

Automating Inference, Learning, and Design using Probabilistic Programming



Tom Rainforth
Wolfson College
University of Oxford

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Acknowledgements

Cheers peeps

Abstract

This work contains science!

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Glossary and Abbreviations

SMC Sequential Monte Carlo. A general purpose inference method using a series of intermediary targets.

1

Introduction

How come a dog is able to catch a frisbee in mid-air? How come a batsman can instinctively predict the flight of a cricket ball moving at over 100km/h sufficiently accurately and quickly to hit it with the bat when there is not even time to consciously make a prediction? Clearly, neither can be based on a deep explicit knowledge of the laws of physics or some hard-coded model for the movement of objects; we are not even born with the knowledge that unsupported objects will fall down [Baillargeon, 2002]. The only reasonable explanation for these abilities is that the batsmen and the dog have *learned from experience*. We do not have all the knowledge we require to survive from birth, but we are born with the ability to learn and adapt, making observations about the world around us and using these to refine our cognitive models for everything from the laws of physics to social interaction. Classically the scientific method has relied on human interpretation of the world to formulate explicit models to explain our internal intuitions, which we then test through experimentation. However, even as a whole scientific society, our models are often terribly inferior to the subconscious models of animals and children, such as for most tasks revolving around social interaction. This leads one to ask, is there something fundamentally wrong with this hand-crafted modeling approach? Is there another approach that better mimics the way humans themselves learn?

Machine learning is an appealing alternative, and often complementary, approach that focuses on constructing algorithms and systems that can adapt, or learn, from data in order to make predictions that have not been explicitly programmed. This is exciting not only because of the potential it brings to automate and improve a wide array of computational tasks, but because it allows us to design systems capable of going beyond the boundaries of human understanding, reasoning about and making predictions for tasks we cannot solve directly ourselves. As a field, machine learning is very wide ranging, straddling computer science, statistics, engineering,

and beyond. It is perhaps most closely related to the field of computational statistics, differing predominantly in its emphasis on prediction rather than understanding. Despite the current hype around the field, most of the core ideas have existed for some time, often under the guise of pattern recognition, artificial intelligence, or computational statistics. Nonetheless, the explosion in the availability of data and in computational processing power in recent years has led to a surge of interest in machine learning by academia and industry alike, particularly in its application to real world problems. This interest alone is enough to forgive the hype as the spotlight is not only driving the machine learning community itself forward, but helping identify huge numbers of applications where existing techniques can be transferred to fantastic effect. From autonomous vehicles [Lefèvre et al., 2014], to speech recognition [Jurafsky and Martin, 2014], and designing new drugs [Burbidge et al., 2001], machine learning is rapidly becoming a crucial component in many technological and scientific advancements.

In many machine learning applications, it is essential to use a principled *probabilistic* approach Ghahramani [2015], incorporating uncertainty and utilizing all the information at hand, particularly when data is scarce. The *Bayesian paradigm* provides an excellent basis upon which to do this: an area specialist constructs a probabilistic model for data generation, conditions this on the actual observations received, and, using Bayes' rule, receives an updated model incorporating this information. This allows information from both existing expertise and data to be combined in a statistically rigorous fashion. As such, it allows us to use machine learning to complement the conventional scientific approach, rather than directly replacing it: we can construct models in a similar way to that which is already done, but then improve and refine these models using data.

Unfortunately, there are two key stumbling blocks that often make it difficult for this idealized view of the Bayesian machine learning approach to be realized in practice. Firstly, a process known as *Bayesian inference* is required to solve the specified problems. This is typically a challenging task, closely related to integration, which is often computationally intensive to solve. Furthermore, it often requires significant statistical expertise to implement effectively, creating a substantial barrier to entry. Secondly, it can be challenging to specify models that are true to the assumptions the user wishes to make and the prior information available. It can again require statistical expertise to abstract application specific knowledge to a valid statistical model. Furthermore, assumptions are often made in the interest of the tractability of inference, rather

than the fidelity of the model. Perhaps because of these drawbacks, there is often a reliance on off-the-shelf solutions, even when these models are somewhat inappropriate for the task at hand.

Probabilistic programming systems (PPS) [Goodman et al., 2008b] are an attempt to overcome this dichotomy between the Bayesian ideal and common practice. Their core philosophy is to decouple model specification and inference, the former corresponding to the user-specified program code, composing of a generative model and statements for conditioning on data, and the latter to an inference engine capable of operating on arbitrary programs. This abstraction barrier allows users with domain specific knowledge to write models naturally, as if they were writing a simulator, without worrying about the inference, which becomes the job of the developer. Informally one can think of PPS as operating as inverse probability engines, outputting the conditional probability distribution implied by the generative model coupled with the observed data. Removing the need for users to worry about the required inference significantly reduces the burden of developing new models, and makes effective statistical methods accessible to non-experts. From a developer's perspective, the abstraction can also aid in the design and testing of new inference algorithms. Furthermore, the availability of the target source code, with known semantics, opens up many opportunities for new methods that would not otherwise be possible.

The underlying theme of this thesis is improving and extending probabilistic programs. However, doing this will require us to make advancements in a number of different research areas such as particle Markov chain Monte Carlo methods [Andrieu et al., 2010a; Rainforth et al., 2016c], Bayesian optimization [Mockus, 1975; Rainforth et al., 2016b], and Monte Carlo fundamentals Metropolis and Ulam [1949]; Rainforth et al. [2016a]. Our aim is to both improve the performance of PPS by improving the underlying inference engines, increasing efficiency and the range of models for which inference can be tractably provided for, and to increase the scope of problems which can be covered by PPS more generally. In particular, we will extend PPS beyond the standard Bayesian inference setting to more general frameworks such as marginal maximum a posteriori estimation and nested estimation. This opens up a number of fascinating opportunities, such as the prospect of constructing systems for automating the design of adaptive experiments and for carrying out principled, probabilistic, engineering simulations that explicitly incorporate the uncertainty in the task at hand.

Build on this a bit so that is a full motivation section. In particular, could do a better job of linking it back to the real world. Could also do more of a linking of my work to the aims, rather than just probabilistic programming in general.

1.1 Thesis Layout

2

A Brief Introduction to Probability Theory

Before going into the main content of the paper, we first provide a quick primer on probability theory, giving some essential background and outlining conventions that we will use throughout the thesis. Readers familiar with the differences between a probability and a probability density and between a random variable and an outcome may want to skip to this chapter, referring back as needed for clarification on any conventions undertaken. Others will hopefully find it to be a gentle introduction to the key concepts that will be needed to be understood to follow the rest of the thesis. Notation has been chosen with accessibility as the primary aim and we will avoid the use measure theory where possible. Nonetheless, we note that a measure theoretic approach to probability is essential for a more rigorous understanding and refer the interested reader to Durrett [2010].

2.1 Random Variables, Outcomes, and Events

A *random variable* is a variable whose realization is currently unknown, such that it can take on multiple different values or *outcomes*.¹ A set of one or more outcomes is known as an *event*. For example, if we roll a fair six-sided dice then the result of the roll is a random variable while rolling a 4 is both a possible outcome and a possible event. Rolling a number greater or equal to 5, on the other hand, is a possible event but not a possible outcome: it is a set of two individual outcomes, namely rolling a 5 and rolling a 6. Outcomes are *mutually exclusive*, i.e. if it not possible for two separate outcomes to occur in a particular trial, but events are not – for example, it is possible for both the events that we roll an even number and we roll a number greater than 3 to occur.

¹Technically speaking, outcomes are points in *sample space* and random variables are measurable functions from outcomes to a measurable space. As we said though, we are trying to avoid the niceties of measure theory when possible...

2.2 Probabilities

A *probability* is the chance of an event occurring. For example, if we denote the output of our dice roll as X , then we can say that $P(X = 4) = 1/6$ or that $P(X \leq 3) = 0.5$. Here $X = 4$ and $X \leq 3$ are events for the random variable X with probabilities of $1/6$ and 0.5 respectively. A probability of 0 indicates that an event has no chance of happening, for example the probability that we role an 8, while a probability of 1 indicates it is certain to happen, for example, the probability that we roll a number less than 7. All probabilities must thus lie (inclusively) between 0 and 1. A *distribution* of a random variable provides the probabilities of each possible outcome for that random variable occurring.

We will regularly use the shorthand $P(x)$ to denote the probability of the event $P(X = x)$. We reiterate the important distinction between the random variable X and the outcome x : the former has an unknown value (e.g. the result of the dice roll) and the latter is a fixed possible realization of the random variable (e.g. rolling a 4). All the same, we will at times be intentionally carefree about delineating between random variables and outcomes, except for when the distinction is explicitly necessary.

Somewhat surprisingly, there are two competing (and often incompatible) formal definitions for what probabilities actually mean. The frequentist definition of probability is that it is the average proportion of the time an event will occur if the trial is repeated infinitely many times. The Bayesian definition of probability is that it is the subjective belief that an event will occur in the process of incomplete information. Both viewpoints have strengths and weaknesses and we will avoid being drawn into one of the biggest debates in science, noting only that the philosophical differences between the two are typically completely detached from the practical differences between the resulting algorithms [Steinhardt, 2012], despite the former all too often being used to argue the superiority of one approach over another.

2.3 Conditioning and Independence

A *conditional probability* is the probability of an event given that another event has occurred. For example, the conditional probability that we roll a 4 with a dice given that we have rolled a 3 or higher is $P(X = 4|X \geq 3) = 0.25$. More typically, we will condition on events that are separate but correlated to the event we care about. For example, the probability of dying of lung cancer is

higher if you smoke. The process of updating a probability using the information from another event is known as conditioning on that event. For example, one can condition the probability that a football team will win the league this season on the results from their first few games.

Events are *independent* if the occurrence of one event does not affect the probability of the occurrence of the other event. Similarly, random variables are independent if the outcome of one random variable does not affect the distribution of the other. Independence of random variables indicates the probability of that variable is the same as the conditional probability given the other variable, i.e. if X and Y are independent, $P(X = x) = P(X = x|Y = y)$ for all possible y . Note that independence does not necessarily carry over when adding or removing a conditioning: if X and Y are independent, this does not necessarily mean that $P(X = x|A) = P(X = x|A, Y = y)$ for some event A . For example, the probability that the next driver to pass a speed camera is speeding and that the speed camera is malfunctioning can be reasonably safely presumed to be independent. However, conditioned on the event that the speed camera is triggered, the two are clearly not independent as if the camera is working, this would indicate that the driver is speeding. If $P(X = x|A) = P(X = x|A, Y = y)$ holds, then X and Y are known as conditionally dependent given A . In the same way that independence does not imply conditional independence, conditional independence does not imply non-conditional independence.

2.4 The Laws of Probability

Though not technically axiomatic, the mathematical laws of probability can be summarized by the *product rule* and the *sum rule*. Remarkably, almost all of probability stems from these two simple rules. The product rule states that the probability of two events occurring is the probability of one of the events occurring times the probability of the other event happening given the first event happened, namely

$$P(A, B) := P(A \cap B) = P(A|B)P(B) = P(B|A)P(A) \quad (2.1)$$

where we have introduced $P(A, B)$ as a shorthand for the probability that both the events A and B occur. An immediate consequence of the product rule is Bayes' rule,

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}, \quad (2.2)$$

which we return at length in Section 3.2. Another is that for independent random variables, the joint distribution is the product of the individual probabilities: $P(A, B) = P(A)P(B)$.

The sum rule has a number of different representations, the most general of which is that the probability that either A or B occurs, $P(A \cup B)$, is given by

$$P(A \cup B) = P(A) + P(B) - P(A, B). \quad (2.3)$$

The intuition of the sum rule is perhaps easiest to see by considering that

$$P(B) - P(A \cap B) = P(B)(1 - P(A|B)) = P(B, \neg A)$$

is the probability of B and not A . $A \cup B$ can only occur if A occurs or if B and not A occurs. As it is not possible for both these events to occur, the probability of either event must be the sum of the probability of each separate event. There are a number of immediate consequences of the sum rule. For example, if A and B are mutually exclusive then $P(A \cup B) = P(A) + P(B)$. As outcomes are mutually exclusive, it follows from the sum rule and the axioms of probability that the sum of the probabilities for each possible outcome is equal to 1. We can also use this to define the concept of *marginalizing* out a random variable Y as

$$P(X = x) = \sum_i P(X = x, Y = y_i) \quad (2.4)$$

where the sum is over all the possible outcomes of Y . Here $P(X = x)$ is known as the *marginal probability* of X and $P(X = x, Y = y)$ as the *joint probability* of X and Y .

Conditional probabilities follow the same key results as unconditional probabilities, but it should be noted that they do not define probability distributions over the conditioning term. For example, $P(A|B)$ is a probability distribution over A with all the corresponding requirements, but is not a distribution over B . Therefore, for example, it is possible to have for example $\sum_i P(A|B = b_i) > 1$.

2.5 Probability Densities

Thus far we have presumed that our random variables are discrete, i.e. that there is some fixed number of possible outcomes.² Things get somewhat more complicated if our variables are

²Technically speaking, discrete random variables can also take on a *countable* number of values. For example, the Poisson distribution is defined over $0, 1, 2, \dots, \infty$ and is a discrete distribution with infinite possible outcomes. However, this countable infinity is much smaller than the *uncountably infinite* number of possible outcomes for continuous random variables.

continuous. Consider for example the probability that a runner takes exactly π hours to run a marathon $P(X = \pi)$. Clearly, the probability of this particular event is zero, $P(X = \pi) = 0$, as is the probability of the runner taking any other exact time to complete the race: we have an infinite number of possible outcomes, each with zero probability (presuming the runner finishes the race). Thankfully, the notion of an event that we previously introduced comes to our rescue. For example, the event that the runner takes between 3 and 4 hours has non-zero probability: $P(3 \leq X \leq 4) \neq 0$. Here our event itself include an infinite number of possible outcomes and even though each individual outcome had zero probability, the combination of *uncountably infinite* many such outcomes need not also have zero probability. To more usefully characterize probability in such cases, we can define a *probability density function* which reflects the relative probability of areas of the space of outcomes. We can define this more precisely by considering the probability of being some small area of the space of size δx . Presuming that the probability density $p_X(x)$ is roughly constant within our small area, we can say that $p_X(x)\delta x \approx P(x \leq X < x + \delta x)$ and thus $p_X(x) = \lim_{\delta \rightarrow 0} \frac{P(x \leq X < x + \delta x)}{\delta x}$. More formally we can define the probability density as satisfying

$$P(X \in \mathcal{A}) = \int_{x \in \mathcal{A}} p_X(x) dx \quad (2.5)$$

where $X \in \mathcal{A}$ means the event that X is in \mathcal{A} . We can further use this to define the *cumulative distribution function* $P(X \leq x)$, which is the probability that X is less than equal to the outcome x

$$P(X \leq x) = \int_{-\infty}^x p_X(u) du, \quad (2.6)$$

where u is a dummy variable.

Most of the key rules of probability theory, such as the sum rule, the product rule, and Bayes rule, apply equally well to continuous and discrete random variables. All that is required is that we replace the summations with integrals over the appropriate variable.

In the rest of the thesis will drop the notation $p_X(x)$, using simply $p(x)$ instead. The main rationale for this is will we regularly use probability density functions that we do not actually sample from. For example, in importance sampling, we will sample from one distribution but evaluate its density under another. In these scenarios, it may not be possible to link a random variable to each density. We will instead make it explicit what distribution of density a random variable is drawn from using the notation $X \sim p(x)$. For the reasons outlined in the next section,

we will also often be carefree at distinguishing between probabilities and probability densities as this oft-used convention will regularly be highly convenient when dealing with variables that could be discrete or continuous. We will also regularly be carefree about distinguishing between random variables and outcomes by using loose notations such as $x \sim p(x)$ when the delineation is not necessary in the context.

2.6 Measures

Consider now if there is also a probability that the runner does not finish the race which we denote as the outcome $X = \infty$. As we have thus-far introduced them, neither the concept of a probability or a probability density seem to be suitable for this case: every outcome other than $X = \infty$ has zero probability, but $X = \infty$ seems to have infinite probability density. To solve this conundrum we have to briefly break our promise to avoid measure theory. A *measure* can be thought of as something that assigns a size to a set of objects. In the context of probability theory, *probability measures* assign probabilities to events, remembering that events represent sets of outcomes, and thus are used to define a more formal notion of probability that we have previously discussed. The measure assigned to event including all possible outcomes is thus 1, while the measure assigned to the empty set is 0.

We can generalize the concept of a probability density to arbitrary random variables by formalizing its defining as being with respect to an appropriate *reference measure*. Somewhat confusingly, this reference measure is typically not a probability measure. Consider the case of the continuous densities examined in Section 2.5. Here we have implicitly used the *Lebesgue measure* as the reference measure, which corresponds to the standard Euclidean notion of size, coinciding with the concepts of length, area, and volume in 1, 2, and 3 dimensions respectively. In (2.5) then dx indicated integration with respect to a Lebesgue measure, with $\int_{x \in \mathcal{A}} dx$ being equal to the hypervolume of \mathcal{A} (e.g. area of \mathcal{A} in two dimensions). We thus clearly have that our reference measure is not a probability measure as $\int_{x \in \mathbb{R}} dx = \infty$. Our probability measure here can be informally thought of as $p(x)dx$, so that $\int_{x \in \mathcal{A}} p(x)dx = P(x \in \mathcal{A})$.³ In the discrete cases, we can define a probability density $p(x) = P(X = x)$ by using the notion of a *counting measure* for reference which simply counts the number of outcomes which lead to a particular

³More formally, the density is derived from the probability measure and reference measure rather than the other way around: it is the Radon-Nikodym derivative of the probability measure with respect to the reference measure.

event. Note that we were not free to choose an arbitrary measure for any given random variable. We cannot use a counting measure as reference for continuous random variables or the Lebesgue measure for discrete random variables because, for example, the Lebesgue measure would assign zero measure to all possible events for the latter. Nonetheless, the reference measure we use is not necessarily unique either. For example, we could apply a constant c scaling the reference measure and then scale the density by $1/c$. For notional convenience, we will refer to dx (or equivalent) as our reference measure elsewhere in the thesis.

For the example where the runner might not finish, we can use a *mixed measure*. Perhaps the easiest way to think about this is to think about the runner's time X as being a deterministic function of two random variables: the first a discrete random variable $Y \in \{0, 1\}$ that dictates where the runner finishes ($Y = 1$) or not ($Y = 0$) and the second a continuous random $Z \in \mathbb{R}^+$ variable that dictates a distribution over run times assuming the runner finishes (such that Z always exists but only equals X if the runner finishes). Now X is a function of Y and Z and we can define the probability of the event $X \in \mathcal{A}$ as follows

$$\begin{aligned} P(X \in \mathcal{A}) &= \sum_{y \in \{0,1\}} \int_{z \in \mathbb{R}} P(Y = y)p(z)\mathbb{I}(X(y, z) \in \mathcal{A})dz \\ &= P(Y = 0)\mathbb{I}(\infty \in \mathcal{A}) + P(Y = 1) \int_{z \in \mathcal{A} \setminus \infty} p(z)dz \end{aligned}$$

where $\mathbb{I}(\cdot)$ is the identity function evaluating to 1 if its input holds true and 0 otherwise, and we have used the independence between Y and Z . By definition of a probability density, we also have that $P(X \in \mathcal{A}) = \int_{x \in \mathcal{A}} p(x)d\mu(x)$ for density $p(x)$ with respect to measure $d\mu(x)$, where we switched notation from dx to $d\mu(x)$ to express the fact that the measure now depends explicitly on the value of x , i.e. our measure is non-stationary in x . For $x \neq \infty$ then it is natural for $d\mu(x)$ to correspond to the Lebesgue measure, noting $\int_{x \in \mathbb{R} \setminus \infty} p(x)d\mu(x) = 1 - P(X = \infty)$. For $x = \infty$ it is natural for $d\mu(x)$ to correspond to some scaling of the counting measure. For discrete distributions it is natural to use the counting measure (i.e. set the scaling to one), but here this could lead to a slightly misleading density given that $X = \infty$ is infinitely times more probable than any other X . For example, this could mean that $\arg \max p(x) \neq \infty$ which could quickly lead to confusion. A more illustrative choice might use the counting measure scaled by an arbitrarily small value (such that the density is scaled by large value), though strictly speaking this scaling should not be 0.

For most applications,⁴ the choice between valid reference measures will turn out to be inconsequential (provided we are consistent in our choice when considering multiple densities) as it does not affect the distribution of random variables themselves or effect things such as expectations (see Section 2.7). The key point we wish to instead make, is that regardless of variable type, we can (implicitly) always define a probability density function.⁵ The generalization also allows us to put probability distributions of variables that are neither discrete or continuous type. For example, we might want to put a distribution over the space of strings. Because of this generalization, we will talk mostly in terms of probability densities throughout this thesis, even though variables may often be discrete.

We finish the section by considering the relationship between random variables which are deterministic functions of one another. This important case is known as a change of *change of variables*. Imagine that a random variable $Y = g(X)$ is a deterministic function of another random variable X . Given a probability density function for X , we can define a probability density function on Y using

$$p(y)dy = p(x)dx = p(g^{-1}(y))dx \quad (2.7)$$

where $p(y)$ and $p(x)$ are the respective probability densities for Y and X respectively with measures dx and dy , the latter of which is known as a *push-forward* measure. Rearranging we see that, for one-dimensional problems,

$$p(y) = \left| \frac{dg^{-1}(y)}{dy} \right| p(g^{-1}(y)). \quad (2.8)$$

For the multidimensional case, the derivative is replaced by the determinant of the Jacobian for the inverse mapping. Note that by (2.5), changing variables does not change the value of actual probabilities or exceptions (see Section 2.7). However, (2.7) still has the important consequence that the optimum of a probability distribution depends on the parameterization. For example, parameterizing the same model with either X or $\log X$ will lead to a different most likely value of the parameter x^* , i.e.

$$x^* = \arg \max_x p(x) \neq g^{-1} \left(\arg \max_{g(x)} p(g(x)) \right) \quad (2.9)$$

in general.

⁴An important exception to this is optimization (see Chapter 8).

⁵Well, almost always. But we are not going to open that can of worms, see e.g. Durrett [2010].

2.7 Expectations and Variances

The *expected value* $\mathbb{E}[X]$, or mean, of a random variable X is the average value that the variable will take if an infinite number of independent draws are made. Its definition is easiest to convey using probability density notation

$$\mathbb{E}[X] = \int xp(x)dx. \quad (2.10)$$

In the discrete case this leads to $\mathbb{E}[X] = \sum_i x_i P(X = x_i)$. Because expectations are defined by a random variable (rather than a density), they average over all the contained randomness, e.g. $\mathbb{E}[f(X, Y)] = \iint f(x, y)p(x, y)dxdy$. However, if we wish to average only with respect to part of the randomness in a system, we can instead use a conditional expectation for example

$$\mathbb{E}[f(X, Y)|Y = y] = \int f(x, y)p(x|y)dx, \quad (2.11)$$

for which we will sometimes use the shorthand $\mathbb{E}[f(X, Y)|Y]$.

It will also sometimes be convenient to implicitly define the random variable and conditioning for an expectation for which we use the slightly loose notation

$$\mathbb{E}_{p(x|y)} [f(x, y, z)] = \int f(x, y, z)p(x|y)dx, \quad (2.12)$$

where we have implicitly defined the random variables $Y \sim p(y)$ and $X \sim p(x|Y = y)$, we are calculating $\mathbb{E}[f(X, Y, z)|Y = y]$, and this resulting expectation is a function of z . One can informally think about this as being the expectation of $f(x, y, z)$ with respect to $p(x|y)dx$: our expectation is only over the randomness associated with drawing from $p(x|y)$. Thus, for example, we are not taking an expectation over nor condition upon z in this example – it is treated as a fixed input, even if it is a random variable externally to this expectation. Depending on the context, we will switch between these different notations for expectation and will sometimes simply use the integral form directly.

Denoting the mean of a random variable X as $\mu = \mathbb{E}[X]$, the *variance* of X is defined using any one of the following equivalent forms

$$\text{Var}(X) = \mathbb{E}[(X - \mu)^2] = \int (x - \mu)^2 p(x)dx = \mathbb{E}[X^2] - \mu^2 = \int x^2 p(x)dx - \mu^2. \quad (2.13)$$

In other words, it is the average squared distance of a variable from its mean. Its square root, the *standard deviation*, informally forms an estimate of the average amount of variation of the

variable from its mean and has units which are the same as the data. We will use the same notational conventions as for expectations when defining variances.

The variance is a particular case of the more general concept of a covariance between two random variables X and Y . Defining $\mu_X = \mathbb{E}[X]$ and $\mu_Y = \mathbb{E}[Y]$ then the covariance is defined by any one of the following equivalent forms

$$\begin{aligned}\text{Cov}(X, Y) &= \mathbb{E}[(X - \mu_X)(Y - \mu_Y)] = \iint (x - \mu_X)(y - \mu_Y)p(x, y)dxdy \\ &= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y] = \iint xy p(x, y)dxdy - \left(\int xp(x)dx\right)\left(\int yp(y)dy\right).\end{aligned}\quad (2.14)$$

The covariance between two variables measures the joint variability of two random variables. It is perhaps easiest to interpret through the definition of correlation (or more specifically, Pearson's correlation coefficient) which is the correlation scaled by the standard deviation of each of the variables:

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)\text{Var}(Y)}}.\quad (2.15)$$

The correlation between two variables is always in the range $[-1, 1]$. Positive correlations indicate that when one variable is relatively larger, the other variable also tends to be larger. The higher the correlation, the more strongly this relationship holds: if the correlation is 1 then one variable is *linearly* dependent on the other. The same hold for negative correlations except that when one variable increases, the other tends to decrease. Independent variables have a correlation (and thus covariance) of zero. Note that correlation is not causation.

3

Probabilistic Machine Learning

In this chapter we will provide a high-level introduction to some of the core approaches to machine learning. We will distinguish between discriminative and generative approaches, outlining some of the key features that indicate when problems are more suited to one approach or the other. Our focus then switches to looking at probabilistic generative approaches that will be the main focus of this thesis. We will explain how the *Bayesian paradigm* provides a powerful framework for generative machine learning that allows us to combine data with existing expertise. We will then go on to show how *graphical models* can be used as a convenient framework to express Bayesian models and how they can be used to extract important features of the model. We continue by introducing one of the main competitors to the Bayesian approach – frequentist modeling – and present arguments for why neither a Bayesian nor a frequentist approach is entirely satisfactory. In particular, we will carefully outline the, oft forgotten, fundamental underlying assumptions made by each approach and demonstrate why the differing suitability of these assumptions to different tasks shows why both approaches are essential tools in the arsenal of machine learning methods, despite the fierce loyalty of many in the community to one approach or the other. Though the focus of this thesis will be on Bayesian approaches, understanding its limitations is essential for understanding when the methods we discuss should be used and critically when they should definitely not be. We finish the chapter by discussing some of the key practical challenges for Bayesian modeling and how we will attempt to address a number of these with this work.

3.1 Discriminative vs Generative Machine Learning

In some machine learning applications, huge quantities of data are available that dwarf the information that can be provided from human expertise. In such situations, the main challenge

is in processing and extracting all the desired information from the data to form a useful characterization, typically an artifact providing accurate predictions at previous unseen inputs. Such problems are typically suited to *discriminative* machine learning approaches [Breiman et al., 2001; Vapnik, 1998], such as neural networks [Rumelhart et al., 1986; Bishop, 1995], support vector machines [Cortes and Vapnik, 1995; Schölkopf and Smola, 2002], and decision tree ensembles [Breiman, 2001; Rainforth and Wood, 2015]. Discriminative machine learning approaches focus on directly learning a predictive model: given training data $\mathcal{D} = \{x_n, y_n\}_{n=1}^N$ they learn a parametrized mapping f_θ from the inputs $x \in \mathcal{X}$ to the outputs $y \in \mathcal{Y}$ that can be used directly to make predictions for new inputs $\tilde{x} \notin \{x_n\}_{n=1}^N$. *Training* uses the data \mathcal{D} to estimate optimal values of the parameters θ^* . *Prediction* at a new input \tilde{x} involves applying the mapping with the optimal parameters given an estimate for the output $\tilde{y} = f_{\theta^*}(\tilde{x})$. Perhaps the simplest example of this is linear regression: one finds the hyperplane that best represents the data and then uses this hyperplane to interpolate or extrapolate to predict the output at previously unseen points. As a more advanced example, in a neural network one uses training to learn the weights of the network, after which prediction can be done by running the network forwards.

There are many intuitive reasons to take a discriminative machine learning approach. Perhaps most compelling is the idea that if our objective is prediction, then it is simplest to solve that problem directly, rather than try and solve some more general problem such as learning an underlying generative process [Vapnik, 1998; Breiman et al., 2001]. Furthermore, if sufficient data is provided, discriminant approaches can be spectacularly successful in term of predictive performance. Methods are typically highly flexible and can capture intricate structure in the data that would be hard or even impossible to establish manually. Many approaches can also be run with little or no input on behalf of the user, delivering state-of-the-art performance when used “out-of-the-box” with default parameters [Rainforth and Wood, 2015].

However, this black-box nature is also often their downfall. Discriminative methods typically make such weak assumptions about the underlying process that is difficult to impart prior knowledge or domain specific expertise. This can be disastrous if insufficient data is available as the data alone is unlikely to possess the required information to make adequate predictions. Even when substantial data is available, there may be significant prior information available that needs to be exploited for effective performance. For example, in time series modelling the sequential nature of the data is critically important information [Liu and Chen, 1998], while in vision

tasks the knowledge that scenes are generated from objects can be invaluable [Kulkarni et al., 2015]. Many problems also increase in complexity as more data is added – “big data” problems are often actually a collection, or sometimes hierarchy, of many small problems, such that the complexity of the required parametrization increases as more data is added. Consider, for example, modeling interactions in a social network. Adding a new user into the model increases the amount of data, but also requires the model to grow and accommodate the new user [Ravasz and Barabási, 2003]. In this situation it is essential to use an approach that respects the structure of the model, while the amount of data available for each individual user is often quite small, such that it will be essential to use prior information by transferring insights gathered from some users to others. Therefore even for such large scale problems, the inflexibility of many discriminative approaches to incorporate known characteristics of the target problem can be problematic.

Not only does the black-box nature of many discriminative methods restrict the level of human input that can be imparted on the system, it often restricts the amount of insight and information that can be extracted from the system once trained. The parameters in most discriminative algorithms do not have physical meaning that can be queried by a user, making their operation difficult to interpret and hampering the process of improving the system through manual revision of the algorithm. Furthermore, this typically makes them inappropriate for more statistics orientated tasks, where it is the parameters themselves which are of interest, rather than the ability for the system itself to make predictions. For example, the parameters may have real world physical interpretations we wish to learn about.

Most discriminative methods are also poor at providing realistic uncertainty estimates. Because they are typically trained in a manner that optimizes the parameters to minimize some loss criterion (e.g. the predictive error), they do not in general encode any uncertainty in either their parameters or the subsequent predictions. Though many methods can produce uncertainty estimates either as a by-product or from a post-processing step, these are typically mostly heuristic based, rather than stemming naturally from a statistically principled estimate of the target uncertainty distribution. The lack of reliable uncertainty estimates can lead to overconfidence and can make discriminative methods inappropriate in many scenarios. This can also reduce the composability of discriminative methods within larger systems, as information is lost when only providing a point estimate. Not representing uncertainty in the parameters

can also restrict the power of the resultant models, compared with approaches that can average over different possible parameter values.

These shortfalls mean that many tasks instead call for a *generative* machine learning approach [Ng and Jordan, 2002; Bishop, 2006]. Rather than directly learning a predictor, generative methods look to explain the observed data using a *probabilistic model*. Whereas discriminative approaches aim only to make predictions, generative approaches model how the data is actually generated; they model the joint probability $p(X, Y)$ of the inputs X and outputs Y . By comparison we can think of discriminative approaches as only modeling the outputs given the inputs $p(Y|X)$.

A key upshot of this difference is that generative approaches generally make stronger modeling assumptions about the problem. Though this can be problematic when the model assumptions are wrong and is often unnecessary in the limit of large data, it is essential for combining prior information with information from data and therefore for constructing systems that exploit application specific human expertise. In the words of the great George Box, “*all models are wrong, but some are useful*” [Box, 1979; Box et al., 1979]. In a way, this is a self-fulfilling statement: a model for any real phenomena is by definition an approximation and so is never exactly correct no matter how powerful. However, it is still an essential point that is all too often forgotten, particularly by academics trying to convince the world that only their approach is correct. Only in artificial situations can we construct exact models and so we must remember, particularly in generative machine learning, that the first, and often largest, error is in our original mathematical abstraction of the problem. On the other hand, real situations have access to finite and often highly restricted data, so it is equally preposterous to suggest that a method is superior simply due to its asymptotic behavior in the limit of large data or that if our approach does not work then the solution is simply to get more data.¹ As such, the ease of which domain specific expertise can be included in generative approaches is often essential to achieving effective performance on real world tasks.

To highlight the difference between discriminative and generative machine learning, we consider the example of the differences between logistic regression (a discriminative classifier)

¹It should, of course, be noted that the availability of data is typically the biggest bottleneck in machine learning. At times, it feels like the machine learning community would be well served to remember that the differences in performance between machine learning approaches is often, if not usually, dominated by variations in the inherently difficult of the problem, which is itself not usually known up front, rather than differences between approaches.

and naïve Bayes (a generative classifier). We will consider the binary classification case for simplicity. Logistic regression is a linear classification where the class label $y \in \{0, 1\}$ is predicted from the input features $x \in \mathbb{R}^D$ using

$$p(y|x, a, b) = \frac{1}{1 + \exp(-y(a + b^T x))} \quad (3.1)$$

where $a \in \mathbb{R}^D$ and $b \in \mathbb{R}^D$ are the parameters of the model. The model is trained by finding the values for a and b that minimize a loss function on the training data. For example, a common approach is to find the *most likely* parameters a^* and b^* by minimizing the negative log-likelihood (which is equivalent to the cross-entropy loss function)

$$\{a^*, b^*\} = \arg \min_{a \in \mathbb{R}^D, b \in \mathbb{R}^D} -\log \left(\prod_{n=1}^N p(y_n|x_n, a, b) \right). \quad (3.2)$$

Once found, a^* and b^* can be used with (3.1) to make predictions at any possible x . Logistic regression is a discriminative approach as we have directly calculated a characterization for the predictive distribution, bypassing any direct reasoning about the joint probability of the inputs and the outputs.

The naïve Bayes classifier on the other hand starts by making the assumption that each feature is *independent* given the class label. As such it reasons about both the distribution over both inputs and outputs, unlike logistic regression which only reasons about the conditional probability of the output given the input. If we let $\{x^1, \dots, x^D\} =: x$ represent the dimensions of x , then the naïve Bayes assumption is that

$$p(x|y) = \prod_{i=1}^D p(x^i|y) \quad (3.3)$$

which in turn leads to the following joint distribution

$$p(x, y) = p(y) \prod_{i=1}^D p(x^i|y). \quad (3.4)$$

Here we are free to choose the form for both $p(x^i|y)$ and $p(y)$ and we will use the data to learn their parameters. This freedom is both a blessing and curse: it allows us to impart our own knowledge about the problem to the model, but we may be forced to make assumptions without proper justification in the interest of tractability, for convenience, in error, or simply because it is challenging to specify a sufficiently general purpose model that can cover all possible cases. Further, even once the forms of $p(x^i|y)$ and $p(y)$ have been defined, there are

still decisions to be made: do we take a Bayesian or frequentist view for making predictions? What is the best way to calculate the information required to make predictions? We will go into these questions in more depth in Section 3.4.

As we have shown, generative approaches are inherently probabilistic. This is highly convenient when it comes to calculating uncertainty estimates or gaining insight from our trained model. They are generally more intuitive than discriminative methods as models denote the probability of events occurring, while the generative model is essence an explanation for how the data is generated. As such, the parameters tend to have physical interpretation in the generative process and therefore provide not only prediction, but insight. Generative approaches will not always be preferable, particularly when there is an abundance of data available, but they provide a very powerful framework that is essential in many scenarios. Perhaps their greatest strength is in allowing the use of so-called Bayesian approaches which we now introduce.

3.2 Learning from Data – the Bayesian Paradigm

At its core, the Bayesian paradigm is simple, intuitive, and compelling: for any task involving learning from data we start with some prior knowledge and then update that knowledge to incorporate information from the data. This process is known as *Bayesian inference*.

Imagine we are trying to reason about some variables or parameters θ . We can encode our initial belief as relative probabilities for different possible instances of θ , this is known as a *prior* $p(\theta)$. Given observed data \mathcal{D} , we can characterize how likely different values of θ are to have given rise to that data using a *likelihood function* $p(\mathcal{D}|\theta)$. These can then be combined using Bayes' rule to give a *posterior*, $p(\theta|\mathcal{D})$ that represents our updated belief about θ once the information from the data has been incorporated

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{\int p(\mathcal{D}|\theta)p(\theta)d\theta} = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}. \quad (3.5)$$

Here the denominator, $p(\mathcal{D})$, is a normalization constant known as the *marginal likelihood* and is necessary to ensure $p(\theta|\mathcal{D})$ is a valid probability distribution (or probability density for continuous problems). One can therefore think of Bayes' rule in the even simpler form of the posterior being proportional to the prior times the likelihood. For such a fundamental theorem, Bayes' rule has a remarkably simple derivation, following directly from the product rule of probability as shown in Chapter 2.

A key feature of Bayes' rule is that it can be used in a self-similar fashion where the posterior from one task becomes the prior when the model is updated with more data, i.e.

$$p(\theta|\mathcal{D}_1, \mathcal{D}_2) = \frac{p(\mathcal{D}_2|\theta, \mathcal{D}_1)p(\theta|\mathcal{D}_1)}{p(\mathcal{D}_2|\mathcal{D}_1)} = \frac{p(\mathcal{D}_2|\theta, \mathcal{D}_1)p(\mathcal{D}_1|\theta)p(\theta)}{p(\mathcal{D}_2|\mathcal{D}_1)p(\mathcal{D}_1)}. \quad (3.6)$$

As a consequence, there is something quintessentially human about the Bayesian paradigm: we learn from our experiences by updating our beliefs after making observations. Our model of the world is constantly evolving over time and is the cumulation of experiences over a lifetime. If we make an observation that goes against our prior experience, we do not suddenly make drastic changes to our underlying belief, but if we see multiple corroborating observations our view will change. Furthermore, once we have developed a strong prior belief about something, we can take substantial convincing to change our mind, even if that prior belief is highly illogical. Perhaps this is why humans seem to have a tendency to develop deep rooted prejudices.

There is similarly something distinctively Bayesian to the scientific process itself. In science we construct models to explain observed phenomena and then run experiments to validate how well our model matches real observations. We then update and improve our model accordingly in a never ending process of increasing understanding for the world around us. We can never hope to truly understand the workings of the universe – after all, it is, at least for practical purposes, fundamentally random [Rainforth, 2013] – and so we can hope only to construct increasingly accurate and pertinent models. This sequential updating, at the very least, shares parallels with the process of Bayesian modeling and could be argued to be a fundamentally Bayesian process in its own right.

To give a more concrete example of Bayesian modeling consider estimating the probability of getting a heads from a weighted coin. Let's call this weighting $\theta \in [0, 1]$ such that the probability of getting a heads (H) when flipping the coin is $p(Y = H|\theta) = \theta$ where Y is the outcome of the flip. This will be our likelihood function, corresponding to a *Bernoulli* distribution, noting that the probability of getting a tails (T) is $p(Y = T|\theta) = 1 - \theta$. Before seeing the coin being flipped we have some prior belief about its weighting. We can therefore define a prior $p(\theta)$, for which we take the beta distribution

$$p(\theta) = \text{BETA}(\theta; \alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta^{\alpha-1}(1 - \theta)^{\beta-1} \quad (3.7)$$

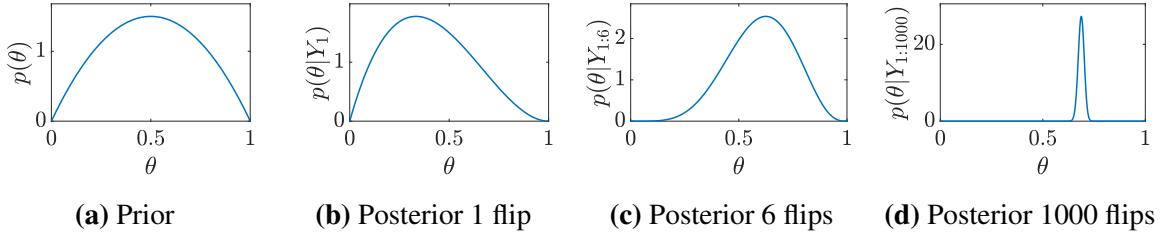


Figure 3.1: Prior and posteriors for coin flip example after different numbers of observations.

where $\Gamma(\cdot)$ is the gamma function and we will take $\alpha = \beta = 2$. A plot for this prior is shown in Figure 3.1a where we see that under our prior then it is more probable that θ is close to 0.5 than the extremes 0 and 1.

Now imagine that we flip the coin and get a tails (T). We can use our prior and likelihood to calculate the posterior

$$\begin{aligned} p(\theta|Y_1 = T) &= \frac{p(\theta)p(Y_1 = T|\theta)}{\int p(\theta)p(Y_1 = T|\theta)d\theta} = \frac{\theta(1-\theta)^2}{\int \theta(1-\theta)^2d\theta} \\ &= \text{BETA}(\theta; 2, 3) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta(1-\theta)^2. \end{aligned} \quad (3.8)$$

Here we have used the fact that a Beta prior is *conjugate* to a Bernoulli likelihood to give an analytic solution. Conjugacy means that the prior-likelihood combination gives a posterior that is of the same form as the prior distribution. More generally, for a prior of $\text{BETA}(\theta; \alpha, \beta)$ then the posterior will be $\text{BETA}(\theta; \alpha + 1, \beta)$ if we observe a heads and $\text{BETA}(\theta; \alpha, \beta + 1)$ if we observe a tails. Figure 3.1b shows that our posterior incorporates the information from the prior and the observed data. Namely, our observations means the distribution has drifted towards it being more probable that $\theta < 0.5$. The posterior also reflects the fact that we are still uncertain about the value of θ , it is not simply the empirical average of our observations which would give $\theta = 0$.

If we now flip the coin again, our previous posterior (3.8) becomes our prior and we can incorporate the new observations in the same way. Through our previous conjugacy result, then if we observe n_H heads and n_T tails and our prior is $\text{BETA}(\theta; \alpha, \beta)$ then our posterior is $\text{BETA}(\theta; \alpha + n_H, \beta + n_T)$. Thus if our sequence of new observations is $HTHHH$ then our new posterior is

$$p(\theta|Y_1, \dots, Y_6) = \frac{p(Y_2, \dots, Y_6|\theta)p(\theta|Y_1)}{\int p(Y_2, \dots, Y_6|\theta)p(\theta|Y_1)d\theta} = \text{BETA}(\theta; 6, 4), \quad (3.9)$$

which is shown in Figure 3.1c. We see now that our belief for the probability of heads has shifted higher and that the uncertainty has reduced because of the increased number of

observations. After seeing a total of 1000 observations as shown in Figure 3.1d, we see that the posterior has predominantly collapsed down to a small range of θ , close to the true value of θ which happens to be 0.7.

Now we have combined our prior information with the information from data, a natural next question is how can we use this to make predictions. In the Bayesian setting this is done with the posterior predictive distribution which marginalizes out over the parameters. For the coin flip case we have

$$\begin{aligned} p(Y_{N+1} = H|Y_{1:N}) &= \int p(Y_{N+1} = H, \theta|Y_{1:N}) d\theta = \int p(Y_{N+1} = H|\theta)p(\theta|Y_{1:N}) d\theta \\ &= \int \theta \text{BETA}(\theta; \alpha + n_H, \beta + n_T) d\theta = \frac{\alpha + n_H}{\alpha + n_H + \beta + n_T} \end{aligned} \quad (3.10)$$

where we have used the known result for the mean of the Beta distribution. The role of the parameters α and β in our prior now become apparent – they take on the role of pseudo observations. Our prediction is in line with the empirical average from seeing $\alpha + n_H$ heads and $\beta + n_T$ tails. The larger $\alpha + \beta$ is then the strong our prior compared to the observations, while we can skew towards heads or tails being more likely by changing the relative values of α and β .

More generally the posterior predictive distribution will depend on a queried input point. To demonstrate this, consider the example of a Bayesian linear regression from inputs $x \in \mathbb{R}^D$ to outputs $y \in \mathbb{R}^D$. Assume that we have seen N observations $\mathcal{D} = \{x_n, y_n\}_{n=1}^N$ and let $\mathbf{x} = [x_1, \dots, x_N]^T$ and $\mathbf{y} = [y_1, \dots, y_N]^T$ respectively be a $N \times D$ matrix and a column vector whose rows correspond to the different data points. Our regression is of the form $y_n = x_n^T \mathbf{w} + b + \epsilon_n$ where $\mathbf{w} \in \mathbb{R}^D$, $b \in \mathbb{R}$ and each $\epsilon_n \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$. This implies a likelihood of

$$p(\mathbf{y}|\mathbf{x}, \mathbf{w}, b, \sigma) = \prod_{n=1}^N p(y_n|x_n, \mathbf{w}, b, \sigma) = \prod_{n=1}^N \mathcal{N}(y_n; x_n^T \mathbf{w} + b, \sigma^2). \quad (3.11)$$

For simplicity we will assume that σ and b are known fixed parameters, but we will put a prior on \mathbf{w} as follows in order to perform inference

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \mathbf{0}, C) \quad (3.12)$$

where C is a fixed covariance matrix. To make predictions, we first calculate the posterior

$$\begin{aligned} p(\mathbf{w}|\mathcal{D}, b, \sigma) &= \mathcal{N}(\mathbf{w}; \mathbf{0}, C) \prod_{n=1}^N \mathcal{N}(y_n; x_n^T \mathbf{w} + b, \sigma^2) \\ &= \mathcal{N}(\mathbf{w}; m, S) \end{aligned} \quad (3.13)$$

$$\text{where } m = S^{-1} \mathbf{x}^T (\mathbf{y} - b) / \sigma^2,$$

$$S = \left(C^{-1} + \frac{\mathbf{x}^T \mathbf{x}}{\sigma^2} \right)^{-1}.$$

We have omitted the necessary linear algebra (see for example Bishop [2006] Sections 2.3.3 and 3.3) but note the conjugacy between the normal distribution and itself. Prediction now uses the posterior predictive, marginalizing over the parameters in the same manner as the coin flip example. Here though, we are interested in predicting the output \tilde{y} at a particular input point \tilde{x} for which we have

$$\begin{aligned} p(\tilde{y}|\tilde{x}, \mathcal{D}, b, \sigma) &= \int p(\tilde{y}|\tilde{x}, \mathbf{w}) p(\mathbf{w}|\mathcal{D}, b, \sigma) d\mathbf{w} = \int \mathcal{N}(\tilde{y}; \tilde{x}^T \mathbf{w} + b, \sigma^2) \mathcal{N}(\mathbf{w}; m, S) d\mathbf{w} \\ &= \mathcal{N}\left(\tilde{y}; \tilde{x}^T m + b, \tilde{x}^T S^{-1} \tilde{x} + \frac{1}{\sigma^2}\right) \end{aligned} \quad (3.14)$$

which again follows from standard results for Gaussian distributions. We therefore have an analytic predictive distribution at any possible input point. Though this linear regression example might seem overly simple for practical purposes, we will see in Section 8.3 that substantially more advanced models, such as Gaussian processes, can be viewed as linear regressions between a set of features on the inputs $\phi(x)$ and the output y .

The models we have introduced so far are specific examples of Bayesian modeling and will clearly only be applicable or appropriate in very particular scenarios. However, the only restrictions we have in order to carry out Bayesian modeling is that the prior and likelihood are valid probability distributions (in practice even these requirements can often be relaxed). Bayesian modeling is at its heart a generative approach and its real power will be when we design a rich and expressive *generative model* that reflects our application specific knowledge. In other words, we can define our model by carefully constructing a stochastic process that describes how the data and parameters are generated. This model then corresponds to the joint distribution $p(\theta, \mathcal{D})$. We can then think of providing real data as refining our model, providing an updated distribution on the parameters and subsequent predictions that incorporate the information from the data. The more flexible we make our generative model, the more

we can make it represent the our data. The less flexible we make the generative model, the more weighting is given to our prior assumptions.

To give an intuitive example of such a generative approach, consider the problem of identifying objects in a visual scene. Here it is relatively straightforward to construct a model for generating images by constructing a sampler for which objects appear in the scene and their respective positions. Such graphics generators are used for computer games all the time. Here our parameters are the objects and the data is the image. Bayesian inference can now be thought of as the process of *inverting* our generator: given objects we can generate images but we want to identify objects from images. We will return to these ideas in Chapter 4 where we show how, using probabilistic programming, one can think of all stochastic simulators as defining Bayesian models and as the process of inference as inverting these simulators.

3.3 Graphical Models

Generative models will typically have many variables and a complex *dependency structure*. In other words, many of variables will be conditionally independent of one another given values for other variables. Graphical models are a ubiquitously used method for representing and reasoning about generative models with a particular focus on the dependency structure. At a high-level, they capture how the joint probability distribution can be broken down into a product of different factors, each defined over a subset of the variables. They are formed of a number of connected nodes, where each node represents a random variable in the model and each variable has its own node. Links between nodes in the model represent dependencies: any two connected nodes have an explicit dependency. Various independence assumptions can be deduced from the graphical model, though the exact nature of these deductions will depend on the type of graphical model – nodes without direct links between them will often still be dependent.

Graphical models can be separated into two distinct classes: directed graphical models and undirected graphical models. Undirected graphical models, also known as Markov random fields, imply no ordering on their factorization and are used only to express conditional independences between variables. They are used in scenarios where it is difficult to specify the target distribution in a structured generative way. For example, if modeling whether it will rain at various locations then there is a clear dependence between nearby locations, but not a natural ordering to the joint

probability distribution of where it will rain. Boltzmann machines are a common example of undirected graphical models [Ackley et al., 1985]. Independence in undirected graphical models can be deduced through the *global Markov property* which states that any two non-intersecting subsets of the variables A and B are conditionally independent given a third, separating, subset C if there is no path between A and B that does not pass through C . This means, for example, that each variable is conditionally independent of all the other variables given its neighbors.

Our main focus, though, will instead be on directed graphical models and in particular directed acyclic graphical models (DAGs), i.e. directed graphical models containing no cycles or loops one can follow and arrive back in the starting position. DAGs, also known as Bayesian networks, are particularly useful in the context of Bayesian modeling because they can be used to express *casual relationships*. As such, they can be used as a piecewise explanation for how the joint distribution is generated. Not only does this form a natural means to describe and design models in the first place, we can carefully order the breakdown to factorize the distribution into only terms we know. For example, in the linear regression model we did not know (at least when the model was first defined) $p(\mathcal{D})$ but we did know $p(\mathbf{w})$ and $p(\mathcal{D}|\mathbf{w})$. Therefore even though we could factorize our joint $p(\mathcal{D}, \mathbf{w})$ as $p(\mathbf{w}|\mathcal{D})p(\mathcal{D})$ and construct a DAG this way, it is much more convenient to factorize and construct the DAG the other way round, namely as $p(\mathcal{D}|\mathbf{w})p(\mathbf{w})$. As a good rule of thumb, when we define a model using a DAG, we need to be able to define the probability of each variable given its *parents*, i.e. all the nodes with links from that node towards the node in question. We will generally not have access to also possible factorizations in an analytic form as otherwise there would be no need to perform inference.

The demonstrate this factorization more explicitly and give a concrete example of a DAG, consider a joint model $p(a, b, c)$. By the product rule, we can break down this joint distribution into a number of different factorizations. However, some will typically be more useful than others. Imagine a medical diagnostic example where a represents lifestyle and genetic factors of a patient such as whether they smoke or have unknown preexisting conditions, b represents the presence of lung cancer, and c represents symptoms such as a persistent cough. Here we have the following natural breakdown of the joint distribution

$$p(a, b, c) = p(a)p(b|a)p(c|a, b). \quad (3.15)$$

The lifestyle and genetic factors will generally either be known or can be estimated from tests or simply prevalence within the population. These factors, the likelihood of somebody developing lung cancer can be modeled using existing data and domain expertise. Given the lifestyle and genetic factors and the knowledge of whether lung cancer is present, we can predict the likelihood of observing the observed symptoms. We can express our model and this factorization using the DAG shown in Figure 3.2. Here we have shaded in c to express the fact that this is observed. The graphical model expresses our dependency structure as we have the probability of each node given its parents. As shown in (3.15), the product of all these factors is equal to our joint distribution. The DAG has thus formed a convenient means of representing our generative process.

Clearly our aim for this problem will be to find the marginal probability $p(b|c)$ which will require Bayesian inference. An important feature of the breakdown of graphical models will become apparent when we consider how we can conduct such inference for more a general class of models where the solution is no analytic in Chapter 5. Here knowing the dependency structure, and in particular the independence relationships, will be essential to many inference schemes such as message passing schemes.

A natural question is now how can we deduce the independence relationships from a DAG? This can be done by introducing the notion of *d-separation* [Pearl, 2014]. Consider three arbitrary, non-intersecting, subsets A , B , and C of our DAG. A and B are conditionally independent given C if there is no *unblocked* paths from A to B (or equivalently from B to A), in which case A is said to be d-separated from B by C . Paths do not need to be in the directions defined by the DAG but are blocked if either

1. Two consecutive arrows in the path both point towards a node that is not in and has no descendants in C , i.e. we cannot get to any of the nodes in C by following the arrows from this node.
2. Two consecutive arrows in the path meet at a node in C and one of them points away from the node.

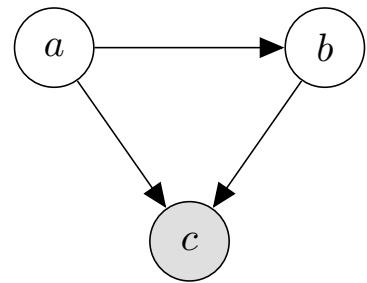


Figure 3.2: Simple example DAG corresponding to (3.15)

Note that only the first of these rules is necessary for establishing marginal independence between nodes as this rule can still be used when C is empty. Examples of blocked paths are shown in Figure 3.3 while examples of unblocked paths are shown in Figure 3.4, explanations for which are given in the captions. For a more comprehensive introduction to establishing independence in DAGs we refer the reader to Section 8.2 of Bishop [2006].

In the simple example of Figure 3.2 there were no independence relationships and so we gain little from working with the DAG compared to just the joint probability distribution. A more advanced example where there are substantial independence relationships which can be exploited is shown in Figure 3.5. This model is known as a hidden Markov model² (HMM) and has T latent variables $x_{1:T}$ and T observations $y_{1:T}$. The joint distribution is as follows

$$p(x_{1:T}, y_{1:T}) = p(x_1)p(y_1|x_1) \prod_{t=2}^T p(x_t|x_{t-1})p(y_t|x_t), \quad (3.16)$$

where each x_t is independent of $x_{1:t-2}$ and $y_{1:t-1}$ given x_{t-1} and of $x_{t+2:T}$ and $y_{t+1:T}$ given x_{t+1} . This is known as the Markov property and means that each latent variable only depends on the other variables and observations through its immediate neighbours. In essence, the model has no memory as information is passed forwards (or backwards) only through the value of the previous latent state. A number of stochastic processes and dynamical systems obey the Markov property and HMMs and their extensions are extensively used for a number of tasks involving sequential data from DNA sequencing [Durbin et al., 1998] to tracking animals [Dhir et al., 2016, 2017]. For example, in a dynamical system, then the next state depends only on the dynamics of the system and its current state (e.g. position velocity etc).

A key part to the appeal of HMMs is that the structure of the DAG can be exploited to give analytic solutions to resulting Bayesian inference whenever each $p(y_t|x_t)$ and $p(x_t|x_{t-1})$ is either a discrete or Gaussian distribution. Even when this does not hold, there are still a number of features of the dependency structure that can make the inference substantially easier. As we will show in Chapter 5, Bayesian inference is generally a challenging problem, often prohibitively so. Therefore the (fast) analytic inference for HMMs is highly convenient. However, it can mean that HMMs are perhaps overused. More generally, simplifying approximations or unjustified assumptions are often made by Bayesian practitioners for tractability, e.g. by using

²The use of the term HMM in the literature (and later in this paper) often also implies that the latent states are discrete variables, with the equivalent continuous model referred to as a (Markovian) state space model.

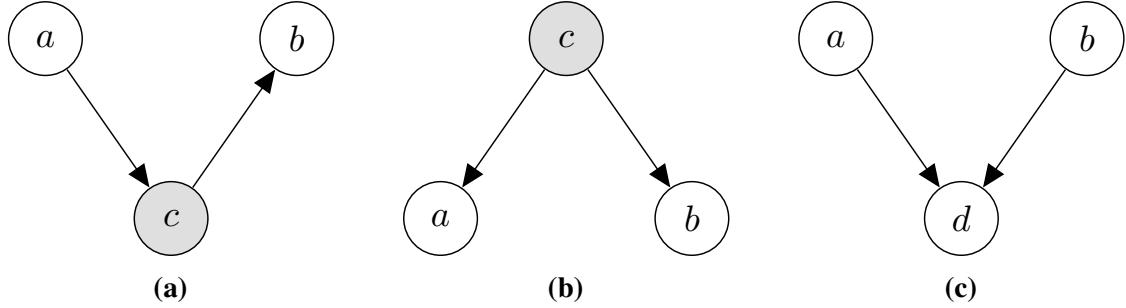


Figure 3.3: Examples of DAGs blocked between a and b . (a) is blocked by the second rule of d-separation. More specifically we have $p(b|a, c) = \frac{p(a,b,c)}{p(a,c)} = \frac{p(a)p(c|a)p(b|c)}{p(a)p(c|a)} = p(b|c)$. (b) is blocked by the first rule of d-separation. Here we have $p(b|a, c) = \frac{p(c)p(a|c)p(b|c)}{p(c)p(a|c)} = p(b|c)$. Consequently, for (a) and (b) then a and b are conditionally independent given c . (c) is an instead example of where a and b are marginally independent. Here the path between a and b is blocked because the the arrows meet head-to-head at d and neither d nor any of its descendants are observed. We thus have $p(b|a) = \frac{p(a)p(b)p(d|a,b)}{p(a)p(d|a,b)} = p(b)$. Note though that a and b are note conditionally independent given d as the path becomes unblocked if this is observed (see Figure 3.4).

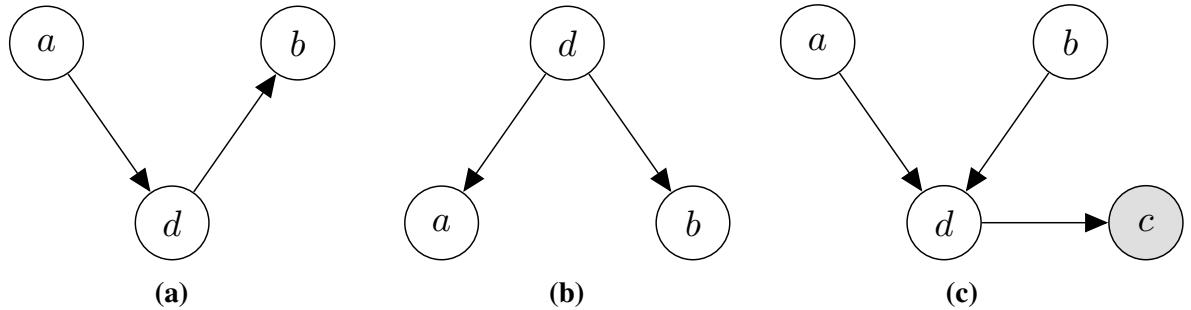
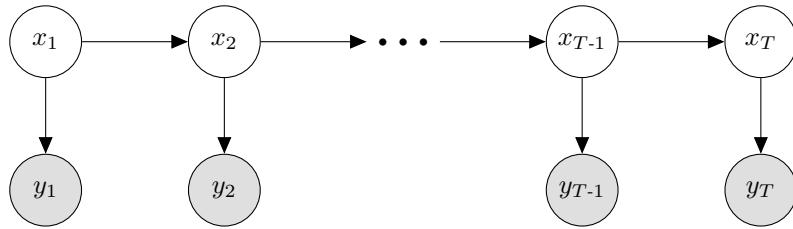


Figure 3.4: Examples of DAGs unblocked between a and b . For (a) then the path from a to b is not blocked by the d-separation rules. Perhaps more intuitively, we have that $p(b|a) = \int p(b, d|a)dd = \int p(b|d)p(d|a)dd \neq p(b)$ unless $p(d|a) = p(d)$. Similarly there is an unblocked path for (b) from a to b as the path that does not pass through any observed nodes or nodes with both arrows points towards it. Here we have $p(b|a) = \frac{p(d)p(a|d)p(b|d)}{p(a)p(d|a,b)} \neq p(b)$ again in general. The path in (c) is unblocked because of the phenomenon of *explaining away*. The first rule of d-separation does not apply here because c is an observed descent of d . We thus have that a and b are marginally independent as per Figure 3.3c, but not conditionally independent given c (and/or d). The rationale for explaining away can thought of in terms of events needing an explanation – if two precursor events (here a and b) can give rise to a third event (here c), then the third event occurring but not the first precursor event implies that the second precursor event occurs. Thus the two precursor events are correlated because one *explains away* the other. As described in Section 2.3, one example of this is that if a speed camera is triggered and the camera is not malfunctioning, this implies the vehicle is speeding, even though the vehicle speeding and the camera malfunctioning are marginally independent.

**Figure 3.5:** DAG for a hidden Markov model.

an off-the-shelf model like a HMM with known analytic solution. Though often necessary, this must be done with extreme care and the implications of the approximations should carefully considered. Unfortunately, quantifying the implications of approximations can be very difficult, given that they are typically made in the interest of tractability in the first place. This is a serious practical weakness of Bayesian modeling and should be factored in to the decision processes of whether taking a Bayesian approach or not. While taking a Bayesian approach for large projects, one should, in general, avoid making approximations or non-clearcut assumptions until absolutely necessary, but also keep in mind that it may be necessary to do so further down the line and account for this appropriately.

3.4 Frequentist vs Bayesian – an Atheist’s View on Two Religions

We have just introduced the Bayesian approach to generative modeling, but this is far from the only possible approach. In this section, we will briefly introduce the alternative, *frequentist*, approach. Unfortunately, there is often a substantial, and sometimes acrimonious, divide between those who advocate Bayesian or frequentist methods within the statistics and machine learning communities. Many people have very strong views one way or another in the debate and it is easy, certainly as a graduate student, to be sufficiently isolated on one side of the divide to completely detract oneself from the considerations of the other. It sometimes feels that the beliefs of some advocates of each side are so deep rooted and fundamental that this is almost a religious, rather than scientific divide. Given the fierceness of the debate, the actual statistical differences between the approaches (rather than the well known philosophical differences we touched on in Section 2.2 which are often dubiously used for justification) are often surprisingly poorly understood. Our aim in this section is not to advocate the use of one approach over the other, but to (hopefully objectively) highlight these statistical differences and demonstrate that *both* approaches have

flaws, such that “head in the sand” mentalities either way can be highly detrimental. We note that whereas Bayesian methods are always, at least in theory, generative [Gelman et al., 2014, Section 14.1], frequentist methods can be either generative or discriminative. As we have already discussed differences between generative and discriminative modeling in Section 3.1 we will omit this difference from our subsequent discussion.

At their root, the difference between Bayesian and frequentist methods stem from distinct fundamental assumptions: frequentist modeling presumes fixed parameters, Bayesian modeling assumes fixed data. In many ways both of these assumptions are actually quite silly. Why assume fixed parameters when we do not have enough information about from the data to be certain of the correct value? Why ignore that fact that other data could have been generated by the underlying process for the same underlying true parameter? Perhaps this is why people have such strong views either way – the arguments against both methods are very strong, so much so that advocates are often, sometimes unintentionally, willing to overlook the shortcomings of their favored approach.

To elucidate the different assumptions further and start looking into why they are made, we will now step into a decision theoretic framework. Lets presume that the universe gives us some data X and some true parameter θ , the former of which we can access but the latter of which is unknown. We can alternatively think about this as X being some information that we actually receive and θ as some underlying truth or oracle from which we could make perfect predictions. There is no need for θ to be some explicit finite parameterization. Any machine learning approach will take this data as input and return some artifact or decision, for example predictions on test data. Lets call this our action, or decision, $a(X)$ and further presume that for a given X , $a(X)$ is deterministic (if we allow our predictions to be probability distributions this assumption is effectively equivalent to assuming we can solve any analysis required by our approach exactly). Presuming that our analysis is not frivolous, there will be some loss function $L(a(X), \theta)$ associated with the action we take and the true parameter θ , even if this loss function is subjective or unknown. At a high level, our aim is always to minimize this loss, but what we mean by minimizing the loss changes between the Bayesian and frequentist settings.

In the frequentist setting, X is a random variable but θ is not. Therefore, one takes an expectation of possible data that could have been generated to give the frequentist risk $R(\theta)$

which is thus a function of theta Vapnik [1998]

$$R(\theta) = \mathbb{E}[L(a(X), \theta)|\theta]. \quad (3.17)$$

The focus is therefore on *repeatability* the generalization of the approach to different datasets that *could* have been generated. Choosing the parameters θ is thus based on optimizing for the best average performance over possible datasets, which common approaches including cross validation and minimax selection of θ . In some ways this is a pessimistic approach and the emphasis is on repeat performance and ensuring satisfactory performance for repeated use on different possible datasets.

In the Bayesian setting, θ is a random variable but X is not. Therefore one takes an expectation over θ to make predictions conditioned on the value of X giving the *posterior expected loss* Robert [2007]

$$\varrho(\pi, X) = \mathbb{E}_{\pi(\theta)}[L(a(X), \theta)|X] \quad (3.18)$$

where $\pi(\theta)$ is a prior distribution on θ . Although $\varrho(\pi, X)$ is a function of the data, the Bayesian approach takes the data as given (after all we have a particular dataset) and so for a given prior, the posterior expected loss is a fixed value and, unlike in the frequentist case, further analysis is not required: the posterior conveys all the information required. The focus of the Bayesian approach is generalizing over all the possible values of the parameters and using all the information at hand. This can be quite an optimistic approach as it does not consider the fact that, even for a given θ , other datasets might have been generated.

3.4.1 Shortcomings of the Frequentist Approach

One of the key criticisms of the frequentist approach is that predictions depend on the experimental procedure and can violate the *likelihood principle*. The likelihood principle is that, for a given model and data, the only information relevant to the parameters θ is conveyed by the likelihood function. In other words, the same data and the same model should always lead to the same conclusions about θ . Though this sounds intuitively obvious, it is actually violated by taking an expectation of X in frequentist methods as this introduces a dependency from the experimental procedure, which is ancillary information to the data and the likelihood function.

As a classic example, imagine that our data from flipping a coin is 3 heads and 9 tails. In a frequentist setting we make different inferences about whether the coin is biased depending on whether our data originated from flipping the coin 12 times and counting the number of heads or if we flipped the coin until we got 3 heads. For example, at the 5% level of a significance test we can reject the null hypothesis that the coin is unbiased in the latter case but not the former case. This is obviously somewhat problematic but can be used to argue both against frequentist methods and the likelihood principle (and thus Bayesian methods). Using it to argue against frequentist methods, and in particular significance tests, is quite straight forward: the subjective differences in our experiment should not effect our conclusions about whether the coin is fair or not. We can also take things further and make the results change for absurd reasons: if our experimenter had intended to flip until she got 3 heads but was then attacked and killed by a bear while the twelfth flip was in the air such that further flips would not have been possible regardless of the outcome, this again changes our conclusions about where the coin is biased. Clearly it is ridiculous that the occurrence or lack of a bear attack during the experiment should change our inferences, but that is need to know information for frequentist approaches, particularly if using p-values.

As we previously suggested though, one can also use this example to again for frequentist methods because it actually suggests the likelihood principle is incorrect. Although p-values are a terribly abused tool whose misuse has had severe detrimental impact on many applied communities [Goodman, 1999; Ioannidis, 2005], they are not incorrect if interpreted correctly and are an extremely important part of the statistical arsenal when used appropriately. If one very carefully considers the definition of a p-value as being the probability that the observed event or one more extreme is observed if the *experiment is repeated*, we see that our bear attack does actually effect the outcome. The chance of getting the same or more extreme data from repeating the experiment of “*flip coins until you get 3 heads or make 12 flips (at which point you will be killed by a bear)*” is different to the chance of getting the same or a more extreme result from repeating the experiment “*flip coins until you get 3 heads*”. As such, one can argue that the apparent absurd changes in conclusions originate from misinterpreting the results and that, in fact, these changes actually demonstrate that the likelihood principle is flawed by demonstrating why the experimental procedure actually matters because otherwise we have no concept of repeatability. Imagine instead the scenario where a suspect researcher stops their experiment early as it looks like the results are likely to support their hypothesis

and they do not want to take the risk that if they keep it running as long as they intended, then the results might no longer be so good. Here the researcher has clearly biased their results in a way that ostensibly violates the likelihood principle.

Whichever view you take, two things are relatively indisputable. Firstly a number of a frequentist concepts, such as p-values, are not compatible with the likelihood principle. Secondly, frequentist methods are not always coherent such that they can return answers that are not consistent with each other or probabilities that do not sum to one. For example, p-values for a hypothesis and its complement do not in general sum to 1.

Another major criticism of the frequentist approach is that it takes a point estimate for θ , rather than averaging over different possible parameters. This can be somewhat inefficient in the finite data case as it limits the information stored in the model to that stored by the parameters and it is clearly wasteful for a model to make predictions based on only one possible set of parameters when our parameter estimates are not known to be correct. Part of the reason that this is done is to actively avoid placing a prior distribution on the parameters, either because this prior distribution might be “wrong”³ or because at a more philosophical level, it is not a random variable under the frequentist definition of probability and so some people object to placing a distribution over it at a fundamental level (we will see this objection mirrored by Bayesians for the data in the next section). For the Bayesian perspective (and a viewpoint we actively argue for elsewhere in the paper), this is itself also a weakness of the frequentist approach as incorporating prior information is often essential for effective modelling.

3.4.2 Shortcomings of the Bayesian Approach

Now we have exposed some shortcomings of the frequentist approach, let's consider if the Bayesian approach does any better. Unfortunately, we find that the Bayesian approach is also not without its shortcomings. We have already discussed one key criticism in the last section in that the Bayesian approach relies on the likelihood principle which itself may not be sound, or at the very least ill-suited for some statistical modeling problems. More generally, it can be seen as foolhardy to not consider other possible datasets that might have been generated. The rationale typically given for this is that we should use all the information available in the data

³Whether a prior can be wrong, or what that even means, is a somewhat open question except in the case where it fails to put any probability mass (or density for continuous problems) on the ground truth value of the parameters.

and by calculating a frequentist risk we are throwing some of this away. For example, cross-validation approaches only ever use a subset of the data when training the model. However, a common key aim of statistics is generalization and repeatability. Bayesian approaches will often reach spectacularly different conclusions for purely random changes between different datasets. Consider for example, a binary classification problem where using parameters θ_1 classifies four billion of five billion points in the dataset correctly while using parameters θ_2 classifies four billion and one thousand of data points correctly. This gives a difference in classification accuracy of 0.00002% but differences in the posterior probabilities for θ_1 and θ_2 will generally be huge. Now presume that we regenerate our data and that each new point is drawn i.i.d., that the probability of it being correctly classified using θ_1 is independent to the probability of being correctly classified by θ_2 , and that these probabilities are equal to the empirical misclassification rates. The probability that θ_1 gives a better misclassification rate for the new dataset is around almost 50%, even though previous posterior suggested that θ_2 was substantially better than θ_1 . Furthermore, if θ_1 does give a much better misclassification rate for the new dataset, it is likely to be assigned a substantially higher mass under the posterior than θ_2 , even though we know that the latter is actually asymptotically preferable. In terms of the posterior expected loss, this is not much of a problem as for most sensible loss functions this will not substantially change. However, if our aim is actually to learn about θ then this is quite worrying. At the very least it shows why we should view posteriors with a degree of skepticism, rather than taking them as ground truth.

Make
this
concrete

Another concern for Bayesian approaches is the choice of the prior ...

write me

Lack of ability to take discriminant approach

Computational intensity, particularly in terms of prediction compared to using point estimate for θ .

3.4.3 Are there Alternatives?

Rewrite and expand the next paragraph

We might now ask, is anything correct? The answer here is probably no, but that this does not really matter. All methods have their strengths and weaknesses and provided we use approaches appropriate to the problem at hand, things should work out. One thing that can be done and should probably be done more often is to use both Bayesian and frequentist approaches concurrently,

by averaging both over data and over parameters, leading to the *Bayes risk*. For example, one could be Bayesian about the results from a cross validation test. Such an approach is still inevitably not universal – we still need to choose a prior,

We argue that the two positions that are completely indefensible are the complete dismissal of Bayesian methods and the complete dismissal of frequentist methods. We have demonstrated that there are shortfalls in both and, in general, there will be some cases where one is preferable and some where the other is. In particular, the Bayesian approach is essential when working with small datasets but where we have substantial prior expertise. On the other hand, a frequentist approach is essential to ensuring repeatability for large datasets with little prior knowledge of note. We will take a Bayesian approach for most of the rest of this thesis, but this is decision based subject matter and to give focus of the work, rather than a point of principle.

Missing points:

Bayesian models are slow in prediction

mean vs median

Both assume some true underlying θ - often inferior to say an ensemble approach, Issues of Bayesian model averaging.

Using the data twice because influences choice of prior

3.5 Challenges of the Bayesian Approach

Di Finetti and i.i.d. assumption of data.

4

Probabilistic Programming – the User’s Perspective

Probabilistic programming systems (PPSs) allow (Bayesian) probabilistic models to be represented in the form of a generative model and statements for conditioning on data [Gordon et al., 2014; Goodman et al., 2008b]. Informally, one can think of the generative model as the definition of a prior, the conditioning statements as the definition of a likelihood, and the output of the program as samples from a posterior distribution. Their core philosophy is to decouple model specification and inference, the former corresponding to the user-specified program code, which implicitly defines a distribution on random variables, and the latter to an inference engine capable of operating on arbitrary programs. Removing the need for users to write inference algorithms significantly reduces the burden of developing new models and makes effective statistical methods accessible to non-experts. The inference/model abstraction barrier further means that some systems allow the definition of models that would be hard, or even impossible, to convey using conventional frameworks like graphical models.

Two key challenges for a PPS are in providing the syntax and semantics to allow easy definition of models, and in designing the solvers, i.e. inference engines, to provide effective inference for those models. In this chapter, we focus on the former of these, providing an introduction to probabilistic programming from a user’s perspective, explaining how it can be used for, and to extend, conventional Bayesian modeling and how it can also be used to reinterpret many computational simulation techniques not usually associated with Bayesian modeling in a more Bayesian mindset. We will mostly ignore the rather major issue of how to construct automated inference engines for probabilistic programs, returning to address this in Chapter 7. Here we will explain how general purpose PPSs aim to provide the *flexibility* to define wide ranging and potentially obscure models, the *expressivity* of a framework for

model definition that is more in line with conventional scientific simulation than mainstream statistical approaches, and the *automation* to run any problem the user might write by decoupling model specification and inference. Together these characteristics produce a framework that allows researchers whose expertise lies elsewhere, to carry out powerful statistical analyses for their application specific tasks. This framework also aids in the development of both inference algorithms and models for those within the machine learning and statistics communities, by removing many of the complications of one while developing the other.

We note that it will be necessary at times during this chapter to refer briefly to some Bayesian inference algorithms that will not be properly introduced until Chapters 5 and 6. We have situated this chapter before those partly in order to emphasize the point that one should not need an intricate knowledge of inference methods to *use* PPSs. Though it is difficult to introduce PPSs while completely omitting reference to inference methods, readers who are not familiar with inference methods should be able to safely ignore which methods are referred to at a first pass, noting only that different inference algorithms have different requirements and sets of problems they perform well on, and thus that the design of a PPS is intricately linked to the inference method(s) used.

Avoiding bugs in code

Relationship with ABC - Church pretty indistinguishable, while modern systems exploit program itself

4.1 Inverting Simulators

Though the use of Bayesian modeling through the sciences and engineering is widespread, it is still dwarfed by the use of simulators more generally. Some simulations are inherently probabilistic, such as many of those used in statistical physics [Landau and Binder, 2014], financial modeling [Jäckel, 2002], and weather prediction Evensen [1994]. Others are deterministic approximations of a truly stochastic world, such as lap time simulation for formula one cars [Perantoni and Limebeer, 2014] and finite element simulations for fluid dynamics [Versteeg and Malalasekera, 2007]. In many of these scenarios, real data is also available, but not in sufficient quantities that the carefully constructed simulations can be done away with entirely and replaced by a purely data driven approach. Imagine the potential utility of general purpose methods for incorporating real data into these simulators to improve them, without having

to throw away the existing carefully constructed models. What about if we could even find methods for automatically inverting these simulators? Given a target lap time, we could return the best car setup; given observations of, and a simulator for, human behavior, we could learn about the underlying cognitive processes; given a climate change model and measurements, we might infer what the driving factors are.

An ambitious long term aim of probabilistic programming is to solve such problems and to do so in an automated fashion so that it requires little or no statistical expertise on the behalf of the user, allowing for simple, widespread usage across many fields. The key realization is that stochastic simulators implicitly define probability distributions. They therefore represent generative models and using probabilistic programming we can reason about, and work with, these generative models explicitly. One typically thinks of Bayesian modeling in terms of the prior and the posterior, but one can also think about it in terms of defining a joint distribution over both parameters and data, then fixing the latter to the actual observations to get a conditional distribution from this joint. Simulators implicitly define such joint distributions, with the outputs of the simulator corresponding to the data, and the inputs and internal variables the parameters. Probabilistic programming allows us to turn this on its head, using the same code as the original simulator but instead providing the observed data as the input and then inverting the simulator through inference, thus learning about possible input parameters and other variables sampled during the program’s forward execution. As well as the clear direct utility of allowing such inversion, this process also allows us to improve our simulator using real data by calculating the posterior predictive distribution that incorporates both the original model and the information from the data.

To explain what we mean by inverting simulators more precisely, we will now consider the example of inferring Captchas [Mansinghka et al., 2013]. Even if the name is not familiar, we should all have come across Captchas before when a website shows us an image, such as those in Figure 4.1a, and asks us to type the characters in that image to demonstrate we are not a robot. We now ask the Machiavellian, but important, question: how might we write an algorithm that breaks this Captcha by automatically predicting these characters directly from the image? In other words, can we build a robot that mimics a human on a task specifically designed to distinguish between the two. If we had access to large supply of training examples, i.e. character-image pairs, we could of course use an off-the-shelf discriminative algorithm:

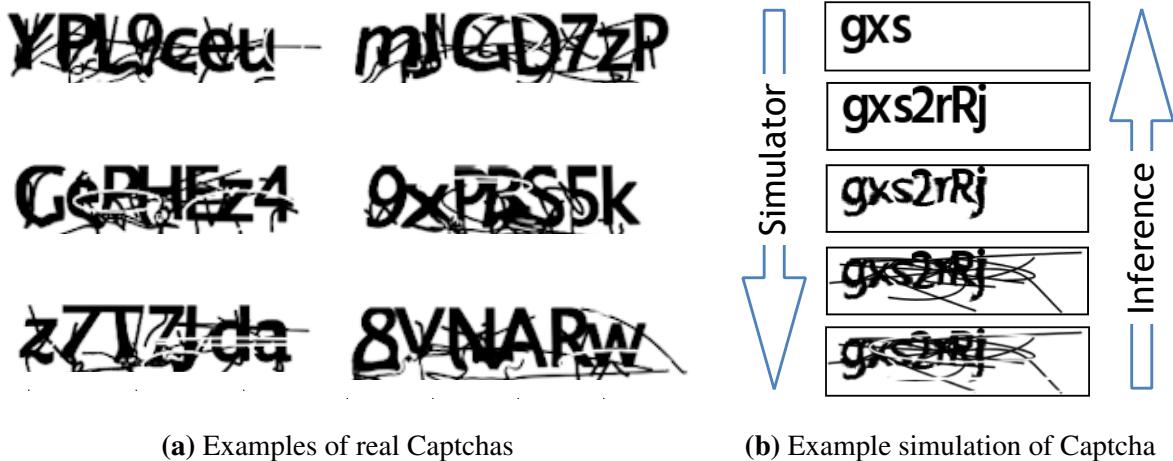


Figure 4.1: Solving Captchas by simulator inversion. (a) gives examples of real Facebook Captchas taken from Le et al. [2017b]. Here the corresponding generating strings going to clockwise from the top left are YPL9ceu, mJGD7zP, 9xPBS5k, 8VNARw, z7T7Jda, and GePHEz4. A user is asked to type in these strings when shown the corresponding image to show they are not a robot. (b) gives an example of the process of simulating Captchas taken by Le et al. [2017a]. Here we see that we can generate a Captcha by first simulating a series of characters, then simulating appropriate manipulations to those characters such as warping and rotating, and finally adding noise. Inverting this simulation process corresponds to an inference problem, where we want to find out the characters that lead to a particular image.

neural networks have been used to try and solve the problem in exactly this way with decent success [Von Ahn et al., 2008]. However, without access to an abundance of data this is a rather challenging task and we will need to exploit our prior knowledge about the problem.

Doing this process in reverse, i.e. simulating a Captcha, on the other hand, is a substantially less daunting process. The true Captchas are actually generated by a simulator and so we can attempt to mimic this original simulation process with our own. For example, as shown in Figure 4.1b we might first sample a number of characters, then a symbol for each character, apply manipulations such as rotations and warpings, simulate some obscuring lines or other noise, and finally render our simulated components into an image. Though admittedly it might make some time and effort to construct a high fidelity simulator that well matches the produced images, the technical requirements for doing this (other than possibly the final rendering) are minimal and so it could be carried out by most people with a reasonable degree of experience in scientific programming. The number of people able to write such a simulator should certainly be substantially larger than the number of people with sufficient experience in Bayesian modeling to construct an equivalent using a graphical model or direct mathematical formulation. The number of people with the expertise to then write an appropriate inference scheme for the problem is

even smaller still. In a PPS, writing this simulator and providing the data is all that is required. Given these, the PPS will carry out the inference required to invert the simulator automatically inferring the characters from the image. More generally, we are estimating the inputs and internal variables of our simulator, given target values for the outputs.

Their are two key factors to realizing our aim of inverting simulators. Firstly we need to provide a language which easily allows users to write down simulators and which has semantics that allows the compiler to extract an appropriate representation of the joint distribution. In other words, we need our language to be sufficiently general purpose and easy to use to not burden the user, while at the same time having syntax and semantics that ensure the corresponding joint distribution is well defined and can be converted into a form where we can run inference. Doing this will require introduction of means for *conditioning* on data and of specially defined *random primitives* whose behavior can be controlled at run time, rather than just always sampling from the same predefined distribution as they would in an ordinary programming language, and primitives. The latter can be thought of as defining terms in the prior and the former as terms in the likelihood as we will discuss in Section 4.3.

Secondly, our language needs a general purpose inference(s) engine capable of working on any program the user writes. Bayesian models are fully defined by their joint distribution and the data. Therefore, once a user has written their simulator and provided the data, this uniquely defines a posterior and the only problem is in solving resulting Bayesian inference. If we can now construct inference engines capable of working on arbitrary code, we can now construct systems for automatic inference on any simulator or model the user defines, creating an abstraction barrier between model definition and solving the model. We will discuss how this can be done in length in Chapter 7.

If we can make a system that successful carry out these tasks, the huge potential applications this could provide should be clear. We would have a system where the user requires no expertise in inference or conventional Bayesian modeling in order to write application specific models and have them solved automatically. Instead, they need only have the ability to write stochastic simulators for the process they wish to model, a skill possessed my most of the scientific community and many of those outside it as well. In a hypothetical future where scientists code all their simulators in extremely powerful PPSs, tasks such as inverting those simulators and improving the simulator by incorporating real data would be automated in the same way current

compilers convert high-level coding languages to machine code. However, this ability is not completely hypothetical – many such problems can already be handled by existing systems. The challenge is improving and scaling such systems to deal effectively with more difficult and more wide ranging models in a tractable manner. The need for such systems to work in an automated manner for a wide array of possible problems makes this a very difficult problem; after all we are somewhat flaunting the no-free-lunch theorem. However, there is a key component that provides hope that this may be possible: we have access to the target source code of the simulator itself, rather than needing to treat it as a black-box. Therefore maybe we can have our cake and eat it by using the source code itself to guide our algorithms, such that they behave in problem specific ways. We will discuss how this can be done at length in Chapters 7 and 9.

Add something about hard / soft constraints and the equivalence between conditioning and constraints. In particular, link back to the fact we talk about deterministic simulators as well as stochastic.

4.2 Differing Approaches

Rather than being a clearly defined particular algorithm, probabilistic programming is more of an umbrella term that covers a spectrum of different approaches, varying from inference toolboxes through to probabilistic programming languages (PPLs) that allow arbitrary probabilistic code to be written, even that which might not correspond to a valid model. Often there is a trade-off between efficiency and expressivity: the more restricted one makes the language, the more those restrictions can be exploited to improve the efficiency of the inference. This leads itself two distinct philosophies when developing a system. Firstly one can start with a particular inference algorithm and then design a system around making it as easy as possible to write models for which that inference algorithm is suitable. Secondly one can start with a general purpose PPL that allows as many model as possible to be written and then try to construct inference engines that are capable of work in such a general framework. Both approaches have their merits and drawbacks, with the distinction typically coming down to the intended use. We will now elucidate each approach more precisely.

4.2.1 Inference Driven Systems

Though there is a plethora of bespoke inference algorithms designed for particular models, the vast majority of these are based around a relatively small number of foundational methods such as importance sampling, sequential Monte Carlo, Metropolis-Hastings, Gibbs sampling, message passing, and variational inference (see Chapter 5 for an introduction to Bayesian inference). The extensive use of these core inference approaches throughout Bayesian statistics and machine learning means that it makes clear sense to write packages for automating them and which make it easy for the user to define an appropriate graphical models for which the inference can be automated. This both improves efficiency of modeling and reduces barriers to effective Bayesian modeling by reducing the required inference expertise for users. This inference-first philosophy is taken by a number of successful PPSs and inference toolboxes (the distinguishing line between which can be a little blurry) such as, amongst many others,

- BUGS (Bayesian inference Using Gibbs Sampling) [Spiegelhalter et al., 1996] and its extensions [Lunn et al., 2000; Plummer et al., 2003; Todeschini et al., 2014] allows finite DAGs to be specified using declarative code or pictorially using a graphical user interface. These are converted to a form that is suitable for inference, the exact nature of which depends on the implementation.
- Infer.Net [Minka et al., 2010] is modeling language for defining, and automating approximate inference in, both DAGs and Markov random fields, using predominantly message-passing algorithms. Distributions are predominantly, though not exclusively, restricted to be exponential families. Branching (i.e. `if` statements) is allowed, but requires enumeration of all possible paths.
- LibBi [Murray, 2013] is a package for doing Bayesian inference for state-space models, using particle-based inference methods (see Chapter 6). There is a strong focus on scalable computation, providing support for multi-core architectures and graphics processing units.
- PyMC3 [Salvatier et al., 2016] is a python framework for carrying out MCMC and variational inference, using Theano [Bergstra et al., 2010] to calculate the gradients required by some inference methods.

- Stan [Carpenter et al., 2015] is a PPS with interfaces to many different languages with a focus on performing Hamiltonian Monte Carlo inference [Duane et al., 1987; Hoffman and Gelman, 2014], though other inference methods such as variational inference are provided as well [Kucukelbir et al., 2015]. As with PyMC3, automatic differentiation is used to calculate required gradients. The need to take derivatives, means that there is limited support for discrete variables or branching.

These systems do not allow users to write models that would be difficult (at least for an expert) to code without a PPS – in general they all can be thought of as defining a graphical model or sometimes factor graph – but they offer substantial utility through ease of model exposition and automating inference.

4.2.2 Universal Probabilistic Programming

As useful as these inference-driven systems are, they do not fit very well with the notion of inverting simulators we introduced in Section 4.1. They are still closely tied to graphical models and are more toolboxes for streamlining the Bayesian modeling process than a means of writing models that would be problematic to define by conventional means. Achieving our long term ambitious aim of making general purpose systems for conducting inference of arbitrary simulators will require us to take a somewhat different approach that instead starts with a general-purpose language and then attempts to design inference algorithms capable of working on arbitrary models and code. It will be necessary for such systems to support models where the set of random variables is dynamically typed, such that it is possible to write programs in which this set, and thus potentially the number of random variables, differs from execution to execution. To avoid hindering the user or restricting the models which can be defined, it will be important to allow things such as branching, recursion, higher-order functions, conditional existence of variables, and arbitrary black-box deterministic functions. Ideally, we would like to provide no restrictions on the code that the user can write, except for eliminating programs that do not define valid probability distributions, such as those that have a non-zero probability of never terminating. In practice catching such cases can be hard or even impossible and so many systems actually adopt a philosophy of applying no restrictions, such that it is perfectly possible to define invalid models. General purpose PPSs actually bring up new theoretical questions about what constitutes

a valid probability model [Heunen et al., 2017], while even the set of valid definable models is a strict super-set of those definable by graphical models for many systems [Goodman, 2013].

In the rest of this thesis, we will predominantly focus on these *universal* PPLs [Goodman et al., 2008a; Staton et al., 2016], so-called because they are based on *Turing complete* languages that can specify any computable distribution [Goodman, 2013]. For our purposes, we further refine this definition to systems that also allow specification for any computable conditioning. We will regularly use the universal PPL Anglican [Wood et al., 2014] as a reference, an introduction to which is provided in Section 4.4. Here we will briefly discuss some other prominent higher order PPLs.

Church is a PPL based on Scheme Goodman et al. [2008a]. The original seminal paper and accompanying system forms a foundation on which many of the prominent existing systems are built through its demonstration that higher-order probabilistic programs define valid probability models, even in the presence of infinite recursion. However, Church predominantly only considers the case of *hard conditioning*,¹ namely a model in Church comprises of a generative sampler and a separate predicate procedure which returns true if the desired conditions are satisfied. This is somewhat restrictive for practical use as one cannot effectively condition on continuous data, given that the generation of that data under the joint distribution has zero probability such that this post-hoc hard constraint application will never be satisfied. This complete separation of the generative process and the conditioning (which is arguably more in line with approximate Bayesian computation [Csilléry et al., 2010] methods than with modern PPLs) can also be wasteful in not allowing the structure of a model to be exploited (see Chapters 6 and 7). Later systems therefore mostly allow soft conditioning statements to be interleaved through the generative progress (in an analogous manner to likelihood terms), increasing the range of models than can be encoded and potentially efficiency of inference algorithms. Inference in Church (and its direct derivatives) is typically carried out using either rejection sampling or MCMC. Church places a particularly strong emphasis on the ability to carry out *nested inference*, something we will look into in depth in Chapter 10 where we demonstrate that only models can either be represented as a single inference, or fall out of the scope of conventional convergence proofs.

Venture [Mansinghka et al., 2014] is a probabilistic programming platform providing a flexible system for both specification of models and inference methods. It has a strong emphasis

¹Some very limited support for soft-conditioning is provided in current implementations through a “noisy equals” that equates to a Gaussian likelihood.

Looks like church might not actually support proper nesting

on being extensible and for allowing the hosting of eternal applications. For example, it allows for user to provide proposals for the inference engine or reprogram the inference strategy entirely. Venture is predominantly used via the VentureScript [Mansinghka et al., 2014] PPL.

WebPPL [Goodman and Stuhlmüller, 2014] is a PPL built using a purely functional subset of Javascript, conveniently allowing for embedding in web pages. It combines the ability to write a generative process using sampling statements and to add in likelihood terms through a *factor* primitive that is analogous to the `observe` primitive that we will introduce in Section 4.3.1. At its back end, WebPPL provides a number of different inference algorithms, such as SMC and MCMC methods.

The price for the expressivity of these general purpose systems is a substantial extra burden on the inference engine as we will discuss in Chapter 7. In general, inference methods for such systems must be formulated in such a manner that they are applicable to models where the density function is intractable and can only be evaluated during forwards simulation of the program. For example, it may not be possible to know if a variable is continuous or discrete except by running the program, while some variables will only exist conditioned on the values of others. This required generality of the inference engine will naturally lead to a drop in performance compared to custom written inference code, but this is often a price worth paying for generality, particularly when considering models that would be challenging to express, let alone do inference in, using more conventional frameworks.

4.3 Bayesian Models as Program Code

In Section 4.1 we showed how one can think of PPS as inverting simulators, predicting internal variables given the outputs. In this section we will take a different perspective and show how we can translate Bayesian modeling into the framework of program code. In Chapter 3 we showed how a Bayesian model is defined by a prior over parameters and a likelihood function for those parameters given the data. This viewpoint will mostly translate into the probabilistic programming setting by equating between the prior and sampling statements and between the likelihood and conditioning statements. However, in Section 4.3.2 we will explain why this is not always true and suggest a formulation, distinct to that commonly used in the literature, for how the density implied by a query can be correctly represented.

A key point to note throughout this section is that probabilistic programs define models rather than procedures. We refer to these models as *queries* [Goodman et al., 2008b] which are analogous to functions in a ordinary language. In a standard programming language, functions take in inputs and then run through a series of commands in order until termination is reached.² Likewise, random sampling statements like `rand`, `randn` etc, make a single independent draw from the same distribution each time they appear in the execution trace. Neither is the case for a probabilistic program query. Instead a query defines a model which is compiled to a form that can be interpreted by an inference engine which then outputs some characterization of the posterior such as a series of samples. Perhaps the easiest way to think about how a probabilistic program language works (though not necessarily what happens for all systems) is that the query is, or sometimes parts of the query are, run many (and potentially millions of) times and the exact behavior of this running is control by the inference engine. For example, the inference engine might sample from a different distribution than specified by the original sampling statement or it might run lots of instances of the query in parallel and then terminate some of the instances performing poorly, while duplicating instances doing well.

4.3.1 A Simplified Probabilistic Programming Setup

We first consider the case of constructing a restricted example PPL. We emphasize that this is by no means the only setup one can use, with design choices made in the interest of exposition. We will presume that our PPL has no branching (i.e. there are no `if` statements or equivalent), recursion, or memoization (i.e. functions are always re-evaluated from scratch when called); is first order (i.e. variables cannot be functions); and that it does not allow any conditioning on internally sampled variables. We will give our language two special constructs, `sample` and `observe`, between which the distribution of the query is defined. We will presume here and throughout that, other than the effects of `sample` and `observe`, functions in our PPL are *pure* such that they always provide the same outputs when called with the same inputs. This restriction naturally means that queries should not have any random components other than dictated by `sample` and `observe`, but also suggests that they should be free from side effects such as modifications of global variables. Informally, `sample` will be used to specify terms in the prior

²In functional programming languages operations are not necessary carried out in the order they are defined, but it still holds that the function takes inputs carries out a series of actions until the desired output is (perhaps lazily) calculated.

and **observe** terms in the likelihood. More precisely, **sample** will be used to make random draws $x_t \sim f_t(x_t|\Xi_t)$, where Ξ_t is a subset the other variables in scope at the point of sampling, and **observe** will use to condition on data $g_s(y_s|\Lambda_s)$ with Λ_s defined in the same way as Ξ_t . For our inference, it will be necessary to control the sampling and so we define the syntax of **sample** to take a *distribution object* as its only input and for **observe** to take a distribution object and an observation as input. We further define each distribution object as containing a sampling procedure and a density function that can be evaluated exactly.³ Our language will be provided with a number of *elementary random procedures* in the form of distribution classes for common sampling distributions such as the normal and Poisson distributions, but will also provide the ability for users to define their own distribution classes. These classes allow a distribution object to be constructed when provided with the required parameters, such that the distribution is fully defined before being passed to a **sample** or **observe**. We complete our syntactic definition of **sample** and **observe** by defining them to return a sample and `nil` respectively.

We distinguish between two types of inputs to our queries: external parameters θ and data $y_{1:S}$. The external parameters are defined as the inputs that are not “observed” at any point but can effect the conditioning through Ξ_t and Λ_s . We presume for our simplified setup that the data terms, defined as the inputs we are observed, appear in neither Ξ_t or Λ_s . We now define both **sample** and **observe** from the probability model perspective as adding a factor to the joint distribution which is therefore given by

$$p(x_{1:T}, y_{1:S}|\theta) = \prod_{t=1}^T f_t(x_t|\Xi_t) \prod_{s=1}^S g_s(y_s|\Lambda_s). \quad (4.1)$$

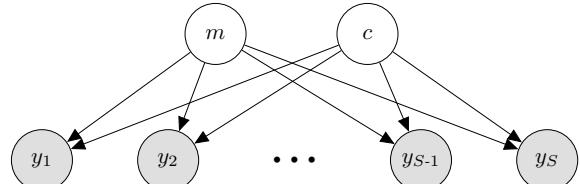
The two vary in whether they define a new random variable or effect the probability of the query given particular instances of the other random variables. Our presumptions for this simplified setup that no y_s terms are present in the Ξ_t or Λ_s and that we do not condition on internally sampled variables, means that the product of the **sample** terms correspond exactly to our prior $\prod_{t=1}^T g_t(x_t|\Xi_t) =: p(x_{1:T}|\theta)$ and that the product of the **observe** terms corresponds exactly to our likelihood $\prod_{s=1}^S g_s(y_s|\Lambda_s) =: p(y_{1:S}|x_{1:T}, \theta)$. Consequently, for our simplified setup, each query defines a finite directed acyclic graphical model (see Section 3.3) where the

³It will actually often be possible to use incomplete distribution objects for both **sample** and **observe** that only contain the sampler and the density function respectively. This former can be permitted by using inference algorithms that use the prior as the proposal, such that only the sampler will be required. The latter is sufficient in the vast majority of scenarios as, unless one is carrying out amortization [Paige and Wood, 2016; Le et al., 2017a], the data is fixed and does not need to be sampled.

Inputs: Student-t degrees of freedom ν , error scale σ , data $y_{1:S} = \{u_s, v_s\}_{s=1}^S$

```

1:  $m \leftarrow \text{sample}(\text{normal}(0,1))$ 
2:  $c \leftarrow \text{sample}(\text{normal}(0,1))$ 
3:  $\text{obs-dist} \leftarrow \text{student-t}(\nu)$ 
4: for  $s = 1, \dots, S$  do
5:    $d \leftarrow (v_s - mu_s - c)/\sigma$ 
6:   observe ( $\text{obs-dist}$ ,  $d$ )
7: end for
8: return  $m, c$ 
```



$$p(m, c, y_{1:S} | \nu, \sigma) = \mathcal{N}(m; 0, 1) \mathcal{N}(c; 0, 1)$$

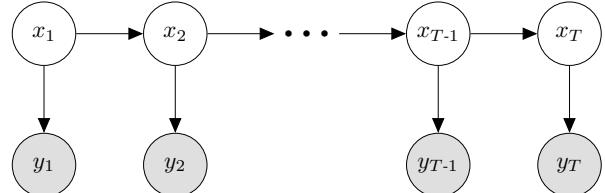
$$\prod_{s=1}^S \text{STUDENT-T} \left(\frac{v_s - mu_s - c}{\sigma}; \nu \right)$$

(a) Bayesian linear regression model with student-t likelihood, namely $v_s = mu_s + c + \sigma\epsilon_s$ where $\epsilon_t \sim \text{STUDENT-T}(\nu)$. We presume that the scaling of the error σ and the number of degrees of freedom ν are fixed input parameters (i.e. $\theta = \{\nu, \sigma\}$), that our fixed data is $y_{1:S} = \{u_s, v_s\}_{s=1}^S$, and that we are trying to infer the slope m and intercept c (we thus have $x_1 = m$, $x_2 = c$ in our general notation), both of which are assigned a unit Gaussian as a prior. Our query first samples m and c (note that `normal(0,1)` generates a unit Gaussian distribution object) and constructs a student-t distribution object `obs-dist`. It then cycles over each datapoint and observes $(v_t - mu_t - c)/\sigma$ using `obs-dist`, before finally returning m and c as outputs. Note that if we instead wished to directly predict the outputs at some untested inputs points $u_{S+1:S+n}$ then we could predict these anywhere in the query (after m and c have been defined) and return these as outputs along with, or instead of, m and c .

Inputs: Transition std-dev σ , output shape α , output rate β , data $y_{1:T}$

```

1:  $x_0 \leftarrow 0$ 
2:  $\text{tr-dist} \leftarrow \text{normal}(0, \sigma)$ 
3:  $\text{obs-dist} \leftarrow \text{gamma}(\alpha, \beta)$ 
4: for  $t = 1, \dots, T$  do
5:    $x_t \leftarrow x_{t-1} + \text{sample}(\text{tr-dist})$ 
6:   observe ( $\text{obs-dist}$ ,  $y_t - x_t$ )
7:    $z_t \leftarrow \mathbb{I}(x_t > 4)$ 
8: end for
9: return  $z_{1:T}$ 
```



$$\begin{aligned}
p(x_{1:T}, y_{1:T} | \sigma, \alpha, \beta) = \\
\mathcal{N}(x_1; 0, \sigma^2) \text{ GAMMA}(y_1 - x_1; \alpha, \beta) \\
\prod_{t=2}^T \mathcal{N}(x_t - x_{t-1}; 0, \sigma^2) \text{ GAMMA}(y_t - x_t; \alpha, \beta)
\end{aligned}$$

(b) State-space model with Gaussian transition and Gamma emission distributions. It is a form of the HMM model given in (3.16) with $p(x_1) = \mathcal{N}(x_1; 0, \sigma^2)$, $p(x_t | x_{t-1}) = \mathcal{N}(x_t - x_{t-1}; 0, \sigma^2)$, and Gamma likelihood model $p(y_t | x_t) = \text{GAMMA}(y_t - x_t; \alpha, \beta)$ with shape parameter α and scale parameter β . We assume that the input parameters $\theta = \{\sigma, \alpha, \beta\}$ are fixed and we want to sample from $p(z_{1:T} | y_{1:T}, \theta)$ given data $y_{1:T}$ where each z_t is an indicator for if x_t exceeds a threshold of 4. Our query, exploiting the equivalence between $p(x_1)$ and $p(x_t | x_{t-1} = 0)$, first initializes $x_0 = 0$ and creates distribution objects for the transitions `tr-dist` and emissions `obs-dist`. It then loops over time steps, sampling each x_t given x_{t-1} , observing y_t given x_t , and deterministically calculating z_t . Finally the $z_{1:T}$ are returned as the desired output.

Figure 4.2: Example pseudo-queries for our simplified probabilistic programming setup with corresponding graphical models and joint distributions.

conditional relationships are defined through the definitions of f_t and g_s . This breakdown into a prior and likelihood and the equivalence to graphical models will not hold in the more general cases we consider later. Our aim will be to perform inference to provide a characterization of $p(x_{1:T}|y_{1:S}, \theta)$ (or the posterior for some deterministic mapping of $x_{1:T}$), typically in the form of (approximate) samples. Figure 4.2 shows two example queries along with the corresponding graphical models and joint distributions they define.

Other than `sample` and `observe` statements, the rest of our query is by construction totally deterministic. Therefore, though it may contain random variables other than $x_{1:T}$, these random variables are deterministic functions of the “raw” random draws $x_{1:T}$ and inputs θ and $y_{1:S}$. We can therefore define the outputs of our query as $\Omega := h(x_{1:T}, y_{1:S}, \theta)$ for some deterministic function h . As we explained in Section 2.6, the change of variables means that the density function on Ω , $p(\Omega|y_{1:S}, \theta)$ can have a different form to the posterior implied by our query, namely $p(x_{1:T}|y_{1:S}, \theta)$. Though this is a serious complication in the context of optimization (we may not in general be able to find $\arg \max_{\Omega} p(\Omega|y_{1:S}, \theta)$ or even evaluate $p(\Omega|y_{1:S}, \theta)$ exactly), it is perfectly acceptable in the context of calculating expectations as

$$\int f(\Omega)p(\Omega|y_{1:S}, \theta)d\Omega = \int f(h(x_{1:T}, y_{1:S}, \theta))p(x_{1:T}|y_{1:S}, \theta)dx_{1:T} \quad (4.2)$$

for implicitly defined measures $d\Omega$ and $dx_{1:T}$. One consequence of this is that we can express any expectations calculated by our query as expectations over $p(x_{1:T}|y_{1:S}, \theta)$ which was fully defined by the joint (4.1). Another is that, provided we are not worried about carrying out optimizations, we do not need to explicitly worry about the implicit measures defined by the definition of our query, other than any potential effects on the inference scheme. In particular, if our aim is to generate samples from $p(\Omega|y_{1:S}, \theta)$ then we can simply generate samples then we can simply generate samples from $p(x_{1:T}|y_{1:S}, \theta)$ and then deterministically convert each sample to the space of Ω . In other words, our inference engine does not need to worry about the consequences of changes of variables if our intended output is just a sequence of samples.

An important point to note is that (4.1) shows that all of our `sample` and `observe` statements are exchangeable, in the sense that their order can be moved around and still define the same joint distribution, up to restrictions about all the required variables (namely the distribution object and, if required, observation in our current setup) existing and being in scope. For example, if all variables remain in scope and are not redefined, we can generally move all our `observe`

statements to the end of the query without changing the joint distribution. Therefore the query given in Figure 4.2b would define the same model if all the x_t were sampled upfront before making any observations. Nonetheless, the position of the `observe` statements can often be important from the perspective of the performance of the inference engine. This exchangeability result will carry over to the non-simplified cases.

4.3.2 A General Probabilistic Programming Setup

Perhaps surprisingly, we do not need to do anything to our language to extend it to a universal PPL other than to relax a number of the restrictions made for our simplified case. Namely, we will allow branching, higher order functions, (potentially infinite) recursion, memoization, conditioning on internally sampled variables, and the use of the “data” inputs $y_{1:T}$ in the definition of our generate model (instead of just allowing them to be observed). We will maintain the syntax of our simplified setup, along with the assumption that functions are pure other than the effect of `sample` and `observe`. An important point to note though for why such a language is universal is that arbitrary distributions with finite parameters can be defined through a series of uniform $[0, 1]$ draws followed by an arbitrary deterministic mapping – after all, this is effectively how all probability distributions are defined from a measure theoretic point of view.⁴

However, these generalizations will have a substantial effect on the intuitions relating our universal PPL to the Bayesian framework, the range of models we can define, and the difficulty of performing general purpose inference. For example, as y_s terms can appear in the Ξ_t terms, it can be the case that $p(x_{1:T}|\theta) \neq \prod_{t=1}^T p(x_t|\Xi_t)$ such that the latter no longer explicitly corresponds to a conventional definition of a prior. Some variables may change type (e.g. between continuous and discrete) or even not exist depending on the value of other variables. The number of variables may change from one execution to the next and it could even be the case that the number of latent variables could be unbounded provided that either the probability that any execution has a finite number of variables is 1 or that only a finite number need to be evaluated to calculate the density, such as is the case for Bayesian non-parametric models such as the Dirichlet process [Ferguson, 1973; Teh, 2011]. Note that the number `sample` and `observe` statements lexically defined within our query must, for obvious reasons, be finite, but recursion or looping may mean that

⁴Interesting, this viewpoint breaks down for distributions over functions for which measure theory itself somewhat breaks down Heunen et al. [2017]. As such, universal PPSs actually go beyond the standard measure-theoretic view of probability.

they are evaluated an uncountable number of times. It is also possible for a variable within a query to itself encode an infinite number of parameters, for example, one might include a Gaussian process within the query (see Section 8.3). These complications make it difficult to mathematically reason about the joint distribution defined by a query in a universal PPS, let alone reason about its breakdown into a prior and a likelihood or represent the query using a graphical model (which might actually not even be possible).

One way to conceptually overcome these difficulties is to reason in terms of *execution paths*. Even though we might not know upfront which `sample` and `observe` statements are invoked by a particular query output, if we execute the query in order, the draws of the `sample` statements made thus far in an *execution trace* uniquely identify which `sample` statement will be invoked next, the value of all the variables up to that `sample` statement, and all `observe` calls prior to the next `sample` statement in the path. In other words, given the outcome of t evaluated `sample` statements, which `sample` statement corresponds to the $(t + 1)$ -th to be evaluated is uniquely defined and the query up to that `sample` statement is completely deterministic, including which path to take at each `if` statement, which variables are defined and their values, and the probability arising from the `observe` conditioning statements. Thus although the distribution of the query is not necessarily statically determinable, it can still be *evaluated through execution* as each `sample` statement provides the information we require, in addition to the information from the previous `sample` statements, to deterministically evaluate up to the next `sample` statement. Consequently, we can evaluate the probability of any particular trace as we run it, even though it might be challenging to evaluate the probability of a predefined configuration of the variables.

Using this idea of execution paths, we can define an expression for the conditional probability a query defines, albeit in a complex and somewhat abstract manner that only really retains meaning in our probability calculation through evaluation mindset, by defining the probability of a particular trace. First let λ denote all the inputs to the query (including both parameters and data as we will now have no explicit distinction between the two). Further let n_x and n_y be the number of `sample` and `observe` statements respectively invoked by the trace, noting that n_x and n_y may themselves be random variables and could potentially be unbounded (e.g. n_x could follow a Poisson distribution). We can now define $x_{1:n_x} = x_1, \dots, x_{n_x}$ and $y_{1:n_y} = y_1, \dots, y_{n_y}$ respectively as the outputs of our n_x `sample` statements and observation inputs for our n_y `observe` statements. Note the key point that each x_j is not in general a variable in our program

and so cannot be overwritten or edited. It is perhaps easiest to think of each x_j as being a new variable that is created whenever a sample statement is invoked. We can use this variable, either directly or by assigning its value to another variable, but the x_j is itself protected and cannot be changed. For example, we can think of $a \leftarrow \text{sample}(\text{dist})$ as creating a protected variable x_j and then immediately assigning its value to a . Because the rest of the program, including the outputs, is a deterministic function of `sample` statement outputs, then, provided this constitutes a measurable function, we can produce samples of, or calculate expectations with respect to, any variable or output of the program by dealing probabilistically only with the $x_{1:n_x}$.

Each x_i is obviously a random variable, but we note that each y_i might also be a random variable. However, for the reasons already explained, each $y_{1:n_y}$ is deterministically calculable given $x_{1:n_x}$ and λ . We continue by defining f_1, \dots, f_{n_s} and g_1, \dots, g_{n_o} respectively as the densities (with respect to an implicitly defined measure) associated with the n_s `sample` and n_o `observe` statements defined lexically within a raw program code (i.e. the distinct `sample` and `observe` statements defined anywhere within the query), noting that n_s and n_o are *not* random variables. To express these densities, we use the notation $f_i(x_j|\phi_j)$ to indicate the density of lexical `sample` statement i returning outputs x_j when provided with distribution object ϕ_j , which is itself a random variable but one which is fully determined by $x_{1:j-1}$ and λ . Similarly, we use the notation $g_i(y_k|\psi_k)$ to express the density of using lexical `observe` g_i to observe output y_k with distribution object ψ_k , which is a random variable fully determined by $x_{1:n_x}$ and λ . We define $a_j \in \{1, \dots, n_s\}$, $\forall j \in \{1, \dots, n_x\}$ and $b_k \in \{1, \dots, n_o\}$, $\forall k \in \{1, \dots, n_y\}$ as the random variables respectively used to index which of the lexical `sample` and `observe` statements correspond to the j^{th} and k^{th} execution trace `sample` and `observe` statement.

To encapsulate the notion of a valid trace, we define the boolean function $\mathcal{B}(x_{1:n_x}, \lambda)$ which returns 1 if the trace is valid and 0 otherwise. This is something we do not need to worry about if we take an evaluation based inference approach, whereby we rely on methods that only simulate from the generative model, but it is necessary to ensure that the density is well defined if we try to evaluate it at a predetermined point, chosen externally to the program. For example, $\mathcal{B}(x_{1:n_x}, \lambda)$ is necessary to ensure that $x_{1:n_x}$ is a “complete” trace: it may be that a certain $x_{1:n_x}$ implies that further `sample` statements are still to be invoked after the n_x^{th} in which case the trace is not valid as these additional outputs are undefined. For example, if the program defines the distribution $\mathcal{N}(x_1; 0, 1)\mathcal{N}(x_2; 0, 1)\mathcal{N}(4; x_2, x_1)$ then the trace $x_1 = 3.2$ is incomplete and

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although there is well defined marginal on x_1 , its density in general not equal to that implied by partial evaluation of the trace. Similarly, we can use $\mathcal{B}(x_{1:n_x}, \lambda)$ to encode that in our example $P(n_x > 2) = 0$. Meanwhile, $\mathcal{B}(x_{1:n_x}, \lambda)$ also ensures that all terms within the trace probability are well defined. For example, if $x_{1:j-1}$ implies that x_j should be a real number but the provided x_j is a string then $f_{a_j}(x_j|\phi_j)$ will, in general, be undefined.

We now finally define the conditional distribution on the trace \mathcal{T} implied by our query as $p(\mathcal{T} = x_{1:n_x}|\lambda) \propto \gamma(x_{1:n_x}, \lambda)$ where

$$\gamma(x_{1:n_x}, \lambda) = \begin{cases} \prod_{j=1}^{n_x} f_{a_j}(x_j|\phi_j) \prod_{k=1}^{n_y} g_{b_k}(y_k|\psi_k) & \text{if } \mathcal{B}(x_{1:n_x}, \lambda) = 1 \\ 0 & \text{otherwise} \end{cases} \quad (4.3)$$

noting that although the a_j , ϕ_j , etc are random variables, they are all deterministically calculable given $x_{1:n_x}$, λ , and our query. Similarly $\mathcal{B}(x_{1:n_x}, \lambda)$ is a deterministic function implied by the program. As a consequence, our program implies a well defined, normalized, conditional distribution, or “posterior, on the produced traces (presuming the normalization constant is finite and non-zero). Note that this definition is explicitly on outcomes of the trace and so, in general, $p(\mathcal{T} = x_{1:j}|\lambda) \neq \int p(\mathcal{T} = x_{1:n_x}|\lambda) dx_{j+1:n_x}$. In fact, it is always necessary that at least one of $p(\mathcal{T} = x_{1:j}|\lambda)$ and $p(\mathcal{T} = x_{1:n_x}|\lambda)$ are equal to zero if they share the same $x_{1:j}$ as a particular value of $x_{1:j}$ deterministically implies whether $n_x = j$ or not.

An illustrative example for calculating the probability of a program through execution traces for a problem that cannot not be expressed using our simplified PPL or a graphical model, but which is simple to write in our universal framework is shown in Figure 4.3. Imagine we want to calculate the unnormalized trace probability $\gamma(x_{1:n_x} = [0.2, 0.07], \lambda = 4)$ which we can do by stepping through the program and accumulating terms (for reference we will be following the cyan path in Figure 4.3a). On our path we first hit $f_1(x_1|\phi_1) = \text{UNIFORM}(0.2; 0, 1) = 1$, we fix $u \leftarrow x_1$ and $p \leftarrow 1 \cdot u$, and test if $p = 0.2 \leq \exp(-4) \approx 0.0183$. This gives false and so we do not break the while loop, instead encountering $g_2(y_1|\psi_1) = \text{BERNOULLI}(1; 0.2) = 0.2$ and so our running value for $\gamma(x_{1:n_x} = [0.2, 0.07], \lambda = 4)$ is $1 \times 0.2 = 0.2$. Updating $k \leftarrow 1$ and going back to the start of the while loop we encounter $f_1(x_2|\phi_2) = \text{UNIFORM}(0.07; 0, 1) = 1$, so our running score is $1 \times 0.2 \times 1 = 0.2$. Reassigning u and p we see that $p = 0.014 \leq \exp(-4)$ is now true and so we take the opposite branch to before with our if statement, thus breaking the while loop. To finish the program we pass through $g_1(y_2|\psi_2) = \text{BERNOULLI}(k > 3; 0.99) = 0.01$ giving the final unnormalized density of $\gamma(x_{1:n_x} = [0.2, 0.07], \lambda = 4) = 0.002$ and an output of $k = 1$. We

finish by checking that our trace was valid, which we can easily see is the case because no terms were undefined and we generated the correct number of sample outputs (i.e. $n_x = 2$ as required).

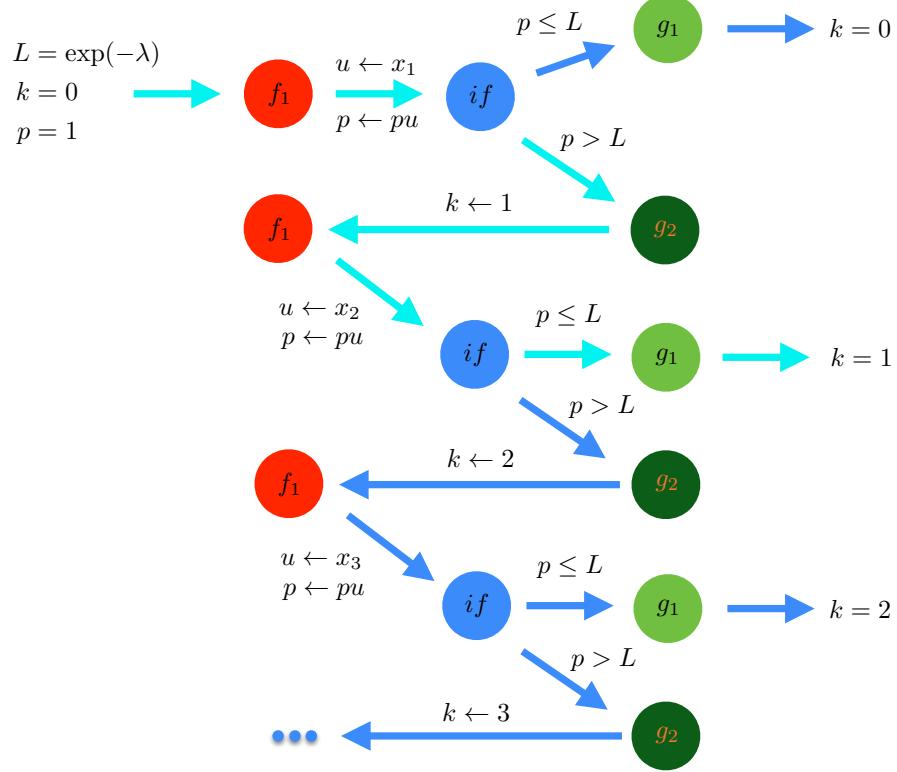
In general, $\gamma(x_{1:n_x}, \lambda)$ is not a normalized joint distribution. This firstly, and most obviously, because λ might contain terms, referred to as θ before, that are not observed and so have no implied density. Secondly, and more critically, even if $\theta = \emptyset$, $\gamma(x_{1:n_x}, \lambda)$ is not necessarily correctly normalized, because of the ability to observe sampled variables and condition the `sample` statements on the observations. As a simple example, our model might consist of a $x_1 \leftarrow \text{sample}(\text{normal}(0,1))$ term followed by an `observe` (`normal`(-1,2), x_1) term. This does not directly define any properly normalized joint distribution on any particular variables (noting $\mathcal{N}(x_1; 0, 1)\mathcal{N}(x_1; 0, 2)$ is an unnormalized distribution with only the variable x_1). Consequently, there is no means of writing down a normalized joint distribution for a general query in our universal PPL setup in closed form – we might actually need to empirically estimate the normalization constant to evaluate the joint. This actually steps outside the conventional Bayesian modeling framework and raises a number of interesting theoretical questions. However, from a practical perspective, we can note that provided the implicitly define normalization constant is finite, the query also implicitly defines a correctly normalized conditional distribution (noting that $\gamma(x_{1:n_x}, \lambda) \geq 0$). This is analogous to knowing the joint but not the posterior in Bayesian inference, but not exactly equivalent because the normalization constant is no longer the marginal likelihood.

As simple example of why it is important to be able to define models up to an unnormalized joint distribution, consider an example where a and b are each sampled from discrete distributions and we want to condition on the value of a and b being equal (see for example Figure 4.6 in the next section). Here the combination of the sample statements and the observation that the two are equal clearly does not lead to a correctly normalized joint (we do not even really have a conventional notion of a likelihood), but it clearly defines an unnormalized conditional distribution as

$$P(a, b|\mathbb{I}(a = b)) = \frac{P(a)P(b|a)\mathbb{I}(a = b)}{\sum_a \sum_b P(a)P(b|a)\mathbb{I}(a = b)}.$$

In such cases where our observation is a hard constraint, we can view the normalizing constant for the conditional defined by the query as the probability of our constraint being satisfied. For more general queries of discrete variables we might have, for example,

$$P(x|\lambda) \propto f(x|\lambda)g(y = \eta(x, \lambda)|x, \lambda)$$



(a) Possible traces for our query. `sample` statements are shown in red, `observe` statements are shown in shades of green, and deterministic computations (given the outputs of the `sample` statements) are shown in shades of blue. Subscripts for the sample and observe statements show the lexical index (i.e. $a_j \in \{1\}$ and $b_k \in \{1, 2\}$), as do the different shades. The cyan arrows correspond to a particular execution path which gives output $k = 1$ and has $n_x = 2$, $n_y = 2$, $b_1 = 2$, and $b_2 = 1$. Valid traces for this path must have $x_1 > \exp(-\lambda)$ and $x_2 \leq \exp(-\lambda)/x_1$.

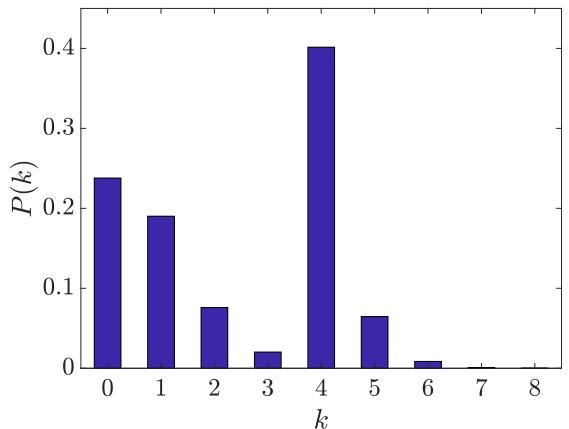
Inputs: Event rate λ

```

1:  $L \leftarrow \exp(-\lambda)$ ,  $k \leftarrow 0$ ,  $p \leftarrow 1$ 
2: while  $p > L$  do
3:    $u \leftarrow \text{sample}(\text{UNIFORM}(0, 1))$ 
4:    $p \leftarrow pu$ 
5:   if  $p \leq L$  then; break while; end if
6:   observe(BERNOULLI(0.2), 1)
7:    $k \leftarrow k + 1$ 
8: end while
9: observe(BERNOULLI(0.99),  $\mathbb{I}(k > 3)$ )
10: return  $k$ 

```

(b) Query code for warped Poisson sampler



(c) Conditional distribution on k for $\lambda = 4$.

Figure 4.3: Demonstration of execution stochastic execution traces using a warper Poisson sampler. The query defined in **(b)** would output k as per a Poisson distribution with event rate λ if it were not for the `observe` statements [Paige, 2016]. As shown in **(c)** though, these `observe` statements warp the distribution to give a lighter tail while discouraging $k \leq 3$. Here both $n_x \in \mathbb{N}^+$ and $n_y \in \mathbb{N}^+$ depend on the trace and are unbounded. Which `observe` we see first is also probabilistic, while it some traces will be invalid, e.g. $x_{1:n_x} = [1, 0.5]$ as $x_1 = 1$ indicates there will be only a single `sample` encountered. Nonetheless, we can calculate the probability of a trace by following its path to completion while accumulating `sample` and `observe` factors.

for some deterministic function η . Here we can view the marginalization as being the probability of the event $y = \eta(x, \lambda)$ under the joint $P(x, y) = f(x|\lambda)g(y|x, \lambda)$. For our previous example we have $x := a$, $y := b$, $\eta(a, \lambda) := a$, $f(a) := p(a)$, and $g(b = a) := p(b = a|a)$. The same intuition applies to continuous cases where we now have the density of the event $y = \eta(x, \lambda)$. We can also think of $f(x|\lambda)g(\eta(x, \lambda)|x, \lambda)$ as defining a unnormalized distribution on x whose normalization constant is $\int f(x|\lambda)g(\eta(x, \lambda)|x, \lambda)dx$. In general, our normalization constant will be a combination of conventional marginal likelihood terms and contributions from these “doubly defined” terms. We coin this normalization constant the *marginal observation density*⁵ and note that it is given by

$$\begin{aligned} Z(\lambda) &= \mathbb{E} \left[\prod_{k=1}^{n_y} g_{b_k}(y_k|\psi_k) | \lambda \right] = \int \gamma(x_{1:n_x}, \lambda) dx_{1:n_x} \\ &= \int_{x_{1:n_x} \in \{x_{1:n_x} : \mathcal{B}(x_{1:n_x}, \lambda) = 1\}} \prod_{j=1}^{n_x} f_{a_j}(x_j|\phi_j) \prod_{k=1}^{n_y} g_{b_k}(y_k|\psi_k) dx_{1:n_x} \end{aligned} \quad (4.4)$$

where the expectation is under running the query forwards (i.e. the distribution implied by simulating from an equivalent query with all the **observe** statements removed) and all terms in the integral are deterministically calculable for the query given λ and $x_{1:n_x}$. Note that for our query to represent a well defined conditional distribution, it is necessary to have $0 < Z(\lambda) < \infty$.

We now see that we can draw a direct analogy to the Bayesian framework whereby the product of the **sample** terms is analogous to the prior, the product of the **observe** terms is analogous to the likelihood, and the marginal observation density is analogous to the marginal likelihood. If observed variables are not sampled within or used elsewhere in the query (e.g. being used as parameters in distribution objects later used for sampling), then this analogy becomes exact as per our simplified setup.⁶ However, as we have explained, it will often be desirable to go beyond this framework to specify some models. When we do, we still have an implicit Bayesian model, in the same way that Bayes’ rule means that a prior and a likelihood implicitly define a posterior, but we may not actually have access to our implicitly defined prior and likelihood.

⁵Note this is not a term that has previously appeared in the literature, where it is usually just referred to as a marginal likelihood. Similarly, it is common in the literature to refer to a query as defining a “normalized joint” density of $p_\theta(x_{1:n_x}, y_{1:n_y}) = \prod_{j=1}^{n_x} f_{a_j}(x_j|\phi_j) \prod_{k=1}^{n_y} g_{b_k}(y_k|\psi_k)$. We have deviated from both of these because, as our examples demonstrate, this viewpoint is technically a little questionable. For example, $p_\theta(x_{1:n_x}, y_{1:n_y})$ defined in this way might not be a correctly normalized distribution and the normalization constant for the conditional distribution might not be a true marginal likelihood. These distinctions will be important in Chapters 9 and 10 where we step outside the standard inference framework. For an even more rigorous treatment of the distributions defined by PPSs, we refer the reader to Staton et al. [2016].

⁶Note that the observed variables should not be used in deterministic elements of the code for this to hold so that they cannot implicitly effect the sampling.

Given our query is now defined to specify a unnormalized conditional distribution rather than a normalized joint distribution, it is natural to ask whether it is necessary for each `observe` term to correspond to a correctly normalized density for its output, instead of just restricting it to be a positive semi-definite function representing an arbitrary soft constraint. The answer is that it is not. In fact, from a theoretical perspective, it perhaps easier to not think of the distribution defined by the query as being a combination of sampling and conditioning terms, but instead the product of the density of a correctly normalized generative model and a positive semi-definite *score function* that applies an unnormalized weighting to any possible sample the generative model can produce. This is exactly the approach taken by [Staton et al., 2016] and [Goodman and Stuhlmüller, 2014] who explicitly use such score functions, calling them `score` and `factor` respectively. We can also allow such functionality in our setup by defining a special distribution class, `factor`, which can only be used with `observe`, takes no parameters, and adds a factor to the trace probability equal to the exponentiation of the observed value. Thus, for example, we could use `observe (factor (), log(g(ψ)))` to factor the trace probability by the output of the function $g(\psi)$. The rationale for factoring by the exponentiation of the observed value rather than the observed value itself is firstly to ensure that the factor is positive and secondly because it will generally be beneficial for our system to work with log probabilities at its back-end for numerical underflow issues. Similarly we will in practice specify distribution objects using there log densities.

Don’t forget to add comments to the BOPP stuff etc about this as the marginal likelihood isn’t really the marginal likelihood...

4.4 The Anglican Probabilistic Programming Language

To allow for a more precise consideration of issues associated with designing and using a universal PPS, we now introduce the particular language *Anglican* [Wood et al., 2014; Tolpin et al., 2016], which we will use for reference throughout the rest of the thesis. Anglican is a universal PPL integrated into *Clojure* [Hickey, 2008], a dynamically-typed, general-purpose, functional programming language (specifically a dialect of Lisp) that runs on the Java virtual machine and uses just-in-time compilation. Anglican inherits most of the syntax of Clojure, but extends it with the key special forms `sample` and `observe` [Tolpin et al., 2015b, 2016], defined in the same way as our example language setup in the previous section, along with a couple of others which aid in defining queries such as `mem`, `store`, and `retrieve`. Despite

using predominantly the same syntax, Anglican has different, probabilistic, semantics to Clojure, i.e. code is written in the same way, but is interpreted differently.

Anglican was the first PPL to introduce particle based inference schemes such as SMC and particle MCMC (see Chapters 6 and 7), which was key advancement for universal PPSs because it allows the structure of the query to be exploited to provide substantially more efficient inference than previous approaches. Though these methods still form the core of the inference in Anglican, there have been a number of advancements and alternative inference approaches introduced since the original work [Paige et al., 2014; Tolpin and Wood, 2015; Tolpin et al., 2015a; van de Meent et al., 2015; Rainforth et al., 2016c,b; Le et al., 2017a]. Another notable feature of Anglican is its support for Bayesian non-parametric modeling, such as providing support for general processes along with primitives for particular models such as Dirichlet processes. Inevitably we can only provide a limited introduction here and so we also refer the interested reader to Tolpin et al. [2016] and to the Anglican website <http://www.robots.ox.ac.uk/~fwood/anglican/> for more information.

4.4.1 Clojure

Before getting into the details of Anglican, we first give a very brief introduction to Clojure [Hickey, 2008], because its syntax may be quite unfamiliar to readers without experience in Lisp based notation or functional programming more generally. There are two key things to get your head around for reading and using Clojure (and Lisp languages more generally): almost everything is a function and brackets evaluate functions. For example, to code $a + b$ in Clojure one would write `(+ a b)` where `+` is a function taking two arguments (here a and b) and the brackets cause the function to evaluate. More generally, Clojure uses prefix notation such that the first term in a bracket is always a function, with the other terms the arguments. Thus `((+ a b))` would be invalid syntax as the result of `(+ a b)` is not a function so cannot be evaluated. Expressions are nested in a tree structure so to code $2(a + b)/c$ one would write `(/ (* 2 (+ a b)) c)`. One can thus think about going outwards in terms of execution order – a function first evaluates its arguments before itself. Functions in Clojure are first class (i.e. they can be variables) and can be declared either anonymously using `(fn [args] body)`, for example `((fn [a b] (/ a b)) 10 5)` evaluates to 2, or using the macro `defn` to declare a named function in the namespace, for example `(defn divide [a b] (/ a b))`. Local

bindings in closure are defined using **let** blocks which are used to denote a number of name value pairs, with the bindings persisting to closure defined by the brackets of the **let** block and the return value being the output of the last element in the **let** block list. Thus for example (**let** [a 2 b 3] (+ a b)) says let *a* be equal to 2, *b* be equal to 3, and then evaluate *a* + *b*, thus returning 5. Note that *a* and *b* remain undefined outside of this let block.

Clojure allows various types of compound literals such as vectors, lists, hash maps and sets. In general, elements in these compound literals are not restricted in there type so it valid to write for example [1 "2" (**fn** [x] (inc x))] to construct a vector whose component terms are different types.

Clojure does not generally use for loops, instead relying the constructs **map** and **reduce**, or the **loop-recur** pairing. **map** applies a function to every value in a list or vector so for example (**map** (**fn** [a] (* a 2)) [2.1 3])) doubles each value in the vector of inputs returning a list (4.2 6), where the brackets in the output now just represent a list rather than a function evaluation, just to be confusing. **reduce** recursively applies a function and so for example to sum up a vector of elements in Clojure one writes for example (**reduce** + 0 [1.2 3.4 2]) which returns 6.6. The **loop-recur** pairing forms a syntax sugar for doing looping through tail recursion. In essence, **loop** defines a function and provides initial bindings for the input arguments. Inside the **loop** function block, **recur** recursively calls the function defined by **loop** with new bindings to the inputs. In general, the **recur** function should only be called depending on a condition holding true to prevent infinite recursion. To give a concrete example,

```
(loop [x 1] (if (> x 10) nil (do (print x) (recur (+ x 1))))))
```

will print out the numbers 1 to 10. Here the syntax of **if** is (**if** test then else) so when *x*>10 it returns **nil**. Otherwise it calls the **do** statement which evaluates each of its arguments in turn, in this case printing out *x* before recalling the body of the **loop** block with *x* reset to (+ *x* 1).

A important feature of Clojure, particularly with regards to Anglican, is its support for (infinite) lazy sequences. Lazy sequences are sequences of terms that are only evaluated as an when they are required. As such, it is valid for them to be infinitely long (typically through recursive definition) because terms are only calculated if they are required, so it is possible to define a term that is theoretically infinite long, but only a finite number of values from which are ever evaluated in practice. For example one can define the function

(**defn** ints [n] (**lazy-seq** (**cons** n (ints (inc n)))) and then call (ints 1) to produce a lazy sequence comprising of all the positive integers. We can evaluate the sequence by explicitly requesting terms with the sequence. For example, we can use (**take** 5 (ints 1)) to return the first 5 elements of our lazy sequence, thus returning (1 2 3 4 5). We could also ask for a particular term in the sequence using, for example, (**nth** 4 (ints 1)) to return 5. Lazy sequences are conceptually useful, amongst other things, for specifying things that are required to be infinitely long to ensure theoretical guarantees (engine an MCMC sampler needs to be run infinitely long to converge), but which are restricted by computational budgets.

4.4.2 Writing Models in Anglican

Anglican queries are written using the macro **defquery**. This allows users to define a model using a mixture of **sample** and **observe** statements and deterministic code in the manner synonymous to that explained in Section 4.3, and bind that model to a variable. As before, Anglican makes use of distribution objects for providing inputs to **sample** and **observe**, for which it provides a number of common constructors corresponding to common elementary random procedures such as **gamma**, **normal**, and **beta**. A distribution object is generated by calling the class constructor with the required parameters, e.g. (**normal** 0 1) for the unit Gaussian. Anglican also allows custom distribution classes to be defined using the **defdist** macro, which requires the user to provide parameterized code for sampling from that distribution class and evaluating the log density at given output.

A simple example of an Anglican query is shown in Figure 4.4, corresponding to a model where we are trying to infer the mean and standard deviation of a Gaussian given some data. The syntax of **defquery** is (**defquery** name [args] body) so in

Figure 4.4 our query is named `my-query` and takes in arguments `data`. The query starts by sampling `mu ~ N(0, 1)` and `sig ~ GAMMA(2, 2)` and constructing a distribution object `lik` to use for the observations. It then maps over each datapoint and observes it under the distribution `lik`, remembering that `fn` defines a function and `map` applies a function to every element of a list

```
(defquery my-query [data]
  (let [mu (sample (normal 0 1))
        sig (sample (gamma 2 2))
        lik (normal mu sig)]
   (map (fn [obs]
             (observe lik obs))
         data)
   [mu sig]))
```

Figure 4.4: A simple Anglican query.

```
(defquery lin-reg [xs ys]
  (let [m (sample (normal 0 10))
        c (sample (normal 0 3))
        s (sample (gamma (1 1)))
        f (fn [x] (+ (* m x) c))]
    (map (fn [x y]
           (observe
             (normal (f x) s) y))
         xs ys)
    [m c s]))
```

```
(defquery discrete-hmm
  [ys x0 trans obs]
  (loop [xs x0 t 0]
    (let
      [x (sample (nth trans (last xs)))]
      (observe (nth obs x)
               (nth ys t))
      (if (= (inc t) (count ys))
          (conj xs x)
          (recur (conj xs x) (inc t))))))
```

(a) Linear regression model with unknown observation variance. Here `xs` and `ys` are the data comprising of the inputs and corresponding outputs of the regression. The query returns estimates for the slope `m`, the intercept `c`, and the observation standard deviation (i.e. noise) `s`.

(b) Hidden Markov model with discrete states. Here `ys` is the data, `x0` is a starting state (which has no associated observation), `trans` is the collection of transition distribution objects for each of the K possible states (index by the value of x_t), and `obs` are the matching emission distributions. Query returns estimates for the latent states `xs`.

Figure 4.5: Example Anglican queries for some simple models. Here `defquery` binds a query to a variable, for which inference can be run using `doquery`. with syntax `(doquery inf-alg model inputs & options)`. For example, we could call `(doquery :ipmcmc lin-reg [xs ys] :number-of-particles 1000)` for some predefined `xs` and `ys` to run iPMCMC inference (see Section 6.3)) on the `lin-reg` model with with 1000 particles.

of vector. Note that `observe` simply returns `nil` and so we are not interested in these outputs – they effect the probability of a program execution trace, but not the calculation of a trace itself. After the observations are made, `mu` and `sig` are returned from the `let` block and then by proxy the query itself. Because the data terms only get used as observations and we do not observe any internal random variables, this query corresponds exactly to a Bayesian model where the `sample` terms form the prior and the `observe` terms form the likelihood as we explained in Section 4.3.2. The query thus defines a correctly normalised joint distribution given by

$$p(\mu, \sigma, y_{1:S}) = \mathcal{N}(\mu; 0, 1) \text{ GAMMA}(\sigma; 2, 2) \prod_{s=1}^S \mathcal{N}(y_s; \mu, \sigma) \quad (4.5)$$

where we have defined $\mu := \text{mu}$, $\sigma := \text{sig}$, and $y_{1:S} := \text{data}$. Other more complicated example Anglican models are given in Figures 4.5 and 4.6.

Compilation of an Anglican program is performed by the macro `query`. Calling `query` invokes a source-to-source compilation from an Anglican query to a continuation-passing style (CPS) Clojure function that can be executed using a particular inference algorithm. We leave discussing what this means in depth to Chapter 7, noting only that the inference algorithms

associated with Anglican are written in pure Clojure (except for the odd bit of Java code) and the aim of the compilation is to produce a model artifact which can be interpreted by that inference code. When `defquery` is called, Anglican internally calls the `query` and assigns the output to the symbol provided by the first argument of `defquery`. Therefore `my-query` in our example is Clojure function that can be read by the Anglican inference engines to produce approximate samples from the conditional distribution. Note that, as a Clojure function, the inputs and body of `my-query` and not as per lexical definition of the Anglican program (e.g. `in` now takes multiple inputs). It is instead a function that encodes all the information required by the inference engine to perform inference and has the corresponding required call structure for the input required by the engine.

Inference on the model is performed using the macro `doquery`, which produces a lazy infinite sequence of approximate samples from the conditional distribution and, for appropriate inference algorithms, an estimate of the marginal observation density. The syntax of `doquery` is `(doquery inf-alg model inputs & options)` where `inf-alg` specifies an inference algorithm, e.g. `:ipmcmc`, `model` is our `query`, `inputs` is a vector of inputs to the query, the `&` represents that there might be multiple additional inputs, and `options` are a series of option-value pairs for the inference engine. For example, to produce 100 samples from our `my-query` model with data `[2.1 5.2 1.1]` using the LMH inference algorithm with no additional options, we can write `(take 100 (doquery :lmh my-query [2.1 5.2 1.1]))`.

Although Anglican mostly inherits Clojure syntax, some complications arise from the compilation to CPS-style Clojure functions. It is thus not possible to naïvely use all Clojure functions inside Anglican without providing appropriate information to the compiler to perform the required transformation. The transformation for many core Clojure functions has been done manually such that they form part of the Anglican syntax and can be used directly. Anglican further allows users to write functions externally to `defquery` using the macro `defm`, which is analogous to `defn` in Clojure and has the same call syntax (except for being restricted to inputs, though as this can be a vector, this places no restrictions on the functions that can be written), which can then be called from inside the query without restrictions. Other deterministic Clojure functions can also be called from inside queries, but must be provided with appropriate wrapping to assist the compiler. Thankfully this is done automatically (except when the function itself is higher order) using the macro `with-primitive-procedures`

```

(defdist strike [volatility] []
  (sample* [this]
    (if (sample* (flip volatility))
        :war :peace))
  (observe* [this value]
    (observe* (flip volatility)
      (= value :war))))
(declare A B)
(with-primitive-procedures [strike]
  (defm A [depth]
    (let [B-strike (B (dec depth))
          A-strike (strike 0.1)]
      (observe A-strike B-strike)
      B-strike)))
  (defm B [depth]
    (let [B-strike (strike 0.2)]
      (if (> depth 0)
          (let [A-strike (A depth)]
            (observe B-strike A-strike)
            A-strike)
          (sample B-strike))))
  (defquery war [depth]
    (or (= (A depth) :war)
        (= (B depth) :war))))

```

Figure 4.6: Anglican code for an example Schelling co-ordination game [Schelling, 1980; Stuhlmüller and Goodman, 2014] modeling if a peace will hold between two volatile countries which we refer to as A and B. This example is adapted from an online Anglican example developed by Brooks Paige and Frank Wood which can be found at <http://www.robots.ox.ac.uk/~fwood/anglican/examples/>, providing a more detailed consideration along with other examples. Our code first defines a custom distribution called `strike` for modeling whether one country will attack the other if it does not reason about the other’s actions. It then constructs a Anglican function for each country using `defm`. Each country has their own volatility and the ability to reason about whether they think the other country will initiate a strike against them. We presume they have access to the exact model of the other country. A’s aim is to match the action it thinks B will do – it would prefer there to be no war, but if there is, it wants to strike first. Its model first samples a draw for B’s action by simulating from B’s model and then observes this action under its own distribution on whether to strike; this is equivalent to sampling both in isolation and constraining them to be the same. However, B can also reason about A and A knows it. It therefore provides the simulation of B’s model with a *meta-reasoning depth*. If this depth is zero, B makes its decision in isolation, simply sampling from `B-strike`. If the depth is greater than zero though, it uses the same approach as A, simulating from A’s model (with a depreciated meta-reasoning depth) and then observing this outcome under `B-strike`. This creates a mutually recursive cycle of reasoning. As an observer, we are interested in establishing the probability that one of the two will strike, as this event leads to a war, and so we define a query which outputs whether the two are the same. The expectation of the output from this query corresponds to the probability of war. Invoking inference using (`doquery :lmh war [depth]`) we see that for a depth of 0, there is roughly a 0.222 chance of war, while depths of 1, 2, and 10 give rough respective chances of 0.052, 0.0021, and 3×10^{-6} . Thus the chance of war goes down the more each country thinks about the reasoning of the other. It is interesting to note that if the volatilities are set to the same value then the critical tipping point, above which things escalate towards war with increased depth, is around 0.38. The mutual recursion involved in the model and the fact that variables are both sampled and observed means that it would be difficult to encode it using a graphical model. It is not even clear how one would go about writing down a well defined joint distribution for the model, without having to empirically calculate a normalization constant. Note though that this not correspond to a nested query example in the manner we discuss in Section XX as there is no inference going on between the nested function calls.

that takes as inputs Clojure functions and creates an environment where these functions have been converted to their appropriate CPS forms.

We finish our introduction by noting the ability of Anglican to *nest* queries within one another. This is somewhat experimental and comes with a number of health warnings because, as we will explain in Chapter 10, it allows users to write so called *nested estimation* problems that fall beyond the scope of the standard proofs of convergence for stand Monte Carlo estimation schemes. Nonetheless, there are problems that cannot be encoded without this ability, such as the Bayesian experimental design equations discussed in Chapter 11. Though **doquery** is not allowed directly within a **defquery** block, one can still nest queries by either using a **doquery** in a Clojure function that is then passed to another query using `with-primitive-procedures`, using a **doquery** within a custom distribution defined by **defdist**, or using the special form `conditional` which takes a query and returns a distribution object constructor, for which the inputs to the query become the parameters. We will return to consider the implications of this at length in Chapter 10.

5

An Introduction to Bayesian Inference

5.1 The Challenge of Bayesian Inference

In Chapter 3 we introduced the concept of Bayesian modeling and showed how we can combine prior information $p(\theta)$ and a likelihood model $p(\mathcal{D}|\theta)$ using Bayes' rule (i.e. (3.5)), to produce a posterior $p(\theta|\mathcal{D})$ on variables θ that characterizes both our prior information and information from the data \mathcal{D} . We now consider the problem of how to calculate (or more typically approximate) this posterior, a process known as Bayesian *inference*. At first this may seem like a straight forward problem: by Bayes' rule we have that $p(\theta|\mathcal{D}) \propto p(\mathcal{D}|\theta)p(\theta)$ and so we already know the relative probability of any one value of θ compared to another. In practice, this could hardly be further from the truth. Bayesian inference for the general class of graphical models is in fact an NP-hard problem [Cooper, 1990; Dagum and Luby, 1993]. We can break it down into key challenges: calculating the normalization constant $p(\mathcal{D}) = \int p(\mathcal{D}|\theta)p(\theta)d\theta$ and providing a useful characterization of the posterior, for example an object we can draw samples from. Many inference schemes, for example Markov chain Monte Carlo (MCMC) methods [Hastings, 1970], will not try to tackle these challenges directly and instead look to generate samples directly from the posterior. However, this breakdown will still prove useful in illustrating the intuitions about the difficulties presented by Bayesian inference.

5.1.1 The Normalization Constant

Calculating the normalization constant in Bayesian inference is essentially a problem of integration. Our target, $p(\mathcal{D})$, is the expectation of the likelihood under the prior, hence the name *marginal likelihood*. When $p(\mathcal{D})$ is known, the posterior can be evaluated exactly at any possible input point using (3.5) directly. When it is unknown, we lack a scaling in the evaluation of any point and so we have no concept of how relatively significant that point is

relative to the distribution as a whole. For example, for a discrete problem then if we know the normalizing constant, we can evaluate the exact probability of any particular θ by evaluating that point alone. If we do not know the normalizing constant, we do not know if there are other substantially more probable events that we have thus-far missed, which would in turn imply that the queried point has a negligible chance of occurring.

To give a more explicit example, consider a model where $\theta \in \{1, 2, 3\}$ with a corresponding uniform prior $P(\theta) = 1/3$ for each θ . Now presume that for some reason that we are only able to evaluate the likelihood at $\theta = 1$ and $\theta = 2$, giving $p(\mathcal{D}|\theta = 1) = 1$ and $p(\mathcal{D}|\theta = 2) = 10$ respectively. Depending on the marginal likelihood $p(\mathcal{D})$, the posterior probability of $P(\theta = 2|\mathcal{D})$ will vary wildly. For example, $p(\mathcal{D}) = 4$ gives $P(\theta = 2|\mathcal{D}) = 5/6$, while $p(\mathcal{D}) = 1000$ gives $P(\theta = 2|\mathcal{D}) = 1/100$. Though this example may seem far-fetched, this is the scenario almost always seen in practice for realistic models, at least those with non-trivial solutions. Typically it is not possible to enumerate all the possible values of θ in reasonable time and we are left wondering - how much probability mass is left that we have not seen? The problem is even worse in the setting where θ is continuous, for which it is naturally impossible to evaluate all possible values for θ . Knowing the posterior only up to a normalization constant is deceptively unhelpful - we never know how much of the probability mass we have missed and therefore whether the probability (or probability density) where we have looked so far is tiny compared to some other dominant region we are yet to explore. At its heart, the problem of Bayesian inference is a problem of where to concentrate our finite computational resources so that we can effectively characterize the posterior. If $p(\mathcal{D})$ is known, then we immediately know whether we are looking in the right place or whether there are places left to look that we are yet to find. This brings us onto our second challenge – knowing the posterior in closed form is often not enough.

5.1.2 Characterizing the Posterior

Once we have the normalization constant, it might seem that we are done; after all we now have the exact form the posterior using Bayes' rule. Unfortunately, it tends to be the case, at least when θ is continuous, that this is insufficient to carry out most tasks that we might want to use our posterior for. There are a number of different, often overlapping, reasons for wanting to calculate a posterior including

- To calculate the posterior probability or probability density for one or more particular instances of the variables.
- To calculate the expected value of some function, $\mu_f = \mathbb{E}_{p(\theta|\mathcal{D})} [f(\theta)]$. For example, we might want to calculate the expected values of the variables themselves $\mu_\theta = E_{p(\theta|\mathcal{D})} [\theta]$ as a point estimate.
- To make predictions. For example, in a supervised learning task then our data typically comprises of a series of input output pairs $\mathcal{D} = \{x_n, y_n\}_{n=1:N}$ and we wish to predict the output at some new input \tilde{x} . In the fully Bayesian framework, one does this using the *posterior predictive distribution*

$$p(\tilde{y}|\tilde{x}) = \int p(\tilde{y}|\tilde{x}, \theta)p(\theta|\mathcal{D})d\theta.$$

Note that this is a particular case of calculating an expectation under the posterior.

- To find the most probable variable values $\theta^* = \arg \max_\theta p(\theta|\mathcal{D})$. This is known as maximum a posteriori estimation and will be discussed in Chapter 8.
- To produce samples from, or form some other useful characterization of, the posterior that can then passed on to another part of a computational pipeline or directly observed by a user.
- To estimate a marginal probability distribution over some variables of particular interest. For example, if $\theta = \{u, v\}$ then we might be interest in the marginal $p(u|\mathcal{D})$.

If θ is continuous or some elements of θ are continuous then only the first of these can be carried out directly using the form of the posterior provided by Bayes' rule with known normalization constant. We, therefore, see that knowing the normalization alone will not be enough to fully solve the Bayesian inference problem in a useful manner. In particular, it will generally not sufficient in order to be able to *sample* from the posterior. As we will see later, the ability to sample will be at the core of most practical uses for the posterior as it allows use of Monte Carlo methods [Metropolis and Ulam, 1949; Robert, 2004; Rubinstein and Kroese, 2016], which can in turn be used to carry out many of the outlined tasks.

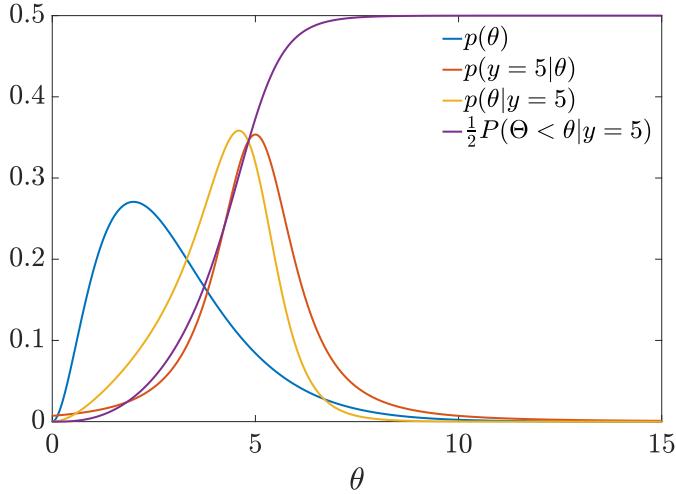


Figure 5.1: Example inference for problem given in (5.1). Also shown is the cumulative distribution for the posterior as per (5.2). This is scaled by a factor of 1/2 for visualization.

To further demonstrate why knowing the normalization constant is insufficient for most Bayesian inference tasks, we consider the following a simple example

$$p(\theta) = \text{GAMMA}(\theta; 3, 1) = \frac{\theta^2 \exp(-\theta)}{2}, \quad \theta \in (0, \infty), \quad (5.1a)$$

$$p(y = 5|\theta) = \text{STUDENT-T}(5 - \theta; 2) = \frac{\Gamma(1.5)}{\sqrt{2\pi}} \left(1 + \frac{(y - \theta)^2}{2}\right)^{-3/2}, \quad (5.1b)$$

$$p(\theta|y = 5) \approx 5.348556 \theta^2 \exp(-\theta) \left(2 + (5 - \theta)^2\right)^{-3/2}. \quad (5.1c)$$

Here we have that the prior on θ is distributed according to a gamma distribution with shape parameter 3 and rate parameter 1. The likelihood function is a student-t distribution on the difference between θ and the output $y = 5$. Using a numerical integration over θ the normalization constant can be calculated to a high accuracy, giving the provided closed-form equation for the posterior. This posterior, along with the prior and likelihood are shown Figure 5.1.

Here knowing the marginal likelihood means that we have a closed-form equation for the posterior. Image though that we wish to sample from it. As it does not correspond to a standard distribution, we cannot simply call a standard sampling procedure. There is, in fact, no way to directly sampling from this distribution without doing further calculations. If we also know the inverse of the cumulative density function of the posterior

$$P(\Theta \leq \theta|y = 5) = \int_{\Theta=0}^{\Theta=\theta} p(\theta = \Theta|y = 5)d\Theta, \quad (5.2)$$

then we can sample from the posterior by sampling $\hat{u} \sim \text{UNIFORM}(0, 1)$ and then taking as our sample $\hat{\theta} = P^{-1}(\hat{u})$ such that $\hat{u} = P(\Theta \leq \hat{\theta}|y = 5)$. However, the cumulative distribution function and its inverse cannot be calculated analytically. Though in this simple one dimensional problem they can be easily estimated numerically, this will prove prohibitively difficult for most problems where θ has more than a few dimensions. Similarly, if we wish to estimate an expectation with respect to this posterior we could do this relatively easily numerically for this simple problem, for example using Simpson's rule, but in higher dimensions this will be impractical.

There are a number of indirect methods we could use instead to sample from the posterior such as rejection sampling, importance sampling, and MCMC. However, as we will show in the Section 5.3, these all only require that we can evaluate an unnormalized version of target distribution, such that they side-step the need to calculate the marginal likelihood. Nonetheless, knowledge of the marginal likelihood can still be helpful in a number of scenarios (e.g. in adapting our inference algorithm) for the reasons outlined in Section 5.1.1.

5.2 Monte Carlo

Monte Carlo [Metropolis and Ulam, 1949] is the characterization of a probability distribution through random sampling. It is the foundation for a huge array of methods for numerical integration, optimization, and scientific simulation; forming the underlying principle for all stochastic computation. Monte Carlo provides us with a means of dealing with complex models and problems in a statistically principled manner. Without it, one would have to resort to deterministic approximation methods whenever the target problem is too complex to permit analytic solution. As we will show, it is a highly composable framework that will allow to output of one system to be input directly to another. For example, the Monte Carlo samples from a joint distribution will also have the correct marginal distribution over any of its individual components, while sampling from the marginal distribution then sampling from the conditional distribution given these samples will give samples distributed according to the joint. As Monte Carlo will be key to most methods for Bayesian inference that we will consider, we take the time in this section key related concepts.

The most common usage of Monte Carlo in this work will be the Monte Carlo estimation of expectations, sometimes known as Monte Carlo integration. The critical importance of Monte

Carlo estimation stems from the fact that most of the example target tasks laid out in 5.1.2 can be formulated as expectations. Even when our intention is simply to generate samples from a target distribution, we can usually think of this as being an implicit expectation of an, as-yet unknown, target function. Here our implicit aims is to minimize the bias and variance of whatever process the samples are eventually used for, even if that process is simply visual inspection.

Consider the problem of calculating the expectation of some function $f(\theta)$ under the distribution $\theta \sim \pi(\theta)$ ($= p(\theta|\mathcal{D})$ for the Bayesian inference case), which we will denote as

$$I := \mathbb{E}_{\pi(\theta)} [f(\theta)] = \int f(\theta)\pi(\theta)d\theta. \quad (5.3)$$

This can be approximated using the Monte Carlo estimator I_N where

$$I \approx I_N := \frac{1}{N} \sum_{n=1}^N f(\hat{\theta}_n) \quad \text{where} \quad \hat{\theta}_n \sim \pi(\theta). \quad (5.4)$$

The first result we note is that (5.4) is an *unbiased* estimator for I . This can be easily shown by noting that

$$\mathbb{E}[I_N] = \mathbb{E}\left[\frac{1}{N} \sum_{n=1}^N f(\hat{\theta}_n)\right] = \frac{1}{N} \sum_{n=1}^N \mathbb{E}[f(\hat{\theta}_n)] = \frac{1}{N} \sum_{n=1}^N \mathbb{E}[f(\hat{\theta}_1)] = I \quad (5.5)$$

where we have first moved the sum outside of expectation using linearity,¹ then the fact that each $\hat{\theta}_n$ is identically distributed to note that each $\mathbb{E}[f(\hat{\theta}_n)] = \mathbb{E}[f(\hat{\theta}_1)]$, and finally that $\mathbb{E}[f(\hat{\theta}_1)] = I$ by the definition of I and the distribution on $\hat{\theta}_1$. This is an important result as it means that Monte Carlo does not introduce any systematic error, i.e. bias, into the approximation: in expectation it does not pathologically overestimate or underestimate the target. This is not to say though that it is equally likely to overestimate or underestimate as it may, for example, typically underestimate by a small amount and then rarely overestimate by a large amount. Instead, it means that if we were to repeat the estimation an infinite number of times and average the results, we would get the true value of I . This now hints at another important question – do we also get recover the true value of I when we conduct one infinitely large estimation, namely if we take $N \rightarrow \infty$? This is known as *consistency* of a statistical estimator, which we will now consider next. Before moving on, we make the important note that many common Monte Carlo inference methods, for example MCMC as discussed in Section 5.3.4), are in fact biased. This

¹Note that this presumes that N is independent of the samples. This is usually the case, but care is necessary in some situations, namely when the number of samples taken is adaptively chosen based on the sample values, for example in adaptive stratified sampling [Etoré and Jourdain, 2010].

is because it is often not possible to $\hat{\theta}_n \sim \pi(\theta)$ exactly as we have assumed in (5.4), with the bias resulting from the approximation. The convergence of such methods relies on the bias diminishing to 0 as $N \rightarrow \infty$, such that they remain unbiased in the limit.

5.2.1 The Law of Large Numbers

A key mathematical idea underpinning the convergence of many Monte Carlo methods is the law of large numbers (LLN). Informally, the LLN states that the empirical average of independent and identically distributed (i.i.d.) random variables converges to the true expected value of the underlying process as the number of samples in the average increases. We can use it to prove the consistency of Monte Carlo estimators where the samples are drawn independently from the same distribution, as is the case in for example rejection sampling and importance sampling. The high level idea for the LLN can be shown by considering the *mean squared error* of a Monte Carlo estimator as follows²

$$\begin{aligned} \mathbb{E}[(I_N - I)^2] &= \mathbb{E}\left[\left(\frac{1}{N} \sum_{n=1}^N f(\hat{\theta}_n) - I\right)^2\right] \\ &= \frac{1}{N^2} \sum_{n=1}^N \mathbb{E}\left[\left(f(\hat{\theta}_n) - I\right)^2\right] + \frac{1}{N(N-1)} \sum_{n=1}^N \sum_{m=1, m \neq n}^N \mathbb{E}\left[\left(f(\hat{\theta}_n) - I\right)\left(f(\hat{\theta}_m) - I\right)\right] \\ &= \frac{1}{N^2} \sum_{n=1}^N \mathbb{E}\left[\left(f(\hat{\theta}_1) - I\right)^2\right] + \frac{1}{N(N-1)} \sum_{n=1}^N \sum_{m=1, m \neq n}^N \underbrace{\left(\mathbb{E}\left[\left(f(\hat{\theta}_1) - I\right)\right]\right)^2}_{\rightarrow 0} \\ &= \frac{\sigma_\theta^2}{N} \quad \text{where} \quad \sigma_\theta^2 := \mathbb{E}\left[\left(f(\hat{\theta}_1) - I\right)^2\right] = \text{Var}[f(\theta)]. \end{aligned} \tag{5.6}$$

Here the second line follows from the first simply by expanding the square and using linearity to move the sum outside of the expectation as in the unbiasedness derivation. The first term in the third line follows from the equivalent term in the second line by again noting that each $\hat{\theta}_n$ has the same distribution. The second term in the third line follows from the assumption that the samples are drawn independently such that

$$\mathbb{E}\left[\left(f(\hat{\theta}_n) - I\right)\left(f(\hat{\theta}_m) - I\right)\right] = \mathbb{E}\left[\left(f(\hat{\theta}_n) - I\right)\right] \mathbb{E}\left[\left(f(\hat{\theta}_m) - I\right)\right].$$

The last line simply notes that $\mathbb{E}\left[\left(f(\hat{\theta}_1) - I\right)^2\right]$ is a constant, namely the variance of $f(\theta)$. Our final result has a simple and intuitive form – the mean squared error for our estimator

²Note here that we use the notation of expectation typically used within the statistics literature, whereby it corresponds to the expectation over all randomness contained in the system.

using N samples, is $1/N$ times the mean squared error of an estimator that only uses a single sample, which is itself equal to the variance of $f(\theta)$. As $N \rightarrow \infty$, we thus have that our expected error goes to 0.

A key upshot of this result is that the difference $I_N - I$ between our empirical estimate and the true value should be of order $O(1/\sqrt{N})$. In some way this is rather slow; deterministic numerical integration schemes of have much fast convergence theoretical convergence rates. For example, Simpson's rule has a a convergence rate of $O(1/n^4)$ for one dimensional functions. However, this requires smoothness assumptions on f and, more critically, the convergence rate diminishes rapidly in higher dimensions. As such, Monte Carlo is often an inferior way of estimating integrals for smooth functions in low dimensions. However, Monte Carlo scales substantially more gracefully to higher dimensions than alternatives. Looking at (5.6), we see that the dimensionality of the problem only effects the Monte Carlo convergence rate through changes in the constant factor σ_θ . Though this will often increase with dimensionality, it will generally do so substantially less aggressively then typical exponential decrease in converge rate of deterministic numerical integration schemes with dimension. Monte Carlo therefore tends to dominate for moderate to high dimensional problems.

5.2.2 Convergence of Random Variables

To introduce the concept the LLN more precisely, we now consider some more formal notations of convergence of random variables. There will be times (in particular in Chapter 10) when mathematical rigour will require us to distinguish between these alternative notations of convergence. However, for most practical purposes, any one of these notions of convergence will be sufficient to informally guarantee that an estimator will return the correct answer if provided with sufficient samples. Therefore those less interested in theoretical details may wish to skip Sections 5.2.2.2, 5.2.2.3 and 5.2.2.4 on first reading.

5.2.2.1 L^p -Convergence

We start by introducing the notion of L^p -convergence, also known as convergence in expectation, as this is the type of convergence we have just alluded to in our informal proof of the LLN. At a

high level, L^p -convergence means that the expected value of the related error metric tends to zero as $N \rightarrow \infty$. More precisely, we first define the L^p -norm for a random variable X as

$$\|X\|_p = (\mathbb{E}[|X|^p])^{\frac{1}{p}} \quad (5.7)$$

where $|\cdot|$ denotes the absolute value. For example, we can write the mean squared error used in (5.6) as the squared L^2 -norm: $\mathbb{E}[(I_N - I)^2] = \|I_N - I\|_2^2$. We further define the notion of L^p -space as being the space of random variables for which $\|X\|_p < \infty$. We can now formally define L^p -convergence as follow.

Definition 5.1 (L^p -convergence). *A sequence of random variables X_N converges in its L^p -norm to X where $p \geq 1$ if $X \in L^p$, each $X_N \in L^p$, and*

$$\lim_{N \rightarrow \infty} \|X_N - X\|_p = 0. \quad (5.8)$$

A key point to note is that $\|X_N - X\|_p \geq 0 \forall X_N, X$ by definition of the L^p -norm and so rather than this simply being a statement of asymptotic unbiasedness, L^p -convergence says that the expected *magnitude* of the error tends to zero as $N \rightarrow \infty$. Different values of p correspond to different metrics for the error, with larger values of p constituting stronger converge guarantees, such that L^{p_1} -convergence implies L^{p_2} -convergence whenever $p_1 > p_2$. Similarly, if a random variable satisfies $X \in L^{p_1}$, then it follows that $X \in L^{p_2}$.

5.2.2.2 Convergence in Probability

At a high level, convergence in probability between two random variables (or between a random variable and a constant) means that they become arbitrary close to one another with high probability. More formally we have the following definition.

Definition 5.2 (Convergence in probability). *A sequence of random variables X_N converges in probability to X if, for every $\varepsilon > 0$,*

$$\lim_{N \rightarrow \infty} P(|X_N - X| \geq \varepsilon) = 0. \quad (5.9)$$

As ε can be made arbitrarily small, this ensures that X_N becomes arbitrarily close to X in the limit of large N . Estimators are *consistent* if they converge in probability. Convergence in probability is, in general, a weaker form of convergence than L^p convergence as L^p convergence for any $p \geq 1$ implies convergence in probability [Williams, 1991].

In (5.6) we demonstrated the L^2 convergence of the Monte Carlo estimator as we have that

$$\lim_{N \rightarrow \infty} \|I_N - I\|_2 = \lim_{N \rightarrow \infty} \frac{\sigma_\theta}{\sqrt{N}} = 0.$$

By the above result we therefore also have the Monte Carlo estimator converges in probability to the expectation and thus that it is consistent. This is known as the *weak law of large numbers*. We can also prove this more explicitly as follows

Theorem 5.1 (Weak law of large numbers). *If I and I_N are defined as per (5.3) and (5.4) respectively, $I \in L^1$, each $I_N \in L^1$, and each $\hat{\theta}_n$ in (5.4) is drawn independently, then I_N converges to I in probability:*

$$\lim_{N \rightarrow \infty} P(|I_N - I| \geq \varepsilon) = 0 \quad \forall \varepsilon > 0. \quad (5.10)$$

Proof. In the interest of exposition, we prove the result in the case where the stronger assumptions that $I \in L^2$ and each $I_N \in L^2$ hold. In practise this is not needed as the theorem can be proved by other means, see for example Theorem 2.2.7 of Durrett [2010].

By (5.5) we have that $\mathbb{E}[I_N] = I$ and by (5.6) we have that $\|I_N - I\|_2^2 = \frac{\sigma_\theta^2}{N}$ where σ_θ^2 is an unknown, but finite, constant by the assumption that $I \in L^2$. Chebyshev's inequality states that if $\mathbb{E}[I_N] = I$, then for any $k > 0$

$$P(|I_N - I| \geq \varepsilon) \leq \frac{\text{Var}(I_N)}{\varepsilon^2}.$$

By further noting that as I_N is unbiased, we have that $\text{Var}(I_N) = \|I_N - I\|_2^2$ and therefore

$$\lim_{N \rightarrow \infty} P(|I_N - I| \geq \varepsilon) \leq \lim_{N \rightarrow \infty} \frac{\sigma_\theta^2}{\varepsilon^2 N} = 0 \quad \forall \varepsilon > 0$$

as required. \square

As an interesting aside, we can prove that convergence in probability follows from L^p convergence more generally in a similar fashion. This can be done by using the more general form of Chebyshev's inequality given in, for example, Theorem 1.6.4 and Lemma 2.2.2 of Durrett [2010] to show that

$$\lim_{N \rightarrow \infty} P(|I_N - I| \geq \varepsilon) \leq \lim_{N \rightarrow \infty} \frac{\mathbb{E}[|I_N - I|^p]}{\varepsilon^p} = \left(\frac{1}{\varepsilon} \lim_{N \rightarrow \infty} \|I_N - I\|_p \right)^p. \quad (5.11)$$

If $I_N \xrightarrow{L^p} I$ then $\lim_{N \rightarrow \infty} \|I_N - I\|_p = 0$ by definition and we have convergence in probability as required.

5.2.2.3 Almost Sure Convergence

Almost sure convergence, also known as strong convergence, is a similar, but stronger, form of convergence than convergence in probability. At a high level the difference between convergence in probability and almost sure converge is a difference in the tail behaviour: convergence in probability suggests the rate at which an event happens tends to zero; almost sure convergence means that there is some point in time after which the event never happens again. More formally we have the following definition

Definition 5.3 (Almost sure convergence). *A sequence of random variables X_N converges almost surely to X if*

$$P\left(\lim_{N \rightarrow \infty} X_N = X\right) = 1. \quad (5.12)$$

Almost sure convergence implies convergence in probability, but not vice-versa – the rate at which events occur might tend to zero without there ever being a point at which the event never occurs again. It does not imply, nor is it implied by, L^p convergence. The *strong law of large numbers* is the dual for the weak law of large numbers as follows.

Theorem 5.2 (Strong law of large numbers). *Assuming the setup of Theorem 5.1 then I_N converges to I almost surely*

$$P\left(\lim_{N \rightarrow \infty} I_N = I\right) = 1. \quad (5.13)$$

The proof is somewhat more complicated than the weak law and so is not provided here, but can be found in, for example, Theorem 2.4.1 of Durrett [2010].

5.2.2.4 Convergence in Distribution

At a high level, convergence in distribution, also known as weak convergence, states that the a sequence of variables become an increasingly closely distributed to a target distribution. Whereas our previous notions of convergence ensure that our sequence of random variables converge to a particular value, convergence in distribution only implies that our sequence of random variables tends towards having a particular distribution. For example, a variable might converge in distribution to having a unit normal distribution, whereas a different variable might converge in probability to zero. More formally, we can define convergence in distribution as follows.

Definition 5.4 (Convergence in distribution). *A sequence of random variables X_N converges in distribution X if*

$$\lim_{N \rightarrow \infty} P(X_N \leq x) = P(X \leq x) \quad (5.14)$$

for every x at which $P(X \leq x)$ is continuous, where $P(X_N \leq x)$ and $P(X \leq x)$ are the cumulative distribution functions for X_N and X respectively.

Because it only requires that a variable has a particular distribution, rather than an exact value, convergence in distribution is a weaker form of convergence than those previously discussed and is implied by any of the other forms of convergence.

5.2.3 The Central Limit Theorem

The central limit theorem (CLT) is a core result in the study of Monte Carlo methods. In its simplest form, it states that the sum of N i.i.d. random variables tends towards a Gaussian in the limit $N \rightarrow \infty$. While the LLN demonstrated the convergence of the average of i.i.d. random variables towards the true mean, the CLT provides a means of constructing consistent confidence intervals of our estimate I_N by exploiting its asymptotic normality. Furthermore, there are variants of the CLT that do not require that the variables are i.i.d., meaning we can use it to demonstrate convergence in scenarios where samples are correlated, such as occurs when doing MCMC inference as shown in Section 5.3.4.

In the i.i.d. case, the CLT is as follows.

Theorem 5.3 (Central Limit Theorem). *Assume X_1, \dots, X_N is a sequence of i.i.d. random variables with $\mathbb{E}[X_i] = I$ and $\mathbb{E}[X_i^2] = \sigma < \infty$ for all $i \in \{1, \dots, N\}$. Let $I_N := \frac{1}{N} \sum_{n=1}^N X_n$ be the sample average of this sequence. Then $\sqrt{N}(I_N - I)/\sigma$ converges in distribution to the unit normal:*

$$\lim_{N \rightarrow \infty} P\left(\frac{\sqrt{N}(I_N - I)}{\sigma} \leq z\right) = \Phi(z) = \int_{-\infty}^z \frac{1}{2\pi} \exp(-\frac{\zeta^2}{2}) d\zeta \quad \forall z \in \mathbb{R} \quad (5.15)$$

where $\Phi(z)$ is the cumulative distribution function for the unit normal. Furthermore, if $\sigma_N^2 = \frac{1}{N-1} \sum_{n=1}^N (X_n - I_N)^2$ is the empirical estimate of the variance of X_N (including Bessel's correction), then $\sqrt{N}(I_N - I)/\sigma_N$ also converges in distribution to the unit normal.

Proof. See, for example, Durrett [2010]. □

The second result here is especially key as it will allow us to calculate consistent confidence intervals on our estimates without needing to know σ as we can instead use our empirical estimate

$$\sigma_N^2 = \frac{1}{N-1} \sum_{n=1}^N (X_n - I_N)^2 \quad \text{where} \quad I_N = \frac{1}{N} \sum_{n=1}^N X_n. \quad (5.16)$$

The form of (5.16) might at first look a bit strange - why is the normalizing term $1/(N-1)$ instead of $1/N$? Although replacing $1/(N-1)$ term with $1/N$ would still lead to a consistent estimator, this estimator turns out to be biased whereas (5.16) is in fact unbiased. The bias correction $N/(N-1)$ is known as Bessel's correction, while the proof that (5.16) is unbiased follows from straightforward algebraic manipulations. Note though that the estimator of the standard deviation, σ_N , is still biased by Jensen's inequality. As a consequence of the unbiasedness, $\sigma_N^2 \xrightarrow{a.s.} \sigma^2$ by the strong LLN, from which the second result in Theorem 5.3 follows from the first by Slutsky's theorem (see Durrett [2010]).

Imagine we want to construct a confidence interval on our estimate I_N such that there is a probability $0 < \alpha < 1$ that I is in the range $[I_N - \varepsilon, I_N + \varepsilon]$. Using the CLT we can do this as follows

$$\begin{aligned} \alpha &:= P(I_N - \varepsilon \leq I \leq I_N + \varepsilon) = P(-\varepsilon \leq I_N - I \leq \varepsilon) \\ &= P\left(-\frac{\sqrt{N}\varepsilon}{\sigma_N} \leq \frac{\sqrt{N}(I_N - I)}{\sigma_N} \leq \frac{\sqrt{N}\varepsilon}{\sigma_N}\right) \\ &\approx \Phi\left(\frac{\sqrt{N}\varepsilon}{\sigma_N}\right) - \Phi\left(-\frac{\sqrt{N}\varepsilon}{\sigma_N}\right) = 2\Phi\left(\frac{\sqrt{N}\varepsilon}{\sigma_N}\right) - 1 \end{aligned} \quad (5.17)$$

where as before $\Phi(\cdot)$ is the cumulative distribution function for the unit normal. Now rearranging for ε we have that

$$\varepsilon = \frac{\sigma_N \Phi^{-1}\left(\frac{\alpha+1}{2}\right)}{\sqrt{N}} \quad (5.18)$$

and therefore the confidence interval on I_N that

$$P\left(I_N - \frac{\sigma_N \Phi^{-1}\left(\frac{\alpha+1}{2}\right)}{\sqrt{N}} \leq I \leq I_N + \frac{\sigma_N \Phi^{-1}\left(\frac{\alpha+1}{2}\right)}{\sqrt{N}}\right) = \alpha. \quad (5.19)$$

Thus for example if we set $\alpha = 0.99$ then $\Phi^{-1}\left(\frac{\alpha+1}{2}\right) \approx 2.576$ and our confidence interval 99% confidence interval for I is $I_N \pm \frac{2.576\sigma_N}{\sqrt{N}}$. We reiterate that these confidence intervals are exact in the limit $N \rightarrow \infty$, but approximate for finite N . As one is often far from the asymptotic

regime, care is often, therefore, required in interpreting them. Nonetheless, the ability to estimate realistic uncertainties for sufficiently large N is an extremely powerful result.

Through most of this section we have assumed that our random variables are i.i.d.. In fact, neither the assumption of identically distributed nor that of independence is actually necessary for the CLT to hold. One can instead use the concept of *strong mixing*, namely that variables sufficiently far apart in the sequence are independent, to generalize beyond the i.i.d. setting [Jones et al., 2004]. This is critical for the numerous Monte Carlo inference schemes, such as MCMC methods, that do not produce independent samples but instead rely on the samples converging in distribution to the target. In most MCMC settings, one can also prove a CLT using reversibility of the Markov chain [Kipnis and Varadhan, 1986]. It is beyond the scope of this thesis to go into these more general forms of the CLT in depth, so we simply note their critical importance and refer the reader to Durrett [2010] for a comprehensive introduction.

5.3 Foundational Monte Carlo Inference Methods

In this section we introduce the key inference methods that form the basis upon which most Monte Carlo inference schemes are based. The key idea at the heart of all Monte Carlo inference methods is to use some form of proposal distribution that we can easily sample from and then make appropriate adjustments to achieve (typically approximate) samples from the posterior. All methods will require only an unnormalized distribution

$$\gamma(\theta) = \pi(\theta)Z \quad (5.20)$$

as a target where $Z = \int \gamma(\theta)d\theta$. As such they will apply to any situation where we desire to sample from an unnormalized (or in some cases normalized) distribution, for which the Bayesian inference setting is a particular case where $\gamma(\theta) = p(\mathcal{D}|\theta)p(\theta)$ and $Z = p(\mathcal{D})$. They will, in general, vary only on how samples are proposal and the subsequent adjustments that are made. However, this will lead to a plethora of different approaches, varying substantially in their motivation, theoretical justification, algorithmic details, and the scenarios for which they are effective.

5.3.1 Rejection Sampling

Add something about usefulness in doing things like defdist

Rejection sampling [Robert, 2004] is one of the simplest Monte Carlo inference methods and one of the only ones to produce exact samples from the target. Before going into the method itself, we first consider an example to demonstrate the underlying intuition. Imagine we want to generate samples distributed uniformly over some arbitrary two dimensional shape. One simple way of doing this would be to sample uniformly from a box enclosing the shape and then only taking the samples which fall within the shape. An example of such sampling by rejection is shown in Figure 5.2. As all the samples within the space are distributed uniformly, they are also uniformly distributed on any subset of the space. Therefore if we sample from a space incorporating the area we care about and then only take the samples that fall within the desired shape, we will generate samples uniformly over that shape. We can also use this method to estimate the area of the shape by using the fact that the probability of any one sample falls within the shape is equal to the ratio of the areas of the shape and the bounding box, namely

$$A_{\text{shape}} = A_{\text{box}} P(\theta \in \text{shape}) \quad (5.21)$$

$$\approx \frac{A_{\text{box}}}{N} \sum_{n=1}^N \mathbb{I}(\hat{\theta}_n \in \text{shape}) \quad \text{where } \hat{\theta}_n \sim \text{UNIFORM(box)} \quad (5.22)$$

where we have used a Monte Carlo estimator for $P(\theta \in \text{shape})$. Note that the value of $P(\theta \in \text{shape})$ will dictate the efficiency of our estimation as it represents the *acceptance rate* of our samples. In other words, we need to generate on average $1/P(\theta \in \text{shape})$ samples from our proposal for each sample created in the target area. As we will show later in Section 5.3.3, $P(\theta \in \text{shape})$ typically becomes very small as θ becomes high dimensional, so this approach will typically only be effective in low dimensions.

The underlying idea for rejection sampling is that we can sample from any distribution by sampling uniformly from the hyper-volume under its unnormalized probability density function. Though this is effectively axiomatic by the definition of a probability density function with respect to the Lebesgue measure, we can get a non measure-theoretic intuition for this by considering augmenting a target distribution with a new variable u such that $p(u|\theta) = \text{UNIFORM}(0, \gamma(\theta))$. Sampling $\hat{\theta} \sim \pi(\theta)$ and then $\hat{u} \sim p(u|\theta)$ corresponds to sampling uniformly from hyper-volume under the probability density function, while we clearly have that the marginal distribution on θ is $\pi(\theta)$.

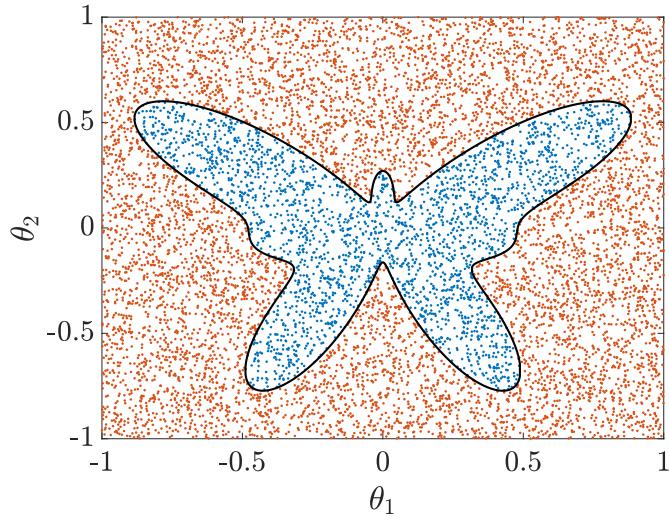


Figure 5.2: Example of sampling uniformly from an arbitrary shape by rejection. Here samples are proposed uniformly from the $[-1, 1]$ square. Any sample falling within the black outline is accepted (blue), otherwise it is rejected (red).

Using this idea, we can sample from any unnormalized distribution by sampling from an appropriate bounding as per our intuitive example and then accepting only samples that fall within the hyper-volume of the probability density function. More specifically, we define a proposal distribution $q(\theta)$ which completely envelopes a scaled version of the unnormalized target distribution $C\gamma(\theta)$ such that $q(\theta) \geq C\gamma(\theta)$ for all values of θ and $C > 0$. We then sample a pair $\{\hat{\theta}, \hat{u}\}$ by first sampling $\hat{\theta} \sim q(\theta)$ and then $\hat{u} \sim \text{UNIFORM}(0, q(\theta))$. The sample is accepted if

$$\hat{u} \leq C\gamma(\hat{\theta}) \quad (5.23)$$

which occurs with an acceptance rate CZ (note that $q(\theta) \geq C\gamma(\theta) \ \forall \theta$ ensures that $C \leq 1/Z$). Note that this can be used to estimate the normalization constant, corresponding to the marginal likelihood for Bayesian models, by calculating the empirical estimate of the acceptance rate and dividing this by C . A graphical demonstration of the rejection sampling process is shown in Figure 5.3.

Rejection sampling can be a highly effective sampling or inference method in low dimensions. In particular, the fact that it generates exact samples from the target distribution can be very useful. For example, this characteristic is used to construct efficient samplers for many common distributions such as in the ziggurat algorithm [Marsaglia et al., 2000] often used for generating Gaussian random variables. However, its efficiency is critically dependent on the value of

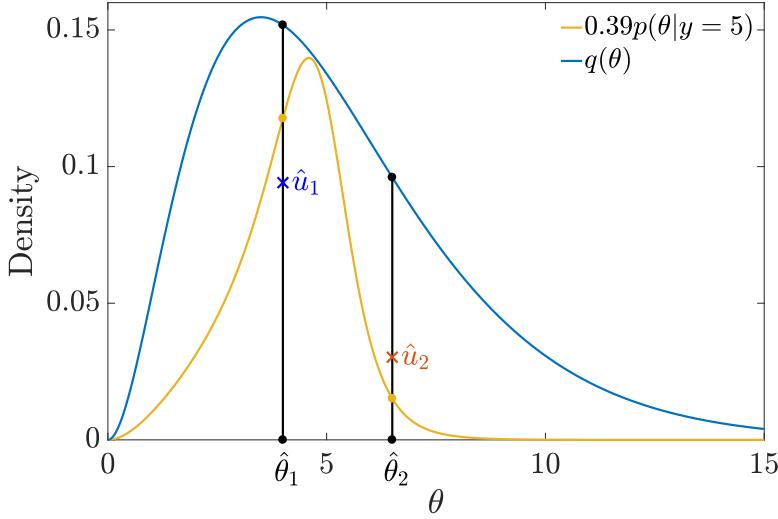


Figure 5.3: Demonstration of rejection sampling for problem shown in (5.1). We first sample $\hat{\theta} \sim q(\theta)$, correspond to the sampling for the distribution shown in blue, and then sample $\hat{u} \sim \text{UNIFORM}(0, q(\theta))$, corresponding to sampling a point uniformly along the black lines for the two shown example values of $\hat{\theta}$. The point is accepted if $\hat{u} \leq C p(\theta|y = 5)$ (i.e. if it below the yellow curve) and is otherwise rejected, where we have taken $C = 0.39$ to ensure $C p(\theta|y = 5) \leq q(\theta)$ for all theta. Here the example sample pair $\{\hat{\theta}_1, \hat{u}_1\}$ is accepted, while $\{\hat{\theta}_2, \hat{u}_2\}$ is rejected. The resulting accepted sample pairs will be uniformly sampled from the region under the unnormalized target distribution given by the yellow curve and therefore the accepted $\hat{\theta}$ will correspond to exact samples from the target.

C because it is directly proportional to the acceptance rate. By proxy, it is also critically dependent on the proposal $q(\theta)$ as this dictates the minimum possible value of C , namely $C_{\min} = \min_{\theta} q(\theta)Z/\pi(\theta)$. Note that if $q(\theta) = \pi(\theta) \forall \theta$ then the acceptance rate will be 1, while the more different they are (in terms of $\min_{\theta} q(\theta)/\pi(\theta)$), the lower the best possible acceptance rate becomes. In low dimensions, adaptive rejection sampling [Gilks and Wild, 1992] often forms an effective method for adaptively learning an effective proposal and corresponding value for C , leading to good acceptance rates. However, the approach will be very prone to the *curse of dimensionality* as we discuss in Section 5.3.3, meaning performance cannot be maintained for higher dimensional problems.

5.3.2 Importance Sampling

Importance sampling is another common sampling method that forms the key building block for many more advanced inference schemes. It is closely related to rejection sampling in that it samples candidate $\hat{\theta}$ from a proposal $q(\theta)$, but instead of going through an accept/reject step,

it assigns an *importance weight* to each sample. These importance weights act like correction factors to account for the fact that we sampled from $q(\theta)$ rather than our target $\pi(\theta)$.

To demonstrate the key idea, consider the problem of calculating an expectation as per (5.3). If we cannot sample exactly from $\pi(\theta)$ then we cannot apply (5.4) directly. However, we can rearrange the form our expectation to generate a different Monte Carlo estimator which we can evaluate directly as follows

$$\begin{aligned} I := \mathbb{E}_{\pi(\theta)} [f(\theta)] &= \int f(\theta)\pi(\theta)d\theta = \int f(\theta)\frac{\pi(\theta)}{q(\theta)}q(\theta)d\theta \\ &\approx \frac{1}{N} \sum_{n=1}^N \frac{\pi(\hat{\theta}_n)}{q(\hat{\theta}_n)} f(\hat{\theta}_n) \quad \text{where } \hat{\theta}_n \sim q(\theta) \end{aligned} \quad (5.24)$$

where $\frac{\pi(\hat{\theta}_n)}{q(\hat{\theta}_n)} =: w_n$ is known as an importance weight. The key trick we have applied is to multiply the integrand by $\frac{\pi(\theta)}{q(\theta)}$, which equals 1 for all points where $q(\theta) \neq 0$. Thus if $q(\theta) \neq 0$ for all θ for which $\pi(\theta) \neq 0$ (to avoid infinite importance weights), this has no effect on the expectation. However, we can informally view the new formulation as being the expectation of $f(\theta)\frac{\pi(\theta)}{q(\theta)}$ under the distribution $q(\theta)$. We can now construct a Monte Carlo estimator for this new formulation, by choosing $q(\theta)$ to be a distribution we can sample from. A graphical demonstration of importance sampling is given in Figure 5.4 in the more general setting where we do not have access to the $\pi(\theta)$ exactly, but only an unnormalized version $\gamma(\theta) = \pi(\theta)Z$. As we will show in detail in Section 5.3.2.1, we can still use importance sampling in this case by *self-normalizing* the weights.

Importance sampling has a number of desirable properties as an inference method. In particular, it is both unbiased and consistent. The former can be shown trivially as follows

$$\begin{aligned} \mathbb{E} \left[\frac{1}{N} \sum_{n=1}^N \frac{\pi(\hat{\theta}_n)}{q(\hat{\theta}_n)} f(\hat{\theta}_n) \right] &= \frac{1}{N} \sum_{n=1}^N \mathbb{E}_{q(\theta_n)} \left[\frac{\pi(\hat{\theta}_n)}{q(\hat{\theta}_n)} f(\hat{\theta}_n) \right] \\ &= \mathbb{E}_{q(\theta_1)} \left[\frac{\pi(\hat{\theta}_1)}{q(\hat{\theta}_1)} f(\hat{\theta}_1) \right] = \mathbb{E}_{\pi(\theta)} [f(\theta)] \end{aligned} \quad (5.25)$$

where we have effectively stepped backwards through (5.24). Given this unbiasedness result, L^2 convergence, and thus convergence in probability, can be shown in the same manner as (5.6) by replacing each $f(\hat{\theta}_n)$ with $\frac{\pi(\hat{\theta}_n)}{q(\hat{\theta}_n)} f(\hat{\theta}_n)$, leading to the same result except that σ_θ is now

$$\sigma_\theta^2 = \mathbb{E}_{q(\theta)} \left[\left(\frac{\pi(\hat{\theta}_n)}{q(\hat{\theta}_n)} f(\hat{\theta}_n) - I \right)^2 \right] = \text{Var}_{q(\theta)} \left[\frac{\pi(\theta)}{q(\theta)} f(\theta) \right]. \quad (5.26)$$

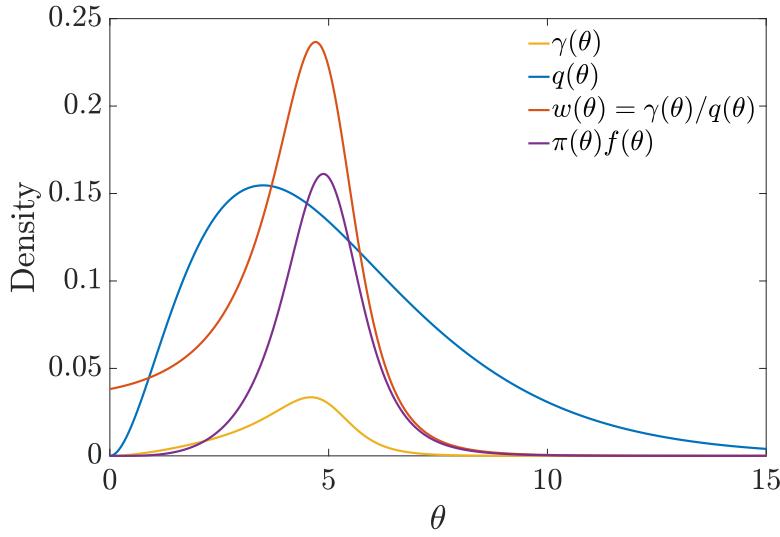


Figure 5.4: Demonstration of importance sampling for problem shown in (5.1) where we are trying to estimate $\mathbb{E}[\pi(\theta)f(\theta)]$: the expectation of the function $f(\theta) := \theta^2/50$ under the posterior $\pi(\theta) := p(\theta|y = 5)$ defined as per (5.1c). We assume the setting where $\pi(\theta)$ is only known up to a normalization constant (see Section 5.3.2.1), namely we only have access to $\gamma(\theta) := p(\theta)p(y = 5|\theta)$ as shown in yellow. Our procedure is to draw samples independently $\hat{\theta}_n \sim q(\theta)$ and then evaluate their weight $w_n = w(\hat{\theta}_n) = \gamma(\hat{\theta}_n)/q(\hat{\theta}_n)$. This produces a set of weighted samples which can then be used to estimate to estimate the expectation using (5.32) (one can also use (5.24) if the normalized $\pi(\theta)$ is used instead of $\gamma(\theta)$).

Almost sure convergence of importance sampling can be similarly shown using the strong law of large numbers.

The form of (5.26) provides substantial insight into how best to set the proposal: we have shown that the mean squared error of an importance sampler is directly proportional to $\text{Var}[f(\theta)\pi(\theta)/q(\theta)]$, thus the lower this term is, the better the expected performance of our estimator. One obvious question is what is the optimal proposal $q^*(\theta)$? It turns out that $q^*(\theta) = \frac{\pi(\theta)|f(\theta)|}{\int \pi(\theta)|f(\theta)|d\theta}$ [Kahn and Marshall, 1953; Owen, 2013], which can be shown as follows where we will make use of Jensen's inequality

$$\begin{aligned} \text{Var}_{q^*(\theta)} \left[\frac{\pi(\theta)}{q^*(\theta)} f(\theta) \right] &= \mathbb{E}_{q^*(\theta)} \left[\left(\frac{\pi(\theta)}{q^*(\theta)} f(\theta) \right)^2 \right] - \left(\mathbb{E}_{q^*(\theta)} \left[\frac{\pi(\theta)}{q^*(\theta)} f(\theta) \right] \right)^2 \\ &= \int \frac{\pi(\theta)^2 f(\theta)^2}{q^*(\theta)} d\theta - I^2 = \left(\int \pi(\theta) |f(\theta)| d\theta \right)^2 - I^2 \end{aligned} \quad (5.27)$$

$$\leq \int \left(\frac{\pi(\theta) f(\theta)}{q(\theta)} \right)^2 q(\theta) d\theta - I^2 = \text{Var}_{q(\theta)} \left[\frac{\pi(\theta)}{q(\theta)} f(\theta) \right]. \quad (5.28)$$

Here we have shown that the variance for $q^*(\theta)$ is less than or equal to the variance using an arbitrary $q(\theta)$. It must therefore be the optimal proposal. A further point of note is

that if $f(\theta) \geq 0 \ \forall \theta$ (or $f(\theta) \leq 0 \ \forall \theta$), then (5.27) will equal zero giving a zero variance estimator: each importance weight will be equal to the $I/f(\theta)$ and thus I can be calculated by evaluating a single point.

Though it will typically be impossible to find $q^*(\theta)$ in practice, it still provides a guide as to what constitutes a good proposal – we want $\pi(\theta) |f(\theta)| / q(\theta)$ to be a close to constant as possible. In particular, we need to be careful to avoid scenarios where $\frac{\pi(\theta) |f(\theta)|}{\int \pi(\theta) |f(\theta)| d\theta} \gg q(\theta)$ as this will cause the ratio to explode, leading to high variances. A consequence of this is that we want $q(\theta)$ to have *light tails* compared to $\pi(\theta) |f(\theta)|$ to ensure that the ratio does not systematically increase as θ moves away from the modes of $q(\theta)$. Aside from the clear practical issues, If this requirement does not hold, then it can easily be the case that $\sigma_\theta = \infty$ and thus that the estimator has infinite variance. Consider, for example, the case where $\pi(\theta) = \mathcal{N}(\theta; 0, 1)$, $f(\theta) = \theta$, and $q(\theta) = \mathcal{N}(\theta; 0, s^2)$ (Example 9.1 from Owen [2013]). Noting that the mean, I , is zero by symmetry and defining $\nu = \frac{1}{2s^2} - 1$, we have that

$$\begin{aligned}\sigma_\theta^2 &= \int_{-\infty}^{\infty} \theta^2 \frac{\left(\exp(-\theta^2/2)/\sqrt{2\pi}\right)^2}{\exp(-\theta^2/(2s^2))/\sqrt{2\pi}s^2} d\theta - I^2 \\ &= \frac{s}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \theta^2 \exp(\theta^2\nu) d\theta.\end{aligned}\tag{5.29}$$

Now this integral is clearly only finite for $\nu < 0$ (as otherwise the integrand is $+\infty$ and $\theta = \pm\infty$ and finite elsewhere). Therefore, σ_θ is only finite when $s^2 > 1/2$. In other words, we only get a finite estimator in this case if the proposal variance is at least half that of the target distribution $\pi(\theta)$. This highlights the pitfalls of having insufficiently heavy tails on our proposal. Overcoming these will typically require careful setup of the proposal on a case-by-case basis, for example, choosing a distribution type for the proposal that is known to have heavier tails than $\pi(\theta)$.

5.3.2.1 Self-Normalized Importance Sampling

In the previous section we presumed that we have access to a normalize version of the target $\pi(\theta)$. Typically this will not be the case and we will only have access to an unnormalized target $\gamma(\theta) = \pi(\theta)Z$ as per (5.20), for example only having access to the joint rather than the posterior in the Bayesian inference setting. In a less common but still plausible situation, it may also only be possible to evaluate the proposal up to a normalization constant. We now show how one can still use importance sampling in these scenarios, by *self-normalizing* the importance weights.

The key idea for self-normalized importance sampling (SNIS) is that the weights provide an unbiased and consistent estimator of the marginal likelihood

$$Z_N = \frac{1}{N} \sum_{n=1}^N w_n, \quad (5.30)$$

$$\mathbb{E}[Z_N] = \frac{1}{N} \sum_{n=1}^N \mathbb{E}[w_n] = \mathbb{E}_{q(\hat{\theta}_1)}[\gamma(\hat{\theta}_1)/q(\hat{\theta}_1)] = Z. \quad (5.31)$$

Now as $\mathbb{E}_{q(\theta)}\left[\frac{\gamma(\theta)}{q(\theta)}f(\theta)\right] = E_{q(\theta)}\left[\frac{\pi(\theta)}{q(\theta)}Zf(\theta)\right] = Z \mathbb{E}_{\pi(\theta)}[f(\theta)]$, we can use our samples to construct Monte Carlo estimators for both Z and $Z \mathbb{E}_{\pi(\theta)}[f(\theta)]$ and use the ratio of our estimates to get an estimate for $\mathbb{E}_{\pi(\theta)}[f(\theta)]$

$$\mathbb{E}_{\pi(\theta)}[f(\theta)] \approx \frac{\sum_{n=1}^N w_n f(\hat{\theta}_n)}{\sum_{n=1}^N w_n} \quad \text{where } \hat{\theta}_n \sim q(\theta), \quad w_n = \frac{\gamma(\hat{\theta}_n)}{q(\hat{\theta}_n)}. \quad (5.32)$$

This can alternatively be expressed as $\mathbb{E}_{\pi(\theta)}[f(\theta)] \approx \sum_{n=1}^N \bar{w}_n f(\hat{\theta}_n)$ where $\bar{w}_n = \frac{w_n}{\sum_n w_n}$ are the normalized importance weights such that $\sum_{n=1}^N \bar{w}_n = 1$.

The consistency of (5.32) follows directly from the individual consistency of both the numerator and the denominator to $Z \mathbb{E}_{\pi(\theta)}[f(\theta)]$ and Z respectively. However, unlike (5.24), (5.32) is biased estimator for finite N . This is because the numerator and denominator are correlated and because even though Z_N is an unbiased estimator of Z , $1/Z_N$ is not an unbiased estimator of $1/Z$. The latter follows directly from Jensen's inequality noting that inversion is a convex function for strictly positive inputs,

$$\mathbb{E}\left[\frac{1}{\sum_{n=1}^N w_n}\right] \geq \frac{1}{\mathbb{E}\left[\sum_{n=1}^N w_n\right]} = \frac{1}{Z}, \quad (5.33)$$

where equality holds only if Z_N is a zero variance estimator for Z (which typically happens only in the limit $N \rightarrow \infty$). However, it can be shown that the bias decreases at a rate $O(1/N)$ (see e.g. Doucet and Johansen [2009]), whereas the standard deviation of the estimate decreases at a rate $O(1/\sqrt{N})$. Thus the bias becomes dominated as $N \rightarrow \infty$. Strangely, even when the normalization constant is known, the self-normalized importance sampler can still be lower variance [Owen, 2013]. Therefore, with the bias becoming dominated, it can actually be preferable to use SNIS even when the normalized target is known. Note also that the optimal proposal in the SNIS case varies slightly from the $q^*(\theta)$ derived earlier in the Section and is instead [Hesterberg, 1988]

$$q_{\text{SNIS}}^*(\theta) = \frac{\pi(\theta) |f(\theta) - I|}{\int \pi(\theta) |f(\theta) - I| d\theta}. \quad (5.34)$$

As a consequence, there is a minimum variance on the SNIS estimator, unlike in the pre-normalized case where $q^*(\theta)$ was a zero variance estimator was possible if $f(\theta) \geq 0 \forall \theta$.

5.3.2.2 Unknown f

So far we have assumed that we are using importance sampling to calculate an expectation of a known function. In practice, there will be many scenarios, particularly in the Bayesian inference setting, where $f(\theta)$ is not known ahead of time and we instead desire to generate samples for some future unknown use. For example, in Section 6.1 we will introduce the concept of *sequential Monte Carlo* where we will typically have multiple importance sampling steps before any target function is itself evaluated. When no $f(\theta)$ is specified we can carry out importance sampling in the same fashion, sampling from $q(\theta)$ and returning a set of *weighted* samples $\{\hat{\theta}_n, w_n\}_{n=1:N}$ where the weights are equal to $\gamma(\hat{\theta}_n)/q(\hat{\theta}_n)$ as before. Here we can think of importance sampling as approximating the posterior with a series of deltas functions, namely

$$\pi(\theta) \approx \hat{\pi}(\theta) := \sum_{n=1}^N \bar{w}_n \delta_{\hat{\theta}_n}(\theta) \quad (5.35)$$

where $\delta_{\hat{\theta}_n}(\theta)$ are delta functions centred at $\hat{\theta}_n$.

Importance weights are multiplicative when doing conditional sampling: if we sample $\hat{\theta}_n \sim q_1(\theta)$ then $\hat{\phi}_n | \hat{\theta}_n \sim q_2(\phi | \hat{\theta}_n)$ when targeting $\gamma_1(\theta)\gamma_2(\phi|\theta)$ then the importance weight is

$$\frac{\gamma_1(\hat{\theta}_n)\gamma_2(\hat{\phi}_n|\hat{\theta}_n)}{q_1(\hat{\theta}_n)q_2(\hat{\phi}_n|\hat{\theta}_n)} = \frac{\gamma_1(\hat{\theta}_n)}{q_1(\hat{\theta}_n)} \times \frac{\gamma_2(\hat{\phi}_n|\hat{\theta}_n)}{q_2(\hat{\phi}_n|\hat{\theta}_n)} = w_{n,1} \times w_{n,2}. \quad (5.36)$$

This is known as sequential importance sampling and means that we can propagate importance weighted samples through a computational system and retain a valid importance sampler with the standard properties such as unbiasedness (presume the weights are not self-normalized) and consistency.³

Again a natural question in this “unknown f ” setting is what is the optimal proposal $q^*(\theta)$? This is a somewhat more challenging and subjective question than when f is known as the optimality will depend on what the samples are eventually used for. In particular, even if we do not know f precisely, it may be the case that we believe some f are more likely than others or we may know that f lives within some space of possible functions, for example functions that have a countable number of discontinuities.

³Note that this does not apply to the *nested estimation* case as we discuss in Chapter 10.

One simple, but insightful approach, is to consider the *minimax* optimal proposal, i.e. the proposal that has the minimum error if f is the most adversarial possible function for that proposal. Imagine that we have N weighted samples $\{\hat{\theta}_n, w_n\}_{n=1:N}$, with N corresponding evaluations $f_n := f(\hat{\theta}_n)$. We use these to calculate an estimate I_N for the target I . Now assume that each $w_n \geq 0$, $\sum_{n=1}^N w_n = 1$, and $\sum_{n=1}^N |f_n - I| = N$ to preclude the ability to provide an improved solution simply by scaling the problem. The error for the estimator is given by

$$|I_N - I| = \left| \sum_{n=1}^N w_n f_n - I \right| = \left| \sum_{n=1}^N w_n (f_n - I) \right|. \quad (5.37)$$

For any given set of weights, the most adversarial set of function evaluations is to have all our error at the largest weight, i.e. $|f_{n^*} - I| = N$ and $|f_n - I| = 0$, $n \neq n^*$ where n^* is the index of the largest weight. For this set of adversarial f_n , the lowest error is achieved when each of the weights are equal. Consequently, we see that the minimax proposal under our assumptions is $q(\theta) = \pi(\theta)$. This result is perhaps not surprising as it effectively states that the best sample representation of $\pi(\theta)$ for an unknown future use is to sample from that distribution directly. As shown in the next section, this proposal will also minimize the variance of the estimator under the assumption that the f_n are independent.

Nonetheless, this point of view is not without criticism in the literature [O'Hagan, 1987; Ghahramani and Rasmussen, 2003; Briol et al., 2015]. Most of this criticism revolves around the valid point that in practice the value of $f(\theta)$ does convey information about $f(\theta + \varepsilon)$ and so the correlation between samples such be taken into account when making an estimation. Though the thrust of this argument is mostly directed towards changing the Monte Carlo method, and in particular importance sampling, at a more fundamental level, the same arguments would still suggest that it is can be beneficial to use a proposal that is more diffuse than the target, thereby reducing the correlation between the produced samples.

5.3.2.3 Effective Sample Size

In this section we consider an important diagnostic for the performance of importance sampling based schemes, the *effective sample size* (ESS). In Section 5.2.3 we showed how an uncertainty estimate for a Monte Carlo estimator can be derived. However, this does cannot be used when f is unknown and even if f is known, it does necessarily convey much information about how effective our proposal is compared to how effective it could be. The ESS instead informally

provides an estimated measure of the amount of information stored in our weighted sample set. The more information stored in the samples, the better our approximation of the posterior, and, at a high level, the more evenly balanced our weights, the more information they encode. Therefore, the ESS is a measure of how many unweighted samples would be required to convey the same information about the posterior as the weighted sample set.

The weighted average of N_e independent evaluations $\{f_n\}_{n=1}^N$, each with individual variance σ^2 , has variance σ^2/N_e as we showed in (5.6). Therefore, we can calculate the ESS of a set of weighted samples by comparing the variance of our weighted estimate to the variance of an estimate using a set of unweighted evaluations. More specifically, the ESS will be the number of unweighted evaluations N_e that gives an equivalent variance to our weighted estimate as follows where we will make use of the assumption that the f_n are independent

$$\begin{aligned}\frac{\sigma^2}{N_e} &= \text{Var} \left[\frac{\sum_{n=1}^N w_n f_n}{\sum_{n=1}^N w_n} \middle| \{w_n\}_{n=1}^N \right] \\ &= \sum_{n=1}^N \left(\frac{\sum_{n=1}^N w_n}{\sum_{n=1}^N w_n} \right)^2 \text{Var}[f_n] \\ &= \frac{\sigma^2 \sum_{n=1}^N w_n^2}{\left(\sum_{n=1}^N w_n \right)^2}.\end{aligned}\tag{5.38}$$

Now rearranging for N_e we get

$$N_e = \frac{\left(\sum_{n=1}^N w_n \right)^2}{\sum_{n=1}^N w_n^2} = \frac{1}{\sum_{n=1}^N \bar{w}_n^2}\tag{5.39}$$

which completes our definition for the effective sample size other than in some scenarios it is necessary to collapse identical weighted samples to a single sample when calculating (5.39), such as when doing resampling (see Section 5.3.2.4). It transpires that N_e is independent of f , so we can still use the ESS as a diagnostic when f is unknown. It is straightforward to show using Jensen's inequality we have that $N_e \leq N$ with equality holding if and only if all the weights are equal. On the other hand, if all but one of the weights is zero, then $N_e = 1$. These two extremes respectively occur when the proposal is equal to the target, $q(\theta) = \pi(\theta)$, and when the proposal provides a very poor representation of the target. The ESS is often therefore used for *proposal adaptation*, as a larger value of the ESS generally indicates a better proposal.

However, the ESS is far from a perfect measure of sample quality. For example, if the proposal perfectly matches one of the modes of the target but completely misses another larger mode,

the ESS will usually be very high, even though the samples provide a very poor representation of the target. It is not uncommon in practice to see the ESS drop drastically as more samples are added, due to the addition of a new dominating sample, typically indicating a region of significant target probability mass that had previously been missed. Nonetheless, the ESS is still a very useful performance metric and is usually a reliable indicator for whether our importance sampling is struggling. In particular, though the possibility of missing modes means that it is possible for the ESS to be high even when the approximation of the posterior is poor, if the ESS is low then the approximation of the posterior will always be poor and any subsequent estimates will, in general, be high variance.

5.3.2.4 Resampling

A useful feature of SNIS is that it can be used to produce unweighted samples by *sampling with replacement* from the set of produced samples in proportion to the sample weights. This procedure is typically known as resampling, because we are resampling samples from the empirical distribution of our original samples. It allows us to generate unweighted samples with importance sampling which are approximately distributed according to $\pi(\theta)$, with this approximation becoming exact in the limit $N \rightarrow \infty$. Resampling on its own always lead to a higher variance estimator than using (5.32) directly. However, in addition to being necessary when unweighted samples are required, it will be a key component in the so-called particle-based inference methods discussed in Chapter 6. For example, when interleaved with sequential importance sampling, this leads to the sequential importance resampling algorithm which is the backbone of sequential Monte Carlo methods.

Mathematically, we can express resampling as producing a set unweighted resampled samples $\{\tilde{\theta}_n\}_{n=1}^N$ using

$$\tilde{\theta}_n = \hat{\theta}_{a_n} \quad \text{where} \quad a_n \sim \text{DISCRETE} \left(\{\bar{w}_n\}_{n=1}^N \right) \quad (5.40)$$

where $\{a_n\}_{n=1}^N$ are known as ancestor indices as they indicate which sample from the original sample set each sample originated from. Note that the a_n need not be drawn independently and typically are not; (5.40) instead conveys the required marginal distribution for each a_n .

Considering the approximation of the posterior provided by importance sampling given in (5.35), we can view resampling as producing the approximation

$$\tilde{\pi}(\theta) := \sum_{n=1}^N \frac{k_n}{N} \delta_{\hat{\theta}_n}(\theta) \quad (5.41)$$

where k_n is the number times the sample $\hat{\theta}_n$ appears in the resampled sample set $\{\tilde{\theta}_n\}_{n=1}^N$. Provided that $\mathbb{E}[k_n | \{w_n\}_{n=1}^N] = Nk_n$, then it directly follows that $\tilde{\pi}(\theta)$ is an unbiased estimator for $\hat{\pi}(\theta)$. Consequently the L^2 convergence, and thus consistency, of SNIS with resampling follows directly from the L^2 convergence of SNIS.

There are a number of different methods one can use for resampling [Douc and Cappé, 2005]. They all share in common the requirements above, but vary in correlations between the a_n . The simplest method, *multinomial resampling*, simply involves sampling each a_n independently, such that each k_n has a multinomial distribution. Though simple, this method is generally inadvisable as it adds unnecessary variation to the resampling compared to methods using randomized quasi-Monte Carlo [L'Ecuyer and Lemieux, 2005], such as systematic resampling Carpenter et al. [1999]; Whitley [1994],⁴ or other variance reduction techniques, such as employed by stratified resampling [Kitagawa, 1996] and residual resampling [Whitley, 1994]. Though residual resampling is a little more complicated (see Douc and Cappé [2005]), stratified and systematic resampling can be viewed as small changes on the underlying random number draws made in multinomial resampling. The typical way to draw from a multinomial distribution with N trials and probabilities p_1, \dots, p_K is to make N independent draws from a unit uniform distribution, $u_n \stackrel{i.i.d.}{\sim} \text{UNIFORM}(0, 1) \ \forall n \in 1, \dots, N$ and then to bin these into the intervals between the cumulative probabilities $P_0 = 0, P_j = \sum_{\ell=1}^j p_\ell, \ \forall j \in 1, \dots, K$. Thus the result of each trial a_n corresponds to which bin the respective u_n falls into:

$$a_n = \{j \in \{1, \dots, K\} : P_{j-1} \leq u_n < P_j\}, \quad \forall n \in \{1, \dots, N\} \quad (5.42)$$

and counts for each event, k_j , is the number of u_n satisfying $P_{j-1} \leq u_n < P_j$. In the context of multinomial resampling, $K = N$ and a_n and k_j are as per (5.40) and (5.41) respectively, noting that the corresponding requirements for their distributions are trivially satisfied. Stratified resampling and systematic resampling differ only in how the u_n are drawn. For stratified

⁴Note that systematic resampling as it is now known is somewhat confusingly referred to as stratified resampling in the former of these papers and universal sampling in the latter.

Algorithm 1 Resampling

Inputs: weighted samples $\{w_n, \hat{\theta}_n\}_{n=1}^N$, method \mathcal{M}

Outputs: unweighted samples $\{\tilde{\theta}_n\}_{n=1}^N$

```

1: switch  $\mathcal{M}$  do
2:   case Multinomial
3:      $u_n \stackrel{i.i.d.}{\sim} \text{UNIFORM}(0, 1), \quad \forall n \in 1, \dots, N$ 
4:   case Stratified
5:      $u_n \sim \text{UNIFORM}\left(\frac{n-1}{N}, \frac{n}{N}\right), \quad \forall n \in 1, \dots, N$ 
6:   case Systematic
7:      $u_1 \sim \text{UNIFORM}\left(0, \frac{1}{N}\right)$ 
8:      $u_n \leftarrow u_1 + \frac{n-1}{N}, \quad \forall n \in 2, \dots, N$ 
9: end switch
10: Normalize weights  $\bar{w}_n \leftarrow w_n / (\sum_{\ell=1}^N w_{\ell}), \quad \forall n \in 1, \dots, N$ 
11:  $P_n \leftarrow \sum_{\ell=1}^n \bar{w}_{\ell}, \quad \forall n \in 1, \dots, N$   $\triangleright P_0 = 0$ 
12:  $a_n = \{\ell \in \{1, \dots, N\} : P_{\ell-1} \leq u_n < P_{\ell}\}, \quad \forall n \in \{1, \dots, N\}$ 
13:  $\tilde{\theta}_n = \hat{\theta}_{a_n}, \quad \forall n \in \{1, \dots, N\}$ 
14: return  $\{\tilde{\theta}_n\}_{n=1}^N$ 

```

resampling, each u_n is independently sampled from a different strata of the full $[0, 1]$ space such that $u_n \sim \text{UNIFORM}(\frac{n-1}{N}, \frac{n}{N})$, which enforces that $u_1 \leq u_2 \leq \dots \leq u_N$. For systematic resampling, the only draw made is $u_1 \sim \text{UNIFORM}(0, \frac{1}{N})$, with all other u_n set deterministically from this point using $u_n = u_1 + \frac{n-1}{N}, \forall n \in 2, \dots, N$. By also randomly permuting $\{u_n\}_{n=1}^N$ before applying (5.42), each u_n after permutation is still uniformly distributed on $[0, 1]$ for both methods and so (5.40) is still satisfied, as is the requirement that $\mathbb{E}[k_n | \{w_n\}_{n=1}^N] = Nk_n$ [Douc and Cappé, 2005]. In practice, the ordering of the samples is usually arbitrary such that this permutation is not necessary. A summary of these three approaches is given in Algorithm 1.

Systematic, stratified, and residual resampling are lower variance than multinomial sampling, with systematic resampling the most widely used due to its simplicity of implementation and generally being the best performing Doucet and Johansen [2009]. It should be noted, however, that there can be theoretical complications with systematic resampling, while stratified and residual resampling can be shown to dominate multinomial resampling [Douc and Cappé, 2005]. To give insight into how these methods reduce the variance of eventual estimation, consider a case where all the weights are equal. Because the ancestor variables are drawn independently for

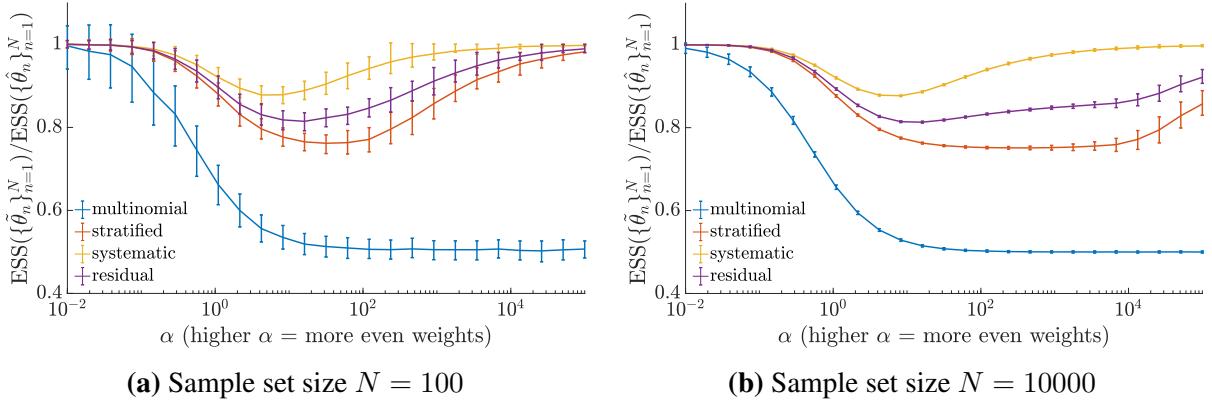


Figure 5.5: Demonstration of performance of different resampling schemes for two different sample set sizes and different levels of variance in the weights. Plots are generated by first sampling a set of N weights from a symmetric Dirichlet distribution with parameter α , $\{\bar{w}_n\}_{n=1}^N \sim \text{DIRICHLET}(\alpha)$, such that the higher α is, the more even the weights are on average. The effective sample size (ESS) as defined in (5.39) is then calculated before and after the resampling is carried out, and the ratio of the ESS after to the ESS before reported. Plots show the mean across 1000 independent trials, with the error bars corresponding to the interquartile range.

multinomial resampling, many of the original samples will not be present in the resampled set. More precisely, the probability of any particular sample being present is given by

$$P(\hat{\theta}_n \in \{\tilde{\theta}\}_{n=1}^N) = 1 - \left(\frac{N-1}{N} \right)^N \xrightarrow{N \rightarrow \infty} 1 - \frac{1}{e} \approx 0.6321.$$

Thus substantial information is lost in the resampling. On the other hand, if we use any of the variance reduction techniques, each of the original samples will appear exactly once in the resampled set so no information is lost in this scenario. In the other extreme, when all the weight is on a single sample, all the resampling schemes will behave the same (returning only the sample with non-zero weight). In most practical scenarios we will be somewhere between these two extremes, but the high level intuition that multinomial resampling throws away more information than the other approaches will remain the same.

An empirical assessment of the methods is shown in Figure 5.5. This shows the relative effective sample size (ESS) before and after resampling as a function of the uniformity of the weights. To calculate the ESS after the resampling, we collapse the identical duplicated particles down to a single sample with the combined weight of the other samples. This is equivalent to replacing w_n with k_n/N in the ESS calculation given in (5.39). Figure 5.5 shows that systematic resampling is clearly preferable to the alternatives, at least in the terms of the ESS after resampling for this particular problem, with this improvement consistent across the different sample size

sets. Similar relatives performances are found if one instead uses the proportion of samples that survive the resampling as a performance metric. As expected, multinomial resampling is significantly worse than the other methods, particularly when the weights are more even. The results also suggest that residual resampling outperforms stratified resampling, though this can come at the cost of being more complicated to implement and potentially slower to run. Note that the reason the ESS sometimes rises above 1 for a particular trial is because it is an imperfect measure of the information stored in the samples and so this simply happens by chance.

5.3.3 The Curse of Dimensionality

In this section we digress from introducing specific inference methods themselves to talk about a common problem faced by most inference methods, the *curse of dimensionality* [Bellman, 1961]. At a high-level the curse of dimensionality is a tendency of modelling and numerical procedures to get substantially harder as the dimensionality increases, often at an exponential rate. If not managed properly, it can cripple the performance of inference methods and it is main reason the two procedures discussed so far, rejection sampling and importance sampling, are in practice only used for very low dimensional problems. At its core, it stems from an increase of the size (in an informal size) of a problem as the dimensionality increases. This is easiest to see for discrete problems. Imagine we are calculating an expectation over a discrete distribution of dimension D where each dimension has K possible values. The cost of enumerating all the possible combinations scales as K^D and thus increases exponentially with D ; even for modest values for K and D this will be prohibitively large.

The curse of dimensionality extends far beyond problems of enumeration. It will be felt to some degree or another by almost all approaches for inference and modelling more generally, but its effect will be most pronounced for methods that try to explicitly model the target space. As a geometrical demonstration of this, consider the effect of dimensionality on the sampling by rejection approach introduced at the start of Section 5.3.1 where to sample uniformly from within some shape we sample uniformly from some bounding shape or box containing the target shape and then take only the samples that fall within the target. For simplicity we will presume that the target shape is a hypersphere and that the bounding shape is the smallest hypercube that encloses that hypersphere. Our acceptance rate, and thus the efficiency of the algorithm, will be equal to the ratio of the two Lebesgue measures, i.e. the ratio of the two

hyper-volumes. For an even number of dimensions the hyper-volume of the D -dimensional hypersphere with radius r is $V_s = \frac{\pi^{D/2} r^D}{(D/2)!}$ and the hyper-volume of the enclosing hypercube is $V_c = (2r)^D$, giving a ratio of $\frac{V_s}{V_c} = \frac{\pi^{D/2}}{(D/2)! 2^D} = \left(\frac{\sqrt{\pi}}{2}\right)^D \frac{1}{(D/2)!}$. The first of these terms decreases exponentially and second super-exponentially with D (noting that $(D/2)! > (D/6)^{(D/2)}$) and thus quickly becomes very small. For example, $D = 10, 20$, and 100 respectively gives ratios of approximately 2.5×10^{-3} , 2.5×10^{-8} , and 1.9×10^{-70} . Consequently, our acceptance rate will diminish super-exponentially with the number of dimensions and our approach will quickly become infeasible in higher dimensions.

An immediate possible criticism of this analysis would be to suggest that approximation of the target shape provided by our bounding shape is simply increasingly poor as the dimensionality increases and that we should choose a better approximation. Although this is true, the key realisation is that achieving a good approximation is increasingly difficult in high dimensions, typically exponentially so. To demonstrate this, imagine we instead use an arbitrary bounding shape defined in polar co-ordinates such that the error on the radius at the any given point is at most ε (i.e. the radius of our bounding shape is between r and $r + \varepsilon$ at all points). The hyper-volume in which our approximation might live for an even number of dimensions is given by

$$V_\varepsilon = \frac{\pi^{D/2}(r + \varepsilon)^D}{(D/2)!} - \frac{\pi^{D/2}r^D}{(D/2)!} = V_s \left((1 + \varepsilon)^D - 1 \right). \quad (5.43)$$

Consequently, we have that the ratio $\frac{V_\varepsilon}{V_s}$ increases exponentially with D and that for sufficiently large D and a fixed ε the amount of space in our tolerance region will become substantially larger than the target hyper-volume, leading to very low acceptance rates.

Flipping this on its head, we can ask the question how does ε need to vary to ensure that V_ε/V_s remains constant? A quick manipulation shows that $\varepsilon = \left(\frac{V_\varepsilon}{V_s} + 1\right)^{1/D} - 1$ and therefore that $\frac{\log\left(\frac{V_\varepsilon}{V_s} + 1\right)}{D} \geq \log(1 + \varepsilon) \approx \varepsilon$ for small values of ε . Thus we only need to decrease ε roughly in proportion to $\frac{1}{D}$ to achieve a fixed ratio. Initially this would not seem so bad. For example, if $D = 1000$ we roughly need $\varepsilon \leq 6.9 \times 10^{-4}$ to get $V_\varepsilon/V_s \leq 1$. However, this misses the key difficulty caused by (5.43): the higher D is, the more difficult it is to accurately model the target shape and keep ε small. It follows from (5.43) that as D increases, the more the hyper-volume of the sphere is concentrated at the surface. This generalized to non-spherical targets and means that accurate modelling the surface of our target is essential in high dimensions. Unfortunately, the this task becomes rapidly more difficult with increasing dimensionality.

Consider, for example, regressing the surface of the target by using a number of inducing points spread over the surface. As the dimensionality increases, these become increasingly far apart from one another and so the more points we need to accurately model the surface. For example, the probability of two points uniformly distributed on the surface of a sphere being within some target distance of one another decreases exponentially with the dimensionality of the sphere. This can be seen by noting that a necessary condition for two points to be within d of each other the discrepancy of each individual dimension must be less than d . In other words, if we denote the overall distance as δ and the distance in each dimension as δ_i then we have

$$P(\delta \leq d) \leq P(\delta_1 \leq d)P(\delta_2 \leq d)\dots P(\delta_D \leq d)$$

and so $P(\delta \leq d)$ must decrease exponentially with D . If the correlation between points is proportional to their euclidean distance, then we will subsequently need an exponentially large number of points in the dimension to model the surface to a given accuracy. Consequently, we see that not only are we increasingly punished for any discrepancies between our approximation and the target as the dimensionality increases, it rapidly becomes harder to avoid these discrepancies in the first place.

One can informally think of the proposals we have introduced thus-far as being approximations to the target distribution: complications with tail behaviour aside, it will generally be the case that the better the proposal approximates the target, the better the inference will perform. This typically leads to catastrophically bad performance for importance sampling and rejection sampling in high dimensions, for which this approximation breaks down for the reasons we have just outlined. To give a simple example, imagine that our target is an isotropic unit Gaussian and we use an independent student-t distribution with $\nu = 2$ in each dimension as the proposal. We have that the weights are as follows

$$w(\theta) = \frac{\pi(\theta)}{q(\theta)} = \prod_{i=1}^D \frac{\exp(-\theta_d^2/2)/\sqrt{2\pi}}{\frac{\Gamma(1.5)}{\sqrt{2\pi}} (1 + \theta_d^2/2)^{-3/2}} = \prod_{i=1}^D \frac{2 \exp(-\theta_d^2/2) (1 + \theta_d^2/2)^{3/2}}{\sqrt{\pi}}. \quad (5.44)$$

It follows that the variance of the weights under the proposal increases exponentially with D as

follows

$$\begin{aligned}
 \text{Var}_{q(\theta)} [w(\theta)] &= \int w^2(\theta)q(\theta)d\theta - \left(\int w(\theta)q(\theta)d\theta \right)^2 \\
 &= -1 + \prod_{i=1}^D \int_{-\infty}^{\infty} w^2(\theta_d)q(\theta_d)d\theta_d \\
 &= -1 + \prod_{i=1}^D \int_{-\infty}^{\infty} \frac{\sqrt{2}\exp(-\theta_d^2)(1+\theta_d^2/2)^{(3/2)}}{\pi} d\theta_d \\
 &\approx 1.1455^D - 1
 \end{aligned} \tag{5.45}$$

where we have used the fact that the integral has a closed form solution. We thus see that our effective sample size will drop exponentially quickly with D and that our inference will break down if the dimensionality is too high.

It is now natural to ask whether we can overcome the curse of dimensionality. Thankfully, the answer in many scenarios is that we can. In many high dimensional scenarios then our target distribution will typically only have significant mass in a small proportion of the total area, often concentrated around a lower dimensional manifold of the larger space. This means that if we use inference methods that in some way exploit the structure of the target distribution and only search the small subset of the space with significant mass, then effective inference can still be performed. When this is not the case, practical inference will typically be futile in high dimensions and so many inference algorithms are geared towards exploiting a particular type of structure. As we will show in the next section, the effectiveness of MCMC methods is mostly based on exploiting single modality in the target by making local moves that cause the algorithm to have hill-climbing style behaviour away from the mode and then sticking close to the mode once it is found. Sequential Monte Carlo methods on the other hand rely on using the structure of the target more explicitly by using a series of stepping-stone distributions and adaptively allocating resources (see Chapter 6). Variational and message passing methods make assumptions or approximations about the structure of the model to break the inference problem down into a number of small problems that can then be combined into an overall estimate. Arguably the key to all advanced inference methods is how well they can exploit structure in higher dimensions, while the relative performance of different methods tends to come down to how suited the target is to their particular form of structure exploitation.

5.3.4 Markov Chain Monte Carlo

This section needs quite a bit of cleaning such as transitioning the notation

Markov chain Monte Carlo (MCMC) methods Metropolis et al. [1953]; Hastings [1970]; Gilks et al. [1995] form one of the key approaches to circumventing the curse of dimensionality and are perhaps the most widely used class of algorithms for Bayesian inference, though they are also used extensively outside the Bayesian inference setting. The key idea is to construct a valid Markov chain that has the target distribution as its equilibrium distribution. They are suitable for Bayesian inference because this can typically done when the target distribution is only known up to a normalization constant.

The reason that they are often able to overcome, or at least alleviate, the curse of dimensionality is that rather than trying to independently sample from the target distribution at each iteration, they instead make *local* moves from their current position. As with rejection sampling and importance sampling, they use a proposal distribution, but unlike these alternatives, the proposal is defined conditionally on the current location, namely they propose according to $x' \sim q(x'|x)$ where x is the current state and x' is the new state to sample. The underlying intuition behind this is that in high dimensions the proportion of the space with significant probability mass is typically very small. Therefore, if the target is single modal (or we have a proposal that is carefully designed to jump between modes), then once we have a sample in the mode, all the other points with significant mass should be close to that point. Therefore we can explore the mode by restricting ourselves to local moves, overcoming the curse of dimensionality by predominantly ignoring the majority of the space as this has insignificant probability mass. As the dimensionality increases, the proportion of the space with significant mass decreases, counteracting many of the other complications that arise from the increasing dimension. When away from a mode, they often behave like hill-climbing algorithms, emphasizing their close links with simulated annealing [Aarts and Korst, 1988] methods for optimization. Therefore they can be highly effective for both finding the mode of a posterior and then sticking to that mode.

5.3.4.1 Markov Chains

We first introduced the concept of the *Markov property* in Section 3.3 in the context of a hidden Markov model, where we explained how in Markovian system is independent of all

the previous states given the last state, i.e.

$$p(X_n = x | X_1 = x_1, \dots, X_{n-1} = x_{n-1}) = p(X_n = x_n | X_{n-1} = x_{n-1}). \quad (5.46)$$

In other words, it transitions from one state to the next based only on the current state. Here the series X_1, \dots, X_n, \dots is known as a Markov chain. We see that a probability of a Markov chain is fully defined by the probability of its initial state $p(X_1 = x_1)$ and the probability of its transitions $p(X_n = x_n | X_{n-1} = x_{n-1})$. If each transition has the same distribution, i.e.

$$p(X_{n+1} = x_{n+1} | X_n = x_n) = p(X_n = x_{n+1} | X_{n-1} = x_n), \quad (5.47)$$

then the Markov chain is known as homogeneous. Most MCMC methods are based on homogeneous Markov chains (the exception being adaptive MCMC methods, see Section 5.3.5) and so we will assume that (5.47) hold from now on. In such situations, $p(X_{n+1} = x_{n+1} | X_n = x_n)$ is typically known as a *transition kernel* $T(x_{n+1} \leftarrow x_n)$.

The marginal probability density of any particular point in a homogenous Markov chain is given by

$$p(x_n) = \int_{x_1, \dots, x_{n-1}} p(x_1) \prod_{i=2}^n T(x_{i-1} \leftarrow x_i) dx_1 \dots dx_{n-1}. \quad (5.48)$$

For a Markov chain to converge to a target distribution $\pi(x)$, we will need that $\lim_{n \rightarrow \infty} p(X_n = x) = \pi(x)$ for any possible starting position x_1 , i.e. that the chain converges in distribution to the target for all possible starting positions. For this to happen we need two things – $\pi(x)$ must be a *stationary distribution* of the Markov chain, such that if $p(X_n = x) = \pi(x)$ then $p(X_{n+1} = x) = \pi(x)$, and all possible starting points x_1 must converge to this distribution. The former of these will be satisfied if

$$\pi(x') = \int_x T(x' \leftarrow x) \pi(x) dx \quad (5.49)$$

where we see that the target distribution is *invariant* under the application of the transition kernel. Thus if $p(x_n) = \pi(x)$ for some n , all subsequent points will have the desired distribution. The requirement that all starting points converge to the desired target distribution is known as *ergodicity* which guarantees both the uniqueness of the stationary distribution and that all points converge to this distribution. Ergodicity requires that the Markov chain is *irreducible*, i.e. all points with non-zero probability can be reached in a finite number of steps, and *aperiodic*, i.e. that no states can only be reached at certain periods of time. We will not delve into the specifics of ergodicity in depth, but note only that homogeneous Markov chains that satisfy (5.49) can be shown to be ergodic under very weak conditions, see for example Neal [1993]; Tierney [1994].

5.3.4.2 Detailed Balance

A common sufficient (but not necessary) condition used for constructing valid Markov chains is to ensure that the chain satisfies the condition of *detailed balance*. Chains that satisfy detailed balance are known as *reversible*.⁵ For a target $\pi(x)$ then detailed balanced is defined as

$$\pi(x)T(x' \leftarrow x) = \pi(x')T(x \leftarrow x'). \quad (5.50)$$

It is straightforward to see that Markov chains satisfying detailed balance will admit $\pi(x)$ as a stationary distribution by noting that

$$\pi(x') = \int_x T(x' \leftarrow x)\pi(x)dx = \pi(x') = \int_x T(x \leftarrow x')\pi(x')dx = \pi(x') \quad (5.51)$$

$$= \int_x p(x|x')\pi(x')dx = \pi(x') \int_x p(x|x')dx = \pi(x') \quad (5.52)$$

as required. Thus any Markov chain we construct that satisfies (5.50) will converge to the target distribution. From an inference perspective, this means that we can eventually generate samples according to our desired target by choosing an arbitrary start point X_1 and then repeated sampling from our transition kernel $T(X_n \leftarrow X_{n-1})$.

5.3.4.3 Metropolis Hastings

One of the simplest and most widely used MCMC methods is Metropolis Hastings (MH) Hastings [1970]. Given an unnormalized target $\gamma(x)$, the MH algorithm then at each iteration one samples a new point x' according to the proposal $x' \sim q(x'|x_n)$ conditioned on the current point x_n and then accepts the new sample with probability

$$P(\text{Accept}) = \min \left(1, \frac{\gamma(x')q(x_n|x')}{\gamma(x_n)q(x'|x_n)} \right). \quad (5.53)$$

At iteration n then we set $x_{n+1} \leftarrow x'$ if the sample is accepted and otherwise set $x_{n+1} \leftarrow x_n$. Critically this process does not require access to the normalized target $\pi(x)$. It is trivial to show

⁵An interesting area of current research is in the study of non-reversible MCMC algorithms Bouchard-Côté et al. [2015]; Bierkens et al. [2016]. These can be beneficial because traditional reversible processes are only able to move by drifting over time – generally at least half of the proposed samples (and generally much more) will be in a direction at odds to this drift. By forcing multiple steps in a particular direction before changing the direction can thus help the chain to mix faster.

that (5.53) satisfies detailed balance and therefore produces a valid Markov chain as follows

$$\begin{aligned}\pi(x_n)T(x_{n+1} \leftarrow x_n) &= \min\left(1, \frac{\gamma(x_{n+1})q(x_n|x_{n+1})}{\gamma(x_n)q(x_{n+1}|x_n)}\right) \pi(x_n)q(x_{n+1}|x_n) \\ &= \min(\gamma(x_n)q(x_{n+1}|x_n), \gamma(x_{n+1})q(x_n|x_{n+1})) / Z \\ &= \min\left(\frac{\gamma(x_n)q(x_{n+1}|x_n)}{\gamma(x')q(x_n|x_{n+1})}, 1\right) \pi(x_{n+1})q(x_n|x_{n+1}) \\ &= \pi(x_{n+1})T(x_n \leftarrow x_{n+1}),\end{aligned}$$

as required.

Though MH is valid for any reasonable choice of the proposal distribution, the practical performance will depend heavily on the choice of the proposal $q(x'|x)$. For example, if $q(x'|x)$ is independent of x then no information is passed from one iteration to the next and gives and one gets an algorithm that is strictly worse than importance sampling because samples are independently generated in the same way, but information is lost in the accept-reject step. Instead, one will generally want to propose points close to the current point so the advantages of *local moves* can be exploited. However, this has complications as explained in the next section, while choosing the a proposal with the right characteristics is still rather challenging. For example, image we use an isotropic Gaussian proposal, corresponding to a random walk without the accept reject step. If the variance of our proposal is too high then we will rarely propose good points and so the acceptance rate will become very low, giving few distinct samples. If the variance is too low, the Markov chain will move very slowly as it can only take small steps. This will increase correlation between all our samples and reduce the fidelity of our estimates. Chain that quickly cover the full probability space are said to *mix* quickly.

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5.3.4.4 Intuitions, Complications, and Practical Considerations

Though MCMC methods can be exceptionally effective, they are not without their weaknesses. Most of these weakness stem from the fact that all the generated samples are correlated, leading to, for example, biased estimates. Clearly this reduces the amount of distinct information conveyed by each sample and this will reduce the accuracy of the estimator. However, it also causes more fundamental issues. Most of the convergence results we have presented so far have relied on samples being generated in a i.i.d. fashion which is clearly not the case in the MCMC setting. MCMC methods therefore require their own unique convergence proofs, based in general on ergodic theory.

Add these, e.g. Birkhoff Ergodic Theorem, pointwise ergodic theorem. Probably worth its own section or at least a paragraph to talk about the requirements for ergodicity

These convergence results show that the bias of MCMC tends to zero as the number of iterations tends to infinity, but it is often very difficult to estimate the magnitude of the bias for finite numbers of iterations. Whereas importance sampling and rejection sampling had reasonable diagnostics for the performance of the inference, such as the effective sample size and the acceptance rate respectively, estimating the bias from MCMC samplers is typically fiendishly difficult and it can often look like an MCMC sampler is performing well (e.g. in terms of its acceptance rate) when in fact it is doing disastrously. One of the most common ways this is manifested is in the sampler becoming stuck in a particular mode of the target. If a target has more than a single mode then using localized proposals can make it prohibitively difficult to move between the modes. Though convergent MCMC samplers must eventually visit every mode infinitely often, it can take arbitrarily long to even visit each mode once. Even worse, getting the correct estimate relies on spending the correct relative proportion of time in each mode which will typically take many orders of magnitude more time to get a reasonable estimate for than just to have the sampler visit each significant mode at least once. The issues associated with multiple modes provides a demonstration of why it is difficult to estimate the bias of an MCMC sampler: we do not in general know or are even able to provide reasonable estimates for if we have missed another mode or whether our sampler has spent an appropriate amount of time in different modes.

Because of these drawbacks, MCMC is rarely used on multi-modal problems unless an appropriate mechanism for transitioning between the modes can be found. Thankfully, many problems become increasingly single-modal in high dimensions CITE SOMETHING and so there are a surprisingly wide array of models that actually fit these restrictions, particularly if we can find an appropriate parameterization of the model. Remembering from section 2.6 that changing the parameterization of a model changes its probability density function in a non-trivial manner, the performance of MCMC methods is often critically dependent on their parameterization. There are two effects at play here. Firstly changing the parameterization will change the concept of what parameter values are close to which other parameter values. In an ideal world we would make moves in the raw sample space where all points are equally probable before calculating the random variables from the position in sample space. Typically this is not practical, but it is still usually the case that some parameterizations will tend to be more

single-modal and more generally have all points of interest close together in the parameter space. Note that there is often an equivalence here between a good proposal, and a good warping of the space to one where an isotropic proposal will be effective.

Secondly, higher dimensional parameterizations are less likely to become stuck in a local mode. At a high level, the more variables that can be changed to some significant effect, the less likely that it is detrimental to change any one of the variables. In essence, projecting into a higher dimensional space provides more degrees of freedom for changes in the proposal and this helps to keep the Markov chain moving and to make distinct moves at each iteration. Though somewhat counter intuitive, projecting to higher dimensional spaces is key to a number of MCMC samplers performing effectively.

Unfortunately MCMC does not provide natural or unbiased estimates for the marginal likelihood in the same manner as importance sampling or rejection sampling ...

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5.3.4.5 Gibbs Sampling

Gibbs sampling is an important special case of Metropolis-Hastings that looks to update only some subset of variables in a joint distribution. Imagine we have target D distributional target distribution $\pi(\theta)$ where $\theta = \{\theta_1, \theta_2, \dots, \theta_D\}$. Gibbs sampling incrementally updates one or more of the variables θ_d at each iteration conditioned on the value of the others. Thus it uses proposals of the form $\theta'_d \sim \pi(\theta'_d | \theta \setminus \theta_d)$ with $\theta \setminus \theta_d$ kept constant from one iteration to the next. There are two reasons for wanting to do this. Firstly changing only of the variables at a time is a form of local proposal and can be a beneficial way to make updates, particularly if random walk proposal are inappropriate, for example because the variables are not continuous. Secondly, if we have access to $\pi(\theta_d | \theta \setminus \theta_d)$ exactly, then we will actually accept every sample as

$$\frac{\pi(\theta)\pi(\theta'_d|\theta \setminus \theta_d)}{\pi(\theta')\pi(\theta_d|\theta' \setminus \theta'_d)} = \frac{\pi(\theta_d|\theta \setminus \theta_d)\pi(\theta \setminus \theta_d)\pi(\theta'_d|\theta \setminus \theta_d)}{\pi(\theta'_d|\theta \setminus \theta_d)\pi(\theta \setminus \theta_d)\pi(\theta_d|\theta' \setminus \theta'_d)}$$

now noting that $\theta' \setminus \theta'_d = \theta \setminus \theta_d$

$$= \frac{\pi(\theta_d|\theta \setminus \theta_d)\pi(\theta \setminus \theta_d)\pi(\theta'_d|\theta \setminus \theta_d)}{\pi(\theta'_d|\theta \setminus \theta_d)\pi(\theta \setminus \theta_d)\pi(\theta_d|\theta \setminus \theta_d)} = 1.$$

In many models it will be possible to sample from $\theta'_d \sim \pi(\theta'_d | \theta \setminus \theta_d)$ exactly and thus carry out Gibbs sampling exactly. We can then cycle through each of the θ_d , either in a random order or in sequence, and apply the appropriate updates. The effectiveness of this approach will depend

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on the level of correlation between the different variables. The more correlated each variable: the smaller the updates will be for each variable conditioned on the values of the others and the slower the chain will mix. In extreme cases, this does impose stricter conditions for convergence for Gibbs samplers than MH [Roberts and Smith, 1994]. For example, consider an exclusive or style problem where $\pi(\theta_1, \theta_2) = 1$ if $0 \leq \theta_1 \leq 1$ and $0 \leq \theta_2 \leq 1$ or $-1 \leq \theta_1 < 0$ and $-1 \leq \theta_2 < 0$ and $\pi(\theta_1, \theta_2) = 0$ otherwise. Here there is no way to move from the $[0, 1]^2$ square to the $[-1, 0]^2$ by updating only one of the variables at a time. As such a Gibbs sampler would end up stuck in either the positive or negative square.

If it is not possible to sample from the conditional distributions exactly or if it is only possible for some of the variables, we can instead use a *Metropolis-within-Gibbs* approach, also known as *component-wise Metropolis-Hastings*, where we use a proposal to approximate one or more $\pi(\theta'_d | \theta \setminus \theta_d)$ with an appropriate proposal. Naturally this means that the acceptance ratio is no longer always 1 and so an accept-reject step becomes necessary. Though the convergence of this approach has been shown by Jones et al. [2014], additional assumptions are required compared to the standard Gibbs or MH cases.

5.3.4.6 Advanced MCMC Algorithms

[Write me](#)

- HMC and typical distance from mode in high dimensional Gaussian
- Slice sampling?
- Estimating the normalization constant

5.3.5 Proposal Adaptation

5.4 Alternatives to Monte Carlo Inference

6

Particle-Based Inference Methods

Particle-based inference methods (PBIM), such as sequential Monte Carlo (SMC) [Gordon et al., 1993; Doucet et al., 2001a] and particle Markov chain Monte Carlo (PMCMC) methods [Andrieu and Roberts, 2009; Rainforth et al., 2016c], are a powerful class of inference algorithms based on propagating populations of samples known as *particles*. By working with populations of samples, also known as *particle systems*, at the same time (rather than individual samples in turn) they allow information to be shared across the population and computational resources to be adaptively reallocated to where they are needed. A common feature of PBIMs is that they make use *intermediate information* available during the inference process and thereby exploit the structure of the problem. For example, SMC uses a series of intermediate target distributions which act a stepping stones to the full posterior. By using the information gathered from these intermediate solutions, they can better allocate computational resources for the next target and combat the curse of dimensionality. As such, PBIMs can be highly effective for problems with rich, exploitable, structures, for example time series models, but are generally less effective for problems that do not lend themselves to a series of intermediate targets.

6.1 Sequential Monte Carlo

6.1.1 Non-Markovian State-Space Models

Although SMC can be used for an arbitrary series of targets as we will explain in Section 6.1.4, we will mostly introduce it in the context of non-Markovian state-space models (NMSSMs). NMSSMs are probabilistic models over a set of latent variables $x_t \in \mathcal{X}_t$, $\forall t = 1 : T$ and observed variables $y_t \in \mathcal{Y}_t$, $\forall t = 1 : T$. They are similar to the HMM introduced in 3.3, but differ by not making the Markov assumption. This leads to the graphical model shown in

Figure 6.1. They are fully defined by an initial density $\mu(x_1)$, a series of transition densities $f_t(x_t|x_{1:t-1})$, and a series of emission densities $g_t(y_t|x_{1:t})$ as follows

$$x_1 \sim \mu(x_1), \quad (6.1a)$$

$$x_t|x_{1:t-1} \sim f_t(x_t|x_{1:t-1}), \quad (6.1b)$$

$$y_t|x_{1:t} \sim g_t(y_t|x_{1:t}). \quad (6.1c)$$

which gives a joint density of

$$p(x_{1:T}, y_{1:T}) = \mu(x_1) \prod_{t=2}^T f_t(x_t|x_{1:t-1}) \prod_{t=1}^T g_t(y_t|x_{1:t}) \quad (6.2)$$

and the standard relationship that this is proportional to the posterior $p(x_{1:T}|y_{1:T})$. Note the key self-similarity relationship: the intermediate posterior of the first t latent variables given the first t observations is

$$p(x_{1:t}|y_{1:t}) \propto \mu(x_1) \prod_{\tau=2}^t f_\tau(x_\tau|x_{1:\tau-1}) \prod_{\tau=1}^t g_\tau(y_\tau|x_{1:\tau}).$$

Perhaps surprisingly, this framework can be almost completely general if the x_t and y_t are allowed to take on arbitrary form. For example, if we set $T = 1$ then $x_1 = \theta$ are our variables, $y_1 = \mathcal{D}$ is our data, $\mu(x_1) = p(\theta)$ is our prior, and $g_1(y_1|x_1) = p(\mathcal{D}|\theta)$ is our likelihood. More generally, the initial density and transition densities form terms in the prior, while the emission densities are terms in the likelihood; all of which can take on arbitrary forms. It will often be the case that each “latent variable” is actually a collection of different variables and each “observed variable” is actually a collection of observations. What the NSMSSM formulation allows us to do is express known structure present in the problem: the earlier we are able to put our observations in the observation structure, and thus express their conditional independence from more of the latent variables, the more will be able to exploit this structure.

There are two common tasks that one wishes to carry out for NMSSMs: *filtering* and *smoothing*. Smoothing corresponds to the standard Bayesian inference task where we want to infer about the latent variables conditioned on all the observations. In filtering we care about the posterior given the observations so far $p(x_t|y_{1:t})$. Filtering is typically done in tasks such as tracking and signal processing where the inference is being done online and the main task is forward prediction. In other words, we do not know all the $y_{1:T}$ upfront but have a series of inference problems where we wish to predict y_{t+1}, y_{t+2}, \dots given the observations so far

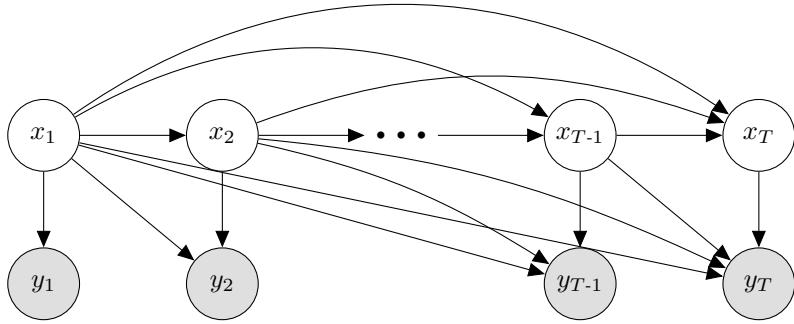


Figure 6.1: DAG for a non-Markovian state space model. Note there are all also multiple dependencies for the nodes summarized in the dots.

$y_{1:t}$. Our focus will be on smoothing, but we note that this is equivalent to the filtering distribution at the last step and so most of the ideas directly transfer.

If the model is in fact Markovian with Gaussian or discrete transition distributions and Gaussian emission distributions, then the solution can be calculated analytically using the *Rauch-Tung-Striebel* smoother [Rauch et al., 1965] and *forward-backward* algorithm [Rabiner and Juang, 1986] respectively. The former corresponds to the class of Kalman filter [Kalman et al., 1960] and Kalman smoother [Rauch et al., 1965] algorithms. These are often used as linear Gaussian approximation for Bayesian modeling dynamic of systems and are a good example of where approximations are often made in Bayesian approaches in the interest of tractability. SMC will allow us to perform inference in similar models, amongst many others, without requiring such assumptions to be made. Naturally this will come at the cost of having access to a closed-form solution.

6.1.2 Sequential Importance Sampling

In Section 5.3.2.2 we showed that importance sampling weights are multiplicative and thus to sample from a joint distribution, one can first importance sample from a marginal distribution and then importance sample from the respective conditional distribution, with the sample weight corresponding to the product of the two individual weights. More generally, one can carry out *sequential importance sampling* (SIS) to carry out inference on a series of target distributions $(\pi_t(x_{1:t}))_{t=1}^T$ of increasing spaces $\mathbb{X}_1, \dots, \mathbb{X}_T$ where each $\mathbb{X}_t = \mathcal{X}_1 \times \dots \times \mathcal{X}_t$ by first making an importance sampling approximation for $\pi(x_1)$ and sequentially update our approximation from $\pi_t(x_{1:t})$ to $\pi_{t+1}(x_{1:t+1})$ by doing importance sampling updates and taking the product of

Algorithm 2 Sequential Importance Sampling

Inputs: model $p(x_{1:T}, y_{1:T})$, data $y_{1:T}$, proposals q_1, \dots, q_T , number of samples N

Outputs: weighted samples $\{x_{1:T}^i, w_T^i\}_{i=1}^N$

```

1: for  $i = 1, \dots, N$  do
2:    $x_1^i \sim q_1(x_1)$ 
3:    $w_1^i = \frac{g_1(y_1|x_1^i)\mu(x_1^i)}{q_1(x_1^i)}$ 
4:   for  $t = 2$  to  $T$  do
5:      $x_t^i \sim q_t(x_t|x_{1:t-1}^i)$ 
6:     Set  $x_{1:t}^i = (x_{1:t-1}^i, x_t^i)$ 
7:      $w_t^i = w_{t-1}^i \frac{g_t(y_t|x_{1:t}^i)f_t(x_t^i|x_{1:t-1}^i)}{q_t(x_t^i|x_{1:t-1}^i)}$ 
8:   end for
9: end for

```

the weights. This is easiest to see in the NMSSM case were we will use the series of targets $p(x_{1:t}|y_{1:t})$ which we can do by first approximating $p(x_1|y_1)$ and then importance sampling each

$$p(x_t|x_{1:t-1}, y_{1:t}) = p(x_t|x_{1:t-1}, y_t) \propto f_t(x_t|x_{1:t-1})g_t(y_t|x_{1:t})$$

noting that x_t is independent of $y_{1:t-1}$ given $x_{1:t-1}$. Presuming a set of proposals $q_1(x_1), q_t(x_t|x_{1:t-1})$, we will calculate importance weights as follows

$$w_1(x_1) = \frac{\mu(x_1)g_t(y_1|x_1)}{q_1(x_1)} \quad (6.3a)$$

$$w_t(x_{1:t}) = w_{t-1}(x_{1:t-1}) \frac{g_t(y_t|x_{1:t})f_t(x_t|x_{1:t-1})}{q_t(x_t|x_{1:t-1})}. \quad (6.3b)$$

Once completed this will produce a set of weighted sample $\{\hat{x}_{1:T}, w_T(\hat{x}_{1:T})\}$ for $p(x_{1:T}|y_{1:T})$. A summary of the SIS process is given in Algorithm 2. Note we do not need the targets to be normalized because we can use self-normalized importance sampling as introduced in 5.3.2.1.

Because SIS produces are pure importance sampling estimate, it will share all the desirable properties of importance sampling introduced in Section 5.3.2, including the ability to use self-normalization. In fact, it is just a particular case of importance sampling because could have produced the same samples and weights by sampling $x_{1:T} \sim q_1(x_1) \prod_{t=2}^T q_t(x_t|x_{1:t-1})$ and then calculating the corresponding importance weight $w_T(x_{1:T})$ in one go. As such, SIS is on its own not very useful. Its utility is realized when it is combined with resampling as we describe next.

6.1.3 SMC for Non-Markovian State Space Models

Sequential Monte Carlo (SMC) [Gordon et al., 1993; Doucet et al., 2001b; Doucet and Johansen, 2009] , or particle filtering as it is sometimes known,¹ is a powerful and general purpose inference algorithm that has been successfully applied to a wide range of fields such as signal processing [Candy, 2016], econometrics [Creal, 2012], and probabilistic programming [Wood et al., 2014]. SMC builds on SIS by interleaving the sampling with resampling steps, the latter of which was introduced in Section 5.3.2.4. The key idea is to exploit the structure of a model by breaking down the overall inference problem into a series of target distributions which get incrementally closer to the distribution of interest. Transitioning from one intermediary distribution to the next typically forms a far simpler inference problem than directly approximating the original target. The critical difference to SIS is that the information gained from approximating these intermediary distributions is exploited by reallocating resources to areas likely to have high posterior mass in the final target distribution through resampling. The simplest, but most common form of SMC, which simply interleaves *propagating* samples from one target to the next and resampling the particle system, is sometimes known as *sequential importance resampling* and will be our main focus. A characterization of the method is shown in Figure 6.2.

To see the intuition of why resampling provides the desired resource reallocation, consider what happens to the relative weights of different particles in a population if they are propagated through the SIS algorithm at the same time. It is easy to see that these weights will quickly diverge, typically exponentially quickly in the number of time steps (see Section 5.3.3), and our effective sample size (see Section 5.3.2.3) will rapidly diminish. It is now rather pointless to continue to propagate the samples with negligible weight through the system as the chance these will have a significant weight by the end of sampling is very low. We therefore desire a principled way of “killing off” these low weight particles and replacing them with higher weight ones. As we showed in Section 5.3.2.4, resampling gives us a method for generating unweighted samples from a population of weighted samples. We explained that if these samples are just going to be used directly for estimation then this is strictly detrimental procedure. However, if we are going to use the samples as a starting point for further sampling this will no longer apply. This is because though resampling itself only duplicates existing particles, rather than producing

¹We avoid the name particle filtering as it often implies that one is only interested in the filtering distribution, whereas most of the tasks we are interested in will target the smoothing distribution.

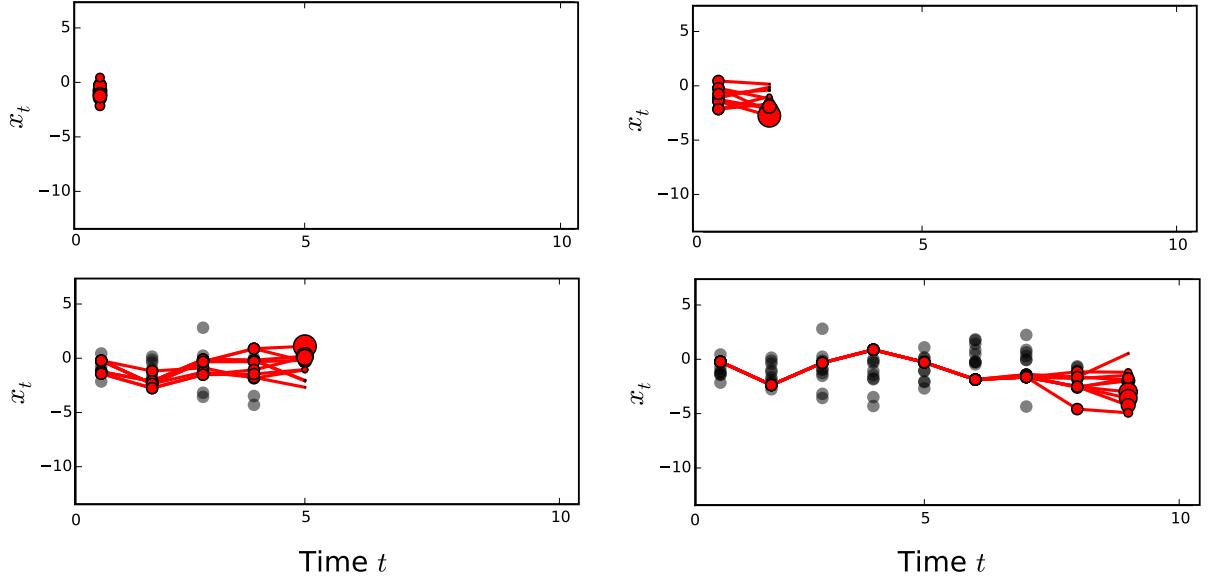


Figure 6.2: Characterization of the SMC method for a non-Markovian state space model. At the first time step (top left) we perform importance sampling to approximate $p(x_1|y_1)$ in the normal way, giving a particle system, or population of weighted samples $\{x_1^i, w_1^i\}_{i=1}^N$. Here each sample is shown by a red blob whose size reflects the weight of the particle. The set of particles are then resampled to produce an unweighted set of particles approximating $p(x_1|y_1)$. For each of these samples, importance sampling is then used again to produce samples for x_2 by sampling from $q_2(x_2|x_1)$ and applying a new importance weight (top right). Note that, unlike for SIS, the importance weights are not propagated from one time step to the next (see Algorithm 3). We now again have a weight particle set $\{x_{1:2}^i, w_2^i\}_{i=1}^N$, for which we again perform a resampling step to produce an unweighted set of particles. The process continues in the same way, eventually returning the final set of samples $\{x_{1:T}^i, \bar{w}_T^i\}_{i=1}^N$, where we have self-normalized the final weights. Note that over time, many of the generated samples are discarded by the system (shown in gray) during the resampling step. A consequence of this, which can be seen in the bottom right, is that many time steps, then our particle set become *degenerate*. Here we have multiple distinct samples for x_9 , but all our samples share the same *ancestors* for $t = 1 : 6$, i.e. each x_t^i in our final sample set is the same for $t \leq 6$. We will return to discuss this further in Section 6.2.3.

new ones, if the duplicate samples are extended independently at the next iteration, this produce distinct samples (albeit heavily correlated ones). In other words if we have two samples $x_{1:t}^1$ and $x_{1:t}^2$ such that $w_t^2/w_t^1 \approx 0$ then it is more beneficial for us to generate both samples at the next stage using $x_{t+1}^i \sim p(x_{t+1}|x_{1:t}^1, y_{1:t})$ for $i = 1, 2$ than to use $x_{1:t}^2$ to sample x_{t+1}^2 . This will not improve our representation of $x_{1:t}$, but it will, in general, give a better representation of the marginal distribution of x_{t+1} and the joint distribution $x_{1:t+1}$. Note that any of the resampling schemes introduced in Section 5.3.2.4 will give rise to valid SMC schemes and so one should, from a practical perspective, generally use systematic resampling.

To introduce the SMC method more formally, we consider approximating a sequence of target distributions in same way as for SIS: in our NMSSM case $p(x_{1:t}|y_{1:t}) = p(y_{1:t})^{-1}p(x_{1:t}, y_{1:t})$, $t =$

Algorithm 3 Sequential Monte Carlo(all for $i = 1, \dots, N$)**Inputs:** data $y_{1:T}$, number of particles N , proposals q_t

- 1: $x_1^i \sim q_1(x_1)$
- 2: $w_1^i = \frac{g_1(y_1|x_1^i)\mu(x_1^i)}{q_1(x_1^i)}$
- 3: **for** $t = 2$ **to** T **do**
- 4: $a_{t-1}^i \sim \text{DISCRETE} \left(\left\{ \bar{w}_{t-1}^\ell \right\}_{\ell=1}^N \right)$
- 5: $x_t^i \sim q_t(x_t|x_{1:t-1}^{a_{t-1}^i})$
- 6: Set $x_{1:t}^i = (x_{1:t-1}^{a_{t-1}^i}, x_t^i)$
- 7: $w_t^i = \frac{g_t(y_t|x_{1:t}^i)f_t(x_t^i|x_{1:t-1}^{a_{t-1}^i})}{q_t(x_t^i|x_{1:t-1}^{a_{t-1}^i})}$
- 8: **end for**

$1, \dots, T$. At each time step t we generate a particle system $\{x_{1:t}^i, w_t^i\}_{i=1}^N$ which provides a weighted approximation to $p(x_{1:t}|y_{1:t})$. Given such a weighted particle system, we convert this to an unweighted particle system by resampling as explained in Section 5.3.2.4. Any of the introduced resampling schemes can be used [Andrieu et al., 2010a, Section 4.1] and so in general one should use systematic resampling. When we later introduce PMCMC methods, it will be useful to think about this in terms of propagating particles each particle by drawing an ancestor variable a_{t-1}^i (as per (5.40)) and then using this to propose the new variable for that particle, i.e. $x_t^i \sim q_t(x_t|x_{1:t-1}^{a_{t-1}^i})$. The particle system is then re-weighted as

$$w_t^i = \frac{g_t(y_t|x_{1:t}^i)f_t(x_t^i|x_{1:t-1}^{a_{t-1}^i})}{q_t(x_t^i|x_{1:t-1}^{a_{t-1}^i})}, \quad (6.4)$$

where $x_{1:t}^i = (x_{1:t-1}^{a_{t-1}^i}, x_t^i)$. Note that after resampling, all the particles have the same weight and therefore, unlike for SIS, the weights at the previous step do not feature in the weights at the current time step. This results in a new particle system $\{x_{1:t}^i, w_t^i\}_{i=1}^N$ that approximates $p(x_{1:t}|y_{1:t})$ and the algorithm continues in a self-similar manner up to time T . The overall process is detailed in Algorithm 3. Once run, we can use our final, self-normalized, particle set $\{x_{1:T}^i, \bar{w}_T^i\}_{i=1}^N$ as a Monte Carlo estimator in the same manner as self-normalized importance sampling:

$$\mathbb{E}_{\pi(x_{1:T})} [f(x_{1:T})] \approx \frac{1}{N} \sum_{i=1}^N \bar{w}_T^i f(x_{1:T}^i). \quad (6.5)$$

Many intuitions from importance sampling transfer over to SMC. For example, we can construct our posterior estimate and calculate expectations in the same way, while we can also

use the effective sample size as a metric of performance (remembering to combine). One of the most important features that translates is that SMC produces the unbiased estimate for the marginal likelihood $p(y_{1:T})$

$$\hat{Z} = \prod_{t=1}^T \frac{1}{N} \sum_{i=1}^N w_t^i. \quad (6.6)$$

as first shown by Del Moral [2004]. Although this original proof requires advanced techniques we will not touch on here, we will later show that this results can also be shown as a consequence of the proof of correctness for the particle independent Metropolis-Hastings method given in Section 6.2.1. Note that although the marginal likelihood estimate is unbiased, the estimator for an general expectation given by (6.5) is biased in the same way as the self-normalized importance sampling estimator given in (5.32) is. Nonetheless, producing unbiased estimates of the marginal likelihood has numerous significant advantages.

Firstly, it means that one can combine results from different SMC runs and still have a consistent estimator for the target and a both unbiased and consistent estimate for the marginal likelihood. This is particularly important as the number of particles N , is typically restricted by the availability of memory and we often want to run more than one *SMC sweep* (i.e. a single run of SMC). To combine our estimates, one simply weights each sample by the marginal likelihood of its sweep times its local, self-normalized, weight \bar{w}_T^i , giving the estimator

$$\mathbb{E}_{\pi(x_{1:T})} [f(x_{1:T})] \approx \frac{1}{RN} \sum_{r=1}^R \sum_{i=1}^N \hat{Z}[r] \bar{w}_T^i[r] f(x_{1:T}^i[r]). \quad (6.7)$$

where the notation $[r]$ is used to indicates samples from sweep r . The ability to do this is known as *proper weighting* [Naesseth et al., 2015a] and we can justify it by thinking in terms of using a proposal that first samples a full particle set, giving importance weight \hat{Z} , and then sampling a particle from this set, giving importance weight \bar{w}_T^i . The product of these separate weights thus gives the weight of each sample.

Secondly, the unbiased marginal likelihood estimate means that we can *nest* SMC within other methods as a unbiased estimate of the likelihood. Methods that make use of such unbiased likelihood estimates are known as pseudo-marginal methods [Andrieu and Roberts, 2009; Andrieu et al., 2015; Naesseth et al., 2015a] and we will discuss them further in Chapter 10, proving the validity of many pseudo-marginal methods on the basis that they form a special case of Theorem 10.2. We note that some PMCMC methods can be interpreted as pseudo-marginal methods.

6.1.4 Sequential Monte Carlo for an Arbitrary Series of Targets

In its most general form, we can use SMC to target an arbitrary series of unnormalized target distributions $\{\gamma_t(x_{1:t})\}_{t=1:T}$, $\gamma_t(x_{1:t}) = Z_t \pi_t(x_{1:t})$ each defined on a space \mathbb{X}_t with strictly increasing dimension² $\dim(\mathbb{X}_{t-1}) < \dim(\mathbb{X}_t)$. Here $Z_t := \int \gamma_t(x_{1:t}) dx_{1:t}$ is the normalization constant and $\pi_t(x_{1:t})$ the corresponding normalized target. The only difference that needs to be made from the NMSSM case is in how the weights are calculated, with them now given by

$$w_1^k = \frac{\gamma_1(x_1^k)}{q_1(x_1^k)} \quad (6.8a)$$

$$w_t^k = \frac{\gamma_t(x_{1:t}^k)}{\gamma_{t-1}(x_{1:t-1}^{a_{t-1}^k}) q_t(x_t^i | x_{1:t-1}^{a_{t-1}^i})}. \quad (6.8b)$$

It can be easily seen that the NMSSM weights are a particular case of this, by plugging in $\gamma_t(x_{1:t}) = p(x_{1:t}, y_{1:t})$ into the above expression.

For posterior inference, then our posterior is the last target, $\pi_T(x_{1:T})$, with corresponding marginal likelihood Z_T . Using this more general SMC formulation, we thus see that any series of targets will lead to a valid inference provided that the final target is the desired posterior and that none of our intermediate targets place zero probability mass on events that have non-zero probability mass under the corresponding marginals of the final target

$$\tilde{\pi}_t(x_{1:t}) = \int_{X_T \setminus X_t} \pi_T(x_{1:T}) dx_{t+1:T} \quad (6.9)$$

$\neq \pi_t(x_{1:t})$ in general. In fact, the series of targets given for the NMSSM case are actually sub-optimal and used because of the fact that $p(x_{1:t}, y_{1:t})$ can, in general, be calculated exactly. It is a well known result (see, for example, the appendices of Le et al. [2017c]) that the optimal series of proposals (complications with computability and proposals aside) is actually the marginals $\tilde{\pi}_t(x_{1:t}) = p(x_{1:t} | y_{1:T})$ for the NMSSM case. To see this, note that at the t^{th} step, we are generating the samples for x_t and that if each of targets is the marginal distribution then the marginal probability of the already sampled variables does not change from one iteration to the next. Conversely, if a different series of targets are used, e.g. $p(x_{1:t} | y_{1:t})$, then the relative marginal probability of already sampled variables changes from one iteration to the next and so we have been wasteful by targeting a different distribution at the previous step. To give an example of this, consider the case where x_1 include global parameters that effect

²This restriction can be avoided by using the SMC samplers approach of Del Moral et al. [2006].

each emission distribution (i.e. likelihood term), for example it could contain the variance for Gaussian likelihood terms. In our NMSSM case we can never regenerate samples for x_1 after the first step and so it is clearly better to at the first step to target $p(x_1|y_{1:T})$ than $p(x_1|y_1)$, i.e. to condition on all the data rather than the first datapoint. Unfortunately, calculating $p(x_1|y_{1:T})$ itself generally requires a marginalization that is as difficult, or potentially even more difficult, than the inference itself. Hence the series of targets we introduced in the NMSSM formulation are those that are usually used in practice. However, we note though that there are some innovative methods for partially alleviating this problem, such as block sampling Doucet et al. [2006], that use a combination of lookahead and *auxiliary weighting* schemes Cappé et al. [2007]. Specifically, they resample using adjusted weights that convey how good the sample is likely to be a few time steps further down the line. The bias this would induce is corrected for by assigning non-even weights to the resampled particles.

Another upshot of the ability to use an arbitrary series of targets is that we can use SMC in lots of scenarios that do not permit a conventional breakdown of the target distribution, but where we can provide guiding distributions to that which we care about. One possible case is when our prior distribution is a generative model that can be evaluated on the target dataset at point in generative process. For example, in Janz et al. [2016], we considered the example of doing inference on the structure of a GP kernel. Here we can define a generative model that produces increasingly kernels, such that all the intermediary kernels in this generation process are themselves valid kernels that can thus be evaluated. Here we can think of expanding our kernel at each time step of the SMC inference and our targets as being the posterior on kernel structure for the GP, subject to increasingly lax restrictions on the kernel complexity.³ Another example is provided by Lakshminarayanan et al. [2013] who use SMC for Bayesian learning of decision trees. Here they use the self-similarity of trees, starting with a basic stump and then adding a new split at each time step. For both these problems, SMC has been used to exploit the fact that the overall problem can be broken down into a series of increasingly difficult problems, namely those with an increasingly large prior, to guide towards good solutions for the final problem.

³Technically in this work actually uses population Monte Carlo Cappé et al. [2004] which is based on using a series of static targets. The intuition, however, predominantly transfers and SMC could have been used instead.

6.1.5 Practical Considerations

6.1.5.1 Use as Many Particles as Possible

The most important practical consideration for SMC, and in most cases for PMCMC methods also, is to *use as many particles as possible*. Although, as we showed in 6.1.1, one can run multiple, say R , SMC sweeps and then combine them using their marginal likelihood estimates, this is almost exclusively a higher variance (and more skew) estimator than carrying out a single SMC sweep with RN particles and often many orders of magnitude so. It is easy to see why a single sweep is preferable from the point of view of the effect of the different marginal likelihood estimates on the effective sample size. The reason the number of particles can be so critical is that if it is too small, the variance of the marginal likelihood estimate explodes and one sweep ends up dominating the estimate. Though the marginal likelihood estimate is unbiased, it has a massive positive skew when insufficient particles are used, such that the probability that a sweep gives a marginal likelihood estimate larger than the true marginal likelihood estimate can be arbitrarily small, after all, the limit $N = 1$ corresponds to importance sampling. As such, if we use insufficient particles and just repeatedly run SMC sweeps, we may have to wait arbitrarily long before getting any useful samples. One way to try and combat this, presuming it is not possible to increase N , is to group the SMC sweeps into a number of islands and then combined estimates in the normal way within the islands, but combined the islands in an unweighted fashion (see for example Lakshminarayanan et al. [2013]). Though often practically useful, this is clearly only trading variance for bias and thus is more of a means of mitigating rather than solving the problem. A more principled means of overcoming this issue is presented by PMCMC methods as discussed later in the Chapter.

6.1.5.2 Adaptive Resampling

Another important practical consideration to note is that it is not always beneficial to resample. Resampling obviously throws away information (by reducing the number of distinct particles) and therefore should not be done spuriously. As the reason for doing resampling is to kill off particles with negligible weight, it is generally preferable to avoid the resampling step when most particles have significant weight. This leads to the development of so-called *adaptive resampling* schemes [Liu and Chen, 1995; Del Moral et al., 2012] that only perform the resampling step if some criterion is met. When the resampling is omitted, the particles remain unweighted, with

their weights at the next iteration updated using (6.3), as per SIS, except that the self normalized weights \bar{w}_t^i should be used so that the marginal likelihood estimate can be carried out in the same manner. That this still informally forms a valid SMC algorithm for posterior inference can be seen by thinking of these as being sequential importance sampling steps, noting the equivalence to standard importance sampling, and then viewing the process as simply skipping some of the intermediate targets, remembering that it is only the final target that we care about. However, it does cause some complications from a theoretical perspective [Del Moral et al., 2012]. A common form for the resampling criteria is to only resample if the effective sample size falls below a certain threshold, for which $N/2$ is a common choice Doucet and Johansen [2009].

6.1.5.3 Proposals

The practical performance os SMC can be critically dependent on the choice of proposal and so we finish our introduction by considering what constitutes a good proposal. We first consider the question of what the theoretically optimal proposal is. Unfortunately it is not generally possible to establish the optimal proposal for the variance of the final estimate in the finite N case, but we can calculate the so-called *one-step optimal proposal* by minimizing the variance of the individual weights (and by proxy the marginal likelihood estimate) at the next iteration. The one-step optimal proposal is given by

$$q_t^*(x_t|x_{1:t-1}) \propto \frac{\gamma_t(x_{1:t})}{\gamma_{t-1}(x_{1:t-1})} \quad (6.10)$$

$= f_t(x_t|x_{1:t-1})g_t(y_t|x_{1:t})$ for the NMSSM formulation. To see why this is optimal we note that by substituting (6.10) into (6.8) (noting that the proposal needs to be correctly normalized) we get weights of

$$w_t(x_{1:t}) = \int_{\mathcal{X}_t} \frac{\gamma_t(x_{1:t})}{\gamma_{t-1}(x_{1:t-1})} dx_t \quad (6.11)$$

$= p(y_t|x_{1:t-1})$ for the NMSSM formulation. Consequently, the weights in the this case are no longer functions of the sampled value and so the marginal likelihood and effective sample size are deterministic functions of the particle system before proposing the x_t , namely of $\{x_{1:t-1}^i, a_{t-1}^i\}_{i=1}^N$. This also means that we can switch the order of sampling from the proposal and doing the resampling when using $q_t^*(x_t|x_{1:t-1})$, which is preferable as it increases the diversity in the final sample set. Note that the weights are not all the same when using the

one-step optimal proposal, because the marginal probability of the particles will change when we incorporate the new observation (or equivalently move to the new target). However, given the expected value of each weight is fixed, i.e. $\mathbb{E}[w_t(x_{1:t})|x_{1:t-1}] = \int_{\mathcal{X}_t} \frac{\gamma_t(x_{1:t})}{\gamma_{t-1}(x_{1:t-1})} dx_t$ regardless of the proposal used, using any proposal other than the optimal one-step proposal only increases the variance of the estimate at the next step. In particular, it is generally not beneficial to use proposals that include some form of lookahead (e.g. approximating $p(x_t|x_{1:t-1}, y_{1:T})$ instead of $p(x_t|x_{1:t-1}, y_{1:t})$) because the resampling step will correct back to the current target and most likely kill off the “good” samples we generated, simply giving us few distinct samples than if we had used the one-step optimal proposal instead.⁴ In both the case where the optimal series of targets (6.9) is used and in the large N case then the *one-step optimal proposal* is optimal more generally for the whole SMC sweep. However, because it is not usually possible to analytically calculate the required normalization for $q_t^*(x_t|x_{1:t-1})$, it is not generally tractable. Nonetheless, it provides a good guide for designing, or adapting for, effective proposal distributions.

Another proposal of note, at least for the state space model case, is the so-called bootstrap proposal which corresponds to sampling from the transition distribution $f_t(x_t|x_{1:t-1})$. The significance of this proposal is that it means that the weight calculation given in (6.4) cancel to

$$w_t^i = g_t(y_t|x_{1:t}^i). \quad (6.12)$$

Consequently, if we use the bootstrap proposal we no need to be able to evaluate the transition distribution at a particular point, only sample from it. Obviously this can be helpful for computational reasons (though it is rare that the effect of this outweighs using a better proposal if one is known), but it is also important because it can be the case that one only has access to a sampler for the transition and not the ability to evaluate the transition probability at an arbitrary point, e.g. when our sampler takes the form of a stochastic simulator. In the absence of other information, the transition can also be a reasonable choice of proposal in its own right as it is almost always more diffuse the one step posterior. Its efficiency will in general depend on how relatively peaked the emission distribution is and the dimensionality of x_t – after all, each step in SMC is in isolation importance sampling. One can usually beneficially use the next observation y_t to help guide the the proposal, but doing this in a general purpose manner can be challenging [Gu et al., 2015].

⁴Note that lookahead in the proposal is distinct from lookahead using auxiliary weights, thus things like block sampling are still useful.

6.2 Particle Markov Chain Monte Carlo Methods

Particle Markov chain Monte Carlo (PMCMC) methods, introduced by Andrieu et al. [2010b], make use of sequential Monte Carlo (SMC) algorithms [Gordon et al., 1993; Doucet et al., 2001b] to construct efficient proposals for an MCMC sampler. This allows them to both utilize the ability of SMC to exploit the structure of the target problem and the hill climbing behavior of MCMC methods. The critical difference from running independent SMC sweeps is that information can be transferred from sweep to the next. Naturally this will come with the drawbacks of MCMC samplers discussed in Section 5.3.4, in particular the loss of unbiasedness or marginal likelihood estimates. However, the advantages will generally outweigh these drawbacks. PMCMC methods will also allow us to explicitly treat global parameters of our system differently to the latent states in a manner that can substantially improve the performance of the model. Though PMCMC can be applied to models with arbitrary series of targets in the same manner as SMC, we will stick to the NMSSM case in this section for notational simplicity.

6.2.1 Particle Independent Metropolis Hastings

Particle independent Metropolis Hastings (PIMH) is the simplest PMCMC algorithm. Although in isolation it is not especially useful (as it strictly worse than running independent SMC sweeps and combining them),⁵ it is an important theoretical stepping stone to more advanced approaches. The idea from a practical perspective is very simple: use an SMC sweep as an independent proposal for an MCMC algorithm targeting $\pi(x_{1:T}) = p(x_{1:T}|y_{1:T})$. From a theoretical perspective, the approach is rather more profound as it can be viewed as a sampler on an *extended space* whose marginal on the returned particles is the target.

The PIMH algorithm is described in Algorithm 4. We see that PIMH is an MCMC algorithm where our proposal involves running an independent SMC sweep and then sampling one of the particles from this set in proportion to the weight of the particle. This sample is then accepted or rejected using a MH accept-reject step that uses the marginal likelihoods of the sweep. To be more precise, let $\xi := \{x_t^i\}_{\substack{i=1:N \\ t=1:T}} \cup \{a_t^i\}_{\substack{i=1:N \\ t=1:T-1}}$ denote all generated particles and ancestor variables of a SMC sampler, and let the associated marginal likelihood estimate be denoted as

⁵There is, though, utility in doing this when also including MCMC steps on global parameters, see Andrieu et al. [2010a].

Algorithm 4 Particle Independent Metropolis Hastings

Inputs: SMC sampler, number of MCMC iterations R, initial output particle $\mathbf{x}'[0]$ and marginal likelihood $\mathbf{Z}'[0]$ (typically both generated from an SMC sweep)

Outputs: MCMC samples $\{\mathbf{x}'[r]\}_{r=1}^R$ where each $\mathbf{x}'[r] \in \mathbb{X}_T$

```

1: for  $r = 1 : R$  do
2:   Run SMC giving candidate  $X_{1:T} = \{x_{1:T}^i, \bar{w}_T^i\}_{i=1}^N$  and  $\hat{Z}$ 
3:   if  $u \leq \min(1, \hat{Z}/\mathbf{Z}'[r-1])$  where  $u \sim \text{UNIFORM}(0, 1)$  then
4:     Sample output particle index  $b$  in proportion to weights as per (6.13)
5:      $\mathbf{x}'[r] \leftarrow x_{1:T}^b$     $\mathbf{Z}'[r] \leftarrow \hat{Z}$                                            ▷ New sweep accepted
6:   else
7:      $\mathbf{x}'[r] \leftarrow \mathbf{x}'[r-1]$ ,    $\mathbf{Z}'[r] \leftarrow \mathbf{Z}'[r-1]$                                                    ▷ New sweep rejected
8:   end if
9: end for

```

\hat{Z} which is calculated as per (6.6). Let $\mathbf{x}^i = x_{1:T,m}^i$ denote one of the final particles and let the index of the final particle we sample be denote as b we is sampled according to

$$b \sim \text{DISCRETE} \left(\left\{ \bar{w}_T^\ell \right\}_{\ell=1}^N \right). \quad (6.13)$$

Sampling a particle also indicates an ancestral path which we denote as $\mathbf{b} = (\beta_1, \dots, \beta_T)$, with $\beta_T = b$ and $\beta_t = a_t^{\beta_{t+1}}$. The result of running a SMC sweep and sampling b thus proposes a $\{\mathbf{x}^b, \mathbf{b}\}$, though in the context of PIMH we only care about the particle \mathbf{x}^b . Given this proposal, the acceptance ratio used for PIMH is given by the ratio of the marginal likelihood estimates for the current point and the SMC used to propose the candidate particle. If we denote the MCMC particle sample at iteration r as $\mathbf{x}'[r]$ and associated marginal likelihood as $\mathbf{Z}'[r]$, then our proposed sample $\{\mathbf{x}^b, \hat{Z}\}$ is accepted with probability

$$P(\text{Accept}) = \min \left(1, \frac{\hat{Z}}{\mathbf{Z}'[r-1]} \right) \quad (6.14)$$

forming a MH sampler. Given our MCMC samples, the resulting Monte Carlo estimator is defined in normal way as

$$\mathbb{E}_{\pi(x_{1:T})} [f(x_{1:T})] \approx \frac{1}{R} \sum_{r=1}^R f(\mathbf{x}'[r]) \quad (6.15)$$

Because our proposal is independent of our current point, this is strictly worse than just running independent SMC sweeps (which can also be thought of as applying waste recycling to PIMH [Frenkel, 2006]). It might seem particularly wasteful to only use one particle from each sweep,

but we will be able to use Rao-Blackwellize to justify returning all the particles at each step as we explain in Section 6.2.5.

The key component of proving the correctness of the PIMH algorithm is in showing that it is a valid MH sampler on an extended target whose marginal is the distribution of interest. The density of the distribution induced by running a SMC sweep is given by

$$q_{\text{SMC}}(\xi) = \prod_{i=1}^N q_1(x_1^i) \cdot \prod_{t=2}^T \prod_{i=1}^N \left[\bar{w}_{t-1}^{a_{t-1}^i} q_t(x_t^i | x_{1:t-1}^{a_{t-1}^i}) \right] \quad (6.16)$$

and the distribution induced by running an SMC sweep and then sampling particle b from the sample set is

$$q_{\text{PIMH}}(\xi, b) = \bar{w}_T^b q_{\text{SMC}}(\xi) \quad \text{where} \quad \bar{w}_t^i = \frac{w_t^i}{\sum_{\ell=1}^N w_t^\ell}. \quad (6.17)$$

The proof for the validity of the PIMH algorithm is now demonstrated by showing that it is a valid MH sampler for an *extended target distribution* whose marginal distribution on \mathbf{x}^b is the distribution of interest $\pi(\mathbf{x}^b)$. To construct our extended target distribution, we consider the following hypothetical sampling process

1. Sample a particle exactly from the target $\mathbf{x}^b \sim \pi(\mathbf{x}^b)$,
2. Sample an ancestral path for the retained particle uniformly at random by independently sampling each $\beta_t \sim \text{UNIFORMDISCRETE}(1, N)$ and setting $\mathbf{b} = (\beta_1, \dots, \beta_T)$,
3. Sample all of the other particles and ancestor indices conditioned on $\{\mathbf{x}^b, \mathbf{b}\}$ using

$$q_{\text{CSMC}}\left(\xi \setminus \{\mathbf{x}^b, \mathbf{b}\} \mid \mathbf{x}^b, \mathbf{b}\right) = \prod_{\substack{i=1 \\ i \neq b_1}}^N q_1(x_1^i) \cdot \prod_{t=2}^T \prod_{\substack{i=1 \\ i \neq b_t}}^N \left[\bar{w}_{t-1}^{a_{t-1}^i} q_t(x_t^i | x_{1:t-1}^{a_{t-1}^i}) \right], \quad (6.18)$$

which corresponds to $q_{\text{SMC}}(\xi)$ as per (6.16) except for having one particle and path, $\{\mathbf{x}^b, \mathbf{b}\}$, already predefined.

We can informally think of this as doing the PIMH process in reverse. Rather than running an SMC sweep and sample one of the produced particles to produce $\{\mathbf{x}^b, \mathbf{b}\}$, we first sample the $\{\mathbf{x}^b, \mathbf{b}\}$ and then the rest of the variables in the SMC sweep conditioned on this particle and accompanying ancestral path. Together these steps induce the distribution

$$\tilde{\pi}(\xi, b) = \frac{\pi(\mathbf{x}^b)}{N^T} \prod_{i=1, i \neq b_1}^N q_1(x_1^i) \cdot \prod_{t=2}^T \prod_{i=1, i \neq b_t}^N \left[\bar{w}_{t-1}^{a_{t-1}^i} q_t(x_t^i | x_{1:t-1}^{a_{t-1}^i}) \right] \quad (6.19)$$

remembering that as ξ includes all the particles and ancestral paths, sampling ξ and choosing one particle b implies a particular $\{\mathbf{x}^b, \mathbf{b}\}$. By construction, the marginal of this distribution is $\pi(\mathbf{x}^b)$. Therefore, although it is not possible to actually sample from $\tilde{\pi}(\xi, b)$ directly (we started the definition by sampling exactly from the distribution of interest), if we can construct a consistent MCMC estimator on (6.19) then this by proxy produces a consistent estimator for $\pi(\mathbf{x}^b)$. We can now show that this is exactly what the PIMH algorithm does by explicitly calculating the importance weight implied by targeting $\tilde{\pi}(\xi, b)$ using the proposal $q_{\text{PIMH}}(\xi, b)$

$$\frac{\tilde{\pi}(\xi, b)}{q_{\text{PIMH}}(\xi, b)} = \frac{\pi(\mathbf{x}^b) q_{\text{CSMC}}(\xi \setminus \{\mathbf{x}^b, \mathbf{b}\} \mid \mathbf{x}^b, \mathbf{b})}{N^T \bar{w}_T^b q_{\text{SMC}}(\xi)} \quad (6.20)$$

$$\begin{aligned} &= \frac{\pi(\mathbf{x}^b)}{N^T \bar{w}_T^b q_1(x_1^{\beta_1}) \prod_{t=2}^T \bar{w}_{t-1}^{\beta_{t-1}} q_t(x_t^{\beta_t} \mid x_{t-1}^{\beta_{t-1}})} \\ &= \left(\frac{\gamma(\mathbf{x}^b)/Z}{q_1(x_1^{\beta_1}) \prod_{t=2}^T q_t(x_t^{\beta_t} \mid x_{t-1}^{\beta_{t-1}})} \right) \cdot \left(\frac{1}{N^T \bar{w}_T^b \prod_{t=2}^T \bar{w}_{t-1}^{\beta_{t-1}}} \right) \\ &= \left(\frac{w_T^b}{Z} \prod_{t=2}^T w_{t-1}^{\beta_{t-1}} \right) \cdot \left(\frac{1}{N^T \bar{w}_T^b \prod_{t=2}^T \bar{w}_{t-1}^{\beta_{t-1}}} \right) \\ &= \left(\frac{w_T^b}{Z} \prod_{t=2}^T w_{t-1}^{\beta_{t-1}} \right) \cdot \left(\frac{\prod_{t=1}^T \frac{1}{N} \sum_{\ell=1}^N w_t^\ell}{w_T^b \prod_{t=2}^T w_{t-1}^{\beta_{t-1}}} \right) \\ &= \frac{1}{Z} \prod_{t=1}^T \frac{1}{N} \sum_{\ell=1}^N w_t^\ell = \frac{\hat{Z}}{Z}. \end{aligned} \quad (6.21)$$

We thus have that \hat{Z} is the importance weight for sampling the unnormalized version of the target $\tilde{\gamma}(\xi, b) = Z \tilde{\pi}(\xi, b)$ and so using the ratio of marginal likelihood estimates provides is exactly the acceptance ratio required for the MH sampler. We have therefore proven that the PIMH algorithm induces a convergent Markov chain for the target $\pi(x_{1:T})$ and therefore our estimator given in (6.15) is consistent. Note that as an aside, this also shows the unbiasedness of the SMC marginal likelihood estimate as we see that

$$\mathbb{E}_{q_{\text{SMC}}(\xi)} [\hat{Z}] = \mathbb{E}_{q_{\text{PIMH}}(\xi, b)} [\hat{Z}] = \mathbb{E}_{\tilde{\pi}(\xi, b)} [Z] = Z. \quad (6.22)$$

6.2.2 Particle Gibbs

One particularly widely used PMCMC algorithm is particle Gibbs (PG). The PG algorithm modifies the SMC step in the PMCMC algorithm to sample the latent variables conditioned on an existing particle trajectory, resulting in what is called a conditional sequential Monte Carlo (CSMC) step. The PG method was first introduced as an efficient Gibbs sampler for

Algorithm 5 Conditional sequential Monte Carlo

Inputs: data $y_{1:T}$, number of particles N , proposals q_t , conditional trajectory $x'_{1:T}$

- 1: $x_1^i \sim q_1(x_1)$, $i = 1, \dots, N - 1$ and set $x_1^N = x'_1$
 - 2: $w_1^i = \frac{g_1(y_1|x_1^i)\mu(x_1^i)}{q_1(x_1^i)}$, $i = 1, \dots, N$
 - 3: **for** $t = 2$ **to** T **do**
 - 4: $a_{t-1}^i \sim \text{DISCRETE} \left(\left\{ \bar{w}_{t-1}^\ell \right\}_{\ell=1}^N \right)$, $i = 1, \dots, N - 1$
 - 5: $x_t^i \sim q_t(x_t|x_{1:t-1}^{a_{t-1}^i})$, $i = 1, \dots, N - 1$
 - 6: Set $a_{t-1}^N = N$ and $x_t^N = x'_t$
 - 7: Set $x_{1:t}^i = (x_{1:t-1}^{a_{t-1}^i}, x_t^i)$, $i = 1, \dots, N$
 - 8: $w_t^i = \frac{g_t(y_t|x_{1:t}^i)f_t(x_t^i|x_{1:t-1}^{a_{t-1}^i})}{q_t(x_t^i|x_{1:t-1}^{a_{t-1}^i})}$, $i = 1, \dots, N$
 - 9: **end for**
-

latent variable models with static parameters [Andrieu et al., 2010b]. Since then, the PG algorithm and the extension by Lindsten et al. [2014] have found numerous applications in e.g. Bayesian non-parametrics [Valera et al., 2015; Tripuraneni et al., 2015], probabilistic programming [Wood et al., 2014; van de Meent et al., 2015] and graphical models [Everitt, 2012; Naesseth et al., 2014, 2015b].

The PG algorithm targets the same extended target $\tilde{\pi}(\xi, b)$ as the PIMH algorithm defined in (6.19), but rather than constructing a MH sampler with independent proposals for this target, it constructs a Gibbs sampler. This is done by iteratively running *conditional* sequential Monte Carlo (CSMC) sweeps. As described in Algorithm 5, a CSMC sweep is similar to a standard, unconditional SMC sweep, except that it starts with an existing *conditional trajectory* $x'_{1:T}$, known as a *retained particle* in the PG context, and runs the sweep conditioned on this conditional trajectory being present in the final sample set. One can think of this as running a SMC sweep conditioned on the predefined particle surviving each of the resampling steps. In other words, the other particles can sample the retained particle as an ancestor but not vice versa, with the values and ancestral path of the retained particle prefixed. Note that running Algorithm 5 corresponds to simulating from q_{CSMC} using a fixed choice for the index variables $b = (N, \dots, N)$. While these indices are used to facilitate the proof of validity of the proposed method, they have no practical relevance (all path are marginally equivalent by symmetry) and can thus be set to arbitrary values, as is done in Algorithm 5, in a practical implementation.

Unlike SMC sweeps, CSMC sweeps can be linked together by conditioning each sweep using a retained particle sampled from the previous sweep with probability proportional to the

final particle weights \bar{w}_T^i . Therefore, once initialized, say using a standard SMC sweep, one can iterate between sampling a retained particle in the same manner ancestor indices are sampled and running CSMC sweeps conditioned on this retained particle. Considerations about global parameters aside (see Section 6.2.4), this is known as iterated CSMC and constitutes the PG algorithm. A characterization is provided in INSERT. Note that the resampling step must always be done for CSMC sweeps (i.e. the techniques introduced in Section 6.1.5.2 cannot be used) as unlike in an SMC sweep, the resampling for a CSMC sweep does not maintain the target distribution. Similarly one cannot do a gratuitous resampling step at the end of a CSMC sweep. to produce unweighted samples as is sometimes done for SMC. Another important difference is that, unlike SMC, a CSMC sweep does not provide an unbiased estimate for the marginal likelihood (expect in the limit $N \rightarrow \infty$).

Add PG characterization figure.

The theoretical justification for the PG algorithm can be shown in a similar manner as the PIMH algorithm. The sampled index b now corresponds the index of the retained particle and we can think of the approach as alternating between Gibbs updates on b and $\xi \setminus \{\mathbf{x}^b, \mathbf{b}\}$. In other words, we alternate between sampling

$$b \sim \tilde{\pi}(b|\xi) = \frac{\tilde{\pi}(\xi, b)}{\int \tilde{\pi}(\xi, b) d\xi} \quad (6.23a)$$

$$\xi \setminus \{\mathbf{x}^b, \mathbf{b}\} \sim \tilde{\pi}(\xi \setminus \{\mathbf{x}^b, \mathbf{b}\} | \mathbf{x}^b, \mathbf{b}) = \frac{\tilde{\pi}(\xi, b)}{\int \int \tilde{\pi}(\xi, b) d\mathbf{x}^b d\mathbf{b}}. \quad (6.23b)$$

The key step to seeing that the PG algorithm samples from these distributions is noting that (6.18) corresponds to the distribution induced by running a CSMC sweep with retained particle $\{\mathbf{x}^b, \mathbf{b}\}$. By construction then $\tilde{\pi}(\xi \setminus \{\mathbf{x}^b, \mathbf{b}\} | \mathbf{x}^b, \mathbf{b}) = q_{\text{CSMC}}(\xi \setminus \{\mathbf{x}^b, \mathbf{b}\} | \mathbf{x}^b, \mathbf{b})$ and so each CSMC sweep samples exactly from (6.23b). To complete the derivation we need to show that $\tilde{\pi}(b|\xi) = \bar{w}_T^b$ so that choosing the retained particle corresponds exactly to sampling from (6.23a). This can be done by noting that

$$\int \tilde{\pi}(\xi, b) d\xi = \int q_{\text{PIMH}}(\xi, b) \frac{\hat{Z}}{Z} d\xi = \bar{w}_T^b \int q_{\text{SMC}}(\xi) \frac{\hat{Z}}{Z} d\xi = \bar{w}_T^b \quad (6.24)$$

as required. We thus have that both (6.23a) and (6.23b) are valid Gibbs updates on our extended target $\tilde{\pi}(\xi, b)$. Now applying each of (6.23a) and (6.23b) once can change all of the variables

in our target as it can change the retained particle, the index b , and all the other particles.⁶ Therefore the combination of the two updates forms a valid Gibbs sampler for the target $\tilde{\pi}(\xi, b)$. Because $\tilde{\pi}(\xi, b)$ has a marginal distribution on the returned samples $\pi(\mathbf{x}^b)$ which is equal to the desired target, we have thus proven that using the PG algorithm and calculating estimates in the manner defined in (6.15) leads to a consistent estimator.

6.2.3 Path Degeneracy

A drawback of particle based methods, and in particular the PG algorithm, is that they can be adversely affected by *path degeneracy* in the (C)SMC sweep. Path degeneracy is the tendency of the number of unique samples to diminish as one follows the ancestry backwards through the sweep. In other words, because of the resampling, there will typically be fewer (and never more) unique instances of x_{t-1} than of x_t in the final particle set $\{x_{1:T}^i, \bar{w}_T^i\}_{i=1}^T$ and therefore there are often few distinct samples for the earlier steps. It is not uncommon for the ancestral paths to collapse back to a single sample for small t , an example of which is demonstrated in the bottom right of Figure 6.2 where there is a collapse to a single trajectory for $t < 7$. This can be especially detrimental when observations late in the sequences have noticeable effect on the early later variables, as it means that these early latent variables are already effectively fixed before the information from these observations is incorporated. This is why observations should be made as early as possible in the state sequence when taking a particle-based inference approach.

For methods that run independent SMC sweeps such as SMC itself and PIMH, the detrimental impact of path degeneracy is generally seen through high variance of the marginal likelihood estimates, resulting in low effective sample sizes and / or slow mixing rates. For PG then path degeneracy can be even more catastrophic. Conditioning on an existing trajectory means that whenever resampling of the trajectories results in a common ancestor, this ancestor must correspond to this trajectory. For a PG sampler, any common ancestor is, by construction, guaranteed to be equal to the retained particle, such that the early part of the trajectory in the retained particle cannot change from one iteration to the next if the particle set has coalesced to a single ancestor. This results in high correlation between the samples, and poor mixing of the Markov chain. In Section 6.3 we introduce the interacting PMCMC algorithm [Rainforth et al., 2016c] which forms one method for trying to overcome this problem.

⁶Note also that applying the update cycle twice can potentially completely remove the retained particle from the system and so one does not need to worry about the possibility of the retained particle simply being “passed around”.

6.2.4 Global Parameters

An important feature of PMCMC methods that we have thus far omitted is that they allow for distinct treatment of global parameters. Imagine we are interested in sampling from $p(\theta, x_{1:T}|y_{1:T})$ where θ are some global parameters that are of particular importance as they directly affect all the other variables, e.g. because they are effect each transition and / or emission distribution. As we explained in Section 6.2.3, SMC / PMCMC methods can do relatively poorly on sampling the earlier parameters, particularly if these have long range dependencies, and so it may be ineffective so simply include them within the SMC inference. One may often therefore wish to use a different sampling scheme for the global parameters, which is possible in PMCMC methods using either Gibbs sampling or Metropolis-within-Gibbs sampling to update θ , rather than including them in the SMC sweep.

Perhaps the simplest way of doing this is using the *particle marginal Metropolis-Hastings* (PMMH) sampler. This extends the PIMH sampler by using a standard MH update proposal $q(\hat{\theta}|\theta = \theta[r-1])$ before each SMCsweep such that the overall proposal is

$$q_{\text{PMMH}}(\xi, \hat{\theta}|\theta[r-1]) = q(\hat{\theta}|\theta[r-1])q_{\text{PIMH}}(\xi) \quad (6.25)$$

and samples are now accepted with probability

$$P(\text{Accept}) = \min \left(1, \frac{\hat{Z}q(\theta[r-1]|\hat{\theta})}{\mathbf{Z}'[r-1]q(\hat{\theta}|\theta[r-1])} \right). \quad (6.26)$$

Typically more effectively, one can also use manual updates for θ in the PG algorithm by alternating between running CSMC sweeps, sampling the index of the retained particle, and updating θ given the retained particle (note the different to PMMH where θ is updated independently of $\mathbf{x}'[r]$). Here one either relies on being able to sample from $\theta \sim p(\theta|x_{1:T} = \mathbf{x}'[r], y_{1:T})$, which is occasionally possible, or uses a MH step to update θ targeting $p(\theta|x_{1:T} = \mathbf{x}'[r], y_{1:T})$ as a Metropolis-with-Gibbs update. In the latter case it is typically preferable to carry out multiple update steps on the parameters between each CSMC to ensure fast mixing, noting that the latter is generally at least a factor of N more times expensive.

6.2.5 Rao-Blackwellization

At each MCMC iteration r , we generate N full particle trajectories. Using only one of these as in (6.15) might seem a bit wasteful. We can however make use of all particles to estimate expectations of interest for all of the PMCMC methods introduced so far by analytically averaging over the possible values of b that could be sampled at each iteration. We can do this by replacing $f(\mathbf{x}'[r])$ in (6.15) by

$$\mathbb{E}[f(\mathbf{x}'[r])|\xi] = \sum_{i=1}^N \bar{w}_{T,m}^i f(\mathbf{x}_m^i), \quad (6.27)$$

where the expectation is over the sampling of b . This procedure is referred to as *Rao-Blackwellization* of a statistical estimator and is (in terms of variance) never worse than the original one. At a high level, we are taking an analytic expectation over part of the randomness of the system (namely the sampling of b) to reduce the variance. We can show the validity of this by noting that

$$\mathbb{E}[f(\mathbf{x}'[r])|\xi] = \mathbb{E}\left[f(x_{1:T}^b) \middle| \xi\right] = \sum_{i=1}^N \bar{w}_{T,m}^i f(\mathbf{x}_m^i) \quad (6.28)$$

where the second equality follows from the definition of the expectation of a discrete distribution, remembering $b \sim \text{DISCRETE}(\{\bar{w}_T^i\}_{i=1}^N)$. When also doing parameter updates, we can think of the samples being returned immediately after sampling b and so that we can still Rao-Blackwellize in the same manner.

6.3 Interacting Particle Markov Chain Monte Carlo

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In this section we introduce *interacting particle Markov chain Monte Carlo* (iPMCMC) [Rainforth et al., 2016c] a PMCMC method based on an interacting pool of standard and conditional sequential Monte Carlo samplers. Like other PMCMC methods, iPMCMC is a Markov chain Monte Carlo sampler on an extended space. In iPMCMC we run a pool of CSMC and unconditional SMC algorithms as parallel processes that we refer to as nodes. After each run of this pool, we apply successive Gibbs updates to the indexes of the CSMC nodes, such that the indices of the CSMC nodes changes. Hence, the nodes from which retained particles are sampled can change from one MCMC iteration to the next, reducing the sensitivity to path degeneracy relative to PG by trading off exploration (SMC) and exploitation (CSMC) to achieve

improved mixing of the Markov chains. Crucially, the pool provides numerous candidate indices at each Gibbs update, giving a significantly higher probability that an entirely new retained particle will be “switched in” than in non-interacting alternatives.

We prove that iPMCMC is a partially collapsed Gibbs sampler on the extended space containing the particle sets for all nodes. In the special case where iPMCMC uses only *one* CSMC node, it can in fact be seen as a non-trivial and unstudied instance of the α -SMC-based [Whiteley et al., 2016] PMCMC method introduced by Huggins and Roy [2015]. However, with iPMCMC we extend this further to allow for an arbitrary number of CSMC and standard SMC algorithms with interaction.

The interaction between nodes requires only minimal communication; each node must report an estimate of the marginal likelihood and receive a new role (SMC or CSMC) for the next sweep. This means that iPMCMC is embarrassingly parallel and can be run in a distributed manner on multiple computers. However, the advantages of iPMCMC go far beyond simple parallelization: our experimental evaluation shows that iPMCMC outperforms both equivalent non-interacting PMCMC samplers as well as a single PG sampler with the same number of particles run longer to give a matching computational budget. An implementation of iPMCMC is provided in the probabilistic programming system *Anglican*⁷ [Wood et al., 2014] as we discuss in Chapter 7. A general purpose toolbox for carrying out iPMCMC and other SMC / PMCMC inference in MATLAB is also provided by the custom made *probabilistic MATLAB* package.⁸

6.3.1 Method

The main goal of iPMCMC is to increase the efficiency of PMCMC, in particular PG. As we explain in Section 6.2.3, PG is especially susceptible to the *path degeneracy* effect of SMC samplers because the early time steps in the state-sequence can become stuck in the same position for long periods if the ancestral paths in the CSMC sweeps typically coalesce to a single sample, which is by construction guaranteed to be the retained particle. This results in high correlation between the samples, and poor mixing of the Markov chain. To counteract this we might need a very high number of particles to get good mixing for all latent variables $x_{1:T}$, which can be infeasible due to e.g. limited available memory. iPMCMC can alleviate

⁷<http://www.robots.ox.ac.uk/~fwood/anglican>

⁸https://github.com/twgr/probabilistic_matlab

Algorithm 6 iPMCMC sampler

Inputs: number of nodes M , conditional nodes P and MCMC steps R , initial $\mathbf{x}'_{1:P}[0]$

- 1: **for** $r = 1$ **to** R **do**
 - 2: Workers $1 : M \setminus c_{1:P}$ run Algorithm 3 (SMC)
 - 3: Workers $c_{1:P}$ run Algorithm 5 (CSMC), conditional on $\mathbf{x}'_{1:P}[r - 1]$ respectively.
 - 4: **for** $j = 1$ **to** P **do**
 - 5: Select a new conditional node by simulating c_j according to (6.29).
 - 6: Set new MCMC sample $\mathbf{x}'_j[r] = \mathbf{x}_{c_j}^{b_j}$ by simulating b_j according to (6.31)
 - 7: **end for**
 - 8: **end for**
-

this issue by, from time to time, switching out a CSMC particle system with a completely independent SMC one, resulting in improved mixing.

iPMCMC, summarized in Algorithm 6, consists of M interacting separate CSMC and SMC algorithms, exchanging only very limited information at each iteration to draw new MCMC samples. We will refer to these internal CSMC and SMC algorithms as nodes, and assign an index $m = 1, \dots, M$. At every iteration, we have P nodes running local CSMC algorithms, with the remaining $M - P$ nodes running independent SMC. The CSMC nodes are given an identifier $c_j \in \{1, \dots, M\}$, $j = 1, \dots, P$ with $c_j \neq c_k$, $k \neq j$ and we write $c_{1:P} = \{c_1, \dots, c_P\}$. Let $\mathbf{x}_m^i = x_{1:T,m}^i$ be the internal particle trajectories of node m .

Suppose we have access to P trajectories $\mathbf{x}'_{1:P}[0] = (\mathbf{x}'_1[0], \dots, \mathbf{x}'_P[0])$ corresponding to the initial retained particles, where the index $[\cdot]$ denotes MCMC iteration. At each iteration r , the nodes $c_{1:P}$ run CSMC (Algorithm 5) with the previous MCMC sample $\mathbf{x}'_j[r - 1]$ as the retained particle. The remaining $M - P$ nodes run standard (unconditional) SMC, i.e. Algorithm 3. Each node m returns an estimate of the marginal likelihood \hat{Z}_m for the internal particle system calculated as per (6.6). Note that whereas for the SMC sweeps this is an unbiased estimate of the marginal likelihood, this a biased estimator for the CSMC sweeps that is being specifically defined for our purposes.

The new conditional nodes are then set using a single loop $j = 1 : P$ of Gibbs updates, sampling new indices c_j where

$$\mathbb{P}(c_j = m | c_{1:P} \setminus j) = \hat{\zeta}_m^j \quad (6.29)$$

$$\text{and } \hat{\zeta}_m^j = \frac{\hat{Z}_m \mathbf{1}_{m \notin c_{1:P} \setminus j}}{\sum_{n=1}^M \hat{Z}_n \mathbf{1}_{n \notin c_{1:P} \setminus j}}, \quad (6.30)$$

defining $c_{1:P \setminus j} = \{c_1, \dots, c_{j-1}, c_{j+1}, \dots, c_P\}$. We thus loop once through the conditional node indices and resample them from the union of the current node index and the unconditional node indices⁹, in proportion to their marginal likelihood estimates. This is the key step that lets us switch completely the nodes from which the retained particles are drawn.

One MCMC iteration r is concluded by setting the new samples $\mathbf{x}'_{1:P}[r]$ by simulating from the corresponding conditional node's, c_j , internal particle system in the same way as b was sampled for the PG algorithm

$$\begin{aligned}\mathbb{P}(b_j = i | c_j) &= \bar{w}_{T,c_j}^i, \\ \mathbf{x}'_j[r] &= \mathbf{x}_{c_j}^{b_j}.\end{aligned}\tag{6.31}$$

The potential to pick from updated nodes c_j , having run independent SMC algorithms, decreases correlation and improves mixing of the MCMC sampler. Furthermore, as each Gibbs update corresponds to a one-to-many comparison for maintaining the same conditional index, the probability of switching is much higher than in an analogous non-interacting system.

The theoretical justification for iP-MCMC is independent of how the initial trajectories $\mathbf{x}'_{1:P}[0]$ are generated. One simple and effective method (that we use in our experiments) is to run standard SMC sweeps for the “conditional” nodes at the first iteration.

The iP-MCMC samples $\mathbf{x}'_{1:P}[r]$ can be used to estimate expectations for test functions $f : \mathcal{X}^T \mapsto \mathbb{R}$ in the standard Monte Carlo sense, with

$$\mathbb{E}[f(\mathbf{x})] \approx \frac{1}{RP} \sum_{r=1}^R \sum_{j=1}^P f(\mathbf{x}'_j[r]).\tag{6.32}$$

However, we can improve upon this if we have access to all particles generated by the algorithm, see Section 6.3.3.

We note that iP-MCMC is suited to distributed and multi-core architectures. In practise, the particle to be retained, should the node be a conditional node at the next iteration, can be sampled upfront and discarded if unused. Therefore, at each iteration, only a single particle trajectory and normalisation constant estimate need be communicated between the nodes, whilst the time taken for calculation of the updates of $c_{1:P}$ is negligible. Further, iP-MCMC should be amenable to an asynchronous adaptation under the assumption of a random execution time, independent of $\mathbf{x}'_j[r-1]$ in Algorithm 6. We leave this asynchronous variant to future work.

⁹Unconditional node indices here refers to all $m \notin c_{1:P}$ at that point in the loop. It may thus include nodes who just ran a CSMC sweep, but have been “switched out” earlier in the loop.

6.3.2 Theoretical Justification

In this section we will give some crucial results to justify the proposed iPAMCMC sampler. This section is due to space constraints fairly brief and it is helpful to be familiar with the proof of PG in Andrieu et al. [2010b]. We start by defining some additional notation, much of which is duplicated from the PG introduction. Let $\xi := \{x_t^i\}_{i=1:N} \cup \{a_t^i\}_{i=1:N} \cup \{c_j\}_{j=1:T}$ denote all generated particles and ancestor variables of a (C)SMC sampler. We write ξ_m when referring to the variables of the sampler local to node m . Let the conditional particle trajectory and corresponding ancestor variables for node c_j be denoted by $\{\mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}\}$, with $\mathbf{b}_{c_j} = (\beta_{1,c_j}, \dots, \beta_{T,c_j})$, $\beta_{T,c_j} = b_j$ and $\beta_{t,c_j} = a_{t,c_j}^{\beta_{t+1,c_j}}$. Let the posterior distribution of the latent variables be denoted by $\pi(\mathbf{x}) := p(x_{1:T}|y_{1:T})$ with normalisation constant $Z := p(y_{1:T})$. Finally we note that the SMC and CSMC algorithms induce the respective distributions over the random variables generated by the procedures are given by (6.16) and (6.18)

Now we are ready to state the main theoretical result.

Theorem 6.1. *The interacting particle Markov chain Monte Carlo sampler of Algorithm 6 is a partially collapsed Gibbs sampler [Van Dyk and Park, 2008] for the target distribution*

$$\tilde{\pi}(\xi_{1:M}, c_{1:P}, b_{1:P}) = \frac{1}{N^{PT} \binom{M}{P}} \prod_{\substack{m=1 \\ m \notin c_{1:P}}}^M q_{SMC}(\xi_m) \cdot \prod_{j=1}^P \left[\pi\left(\mathbf{x}_{c_j}^{b_j}\right) \mathbb{1}_{c_j \notin c_{1:j-1}} q_{CSMC}\left(\xi_{c_j} \setminus \{\mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}\} \mid \mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}\right) \right]. \quad (6.33)$$

Proof. The proof follows similar ideas as our derivation for the PIMH and PG samplers and thus follows similar ideas to those introduced by Andrieu et al. [2010a]. We prove that the interacting particle Markov chain Monte Carlo sampler is in fact a standard partially collapsed Gibbs sampler [Van Dyk and Park, 2008] on an extended space

$$\Upsilon := \mathcal{X}^{\otimes MTN} \times [N]^{\otimes M(T-1)N} \times [M]^{\otimes P} \times [N]^{\otimes P}.$$

With $\tilde{\pi}(\cdot)$ with as per (6.33), we will show that the Gibbs sampler on the extended space, Υ , defined as follows

$$\xi_{1:M} \setminus \{\mathbf{x}_{c_{1:P}}^{b_{1:P}}, \mathbf{b}_{c_{1:P}}\} \sim \tilde{\pi}(\cdot \mid \mathbf{x}_{c_{1:P}}^{b_{1:P}}, \mathbf{b}_{c_{1:P}}, c_{1:P}, b_{1:P}), \quad (6.34a)$$

$$c_j \sim \tilde{\pi}(\cdot \mid \xi_{1:M}, c_{1:P \setminus j}), \quad j = 1, \dots, P, \quad (6.34b)$$

$$b_j \sim \tilde{\pi}(\cdot \mid \xi_{1:M}, c_{1:P}), \quad j = 1, \dots, P, \quad (6.34c)$$

is equivalent to the iPMCMC method in Algorithm 6.

First, the initial step (6.34a) corresponds to sampling from

$$\begin{aligned} \tilde{\pi}(\xi_{1:M} \setminus \{\mathbf{x}_{c_{1:P}}^{b_{1:P}}, \mathbf{b}_{c_{1:P}}\} | \mathbf{x}_{c_{1:P}}^{b_{1:P}}, \mathbf{b}_{c_{1:P}}, c_{1:P}, b_{1:P}) = \\ \prod_{\substack{m=1 \\ m \notin c_{1:P}}}^M q_{\text{SMC}}(\xi_m) \prod_{j=1}^P q_{\text{CSMC}}(\xi_{c_j} \setminus \{\mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}\} | \mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}, c_j, b_j). \end{aligned}$$

This, excluding the conditional trajectories, just corresponds to steps 3–4 in Algorithm 6, i.e. running P CSMC and $M - P$ SMC algorithms independently.

We continue with a reformulation of (6.33) which will be useful to prove correctness for the other two steps. Here we first note that

$$\begin{aligned} \tilde{\pi}(\xi_{1:M}, c_{1:P}, b_{1:P}) = \frac{1}{\binom{M}{P}} \prod_{m=1}^M q_{\text{SMC}}(\xi_m) \\ \cdot \prod_{j=1}^P \left[\mathbb{1}_{c_j \notin c_{1:j-1}} \bar{w}_{T,c_j}^{b_j} \frac{\pi(\mathbf{x}_{c_j}^{b_j}) q_{\text{CSMC}}(\xi_{c_j} \setminus \{\mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}\} | \mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}, c_j, b_j)}{N^T \bar{w}_{T,c_j}^{b_j} q_{\text{SMC}}(\xi_{c_j})} \right]. \end{aligned} \quad (6.35)$$

Now by self similarity to importance weight calculated for the PIMH derivation in (6.21) we have that

$$\frac{\pi(\mathbf{x}_{c_j}^{b_j}) q_{\text{CSMC}}(\xi_{c_j} \setminus \{\mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}\} | \mathbf{x}_{c_j}^{b_j}, \mathbf{b}_{c_j}, c_j, b_j)}{N^T \bar{w}_{T,c_j}^{b_j} q_{\text{SMC}}(\xi_{c_j})} = \frac{\hat{Z}_{c_j}}{Z} \quad (6.36)$$

and therefore

$$\tilde{\pi}(\xi_{1:M}, c_{1:P}, b_{1:P}) = \frac{1}{\binom{M}{P}} \prod_{m=1}^M q_{\text{SMC}}(\xi_m) \cdot \prod_{j=1}^P \frac{\hat{Z}_{c_j}}{Z} \mathbb{1}_{c_j \notin c_{1:j-1}} \bar{w}_{T,c_j}^{b_j}. \quad (6.37)$$

By marginalizing this reformulation over $b_{1:P}$ we get

$$\tilde{\pi}(\xi_{1:M}, c_{1:P}) = \frac{1}{\binom{M}{P}} \prod_{m=1}^M q_{\text{SMC}}(\xi_m) \prod_{j=1}^P \frac{\hat{Z}_{c_j}}{Z} \mathbb{1}_{c_j \notin c_{1:j-1}}.$$

From this it is easy to see that $\tilde{\pi}(c_j | \xi_{1:M}, c_{1:P \setminus j}) = \hat{\zeta}_{c_j}^j$, which corresponds to sampling the conditional node indices, i.e. step 6 in Algorithm 6. Finally, from (6.37) we can see that simulating $b_{1:P}$ can be done independently as follows

$$\tilde{\pi}(b_{1:P} | \xi_{1:M}, c_{1:P}) = \frac{\tilde{\pi}(b_{1:P}, \xi_{1:M}, c_{1:P})}{\tilde{\pi}(\xi_{1:M}, c_{1:P})} = \prod_{j=1}^P \bar{w}_{T,c_j}^{b_j}.$$

This corresponds to step 7 in the iPMCMC sampler, Algorithm 6. So the procedure defined by (6.34) is a partially collapsed Gibbs sampler, derived from (6.33), and we have shown that it is exactly equal to the iPMCMC sampler described in Algorithm 6. \square

Remark 1. The marginal distribution of $(\mathbf{x}_{c_{1:P}}^{b_{1:P}}, c_{1:P}, b_{1:P})$, with $\mathbf{x}_{c_{1:P}}^{b_{1:P}} = (\mathbf{x}_{c_1}^{b_1}, \dots, \mathbf{x}_{c_P}^{b_P})$, under (6.33) is by construction given by

$$\tilde{\pi}(\mathbf{x}_{c_{1:P}}^{b_{1:P}}, c_{1:P}, b_{1:P}) = \frac{\prod_{j=1}^P \pi(\mathbf{x}_{c_j}^{b_j}) \mathbb{1}_{c_j \notin c_{1:j-1}}}{N^{PT} \binom{M}{P}} \quad (6.38)$$

because our extended target is formulated as being the process of sampling exactly from (6.38) and then running the P CSMC sweeps and $M - P$ SMC sweeps. This means that each trajectory $\mathbf{x}_{c_j}^{b_j}$ is marginally distributed according to the posterior distribution of interest, π . Indeed, the P retained trajectories of iPMCMC will in the limit $R \rightarrow \infty$ be independent draws from π . Note similarly that it follows that (6.32) is a consistent estimator (converging in the limit $R \rightarrow \infty$ provided the standard assumptions for convergence of Gibbs samplers are satisfied (see e.g. [Roberts and Smith, 1994]).

Note that adding a backward or ancestor simulation step can drastically increase mixing when sampling the conditional trajectories $\mathbf{x}'_j[r]$ [Lindsten and Schön, 2013]. In the iPMCMC sampler we can replace simulating from the final weights on line 7 by a backward simulation step. Another option for the CSMC nodes is to replace this step by internal ancestor sampling [Lindsten et al., 2014] steps and simulate from the final weights as normal.

6.3.3 Using All the Particles

As we discussed for the PIMH and PG cases in Section 6.2.5, it can be wasteful to throw away most of our generated samples. Thankfully we can again carry out a Rao-Blackwellization for iPMCMC to make use of all particles when estimating expectations of interest. To do this we will at each Gibbs update j , averaging over the possible new values for the conditional node index c_j and corresponding particle index b_j . We can do this by replacing $\frac{1}{P} \sum_{j=1}^P f(\mathbf{x}'_j[r])$ in (6.32) by

$$\frac{1}{P} \sum_{j=1}^P \mathbb{E}[f(\mathbf{x}'_j[r]) | \xi_{1:M}, c_{1:P \setminus j}] = \frac{1}{P} \sum_{m=1}^M \left[\left(\sum_{j=1}^P \hat{\zeta}_m^j \right) \cdot \left(\sum_{i=1}^N \bar{w}_{T,m}^i f(\mathbf{x}_m^i) \right) \right]$$

where the expectation is over b_j and c_j . We highlight that each $\hat{\zeta}_m^j$, as defined in (6.30), depends on which indices are sampled earlier in the index reassignment loop.

To derive this we first note that for iteration r we calculate $\frac{1}{P} \sum_{j=1}^P f(\mathbf{x}'_j[r]) = \frac{1}{P} \sum_{j=1}^P f(\mathbf{x}_{c_j}^{b_j})$ where we can Rao-Blackwellize the selection of the retained particle along with each individual

Gibbs update and thereby replace $f(\mathbf{x}_{c_j}^{b_j})$ with its expectation over c_j and b_j given all the other variables as follows

$$\begin{aligned}\frac{1}{P} \sum_{j=1}^P \mathbb{E} \left[f(\mathbf{x}_{c_j}^{b_j}) \middle| \xi_{1:M}, c_{1:P \setminus j} \right] &= \frac{1}{P} \sum_{j=1}^P \mathbb{E} \left[\sum_{i=1}^N \bar{w}_{T,c_j}^i f(\mathbf{x}_{c_j}^i) \middle| \xi_{1:M}, c_{1:P \setminus j} \right] \\ &= \frac{1}{P} \sum_{j=1}^P \sum_{i=1}^N \sum_{m=1}^M \hat{\zeta}_m^j \bar{w}_{T,m}^i f(\mathbf{x}_m^i) \\ &= \frac{1}{P} \sum_{m=1}^M \left[\left(\sum_{j=1}^P \hat{\zeta}_m^j \right) \cdot \left(\sum_{i=1}^N \bar{w}_{T,m}^i f(\mathbf{x}_m^i) \right) \right].\end{aligned}$$

Here we have made use of the knowledge that the internal particle system $\{(\mathbf{x}_m^i, \bar{w}_{T,m}^i)\}$ does not change between Gibbs updates of the c_j 's, whereas the $\hat{\zeta}_m^j$ do. We emphasise that this is a separate Rao-Blackwellization of each Gibbs update of the conditional node indices, such that each is conditioned upon the actual update made at $j - 1$, rather than a simultaneous Rao-Blackwellization of the full batch of P updates. Though the latter also has analytic form and should theoretically be lower variance, it suffers from inherent numerical instability and so is difficult to calculate in practise. We found that empirically there was not a noticeable difference between the performance of the two procedures. Furthermore, one can always run additional Gibbs updates on the c_j 's and obtain an improve estimate on the relative sample weightings if desired.

6.3.4 Choosing \mathbf{P}

Before jumping into the full details of our experimentation, we quickly consider the choice of P . Intuitively we can think of the independent SMC's as particularly useful if they are selected as the next conditional node. The probability of the event that at least one conditional node switches with an unconditional, is given by

$$\mathbb{P}(\{\text{switch}\}) = 1 - \mathbb{E} \left[\prod_{j=1}^P \frac{\hat{Z}_{c_j}}{\hat{Z}_{c_j} + \sum_{m \notin c_{1:P}}^M \hat{Z}_m} \right]. \quad (6.39)$$

There exist theoretical and experimental results [Pitt et al., 2012; Bérard et al., 2014; Doucet et al., 2015] that show that the distributions of the normalisation constants are well-approximated by their log-Normal limiting distributions. Now, with $\sigma^2 (\propto \frac{1}{N})$ being the variance of the (C)SMC estimate, it means we have $\log(Z^{-1} \hat{Z}_{c_j}) \sim \mathbb{N}(\frac{\sigma^2}{2}, \sigma^2)$ and $\log(Z^{-1} \hat{Z}_m) \sim \mathbb{N}(-\frac{\sigma^2}{2}, \sigma^2)$, $m \notin c_{1:P}$ at stationarity, where Z is the true normalization constant. Under this assumption,

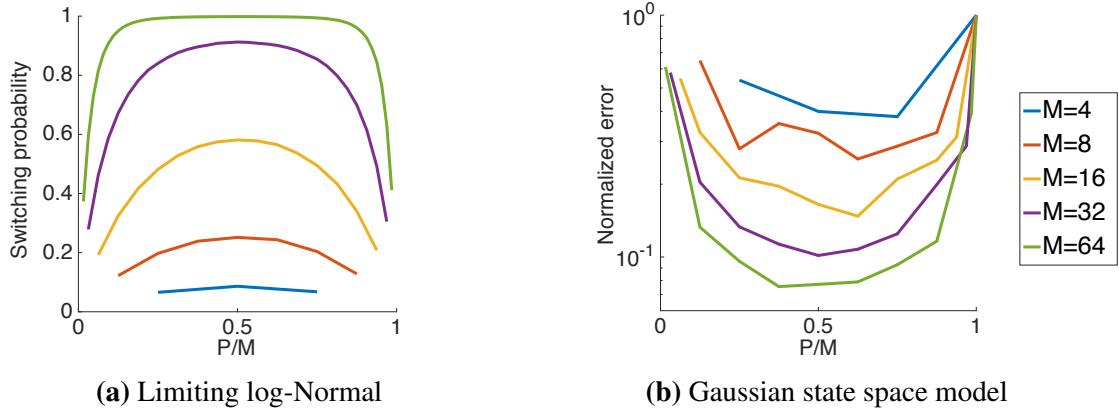


Figure 6.3: a) Estimation of switching probability for different choices of P and M assuming the log-Normal limiting distribution for \hat{Z}_m with $\sigma = 3$. b) Median error in mean estimate for different choices of P and M over 10 different synthetic datasets of the linear Gaussian state space model given in (6.40) after 1000 MCMC iterations. Here errors are normalized by the error of a multi-start PG sampler which is a special case of iPMCMC for which $P = M$ (see Section 6.3.5).

we can accurately estimate the probability (6.39) for different choices of P an example of which is shown in Figure 6.3a along with additional analysis given in the supplementary material of Rainforth et al. [2016c]. These provide strong empirical evidence that the switching probability is maximised for $P = M/2$.

In practice we also see that best results are achieved when P makes up roughly half of the nodes, see Figure 6.3b for performance on the state space model introduced in (6.40). Note also that the accuracy seems to be fairly robust with respect to the choice of P . Based on these results, we set the value of $P = \frac{M}{2}$ for the rest of our experiments.

6.3.5 Experiments

To demonstrate the empirical performance of iPMCMC we report experiments on two state space models. Although both the models considered are Markovian, we emphasise that iPMCMC goes far beyond this and can be applied to arbitrary graphical models. We will focus our comparison on the trivially distributed alternatives, whereby M independent PMCMC samplers are run in parallel—these are PG, particle independent Metropolis-Hastings (PIMH) Andrieu et al. [2010b] and the alternate move PG sampler (APG) Holenstein [2009]. Comparisons to other alternatives, including independent SMC, serialized implementations of PG and PIMH, and running a mixture of independent PG and PIMH samplers, are provided in the supplementary material of Rainforth et al. [2016c]. None outperformed the methods considered here, with the exception of running

a serialized PG implementation with an increased number of particles, requiring significant additional memory ($O(MN)$ as opposed to $O(M + N)$).

In PIMH a new particle set is proposed at each MCMC step using an independent SMC sweep, which is then either accepted or rejected using the standard Metropolis-Hastings acceptance ratio. APG interleaves PG steps with PIMH steps in an attempt to overcome the issues caused by path degeneracy in PG. We refer to the trivially distributed versions of these algorithms as multi-start PG, PIMH and APG respectively (mPG, mPIMH and mAPG). We use Rao-Blackwellization, as described in 6.3.3, to average over all the generated particles for all methods, weighting the independent Markov chains equally for mPG, mPIMH and mAPG. We note that mPG is a special case of iPMCMC for which $P = M$. Because our interest is in alleviating degeneracy multinomial resampling was used in the experiments,¹⁰ with the prior transition distribution of the latent variables taken for the proposal. $M = 32$ nodes and $N = 100$ particles were used unless otherwise stated. Initialization of the retained particles for iPMCMC and mPG was done by using standard SMC sweeps.

6.3.5.1 Linear Gaussian State Space Model

We first consider a linear Gaussian state space model (LGSSM) with 3 dimensional latent states $x_{1:T}$, 20 dimensional observations $y_{1:T}$ and dynamics given by

$$x_1 \sim \mathcal{N}(\mu, V) \quad (6.40a)$$

$$x_t = \alpha x_{t-1} + \delta_{t-1} \quad \delta_{t-1} \sim \mathcal{N}(0, \Omega) \quad (6.40b)$$

$$y_t = \beta x_t + \varepsilon_t \quad \varepsilon_t \sim \mathcal{N}(0, \Sigma). \quad (6.40c)$$

We set $\mu = [0, 1, 1]^T$, $V = 0.1 \mathbf{I}$, $\Omega = \mathbf{I}$ and $\Sigma = 0.1 \mathbf{I}$ where \mathbf{I} represents the identity matrix. The constant transition matrix, α , corresponds to successively applying rotations of $\frac{7\pi}{10}$, $\frac{3\pi}{10}$ and $\frac{\pi}{20}$ about the first, second and third dimensions of x_{t-1} respectively followed by a scaling of 0.99 to ensure that the dynamics remain stable. A total of 10 different synthetic datasets of length $T = 50$ were generated by simulating from (6.40a)–(6.40c), each with a different emission matrix β generated by sampling each column independently from a symmetric Dirichlet distribution with concentration parameter 0.2.

¹⁰We recommend using systematic resampling,, as is the default in the provided implementations, and setting N as large as possible for iPMCMC in general.

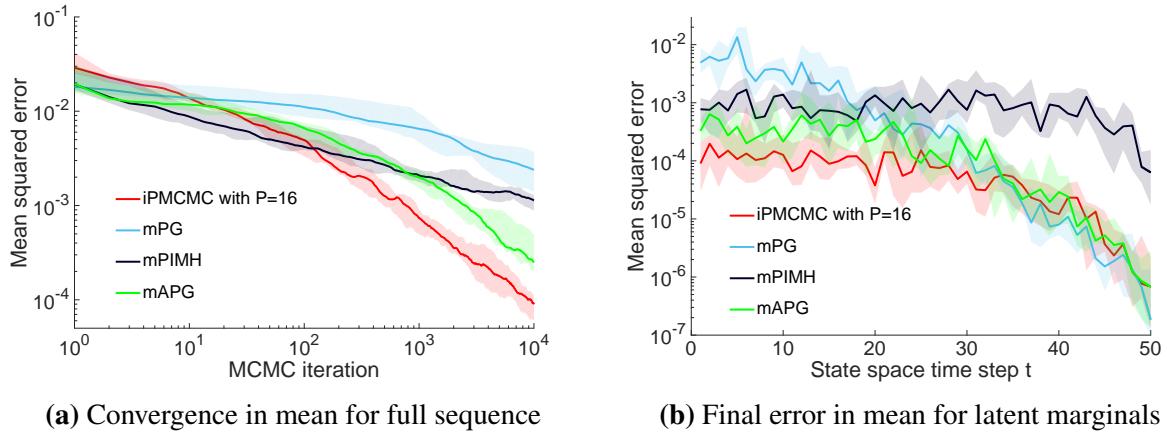


Figure 6.4: Mean squared error averaged over all dimensions and steps in the state sequence as a function of MCMC iterations (left) and mean squared error after 10^4 iterations averaged over dimensions as function of position in the state sequence (right) for (6.40) with 50 time sequences. The solid line shows the median error across the 10 tested synthetic datasets, while the shading shows the upper and lower quartiles. Ground truth was calculated using the Rauch–Tung–Striebel smoother algorithm Rauch et al. [1965].

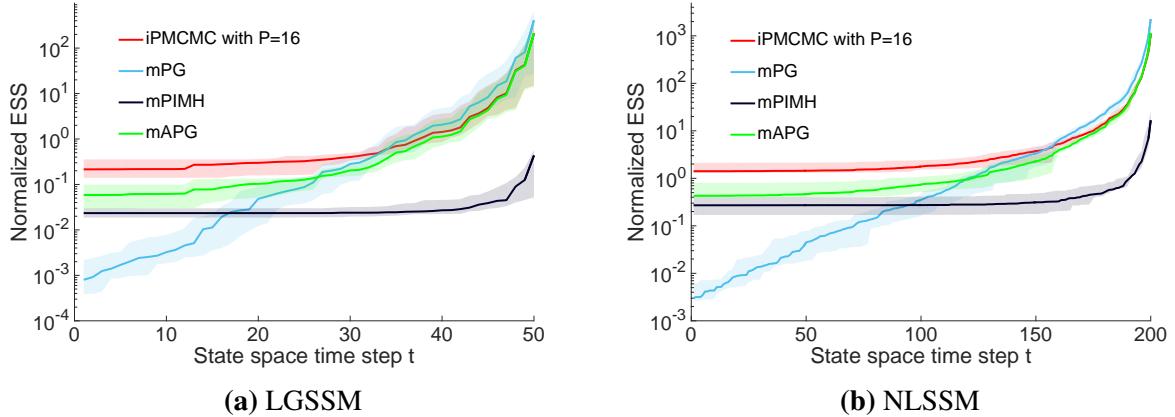


Figure 6.5: Normalized effective sample size (NESS) for LGSSM (left) and NLSSM (right).

Figure 6.4a shows convergence in the estimate of the latent variable means to the ground-truth solution for iPMCMC and the benchmark algorithms as a function of MCMC iterations. It shows that iPMCMC comfortably outperforms the alternatives from around 200 iterations onwards, with only iPMCMC and mAPG demonstrating behaviour consistent with the Monte Carlo convergence rate, suggesting that mPG and mPIMH are still far from the ergodic regime. Figure 6.4b shows the same errors after 10^4 MCMC iterations as a function of position in state sequence. This demonstrates that iPMCMC outperformed all the other algorithms for the early stages of the state sequence, for which mPG performed particularly poorly. Toward the end of state sequence, iPMCMC, mPG and mAPG all gave similar performance, whilst

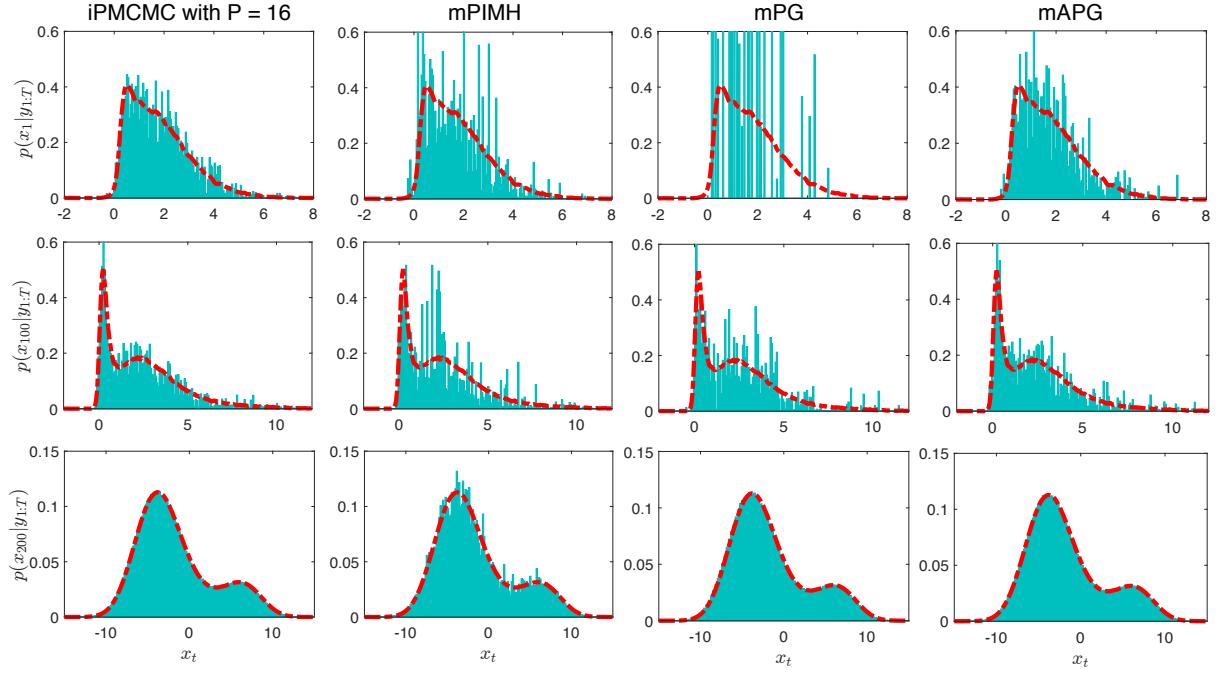


Figure 6.6: Histograms of generated samples at $t = 1, 100$, and 200 for a single dataset generated from (6.41) with $T = 200$. Dashed red line shows an approximate estimate of the ground truth, found by running a kernel density estimator on the combined samples from a small number of independent SMC sweeps, each with 10^7 particles.

that of mPIMH was significantly worse.

6.3.5.2 Nonlinear State Space Model

We next consider the one dimensional nonlinear state space model (NLSSM) considered by, among others, Gordon et al. [1993]; Andrieu et al. [2010b]

$$x_1 \sim \mathcal{N}(\mu, v^2) \quad (6.41a)$$

$$x_t = \frac{x_{t-1}}{2} + 25 \frac{x_{t-1}}{1+x_{t-1}^2} + 8 \cos(1.2t) + \delta_{t-1} \quad (6.41b)$$

$$y_t = \frac{x_t^2}{20} + \varepsilon_t \quad (6.41c)$$

where $\delta_{t-1} \sim \mathcal{N}(0, \omega^2)$ and $\varepsilon_t \sim \mathcal{N}(0, \sigma^2)$. We set the parameters as $\mu = 0$, $v = \sqrt{5}$, $\omega = \sqrt{10}$ and $\sigma = \sqrt{10}$. Unlike the LGSSM, this model does not have an analytic solution and therefore one must resort to approximate inference methods. Further, the multi-modal nature of the latent space makes full posterior inference over $x_{1:T}$ challenging for long state sequences.

To examine the relative mixing of iPIMCMC we calculate an effective sample size (ESS) for different steps in the state sequence as described in Section 5.3.2.3, taking care to condense

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identical samples. To be precise, let

$$u_t^k \in \{x_{t,m}^i[r]\}_{m=1:M}^{i=1:N, r=1:R}, \quad \forall k \in 1 \dots K, t \in 1 \dots T$$

denote the unique samples of x_t generated by all the nodes and sweeps of particular algorithm after R iterations, where K is the total number of unique samples generated. The weight assigned to these unique samples, v_t^k , is given by the combined weights of all particles for which x_t takes the value u_t^k :

$$v_t^k = \sum_{r=1}^R \sum_{m=1}^M \sum_{i=1}^N \bar{w}_{t,m}^{i,r} \eta_m^r \delta_{x_{t,m}^i[r]}(u_t^k) \quad (6.42)$$

where $\delta_{x_{t,m}^i[r]}(u_t^k)$ is the Kronecker delta function and η_m^r is a node weight. For iPMCMC the node weight is given by as per the Rao-Blackwellized estimator described in Section 6.3.3. For mPG and mPIMH, η_m^r is simply $\frac{1}{RM}$, as samples from the different nodes are weighted equally in the absence of interaction. Finally we define our effective sample size as $\text{ESS}_t = \left(\sum_{k=1}^K (v_t^k)^2 \right)^{-1}$.

Figure 6.5 shows the ESS for the LGSSM and NLSSM as a function of position in the state sequence. For this, we omit the samples generated by the initialization step as this SMC sweep is common to all the tested algorithms. We further normalize by the number of MCMC iterations so as to give an idea of the rate at which unique samples are generated. These show that for both models the ESS of iPMCMC, mPG and mAPG is similar towards the end of the space sequence, but that iPMCMC outperforms all the other methods at the early stages. The ESS of mPG was particularly poor at early iterations. PIMH performed poorly throughout, reflecting the very low observed acceptance ratio of around 7.3% on average.

It should be noted that the ESS is not a direct measure of performance for these models. For example, the equal weighting of nodes is likely to make the ESS artificially high for mPG, mPIMH and mAPG, when compared with methods such as iPMCMC that assign a weighting to the nodes at each iteration. To acknowledge this, we also plot histograms for the marginal distributions of a number of different position in the state sequence as shown in Figure 6.6. These confirm that iPMCMC and mPG have similar performance at the latter state sequence steps, whilst iPMCMC is superior at the earlier stages, with mPG producing almost no more new samples than those from the initialization sweep due to the degeneracy. The performance of PIMH was consistently worse than iPMCMC throughout the state sequence, with even the final step exhibiting noticeable noise.

6.3.6 Discussion

The iPMCMC sampler overcomes degeneracy issues in PG by allowing the newly sampled particles from SMC nodes to replace the retained particles in CSMC nodes. Our experimental results demonstrate that, for the models considered, this switching in rate is far higher than the rate at which PG generates fully independent samples. Moreover, the results in Figure 6.3b suggest that the degree of improvement over an mPG sampler with the same total number of nodes increases with the total number of nodes in the pool.

The mAPG sampler performs an accept reject step that compares the marginal likelihood estimate of a single CSMC sweep to that of a single SMC sweep. In the iPMCMC sampler the CSMC estimate of the marginal likelihood is compared to a population sample of SMC estimates, resulting in a higher probability that at least one of the SMC nodes will become a CSMC node.

Since the original PMCMC paper in 2010 there have been several papers studying [Chopin and Singh, 2015; Lindsten et al., 2015] and improving upon the basic PG algorithm. Key contributions to combat the path degeneracy effect are backward simulation [Whiteley et al., 2010; Lindsten and Schön, 2013] and ancestor sampling [Lindsten et al., 2014]. These can also be used to improve the iPMCMC method ever further.

6.4 Other Methods and Extensions

- Backwards / ancestral sampling
- Resample-move stuff
- Rejuvenation

7

General Purpose Inference for Probabilistic Programs

In Chapter 4 we showed how probabilistic programming systems (PPSs) provide an expressive framework for specifying probabilistic models. We now consider the other major component for PPSs: automating inference for any model the user is allowed to specify using general-purpose inference engines. For most PPSs this requires two things – the inference engine itself and either an interpreter controlling the probabilistic semantics or a compiler to convert the *query* to a suitable form for input to the inference engine. Our focus will be on the compiled case.

For the inference driven systems discussed in Section 4.2.1, the inference engine typically comprises of a standard Bayesian inference method for graphical models such as those discussed in Chapters 3 and 6. Developing these in a way to robustly work for a wide range of problems typically requires careful engineering and algorithmic innovation – e.g. because many inference methods require the definition of a proposal, upon which performance can critically depend – but does not generally require the development of approaches distinct to those used outside a probabilistic programming context. In these systems, the inference algorithm(s) is/are usually chosen first, with the language and its restrictions built around it. Therefore the challenges of the designing the system are generally rooted in generalizing and increasing the robustness of the specific inference method(s) used. Similarly, the language itself and associated compiler is generally built around providing the easiest representation to work with the target model class, while the fact that most of these such systems to not support higher order functions usually substantially simplifies the compilation process.

Because the design of these systems is very much driven by the particular inference algorithm used, it beyond the scope of this thesis to do the associated literature justice. Our focus will instead mostly be on conducting inference for universal PPSs, though some of what we introduce

will apply to both. Unfortunately, we will find that there are very few (known) inference methods which can actually cope with the most general possible models as we introduced in Section 4.3.2, all of which suffer particularly badly from the curse of dimensionality. Consequently, it will be necessary to make certain (mostly very small) concessions in generality to achieve any reasonable performance on non-toy models. We will focus on conducting inference in Anglican [Wood et al., 2014; Tolpin et al., 2016] to give us a basis for explanation, but much of what we discuss will still be relevant to other universal systems, in particular, those which are also built around `sample`-`observe` syntaxes, such as VentureScript [Mansinghka et al., 2014], WebPPL [Goodman and Stuhlmüller, 2014], and Probabilistic C [Paige and Wood, 2014].

7.1 A High-Level Introduction to General Purpose Inference

Before getting into the nitty-gritty of designing a compiler and inference engine for a universal PPL, we first consider at a high-level how we might hope to do inference in such systems. The simplest thing we could do is self normalized importance sampling (SNIS) using the generative model specified by the `sample` statements as a proposal. This strategy is sometimes known as *likelihood weighting* in the probabilistic programming literature and simple involves directly sampling from the forward model an accumulating weights from the `observe` conditioning statements in a sequential importance sampling fashion (see Section 6.1.2). In Section 4.3.2, we specified with (4.3) the unnormalized conditional distribution of the program using execution traces generated by the program. If we sample from the generative model then it is clear that all samples will satisfy $\mathcal{B}(x_{1:n_x}, \lambda) = 1$ while our the support of our proposal will clearly cover that of the posterior provided the conditioning density terms are always finite. This is also a proposal we can always sample from because our `observe` terms will only effect the probability of a trace, not the variables it generates. Using the notation from Section 4.3.2 this approach leads to the following SNIS characterization of the posterior

$$p(x_{1:n_x}|\lambda) \approx \hat{p}(x_{1:n_x}|\lambda) := \sum_{n=1}^N \bar{w}_n \delta_{\hat{x}_{1:n_x}^n}(x_{1:n_x}) \quad \text{where} \quad (7.1)$$

$$\hat{x}_{1:n_x}^n \sim \prod_{j=1}^{n_x} f_{a_j}(x_j|\phi_j); \quad \bar{w}_n = \frac{w_n}{\sum_{n=1}^N w_n}; \quad w_n = \prod_{k=1}^{\hat{n}_y^n} g_{\hat{b}_k^n}(\hat{y}_k^n|\hat{\psi}_k^n); \quad (7.2)$$

$\delta_{\hat{x}_{1:n_x}^n}(\cdot)$ is a delta function centered at $\hat{x}_{1:n_x}^n$; ϕ_j and a_j are deterministic functions of $\hat{x}_{1:n_x}^n$ and λ ; and \hat{n}_y^n , \hat{b}_k^n , \hat{y}_k^n , and $\hat{\psi}_k^n$ are random variables that are deterministic functions of $\hat{x}_{1:n_x}^n$

and λ . Here we are sampling $\hat{x}_{1:n_x}^n$ from the generative model defined by the program which is equivalent to running the forward program ignoring all of the `observe` statements. Our unnormalized likelihood weights w_n correspond to product of all the probabilities accumulated from the `observe` terms. We remind the reader that each x_j corresponds to the direct output of a sample statement, not an explicit variable in the program, with the program variables and outputs being deterministic functions of $x_{1:n_x}$ (see Section 4.4.2). In addition to providing a characterization of the conditional distribution through $\hat{p}(x_{1:n_x}|\lambda)$, we can also use our samples to construct consistent estimates from the outputs of program Ω , remembering that these are a deterministic function of $x_{1:n_x}$ and so an expectation over Ω can be represented as an expectation over $x_{1:n_x}$. This convergence follows in the standard way for SNIS provided our program terminates with probability 1.

In practice, we will not sample a full $\hat{x}_{1:n_x}^n$ before evaluating its weight in one go – we will use sequential importance sampling strategy whereby we sample directly from any `sample` statement as we encounter it and accumulate weights from `observe` statements as we go (see Figure 4.3 in Section 4.3.2). Another way of viewing this is that we will repeatedly run our query as if it were an ordinary program, except for the fact that we accumulate a weight as a side effect that is then returned with the produced sample. Such a guess and check strategy will obviously be ineffective except in very low dimensions. However, it will both be a go-to strategy for the most extreme possible problems that fail to satisfy any of the required assumptions for more advanced methods and a basis for more complex inference strategies. For example, as we will show in Section 7.4, we can convert this to an SMC strategy, provided n_y is fixed, by running a number of separate executions in parallel and performing resampling at each of the `observe` statements. Alternatively, we can develop component-wise MCMC strategies by proposing changes to individual x_j and then re-evaluating the weights. However, doing so will require our inference strategy to have more control than simply running the program forwards in its entirety and this will require both a compilation and an interface for inference, which will be the focus of the next two sections.

7.2 Compiling Queries

Non-probabilistic languages can be either compiled, whereby high-level source code is converted to a lower level language (e.g. byte-code) before being evaluated, or interpreted, whereby an

interpreter reads the program and directly evaluates it based on the language semantics. The same is true for PPLs, for which compilation using comprises of converting the query to a model artifact in a host language in which the inference algorithm itself is written. Though its original implementation was interpreted, the current version of Anglican is compiled and our focus will be on this compiled approach. Rather than just being a technical hurdle, compilation is also often an important tool in the ability of probabilistic programming systems to perform effective inference as, in addition to offering potential speed improvements, it can often be used to establish helpful salient features in the model, such as dependency structures, variable types, and features of the model that can guide which inference algorithm is likely to be most successful or even elements of the model that can be calculated analytically. Hakaru [Narayanan et al., 2016] is a good example of what can be achieved in probabilistic programming through compilation alone, as it, for example, uses the computer algebra system Maple to automatically simplify models when possible. Once a compiler is written for a PPL, this often substantially simplifies the process of writing new inference algorithms by providing a common representation of models and allowing inheritance from existing algorithms.

7.2.1 What do we want to Achieve through Compilation?

So what are the aims of our PPL compiler? First and foremost, we need to perform a source-to-source transformation of the program to produce some representation in the conventional programming language in which the inference engine is written so that execution of the program is possible and inference can be carried out. As a simple example, consider the case of an Anglican program where we wish only to run importance sampling using the generative model as a proposal (i.e. the query with all the `observe` statements removed). Here we need only produce a Clojure program that samples directly from the generative model and accumulates weights from the `observe` terms as a side-effect. We can then rerun this program arbitrarily many times, each returning a sampled output and accompanying weight, to produce a sequence of importance samples which can then be used to make consistent Monte Carlo estimations. Such a strategy would be naïve though as we would be able to use our Clojure program for little else than importance sampling with this particular proposal. Clearly, we want to compile to a more general purpose representation that permits a wider array inference algorithms and proposals, and which ideally allows features of the model, such as its dependency structure, to be exploited.

One desirable feature of our compiled representation is an ability to make partial program evaluations. This will allow us to re-evaluate elements of the program in isolation in a Gibbs sampling style fashion and it will allow us to interrupt the execution of the program, giving us the ability to add in things such as the resampling step in SMC. Supporting partial evaluation can also allow us to avoid gratuitous re-executions of elements of the program whose result is already known by using databases to store and recall the effect of previous executions.

Another desirable feature is to avoid being restricted to only directly sampling from `sample` statements. We may wish to sample from a different distribution as a proposal or to evaluate the probability density of the `sample` statement producing a particular output, e.g. as part of an acceptance ratio calculation for an MCMC scheme. The key requirement for both of these is the knowledge of density function associated with the `sample` statement, rather than just access to a black-box sampling scheme. This is the motivation behind why we defined the syntax of `sample` as taking as input a distribution object which encodes both the density function and means of sampling from that density.

It will also often be helpful for our compiler to delineate between probabilistic and deterministic elements of the code. Other than potentially trying to make efficiency gain by avoiding repeated computation, we know that any deterministic parts of our code (namely code in between consecutive `sample` and/or `observe` statements) can be safely run without the need to worry about the implications this has on the inference. The execution of these segments of the program in isolation can thus be per the language being compiled to, without needing to worry about the probabilistic semantics. On the other hand, we will generally desire the identification of *checkpoints* for positions in the program where `sample` or `observe` statements are made so that the behavior of the program at these points can be handed over to the inference engine.

The compiler will in general also play an important role in the interaction between the PPL as its integrated language on the behalf of the user. Any PPL that does not provide produce outputs in a helpful form that can be manipulated by the user will be somewhat impractical, while for general purpose systems it is essential to allow the user to link in external deterministic code packages specific their particular problem.

This example list of desirable features for our compiler is far from exhaustive. In particular, there will be many inference specific features required for some systems, such as the need to have a representation of the derivations, e.g. calculated through automatic differentiation Baydin

et al. [2015], to carry out Hamiltonian Monte Carlo inference Carpenter et al. [2015] or common variational inference methods [Kucukelbir et al., 2015]. As we said earlier, we will often also want our compilation to, when possible, pick out salient features of the model, carry out simplifications, and even automatically establish the most suitable inference algorithm for a particular problem. The compiler is an integral part of any PPL and there is no one best approach for all situations. One of the key distinguishing features between different PPLs is how they approach this compilation problem, with different design choices inevitably lead to systems geared towards different models or inference algorithms.

7.2.2 Compilation of Anglican Queries

As it is inevitably infeasible to detail the inner workings of a PPL compiler in a general manner, we now provide a more in depth introduction to compilation method employed by Anglican. Our introduction is inevitably not exhaustive, focusing more on intuition than being exactly true to the implementation details; we refer the reader to [Tolpin et al., 2016] for a more complete and rigorous introduction.

As we explain in Section 4.4.2, Anglican programs, or queries, are compiled using the macro `query` which provides a Clojure function that can be passed to one of the provided inference algorithms. The key element of this compilation for providing the desirable properties discussed in the last section and a convenient interface for the inference algorithms is that Anglican compiles queries to *continuation passing style* (CPS) [Appel and Jim, 1989] Clojure functions.¹ At a high level, a continuation is a function that represents the rest of the program. CPS is a style of functional programming that uses a series of continuations to represent the program through a series of nested function calls, where the program is run by evaluating each function and then passing the output to the continuation which invokes the rest of the program. This is perhaps easiest to see through example. Consider the simple function `+`, which in Clojure has syntax `(+ a b)`. The CPS transformed version of `+`, which we will call `+&` takes an extra input of the continuation \mathcal{P} and invokes it after evaluation such that we have `(defn +& [a b P] (P (+ a b)))`. More generally, for any simple function f , we have that its the CPS transformation is `(defn f& [args P] (P (f args)))`.² We will use this notation of adding an `&` to an

¹WebPPL also does a CPS style transformation, namely to a purely functional subset of Javascript.

²Note that in practice, the continuation is usually set to be the first argument in order to provide support for functions with a variable number of inputs.

expression name to denote its CPS transformation throughout. To give a more detailed example, the CPS transform of the program (`max 6 (* 4 (+ 2 3))`) would be

```
(fn [P] (+& 2 3 (fn [x] (*& 4 x (fn [y] (max& 6 y P))))))
```

where `*&` and `max&` are analogous to `+` and `max` defined as before. Here our first continuation is

```
(fn [x] (*& 4 x (fn [y] (max& 6 y))))
```

Note that the CPS transformed code is itself a function because it itself takes a continuation.

Things are a little trickier for general expression that are neither literals nor simple first order functions, for example, binding forms like `let`, Anglican special forms like `sample`, and branching statements like `if`. For these expressions, the high-level idea is the same, but the CPS transformation is, unfortunately, expression specific and must, in general, be implemented on a case-by-case basis. For example, one can CPS transform `let` by going from

```
(let [x (foo1 1) y (foo2 2)] (foo3 x y)) to  
(fn [P] (foo1& 1 (fn [x] (foo2& 2 (fn [y] (foo3& x y P)))))).
```

noting that within the `(fn [x] .)` closure, `x` is bound to the input of the function, giving behavior synonymous to the original `let` block. Another special case of particular note is `loop-recur` blocks. These can be CPS transformed by explicitly redefining them as a self-recursive function which can then be transformed in the normal way. For example,

```
(loop [x 10] (if (> x 1) (recur (- x 2)) x)) becomes  
(fn [P] ((fn foo [x] (if (> x 1) (foo (- x 2)) (P x))) 10))
```

where we have exploited the fact that `fn` allows the function to be named (in this case to `foo`) so that it can call itself.

In CPS style code, functions never return (until the final tail call) and every function takes an extra input corresponding to the continuation. This would be a somewhat awkward method for writing programs, as the whole program must be written as a single nested function. However, it can be a very useful form to compile to as the execution of the program becomes exceptionally simple and just involves evaluating functions and passing the output to the next continuation – it explicitly linearizes the computation. For our purposes, having access to functions representing the rest of the program in the form of continuations will be particularly useful as it will allow for partial program evaluations. It will also be convenient for adding checkpoints at particular points in the program – namely at the `sample` and `observe` calls – where control is handed over to the inference algorithm.

Compilation of an Anglican query, triggered through the `query` macro, is done in recursively in a top down manner. The key function in doing this, called `cps-of-expression`, dispatches to the individual CPS transformations by matching types of expression, or, if necessary, directly by key-word. Individual CPS transformations then recursively call `cps-of-expression` or themselves if necessary, e.g. if the top level call is a `let` block, until the full query is transformed.

The individual CPS transformations in Anglican are marginally more complicated than the framework we have laid out thus far. This is because it is necessary to not just run the program, but also track its state from a probabilistic perspective, storing things such as sample weights and other probabilistic side-effects. To deal with this, the transformed Anglican continuations take as input an *internal state*, which we will denote as `$state`, in addition to the computed value. Thus, for example, the transformation for a simple function becomes³

```
(defn f& [args P $state] (P (f args) $state)).
```

More generally, we will simply pass on `$state` unchanged except for the Anglican special forms which can use and/or manipulate the internal state. `$state` itself is defined to be a hash map, initialized as follows

```
(def initial-state {:log-weight 0.0 :result nil ...})
```

where `...` includes some fields we will not directly consider at the moment and some algorithm specific fields (e.g. information required to the retained particle in PMCMC methods). Here the field `:log-weight` allows the program to be assigned a (relative) weight as accumulated by, for example, `observe` statements or importance weights when sampling from a different distribution than that provided to the `sample` statement. The return for each sample in our inference will effectively be the `$state`, hence the inclusion of the `:result` field which is set to the output of the query at its tail call.

One of the key components of the Anglican compilation is the transformation applied to the special forms and in particular the probabilistic forms `sample` and `observe`. These are respectively transformed to the Clojure record constructors `->sample` and `->observe` which have the call syntaxes of `(->sample id dist P $state)` and `(->observe id dist value P $state)`, where `id` is a unique checkpoint identifier (e.g. the $\{1, \dots, n_s\}$ and $\{1, \dots, n_o\}$ identifiers we used in 4.3.2) set at compilation time, and `dist` and `value` are the original inputs

³As before, the original arguments are actually last in the argument list for the true implementation.

to the `sample` and `observe` statements. The final return of the program is similarly transformed to the record constructor (`->result $state`). At a high level, one can think of a Clojure record as defining a new class type (here `trap.sample`, `trap.observe`, and `trap.result` respectively) with given fields (here `:id`, `:dist` etc). Our constructors thus create an object of the given type with appropriately set fields. The significance of this is that it allows definition of a multimethod, which we call `checkpoint`, to provide a runtime polymorphism (i.e. single interface) for dispatching depending on the checkpoint type and the inference algorithm. In other words, we will have one function, `checkpoint`, whose behavior can be redefined for different checkpoint types and inference types. There are many consequences of this. Firstly, our compiler does not need to be inference algorithm specific because we can use `checkpoint` to distribute the behavior to the required inference algorithm at run time. Secondly, it creates an abstraction barrier for writing inference algorithms – implementing an inference algorithm now only requires us to implement, along with a top level function `infer` that we will discuss later, new methods describing the behavior of `checkpoint` at `sample` and `observe` checkpoints. Furthermore, these can be inherited from other inference algorithms, for example, the `observe` checkpoints for particle Gibbs are inherited from SMC in Anglican’s implementation.

A slightly more subtle consequence of compiling to a constructor with typed output is that we will use this to catch the checkpoints themselves. Once compiled, individual instances of a program in the Anglican inference engines are run using the `exec` function. The role of `exec` is to run the program until it reaches a checkpoint that requires control to be transferred to the top level inference function of a particular method, i.e. the `infer` function, such as when a particular trace has finished running or when interaction is required between different samples, e.g. the resampling step in SMC. In Anglican this is achieved using *trampolining*. In functional programming languages, trampolining is a process of looping execution where if an iteration of a loop returns a function, that function is immediately evaluated without passing forward any arguments, with this process continuing until a non-functional output is returned. The primary use of trampolining is for managing stack sizes by constructing a nested call structure of *thunks* (i.e. functions which require no input arguments) that when called by the trampolining function (called `trampoline` in Clojure) invoked the full set of nested calls without requiring a stack to be constructed or stored, as would be necessary for an ordinary nested function structure. In the context of our CPS transformations, we can do this by simply wrapping each call with an

anonymous function, namely converting `(foo args \mathcal{P} $state)` to `(fn [] (foo args \mathcal{P} $state))`, which will be carried out for all continuations except the checkpoints. Though a large part of the motivation for doing this in Anglican is similarly to maintain the stack size, it is also highly useful for using the checkpoints to trigger control to be transferred to the `infer` function. To be precise, the `exec` function is defined as

```
(defn exec [algorithm prog value $state]
  (loop [step (trampoline prog value $state)]
    (let [next (checkpoint algorithm step)]
      (if (fn? next) (recur (trampoline next)) next))))
```

where `algorithm` specifies the inference algorithm; `prog` is the program to call, comprising of either the full CPS compiled program output by `query` or a continuation representing the rest of the program; `value` is the input required by `prog`, comprising of either the original program inputs or the value passed to the continuation; and `$state` is the program state as before. Here we see that `exec` first creates the variable `step` by making a trampolined call to `prog`. As all continuations are now represented by anonymous functions with no inputs except for our checkpoints, this will run until it hits one of those checkpoints, returning the corresponding constructed checkpoint object. In other words, this causes the program to run until it reaches a `sample` or `observe` statements, or it reaches the end of the program. This is a highly desirable behavior, as it means the deterministic elements of our program are run as normal. Once returned, our multimethod `checkpoint` is called using `algorithm` and `step`, which distributes to the appropriate `checkpoint` implementation based on the value of `algorithm` and the type of `step` (e.g. calling to the `sample` checkpoint method of an algorithm if it is of type `trap.sample`). Note that individual `checkpoint` implementations are based on using `step` as the only input of note, which, as we remember, is a Clojure record containing fields providing information on the distribution object, the state, etc. Invoking the appropriate checkpoint method will cause inference algorithm specific behavior, e.g. updating a weight in `$state`, and provide a return value `next`. If `next` is a function, the loop is recurred, with `step` now replaced by the output of a trampolined call of `next`. If `next` is not a function, the `exec` function terminates, returning `next`. The reason for this looping is that it allows different inference algorithms to specify different occurrences for when control needs to be passed back to the `infer` function in an algorithm specific way, by defining the checkpoint methods to either return a checkpoint object (for which the `exec` call will terminate) or the continuation wrapped

```
(query [y]
  (let [s (sample (gamma 1 2)) ]
    (observe (normal 0 s) y)
    s))
```

Figure 7.1: Example compilation of an Anglican query (above) to a CPS Clojure function (right). Here '`S30744`' and '`O30742`' provide unique identifiers for the (lexical) sample and observe statement respectively, while `var30743` and `do30741` are function identifiers.

```
(fn [y $state]
  (->sample 'S30744
    (gamma 1 2)
    (fn var30743 [s $state]
      (->observe 'O30742
        (normal 0 s)
        y
        (fn do30741 [_ $state]
          (->result s $state))
        $state)))
    $state))
```

in a thunk (for which execution will continue). For example, when running SMC, action distinct to running the program forwards only needs to be taken at the `observe` statement checkpoints. As different traces may have a different number of `sample` statements between observations, it is therefore convenient to have a function that does not terminate at the `sample` checkpoints, returning only once an `observe` or the end of the program is reached. On the other hand, for MCMC samplers, we will need to externally control the sampling behavior and so it may be necessary to return control at each `sample` statement.

We have now demonstrated how an Anglican query is compiled, a summarizing example for which is provided in Figure 7.1. We have also laid out a framework for writing inference algorithms in Anglican: we need to implement methods of the `checkpoint` multimethod and a top level inference function `infer`. In the rest of this Chapter we will explain how this abstraction allows us to write inference algorithms suitable for arbitrary programs.

7.3 Writing Inference Algorithms in Anglican

Taking stock, what has our compilation given access to and what do we not have access to? The key upshots of our compilation are that we have access to a continuation representing the rest of the program at any point during the execution and the interactions between the inference back-end and the query code happens only through the `sample` and `observe` statements and the final returned `$state` of each execution. Consequently, we have means of running the program forwards and controlling the behavior at each `sample` and `observe` statement. We can stop or restart the program at any one of our checkpoints and choose whether to do so adaptively, for example, by killing off certain evaluations or duplicating others. Once a program is run, we can test the effect of changing one or more of our sampled variables in an MCMC fashion, though it

may be difficult to statically determine an appropriate global proposal as we can only establish the structure of the target through evaluation. Although we might be able to do so with other code analysis, we do not directly have access to any information about independence relationships or even knowledge under what conditions a certain variable will exist. We can transfer information from one sampling iteration to the next using a database, giving us the potential to avoid repeated computation or adaptively learn proposals. In theory, we can query the unnormalized density $\gamma(x_{1:n_x}, \lambda)$ of any fixed set of parameter values $x_{1:n_x}$, given fixed inputs λ , by effectively making `sample` operate as an `observe` statement. However, it may be difficult, or even impossible, to find values of $x_{1:n_x}$ that have non-zero probability unless they are generated by running the program forwards. In particular, it might be arbitrarily hard to find a trajectory that satisfies $\mathcal{B}(x_{1:n_x}, \lambda) = 1$ without forward sampling from the program. It is liable to be even more difficult to externally construct a valid proposal to generate consistent estimates through, for example, importance sampling based schemes or that will lead to ergodic Markov chains, particularly if the program contains a potentially unbounded number of variables.

These availabilities and restrictions suggest that Anglican is, and universal PPSs more generally are, best suited to *evaluation based* inference methods. At a high level, we can think of such methods as acting like a controller wrapping around the standard program execution (or potentially multiple simultaneous executions). When the program hits a checkpoint, control is transferred to the inference engine, providing information about the current state through `$state` and about the current checkpoint command (i.e. checkpoint type, distribution object, etc). The inference engine then decides exactly how the checkpoint command should be executed (e.g. how to sample the new variable for a `sample` statement), updates the `$state` appropriately, and decides if and how the execution should continue. Once an execution is complete (i.e. the return checkpoint is reached), the inference controller decides what to run next, which could, for example, be an entirely new independent execution or an MCMC update to the current execution. Two important things the inference controller does not do is alter the deterministic elements of the program (which we can think of as being single deterministic functions from one checkpoint to the next because our collapsing through trampolining) or do further analysis on the program source code itself.

There are four functions required to define an Anglican inference algorithm more generally: a top level `infer` function and three `checkpoint` implementations for types `trap.sample`,

`trap.observe`, and `trap.return`. The `infer` implementation must always be written anew, but the `checkpoint` implementations can be inherited from another inference algorithm of default behavior. Other than some top level book keeping, the user inference command `doquery` directly calls the `infer` function of the specified inference algorithm, providing as input the CPS-transformed query, the fixed query inputs, and inference algorithm specific options. The `infer` function is required to then return a lazy infinite sequence of samples, each in the form of a `$state`. To carry out inference, `infer` uses the `exec` function introduced earlier to run (partial) executions of the program, which will run until they hit a checkpoint that returns something other than a thunk (see below).

All of the `checkpoint` implementations take as their only input of note an instance of the relevant Clojure record. Here `trap.sample` has fields `:id` which is a unique identifier for the corresponding lexical `sample` statement, `:dist` which is the distribution object input, `:cont` which is the continuation function \mathcal{P} , and `:state` which is the current instance of `$state`. Meanwhile, `trap.observe` has the same fields and additionally a `:value` field giving the observation and `trap.result` has only the `:state` field. Each `checkpoint` method should either return a thunk, in which case the `exec` function will resume running, or an instance of the relevant Clojure record, in which case `exec` terminates and returns control to the `infer` function (or some intermediary function used by the `infer` function). For example, in SMC methods then we will want to return control to `infer` at an `observe` point to do the resampling, while all methods return control for a `return` checkpoint. Default behaviors are provided for each checkpoint that dictate their behavior unless overwritten by a particular inference algorithm. The default behavior of `sample` is to sample from the distribution object and return a thunk that calls the continuation with this sample and `$state` as input arguments. The default behavior of `observe` is to update the `:log-weight` field in `$state` with the current observation term and then call the continuation with inputs `nil` and `$state`. The default behavior of `return` simply returns the `trap.result` object.

7.4 General Purpose Inference Strategies

As we previously alluded to, the simplest inference strategy we can carry out is importance sampling. This is in fact so simple in a current framework that it uses the default behavior of all the checkpoints, while the `infer` function only involves constructing a lazy infinite sequence of the output from independent calls of `exec` on the full program.

7.4.1 MCMC Strategies

We have already explained why it might be difficult to construct a global MH proposal for our program due to the difficulties in varying dimensionality and unknown variable supports. One solution to this is to try and use compilation to establish this support so that a valid proposal can be specified. However, doing this in general manner is a somewhat challenging and remains an open problem in field. Another, more immediately viable, approach is to use a proposal that looks to update particular x_j in the trace in a component-wise MH manner (see Section 5.3.4.5), potentially rerunning the rest of the program after that choice if necessary. In the context of PPSs such approaches are generally known as either single-site MH, random database sampling, or lightweight MH (LMH) and were originally suggested by [Wingate et al., 2011].⁴ There are two key factors that make such approaches viable. Firstly, if we update term x_j in our trace, there is no need to update any of the factors in our trace probability that occur before the sampling x_j , while we may be able to avoid evaluating many of those after as well by establishing conditional independence. Secondly, the support for a particular x_j is typically known (as we have access to the appropriate distribution object) and so it is generally possible to specify an appropriate proposal for an individual x_j . Even if that transpired not to be possible, simply using the prior as the proposal is still often reasonable as individual x_j will typically be low dimensional. However, a key downside of this approach is that changing a particular x_j might lead to an invalid trace and checking might require revaluation of the entire rest of the trace, making it an $O(n_x + n_y)$. Perhaps even more problematically, if n_x is not fixed then, unless we make adjustments to the algorithm, the approach will not produce a valid Markov chain. Similarly, as we showed in Section 5.3.4.5, there are models for which component-wise MH approaches lead to reducible Markov chains that no longer admit the correct target. The emphasis on branching in universal PPSs further means that the chance of falling into this category of invalid models is relatively high. As noted by [Kiselyov, 2016]), this is a rather serious issue missed (or at least not acknowledged) by Wingate et al. [2011] and various follow-up implementations. See also issues highlighted by [Hur et al., 2015] in other implementations. The problem is not shared by all implementations though, with the Anglican LMH method, amongst others, not suffering from the issue. More generally, there are means

⁴The MH acceptance ratio in the original version of this work is incorrect so we point the reader to the following updated version <https://stuhlmuller.org/papers/lightweight-mcmc-aistats2011.pdf>.

of potentially overcoming both the reducibility and computational issues of LMH as we will discuss later, but they still represent noticeable practical and theoretical hurdles.

As a simple illustrative approach that avoids some of the theoretical pitfalls associated with LMH approaches [Wood et al., 2014], consider an MH sampler whose proposal is simply to choose one of the **sample** statements, m , uniformly at random from $\{1, \dots, n_x\}$, propose a new x'_m using a local reversible MH kernel for that **sample** statement $\kappa(x'_m|x_m)$ (which can always be independently sampling from $f_m(x_m|\phi_m)$ if necessary) and then rerun the entire rest of the program from that point. This equates to using the proposal (omitting our trace validity term on the basis that this always holds because we are sampling from the generative model)

$$\begin{aligned} q(x'_{1:n'_x}|x_{1:n_x}) &= q(m|x_{1:n_x})q(x'_m|x_m, m)q(x'_{m+1:n_x}|x_{1:m-1}, m, x'_m)\mathbb{I}(x'_{1:m-1}=x_{1:m-1}) \\ &= \frac{1}{n_x}\kappa(x'_m|x_m)\mathbb{I}(x'_{1:m-1}=x_{1:m-1}) \prod_{j=m+1}^{n'_x} f_{a'_j}(x'_j|\phi'_j) \end{aligned} \quad (7.3)$$

which in turn gives an acceptance probability of

$$\begin{aligned} P(\text{Accept}) &= \min \left(1, \frac{\gamma(x'_{1:n'_x}, \lambda)q(x_{1:n_x}|x'_{1:n'_x})}{\gamma(x_{1:n_x}, \lambda)q(x'_{1:n'_x}|x_{1:n_x})} \right) \\ &= \min \left(1, \frac{\kappa(x_m|x'_m)f_{a_m}(x'_m|\phi_m)}{\kappa(x'_m|x_m)f_{a_m}(x'_m|\phi_m)} \frac{n_x}{n'_x} \frac{\prod_{k=k_0(x_{1:m})+1}^{n'_y} g_{b'_k}(y'_k|\psi'_k)}{\prod_{k=k_0(x_{1:m})+1}^{n_y} g_{b_k}(y_k|\psi_k)} \right) \end{aligned} \quad (7.4)$$

where $k_0(x_{1:m})$ is equal to the number of **observe** statements encountered by the partial trace $x_{1:m}$. Here we have used the fact that the trace probability factors before x_m cancel exactly, while the **sample** terms for $m + 1$ onwards cancel between the target and the proposal. We can intuitively break down the terms in (7.4) by first noting that the first ratio of terms is what we would get from doing MH targeting $f_{a_m}(x_m|\phi_m)$ (note also that these terms cancel if we propose “from the prior” by just independently sampling a new x'_m from the **sample** statement). The next ratio of terms, n_x/n'_x reflect the fact that if our new trace is longer it is less likely that we would have chosen the point m to resample and vice versa. The final ratio of terms reflects the ratio of the likelihood weight for the new generated section of the trace over the existing section of the trace.

This approach avoids the reducibility issues because it includes as a possible step generating a completely new trace from the generative model. However, it will clearly be heavily limited in practical performance because, for modest typical n_x , each iteration is effectively using importance sampling in $n_x - m$ dimensions such that, once the sampler has burnt in, its acceptance

rate will typically decrease dramatically with dimension. Each iteration is also $O(n_x + n_y)$ as the complete new trace needs to be proposed each time. To get around these issues, we would like to have some concept of whether we can update x_m without invalidating the trace. When possible, we could solve this problem using code analysis or compilation to establish the Markov blanket of x_m in order to know immediately which terms will be unaffected and so do not need re-proposing or re-calculating. This can be an effective approach and is the underlying principle in a number of LMH approaches Yang et al. [2014]; Mansinghka et al. [2014]; Ritchie et al. [2016]. One needs to be careful, however, not to reintroduce reducibility issues and, in general, correctness of LMH schemes is far from trivial and perhaps requires further consideration in the literature.

Even if we do not have a convenient means of extract Markov blankets, we will still generally desire to reuse $x_{m+1:n_x}$ if it produces a valid trace, i.e. if $\mathcal{B}([x_{1:m-1}, x'_m, x_{m+1:n_x}], \lambda) = 1$, and reducibility issues can be guarded against, in order to avoid the terrible scaling in the acceptance rate of 7.4 with $n_x - m$. One way to do this would be to propose a new x'_m in the same way but then deterministically run the program forward with the old $x_{m+1:n_x}$ to evaluate whether the trace is valid, noting that if it is, it must also be the case that any extension or reduction of this (i.e. increasing or decreasing n_x) is invalid as the program is deterministic given $x_{1:n_x}$ (remembering that we have defined $x_{1:n_x}$ as be the raw **sample** outputs not program variables). If $x_m \rightarrow x'_m$ gives a valid trace, then $\gamma([x_{1:m-1}, x'_m, x_{m+1:n_x}], \lambda)$ will be well defined (though not necessarily non-zero) and we can use the update as a proposal with needing to regenerate $x_{m+1:n_x}$. Note though that as the a_j , b_k , ϕ_j , and ψ_k terms downstream of m can change, the probability of the new trace still needs recalculating. In this scenario, our acceptance ratio becomes

$$P(\text{Accept}) = \min \left(1, \frac{\gamma(x'_{1:n_x}, \lambda) \kappa(x_m | x'_m)}{\gamma(x_{1:n_x}, \lambda) \kappa(x'_m | x_m)} \right) \quad (7.5)$$

where all terms in $\gamma(x'_{1:n_x}, \lambda)$ (i.e. both **sample** and **observe**) will need to be evaluated for $j \geq m$, as will $\gamma(x_{1:n_x}, \lambda)$ if these are not already known.

If, on the other hand, our trace becomes invalid at any point (noting that we can evaluate the validity of sub traces as we rerun them), we can resort to resampling the trace anew from the required point onwards. Note that we can do this validity evaluation and regeneration during the same single forward pass through trace and that whether we do regeneration is deterministic

for given $x_m - x'_m$ pair (and thus does not affect the MH acceptance ratio by symmetry). If we regenerate from `sample` ℓ onwards then we now have

$$P(\text{Accept}) = \min \left(1, \frac{\gamma(x'_{1:n_x}, \lambda) \kappa(x_m | x'_m) n_x \prod_{j=\ell}^{n_x} f_{a_j}(x_j | \phi_j)}{\gamma(x_{1:n_x}, \lambda) \kappa(x'_m | x_m) n'_x \prod_{j=\ell}^{n'_x} f_{a'_j}(x'_j | \phi'_j)} \right). \quad (7.6)$$

We can further overcome reducibility issues with such a scheme by forcing a fresh trace generation not only when we realize the trace is invalid, but also when we find a term in our trace with probability zero. Once this occurs, it is clear the that full trace probability must be zero, even if it produces a valid path. We could just immediately reject the trace, but we would then fall foul of reducibility problems. By instead regenerating the rest of the trace in this scenario, then at each iteration we can propose any value of x_1 that has non-zero marginal mass under $\gamma(x_{1:n_x}, \lambda)$ regardless of our current state, so we clearly have mixing on x_1 . For a given value of x_1 , we can similarly propose any value of x_2 with non-zero density under the marginal conditional distribution of $x_2 | x_1$. As we have mixing of x_1 , this now implies we have mixing on $x_{1:2}$ as well. By induction, of method now leads to mixing on all of $x_{1:n_x}$, which coupled with detailed balance provides an informal demonstration of the consistency of the method.

We can refine this process by using the concept of a database. To do this we mark each `sample` statement in the trace with a unique identifier that is common for all traces that evaluate the same `sample` statement at the same point, i.e. points in the trace for which both the `sample` number j and the lexical `sample` identifier a_j are the same. In our database then we can store previous sample and deterministically return when returning to the `sample` statement with the same identifier, keeping the sample if it still produces a valid partial trace with non-zero probability, regenerating it if not. Thus triggering regeneration of x_j no longer necessarily requires regeneration of x_{j+1} . Note the importance of points in the database being defined by both j and a_j – if we hit the same sample lexical sample statement at a different point in the program, we always need to redraw it. Care is needed to ensure superfluous terms are removed from the database at each iteration – it should contain only terms from the current trace. If we use $\mathbb{D}(j) = 0$ to denote terms taken from the database and $\mathbb{D}(j) = 1$ to indicate terms that are redrawn, then our acceptance ratio now becomes

$$P(\text{Accept}) = \min \left(1, \frac{\gamma(x'_{1:n_x}, \lambda) \kappa(x_m | x'_m) n_x \prod_{j=m+1}^{n_x} \left(f_{a_j}(x_j | \phi_j) \right)^{\mathbb{D}(j)}}{\gamma(x_{1:n_x}, \lambda) \kappa(x'_m | x_m) n'_x \prod_{j=m+1}^{n'_x} \left(f_{a'_j}(x'_j | \phi'_j) \right)^{\mathbb{D}(j)}} \right). \quad (7.7)$$

We finish by noting that our identifies for points in the database, namely both j and a_j being the same, is potentially stronger than necessary and there may be more useful addressing schemes. Remembering back to Section 4.3.2, each of `sample` and `observe` statements is exchangeable up to the required inputs being in scope. Now consider the case where the update $x'_m \leftarrow x_m$ triggers an inconsequential extra `sample` to be invoked between points j and $j + 1$, with everything else staying the same. Under our current system then all points after j would need to be resampled. However, our program would define the same distribution if this superfluous `sample` statement came at the end of the program, in which case our method would mean that $x_{j+1:n_x}$ no longer necessarily need updating. From a more practical perspective, we can consider using more useful naming strategies for our database entries that exploit this exchangeability such that x'_{j+2} could, for example, inherit from x_{j+1} [Wingate et al., 2011]. Though this should intuitively not effect the convergence of estimates based on the program output, the formal proof is not immediately trivial and is perhaps missing from the literature.

Anglican's implementations including RMH and ALMH

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7.4.2 Particle Based Inference Strategies

7.4.2.1 Sequential Monte Carlo

Going from importance sampling to SMC in our framework is remarkably simple from an implementation perspective [Wood et al., 2014]. The behavior of the `sample` and `result` checkpoints is kept as per the default. Keeping the default behavior for the former implicitly means that our inference will use a bootstrap proposal (i.e. the generative model is taken as the proposal). Though not technical required, this is still a highly convenient choice of proposal as amongst other things, this ensures that we can always sample from the proposal and that the proposal is valid in terms of its tail behavior (presuming the conditional probabilities are bounded). The `observe` checkpoints are redefined to carry out the same operations, but return a `trap.observe` record rather than a thunk, returning control to the `infer` function. This means that calling `exec` for the SMC checkpoint setup will run the program up to and including the next `observe` statement. Consequently, if we run multiple threads of `exec` at once, each corresponding to a separate particle, these will all stop exactly when the next resampling point is required for SMC. Thus all the `infer` function needs to do for SMC, other than some bookkeeping to e.g. check when the sweep is complete, is alternate between mapping an `exec`

call across all of the particles and performing resampling steps (remembering to reset the internal weights for the traces to be the same). The marginal likelihood estimate can also be calculated in the standard way, therefore the SMC algorithm can produce the required lazy infinite sequence of output samples by running independent SMC sweeps and setting the weights in the returned samples to include the factor from both the sweep and the sample.

From a theoretical perspective, running SMC in Anglican requires us to make one small model assumption – that the value of n_y is fixed. In practice, this assumption is usually satisfied, particularly if there are no observations of internally sampled variables. Violations of the assumption are caught at run time. Given a fixed n_y , then we are able to define the series of targets for SMC as being distributions induced by running the program up to the t^{th} `observe` statement for $t \in \{1, \dots, n_y\}$, namely

$$\gamma_t(x_{1:n_x}, \lambda) = \begin{cases} \prod_{j=1}^{n_x} f_{a_j}(x_j | \phi_j) \prod_{k=1}^t g_{b_k}(y_k | \psi_k) & \text{if } \mathcal{B}_t(x_{1:n_x}, \lambda) = 1 \\ 0 & \text{otherwise} \end{cases} \quad (7.8)$$

where $\mathcal{B}_t(x_{1:n_x}, \lambda)$ is a function establishing the validity of the partial program trace. More formally, we can define $\mathcal{B}_t(x_{1:n_x}, \lambda)$ as being a function indicating validity of a trace for transformation of the original program that terminates after making its t^{th} `observe`. It may be that executions corresponding to different particles have not gone through the same `sample` and `observe` statements at any particular point, but this is not a problem⁵. As provided that n_y is fixed, (7.8) still defines an appropriate series of targets for SMC inference.

A point of note here is that although changing the position of the `observe` statements in our program does not change the final distribution targeted by running SMC, it can change the intermediate target distributions, by adjusting at what point during the series of targets the `sample` statements are introduced. Consequently, changing the position of the `observe` statements can have a dramatic effect on the practical performance of the inference, after all, placing all the `observe` statements just before the program returns will cause the algorithm to reduce to basic importance sampling. The earlier the `observe` statements are in the program, or more precisely the later variables are sampled relative to the `observe` statements, the better inference will perform as the better the information can be incorporated into the resampling. Tricks such as lazily sampling variables (such that the `sample` statement only gets invoked when the variable is actually used) can, therefore, lead to substantial performance gains.

⁵A least not a theoretic problem. This could still be somewhat detrimental to practical performance

7.4.2.2 Particle Gibbs

Provide one does not try to support the special treatment of global variables that particle gibbs allows (i.e. restricting to the iterated CSMC case), extending SMC to particle gibbs is relatively straightforward in our framework. From a theoretical perspective, the algorithm extends from the SMC case in the same way as outside of the probabilistic programming framework. From a practical perspective there are two distinct challenges. Firstly, resampling for CSMC sweeps does not maintain the target distribution in the same way as SMC and so one has to be careful that there is no possibility for gratuituous resampling. At first this would make it seem like one would need to take care not to resample after the n_y^{th} observe. However, as resampling and choosing the retained particle uniformly at random from the present particles turns out to be identical to sampling the retained particle in proportion to weight and as so it turns out that this is actually fine. Secondly, we need a method of storing and retrieving the state of the retained particle in a manner that allows other particles to inherit from it. Given our inference methods do not use a stack, this is done by storing the raw $x_{1:n_x}$ samples within `$state` for each particle and then retrieving them for the retained particle. The retained particle is thus re-run in a deterministic fashion from a stored $x_{1:n_x}$, regenerating all the variables in the program and the continuation. This is achieved by editing the `sample` checkpoint so that it deterministically retrieves the x_j for the retained particle, but samples normally for other particles. For both it is also stores the current x_j for each particle in case this particle becomes the retained particle at the next sweep. Provided one is running a reasonably large number of particles the extra computational cost for re-running the retained particle is negligible, but the need to store all the $\{\hat{x}_{1:n_x}^n\}_{n=1}^N$ can noticeably increase the memory requirements. Other than these minor complications, the extension from SMC to particles Gibbs in the probabilistic programming setting is identical to that for conventional settings as disucssed in Section 6.2.2.

7.4.2.3 Interacting PMCMC

Given the particle Gibbs and SMC implementations, Interacting PMCMC can be implemented relatively simply by using those implementations for the CSMC and SMC sweeps respectively. All checkpoint implementations are inherited from particle Gibbs and the extension does not have any distinct challenges unique to probabilistic programming. We note though that the Anglican implementation of iPMCMC exploits the algorithmic ability for parallelization by

creating a pool of threads to distribute computation of the different nodes. Consequently, the implementation has substantial computational benefits over say particle Gibbs, in addition to the improved per-sample performance demonstrated in Section 6.3.

7.4.3 Other Methods

Though it would be impractical to do justice to all of the methods one can use for general purpose in universal PPSs, some other algorithms of particular note include.

- The particle cascade [Paige et al., 2014] is an asynchronous and anytime variant of SMC. This can provide improved in-sweep parallelization compared to SMC / PMCMC methods and provides an alternative to PMCMC methods for overcoming memory restrictions in SMC. It has the crucial advantage over PMCMC methods of maintaining an unbiased estimate of the marginal likelihood, but can suffer issues in instability in the number of particles produced by the schedule strategy during a sweep and it does not permit any distinct treatment of global variables.
- Particle Gibbs with ancestor sampling (PGAS) [Lindsten et al., 2014; van de Meent et al., 2015] looks to alleviate degeneracy for the particle Gibbs algorithm by performing ancestor sampling for the retained particle. This can substantially improve mixing for the early samples, but can result in very large computational overheads, sometimes requiring $O(Nn_y^2)$ computation (compared to $O(Nn_y)$). This can be partly mitigated by using database techniques van de Meent et al. [2015] to avoid unnecessary repeated computation, but still typically is substantially more computationally intensive than standard particle Gibbs.
- Some black-box variational methods [Ranganath et al., 2014; Kucukelbir et al., 2015] have been developed for general purpose PPSs [Wingate and Weber, 2013] including Anglican Vandemeent et al. [2016]; Paige [2016]. Though these can suffer from difficulties in finding effective addressing schemes and or high variance of the ELBO gradients, they can still form an effective approximate approach for certain problems, see e.g. [Paige, 2016].

7.4.4 Which inference algorithm should I use?

The question of which algorithm one should use is a critical, but somewhat subjective and problem dependent question. We now provide some (inevitably biased) recommendations for which inference algorithms to use in Anglican that should be taken as a very rough guide rather than clear cut truth.

Firstly, except for very low dimensional problems, importance sampling should be avoided as it is almost universally worse than, e.g. SMC. Similarly, there is very little reason to use PIMH or vanilla LMH over more advanced approaches. The relative performance of the MCMC based and particle based (including PMCMC) methods will depend on the amount of structure that can be exploited in the system by the respective approaches. The particle based approaches will generally be substantially preferable when the `observe` statements are interlaced with the `sample` statements so that the intermediate information can be exploited. However, if all the variables need to be sampled before making observations or if all the variables are completely independent of one another given the data, SMC will reduce to importance sampling, while the MCMC methods can still take advantage of hill-climbing effects.

If using SMC or PMCMC based methods, then, as per Section 6.1.5.1, the most important thing is not the exact algorithm, but ensuring that sufficient particles are used. Because PMCMC methods in probabilistic programming do not use separate updates for global parameters, using enough particles can be even more important than in conventional settings. Presume that your computational budget is M particles and your memory budget is N particles. Our recommendation is that If $M < N$, you should just run a single SMC sweep with M particles – all the more advanced algorithms are mostly setup to avoid issues that are easily solved by running more particles when you can. For larger values of M , then you should keep the number of particles as high as possible (ideally N). If M is less than around $20N$, most methods will give similar per sample performance. For larger values of M , then our recommendation is to use iPMCMC as the go-to algorithm as this will rarely be noticeably worse than other PMCMC approaches and sometimes substantially better. Two possible exceptions to this are that PGAS and the particle cascade can sometimes still be better in such settings. For example, PGAS can be relatively very effective in models whether there is very extreme restriction on the number of particles that can be run.

8

A Predominantly Bayesian Approach to Optimization

8.1 Introduction

From designing engineering components to managing portfolios and tuning control systems, optimization is used ubiquitously throughout engineering and the sciences. Whereas inference dealt with cases where we desire to calculate an expectation or approximate a probability distribution given data, optimization considers cases where only a single output is desired. For example, in a decision problem only a single action can be taken, meaning a single optimal action must be found. It it is also often used in machine learning as a tractable alternative when full inference is infeasible Murphy [2012].

In general, all optimization problems can be expressed in the form

$$\begin{aligned} \theta^* &= \arg \max_{\theta \in \vartheta} f(\theta) \\ \text{s.t. } g_i(\theta) &= c_i \quad \forall i \in \{1, \dots, n_e\} \\ h_i(\theta) &\geq d_i \quad \forall i \in \{1, \dots, n_i\} \end{aligned} \tag{8.1}$$

where $f: \vartheta \rightarrow \mathbb{R}$ is the target function with input variables θ , ϑ is the space of permissible solutions, $g_i(\theta) = c_i$ are equality constraints, $h_i(\theta) \geq d_i$ are inequality constraints, and θ^* is the optimum value of θ . We note that careful definition of ϑ can remove the need to define constraints explicitly, a fact which we exploit in Chapter 9, while minimization problems can be dealt with by maximizing $-f(\theta)$.

A large range of problems are covered by (8.1). For example, there are arbitrary different types ϑ might correspond to from the set of real values to the setup of race car. There is also a wide range of information that might be known about f - we might have access to the exact function and all its derivatives, or it might be that the only way to evaluate it is to conduct an

expensive real world experiment with stochastic results at a given value of θ . Naturally this leads to a plethora of different techniques to suit the different problems at hand such as dynamic programming [Bellman, 2013], evolutionary algorithms [Bäck, 1996], combinatorial optimization methods [Papadimitriou and Steiglitz, 1982], gradient based methods [Boyd and Vandenberghe, 2004], and Monte Carlo based methods [Robert, 2004]. Such optimization algorithms can be split into two key categories: local optimization approaches and global optimization approaches. The latter strictly aims to solved the true target as laid out in (8.1), but is in often infeasible in practice. The former instead only tries to find a point where there is no better point in its immediate vicinity. Local optimization is generally used either when the problem is known or expected to be convex (such that there is only one such local optimum), or when global optimization is infeasible and a local optimum is expected to still for a good approximate solution.

In a probabilistic machine learning context, common optimization problems include maximum likelihood (ML) estimation, maximum a posterior (MAP) estimation, maximum marginal likelihood (MML) estimation, marginal maximum a posteriori (MMAP) estimation, and risk minimization.

ML estimation looks to find the most probable set of parameters for a given distribution, namely given data Y they look to find

$$\theta^* = \arg \max_{\theta \in \vartheta} p(Y|\theta). \quad (8.2)$$

Many classical statistical and machine learning techniques on based on ML estimation [Hastie et al., 2001] as it is intuitively the most probable set of parameters given data and a model. However, this can be prone to overfitting and so it is typically requires the inclusion of regularization terms.

MAP estimation extends ML estimation to also include a prior term

$$\theta^* = \arg \max_{\theta \in \vartheta} p(Y|\theta)p(\theta). \quad (8.3)$$

This provides regularization compared to ML estimation (indeed many priors and ML regularization methods are exactly equivalent [Bishop, 2006]), but still has a number of drawbacks compared to full inference when the latter is possible. For example, the position of the MAP estimate is dependent of the parametrization of the problem: if some mapping to input variables is provided $\phi = \eta(\theta)$, this changes the position of the optimum, i.e. in general $\phi^* \neq \eta(\theta^*)$. Using

a MAP estimate also of course incorporates less information into the predictive distribution than using a fully Bayesian approach. Nonetheless, MAP estimation is still an important tool of Bayesian machine learning, necessary when a single estimate or decision is required, or when inference is infeasible. Note that when ϑ is bounded or takes on only finite values, then ML estimation is recovered from MAP estimation by using a uniform prior.

MML estimation is often referred to using a number of different names such as expectation maximization, type-II maximum likelihood estimation, hyperparameter optimization, and empirical Bayes. Despite the multitude of names, which originate from different application areas, the aim of all these methods is the same: to maximize the likelihood of a model marginalized over some latent variables X , namely

$$\theta^* = \arg \max_{\theta \in \vartheta} p(Y|\theta) = \arg \max_{\theta \in \vartheta} \mathbb{E}[p(Y, X|\theta)|Y, \theta] \quad (8.4)$$

where the above expectation is with respect to $p(X|\theta)$. Common examples of MML problems include parameter tuning, decision making, and model learning.

MMAP estimation varies from MML in the same manner as MAP from ML: the inclusion of a prior on the target parameters. Specifically it aims to optimize

$$\theta^* = \arg \max_{\theta \in \vartheta} p(Y, \theta) = \arg \max_{\theta \in \vartheta} \mathbb{E}[p(Y, X|\theta)p(\theta)|Y, \theta]. \quad (8.5)$$

As with MAP estimation compared with ML estimation, MMAP estimation problems extend MML by allowing for prior information or regularization to be included.

As with MML and MMAP estimation, risk minimization problems consider the optimization of an expectation. The key difference is in the fact that they are a *minimization* rather than a *maximization*, namely they look to find

$$\theta^* = \arg \min_{\theta \in \vartheta} \mathbb{E}[L(X, Y; \theta)] \quad (8.6)$$

for some loss function L which is parametrized by θ and is typically positive only. Depending on the context, Y can either be taken as fixed, or the expectation can be over both X and Y . The latter corresponds to the classical risk taken in the frequentist view of supervised. At first the change from maximization to minimization might seem trivial. However, the fact that probabilities are positive only means that the two problems behave very differently. For example, imagine the problem of designing a bridge and let $Y = \emptyset$, X be the loadings the bridge will see in its

lifetime, and θ the design. Even though the probability of failure will generally be very low, the loss in the case where the bridge collapses is very large. Therefore the expected loss is dominated by rare adversarial events and the desire is to choose a “safe” value for θ . Such a problem cannot be encoded effectively as a MML or MMAP estimation problem where we maximizing the probability of the bridge not collapsing, as this expected probability cannot be dominated by the rare adversarial loading cases. In essence, expectations over probabilities are “optimistic” and by construction focus on the more probable cases.

In the rest of this chapter we will consider in more depth two approaches that have been used extensively through machine learning to solve optimization problems such as those discussed: stochastic gradient ascent and Bayesian optimization. As we will see, these represent quite starkly different approaches and are thus suited to very different problems.

8.2 Stochastic Gradient Ascent

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8.3 Gaussian Processes

Before introducing Bayesian optimization (BO), we first digress to introduce Gaussian processes (GPs) as they are an essential precursor to much of the BO literature. As we will show in the next section, BO relies on modelling the target with a surrogate, which can be used to estimate the expected value and uncertainty estimates for the value of a function away from points that have been evaluated. The most common surrogate taken in the BO literature is a GP and the one we will use later in Chapter 9, hence their central importance to the BO method.

Informally one can think of a GP [Rasmussen and Williams, 2006] as being a nonparametric distribution¹ over functions. Equivalently, one can think of it as a generalization of a Gaussian distribution to (uncountably) infinite dimensions. Practically, they are powerful tool for regression, classification Kuss and Rasmussen [2005], and feature extraction Lawrence [2004]. We focus here on regression as it is generally the simplest usage and the most relevant to our needs.

¹Technically speaking they are a stochastic process not a distribution.

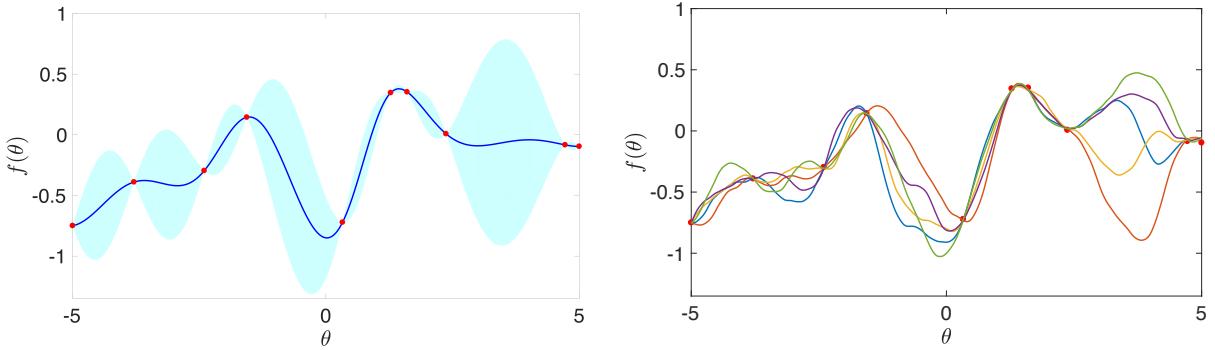


Figure 8.1: Example GP regression for points shown in left dots. Shown left is GP where the solid dark blue line is the mean of the GP and the light blue shading is the mean ± 2 standard deviations. Shown right is 4 example functions drawn from the GP which uses a mixture of Matérn-3/2 and Matérn-5/2 kernels as per Section 9.3.2.

8.3.1 Function-Space View

A GP is fully specified by a mean function $\mu: \vartheta \rightarrow \mathbb{R}$ and covariance function $k: \vartheta \times \vartheta \rightarrow \mathbb{R}$, the latter of which must be a bounded (i.e. $k(\theta, \theta') < \infty, \forall \theta, \theta' \in \vartheta$) and reproducing kernel (we will return to this in depth later in Section 8.3.3). We can informally describe a function f as being distributed according to a GP:

$$f(\theta) \sim GP(\mu(\theta), k(\theta, \theta')) \quad (8.7)$$

which by definition means that the functional evaluations realized at any finite number of sample points is distributed according to a multivariate Gaussian. Note that the inputs to μ and k need not be numeric and as such a GP can be defined over anything for which kernel can be defined.

Figure 8.1 shown an example of a GP regression with a small number of data points $\{\theta_j, v_j\}_{j=1:m}$. Here we wish to regress a function f from θ to y . We place a GP prior on f

$$f_{\text{prior}}(\theta) \sim GP(\mu_{\text{prior}}(\theta), k_{\text{prior}}(\theta, \theta')),$$

and take $\mu_{\text{prior}}(\theta) = 0 \ \forall \theta$, noting the generality of this choice as one can simply regress $y - \mu_{\text{prior}}(\theta)$ if a different μ_{prior} is desired. We further take for the covariance function

$$\begin{aligned} k_{\text{prior}}(\theta, \theta') = & \sigma_{3/2}^2 \left(1 + \sqrt{3} \frac{\theta - \theta'}{\rho_{3/2}} \right) \exp \left(-\sqrt{3} \frac{\theta - \theta'}{\rho_{3/2}} \right) + \\ & \sigma_{5/2}^2 \left(1 + \sqrt{5} \frac{\theta - \theta'}{\rho_{5/2}} + \frac{5}{3} \left(\frac{\theta - \theta'}{\rho_{5/2}} \right)^2 \right) \exp \left(-\sqrt{5} \frac{\theta - \theta'}{\rho_{5/2}} \right) \end{aligned} \quad (8.8)$$

which corresponds to a combination of a Matérn-3/2 and Matérn-5/2 kernel with hyperparameters $\sigma_{3/2}, \sigma_{5/2}, \rho_{3/2}$, and $\rho_{5/2}$. We will return to how to choose the kernel function and these parameters later, the latter of which are set to $\sigma_{3/2} = 0.04, \sigma_{5/2} = 0.47, \rho_{3/2} = 1.89$, and $\rho_{5/2} = 0.98$ in Figure 8.1. For now we simply note that the choice of covariance function and its parameters will heavily influence the nature of functions generated by the GP, dictating things such as smoothness and characteristic lengths scales of variation.

An important property of a GP that we now exploit is that it is conjugate with a Gaussian likelihood. Let $\Theta = \{\theta_j\}_{j=1:m}$ and $V = \{v_j\}_{j=1:m}$ be the set of observed inputs and outputs respectively. We use a separable Gaussian likelihood function

$$p(V|\Theta, f) = \prod_{j=1}^m p(v_j|f(\theta_j)) = \prod_{j=1}^m \frac{1}{\sigma_n \sqrt{2\pi}} \exp\left(-\frac{(v_j - f(\theta_j))^2}{2\sigma_n^2}\right) \quad (8.9)$$

where σ_n is an observation noise. It is set to 0.001 in our example. Combining this with the GP prior we previously defined leads to GP process posterior and predictive distribution. To see this we can consider the joint distribution between the points we have considered so far, and a new set of points $\{\Theta^*, V^*\}$. Introducing the shorthand $k_{\text{prior}}(\Theta, \Theta^*) = \begin{bmatrix} k_{\text{prior}}(\theta_1, \theta_1^*) & k_{\text{prior}}(\theta_1, \theta_2^*) & \dots \\ k_{\text{prior}}(\theta_2, \theta_1^*) & k_{\text{prior}}(\theta_2, \theta_2^*) & \dots \\ \dots & \dots & \dots \end{bmatrix}$ then we have by the fact that any finite realisations of points is Gaussian

$$\begin{bmatrix} V \\ f^* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} k_{\text{prior}}(\Theta, \Theta) + \sigma_n^2 I & k_{\text{prior}}(\Theta, \Theta^*) \\ k_{\text{prior}}(\Theta^*, \Theta) & k_{\text{prior}}(\Theta^*, \Theta^*) \end{bmatrix}\right) \quad (8.10)$$

where I is the identity matrix, $\mathbf{0}$ is a vector of zeros, f^* is the true function values at Θ^* (such that $V^* - f^* \sim \mathcal{N}(0, \sigma_n^2 I)$). We can now use standard results for Gaussians (see e.g. Petersen et al. [2008]) to get the conditional distribution for f^* given all the other variables

$$\begin{aligned} f^* | \Theta, V, \Theta^* &\sim \mathcal{N}(\mu_{\text{post}}(\Theta^*), k_{\text{post}}(\Theta^*, \Theta^*)) \quad \text{where} \\ \mu_{\text{post}}(\Theta^*) &= k_{\text{prior}}(\Theta^*, \Theta) \left[k_{\text{prior}}(\Theta, \Theta) + \sigma_n^2 I \right]^{-1} V \\ k_{\text{post}}(\Theta^*, \Theta^*) &= k_{\text{prior}}(\Theta^*, \Theta^*) - k_{\text{prior}}(\Theta^*, \Theta) \left[k_{\text{prior}}(\Theta, \Theta) + \sigma_n^2 I \right]^{-1} k_{\text{prior}}(\Theta, \Theta^*). \end{aligned} \quad (8.11)$$

Now as Θ^* are arbitrary points, this corresponds to our predictive distribution. Further, as the predictive distribution is still a GP, we can refer to our model as having a GP posterior

$$f_{\text{post}}(\theta) | \Theta, V \sim \text{GP}(\mu_{\text{post}}(\theta), k_{\text{post}}(\theta, \theta')).$$

Going back to Figure 8.1, we see the result of this process. Our GP regression gives us a posterior mean function that represents the expected value at every possible input points,

along with variance that represents our subjective uncertainty in the value of the function at that point. It is important to note that, as is always the case in Bayesian modelling, these uncertainty estimates are generally an underestimate, as they do not account for the “unknown unknowns”. Figure 8.1 also shows that we can draw from the GP by choosing some set of evaluation points Θ^* and then drawing from (8.11). We see that there is larger variation in the function values away from the points that have been evaluated, as would be expected.

We finish our introduction to GPs from the function space point of view by noting that the marginal likelihood for our model is also analytic. Specifically we have

$$\begin{aligned} \log p(V|\Theta) = & -\frac{1}{2}V^T \left[k_{\text{prior}}(\Theta, \Theta) + \sigma_n^2 I \right]^{-1} V \\ & -\frac{1}{2} \log |k_{\text{prior}}(\Theta, \Theta) + \sigma_n^2 I| - \frac{m}{2} \log 2\pi \end{aligned} \quad (8.12)$$

where m is the number of points in Θ . This is important as it means it will be tractable to optimize or do inference over the GP hyperparameters.

8.3.2 Kernels and Hyperparameters

As we showed in the last section, GPs form powerful and expressive priors over functions. In this section we show that their practical behaviour varies substantially depending on the choice of the covariance function, aka kernel, and the hyperparameters. Informally, we can think of the kernel as expressing the similarity between the evaluation of the function at two different input points θ and θ' . When $k(\theta, \theta')$ is large, these evaluations are strongly correlated such that the evaluations will have similar values. When it is small, there is little correlation between the points and so their evaluations will be roughly independent. Note that it is possible for $k(\theta, \theta') < 0$ provided $\theta \neq \theta'$, but as kernels must be positive definite functions as explained in the next section, $k(\Theta, \Theta)$ is always a positive definite matrix. Though it is not necessary for the kernel to be stationary (i.e. that it only depends on $\theta - \theta'$ rather than the absolute values), we will not consider non-stationary cases further here (see Rasmussen and Williams [2006] for further information).

Figure 8.2 shows some simple example kernels. Note x here is equivalent to θ in our notation. The figure shows that the qualitative behaviour of the GP changes substantially with changes to the kernel. All of these kernels also behave substantially differently to the compound Matérn kernel we considered in the last section. The choice of kernel is therefore critical to the performance of GPs. Though there is work, including some of our own, that examines

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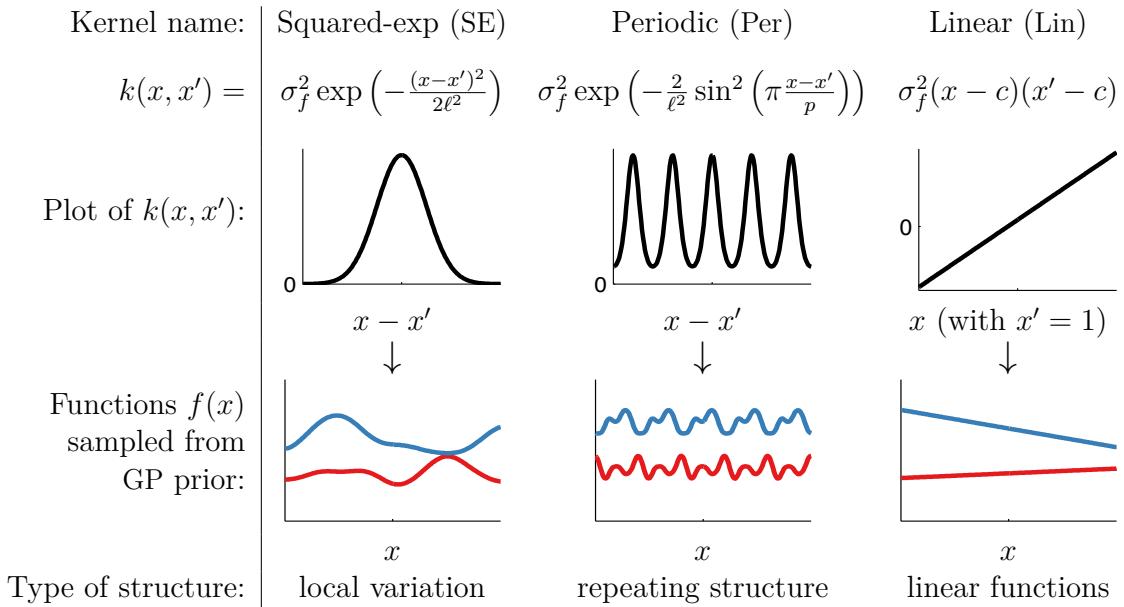


Figure 8.2: Example basic kernels. Figure taken from David Duvenaud's PhD Thesis.

methods for learning the kernel directly Duvenaud et al. [2013]; Lloyd et al. [2014]; Wilson et al. [2014]; Janz et al. [2016], this is typically too computationally intensive to carry out in practice. One must therefore either use prior knowledge about the problem, or use an relatively general purpose to ensure that the nuances of the data are not overwhelmed.

A particularly common problem in the choice of kernel is in the desired level of smoothness. At the one extreme, one can use the squared exponential kernel

$$k_{\text{se}}(\theta, \theta') = \sigma_f^2 \exp\left(-\frac{\|\theta - \theta'\|_2^2}{2\rho^2}\right) \quad (8.13)$$

which is infinitely differentiable. It is also sometimes known as the exponentiated quadratic kernel. Here σ_f^2 is the “signal standard deviation” - a hyperparameter that effects the scaling of the output from the GP: the larger σ_f , the higher the average standard deviation of the function. ρ is a hyperparameter that dictates the characteristic length scale of variation for the function - the higher ρ is, the slower the correlation decreases as one moves away from the current point, and therefore the less “wiggly” the function is. Both these hyperparameters are common to most commonly used kernels. Although the presented kernel is isotropic, this is easily relaxed by having a different ρ for each dimension.

In many practical problems, the squared exponential kernel is too smooth. One possible

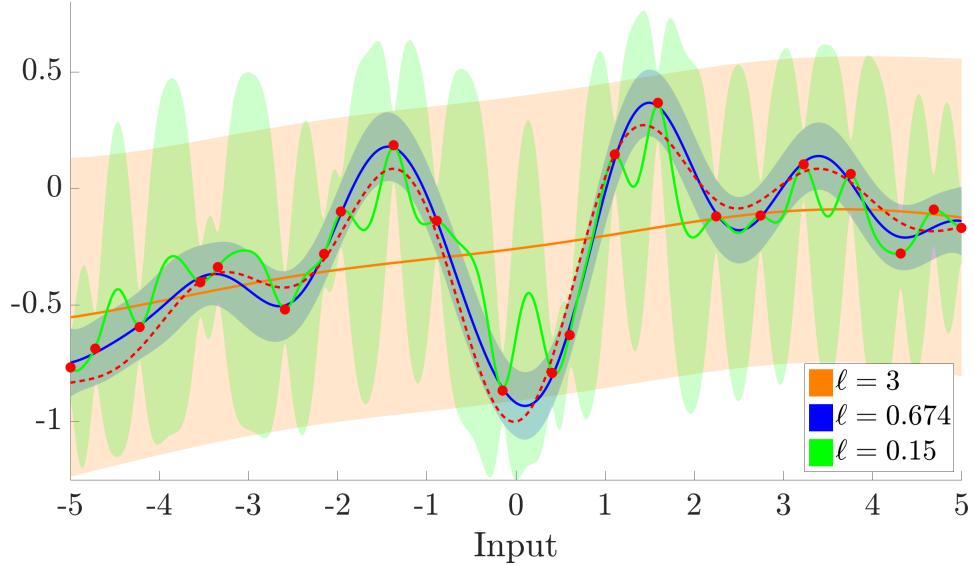


Figure 8.3: Effect of changing the length scale for Matérn-5/2 kernel. NEEDS CLEANING

alternative in these scenarios are the Matérn kernels. The Matérn- ν kernel given by

$$k_\nu(\theta, \theta') = \sigma_f \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{\rho} \|\theta - \theta'\| \right)^\nu K_\nu \left(\frac{\sqrt{2\nu}}{\rho} \|\theta - \theta'\| \right) \quad (8.14)$$

where K_ν is the modified Bessel function of second kind order ν and $\Gamma(\cdot)$ is the gamma function, is $\lfloor \nu - 1 \rfloor$ times differentiable and therefore different values of ν can be used to express different levels of smoothness. Typically ν is set to $n + 1/2$ for some integer n , for which it has a simple closed form Rasmussen and Williams [2006].

Though the choice of kernel function is critical input for a GP, the choice of hyperparameters such as the scaling and length scale can have equally significant impact on the behaviour. Figure 8.3 shows the effect of changing the length scale of a Matérn-5/2 kernel. When the length scale is too large as shown in red, the regressed function is overly smooth and does not capture the data. When the length scale is too small, as shown in green, wild fluctuations are permitted in between the datapoints such that there is very high uncertainty between points, but also potentially overfitting as the regressor can model all the fluctuations in the data including those originating simply from noisy evaluations. As the hyperparameters are rarely known upfront, one must typically either optimize them, or perform inference over them to produce a mixture of GPs output.

8.3.3 Weight-Space View, Reproducing Kernel Hilbert Space, and Derivation of a Gaussian Process

One of the key advantages of GPs is that they can be used effectively without needing to know the intricacies for why they work. The derivations we introduced in the last section and in particular the calculations required to derive the GP posterior were spectacularly simple, albeit computationally intensive (the need for a matrix inversion to calculate (8.11) means that training is $O(m^3)$ for m training points). However, what is going on beneath the surface is substantially more complicated, which is perhaps not surprising when one remembers that they are defined over uncountably infinitely many variables. To truly understand the underlying rational and assumptions for GPs, and to properly appreciate the restrictions on possible kernels, it is necessary to delve into GPs more formally, taking the so called weight-space view. In this section we therefore outline a more formal derivation of a GP from the viewpoint of reproducing kernels Hofmann et al. [2008] and show how they can be thought of as Bayesian linear regression using an infinite number of features. We start with the following definitions.

Definition 8.1. Let \mathcal{H} denote a vector space over \mathbb{R} . An inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is a function $\mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$ that is:

1. Linear $\langle au_1 + bu_2, v \rangle_{\mathcal{H}} = a\langle u_1, v \rangle_{\mathcal{H}} + b\langle u_2, v \rangle_{\mathcal{H}}$
2. Symmetric $\langle u, v \rangle_{\mathcal{H}} = \langle v, u \rangle_{\mathcal{H}}$
3. Has the properties $\langle u, u \rangle_{\mathcal{H}} \geq 0$ and $\langle u, u \rangle_{\mathcal{H}} = 0$ only if $u = \mathbf{0}$

Definition 8.2. A Hilbert space, \mathcal{H} , is a potentially uncountably infinite, vector space associated with an inner product and which contains Cauchy sequence limits.

Consider now the linear (in the weights \mathbf{w}) model

$$f(\theta) = \mathbf{w}^T Z(\theta) + \mu(\theta), \quad \mathbf{w} \sim \mathcal{N}(\mathbf{0}, C) \quad (8.15)$$

where $Z(\cdot) = [\zeta_1(\cdot), \dots, \zeta_m(\cdot)]^T$, $\zeta_a: \vartheta \rightarrow \mathbb{R}$ for $a = 1, \dots, m$ is a feature map in m -dimensional Hilbert space \mathcal{H} . For any set of points $\theta_1, \dots, \theta_t$ then $F = [f(\theta_1), \dots, f(\theta_t)]^T$

will be distributed according to a t -dimensional Gaussian with mean $[\mu(\theta_1), \dots, \mu(\theta_t)]^T$ and covariance $k(\theta_i, \theta_j) = Z(\theta_i)^T C Z(\theta_j)$, $\forall i, j \in \{1, \dots, t\}$. Note that

$$Z(\theta)^T C Z(\theta') = \sum_{a=1}^m \sum_{b=1}^m C_{ab} \zeta_a(\theta) \zeta_b(\theta') \geq 0, \quad \forall \theta, \theta' \in \vartheta \quad (8.16)$$

as C must be positive semi-definite for the distribution on \mathbf{w} to be well defined². This also means that the Cholesky decomposition $C^{1/2}$ exists and we can define $\Psi(\cdot) = C^{1/2} Z(\cdot) = [\psi_1(\cdot), \dots, \psi_m(\cdot)]^T$ to give a covariance function $k: \vartheta \times \vartheta \rightarrow \mathbb{R}$ in the form

$$k(\theta, \theta') = \langle \Psi(\theta), \Psi(\theta') \rangle_{\mathcal{H}} = \sum_{a=1}^m \psi_a(\theta) \psi_a(\theta') \leq \sqrt{\sum_{a=1}^m (\psi_a(\theta))^2} \sqrt{\sum_{a=1}^m (\psi_a(\theta'))^2} \quad (8.17)$$

where the inequality can be trivially shown using Cauchy-Schwarz. Now consider the case where m is uncountably infinite such that \mathcal{H} represents a functional space along with an inner product. Note that if $\Psi(\cdot)$ remains in ℓ_2 space, i.e.

$$\sum_{a=1}^{\infty} (\psi_a(\theta))^2 < \infty, \quad \forall \theta \in \vartheta, \quad (8.18)$$

then $k(\theta, \theta') < \infty$, $\forall \theta, \theta' \in \vartheta$ using the inequality from equation (8.17) and our covariance will remain bounded with infinitely many basis functions.

A key realisation is that the distribution of F only depends on Z and C through the inner product $\langle \Psi(\theta), \Psi(\theta') \rangle_{\mathcal{H}}$ such that we need never compute the potential high dimensional feature mappings if we can find a way to implicitly compute the inner product, for example if k has the reproducing property

$$\langle u(\cdot), k(\cdot, \theta) \rangle_{\mathcal{H}} = u(\theta), \quad \forall \theta \in \vartheta, \quad \forall u(\cdot) \in \mathcal{H}. \quad (8.19)$$

This is called the kernel trick, where we have used the representation $\Psi(\theta) = k(\cdot, \theta)$ noting that any feature map can also be thought of as parametrizing a mapping $\mathcal{H} \rightarrow \mathbb{R}$.

Definition 8.3. Let \mathcal{H} be a Hilbert space of functions on a space ϑ , the evaluations of which are in \mathbb{R} . A reproducing kernel of \mathcal{H} is a function $k: \vartheta \times \vartheta \rightarrow \mathbb{R}$ satisfying

1. $k(\cdot, \theta) \in \mathcal{H}, \quad \forall \theta \in \vartheta,$
2. k satisfies the reproducing property described in equation (8.19).

² $Z(\theta_i)^T C Z(\theta_j) = 0$ is only possible if \mathbf{w} lives in a lower dimensional subspace of \mathbb{R}^m

If k is a reproducing kernel then \mathcal{H} is reproducing kernel Hilbert space (RKHS). As $k(\theta, \theta') = \langle k(\cdot, \theta), k(\cdot, \theta') \rangle = k(\theta', \theta)$, all reproducing kernels are symmetric.

For the realisation of $k(\theta, \theta')$ at a finite number of points to be a valid covariance matrix we further require it to be positive definite, i.e:

$$\sum_{i=1}^n \sum_{j=1}^n \beta_i \beta_j k(\theta_i, \theta_j) \geq 0, \quad \forall n \geq 1, \forall \{\beta_1, \dots, \beta_n\} \in \mathbb{R}^n, \forall \{\theta_1, \dots, \theta_n\} \in \vartheta^n \quad (8.20)$$

which can be proved to be the case given the restrictions we have placed on k by noting

$$\sum_{i=1}^n \sum_{j=1}^n \beta_i \beta_j k(\theta_i, \theta_j) = \sum_{i=1}^n \beta_i \Psi(\theta_i)^T \sum_{j=1}^n \beta_j \Psi(\theta_j) = \left\| \sum_{i=1}^n \beta_i \Psi(\theta_i) \right\|_{\mathcal{H}}^2 \geq 0. \quad (8.21)$$

Consequently, (8.18) is a sufficient condition for the distribution of F to be a multivariate t -dimensional Gaussian with a valid and finite covariance matrix when we consider an uncountable infinite number of basis functions. Furthermore, we note that many choices for Ψ will lead to closed form analytic expressions of $\langle \Psi(\theta), \Psi(\theta') \rangle_{\mathcal{H}}$ without the need to ever calculate $\Psi(\theta)$ explicitly.

To show a simple example of this consider the one-dimensional case were $\theta \in \mathbb{R}$ and basis functions of the form $\psi_a = \sigma_w \exp\left(-\frac{(\theta - c_a)^2}{2\rho^2}\right)$ where $c_a \in [c_{\min}, c_{\max}]$ represents the centre of the basis function and ρ is a common length scale. Further specify that $\sigma_w^2 = \frac{\beta(c_{\max} - c_{\min})}{m}$, i.e. that σ_w^2 is proportional to the number of functions per unit length then we have

$$k(\theta, \theta') = \sum_{a=1}^m \frac{\beta(c_{\max} - c_{\min})}{m} \exp\left(-\frac{(\theta - c_a)^2}{2\rho^2}\right) \exp\left(-\frac{(\theta' - c_a)^2}{2\rho^2}\right). \quad (8.22)$$

Now assume that the basis functions are evenly space in $[c_{\min}, c_{\max}]$ and consider $m \rightarrow \infty$ then we recover the integral

$$k(\theta, \theta') = \beta \int_{c_{\min}}^{c_{\max}} \exp\left(-\frac{(\theta - c)^2}{2\rho^2}\right) \exp\left(-\frac{(\theta' - c)^2}{2\rho^2}\right) dc. \quad (8.23)$$

Now if we further take $c_{\min} \rightarrow -\infty$ and $c_{\max} \rightarrow \infty$ then the integral becomes analytic with solution:

$$k(\theta, \theta') = \sqrt{\pi} \rho \beta \exp\left(-\frac{(\theta - \theta')^2}{4\rho^2}\right). \quad (8.24)$$

which is the common squared exponential kernel in one dimension. Thus we have managed to analytically marginalize over all basis functions and are left with a simple expression that can be used to evaluate the covariance between any two given points that implicitly uses an uncountably infinite number of basis functions.

More generally, the Moore-Aronszajin theorem Aronszajn [1950] states that

Theorem 8.1. Any symmetric, positive definite kernel $k: \vartheta \times \vartheta \rightarrow \mathbb{R}$ has a unique RKHS for which k is a reproducing kernel.

In other words, if we define a kernel function that is symmetric $k(\theta, \theta') = k(\theta', \theta)$ and positive definite as per (8.20), then at least one corresponding feature map $\Psi: \vartheta \rightarrow \mathcal{H}$ must exist. Therefore a corresponding $Z: \vartheta \rightarrow \mathcal{H}$ and C must also exist (for example we can trivially take C as the identity matrix and $Z = \Psi$), and if we further ensure that k is bounded $k(\theta, \theta') < \infty, \forall \theta, \theta' \in \vartheta$, then finite realisations $[f(\theta_1), \dots, f(\theta_t)]^T$ of equation (8.15) must be distributed to a finite multivariate Gaussian distribution with mean $[\mu(\theta_1), \dots, \mu(\theta_t)]^T$ and covariance $k(\theta_i, \theta_j) \forall i, j \in 1, \dots, t$. We have therefore arrived at the following formal definition of a GP.

Definition 8.4. A Gaussian process describes the probability distribution for the functional realisations $f: \vartheta \rightarrow \mathbb{R}$ of (8.15) in the limit of uncountably many basis functions, noting that this distribution is fully defined by a mean function $\mu: \vartheta \rightarrow \mathbb{R}$ and a covariance function $k: \vartheta \times \vartheta \rightarrow \mathbb{R}$, the latter of which must be a positive definite (or equivalently reproducing), bounded kernel.

We can therefore think of GP regression as Bayesian linear regression using a feature mapping to a RKHS. This shows the power of a GP - for appropriate choices of kernel it uses an uncountable number of features - but also highlights the assumptions - the co-Gaussianity of the weights and reliance of the target function to fall in RKHS represented by the covariance function.

8.4 Bayesian Optimization

Bayesian optimization (BO, Mockus [1975]; Jones et al. [1998]; Osborne et al. [2009]; Brochu et al. [2010]; Shahriari et al. [2016b]) is a global optimization scheme that requires only that the target function can be evaluated (noisily) at any given point. It is derivative-free, naturally incorporates noisy evaluations, and is typically highly efficient in the number of function evaluations. It is therefore suited to problems where the target function corresponds to the output of a simulator, estimation scheme, algorithm performance evaluation, or other cases where the target is not known in closed form. It has been successfully applied to a number of applications and remains a fast growing area of active research.

ADD

The key idea of BO is to place a prior on f that expresses belief about the space of functions within which f might live. When the function is evaluated, the resultant information is incorporated by conditioning upon the observed data to give a posterior over functions. This allows estimation of the expected value and uncertainty in $f(\theta)$ for all $\theta \in \vartheta$. From this, an acquisition function $\zeta : \vartheta \rightarrow \mathbb{R}$ is defined, which assigns an expected utility to evaluating f at particular θ , based on the trade-off between exploration and exploitation in finding the maximum. When direct evaluation of f is expensive, the acquisition function constitutes a cheaper to evaluate substitute, which is optimized to ascertain the next point at which the target function should be evaluated in a sequential fashion. By interleaving optimization of the acquisition function, evaluating f at the suggested point, and updating the surrogate, BO forms a global optimization algorithm that is typically very efficient in the required number of function evaluations, whilst naturally dealing with noise in the outputs.

Although alternatives such as random forests [Bergstra et al., 2011; Hutter et al., 2011] or neural networks [Snoek et al., 2015] exist, the most common surrogate model used for f is a Gaussian process (GP) [Rasmussen and Williams, 2006]. Their are a number of characteristics that make GPs suitable for the surrogate model. For example, they are very powerful regressors that can accurately represent the function from relatively few evaluations, especially for low-dimensional smooth functions. They also naturally produce uncertainty estimates that are typically more accurate than those produced by alternatives which often have to resort to post-processing or heuristics to estimate uncertainty. It also leads to simple and tractable acquisition functions. Similarly, their ability to incorporate noisy observations is often helpful, though because GP inference is only analytic for Gaussian likelihoods, it is often impractical to incorporate non-Gaussian noise. This problem can be particularly manifest when the observations are bounded, such as when the target is a probability and thus always positive. A common way of dealing with this is to optimize a mapping of the original function, for example optimizing the log probability in MAP problem [Osborne, 2010].

When prior information is known about the function, the flexibility in choosing the covariance kernel can also be very helpful, for example allowing known smoothness to be incorporated. However, this can also be a curse as an inappropriate choice of kernel can severely happen the performance. In particular, it will typically be necessary to do inference over, or at least optimize, the GP hyperparameters. Another drawbacks to using GPs is poor scaling in the

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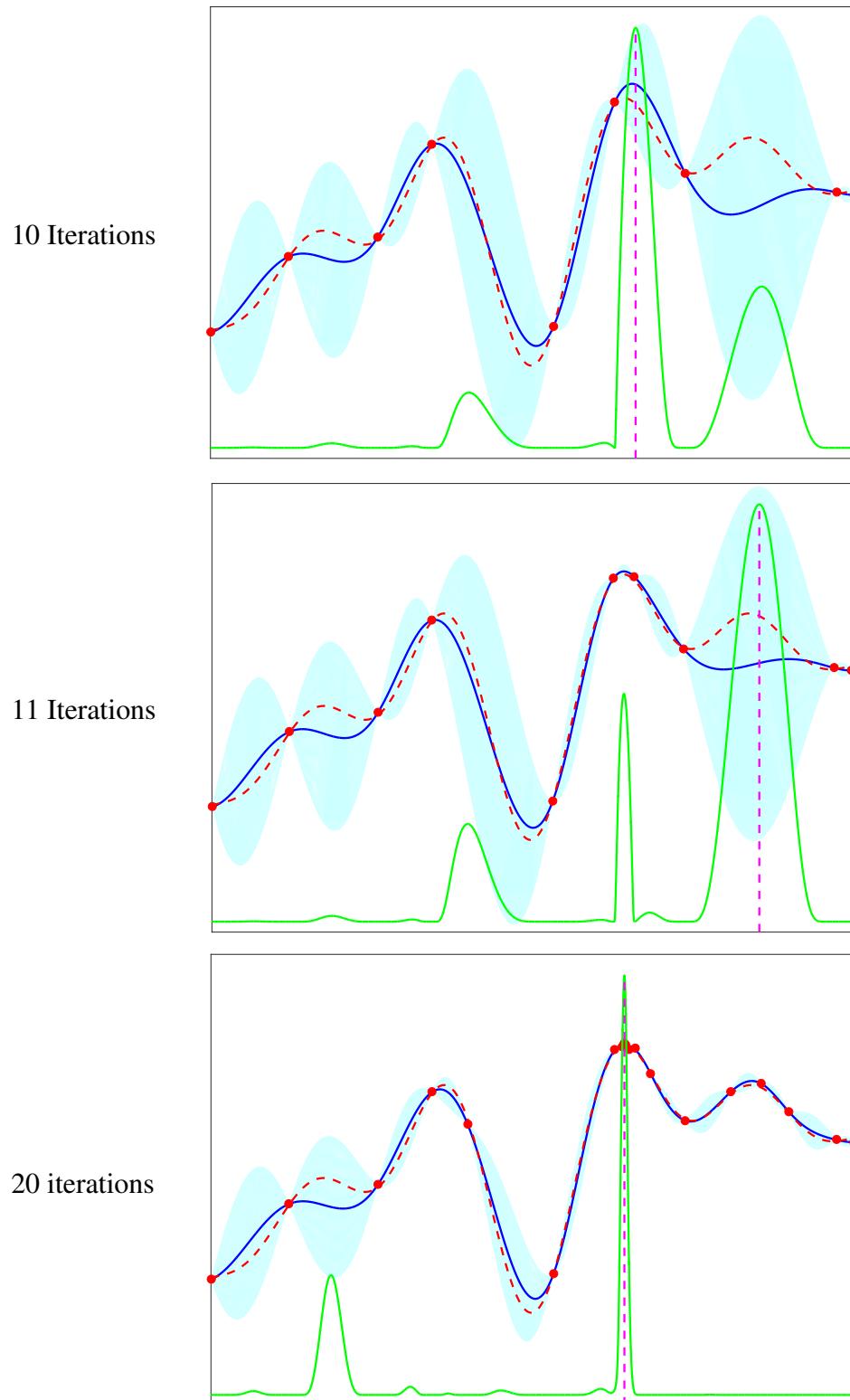


Figure 8.4: Illustration of using Bayesian optimization method to optimize the toy one dimensional problem given in (8.25). Red dots show the function evaluations, the dotted red line shows the true function, the solid blue line is the GP mean, the shaded region is the GP mean ± 2 standard deviations, the green line is the acquisition function, and the dotted purple line is the location of the maximum of the acquisition function. See main text for further description.

number of iterations - training is a $O(N^3)$ operation due to the required matrix inversion. This typically restricts BO using GPs to using at most hundreds of iterations unless appropriate approximations are made [Snelson and Ghahramani, 2006; Hensman et al., 2013]. Another drawback can be poor scaling in the dimensionality of the inputs - most common kernels rely on local modelling which can break down in high dimensions because points are typically far away from one another [Bengio et al., 2006].

Figure 8.4 shows BO being used to optimize the following simple one dimensional function

$$f(\theta) = \frac{\theta}{15} - \frac{\theta^2}{50} - \frac{\sin \theta}{\theta}, \quad -5 \leq \theta \leq 5 \quad (8.25)$$

with noisy observations $v \sim \mathcal{N}(f(\theta), 0.01^2)$. As we explained before, BO employs only point-wise function evaluations and so the optimization problem boils down to deciding

1. What input point should be evaluated at each iteration?
2. Which point of those evaluated is most optimal?

Both of these are done using a GP regressed to the existing evaluations, which therefore forms the first step of each BO iteration. As shown in Figure 8.4, this gives an estimated value and uncertainty for the function at every point in the form of the GP posterior mean $\mu_{\text{post}}(\theta)$ and marginal standard deviation $\sigma_{\text{post}}(\theta) = \sqrt{k_{\text{post}}(\theta, \theta)}$ where μ_{post} and k_{post} are as per (8.11). We will drop the $_{\text{post}}$ subscript in the rest of this chapter to avoid clutter. The second decision is now straight forward - our estimate for the most optimal point of those evaluated is simply the point with the highest mean.

To solve the first decision - where to evaluate next - we specify a so-called *acquisition function* $\zeta : \vartheta \rightarrow \mathbb{R}$ that encodes the relative utility of evaluating a new point. The optimum of this acquisition function is then the optimal point to evaluate at the next iteration. At a high level, the utility of a point is based on a trade off between *exploration*, namely the desire to evaluate points where our uncertainty is high to reduce the uncertainty in those regions, and *exploitation*, namely the desire to evaluate points where the expected function value is high so that we get a good characterization of the function in promising regions. One could alternatively think about this as wanting to refine the estimates of promising local optima and sample in places that are likely to contain a missing mode. We will return to discuss specific acquisition functions in depth in the next section and for now we simply note that the most desirable points to evaluate

will be those that provide both exploration and exploitation. For example, consider the expected improvement acquisition function (see (8.29)) after 10 iterations shown in green in Figure 8.4. This is reasonably large in the two regions of highest uncertainty, but it is highest in the region near the true global optima where both the expected value and uncertainty are high. After 11 iterations on the other hand, the uncertainty in this region has dropped dramatically and the point with the highest uncertainty now has the largest value for the acquisition function. Note that the scales for the acquisition functions are different for the different iterations and that the acquisition function typically decreases as more points are observed.

At first it might seem strange to replace our original optimization problem with another in the form of optimizing the acquisition function to choose the point to evaluate next. This new optimization problem is itself a global optimization of a typically highly multi-modal function and we need to carry it out at each iteration of the BO algorithm. Indeed if the target function f is cheap to evaluate, taking such an approach would be rather foolish. The key difference though is that the surrogate optimization problem can be solved without the need to evaluate the original target function. Therefore, if f is expensive to evaluate, this additional computation can be justified if it keeps the number of required evaluations of f to a minimum. There are also a number of other features that mean the problem of optimizing the acquisition function is typically much easier than the original target – it can be evaluated exactly, derivatives are often available, and provided an appropriate kernel is used then it is guaranteed to be smooth. It is also not typically necessary to ensure that the acquisition function is optimized exactly, as evaluating a point that is sub-optimal under the acquisition function simply means that a point expected to be less helpful is evaluated at the next iteration. This can be useful when the time for a BO iteration is comparable to a function evaluation as the amount of computational effort undertaken by the BO can be tuned to the problem at hand. It is also worth noting that the computational complexity for optimizing the acquisition function is theoretically less (in terms of BO iterations) than the GP training ($O(N^2)$ instead of $O(N^3)$), though in practice the two are typically comparable for the modest number of iterations BO is generally run for.

Going back to Figure 8.4, we see that BO works by interleaving regressing a GP to the evaluations, optimizing the acquisition function to find the next point to evaluate, evaluating the target function at that point, and the updating the GP regression again. After 20 iterations for our simple problem, the GP regression around the optimum has become very accurate, while

it is less accurate elsewhere. This highlights the sample efficiency of BO as it shows how computational resources are focussed on where they are required.

8.4.1 Acquisition Functions

As we previously explained, the GP posterior provides convenient analytic representations for the expected value and uncertainty in the function in the form of the GP posterior mean $\mu(\theta)$ and marginal standard deviation $\sigma(\theta)$ respectively. We now introduce a number of common acquisition functions, many, but not all, of which will use these representations directly.

The choice of acquisition function can be critical to the performance of Bayesian optimization and its choice forms a basis for a significant proportion of the Bayesian optimization literature [Shahriari et al., 2016b]. In particular, some acquisition functions have pathologies, for example a tendency to insufficiently explore, which can severely impede the performance of BO. This has lead to the development of some very powerful, but computationally intensive and algorithmically complicated, acquisition strategies (e.g. Hernández-Lobato et al. [2014]), such that there is often a speed / simplicity vs per iteration performance trade-off in their selection.

8.4.1.1 Probability of Improvement

One of the conceptually simplest acquisition functions is the probability of improvement (PI, Kushner [1964]), namely the probability that the function value at a point is higher than the current estimated optimum. A characterization of this is shown in Figure 8.5. As shown by, for example, Brochu et al. [2010], the probability of improvement has a simple analytic form because the marginal distributions for function evaluations are Gaussian. Specifically, let

$$\mu^+ = \max_{j \in \{1, \dots, m\}} \mu(\theta_j) \quad (8.26)$$

denote the point with the highest expected value and define

$$\gamma(\theta) = \frac{\mu(\theta) - \mu^+ - \xi}{\sigma(\theta)}, \quad (8.27)$$

where $\xi \geq 0$ is a user set parameter ($\xi = 0$ in Figure 8.5). The probability of improvement is then defined as the probability of improving the objective function by at least an amount ξ

$$\text{PI}(\theta) = p(f(\theta) \geq \mu^+ + \xi) = \Phi(\gamma(\theta)) \quad (8.28)$$

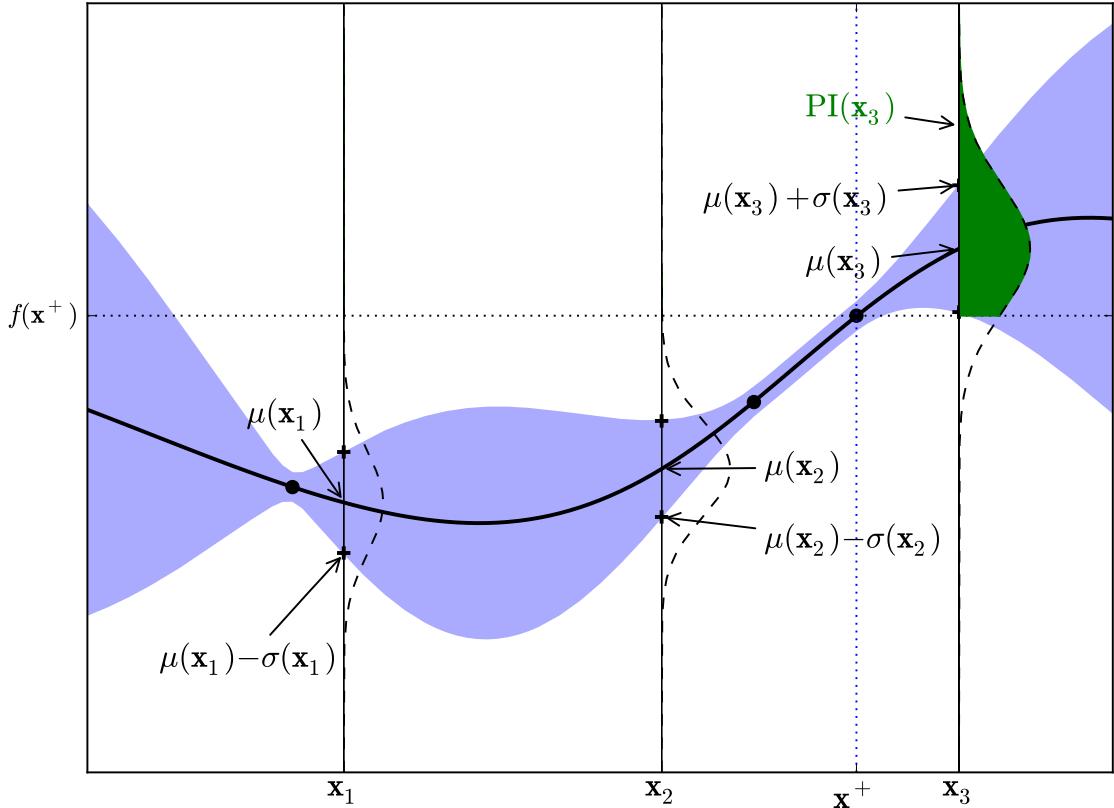


Figure 8.5: Explanation figure for probability of improvement, taken from Brochu et al. [2010]. The best point so far (i.e. evaluated point with the highest GP mean) occurs at \mathbf{x}^+ , with corresponding GP mean $\mu(\mathbf{x}^+)$ (for some reason $f(\mathbf{x}^+)$ is shown instead). The probability of improvement at any point corresponds to the marginal probability that the true function value at that point is larger than $\mu(\mathbf{x}^+)$. An example of which is shown at the point \mathbf{x}_3 , corresponding to the green shaded region, which is clearly substantially larger than at two other hypothetical points \mathbf{x}_1 and \mathbf{x}_2 . Note also that the expected improvement of \mathbf{x}_3 corresponds to the expectation of $\mathbf{x}_3 - \mathbf{x}^+$ under the distribution of the green shaded region, while the point $\mu(\mathbf{x}_3) + \sigma(\mathbf{x}_3)$ corresponds to the UCB acquisition function with $\kappa = 1$. REPLACE WITH OWN FIGURE

where $\Phi(\cdot)$ represents the unit normal cumulative distribution function. Note that $\xi = 0$ corresponds to pure exploitation and $\xi \rightarrow \infty$ corresponds to pure exploration. Typically for PI, one will employ a cooling schedule for ξ to incorporate the intuitive idea that one should first explore and then exploit. However, as shown by for example Jones [2001], the performance of the PI acquisition function is sensitive to the choice of ξ and therefore the cooling strategy requires careful tuning. Doing this in effectively in a general purpose way is very challenging, meaning that PI is rarely used in practice.

8.4.1.2 Expected Improvement

A method less sensitive to tuning is the expected improvement [Mockus, 1975]. It is conceptually similar to PI, but incorporates the idea that large improvements are more beneficial to small improvements. It therefore better represents the importance of exploration and is less prone to over-exploitation. It can also be calculated analytically for a GP (see e.g. Brochu et al. [2010]) leading to the following definition

$$\begin{aligned} EI(\theta) &= \int_{\mu^+ + \xi}^{\infty} p(f(\theta) | \mu(\theta), \sigma(\theta)) (f(\theta) - \mu^+ - \xi) df(\theta) \\ &= \begin{cases} (\mu(\theta) - \mu^+ - \xi) \Phi(\gamma(\theta)) + \sigma(\theta) \phi(\gamma(\theta)), & \sigma(\theta) > 0 \\ 0, & \sigma(\theta) = 0 \end{cases} \end{aligned} \quad (8.29)$$

where $\phi(\cdot)$ represents the probability density function of the unit normal distribution. The parameter ξ plays a similar role as for the PI, but in this case $\xi = 0$ no longer corresponds to pure exploitation. Lizotte [2008] suggests that cooling schedules on ξ are not helpful for EI and that $\xi = 0.01\mathbb{E}[\sigma(\theta)]$ where $\mathbb{E}[\sigma(\theta)]$ is signal standard deviation works well in almost all cases. Simply setting $\xi = 0$ is also a common choice, but it can be prone to doing insufficient exploration. Convergence rates for EI have been demonstrated by Bull [2011].

8.4.1.3 Upper Confidence Bounding

Another possible acquisition strategy is to maximize the upper confidence bound (UCB) for the function value [Lai and Robbins, 1985; Srinivas et al., 2009], namely

$$UCB(\theta) = \mu(\theta) + \kappa\sigma(\theta) \quad (8.30)$$

where $\kappa \geq 0$ is again a parameter that will control the exploration / exploitation trade off. This bound represents point at which the probability the function is less than this value is $\Phi(\kappa)$. A particularly nice feature of the UCB acquisition function is that given certain constraints on ϑ and k , κ can be chosen in a manner such that acquisition has bounded cumulative regret with high probability, this is known as GP-UCB [Srinivas et al., 2009]. However, the need to (often adaptively) set κ can be a noticeable drawback.

8.4.1.4 Information-Based Policies

At the end of the day, the aim of BO is to find the location of the optimum. The true utility of evaluating a new point is, therefore, in the information it provides about the location of the true maximum θ^* and the assistance it provides in guiding future evaluations. Though the latter of these is difficult to actively incorporate, the former is something that can be target in a principled manner by considering the distribution on the location of the maximum $p(\theta^*|\Theta, V)$ where Θ and V are the previously evaluated input and output points as per Section 8.3.

The simplest way this can be done is using Thompson sampling [Thompson, 1933], where instead of optimizing an acquisition function directly, one looks to sample the next point to evaluate from $p(\theta^*|\Theta, V)$ [Shahriari et al., 2014; Kandasamy et al., 2017]. In the GP setting, this is equivalent to sampling a particular function realisation f and then taking θ_{next} as the optimum of this particular realisation. This can prove surprisingly expensive, as sampling a joint realisation of a GP at M points is an $O(M^3)$ operation.

A more complicated, but theoretically more powerful approach, is to try and directly optimize for the point that will, in expectation, most reduce the uncertainty about the location of the maximum. These so called entropy search (ES) methods [Villemonteix et al., 2009; Hennig and Schuler, 2012; Hernández-Lobato et al., 2014] use as an acquisition function the expected gain in Shannon information about the location of the optimum, or equivalently the reduction in entropy of the location of the maximum. Namely they take

$$\zeta(\theta) = H[p(\theta^*|\Theta, V, \theta)] - \mathbb{E}_{p(v|\Theta, V, \theta)}[H[p(\theta^*|\Theta, V, \theta, v)]] \quad (8.31)$$

where $H[p(x)] = - \int p(x) \log p(x) dx$ is the differential entropy of its argument and $p(v|\Theta, V, \theta)$ is the predictive distribution of the GP such that $v \sim \mathcal{N}(\mu(\theta), \sigma(\theta)^2 + \sigma_n^2)$ as explained in Section 8.3.1. Entropy search methods are closely linked to the idea of Bayesian experimental design, in which an equivalent target has been used for some time Chaloner and Verdinelli [1995]. We return to Bayesian experimental design in detail in Chapter INSERT.

Unfortunately, (8.31) is not analytically tractable and so entropy search methods must rely on methods for approximately solving (8.31). This can be particularly difficult as (8.31) represents a nested estimation problem that cannot be solved simply by, for example, Monte Carlo [Rainforth et al., 2016a]. An important advancement in this regard was the development of an estimation scheme by Hernández-Lobato et al. [2014] that uses a combination of analytic approximations

and Monte Carlo sampling. Despite these approximations, the resulting predictive ES algorithm provides excellent empirical performance in terms of the number of function evaluations and remains arguably the state-of-the-art acquisition function for BO.

8.4.1.5 Other Acquisition Functions

Many more acquisition strategies have been developed than we have space to cover here. However, some of other strategies of particular note include

- Contal et al. [2014] construct an acquisition function from a combination of the GP mean and an approximation of the mutual information between the function and the noisy evaluations at the chosen input points. This leads to impressive theoretical and empirical results.
- Osborne et al. [2009]; González et al. [2016b] develop non-myopic methods that incorporate the effect of future hypothetical evaluations on the relative optimality of evaluating a point at the current iteration. Such lookahead methods can improve performance, but at the expense of substantially increased computational cost.
- Wang et al. [2016] introduce a strategy explicitly estimating then using the value of function maximum $f(\theta^*)$ and establish links connections between their approach, UCB, and PI.
- Swersky et al. [2013]; Shah and Ghahramani [2016]; Hernández-Lobato et al. [2016]; Feliot et al. [2017] introduce various acquisition functions for dealing with multi-objective problems where we wish to optimize many functions simultaneously. For example, they may try to approximate the so-called Pareto front, constituting of the set of non-dominated solutions.

8.4.2 GP Hyperparameters

Generally the performance of BO will be strongly dependent on the choice of GP hyperparameters α . Rather than optimizing for α it is natural, when tractable, to take a fully Bayesian view and marginalize over α Osborne et al. [2009]; Snoek et al. [2012], leading to mixture of GPs posterior. This was shown by Snoek et al. [2012] to substantially improve the performance

of BO. An easy way to do this for simple acquisition functions is to consider an integrated acquisition function corresponding to the expectation of the acquisition function over the GP hyperparameters [Snoek et al., 2012]

$$\bar{\zeta}(\theta) = \mathbb{E}_{p(\alpha|\Theta, V)} [\zeta(\theta; \alpha)] \quad (8.32)$$

$$= \frac{1}{p(V|\Theta)} \mathbb{E}_{p(\alpha)} [\zeta(\theta; \alpha) p(V|\Theta, \alpha)] \quad (8.33)$$

where $p(\alpha)$ is a prior over the hyperparameters, $p(V|\Theta)$ is a constant that can be ignored as it does not effect the position of the optimum, and $p(V|\Theta, \alpha)$ is the GP marginal likelihood as given in (8.12). The expectation can be approximated using Monte Carlo inference, with slice sampling [Neal, 2003; Murray and Adams, 2010] and Hamiltonian Monte Carlo [Duane et al., 1987; Hensman et al., 2015] being common choices.

8.4.3 Constraints

Bayesian optimization approaches mostly assume that the target function is constrained by a bounding box, i.e. that each input is independently constrained. In practice, this assumption is rarely fulfilled, though for technically unbounded problems then it is not uncommon for the user to be able to specify a box conveying the region where it is reasonable to assume the true optimum falls within the box. To go beyond this assumption, it is necessary to design strategies that can deal with constraints and strategies that deal with unbounded problems. Dealing with the former when using a GP surrogate can be particularly challenging, as simply setting the points that violate the constraints to have very low objective function evaluations will severely undermine the GP regression.

Known inequality constraints with simple closed forms can easily be incorporated into most BO methods by adapting the acquisition function to be arbitrarily bad when the constraints are violated [Gramacy and Lee]. In other words, the constraints can be incorporated by optimizing the acquisition function as a constrained optimization problem. If the constraints are not known a-priori and expensive to evaluate, then it is typically also necessary to model the constraints as well as the target function. Gardner et al. [2014] introduced a method for carrying out BO in the scenario where the constraint function is evaluated concurrently to the target function. Their approach learns the constraint function in a similar way as the target function using a Gaussian process and they then adapt the EI acquisition function to incorporate this constraint

information. In independently developed work, Gelbart et al. [2014] introduce a similar, but more general, approach where the constraints can be evaluated independently and the constraint evaluations may be noisy. Hernández-Lobato et al. [2016] take this further by showing that the trade-off between improving the models of the target and constraints respectively can be dealt with naturally by ES based acquisition strategies.

A weakness of all these approaches is that they do not allow for dealing with equality constraints and will similarly perform poorly for constraint functions that are not well modelled by a GP. They also do not guarantee that the target function will only be evaluated at places where the constraints are satisfied. This can be inefficient as evaluations are wasted and makes the method inappropriate for scenarios where it is essential that the constraints are never violated, for example if the constraints correspond to the failure of a component. In recent work that will be discussed at length in Chapter 9 [Rainforth et al., 2016b], we show how probabilistic programming can be used to overcome both these problems, creating a BO strategy that automatically satisfies the problem constraints at every evaluation, even when these constraints are equality constraints. Our method also introduces an approach for dealing with unconstrained BO problems.

8.4.4 Parallelization

In recent years there has been increased interest in performing Bayesian optimization in the setting where function evaluations can be performed in parallel [Contal et al., 2013; Desautels et al., 2014; González et al., 2016a; Kathuria et al., 2016]. Such methods usually predict a batch of evaluation points that are then evaluated simultaneously. It is desirable for the batch to both include points that have high acquisition functions values, but which are well separated to minimize the correlation between their outputs. Recent work by Kandasamy et al. [2017] has also looked at the case where evaluation times can vary greatly, such that it is desirable to carry out evaluations asynchronously in parallel, rather than in batches.

9

Automating Learning – Bayesian Optimization for Probabilistic Programs

We present the first general purpose framework for marginal maximum a posteriori estimation of probabilistic program variables. By using a series of code transformations, the evidence of any probabilistic program, and therefore of any graphical model, can be optimized with respect to an arbitrary subset of its sampled variables. To carry out this optimization, we develop the first Bayesian optimization package to directly exploit the source code of its target, leading to innovations in problem-independent hyperpriors, unbounded optimization, and implicit constraint satisfaction; delivering significant performance improvements over prominent existing packages. We present applications of our method to a number of tasks including engineering design and parameter optimization.

9.1 Introduction

Move this first paragraph to the prob prog section to make a better opening

Probabilistic programming systems (PPS) allow probabilistic models to be represented in the form of a generative model and statements for conditioning on data [Carpenter et al., 2015; Goodman et al., 2008a; Goodman and Stuhlmüller, 2014; Mansinghka et al., 2014; Minka et al., 2010; Wood et al., 2014]. Their core philosophy is to decouple model specification and inference, the former corresponding to the user-specified program code and the latter to an inference engine capable of operating on arbitrary programs. Removing the need for users to write inference algorithms significantly reduces the burden of developing new models and makes effective statistical methods accessible to non-experts.

Although significant progress has been made on the problem of general purpose *inference* of program variables, less attention has been given to their *optimization*. Optimization is an

essential tool for effective machine learning, necessary when the user requires a single estimate. It also often forms a tractable alternative when full inference is infeasible [Murphy, 2012]. Moreover, coincident optimization and inference is often required, corresponding to a marginal maximum a posteriori (MMAP) setting where one wishes to maximize some variables, while marginalizing out others. Examples of MMAP problems include hyperparameter optimization, expectation maximization, and policy search [van de Meent et al., 2016].

In this paper we develop the first system that extends probabilistic programming (PP) to this more general MMAP framework, wherein the user specifies a model in the same manner as existing systems, but then selects some subset of the sampled variables in the program to be optimized, with the rest marginalized out using existing inference algorithms. The *optimization query* we introduce can be implemented and utilized in any PPS that supports an inference method returning a marginal likelihood estimate. This framework increases the scope of models that can be expressed in PPS and gives additional flexibility in the outputs a user can request from the program.

MMAP estimation is difficult as it corresponds to the optimization of an intractable integral, such that the optimization target is expensive to evaluate and gives noisy results. Current PPS inference engines are typically unsuited to such settings. We therefore introduce BOPP¹ (Bayesian optimization for probabilistic programs) which couples existing inference algorithms from PPS, like *Anglican* [Wood et al., 2014], with a new Gaussian process (GP) [Rasmussen and Williams, 2006] based Bayesian optimization (BO) package [Gutmann and Corander, 2016; Jones et al., 1998; Osborne et al., 2009; Shahriari et al., 2016a].

To demonstrate the functionality provided by BOPP, we consider an example application of engineering design. Engineering design relies extensively on simulations which typically have two things in common: the desire of the user to find a single best design and an uncertainty in the environment in which the designed component will live. Even when these simulations are deterministic, this is an approximation to a truly stochastic world. By expressing the utility of a particular design-environment combination using an approximate Bayesian computation (ABC) likelihood [Csilléry et al., 2010], one can pose this as a MMAP problem, optimizing the design while marginalizing out the environmental uncertainty.

¹Code available at <http://www.github.com/probprog/bopp/>

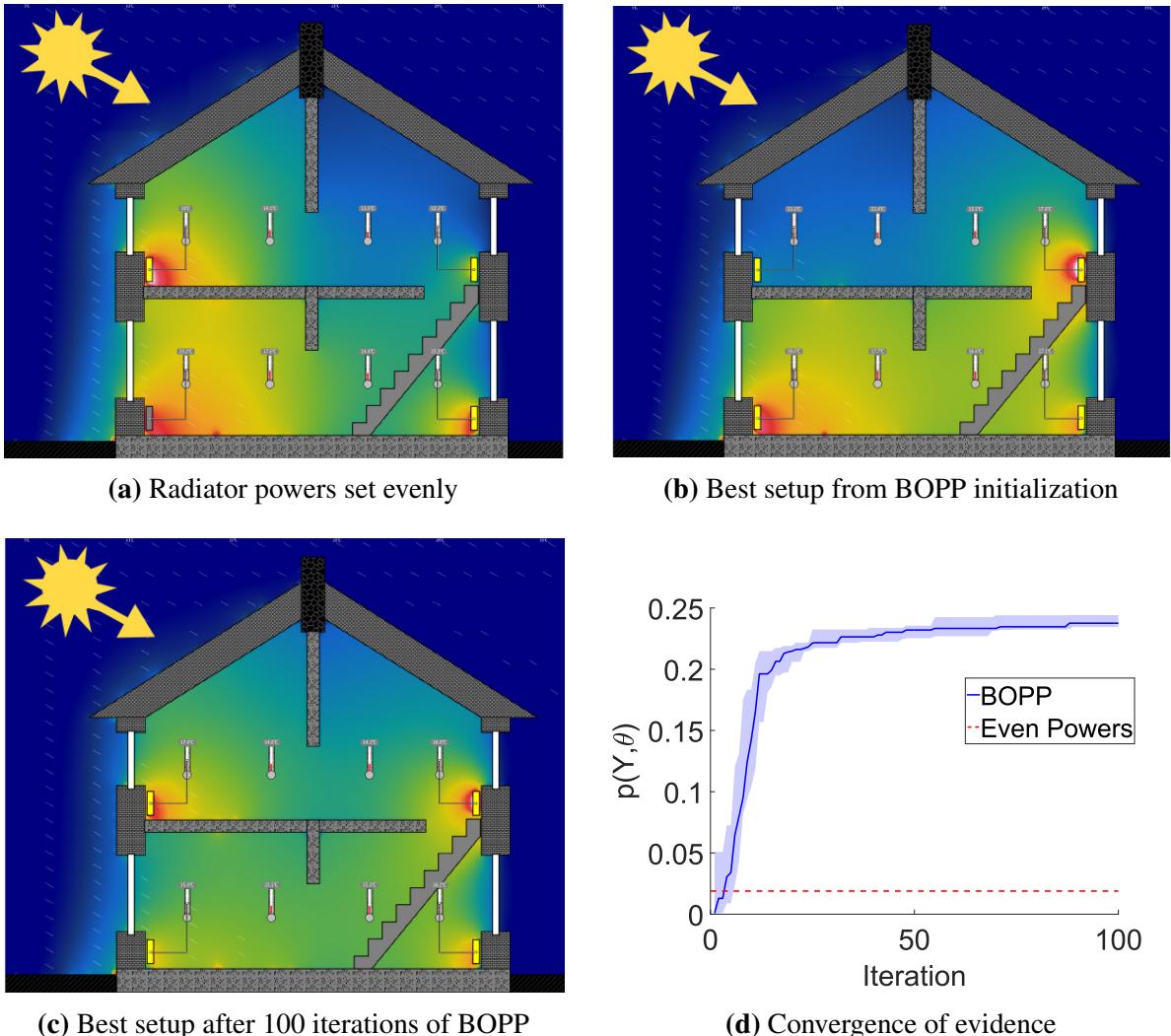


Figure 9.1: Simulation-based optimization of radiator powers subject to varying solar intensity. Shown are output heat maps from Energy2D [Xie, 2012] simulations at one intensity, corresponding to setting all the radiators to the same power (*top left*), the best result from a set of 5 randomly chosen powers used for initializing BOPP (*top right*), and the best setup found after 100 iterations of BOPP (*bottom left*). The bottom right plot shows convergence of the evidence of the respective model, giving the median and 25/75% quartiles.

Figure 9.1 illustrates how BOPP can be applied to engineering design, taking the example of optimizing the distribution of power between radiators in a house so as to homogenize the temperature, while marginalizing out possible weather conditions and subject to a total energy budget. The probabilistic program shown in Figure 9.2 allows us to define a prior over the uncertain weather, while conditioning on the output of a deterministic simulator (here Energy2D [Xie, 2012]-a finite element package for heat transfer) using an ABC likelihood. BOPP now allows the required coincident inference and optimization to be carried out automatically, directly returning increasingly optimal configurations.

```
(defopt house-heating [alphas target-temperatures] [powers]
  (let [solar-intensity (sample weather-prior)
    powers (sample (dirichlet alphas))
    temperatures (simulate solar-intensity powers)]
  (observe (abc-lielihood temperatures) target-temperatures)))
```

Figure 9.2: BOPP query for optimizing the power allocation to radiators in a house. Here `weather-prior` is a distribution over the solar intensity and a uniform Dirichlet prior with concentration alpha is placed over the powers. Calling `simulate` performs an Energy2D simulation of house temperatures. The utility of the resulting output is incorporated using `abc-lielihood`, which measures a discrepancy from the `target-temperatures`. Calling `doopt` on this query invokes the BOPP algorithm to perform MMAP estimation, where the second input `powers` indicates the variable to be optimized.

BO is an attractive choice for the required optimization in MMAP as it is typically efficient in the number of target evaluations, operates on non-differentiable targets, and incorporates noise in the target function evaluations. However, applying BO to probabilistic programs presents challenges, such as the need to give robust performance on a wide range of problems with varying scaling and potentially unbounded support. Furthermore, the target program may contain unknown constraints, implicitly defined by the generative model, and variables whose type is unknown (i.e. they may be continuous or discrete).

On the other hand, the availability of the target source code in a PPS presents opportunities to overcome these issues and go beyond what can be done with existing BO packages. BOPP exploits the source code in a number of ways, such as optimizing the acquisition function using the original generative model to ensure the solution satisfies the implicit constraints, performing adaptive domain scaling to ensure that GP kernel hyperparameters can be set according to problem-independent hyperpriors, and defining an adaptive non-stationary mean function to support unbounded BO.

Together, these innovations mean that BOPP can be run in a manner that is fully black-box from the user’s perspective, requiring only the identification of the target variables relative to current syntax for operating on arbitrary programs. We further show that BOPP is competitive with existing BO engines for direct optimization on common benchmarks problems that do not require marginalization.

9.2 Problem Formulation

Given a program defining the joint density $p(Y, X, \theta)$ with fixed Y , our aim is to optimize with respect to a subset of the variables θ whilst marginalizing out latent variables X

$$\theta^* = \arg \max_{\theta \in \vartheta} p(\theta|Y) = \arg \max_{\theta \in \vartheta} p(Y, \theta) = \arg \max_{\theta \in \vartheta} \int p(Y, X, \theta) dX. \quad (9.1)$$

To provide syntax to differentiate between θ and X , we introduce a new query macro **defopt**. The syntax of **defopt** is identical to **defquery** except that it has an additional input identifying the variables to be optimized. To allow for the interleaving of inference and optimization required in MMAP estimation, we further introduce **doopt**, which, analogous to **doquery**, returns a lazy sequence $\{\hat{\theta}_m^*, \hat{\Omega}_m^*, \hat{u}_m^*\}_{m=1,\dots}$ where $\hat{\Omega}_m^* \subseteq X$ are the program outputs associated with $\theta = \hat{\theta}_m^*$ and each $\hat{u}_m^* \in \mathbb{R}^+$ is an estimate of the corresponding log marginal $\log p(Y, \hat{\theta}_m^*)$ (see Section 9.3.2). The sequence is defined such that, at any time, $\hat{\theta}_m^*$ corresponds to the point expected to be most optimal of those evaluated so far and allows both inference and optimization to be carried out online.

Although no restrictions are placed on X , it is necessary to place some restrictions on how programs use the optimization variables $\theta = \phi_{1:K}$ specified by the optimization argument list of **defopt**. First, each optimization variable ϕ_k must be bound to a value directly by a **sample** statement with fixed measure-type distribution argument. This avoids change of variable complications arising from nonlinear deterministic mappings. Second, in order for the optimization to be well defined, the program must be written such that any possible execution trace binds each optimization variable ϕ_k exactly once. Finally, although any ϕ_k may be lexically multiply bound, it must have the same base measure in all possible execution traces, because, for instance, if the base measure of a ϕ_k were to change from Lebesgue to counting, the notion of optimality would no longer admit a conventional interpretation. Note that although the transformation implementations shown in Figure 9.3 do not contain runtime exception generators that disallow continued execution of programs that violate these constraints, those actually implemented in the BOPP system do.

9.3 Bayesian Program Optimization

In addition to the syntax introduced in the previous section, there are five main components to BOPP:

- A program transformation, $q \rightarrow q\text{-marg}$, allowing estimation of the evidence $p(Y, \theta)$ at a fixed θ .
- A high-performance, GP based, BO implementation for actively sampling θ .
- A program transformation, $q \rightarrow q\text{-prior}$, used for automatic and adaptive domain scaling, such that a problem-independent hyperprior can be placed over the GP hyperparameters.
- An adaptive non-stationary mean function to support unbounded optimization.
- A program transformation, $q \rightarrow q\text{-acq}$, and annealing maximum likelihood estimation method to optimize the acquisition function subject the implicit constraints imposed by the generative model.

Together these allow BOPP to perform online MMAPE estimation for arbitrary programs in a manner that is black-box from the user's perspective - requiring only the definition of the target program in the same way as existing PPS and identifying which variables to optimize. The BO component of BOPP is both probabilistic programming and language independent, and is provided as a stand-alone package.² It requires as input only a target function, a sampler to establish rough input scaling, and a problem specific optimizer for the acquisition function that imposes the problem constraints.

Figure 9.3 provides a high level overview of the algorithm invoked when `doopt` is called on a query q that defines a distribution $p(Y, a, \theta, b)$. We wish to optimize θ whilst marginalizing out a and b , as indicated by the the second input to q . In summary, BOPP performs iterative optimization in 5 steps

- Step 1 (blue arrows) generates unweighted samples from the transformed prior program $q\text{-prior}$ (*top center*), constructed by removing all conditioning. This initializes the domain scaling for θ .

²Code available at <http://www.github.com/probprog/deodorant/>

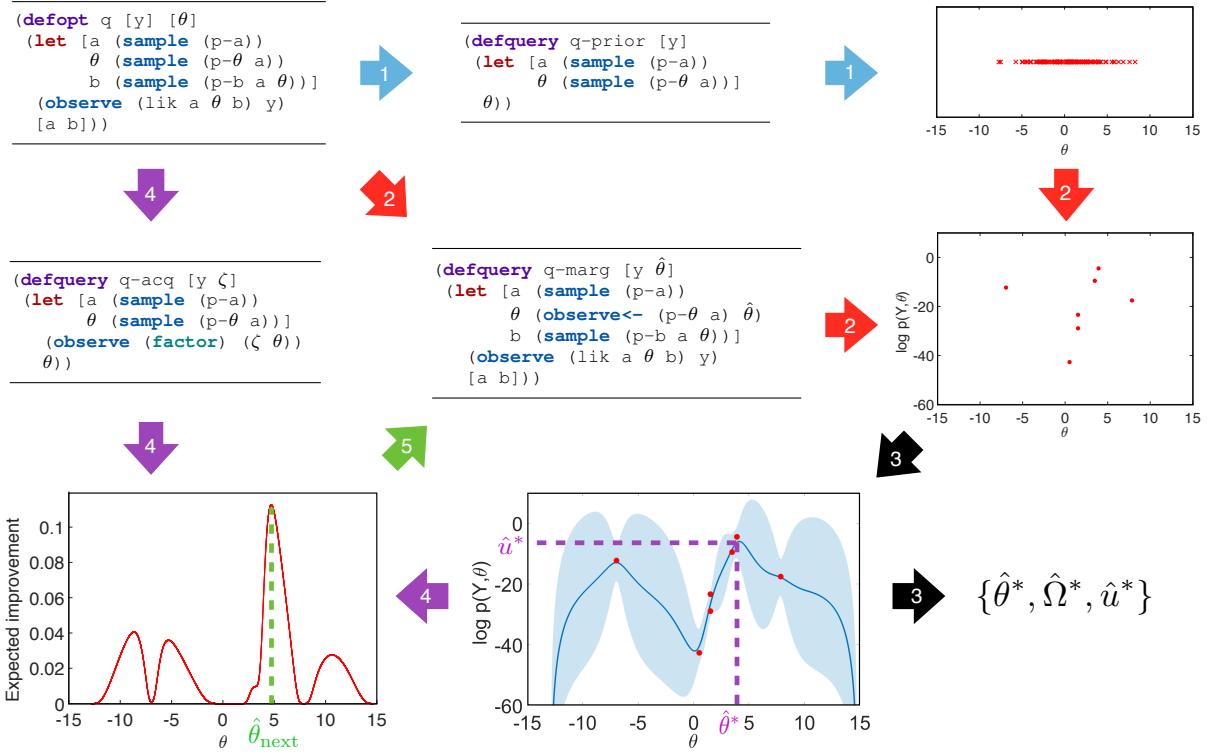


Figure 9.3: Overview of the BOPP algorithm, description given in main text. $p-a$, $p-\theta$, $p-b$ and lik all represent distribution object constructors. **factor** is a special distribution constructor that assigns probability $p(y) = y$, in this case $y = \zeta(\theta)$.

- Step 2 (red arrows) evaluates the marginal $p(Y, \theta)$ at a small number of the generated $\hat{\theta}$ by performing inference on the marginal program $q\text{-marg}$ (*middle centre*), which returns samples from the distribution $p(a, b|Y, \theta)$ along with an estimate of $p(Y, \theta)$. The evaluated points (*middle right*) provide an initial domain scaling of the outputs and starting points for the BO surrogate.
- Step 3 (black arrow) fits a mixture of GPs posterior Rasmussen and Williams [2006] to the scaled data (*bottom centre*) using a problem independent hyperprior. The solid blue line and shaded area show the posterior mean and ± 2 standard deviations respectively. The new estimate of the optimum $\hat{\theta}^*$ is the value for which the mean estimate is largest, with \hat{u}^* equal to the corresponding mean value.
- Step 4 (purple arrows) constructs an acquisition function $\zeta: \vartheta \rightarrow \mathbb{R}^+$ (*bottom left*) using the GP posterior. This is optimized, giving the next point to evaluate $\hat{\theta}_{next}$, by performing annealed importance sampling on a transformed program $q\text{-acq}$ (*middle left*) in which

all `observe` statements are removed and replaced with a single `observe` assigning probability $\zeta(\theta)$ to the execution.

- Step 5 (green arrow) evaluates $\hat{\theta}_{\text{next}}$ using `q-marg` and continues to step 3.

9.3.1 Program Transformation to Generate the Target

Consider the `defopt` query `q` in Figure 9.3, the body of which defines the joint distribution $p(Y, a, \theta, b)$. Calculating (9.1) (defining $X = \{a, b\}$) using a standard optimization scheme presents two issues: θ is a random variable within the program rather than something we control and its probability distribution is only defined conditioned on a .

We deal with both these issues simultaneously using a program transformation similar to the disintegration transformation in Hakaru [Zinkov and Shan, 2016]. Our *marginal* transformation returns a new `query` object, `q-marg` as shown in Figure 9.3, that defines the same joint distribution on program variables and inputs, but now accepts the value for θ as an input. This is done by replacing all `sample` statements associated with θ with equivalent `observe<-` statements, taking θ as the observed value, where `observe<-` is identical to `observe` except that it returns the observed value. As both `sample` and `observe` operate on the same variable type - a distribution object - this transformation can always be made, while the identical returns of `sample` and `observe<-` trivially ensures validity of the transformed program.

9.3.2 Bayesian Optimization of the Marginal

The target function for our BO scheme is $\log p(Y, \theta)$, noting $\arg \max f(\theta) = \arg \max \log f(\theta)$ for any $f : \vartheta \rightarrow \mathbb{R}^+$. The log is taken because GPs have unbounded support, while $p(Y, \theta)$ is always positive, and because we expect variations over many orders of magnitude. PPS with importance sampling based inference engines, e.g. sequential Monte Carlo [Wood et al., 2014] or the particle cascade [Paige et al., 2014], can return noisy estimates of this target given the transformed program `q-marg`.

Our BO scheme uses a GP prior and a Gaussian likelihood. Though the rationale for the latter is predominantly computational, giving an analytic posterior, there are also theoretical results suggesting that this choice is appropriate [Bérard et al., 2014]. We use as a default

covariance function a combination of a Matérn-3/2 and Matérn-5/2 kernel. Specifically, let $D = \|\theta\|_0$ be the dimensionality of θ and define

$$d_{3/2}(\theta, \theta') = \sqrt{\sum_{i=1}^D \frac{\theta_i - \theta'_i}{\rho_i}} \quad (9.2a)$$

$$d_{5/2}(\theta, \theta') = \sqrt{\sum_{i=1}^D \frac{\theta_i - \theta'_i}{\varrho_i}} \quad (9.2b)$$

where i indexes a dimension of θ and ρ_i and ϱ_i are dimension specific length scale hyperparameters. Our prior covariance function is now given by

$$\begin{aligned} k_{\text{prior}}(\theta, \theta') = & \sigma_{3/2}^2 \left(1 + \sqrt{3} d_{3/2}(\theta, \theta') \right) \exp \left(-\sqrt{3} d_{3/2}(\theta, \theta') \right) + \\ & \sigma_{5/2}^2 \left(1 + \sqrt{5} d_{5/2}(\theta, \theta') + \frac{5}{3} (d_{5/2}(\theta, \theta'))^2 \right) \exp \left(-\sqrt{5} d_{5/2}(\theta, \theta') \right) \end{aligned} \quad (9.3)$$

where $\sigma_{3/2}$ and $\sigma_{5/2}$ represent signal standard deviations for the two respective kernels. The full set of GP hyperparameters is defined by $\alpha = \{\sigma_n, \sigma_{3/2}, \sigma_{5/2}, \rho_{i=1:D}, \varrho_{i=1:D}\}$. A key feature of this kernel is that it is only once differentiable and therefore makes relatively weak assumptions about the smoothness of f . The ability to include branching in a probabilistic program means that, in some cases, an even less smooth kernel than (9.3) might be preferable. However, there is clear a trade-off between generality of the associated reproducing kernel Hilbert space and modelling power.

As noted by [Snoek et al., 2012], the performance of BO using a single GP posterior is heavily influenced by the choice of these hyperparameters. We therefore exploit the automated domain scaling introduced in Section 9.3.3 to define a problem independent hyperprior $p(\alpha)$ and perform inference to give a mixture of GPs posterior. Details on this hyperprior are given in Appendix 9.3.6.

Inference over α is performed using Hamiltonian Monte Carlo (HMC) [Duane et al., 1987], giving an unweighted mixture of GPs. Each term in this mixture has an analytic distribution fully specified by its mean function $\mu_m^i : \vartheta \rightarrow \mathbb{R}$ and covariance function $k_m^i : \vartheta \times \vartheta \rightarrow \mathbb{R}$, where m indexes the BO iteration and i the hyperparameter sample. HMC was chosen because of the availability of analytic derivatives of the GP log marginal likelihoods. As we found that the performance of HMC was often poor unless a good initialization point was used, BOPP runs a small number of independent chains and allocates part of the computational budget to their initialization using a L-BFGS optimizer [Broyden, 1970].

The inferred posterior is first used to estimate which of the previously evaluated $\hat{\theta}_j$ is the most optimal, by taking the point with highest expected value, $\hat{u}_m^* = \max_{j \in 1 \dots m} \sum_{i=1}^N \mu_m^i(\hat{\theta}_j)$. This completes the definition of the output sequence returned by the `doopt` macro. Note that as the posterior updates globally with each new observation, the relative estimated optimality of previously evaluated points changes at each iteration. Secondly it is used to define the acquisition function ζ , for which we take the expected improvement [Snoek et al., 2012], defining $\sigma_m^i(\theta) = \sqrt{k_m^i(\theta, \theta)}$ and $\gamma_m^i(\theta) = \frac{\mu_m^i(\theta) - \hat{u}_m^*}{\sigma_m^i(\theta)}$,

$$\zeta(\theta) = \sum_{i=1}^N (\mu_m^i(\theta) - \hat{u}_m^*) \Phi(\gamma_m^i(\theta)) + \sigma_m^i(\theta) \phi(\gamma_m^i(\theta)) \quad (9.4)$$

where ϕ and Φ represent the pdf and cdf of a unit normal distribution respectively. We note that more powerful, but more involved, acquisition functions, e.g. [Hernández-Lobato et al., 2014], could be used instead.

9.3.3 Automatic and Adaptive Domain Scaling

Domain scaling, by mapping to a common space, is crucial for BOPP to operate in the required black-box fashion as it allows a general purpose and problem independent hyperprior to be placed on the GP hyperparameters. BOPP therefore employs an affine scaling to a $[-1, 1]$ hypercube for both the inputs and outputs of the GP. To initialize scaling for the input variables, we sample directly from the generative model defined by the program. This is achieved using a second transformed program, `q-prior`, which removes all conditioning, i.e. `observe` statements, and returns θ . This transformation also introduces code to terminate execution of the query once all θ are sampled, in order to avoid unnecessary computation. As `observe` statements return `nil`, this transformation trivially preserves the generative model of the program, but the probability of the execution changes. Simulating from the generative model does not require inference or calling potentially expensive likelihood functions and is therefore computationally inexpensive. By running inference on `q-marg` given a small number of these samples as arguments, a rough initial characterization of output scaling can also be achieved. If points are observed that fall outside the hypercube under the initial scaling, the domain scaling is appropriately updated³ so that the target for the GP remains the $[-1, 1]$ hypercube.

³An important exception is that the output mapping to the bottom of the hypercube remains fixed such that low likelihood new points are not incorporated. This ensures stability when considering unbounded problems.

9.3.4 Unbounded Bayesian Optimization via Non-Stationary Mean Function Adaptation

Unlike standard BO implementations, BOPP is not provided with external constraints and we therefore develop a scheme for operating on targets with potentially unbounded support. Our method exploits the knowledge that the target function is a probability density, implying that the area that must be searched in practice to find the optimum is finite, by defining a non-stationary prior mean function. This takes the form of a bump function that is constant within a region of interest, but decays rapidly outside. Specifically we define this bump function in the transformed space as

$$\mu_{\text{prior}}(r; r_e, r_\infty) = \begin{cases} 0 & \text{if } r \leq r_e \\ \log\left(\frac{r-r_e}{r_\infty-r_e}\right) + \frac{r-r_e}{r_\infty-r_e} & \text{otherwise} \end{cases} \quad (9.5)$$

where r is the radius from the origin, r_e is the maximum radius of any point generated in the initial scaling or subsequent evaluations, and r_∞ is a parameter set to $1.5r_e$ by default. Consequently, the acquisition function also decays and new points are never suggested arbitrarily far away. Adaptation of the scaling will automatically update this mean function appropriately, learning a region of interest that matches that of the true problem, without complicating the optimization by over-extending this region. We note that our method shares similarity with the recent work of Shahriari et al [Shahriari et al., 2016a], but overcomes the sensitivity of their method upon a user-specified bounding box representing soft constraints, by initializing automatically and adapting as more data is observed.

9.3.5 Optimizing the Acquisition Function

Optimizing the acquisition function for BOPP presents the issue that the query contains implicit constraints that are unknown to the surrogate function. The problem of unknown constraints has been previously covered in the literature [Gardner et al., 2014; Hernández-Lobato et al., 2016] by assuming that constraints take the form of a black-box function which is modeled with a second surrogate function and must be evaluated in guess-and-check strategy to establish whether a point is valid. Along with the potentially significant expense such a method incurs, this approach is inappropriate for *equality* constraints or when the target variables are potentially discrete. For example, the Dirichlet distribution in Figure 9.2 introduces an equality constraint on powers, namely that its components must sum to 1.

We therefore take an alternative approach based on directly using the program to optimize the acquisition function. To do so we consider a transformed program `q-acq` that is identical to `q-prior` (see Section 9.3.3), but adds an additional `observe` statement that assigns a weight $\zeta(\theta)$ to the execution. By setting $\zeta(\theta)$ to the acquisition function, the maximum likelihood corresponds to the optimum of the acquisition function subject to the implicit program constraints. We obtain a maximum likelihood estimate for `q-acq` using a variant of annealed importance sampling [Neal, 2001] in which lightweight Metropolis Hastings (LMH) [Wingate et al., 2011] with local random-walk moves is used as the base transition kernel.

9.3.6 Problem Independent Gaussian Process Hyperprior

Remembering that the domain scaling introduced in Section 9.3.3 means that both the input and outputs of the GP are taken to vary between ± 1 , we define the problem independent GP hyperprior as $p(\alpha) = p(\sigma_n)p(\sigma_{3/2})p(\sigma_{5/2})\prod_{i=1}^D p(\rho_i)p(\varrho_i)$ where

$$\log(\sigma_n) \sim \mathcal{N}(-5, 2) \quad (9.6a)$$

$$\log(\sigma_{3/2}) \sim \mathcal{N}(-7, 0.5) \quad (9.6b)$$

$$\log(\sigma_{5/2}) \sim \mathcal{N}(-0.5, 0.15) \quad (9.6c)$$

$$\log(\rho_i) \sim \mathcal{N}(-1.5, 0.5) \quad \forall i \in \{1, \dots, D\} \quad (9.6d)$$

$$\log(\varrho_i) \sim \mathcal{N}(-1, 0.5) \quad \forall i \in \{1, \dots, D\}. \quad (9.6e)$$

The rationale of this hyperprior is that the smoother Matérn 5/2 kernel should be the dominant effect and model the higher length scale variations. The Matérn 3/2 kernel is included in case the evidence suggests that the target is less smooth than can be modelled with the Matérn 5/2 kernel and to provide modelling of smaller scale variations around the optimum.

9.4 Experiments

We first demonstrate the ability of BOPP to carry out unbounded optimization using a 1D problem with a significant prior-posterior mismatch as shown in Figure 9.4. It shows BOPP adapting to the target and effectively establishing a maxima in the presence of multiple modes. After 20 evaluations the acquisitions begin to explore the right mode, after 50 both modes have been fully uncovered.

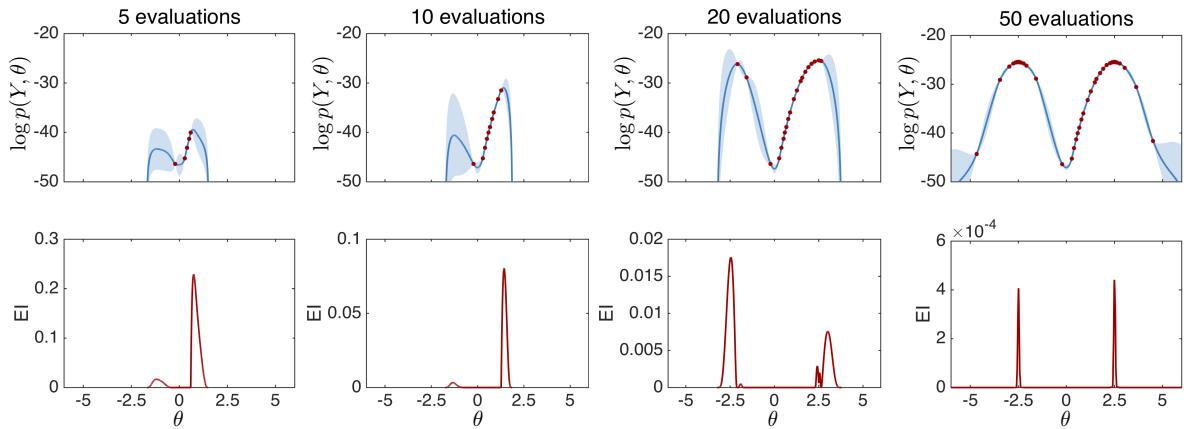


Figure 9.4: Convergence on an unconstrained bimodal problem with $p(\theta) = \text{Normal}(0, 0.5)$ and $p(Y|\theta) = \text{Normal}(5 - |\theta|, 0.5)$ giving significant prior misspecification. The top plots show a regressed GP, with the solid line corresponding to the mean and the shading shows ± 2 standard deviations. The bottom plots show the corresponding acquisition functions.

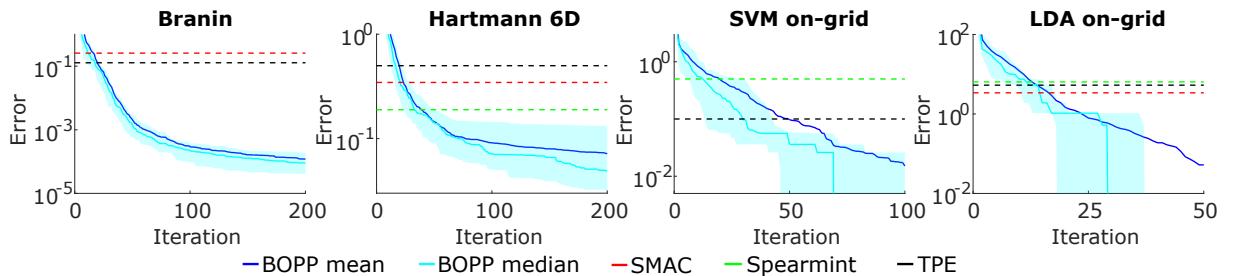


Figure 9.5: Comparison of BOPP used as an optimizer to prominent BO packages on common benchmark problems. The dashed lines shows the final mean error of SMAC (red), Spearmint (green) and TPE (black) as quoted by Eggensperger et al. [2013]. The dark blue line shows the mean error for BOPP averaged over 100 runs, whilst the median and 25/75% percentiles are shown in cyan. Results for Spearmint on Branin and SMAC on SVM on-grid are omitted because both BOPP and the respective algorithms averaged zero error to the provided number of significant figures in Eggensperger et al. [2013].

9.4.1 Classic Optimization Benchmarks

Next we compare BOPP to the prominent BO packages SMAC Hutter et al. [2011], Spearmint Snoek et al. [2012] and TPE Bergstra et al. [2011] on a number of classical benchmarks as shown in Figure 9.5. These results demonstrate that BOPP provides substantial advantages over these systems when used simply as an optimizer on both continuous and discrete optimization problems. In particular, it offers a large advantage over SMAC and TPE on the continuous problems (Branin and Hartmann), due to using a more powerful surrogate, and over Spearmint on the others due to not needing to make approximations to deal with discrete problems.

```
(defopt mvn-mixture [data mu0 kappa psi] [nu alpha]
  (let [[n d] (shape data)
        alpha (sample (uniform-continuous 0.01 100))
        nu (sample (uniform-continuous (- d 1) 100))
        obs-proc0 (mvn-niw mu0 kappa nu psi)]
    (loop [data data
           obs-procs {}
           mix-proc (dirichlet-discrete
                      (vec (repeat d alpha)))]
      (let [y (first data)]
        (if y
            (let [z (sample (produce comp-proc))
                  obs-proc (get obs-procs z obs-proc0)
                  obs-dist (produce obs-proc)]
              (observe obs-dist y)
              (recur (rest data)
                     (assoc obs-procs z (absorb obs-proc y)))
              (absorb mix-proc z)))
            mix-proc)))))
```

Figure 9.6: Anglican query for hyperparameter optimization of a Gaussian mixture model, defined in terms of two parameters nu and alpha. A `mvn-niw` process is used to represent the marginal likelihood of observations under a Gaussian-inverse-Wishart prior, whereas a `dirichlet-discrete` process models the prior probability of cluster assignments under a Dirichlet-discrete prior. The command `produce` returns the predictive distribution for the next sample from a process. `absorb` conditions on the value of the next sample.

9.4.2 Marginal Maximum a Posteriori Estimation Problems

We now demonstrate application of BOPP on a number of MMAP problems. Comparisons here are more difficult due to the dearth of existing alternatives for PPS. In particular, simply running inference on the original query does not return estimates for $p(Y|\theta)$. We consider the possible alternative of using our conditional code transformation to design a particle marginal Metropolis Hastings (PMMH, Andrieu et al. [2010a]) sampler which operates in a similar fashion to BOPP except that new θ are chosen using a MH step instead of actively sampling with BO. For these MH steps we consider both LMH [Wingate et al., 2011] with proposals from the prior and the random-walk MH (RMH) variant introduced in Section 9.3.5.

9.4.2.1 Hyperparameter Optimization for Gaussian Mixture Model

We start with an illustrative case study of optimizing the hyperparameters in a multivariate Gaussian mixture model. We consider a Bayesian formulation with a symmetric Dirichlet prior on the mixture weights and a Gaussian-inverse-Wishart prior on the likelihood parameters:

$$\pi \sim \text{Dir}(\alpha, \dots, \alpha) \quad (9.7)$$

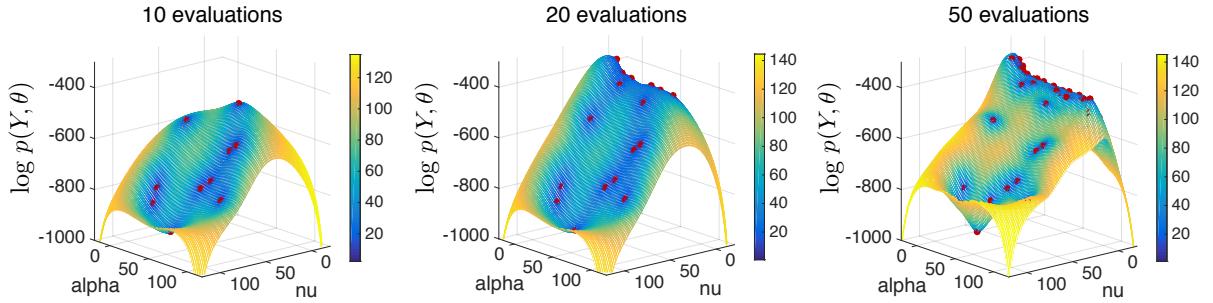


Figure 9.7: Bayesian optimization of hyperparameters in a Gaussian mixture model evaluated on the Iris dataset. Panels show the GP posterior as a function of number of evaluations, with the surface corresponding to the posterior mean and the color bars the posterior standard deviation. Optimization is performed over the parameter α of a 10-dimensional symmetric Dirichlet distribution and the degrees of freedom ν of the inverse-Wishart prior. At each evaluation we obtain an estimate of the log marginal $\log p(Y, \theta)$ obtained by performing sequential Monte Carlo inference with 1000 particles. The apparent maximum after initialization with 10 randomly sampled points lies at $\nu = 31$, $\alpha = 60$, and $\log p(Y, \theta) = -456.3$ (left). The surface after 10 optimization steps shows a new maximum at $\nu = 9.2$, $\alpha = 0.8$, and $\log p(Y, \theta) = -364.2$ (middle). After 40 steps and 50 total evaluations this optimum is refined to $\nu = 16$, $\alpha = 0.2$, and $\log p(Y, \theta) = -352.5$ (right).

$$(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \sim \text{NIW}(\boldsymbol{\mu}_0, \kappa, \boldsymbol{\Psi}, \nu) \quad \text{for } k = 1, \dots, K \quad (9.8)$$

$$z_n \sim \text{Disc}(\boldsymbol{\pi}) \quad (9.9)$$

$$\mathbf{y}_n \sim \text{Norm}(\boldsymbol{\mu}_{z_n}, \boldsymbol{\Sigma}_{z_n}) \quad \text{for } n = 1, \dots, N \quad (9.10)$$

Anglican code for this model is shown in Figure 4. Anglican provides stateful objects, which are referred to as random processes, to represent the predictive distributions for the cluster assignments z and the observations \mathbf{y}^k assigned to each cluster

$$z_{n+1} \sim p(\cdot | z_{1:n}, \alpha), \quad (9.11)$$

$$\mathbf{y}_{m+1}^k \sim p(\cdot | \mathbf{y}_{1:m}^k, \boldsymbol{\mu}_0, \kappa, \boldsymbol{\Psi}, \nu). \quad (9.12)$$

In this collapsed representation marginalization over the model parameters $\boldsymbol{\pi}$, $\boldsymbol{\mu}_{k=1:K}$, and $\boldsymbol{\Sigma}_{k=1:K}$ is performed analytically. Using the Iris dataset, a standard benchmark for mixture models that contains 150 labeled examples with 4 real-valued features, we optimize the marginal with respect to the subset of the parameters ν and α under uniform priors over a fixed interval. For this model, BOPP aims to maximize

$$\begin{aligned} & p(\nu, \alpha | \mathbf{y}_{n=1:N}, \boldsymbol{\mu}_0, \kappa, \boldsymbol{\Psi}) \\ &= \iiint p(\nu, \alpha, z_{n=1:N}, \boldsymbol{\pi}, \boldsymbol{\mu}_{k=1:K}, \boldsymbol{\Sigma}_{k=1:K} | \mathbf{y}_{n=1:N}, \boldsymbol{\mu}_0, \kappa, \boldsymbol{\Psi}) dz_{n=1:N} d\boldsymbol{\pi} d\boldsymbol{\mu}_{k=1:K} d\boldsymbol{\Sigma}_{k=1:K}. \end{aligned} \quad (9.13)$$

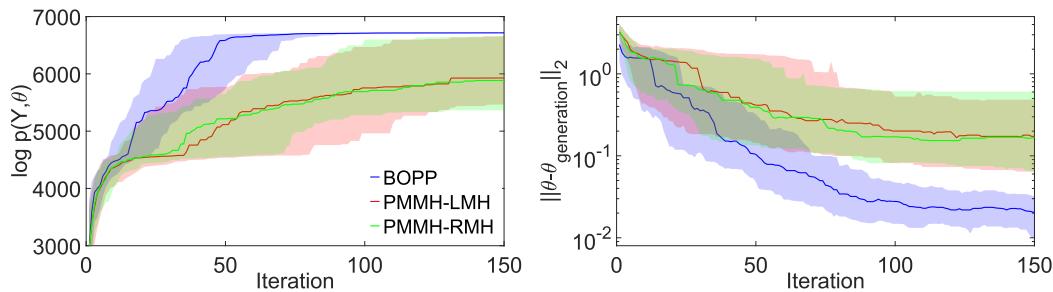


Figure 9.8: Convergence for transition dynamics parameters of the pickover attractor in terms of the cumulative best $\log p(Y, \theta)$ (*left*) and distance to the “true” θ used in generating the data (*right*). Solid line shows median over 100 runs, whilst the shaded region the 25/75% quantiles.

Figure 9.7 shows GP regressions on the evidence after different numbers of the SMC evaluations have been performed on the model. This demonstrates how the GP surrogate used by BO builds up a model of the target, used to both estimate the expected value of $\log p(Y, \theta)$ for a particular θ and actively sample the θ at which to undertake inference.

9.4.2.2 Extended Kalman Filter for the Pickover Chaotic Attractor

We next consider the case of learning the dynamics parameters of a chaotic attractor. Chaotic attractors present an interesting case for tracking problems as, although their underlying dynamics are strictly deterministic with bounded trajectories, neighbouring trajectories diverge exponentially⁴. Therefore regardless of the available precision, a trajectory cannot be indefinitely extrapolated to within a given accuracy and probabilistic methods such as the extended Kalman filter must be incorporated [Fujii, 2013; Ruan et al., 2003]. From an empirical perspective, this forms a challenging optimization problem as the target transpires to be multi-modal, has variations at different length scales, and has local minima close to the global maximum.

Suppose we observe a noisy signal $y_t \in \mathbb{R}^K$, $t = 1, 2, \dots, T$ in some K dimensional observation space where each observation has a lower dimensional latent parameter $x_t \in \mathbb{R}^D$, $t = 1, 2, \dots, T$ whose dynamics correspond to a chaotic attractor of known type, but with unknown parameters. Our aim will be to find the MMAP values for the dynamics parameters θ , marginalizing out the latent states. The established parameters can then be used for forward simulation or tracking.

⁴It is beyond the scope of this paper to properly introduce chaotic systems. We refer the reader to Devaney et al. [1989] for an introduction.

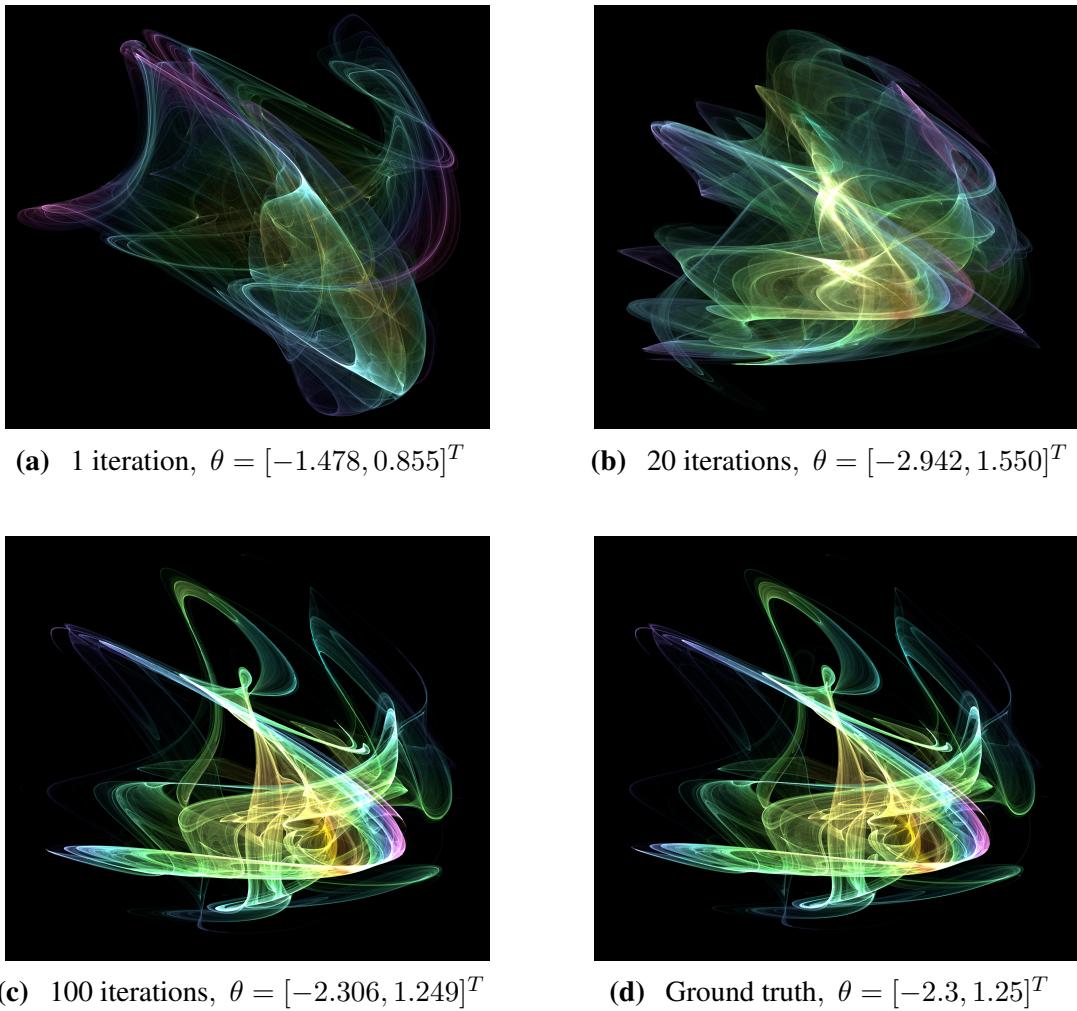


Figure 9.9: A series of trajectories for different parameters, demonstrating convergence to the true attractor. The colormap is based on the speed and curvature of the trajectory, with rendering done using the program Chaoscope (available at <http://www.chaoscope.org/>).

To carry out the required MMAP estimation, we apply BOPP to the extended Kalman smoother

$$x_1 \sim \mathcal{N}(\mu_1, \sigma_1 I) \quad (9.14)$$

$$x_t = A(x_{t-1}, \theta) + \delta_{t-1}, \quad \delta_{t-1} \sim \mathcal{N}(0, \sigma_q I) \quad (9.15)$$

$$y_t = Cx_t + \varepsilon_t, \quad \varepsilon_t \sim \mathcal{N}(0, \sigma_y I) \quad (9.16)$$

where I is the identity matrix, C is a known $K \times D$ matrix, μ_1 is the expected starting position,

and σ_1 , σ_q and σ_y are all scalars which are assumed to be known. The transition function $A(\cdot, \cdot)$

$$x_{t,1} = \sin(\beta x_{t-1,2}) - \cos\left(\frac{5x_{t-1,1}}{2}\right) x_{t-1,3} \quad (9.17a)$$

$$x_{t,2} = -\sin\left(\frac{3x_{t-1,1}}{2}\right) x_{t-1,3} - \cos(\eta x_{t-1,2}) \quad (9.17b)$$

$$x_{t,3} = \sin(x_{t-1,1}) \quad (9.17c)$$

corresponds to a Pickover attractor [Pickover, 1995] with unknown parameters $\theta = \{\beta, \eta\}$ which we wish to optimize. Note that η and $-\eta$ will give the same behaviour.

Synthetic data was generated for 500 time steps using the parameters of $\mu_1 = [-0.2149, -0.0177, 0.7630]^T$, $\sigma_1 = 0$, $\sigma_q = 0.01$, $\sigma_y = 0.2$, a fixed matrix C where $K = 20$ and each column was randomly drawn from a symmetric Dirichlet distribution with parameter 0.1, and ground truth transition parameters of $\beta = -2.3$ and $\eta = 1.25$ (note that the true global optimum for finite data need not be exactly equal to this).

MMAP estimation was performed on this data using the same model and parameters, with the exceptions of θ , μ_1 and σ_1 . The prior on θ was set to a uniform in over a bounded region such that

$$p(\beta, \eta) = \begin{cases} 1/18, & \text{if } -3 \leq \beta \leq 3 \cap 0 \leq \eta \leq 3 \\ 0, & \text{otherwise} \end{cases}. \quad (9.18)$$

The changes $\mu_1 = [0, 0, 0]$ and $\sigma_1 = 1$ were further made to reflect the starting point of the latent state being unknown. For this problem, BOPP aims to maximize

$$p(\beta, \eta | y_{t=1:T}) = \int p(\beta, \eta, x_{t=1:T} | y_{t=1:T}) dx_{t=1:T}. \quad (9.19)$$

Inference on the transformed marginal query was carried out using SMC with 500 particles. Convergence results are given in Figure 9.8 showing that BOPP comfortably outperforms the PMMH variants, while Figure 9.9 shows the simulated attractors generated from the dynamics parameters output by various iterations of a particular run of BOPP.

9.4.2.3 Hidden Markov Model with Unknown Number of States

We finally consider a hidden Markov model (HMM) with an unknown number of states. This example demonstrates how BOPP can be applied to models which conceptually have an unknown number of variables, by generating all possible variables that might be needed, but then leaving some variables unused for some execution traces. This avoids problems of varying base measures

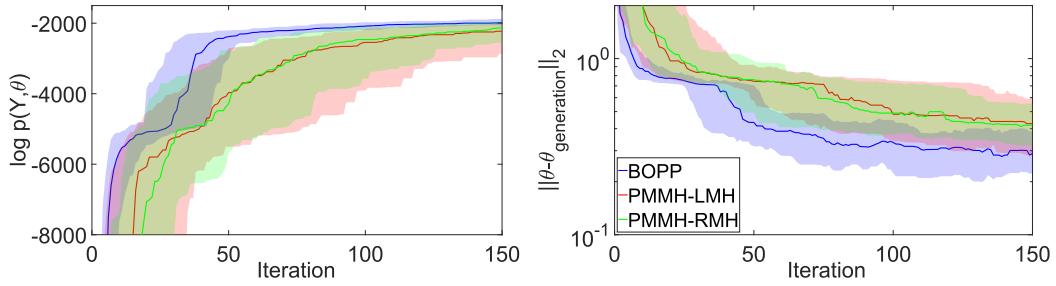


Figure 9.10: Convergence for HMM in terms of the cumulative best $\log p(Y|\theta)$ (left) and distance to the “true” θ used in generating the data (right). Solid line shows median over 100 runs, whilst the shaded region the 25/75% quantiles. Note that for the distance to true θ was calculated by selecting which three states (out of the 5 generates) that were closest to the true parameters.

so that the MMAP problem is well defined and provides a function with a fixed number of inputs as required by the BO scheme. From the BO perspective, the target function is simply constant for variations in an unused variable.

HMMs are Markovian state space models with discrete latent variables. Each latent state $x_t \in \{1, \dots, K\}$, $t = 1, \dots, T$ is defined conditionally on x_{t-1} through a set of discrete transition probabilities, whilst each output $y_t \in \mathbb{R}$ is considered to be generated i.i.d. given x_t . We consider the following HMM, in which the number of states K , is also a random variable:

$$K \sim \text{Discrete}\{1, 2, 3, 4, 5\} \quad (9.20)$$

$$T_k \sim \text{Dirichlet}\{1_{1:K}\}, \quad \forall k = 1, \dots, K \quad (9.21)$$

$$\phi_k \sim \text{Uniform}[0, 1], \quad \forall k = 1, \dots, K \quad (9.22)$$

$$\mu_0 \leftarrow \min\{y_{1:T}\} \quad (9.23)$$

$$\mu_k \leftarrow \mu_{k-1} + \phi_k \cdot (\max\{y_{1:T}\} - \mu_{k-1}), \quad \forall k = 1, \dots, K \quad (9.24)$$

$$x_1 \leftarrow 1 \quad (9.25)$$

$$x_t|x_{t-1} \sim \text{Discrete}\{T_{x_{t-1}}\} \quad (9.26)$$

$$y_t|x_t \sim \mathcal{N}(\mu(x_{t-1}), 0.2). \quad (9.27)$$

Our experiment is based on applying BOPP to the above model to do MMAP estimation with a single synthetic dataset, generated using $K = 3$, $\mu_1 = -1$, $\mu_2 = 0$, $\mu_3 = 4$, $T_1 = [0.9, 0.1, 0]$, $T_2 = [0.2, 0.75, 0.05]$ and $T_3 = [0.1, 0.2, 0.7]$.

We use BOPP to optimize both the number of states K and the stick-breaking parameters ϕ_k , with full inference performed on the other parameters. BOPP therefore aims to maximize

$$p(K, \phi_{k=1:5}|y_{t=1:T}) = \iint p(K, \phi_{k=1:5}, x_{t=1:T}, T_{k=1:K}|y_{t=1:T}) dx_{t=1:T} dT_{k=1:K}. \quad (9.28)$$

As with the chaotic Kalman filter example, we compare to two PMMH variants using the same code transformations. The results, given in Figure 9.10, again show that BOPP outperforms these PMMH alternatives.

9.4.3 Full Details for House Heating Experiment

In this case study, illustrated in Figure 9.1, we optimize the parameters of a stochastic engineering simulation. We use the Energy2D system from Xie [2012] to perform finite-difference numerical simulation of the heat equation and Navier-Stokes equations in a user-defined geometry.

In our setup, we designed a 2-dimensional representation of a house with 4 interconnected rooms using the GUI provided by Energy2D. The left side of the house receives morning sun, modelled at a constant incident angle of 30° . We assume a randomly distributed solar intensity and simulate the heating of a cold house in the morning by 4 radiators, one in each of the rooms. The radiators are given a fixed budget of total power density P_{budget} . The optimization problem is to distribute this power budget across radiators in a manner that minimizes the variance in temperatures across 8 locations in the house.

Energy2D is written in Java, which allows the simulation to be integrated directly into an Anglican program that defines a prior on model parameters and an ABC likelihood for evaluating the utility of the simulation outputs. Figure 9.2 shows the corresponding program query. In this, we define a Clojure function `simulate` that accepts a solar power intensity I_{sun} and power densities for the radiators P_r , returning the thermometer temperature readings $\{T_{i,t}\}$. We place a symmetric Dirichlet prior on $\frac{P_r}{P_{\text{budget}}}$ and a gamma prior on $\frac{I_{\text{sun}}}{I_{\text{base}}}$, where P_{budget} and I_{base} are constants. This gives the generative model:

$$p_r \sim \text{Dirichlet}([1, 1, 1, 1]) \quad (9.29)$$

$$P_r \leftarrow P_{\text{budget}} \cdot p_r \quad (9.30)$$

$$v \sim \text{Gamma}(5, 1) \quad (9.31)$$

$$I_{\text{sun}} \leftarrow I_{\text{base}} \cdot v. \quad (9.32)$$

After using these to call `simulate`, the standard deviations of the returned temperatures is calculated for each time point,

$$\omega_t = \sqrt{\sum_{i=1}^8 T_{i,t}^2 - \left(\sum_{i=1}^8 T_{i,t} \right)^2} \quad (9.33)$$

and used in the ABC likelihood `abc-likelihood` to weight the execution trace using a multivariate Gaussian:

$$p(\{T_{i,t}\}_{i=1:8, t=1:\tau}) = \text{Normal}(\omega_{t=1:\tau}; \mathbf{0}, \sigma_T^2 \mathbf{I})$$

where \mathbf{I} is the identity matrix and $\sigma_T = 0.8^\circ\text{C}$ is the observation standard deviation.

Figure 9.1 demonstrates the improvement in homogeneity of temperatures as a function of total number of simulation evaluations. Visual inspection of the heat distributions also shown in Figure 9.1 confirms this result, which serves as an exemplar of how BOPP can be used to estimate marginally optimal simulation parameters.

9.5 Discussion and Future Work

We have introduced a new method for carrying out MMAP estimation of probabilistic program variables using Bayesian optimization, representing the first unified framework for optimization and inference of probabilistic programs. By using a series of code transformations, our method allows an arbitrary program to be optimized with respect to a defined subset of its variables, whilst marginalizing out the rest. To carry out the required optimization, we introduce a new GP-based BO package that exploits the availability of the target source code to provide a number of novel features, such as automatic domain scaling and constraint satisfaction.

The concepts we introduce lead directly to a number of extensions of interest, including but not restricted to smart initialization of inference algorithms, adaptive proposals, and nested optimization. Further work might consider maximum marginal likelihood estimation and risk minimization. Though only requiring minor algorithmic changes, these cases require distinct theoretical considerations.

9.6 Program Transformations in Detail

In this section we give a more detailed and language specific description of our program transformations, code for which can be found at <http://www.github.com/probprog/bopp>.

9.6.1 Anglican

Anglican is a probabilistic programming language integrated into Clojure (a dialect of Lisp) and inherits most of the corresponding syntax. Anglican extends Clojure with the special forms `sample` and `observe` [Tolpin et al., 2015b]. Each random draw in an Anglican program corresponds to a `sample` call, which can be thought of as a term in the prior. Each `observe` statement applies weighting to a program trace and thus constitutes a term in the likelihood. Compilation of an Anglican program, performed by the macro `query`, corresponds to transforming the code into a variant of continuation-passing style (CPS) code, which results in a function that can be executed using a particular inference algorithm.

Anglican program code is represented by a nested list of expressions, symbols, non-literals for constructing data structures (e.g. `[...]` for vectors), and command dependent literals (e.g. `[...]` as a second argument of a `let` statement which is used for binding pairs). In order to perform program transformations, we can recursively traverse this nested list which can be thought of as an abstract syntax tree of the program.

Our program transformations also make use of the Anglican forms `store` and `retrieve`. These allow storing any variable in the probabilistic program’s execution trace in a state which is passed around during execution and from which we can retrieve these stored values. The core use for this is to allow the outer query to return variables which are only locally scoped.

To allow for the early termination that will be introduced in Section 9.6.5, it was necessary to add a mechanism for non-local returns to Anglican. Clojure supports non-local returns only through Java exception handling, via the keywords `try throw`, `catch` and `finally`. Unfortunately, these are not currently supported by Anglican and their behaviour is far from ideal for our purposes. In particular, for programs containing nested `try` statements, throwing to a particular `try` in the stack, as opposed to the most recently invoked, is cumbersome and error prone.

We have instead, therefore, added to Anglican a non-local return mechanism based on the Common Lisp control form `catch/throw`. This uses a *catch tag* to link each `throw` to a particular `catch`. For example

```
(catch :tag
  (when (> a 0)
    (throw :tag a))
  0)
```

is equivalent to `(max a 0)`. More precisely, `throw` has syntax `(throw tag value)` and will cause the `catch` block with the corresponding `tag` to exit, returning `value`. If a `throw` goes uncaught, i.e. it is not contained within a `catch` block with a matching `tag`, a custom Clojure exception is thrown.

9.6.2 Representations in the Main Paper

In the main paper we presented the code transformations as static transformations as shown in Figure 9.3. Although for simple programs, such as the given example, these transformations can be easily expressed as static transformations, for more complicated programs it would be difficult to actually implement these as purely static generic transformations in a higher-order language. Therefore, even though all the transformations dynamically execute as shown at runtime, in truth, the generated source code for the prior and acquisition transformations varies from what is shown and has been presented this way in the interest of exposition. Our true transformations exploit `store`, `retrieve`, `catch` and `throw` to generate programs that dynamically execute in the same way at run time as the static examples shown, but whose actual source code varies significantly.

9.6.3 Prior Transformation

The prior transformation recursively traverses the program tree and applies two local transformations. Firstly it replaces all `observe` statements by `nil`. As `observe` statements return `nil`, this trivially preserves the generative model of the program, but the probability of the execution changes. Secondly, it inspects the binding variables of `let` forms in order to modify the binding expressions for the optimization variables, as specified by the second input of `defopt`, asserting that these are directly bound to a `sample` statement of the form `(sample dist)`. The transformation then replaces this expression by one that stores the result of this sample in Anglican’s `store` before returning it. Specifically, if the binding variable in question is `phi-k`, then the original binding expression `(sample dist)` is transformed into

```
(let [value (sample dist)]
  ;; Store the sampled value in Anglican's store
  (store OPTIM-ARGS-KEY
    'phi-k
    value)
  value)
```

After all these local transformation have been made, we wrap the resulting query block in a `do` form and append an expression extracting the optimization variables using Anglican’s `retrieve`. This makes the optimization variables the output of the query. Denoting the list of optimization variable symbols from `defopt` as `optim-args` and the query body after applying all the above location transformations as `...`, the prior query becomes

```
(query query-args
  (do
    ...
    (map (fn [x] (retrieve OPTIM-ARGS-KEY x))
      optim-args)))
```

Note that the difference in syntax from Figure 9.3 is because `defquery` is in truth a syntactic sugar allowing users to bind `query` to a variable. As previously stated, `query` is macro that compiles an Anglican program to its CPS transformation. An important subtlety here is that the order of the returned samples is dictated by `optim-args` and is thus independent of the order in which the variables were actually sampled, ensuring consistent inputs for the BO package.

We additionally add a check (not shown) to ensure that all the optimization variables have been added to the store, and thus sampled during the execution, before returning. This ensures that our assumption that each optimization variable is assigned for each execution trace is satisfied.

9.6.4 Acquisition Transformation

The acquisition transformation is the same as the prior transformation except we append the acquisition function, `ACQ-F`, to the inputs and then `observe` its application to the optimization variables before returning. The acquisition query is thus

```
(query [query-args ACQ-F]
  (do
    ...
    (let [theta (map (fn [x] (retrieve OPTIM-ARGS-KEY x))
      optim-args)]
      (observe (factor) (ACQ-F theta))
      theta)))
```

9.6.5 Early Termination

To ensure that `q-prior` and `q-acq` are cheap to evaluate and that the latter does not include unnecessary terms which complicate the optimization, we wish to avoid executing code that is not required for generating the optimization variables. Ideally we would like to directly

remove all such redundant code during the transformations. However, doing so in a generic way applicable to all possible programs in a higher order language represents a significant challenge. Therefore, we instead transform to programs with additional early termination statements, triggered when all the optimization variables have been sampled. Provided one is careful to define the optimization variables as early as possible in the program (in most applications, e.g. hyperparameter optimization, they naturally occur at the start of the program), this is typically sufficient to ensure that the minimum possible code is run in practise.

To carry out this early termination, we first wrap the query in a `catch` block with a uniquely generated tag. We then augment the transformation of an optimization variable’s binding described in Section 9.6.3 to check if all optimization variables are already stored, and invoke a `throw` statement with the corresponding tag if so. Specifically we replace relevant binding expressions (`sample dist`) with

```
(let [value (sample dist)]
  ;; Store the sampled value in Anglican's store
  (store OPTIM-ARGS-KEY
    'phi-k
    value)
  ;; Terminate early if all optimization variables are sampled
  (if (= (set (keys (retrieve OPTIM-ARGS-KEY)))
    (set optim-args))
    (throw BOPP-CATCH-TAG prologue-code)
    value))
```

where `prologue-code` refers to one of the following expressions depending on whether it is used for a prior or an acquisition transformation

```
;; Prior query prologue-code
(map (fn [x] (retrieve OPTIM-ARGS-KEY x))
  optim-args)

;; Acquisition query prologue-code
(do
  (let [theta (map (fn [x] (retrieve OPTIM-ARGS-KEY x))
    optim-args)]
    (observe (factor) (ACQ-F theta))
    theta))
```

We note that valid programs for both `q-prior` and `q-acq` should always terminate via one of these early stopping criteria and therefore never actually reach the appending statements in the `query` blocks shown in Sections 9.6.3 and 9.6.4. As such, these are, in practise, only for exposition and error catching.

9.6.6 Marginal/MMAP Transformation

The marginal transformation inspects all **let** binding pairs and if a binding variable `phi-k` is one of the optimization variables, the binding expression (**sample** `dist`) is transformed to the following

```
(do (observe dist phi-k-hat)
    phi-k-hat)
```

corresponding to the **observe**`<-` form used in the main paper.

9.6.7 Error Handling

During program transformation stage, we provide three error-handling mechanisms to enforce the restrictions on the probabilistic programs described in Section 9.2.

1. We inspect **let** binding pairs and throw an error if an optimization variable is bound to anything other than a **sample** statement.
2. We add code that throws a runtime error if any optimization variable is assigned more than once or not at all.
3. We recursively traverse the code and throw a compilation error if **sample** statements of different base measures are assigned to any optimization variable. At present, we also throw an error if the base measure assigned to an optimization variable is unknown, e.g. because the distribution object is from a user defined **defdist** where the user does not provide the required measure type meta-information.

9.7 Particle Methods for Model Learning

10

Nested Estimation – when Inference Alone is Not Enough

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Voting probprog example?

We present a formalization of nested Monte Carlo (NMC) estimation, whereby terms in an outer estimator are themselves the output of separate, nested, Monte Carlo (MC) estimators. We demonstrate that NMC can provide consistent estimates of nested expectations under mild conditions, establish corresponding rates of convergence, and provide empirical evidence that suggests these rates are observed in practice. We further establish a number of pitfalls that can arise from naïve nesting of MC estimators and provide guidelines about how they can be avoided. Finally, we derive a new estimator for use in discrete Bayesian experimental design problems, which has a better convergence rate than existing methods.

10.1 Introduction

Monte Carlo (MC) methods [Metropolis and Ulam, 1949; Robert, 2004] are used throughout the quantitative sciences. For example, they have become a ubiquitous means of carrying out approximate Bayesian inference [Doucet et al., 2001a; Gilks et al., 1995], generating approximate samples from a posterior from which an expectation can be calculated. Although interesting alternatives have been suggested recently [Briol et al., 2015], MC integration is used almost exclusively for calculating these expectations from the produced samples.

Though the convergence of MC integration has been considered extensively in literature [Gilks, 2005; Robert, 2004], the theoretical implications arising from the *nesting* of MC schemes, where terms in the integrand depend on the result of separate, nested, MC estimators,

is generally less well known. This paper examines the convergence of such nested Monte Carlo (NMC) methods.

There are various problems involving nested expectations that require the use of nested estimation schemes such as NMC. For example, the expected information gain used in Bayesian experimental design [Chaloner and Verdinelli, 1995; Sebastiani and Wynn, 2000] requires the calculation of an entropy of a marginal distribution, and therefore includes the expectation of the logarithm of an expectation. By extension, any Kullback-Leibler divergence where one of the terms is a marginal distribution also involves a nested expectation. Hence, our results have important implications for relaxing mean field assumptions in variational inference [Hoffman and Blei, 2015] and deep generative models [Burda et al., 2015; Maaløe et al., 2016].

Another important reason for studying the properties of NMC comes from probabilistic programming systems (PPS) [Goodman et al., 2008b; Wood et al., 2014]. PPS allow a decoupling of model specification and inference, with the latter being carried out by a back-end engine that can operate on arbitrary programs. Some PPS allow for arbitrary nesting of queries so that it is easy to define and run nested inference problems, which has already begun to be exploited in application-specific work [Ouyang et al., 2016]. However, these nested inference problems fall outside the scope of the conventional proof of the convergence of MC estimation. Thus additional work is required to prove the validity of the corresponding back-end inference engines.

Outside the Bayesian inference framework, NMC can also arise in contexts demanding the use of direct MC simulations, for example in portfolio risk management [Gordy and Juneja, 2010] and stochastic control [Belomestny et al., 2010].

Certain nested estimation problems can be tackled by so-called pseudo-marginal methods [Andrieu and Roberts, 2009; Andrieu et al., 2010a, 2015; Naesseth et al., 2015a]. These consider cases of Bayesian inference where the likelihood is intractable, such as when it originates from an Approximate Bayesian Computation (ABC) [Csilléry et al., 2010], and involve reformulating the problem in an extended space with auxiliary variables that are used to represent the stochasticity in the likelihood computation. This then enables the problem to be expressed as a single expectation. Our work goes beyond this by also considering cases in which a non-linear mapping is applied to the output of the inner expectation (such as the logarithm in the experimental design case), so that this reformulation to a single expectation is no longer possible.

NMC with non-linear mappings of the inner expectation has been previously considered in the financial statistics literature, for example in the pricing of American options [Longstaff and Schwartz, 2001]. Though most of this literature focuses on particular application-specific non-linear mappings [Broadie et al., 2011; Gordy and Juneja, 2010], convergence bounds for a more general class of models has been shown by Hong and Juneja [2009].

We build on these results and outline the opportunities and pitfalls of nesting Monte Carlo estimators in a machine learning context. We demonstrate that the construction of consistent NMC algorithms is possible, establish convergence rates, and provide empirical evidence that these rates are observed in practice. Our proofs apply to a more general class of problems than existing approaches. In particular, we provide the first convergence bounds for cases of multiple levels of estimator nesting as might occur in, for example, a probabilistic programming system. Our results show that whenever an outer estimator depends nonlinearly on an inner estimator, then the number of samples used in *both* the inner and outer estimators must, in general, be driven to infinity for convergence. We provide theoretical results showing that in such scenarios any MC estimator using imperfect nested estimates is, in general, biased. We also lay out novel methods for reformulating certain classes of nested expectation problems into a single expectation, allowing the use of conventional MC estimation schemes with superior convergence rates than the naïve use of NMC. Finally, we use one of these results to derive a new estimation scheme for Bayesian experimental design with discrete outputs that has a superior convergence rate to existing approaches.

10.2 Problem Formulation

The key idea of MC is that the expectation of an arbitrary function $\lambda: \mathcal{Y} \rightarrow \mathcal{F} \subseteq \mathbb{R}$ under a probability distribution $p(y)$ for its input $y \in \mathcal{Y}$ can be approximately calculated using:

$$I = \mathbb{E}_{p(y)} [\lambda(y)] \approx \frac{1}{N} \sum_{n=1}^N \lambda(y_n) \quad \text{where} \quad y_n \stackrel{i.i.d.}{\sim} p(y). \quad (10.1)$$

In this paper, we consider the case that λ is itself intractable, defined only in terms of a functional mapping of an expectation. Specifically, $\lambda(y) = f(y, \gamma(y))$ where we can evaluate $f: \mathcal{Y} \times \Phi \rightarrow \mathcal{F}$ exactly for a given y and $\gamma(y)$, but $\gamma(y)$ is the output of the following intractable

expectation of another variable $z \in \mathcal{Z}$:

$$\text{either } \gamma(y) = \mathbb{E}_{p(z|y)} [\phi(y, z)] \quad (10.2a)$$

$$\text{or } \gamma(y) = \mathbb{E}_{p(z)} [\phi(y, z)] \quad (10.2b)$$

depending on the problem, with $\phi: \mathcal{Y} \times \mathcal{Z} \rightarrow \Phi \subseteq \mathbb{R}^{D_\phi}$. All our results apply to both cases, but we will focus on (10.2a) for clarity. Estimating I involves computing two integrals, one for y and the other for z . We call the approach of tackling both integrations using Monte Carlo as *nested Monte Carlo (NMC)*:

$$I \approx I_{N,M} = \frac{1}{N} \sum_{n=1}^N f(y_n, (\hat{\gamma}_M)_n) \quad \text{where } y_n \stackrel{i.i.d.}{\sim} p(y) \text{ and} \quad (10.3a)$$

$$(\hat{\gamma}_M)_n = \frac{1}{M} \sum_{m=1}^M \phi(y_n, z_{n,m}) \quad \text{where each } z_{n,m} \sim p(z|y_n) \text{ independently.} \quad (10.3b)$$

In Section 10.4 we will build on this further by considering cases with multiple levels of nesting, where computing $\phi(y, z)$ requires the computation of an intractable (nested) expectation.

The rest of this paper proceeds as follows. In Section 10.3, we consider special cases that allow recovery of the standard MC convergence rate. In Section 10.4, we establish convergence results for $I_{N,M}$ given a general class of f . In Section 10.5, we establish results demonstrating the inevitable bias of most possible general-purpose NMC schemes. Finally, in Section 10.6, we present empirical results demonstrating the applicability of NMC and suggesting that our theoretical convergence rates are observed in practice.

10.3 Special Cases

We begin by discussing some special cases where it is possible to achieve a convergence rate of $O(1/N)$ in the mean square error (MSE) as per conventional MC estimation [Robert, 2004]. Establishing these cases is important because it identifies what problems we can use existing results for, when we can achieve an improved convergence rate, and what precautions we must take to ensure this. The first case is that the top-level integrand f in our estimation problem is linear. Section 10.3.1 summarizes the well-known result in this case, which forms the basis for pseudo-marginal, nested sequential MC [Naesseth et al., 2015a], and ABC methods. The next is that y has finite possible realisations. The result for this case is given in Section 10.3.2. Though intuitively straight-forward, it requires significant care to prove. The third case in

Section 10.3.3 is concerned with the product of expectations. Our result for this case is, to the best of our knowledge, new and applies to many latent variable models and a number of probabilistic program examples, e.g. when the probability of a program trace is weighted by marginal likelihood estimates from other programs. The last case is that the integrand f is a polynomial (Section 10.3.4). It covers cases such as moment estimation and opens up interesting possibilities in using tractable approximations to the integrand f .

10.3.1 Linear f

Suppose that f is integrable and linear in its second argument, i.e. $f(y, \alpha v + \beta w) = \alpha f(y, v) + \beta f(y, w)$. In this case, we can rearrange the problem to a single expectation:

$$\begin{aligned} I &= \mathbb{E}[f(y, \gamma(y))] = \mathbb{E}[f(y, \mathbb{E}[\phi(y, z)|y])] = \mathbb{E}[\mathbb{E}[f(y, \phi(y, z))|y]] \\ &= \mathbb{E}[f(y, \phi(y, z))] \approx \frac{1}{N} \sum_{n=1}^N f(y_n, \phi(y_n, z_n)) \end{aligned}$$

where $(y_n, z_n) \sim p(y)p(z|y)$ if $\gamma(y)$ is of the form of (10.2a) and $y_n \sim p(y)$ and $z_n \sim p(z)$ are independently drawn if $\gamma(y)$ is of the form of (10.2b).

10.3.2 Finite Possible Realisations of y

If y must take one of finitely many values y_1, \dots, y_C , then it is possible to use another approach to ensure the same convergence rate as standard MC. The key observation is to note that in this case we can convert the nested problem (10.1) into C separate non-nested problems

$$I = \sum_{c=1}^C P(y = y_c) f(y_c, \gamma(y_c)) \quad (10.4)$$

which can then be estimated using

$$I_N = \sum_{c=1}^C (\hat{P}_N)_c (\hat{f}_N)_c \quad \text{where} \quad (10.5)$$

$$P(y = y_c) \approx (\hat{P}_N)_c = \frac{1}{N} \sum_{n=1}^N \mathbb{1}(y_n = y_c) \quad (10.6)$$

$$f(y_c, \gamma(y_c)) \approx (\hat{f}_N)_c = f\left(y_c, \frac{1}{N} \sum_{n=1}^N \phi(y_c, z_{n,c})\right), \quad (10.7)$$

with $y_n \stackrel{i.i.d.}{\sim} p(y)$ and $z_{n,c} \sim p(z|y_c)$ or $z_{n,c} \sim p(z)$ depending on whether our formulation uses (10.2a) or (10.2b). We can now show the following result, noting that as the same set of y_n 's is used for every $(\hat{P}_N)_c$, calculating I_N requires N samples of y , CN samples of z (each drawn independently to the samples of y), CN evaluations of ϕ , and C evaluations of f .

Theorem 10.1. *If f is Lipschitz continuous, then the mean squared error of I_N as an estimator for I converges at rate $O(1/N)$.*

Proof. See Appendix 10.8.1. □

10.3.3 Products of Expectations

In this section we consider the scenario where $\gamma(y)$ is equal to the product of multiple expectations, rather than just a single expectation as per (10.2a). That is,

$$I = \mathbb{E}_{p(y)} \left[f \left(y, \prod_{\ell=1}^L \mathbb{E}_{p(z_\ell|y)} [\psi_\ell(y, z_\ell)] \right) \right]. \quad (10.8)$$

This product of expectations can be rearranged to a single expectation and so the estimation of I corresponds to the formulation laid out in Section 10.2. To see this, consider the set of random variables $\{z'_\ell\}_{\ell=1:L}$ such that each $z'_\ell|y \sim p(z_\ell|y)$ and the z'_ℓ are independent of one another. This can be achieved by, for example, taking L independent samples from the joint $Z_\ell \stackrel{i.i.d.}{\sim} p(z_{1:L}|y)$ and using the ℓ^{th} such draw for the ℓ^{th} dimension of z' , i.e. setting $z'_\ell = \{Z_\ell\}_\ell$. For every $y \in \mathcal{Y}$ we now have

$$\prod_{\ell=1}^L \mathbb{E}_{p(z_\ell|y)} [\psi_\ell(y, z_\ell)] = \prod_{\ell=1}^L \mathbb{E}_{p(z'_\ell|y)} [\psi_\ell(y, z'_\ell)] = \mathbb{E}_{p(\{z'_\ell\}_{\ell=1:L}|y)} \left[\prod_{\ell=1}^L \psi_\ell(y, z'_\ell) \right]$$

which is a single expectation on an extended space and implies that (10.8) fits the NMC formulation. Furthermore, we can now show that if f is linear, the MSE of the NMC estimator (10.8) converges at the standard MC rate $O(1/N)$, provided that the number of samples used in the inner estimators remains fixed.

Theorem 10.2. *Consider the NMC estimator*

$$I_N = \frac{1}{N} \sum_{n=1}^N f \left(y_n, \prod_{\ell=1}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y_n, z'_{n,\ell,m}) \right)$$

where each $y_n \in \mathcal{Y}$ and $z'_{n,\ell,m} \in \mathcal{Z}_\ell$ are independently drawn from $y_n \sim p(y)$ and $z'_{n,\ell,m}|y_n \sim p(z_\ell|y_n)$, respectively. If f is linear, the estimator converges almost surely to I , with a convergence rate of $O(1/N)$ in the mean square error for any fixed choice of $\{M_\ell\}_{\ell=1:L}$.

Proof. See Appendix 10.8.2. □

As this result holds in the case $L = 1$, an important consequence is that whenever f is linear, the same convergence rate is achieved regardless of whether we reformulate the problem to a single expectation or not, provided that the number of samples used by the inner estimator remains fixed. This, for example, demonstrates that pseudo-marginal methods where the outer estimator uses importance sampling or direct MC estimation converge at the standard MC error rate. Conversely, as we will show in Section 10.4, if f is nonlinear, it will be necessary for the number of samples in *both* the inner and the outer estimators to increase in order to achieve the convergence of (10.3).

10.3.4 Polynomial f

Perhaps surprisingly, when f is of the form

$$f(y, \gamma(y)) = \sum_{j=1}^J g_j(y) \gamma_j(y)^{\alpha_j} \quad \text{where } \alpha_j \in \mathbb{Z}_{\geq 0}, \forall j \in \{1, \dots, J\} \quad (10.9)$$

then it is also be possible to construct a standard MC estimator by building on the ideas introduced in Section 10.3.3 and those introduced by Goda [2016]. The key idea is to note that

$$(\mathbb{E}[z])^2 = \mathbb{E}[z] \mathbb{E}[z'] = \mathbb{E}[zz']$$

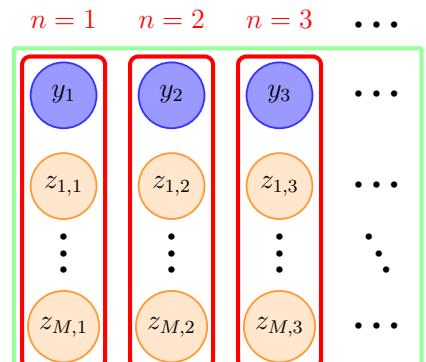
where z and z' are i.i.d. Therefore, assuming appropriate integrability requirements, we can construct the following non-nested MC estimator:

$$\begin{aligned} \mathbb{E}\left[\sum_{j=1}^J g_j(y) \gamma_j(y)^{\alpha_j}\right] &= \sum_{j=1}^J \mathbb{E}[g_j(y) \mathbb{E}[\phi(y, z_j)|y]^{\alpha_j}] = \sum_{j=1}^J \mathbb{E}\left[g_j(y) \mathbb{E}\left[\prod_{\ell=1}^{\alpha_j} \phi(y, z_{j,\ell}) \middle| y\right]\right] \\ &= \sum_{j=1}^J \mathbb{E}\left[g_j(y) \prod_{\ell=1}^{\alpha_j} \phi(y, z_{j,\ell})\right] \approx \frac{1}{N} \sum_{n=1}^N \sum_{j=1}^J g(y_n) \prod_{\ell=1}^{\alpha_j} \phi(y_n, z_{j,\ell,n}). \end{aligned} \quad (10.10)$$

Here each $z_{j,\ell,n} \sim p(z_j|y)$ is drawn i.i.d. from the corresponding conditional distribution.

10.4 Convergence of Nested Monte Carlo

Since we cannot always unravel the target estimation using one of the special cases in the previous section, we must resort to NMC (or another nested estimation scheme) in order to compute I in general. Our aim



here is to show that approximating $I \approx I_{N,M}$ is in principle possible, at least when f is well-behaved. In particular, we establish a convergence rate of the mean squared error of $I_{N,M}$ and prove a form of almost sure convergence to I . We further generalize our convergence rate to apply to the case of multiple levels of estimator nesting.

Before providing a formal examination of the convergence of NMC, we first provide more intuition about how we might expect to construct a convergent NMC estimator. Consider the diagram shown in Figure 10.1, and suppose that we want our error to be less than some arbitrary ε . Assume that f is sufficiently smooth that we can choose M large enough to make $|I - \mathbb{E}[f(y_n, (\hat{\gamma}_M)_n)]| < \varepsilon$ (we will characterize the exact requirements for this later). For this fixed M , we have a standard MC estimator on an extended space y, z_1, \dots, z_M such that each sample constitutes one of the red boxes. As we take $N \rightarrow \infty$, i.e. taking all the samples in the green, this estimator converges such that $I_{N,M} \rightarrow \mathbb{E}[f(y_n, (\hat{\gamma}_M)_n)]$ as $N \rightarrow \infty$ for fixed M . As we can make ε arbitrarily small, we can also achieve an arbitrarily small error.

Convergence bounds for NMC have previously been shown by Hong and Juneja [2009] in the financial statistics literature. Under the assumption that $\hat{\gamma}$ is Gaussian distributed (which is often reasonable due to the central limit theorem) and that f is thrice differentiable other than at some finite number of points, they have shown that it is possible to achieve a converge rate of $O(1/N + 1/M^2)$. We now show that these assumptions can be relaxed to only requiring f to be Lipschitz continuous, at the expense of weakening this bound to $O(1/N + 1/M)$.

Theorem 10.3. *If f is Lipschitz continuous and $f(y_n, \gamma(y_n)), \phi(y_n, z_{n,m}) \in L^2$, the mean squared error of $I_{N,M}$ converges to 0 at rate $O(1/N + 1/M)$.*

Proof. See Appendix 10.8.3 □

Inspection of the convergence rate above shows that, given a total number of samples $T = MN$, our bound is tightest when $N \propto M$, with a corresponding rate $O(1/\sqrt{T})$ (see Appendix 10.9). When the additional assumptions of Hong and Juneja [2009] apply, this rate can be lowered to $O(1/T^{2/3})$ by setting $N \propto M^2$. We note that the result of Theorem 10.3 was recently independently derived by Fort et al. [2017]. They also show that if f is continuously

differentiable in its second variable and this derivative is bounded and Lipschitz continuous, then the $O(1/N + 1/M^2)$ bound is achieved.

We now consider the question of what is the minimal requirement on f to ensure some form of convergence? For a fixed single y_1 , we have that $(\hat{\gamma}_M)_1 = \frac{1}{M} \sum_{m=1}^M \phi(y_1, z_{1,m}) \rightarrow \gamma(y_1)$ almost surely as $M \rightarrow \infty$, because the left-hand side is a MC estimator. If f is continuous around y_1 , this also implies $f(y_1, (\hat{\gamma}_M)_1) \rightarrow f(y_1, \gamma(y_1))$. Our candidate requirement is that this holds in expectation, i.e. that it holds when we incorporate the effect of the outer estimator. More precisely, we define $(\epsilon_M)_n = |f(y_n, (\hat{\gamma}_M)_n) - f(y_n, \gamma(y_n))|$ and require that $\mathbb{E}[(\epsilon_M)_1] \rightarrow 0$ as $M \rightarrow \infty$ (noting that $(\epsilon_M)_n$ are i.i.d. and so $\mathbb{E}[(\epsilon_M)_1] = \mathbb{E}[(\epsilon_M)_n], \forall n \in \mathbb{N}$). Informally, this “expected continuity” requirement is weaker than uniform continuity because it does allow (potentially infinitely many) discontinuities in f . More formally we have the following result.

Theorem 10.4. *For $n \in \mathbb{N}$, let*

$$(\epsilon_M)_n = |f(y_n, (\hat{\gamma}_M)_n) - f(y_n, \gamma(y_n))|.$$

Assume that $\mathbb{E}[(\epsilon_M)_1] \rightarrow 0$ as $M \rightarrow \infty$. Denote by Ω the sample space of our underlying probability space, so that $I_{\tau_\delta(M), M}$ can be thought of as a map from Ω to \mathbb{R} . Then, for every $\delta > 0$, there exists a measurable $A_\delta \subseteq \Omega$ with $\mathbb{P}(A_\delta) < \delta$, and a function $\tau_\delta : \mathbb{N} \rightarrow \mathbb{N}$ such that, for all $\omega \notin A_\delta$,

$$I_{\tau_\delta(M), M}(\omega) \rightarrow I \quad \text{as } M \rightarrow \infty.$$

Proof. See Appendix 10.8.4 □

As this convergence is in M , it suggests (and is reinforced by the convergence rate) that in order to achieve convergence for most f , we should increase not just the number of samples in the outer estimator but also the number of samples in the inner estimator. Theorem 10.3 gives an intuitive reason for why this should be the case; it says that if M is fixed, the bias on each inner term will remain non-zero even when N tends to ∞ .

We next consider the case of multiple levels of nesting. This case is particularly important for analysing probabilistic programming languages, which provide mechanisms for nesting probabilistic submodules to enable flexible compositionality. To formalise what we mean by

arbitrary nesting, we first assume some fixed integral depth $D > 0$, and real-valued functions f_0, \dots, f_D . We then define

$$\begin{aligned}\gamma_D(y^{(0:D-1)}) &= \mathbb{E} [f_D(y^{(0:D)}) | y^{(0:D-1)}] \quad \text{and} \\ \gamma_k(y^{(0:k-1)}) &= \mathbb{E} [f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)})) | y^{(0:k-1)}],\end{aligned}$$

for $0 \leq k < D$, where $y^{(k)} \sim p(y^{(k)} | y^{(0:k-1)})$. Note that our single nested case corresponds to the setting of $D = 1$, $f_0 = f$, $f_1 = \phi$, $y^{(0)} = y$, $y^{(1)} = z$, $\gamma_0 = I$, and $\gamma_1 = \gamma$. Our goal is to estimate $\gamma_0 = \mathbb{E} [f_0(y^{(0)}, \gamma_1(y^{(0)}))]$. To do so we will use the following NMC scheme:

$$\begin{aligned}I_D(y^{(0:D-1)}) &= \frac{1}{N_D} \sum_{n=1}^{N_D} f_D(y^{(0:D-1)}, y_n^{(D)}) \quad \text{and} \\ I_k(y^{(0:k-1)}) &= \frac{1}{N_k} \sum_{n=1}^{N_k} f_k(y^{(0:k-1)}, y_n^{(k)}, I_{k+1}(y^{(0:k-1)}, y_n^{(k)}))\end{aligned}$$

for $0 \leq k < D$, where each $y_n^{(k)} \sim p(y^{(k)} | y^{(0:k-1)})$ is drawn independently. The theorem below gives a rate of convergence of NMC in this case.

Theorem 10.5. *Assume that f_0, \dots, f_D are all Lipschitz continuous, and that*

$$f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)})), I_k(y^{(0:k-1)}) \in L^2$$

for $0 \leq k \leq D$. Then, the mean squared error $\mathbb{E} [(\gamma_0 - I_0)^2]$ converges to 0 at rate $O\left(\sum_{k=0}^D \frac{1}{N_k}\right)$.

Proof. See Appendix 10.8.5 □

As this estimation scheme requires drawing ($T = \prod_{k=0}^D N_k$)-many samples, the result shows that the convergence speed rapidly diminishes with repeated nesting.

10.5 The Inevitable Bias of Nested Estimation

The previous section confirmed the capabilities of NMC; in this section we establish a limitation by proving that NMC schemes must produce biased estimates of $I(f)$ for certain functions f . In fact, our result applies more generally: we show that this holds for any Monte Carlo scheme that makes use of imperfect estimates $\hat{\zeta}_n$ of $\gamma(y_n)$, either via a nested Monte Carlo procedure (e.g. $\hat{\zeta}_n = (\hat{\gamma}_M)_n$), or when these inner estimates are generated by some other potentially deterministic methods such as a variational approximation [Blei et al., 2016] or Bayesian quadrature [O’Hagan, 1991].

Theorem 10.6. Suppose that the random variables $\hat{\zeta}_n$ satisfy $\mathbb{P}(\hat{\zeta}_n \neq \gamma(y_n)) > 0$. Then we can choose f such that if $y_n \sim p(y)$, $\mathbb{E} \left[\frac{1}{N} \sum_{n=1}^N f(y_n, \hat{\zeta}_n) \right] \neq I(f)$ for any N (including the limit $N \rightarrow \infty$).

Proof. Take $f(y, w) = (\gamma(y) - w)^2$. Then $f(y, \gamma(y)) = 0$, so that $I(f) = 0$. On the other hand, $f(y_n, \hat{\zeta}_n) \geq 0$ since f is non-negative. Moreover, $f(y_n, \hat{\zeta}_n) > 0$ on the event $\{\hat{\zeta}_n \neq \gamma(y_n)\}$. Since we assumed this event has nonzero probability, it follows that $\mathbb{E} [f(y_n, \hat{\zeta}_n)] > 0$ and hence

$$\mathbb{E} \left[\frac{1}{N} \sum_{n=1}^N f(y_n, \hat{\zeta}_n) \right] = \frac{1}{N} \sum_{n=1}^N \mathbb{E} [f(y_n, \hat{\zeta}_n)] > 0 = I(f)$$

which gives the required result. \square

We now show that *any* strictly convex or concave f entails a biased estimator when $\hat{\zeta}_n$ is unbiased but has non-zero variance given y_n . This covers the case where $\hat{\zeta}_n$ is a MC estimate.

Theorem 10.7. Suppose that $y_n \sim p(y)$ and that each $\hat{\zeta}_n$ satisfies $\mathbb{E} [\hat{\zeta}_n | y_n] = \gamma(y_n)$. Define $\mathcal{A} \subseteq \mathcal{Y}$ as $\mathcal{A} = \{y \in \mathcal{Y} \mid \text{Var}(\hat{\zeta}_n | y_n = y) > 0\}$ and assume that $\mathbb{P}(y_n \in \mathcal{A}) > 0$. Then for any f that is strictly convex in its second argument,

$$\mathbb{E} \left[\frac{1}{N} \sum_{n=1}^N f(y_n, \hat{\zeta}_n) \right] > I(f).$$

Similarly for any f that is strictly concave in its second argument,

$$\mathbb{E} \left[\frac{1}{N} \sum_{n=1}^N f(y_n, \hat{\zeta}_n) \right] < I(f).$$

Proof. We prove our claim for the case that f is strictly convex; our proof for the other concave case is symmetrical. We have

$$\mathbb{E} \left[\frac{1}{N} \sum_{n=1}^N f(y_n, \hat{\zeta}_n) \right] = \mathbb{E} [f(y_1, \hat{\zeta}_1)] = \mathbb{E} [\mathbb{E} [f(y_1, \hat{\zeta}_1) | y_1]] \geq \mathbb{E} [f(y_1, \mathbb{E} [\hat{\zeta}_1 | y_1])] = I(f)$$

where the \geq is a result of Jensen's inequality on the inner expectation. Since f is strictly convex and therefore nonlinear, equality holds if and only if $\hat{\zeta}_1$ is almost surely constant given y_1 . This is violated whenever $y_1 \in \mathcal{A}$, which by assumption has a non-zero probability of occurring. Consequently, the inequality must be strict, giving the desired result. \square

For certain nonlinear f , it may still be possible to develop unbiased estimation schemes using Russian roulette sampling [Lyne et al., 2015] or other debiasing techniques. However, this induces its own complications: for some problems the resultant estimates have infinite variance [Lyne et al., 2015] and as shown by Jacob et al. [2015], there are no general purpose “ f -factories” that produce both non-negative and unbiased estimates for non-constant, positive output functions $f : \mathbb{R} \rightarrow \mathbb{R}^+$, given unbiased estimates for the inputs.

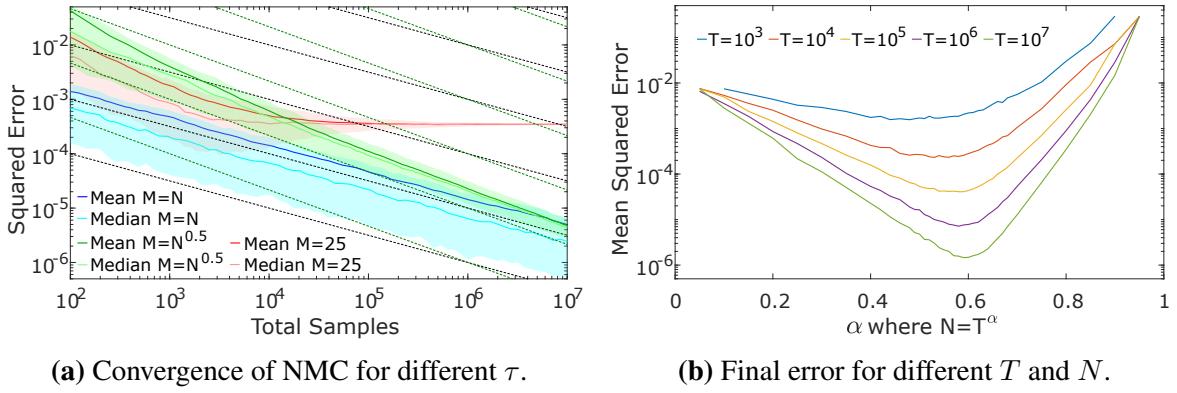


Figure 10.2: Empirical convergence of NMC for (10.11). Shown left is the convergence in total samples for different ways of setting M and N . Results are averaged over 1000 independent runs, while shaded regions give the 25%-75% quantiles. We see that the theoretical convergence rates (as shown by the dash lines) are observed. The fixed M case converges at the MC error rate, but to a biased solution. Shown right is the final error for different total sample budgets as a function of α where $N = T^\alpha$ and $M = T^{1-\alpha}$ iterations are used for the outer and inner estimators respectively. This shows that even though $\alpha = 2/3$ is the asymptotically optimal allocation strategy, this is not the optimal solution for finite T . Nonetheless, as T increases, the optimum value of α increases, starting at around 0.5 for $T = 10^3$ and reaching around 0.6 for $T = 10^7$.

10.6 Empirical Verification and Applications

The convergence rates proven in Section 10.4 are only *upper bounds* on the worst case performance we can expect. We will now examine whether these convergence rates are tight in practice, investigate what happens when our guidelines are not followed, and outline some possible applications of NMC.

We start with the following simple model where the exact solution for I can be calculated analytically:

$$\begin{aligned} y &\sim \text{Uniform}(-1, 1), & z &\sim \mathcal{N}(0, 1), \\ \phi(y, z) &= \sqrt{2/\pi} \exp\left(-2(y-z)^2\right), & f(y, \gamma(y)) &= \log(\gamma(y)) = \log(\mathbb{E}_z[\phi(y, z)]). \end{aligned} \tag{10.11}$$

Figure 10.2a shows the corresponding empirical convergence obtained by applying (10.3) to (10.11) directly. It shows that, at least in this case, the theoretical convergence rates from Theorem 10.3 are indeed realised. The figure also demonstrates the danger of not increasing M with N , showing that the NMC estimator converges to an incorrect solution when M is held constant. Figure 10.2b shows the effect of varying N and M for various fixed sample budgets T and demonstrates that the asymptotically optimal strategy can be suboptimal for finite budgets. An extension of this model to a case with multiple levels of nesting is shown in Appendix 10.10.

10.6.1 Planning Cancer Treatment

We now introduce a real-world example to show the applicability of NMC in a scenario where the solution is not analytically tractable and conventional MC is insufficient. Consider a treatment centre assessing a new policy for planning cancer treatments, subject to a budget. Clinicians must decide on a patient-by-patient basis whether to administer chemotherapy in the hope that their tumour will reduce in size sufficiently to be able to perform surgery at a later date. A treatment is considered to have been successful if the size of the tumour drops below a threshold value in a fixed time window. The clinicians have at their disposal a simulator for the evolution of tumours with time, parameterized by both observable values, y , such as tumour size, and unobservable values, z , such as the patient-specific response to treatment. Given a set of input parameters, the simulator deterministically returns a binary response $\phi(y, z) \in \{0, 1\}$, with $\phi(y, z) = 1$ indicating a successful treatment. To estimate the probability of a successful treatment for a given patient, the clinician must calculate the expected success over these unobserved variables, namely $\mathbb{E}_{p(z|y)}[\phi(y, z)]$ where $p(z|y)$ represents a probabilistic model for the unobserved variables, which could, for example, be constructed based on empirical data. The clinician then decides whether to go ahead with the treatment for that patient based on whether the calculated probability of success exceeds a certain threshold T_{treat} .

The treatment centre now wishes to estimate the expected number of patients that will be treated for a given T_{treat} so that it can minimize this threshold without exceeding its budget. To do this, it needs to calculate the expectation of the clinician's decisions to administer treatment, giving the complete nested expectation for calculating the number of treated patients as

$$I(T_{\text{treat}}) = \mathbb{E}_{p(y)} \left[\mathbb{I} \left(\mathbb{E}_{p(z|y)}[\phi(y, z)] > T_{\text{treat}} \right) \right], \quad (10.12)$$

which we propose to estimate using NMC. Full details on ϕ , $p(y)$, and $p(z|y)$ are provided in Appendix 10.11.

To verify the convergence rate, we repeat the analysis from Section 10.4 for the problem defined by (10.12) at a fixed value of $T_{\text{treat}} = 0.35$. The results, shown in Figure 10.3a, again verify the theoretical rates. By further testing different values of T_{treat} , we found $T_{\text{treat}} \geq 0.125$ (i.e. go ahead with treatment if the probability of success is 0.125 or greater) to be the optimal under the budget.

10.6.2 Bayesian Experimental Design

In this section we show how our results can be used to derive an improved estimator for the problem of Bayesian experimental design (BED) in the case where the experiment outputs are discrete. Due to space restrictions, this section is necessarily brief, with a full introduction to BED, the derivation of all the introduced estimators, and additional results provided in Appendix 11.1.

Bayesian experimental design provides a framework for designing experiments in a manner that is optimal from an information-theoretic viewpoint [Chaloner and Verdinelli, 1995; Sebastiani and Wynn, 2000]. Given a prior $p(\theta)$ on parameters θ and a corresponding likelihood $p(y|\theta, d)$ for experiment outcomes y given a design d , the Bayesian optimal design d^* is given by maximizing the mutual information between θ and y defined as follows

$$\bar{U}(d) = \int_y \int_{\Theta} p(y, \theta|d) \log \left(\frac{p(\theta|y, d)}{p(\theta)} \right) d\theta dy. \quad (10.13)$$

Finding d^* is challenging as the posterior $p(\theta|y, d)$ is rarely known in closed form. However, after appropriate algebraic manipulation, it can be shown that (10.13) is consistently estimated by

$$\hat{U}_{\text{NMC}}(d) = \frac{1}{N} \sum_{n=1}^N \left[\log(p(y_n|\theta_{n,0}, d)) - \log \left(\frac{1}{M} \sum_{m=1}^M p(y_n|\theta_{n,m}, d) \right) \right] \quad (10.14)$$

where $\theta_{n,m} \sim p(\theta)$ for each $(m, n) \in \{0, \dots, M\} \times \{1, \dots, N\}$, and $y_n \sim p(y|\theta = \theta_{n,0}, d)$ for each $n \in \{1, \dots, N\}$. This naïve NMC estimator has been implicitly used by Myung et al. [2013] and Ouyang et al. [2016] amongst others and gives a convergence rate $O(1/M^2 + 1/N)$ as per Section 10.4.

When y can only take on finitely many realisations y_1, \dots, y_c , we use the ideas introduced in Section 10.3.2 to derive the following estimator

$$\begin{aligned} \hat{U}_R(d) &= \frac{1}{N} \sum_{n=1}^N \sum_{c=1}^C p(y_c|\theta_n, d) \log(p(y_c|\theta_n, d)) \\ &\quad - \sum_{c=1}^C \left[\left(\frac{1}{N} \sum_{n=1}^N p(y_c|\theta_n, d) \right) \log \left(\frac{1}{N} \sum_{n=1}^N p(y_c|\theta_n, d) \right) \right] \end{aligned} \quad (10.15)$$

where $\theta_n \sim p(\theta)$ for each $n \in \{1, \dots, N\}$. As C is a fixed constant, (10.15) converges at the standard MC error rate of $O(1/N)$. This constitutes a substantially faster convergence as (10.14) requires a total of MN samples compared to N for (10.15). To the best of our knowledge, this estimator for this experimental design problem with its superior convergence guarantee has not been introduced in the literature.

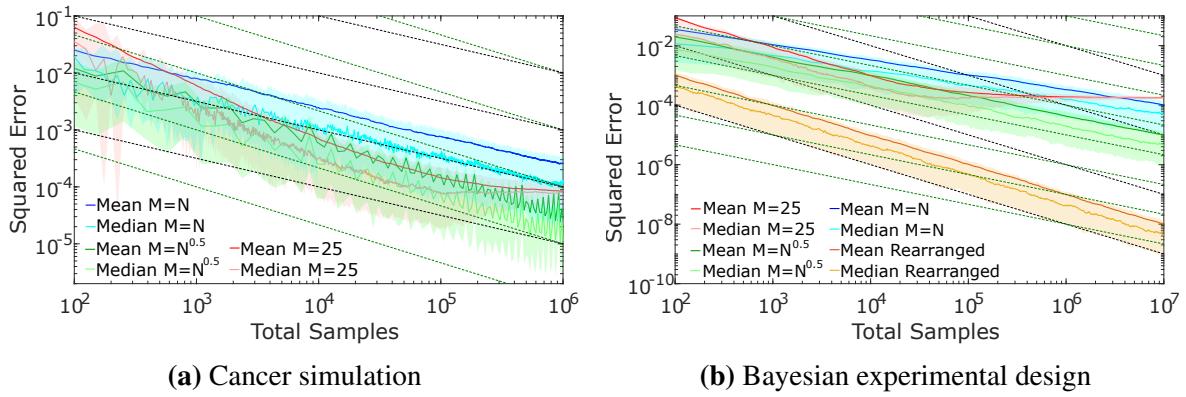


Figure 10.3: Convergence of NMC for cancer simulation and of both NMC and our reformulated estimator (10.15) for the BED problem. A ground truth estimate for the cancer simulation was calculated using a single run with $M = 10^5$ and $N = 10^5$ and using a single run of the reformulated estimator with 10^{10} for the BED problem. Results are averaged over 1000 independent runs, while shaded regions give the 25%-75% quantiles. We see that the theoretical convergence rates are observed in all cases, with the advantages of the reformulated estimator particularly pronounced. On the cancer example when $M = \sqrt{N}$ an interesting fluctuation behaviour is observed. Further testing suggests that this originates because the bias of the estimator depends in a fluctuating manner on the value of M as the binary output of $\phi(y, z)$ creates a quantization effect on the possible estimates for $\hat{\gamma}$. This effect is also observed for the $M = N$ case, but is less pronounced.

We finish by showing that the theoretical advantages of this reformulation also lead to empirical gains in the estimation of $\bar{U}(d)$. For this we consider a model used in psychology experiments for delay discounting introduced by Vincent [2016], details of which are given in Appendix 11.1. Convergence results shown in Figure 10.3b demonstrate that the theoretical convergence rates are observed while results given in Appendix 11.1 show that this leads to significant practical gains in estimating $\bar{U}(d)$.

10.7 Conclusions

We have introduced a formal framework for nested Monte Carlo (NMC) estimation and shown that it can be used to yield a consistent estimator for problems that cannot be tackled with conventional MC alone. We have demonstrated convergence rates and that NMC is, in general, biased. We have introduced a number of techniques for converting certain classes of NMC problems to conventional MC ones, allowing for improved convergence rates on these problems. We used one of these to derive a new estimator for Bayesian experimental design with a superior convergence rate to existing schemes. For problems that do not satisfy these special cases, we have highlighted the importance of increasing the number of samples in both the inner

and the outer estimators to ensure convergence. Our results have implications for numerous applications, for example probabilistic programming, and serve both as an invitation for further inquiry and a caveat against careless use.

10.8 Proofs

10.8.1 Proof of Theorem 10.1 - Convergence Rate for Finite Realisations of y

Theorem 10.1. *If f is Lipschitz continuous, then the mean squared error of I_N as an estimator for I converges at rate $O(1/N)$.*

Proof. Denote $P_c = P(y = y_c)$ and $f_c = f(y_c, \gamma(y_c))$ noting that as the y_c are fixed values, so are P_c and f_c . Then, Minkowski's inequality allows us to bound the mean squared error as

$$\mathbb{E}[(I_N - I)^2] = \|I_N - I\|_2^2 \leq \left(\sum_{c=1}^C W_c\right)^2 \quad \text{where} \quad W_c := \left\|(\hat{P}_N)_c (\hat{f}_N)_c - P_c f_c\right\|_2.$$

Moreover, again by Minkowski, we have $W_c \leq U_c + V_c$ where

$$U_c = \left\|(\hat{P}_N)_c (\hat{f}_N)_c - (\hat{P}_N)_c f_c\right\|_2, \quad V_c = \left\|(\hat{P}_N)_c f_c - P_c f_c\right\|_2.$$

Factoring out $(\hat{P}_N)_c$ in U_c and noting that each y_n and $z_{n,c}$ are sampled independently gives

$$U_c = \sqrt{\mathbb{E}\left[(\hat{P}_N)_c^2 \left((\hat{f}_N)_c - f_c\right)^2\right]} = \sqrt{\mathbb{E}\left[(\hat{P}_N)_c^2\right]} \sqrt{\mathbb{E}\left[\left((\hat{f}_N)_c - f_c\right)^2\right]}.$$

Using Minkowski's inequality, we may write the first right-hand term as

$$\begin{aligned} \sqrt{\mathbb{E}\left[(\hat{P}_N)_c^2\right]} &= \left\|(\hat{P}_N)_c\right\|_2 \leq \frac{1}{N} \sum_{n=1}^N \|\mathbb{1}(y_n = y_c)\|_2 \\ &= \frac{1}{N} \sum_{n=1}^N \mathbb{E}\left[\mathbb{1}(y_n = y_c)^2\right] = \frac{1}{N} \sum_{n=1}^N P_c = P_c. \end{aligned}$$

For the second term, note that by Lipschitz continuity, we have for some constant $K > 0$

$$\begin{aligned} \sqrt{\mathbb{E}\left[\left((\hat{f}_N)_c - f_c\right)^2\right]} &= \left\|(\hat{f}_N)_c - f_c\right\|_2 \leq K \left\|\frac{1}{N} \sum_{n=1}^N \phi(y_c, z_{n,c}) - \gamma(y_c)\right\|_2 \\ &= K \cdot O(1/\sqrt{N}) = O(1/\sqrt{N}), \end{aligned}$$

since $\frac{1}{N} \sum_{n=1}^N \phi(y_c, z_{n,c})$ is a Monte Carlo estimator for $\gamma(y_c)$. Altogether then, we have that

$$U_c = P_c \cdot O(1/\sqrt{N}) = O(1/\sqrt{N}).$$

We can also factor out f_c in V_c to obtain

$$V_c = |f_c| \cdot \left\|(\hat{P}_N)_c - P_c\right\|_2 = |f_c| \cdot O(1/\sqrt{N}) = O(1/\sqrt{N}),$$

since $(\hat{P}_N)_c$ is a Monte Carlo estimator for P_c . Now by noting that $(A + B)^2 \leq 2(A^2 + B^2)$ for any $A, B \in \mathbb{R}$, an inductive arguments shows that

$$\left(\sum_{\ell=1}^L A_\ell \right)^2 \leq 2^{\lceil \log_2 L \rceil} \sum_{\ell=1}^L A_\ell^2$$

for all $A_1, \dots, A_L \in \mathbb{R}$. We can now show that our asymptotic bounds for U_c and V_c entail that our overall mean squared error satisfies

$$\begin{aligned} \mathbb{E}[(I_N - I)^2] &\leq 2^{\lceil \log_2 C \rceil} \sum_{c=1}^C W_c^2 \leq 2^{\lceil \log_2 C \rceil} \sum_{c=1}^C (U_c + V_c)^2 \leq 2^{\lceil \log_2 C \rceil + 1} \sum_{c=1}^C U_c^2 + V_c^2 \\ &= 2^{\lceil \log_2 C \rceil + 1} \sum_{c=1}^C O(1/N) + O(1/N) = O(1/N), \end{aligned}$$

as desired. \square

10.8.2 Proof for Theorem 10.2 - Products of Expectations

Theorem 10.2. Consider the NMC estimator

$$I_N = \frac{1}{N} \sum_{n=1}^N f \left(y_n, \prod_{\ell=1}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y_n, z'_{n,\ell,m}) \right)$$

where each $y_n \in \mathcal{Y}$ and $z'_{n,\ell,m} \in \mathcal{Z}_\ell$ are independently drawn from $y_n \sim p(y)$ and $z'_{n,\ell,m} | y_n \sim p(z_\ell | y_n)$, respectively. If f is linear, the estimator converges almost surely to I , with a convergence rate of $O(1/N)$ in the mean square error for any fixed choice of $\{M_\ell\}_{\ell=1:L}$.

Proof. Consider fixed sizes of nested sample sets, $\{M_\ell\}_{\ell=1:L}$. For each $y \in \mathcal{Y}$ and

$$x = \{\{z'_{\ell,m}\}_{m=1:M_\ell}\}_{\ell=1:L} \in \mathcal{X} = \mathcal{Z}_1^{M_1} \otimes \cdots \otimes \mathcal{Z}_L^{M_L},$$

define

$$\eta(y, x) = f \left(y, \prod_{\ell=1}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y, z'_{\ell,m}) \right).$$

Now, $I_N = \frac{1}{N} \sum_{n=1}^N \eta(y_n, x_n)$ is a standard MC estimator on the space $\mathcal{Y} \otimes \mathcal{X}$. Thus, $I_N \xrightarrow{a.s.} \mathbb{E}[I_N]$ with convergence properties and rate as per standard MC. We finish the proof by showing that $\mathbb{E}[I_N] = I$ when f is linear:

$$\mathbb{E}[I_N] = \mathbb{E} \left[\frac{1}{N} \sum_{n=1}^N f \left(y_n, \prod_{\ell=1}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y_n, z'_{n,\ell,m}) \right) \right]$$

$$\begin{aligned}
&= \mathbb{E} \left[f \left(y_1, \prod_{\ell=1}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y_1, z'_{1,\ell,m}) \right) \right] \\
&= \mathbb{E} \left[\mathbb{E} \left[f \left(y_1, \prod_{\ell=1}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y_1, z'_{1,\ell,m}) \right) \middle| y_1 \right] \right],
\end{aligned}$$

now using the linearity of f

$$= \mathbb{E} \left[f \left(y_1, \mathbb{E} \left[\prod_{\ell=1}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y_1, z'_{1,\ell,m}) \middle| y_1 \right] \right) \right],$$

and using the fact that terms for different ℓ are by construction independent

$$\begin{aligned}
&= \mathbb{E} \left[f \left(y_1, \prod_{\ell=1}^L \mathbb{E} \left[\frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \psi_\ell(y_1, z'_{1,\ell,m}) \middle| y_1 \right] \right) \right] \\
&= \mathbb{E} \left[f \left(y_1, \prod_{\ell=1}^L \mathbb{E} [\psi_\ell(y_1, z'_{1,\ell,1}) \mid y_1] \right) \right] \\
&= I,
\end{aligned}$$

as required. \square

10.8.3 Proof of Theorem 10.3 - Convergence Rate

Theorem 10.3. *If f is Lipschitz continuous and $f(y_n, \gamma(y_n)), \phi(y_n, z_{n,m}) \in L^2$, the mean squared error of $I_{N,M}$ converges to 0 at rate $O(1/N + 1/M)$.*

Proof. Though the proof follows directly from Theorem 10.5, we also provide the following proof for this simplified case as a stepping stone to aid in understanding the more general proof.

Using Minkowski's inequality, we can bound the mean squared error of $I_{N,M}$ by

$$\mathbb{E}[(I - I_{N,M})^2] = \|I - I_{N,M}\|_2^2 \leq U^2 + V^2 + 2UV \leq 2(U^2 + V^2) \quad (10.16)$$

$$\text{where } U = \left\| I - \frac{1}{N} \sum_{n=1}^N f(y_n, \gamma(y_n)) \right\|_2 \quad \text{and} \quad V = \left\| \frac{1}{N} \sum_{n=1}^N f(y_n, \gamma(y_n)) - I_{N,M} \right\|_2.$$

We see immediately that $U = O(1/\sqrt{N})$, since $\frac{1}{N} \sum_{n=1}^N f(y_n, \gamma(y_n))$ is a MC estimator for I , noting our assumption that $f(y_n, \gamma(y_n)) \in L^2$. For the second term,

$$\begin{aligned}
V &= \left\| \frac{1}{N} \sum_{n=1}^N f(y_n, (\hat{\gamma}_M)_n) - f(y_n, \gamma(y_n)) \right\|_2 \\
&\leq \frac{1}{N} \sum_{n=1}^N \|f(y_n, (\hat{\gamma}_M)_n) - f(y_n, \gamma(y_n))\|_2 \leq \frac{1}{N} \sum_{n=1}^N K \|(\hat{\gamma}_M)_n - \gamma(y_n)\|_2
\end{aligned}$$

where K is a fixed constant, again by Minkowski and using the assumption that f is Lipschitz.

We can rewrite

$$\|(\hat{\gamma}_M)_n - \gamma(y_n)\|_2^2 = \mathbb{E} [\mathbb{E} [((\hat{\gamma}_M)_n - \gamma(y_n))^2 | y_n]].$$

by the tower property of conditional expectation, and note that

$$\mathbb{E} [((\hat{\gamma}_M)_n - \gamma(y_n))^2 | y_n] = \text{Var} \left(\frac{1}{M} \sum_{m=1}^M \phi(y_n, z_{n,m}) \middle| y_n \right) = \frac{1}{M} \text{Var} (\phi(y_n, z_{n,1}) | y_n)$$

since each $z_{n,m}$ is i.i.d. and conditionally independent given y_n . As such

$$\|(\hat{\gamma}_M)_n - \gamma(y_n)\|_2^2 = \frac{1}{M} \mathbb{E} [\text{Var} (\phi(y_n, z_{n,1}) | y_n)] = O(1/M),$$

noting that $\mathbb{E} [\text{Var} (\phi(y_n, z_{n,1}) | y_n)]$ is a finite constant by our assumption that $\phi(y_n, z_{n,m}) \in L^2$.

Consequently,

$$V \leq \frac{NK}{N} O(1/\sqrt{M}) = O(1/\sqrt{M}).$$

Substituting these bounds for U and V in (10.16) gives

$$\|I - I_{N,M}\|_2^2 \leq 2 \left(O(1/\sqrt{N})^2 + O(1/\sqrt{M})^2 \right) = O(1/N + 1/M)$$

as desired. □

10.8.4 Proof of Theorem 10.4 - “Almost almost sure” convergence

Theorem 10.4. For $n \in \mathbb{N}$, let

$$(\epsilon_M)_n = |f(y_n, (\hat{\gamma}_M)_n) - f(y_n, \gamma(y_n))|.$$

Assume that $\mathbb{E}[(\epsilon_M)_1] \rightarrow 0$ as $M \rightarrow \infty$. Denote by Ω the sample space of our underlying probability space, so that $I_{\tau_\delta(M),M}$ can be thought of as a map from Ω to \mathbb{R} . Then, for every $\delta > 0$, there exists a measurable $A_\delta \subseteq \Omega$ with $\mathbb{P}(A_\delta) < \delta$, and a function $\tau_\delta : \mathbb{N} \rightarrow \mathbb{N}$ such that, for all $\omega \notin A_\delta$,

$$I_{\tau_\delta(M),M}(\omega) \rightarrow I \quad \text{as } M \rightarrow \infty.$$

Proof. For all N, M , we have by the triangle inequality that

$$|I_{N,M} - I| \leq V_{N,M} + U_N, \quad \text{where}$$

$$V_{N,M} = \left| \frac{1}{N} \sum_{n=1}^N f(y_n, \gamma(y_n)) - I_{N,M} \right| \quad \text{and} \quad U_N = \left| I - \frac{1}{N} \sum_{n=1}^N f(y_n, \gamma(y_n)) \right|.$$

A second application of the triangle inequality then allows us to write

$$V_{N,M} \leq \frac{1}{N} \sum_{n=1}^N (\epsilon_M)_n \tag{10.17}$$

where we recall that $(\epsilon_M)_n = |f(y_n, \gamma(y_n)) - f(y_n, \hat{\gamma}_n)|$. Now, for all fixed M , each $(\epsilon_M)_n$ is i.i.d. Furthermore, since $\mathbb{E}[(\epsilon_M)_1] \rightarrow 0$ as $M \rightarrow \infty$ by our assumption and $(\epsilon_M)_n$ is nonnegative, there exists some $L \in \mathbb{N}$ such that $\mathbb{E}[|(\epsilon_M)_n|] < \infty$ for all $M \geq L$. Consequently, the strong law of large numbers means that for all $M \geq L$,

$$\frac{1}{N} \sum_{n=1}^N (\epsilon_M)_n \xrightarrow{a.s.} \mathbb{E}[(\epsilon_M)_1]$$

as $N \rightarrow \infty$.

Fix $\delta > 0$. By repeatedly applying Ergorov's theorem to each $M \geq L$, we can find a sequence of events

$$B_L, B_{L+1}, B_{L+2}, \dots$$

such that for every $M \geq L$,

$$\mathbb{P}(B_M) < \frac{\delta}{4} \cdot \frac{1}{2^{M-L}}$$

and outside of B_M , the sequence $\frac{1}{N} \sum_{n=1}^N (\epsilon_M)_n$ converges uniformly to $\mathbb{E}[(\epsilon_M)_1]$. Pick a function $\tau_\delta^1 : \mathbb{N} \rightarrow \mathbb{N}$ such that

$$\left| \frac{1}{M'} \sum_{n=1}^{M'} (\epsilon_M)_n(\omega) - \mathbb{E}[(\epsilon_M)_1] \right| < \frac{1}{M}$$

for all $M \geq L$, $M' \geq \tau_\delta^1(M)$, and $\omega \notin B_M$. Such a τ_δ^1 exists because of the uniform convergence guarantee that we just mentioned. Let

$$B_\delta = \bigcup_{M \geq L} B_M.$$

Then, for all $M \geq M_0$, $M' \geq \tau_\delta^1(M)$, and $\omega \notin B_\delta$,

$$\left| \frac{1}{M'} \sum_{n=1}^{M'} (\epsilon_M)_n(\omega) - \mathbb{E}[(\epsilon_M)_1] \right| < \frac{1}{M}.$$

Consequently, for all such M , M' and ω ,

$$V_{M',M}(\omega) \leq \frac{1}{M'} \sum_{n=1}^{M'} (\epsilon_M)_n(\omega) < \frac{1}{M} + \mathbb{E}[(\epsilon_M)_1]. \tag{10.18}$$

Furthermore,

$$\mathbb{P}(B_\delta) = \mathbb{P}\left(\bigcup_{M \geq L} B_M\right) \leq \sum_{M \geq L} \mathbb{P}(B_M) < \sum_{M \geq L} \frac{\delta}{4} \cdot \frac{1}{2^{M-L}} = \frac{\delta}{2}. \quad (10.19)$$

To complete the proof, we must remove the dependence of U_N on N as well. This is straightforward once we observe that $U_N \xrightarrow{a.s.} 0$ as $N \rightarrow \infty$ by the strong law of large numbers. So, by Ergorov's theorem again, there exists an event C_δ such that

$$\mathbb{P}(C_\delta) < \frac{\delta}{2} \quad (10.20)$$

and outside of C_δ , the sequence U_N converges uniformly to 0. This uniform convergence, in turn, ensures the existence of a function $\tau_\delta^2 : \mathbb{N} \rightarrow \mathbb{N}$ such that

$$U_{M'}(\omega) < \frac{1}{M} \quad (10.21)$$

for all $M \in \mathbb{N}$, $M' \geq \tau_\delta^2(M)$, and $\omega \notin C_\delta$.

We can now define $\tau_\delta(M) = \max(\tau_\delta^1(M), \tau_\delta^2(M))$, and $A_\delta = B_\delta \cup C_\delta$. By inequalities in (10.19) and (10.20),

$$\mathbb{P}(A_\delta) \leq \mathbb{P}(B_\delta) + \mathbb{P}(C_\delta) < \delta.$$

Also, by the inequalities in (10.18) and (10.21),

$$\left| I - I_{\tau_\delta(M), M}(\omega) \right| \leq V_{\tau_\delta(M), M}(\omega) + U_{\tau_\delta(M)}(\omega) \leq \frac{1}{M} + \frac{1}{M} + \mathbb{E}[(\epsilon_M)_1]$$

for all $M \geq L$ and $\omega \notin A_\delta$. Since $\mathbb{E}[(\epsilon_M)_1] \rightarrow 0$, we have here that $I_{\tau_\delta(M), M}(\omega) \rightarrow I$ as desired. \square

10.8.5 Proof of Theorem 10.5 - Convergence for Repeated Nesting

Below we provide a proof of Theorem 10.5 from the main paper. We note that this covers Theorem 10.3 as a special case. A separate proof for Theorem 10.3 was provided in Appendix 10.8.3. This may make easier reading on a first pass as it constitutes a simplified version of the following proof.

Theorem 10.5. *Assume that f_0, \dots, f_D are all Lipschitz continuous, and that*

$$f_k \left(y^{(0:k)}, \gamma_{k+1} \left(y^{(0:k)} \right) \right), I_k \left(y^{(0:k-1)} \right) \in L^2$$

for $0 \leq k \leq D$. Then, the mean squared error $\mathbb{E}[(\gamma_0 - I_0)^2]$ converges to 0 at rate $O\left(\sum_{k=0}^D \frac{1}{N_k}\right)$.

Proof. To establish this claim, we show that for all $0 \leq k \leq D$, the mean squared error

$$\left\| \gamma_k \left(y^{(0:k-1)} \right) - I_k \left(y^{(0:k-1)} \right) \right\|_2^2 = O \left(\sum_{\ell=k}^D \frac{1}{N_\ell} \right). \quad (10.22)$$

Our theorem corresponds to the case that $k = 0$.

We proceed by applying Minkowski's inequality, which allows us to bound

$$\left\| \gamma_k \left(y^{(0:k-1)} \right) - I_k \left(y^{(0:k-1)} \right) \right\|_2^2 \leq U_k^2 + V_k^2 + 2U_k V_k \leq 2(U_k^2 + V_k^2),$$

where

$$\begin{aligned} U_k &= \left\| \gamma_k \left(y^{(0:k-1)} \right) - J_k \left(y^{(0:k-1)} \right) \right\|_2 \\ V_k &= \left\| J_k \left(y^{(0:k-1)} \right) - I_k \left(y^{(0:k-1)} \right) \right\|_2 \end{aligned}$$

and we define

$$J_k \left(y^{(0:k-1)} \right) = \frac{1}{N_k} \sum_{n=1}^{N_k} f_k \left(y^{(0:k-1)}, y_n^{(k)}, \gamma_{k+1} \left(y^{(0:k-1)}, y_n^{(k)} \right) \right)$$

for $0 \leq k < D$, and

$$J_D \left(y^{(0:D-1)} \right) = I_D \left(y^{(0:D-1)} \right).$$

Intuitively, $J_k \left(y^{(0:k-1)} \right)$ corresponds to applying an MC approximation to $\gamma_k \left(y^{(0:k-1)} \right)$ only to the outermost expectation, and exactly computing the expectations nested within.

We show below that

$$U_k^2 = O \left(\frac{1}{N_k} \right) \quad (10.23)$$

for all k , which, since $V_D = 0$, establishes (10.22) for the case $k = D$. For the remaining k , we note that

$$\begin{aligned} V_k &\leq \frac{1}{N_k} \sum_{n=1}^{N_k} \left\| f_k \left(y^{(0:k-1)}, y_n^{(k)}, \gamma_{k+1} \left(y^{(0:k-1)}, y_n^{(k)} \right) \right) \right. \\ &\quad \left. - f_k \left(y^{(0:k-1)}, y_n^{(k)}, I_{k+1} \left(y^{(0:k-1)}, y_n^{(k)} \right) \right) \right\|_2 \\ &\leq \frac{K}{N_k} \sum_{n=1}^{N_k} \left\| \gamma_{k+1} \left(y^{(0:k-1)}, y_n^{(k)} \right) - I_{k+1} \left(y^{(0:k-1)}, y_n^{(k)} \right) \right\|_2, \end{aligned}$$

for some $K > 0$, by Minkowski's inequality and using the assumption that f_k is Lipschitz. Since the $y_n^{(k)} \sim p(y^{(k)} | y^{(0:k-1)})$ are i.i.d., we can rewrite this inequality as

$$V_k \leq K \left\| \gamma_{k+1} \left(y^{(0:k)} \right) - I_{k+1} \left(y^{(0:k)} \right) \right\|_2$$

so that

$$V_k^2 \leq K^2 \left\| \gamma_{k+1} (y^{(0:k)}) - I_{k+1} (y^{(0:k)}) \right\|_2^2.$$

We see that the second term on the right-hand side has the same form as (10.22), and so recursing on k (until the base case $k = D$) allows us to bound

$$V_k^2 \leq K^2 O \left(\sum_{\ell=k+1}^N \frac{1}{N_\ell} \right).$$

This then yields

$$\left\| \gamma_k (y^{(0:k-1)}) - I_k (y^{(0:k-1)}) \right\|_2^2 \leq 2 \left(O \left(\frac{1}{N_k} \right) + K^2 O \left(\sum_{\ell=k+1}^N \frac{1}{N_\ell} \right) \right) = O \left(\sum_{\ell=k}^D \frac{1}{N_\ell} \right)$$

as desired.

It remains to show (10.23). To do so, we first observe that

$$U_k^2 = \mathbb{E} \left[\mathbb{E} \left[(\gamma_k (y^{(0:k-1)}) - J_k (y^{(0:k-1)}))^2 \middle| y^{(0:k-1)} \right] \right]$$

by the tower property of conditional expectation. Now,

$$\begin{aligned} \mathbb{E} \left[(\gamma_k (y^{(0:k-1)}) - J_k (y^{(0:k-1)}))^2 \middle| y^{(0:k-1)} \right] &= \text{Var} [J_k (y^{(0:k-1)}) \mid y^{(0:k-1)}] \\ &= \frac{1}{N_k} \text{Var} [f_k (y^{(0:k)}, \gamma_{k+1} (y^{(0:k)})) \mid y^{(0:k-1)}] \end{aligned}$$

(omitting the γ_{k+1} term when $k = D$), since each $y_n^{(k)}$ in $J_k (y^{(0:k-1)})$ is conditionally independent given $y^{(0:k-1)}$. Consequently,

$$U_k^2 = \frac{1}{N_k} \mathbb{E} \left[\text{Var} [f_k (y^{(0:k)}, \gamma_{k+1} (y^{(0:k)})) \mid y^{(0:k-1)}] \right] = O \left(\frac{1}{N_k} \right),$$

noting that $\mathbb{E} [\text{Var} [f_k (y^{(0:k)}, \gamma_{k+1} (y^{(0:k)})) \mid y^{(0:k-1)}]]$ is a finite constant by our assumption that $f_k (y^{(0:k)}, \gamma_{k+1} (y^{(0:k)})) \in L^2$ (and where once again we omit the γ_{k+1} terms when $k = D$). \square

Theorem 10.8. *If f_0, \dots, f_D are all Lipschitz continuous with Lipschitz constants¹*

$$K_k = \sup_{y^{(0:k)}} \left| \frac{\partial f_k (y^{(0:k)}, \gamma_{k+1} (y^{(0:k)}))}{\partial \gamma_{k+1}} \right|, \quad \forall k \in 0, \dots, D-1$$

and if

$$\varsigma_k^2 = \mathbb{E} \left[(f_k (y_1^{(0:k)}, \gamma_{k+1} (y_1^{(0:k)})) - \gamma_k (y_1^{(0:k-1)}))^2 \right] \leq \infty \quad \forall k \in 0, \dots, D$$

¹Note that these are the Lipschitz constants corresponding to the definition of Lipschitz continuity and not an extra requirement.

then the mean squared error converges to 0 with the following rate

$$\mathbb{E} [(I_0 - \gamma_0)^2] \leq \frac{\varsigma_0^2}{N_0} + \sum_{k=1}^D \left(\prod_{\ell=0}^{k-1} K_\ell^2 \right) \frac{\varsigma_k^2}{N_k} + O(\epsilon) \quad (10.24)$$

where $O(\epsilon)$ represents terms that become dominated as $N_0, \dots, N_D \rightarrow \infty$. If f_0, \dots, f_D are also continuously differentiable with first derivative bounds K_0, \dots, K_D and second derivative bounds $C_k = \sup_{y^{(0:k)}} \left| \frac{\partial^2 f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)}))}{\partial \gamma_{k+1}^2} \right|$, $\forall k \in \{0, \dots, D-1\}$, then this mean square error bound can be tightened to

$$\mathbb{E} [(I_0 - \gamma_0)^2] \leq \frac{\varsigma_0^2}{N_0} + \frac{1}{4} \left(\frac{C_0 \varsigma_1^2}{N_1} + \sum_{k=0}^{D-2} \left(\prod_{d=0}^k K_d \right) \frac{C_{k+1} \varsigma_{k+2}^2}{N_{k+2}} \right)^2 + O(\epsilon). \quad (10.25)$$

In the case of a single nesting we can further characterize $O(\epsilon)$ to give

$$\mathbb{E} [(I_0 - \gamma_0)^2] \leq \frac{\varsigma_0^2}{N_0} + \frac{4K_0^2 \varsigma_1^2}{N_0 N_1} + \frac{2K_0 \varsigma_0 \varsigma_1}{N_0 \sqrt{N_1}} + \frac{K_0^2 \varsigma_1^2}{N_1} \quad (10.26)$$

$$\mathbb{E} [(I_0 - \gamma_0)^2] \leq \frac{\varsigma_0^2}{N_0} + \frac{4K_0^2 \varsigma_1^2}{N_0 N_1} + \frac{2K_0 \varsigma_0 \varsigma_1}{N_0 \sqrt{N_1}} + \frac{C_0^2 \varsigma_1^4}{4N_1^2} + O\left(\frac{1}{N_1^3}\right). \quad (10.27)$$

for when the continuous differentiable assumption does not hold and holds respectively.

Proof. As this is a long and involved proof, we start by defining a number of terms that will be useful throughout the proof. Unless otherwise stated, these definitions hold for all $k \in \{0, \dots, D\}$.

$$E_k(y_1^{(0:k-1)}) := \mathbb{E} \left[(I_k(y_1^{(0:k-1)}) - \gamma_k(y_1^{(0:k-1)}))^2 \middle| y_1^{(0:k-1)} \right] \quad (10.28)$$

$$A_k(y_1^{(0:k-1)}) := \mathbb{E} \left[(f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)})) - f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)})))^2 \middle| y_1^{(0:k-1)} \right] \quad (10.29)$$

$$A_D := 0 \quad (10.30)$$

$$s_k^2(y_1^{(0:k-1)}) := \mathbb{E} \left[(f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)})) - \gamma_k(y_1^{(0:k-1)}))^2 \middle| y_1^{(0:k-1)} \right] \quad (10.31)$$

$$s_D^2(y_1^{(0:D-1)}) := \mathbb{E} \left[(f_D(y_1^{(0:D)}, \gamma_D(y_1^{(0:D)})) - \gamma_D(y_1^{(0:D-1)}))^2 \middle| y_1^{(0:D-1)} \right] \quad (10.32)$$

$$\begin{aligned} \zeta_{d,k}^2(y_1^{(0:k-1)}) &:= \mathbb{E} [s_d^2(y_1^{(0:d-1)}) \mid y_1^{(0:k-1)}] \\ &= \mathbb{E} \left[(f_d(y_1^{(0:d)}, \gamma_{d+1}(y_1^{(0:d)})) - \gamma_d(y_1^{(0:d-1)}))^2 \middle| y_1^{(0:k-1)} \right] \end{aligned} \quad (10.33)$$

$$\varsigma_k^2 := \zeta_{k,0}^2 = \mathbb{E} \left[(f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)})) - \gamma_k(y_1^{(0:k-1)}))^2 \right] \quad (10.34)$$

$$\bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)}) := \mathbb{E} [f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)})) \mid y_1^{(0:k-1)}] \quad \forall k \in \{0, \dots, D-1\} \quad (10.35)$$

$$\begin{aligned} v_k^2(y_1^{(0:k-1)}) &:= \text{Var}[I_k(y_1^{(0:k-1)})|y_1^{(0:k-1)}] \\ &= \mathbb{E}\left[\left(I_k(y_1^{(0:k-1)}) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)})\right)^2 | y_1^{(0:k-1)}\right] \end{aligned} \quad (10.36)$$

$$\begin{aligned} \sigma_k^2(y_1^{(0:k-1)}) &:= \text{Var}[f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)}))|y_1^{(0:k-1)}] \\ &= \mathbb{E}\left[\left(f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)})) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)})\right)^2 | y_1^{(0:k-1)}\right] \end{aligned} \quad (10.37)$$

$$\sigma_D^2(y_1^{0:D-1}) := s_D^2(y_1^{0:D-1}) \quad (10.38)$$

$$\begin{aligned} \beta_k(y_1^{(0:k-1)}) &:= \mathbb{E}[I_k(y_1^{(0:k-1)}) - \gamma_k(y_1^{(0:k-1)})|y_1^{(0:k-1)}] \\ &= \mathbb{E}\left[f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)})) - f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)}))|y_1^{(0:k-1)}\right] \end{aligned} \quad (10.39)$$

$$\begin{aligned} \omega_k(y_1^{(0:k-1)}) &:= \mathbb{E}[E_{k+1}(y_1^{(0:k)})|y_1^{(0:k-1)}] \\ &= \mathbb{E}\left[\left(I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)})\right)^2 | y_1^{(0:k-1)}\right] \end{aligned} \quad (10.40)$$

$$\omega_D(y_1^{(0:D-1)}) := 0 \quad (10.41)$$

$$\begin{aligned} \lambda_k(y_1^{(0:k-1)}) &:= \mathbb{E}\left[\left|\beta_{k+1}(y_1^{(0:k)})\right| | y_1^{(0:k-1)}\right] \\ &= \mathbb{E}\left[\left|\mathbb{E}\left[\left(I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)})\right) | y_1^{(0:k)}\right]\right| | y_1^{(0:k-1)}\right] \end{aligned} \quad (10.42)$$

$$\lambda_D(y_1^{(0:D-1)}) := 0 \quad (10.43)$$

We note that s_k , $\zeta_{d,k}$, and ς_d are independent of the number of samples used and are thus constants for a particular problem.

Given these definitions, we start by breaking the error down into a variance and bias term.

Using the standard bias-variance decomposition we have

$$\begin{aligned} E_k(y_1^{(0:k-1)}) &= \mathbb{E}\left[\left(I_k(y_1^{(0:k-1)}) - \gamma_k(y_1^{(0:k-1)})\right)^2 | y_1^{(0:k-1)}\right] \\ &= v_k^2(y_1^{(0:k-1)}) + (\beta_k(y_1^{(0:k-1)}))^2 \end{aligned} \quad (10.44)$$

It is immediately clear from its definition in (10.39) that the bias term $(\beta_k(y_1^{(0:k-1)}))^2$ is independent of N_0 . On the other hand we will show later that the dominant components of the variance term for large $N_{0:D}$ depend only on N_0 . We can thus think of increasing N_0 as reducing the variance of the estimator and increasing $N_{1:D}$ as reducing the bias.

We first consider the variance term

$$\begin{aligned}
v_k^2(y_1^{(0:k-1)}) &= \mathbb{E} \left[\left(\frac{1}{N_k} \sum_{n=1}^{N_k} f_k(y_n^{(0:k)}, I_{k+1}(y_n^{(0:k)})) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)}) \right)^2 \middle| y_1^{(0:k-1)} \right] \\
&= \mathbb{E} \left[\frac{1}{N_k^2} \sum_{n=1}^{N_k} \left(f_k(y_n^{(0:k)}, I_{k+1}(y_n^{(0:k)})) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)}) \right)^2 \middle| y_1^{(0:k-1)} \right] \\
&\quad + \mathbb{E} \left[\frac{1}{N_k^2} \sum_{n=1}^{N_k} \sum_{m=1, m \neq n}^{N_k} \left(f_k(y_n^{(0:k)}, I_{k+1}(y_n^{(0:k)})) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)}) \right) \right. \\
&\quad \cdot \left. \left(f_k(y_m^{(0:k)}, I_{k+1}(y_m^{(0:k)})) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)}) \right) \middle| y_1^{(0:k-1)} \right]
\end{aligned}$$

Now noting that each $y_n^{(0:k)}$ are drawn i.i.d., the cross terms are independent and the distribution is the same for each m and n and so we have

$$\begin{aligned}
v_k^2(y_1^{(0:k-1)}) &= \frac{1}{N_k} \mathbb{E} \left[\left(f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)})) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)}) \right)^2 \middle| y_1^{(0:k-1)} \right] \\
&\quad + \frac{N_k - 1}{N_k} \left(\mathbb{E} \left[f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)})) - \bar{f}_{k,N_{k+1:D}}(y_1^{(0:k-1)}) \middle| y_1^{(0:k-1)} \right] \right)^2 \\
&= \frac{\sigma_k^2(y_1^{(0:k-1)})}{N_k}
\end{aligned}$$

where the second equality follows directly from the definitions of σ_k and $\bar{f}_{k,N_{k+1:D}}$. We have now have using Minkowski's inequality

$$\begin{aligned}
\sigma_k^2(y_1^{(0:k-1)}) &\leq \left(A_k(y_1^{(0:k-1)}) \right)^{\frac{1}{2}} + \left(\mathbb{E} \left[\left(f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)})) - \bar{f}_{k,N_{k+1:D}} \right)^2 \right] \right)^{\frac{1}{2}} \\
&= \left(A_k(y_1^{(0:k-1)}) \right)^{\frac{1}{2}} + \left(s_k^2(y_1^{(0:k-1)}) + \left(\beta_k(y_1^{(0:k-1)}) \right)^2 \right)^{\frac{1}{2}}
\end{aligned}$$

where the equality stems from using another bias-variance decomposition. The first thing to now notice is that s_0^2 is independent of the number of samples used at any level of the estimate, while A_k and β_k^2 are independent of $N_d \forall d \leq k$. Therefore, presuming that A_k and $\beta_k^2 (\leq A_k)$ by Jensen's inequality do not increase with $N_d \forall d > k$, the variance term will converge to zero with rate $O(1/N_k)$. Further, if $A_k \rightarrow 0$ as $N_{k+1}, \dots, N_D \rightarrow \infty$, then for a large number of inner samples $\sigma_k^2 \rightarrow s_k^2$ and thus we will have $v_k^2(y_1^{(0:k-1)}) \leq \frac{s_0^2}{N_0} + O(\epsilon)$ where $O(\epsilon)$ represents higher order terms that are dominated in the limit $N_k, \dots, N_D \rightarrow \infty$.

We now show that Lipschitz continuity is sufficient for $A_k \rightarrow 0$ and derive a concrete bound on the variance by bounding A_k . We found that there was no noticeably tighter bound to be

found for A_k using the continuity assumption and therefore this result will be used for both cases (10.24) and (10.25). First by definition of Lipschitz continuity we have that

$$\begin{aligned} \left(A_k \left(y_1^{(0:k-1)} \right) \right)^{\frac{1}{2}} &\leq K_k \left(\mathbb{E} \left[\left(I_{k+1} \left(y_1^{(0:k)} \right) - \gamma_{k+1} \left(y_1^{(0:k)} \right) \right)^2 \middle| y_1^{(0:k-1)} \right] \right)^{\frac{1}{2}} \\ &= K_k \left(\omega_k \left(y_1^{(0:k-1)} \right) \right)^{\frac{1}{2}} \end{aligned}$$

where we remember that $\omega_k \left(y_1^{(0:k-1)} \right) = \mathbb{E} \left[E_{k+1} \left(y_1^{(0:k)} \right) \middle| y_1^{(0:k-1)} \right]$ is the expected error of the next level estimator. Once we also have an expression for the bias, we will thus be able to use this bound on A_k to inductively derive a bound on the variance.

For the case where we only assume Lipschitz continuity then we will simply use Jensen's inequality to bound the bias

$$\left(\beta_k \left(y_1^{(0:k-1)} \right) \right)^2 \leq A_k \left(y_1^{(0:k-1)} \right)$$

noting that the only difference in the definition of $\left(\beta_k \left(y_1^{(0:k-1)} \right) \right)^2$ and $A_k \left(y_1^{(0:k-1)} \right)$ is whether the squaring occurs inside or outside the expectation. Putting this together we now have that

$$E_k \left(y_1^{(0:k-1)} \right) \leq \frac{\sigma_k^2 \left(y_1^{(0:k-1)} \right)}{N_k} + A_k \left(y_1^{(0:k-1)} \right). \quad (10.45)$$

$$\begin{aligned} &\leq \frac{s_k^2 \left(y_1^{(0:k-1)} \right) + 2A_k \left(y_1^{(0:k-1)} \right) + 2 \left(A_k \left(y_1^{(0:k-1)} \right) \right)^{\frac{1}{2}} \left(s_k^2 \left(y_1^{(0:k-1)} \right) + A_k \left(y_1^{(0:k-1)} \right) \right)^{\frac{1}{2}}}{N_k} \\ &\quad + A_k \left(y_1^{(0:k-1)} \right) \\ &\leq \frac{s_k^2 \left(y_1^{(0:k-1)} \right) + 4K_k^2 \omega_k \left(y_1^{(0:k-1)} \right) + 2K_k \left(\omega_k \left(y_1^{(0:k-1)} \right) \right)^{\frac{1}{2}} s_k \left(y_1^{(0:k-1)} \right) + K_k^2 \omega_k \left(y_1^{(0:k-1)} \right)}{N_k} \end{aligned} \quad (10.46)$$

which fully defines a bound on conditional the variance of one layer given the mean squared error of the layer below. In particular as $\omega_D \left(y_1^{(0:D-1)} \right) = 0$ we now have

$$E_D \left(y_1^{(0:D-1)} \right) \leq \frac{s_D^2 \left(y_1^{(0:D-1)} \right)}{N_D} = \frac{\mathbb{E} \left[\left(f_D \left(y_1^{(0:D)} \right) - \gamma_D \left(y_1^{(0:D)} \right) \right)^2 \middle| y_1^{(0:D-1)} \right]}{N_D}$$

which is the standard error for Monte Carlo convergence. We further have

$$\omega_{D-1} \left(y_1^{(0:D-2)} \right) = \mathbb{E} \left[E_D \left(y_1^{(0:D-1)} \right) \middle| y_1^{(0:D-2)} \right] = \frac{\zeta_{D,D-1}^2 \left(y_1^{(0:D-2)} \right)}{N_D}.$$

and thus

$$\begin{aligned} E_{D-1}(y_1^{(0:D-2)}) &\leq \frac{s_{D-1}^2(y_1^{(0:D-2)})}{N_{D-1}} + \frac{4K_{D-1}^2\zeta_{D,D-1}^2(y_1^{(0:D-2)})}{N_D N_{D-1}} \\ &+ \frac{2K_{D-1}s_{D-1}(y_1^{(0:D-2)})\zeta_{D,D-1}(y_1^{(0:D-2)})}{N_{D-1}\sqrt{N_D}} + \frac{K_{D-1}^2\zeta_{D,D-1}^2(y_1^{(0:D-2)})}{N_D}. \end{aligned} \quad (10.47)$$

This leads to following result for the single nesting case

$$E_0 \leq \frac{\varsigma_0^2}{N_0} + \frac{4K_0^2\varsigma_1^2}{N_0 N_1} + \frac{2K_0\varsigma_0\varsigma_1}{N_0\sqrt{N_1}} + \frac{K_0^2\varsigma_1^2}{N_1} \approx \frac{\varsigma_0^2}{N_0} + \frac{K_0^2\varsigma_1^2}{N_1} = O\left(\frac{1}{N_0} + \frac{1}{N_1}\right) \quad (10.48)$$

where the approximation becomes exact as $N_0, N_1 \rightarrow \infty$. Note that there is no $O(\epsilon)$ term as this bound is exact in the finite sample case.

Things quickly get messy for double nesting and beyond so we will ignore non-dominant terms in the limit $N_0, \dots, N_D \rightarrow \infty$ and resort to using $O(\epsilon)$ for these terms instead. We first note that (10.46) can be simplified to

$$E_k(y_1^{(0:k-1)}) \leq \frac{s_k^2}{N_k} + K_k^2\omega_k(y_1^{(0:k-1)}) + O(\epsilon) \quad (10.49)$$

as s_k^2 does not decrease with increasing $N_{k+1:D}$ whereas the other terms do. We therefore also have that

$$\omega_k^2(y_1^{(0:k-1)}) = \mathbb{E}\left[\frac{s_{k+1}^2(y_1^{(0:k)})}{N_{k+1}} + K_{k+1}^2\omega_{k+1}(y_1^{(0:k)}) \middle| y_1^{(0:k-1)}\right] + O(\epsilon) \quad (10.50)$$

and therefore

$$E_k(y_1^{(0:k-1)}) \leq \frac{s_k^2(y_1^{(0:k-1)})}{N_k} + \sum_{d=k+1}^D \frac{(\prod_{\ell=k}^{d-1} K_\ell^2) \mathbb{E}[s_d^2(y_1^{(0:d-1)}) \mid y_1^{(0:k-1)}]}{N_d} + O(\epsilon) \quad (10.51)$$

$$= \frac{s_k^2(y_1^{(0:k-1)})}{N_k} + \sum_{d=k+1}^D \frac{(\prod_{\ell=k}^{d-1} K_\ell^2) \zeta_{d,k}^2(y_1^{(0:k-1)})}{N_d} + O(\epsilon) \quad (10.52)$$

Now from its definition we have that $\zeta_{0,0}^2 = s_0^2$ and $\zeta_{d,0}^2 = \varsigma_d^2$ and as (10.52) holds in the case $k = 0$, the mean squared error of the overall estimator is as follows

$$\mathbb{E}[(I_0 - \gamma_0)^2] = E_0 \leq \frac{\varsigma_0^2}{N_0} + \sum_{k=1}^D \frac{(\prod_{\ell=0}^{k-1} K_\ell^2) \varsigma_k^2}{N_k} + O(\epsilon) \quad (10.53)$$

and we have the desired result for the Lipschitz case.

We now revisit the bound for the bias in the continuously differentiable case to show that a tighter bound can be found. We first remember that

$$\beta_k(y_1^{(0:k-1)}) = \mathbb{E}\left[f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)})) - f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)})) \middle| y_1^{(0:k-1)}\right].$$

We now use a Taylor expansion for $f_k(y_1^{(0:k)}, I_{k+1}(y_1^{(0:k)}))$ about the point $f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)}))$ as follows where all derivatives are with respect to the second input. First we define

$$\delta_1 = \mathbb{E} \left[\frac{\partial f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)}))}{\partial \gamma_{k+1}} (I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)})) \middle| y_1^{(0:k-1)} \right]$$

$$\delta_2 = \mathbb{E} \left[\frac{\partial^2 f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)}))}{\partial \gamma_{k+1}^2} (I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)}))^2 \middle| y_1^{(0:k-1)} \right]$$

then we have from the Taylor expansion

$$\begin{aligned} \beta_k^2(y_1^{(0:k-1)}) &= \left(\mathbb{E} [f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)})) \mid y_1^{(0:k-1)}] + \delta_1 + \frac{\delta_2}{2} + O(\epsilon) \right. \\ &\quad \left. - \mathbb{E} [f_k(y_1^{(0:k)}, \gamma_{k+1}(y_1^{(0:k)})) \mid y_1^{(0:k-1)}] \right)^2 \\ &= \delta_1^2 + \frac{\delta_2^2}{4} + \delta_1 \delta_2 + O(\epsilon). \end{aligned}$$

Now considering δ_1 we have by the tower property

$$\begin{aligned} \delta_1 &= \mathbb{E} \left[\mathbb{E} \left[\frac{\partial f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)}))}{\partial \gamma_{k+1}} (I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)})) \middle| y_1^{(0:k)} \right] \middle| y_1^{(0:k-1)} \right] \\ &= \mathbb{E} \left[\frac{\partial f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)}))}{\partial \gamma_{k+1}} \mathbb{E} [(I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)})) \mid y_1^{(0:k)}] \middle| y_1^{(0:k-1)} \right] \end{aligned}$$

and so by noting that $a \leq |a|$ where $|a|$ is the absolute value of a we have

$$\begin{aligned} \delta_1 &\leq \mathbb{E} \left[\left| \frac{\partial f_k(y^{(0:k)}, \gamma_{k+1}(y^{(0:k)}))}{\partial \gamma_{k+1}} \right| \left| \mathbb{E} [(I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)})) \mid y_1^{(0:k)}] \right| \middle| y_1^{(0:k-1)} \right] \\ &\leq K_k \mathbb{E} \left[\left| \mathbb{E} [(I_{k+1}(y_1^{(0:k)}) - \gamma_{k+1}(y_1^{(0:k)})) \mid y_1^{(0:k)}] \right| \middle| y_1^{(0:k-1)} \right] \\ &= K_k \lambda_k(y_1^{(0:k-1)}) \end{aligned}$$

Similarly we have

$$\delta_2 \leq C_k \omega_k(y_1^{(0:k-1)})$$

and therefore

$$\begin{aligned} \beta_k^2(y_1^{(0:k-1)}) &\leq K_k^2 \lambda_k^2(y_1^{(0:k-1)}) + \frac{C_k^2}{4} \omega_k^2(y_1^{(0:k-1)}) + K_k C_k \lambda_k(y_1^{(0:k-1)}) \omega_k(y_1^{(0:k-1)}) + O(\epsilon) \\ &= \left(K_k \lambda_k(y_1^{(0:k-1)}) + \frac{C_k}{2} \omega_k(y_1^{(0:k-1)}) \right)^2 + O(\epsilon). \end{aligned}$$

Now remembering that our overall error is of the form $E_k(y_1^{(0:k-1)}) = \frac{\sigma_k^2(y_1^{(0:k-1)})}{N_k} + \beta_k^2(y_1^{(0:k-1)})$,

we can again recursively define the error bound. We can immediately see that, as $\beta_D = 0$ without any nesting, we recover the bound from the Lipschitz case for the inner most estimator as expected. As the innermost estimator is unbiased we also have $\lambda_{D-1}(y_1^{(0:D-2)}) = 0$ and so

$$\begin{aligned}\beta_{D-1}^2(y_1^{(0:D-2)}) &\leq \frac{C_{D-1}^2}{4} \omega_{D-1}^2(y_1^{(0:D-2)}) + O(\epsilon) \\ &\leq \frac{C_{D-1}^2}{4} \left(\mathbb{E} \left[\frac{s_D^2(y_1^{(0:D-1)})}{N_D} \middle| y_1^{(0:D-2)} \right] \right)^2 + O(\epsilon) \\ &= \frac{C_{D-1}^2 \zeta_{D,D-1}^4(y_1^{(0:D-2)})}{4N_D^2} + O(\epsilon).\end{aligned}$$

Using the full expansion of $\sigma_{D-1}^2(y_1^{(0:D-2)})$ derived in the Lipschitz case we have

$$\begin{aligned}E_{D-1}(y_1^{(0:D-2)}) &\leq \frac{s_{D-1}^2(y_1^{(0:D-2)})}{N_{D-1}} + \frac{4K_{D-1}^2 \zeta_{D,D-1}^2(y_1^{(0:D-2)})}{N_D N_{D-1}} \\ &+ \frac{2K_{D-1} s_{D-1}(y_1^{(0:D-2)}) \zeta_{D,D-1}(y_1^{(0:D-2)})}{N_{D-1} \sqrt{N_D}} + \frac{C_{D-1}^2 \zeta_{D,D-1}^4(y_1^{(0:D-2)})}{4N_D^2} + O(\epsilon).\end{aligned}\tag{10.54}$$

Therefore for the single nesting case we now have

$$E_0 \leq \frac{\varsigma_0^2}{N_0} + \frac{4K_0^2 \varsigma_1^2}{N_0 N_1} + \frac{2K_0 \varsigma_0 \varsigma_1}{N_0 \sqrt{N_1}} + \frac{C_0^2 \varsigma_1^4}{4N_1^2} + O(\epsilon) \approx \frac{\varsigma_0^2}{N_0} + \frac{C_0^2 \varsigma_1^4}{4N_1^2} = O\left(\frac{1}{N_0} + \frac{1}{N_1^2}\right)\tag{10.55}$$

where again the approximation becomes tight when $N_0, N_1 \rightarrow \infty$. We can further note that in this case the only contribution to the $O(\epsilon)$ term is from higher order terms in the Taylor expansion of the bias term. As $\delta_1 = 0$ for the single nesting case by unbiasedness, The largest of these

terms is $\frac{\delta_2 \delta_3}{3}$ where

$$\begin{aligned}
\delta_3 &= \mathbb{E} \left[\frac{\partial^3 f_0(y^{(0)}, \gamma_1(y^{(0)}))}{\partial \gamma_1^3} (I_1(y_1^{(0)}) - \gamma_1(y_1^{(0)}))^3 \right] \\
&\leq \sup_{y_1^{(0)}} \left| \frac{\partial^3 f_0(y^{(0)}, \gamma_1(y^{(0)}))}{\partial \gamma_1^3} \right| \mathbb{E} \left[\left| \mathbb{E} \left[(I_1(y_1^{(0)}) - \gamma_1(y_1^{(0)}))^3 \middle| y_1^{(0)} \right] \right| \right] \\
&= \frac{1}{N_1^3} \sup_{y_1^{(0)}} \left| \frac{\partial^3 f_0(y^{(0)}, \gamma_1(y^{(0)}))}{\partial \gamma_1^3} \right| \mathbb{E} \left[\left| \mathbb{E} \left[\sum_{n=1}^{N_1} (f_1(y_1^{(0)}, y_n^{(1)}) - \gamma_1(y_1^{(0)}))^3 \middle| y_1^{(0)} \right] \right| \right] + \\
&\quad \mathbb{E} \left[\left| \sum_{n=1}^{N_1} \sum_{m=1, m \neq n}^{N_1} (f_1(y_1^{(0)}, y_n^{(1)}) - \gamma_1(y_1^{(0)})) (f_1(y_1^{(0)}, y_m^{(1)}) - \gamma_1(y_1^{(0)}))^2 \middle| y_1^{(0)} \right| \right] \\
&= \frac{1}{N_1^3} \sup_{y_1^{(0)}} \left| \frac{\partial^3 f_0(y^{(0)}, \gamma_1(y^{(0)}))}{\partial \gamma_1^3} \right| \mathbb{E} \left[\left| \mathbb{E} \left[\sum_{n=1}^{N_1} (f_1(y_1^{(0)}, y_n^{(1)}) - \gamma_1(y_1^{(0)}))^3 \middle| y_1^{(0)} \right] \right| \right] \\
&= \frac{1}{N_1^2} \sup_{y_1^{(0)}} \left| \frac{\partial^3 f_0(y^{(0)}, \gamma_1(y^{(0)}))}{\partial \gamma_1^3} \right| \mathbb{E} \left[\left| \mathbb{E} \left[(f_1(y_1^{(0)}, y_1^{(1)}) - \gamma_1(y_1^{(0)}))^3 \middle| y_1^{(0)} \right] \right| \right] \\
&= O\left(\frac{1}{N_1^2}\right)
\end{aligned}$$

Therefore $\frac{\delta_2 \delta_3}{3} = O\left(\frac{1}{N_1^3}\right)$ which confirms that the $O(\epsilon)$ term is asymptotically negligible as required and allows us to better characterize the bound in the single nesting case as we have

$$E_0 \leq \frac{\varsigma_0^2}{N_0} + \frac{4K_0^2 \varsigma_1^2}{N_0 N_1} + \frac{2K_0 \varsigma_0 \varsigma_1}{N_0 \sqrt{N_1}} + \frac{C_0^2 \varsigma_1^4}{4N_1^2} + O\left(\frac{1}{N_1^3}\right). \quad (10.56)$$

For the repeated nesting case we first note that

$$\begin{aligned}
\omega_k(y_1^{(0:k-1)}) &= \mathbb{E} \left[\frac{s_{k+1}^2(y_1^{(0:k)})}{N_{k+1}} + \beta_{k+1}^2(y_1^{(0:k)}) \middle| y_1^{(0:k-1)} \right] + O(\epsilon) \\
&= \frac{\zeta_{k+1,k}^2}{N_{k+1}} + \mathbb{E} [\beta_{k+1}^2(y_1^{(0:k)}) \mid y_1^{(0:k-1)}] + O(\epsilon)
\end{aligned}$$

and that except at $k = D - 1$ and $k = D$ (for which both are zero), then

$$\lambda_k(y_1^{(0:k-1)}) = \mathbb{E} \left[|\beta_{k+1}(y_1^{(0:k-1)})| \middle| y_1^{(0:k)} \right] \gg \mathbb{E} [\beta_{k+1}^2(y_1^{(0:k)}) \mid y_1^{(0:k-1)}]$$

for sufficiently large N_{k+1}, \dots, N_D . We can therefore ignore the latter term in ω_k as follows

$$\begin{aligned}
E_k(y_1^{(0:k-1)}) &= \frac{s_k^2(y_1^{(0:k-1)})}{N_k} + \beta_k^2(y_1^{(0:k-1)}) + O(\epsilon) \\
&\leq \frac{s_k^2(y_1^{(0:k-1)})}{N_k} + \left(K_k \lambda_k(y_1^{(0:k-1)}) + \frac{C_k}{2} \omega_k(y_1^{(0:k-1)}) \right)^2 + O(\epsilon) \\
&= \frac{s_k^2(y_1^{(0:k-1)})}{N_k} + \left(K_k \lambda_k(y_1^{(0:k-1)}) + \frac{C_k \zeta_{k+1,k}^2}{2N_{k+1}} \right)^2 + O(\epsilon).
\end{aligned}$$

Now we have

$$\begin{aligned}
\lambda_k(y_1^{(0:k-1)}) &= \mathbb{E} \left[\sqrt{E_{k+1}(y_1^{(0:k)}) - \frac{s_{k+1}^2(y_1^{(0:k)})}{N_{k+1}}} \middle| y_1^{(0:k-1)} \right] + O(\epsilon) \\
&\leq \mathbb{E} \left[K_{k+1} \lambda_{k+1}(y_1^{(0:k)}) + \frac{C_{k+1} \zeta_{k+2,k+1}^2}{2N_{k+2}} \middle| y_1^{(0:k-1)} \right] + O(\epsilon) \\
&= \frac{C_{k+1} \zeta_{k+2,k}^2}{2N_{k+2}} + K_{k+1} \mathbb{E} [\lambda_{k+1}(y_1^{(0:k)}) \mid y_1^{(0:k-1)}] + O(\epsilon) \\
&\leq \frac{C_{k+1} \zeta_{k+2,k}^2}{2N_{k+2}} + \sum_{d=k+1}^{D-2} \mathbb{E} \left[\left(\prod_{\ell=k+1}^d K_\ell \right) \frac{C_{d+1} \zeta_{d+2,d}^2}{2N_{d+2}} \middle| y_1^{(0:k-1)} \right] + O(\epsilon) \\
&\leq \frac{C_{k+1} \zeta_{k+2,k}^2}{2N_{k+2}} + \sum_{d=k+1}^{D-2} \left(\prod_{\ell=k+1}^d K_\ell \right) \frac{C_{d+1} \zeta_{d+2,k}^2}{2N_{d+2}} + O(\epsilon)
\end{aligned}$$

and thus

$$E_k(y_1^{(0:k-1)}) \leq \frac{s_k^2(y_1^{(0:k-1)})}{N_k} + \frac{1}{4} \left(\frac{C_k \zeta_{k+1,k}^2}{N_{k+1}} + \sum_{d=k}^{D-2} \left(\prod_{\ell=k}^d K_\ell \right) \frac{C_{d+1} \zeta_{d+2,k}^2}{N_{d+2}} \right)^2 + O(\epsilon).$$

and therefore

$$\mathbb{E} [(I_0 - \gamma_0)^2] = E_0 \leq \frac{\varsigma_0^2}{N_0} + \frac{1}{4} \left(\frac{C_0 \varsigma_1^2}{N_1} + \sum_{k=0}^{D-2} \left(\prod_{d=0}^k K_d \right) \frac{C_{k+1} \varsigma_{k+2}^2}{N_{k+2}} \right)^2 + O(\epsilon)$$

as required and we are done. \square

10.9 Optimizing the Convergence Rates

We have shown that the mean squared error converges at a rate $O(1/N + 1/M)$ or $O(1/N + 1/M^2)$ depending on the smoothness assumptions that can be made about f . Here we show that given a sample budget $T = MN$, then these bounds are optimized by setting $N \propto M$ and $N \propto M^2$ respectively and that this gives bounds of $O(1/\sqrt{T})$ and $O(1/T^{2/3})$ respectively.

Consider setting $N = \tau(M)$ then $T = \tau(M) \cdot M$ and our bounds become $O(R)$, where

$$R = 1/\tau(M) + 1/M \quad \text{and} \quad R = 1/\tau(M) + 1/M^2.$$

for the two cases respectively.

In this first case supposing $\tau(M) = O(M)$ easily gives

$$T = M\tau(M) = O(M^2)$$

and as such

$$R = O\left(\frac{1}{M}\right) = O\left(\frac{1}{\sqrt{T}}\right) \quad (10.57)$$

as $M \rightarrow \infty$. In contrast, consider the case that $\tau(M) \gg M$ as $M \rightarrow \infty$. We then have

$\frac{1}{\sqrt{M}} \gg \frac{1}{\sqrt{\tau(M)}}$ as $M \rightarrow \infty$, so that

$$R = O\left(\frac{1}{M}\right) \gg \frac{1}{\sqrt{M}} \frac{1}{\sqrt{\tau(M)}} = \frac{1}{\sqrt{T}}.$$

Comparing with (10.57), we observe that, for the same total budget of samples T , this choice of τ provides a strictly weaker convergence guarantee than in the previous case. When $M \gg \tau(M)$ also then we have $\frac{1}{\sqrt{\tau(M)}} \gg \frac{1}{\sqrt{M}}$ as $M \rightarrow \infty$ and so

$$R = O\left(\frac{1}{\tau(M)}\right) \gg \frac{1}{\sqrt{M}} \frac{1}{\sqrt{\tau(M)}} = \frac{1}{\sqrt{T}}$$

which is again a weaker bound. We thus see that the $O(1/N + 1/M)$ bound is optimized when $N \propto M$, giving a convergence rate of $O(1/\sqrt{T})$.

In the second case suppose that $\tau(M) = O(M^2)$ as $M \rightarrow \infty$. This now gives

$$T = M\tau(M) = O(M^3)$$

and therefore

$$R = O\left(\frac{1}{M^2}\right) = O\left(\frac{1}{T^{2/3}}\right)$$

as $M \rightarrow \infty$. Now considering the cases $\tau(M) \gg M^2$ leads to $\frac{1}{M^{4/3}} \gg \frac{1}{\tau(M)^{2/3}}$ and thus

$$R = O\left(\frac{1}{M^2}\right) \gg \frac{1}{M^{2/3}} \frac{1}{\tau(M)^{2/3}} = \frac{1}{T^{2/3}}.$$

Similarly, if $\tau(M) \ll M^2$ then $\frac{1}{\tau(M)^{1/3}} \gg \frac{1}{M^{2/3}}$ and thus

$$R = O\left(\frac{1}{\tau(M)}\right) \gg \frac{1}{M^{2/3}} \frac{1}{\tau(M)^{2/3}} = \frac{1}{T^{2/3}}.$$

Both of these cases lead to weaker bounds and so we see that the $O(1/N + 1/M^2)$ bound is tightest when $N \propto M^2$, giving a convergence rate of $O(1/T^{2/3})$.

10.10 Empirical Confirmation for Repeated Nesting

In this section we consider a simple model with multiple levels of nesting. The model is extended from the one shown at the start of Section 6 in the main paper. Specifically we consider the following model

$$\begin{aligned}
 y^{(0)} &\sim \text{Uniform}(-1, 1), \\
 y^{(1)} &\sim \mathcal{N}(0, 1), \\
 y^{(2)} &\sim \mathcal{N}(0, 1), \\
 f_0(y^{(0)}, \gamma_1(y^{(0)})) &= \log \gamma_1(y^{(0)}) \\
 f_1(y^{(0:1)}, \gamma_2(y^{(0:1)})) &= \exp\left(-\left(y^{(0)} - y^{(1)} - \log \gamma_2(y^{(0:1)})\right)\right) \\
 f_2(y^{(0:2)}) &= \exp\left(-\left(y^{(0)} - y^{(1)} - y^{(2)}\right)\right), \\
 f_1(y^{(0:1)}, \gamma_2(y^{(0:1)})) &= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(y^{(0)} - y^{(1)} - \log \gamma_2(y^{(0:1)}))^2}{2}\right) \\
 f_2(y^{(0:2)}) &= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(y^{(0)} - y^{(1)} - y^{(2)})^2}{2}\right), \\
 \phi_1(y, z_1, \gamma_2) &= \sqrt{2/\pi} \exp\left(-2(y - z_1)^2\right), \\
 \phi_2(y, z_1, z_2) &= \sqrt{2/\pi} \exp\left(-2(y - z_1 - z_2)^2\right), \\
 I &= \mathbb{E}_{p(y)} \left[\log \left(\mathbb{E}_{p(z_1)} \left[\phi_1 \left(y, \log \left(\mathbb{E}_{p(z_2)} [\phi_2(y, z_1, z_2)] \right) \right) \right] \right) \right]. \tag{10.58}
 \end{aligned}$$

Unlike the model in the main paper, this no longer has an analytical solution, but we generate a ground truth estimate using a large run where $N_0 = 25000$, $N_1 = 5000$, and $N_2 = 1000$ giving a total of 1.25×10^{11} samples. The converge plot shown in Figure 10.4 shows that the theoretically expected convergence rates are observed.

Move these experimental section mostly into the main paper

10.11 Additional details pertaining to cancer simulator

In this section we elucidate some more details about the cancer simulator described in the manuscript, provide more rigorous mathematical definitions for the relevant terms using the same nomenclature, and also include more results figures.

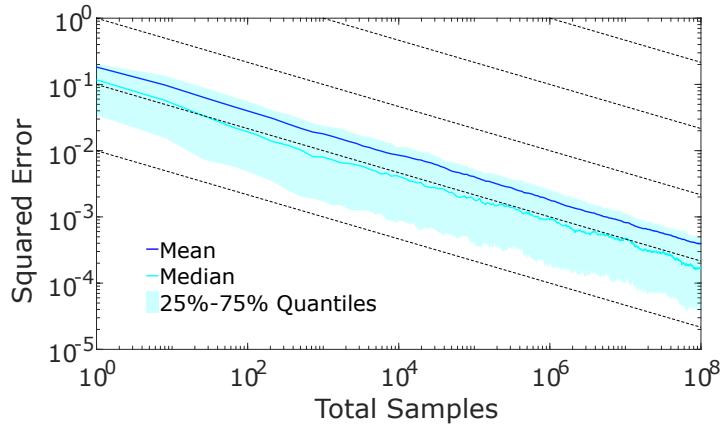


Figure 10.4: Empirical convergence of NMC for (10.58). We set $N_0 = N_1 = N_2$ and observe the convergence with increasing number of total samples $T = N_0 N_1 N_2$. We see the that the convergence rate suggested by our bounds of $O(T^{1/3})$ is observed as expected. Results shown are from 1000 independent runs.

10.11.1 Simulator details

We define $I(T_{treat})$ to be the expected proportion of patients who receive treatment. A particular patient is represented by $y \in \mathcal{R}^d$. Specifically, y consists of only a single real number ($d = 1$) representing the size of the tumour upon discovery. Initial tumour size is drawn from a scaled Rayleigh distribution. The outcome of the simulator is then $\phi(y, z) \in \{0, 1\}$, and is the binary outcome of whether that particular patient and sample of unobserved parameters yield an expected tumour size below the threshold, T_{opp} , after a fixed time duration, t_{max} . The simulator is a pair of coupled, parameterized differential equations for the action of an anti-tumour treatment such as chemotherapy, as described in Enderling and Chaplain [2014]:

$$\frac{dc}{dt} = -\lambda c \log\left(\frac{c}{K}\right) - \xi c \quad (10.59)$$

$$\frac{dK}{dt} = \phi c - \psi K c^{2/3}, \quad (10.60)$$

where $c(t, x) \in \mathcal{R}_+$ represents tumour size, with initial size y_n . Similarly, $K(t, x) \in \mathcal{R}_+$ represents the notion of a carrying capacity, with the initial carrying capacity, $K(0, z)$, set to a known constant K_0 . The magnitude of the patient response to an anti-tumour treatment (such as chemotherapy) is represented by $\xi \in [0, 1]$, drawn from a beta distribution. $\{\lambda, \psi, \phi\} \in \mathcal{R}_+^3$ represent the parameters of the simulator. We also define $x_{n,m} = \{\lambda, \psi, \phi, K_0, \xi\}$ and $z_{n,m} = \{x_{n,m}, T_{opp}, t_{max}\}$, where all but ξ are set to constant values. Expanding this to condition all

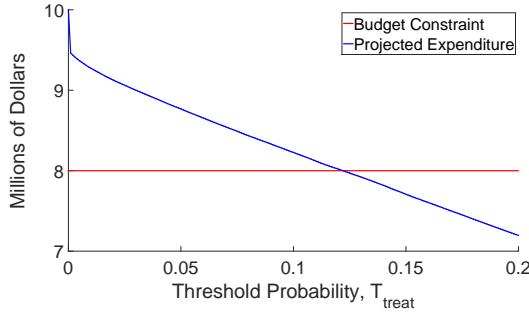


Figure 10.5: Projected expenditure (proportional to $I_{N,M}$) evaluated at different values of T_{treat} . The budget constraint is shown by the horizontal red line. The optimal value of T_{treat} is found by the intersection and occurs at $T_{treat} = 12.5\%$. Evaluated was carried out at 100 T_{treat} s. Only the bottom 20% is pictured as this is the operating range for most treatment centres.

values on y_n is trivial given domain knowledge. Alternatively, they could also be drawn at random, but not be conditioned on y_n . Such relations are omitted here for simplicity.

We can now fully define ϕ as:

$$\phi(y_n, z_{n,m}) = \mathbb{1}(c(t_{max}, x_{n,m}) < T_{opp}). \quad (10.61)$$

Taking the expectation of ϕ over M different realisations of z yields the estimate $(\hat{\gamma}_M)_n$. This value is the probability that treatment will be successful for a particular patient, marginalizing over possible unobserved dynamics. This is the point at which clinician decides whether initiate the treatment plan. This decision is represented $f(y_n, (\hat{\gamma}_M)_n) \in [0, 1]$ as:

$$f(y_n, (\hat{\gamma}_M)_n) = \mathbb{1}((\hat{\gamma}_M)_n > T_{treat}) \quad (10.62)$$

where T_{treat} is the minimum probability of success required for that patient to receive the treatment, and again, could be conditioned on y also. Taking the expectation of f over patients yields the expected frequency with which the treatment will be delivered, given a value of T_{treat} . The hospital wishes to estimate the value T_{treat} that maximizes the number of patients treated, while only treating those patients with the highest probability of success, and (in expectation) staying within the budgetary constraint.

The model is completed by the definition of the following distributions and parameters.

$$K_0 = 100000000, \quad \phi = 0.001, \quad \psi = 0.05, \quad \lambda = 0.5, \quad \xi \sim \text{Beta}(5, 2),$$

$$c_0 \sim 1000 * \text{Rayleigh}(10), \quad T_{opp} = 2000, \quad T_{treat} = 0.35, \quad t_{max} = 250, \quad t_{step} = 0.01$$

10.11.2 Budget result

In the example outlined above, the treatment centre is not actually attempting to evaluate the value of I , but to find the optimal value of T_{treat} subject to a budgetary constraint. A simplistic way of evaluating the optimal value is to perform a dense search over different values of the parameter, each time evaluating the estimated expenditure, and select the best performing value.

Figure 10.5 shows the variation of predicted expenditure against the threshold probability, as well as the budget constraint. The intersection of these curves is the optimal setting of T_{opp} , here evaluated to be 12.5%. From the blue line, it is clear that the relationship between expenditure and treatment probability is non-linear, especially at the extrema of the distribution, and hence the use of NMC was necessarily for evaluating the optimal value.

11

A Statistically Principled Approach to Automating Design

11.1 Bayesian Experimental Design

Bayesian experimental design provides a framework for designing experiments in a manner that is optimal from an information-theoretic viewpoint [Chaloner and Verdinelli, 1995; Sebastiani and Wynn, 2000]. By minimizing the entropy in the posterior distribution of the parameters of interest, one can maximize the information gathered by the experiment.

Let the parameters of interest be denoted by $\theta \in \Theta$ for which we define a prior distribution $p(\theta)$. Let the probability of achieving outcome $y \in \mathcal{Y}$, given parameters θ and a design $d \in \mathcal{D}$, be defined by likelihood model $p(y|\theta, d)$. Under our model, the outcome of the experiment given a chosen d is distributed according to

$$p(y|d) = \int_{\Theta} p(y, \theta|d) d\theta = \int_{\Theta} p(y|\theta, d)p(\theta)d\theta. \quad (11.1)$$

where we have used the fact that $p(\theta) = p(\theta|d)$ because θ is independent of the design. Our aim is to choose the optimal design d under some criterion. We therefore define a utility function, $U(y, d)$, representing the utility of choosing a design d and getting a response y . Typically our aim is to maximize information gathered from the experiment, and so we set $U(y, d)$ to be the gain in Shannon information between the prior and the posterior:

$$U(y, d) = \int_{\Theta} p(\theta|y, d) \log(p(\theta|y, d)) d\theta - \int_{\Theta} p(\theta) \log(p(\theta)) d\theta \quad (11.2)$$

However, we are still uncertain about the outcome. Thus, we use the expectation of $U(y, d)$

with respect to $p(y|d)$ as our target:

$$\begin{aligned}\bar{U}(d) &= \int_{\mathcal{Y}} U(y, d)p(y|d)dy \\ &= \int_{\mathcal{Y}} \int_{\Theta} p(y, \theta|d) \log(p(\theta|y, d))d\theta dy - \int_{\Theta} p(\theta) \log(p(\theta))d\theta \\ &= \int_{\mathcal{Y}} \int_{\Theta} p(y, \theta|d) \log\left(\frac{p(\theta|y, d)}{p(\theta)}\right) d\theta dy.\end{aligned}\quad (11.3)$$

noting that this corresponds to the mutual information between the parameters θ and the observations y . The Bayesian-optimal design is then given by

$$d^* = \arg \max_{d \in \mathcal{D}} \bar{U}(d). \quad (11.4)$$

Finding d^* is challenging because the posterior $p(\theta|y, d)$ is rarely known in closed form. To solve the problem, we proceed by rearranging (11.3) using Bayes' rule (remembering that $p(\theta) = p(\theta|d)$):

$$\begin{aligned}\bar{U}(d) &= \int_{\mathcal{Y}} \int_{\Theta} p(y, \theta|d) \log\left(\frac{p(\theta|y, d)}{p(\theta)}\right) d\theta dy \\ &= \int_{\mathcal{Y}} \int_{\Theta} p(y, \theta|d) \log\left(\frac{p(y|\theta, d)}{p(y|d)}\right) d\theta dy \\ &= \int_{\mathcal{Y}} \int_{\Theta} p(y, \theta|d) \log(p(y|\theta, d))d\theta dy - \int_{\mathcal{Y}} p(y|d) \log(p(y|d))dy.\end{aligned}\quad (11.5)$$

The first of these terms can now be evaluated using standard MC approaches as the integrand is analytic. In contrast, the second term is not directly amenable to standard MC estimation as the marginal $p(y|d)$ represents an expectation and taking its logarithm represents a nonlinear functional mapping.

To derive an estimator, we will now consider these terms separately. Starting with the first term,

$$\bar{U}_1(d) = \int_{\mathcal{Y}} \int_{\Theta} p(y, \theta|d) \log(p(y|\theta, d))d\theta dy \approx \frac{1}{N} \sum_{n=1}^N \log(p(y_n|\theta_n, d)) \quad (11.6)$$

where $\theta_n \sim p(\theta)$ and $y_n \sim p(y|\theta = \theta_n, d)$. We note that evaluating (11.6) involves both sampling from $p(y|\theta, d)$ and directly evaluating it point-wise. The latter of these cannot be avoided, but in the scenario where we do not have direct access to a sampler for $p(y|\theta, d)$, we can use the standard importance sampling trick, sampling instead $y_n \sim q(y|\theta = \theta_n, d)$ and weighting the samples in (11.6) by $w_n = \frac{p(y_n|\theta_n, d)}{q(y_n|\theta_n, d)}$.

Now considering the second term we have

$$\bar{U}_2(d) = \int_{\mathcal{Y}} p(y|d) \log(p(y|d)) dy \approx \frac{1}{N} \sum_{n=1}^N \log \left(\frac{1}{M} \sum_{m=1}^M p(y_n|\theta_{n,m}, d) \right) \quad (11.7)$$

where $\theta_{n,m} \sim p(\theta)$ and $y_n \sim p(y|d)$. Here we can sample the latter by first sampling an otherwise unused $\theta_{n,0} \sim p(\theta)$ and then sampling $y_n \sim p(y|\theta_{n,0}, d)$. Again we can use importance sampling if we do not have direct access to a sampler for $p(y|\theta_{n,0}, d)$.

Putting (11.6) and (11.7) together (and renaming θ_n from (11.6) as $\theta_{n,0}$ for notational consistency with (11.7)) we now have the following complete estimator given in the main paper and implicitly used by Myung et al. [2013] and Ouyang et al. [2016] amongst others

$$\bar{U}(d) \approx \frac{1}{N} \sum_{n=1}^N \left[\log(p(y_n|\theta_{n,0}, d)) - \log \left(\frac{1}{M} \sum_{m=1}^M p(y_n|\theta_{n,m}, d) \right) \right] \quad (11.8)$$

where $\theta_{n,m} \sim p(\theta) \forall m \in 0 : M, n \in 1 : N$ and $y_n \sim p(y|\theta = \theta_{n,0}, d) \forall n \in 1 : N$.

We now show that if y can only take on one of C possible values (y_1, \dots, y_C) , we can achieve significant improvements in the convergence rate by using a similar to that introduced in Section 3.2 to convert to single MC estimator:

$$\begin{aligned} \bar{U}(d) &= \int_{\mathcal{Y}} \int_{\Theta} p(y, \theta|d) \log(p(y|\theta, d)) d\theta dy - \int_{\mathcal{Y}} p(y|d) \log(p(y|d)) dy \\ &= \int_{\Theta} \left[\sum_{c=1}^C p(\theta) p(y_c|\theta, d) \log(p(y_c|\theta, d)) \right] d\theta - \sum_{c=1}^C p(y_c|d) \log(p(y_c|d)) \\ &\approx \frac{1}{N} \sum_{n=1}^N \sum_{c=1}^C p(y_c|\theta_n, d) \log(p(y_c|\theta_n, d)) \\ &\quad - \sum_{c=1}^C \left[\left(\frac{1}{N} \sum_{n=1}^N p(y_c|\theta_n, d) \right) \log \left(\frac{1}{N} \sum_{n=1}^N p(y_c|\theta_n, d) \right) \right] \end{aligned} \quad (11.9)$$

where $\theta_n \sim p(\theta) \forall n \in 1, \dots, N$. As C is a fixed constant, the MSE for first term clearly converges at the standard MC error rate of $O(1/N)$. Similarly each $\hat{P}_N(y_c|d) = \frac{1}{N} \sum_{n=1}^N p(y_c|\theta_n, d)$ term also converges at a rate $O(1/N)$ to $p(y_c|d)$. Now noting that $\hat{P}_N(y_c|d) \leq 1$ and that $f(x) = x \log x$ is Lipschitz continuous in the range $(0, 1]$, each $\hat{P}_N(y_c|d) \log(\hat{P}_N(y_c|d))$ term must also converge at the MC error rate if $p(y_c|d) > 0 \forall c = 1, \dots, C$. Finally if we assume that when $p(y_c|d) = 0$ then $\hat{P}_N(y_c|d) = 0$ almost surely for sufficiently large N , then the second term also converges at the MC error when $p(y_c|d) = 0$. We now have a finite sum of terms which each converge to $\bar{U}(d)$ with MC MSE rate $O(1/N)$, and so the overall estimator (11.9) must also converge at this rate. This compares to $O(1/T^{2/3})$ for (11.8) (assuming we take

$N \propto M^2$), noting that generating T samples for (11.8) has the same cost up to a constant factor as generating N for (11.9). To the best of our knowledge, this is the first introduction of this superior estimator in the literature.

We finish by showing that the theoretical advantages of this reformulation also leads to empirical gains in the estimation of $\bar{U}(d)$. For this we consider a model used in psychology experiments for delay discounting introduced by Vincent [2016]. Our experiment comprises of asking questions of the form “*Would you prefer £A now, or £B in D days?*” and we wish to choose the question variables $d = \{A, B, D\}$ in the manner that will give the most incisive questions. The target participant is presumed to have parameters $\theta = \{k, \alpha\}$ and the following response model

$$y \sim \text{Bernoulli} \left(0.01 + 0.98 \cdot \Phi \left(\frac{1}{\alpha} \left(\frac{B}{1 + e^{kD}} - A \right) \right) \right) \quad (11.10)$$

where $y = 1$ indicates choosing the delayed response and Φ represents the cumulative normal distribution. As more questions are asked, the distribution over the parameters θ is updated, such that the most optimal question to ask at a particular time depends on the previous questions and responses. For the sake of brevity, when comparing the performance of (11.8) and (11.9) we will neglect the problem of how best to optimize the design, and consider only the problem of evaluating $\bar{U}(d)$. We will further consider the case where $B = 100$ and $D = 50$ are fixed and we are only choosing the delayed value A . We presume the following distribution on the parameters

$$k \sim \mathcal{N}(-4.5, 0.5^2)$$

$$\alpha \sim \Gamma(2, 2).$$

We first consider convergence in the estimate of $\bar{U}(d)$ for the case $A = 70$ for our suggested method (11.9) and the naïve solution (11.8), the results of which are shown in Figure 2a in the main paper. Here we see that the convergence rates of the two methods are both as expected and that our suggested method offers significant empirical performance improvements.

We next consider setting a total sample budget $T = 10^4$ and look at the variation in the estimated values of $\bar{U}(d)$ for different values of A for the two methods as shown in Figure 11.1. This shows that the improvement in MSE leads to clearly visible improvements in the characterization of $\bar{U}(d)$ that will translate to improvements in seeking the optimum.

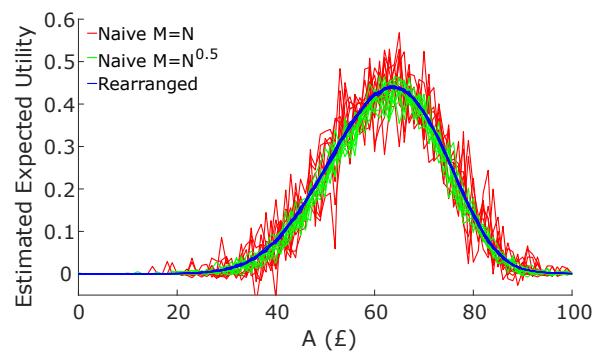


Figure 11.1: Estimated expected utilities $\bar{U}(d)$ for different values of one of the design parameters $A \in \{1, 2, \dots, 100\}$ given a fixed total sample budget of $T = 10^4$. Here the lines correspond to 10 independent runs, showing that the variance of (11.8) is far higher than (11.9).

11.2 Automating Adapting Designs

11.3 Application to Psychological Trials

12

Challenges, Criticisms, and Future Directions

- Relationships with ABC
- Reinvention of priors in deep learning by generating data
- Is amortization just a learning a different decomposition of the joint $p(\theta|\mathcal{D}_1)p(\mathcal{D}_2|\theta)$ that shifts more to the prior to make inference easier? Does it actually implicitly define a different joint distribution that is otherwise difficult to express or is it just proposal adaptation as Tuan Anh's paper says.
- Randomness vs no randomness - blog post for Michi

12.1 Do we need Random Numbers?

Random numbers are a fundamental tool in the arsenal of all the mathematical sciences, especially in the realm of probabilistic numerics. From basic cross-validation to advanced MCMC methods, randomness is at the core of many of our most prevalent and highest performance algorithms. In his related post, Michael will try to convince you why we should eventually try and do away with randomness; here I will do my best to explain why `if (rand<1-ε) {we should not}.`

My argument can be broken down into four main reasons that we need, and always will need, random numbers:

1. Speed and simplicity - sometimes even if there is the information available to improve a computation, uncovering or incorporating that information in a principled manner may require substantially more computational power than not doing so.
2. Honesty and reliability - the alternative to randomness is almost always approximation, introducing bias and an error whose uncertainty is inherently subjective.

3. Compossibility - methods such as Monte Carlo are ambivalent to how the samples are to be used, creating a scalable ability to modularize, compose and reuse. Non-compossible systems, on the other hand, are doomed to fail for large frameworks through the curse of repeated nested of estimators [Rainforth et al., 2016a]
4. Lack of repeatability - though it is always convenient when an experiment is repeatable, systematically returning the same incorrect answer is far more dangerous.

Update
to new
paper

Of these, the speed and simplicity argument is perhaps the most commonly used to support the use of random numbers and is certainly a core reason for their prevalence. However, I believe it is the other three, and in particular the honesty of random numbers, that is most critical for why random numbers are, will remain to be, fundamental to numerical computation. All of these arguments are related to the following principle:

Once we have imparted all possible information upon a system, we must treat what is left as truly stochastic or introduce bias.

In other words, imagine we can construct a problem in a manner that utilizes all available prior information, both in terms of the model and in how best to solve the model. Any remaining uncertainty is now, at least for all practical purposes, inherent to the problem and so any further attempt to remove randomness from the system is indirectly adding in further prior information we did not want to impart. Furthermore, when things we kept random, we can gauge the error in our approximation or the level of our uncertainty by simply rerunning the system. As soon as we replace this with an approximation or fix the random number seed, we lose calibration of the uncertainty in our estimate because we can estimate the variance resulting from randomness, but typically not the bias resulting from approximation.

Putting our frequentist hat on for the moment, then the notion of doing away with randomness is scary. Frequentist statistics is all about *repeatability* and focuses on the fact that any data we collect is random in a many-worlds point of view, because even with the same ground-truth underlying generative process, the inherent randomness of the universe (or at least effective randomness if you have philosophical objections to this) means that multiple possible datasets *could* have been generated. Regardless of your philosophical position on the Bayesian vs frequentist divide, there are many times when such a frequentist approach is absolutely essential from a practical viewpoint. For example, in medical tasks we need to make sure that our

confidence intervals are actually correct when we repeat a procedure – we need guarantees on their *calibration*. This simply is not possible in a Bayesian framework as by its very nature it presumes the data is fixed and thus permits no concept of repetition. Once we realize that we sometimes need to take a frequentist approach, the need for randomness becomes obvious, as in the frequentist framework probability originates only through random variables. In other words, as powerful as the Bayesian framework is, it is inherently optimistic and subjective (e.g. there are always unknown unknowns), and as such it can never really be the whole story. If we try and do away with randomness completely it is impossible to be objective – we have to choose our approximation, sometimes in an arbitrary fashion (e.g. by setting the random number seed) – and so we can never provide properly calibrated confidence intervals that are not prone to subjective interpretation.

This honesty of Monte Carlo goes beyond specific applications. One of its most powerful consequences is the compossibility of Monte Carlo estimates: give a sample from a marginal, I can generate a valid sample of the joint by sampling from the conditional. Similarly, if I have samples from a joint, I also have samples from the marginal distributions. This behavior is essential when composing different components into a greater system as one can ensure each component takes in samples as inputs and outputs corresponding samples as output that can be used by the next process in the pipeline. If we instead make some deterministic approximation at each stage, we flaunt the flaw of averages and our biases will conflagulate to give a result that might be substantially different to the truth. Sticking with unbiased Monte Carlo estimation (e.g. using importance sampling or sequential Monte Carlo [Doucet and Johansen, 2009]) then although it is of course possible that our variance will explode, we at least know that if our estimate has a poor accuracy. If we do away with randomness, we might generate large errors without even knowing we have.

This lack of repeatability is actually an essential advantage of Monte Carlo. It is better for a system to give you a different wrong answer each time it is queried than to always give the same wrong answer, particularly if the average of the different answers is in fact the truth, as is often the case. When we write scientific papers we run our experiments multiple times to show the variability in the results. Systems that always give the same answer and instead return a single subjective uncertainty estimate (e.g. a Gaussian process) are not generally trustworthy because there is no true calibration or sense of whether the experimenter simply got lucky with a

system that does not actually work well in practice. Furthermore, such a setting it very open to intentional or unintentional abuse. If we fix our randomness *a priori* and then adapt our algorithm until it works, we may well simply be over-fitting to what works best for that random number seed or approximation. It horrifies me that some people fix their random number seeds when tuning or improving an algorithm and I expect that this practice has actually led to a plethora of statistically incorrect results. If we want to maintain scientific integrity then we have to report results on experiments that have not been tested during the design of our algorithm and which are tested with multiple different choices for arbitrary or subjective decisions, to show that those results are actually stable and representative. If we do away with randomness, we lose, or at the very least seriously hamper, this ability to repeat experiments in an objective manner.

To summarize, we need randomness because we do not know everything. In the Bayesian framework we place distributions on what we are not sure about to reflect this lack of knowledge. A key part of this process is acknowledging that once we have done this, what is left is random. After all, this uncertainty is where the Bayesian definition of probability actually comes from and what does it mean to have probability without randomness? Yes we might be able to impart more knowledge on problems that we currently do, such as by decorrelating our samples, but there always become a point where we have imparted everything we know, after which what is left is truly random by the Bayesian definition of probability. If we go outside the Bayesian framework, the need for randomness becomes even more pronounced. In frequentist settings even our data is a random variable and probability is defined through variations in repeating an experiment. In short, regardless of whether we take a Bayesian or frequentist viewpoint, arguing for the removal of all randomness from our system is tantamount to arguing that we should do away with probability theory entirely.

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