Nonparametric Bayesian Methods in Robotics

PROEFSCHRIFT

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INTRODUCTION

Contents   The thesis addresses nonparametric Bayesian methods in robotic vision. Nonparametric Bayesian models simultaneously employed to perform inference over the number of entities observed and over the shape or nature of these entities. This chapter introduces nonparametric Bayesian models, the research methodology based on the Bayesian methodology, the main contribution towards robotic vision, and the general organization of this thesis.

Outline   The scope of thesis is to apply nonparametric Bayesian methods to robotic vision (Sect. 1.1). Bayesian nonparametric models define entities together with noise in such a way that inference can be performed in an optimal manner (Sect. 1.2). Particular problems in robotic vision that can benefit from Bayesian nonparametric methods are detailed (Sect. 1.3). The research methodology is introduced (Sect. 1.4). Our main contribution is to introduce nonparametric Bayesian models in robotic vision (Sect. 1.5). At the end of this chapter the organization of this thesis is given (Sect. 1.6).

1.1   Scope of the Thesis

In this thesis, modern Bayesian nonparametric methods are used to answer outstanding questions within computer vision and robotics. Is there a Bayesian form of line detection rather than applying the traditional Hough transform? Which of the nonparametric Bayesian priors can be used to detect multiple features simultaneously? What are efficient inference methods for these priors?

The scope of this thesis is the transfer of knowledge on Bayesian nonparametrics to well-described application domains. It will not establish a new body of work around a new family of stochastic processes. The detailed application of complex models towards robotic vision is expected to help and encourage people in entirely different application domains, such as

collaborative filtering, search engine optimization, and audio processing. All these different applications do not always need dedicated algorithms, but do deserve and can exploit the same optimal general inference techniques from Bayesian nonparametrics.

1.2   Bayesian Nonparametrics

In robotic vision (computer vision and depth perception) traditionally custom-made algorithms have been developed for a given task at hand. There are specific methods to detect corners (e.g. Harris and Stephens, 1988; Shi and Tomasi, 1994; Förstner and Gülch, 1987), to detect edges (e.g. Canny, 1986; Sobel, 1970), to detect features (e.g. Hough, 1962), and to describe features (e.g. Lowe, 1999; Bay et al., 2006; Dalal and Triggs, 2005).

On the one hand, it is desirable that such sophisticated methods are generalized to other application domains. On the other hand, it is important to take particular information about an application domain into account. The methods described in the previous paragraph are limited to their specific task. An example of limited generalizability can be found in the Hough transform. The Hough transform can be used to detect lines, but the way inference is performed in the algorithm does limit its application to basic forms of object detection. An example of limited specificity can be found in linear regression. Linear regression does not take into account real-world statistics.

Both generalization and specificity are formalized by a Bayesian model. A Bayesian model is general because it can be solved with general inference methods. One of such general inference methods is a Markov-Chain Monte Carlo method. It does not know anything about real-world statistics. A Bayesian model is also specific in that it can incorporate application-specific know-how by the definition of priors.

Typical problems in robotic vision will be about the recognition of several objects, multiple shapes, or objects that have multiple parts. Models that represent such objects do not have knowledge about the number of such objects, shapes, or parts. To incorporate application-specific know-how on the number of objects it is possible to define a prior that assigns a probability to this quantity. The number of objects can even be potentially infinite. The Bayesian models that define a prior on the number of objects, shapes, or parts are called nonparametric Bayesian models. This means that in contrast with conventional methods like k-means clustering (Forgy, 1965; **?**) the number of objects do not have to be predefined.

1.3   Problem Statement and Research Questions

Many methods in robotics - and in particular in robotic vision - have been developed in times where computational resources were limited. Then, highly optimized algorithms have been developed, leveraging pecularities of the application domain. Recent advances in Bayesian methods, both with respect to concept development, as well as computational efficient solution strategies, now open up new ways to solve old problems. Extending only the old

methods themselves would lead to ad-hoc solution strategies that will miss benefits from potential optimal and more widely applicable algorithms.

This observation leads us to the formulation of our problem statement (PS).

> **PS:** *How can robotic problems effectively be generalized and their structure exploited in a wider Bayesian framework?*

This problem statement is divided into three research questions (RQs).

> **RQ 1** How can we estimate the number of objects simultaneously with the fitting of these objects?

> **RQ 2** How can we estimate the number of lines simultaneously with line fitting in computer vision?

> **RQ 3** How can we estimate the number of user types simultaneously with user fitting in recommendation systems?

1.4 Research Methodology

The research methodology advocated in this thesis follows (Savage, 1972; Jaynes, 2003) the Bayesian methodology. Given (1) a definition of a model, (2) a definition of the noise, (3) the data, the Bayesian methodology dictates all remaining unknowns, from the number of parameters to the values of the parameters.

The Bayesian methodology aims to establish the rationale for practical questions. The following four questions are clear examples. If a person did never exercise before, at what time should we recommend her to exercise? If a person did only run once, at what time should we recommend her to exercise? If we observe a single point in an image, can we expect it to be part of a line? If we have two lines and we live in a world with squares, what are we able to infer?

The four questions tap into our capabilities to define models that makes our prior knowledge explicit. Moreover, if we are able to quickly assign people to groups, points to lines, objects to categories, we can enrich it with all corresponding group properties without the need to have them observed for this individual.

In robotic vision, for example for the task of line detection, the Hough transform (Hough, 1962) or RANSAC method (Bolles and Fischler, 1981) , does detect lines, but does not explicitly take noise into account. By introducing Bayesian methodology the inference method becomes optimal in an information-theoretic sense. Also frequentists agree that nonparametric Bayesian models are consistent in the sense that they approach the underlying true distribution (Wasserman, 1998). There is no need to search for another method to infer lines in a line detection task. If someone would find a method that outperforms a Bayesian

method it is either (1) because the signal or noise has not been correctly modeled after all or (2) because the method overfits with respect to the data at hand. If approximations are used with respect to optimal Bayesian inference, either variational approximations or Markov-Chain Monte Carlo, there are theoretical guarantuees on convergence.

A well known problem with nonparametric Bayesian models is the curse of dimensionality. Compared to maximum likelihood methods or other non-probabilistic methods that do not take noise into account at all, the nonparametric Bayesian models require significant computational resources. Our research methodology first establishes the correct models, even if solving them seems computationally infeasible. Our approach is to develop subsequently approximations using more sophisticated samplers, so that the theoretical guarantuees on convergence are preserved.

Due to the fact that the models are optimal by construction, this does not require experiments to address the optimality in particular. However, experiments are still required to establish if the models make sense. The methodology does have limitations. We will not search over different noise models and limit priors to a particular hierarchical level.

1.5 Main Contribution

The main contribution of this thesis is a fundamental approach to inference in robotic vision and depth perception. This contribution can be subdivided into three parts.

The first part addresses the problem of contemporary methods in robotic vision not allowing for astute statements about their performance. In practice, this means that when using computer vision to detect cells under a microscope, someone cannot be confident about the number of detected cells. A self-driving car cannot be confident about the shape of other cars or bikes on the road. An autonomous cleaning robot in a supermarket cannot be confident about the isle it is driving into. To be able to properly take into account models and uncertainty simultaneously, Bayesian models have found mainstream adoption. State-of-the-art Bayesian methods that reason about the number of objects alongside object models are a recent object of study. This thesis applies such nonparametric Bayesian models towards the applications of robotic vision and depth perception. An Infinite Line Model and an Infinite Line Segment Model are introduced.

The second part addresses the problem of high-dimensional data, typified by the applications at hand. To efficiently sample more complex geometric structures, new MCMC (Markov-Chain Monte Carlo, Sect. 2.3.4) methods are required. This thesis also introduces the Infinite Box Model and applies the new MCMC methods to this challenging application.

The third part addresses the generality of the new MCMC sampler for nonparametric Bayesian methods by applying it to a different field, namely that of recommender engines. An exercise recommendation engine groups people on their exercise schedules to subsequently be able to hand out recommendations depending on the time of day.

1.6 Organization of the Thesis

Chapter 1 (this chapter) introduces the problem of contemporary methods in computer vision and depth perception. Due to the fact that these methods are not optimal by construction, it is hard to articulate how they perform. The need for a Bayesian methodology is sketched briefly.

Chapter 2 describes (1) probability theory using measure theory, (2) random measures known as random processes of which five are described as nonparametric Bayesian models, and (3) six inference methods that infer model parameters of such nonparametric Bayesian models given the data. It is followed by a dicussion that indicates which parts will be most useful for chapters 3 and 4.

Chapter 3 introduces a first nonparametric Bayesian model, the infinite line model. The infinite line model represents a countably infinite set of lines. Gibbs sampling is used to perform simultaneous inference over the number of lines and line parameter values such as slope and intercept.

Chapter 4 introduces a second nonparametric Bayesian model, the infinite line segment model. The infinite line segment model represents a countably infinite set of line segments. A split-merge MCMC sampling method is used to perform simultaneous inference over the number of line segments and line segment parameter values such as slope, intercept, and segment size.

Chapter 5 introduces a new MCMC method that accelerates inference of the models in chapter **??** by making use of hierarchical sampling.

Chapter ?? introduces a third nonparametric Bayesian model, the infinite box model for volumetric inference. The infinite box model represents a countably infinite set of 3D boxes. An MCMC method is used to perform simultaneous inference over the number of boxes and the box parameter values such as center, orientation, and size.

Chapter 7 applies the hierarchical sampling method to the domain of recommender engines. It estimates simultaneously the number of user types with a fitting procedure for the invididual user.

Chapter 8 discusses the relevance of the developed models and inference methods. Finally, conclusions are formulated.

RELATED WORK

Contents   In robotics depth sensors generate point clouds. The tasks of robotic object recognition, positioning, and navigation require models that represent such point clouds. It is unclear if the current methods to perform inference over point clouds are appropriate for these tasks. The current models do not model uncertainty explicitly. This chapter presents models that can be used for point cloud modeling and that represent uncertainty. This (partially) answers research question RQ1. This chapter concludes with recommendations for the development of point cloud inference models. These are implemented in a new model for line inference in Chapter 3 and line segment inference in Chapter 4.

Outline   Probability theory has a theoretical basis in measure theory. It is based on the notion of random measures and defines uncertainty rigorously (Sect. 2.1). Random processes are random measures that model uncertainty (Sect. 2.2). Inference in models represented by random processes is done by sampling (Sect. 2.3). Inference about point clouds in the next chapters will use adaptations of the described models and inference methods for which some recommendations are given (Sect. 2.4).

2.1 Probability Theory

Modern probability is based on measure theory (Sect. 2.1.1). Measure theory will provide the means to formally describe random variables, random processes, and most generally, random measures. A model represented by random measures can be fitted with data using Bayesian inference (Sect 2.1.2).

2.1.1 Measure Theory

A random variable is a *function* that assigns values to a *set* of possible outcomes. The formal definition requires concepts such as "measurable function" and "probability space" from *measure theory* (Feller, 1950). Measure theory is used to generalize the notion of a random variable to that of a "random process".

Informally, a measure generalizes the notion of size of Euclidean objects to sets and subsets. To definition of a measure is based on the definition of a σ-algebra. A σ-algebra ascribes a value to a sum of individual disjoint sets, even if they are infinite in number.

Definition 2.1. A σ-**algebra** is a *subset* $\Sigma \in 2^X$, with X a set and 2^X its powerset, with three requirements:

- Σ is non-empty: at least one $A \in X$ is in Σ

- Σ is closed under complementation: if A in Σ, so is its complement A^c

- Σ is closed under countable unions: if $A_1, A_2, \ldots$ in Σ, so is $A = A_1 \cup A_2 \cup \ldots$

The members of Σ are called *measurable sets*. Let $X = \{1, 2, 3, 4\}$ and let us define a σ-algebra $\Sigma = \{\varnothing, \{1\}, \{4\}, \{2, 3\}, \{1, 4\}, \{1, 2, 3\}, \{2, 3, 4\}, \{1, 2, 3, 4\}\}$. Here $\varnothing$ denotes the empty set. The complement of A is defined with respect to X. $A \cup A^c = X$ or $A^c = X\,A$. An example of closure under complementation: let $A_1 = \{1\}$, then $A_1^c = \{2, 3, 4\}$ and $A_1^c \in \Sigma$. An example of closure under countable unions: let $A_1 = \{1\}$ and $A_2 = \{2, 3\}$, then $A_1 \cup A_2 = \{1, 2, 3\}$ and $A_1 \cup A_2 \in \Sigma$.

Definition 2.2. A **generated** σ-**algebra**, with X a set and $B \in 2^X$, is the smallest σ-algebra $\sigma(B)$ that contains all sets of B.

Let $X = \{1, 2, 3, 4\}$ and $B = \{\{1\}, \{2, 3\}\}$, then $\sigma(B) = \{\varnothing, \{1\}, \{2, 3\}, \{1, 4\}, \{2, 3, 4\}, \{1, 2, 3, 4\}\}$. The sets in $\sigma(B)$ that are not in B follow from the requirements of a σ algebra of closure under complementation and countable unions.

The notion of a σ-algebra (Fremlin, 2000) is necessary to prevent the so-called Banach-Tarski paradox (Banach and Tarski, 1924). This paradox describes how a unit-ball in $\mathbf{R}^3$ can be reassembled into two unit-balls, violating the intuitive notion of preservation of volume. If the measure μ of the union of two disjoint sets is equal to the sum of the measures of the two sets, this is called *finite additivity*: $\mu(\bigcup_{i=1}^{N} A_i) = \sum_{i=1}^{N} \mu(A_i)$. In probability theory σ-*additivity* extends this to infinite disjoint sets: $\mu(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \mu(A_i)$. Measure theory solves the Banach-Tarski paradox by only assigning a measure to subsets that are measurable sets (Tao, 2011).

A *measure* assigns values to subsets of Σ.

Definition 2.3. A **measure** μ is a function from Σ to $[-\infty, +\infty]$, with three requirements:

○ μ is non-negative: $\mu(A) \geq 0$ for $\forall A \in \Sigma$

○ μ has a null empty set: $\mu(\emptyset) = 0$

○ μ is σ-additive: $\mu(\bigcup_{i \in I_\Sigma} A_i) = \sum_{i \in I_\Sigma} \mu(A_i)$ for A_i disjoint

The first statement defines that a measure μ only assigns non-negative values to sets in Σ. The second statement equals the measure of the empty set $\emptyset$ to 0. The third statement defines that σ-additivity is required. For any two sets in Σ the measure of the union of the sets equals the sum of the measures of the individual sets. Here I_Σ defines an index over sets in Σ.

Informally, a measure relates the concepts of *sets* and *subsets* to notions of size. A measure can be seen as a *monotonically* increasing function. Let the set A in X be the interval $[0,1)$, an uncountable (infinite) set of real numbers. Define the σ-algebra $\{\emptyset, A\}$. The empty set has measure 0, the set A has measure 1. Let us define the σ-algebra $\{\emptyset, A_{0,0.5}, A_{0.5,1}, A\}$. The set $A_{0,0.5}$ corresponds to the interval $[0, 0.5)$ and $A_{0.5,1}$ to $[0.5, 1)$. Both sets are assigned measure 0.5 and their union has measure 1. This examples shows that with σ-additive unions measures can be assigned to sets that are uncountable.

A *measurable space* (X, Σ) is defined as a pair.

Definition 2.4. A **measurable space** (X, Σ) is a pair with:

○ X a set

○ Σ a σ-algebra over X.

A *measure space* (X, Σ, μ) is defined as a triple.

Definition 2.5. A **measure space** (X, Σ, μ) is a triple with:

○ X a set

○ Σ a σ-algebra over X.

○ μ a measure from Σ to $[-\infty, \infty]$.

A finite measure μ assigns a finite real number to all A.

Definition 2.6. A **finite measure** μ is a measure from Σ to $[0, \infty)$:

○ μ is non-negative: $\mu(A) \geq 0$ for $\forall A \in \Sigma$

○ μ has a null empty set: $\mu(\emptyset) = 0$

○ μ is σ-additive: $\mu(\bigcup_{i \in I_\Sigma} A_i) = \sum_{i \in I_\Sigma} \mu(A_i)$ for A_i disjoint

○ μ for the whole sample space, X, is finite: $\mu(X) = N$

A σ-finite measure allows A to be a countable union of sets with finite measure.

Definition 2.7. A σ-**finite measure** μ is a finite measure with:

- X is a countable union of sets with finite measures

We will now define three measures: the *probability measure,* the *counting measure*, and the *Lebesgue measure*.

A *probability measure*, $\mathbb{P}$, is a finite measure which satisfies the following requirements:

Definition 2.8. A **probability measure** $\mathbb{P}$ is a measure μ with:

- $\mathbb{P}$ is non-negative: $\mathbb{P}(A) \geq 0$ for $\forall A \in \Sigma$

- $\mathbb{P}$ has a null empty set: $\mathbb{P}(\varnothing) = 0$

- $\mathbb{P}$ is σ-additive: $\mathbb{P}(\bigcup_{i \in I_\Sigma} A_i) = \sum_{i \in I_\Sigma} \mu(A_i)$ for A_i disjoint

- $\mathbb{P}$ for the whole sample space, X, is unity: $\mathbb{P}(X) = 1$

These requirements are called the Kolmogorov axioms (Kolomogoroff, 1933). The probability measure is a measure and therefore obeys the same three requirements of a non-negative measure for each set, the existence of a null empty set, and σ-additivity. A fourth requirement restricts the measure for the whole space X to 1.

In Fig. 2.1 the probability measure is visualized as a mapping from the probability space to the unit interval $[0, 1]$.
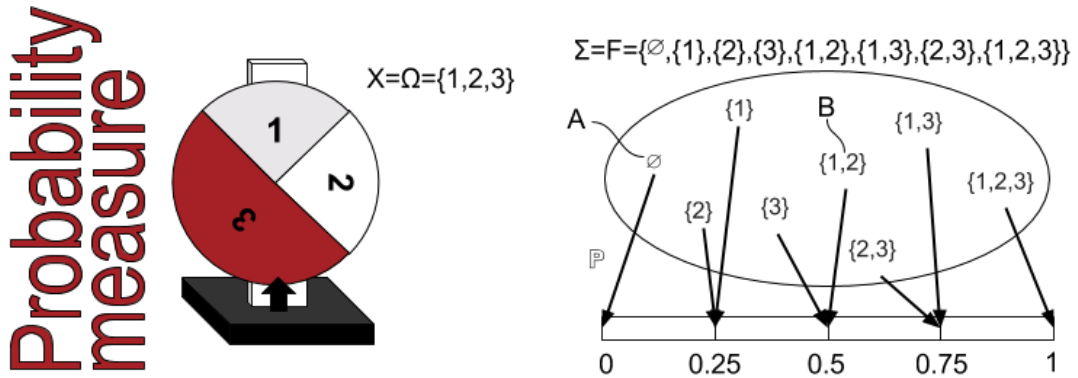
Figure 2.1: A probability measure $\mathbb{P}$ mapping the probability space for 3 events to the unit interval. Left: a turning wheel representing three possible outcomes of which the third is twice as likely as the other two outcomes. Right: a probability measure $\mathbb{P}$ assigned to each outcome. The empty set, $A = \varnothing$, has probability measure 0. The set of encountering either 1 or 2, $B = \{1, 2\}$, has probability measure 0.5. Adapted from Wikipedia.

A *probability space* $(X, \Sigma, \mathbb{P})$ is a measure space (X, Σ, μ) with the probability measure $\mathbb{P}$ as its measure μ.

Definition 2.9. A **probability space** $(X, \Sigma, \mathbb{P})$ is a triple with:

- X a set

- Σ a σ-algebra over X.

- $\mathbb{P}$ a probability measure from Σ to $[0, 1]$.

The triple for the probability space $(X, \Sigma, \mathbb{P})$ is also written as $(\Omega, \mathbb{F}, \mathbb{P})$. The space X is the event space Ω, the set of *elementary outcomes*. The σ-algebra over subsets of Ω is denoted by $\mathbb{F}$. The probability measure $\mathbb{P}$ assigns a value on the unit interval $[0, 1]$ to every event in $\mathbb{F}$.

The *counting measure* forms the basis for the definition of discrete probabilities (Schilling, 2005).

Definition 2.10. A **counting measure** ν on a space X is a measure μ with:

- ν is non-negative and integer-valued for $\forall A \in \Sigma$

- $\nu < \infty$ for $\forall A \in \Sigma$ if A bounded (of finite size)

- $\nu = \infty$ if $\exists A \in \Sigma$ with A unbounded (infinite)

A counting measure is a measure that is integer-valued. Every set A has a measure that is a positive integer or zero. If and only if the set A is unbounded is its counting measure infinite.

The *Borel σ-algebra* defines a σ-algebra for the real line $\mathbb{R}$.

Definition 2.11. A **Borel σ-algebra** $\mathbb{B}_\sigma$ on $\mathbb{R}$ is the smallest σ-algebra that contains all open subsets of $\mathbb{R}$:

- $\mathbb{B} = \Sigma(U)$ with $U = U \subseteq \mathbb{R}$: U is open

The Borel σ-algebra contains all open subsets of $\mathbb{R}$. The property of closure under complementation of a σ-algebra means that it also contains the closed subsets of $\mathbb{R}$. If $A = (0, 1)$, then $A^c = \{[-\infty, 0], [1, \infty]\}$.

A *Borel measure* assigns values to subsets of $\mathbb{B}_\sigma$.

Definition 2.12. A **Borel measure** μ is a function from $\Sigma = \mathbb{B}_\sigma$ to $[-\infty, +\infty]$, with the three measure requirements:

- μ is non-negative: $\mu(A) \geq 0$ for $\forall A \in \Sigma$

- μ has a null empty set: $\mu(\varnothing) = 0$

- μ is σ-additive: $\mu(\bigcup_{i \in I_\Sigma} A_i) = \sum_{i \in I_\Sigma} \mu(A_i)$ for A_i disjoint

The *Borel space* is a measureable space with a Borel σ-algebra rather than a general σ-algebra.

Definition 2.13. A **Borel space** $(X, \mathbb{B}_\sigma)$ is a pair with:

- X a set

- $\mathbb{B}_\sigma$ a Borel σ-algebra over X.

A *complete measure space* is a measure space in which every subset of every null set is measurable.

Definition 2.14. A **complete measure space** (X, Σ, μ):

- $S \subseteq N \in \Sigma$ and $\mu(N) = 0 \Rightarrow S \in \Sigma$

The Borel space is not a complete measure space. There are sets in the Borel σ-algebra that are of measure zero and that have subsets that are undefined.

The *Lebesgue measure* defines a size to subsets of $\mathbb{R}^n$ that completes the Borel measure (Lebesgue, 1902). It makes use of the notion of an *outer measure*.

Definition 2.15. An **outer measure** ϕ on a space $\mathbb{R}$ is a measure μ with:

- ϕ is non-negative and real-valued for $\forall A \in \Sigma$

- ϕ has a null empty set: $\phi(\emptyset) = 0$

- ϕ is σ-subadditive: $\phi(\bigcup_{i \in I_\Sigma} A_i) < \sum_{i \in I_\Sigma} \mu(A_i)$ for $\forall A_i$

- ϕ is monotone: $A \subseteq B$ implies $\phi(A) \leq \phi(B)$

- ϕ is translation-invariant: $\phi(A + x) = \phi(A)$ for $\forall A \in \Sigma$ and $\forall x \in \mathbb{R}$

An outer measure relaxes σ-additivity of disjoint sets of X to σ-subadditivity for any sequence of sets. Intuitively, the outer measure of a set is an upper bound on the size of a set.

Definition 2.16. A **Lebesgue outer measure** λ on a space $\mathbb{R}^n$ is an outer measure ϕ with:

- $\lambda(A) = \inf \left\{ \sum_{k=1}^\infty l(I_k) : (I_k)_{k \in \mathbb{N}} \text{ is a sequence of open intervals with } A \subseteq \bigcup_{k=1}^\infty I_k \right\}$

Here $A \subseteq \mathbb{R}$ is a subset of the real line. The Lebesgue outer measure λ is the infimum (greatest lower bound) of the sum of the lengths $l(I) = b - a$ of the intervals $I = [a, b]$.

The *Lebesgue measure* is defined through the Lebesgue outer measure.

Definition 2.17. A **Lebesgue measure** m on a space $\mathbb{R}^n$ is a Lebesgue outer measure λ with:

○ $m(B) = \lambda(B \cup A) + \lambda(B \cup A^c)$

A measurable function is defined between two measurable spaces.

Definition 2.18. A **measurable function** $f : X \rightarrow Y$ fulfills:

○ $f^{-1}(E) \in \Sigma$ for $\forall E \in T$

with both (X, Σ) and (Y, T) measurable spaces.

> A measurable function *preserves the structure* of the corresponding measurable spaces (captured through the σ-algebras).

A random variable is a measurable function between two measurable space, with as domain a measurable space that is a probability space.

Definition 2.19. A (X, Σ)-valued **random variable** X is a measurable function from probability space $(\Omega, \mathbb{F}, \mathbb{P})$ to measurable space (X, Σ).

A random variable is a (X, Σ)-valued random variable with the following choice for the codomain and σ-algebra:

Definition 2.20. A **random variable** X is a measurable function from probability space $(\Omega, \mathbb{F}, \mathbb{P})$ to the real line with the Borel σ-algebra $(\mathbb{R}, \mathbb{B}_{\mathbb{R}})$.

The codomain is the real line $\mathbb{R}$ and the Borel σ-algebra.

> Random variables can be generalized to complex random variables or random elements of any type. A *complex random variable* is a measurable function from Ω to $\mathbb{C}$. A *random elephant* is a measurable function from Ω to a suitable space of elephants (Kingman, 1993).

Definition 2.21. A **random measure** is a function $\xi : \Omega \times X \rightarrow [0, +\infty]$ from probability space $(\Omega, \mathbb{F}, \mathbb{P})$ to measurable space (X, Σ) such that $\xi(\cdot, X)$ is a random variable on $(\Omega, \mathbb{F}, \mathbb{P})$ and $\xi(\omega, \cdot)$ is a measure on Σ.

We have encountered a random variable, and a probability measure $\mathbb{P}$ on the original probability space. Now, one might wonder, are probabilities not logically assigned to elements on the measurable space that is the codomain of this random variable? Why does it map to a measurable space and not a measure space actually? This is because (through the σ-algebras of both spaces, or more precisely the random variable itself) the probability measure is *induced* on the target space. This is known as a *probability distribution*:

Definition 2.22. Given a random variable X from $(\Omega, \mathbb{F}, \mathbb{P})$ to $(\mathbb{R}, \mathbb{B}_{\sigma})$, the **probability distribution** μ is the induced probability measure: $\mu(B) = \mathbb{P}(X^{-1}(B))$ for all Borel sets $B \in \mathbb{B}_{\sigma}$.

The measurable *function X* is inverted: $X^{-1}(\cdot)$. The measure μ exists on $(\mathbb{R}, \mathbb{B}_\sigma)$ just as $\mathbb{P}$ exists on $(\Omega, \mathbb{F})$. The notation for the measure μ does not include the original probability space or σ-algebra. The complete notation for the probability distribution μ can be written as a function f of X:

$$f_X(x) = f_{X,(\Omega,\mathbb{F},\mathbb{P}),(\mathbb{R},\mathbb{B}_\sigma)}(x) \tag{2.1}$$

At the left X denotes the random variable, $x \in \Omega$ are the (elementary) outcomes on the sample space Ω. At the right the complete notation adds $\mathbb{F}, \mathbb{P}$ and $\mathbb{R}, \mathbb{B}_\sigma$. The shorthand notation at the left will be used to indicate the real line with a Borel σ-algebra as codomain.

A random variable X is *distributed as $f_X(x)$*, notation:

$$X \sim f_X(x) \tag{2.2}$$

A *random process* is an *ordered* set of random variables. The set can be a sequence of random variables in a time series. It can be a series of steps in the spatial domain, called a random field.

Definition 2.23. A **random process** X is a collection $\{X_t : t \in T\}$ with X_t an (S, Σ)-valued random variable on Ω and $(\Omega, \mathbb{F}, \mathbb{P})$ a probability space, (S, Σ) a measurable space, and T a totally *ordered* set.

A random process is a probability distribution with a domain that is a set of probability distributions. A random process is a distribution over distributions, a hierarchy over distribution.

2.1.2 Bayesian Inference

Let x be a (S, Σ_S, μ_S)-valued random variable[1], y a (T, Σ_T, μ_T)-valued random variable, then we can construct z, a (C, Σ_C, μ_C)-valued random variable with the latter being a subset of the product set of x and y: $C \in S \otimes T$.

Definition 2.24. A **product space** $(S \otimes T, \Sigma_{S \otimes T})$ and **product measure** $\mu_{S \otimes T}$ has σ-algebra $\Sigma_{S \otimes T} = \sigma(F \otimes G : F \in \Sigma_S, G \in \Sigma_T)$ and $\mu_{S \otimes T}(F \otimes G) = \mu_S(F) \otimes \mu_T(G)$ with (S, Σ_S, μ_S) and (T, Σ_T, μ_T) two σ-finite measure spaces.

The **joint probability distribution** P_C is a probability measure on the product σ-algebra Σ_C. As function of the random variables x and y the joint probability distribution is written as $_{X,Y}(x, y)$, $f(x, y)$, or $p(x, y)$.

A σ-algebra is *independent* in the following sense.

Definition 2.25. Let $(\Omega, \mathbb{F}, P)$ be a probability space and $\mathbb{A}$ and $\mathbb{B}$ be a sub-σ-algebras of $\mathbb{F}$. $\mathbb{A}$ and $\mathbb{B}$ are **independent σ-algebras** if:

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[1]The lowercase x is used instead of X in the context of probability distributions as in Eq. 2.1.

o $P(A \cap B) = P(A)P(B) \ \forall A \in \mathbb{A}$ and $B \in \mathbb{B}$

Two random variables x and y are independent if and only if the σ-algebras that they generate are independent.

Definition 2.26. Let $(\Omega, \mathbb{F}, P)$ be a probability space, $\mathbb{G} \subseteq \mathbb{F}$ a sub-σ-algebra of $\mathbb{F}$, and $X :$ $\Omega \to \mathbb{R}$ a real-valued random variable ($\mathbb{F}$-measurable with respect to the Borel σ-algebra $\mathbb{B}_\sigma$ on $\mathbb{R}$). There exists a function $\mu : \mathbb{B}_\sigma \times \Omega \to \mathbb{R}$ such that $\mu(\cdot, \omega)$ is a probability measure on $\mathbb{B}_\sigma$ for each $\omega \in \Omega$ and $\mu(H, \cdot) = P(X \in H | \mathbb{G})$ (almost surely) for every $H \in \mathbb{B}_\sigma$. For any $\omega \in \Omega$, the function $\mu(\cdot, \omega) : \mathbb{B}_\sigma \to \mathbb{R}$ is called a **conditional probability distribution** of X given $\mathbb{G}$.

Informally, a conditional probability is described with a sub-σ-algebra which only presents part of the structure of the full σ-algebra. As function of the random variables x and y the conditional probability distribution of y given x is written as $f_{Y|X}(y|x)$, $f(y|x)$, or $p(y|x)$.

The random variables x and θ define a Bayesian model with observations x and parameters θ.

Definition 2.27. A **Bayesian model** $f(x, \theta)$ defines a function between observations x and state or parameters θ with both x and θ random variables.

In a **supervised learning** task both θ and x are known. In an **unsupervised learning** task x is known, but θ is unknown. The random variable θ is called a hidden or latent variable. The random variable θ can be any random element: a random vector, a random matrix.

Let the observations x be a sequence $x_0, x_1, \ldots$, then the observations x_i can be distributed *independent and identically*:

Definition 2.28. A collection of random variables $x = \{x_0, x_1, \ldots\}$ is **independent and identically distributed (i.d.d.)** if:

o the probability distribution $p(x_i)$ is the same for $\forall x_i \in x$

o each x_i is independent with respect to x_j with $i \neq j$

The observations x_i can be distributed in an *exchangeable* sequence in which any order is equally likely:

Definition 2.29. A sequence of random variables $x = \{x_0, x_1, \ldots\}$ is **exchangeable** if for any finite permutation ρ of the indices $0, 1, \ldots$:

o the joint probability distribution of the permuted sequence $p(x_{\rho(0)}, x_{\rho(1)}, \ldots)$ equals that of the original sequence $p(x_0, x_1, \ldots)$

The joint probability distribution of i.d.d. observations given parameters can be written as a product:

$$p(x_0, \ldots, x_{k-1} | \theta) = \prod_{i=0}^{k-1} p(x_i | \theta) \tag{2.3}$$

Definition 2.30. The **likelihood function** is defined as:

$$\mathscr{L}(\theta | x) = p(x | \theta) \tag{2.4}$$

The likelihood of the parameters θ given observations x is the probability of these observations given the parameter values.

The likelihood function definition allows us to find an optimal set of parameter values given the observations. The probability $p(x|\theta)$ can be maximized (Aldrich and Others, 1997):

Definition 2.31. Maximum Likelihood is defined as:

$$\theta^* \in \underset{\theta}{\operatorname{argmax}} \prod_{i=0}^{k-1} p(x_i | \theta) \tag{2.5}$$

The Maximum Likelihood method finds the maximum of $\prod_{i=0}^{k-1} p(x|\theta)$ for all possible parameter values θ. The maximum in Maximum Likelihood does not need to be unique (Steel, 1994). The notation makes this explicit by writing θ^* as a member (denoted by the $\in$ symbol) of the outcomes of the argmax operation (and does not use the equal sign).

A function $f(\cdot)$ and the logarithm of a function $\log f(\cdot)$ have the same maxima. This is due to the fact that the logarithm is a monotonic function (a monotonically increasing function). The log of a product of logarithms is equal to the sum of the individual logarithms.

Definition 2.32. Maximum log-Likelihood is defined as:

$$\theta^* \in \underset{\theta}{\operatorname{argmax}} \sum_{i=0}^{k-1} \log p(x_i | \theta) \tag{2.6}$$

In the case we have information about the parameters θ we can model this with a probability distribution.

Definition 2.33. A **prior probability distribution** defines a probability distribution $p(\theta)$ to parameters θ without a dependency on the observations x.

Given the definition of a prior probability distribution, we can define *Maximum A Posteriori* estimation.

Definition 2.34. Maximum A Posteriori estimation:

$$\theta^* \in \underset{\theta}{\operatorname{argmax}} \sum_{i=0}^{k-1} \log p(x_i | \theta) + \log p(\theta) \tag{2.7}$$

If we are not only interested in the parameter θ^* that maximizes $p(x|\theta)$ and $p(\theta)$, but in the complete distribution for $p(\theta)$ we need Bayes' theorem described by Laplace (marquis de Laplace, 1820).

Definition 2.35. Bayesian inference uses Bayes' theorem:

$$f(\theta|x) = p(\theta|x) = \frac{\overbrace{p(x|\theta)}^{\text{likelihood}} \overbrace{p(\theta)}^{\text{prior}}}{\underbrace{p(x)}_{\text{normalization constant}}} = \frac{p(x|\theta)p(\theta)}{\int p(x|\theta)p(\theta)d\theta} \qquad (2.8)$$

Bayes' theorem describes the posterior probability $p(\theta|x)$ as the likelihood times the prior probability distribution divided by a normalization constant, also called the evidence. The normalization constant is not a function of the parameters θ. If a function is known except for the normalization constant this is indicates by the "proportional to" symbol $\propto$.

$$f(\theta|x) \propto p(x|\theta)p(\theta) \qquad (2.9)$$

In Bayesian inference $p(\theta|x)$ is calculated. In contrast, in Maximum Likelihood and Maximum A Posteriori only parts of Eq. 2.8 are calculated, respectively $p(x|\theta)$ and $p(x|\theta)p(\theta)$. In Section 2.3 inference methods will be described that approximate Bayesian inference. Approximation is required in the case closed-form expressions are not available. If the inference task only requires Maximum A Posteriori, approximation methods are also available (Daume, 2007), but this is outside of the scope of the current thesis.

There are two supervised learning models, a generative model and a distriminative model.

Definition 2.36. A **generative** model defines the joint probability distribution $p(x, \theta)$ and uses Bayes rule to define $p(x|\theta)$.

Definition 2.37. A **discriminative** model defines the conditional probability distribution $p(x|\theta)$ directly.
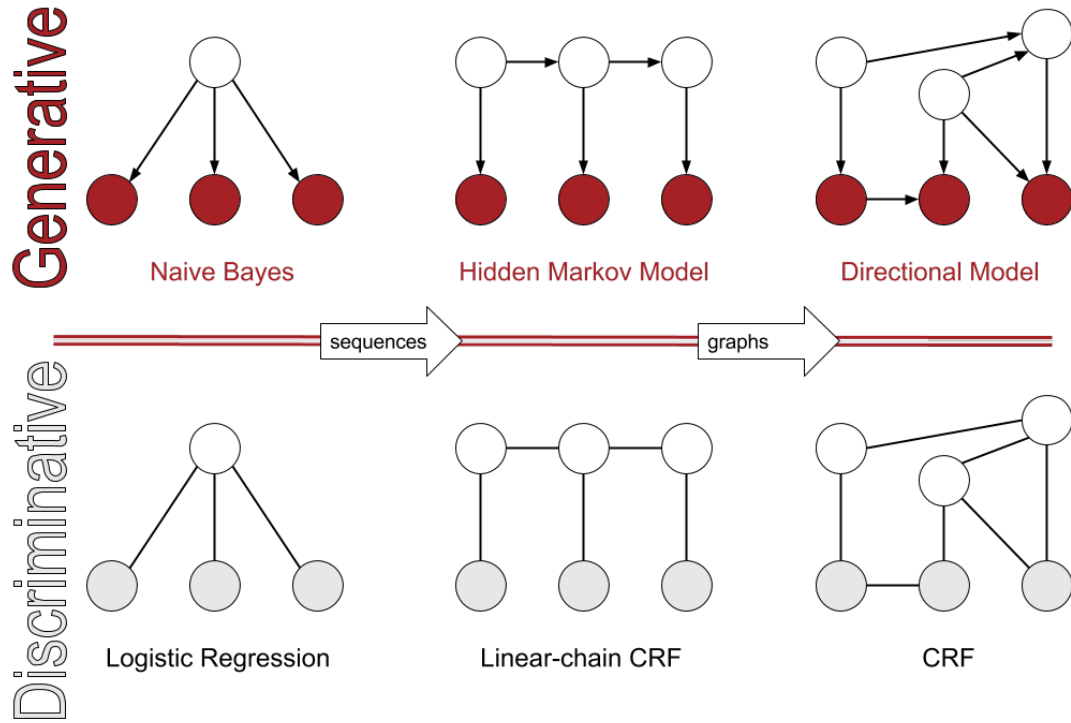
Figure 2.2: Generative models: Naive Bayes (Russell et al., 1995), Hidden Markov Models (Baum and Petrie, 1966), and Directional Models (Koller and Friedman, 2009). Discriminative models: Logistic Regression, Linear-chain Conditional Random Fields, and (general) Conditional Random Fields. Figure adapted from Sutton and McCallum (2011).

Fig. 2.2 shows generative and discriminative models. There is no definitive reason to use a generative model above a discriminative model or vice-versa. First, a discriminative model has lower asymptotic error, but a generative model approaches its asymptotic error faster in the case of a Naive Bayes classifier versus Logistic Regression (Jordan, 2002), but see also (Xue and Titterington, 2008) which doubts the existence of such precisely defined regimes. Asymptotic error denotes the error with an increasing number of samples. Second, the prior $p(\theta)$ in the generative model provides a principled way to handle missing information, while the direct modeling of decision boundaries in a discriminative model often leads to better performance in a classification task (Jaakkola et al., 1999). Apart from generative models and discriminative models, there are hybrid models (Bouchard and Triggs, 2004; Raina et al., 2003; Bosch et al., 2008). In this thesis we will limit ourselves to generative models.

2.2 Nonparametric Bayesian Models

A model can be composed out of a finite set of probability distibutions. An example of such a model is the Naive Bayes model.

Definition 2.38. The **Naive Bayes model** is a product over a finite number $k \neq \infty$ of probability distributions $p(x_i|\theta)$ multiplied by the prior distribution $p(\theta)$:

$$p(\theta|x) \propto p(\theta) \prod_{i=0}^{k-1} p(x_i|\theta) \tag{2.10}$$

A finite mixture model is a sum over a finite number of probability distributions:

Definition 2.39. A **finite mixture model** is a sum over a finite number $k \neq \infty$ of probability distributions $p(x_i)$, with each distribution weighted by a factor w_i with $\sum_i w_i = 1$.

$$p(x) = \sum_{i=0}^{k-1} w_i p(x_i) \tag{2.11}$$

The mixture model is finite in the sense that there are only $k \neq \infty$ distributions summed up. The weights of the individual distributions $p(x_i)$ are normalized (sum up to one) such that the weighted sum of probability distributions is itself a probability distribution.

An infinite mixture model is a sum over an infinite number of probability distributions:

Definition 2.40. A **infinite mixture model** is a sum over an infinite number of probability distributions $p(x_i)$, with each distribution weighted by a factor w_i with $\sum_i w_i = 1$.

$$p(x) = \sum_{i=0}^{\infty} w_i p(x_i) \tag{2.12}$$

The infinite mixture model is a sum over an infinite number of probability distributions with weights that sum up to one. In this way it assigns a finite value to a countably infinite set of functions.

In section 2.1.1 random elements are described in general. Random elements can vary from random vectors, random distributions, random clusters (partitions), to random trees. Table 2.1 describes the random elements and the corresponding examples of random processes in the literature.

The Gaussian Process (Rasmussen and Williams, 2006) describes a distribution on functions. The Beta Process (Hjort, 1990), the Gamma Process (Ferguson, 1974), the Dirichlet Process and the Polya Tree (Ferguson, 1973) describe a distribution on distributions. The Chinese Restaurant Process (Aldous, 1985) and Pitman-Yor Process (Pitman and Yor, 1997) describe a distribution on partitions. The Dirichlet Diffusion Tree (Neal, 2001) and Kingman's coalescence (Kingman, 1965) describe a distribution on hierarchical partitions. The Indian Buffet Process (Ghahramani and Griffiths, 2005) describes a distribution over sparse binary matrices. The Gamma-Poisson Process (Titsias, 2008) describes a distribution over integer-valued matrices. The Mondrian Process (Roy and Teh, 2009) describes a distribution over kd-trees.

Random processes and mixture models are visually represented by a method called *plate notation* (Koller and Friedman, 2009). Sets of variables are represented in a plate, a rectangular region (see Fig. 2.3).

Table 2.1: A list of mathematical structures and random processes that can be used to generate them.

Structure	Example
Distribution on functions	Gaussian Process
Distribution on distributions	Beta Process
	Gamma Process
	Dirichlet Process
	Polya Tree
Distribution on partitions	Chinese Restaurant Process
	Pitman-Yor Process
Distribution on hierarchical partitions	Dirichlet Diffusion Tree
	Kingman's coalescence
Distribution on sparse binary matrices	Indian Buffet Process
Distribution on integer-valued matrices	Gamma-Poisson Process
Distribution on kd-trees	Mondrian Process
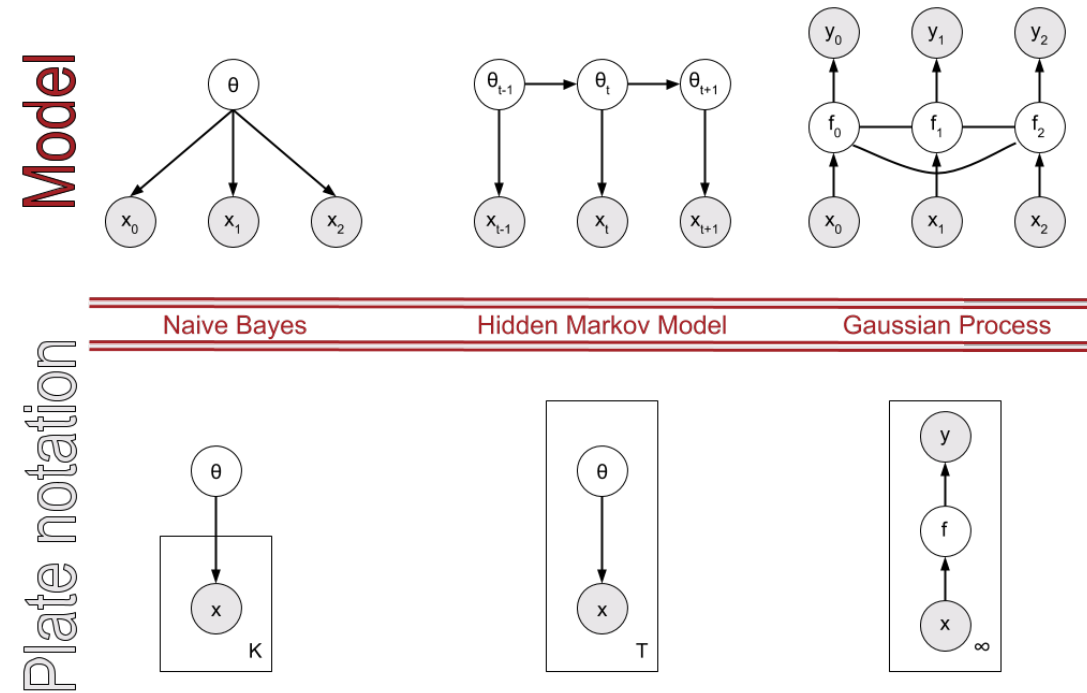
Figure 2.3: Top: graphical model of a Naive Bayes, Hidden Markov Model, and Gaussian Process. Bottom: corresponding plate notation of the Naive Bayes, Hidden Markov Model, and Gaussian Process. Observed variables are denoted by a circle that is shaded. The plate notation is a representation that does not capture all dependencies. The dependencies between the states θ_0 and θ_1 in the Hidden Markov Model are not represented for example.

Plate notation is a representation that does not preserve all dependencies between variables. The dependencies between the states in the Hidden Markov Model are not represented for example.

Some random process are mathematically represented by a completely random measure (Kingman, 1967), which is defined as follows:

Definition 2.41. A **completely random measure** is a random measure $\mu : \Omega \times X \to [0, +\infty]$ from probability space $(\Omega, \mathbb{F}, \mathbb{P})$ to measurable space (X, Σ) with

- for any collection of disjoint sets $A_1, \ldots, A_k \in \Sigma$ and $A_i \cap A_j = \emptyset$ for $i \neq j$ a mutual independency between $\mu(A_1), \ldots, \mu(A_k)$.

It is shown (Kingman, 1967) that a completely random measure can be decomposed into three components:

1. a deterministic function

2. a countable set of non-negative random masses at deterministic locations

3. a countable set of non-negative random masses at random locations

The first component is a deterministic function. The second component has non-negative random masses, also called atoms, on deterministic locations. The third component is the one of interest. It has a set of random masses (atoms) that can be represented as a Poisson random measure on $\mathbb{R}^+ \otimes X$ with mean measure ν which is known as the Lévy intensity measure (Favaro et al., 2013).

Table 2.2: Lévy measure of the Beta Process (Wang and Carin, 2012), Gamma Process (Knowles et al., 2014), the Dirichlet Process (Lijoi and Prünster, 2010) (indirectly through $F = 1 - e^{-\nu}$) .

Random Process	Lévy measure
Beta Process	$\nu(da, dw) = H(da)\alpha w^{-1}(1-w)^{\alpha-1}dw$
Gamma Process	$\nu(da, dw) = H(da)w^{-1}e^{-\alpha w}dw$
Dirichlet Process	$\nu(da, dw) = H(da)\frac{e^{-w\alpha(x,\infty)}}{1-e^{-w}}dw$

For Lévy measure decompositions of other processes such as the Indian Buffet Process, see Wang and Carin (2012).

Recall definition 2.29 for exchangeable sequences. There is a theorem (**?**) that states that there is parameter θ such that the data x_i is conditionally independent given this parameter for exchangeable sequences.

Definition 2.42. de Finetti's theorem. A sequence $\{x_0, x_1, \ldots\}$ of (X, Σ_X)-valued random variables is an infinitely exchangeable sequence if and only if there exist a measure $\mu(d\theta)$ on θ such that

$$p(x_0, \ldots, x_{k-1}) = \int_{\Sigma_X(X)} \prod_{i=0}^{k-1} p(x_i | \theta)\mu(d\theta) \qquad \forall k \geq 1 \qquad (2.13)$$

De Finetti's theorem states that if we have exchangeable data, we have a parameter θ, a likelihood $p(x|\theta)$ and some measure μ on θ, such that the data $(x_0, \ldots, x_{k-1})$ is conditionally independent.

De Finetti's theorem is not limited to exchangeable sequences. There are corresponding theorem's for other exchangeable objects (Orbanz and Roy, 2015):

Table 2.3: Several exchangeable structures have a theorem that describes an underlying measure that can be sampled i.i.d. Exchangeable sequences (de Finetti, 1930), increments (Bühlmann, 1960), partitions (Kingman, 1978), arrays (Aldous, 1981), and Markov chains (Diaconis and Freedman, 1980).

| Mathematical Objects	Theorem
Exchangeable Sequences	de Finetti
Exchangeable Increments	Bühlmann
Exchangeable Partitions	Kingman
Exchangeable Arrays	Aldous-Hoover
Exchangeable Markov Chains	Diaconis-Freedman

The *stick-breaking presentation* (Freedman and Diaconis, 1983) or residual allocation model (Hoppe, 1986; Sawyer and Hartl, 1985)

Definition 2.43. An infinite sequence of random variables $\phi = \{\phi_0, \phi_1, \ldots\}$ has a **stick-breaking presentation** with parameters α and β denoted by $\phi \sim GEM(\alpha, \beta)$.

$$w_k \overset{i.i.d.}{\sim} Beta(1-\beta, \alpha + k\beta) \qquad k = 1, \ldots, K \qquad (2.14)$$

$$\phi_k = w_k \prod_{i=1}^{k-1}(1-w_i) \qquad (2.15)$$

The stick-breaking presentation samples repeatedly from a $Beta(1-\beta, \alpha+k\beta)$ distribution. The result of the process is a vector of k weights ϕ_k. The abbrevation GEM stands for Griffiths, Engen, and McCloskey (Ewens, 1990; Ethier, 1990). There is also a variant of GEM with a single parameter α which can be obtained by setting $\beta = 0$. In that case w_k are drawn from a $Beta(1, \alpha)$ distribution.

Stick Breaking   Stick Breaking Process
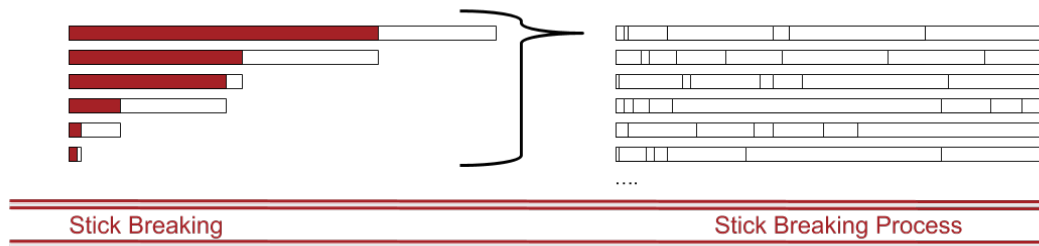
Figure 2.4: The stick-breaking presentation. Left: at the first row, the stick is broken at x_0, at the next rows the remaining part of the stick is broken x_i with $i > 0$. Only six iterations are shown. Right: samples of a stick-breaking process. The first row shows the stick ratios from the stick-breaking presentation at the left. The next rows show other samples from the same process.

Fig. 2.4 visualized the stick-breaking process. A stick of fixed length 1 gets broken at a position sampled from a Beta distribution. An infinite number of times it is broken. A stick-breaking process generates many of these broken sticks. The stick-breaking presentation is convenient for extensions that allow the atoms to vary according to some other stochastic process (Dunson et al., 2012) and for approximations by truncating the stick-breaking to a limited number of times (Kurihara et al., 2007).

2.2.1 Beta Process

A Beta Process (Hjort, 1990) is a random process with a countably infinite collection of weighted atoms in a space $(X, \mathbb{B})$ with weights that are in between $[0, 1]$ (Hjort, 1990).

Definition 2.44. Let $(X, \mathbb{B})$ be a Borel space, ν a finite measure, and $\alpha > 0$ a scale parameter, then a **Beta Process** is a Lévy process on $(X, \mathbb{B})$ with its Lévy measure ν corresponding to the density:

$$\nu(dw) = \alpha w^{-1}(1-w)^{\alpha-1}dw \qquad (2.16)$$

with $w > 0$.
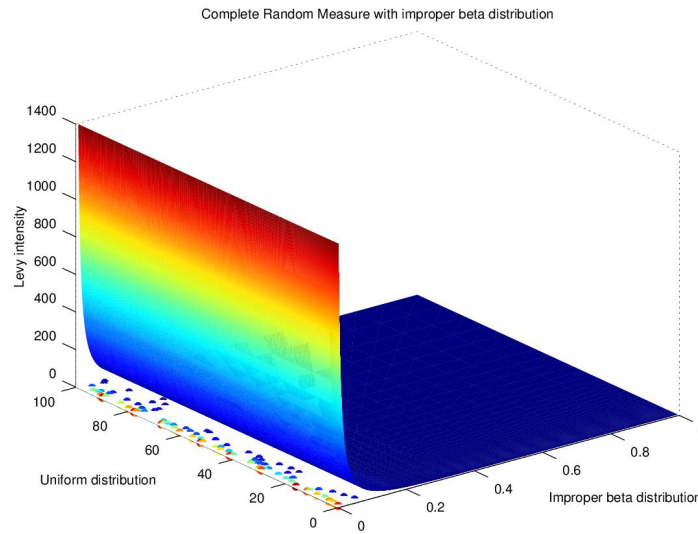
Figure 2.5: A Completely Random Measure with a Lévy intensity defined on the product space $\Omega \otimes (0,1)$. Here Ω is a bounded interval on which the base measure $B_0 = U(0,100)$ is defined. On $(0,1)$ we define an improper beta distribution $\alpha w^{-1}(1-w)^{\alpha-1}$. In this example $\alpha = 10$. This is how a Beta Process can be generated from a nonhomogeneous spatial Poisson point process. This has been visualized before (Jordan, 2010). The image is produced by rejection sampling using a homogeneous Poisson point process at $\max(\nu)$ over $w = [0.01, 0.9]$. For $w \to 0$ this maximum would go to ∞ and all points would be rejected. Hence, the points should be denser for w around 0 and should be seen as an approximation of the actual process.

In Fig. 2.5 the Beta Process is generated from a Completely Random Measure with a Lévy intensity defined on $\Omega \otimes (0,1)$ (Thibaux and Jordan, 2007). In this case Ω is the so-called base measure B_0 and is assumed uniform over a bounded region. The $(0,1)$ space is equipped

with an improper Beta distribution. It is called improper or degenerate because the scale parameter of the standard Beta distribution is set to zero. This has the consequence that the integral is infinite: $\nu(\Omega \otimes (0,1)) = \infty$. It is due to the fact that the density $w^{-1}(1-w)^{\alpha-1}$ goes to infinity for $w \to 0$. That means that a countable infinite number of points can be obtained from the Poisson process.

The Beta Process has a sequential representation in the form of the Indian Buffet Process:

Definition 2.45. An **Indian Buffet Process** is a sequential process that is an exchangeable distribution over matrices:

$$p(z_{i,j} = k | z_{0,0}, \ldots, z_{i-1,K_+}) = \begin{cases} \frac{n_{-i,k}}{i} & \text{if } k \leq K_+ \\ \frac{\lambda^{k_{new}}e^{-\lambda}}{k_{new}!} & \text{if } k > K_+ \end{cases} \tag{2.17}$$

Here $\lambda = \alpha/i$, $k_{new} = K_+ - k$. The i'th data item samples an existing column with a probability of the number of times it has been sampled before divided by its index, $n-i,k/i$. It samples a new column with a probability according to a Poisson distribution, $\lambda^{k_{new}}e^{-\lambda}/k_{new}!$. The conditional form of the sequential presentation describes a closed-form solution for Gibbs sampling, section 2.3.4 (**?**).

The Beta Process (BP) is used in linguistics (He et al., 2013; Vanhainen and Salvi, 2012), computer vision (Zhou et al., 2011; Gao and Sun, 2013),

2.2.2 Gamma Process

A Gamma process is a random process with independent gamma distributed increments (Ferguson, 1974), formally:

Definition 2.46. Let $(X, \mathbb{B})$ be a Borel space, ν a finite measure, and $\alpha > 0$ a scale parameter, then a **Gamma Process** is a Lévy process on $(X, \mathbb{B})$ with its Lévy measure ν corresponding to the density:

$$\nu(dw) = w^{-1}e^{-\alpha w}dw \tag{2.18}$$

with $w > 0$.

The Gamma Process is used in risk theory (Dufresne et al., 1991), spatial statistics (Wolpert and Ickstadt, 1998; Rao and Teh, 2009), erosion (Singpurwalla, 1997; Abdel-Hameed, 2012), and finance (Madan and Seneta, 1990; Küchler and Tappe, 2008).

2.2.3 Dirichlet Process

The Dirichlet Process (DP) is, just as the Beta Process and the Gamma Process, a distribution over distributions (Ferguson, 1973).

Definition 2.47. A **Dirichlet process** DP over a set S can be used to draw sample paths X:

$$X \sim DP(\alpha, H)$$
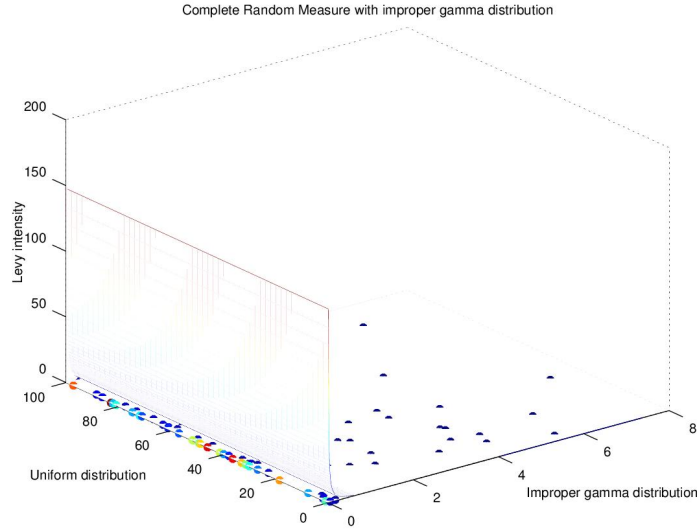
Figure 2.6: A Completely Random Measure with a Lévy intensity defined on the product space $\Omega \otimes \mathbb{R}$. Here Ω is a bounded interval on which the base measure $B_0 = U(0,100)$ is defined. On $\mathbb{R}$ we define an improper gamma distribution $w^{-1}e^{-\alpha w}$. In this example $\alpha = 1$. This is how a Gamma Process can be generated from a nonhomogeneous spatial Poisson point process. The image is produced by rejection sampling in the same way as Fig. 2.5.

with α the dispersion parameter and H a measure on S and for which any measurable partition $\{B_0, \ldots, B_{n-1}\} \in S$ is drawn from a Dirichlet distribution:

$$(X(B_0), \ldots, X(B_{n-1})) \sim \text{Dirichlet}(\alpha H(B_0), \ldots, \alpha H(B_{n-1}))$$

The Lévy intensity of the Dirichlet Process is complicated, because it is a so-called normalized process, see Regazzini et al. (2003).

De Finetti's theorem can be used to define the so-called Chinese Restaurant Process (CRP). This is a *distribution over partitions*. The Dirichlet Process has with the Chinese Restaurant Process a sequential representation:

Definition 2.48. A **Chinese Restaurant Process** is a sequential process that is an exchangeable distribution over partitions:

$$p(z_i = k | z_0, \ldots, z_{i-1}) = \begin{cases} \frac{n_k}{\alpha + i} & \text{if } k \leq K_+ \\ \frac{\alpha}{\alpha + i} & \text{if } k > K_+ \end{cases} \tag{2.19}$$

The conditional probability of a cluster assignment z_i for data item y_i given the cluster assignments $z_0, \ldots, z_{i-1}$ is proportional to the number of data items n_k assigned to an existing cluster k, or proportional to α for a new cluster.

The Chinese Restaurant Process is visualized in Fig. 2.8.
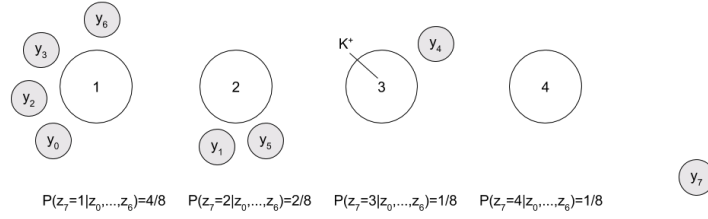
Figure 2.7: The Chinese Restaurant Process with i customers already sitting down. A new customer $y_{i=7}$ arrives and gets assigned, z_i. This is an existing table $\{1, 2, 3\}$ with a probability proportional to the number of customers n_i sitting at that table: $n_i/(\alpha + i)$, or a new, empty table 4 with probability $1/(\alpha + i)$. In the visualized Chinese Restaurant Process the dispersion factor $\alpha = 1$.
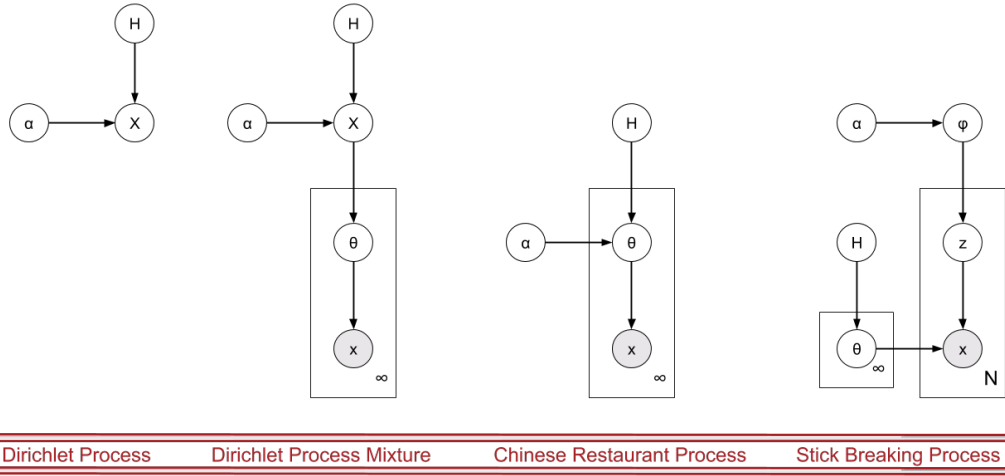
Figure 2.8: The Dirichlet Process $X \sim DP(\alpha, H)$. The Dirichlet Mixture Model where X is a prior for a sum $\sum_i w_i p(x_i | \theta_i)$, a Chinese Restaurant Process with X marginalized out, and the Stick Breaking Process with a distribution over partition sizes π and indicator variables z_i.

Definition 2.49. The **stick-breaking presentation** of the Dirichlet Process states that if

$$\phi_k \sim GEM(\alpha, 0) \tag{2.20}$$

$$\theta_k \sim H \tag{2.21}$$

$$G = \sum_{k=1}^{\infty} \phi_k \delta(\theta, \theta_k) \tag{2.22}$$

then $G \sim DP(\alpha, H)$.

The weights ϕ_k are sampled from the stick-breaking process $GEM(\alpha, 0)$. The parameter values θ_k are sampled from the base measure H. To sample from the Dirichlet Process we have to sample these parameters with the given weights.

If the stick-breaking process is used as a prior for a mixture, then the cluster assignments z_i are sampled according to the mixing proportions ϕ:

$$\phi \sim GEM(\alpha, 0) \tag{2.23}$$

$$\theta_k \sim H \tag{2.24}$$

$$G = \sum_{k=1}^{\infty} \phi_k \delta(\theta, \theta_k) \tag{2.25}$$

$$z_i \sim Mult(\phi) \tag{2.26}$$

$$x_i \sim F(\theta_{z_i}) \tag{2.27}$$

Here $\theta_k = \theta_{z_i}$ for observation with index i and cluster assignment k: $z_i = k$.

2.2.4 Pitman-Yor Process

The Pitman-Yor Process introduces another parameter d with respect to the Dirichlet Process. It has been developed by Pitman and Yor as the two-parameter Poisson-Dirichlet distribution (Pitman and Yor, 1997). The Pitman-Yor Process has the following definition:

Definition 2.50. A Pitman-Yor process PY over a set S can be used to draw sample paths X:

$$X \sim PY(d, \alpha, H)$$

with $\alpha > -d$ a strength parameter, $0 \le d < 1$ a discount parameter, and H a measure on S.

The Pitman-Yor Process (PYP) generalizes the DP. The Pitman-Yor Process has a stick-breaking presentation in which sticks are drawn from $GEM(\alpha, \beta)$. The Dirichlet Process has a stick-breaking presentation in which sticks are drawn from $GEM(\alpha, 0)$, see Def. 2.49.

Definition 2.51. The **stick-breaking presentation** of the PYP states that if

$$\phi_k \sim GEM(\alpha, \beta) \tag{2.28}$$

$$\theta_k \sim H \tag{2.29}$$

$$G = \sum_{k=1}^{\infty} \phi_k \delta(\theta, \theta_k) \tag{2.30}$$

then $G \sim PYP(\alpha, H)$.

The Pitman-Yor Process is used in quite a few applications, such as language models (Teh et al., 2006), scene segmentation (Sudderth and Jordan, 2009), speech induction (Blunsom and Cohn, 2011), and time series (Bassetti et al., 2014).

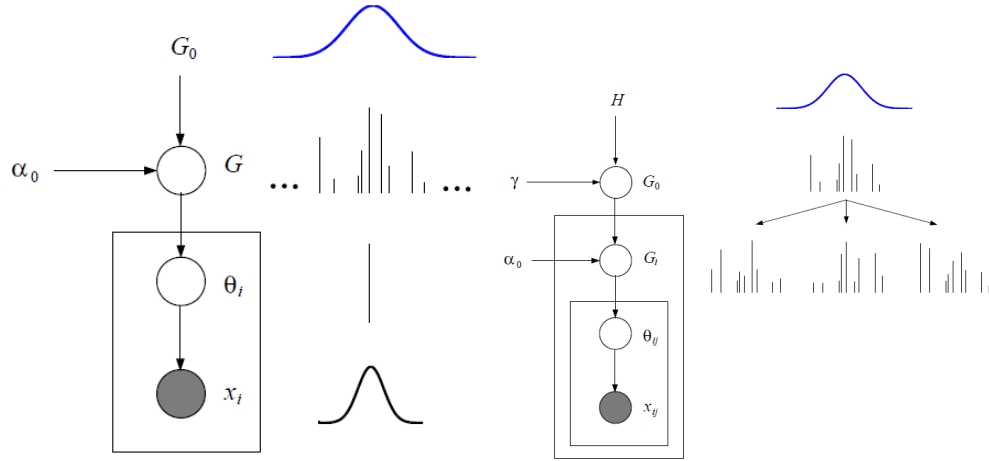### 2.2.5 Hierarchical Dirichlet Process

The Hierarchical Dirichlet Process (HDP) extends the Dirichlet Mixture Model with a hierarchical structure (Teh et al., 2006).

Definition 2.52. A Hierarchical Dirichlet process *HDP* over a set S can be used to draw sample paths X:

$$G_0 \sim DP(\gamma, H)$$
$$X_i \sim DP(\alpha_0, G_0) \text{ for each group } i$$

with a Dirichlet Process with a general γ dispersion parameter and base distribution H as a measure on S of which the generated distributions G_0 are used as base distribution for each group distribution X_i.

(a) Dirichlet Process Mixture Model. Each draw from the process corresponds to a parameter. Each parameter is associated with a distribution (in this case a Gaussian).

(b) Hierarchical Dirichlet Process. Observe that the location of the atoms are fixed through the highest layer G_0. The only freedom left to express by G_i is in the weights of those atoms. This reflects a decomposition in a structural and non-structural component.

Figure 2.9: The difference visualized between a Dirichlet Process mixture and a Hierarchical Dirichlet Process. It illustrates also that the input of a Dirichlet process does not have to be a continuous function. If it is a continuous distribution it will become a discrete distributed almost surely. If it is a discrete distribution, it will have atoms at the locations where the discrete distribution had its probability mass concentrated.

The Hierarchical Dirichlet Process uses the outcome of a Dirichlet Process as a starting point to define multiple distributions with atoms at the same locations, while they come equipped with different weights. So, the Dirichlet Process on the lower level uses not a continuous distribution as input, but a discrete one, generated by the DP at the top layer. Note, that the Dirichlet Process will create an a.s. discrete distribution, but it can be fed a discrete distribution as prior just fine.

2.3   Inference

There will be six inference methods described, all sampling methods. Section 2.3.1 describes inverse transform sampling. Section 2.3.2 describes rejection sampling. Section 2.3.3 describes approximate Bayesian computation. Section 2.3.4 describes Gibbs sampling. Section 2.3.5 describes Metropolis-Hastings. Section 2.3.6 describes Split-Merge MCMC.

2.3.1   Inverse Transform Sampling

Let $p_f(x)$ and $p_g(x)$ be two probability distributions with $p_f(x) + p_g(x) = 1$. Sample with probability $p_f(x)$ by drawing from a uniform distribution $u \sim U(0,1)$, then if $u < p_f(x)$, accept x, if not reject x. This can be generalized to more than two probability distributions.

Let $p_f(x), p_g(x), p_h(x)$ be multiple probability distributions. Draw u from the uniform distribution $U(0,1)$. If $u < p_f(x)$ we select f, else if $u < p_f(x) + p_g(x)$ we select g, and otherwise we select g. The procedure is called inverse transform sampling. The term "inverse" stems from the fact that we return x (or $f(x)$) given u. Inverse transform sampling is common to a lot of sampling methods. Often when there are samples from a uniform distribution this is an inverse transform sampling step.

2.3.2   Rejection Sampling

Let $f(x)$ be a complicated function from which it is hard to take samples. Let $g(x)$ be a simple function that is easy to sample from. Then we can sample from $f(x)$ by making sure $Mg(x) > f(x)$:

$$X = S(f(x), g(x)) \tag{2.31}$$

The rejection sampling method (Halperin and Burrows, 1960) for $f(x)$ is described in algorithm 1:

Algorithm 1 Rejection sampling for $f(x)$

1: **procedure** Rejection Sampling$(f(x), g(x))$ ▷ Target and proposal distribution.
2:     **for** $t = 1 \rightarrow T$ **do**
3:         $x^t \sim g(x)$ ▷ Generate x^t from $g(x)$
4:         $u \sim U(0,1)$ ▷ Inverse transform sampling
5:         $p_0 = f(x)/(Mg(x))$
6:         **if** $u < p_0$ **then**
7:             $X = X \cup x^t$ ▷ Accept
8:         **end if**
9:     **end for**
10:     **return** X ▷ X will have the distribution of $f(x)$
11: **end procedure**

We can also use rejection sampling to sample from the posterior $f(\theta|x)$ given that we know the form of the likelihood function and that we can sample from the prior. We know that we can sample from the posterior by sampling from $p(\theta)p(x \mid \theta)$. We also know that the prior $p(\theta)$ necessarily has to be larger than $p(\theta)p(x \mid \theta)$ for any observation, because $p(x \mid \theta)$ is a probability, hence smaller than one.

$$\Theta = S(\sim p(\theta), p(x|\theta), x) \tag{2.32}$$

In our notation we make explicit that we need $p(x|\theta)$ for each combination of observations and parameters, but that we only need to sample $\sim$ from the prior $p(\theta)$.

Algorithm 2 Rejection sampling for $f(\theta \mid x)$

1: **procedure** REJECTION SAMPLING$(p(\theta), p(x|\theta), x)$ ▷ Requires prior, likelihood and observations.
2:   **for** $t = 1 \rightarrow T$ **do**
3:     $\theta^t \sim p(\theta)$ ▷ Generate θ^t from prior
4:     $u \sim U(0,1)$ ▷ Inverse transform sampling
5:     $p_0 = p(x \mid \theta)$
6:     **if** $u < p_0$ **then**
7:       $\Theta = \Theta \cup \theta^t$ ▷ Accept
8:     **end if**
9:   **end for**
10:   **return** Θ ▷ Θ will have the distribution of $f(\theta|x)$
11: **end procedure**

In algorithm 2 the envelope distribution $p(\theta)$ and the target distribution $p(\theta)p(x \mid \theta)$, cancel in such way that only $p(x \mid \theta)$ remains.

Most examples illustrate rejection sampling by estimating the area of a circle, but let us visualize the method in the context of sampling (Fig. 2.10).
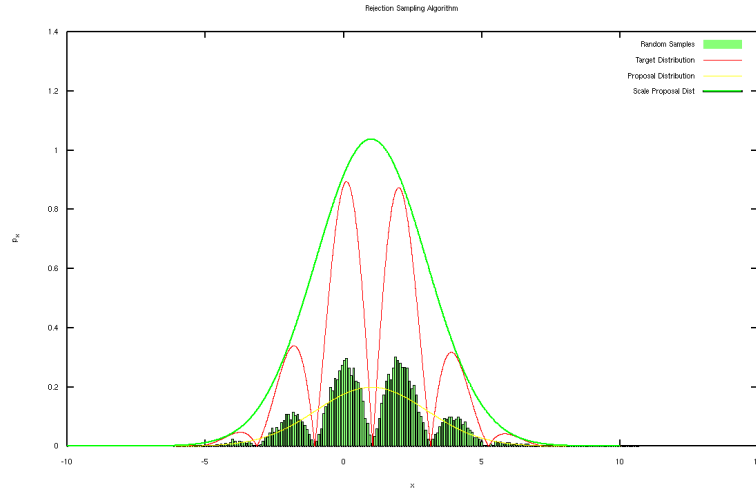
Figure 2.10: A Gaussian is placed over the complex target probability density function. Subsequently the samples that fall in between these two 'envelopes' are rejected. This results in a sampling scheme that follows exactly the more complicated probability density function. Note that if the function is scaled by a factor, the sampling scheme stays the same. Such a scaling factor is only important if we want, for example, to know the area under the graph.

2.3.3 Approximate Bayesian Computation

In Approximate Bayesian Computation (ABC) (Rubin and Others, 1984) the likelihood function does not need to be calculated[2] (Sisson and Fan, 2011). In contrast, it is assumed that there is a model available that allows to generate observations given the (searched for) parameters. In ABC for each configuration of parameters a set of observations is generated.

$$\Theta = S(\sim p(\theta), X, \sim M(\theta), d(X^t, X), \epsilon) \tag{2.33}$$

Approximate Bayesian computation uses many tuning parameters. It most salient characteristic though is that it generates pseudo-observations through $\sim M(\theta)$.

---

[2]ABC is also called likelihood-free computation

Algorithm 3 Approximate Bayesian computation

1: **procedure** ABC APPROXIMATE BAYESIAN COMPUTATION$(p(\theta), X, M, d, \epsilon)$ ▷ Requires prior, observations, model, distance function, and threshold.

2:     **for** $t = 1 \rightarrow T$ **do**

3:        $\theta^t \sim p(\theta)$ ▷ Generate θ from prior

4:        $X^t \sim M(\theta)$ ▷ Simulate observations X^t from model M

5:        $\rho = d(X^t, X)$ ▷ Calculate distance between simulated and actual observations

6:        **if** $\rho \leq \epsilon$ **then**

7:           $\Theta = \Theta \cup \theta^t$ ▷ Accept θ^t if distance falls under threshold ϵ.

8:        **end if**

9:     **end for**

10:     **return** Θ ▷ Θ will have the distribution of $f(\theta|X)$

11: **end procedure**

The term Bayesian reflects the fact that a prior is involved. The weight of this prior can be manipulated by the threshold ϵ. If this threshold is set very low, the prior plays no role and only observations are taken into account. If ϵ is set extremely high, all θ coming from the prior will be accepted, and the actual observations are not used in the process. There are several disadvantages to approximate Bayesian computation:

- A set of simulated observations has to be compared with the actual observations. This becomes unwieldly if there are many observations.

- It is possible to use summary statistics rather than the observations themselves. If these are sufficient statistics there will be no information lost. If not, there will be information loss in practice

- The distance function suffers from the curse of dimensionality. In the case that the dimensionality of the individual observations becomes high, or the number of parameters becomes large, it gets increasingly difficult to come up with a distance function which is efficient and accurate at the same time.

2.3.4 Gibbs Sampling

Gibbs sampling (Geman and Geman, 1984) is similar to the *coordinate descent* optimization algorithm (Wright, 2015). In coordinate descent a local minimum of a function is found by iteratively performing a line search along one coordinate direction at a time. Gibbs sampling is named after the physicist Gibbs and belongs to the family of Markov chain Monte Carlo (MCMC) methods. Gibbs sampling optimizes over one variate in the multivariate probability distribution at a time. The update value is set and fixed. Then, the next variate is chosen in a round-robin like manner.

$$\Theta = S(X, \sim p(\theta_i | \theta_{-i}, X), \sim p(\theta), B) \tag{2.34}$$

The multiple parameters in the multivariate probability distribution are denoted by θ. The parameters are denoted individually with θ_i. The set of all parameters except for i is denoted by θ_{-i}. If we sample a parameter we write θ^t with t the iteration or sampling round. The set of parameter samples has capital letter Θ.

Algorithm 4 Gibbs sampling

1: **procedure** Gibbs Sampling$(p(\theta_i|\theta_{-i},X),p(\theta),X,B)$ ▷ Requires parameters, observations and burn-in.

2:     $\theta^0 \sim p(\theta)$ ▷ Set parameters to some initial value

3:     **for** $t = 1 \rightarrow T$ **do**

4:        **for** $i = 1 \rightarrow k$ **do**

5:           $\theta_i^t \sim p(\theta_i^{t-1}|\theta_{-i}^t,X)$ ▷ Generate θ_i^t from the full conditional probability

6:        **end for**

7:        $\Theta = \Theta \cup \theta^t$

8:     **end for**

9:     $\Theta_{B:T} \in \Theta$ ▷ Get Θ_T set, from burn-in B to end of run T

10:    $\Theta \sim \Theta_{B:T}$ ▷ Sample Θ from correlated $\Theta_{B:T}$

11:    **return** Θ

12: **end procedure**

Gibbs samples are Markovian, the conditional probability only takes into account values at the previous time step $t - 1$. When running the Gibbs sampling algorithm long enough, it will visit all possible states eventually. The Markovian property makes subsequent steps correlated, hence when finally extracting the parameter probabilities, it is important not to consider subsequent steps. It is also important to run the algorithm for a while, so it does not suffer from a bad choice of initial parameter values, this is called burn-in. Gibbs sampling works properly because the time the algorithm spends in parts of the space is directly related to the probability of getting into that part of the space.

In the physics literature Gibbs sampling is known as Glauber dynamics or the heat bath algorithm. Observe that Gibbs sampling does not necessary require an actual calculation of the conditional probability in all cases. The obvious exception is for the observations, which are already known. Another, neat optimization procedure arises when conjugate priors are used. A conjugate prior leads to a posterior distribution that can be described analytically. In such a case it is computationally unnecessary to perform sampling. It is much faster to use the actual available analytic description. This is commonly called collapsed Gibbs sampling.

2.3.5 Metropolis-Hastings Sampling

Another MCMC algorithm is Metropolis-Hastings (Metropolis et al., 1953), likewise used for high-dimensional distributions. Metropolis-Hastings calculates an acceptance factor α which takes into account if a step should be taken according to a predefined proposal distribution. In case this step is not accepted, the current sample is resampled.

$$\Theta = S(X, \theta^0, Q(\theta^{t+1}|\theta^t), f(\theta, X))$$ (2.35)

Here we need $Q(\theta^{t+1}|\theta^t)$ explicitly as well as samples from it.

Algorithm 5 Metropolis-Hastings sampling

1: **procedure** METROPOLIS-HASTINGS SAMPLING(θ^0, X, Q, f) ▷ Requires initial parameters, observations, proposal distribution, and function proportional to desired distribution

2:     **for** $t = 1 \to T$ **do**

3:         $\theta^{t+1} \sim Q(\theta^{t+1}|\theta^t)$ ▷ Sample from proposal distribution Q

4:         $\alpha = \frac{f(\theta^{t+1}, X^{t+1})Q(\theta^{t+1}|\theta^t)}{f(\theta^t, X^t)Q(\theta^t|\theta^{t+1})}$ ▷ Calculate acceptance

5:         $u \sim U(0, 1)$ ▷ Inverse transform sampling

6:         **if** $\alpha > u$ **then**

7:             $\Theta = \Theta \cup \theta^{t+1}$ ▷ Accept θ^{t+1}

8:         **else**

9:             $\Theta = \Theta \cup \theta^t$ ▷ Reuse previous sample (note, different from rejection)

10:        **end if**

11:     **end for**

12:     **return** Θ ▷ Θ will be samples from the distribution $f(\theta|x)$

13: **end procedure**

A particular choice of a Metropolis-Hastings step is that of a proposal distribution that does not depend on the state of the chain. This is already suggested by Hastings and is called the independence sampler.

2.3.6 Split-Merge MCMC Sampling

The discussed sampling methods do not assume much structure in the model. This means that in hierarchical models sampling either occurs through updating the to be estimated quantities observation by observation or cluster by cluster. Splitting a cluster in two requires moving data points one by one to this new cluster. Much more efficient sampling methods can be obtained if we would be able to reason about larger chunks of cluster assignments.

Split-merge sampling can update cluster assignments for multiple observations at once. It is an adaptation of acceptance method in the Metropolis-Hastings algorithm.

Algorithm 6 Split-Merge MCMC sampling

1: **procedure** SPLIT-MERGE MCMC SAMPLING(θ^0, X, Q, f)   ▷ Requires initial parameters, observations, proposal distribution, and function proportional to desired distribution
2:     **for** $t = 1 \rightarrow T$ **do**
3:         $i \sim D(0, N-1)$ ▷ Sample observation i discretely
4:         $j \sim D(0, N-1)$ ▷ Sample observation j discretely
5:         **if** $c_i == c_j$ **then**
6:             $c_{old} = c_i$
7:             $\theta^{t+1}_{c_{new}} \sim Q(\theta^{t+1} | \theta^t)$ ▷ Sample from proposal distribution Q
8:             **for** $k \in c_{old}$ **do**
9:                 $c_k \sim C(c_{old}, c_{new})$ ▷ Assign to new cluster categorically
10:             **end for**
11:         **else**
12:             $c_{merge} = c_i$
13:             **for** $k \in c_j$ **do**
14:                 $c_k = c_{merge}$ ▷ Assign all to first cluster
15:             **end for**
16:         **end if**
17:         $\alpha = \frac{f(\theta^{t+1}, X^{t+1}) Q(\theta^{t+1} | \theta^t)}{f(\theta^t, X^t) Q(\theta^t | \theta^{t+1})}$ ▷ Calculate acceptance
18:         $u \sim U(0, 1)$ ▷ Inverse transform sampling
19:         **if** $\alpha > u$ **then**
20:             $\Theta = \Theta \cup \theta^{t+1}$ ▷ Accept θ^{t+1}
21:         **else**
22:             $\Theta = \Theta \cup \theta^t$ ▷ Reuse previous sample (note, different from rejection)
23:         **end if**
24:     **end for**
25:     **return** Θ ▷ Θ will be samples from the distribution $f(\theta | x)$
26: **end procedure**

The exact acceptance probability depends on the model at hand. For the mixture model with a Dirichlet Process as prior, its performance is further improved by adjusting the assignment process from random to observation-supported by introducing intermediate restricted Gibbs sampling steps (Jain and Neal, 2004, 2007). Similarly, there are other variants that incorporate data fit to the splitting step. Labels can for example be calculated sequentially (Dahl, 2003) or methods can be used that postulate subcluster structure within clusters to streamline reasoning over split and merge sets (**?**).

2.4   Chapter Conclusions

This chapter described in section 2.1 probability theory, and in particular, measure theory underlying random processes. In section 2.2 five random processes are described, the Beta Process, the Gamma Process, the Dirichlet Process, the Pitman-Yor Process, and the Hierarchical Dirichlet Process.

The random measures have been presented as a Poisson process with a Lévy measure, a stick-breaking construction, and a sequential presentation. These representations give rise to different inference methods.

In section 2.3 six inference methods are described. Inverse transform sampling, rejection sampling, approximate Bayesian computation, Gibbs sampling, Metropolis-Hastings, and Split-Merge MCMC.

Chapter 3 describes Gibbs sampling to perform inference over an infinite set of lines. Gibbs sampling requires conditional probabilities. These are given in closed-form because there is a conjugate description of the line parameters given the points that form the lines in this application.

Chapter 4 describes Split-Merge MCMC sampling to perform inference over an infinite set of line segments. The parameters for line segments do not have a conjugate description. Metropolis-Hastings can be used to perform inference over the line segments, but the search space is quite large. The Split-Merge MCMC method performs faster inference than Metropolis-Hastings because it is able to split and merge line segments (with multiple points ascribed to them) at once.

NONPARAMETRIC BAYESIAN LINE DETECTION

Contents   The nonparametric Bayesian models from the literature (Chapter 2) can be applied to perform inference over point clouds. An example of a point cloud are points distributed over lines in a two-dimensional space. Traditionally, RANSAC and the Hough transform have been used to perform inference over such lines. This chapter uses a nonparametric Bayesian model to perform inference over a countably infinite number of lines. Given a prior with respect to the noise and distribution of points over the lines, Bayesian inference describes the optimal procedure to perform line fitting.

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A.C. van Rossum, H.X. Lin, J. Dubbeldam, and H.J. van den Herik. Fundamentals of Nonparametric Bayesian Line Detection. Springer, 2017.

Outline   The infinite line model describes a collection of lines with a Dirichlet Process as prior (Sect. 3.1). Inference in the infinite line model is performed through Gibbs sampling. (Sect. 3.2). Gibbs sampling over parameters converges slowly. It can be accelerated through sampling over clusters (Sect. 3.3). The inference method results are measured using clustering performance measures (Sect. 3.4). The chapter summarizes the findings (Sect. 3.5) and introduces extensions which will be handled in the next chapters.

In computer vision and particularly in robotics, traditionally the task of line detection has been performed through sophisticated, but ad-hoc methods. We will give two examples

of such methods. RANSAC (Bolles and Fischler, 1981) is a method that iteratively tests a hypothesis. A line is fitted through a subset of points. Then other points that are in consensus with this line (according to a certain loss function) are added to the subset. This procedure is repeated till a certain performance level is obtained. The Hough transform (Hough, 1962) is a deterministic approach which maps points in the image space to curves in the so-called Hough space of slopes and intercepts. A line is extracted by getting the maximum in the Hough space.

There are four main problems with these methods. First, the extension of RANSAC or Hough to the detection of multiple lines is nontrivial (Zhang and Kŏsecká, 2007; Gallo et al., 2011; Chen et al., 2001). Second, the noise level is hardcoded into model parameters and it is not possible to incorporate knowledge about the nature of the noise. Third, it is hard to extend the model to hierarchical forms, for example, to lines that form more complicated structures such as squares or volumetric forms. Fourth, there are no results known with respect to any form of optimality of the mentioned algorithms.

In this chapter we postulate a method to perform inference over the number of lines and over the fitting of points on that line using the nonparametric Bayesian methods from chapter 2.

3.1 Infinite Line Model

The Dirichlet Process described as prior for a mixture distribution (Fig. 2.8 in section 2.2.3) can be used in this particular case as a prior for the distribution of points over a countably infinite set of lines.
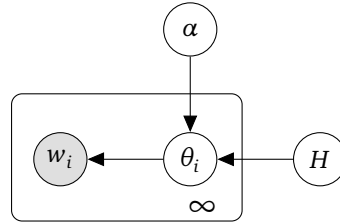
Figure 3.1: The Infinite Line Model in the Chinese Restaurant Process representation (compare with Fig. 2.8). Top: α, the concentration parameter of the Dirichlet Process. Bottom, left to right: w_i, the observation, an individual point in a 2D space; θ_i, the parameters (intercept, slope) of the line belonging to observation w_i; H, the base distribution from which line parameter values are sampled.

The infinite line model is visualized (Fig. 3.2) through plate notation (Buntine, 1994). In section 3.1.1 it is described how θ_i is sampled from H and α. In section 3.1.2 it is described how w_i is sampled from θ_i. In section 3.1.3 the prior H for θ_i is described.

3.1.1 Posterior Predictive for a Line given Other Lines

Let us reiterate the definition of the Dirichlet Process. Let H be a distribution over Θ, let α be scalar. The Dirichlet Process generates a distribution $G \sim DP(\alpha, H)$:

$$G(\theta_1, \ldots, \theta_\infty) \sim DP(\alpha, H(\theta_1, \ldots, \theta_\infty)) \tag{3.1}$$

A Dirichlet Process assigns a Dirichlet distribution to every parameter partition $\Theta_1, \ldots, \Theta_r$:

$$(G(\Theta_1), \ldots, G(\Theta_r)) \sim Dir(\alpha H(\Theta_1), \ldots, \alpha H(\Theta_r)) \tag{3.2}$$

The Dirichlet is conjugate to the categorical:

$$(G(\Theta_1), \ldots, G(\Theta_r)) \mid \theta_1, \ldots, \theta_n \sim Dir(\alpha H(\Theta_1) + n_1, \ldots, \alpha H(\Theta_r) + n_r)$$
$$n_k = \sum_{j=1}^{n} \delta_{\theta_j}(\Theta_k) \tag{3.3}$$

In the above notation, $\delta_{\theta_j}(\Theta_k)$ is a Dirac measure (a generalization of the Dirac delta function), also known as an indicator function. Given a set Θ_k with a σ-algebra over subsets of Θ:

$$\delta_{\theta_j}(\Theta_k) = 1_{\Theta_k}(\theta_k) = \begin{cases} 1 & \text{if } \theta_j \in \Theta_k \\ 0 & \text{if } \theta_j \notin \Theta_k \end{cases} \tag{3.4}$$

The posterior for the Dirichlet Process base distribution and dispersion parameter is a Dirichlet Process with adjusted parameters:

$$G(\cdot) \mid \theta_1, \ldots, \theta_n \sim DP\left(\alpha + n, \frac{\alpha}{\alpha + n} H(\cdot) + \frac{n}{\alpha + n} \frac{\sum_{j=1}^{n} \delta_{\theta_j}(\cdot)}{n}\right) \tag{3.5}$$

The posterior base distribution G is a weighted average between the prior base distribution H and the empirical distribution $n^{-1} \sum_{j=1}^{n} \delta_{\theta_j}$ with the weights respectively α and n (normalized). The dispersion parameter α is updated to $\alpha + n$. Note that $\delta_{\theta_j}(\cdot)$ is a distribution, the Dirac measure Eq. 3.4.

The posterior predictive for a new parameter θ_{n+1} has the form:

$$P(\theta_{n+1} \in \Theta_k \mid \theta_1, \ldots, \theta_n) = \frac{1}{\alpha + n}\left(\alpha H(\Theta_k) + \sum_{j=1}^{n} \delta_{\theta_j}(\Theta_k)\right) \tag{3.6}$$

In other words, the posterior predictive of θ_{n+1} given the parameters $\theta_1, \ldots, \theta_n$ in Eq. 3.6 has exactly the same form as the posterior base distribution G given the parameters $\theta_1, \ldots, \theta_n$ (Blackwell and MacQueen, 1973) in Eq. 3.5, namely:

$$\theta_{n+1} \mid \theta_1, \ldots, \theta_n \sim \frac{1}{\alpha + n}\left(\alpha H(\theta_{n+1}) + \sum_{j=1}^{n} \delta(\theta_j - \theta_{n+1})\right) \tag{3.7}$$

A normal Dirac delta function $\delta(\theta_j - \theta_{n+1})$ can be used here, which is only non-zero when θ_j is equal to θ_{n+1}.

Equivalently, if we describe θ_n conditioned on $\theta_1, \ldots, \theta_{n-1}$ we have to run over $n-1$ rather than n parameters:

$$\theta_n \mid \theta_1, \ldots, \theta_{n-1} \sim \frac{1}{\alpha + n - 1}\left(\alpha H(\theta_n) + \sum_{j=1}^{n-1} \delta(\theta_j - \theta_n)\right) \tag{3.8}$$

Due to the exchangeability property we can also consider any other parameter update (Neal, 2000):

$$\theta_i \mid \theta_{-i} \sim \frac{1}{\alpha + n - 1}\left(\alpha H(\theta_i) + \sum_{j \neq i} \delta(\theta_j - \theta_i)\right) \tag{3.9}$$

The notation θ_{-i} means every parameter θ except for the one equal to θ_i.

3.1.2 Likelihood of Data given a Line

The likelihood of data given line parameters is defined to be according to the **Bayesian linear regression** model. The Bayesian linear regression model for a single line (Box and Tiao, 2011) assumes a linear relationship between the independent x_i and dependent variables y_i with Gaussian noise added in the y-direction. The individual points i are drawn from a Normal distribution:

$$y_i \sim \mathcal{N}(x_i\beta, \sigma^2) \tag{3.10}$$

The (column) vector β maps the (row) vector with independent variables x_i to the dependent variable y_i. The noise is normally distributed with standard deviation σ along the dimension of the dependent variable.

In a 2D point cloud the point p is represented by (x_p, y_p). The points are mapped into an intercept-slope representation through defining $X_i = [1, x_p]$ and $y_i = y_p$. The vector β will then contain the y-intercept as the first value, the slope as the second value.

All observations that belong to the same single line lead to a likelihood function that corresponds to a normally distributed random variable with y and X as parameters:

$$p(y \mid X, \beta, \sigma^2) \propto \sigma^{-n} \exp\left(-\frac{1}{2\sigma^2}(y - X\beta)^T(y - X\beta)\right) \tag{3.11}$$

The dependent variable is now a column vector of values y and each observation has a row of independent variables in X. The vector β and the standard deviation σ are shared across all observations. The term $y - X\beta$ is written out like this:

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} - \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} \tag{3.12}$$

Note that Eq. 3.11 has exactly the same form for a single point or multiple points that belong to the same line. Hence, we have the probability of a point w_i given the line parameters $\theta_k = (\beta_k, \sigma_k)$:

$$F(w_i, \theta_k) = p(w_i \mid \theta_k) = p(w_i \mid \beta_k, \sigma_k^2) = p(y_i \mid X_i, \beta_k, \sigma_k^2) \tag{3.13}$$

To get the full distribution $p(w_i, \beta, \sigma^2)$ we will need also $p(\beta, \sigma^2)$.

3.1.3 Conjugate Prior for a Line

The conjugate prior for the likelihood in Eq. 3.11 is a product of a prior for the standard deviation $p(\sigma)$ and the conditional probability of the line coefficients given the standard deviation $p(\beta \mid \sigma^2)$.

$$p(\sigma^2, \beta) = p(\sigma^2)p(\beta \mid \sigma^2) \tag{3.14}$$

The standard deviation σ is sampled from an Inverse-Gamma (IG) distribution:

$$p(\sigma) \propto (\sigma^2)^{-(\nu_0/2+1)} \exp(-\frac{1}{2\sigma^2} \nu_0 s_0^2) \tag{3.15}$$

This is an $IG(a_0, b_0)$ with $a_0 = \nu_0/2$ and $b_0 = 1/2 \nu_0 s_0^2$. The conditional with respect to the line coefficients has a normal distribution as prior:

$$p(\beta \mid \sigma^2) \propto \sigma^{-n} \exp\left(-\frac{1}{2\sigma^2}(\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0)\right) \tag{3.16}$$

Let us collect $\Lambda_0, \mu_0, a_0, b_0$ into λ_0, we have now a description of our base distribution H:

$$H(\theta_k) = NIG(\theta_k; \lambda_0) \tag{3.17}$$

NIG is an abbrevation of the Normal-Inverse-Gamma distribution. The standard deviation is sampled from the Gamma distribution with a_0 and b_0 as hyperparameters and the line coefficients from a Normal distribution:

$$\begin{aligned} \sigma_k = \tau_k^{-1/2} \qquad \tau_k &\sim \mathcal{G}(a_0, b_0) \\ \mu_k &\sim \mathcal{N}(\mu_0, \sigma^2 \Lambda_0^{-1}) \end{aligned} \tag{3.18}$$

3.1.4 Posterior Predictive for a Line given Data

Due to the fact that it is a conjugate distribution we have a simplified description for updating the parameters at once, given a set of observations. The sufficient statistics are updated (Minka, 2000) according to:

$$
\begin{aligned}
\Lambda_n &= (X^T X + \Lambda_0) \\
\mu_n &= \Lambda_n^{-1}(\Lambda_0\mu_0 + X^T y) \\
a_n &= a_0 + n/2 \\
b_n &= b_0 + 1/2(y^T y + \mu_0^T \Lambda_0\mu_0 - \mu_n^T \Lambda_n\mu_n)
\end{aligned}
\tag{3.19}
$$

Let us collect $\Lambda_0, \mu_0, a_0, b_0$ into λ_0 and $\Lambda_n, \mu_n, a_n, b_n$ into λ_n. Let us collect a set of our observations and $(X, y)_k$ into w_k. The update for the sufficient statistics can then be summarized as:

$$
\lambda_n = U_{ss}(\lambda_0, w)
\tag{3.20}
$$

If we combine this update with sampling θ_k from λ_n according to Eq. 3.17, then we obtain:

$$
p(\theta_k \mid \lambda_0, w_k) \propto F(w_k, \theta_k)H(\theta_k; \lambda_0) = p(\theta_k \mid \lambda_n) = NIG(\theta_k; \lambda_n)
\tag{3.21}
$$

Sampling of $NIG(\theta_k; \lambda_n)$ is as in Eq. 3.18, but with λ_n rather than λ_0.

Let us integrate over θ (through the function H):

$$
Q(w_k, \lambda_0) = \int_\Theta F(w_k, \theta)dH(\theta; \lambda_0)
\tag{3.22}
$$

3.2 Inference for the Infinite Line Model

The posterior predictive for parameters (see Eq. 3.9) combined with observations w_i is described by:

$$
p(\theta_i \mid \theta_{-i}, w_i) \propto r_i H_i(\theta_i) + \sum_{j \neq i} L_{i,j}\delta(\theta_j - \theta_i)
\tag{3.23}
$$

The posterior is proportional (indicated by $\propto$) to three terms. First, the α weighted posterior predictive r_i for a new cluster. Second, the posterior to sample from $H_i(\theta_i)$ with probability r_i. Third, the likelihood of an observation given a line $L_{i,j}$:

$$
r_i = \alpha Q(w_i, \lambda_0) = \alpha \int_\Theta F(w_i, \theta)dH(\theta)
\tag{3.24}
$$

The posterior $H_i(\theta)$ is the normalized product of the prior distribution $H(\theta_i)$ with the likelihood $F(w_i, \theta_i)$ for a single observation w_i.

$$H_i(\theta_i) \propto H(\theta_i)F(w_i, \theta_i) \tag{3.25}$$

$$L_{i,j} = F(w_i, \theta_j) \tag{3.26}$$

Sampling a new cluster parameter from $H_i(\theta_i)$ is done with probability:

$$p(\theta_{new}) = \frac{r_i}{r_i + \sum_{j \neq i} L_{i,j}} \tag{3.27}$$

We can use this to derive the parameters θ_i.

Algorithm 7 Gibbs sampling over parameters θ_i

1: **procedure** GIBBS ALGORITHM 1(w, λ_0, α) ▷ Accepts points w, hyperparameters λ_0, α and returns k line coordinates
2:   **for all** $t = 1 : T$ **do**
3:     **for all** $i = 1 : N$ **do**
4:       $r_i = \alpha Q(w_i, \lambda_0)$ ▷ Posterior predictive of w_i given hyper parameters (Eq. 3.24)
5:       **for all** $j = 1 : N, j \neq i$ **do**
6:         $L_{i,j} = F(w_i, \theta_j)$ ▷ Likelihood for a line given observation (Eq. 3.26)
7:       **end for**
8:       $p(\theta_{new}) = \frac{r_i}{r_i + \sum_{j \neq i} L_{i,j}}$ ▷ Probability of sampling a new parameter (Eq. 3.27)
9:       $u \sim U(0, 1)$
10:       **if** $p(\theta_{new}) > u$ **then** ▷ Sample with probability $p(\theta_{new})$
11:         $\lambda_n = U_{ss}(w_i, \lambda_0)$ ▷ Update sufficient statistics with w_i (Eq. 3.20)
12:         $\theta_i \sim NIG(\theta_i; \lambda_n)$ ▷ Sample θ_i from NIG (Eq. **??**)
13:       **else**
14:         θ_i sampled from existing clusters ▷ Sample old cluster
15:       **end if**
16:     **end for**
17:   **end for**
18:   **return** summary on θ_k for k lines
19: **end procedure**

This Gibbs algorithm is described in its general form before (Neal, 2000) (Algorithm 1). We perform a loop in which for T iterations each θ_i belonging to observation w_i is updated in sequence. First, the posterior predictive for w_i given the hyperparameters $p(w_i \mid \lambda_0)$ is calculated. Second, the likelihood $L_{i,j}$ for all θ_j given w_i (with $j \neq i$) is calculated. Third, the fraction with r_i defines if θ_i will be sampled from a new cluster or if one of the existing clusters will be sampled. Fourth, a new cluster is sampled, the sufficient statistics are updated with information on w_i and thereafter θ is sampled from a Normal-Inverse-Gamma distribution with the updated hyperparameters. That, or an existing cluster will be sampled.
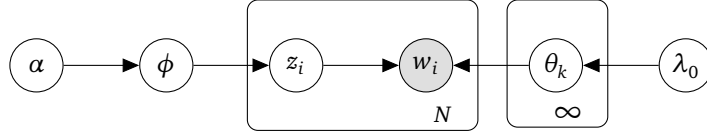
Figure 3.2: The Infinite Line Model in the stick-breaking representation (compare with Fig. 2.8). From left to right: α, the concentration parameter of the Dirichlet Process; $(\phi_1, \ldots, \phi_k)$, the partition of points over lines; z_i, the assignment parameters that link observation w_i with line k; w_i, the observation, an individual point with x and y coordinates; θ_k, the parameters of line k; λ_0, the base measure from which the line parameter values are sampled.

3.3 Accelerating Inference for the Infinite Line Model

It is also possible to iterate only over the clusters. The derivation takes a few steps (Neal, 2000) but leads to a simple update for the component indices that only depends on the number of data items per cluster, the parameter α, and the data at hand.

Algorithm 8 Gibbs sampling over clusters c_k

1: **procedure** GIBBS ALGORITHM 2(w, λ_0, α) ▷ Accepts points w and hyperparameters λ_0 and α, returns k line coordinates
2:    **for all** $t = 1 : T$ **do**
3:       **for all** $i = 1 : N$ **do**
4:          $c = \text{cluster}(w_i)$ ▷ Get cluster c currently assigned to observation w_i
5:          $\lambda_c = \text{downdate}(w_i, \lambda_c)$ ▷ Adjust sufficient statistics for cluster c by removing observation w_i
6:          $m_c = m_c - 1$ ▷ Adjust cluster size m_c (observation w_i removed reduces it with one)
7:          **for all** $k = 1 : K$ **do**
8:             $L_k = m_k \, \text{F}(w_i, \theta_k)$ ▷ Update likelihood for cluster k given observation w_i
9:          **end for**
10:         $r_i = \text{Q}(w_i, \lambda_0)$ ▷ Posterior predictive of w_i given hyper parameters
11:         $p(new) = \frac{r_i}{r_i + \sum_k L_k}$ ▷ Sample new or old?
12:         **if** $p(new)$ **then**
13:             $\lambda_k = U_{ss}(w_i, \lambda_0)$ ▷ Update sufficient statistics with observation w_i
14:             $\theta_i \sim NIG(\lambda)$ ▷ Sample θ_i from NIG
15:         **else**
16:             k sampled from existing clusters
17:             $\lambda_k = \text{update}(w_i, \lambda_k)$ ▷ Restore sufficient statistics with observation w_i
18:         **end if**
19:         $m_k = m_k + 1$ ▷ Increment cluster size m_k
20:       **end for**
21:       **for all** $k = 1 : K$ **do**
22:          $\theta_k \sim NIG(\lambda_k)$ ▷ Sample θ_k from NIG
23:       **end for**
24:    **end for**
25:    **return** summary on θ_k for k lines
26: **end procedure**

The probability to sample from a cluster depends on the number of items in that cluster (except the data item at hand). This is expressed in equation 3.28.

$$p(c_i = c \text{ and } c_i = c_j \text{ and } i \neq j \mid c_{-i}, w_i, \alpha, \theta) \propto \frac{n_{c,-i}}{\alpha + n - 1} F(w_i \mid \theta_i) \tag{3.28}$$

The probability to sample a new cluster only depends on α and the total number of data items. This is described in equation 3.29.

$$p(c_i \in \Omega(c) \text{ and } c_i \neq c_j \text{ and } i \neq j \mid c_{-i}, \alpha) \propto \frac{\alpha}{\alpha + n - 1} \int F(w_i \mid \theta_i) dH(\theta) \qquad (3.29)$$

Here $\Omega(c)$ denotes all admitted values for c_i.

The importance of conjugacy is obvious from Eq. 3.29, it will lead to an analytic form of the integral. The inference method using equations 3.28 and 3.29 is described in section **??**.

Directly sampling over the clusters is described in its general form (Neal, 2000) (Algorithm 2).

Rather than updating each θ_i per observation w_i, an entire cluster θ_k is updated. In Algorithm 7 the update of a cluster would require a first observation to generate a new cluster at θ_j and then moving all observations of the old cluster θ_i to θ_j.

Algorithm 8 follows the same procedure in excluding w_i from calculating the likelihood. This requires the previously mentioned "downdate" from the corresponding sufficient statistics. In Algorithm 8 after all observations have been iterated over and assigned the corresponding cluster k, an outer loop iterates over all clusters to obtain new parameters θ from the NIG prior.

3.4 Performance of the Infinite Line Model

The Infinite Line Mixture Model (see section **??**) is able to fit an infinite number of lines through a point cloud in two dimensions. These lines are no line segments, but infinite lines. However, to test the model a variable number of lines are generated of a length that is considerably larger compared to the spread caused by the standard deviation of points from that line.

As described before, Gibbs sampling leads to correlated samples. We choose to get the Maximum A Posterior estimates for our clusters by picking the median values for all the parameters involved.

3.4.1 Clustering Performance

The results are measured using conventional metrics for clustering performance. For example the Rand Index describes the accuracy of cluster assignments (Rand, 1971):

$$R = \frac{a + b}{a + b + c + d} \qquad (3.30)$$

Here a numbers the pair of points that belong to the same cluster, both at ground truth as well as after the inference procedure. Likewise b numbers the pair of points that belong to different clusters in both sets. The values c and d describe discrepancies between the ground truth and the results after inference. A Rand Index of one means that there have been no mistakes.

The clustering performance is separate from the line estimation performance. If the points are not properly assigned, the line will not be estimated correctly. Due to the fact that line estimation has this secondary effect, this performance is not taken into account. Moreover, from lines that generated only a single, or very few points, we can extract point assignments, but line coefficients are impossible to derive. This would lead to introducing a threshold for the number of points per cluster. Moreover, the performance would then need to be measured by weighting the fitting versus the assignment.

The performance of Algorithm 1 can be seen in Fig. 3.3 and is rather disappointing. On average the inference procedure agrees upon the ground truth for 75% of the cases considering the Rand Index. Moreover, if we adjust for chance as with the Adjusted Rand Index, the performance drops to only having 25% correct!

Algorithm 2 leads to stellar performance measures (Fig. 3.4). Apparently updating entire clusters at once with respect to their parameter values leads at times to perfect clustering, bringing the performance metrics close to their optimal values.

The lack of performance of Algorithm 1 is not only caused by slower mixing (time required to reach the steady state distribution). Also when allowing it ten times the number of iterations of Algorithm 2, it still does not reach the same performance levels. A line seems to form local regions of high probability making it difficult for points to postulate slightly changed line coordinates.

3.4.2   Some Examples

In the following we show a few examples to understand the inference process better. Figure 3.5 shows the assignment after a single Gibbs step in Algorithm 1. There is a single line that is represented by two clusters. Algorithm 1 does not have merge or split steps to group these clusters at once, it thus has to move each data point one by one. By the way, there are split-merge algorithms that take these more sophisticated Gibbs steps into account (Jain and Neal, 2004).

The example in Fig. 3.6 shows that a single point as an outlier is not a problem for our method. A single point might throw off Bayesian linear regression, but because there are multiple lines to be estimated in our Infinite Line Mixture Model, this single point is assigned its own line.

The extension to more points as outliers would of course require us to postulate a distribution for these outlier points as well. A uniform distribution might for example be used in tandem with the proposed model. This however would lead to a non-conjugate model and hence different inference methods.
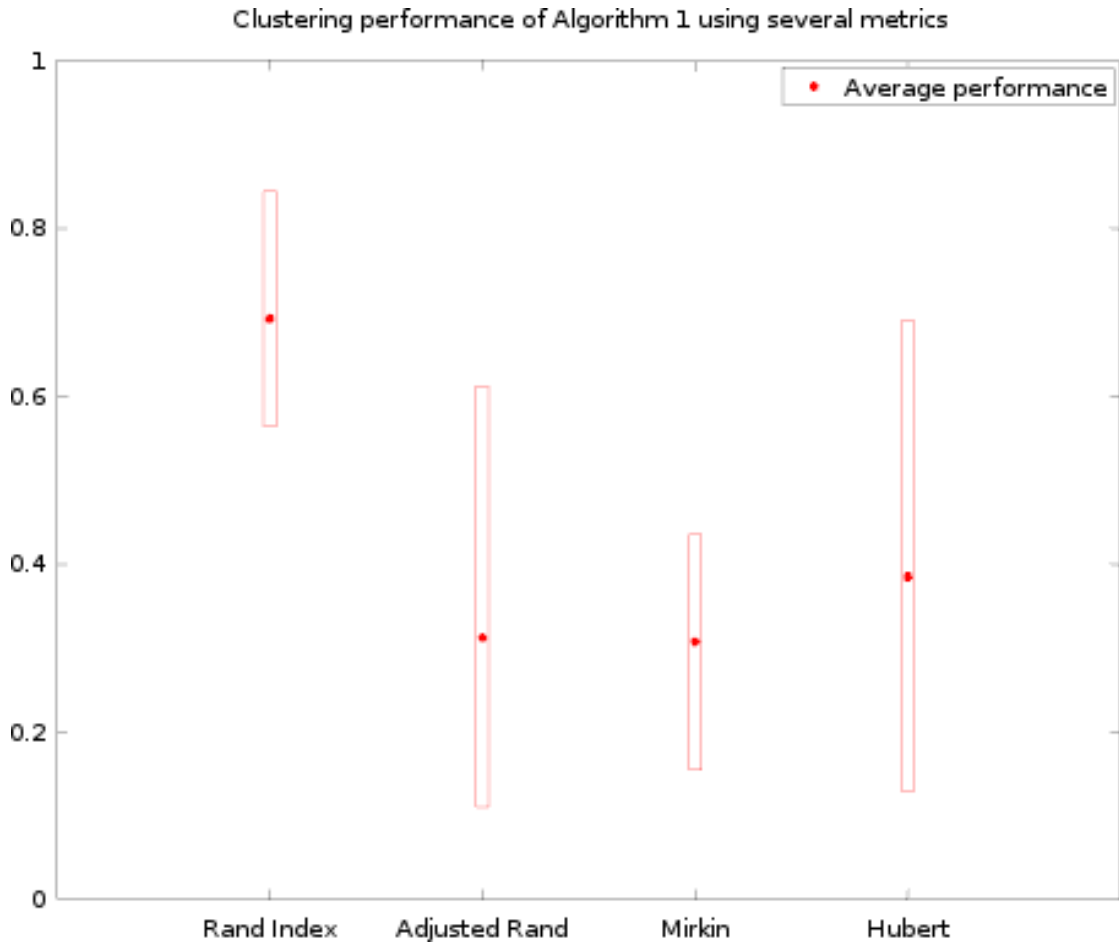
Figure 3.3: The performance of Algorithm 1 with respect to clustering is measured using the Rand Index, the Adjusted Rand Index, the Mirvin metric, and the Hubert metric. A figure of 1 means perfect clustering for all metrics, except Mirvin's where 0 denotes perfect clustering.

3.5 Chapter Conclusions

The Infinite Line Mixture Model that is proposed extends the familiar Bayesian linear regression model to an infinite number of lines using a Dirichlet Process as prior. The model is a full Bayesian method to detect multiple lines. A full Bayesian method, in contrast to ad-hoc methods such as the Hough transform or RANSAC, means optimal inference (Zellner, 1988) given the model and noise definition.

Results in section **??** show high values for difference performance metrics for clustering, such as the Rand Index, the Adjusted Rand Index, and other metrics. The Bayesian model is solved through two types of algorithms. Algorithm 7 iterates over all observations and suffers from slow mixing. The individual updates makes it hard to reassign large number of points at the same time. Algorithm 8 iterates over entire clusters. This allows updates for groups of points leading to much faster mixing. Note, that even optimal inference results in occasional misclassifications. The dataset is generated by a random process. Hence,
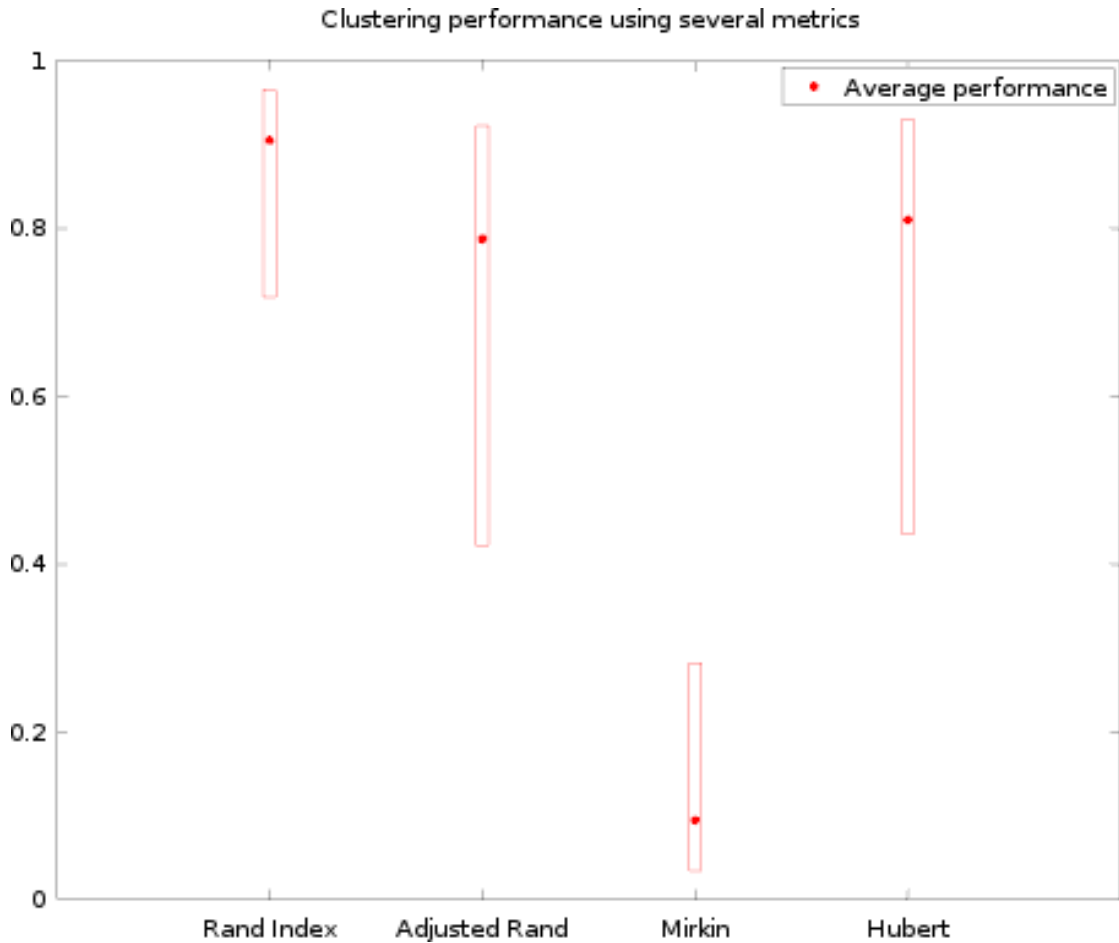
Figure 3.4: The performance of Algorithm 2 with respect to clustering is measured using the Rand Index, the Adjusted Rand Index, the Mirvin metric, and the Hubert metric. A figure of 1 means perfect clustering for all metrics, except Mirvin's where 0 denotes perfect clustering.

occassionally two lines are generated with almost the same slope and intercept. Points on these lines are impossible to assign to the proper line.

The essential contribution in this chapter is the introduction of a fully Bayesian method to infer lines and there are two ways in which the postulated model can to be extended for full-fledged inference in computer vision as required in robotics. First, the extension of lines in 2D to planes in 3D. This is quite a trivial extension that does not change anything of the model except for the dimension of the data points. Second, somehow a prior needs to be incorporated to limit the lines of infinite length, to line segments. To restrict points on the lines to a uniform distribution of points over a line segment, a symmetric Pareto distribution can be used as prior (for the end points). This would subsequently allow for a hierarchical model in which these end points are in their turn part of more complicated objects. Hence, the Infinite Line Mixture Model is an essential step towards the use of Bayesian methods (and thus properly formulated priors) for robotic computer vision.
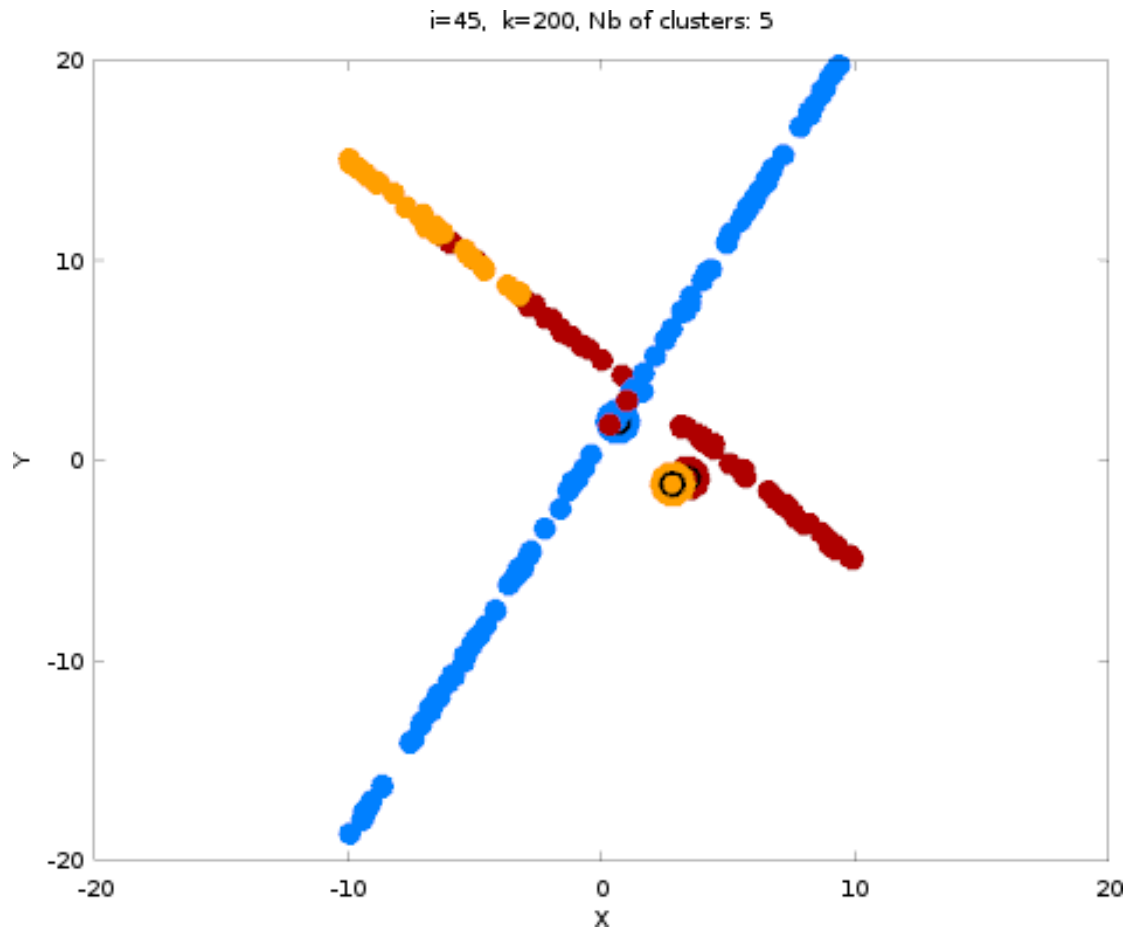
Figure 3.5: One of the Gibbs steps in the inference of two particular lines. The points are more or less distributed according to the lines, but one line exists out of two large clusters. The line coordinates are visualized by a double circle. The x-coordinate is the y-intercept of the line, the y-coordinate is the slope.
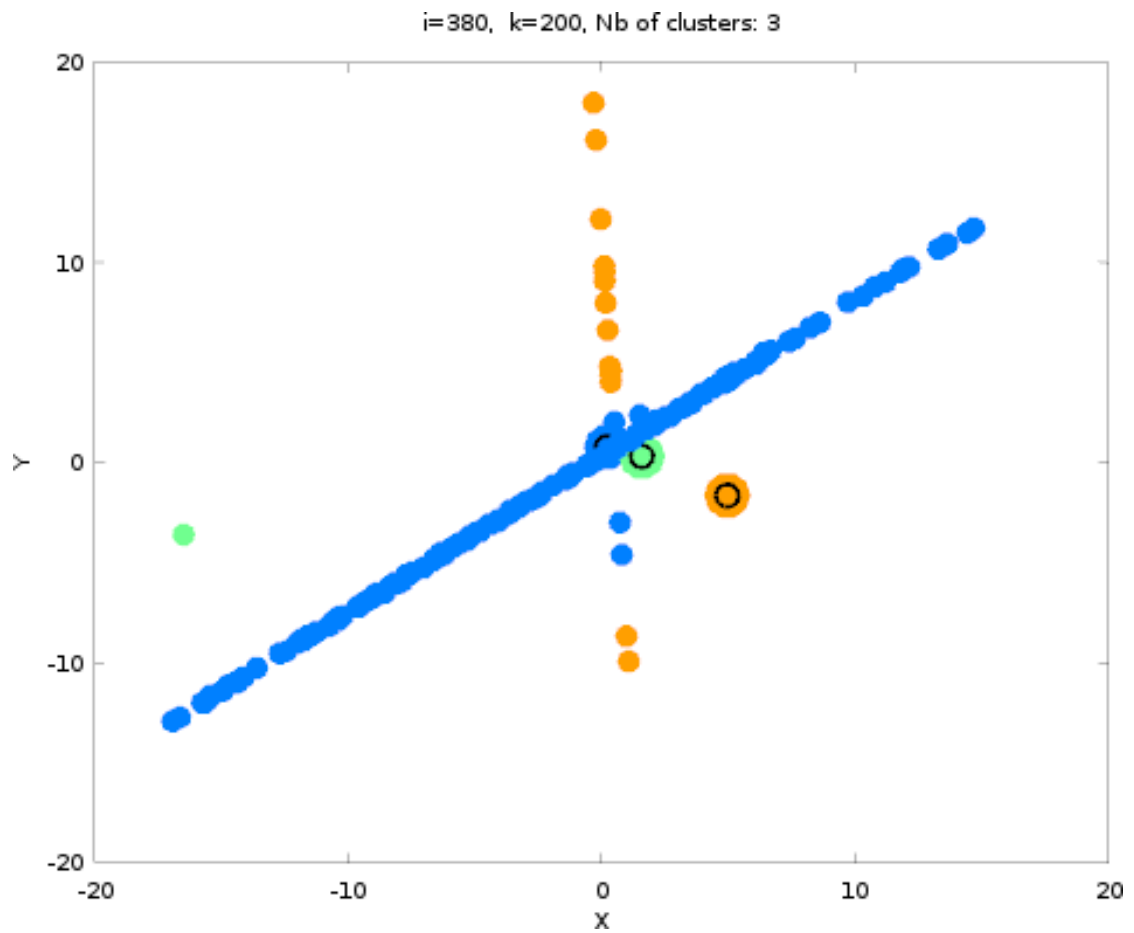
Figure 3.6: The assignment of a line to a single point. There are three clusters found, rather than only the obvious two.

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NONPARAMETRIC BAYESIAN SEGMENT ESTIMATION

Contents　The nonparametric Bayesian model for line estimation (Chapter 3) does not take into account lines that are of finite length. In this chapter, we introduce a Bayesian method to perform inference over such line segments. In this model our prior for the extend of the line segment is a symmetric Pareto distribution. Due to the fact that the prior and likelihood is not a conjugate pair a more general inference method is used, namely Gibbs sampling with auxiliary variables.

Published in　A.C. van Rossum, H.X. Lin, J. Dubbeldam, and H.J. van den Herik. Nonparametric Segment Detection. *Proceedings of the Eighth European Starting AI Researcher Symposium*, STAIRS 2016, The Hague, Netherlands, August 26-September 2, 2016.

Outline　The model is using a Normal-Inverse-Gamma and a Pareto prior for an individual line segment (Sect. 4.1). These line segments are generated using a Dirichlet Process (Sect. 4.2). This generative process is used to perform inference using Gibbs sampling over auxiliary variables (Sect. 4.3). The results for inference over line segments are compared with these for lines. (Sect. 4.4). Finally, weak aspects of the current MCMC method are established (Sect. 4.5) which will form the basis for new inference methods in the next chapters.

4.1　Pareto pairs

.

Lines in a two-dimensional space are mathematical objects that can be described by two parameters. To limit a line to a line segment, four parameters are required. There are

two parametrizations that come to mind. First, a center-point parametrization, in which parameters describe the center of a line segment, the slope of the line through the center, and the size of the line segment. Second, an endpoint parametrization, in which parameters describe the locations of the two endpoints. These parametrizations are equivalent, but generalizations can be intuitive or cumbersome. The generalization to a line segment from a two-dimensional space to a three-dimensional space, requires the endpoints to be positions in a 3D space. The center-point parametrization would require a nonintuitive description of the angles in particular directions. The generalization to squares and rectangles or shapes with many endpoints, might benefit from the center-point parametrization.

There seems to be no statistical description of data points distributed over a line segment that has a conjugate prior form. A line segment itself, however, has a conjugate form! Suppose that we have a prior for the location of endpoints on the x-axis. Given the data we want to update the location of the endpoints. By leaving out the spread of the data over the segment, we can do this using a conjugate Bayesian construction.

The data is distributed according to a symmetric uniform distribution. Hence the likelihood is given by:

$$p(x \mid a) \sim \mathcal{U}(-a, a) = \begin{cases} \frac{1}{2a} & \text{for } x \leq |a| \\ 0 & \text{otherwise} \end{cases} \tag{4.1}$$

Here the uniform distribution is centered around 0 and extends with size a in both directions. It is possible to shift the entire distribution with b. For now, let's continue with one endpoint at a and one endpoint at $-a$.

A prior for the (endpoints of a) symmetric uniform distribution is a symmetric Pareto distribution:

$$p(a) \sim \mathcal{P}_s(\lambda, k) = \begin{cases} \frac{1}{2} k \lambda^k |a|^{-k-1} & |a| \geq \lambda \\ 0 & \text{otherwise} \end{cases} \tag{4.2}$$

The factor $\frac{1}{2}$ stems from the fact that the symmetric Pareto distribution is now mirrored across the y-axis. Hence, the probability density is half of that of the normal Pareto distribution for the positive x-axis.

If we would just sample from a symmetric Pareto distribution, we can sample multiple times from the positive x-axis. To actually sample endpoints of segments we have to sample pairs of points.

$$p(a, b) \sim \mathcal{P}_p(\lambda_m, \lambda_n, k) \tag{4.3}$$

We can describe this process as first sampling a and b from a categorical distribution to decide which one will be the left endpoint and which one the right endpoint. Then we sample the right endpoint from a normal Pareto distribution and the left endpoint from a mirrored Pareto distribution.

The sampling of Pareto pairs is visualized in Fig. 4.1.
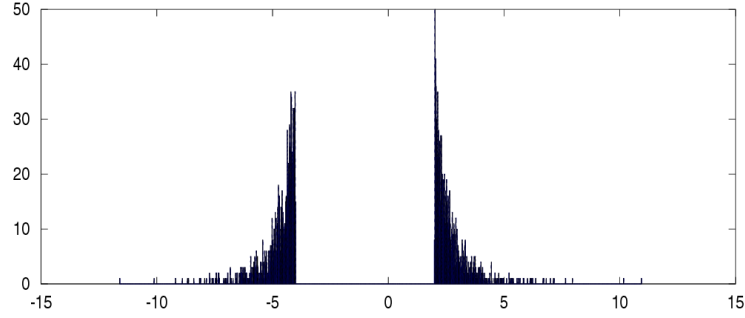
Figure 4.1: Sampling of Pareto pairs. The parameters are $\lambda_m = 2$, $\lambda_n = -2$, $k = 5$, and we have sampled $N = 1000$ pairs.

The Pareto distribution is a conjugate prior for the uniform distribution, with updated hyperparameters:

$$p(a \mid D) = \mathscr{P}(c, N + k) \qquad (4.4)$$

The data is denoted by $D = \{x_0, \ldots, x_{N-1}\}$, the parameter k is adjusted with the number of data points N, and the parameter c is the maximum of $\{m, \lambda\}$ with m the maximum value in D.

Given this description for the posterior for a single point, the posterior for a Pareto pair can be found by sampling in parallel from a Pareto distribution $\mathscr{P}(c_n, N + k_n)$ with c_n the maximum of the data points D and λ_n, N the number of Pareto pairs, and k_n the hyperprior for the endpoint at the right. Plus sampling fom a Pareto distribution $\mathscr{P}(c_m, N + k_m)$ with c_m the minimum of the data points D and λ_m, N the same, and k_m the hyperprior for the endpoint at the left.

If $k_n \neq -k_m$ the distribution is shifted such that $k'_n = -k'_m$. This makes the form of the probability distribution symmetric with respect to the y axis. In the end the results are shifted back. This transformation makes sense for pairs of points. We do not want the two scale parameters of the Pareto distribution to influence the symmetry of the overall distribution.

Sampling from the Pareto distribution is through inverse transform sampling. By sampling from $U(0, 1)$ with 1 included, we transform according to $k/U^{1/a}$.

Fig. 4.2 shows how the endpoints are updated given the data. An uninformative prior is used. In this case the hyperparameters k_n and k_m are set close to 0, thus the data will wash out the prior immediately. Naturally, it is possible to set them quite large. In that case it
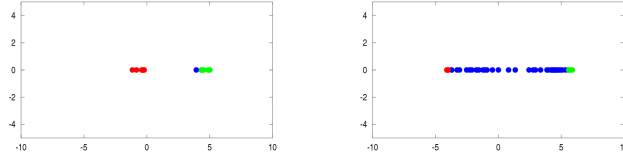
Figure 4.2: Consider the data uniformly distributed on a line segment and a symmetric Pareto prior for both the endpoints, then we can update the estimate for the endpoints given the data as visualized. Each subfigure shows an adjustment of the endpoints given more data points (1, 3, 10, and 100 data points).
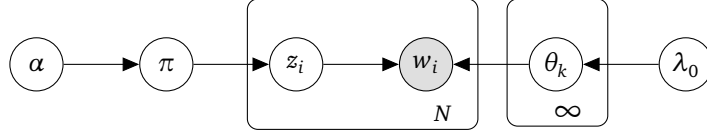
Figure 4.3: The Bayesian linear regression model for multiple line segments in plate notation is the same as for the Infinite Line Model. The Dirichlet process is defined at the left with concentration parameter α. It generates the partitions $(\pi_1, \ldots, \pi_k)$ with assignment parameters z_i that denote which observation w_i belongs to which cluster k. The cluster is summarized through the parameter set θ_k and has λ_0 as its hyperparameter. The parameter set θ_k includes parameters that signify the line itself such as slope and y-intercept, plus the parameters that denote the extend of the segment.

must be noted that the data will never be able to "correct for" this prior. Note also that the maximum and minimum operators are quite sensitive to outliers as well.

4.2 Generative Process to Create a Line Segment

To be able to perform inference over a line segment in a two-dimensional space, we'll have to map somehow these points to a one-dimensional space.

In the case of a line we can sample θ_i from a Normal-Inverse-Gamma with hyperparameter λ_{temp}. The latter we have in closed form given observations through a single update.

In the case of a line segment there is no known conjugate prior available. Let's reiterate the Dirichlet Process basis for our nonparametric model:

$$G \sim DP(\alpha, H)$$
$$\theta_i \mid G \sim G \tag{4.5}$$
$$w_i \mid \theta_i \sim F(\theta_i)$$

Again F describes the mapping from parameters θ_i to observations w_i. As described, for line segments this mapping is different from that of lines.

$$F(\theta_i) = \mathcal{N}(\mu_i + H(\nu_i), \Sigma_i)$$
$$H(\nu_i) = \mathcal{N}(\nu_i, 1)\gamma_i \tag{4.6}$$
$$\gamma_i \sim \mathcal{N}(0, 1)$$

The probability density F is a Gaussian with a mean that is additively distributed according to another distribution H. The latter distribution originates from the product of a normal distribution with a value sampled from a normal distribution. Fig. 4.4 shows how points are generated from the described distribution.
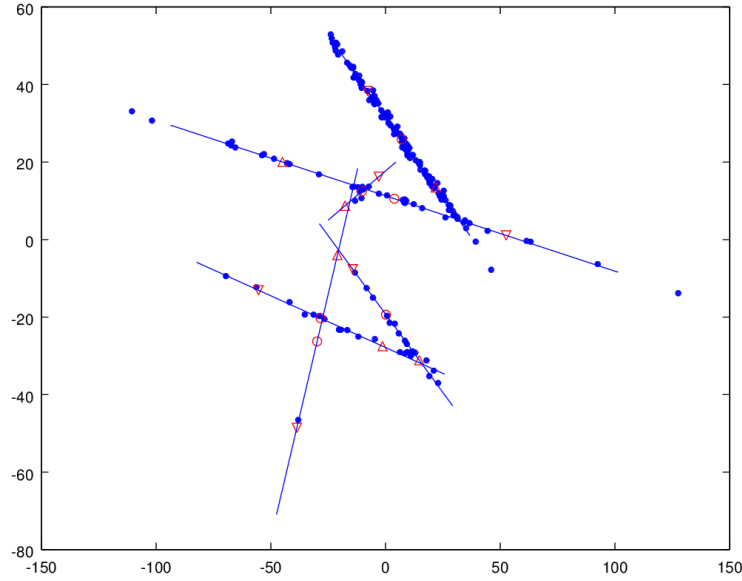
Figure 4.4: Line segments generated through a Dirichlet Process. The Dirichlet Process itself is again the same. But now four parameters are generated. A normal-inverse-Wishart distribution is used to generate the center of the line segment, and an inverse-Wishart distribution to generate one of the endpoints of the line segments (the other end point is mirrored through its center). Points are generated normally over the line segments, with an additional Gaussian component to indicate the deviation from the line segment from the normal-inverse-Wishart.

To generate lines uniformly, only γ_i needs adjustment:

$$F(z_i) = \mathcal{N}(\mu_i + H_i(\nu_i), \Sigma_i)$$
$$H(\nu_i) = \mathcal{N}(\nu_i, 1)\gamma_i \qquad (4.7)$$
$$\gamma_i \sim \mathcal{U}(-1, 1)$$

Fig. 4.5 displays the adjustment with points generated uniformly over the line segment.

The descriptions in Eq. 4.6 and 4.7 are clearly not conjugate setups. This means that inference over line segments requires more complicated sampling strategies.

4.3 Inference over a Line Segment

To perform inference over a line segment our model is not conjugate anymore. This requires a sampling algorithm that does not make use of conjugacy. An algorithm that does
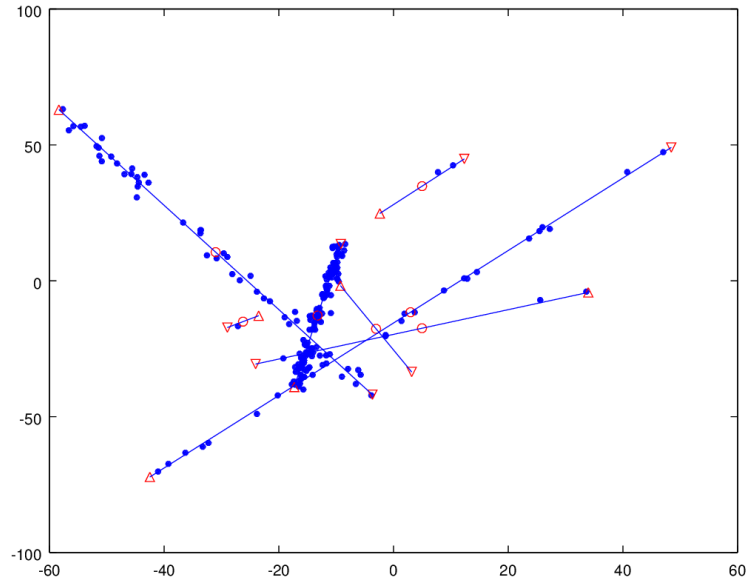
Figure 4.5: Line segments generated through a Dirichlet Process. Compared to Fig. 4.4 the points are generated uniformly over the line segments: points are not generated outside of the line segments.

not assume conjuacy is described in its general form before (Neal, 2000) (Algorithm 8). The sampling process proposes m new values for the parameters directly from the hyperparameters. These are called auxiliary parameters. Now, to establish to which cluster a certain observation w_i need to be assigned, the likelihood of each existing and new clusters alike are compared. The weight of an old cluster is defined through the number of data points assigned to it. The weight of a new cluster is defined through $alpha/m$.

After every data item is assigned a cluster, the cluster parameters themselves are updated given the assigned data items. In a conjugate model the sufficient statistics can be updated at once, given such observations. In a nonconjugate model we will need to update θ_j by sampling from $p(\theta_j \mid y)$.

Algorithm 9 Gibbs sampling over auxiliary variables (a θ_i)

1: **procedure** Gibbs Algorithm with auxiliary variables(w, λ_0, α) ▷ Accepts points w, hyperparameters λ_0, α, number of auxiliary variables m, and returns k line coordinates
2:     **for all** $t = 1 : T$ **do**
3:         **for all** $i = 1 : N$ **do**
4:             **for all** $j = 1 : m$ **do**
5:                 $\theta_j \sim NIG(\lambda_0)$ ▷ Sample θ_j from NIG
6:             **end for**
7:             **for all** $j = 1 : K + m, j \neq i$ **do**
8:                 $L_j = \text{likelihood}(w_i, \theta_j)$ ▷ Update likelihood for all theta (except θ_i) given observation w_i
9:             **end for**
10:             $P_{-i=1:K} = b \sum_{-i} L_{-i}$ ▷ Calculate probability of existing cluster
11:             $P_{-i=K:K+m} = b\alpha/mL_mL_{-i}$ ▷ Calculate probability of new cluster
12:             $\theta_i = \theta_j$ according to above P_{-i} ▷ Sample θ_i accord. to above prob
13:             Remove unused clusters
14:         **end for**
15:         **for all** $j = 1 : K$ **do**
16:             $\theta_j \sim p(\theta_j \mid y)$ ▷ Update θ_j
17:         **end for**
18:     **end for**
19:     **return** summary on θ_k for k line segments
20: **end procedure**

4.4 Results
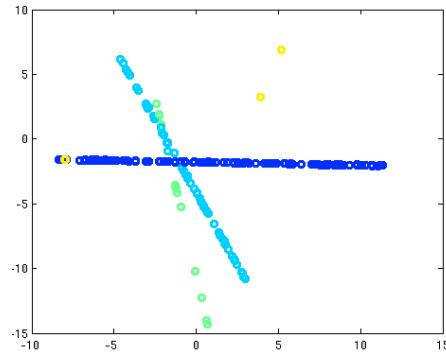
(a) Correctly sampled. Only one outlier to the left.
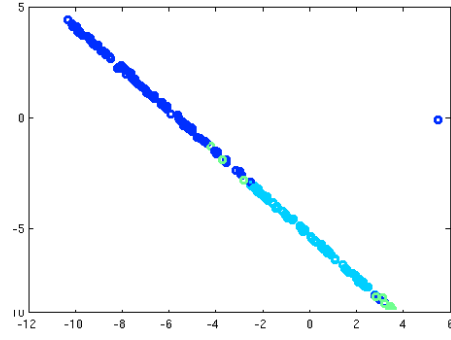
(b) Incorrectly sampled. The line is recognized as multiple segments.
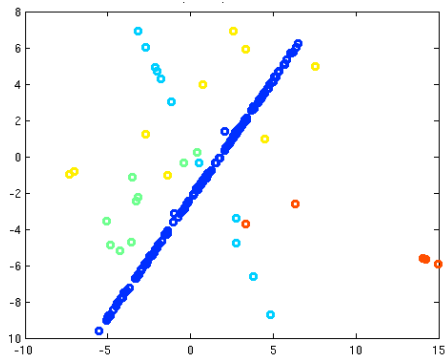
(c) More or less correct. The segments with fewer observations are recognized poorly.
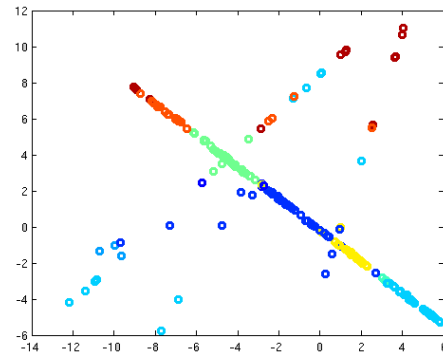
(d) Completely incorrect. Line segments are chosen to be orthogonal to the lines.

Figure 4.6: Bayesian point estimates of the sampling process with varying outcomes.

There is one phenomenon that is very noticable in Fig. 4.6. Line segments that form a larger line segment are not recognized as such by the inference method.

The results over a larger dataset can be measured with clustering metrics as visualized in Fig. 4.7. The Rand Index, Adjusted Rand Index, and Hubert metrics show all reduced performance compared to line detection where there are no constraints on segment size.

(a) Segment detection.

(b) Line detection.

Figure 4.7: Segment detection performs much worse than line detection across all three clustering performance indicators. Perfect clustering is indicated by 1.0 for Rand Index, Adjusted Rand Index, and Hubert.

4.5 Chapter Conclusions

Segment estimation is a much harder problem than line estimation (Chap. 3). In this chapter we used an advanced method, namely MCMC sampling with auxiliary variables to perform inference over an infinite set of line segments. The parameters for line segments do not have a conjugate description. Metropolis-Hastings has been used to perform inference over the line segments, but the search space is quite large. The auxiliary variable MCMC method is indeed faster than ordinary Metropolis-Hastings thanks to postulating multiple new lines than only one.

However, the segment estimation problem is a challenge for the current inference methods. The target probability density has a lot of modes that each needs to be found and are separated by very low probability regions. In Chapter 5 we will introduce new sampling methods that will cope with these challenges.

TRIADIC SPLIT-MERGE SAMPLER

Contents   The nonparametric Bayesian model for line estimation, the infinite line model (Chapter 3) thanks to its conjugate properties has been solved with moderately straightforward sampling methods. The additional constraints that limit lines to line segments (Chapter 4) reduced convergence of the underlying MCMC sampling method (a Gibbs method with auxiliary variables) to sub-par results.

   This chapter introduces a new sampling method called the triadic split-merge sampler.

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Outline   The class of split-merge samplers, part of MCMC samplers, are introduced (Sect. 5.1). A conventional split-merge sampler, labeled the dyadic split-merge sampler is detailed (Sect. 5.2). The new split-merge sampler, the triadic split-merge sampler is introduced (Sect. 5.3). The results for inference over lines is compared between the conventional and the new sampler (Sect. 5.4). Finally, although this sampler already improves on the state-of-the-art we see in the chapter conclusions (Sect. 5.5) how we further improve the inference procedure, which will be the basis of the next chapter.

5.1   Introduction

We will consider a Dirichlet process as a prior on the distribution over parameters G. The form of this model is:

$$y_i|\theta_i \sim F(\theta_i)$$
$$\theta_i|G \sim G \qquad\qquad (5.1)$$
$$G \sim DP(H, \alpha)$$

5.2 Conventional split-merge sampler

The conventional split-merge sampler Jain and Neal (2004) splits a single cluster into two clusters, and merges two clusters into a single cluster. Hence, this split-merge sampler operates on two clusters at each time step, for which reason we will call it a dyadic split-merge sampler in constrast with our approach.

Algorithm 10 Dyadic split-merge sampler

1: **procedure** DYADIC SPLIT-MERGE SAMPLER(c)　　　　　▷ Accepts cluster assignments c of length N (besides Metropolis-Hastings acceptance factors $a(c', c)$ and a split procedure e.g. SIMPLERANDOMSPLIT) and returns a (potentially) updated cluster assignment vector c'.

2:　　$i \sim U(1, N)$　　　　　　　　　　　▷ Sample i random uniformly over cluster assignments.

3:　　$j \sim U(1, N) \cap i$　　　　　　　　　　▷ Sample j also random uniformly, but with $j \neq i$.

4:　　$S_R = \{c_i, c_j\}$　　　　　　　　　　　　　　　▷ Sampled clusters c_i, c_j.

5:　　$S_I = \{c_x\}$ with $c_x \in S_R$ for $x \in \{1, \ldots, N\}$　　　　　▷ All data in clusters c_i, c_j.

6:　　$S_E = S \cap S_R$　　　　　　　　　　　▷ All data in clusters c_i, c_j excluding S_R.

7:　　$N_S = \text{unique}(S_R)$

8:　　**if** $N_S = 1$ **then**　　　　　　　　　　▷ Case: i, j belong to the same cluster.

9:　　　　$c_i^{(2)} = c_k$ with $c_k \notin \{c_1, \ldots, c_N\}$　　　　　　▷ Sample new cluster for $c_i^{(2)}$.

10:　　　　$c_j^{(2)} = c_j^{(1)}$　　　　　　　　　　　　　▷ Keep c_j the same.

11:　　　　$c_e^{(2)} = \text{SPLITPROCEDURE}(S_E, c_i^{(2)}, c_j^{(2)})$　　　　▷ After $c_i^{(2)}, c_j^{(2)}$ assign S_E.

12:　　　　**for all** $m \notin S_I$ **do**

13:　　　　　　$c_m^{(2)} = c_m^{(1)}$　　　　　▷ Data points in clusters other than c_i, c_j are not adjusted.

14:　　　　**end for**

15:　　　　$c' = \{c_i^{(2)}, c_j^{(2)}, c_e^{(2)}, c_m^{(2)}\}$

16:　　　　$a = a_{split}(c', c)$ according to Eq. 5.3　　　　　▷ MH acceptance for a split.

17:　　**else**　　　　　　▷ Case: i, j belong to different clusters $c_i \neq c_j$ ($N_S = 2$).

18:　　　　**for all** $q \in S_I$ **do**

19:　　　　　　$c_q^{(1)} = c_j^{(2)}$　　　　　　　　　▷ Assign all data points in c_i and c_j to c_j.

20:　　　　**end for**

21:　　　　**for all** $m \notin S_I$ **do**

22:　　　　　　$c_m^{(1)} = c_m^{(2)}$　　　　▷ Data points in clusters other than c_i, c_j are not adjusted.

23:　　　　**end for**

24:　　　　$c' = \{c_q^{(1)}, c_m^{(1)}\}$

25:　　　　$a = a_{merge}(c', c)$ according to Eq. 5.10　　　　　▷ MH acceptance for a merge.

26:　　**end if**

27:　　$u \sim U(0, 1)$　　　　　　　　　　　▷ Sample u between 0 or 1 uniformly.

28:　　**if** $a < u$ **then**

29:　　　　$c' = c$　　　　　　　　　　　　▷ Reject c' by setting it to c

30:　　**end if**

31:　　**return** c', the (updated) cluster assignment vector: $c \to c'$.

32: **end procedure**

In algorithm 10 the notation $c_i^{(2)}$ is used to signify that the cluster assignment c_i has 2 clusters under consideration. In the dyadic algorithm we could have used c_i^{merge} and c_i^{split}, however in the triadic algorithm (see algorithm 13) with multiple split and merge operations the latter notation would become confusing.

Algorithm 11 Simple random split

1: **procedure** SIMPLERANDOMSPLIT(S, c_0, c_1)   ▷ Accepts unassigned set S and cluster indices c_0, c_1, returns cluster assignment c_m'.
2:     **for all** $m \in S$ **do**
3:         $c_m' \sim Cat(c_0, c_1)$ with equiprobable $p(c_0) = p(c_1) = \frac{1}{2}$.
4:     **end for**
5:     **return** c_m', the cluster assignment for S.
6: **end procedure**

The dyadic split-merge sampler in Algorithm 10 samples two distinct data items. If the data items belong to the same cluster a split step is attempted. If the data items belong to different clusters a merge step is attempted. The split procedure itself is the so-called simple random split (Algorithm 11) that assigns data items with the same probability to one of the parts of the splitted cluster without consideration for data fit.

5.2.1   Acceptance for the split step

The acceptance ratio contains the Metropolis ratio to step from c to c':

$$\frac{P(c')L(c'|y)}{P(c)L(c|y)} \tag{5.2}$$

Additionally, the Hastings correction is applied because of the asymmetry of the proposal distribution in the form of $q(c|c')/q(c'|c)$:

$$a_{split}(c^{(2)}, c^{(1)}) = \min\left[1, \frac{q(c^{(1)}|c^{(2)})}{q(c^{(2)}|c^{(1)})} \frac{P(c^{(2)})}{P(c^{(1)})} \frac{L(c^{(2)}|y)}{L(c^{(1)}|y)} \right] \tag{5.3}$$

The notation $c^{(2)}$ is used to indicate that the cluster index vector is referencing 2 unique clusters (in this case after the split step).

The prior distribution is represented by a Chinese Restaurant Process with concentration parameter α and no discount factor. Data not yet assigned is assigned with probability $\alpha/(n+\alpha)$ to a new cluster and with probability $n_c/(n+\alpha)$ to an existing cluster c. Here n are the total number of assigned data points, n_c are the number of data points assigned to cluster c. There are D clusters. Hence, the prior over clusters:

$$P(c) = \frac{\Gamma(\alpha)}{\Gamma(\alpha+n)} \alpha^D \prod_{c_l} \Gamma(n_{c_l}) = \alpha^D \frac{\prod_{c_l}(n_{c_l}-1)!}{\prod_{k=1}^n(\alpha+k-1)} \tag{5.4}$$

In the prior distribution ratio before and after the split step many of the factors drop out. There is one factor α remaining and the number of data points in the splitted cluster is part

of the equation. There is no dependency on other clusters or the total number of data points and we can simplify the formula using the beta function $B(a, b)$:

$$\frac{P(c^{(2)})}{P(c^{(1)})} = \alpha \frac{(n_{c_i^{(2)}} - 1)!(n_{c_j^{(2)}} - 1)!}{(n_{c_i^{(1)}} - 1)!} = \alpha B(n_{c_i^{(2)}}, c_j^{(2)}) \tag{5.5}$$

The likelihood can be written as:

$$L(c|y) = \prod_{c=1}^{D} \prod_{k:c_k=c} p(y_k|\phi) \tag{5.6}$$

Here we assume no conjugacy between $F(y_k, \phi)$ and prior distribution $H(\phi)$ and hence write $p(y_k|\phi)$ rather than the conjugate construction $\int F(y_k, \phi)dH_{k,c}(\phi)$ (see Dahl (2005)). The likelihood ratio becomes:

$$\frac{L(c^{(2)}|y)}{L(c^{(1)}|y)} = \frac{\prod_{k:c_k^{(2)}=c_i^{(2)}} p(y_k|\phi) \prod_{k:c_k^{(2)}=c_j^{(2)}} p(y_k|\phi)}{\prod_{k:c_k^{(1)}=c_i^{(1)}} p(y_k|\phi)} \tag{5.7}$$

The split step determines the probability of a particular split. Given that already two data points are assigned to distinct clusters, only the remaining ones have to be assigned with equal probability to $c_i^{(2)}$ and $c_j^{(2)}$:

$$q(c^{(2)}|c^{(1)}) = \left(\frac{1}{2}\right)^{-2+n_{c_i^{(2)}}+n_{c_j^{(2)}}} = \left(\frac{1}{2}\right)^{-2+n_{c_i^{(1)}}} \tag{5.8}$$

The probability of the reverse of the split operation is exactly 1. There is only one way in which a single cluster could have risen from a split cluster, hence:

$$\frac{q(c^{(1)}|c^{(2)})}{q(c^{(2)}|c^{(1)})} = \frac{1}{\left(\frac{1}{2}\right)^{n_{c_i^{(2)}}+n_{c_j^{(2)}}-2}} = 2^{-2+n_{c_i^{(1)}}} \tag{5.9}$$

5.2.2 Acceptance for the merge step

Acceptance of a merge step consists of the same components as that of the split step.

$$a_{merge}(c^{(1)}, c^{(2)}) = \min\left[1, \frac{q(c^{(2)}|c^{(1)})}{q(c^{(1)}|c^{(2)})} \frac{P(c^{(1)})}{P(c^{(2)})} \frac{L(c^{(1)}|y)}{L(c^{(2)}|y)}\right] \tag{5.10}$$

$$\frac{P(c^{(1)})}{P(c^{(2)})} = \alpha^{-1} \frac{(n_{c_i^{(1)}} - 1)!}{(n_{c_i^{(2)}} - 1)!(n_{c_i^{(2)}} - 1)!} = \frac{1}{\alpha B(n_{c_i^{(2)}}, c_j^{(2)})} \tag{5.11}$$

$$\frac{L(c^{(1)}|y)}{L(c^{(2)}|y)} = \frac{\prod_{k:c_k^{(1)}=c_i^{(1)}} p(y_k|\phi)}{\prod_{k:c_k^{(2)}=c_i^{(2)}} p(y_k|\phi) \prod_{k:c_k^{(2)}=c_j^{(2)}} p(y_k|\phi)} \tag{5.12}$$

$$\frac{q(c^{(2)}|c^{(1)})}{q(c^{(1)}|c^{(2)})} = \left(\frac{1}{2}\right)^{-2+n_{c_i^{(1)}}} = 2^{2-n_{c_i^{(1)}}} \tag{5.13}$$

The ratios of the merge step are the inverse of the ratios of the split step.

5.2.3 Sequentially-Allocated Merge-Split sampler

A variant on the conventional split-merge sampler is the Sequentially Allocated Merge-Split[1] (SAMS) sampler Dahl (2003). The simple random split procedure of Algorithm 11 is replaced by a procedure that sequentially assigns observations to clusters rather than splitting the data random uniformly over the splitted clusters.

Algorithm 12 Sequentially Allocated Merge-Split

1: **procedure** SAMS(S, c_0, c_1) ▷ Accepts unassigned set S, cluster indices c_i, and $p(y_k|\theta_{c_i})$ with $i = 0, 1$, returns cluster assignment c'_m.
2:    $T = \text{random\_shuffle}(S)$
3:    **for all** $m \in T$ **do**
4:        $p(c_m = c_0|c_0, c_1, \theta_{c_0}, \theta_{c_1}) = \frac{N_0 p(y_k|\theta_0)}{N_0 p(y_k|\theta_0) + N_1 p(y_k|\theta_1)}$
5:        $p(c_m = c_1|c_0, c_1, \theta_{c_0}, \theta_{c_1}) = 1 - p(c_m = c_0|c_0, c_1, \theta_{c_0}, \theta_{c_1})$
6:        $c'_m \sim p(c_m|c_0, c_1, \theta_{c_0}, \theta_{c_1})$
7:    **end for**
8:    **return** c'_m, the cluster assignment for S.
9: **end procedure**

In contrast to the simple random split, observations y_k are used in the SAMS to obtain cluster assignments that correspond with the data rather than cluster assignments independent of the data.

5.3 Triadic split-merge sampler

The triadic split-merge sampler uses up to three clusters for a split or merge step (Fig. 5.1).
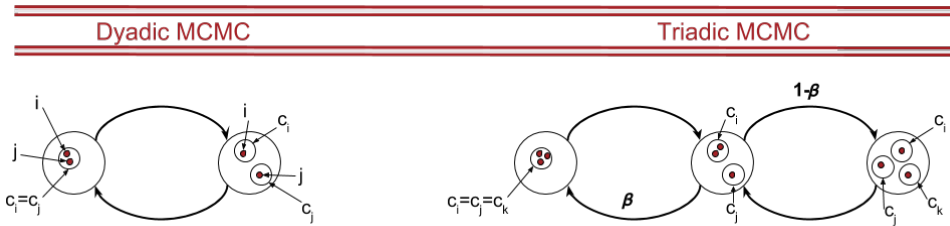
Figure 5.1: Right: dyadic MCMC picks two data items i, j random uniformly. If both are in the same cluster a split towards two clusters is attempted. If both are in distinct clusters a merge towards one cluster is attempted. Left: triadic MCMC picks three data items i, j, k random uniformly. If all three are in the same cluster a split towards two clusters is attempted. If the three items are in two clusters either a split into three (with probability $1 - \beta$) or a merge into a single cluster (with probability β) is attempted. If the three data items are in three distinct clusters a merge is attempted. There are no direct transitions from a single cluster to three clusters or the other way around.

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[1]In the naming of split-merge or merge-split samplers, the order of merge split does not bear any significance.

The intuition behind the triadic split-merge sampler is twofold:

- In the dyadic sampler there is a large asymmetry between split and merge steps. There is only one way in which two clusters can be merged into one single cluster, while there are many ways in which one single cluster can be split into two clusters. This asymmetry is reduced by transitioning between two and three clusters. This is a straightforward improvement in balancing split and merge steps (for alternatives, see Wang and Russell (2015)).

- In practical optimization problems it might be useful to form a third cluster out of subsets of two other clusters. The dyadic MCMC sampler requires immediate steps in which (1) one of these clusters is split into two, (2) the other is split into two, and (3) the two new clusters are merged. This means that (a) mixing and hence convergence will be slow and (b) the intermediate steps might have very low probability and function as an unnecessary barrier between high probable states.

Sampling random uniformly for three unique items is implemented through a random shuffle algorithm, in particular the modern version of the Fisher-Yates shuffle introduced by Durstenfeld Durstenfeld (1964) and picking the first three items.

5.3.1 Acceptance for the split step

In the triadic split-merge sampler there are two splitting steps. It is possible to split according to the dyadic split-merge sampler. However, given two clusters there are (split) jumps to three states as well as (merge) jumps to single states again. To account for this asymmetry another Hastings correction is applied to establish detailed balance.

$$a_{split}(c^{(2)}, c^{(1)}) = \min\left[1, \frac{r(c^{(1)}|c^{(2)})}{r(c^{(2)}|c^{(1)})} \frac{q(c^{(1)}|c^{(2)})}{q(c^{(2)}|c^{(1)})} \frac{P(c^{(2)})}{P(c^{(1)})} \frac{L(c^{(2)}|y)}{L(c^{(1)}|y)}\right] \tag{5.14}$$

Here we have one additional term compared to the split step from one cluster to two clusters:

$$\frac{r(c^{(1)}|c^{(2)})}{r(c^{(2)}|c^{(1)})} = \frac{\beta}{1} \tag{5.15}$$

The parameter β is free to control, as long as $0 < \beta < 1$ (to maintain ergodicity). The transition from two states to three states is another split step:

$$a_{split}(c^{(3)}, c^{(2)}) = \min\left[1, \frac{r(c^{(2)}|c^{(3)})}{r(c^{(3)}|c^{(2)})} \frac{q(c^{(2)}|c^{(3)})}{q(c^{(3)}|c^{(2)})} \frac{P(c^{(3)})}{P(c^{(2)})} \frac{L(c^{(3)}|y)}{L(c^{(2)}|y)}\right] \tag{5.16}$$

The fraction with r:

$$\frac{r(c^{(2)}|c^{(3)})}{r(c^{(3)}|c^{(2)})} = \frac{1}{1-\beta} \tag{5.17}$$

Algorithm 13 Triadic split-merge sampler

1: **procedure** TRIADIC SPLIT-MERGE SAMPLER(c) ▷ Accepts cluster assignments c of length N (besides Metropolis-Hastings acceptance factors $a(c',c)$ and a split procedure) and returns a (potentially) updated cluster assignment vector c'.

2:    $i \sim U(1,N)$ ▷ Sample i random uniformly over cluster assignments.

3:    $j \sim U(1,N) \cap i$ ▷ Sample j also random uniformly, but with $j \neq i$.

4:    $k \sim U(1,N) \cap \{i,j\}$ ▷ Sample k random uniformly, but with $k \neq j$, $k \neq i$.

5:    $S_R = \{c_i, c_j, c_k\}$ ▷ Sampled clusters c_i, c_j, c_k.

6:    $S_I = \{c_x\}$ with $c_x \in S_R$ for $x \in \{1,\dots,N\}$ ▷ All data in clusters c_i, c_j, c_k.

7:    $S_E = S_I \cap S_R$ ▷ All data in clusters c_i, c_j, c_k excluding S_R.

8:    $N_S = \text{unique}(S_R)$

9:    $u \sim U(0,1)$ ▷ Sample u between 0 or 1 uniformly.

10:    **if** $N_S = 1$ **then** ▷ Case: i, j, k belong to the same cluster.

11:       **return** $c' = $ DYADIC SPLIT-MERGE SAMPER(c)

12:    **else if** $N_S = 2$ and $u < \beta$ **then** ▷ Case: a cluster with one item and one with two items and $u < \beta$.

13:       **return** $c' = $ DYADIC SPLIT-MERGE SAMPER(c)

14:    **else if** $N_S = 2$ and $u \geq \beta$ **then** ▷ Case: a cluster with one item and one with two items and $u \geq \beta$.

15:       $c_i^{(3)} = c_k$ with $c_k \notin \{c_1,\dots,c_N\}$ ▷ Sample new cluster for $c_i^{(3)}$.

16:       $c_j^{(3)} = c_j^{(2)}$ ▷ Keep c_j the same.

17:       $c_e^{(3)} = $ SPLITPROCEDURE($S_E, c_i^{(3)}, c_j^{(3)}$) ▷ After $c_i^{(3)}, c_j^{(3)}$ assign S_E.

18:       **for all** $m \notin S_I$ **do**

19:          $c_m^{(3)} = c_m^{(2)}$ ▷ Data points in clusters other than c_i, c_j are not adjusted.

20:       **end for**

21:       $c' = \{c_i^{(3)}, c_j^{(3)}, c_e^{(3)}, c_m^{(3)}\}$

22:       $a = a_{split}(c',c)$ according to Eq. 5.14 ▷ MH acceptance for a split.

23:    **else** ▷ Case: i, j, k belong to thee different clusters $c_i \neq c_j \neq c_k$ ($N_S = 3$).

24:       $S_L = S_I \cap \{c_i^{(3)}, c_j^{(3)}\}$ ▷ Data in clusters c_i, c_j, c_k except for i and j itself.

25:       $\{c_i^{(2)}, c_j^{(2)}\} = $ SAMS($S_L, c_i^{(3)}, c_j^{(3)}$) ▷ Assign data points in c_i, c_j, c_k to c_i, c_j.

26:       **for all** $m \notin S_L$ **do**

27:          $c_m^{(2)} = c_m^{(3)}$ ▷ Data points in clusters other than S_L are not adjusted.

28:       **end for**

29:       $c' = \{c_i^{(2)}, c_j^{(2)}, c_m^{(2)}\}$

30:       $a = a_{merge}(c',c)$ according to Eq. 5.21 ▷ MH acceptance for a merge.

31:    **end if**

32:    $u \sim U(0,1)$ ▷ Sample u between 0 or 1 uniformly.

33:    **if** $a < u$ **then**

34:       $c' = c$ ▷ Reject c' by setting it to c

35:    **end if**

36:    **return** c', the (updated) cluster assignment vector: $c \rightarrow c'$.

37: **end procedure**

The fraction with q uses the total number of data points n_c in the clusters:

$$\frac{q(c^{(2)}|c^{(3)})}{q(c^{(3)}|c^{(2)})} = \frac{\left(\frac{1}{2}\right)^{n_c-2}}{\left(\frac{1}{3}\right)^{n_c-3}} = \left(3^{n_c-3}\right)\left(2^{2-n_c}\right) = \left(\frac{3}{2}\right)^{n_c}\frac{2^2}{3^3} \tag{5.18}$$

To move from 2 clusters to 3 clusters the probability is a 1/3 for each cluster index in vector c (except for the three data items already selected randomly, hence $n_c - 3$). To move back, the probability is a 1/2 and there are only two data items randomly assigned beforehand. The fraction with P uses the number of data points in each of the clusters before and after the step:

$$\frac{P(c^{(3)})}{P(c^{(2)})} = \alpha \frac{(n_{c_i^{(3)}} - 1)!(n_{c_j^{(3)}} - 1)!(n_{c_k^{(3)}} - 1)!}{(n_{c_i^{(2)}} - 1)!(n_{c_j^{(2)}} - 1)!} = \alpha \frac{B(n_{c_i^3}, n_{c_j^3}, n_{c_k^3})}{B(n_{c_i^2}, n_{c_j^2})} \tag{5.19}$$

Here we introduced a generalized Beta function $B(a, b, c) = \Gamma(a)\Gamma(b)\Gamma(c)/\Gamma(a + b + c)$ with $\Gamma(x) = (x - 1)!$ the Gamma function. The likelihood ratio becomes:

$$\frac{L(c^{(3)}|y)}{L(c^{(2)}|y)} = \frac{\prod_{m:c_m^{(3)}=c_i^{(3)}} p(y_m|\phi) \prod_{m:c_m^{(3)}=c_j^{(3)}} p(y_m|\phi) \prod_{m:c_m^{(3)}=c_k^{(3)}} p(y_m|\phi)}{\prod_{m:c_m^{(2)}=c_i^{(2)}} p(y_m|\phi) \prod_{m:c_m^{(2)}=c_j^{(2)}} p(y_m|\phi)} \tag{5.20}$$

5.3.2 Acceptance for the merge step

The merge step from two to one cluster is analogous to the split step:

$$a_{merge}(c^{(1)}, c^{(2)}) = \min\left[1, \frac{r(c^{(2)}|c^{(1)})}{r(c^{(1)}|c^{(2)})} \frac{q(c^{(2)}|c^{(1)})}{q(c^{(1)}|c^{(2)})} \frac{P(c^{(1)})}{P(c^{(2)})} \frac{L(c^{(1)}|y)}{L(c^{(2)}|y)}\right] \tag{5.21}$$

The merge step from three clusters to two clusters is:

$$a_{merge}(c^{(2)}, c^{(3)}) = \min\left[1, \frac{r(c^{(3)}|c^{(2)})}{r(c^{(2)}|c^{(3)})} \frac{q(c^{(3)}|c^{(2)})}{q(c^{(2)}|c^{(3)})} \frac{P(c^{(2)})}{P(c^{(3)})} \frac{L(c^{(2)}|y)}{L(c^{(3)}|y)}\right] \tag{5.22}$$

Note that all the fractions in Eq. 5.22 are the reverse of the fractions in Eq. 5.16. Inverting Eq. 5.17–5.20 will be left to the reader.

One additional issue we have to consider. When merging three clusters into two we can (1) distribute the data over all three clusters or (2) alternatively, keep the data in two clusters assigned to these clusters and only distribute the data in the third cluster over the other two clusters. The second and alternative option however would introduce unnecessary asymmetry with the merge step. In other words, Eq. 5.23 is not the inverse of Eq. 5.18. In contrast, the equation is similar to splitting one cluster across two as in Eq. 5.9:

$$\frac{q_{alt}(c^{(3)}|c^{(2)})}{q_{alt}(c^{(2)}|c^{(3)})} = 2^{-2+n_c} \tag{5.23}$$

Hence the first option is entertained and the q-fraction is exactly the inverse of Eq. 5.18.

Another choice has been made, namely to exclude direct operations between a single cluster and three clusters. This is because factors like:

$$\frac{P(c^{(3)})}{P(c^{(1)})} = \alpha^2 \frac{(n_{c_i^{(3)}} - 1)!(n_{c_j^{(3)}} - 1)!(n_{c_k^{(3)}} - 1)!}{(n_{c_i^{(1)}} - 1)!} \tag{5.24}$$

become very small and although compensated by a large q fraction, remain further away from an acceptance factor of 1. Note that by the ability to split a single cluster into two and then into three, there is no ergodic argument to introduce also the immediate step.

5.4 Results

The problem we use to test our sampler is a well-known problem in computer vision, namely that of the inference of line parameters (slope and intercept) given data points. Rather than ordinary linear regression, in computer vision there is a mixture of lines that have to be estimated. Moreover, the number of lines is not known beforehand. To solve this problem we use the Dirichlet process mixture (Eq. 5.1) with a normal distribution $N(0, \sigma_0)$ to generate the line parameters and a likelihood function that defines points to be uniformly distributed across a line of length 20 and deviating from the line according to a normal distribution $N(0, \sigma_1)$.
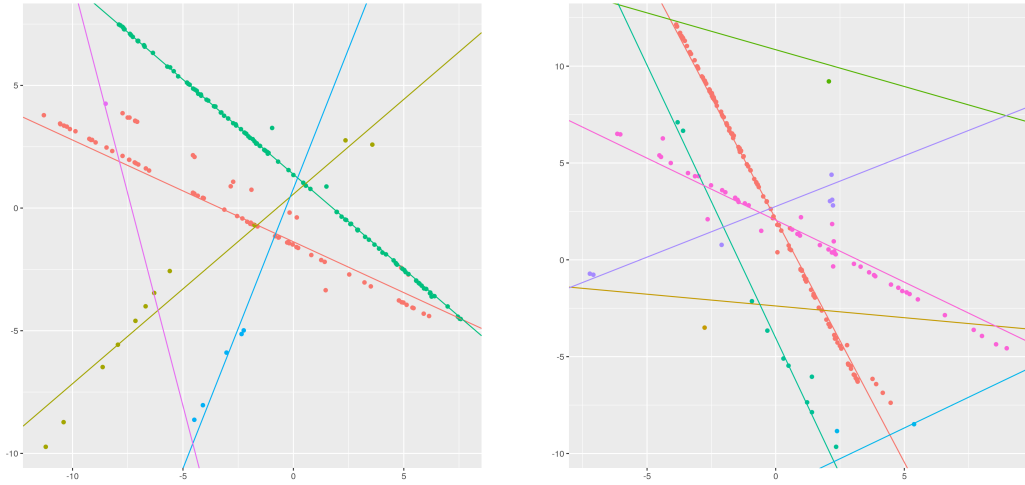
Figure 5.2: Two examples of fitting a mixture of lines to data items scattered over a two-dimensional space. The lines drawn are inferred using one of the methods in this paper. The lines are not the ground truth, but are meant to demonstrate the typical errors made by fitting methods. Note for example that there are mistakes in both the assignment of points to lines as well as the line parameters (slope and intercept).

5.4.1 Implementation

The sampler is open-source[2] implemented in C++ which means that (a) it is computationally fast, (b) it can be run on embedded devices if a cross-compiler is available and the Eigen3 library is ported. Note, that due to the fact that the simulator uses a lot of randon numbers the system should use a modern compiler (g++-6 or newer) and should have enough entropy available[3]. Rather than a random scan, the implementation uses a fixed scan as advocated in the literature MacEachern (2007).

To speed up the sampler most calculations are done in log-space. Consider $v = u + 1$. The ratio with probabilities (Eq. 5.5 and 5.19) becomes:

$$\log \frac{P(c^{(v)})}{P(c^{(u)})} = \log(\alpha) + \sum_i \log \Gamma(n_{c_i^{(v)}}) - \sum_i \log \Gamma(n_{c_i^{(u)}}) \tag{5.25}$$

The fraction with $q(\cdot)$ (Eq. 5.9 and 5.18) becomes:

$$\log \frac{q(c^{(v-1)}|c^{(v)})}{q(c^{(v)}|c^{(v-1)})} = (v - n_c - 1)\log(v-1) - (v - n_c)\log(v) \tag{5.26}$$

The fraction with r becomes for example (Eq. 5.17):

$$\log \frac{r(c^{(2)}|c^{(3)})}{r(c^{(3)}|c^{(2)})} = -\log(1 - \beta) \tag{5.27}$$

The log-probability to calculate the likelihood given by a multivariate Normal distribution is well-known.

5.4.2 Comparison

The Triadic sampler using SAMS is compared with the Jain-Neal Dyadic sampler using SAMS and an auxiliary variable sampler with $m = 3$ (see algorithm 8 in Neal (2000)).

Method	Purity	Rand Index	Adjusted Rand Index
Dyadic sampler	0.80960	0.80580	0.56382
Auxiliary variables	0.87235	0.85879	0.68224
Triadic sampler	0.86405	0.87188	0.71067

Table 5.1: The purity, rand index, and adjusted rand index establishing the quality of the clustering method. The closer the values to one, the better the method performed. The purity metric assigns high values to clusters that do not have data points from other clusters (but does not penalize the number of clusters). The rand index index computes similarity between clusters taking false negatives and false positives into account. The adjusted rand index accounts for chance. The adjusted rand index is most useful in our comparison.

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[2]Code can be found at https://code.annevanrossum.nl/noparama.
[3]On Linux this can be checked in /proc/sys/kernel/random/entropy_avail.

In Table 5.1 the line estimation problem is compared for the dyadic sampler, an auxiliary variables sampler, and the proposed triadic sampler. The simulation is run with $\beta = 0.1$ so that a significant number of steps are tried between two and three clusters (rather than only between one and two clusters).
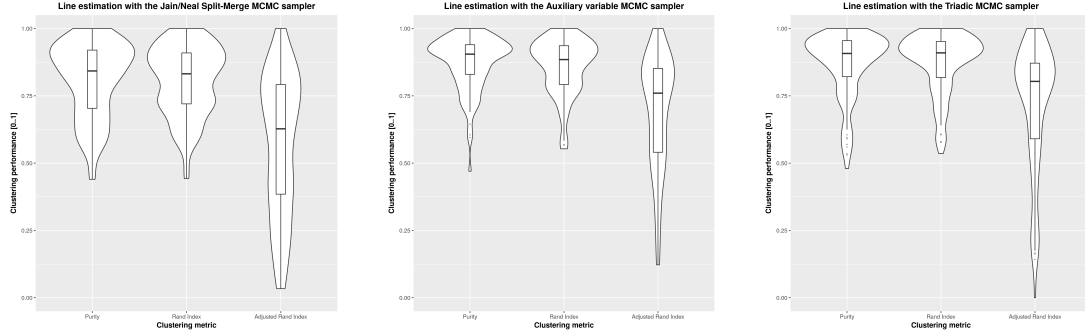
Figure 5.3: The same results as in Table 5.1, but visualized in a violin plot. The distribution over metric values are displayed in a vertical fashion. From left to right the distribution shifts to one, signifying better clustering performance.

In Fig. 5.3 the different metrics are visualized in the form of violin plots. The improvement in clustering is especially visible with the adjusted rand index.

5.5   Chapter Conclusions

A new split-merge sampler has been introduced, implemented, and applied to the computer vision problem of line estimation. The sampler outperforms existing samplers, such as the ordinary (dyadic) split-merge sampler Jain and Neal (2004) and auxiliary variable sampler Neal (2000).

Although the proposed split-merge sampler is able to mix considerably faster through a mixture model, it does not use global jumps directly based on the data at hand. It is reasonable to suggest that MCMC methods benefit from combining the local jumps with global jumps, for example by a mixture of the local Metropolis-Hastings sampler with a Metropolized independence sampler Jampani et al. (2015). We will introduce such a sampler in chapter **??**.

ADVERSARIALLY TRAINED MCMC KERNELS

Contents   To use MCMC for volumetric inference it is necessary to be able to accelerate the algorithms even further. Volumetric objects exhibit more structure, which is reflected by symmetry.

Outline   We describe MCMC methods that cope with symmetric objects.

6.1 Introduction

There are three aspects we would like to address in our inference engine.

The first aspect aims to have structure within our inference engine. The proposal distribution in a Markov chain, although moderately complex in the previous chapter, does not have much knowledge about the model at hand. An artificial border is maintained that does not allow the inference engine to have knowledge about the model. The purpose of this is never articulated in particular. However, it is logical from a separation of concern. Such an inference engine (1) does not need to receive any information about the model and (2) is guaranteed to be general in the sense that it is not tailored to a particular model. This is nicely articulated by Tran et al. (2017) from which we quote.

> *Many existing probabilistic programming languages treat the inference engine as a black box, abstracted away from the model. These cannot capture probabilistic inferences that reuse the model's representation - a key idea in recent advances in variational inference, generative adversarial networks, and also in more classic inference.*

The second aspect concerns the data at hand. In MCMC the position for the chain is driven by (1) the prior, (2) the prior and the likelihood, (3) a sequence of priors and likelihood, (4)

a sequence of priors, likelihood and proposal distributions, basically anything, except for the data itself. Data-driven approaches would namely destroy the convergence of the Markov chain. To start an MCMC sampler in a data-driven manner and continue in a data-oblivious manner is a possible solution (Zhang and Perez-Cruz, 2017). Even better, it is possible to use a Metropolized independence sampler Jampani et al. (2015). Such a sampler samples independently from the previous state and uses global information. However, to work well its proposal distribution needs to match the target distribution quite well. Although, when combined with a local sampler, it might be sufficient to just be able to match the modes of the target distribution well.

The third aspect concerns the way we build our MCMC engine. The split-merge sampler of the previous chapter has been meticulously designed. If we admit a data-driven approach, we might as well adjust our MCMC engine using training samples. Note, that this training will be across a set of line, box, or scenes mixtures. The MCMC engine will not be able to learn just the parameters of a particular visual object. It will learn how to jump around (optionally, adaptively) from one visual object to the next or from one cluster configuration to the next. In other words, it will be able to teach itself to become a Triadic Split-Merge sampler if that happens to be a good engine. Is it possible to constrain the search through MCMC kernels such that its result is always converging in an MCMC sense? If we aim to learn the transition operator of our Markov chains, there is new literature at hand that makes use of deep nets.

6.2 Learning the Transition Operator

There are multiple methods that can be used in a generative setting. We will discuss the three most prominent ones: (1) generative adversarial networks, (2) variational autoencoders, and (3) infusion training. This is far from an extensive categorization, worth studying are variational walkback (Goyal et al., 2017), stacked generative adversarial networks (Huang et al., 2016), generative latent optimization (Bojanowski et al., 2017), deep learning through the use of non-equilibrium thermodynamics (Sohl-Dickstein et al., 2015), denoising autoencoders, or generative stochastic networks, to name just a few.

6.2.1 Adversarial training

Adversarial training has been extensively studied since the article on generative adversarial networks by Goodfellow et al. (2014). A particular adversarial setup for training an MCMC has been suggested as well (Song et al., 2017). The generator samples from a Markov chain. A discriminator subsequently needs to judge if its incoming data comes from the generator or if it is sampled from the actual data set. To start the process, the generator can run the chain from the model as well as from the data.
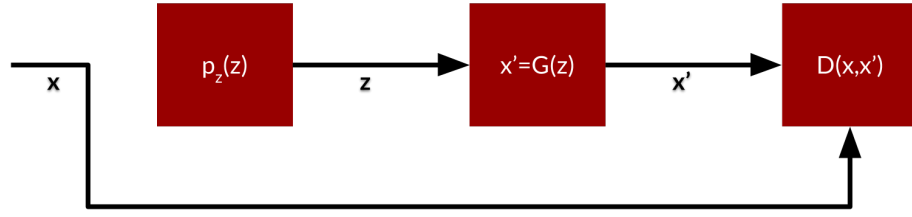
Figure 6.1: Left: $p_z(z)$ is a (prior) random distribution that generates random variables z. Middle: the generator G maps the random variables z to simulated data points x'. Right: the discriminator $D(x, x')$ compares the simulated data x' with the real data x. The generator tries to generate samples in such way that the discriminator has difficulties distinguishing the simulated from the real data.

6.2.2 Variational encoders

Variational autoencoders (Kingma and Welling, 2013; Rezende et al., 2014) are ordinary autoencoders with additional constraints on the latent variables. The latent variables in autoencoder parlance are called the code. In a variational autoencoder the latent variables are forced to approximately describe a unit Gaussian distribution. The autoencoder is trained using a loss function that is composed out of (1) a generative loss, a mean squared error that measures how accurately the network reconstructs its input, and (2) a latent loss, a KL-divergence that measures how closely the latent variables match a unit Gaussian. To optimize the KL divergence a reparameterization trick is applied. The encoder does not generate a vector with real values, but generates a vector with means and standard deviations instead.
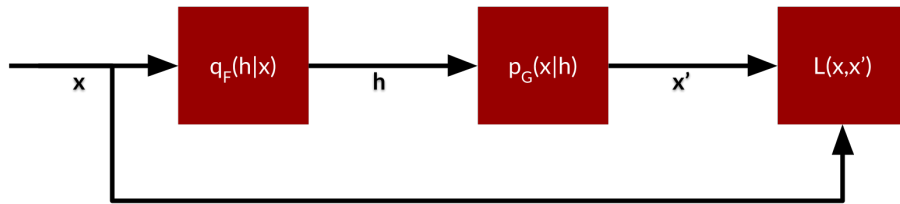
Figure 6.2: Left: $q_F(h|x)$ maps the data x to (hidden) random variables h. Middle: $p_G(x|h)$ maps the hidden random variables to reconstructed data x'. Right: $L(x, x')$ measures the similarity between x and x'.

6.2.3 Infusion training

The transition operator can also be learned directly through infusion training. In infusion training we gradually adjust totally unstructured noise to a target distribution as well. In this method a particular data point is 'infused' into the Markov chain to bias the model sampling to move towards this particular data point (and not another). In contrast to a generative loss that is a mean squared error, this promises to have less blurry reconstructions.

6.3 Volumetric models

In image processing autoencoders have been used for 2D shape recognition. To apply the same type of models to 3D point louds, these point clouds are represented through voxels. The application of data-driven deep learning techniques, be it autoencoders, generative adversarial networks, or adversarial autoencoders promises similar good results in these 3D settings than in the current computer vision tasks.

The 3D ShapeNet model (Wu et al., 2015) exists of 3D voxel input that is piped through several stages with an increasing number of filters. The used voxel representation is a binary tensor. It assigns a value of 1 to each voxel that is inside the 3D object mesh and a value 0 to each voxel outside the mesh (empty space). The voxel sizes are fixed as well as the grid size (in this particular model the grid exists of 30x30x30 voxels). The inference model is a Deep Belief Network (DBN). Convolution operators, in the form of filters over small neighbourhoods, are used to reduce the number of model parameters (30x30x30 fully connected would be really many weights). The DBN is used in a supervised setting where shapes are trained with object labels. The model subsequently learns to generate shapes given an object label.

An unsupervised method in the form of a convolutional (volumetric) autoencoder (Sharma et al., 2016) has been applied to the same type of data. This (denoising) autoencoder, coined VConv-DAE maps from an entire voxel grid to another voxel grid. This work uses a combination of standard techniques, a dropout layer, a deconvolution layer, ReLu as well as sigmoid activation, but it is not in particular tailored to 3D point clouds.

Other representations than voxels are used. For example collections of 2D views and transformation parameters (Dosovitskiy et al., 2017). The most interesting are methods that work with raw data, the point cloud themselves. This alleviate the need to process the data and does not inadvertently increase the data dimensions, for example by artificially introduce voxels where there is no object present.

PointNet (**?**) directly operates on point clouds. To handle the input as a set of points (unordered), it uses a symmetric function over n input vectors and outputs a vector that is invariant to the input order. Typically sum and multiplication operators are such symmetric functions. After input and feature transforms by multi-layer perceptrons, a max pooling operator is used to map the input to a global feature. In the ModelNet40 shape classification benchmark there are more than 12000 CAD models from 40 object categories. PointNet achieves state of the art results compared to volumetric methods for a fraction of the computational costs.

Point clouds are also directly used in so-called deep kd-networks (Klokov and Lempitsky, 2017). A kd-tree is constructed by recursively picking the coordinate axis with the largest range of point coordinates and splitting the set of points into two subsets of equal size. These subsets are recursed into successively. The recursion stops at a particular level, depth D. The kd-networks are purported to outperform for example PointNet amongst other model architectures.

A deep permutation equivariant (for semisupervised learning) and permutation invariant (for supervised learning) network has also bee directly applied to point clouds (Ravanbakhsh et al., 2016). It does not reach the ModelNet40 accuracy levels from PointNet or the kd-networks though.

PointNet++ Qi et al. (2017) introduces hierarchical structure to PointNet. This fits better non-uniform point distributions and seems to surpass kd-nets again on the ModelNet40 task.

RECOMMENDER ENGINE

Contents The described nonparametric Bayesian models (Chapter 3, 4, 5, and 6) are not limited to computer vision tasks. This chapter describes a recommender engine in which groups of runners are extracted from data collected from social media.

Outline We (1) introduce the form of the data at hand, (2) describe a multi-modal Von Mises-Uniform distribution to model the individual runners, (3) use a Dirichlet Process prior to group people, (4) use the previously described MCMC methods to perform inference, (5) show the results on an artificial and real-world data set, and (6) discuss ways with which the model can be expanded.

7.1 Application

The data of people exercising can be considered binary (someone is either exercising or not in a particular timeslot). We do have however more information available. We know how often people have been exercising in a timeslot. This data has the form as visualized in Table 7.1.

Table 7.1: Example of the type of data about the timing of exercising. A person is represented by row, her preferences by column. There is not a predefined number of users or groups of users.

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
0	0	0	0	4	23	38	9	12	6	2	7	2	3	2	7	5	3	2	0	3	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	11	4	4	2	1	2	0	0	0
0	0	0	0	0	1	0	0	1	2	0	0	0	1	0	2	3	1	1	3	2	0	0	0
0	0	0	0	0	0	5	4	1	3	11	3	7	3	3	4	3	10	23	3	0	0	0	0
0	0	0	0	0	0	8	35	23	12	4	41	14	11	8	7	14	38	36	6	5	1	2	0
0	0	0	0	0	0	0	1	9	2	0	3	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	29	9	8	7	5	3	0	2	0	1	8	6	1	4	1	2	0	0
0	0	0	0	0	2	14	12	7	1	0	2	0	2	0	3	4	6	4	3	9	2	0	1
0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	3	3	2	0	1	0	0	0
0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	2	1	2	3	0	1	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	2	0	4	5	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1	3	2	1	0	1	1	0	0	0	0	3	11	12	0	0	0
0	0	0	0	0	0	0	0	0	2	1	0	0	0	1	0	3	5	4	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	18	4	0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	2	0	0	1	9	14	14	2	1	4	15	4	0	0
0	0	0	0	0	0	0	0	2	4	2	1	3	5	2	0	1	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1	0	1	1	0	0	0	1	1	3	3	1	3	2	3	0	0
0	0	0	0	0	0	0	1	2	1	3	2	0	1	2	0	0	0	0	1	2	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	8	4	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	4	6	2	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1	0	1	1	6	2	1	0	0	0	0	1	1	0	0	0	0
0	0	0	0	0	0	2	2	3	12	18	12	12	2	4	3	5	6	43	37	16	1	2	0

The first row defines the time of day, starting at midnight till the last timeslot from 23.00 till 00.00. In this particular case it shows that nobody is running from midnight to four o'clock in the morning, understandably so.

7.2 Model of Individuals

7.2.1 Multi-modal Normal-Uniform Distribution Model

We first postulate the likelihood function for the moments at which people exercise through the day as defined in Eq. 7.1.

$$f(x|\theta) = w_0 \mathcal{U}(a, b) + \sum_{i=1}^{2} w_i \mathcal{N}(\mu_i, \sigma_i) \tag{7.1}$$

The likelihood (Eq. 7.1 is built up out of three probability density functions: one Uniform distribution $\mathcal{U}(a, b)$ with a and b as parameters and two Normal distributions $\mathcal{N}(\mu_i, \sigma_i)$ with mean μ_i and σ_i. The distributions are weighted by the factors w_0, w_1, w_2. The collection of parameters for the likelihood function is referred to by $\theta = \{a, b, \mu_1, \sigma_1, \mu_2, \sigma_2, w_0, w_1, w_2\}$.

This probability density function $f(x|\theta)$ will have the form as in Fig. 7.1. The uniform distribution generates values here between 00:00 and 24:00. There are on top of that the two Normal distributions that form peaks at certain moments during the day.

(a) People who like to run late in the evening.

(b) People who run before work, early in the morning and occasionally during the day.

(c) People who exclusively run before work.

(d) People who run right after dinner.

Figure 7.1: The likelihood function for the moments at which people decide to exercise during the day. On the horizontal axis time, on the vertical axis the frequency of exercising.

There is something noticable in Fig. 7.1, namely that the 24 hours of a day cause the Normal distribution to be cut off. Especially in Fig. 7.1 (a) there should be some considerable likelihood of running in the wee hours of the morning between 00:00 and 01:00.

7.2.2 Multi-modal Von-Mises-Uniform Distribution Model

There are several options to define a distribution over a limited range T. A so-called wrapped distribution is a distribution defined over the unity circle. By just multiplying it with $T/(2pi)$ it can be used to define a probability density function over a day ($T = 24$).

$$f(x|\theta) = w_0 \mathcal{U}(a, b) + \sum_{i=1}^{2} w_i \mathcal{VM}(\mu_i, \kappa_i) \tag{7.2}$$

The likelihood (Eq. 7.2) is again built up out of three probability density functions: one Uniform distribution $\mathcal{U}(a, b)$ with a and b as parameters and two Von Mises distributions $\mathcal{VM}(\mu_i, \kappa_i)$ with mean μ_i and κ_i. The parameters μ_i will be scaled and shifted with $[a, b]$ so all variables within this range fall on the unity circle. The parameter κ_i plays the same role as σ_i for the Normal distribution. The distributions are weighted by the factors w_0, w_1, w_2. The collection of parameters for the likelihood function is referred to by $\theta = \{a, b, \mu_1, \kappa_1, \mu_2, \kappa_2, w_0, w_1, w_2\}$.

(a) People who like to run late in the evening

(b) People who run before work, early in the morning and later in the evening.
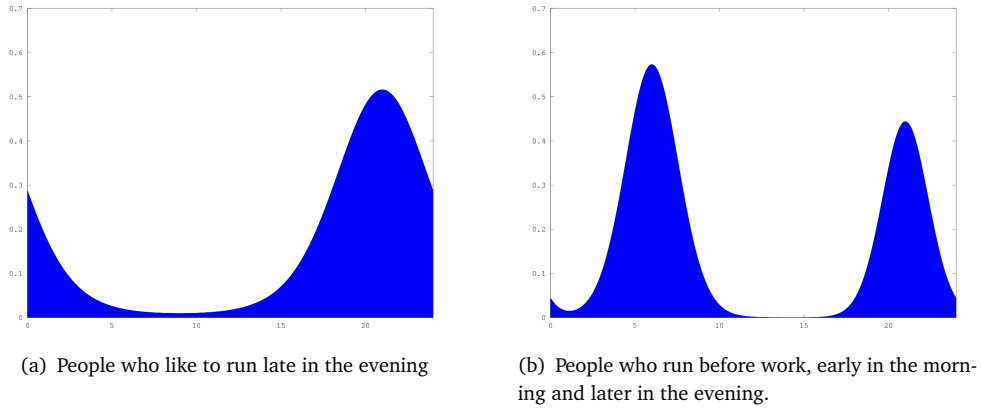
Figure 7.2: The improved likelihood function for the moments at which people decide to exercise during the day using the Von Mises distribution. On the horizontal axis time, on the vertical axis the frequency of exercising.

The likelihood with Von Mises distributions rather than Normal distributions is visualized in Fig. 7.2. The Von Mises distributions capture behavior in deviations from a standard exercise time. It does not take into account structured deviations, for example running late from work every Thursday, or weekends, or a person either running in the morning or in the evening, but never both at the same day.

7.2.3 Hyperparameters

The parameters θ for each user j are either fixed or generated from prior distributions. The hyperparameters a and b for the Uniform distribution are set to 0 and 24. People can run potentionally any time of the day. The hyperparameters μ_i, κ_i for the Von Mises distributions are generated from a Uniform-Exponential distribution (Eq. 7.3). The Uniform distribution reflects the fact that if people run on regular times, this time can be any time of the day. The Exponential distribution defines a prior on how much people deviate from such a regular time to exercise.

$$
\begin{aligned}
f(\mu_i|a,b) &= \mathcal{U}(a,b) \\
f(\kappa_i|\lambda) &= \mathcal{E}(\lambda)
\end{aligned}
\tag{7.3}
$$

The Uniform distribution generates μ_i between a and b. The parameter κ_i is generated from an Exponential distribution with hyperparameter λ. If λ is set to be small (< 0.5) we have a high likelihood that κ can be large and we have pronounced peaks. In contrary, if λ is set to be large, the Von Mises distribution likely approaches the Uniform distribution due to a higher chance of sampling a small value for κ.

The weights we sample from a normalized product of a zero-deflated Bernoulli distribution and a Dirichlet distribution (Eq. 7.4).

$$f(w_i|p, \alpha_i) = \mathscr{B}(p)\mathscr{D}(\alpha_i)/Z \tag{7.4}$$

The Bernoulli distribution samples zeros and ones with probability of $p = 0.5$, leading to 3-vectors like 001, 101, etc. The distribution is corrected in such way that the chance to sample 000 is zero. The Bernoulli distribution only gives weights $w_i = 0$ or $w_i = 1$, hence it is multiplied with a Dirichlet distribution. The Dirichlet samples a 3-vector with weights between zero and one where the weights $\sum_i w_i = 1$. A symmetric Dirichlet distribution with $\alpha = 1$ is similar to the Uniform distribution over the simplex. It is set slightly more towards favoring particular distributions with $\alpha_i = 1/3$ (we assume that people sample one or two distributions, and rarely from all three). The product with the zero-deflated Bernoulli distribution is made up to sum up to one again by normalizing the result.

We can combine Eq. 7.3 and Eq. 7.4 in Eq. 7.5:

$$\theta \sim \mathscr{U}(a, b)\mathscr{E}(\lambda)\mathscr{B}(p)\mathscr{D}(\alpha_i)/Z \tag{7.5}$$

To sample the parameters θ this is the base distribution we will encounter in the next section 7.3.

7.3 Model of Groups

Each person's exercise schedule is represented by a Von-Mises-Uniform distribution. People that are similar do have exercise schedules that can be represented by the same Von-Mises-Uniform distribution. To group similar schedules we define a nonparametric discrete distribution over a potentially infinite number of groups with each person assigned to a group.

A Dirichlet Process (Eq. 7.6) is a distribution over distributions that can be used as a prior for such a nonparametric discrete distribution.

$$DP(\alpha, H) \tag{7.6}$$

The Dirichlet Process has (1) a hyperparameter α, which defines the likelihood that there are many clusters versus few clusters (although it doesn't say anything about its actual count), and (2) a base distribution H, the distribution that generates θ (Eq.7.5).

7.4 Inference

The implementation of the model makes use of Gibbs sampling with auxiliary variables Jain and Neal (2007).

Details on this algorithm can be found in Jain and Neal (2007) and previous work of the authors van Rossum et al. (2016a,b).

Algorithm 14 Gibbs sampling over auxiliary variables

1: **procedure** GIBBS ALGORITHM WITH AUXILIARY VARIABLES(w, λ_0, α)   ▷ Accepts schedule w, hyperparameters λ_0, α, number of auxiliary variables m, and returns k groups

2:      **for all** $t = 1 : T$ **do**

3:          **for all** $i = 1 : N$ **do**

4:              **for all** $j = 1 : m$ **do**

5:                  $\theta_j \sim H(\lambda_0)$ ▷ Sample θ_j from base distribution H in Eq. 7.5

6:              **end for**

7:              **for all** $j = 1 : K + m, j \neq i$ **do**

8:                  $L_j = \text{likelihood}(w_i, \theta_j)$ ▷ Update likelihood for all theta (except θ_i) given w_i

9:              **end for**

10:              $P_{-i=1:K} = b \sum_{-i} L_{-i}$ ▷ Calculate probability of existing cluster

11:              $P_{-i=K:K+m} = b\alpha/mL_m L_{-i}$ ▷ Calculate probability of new cluster

12:              $\theta_i = \theta_j$ according to above P_{-i} ▷ Sample θ_i accord. to above prob

13:              Remove unused clusters

14:          **end for**

15:          **for all** $j = 1 : K$ **do**

16:              $\theta_j \sim p(\theta_j \mid y)$ ▷ Update θ_j

17:          **end for**

18:      **end for**

19:      **return** summary on θ_k for k groups of runners

20: **end procedure**

7.5 Results

The algorithm is run first on an artificial dataset of which we know the ground truth (Sect. 7.5.1) and next on the real-world dataset from Twitter (Sect. 7.5.2).

7.5.1 Artificial Dataset

The algorithm has been used on a self-generated dataset (generated from the probability density function as in Fig. 7.2). In this case we have the ground truth that establishes which exercise schedule comes from which probability density function. Using this ground truth we can calculate how often our algorithm makes a mistake, grouping a person with people that belong to another group. The results with this dataset are perfect (Rand Index equal to one: perfect clustering). The results are of the form of Table 7.2 (except by a permutation of indices), hence are not shown (the indices have no intrinsic meaning).

Table 7.2: Top row: A sequence of cluster indices indicates the ground truth. Each cluster index represents a multi-modal Von-Mises-Uniform distribution with different parameters θ. Bottom row: A sequence of cluster indices that are the result of the described algorithm. Each cluster index represents again a multi-modal Von-Mises distribution. Errors would be represented by an inconsistent mapping from the top row to the bottom row.

1	4	4	5	2	2	2	1	3	2	1	5	1	1	4	4	3	1	3	1	2	...
4	5	5	1	2	2	2	4	3	2	4	1	4	4	5	5	3	4	3	4	2	...

7.5.2 Real-world Dataset

The results when we actually use the collected Twitter dataset can be best visualized (Fig. 7.3). This dataset consists of around 4000 moments at which people decide to run. The dataset is subsequently filtered on regulars, people that at least have run a few times.

(a) People who predemominally seem to like to run in the early evening.

(b) People who run during the day, not later than at 20:00 o'clock.

(c) People who seem to run all the time (interesting collection though!).

(d) People who run early in the morning.

(e) People who run around 16:00 o'clock and almost never run at another time.
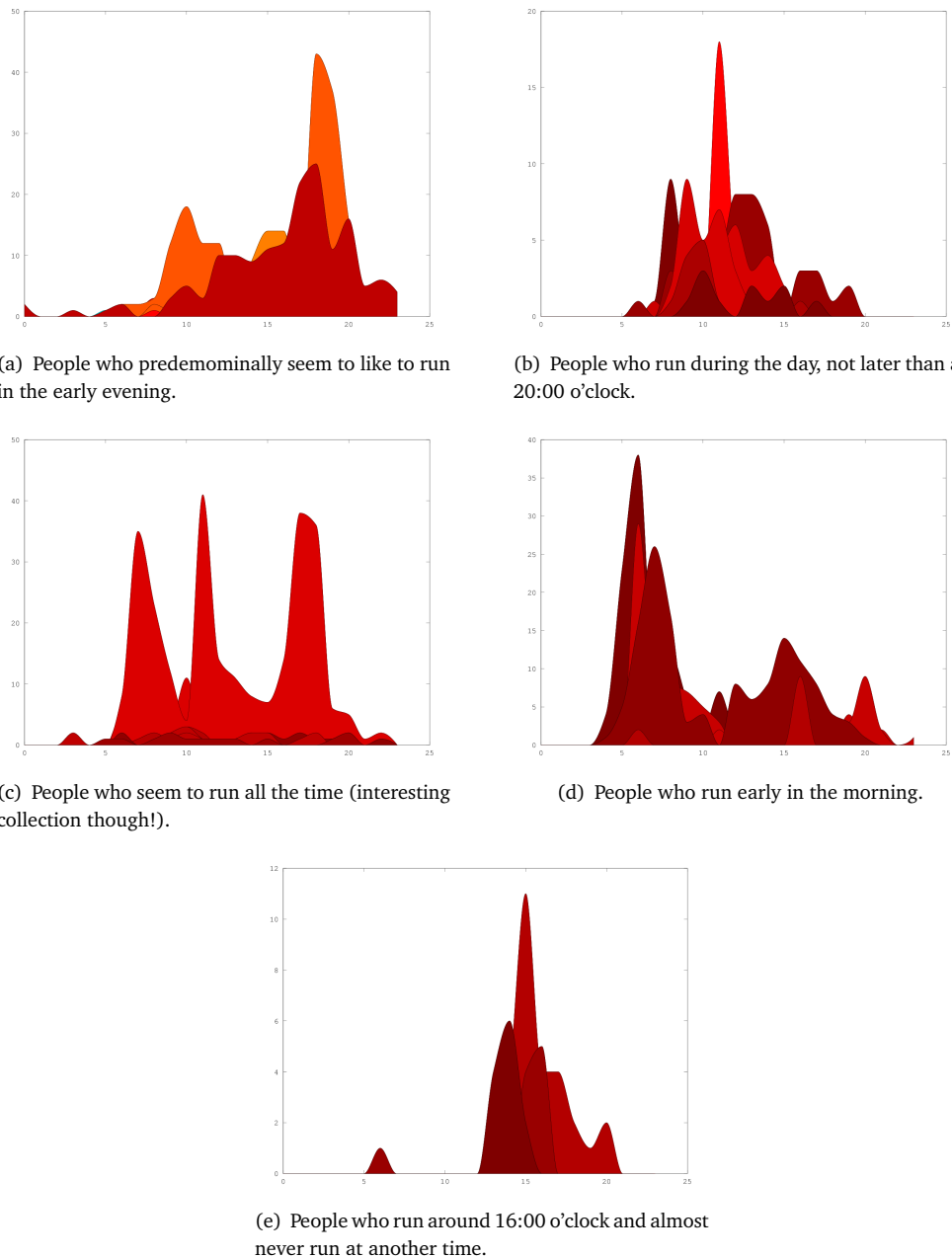
Figure 7.3: After running the algorithm, the above figures show the different categories of runners that have been found.

The results in Fig. 7.3 show that there is a categorization of people indeed. After the algorithm has done its work it is possible to assign a certain label in a post-hoc manner, e.g. "People who run around 16:00 o'clock and almost never run at another time.".

7.6 Discussion

The postulated model allows to reason about groups of people performing exercising, without predefining what these groups constitute apart from very general characteristics such as that there might be preferred times of day to exercise. A Dirichlet process is used as a nonparametric Bayesian model in which both the number of groups and the assignment of people exercising are learnt from the data.

There are several directions in which this research can be extended. First, more data would be very helpful. Only a limited number of people are posting consistently their training data online. Tapping into the data of current fitness promoting companies would allow the model to wash out the prior a bit more and adjust to the data. Second, we also collected weather data over this time period and also expect the day of the week to have significant influence. When there will be more data available these are logically dimensions to include in the dataset. Third, it would be interesting to study if people relate to the group of people they have been categorized with. Can this help or support their exercise regime?

DISCUSSION AND CONCLUSIONS

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PROBABILISTIC CONCEPTS

> **TODO**: What follows down here is old and has to be adapted to the measure-theoretic realizations.

Let us introduce the notation of expectation for random variable X:

$$E_p[X] = \sum_i^k p(X = x_i)x_i \tag{A.1}$$

For the continuous case, if $f_X(x)$ is a properly defined probability density function, the expected value becomes:

$$E_f[X] = \int_{-\infty}^{\infty} x f_X(x)dx \tag{A.2}$$

From the context it can be seen that the object X at the left is a different object than x at the right. The former is random variable (a one-dimensional function, an (in)finite vector), the latter is a value of a random variable (a scalar). The term dx is a measure, in this case it assigns volume to *subsets of random variables values*. A proper notation would incorporate this aspect, but not much will be gained by creating such complex notations.

Let us also introduce the conditional probability:

$$p(X|Y) = \frac{p(X,Y)}{p(Y)} \tag{A.3}$$

Suppose X is a discrete random variable, then the object $p(X)$ is a vector of finite size k, $p(Y)$ is a vector of finite size l, and $p(X|Y)$ as well as $p(X,Y)$ are matrices of size $k \times l$. A conditional probability hence 'divides' a matrix by a vector. It is a proper measure if $p(Y) \neq 0$ (for all values of - or events in - Y).

In for example importance sampling (Sect. **??**), the expectation is taken over a function of a random variable. A function, if measurable, can be taken the expectation over using the so-called law of the unconscious statistician:

$$E_f[g(X)] = \int_{-\infty}^{\infty} g(x)f_X(x)dx \tag{A.4}$$

Here $g(X)$ is a general measurable function, and not restricted to a probability density function.

The notation above is an indefinite integral. We can approach this integral by Monte Carlo integration (Sect. **??**).

$$E_f[g(X)] = \frac{1}{k}\sum_{i=1}^{k} g(x_i) \qquad \text{with} \qquad x_i \sim f_X(x) \tag{A.5}$$

Rather than summing over $f_X(x_i)$, we now sample $x_i \sim f_X(x)$.

A.1 Common Inequalities

A.1.1 Markov's Inequality

Markov's inequality comes up with an upper bound for the probability that an non-negative random variable X exceeds some constant positive threshold a.

$$p(X \geq a) \leq \frac{E[X]}{a} \tag{A.6}$$

The proof in classical probability theory uses an indicator variable:

$$aI(X \geq a) \leq X \tag{A.7}$$

Here $I(X \geq a) = 1$ if the event $X \geq a$ occurs, setting the left-hand side to a (which is of course smaller than X). And $I(X \geq a) = 0$ on the event $X < a$, which is naturally smaller than the non-negative X.

Expectations obey the inequality: if $(X \leq Y)$, then $E[X] \leq E[Y]$, hence:

$$E[aI(X \geq a)] \leq E[X] \tag{A.8}$$

And because expectations add up linearly:

$$E[aI(X \geq a)] = aE[I(X \geq a)] = a(1 \cdot p(X \geq a) + 0 \cdot p(X < a)) = a \cdot p(X \geq a) \tag{A.9}$$

So, we have Markov's inequality combining Eq. A.8 and A.9:

$$a \cdot p(X \geq a) \leq E[X] \tag{A.10}$$

A.1.2   Chebyshev's Inequality

Now, Chebyshev's inequality defines in a simular way (Chebyshev was a teacher of Markov[1]) an upper bound on the deviation from the mean for a random variable. Recall the definition of the variance of X and assume it is finite:

$$Var(X) = E[(X - E[X])^2] = \sigma^2 \tag{A.11}$$

Consider now the random variable $(X - E[X])^2$ and constant $a = (\sigma k)^2$ and write down Markov's inequality:

$$p((X - E[X])^2 \geq (\sigma k)^2) \leq \frac{E[(X - E[X])^2]}{(\sigma k)^2} \tag{A.12}$$

Taking the square root of the unequality at the left, and using the definition of σ^2 at the right, leads to:

$$p(|X - E[X]| \geq \sigma k) \leq \frac{1}{k^2} \tag{A.13}$$

A.1.3   Weak Law of Large Numbers

Chebyshev's inequality can be used to prove the weak law of large numbers. Given that we have a series of random variables, all with the same finite expectation, $E[X_i] = \mu$, then this law states that the sample average $\bar{X} = \frac{1}{n}(X_1 + \cdots + X_n)$ converges in probability towards the expected value:

$$\bar{X} \xrightarrow{P} \mu \qquad \text{for} \qquad n \to \infty \tag{A.14}$$

We can use the independence assumption between variables X_i to write down the variance and expectation of $\bar{X}$:

$$Var(\bar{X}) = Var(\frac{1}{n}(X_1 + \cdots + X_n)) = \frac{1}{n^2} Var(X_1 + \cdots + X_n) = \frac{\sigma^2}{n} E[\bar{X}] = \mu \tag{A.15}$$

---

[1]There were many mathematically gifted Markov's. This is Andrey Andreyevich Markov Sr., known from the Markov chains and Markov processes. Jr. is known from Markov's principle, Markov's rule and the Markov algorithm.

And now we can apply Chebyshev's inequality on $\bar{X}$:

$$p(|\bar{X} - \mu| \geq \epsilon) \leq \frac{\sigma^2}{n\epsilon^2} \tag{A.16}$$

Convergence in probability towards X is the case if for all ϵ:

$$\lim_{n \to \infty} p(|\bar{X} - X| \geq \epsilon) = 0 \tag{A.17}$$

This is the case for $n \to \infty$ indeed.

A.1.4 Strong Law of Large Numbers

The strong law incorporates the weak law. Rather than convergence *in probability*, it states convergence *almost surely* towards the expected value.

$$\bar{X} \xrightarrow{a.s.} \mu \qquad \text{for} \qquad n \to \infty \tag{A.18}$$

The strong law states that with probability 1, for any $\epsilon > 0$, the inequality $|X - \mu| < \epsilon$ holds for large enough n. The weak law states only that the average $\bar{X}$ is likely near μ, but $|X - \mu| \geq \epsilon$ can still happen, even for large n.

A.1.5 Common Distributions

One of the probability distributions that is interesting to us is the beta-distribution. A normal distribution might be a reasonable prior for a continuous variable such as human heights in a population. If this variable however is itself a probability, a reasonable prior is the beta-distribution. The beta-distribution can be described as:

$$f(x, \alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1}(1-x)^{\beta-1} = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1} \tag{A.19}$$

Here B is the beta function and Γ is the gamma function, the continuous extension of the factorial function: $\Gamma(n) = (n-1)!$. Naturally, there are many of such extensions. The gamma function extends the factorial in a specific sense. It obeys the recurrence relation $f(x+1) = x f(x)$ with $f(1) = 1$. Its description is defined with an improper integral:

$$\Gamma(t) = \int_0^\infty x^{t-1} e^{-x} dx \tag{A.20}$$

The expected value of a random variable X with a beta-distribution:
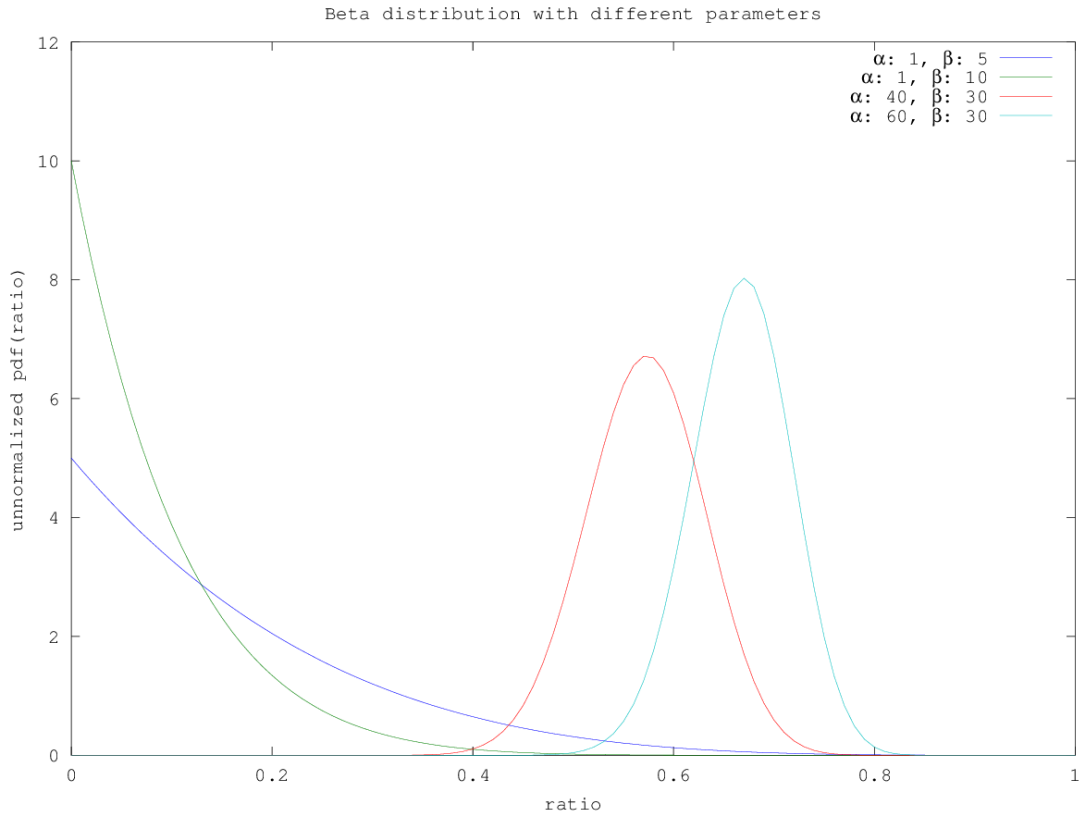
Figure A.1: The beta-distribution with different parameters. The x-axis is the quantity modelled, for example a ratio between wins and losses in a soccer season. The y-axis is the corresponding unnormalized density function. Setting $\alpha = 1$ shows a monotonically decreasing density function. Having a variable α allows probability mass to shift to the end.

$$E_f[X] = \int_0^1 x f(x, \alpha, \beta) dx = \int_0^1 \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^\alpha (1-x)^{\beta-1} dx = \frac{\alpha}{\alpha + \beta} \tag{A.21}$$

Let us illustrate the effects of the parameters of the beta-distribution.

The stick-breaking presentation shows that a Dirichlet process consists of beta processes with $\alpha = 1$. The Pitman-Yor process has α left variable. Informally, the location where the stick will be broken (iteratively) for the Dirichlet process is 'quite close to the beginning' with high probability. In the case α becomes larger, the breaking can also occur likely at the end of the stick. This means for breaking a stick, say 20 times, the distribution of stick lengths for the Pitman-Yor process has a much larger support. The difference between the large and small sticks is much larger.

DIRICHLET-MULTINOMIAL

There is confusion in the literature with respect to the Dirichlet-multinomial. There are three ways to interpret this.

B.1 Categorical Distribution

Often, the Dirichlet-multinomial is actually not a compound Dirichlet and a multinomial, but a compound Dirichlet and **categorical** distribution:

$$p(z|\theta) = \prod_i \theta_i^{z_i} \tag{B.1}$$

This means that this is about only one categorical variable, not a set. The notation of above would for dice assign the vector $[1, 0, 0, 0, 0, 0]$ to the face with one pip, $[0, 1, 0, 0, 0, 0]$ to the face with two pips, etc. Naturally, this means that $\sum_i z_i = 1$.

This gets rid off the $\frac{n!}{\prod_i z_i!}$ factor and leads to the much shorter:

$$p(z|\theta)p(\theta|\alpha) = \frac{1}{B(\alpha)} \prod_i \theta_i^{z_i + \alpha_i - 1} \tag{B.2}$$

To subsequently derive at the Dirichlet-multinomial, you'll have to integrate over:

$$\int p(z|\theta)p(\theta|\alpha)d\theta = \frac{1}{B(\alpha)} \int \prod_i \theta_i^{z_i + \alpha_i - 1} d\theta \tag{B.3}$$

Now, the Dirichlet didn't come from nowhere... The factor $B(\alpha)$ is a normalization factor:

$$p(\theta|\alpha) = \frac{1}{B(\alpha)}\prod_i \theta_i^{\alpha_i-1} = \frac{\prod_i \theta_i^{\alpha_i-1}}{\int_{\Delta^n}\prod_i \theta_i^{\alpha_i-1}d\theta} \tag{B.4}$$

with $\int_{\Delta^n}$ corresponding to the condition $\sum_i \theta_i = 1$.

In other words, the multivariate Beta function is actually this integral directly from the definition:

$$\int_{\Delta^n}\prod_i \theta_i^{\alpha_i-1}d\theta = B(\alpha) \tag{B.5}$$

And hence the integral:

$$\int \prod_i \theta_i^{z_i+\alpha_i-1}d\theta = B(\alpha+z) \tag{B.6}$$

Hence:

$$\int p(z|\theta)p(\theta|\alpha)d\theta = \frac{B(\alpha+z)}{B(\alpha)} \tag{B.7}$$

Or to end up with something commonly stated as the Dirichlet-multinomial:

$$\int p(z|\theta)p(\theta|\alpha)d\theta = \frac{\prod_i \Gamma(\alpha_i+z_i)}{\Gamma(\sum_i(\alpha_i+z_i))}\frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \tag{B.8}$$

Collecting terms:

$$\int p(z|\theta)p(\theta|\alpha)d\theta = \frac{\Gamma(\sum_i \alpha_i)}{\Gamma(\sum_i \alpha_i + \sum_i z_i)}\prod_i \frac{\Gamma(\alpha_i+z_i)}{\Gamma(\alpha_i)} \tag{B.9}$$

Note, however that we run i here over the entries in our categorical variable z represented as a vector! This is very different from a multinomial distribution over a set of variables!

B.2 Multinomial Distribution

In case of an actual multinomial distribution, counts of z, let's write them $n(z)$ are actually the topic of consideration, not z itself.

$$p(z|\theta) = \frac{(\sum_k n(z_k))!}{\prod_k(n(z_k)!)}\prod_k \theta_k^{n(z_k)} \tag{B.10}$$

We now run over k unique variables, not over a vectorized categorical variable.

Of course, we can know again multiply with a Dirichlet distribution and the derivation is along the lines as described before. The result:

$$\int p(z|\theta)p(\theta|\alpha)d\theta = \frac{(\sum_k n(z_k))!}{\prod_k (n(z_k)!)} \frac{\Gamma(\sum_k \alpha_k)}{\Gamma(\sum_k \alpha_k + \sum_k n(z_k))} \prod_k \frac{\Gamma(\alpha_k + n(z_k))}{\Gamma(\alpha_k)} \tag{B.11}$$

This might not be pretty, but it is the actual full Dirichlet-multinomial.

B.3 N Categorical Distributions

The third option, and this is meant most times is the distribution of a **sequence** of categorical variables. Recall that the multinomial assigns probabilities to the **number** of extracted balls (in an experiment getting n balls out of a bag with k ball types). A sequence of categorical variables assigns a probability to a **sequence** and has a form without the normalization factor:

$$p(z|\theta) = \prod_k \theta_k^{z_k} \tag{B.12}$$

Here k runs over the categories. We can now follow the derivation as with the single categorical variable.

C

GIBBS SAMPLING

Notation:

$$\int dF(x) = F(x) \tag{C.1}$$

A mixture model:

$$L(x) = \int dF(x)\mu(x) \tag{C.2}$$

If we have a particular form of $F(x)$, namely it admits a decomposition of a sum of individual values x_i:

$$F(x) = \sum_i \delta_{x_i} = \delta(x = x_0) + \delta(x = x_1) + \dots \tag{C.3}$$

Then our mixture model can be written as:

$$L(x) = \int dF(x)\mu(x) = \sum_i \mu(x_i) \tag{C.4}$$

Let $x_0 = 3$, $x_1 = 4$, $\mu(x) = x^2$, then $L(x) = 3^2 + 4^2 = 25$.

Walker with $P = F$, $\mu(x) = N(y|\theta)$, $i = j$ and giving each θ_j a weight ω_j:

$$f_P(y) = \int dP(\theta)N(y|\theta) \qquad P = \sum_j \omega_j \delta_{\theta_j} \tag{C.5}$$

Then:

$$f_{\omega,j}(y) = \sum_j \omega_j N(y|\theta_j) \tag{C.6}$$

The likelihood:

$$L(w \mid \alpha, \lambda_0) = p(\phi \mid \alpha) \prod_{i=0}^{N-1} \int p(w_i \mid \theta_i, \phi) dG_0(\theta_i) \tag{C.7}$$

Here the index runs over all data points w_i. Each data point corresponds to a line with parameters θ_i. Here the parameters θ_i and θ_j for data point w_i and w_j can be the same and thus reflect the same line. The index for θ runs over the N data points, not over the K lines.

The distribution G_0 does have hyperparameters λ_0.

We can also group all data points that belong to the same line k together by reordering the product terms:

$$L(w \mid \alpha, \lambda_0) = p(\phi \mid \alpha) \prod_k \prod_{i:z_i=k} \int p(w_i \mid \theta_i, \phi) dG_0(\theta_i) \tag{C.8}$$

Here the factors that belong to line k are multiplied. The index still runs over the data points.

It is also possible not to limit the second product to only the data points i that are assigned to line k.

$$L(w \mid \alpha, \lambda_0) = p(\phi \mid \alpha) \prod_k \prod_i p(z_i|\phi) \int p(w_i \mid \theta_i, \phi) dG_0(\theta_i) \tag{C.9}$$

Now, we are gonna introduce the stick-breaking sum, which turns our integral into a discrete sum.

$G = \sum_l p_l \delta_{Z_l}$ with Z_l iid from G_0 and p_l defined as a product of beta distributions.

$$L(w \mid \alpha, \lambda_0) = p(\phi \mid \alpha) \sum_k \prod_i p(z_i \mid \phi) p(w_i \mid \theta_k) p(\theta_k \mid \lambda_0) \tag{C.10}$$

The first term at the right hand side, $p(\phi \mid \alpha)$, generates the partition ϕ by the Dirichlet Process with concentration parameter α. The second term $p(z_i \mid \phi)$ defines indices $z_0, \ldots, z_N$ to link observations $w_0, \ldots, w_N$ with the parameters $\theta_0, \ldots, \theta_K$. The probability $p(w_i \mid \theta_k)$ corresponds to the likelihood equations 3.10 and 3.11 with w_i the tuple of x_i and y_i and θ_k the line parameters σ_k^2 and β_k. The probability $p(\theta_k \mid \lambda_0)$ corresponds to the prior from equation 3.14. The parameters θ_k (that is, σ_k^2 and β_k) are generated from hyperparameters λ_0. The hyperparameters $\lambda_0 = \{\mu_0, \Lambda_0, a, b\}$ are the parameters from the Normal-Inverse-Gamma prior.

The Dirichlet process can be used as a mixture model (Antoniak, 1974; Escobar and West, 1995; MacEachern and Müller, 1998) in which it generates (non-unique) parameters that subsequently generate observations:

$$G \sim DP(\alpha, G_0)$$
$$\theta_i \mid G \sim G \qquad \text{(C.11)}$$
$$w_i \mid \theta_i \sim F(\theta_i)$$

Here F describes the mapping from parameters θ_i to observations w_i. It is possible to integrate over G and sample the parameters directly from the base distribution G_0.

It is possible to integrate over G and get a description in the form of conditionals over the parameters (Blackwell and MacQueen, 1973):

$$\theta_{n+1} \mid \theta_1 \ldots \theta_{n-1} \sim \frac{1}{\alpha + n}\left(\alpha G_0 + \sum_{i=1}^{n} \delta_{\theta_i}\right) \qquad \text{(C.12)}$$

C.1 Gibbs Sampling of Parameters

Algorithm, we will draw $\theta_i | \theta_{-i}, y_i$ for all i.

And that continuously. So, that's how we get theta.

Gibbs sampling requires the conditional probabilities of all entities involved (Geman and Geman, 1984). Gibbs sampling just as other Markov chain Monte Carlo methods generates a sequence of correlated samples. Subsequently, if necessary, the Maximum A Posteriori estimation of a value can be found through picking the mode (most common occurring value) of a parameter.

The derivation of the conditional probabilities of parameters with respect to the remaining parameters has been described in the literature (Neal, 2000). Such a derivation uses an important property of the Dirichlet process, namely that it is the conjugate prior of the multinomial distribution. Thanks to conjugacy the following equations have closed-form descriptions. The conditional probabilities are sampled from the base distribution G_0 and the other parameters θ_i in the following way:

$$\theta_{n+1} \mid \theta_1 \ldots \theta_{n-1} \sim \frac{1}{\alpha + n}\left(\alpha G_0 + \sum_{i=1}^{n} \delta_{\theta_i}\right) \qquad \text{(C.13)}$$

If we include the observations themselves, we need to include the likelihood as well:

$$\theta_i \mid \theta_{-i}, w_i \sim C\left\{\sum_{j,j \neq i} F(w_i, \theta_j)\delta_{\theta_j} + \alpha H_i \int F(w_i, \theta)dG_0(\theta)\right\} \qquad \text{(C.14)}$$

The constant C is a normalization factor to make the above a proper probability density (summing to one). The entity H_i is the posterior density of θ given G_0 as prior and y_i as observation. The notation θ_{-i} describes the set of all parameters Θ with θ_i excluded. The integral over $dG_0(\theta)$ is a Lebesgue-Stieltjes integral that weighs the contribution of $F(w_i, \theta)$ with the base distribution $G_0(\theta)$.

Equation C.14 can be used to perform inference directly with all (non-unique) parameters θ_i tied to observations w_i. Details on inference will be provided in Sect. **??**.

GLOSSARY

burn-in running a Markov chain Monte Carlo for a while before starting to sample from it, so the results are not depending on its initial random starting position. 33

collapsed Gibbs sampling Rao-Blackwellized Gibbs sampling. Certain sampling steps are replaced by steps where one or more variables are integrated out. This is can be thanks to analytic descriptions that arise from the use of conjugate priors. 33

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LIST OF ABBREVIATIONS

AIC   **A**kaike **I**nformation **C**riterion

BIC   **B**ayesian **I**nformation **C**riterion

DP   **D**irichlet **P**rocess

Summary

Summary....

SAMENVATTING

Samenvatting...

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Anne van Rossum ....

PUBLICATIONS

The investigations performed during my Ph.D. research resulted in the following publications.

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[1]Abbreviations: SIKS - Dutch Research School for Information and Knowledge Systems; CWI - Centrum voor Wiskunde en Informatica, Amsterdam; EUR - Erasmus Universiteit, Rotterdam; KUB - Katholieke Universiteit Brabant, Tilburg; KUN - Katholieke Universiteit Nijmegen; OU - Open Universiteit; RUL - Rijksuniversiteit Leiden; RUN - Radboud Universiteit Nijmegen; TUD - Technische Universiteit Delft; TU/e - Technische Universiteit Eindhoven; UL - Universiteit Leiden; UM - Universiteit Maastricht; UT - Universiteit Twente, Enschede; UU - Universiteit Utrecht; UvA - Universiteit van Amsterdam; UvT - Universiteit van Tilburg; VU - Vrije Universiteit, Amsterdam.

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