Probabilistic Programming with Gaussian Process Memoization

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Abstract

This paper describes the *Gaussian process memoizer*, a probabilistic programming technique that uses Gaussian processes to provides a statistical alternative to memorization. Memoizing a target procedure results in a self-caching wrapper that remembers previously computed values. Gaussian process memoization additionally produces a statistical emulator based on a Gaussian process whose predictions automatically improve whenever a new value of the target procedure becomes available. This paper also introduces an efficient implementation, named `gpmem`, that can use kernels given by a broad class of probabilistic programs. The flexibility of `gpmem` is illustrated via three applications: (i) GP regression with hierarchical hyper-parameter learning, (ii) Bayesian structure learning via compositional kernels generated by a probabilistic grammar, and (iii) a bandit formulation of Bayesian optimization with automatic inference and action selection. All applications share a single 50-line Python library and require fewer than 20 lines of probabilistic code each.

1 Introduction

Probabilistic programming could be revolutionary for machine intelligence due to universal inference engines and the rapid prototyping for novel models (Ghahramani, 2015). This levitates the design and testing of new models as well as the incorporation of complex prior knowledge which currently is a difficult and time consuming task. Probabilistic programming languages aim to provide a formal language to specify probabilistic models in the style of computer programming and can represent any computable probability distribution as a program. In this work, we will introduce new features of Venture, a recently developed probabilistic programming language. We consider Venture the most compelling of the probabilistic programming languages because it is the first probabilistic programming language suitable for general purpose use (Mansinghka et al., 2014). Venture comes with scalable performance on hard problems and with a general purpose inference engine. The inference engine deploys Markov Chain Monte Carlo (MCMC) methods (for an introduction, see Andrieu et al. (2003)). MCMC lends itself to models with complex structures such as probabilistic programs or hierarchical Bayesian non-parametric models since they can provide a vehicle to express otherwise intractable integrals necessary for a fully Bayesian representation. MCMC is scalable, often distributable and also compositional. That is, one can arbitrarily chain MCMC kernels to infer over several hierarchically connected or nested models as they will emerge in probabilistic programming.

One very powerful model yet unseen in probabilistic programming languages are Gaussian Processes (GPs). GPs are gaining increasing attention for representing unknown functions by posterior probability distributions in various fields such as machine learning, signal processing, computer vision and bio-medical data analysis. Making GPs available in probabilistic programming is crucial to allow a language to solve a wide range of problems. Hard problems include but are not limited to hierarchical prior construction (Neal, 1997), Bayesian Optimization Snoek et al. (2012) and systems for inductive learning of symbolic expressions such as the one introduced in the Automated Statistician project Duvenaud et al. (2013); Lloyd et al. (2014). Learning such symbolic expressions is a hard problem that requires careful design of approximation techniques since standard inference method do not apply.

In the following, we will present `gpmem` as a novel probabilistic programming technique that solves such hard problems. `gpmem` introduces a statistical alternative to standard memoization. Our contribution is threefold:

- we introduce an efficient implementation of `gpmem` in form of a self-caching wrapper that remembers previously computed values;
- we illustrate the statistical emulator that `gpmem` produces and how it improves with every data-point that becomes available; and
- we show how one can solve hard problems of state-of-the-art machine learning related to GP using `gpmem` in a Bayesian fashion and with only a few lines of Venture code.

We evaluate the contribution on problems posed by the GP community using real world and synthetic data by assessing quality in terms of posterior distributions of symbolic outcome and in terms of the residuals produced by our probabilistic programs. The paper is structured as follows, we will first provide some background on memoization. We will explain programming in Venture and provide a brief introduction to GPs. We introduce `gpmem` and its use in probabilistic programming and Bayesian modeling. Finally, we will show how we can apply `gpmem` on problems of causally structured hierarchical priors for hyper-parameter inference, structure discovery for Gaussian Processes and Bayesian Optimization including experiments with real world and synthetic data.

2 Background

2.1 Memoization

Memoization is the idea of computing the value of a function given an input once and then store it. If the function is called again at the same input, we return the stored value without evaluating the function body again. Research on the Church language (Goodman et al., 2008) pointed out that although memoization does not change the semantics of a program for determinstic programs it does for stochastic ones. This implies that one can stochastically decide on each function evaluation whether to use a stored value or a new function evaluation. Here, memoization induces random world semantics (Poole, 1993; Sato, 1995) over the probabilistic program: we interpret a specific mapping from function input to function output as a single possible world (**?**).

2.2 Venture

Venture is a compositional language for custom inference strategies that comes with a Scheme- and Java-Script-like front-end syntax. Its implementation is based on on three concepts. (i) stochastic procedure interfaces that specify and encapsulate random variables, analogously to conditional probability tables in a Bayesian network; (ii) probabilistic execution traces that represent execution histories and capture conditional dependencies; and (iii) scaffolds that partition execution histories and factor global inference problems into sub-problems. These building blocks provide a powerful way to represent probability distributions; some of which cannot be expressed with density functions. For the purpose of this work the most important Venture directives that operate on these building blocks to understand are ASSUME, OBSERVE, SAMPLE and INFER. ASSUME induces a hypothesis space for (probabilistic) models including random variables by binding the result of an expression to a symbol. SAMPLE simulates a model expression and returns a value. OBSERVE adds constraints to model expressions. INFER instructions incorporate observations and cause Venture to find a hypothesis that is probable given the data.

INFER is most commonly done by deploying the Metropolis-Hastings algorithm (MH) (Metropolis et al., 1953). Many algorithms used in the MCMC world can be interpreted as special cases of MH (Andrieu et al., 2003). We can outline the MH algorithm as follows. For T steps we sample x^*

from a proposal distribution q:

$$x^* \sim q(x^* \mid x^{(t)}) \tag{1}$$

which we accept ($x^{t+1} \leftarrow x^*$) with ratio:

$$\alpha = min\left\{1, \frac{p(x^*)q(x^t \mid x^*)}{p(x^{(t)})q(x^* \mid x^t)}\right\} \tag{2}$$

Venture implements an MH transition operator for probabilistic execution traces.

2.3 Gaussian Processes

In the following, we will introduce GP related theory and notations. We will exclusively work on two variable regression problems. Let the data be real-valued scalars $\{x_i, y_i\}_{i=1}^n$ (complete data will be denoted by column vectors $\mathbf{x}, \mathbf{y}$). GPs present a non-parametric way to express prior knowledge on the space of possible functions f that we assume to have generated the data. f is assumed latent and the GP prior is given by a multivariate Gaussian $f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(x_i, x_i'))$, where $m(\mathbf{x})$ is a function of the mean of all functions that map to y_i at x_i and $k(x_i, x_i')$ is a kernel or covariance function that summarizes the covariance of all functions that map to y_i at x_i. We can absorb the mean function into the covariance function so without loss of generality we can set the mean to zero. The marginal likelihood can be expressed as:

$$p(\mathbf{y}|\mathbf{x}) = \int p(\mathbf{y}|\mathbf{f}, \mathbf{x})\, p(\mathbf{f}|\mathbf{x})\, d\mathbf{f} \tag{3}$$

where the prior is Gaussian $\mathbf{f}|\mathbf{x} \sim \mathcal{N}\big(0, k(\mathbf{x}, \mathbf{x}')\big)$. We can sample a vector of unseen data from the predictive posterior with

$$\mathbf{y}^* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \tag{4}$$

for a zero mean prior GP with a posterior mean of:

$$\boldsymbol{\mu} = \mathbf{K}(\mathbf{x}, \mathbf{x}^*)\, \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1}\, \mathbf{y} \tag{5}$$

and covariance

$$\boldsymbol{\Sigma} = \mathbf{K}(\mathbf{x}, \mathbf{x}) - \mathbf{K}(\mathbf{x}, \mathbf{x}^*)\mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1}\mathbf{K}(\mathbf{x}^*, \mathbf{x}). \tag{6}$$

$\mathbf{K}$ is a covariance function. The log-likelihood is defined as:

$$\log P(\mathbf{y} \mid \mathbf{X}) = -\frac{1}{2}\mathbf{y}^\top(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{y} - \frac{1}{2}\log|\mathbf{K} + \sigma^2 I| - \frac{n}{2}\log 2\pi \tag{7}$$

with n being the number of data-points and sigma the independent observation noise. Both log-likelihood and predictive posterior can be computed efficiently in a Venture SP with an algorithm that resorts to Cholesky factorization(Rasmussen and Williams, 2006, chap. 2) resulting in a computational complexity of $\mathcal{O}(n^3)$ in the number of data-points.

The covariance function covers general high-level properties of the observed data such as linearity, periodicity and smoothness. The most widely used type of covariance function is the squared exponential covariance function:

$$k(x, x') = \sigma^2 \exp(-\frac{(x - x')^2}{2\ell^2}) \tag{8}$$

where σ and ℓ are hyper-parameters. σ is a scaling factor and ℓ is the typical length-scale. Smaller variations can be achieved by adapting these hyper-parameters.

Larger variations are achieved by changing the type of the covariance function structure. Note that covariance function structures are compositional. We can add covariance functions if we want to model globally valid structures

$$k_3(x, x') = k_1(x, x') + k_2(x, x') \tag{9}$$

and we can multiply covariance functions if the data is best explained by local structure

$$k_4(x, x') = k_1(x, x') \times k_2(x, x'); \tag{10}$$

both, k_3 and k_4 are valid covariance function structures.

3 Venture GPs

Given a stochastic process that implements the GP algebra above we can implement a GP sampler (4) to perform GP inference in a few lines of code. We can express simple GP smoothing with fixed hyper-parameters or a prior on hyper-parameters and perform MH on it while allowing users to custom design covariance functions. Throughout the paper, we will use the Scheme-like front-end syntax.

```
[ASSUME l  (gamma 1 3)] ∈ {hyper-parameters}
[ASSUME sf (gamma 1 3)] ∈ {hyper-parameters}
```

$$k(x, x') := \sigma^2 \exp(-\frac{(x-x')^2}{2\ell^2})$$

```
[ASSUME f VentureFunction(k,σ,ℓ) ]
[ASSUME SE make-se (apply-function f l sf) ]
[ASSUME (make-gp 0 SE) ]

[SAMPLE GP (array 1 2 3)] % Prior
[OBSERVE GP D]
[SAMPLE GP (array 1 2 3)]
[INFER  (MH {hyper-parameters} one 100) ]
[SAMPLE GP (array 1 2 3)] % Posterior
```

Listing 1: Bayesian GP Smoothing

The first two lines depict the hyper-parameters. We tag both of them to belong to the set {hyper-parameters}. Every member of this set belongs to the same inference scope. This scope controls the application of the inference procedure used. In this paper, we use MH throughout. Each scope is further subdivided into blocks that allow to do block-proposals. In the following we omit the block notation for readability, since we always choose the block of a certain scope at random.

The ASSUME directives describe the assumptions we make for the GP model, we assume the hyper-parameters l and sf (corresponding to ℓ, σ) to be 1 and 2. The squared exponential covariance function can be defined outside the Venture code with foreign conventional programming languages, e.g. Python. In that way, the user can define custom covariance functions without being restricted to the most common ones. We then integrate the foreign function into Venture as VentureFunction. In the next line this function is associated with the hyper-parameters. Finally, we assume a Gaussian Process SP with a zero mean and the previously assumed squared exponential covariance function.

In the case where hyper-parameters are unknown they can be found deterministically by optimizing the marginal likelihood using a gradient based optimizer. Non-deterministic, Bayesian representations of this case are also known (Neal, 1997).

We have already implemented this in listing 1. We draw the hyper-parameters from a Γ-prior for a Bayesian treatment of hyper-parameters. This is simple using the build in stochastic procedure that simulates drawing samples from a gamma distribution. The program gives rise to a Bayesian representation of GPs, which we will explore in the following.

3.1 A Bayesian interpretation

3.1.1 Data modelling as a special case of `gpmem`

From the standpoint of computation, a data set of the form $\{(x_i, y_i)\}$ can be thought of as a function $y = f_{\text{restr}}(x)$, where f_{restr} is restricted to only allow evaluation at a specific set of inputs x. Modelling the data set with a GP then amounts to trying to learn a smooth function f_{emu} ("emu" stands for "emulator") which extends f to its full domain. Indeed, if f_{restr} is a foreign procedure made available as a black-box to Venture, whose secret underlying source code is:

```
def f_restr(x):
  if x in D:
    return D[x]
  else:
    raise Exception('Illegal input')
```

Then the `OBSERVE` code in Listing 1 can be rewritten using `gpmem` as follows (where here the data set `D` has keys `x[1]`,...,`x[n]`):

```
[ASSUME (list f_compute f_emu) (gpmem f_restr)]
for i=1 to n:
  [PREDICT (f_compute x[i])]
  [INFER (MH {hyper-parameters} one 100)]
[SAMPLE (f_emu (array 1 2 3))]
```

This rewriting has at least two benefits: (i) readability (in some cases), and (ii) amenability to active learning. As to (i), the statistical code of creating a Gaussian process is replaced with a memoization-like idiom, which will be more familiar to programmers. As to (ii), when using `gpmem`, it is quite easy to decide incrementally which data point to sample next: for example, the loop from `x[1]` to `x[n]` could be replaced by a loop in which the next index `i` is chosen by a supplied decision rule. In this way, we could use `gpmem` to perform online learning using only a subset of the available data.

3.1.2 The efficacy of learning hyperparameters

The probability of the hyper-parameters of a GP with assumptions as above and given covariance function structure $\mathbf{K}$ can be described as:

$$P(\boldsymbol{\theta} \mid \mathbf{D}, \mathbf{K}) = \frac{P(\mathbf{D} \mid \boldsymbol{\theta}, \mathbf{K}) P(\boldsymbol{\theta} \mid \mathbf{K})}{P(\mathbf{D} \mid \mathbf{K})}. \tag{11}$$

Let the $\mathbf{K}$ be the sum of a smoothing and a white noise (WN) kernel. For this case, Neal suggested the problem of outliers in data as a use-case for a hierarchical Bayesian treatment of Gaussian processes (1997)[1]. The work suggests a hierarchical system of hyper-parameterization (Fig. 1a). Here, we draw hyper-parameters from a Γ distributions:

$$\ell^{(t)} \sim \Gamma(\alpha_1, \beta_1),\ \sigma^{(t)} \sim \Gamma(\alpha_2, \beta_2) \tag{12}$$

and in turn sample the α and β from Γ distributions as well:

$$\alpha_1^{(t)} \sim \Gamma(\alpha_\alpha^1, \beta_\alpha^1),\ \alpha_2^{(t)} \sim \Gamma(\alpha_\alpha^2, \beta_\alpha^2), \cdots \tag{13}$$

[1] In (Neal, 1997) the sum of an SE plus a constant kernel is used. We stick to the WN kernel for illustrative purposes.

Assuming the covariance structure is an additive comprised of a smoothing and a white noise kernel, one can represent this kind of model using gpmem with only a few lines of code:

```
[ASSUME alpha (mem (lambda (i)  (gamma  1 3 )))] ∈ {hyper-parameters-Γ}
[ASSUME beta  (mem (lambda (i)  (gamma  1 3 )))] ∈ {hyper-parameters-Γ}

[ASSUME l  (gamma (alpha 1) (beta 1))]    ∈ {hyper-parameters}
[ASSUME sf (gamma (alpha 2) (beta 2))]    ∈ {hyper-parameters}
[ASSUME sigma (uniform 0 5 )]             ∈ {hyper-parameters} % Fig. 2
% above: structured prior, Fig. 1a

k1(x,x') := θ^2 exp(-(x-x')^2/(2ℓ^2))
k2(x,x') := σ^2 δ_{x,x'}

[ASSUME k1 VentureFunction(k1,θ,ℓ) ]
[ASSUME k2 VentureFunction(k2,σ) ]

[ASSUME SE make-se (apply-function k1 l sf) ]
[ASSUME WN make-se (apply-function k1 sigma) ]

[ASSUME (list f_compute f_emu) (gpmem f_restr (function-plus SE WN) )]
[SAMPLE (f_emu (array 1 2 3))]  % prior, Fig. 1b

for i=1 to n:
  [PREDICT (f_compute x[i])] % observing with a look-up function
[SAMPLE (f_emu (array 1 2 3))]  % after observation, Fig. 1c

[INFER (REPEAT 100
  (DO (MH {hyper-parameters} one 2)
      (MH {hyper-parameters-Γ} one 2) ))]
[SAMPLE (f_emu (array 1 2 3))]  % posterior , Fig. 1d
```

Listing 2: Hierarchical GP Smoothing

Neal provides a custom inference algorithm setting and evaluates it using the following synthetic data problem. Let f be the underlying function that generates the data:

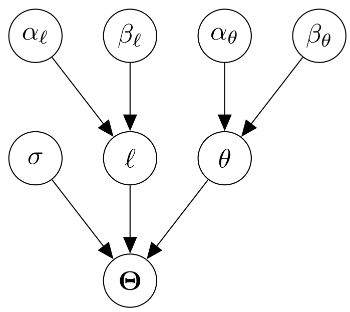
$$f(x) = 0.3 + 0.4x + 0.5\sin(2.7x) + \frac{1.1}{(1+x^2)} + \eta \quad with \;\; \eta \sim \mathcal{N}(0,\sigma) \tag{14}$$

We synthetically generate outliers by setting $\sigma = 0.1$ in 95% of the cases and to $\sigma = 1$ in the remaining cases. gpmem can capture the true underlying function within only 100 MH steps on the hyper-parameters to get a good approximation for their posterior (see Fig. 1). Note that Neal devices an additional noise model and performs large number of Hybrid-Monte Carlo and Gibbs steps. We illustrate the hyper-parameter by showing the shift of the distribution on the noise parameter σ (Fig. 2). We see that gpmem learns the posterior distribution well, the posterior even exhibits a bimodal histogram when sampling σ 100 times reflecting the two modes of data generation, that is normal noise and outliers[2].

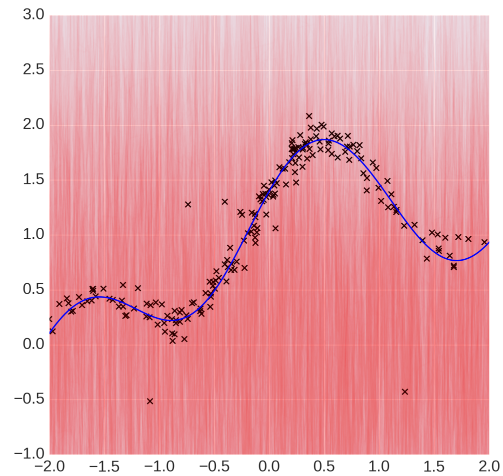
3.1.3 Broader applicability of gpmem

More generally, gpmem is relevant not just when a data set is available, but also whenever we have at hand a function f_{restr} which is expensive or impractical to evaluate many times. gpmem allows us to model f_{restr} with a GP-based emulator f_{emu}, and also to use f_{emu} during the learning process to choose, in an online manner, an effective set of probe points $\{x_i\}$ on which to use our few evaluations of f_{restr}. This idea is illustrated in detail in Section 4. Before doing this, we will illustrate another benefit of having a probabilistic programming apparatus for GP modelling: the linguistically unified treatment of inference over structure and inference over parameters. This unification makes interleaved joint inference over structure and parameters very natural, and allows us to give a short, elegant description of what it means to "learn the covariance function," both in prose and in code.

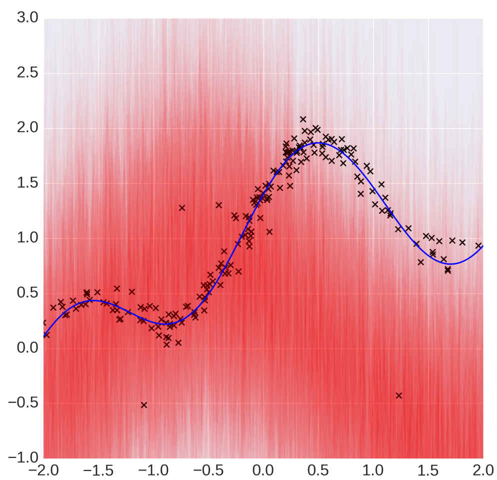
[2] For this pedagogical example we have increased the probability for outliers in the data generation slightly from 0.05 to 0.2



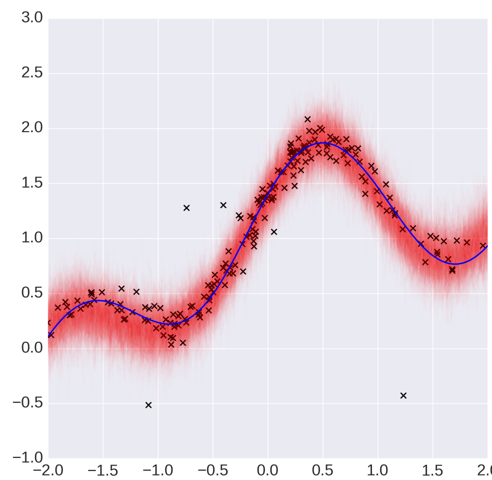
(a) Hierarchical Prior



(b) Prior Inference

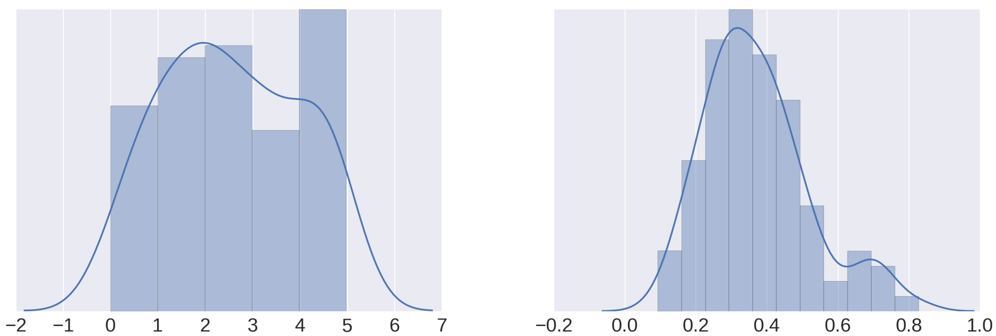


(c) Observed



(d) Inferred

Figure 1: (a) depicts the hierarchical structure of the hyper-parameter as constructed in the work by Neal as a Bayesian Network. (b)-(d) shows a Venture GP on Neal's example. We see that prior renders functions all over the place (a). After `gpmem` observes a some data-points an arbitrary smooth trend with a high level of noise is sampled. After running inference on the hierarchical system of hyper-parameters we see that the posterior reflects the actual curve well. Outliers are treated as such and do not confound the GP.



(a) σ Before (b) σ After

Figure 2: Hyper-parameter inference on the parameter of the noise kernel. We show a 100 samples drawn from the distribution on σ. One can clearly recognise the shift from the uniform prior $\mathcal{U}(0, 5)$ to a double peak distribution around the two modes - normal and outlier.

Furthermore, the example in Section 3.2 below recovers the performance of current state-of-the-art GP-based models.

3.2 Structure Learning

The space of possible kernel composition is infinite. Combining inference over this space with the problem of finding a good parameterization that could potentially explain the observed data best poses a hard problem. The natural language interpretation of the meaning of a kernel and it's composition renders this a problem of symbolic computation. Duvenaud and colleagues note that sum of kernels can be interpreted as logical OR operations and kernel multiplication as logical AND (2013). This is due to the kernel rendering two points similar if k_1 OR k_2 outputs a high value in the case of a sum. Respectively, multiplication of two kernel results in high values only if k_1 AND k_2 have high values (see Fig. 3 for examples how to interpret global vs. local aspects and its symbolic analog respectively).

In the following, we will refer to covariance functions that are not composite as base covariance functions. Note that this form of composition can be easily expressed in Venture, for example if one wishes to add a linear and a periodic kernel:

```
[ASSUME l (gamma 1 3)]
[ASSUME sf (gamma 1 2)]
[ASSUME a (gamma 2 2)]

k_LIN(x,x') := σ_1^2 (x − ℓ)(x' − ℓ)
k_PER(x,x') := σ_2^2 exp(− 2 sin^2(π(x−x')/p) / ℓ^2)

[ASSUME f_LIN VentureFunction(k_LIN,σ_1) ]
[ASSUME f_PER VentureFunction(k_PER,σ_2,ℓ,p) ]
[ASSUME LIN (make-LIN (apply-function f_LIN a)) ]
[ASSUME PER (make-PER (apply-function f_PER l sf)) ]
[ASSUME (make-gp 0 (function-times LIN PER)) ]
```

Listing 3: LIN $\times$ PER

Knowledge about the composite nature of covariance functions is not new, however, until recently, the choice and the composition of covariance functions were done ad-hoc. The Automated Statistician Project came up with an approximate search over the possible space of kernel structures (Duvenaud et al., 2013; Lloyd et al., 2014). However, a fully Bayesian treatment of this was not done before. The case where the covariance structure is not given is even more interesting. Our probabilistic programming based MCMC framework approximates the following intractable integrals of the expectation for the prediction:

$$\mathbb{E}[y^* \mid x^*, \mathbf{D}, \mathbf{K}] = \iint f(x^*, \boldsymbol{\theta}, \mathbf{K})\, P(\boldsymbol{\theta} \mid \mathbf{D}, \mathbf{K})\, P(\mathbf{K}|\boldsymbol{\Omega}, s, n)\, \mathbf{d}\boldsymbol{\theta}\mathbf{d}\mathbf{K}. \tag{15}$$

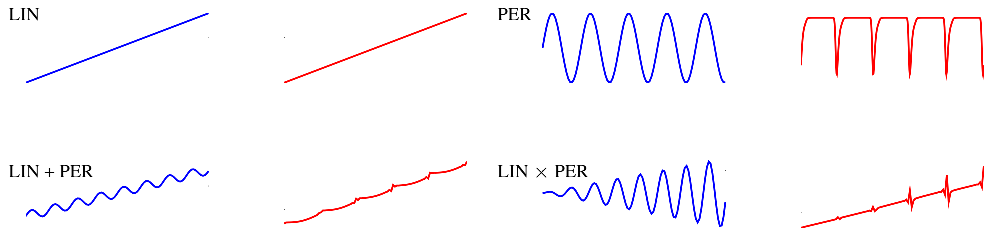


Figure 3: Composition of covariance functions (blue, left) and samples from the distribution of curves they can produce (red, right).

This is done by sampling from the posterior probability distribution of the hyper-parameters and the possible kernel:

$$y^* \approx \frac{1}{T} \sum_{t=1}^{T} f(x^* | \boldsymbol{\theta}^{(t)}, \mathbf{K}^{(t)}). \tag{16}$$

In order to provide the sampling of the kernel, we introduce a stochastic process to the SP that simulates the grammar for algebraic expressions of covariance function algebra:

$$\mathbf{K}^{(t)} \sim P(\mathbf{K} \mid \boldsymbol{\Omega}, s, n) \tag{17}$$

Here, we start with a set of possible kernels and draw a random subset. For this subset of size n, we sample a set of possible operators that operate on the base kernels.

The marginal probability of a kernel structure which allows us to sample is characterized by the probability of a uniformly chosen subset of the set of n possible covariance functions times the probability of sampling a global or a local structure which is given by a binomial distribution:

$$P(\mathbf{K} \mid \boldsymbol{\Omega}, s, n) = P(\boldsymbol{\Omega} \mid s, n) \times P(s \mid n) \times P(n), \tag{18}$$

with

$$P(\boldsymbol{\Omega} \mid s, n) = \binom{n}{r} p_{+\times}^{k} (1 - p_{+\times})^{n-k} \tag{19}$$

and

$$P(s \mid n) = \frac{n!}{\mid s \mid !} \tag{20}$$

where $P(n)$ is a prior on the number of base kernels used which can sample from a discrete uniform distribution. This will strongly prefer simple covariance structures with few base kernels since individual base kernels are more likely to be sampled in this case due to (20). Alternatively, we can approximate a uniform prior over structures by weighting $P(n)$ towards higher numbers. It is possible to also assign a prior for the probability to sample global or local structures, however, we have assigned complete uncertainty to this with the probability of a flip $p = 0.5$.

Many equivalent covariance structures can be sampled due to covariance function algebra and equivalent representations with different parameterization (Lloyd et al., 2014). Certain covariance functions can differ in terms of the hyper-parameterization but can be absorbed into a single covariance function with a different parameterization. To inspect the posterior of these equivalent structures we convert each kernel expression into a sum of products and subsequently simplify expressions using the following grammar:

```
SE × SE                    → SE
{SE,PER,C,WN} × WN         → WN
LIN + LIN                  → LIN
{SE,PER,C,WN,LIN} × C      →  {SE,PER,C,WN,LIN}
```

Listing 4: Grammar to simplify expressions

For reproducing results from the Automated Statistician Project in a Bayesian fashion we first define a prior on the hypothesis space. Note that, as in the implementation of the Automated Statistician, we upper-bound the complexity of the space of covariance functions we want to explore. We also put vague priors on hyper-parameters.

```
[ASSUME base_kernels (list K1,K2,···,Kn)] % defined as above
[ASSUME pn (uniform_structure n)]         % prior on the number of kernels
[ASSUME SK (subset  base_kernels pn)]     % sampling a subset of size n
[ASSUME composition (lambda (l)           % kernel composition
                     (if (lte ( size l) 1)
                         (first l)
                          (if (flip)
                              (func_plus (first l) (cov_compo (rest l)))
                              (func_times (first l) (cov_compo (rest l)))
                          )
                     )
              )

[ASSUME K (composition  SK)]

[ASSUME (list f_compute f_emu) (gpmem f_restr K )]

for i=1 to n:
  [PREDICT (f_compute x[i])] % observing with a look-up function

[INFER  (REPEAT 2000 (DO
                        (MH pn one 1)
                        (MH SK one 1)
                        (MH K* one 1)
                        (MH {hyper-parameters} one 10)) ]
```

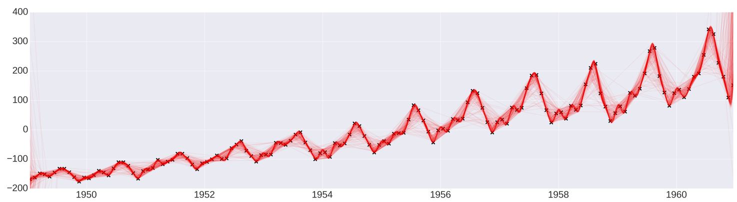
Listing 5: Venture Code for Bayesian GP Structure Learning

We defined the space of covariance structures in a way allowing us to reproduce results for covariance function structure learning as in the Automated Statistician. This lead to coherent results, for example for the airline data set. We will elaborate the result using a sample from the posterior (Fig. 4). The sample is identical with the highest scoring result reported in previous work using a search-and-score method (Duvenaud et al., 2013) for the CO_2 data set () and the predictive capability is comparable. However, the components factor in a different way due to different parameterization of the individual base kernels.

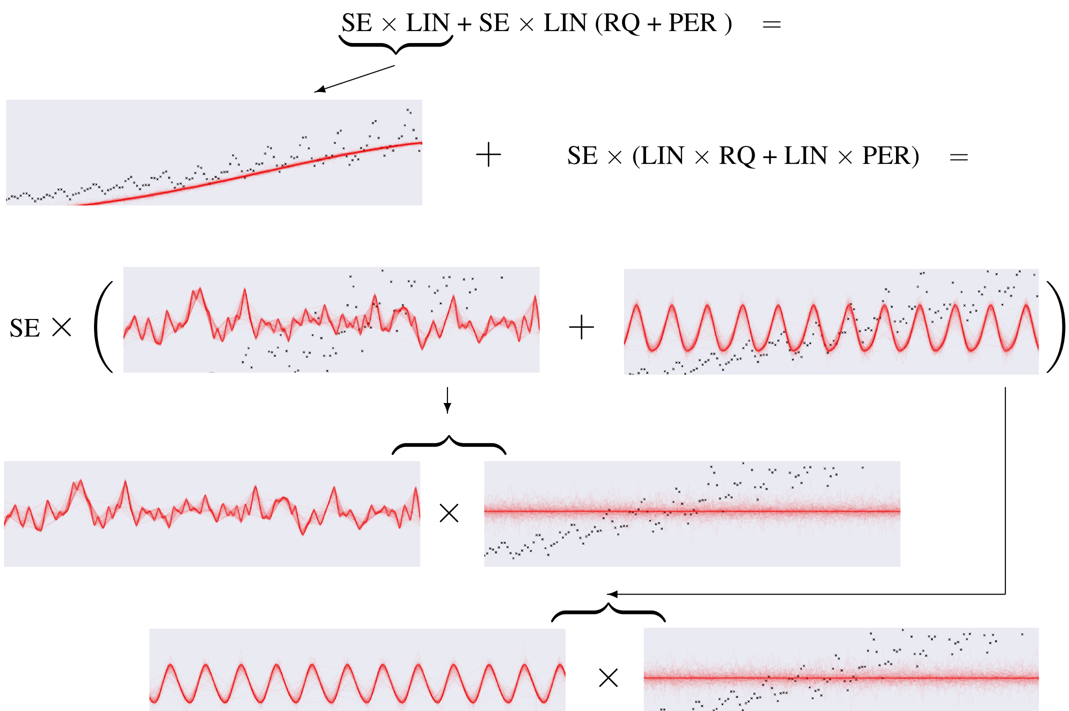
We further investigated the quality of our stochastic processes by running a leave one out cross-validation to gain confidence on the posterior. This resulted in 545 independent runs of the Markov chain that produced a coherent posterior: our Bayesian interpretation of GP structure and GPs produced a posterior of structures that is in line with previous results on this data set (Duvenaud et al., 2013; see Fig. 5).

We ran similar evaluation on the airline data set () resulting in a similar structure to what was previously reporte (Fig. 6, residuals and log-score along the Markov chain see Fig. 7).

We found the final sample of multiple runs to be most informative. This kind of Markov Chain seems to produce samples that are highly auto-correlated.



(a) The predictive posterior using the full grammar structure.



(b) Compositional Structure

Figure 4: a) We see the predictive posterior as a result 1000 nested MH steps on the airline data set. b) depicts a decomposition of this posterior for the structures sampled by Venture. RQ is the rational quadratic covariance function. The first line shows the global trend and denotes the rest of the structure that is shown above. In the second line, the see the periodic component on the right hand side. The left hand side denotes short term deviations both multiplied by a smoothing kernel. The third and fourth lines denote how we reach the second line: both periodic and rational quadratic covariance functions are multiplied by a linear covariance function with slope zero.

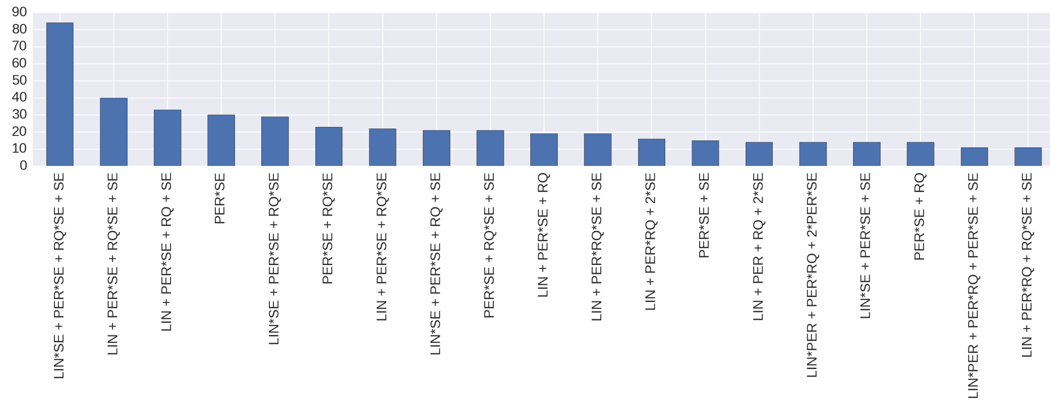


Figure 5: Posterior on structure of the CO_2 data. We have cut the tail of the distribution for space reasons since the number of possible structures is large. We see the final sample of the each of the 545 chains with 2000 nested steps each. Note that Duvenaud et al. (2013) report LIN $\times$ SE + PER $\times$ SE + RQ $\times$ SE.

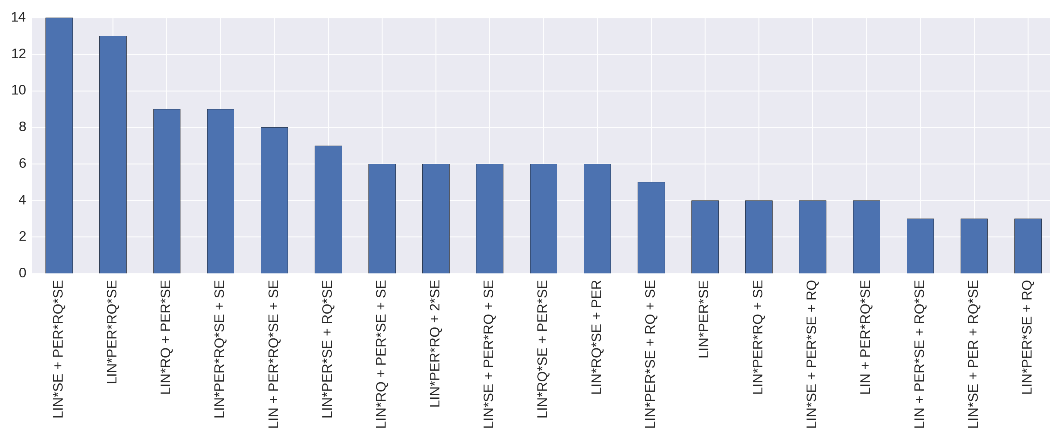
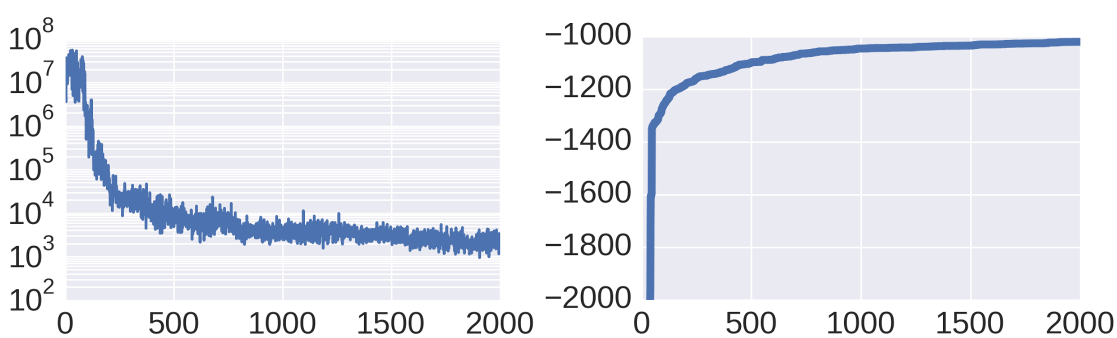


Figure 6: Posterior on structure of airline data set. We have cut the tail of the distribution for space reasons since the number of possible structures is large. We see the final sample of the each of the 144 chains with 2000 nested steps each. Note that Duvenaud et al. (2013) report LIN $\times$ SE + (PER + RQ) $\times$ SE $\times$ LIN



(a) Residuals

(b) Log Likelihood

Figure 7: 2000 steps along the Markov Chain.

4 Bayesian Optimization

Bayesian optimization casts the problem of finding the global maximum of an unknown function as a hierarchical decision problem (Ghahramani, 2015). Evaluating the actual function may be very expensive, either in computation time or in some other resource. For one example, when searching for the best configuration for the learning algorithm of a large convolutional neural network, a large amount of computational work is required to evaluate a candidate configuration, and the space of possible configurations is high-dimensional. Another common example, alluded to in Section 3.1.3, is data acquisition: for machine learning problems in which a large body of data is available, it is often desirable to choose the right queries to produce a data set on which learning will be most effective. In continuous settings, many Bayesian optimization methods employ GPs (e.g. Snoek et al., 2012).

We have implemented a version of Thompson sampling using GPs in Venture. Thompson sampling Thompson (1933) is a widely-used Bayesian framework for solving exploration-exploitation problems. Our implementation has two notable features: (i) the ability to search over a broader space of contexts than the parametric families that are typically used, and (ii) the parsimony of the resulting probabilistic program.

4.1 Thompson sampling framework

We now lay out the setup of Thompson sampling for Markov decision processes (MDPs). An agent is to take a sequence of actions $a_1, a_2, \ldots$ from a (possibly infinite) set of possible actions $\mathcal{A}$. After each action, a reward $r \in \mathbb{R}$ is received, according to an unknown conditional distribution $P_{\text{true}}(r|a)$. The agent's goal is to maximize the total reward received for all actions. In Thompson sampling, the Bayesian agent accomplishes this by placing a prior distribution $P(\theta)$ on the possible "contexts" $\theta \in \Theta$. Here a context is a believed model of the conditional distributions $\{P(r|a)\}_{a\in\mathcal{A}}$, or at least, a believed statistic of these conditional distributions which is sufficient for deciding an action a. One example of such a sufficient statistic is the conditional mean $V(a|\theta) = \mathbb{E}\left[r|a,\theta\right]$, which can be thought of as a value function. Thompson sampling thus has the following steps, repeated as long as desired:

1. Sample a context $\theta \sim P(\theta)$.

2. Choose an action $a \in \mathcal{A}$ which (approximately) maximizes $V(a|\theta) = \mathbb{E}\left[r|a,\theta\right]$.

3. Let r_{true} be the reward received for action a. Update the believed distribution on θ, i.e., $P(\theta) \leftarrow P_{\text{new}}(\theta)$ where $P_{\text{new}}(\theta) = P\left(\theta \mid a \mapsto r_{\text{true}}\right)$.

Note that when $\mathbb{E}\left[r|a,\theta\right]$ (under the sampled value of θ for some points a) is far from the true value $\mathbb{E}_{P_{\text{true}}}\left[r|a\right]$, the chosen action a may be far from optimal, but the information gained by probing action a will improve the belief θ. This amounts to "exploration." When $\mathbb{E}\left[r|a,\theta\right]$ is close to the true value except at points a for which $\mathbb{E}\left[r|a,\theta\right]$ is low, exploration will be less likely to occur, but the chosen actions a will tend to receive high rewards. This amounts to "exploitation." Roughly speaking, exploration will happen until the context θ is reasonably sure that the unexplored actions are probably not optimal, at which time the sampler will exploit by choosing actions in regions it knows to have high value.

Typically, when Thompson sampling is implemented, the search over contexts $\theta \in \Theta$ is limited by the choice of representation. In traditional programming environments, θ often consists of a few numerical parameters for a family of distributions of a fixed functional form. With work, a mixture of a few functional forms is possible; but without probabilistic programming machinery, implementing a rich context space Θ would be an unworkably large technical burden. In a probabilstic programing language, however, the representation of heterogeneously structured or infinite-dimensional context spaces is quite natural. Any computable model of the conditional distributions $\{P(r|a)\}_{a\in\mathcal{A}}$ can be represented as a stochastic procedure $(\lambda(a)\ldots)$. Thus, for computational Thompson sampling, the most general context space $\widehat{\Theta}$ is the space of program texts. Any other context space Θ has a natural embedding as a subset of $\widehat{\Theta}$.

4.2 Thompson sampling in Venture

Because Venture supports sampling and inference on (stochastic-)procedure-valued random variables (and the generative models which produce those procedures), Venture can capture arbitrary context spaces as described above. To demonstrate, we have implemented Thompson sampling in Venture in which the contexts θ are Gaussian processes over the action space $\mathcal{A} = \mathbb{R}$. That is, $\theta = (\mu, K)$, where the mean μ is a computable function $\mathcal{A} \to \mathbb{R}$ and the covariance K is a computable (symmetric, positive-semidefinite) function $\mathcal{A} \times \mathcal{A} \to \mathbb{R}$. This represents a Gaussian process $\{R_a\}_{a \in \mathcal{A}}$, where R_a represents the reward for action a. Computationally, we represent a context not as a pair of infinite lookup tables for μ and K, but as a finite data structure $\theta = (K_{\text{prior}}, \sigma, \ell, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}})$, where

- $K_{\text{prior}} = K_{\text{prior},\sigma,\ell}$ is a procedure, with parameters σ, ℓ, to be used as the prior covariance function: $K_{\text{prior}}(a, a') = \sigma^2 \exp\left(-\frac{(a-a')^2}{2\ell^2}\right)$
- σ and ℓ are (hyper)parameters for K_{prior}
- $\mathbf{a}_{\text{past}} = (a_i)_{i=1}^n$ are the previously probed actions
- $\mathbf{r}_{\text{past}} = (r_i)_{i=1}^n$ are the corresponding rewards

To simplify the treatment, we take prior mean $\mu_{\text{prior}} \equiv 0$. The mean and covariance for θ are then gotten by the usual conditioning formula:

$$\begin{aligned}
\mu(\mathbf{a}) &= \mu\left(\mathbf{a} \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}\right) \\
&= K_{\text{prior}}(\mathbf{a}, \mathbf{a}_{\text{past}})\, K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}})^{-1}\, \mathbf{r}_{\text{past}} \\
K(\mathbf{a}, \mathbf{a}) &= K\left(\mathbf{a}, \mathbf{a} \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}\right) \\
&= K_{\text{prior}}(\mathbf{a}, \mathbf{a}) - K_{\text{prior}}(\mathbf{a}, \mathbf{a}_{\text{past}})\, K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}})^{-1}\, K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}).
\end{aligned}$$

Note that even in this simple example, the context space Θ is not a finite-dimensional parametric family, since the vectors $\mathbf{a}_{\text{past}}$ and $\mathbf{r}_{\text{past}}$ grow as more samples are taken. Θ is, however, quite easily representable as a computational procedure together with parameters and past samples, as we do in the representation $\theta = (K_{\text{prior}}, \sigma, \ell, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}})$.

4.3 Implementation with `gpmem`

As a demonstration, we use Thompson sampling to optimize an unknown function $V(x)$ (the value function) using `gpmem`. (**TODO** we should not assume V is deterministic, it would be easy enough to make it random or have it give noisy samples.) We assume V is made available to Venture as a black-box. The code for optimizing V is given in Listing 6. For step 3 of Thompson sampling, the Bayesian update, we not only condition on the new data (the chosen action a and the received reward r), but also perform inference on the hyperparameters σ, ℓ using a Metropolis–Hastings sampler. These two inference steps take 1 line of code: 0 lines to condition on the new data (as this is done automatically by `gpmem`), and 1 line to call Venture's built-in `MH` operator. The results are shown in Figure 8. We can see from the figure that, roughly speaking, each successive probe point a is chosen either because the current model V_{emu} thinks it will have a high reward, or because the value of $V_{\text{emu}}(a)$ has high uncertainty. In the latter case, probing at a decreases this uncertainty and, due to the smoothing kernel, also decreases the uncertainty at points near a. We thus see that our Thompson sampler simultaneously learns the value function and optimizes it.

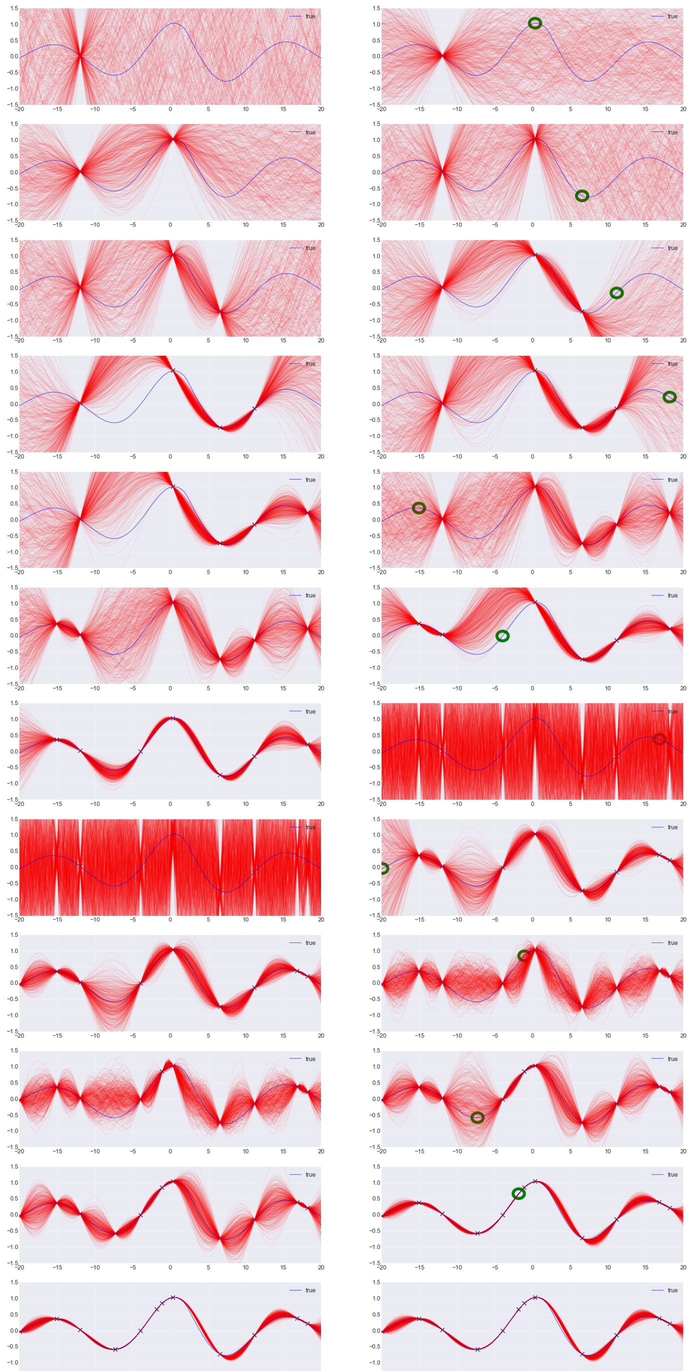


Figure 8: Dynamics of Thompson sampling in Venture. The blue curve is the true function V, and the red region is a blending of 100 samples of the curve generated (jointly) by a GP-based emulator V_{emu}. The left and right columns show the state of V_{emu} before and after hyperparameter inference is run on the new data, respectively. (We can see, for example, that after the seventh probe point, the Metropolis–Hastings sampler chose a "crazy" set of hyperparameters, which was corrected at the next inference step.) In the right column, the next chosen probe point is circled in green. Each successive probe point a is the (stochastic) maximum of V_{emu}, sampled pointwise and conditioned on the values of the previously probed points. Note that probes tend to happen at points either where the value of V_{emu} is high, or where V_{emu} has high uncertainty.

```
[ASSUME sigma (sigma-prior)]
[ASSUME l (l-prior)]
[ASSUME K (make-squared-exponential sigma l)]
[ASSUME (list V_compute V_emu) (gpmem V K)]
[ASSUME V_emu_pointwise (lambda (a) (first (V_emu (array a))))]
[ASSUME mc_sampler (uniform_sampler -20 20)]

for i=1 to 15:
  [PREDICT (V_compute (mc_argmax V_emu_pointwise mc_sampler))]
  [INFER (MH 'hypers one 50)

[INFER (extract_stats V_emu)]
```

Listing 6: Code for Bayesian optimization using `gpmem`. In the loop, `V_compute` is called to probe the value of `V` at a new argument. The new argument, `(mc_argmax V_emu_pointwise mc_sampler)`, is a Monte Carlo estimate of the maximum pointwise sample of `V_emu` (itself a stochastic quantity), with the Monte Carlo samples being drawn in this case uniformly between -20 and 20. After each new call to `V_compute`, the Metropolis–Hastings algorithm is used to perform inference on the hyperparameters of the covariance function in the GP model in light of the new conditioning data. Once enough calls to `V_compute` have been made (in our case we stopped at 15 calls), we can inspect the full list of probed (a, r) pairs with `extract_stats`. The answer to our maximization problem is simply the pair having the highest r; but our algorithm also learns more potentially useful information.

5 Conclusion

We have shown Venture GPs. We have introduced novel stochastic processes for a probabilistic programming language. We showed how flexible non-parametric models can be treated in Venture in only a few lines of code. We evaluated our contribution on a range of hard problems for state-of-the-art Bayesian non-parametrics. Venture GPs showed competitive performance in all of them.

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