Other topics

Mauricio A. Álvarez, PhD

Curso de entrenamiento ArcelorMittal

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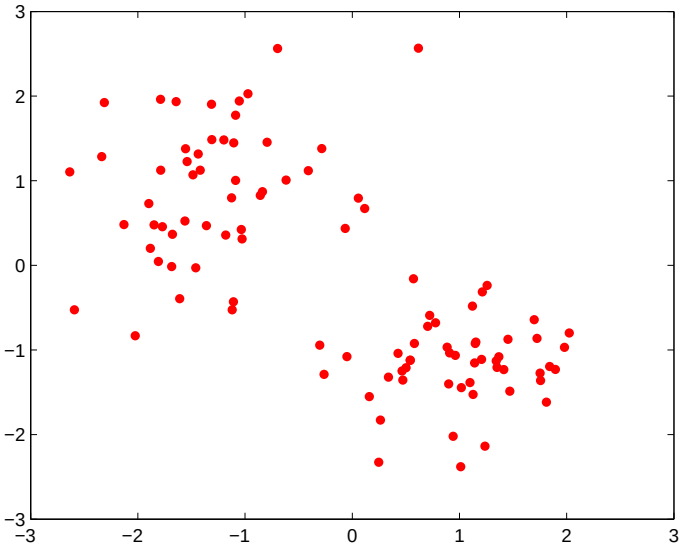
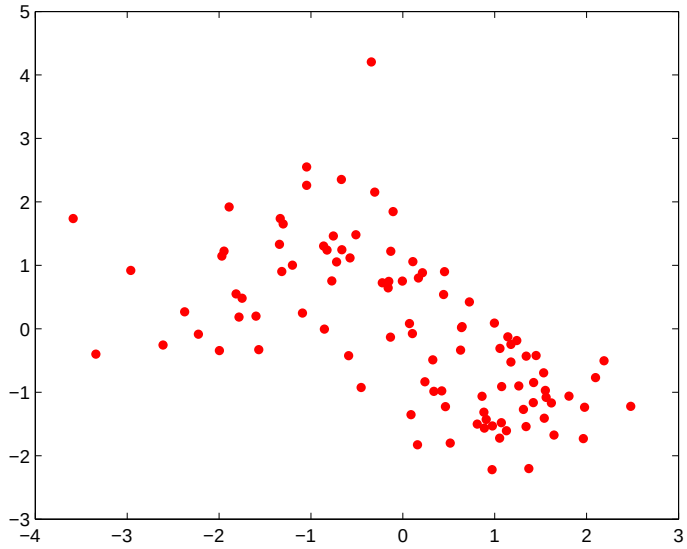
Clustering





Mixture of probability functions

- One way to approximate multimodal probability functions is through a mixture of probability functions.

- From the mixtures of probability functions, the Gaussian mixture model (GMM) is one of the best known,

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k),$$

where K is the number of components in the mixture and the parameters π_k are probabilities that satisfy

$$0 \leq \pi_k \leq 1, \quad \sum_{k=1}^{K} \pi_k = 1.$$

Contents

Introduction

- The goal of the EM (Expectation - Maximization) algorithm is to find maximum likelihood solutions for models that use latent variables.
- Let $\mathbf{X} = \{\mathbf{x}_n\}_{n=1}^N$ be the set of observations and $\mathbf{Z} = \{\mathbf{z}_n\}_{n=1}^N$, the sequence of latent variables.
- The log-likelihood function is given as

$$\ln p(\mathbf{X}|\theta) = \ln \left\{ \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta) \right\}.$$

- The presence of the sum prevents the logarithm from acting directly on the joint distribution, which results in complex expressions for the maximum likelihood solution.

Incomplete data

- The set $\{\mathbf{X}, \mathbf{Z}\}$ is known as the set of complete data.
- The observed data $\mathbf{X}$ is known as incomplete data.
- From the set $\{\mathbf{X}, \mathbf{Z}\}$ we only know $\mathbf{X}$. The only information we have about $\mathbf{Z}$ is in the probability density function $p(\mathbf{Z}|\mathbf{X}, \theta)$.

What is the logic of the EM algorithm? (I)

- Since the complete data likelihood function cannot be used, consider using its expected value under the posterior distribution of the latent variables, which corresponds to step E of the EM algorithm.
- In step M, this expectation is maximized with respect to the parameters of interest.
- If the current estimate of the parameters is θ^{old}, a successive pair of steps E and M, give rise to a new estimate θ^{new}.

What is the logic of the EM algorithm? (II)

- In step E, the current parameters are used $\boldsymbol{\theta}^{\text{old}}$, to find the posterior distribution of the latent variables given by $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$.

- This posterior distribution is then used to find the expected logarithmic likelihood of the complete data evaluated for a general parameter vector $\boldsymbol{\theta}$.

- This expectation, denoted by $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$, is given as

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}).$$

- In step M, a new vector of parameters is determined by maximizing $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}).$$

Pseudo-code for the EM algorithm

Given a joint distribution $p(\mathbf{X}, \mathbf{Z}|\theta)$, the goal is to maximize the likelihood function $p(\mathbf{X}|\theta)$ wrt the parameters θ.

1. Initialize the parameter vector θ^{old}.
2. **E step**. Compute $p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}})$.
3. **M step**. Compute θ^{new} given as

$$\theta^{\text{new}} = \arg\max_{\theta} \mathcal{Q}(\theta, \theta^{\text{old}}),$$

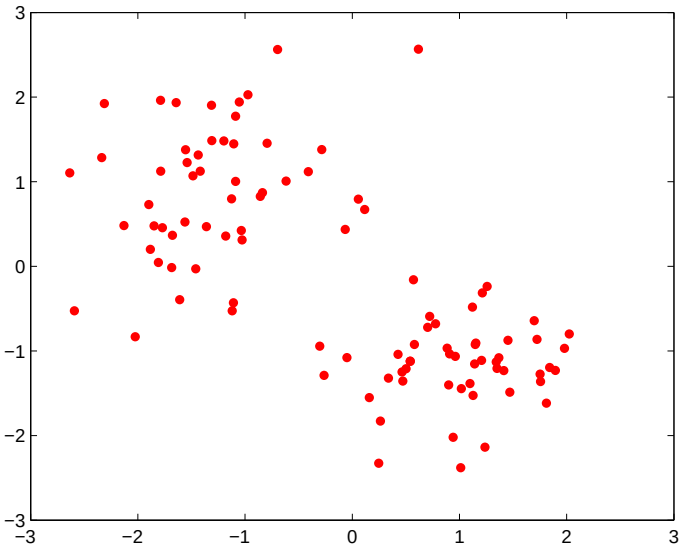
   where

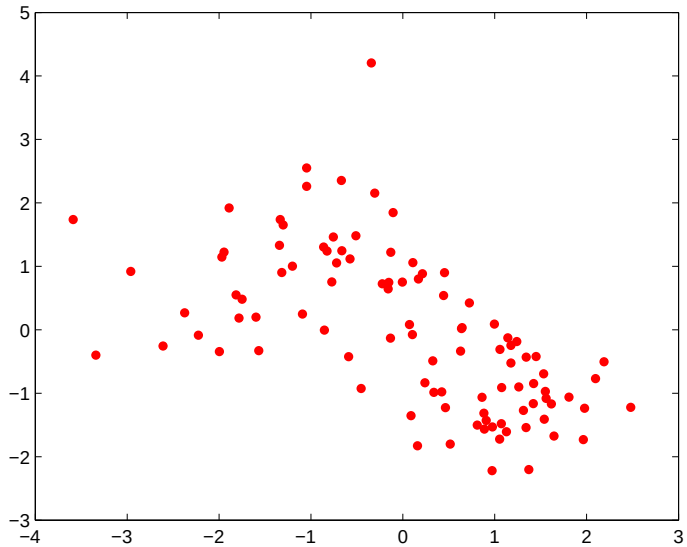
$$\mathcal{Q}(\theta, \theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\theta).$$

4. Check the convergence of the likelihood function or the parameters. If the convergence criterion is not satisfied, then $\theta^{\text{old}} \leftarrow \theta^{\text{new}}$ and go back to Step 2.

Contents

Clustering





Mixture of probability functions

- One way to approximate multimodal probability functions is through a mixture of probability functions.
- From the mixtures of probability functions, the Gaussian mixture model (GMM) is one of the best known,

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k),$$

where K is the number of components in the mixture and the parameters π_k are probabilities that satisfy

$$0 \leq \pi_k \leq 1, \quad \sum_{k=1}^{K} \pi_k = 1.$$

Latent variable $\mathbf{z}$

- Let $\mathbf{z}$ be a random binary vector of K dimensions with 1-of-K representation.
- The vector $\mathbf{z}$ can only take K states, according to which of its inputs is different from zero.
- The marginal distribution over $\mathbf{z}$ is given as

$$p(z_k = 1) = \pi_k.$$

- This distribution can be written in short as

$$p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}.$$

Conditional distribution of **x** given **z**

- The conditional distribution of **x** given **z**, is Gaussian

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- It can also be expressed as,

$$p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}$$

Marginal distribution for $\mathbf{x}$

- The joint distribution is given as $p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$.
- The marginal distribution for $\mathbf{x}$ follows as

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

- For each observed value $\mathbf{x}_n$ there is a corresponding latent variable $\mathbf{z}_n$.
- This is a new formulation of the mixture of distributions using latent variables, which allows working with the joint distribution $p(\mathbf{x}, \mathbf{z})$.

Conditional distribution of **z** given **x**

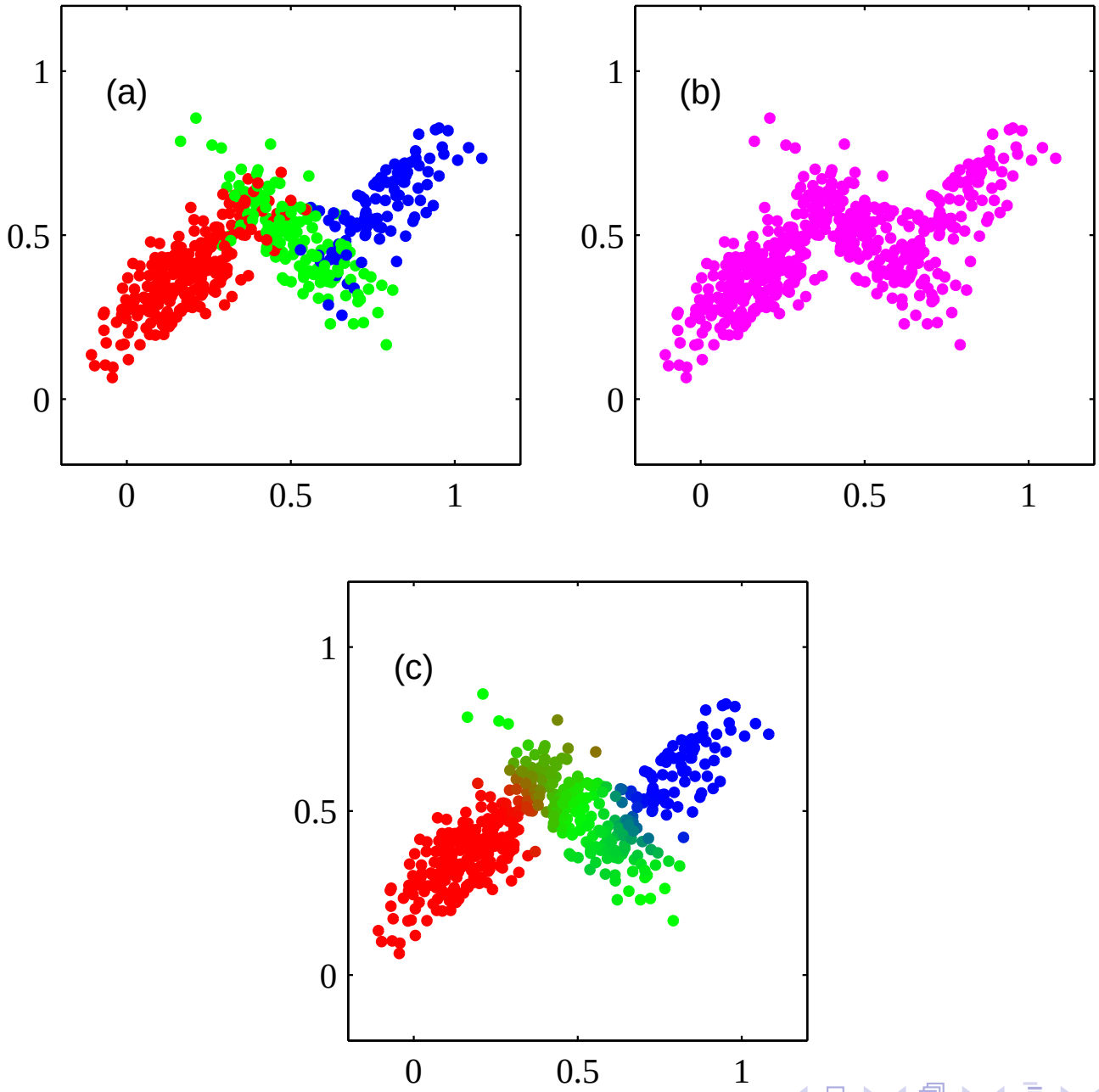
- Another quantity that plays an important role is the conditional probability of **z** given **x**.
- The probability is given as

$$\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)}$$

$$= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

- The probability π_k can be seen as the prior probability $p(z_k = 1)$ and $\gamma(z_k)$ as the corresponding posterior probability once **x** has been observed.
- This quantity can be seen as the *responsibility* that the component k assumes to explain the observation **x**.

Incomplete and complete data



Log-likelihood function

- We start with a set of observations $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ that we want to model using a mixture of Gaussians.
- These observations are represented with a matrix $\mathbf{X}$ of dimensions $N \times D$ and row vectors $\mathbf{x}_n^\top$.
- Similarly, the corresponding latent variables are denoted by a matrix $\mathbf{Z}$ with row vectors $\mathbf{z}_n^\top$ and dimensions $N \times K$.
- The log-likelihood function is given as

$$\ln p(\mathbf{X}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k) \right\}$$

- We want to find the parameters $\theta = \{\{\pi_k\}_{k=1}^K, \{\mu_k\}_{k=1}^K, \{\Sigma_k\}_{k=1}^K\}$, that maximize the likelihood of the incomplete data.

E step

- Starting with a value of θ^{old}, the posterior probability of the latent variables $\mathbf{Z}$ is calculated given the data $\mathbf{X}$ and the parameters θ^{old}.
- The probability function $p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}})$ has elements $\gamma(z_{n,k})$.
- The probabilities $\gamma(z_{n,k})$ are given as

$$\gamma(z_{n,k}) \equiv p(z_{n,k} = 1|\mathbf{x}_n) = \frac{p(z_{n,k} = 1)p(\mathbf{x}_n|z_{n,k} = 1)}{\sum_{j=1}^{K} p(z_{n,j} = 1)p(\mathbf{x}_n|z_{n,j} = 1)}$$

$$= \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

- $p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}})$ is a table of dimensions $N \times K$.

M step (I)

- We first compute the function $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$.
- $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$ is given as

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})]$$

- The complete likelihood function for the Gaussian mixture is given as

$$p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{z_{nk}} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_{nk}}$$

- The log-likelihood is given as

$$\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\}.$$

M step (II)

- $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$ is given as

$$\begin{aligned}\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) &= \mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})] \\ &= \sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(z_{nk}) \left\{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right\}.\end{aligned}$$

- Notice from the equation above that $\mathbb{E}_{\mathbf{Z}}[z_{nk}]$ corresponds to $\gamma(z_{nk})$,

$$\mathbb{E}_{\mathbf{Z}}[z_{nk}] = \sum_{z_{nk}} z_{nk} p(z_{nk}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) = p(z_{nk} = 1|\mathbf{x}_n, \boldsymbol{\theta}^{\text{old}}) = \gamma(z_{nk}).$$

- Given $\gamma(z_{nk})$, we maximize $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$ with respect to the parameters $\boldsymbol{\theta} = \{\{\pi_k\}_{k=1}^K, \{\boldsymbol{\mu}_k\}_{k=1}^K, \{\boldsymbol{\Sigma}_k\}_{k=1}^K\}$.

M step (III)

- Maximizing $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$ wrt π_k leads to

$$\pi_k^{\text{new}} = \frac{1}{N} \sum_{n=1}^{N} \gamma(z_{nk}) = \frac{N_k}{N},$$

  where $N_k = \sum_{n=1}^{N} \gamma(z_{nk})$.

- Maximizing $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$ wrt $\boldsymbol{\mu}_k$ leads to

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

- Maximizing $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$ wrt $\boldsymbol{\Sigma}_k$ leads to

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^{\top}.$$

EM algorithm for the GMM

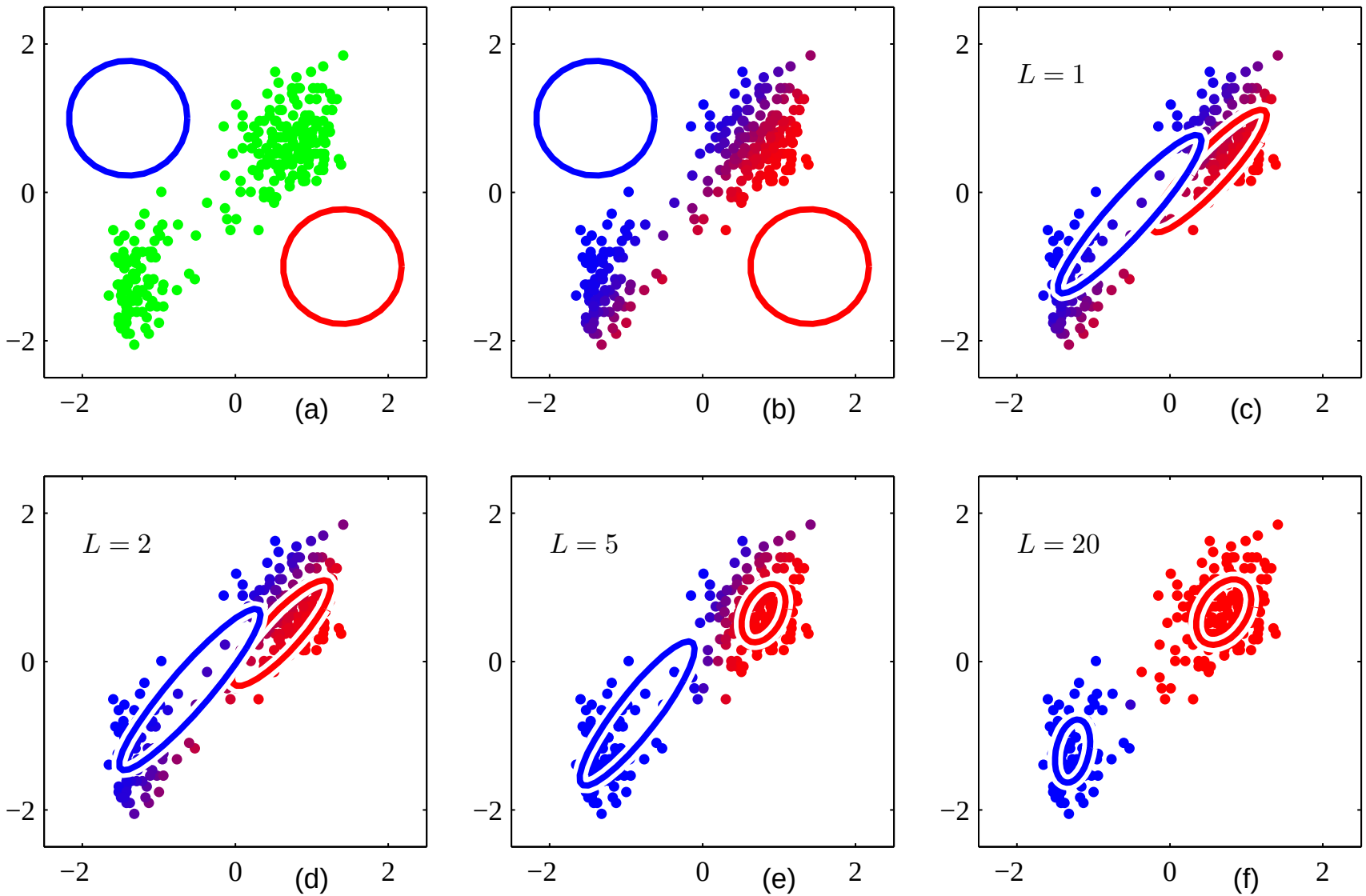
1. Initialize θ^{new}.

2. **E** step. Compute $\gamma(z_{nk})$, for $n = 1, \ldots, N$ y $k = 1, \ldots, K$.

3. **M** step. Use the update equations for π_k^{new}, μ_k^{new} and Σ_k^{new}, for $k = 1, \ldots, K$.

4. The convergence of the likelihood function or the parameters is verified. If the convergence criterion is not satisfied, then $\theta^{\text{old}} \leftarrow \theta^{\text{new}}$ and repeats from step 2.

Example



Contents

Infinite mixture models

- The simplest approach to (flat) clustering is to use a finite mixture model.
- The principle problem with finite mixture models is how to choose the number of components K.
- We discuss **infinite mixture models**, in which we do not impose any a priori bound on K.
- To do this, we will use a **non-parametric prior** based on the **Dirichlet process** (DP).
- This allows the number of clusters to grow as the amount of data increases.

From finite to infinite mixture models

- The representation for the finite mixture model that we saw before follows

$$p(\mathbf{x}_i|z_i = k, \theta) = p(\mathbf{x}_i|\theta_k)$$
$$p(z_i = k|\boldsymbol{\pi}) = \pi_k.$$

- We can additionally consider a distribution over the parameters π_k, e.g. the Dirichlet distribution

$$p(\boldsymbol{\pi}|\alpha) = \text{Dir}(\boldsymbol{\pi}|(\alpha/K)\mathbf{1}_K),$$

where $\alpha > 0$ and $\mathbf{1}_K$ is a vector of ones of dimension K.

Dirichlet distribution (I)

- A multivariate generalization of the beta distribution is the Dirichlet distribution.
- It has support over the **probability simplex**, defined by

$$S_K = \left\{ \mathbf{x} : 0 \leq x_k \leq 1, \sum_{k=1}^{K} x_k = 1 \right\}.$$

- The pdf is defined as follows:

$$\text{Dir}(\mathbf{x}|\boldsymbol{\alpha}) \triangleq \frac{1}{B(\boldsymbol{\alpha})} \prod_{k=1}^{K} x_k^{\alpha_k - 1} \mathbb{I}(\mathbf{x} \in S_K),$$

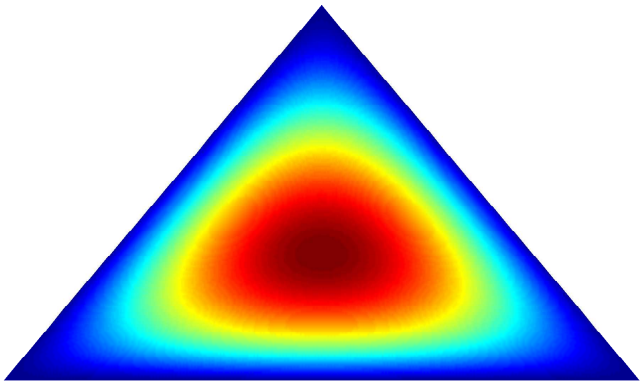
where $B(\alpha_1, \ldots, \alpha_K)$ is the natural generalization of the beta function to K variables

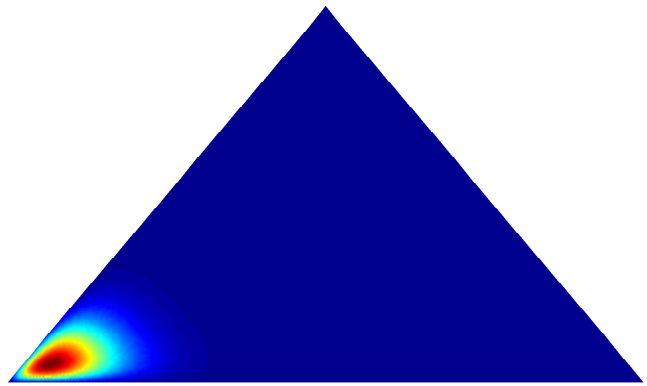
$$B(\boldsymbol{\alpha}) \triangleq \frac{\prod_{k=1}^{K} \Gamma(\alpha_k)}{\Gamma(\alpha_0)},$$

with $\alpha_0 \triangleq \sum_{k=1}^{K} \alpha_k$.

Dirichlet distribution (II)

Examples of the distribution





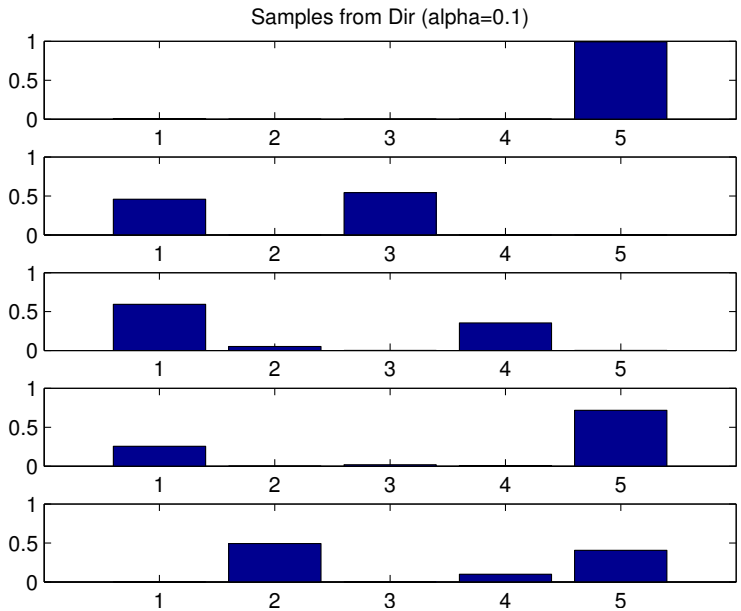
$$\boldsymbol{\alpha} = (2, 2, 2), \text{ y } \boldsymbol{\alpha} = (20, 2, 2).$$

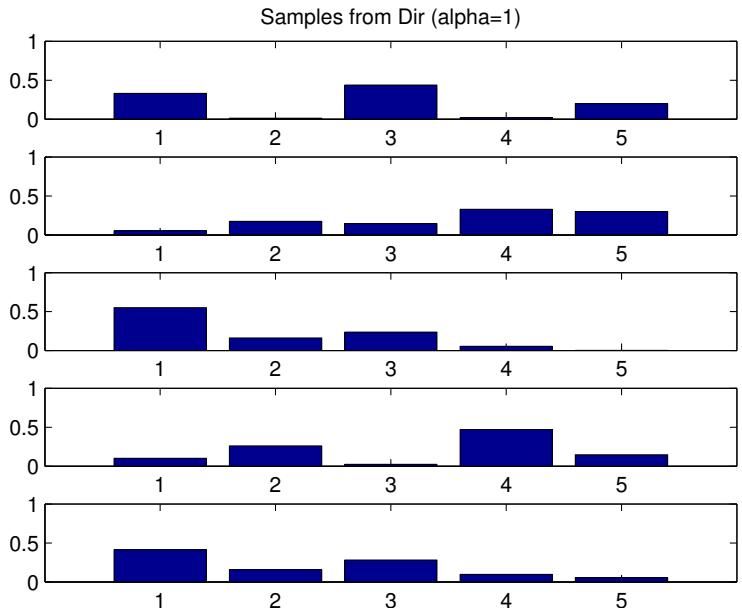
Properties

$$\mathbb{E}[x_k] = \frac{\alpha_k}{\alpha_0}, \text{mode}[x_k] = \frac{\alpha_k - 1}{\alpha_0 - K}, \text{var}[x_k] = \frac{\alpha_k(\alpha_0 - \alpha_k)}{\alpha_0^2(\alpha_0 + 1)}$$

Often we use a symmetric Dirichlet prior of the form $\alpha_k = \alpha/K$. In this case, the mean becomes $1/K$ and the variance becomes $\text{var}[x_k] = \frac{K-1}{K^2(\alpha+1)}$.

Samples from a Dirichlet distribution

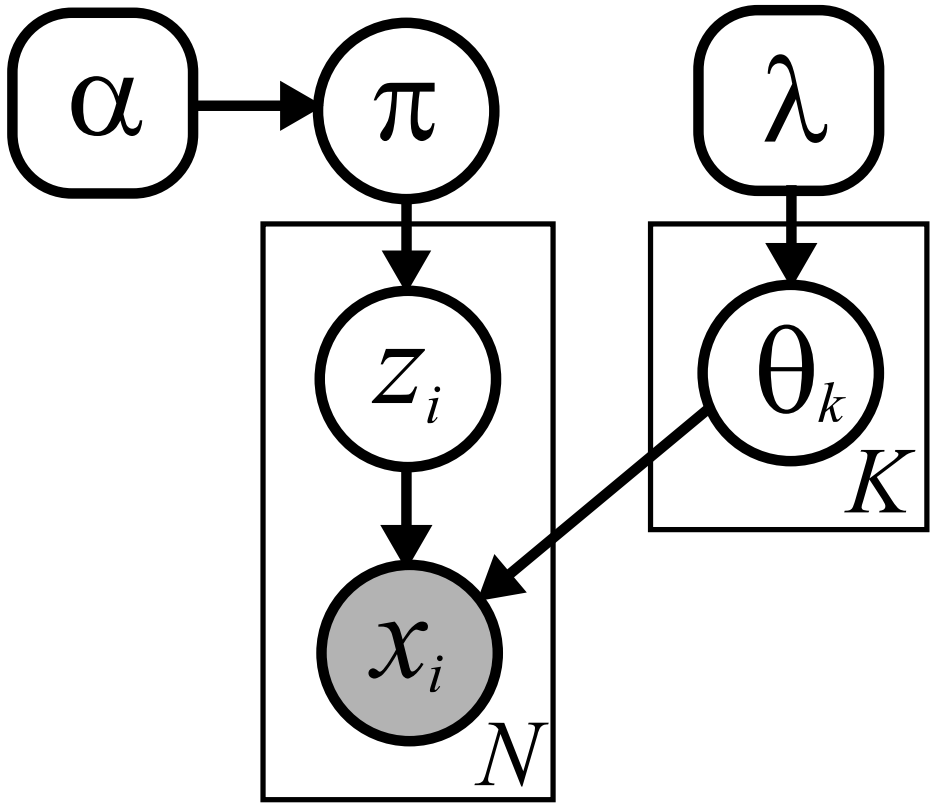




From finite to infinite mixture models

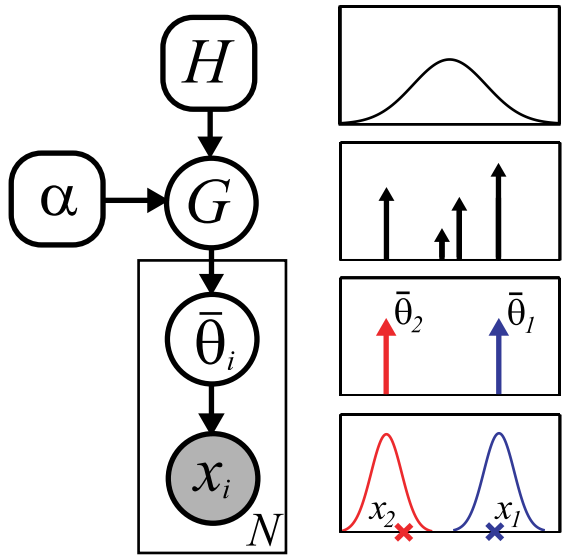
- We can also place priors over θ_k.
- The form of $p(\theta_k|\lambda)$ is chosen to be conjugate to $p(\mathbf{x}_i|z_i = k, \theta)$.
- We can write $p(\mathbf{x}_i|\theta_k)$ as $\mathbf{x}_i \sim F(\theta_{z_i})$, where F is the observation distribution.
- Similarly, we can write $\theta_k \sim H(\lambda)$ where H is the prior.

Graphical model



Alternative representation of the finite mixture model

- Another representation for the finite mixture model is shown here



- $\bar{\theta}_i$ is the parameter used to generate observation $\mathbf{x}_i$
- These parameters are sampled from distribution G,

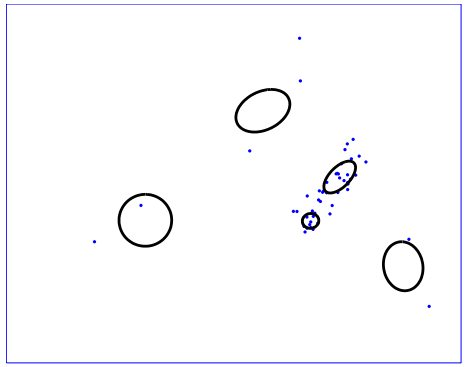
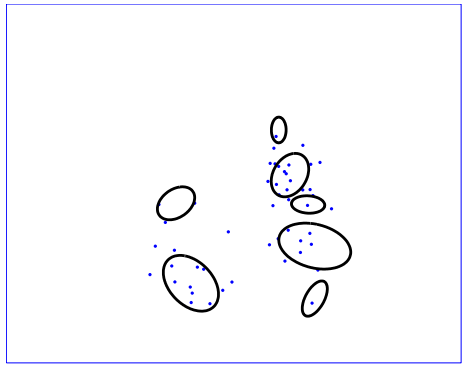
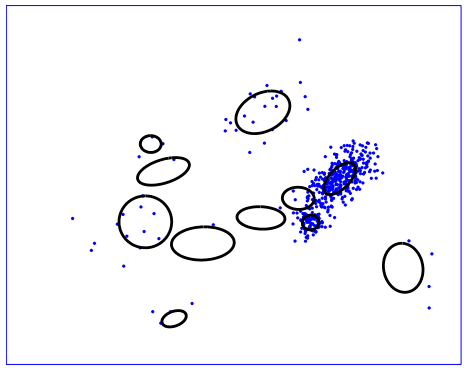
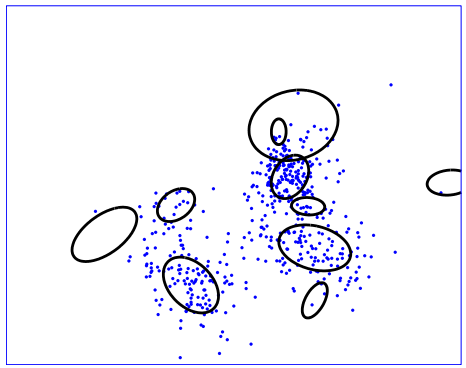
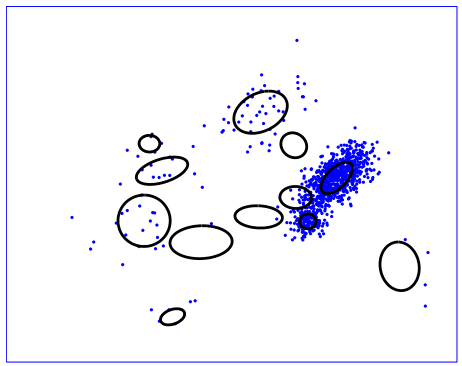
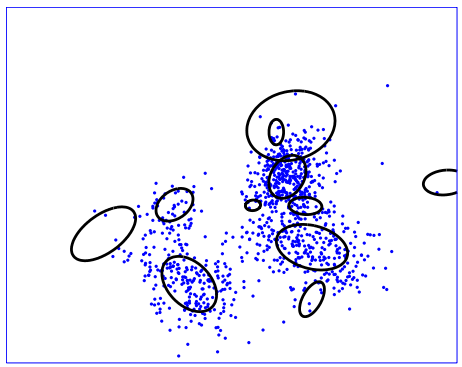
$$G(\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k \delta_{\boldsymbol{\theta}_k}(\boldsymbol{\theta}),$$

  where $\boldsymbol{\pi} \sim \text{Dir}\left(\frac{\alpha}{K}\mathbf{1}\right)$ and $\boldsymbol{\theta}_k \sim H$.
- G is a finite mixture of delta functions, centered on $\boldsymbol{\theta}_k$.
- The probability that $\bar{\theta}_i$ is equal to $\boldsymbol{\theta}_k$ is exactly π_k, the prior probability for that cluster.

Alternative representation of the finite mixture model

- If we sample from this model, we will always get exactly K clusters, with data points scattered around the cluster centers.
- We would like a more flexible model, that can generate a variable number of clusters
  - the more data we generate, the more likely we should be to see a new cluster.
- The way to do this is to replace the discrete distribution G with a random probability measure.
- The Dirichlet process, denoted $G \sim \text{DP}(\alpha, H)$, is one way to do this.

Infinite mixture model ($N = 50, 500, 1000$)

The Dirichlet process

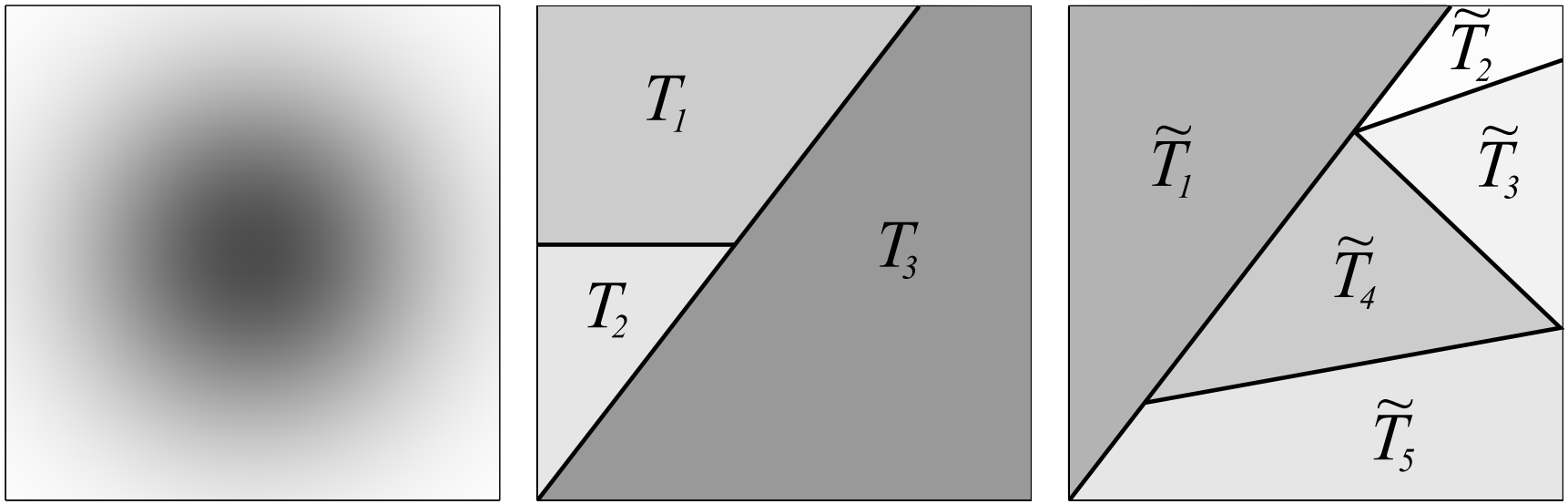
- A Dirichlet process is a distribution over probability measures $G : \Theta \to \mathbb{R}^+$.
- It is required that $G(\theta) \geq 0$ and $\int_\Theta G(\theta) d\theta = 1$.
- The DP is defined implicitly by the requirement that $(G(T_1), \ldots, G(T_K))$ has a joint Dirichlet distribution

$$\text{Dir}(\alpha H(T_1), \ldots, \alpha H(T_K)),$$

for any finite partition $(T_1, \ldots, T_K)$ of Θ.

- We write $G \sim \text{DP}(\alpha, H)$ where α is the **concentration parameter** and H is called the **base measure**.

Example



The base measure is a 2d Gaussian.

Dirichlet distribution as a prior distribution

- The Dirichlet distribution is commonly used as a prior over the parameters of a categorical or discrete distribution.

- The categorical distribution for a vector $\mathbf{z}$ with 1-of-K representation is given as

$$\mathrm{Cat}(\mathbf{z}|\boldsymbol{\pi}) = \prod_{j=1}^{K} \pi_j^{\mathbb{I}(z_j=1)},$$

  where $\pi_j = p(z_j = 1)$

- If $\boldsymbol{\pi} \sim \mathrm{Dir}(\boldsymbol{\alpha})$, the updated posterior for $\boldsymbol{\pi}$ given one observation is given by

$$\boldsymbol{\pi}|z \sim \mathrm{Dir}\left(\alpha_1 + \mathbb{I}(z = 1), \ldots, \alpha_K + \mathbb{I}(z = K)\right).$$

Dirichlet process as a prior distribution

- The DP generalizes the concept we saw before to arbitrary partitions.
- If $G \sim \mathrm{DP}(\alpha, H)$, then $p(\theta \in T_i) = H(T_i)$ and the posterior is

$$\begin{aligned} & p(G(T_1), \ldots, G(T_K) \mid \theta, \alpha, H) \\ & = \mathrm{Dir}(\alpha H(T_1) + \mathbb{I}(\theta \in T_1), \ldots, \alpha H(T_K) + \mathbb{I}(\theta = T_K)) \end{aligned}$$

- This holds for any set of partitions.
- If there are multiple samples $\overline{\theta}_i \sim G$, the new posterior is given by

$$G \mid \overline{\theta}_1, \ldots, \overline{\theta}_N, \alpha, H \sim \mathrm{DP}\left(\alpha + N, \frac{1}{\alpha + N}\left(\alpha H + \sum_{i=1}^{N} \delta_{\theta_i}\right)\right).$$

- The DP effectively defines a conjugate prior for arbitrary measurable spaces.

Stick breaking construction of the DP

- The stick-breaking construction provides a concrete way to build a DP.

- Let $\pi = \{\pi_k\}_{k=1}^{\infty}$ be an infinite sequence of mixture weights derived from the following process:

$$\beta_k \sim \text{Beta}(1, \alpha)$$

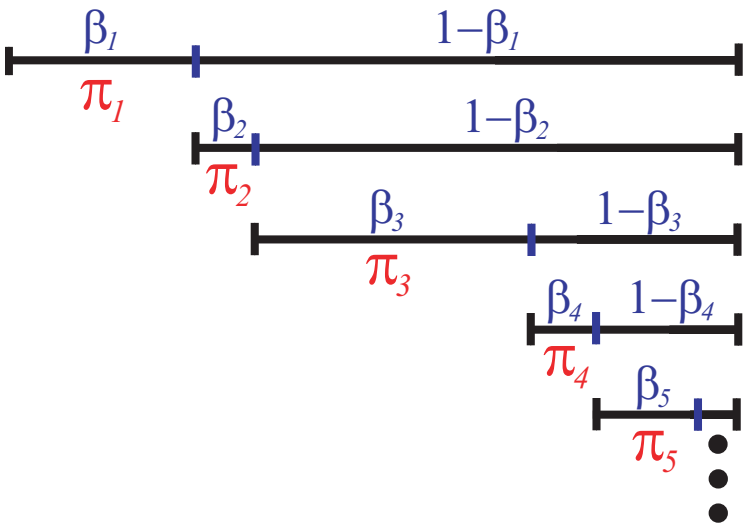
$$\pi_k = \beta_k \prod_{l=1}^{k-1} (1 - \beta_l) = \beta_k \left(1 - \sum_{l=1}^{k-1} \pi_l\right)$$

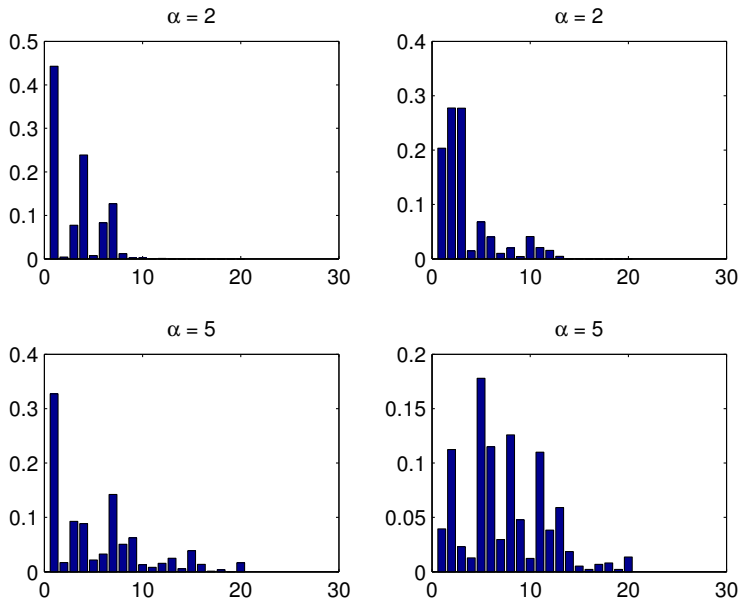
- This is often denoted by

$$\pi \sim \text{GEM}(\alpha)$$

where GEM stands for Griffiths, Engen and McCloskey (this term is due to (Ewens 1990)).

Illustration





Stick breaking construction of the DP

- We define

$$G(\theta) = \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k}(\theta),$$

where $\pi \sim \text{GEM}(\alpha)$ and $\theta_k \sim H$.

- Then one can show that $G \sim \text{DP}(\alpha, H)$.

- As a consequence of this construction, we see that samples from a DP are discrete with probability one.

- In other words, if you keep sampling it, you will get more and more repetitions of previously generated values.

Chinese restaurant processes (I)

- As the Dirichlet process assigns observations $\bar{\theta}_i$ to distinct values θ_k, it implicitly partitions the data.

- Let z_i indicate the subset, or cluster, associated with the i-th observation, so that $\bar{\theta}_i = \theta_{z_i}$.

- The predictive distribution of z_{N+1} given $\mathbf{z}_{1:N}$ is given as

$$p\left(z_{N+1} = z | \mathbf{z}_{1:N}, \alpha\right) = \frac{1}{\alpha + N}\left(\alpha \mathbb{I}\left(z = k^*\right) + \sum_{k=1}^{K} N_k \mathbb{I}(z = k)\right),$$

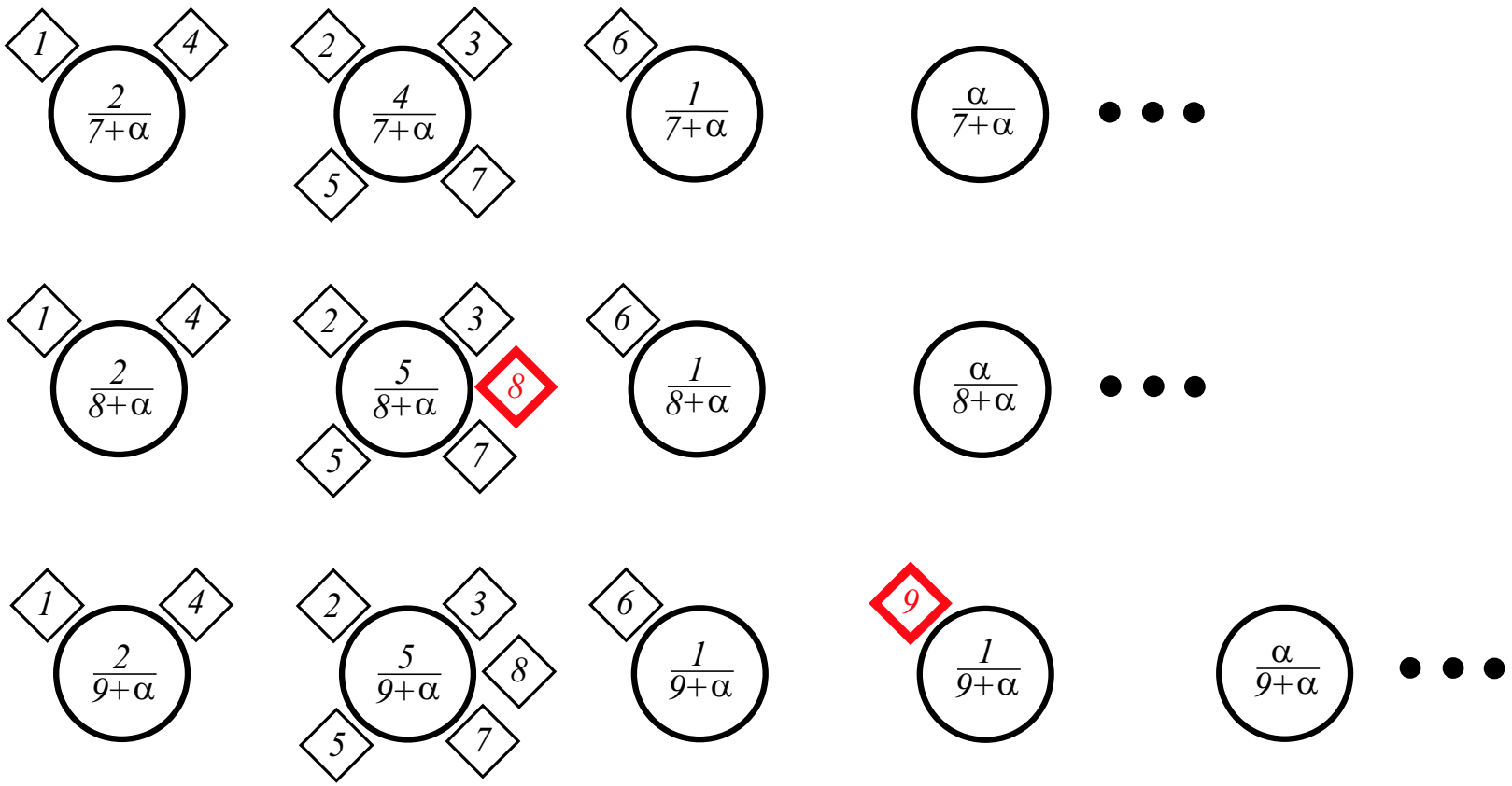
where N_k is the number of previous observations associated to the discrete variable $z = k$ and k^* represents a new cluster index that has not yet been used.

Chinese restaurant processes (II)

- Inspired by the seemingly infinite seating capacity of restaurants in San Francisco's Chinatown, Pitman and Dubins (2002) called this distribution over partitions the *Chinese restaurant process*.

- Dirichlet processes extend this construction by serving each table a different, independently chosen dish (parameter) θ_k.

Illustration



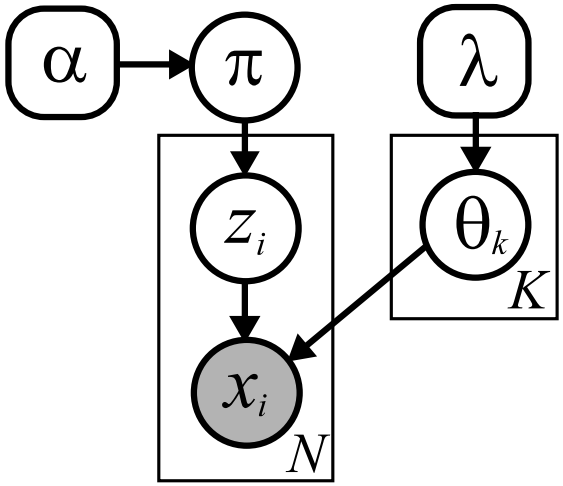
Taken from Erik B. Sudderth's PhD thesis (2006), figure 2.23.

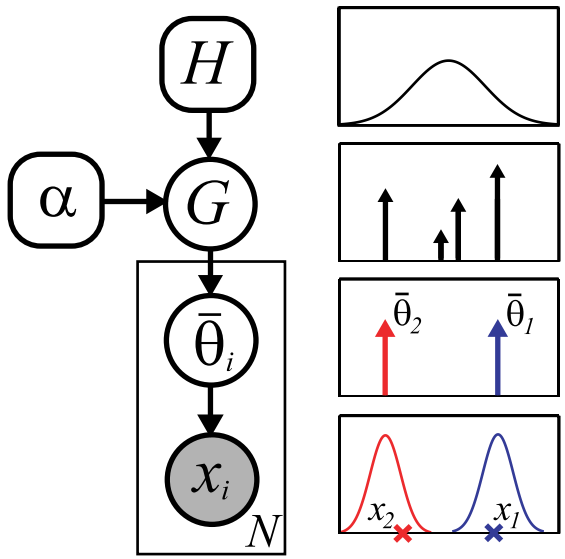
Applying Dirichlet processes to mixture modeling

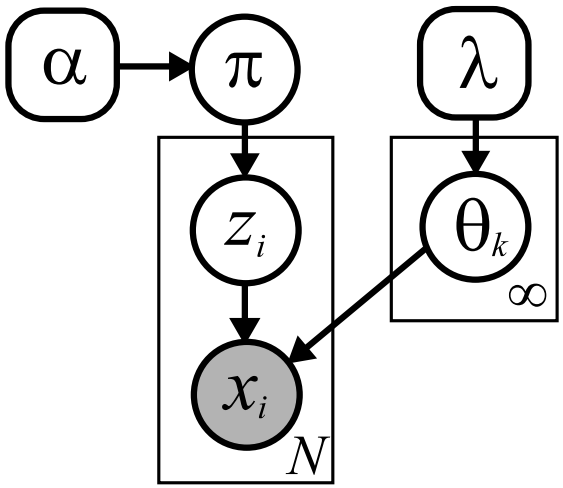
- The DP is not particularly useful as a model for data directly, since data vectors rarely repeat exactly.
- However, it is useful as a prior for the parameters of a stochastic data generating mechanism, such as a mixture model.
- We can write the model as follows

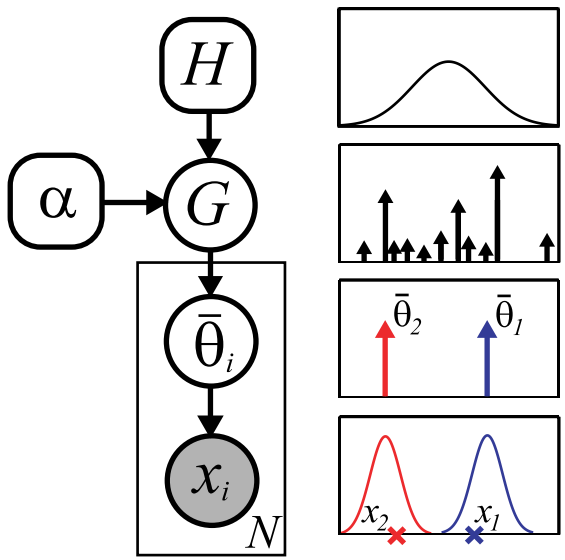
$$\begin{aligned}
\boldsymbol{\pi} &\sim \text{GEM}(\alpha) \\
z_i &\sim \boldsymbol{\pi} \\
\boldsymbol{\theta}_k &\sim H(\lambda) \\
\mathbf{x}_i &\sim F(\boldsymbol{\theta}_{z_i})
\end{aligned}$$

Finite vs infinite mixture models





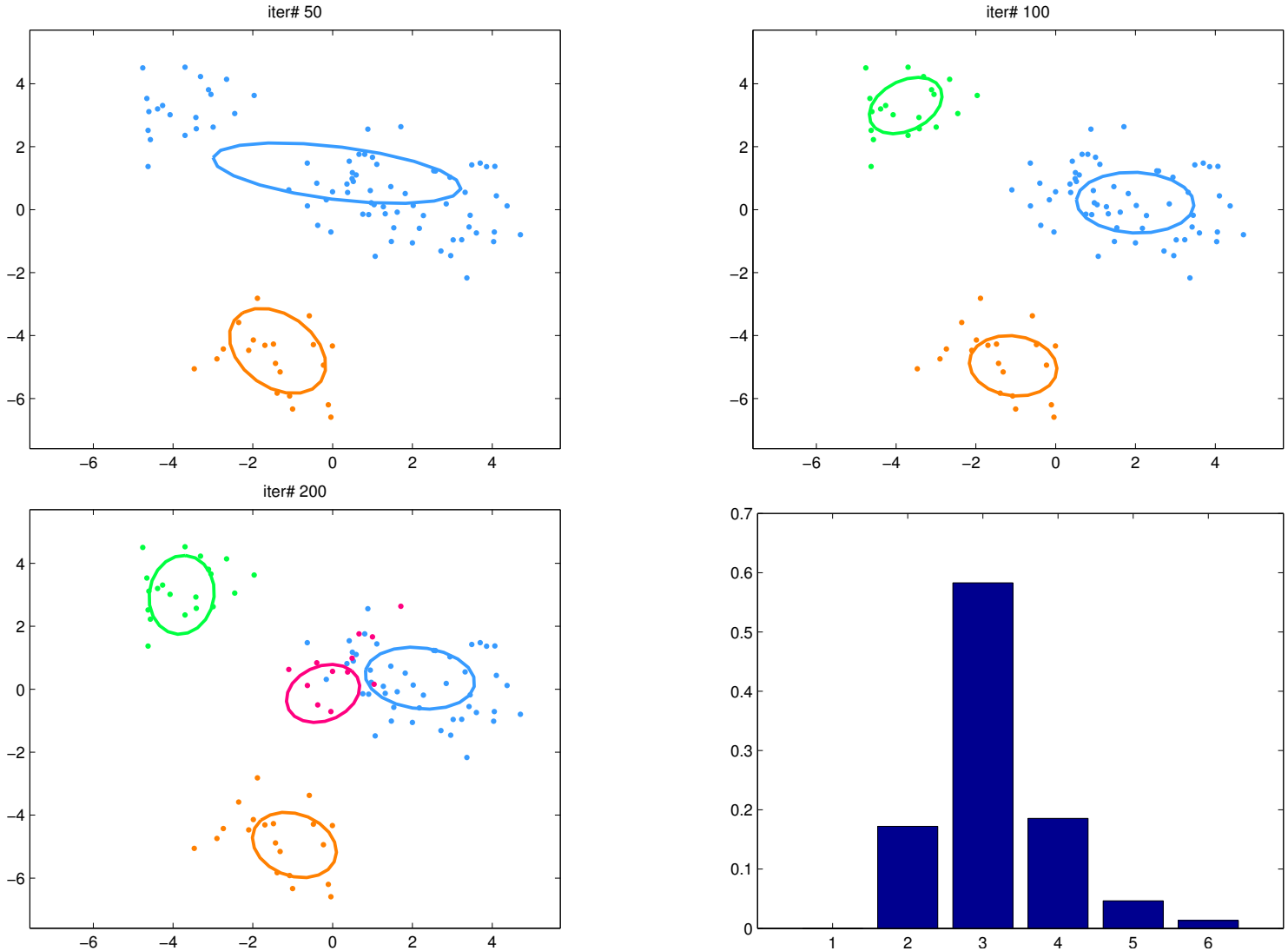




Fitting a DP mixture model

Given a dataset $\mathbf{X}$, we can uncover $\mathbf{Z}$ either by Gibbs sampling (Murphy, 2013) or variational inference (Blei and Jordan, 2005).

Example



100 data points in 2d are clustered using a DP mixture fit with collapsed Gibbs sampling. Samples from the posterior after 50,100, 200 samples.

Posterior over K, based on 200 samples, discarding the first 50 as burnin.

Contents

Introduction

- The original ME model can be viewed as a tree-structured architecture, based on the principle of divide and conquer.

- It has three main components:
  - several experts that are either regression functions or classifiers.
  - a gate that makes soft partitions of the input space and defines those regions where the individual expert opinions are trustworthy.
  - a probabilistic model to combine the experts and the gate.

Model (I)

- The basic expression for the ME is given as

$$p(y|\mathbf{x},\theta) = \sum_{k=1}^{K} \pi_k(\mathbf{x}|\theta) p_k(y|\mathbf{x},\theta),$$

  where $\pi_k(\mathbf{x})$ is known as *gating* functions and the individual component densities $p_k(\mathbf{y}|\mathbf{x})$ are called *experts*.

- More specifically,

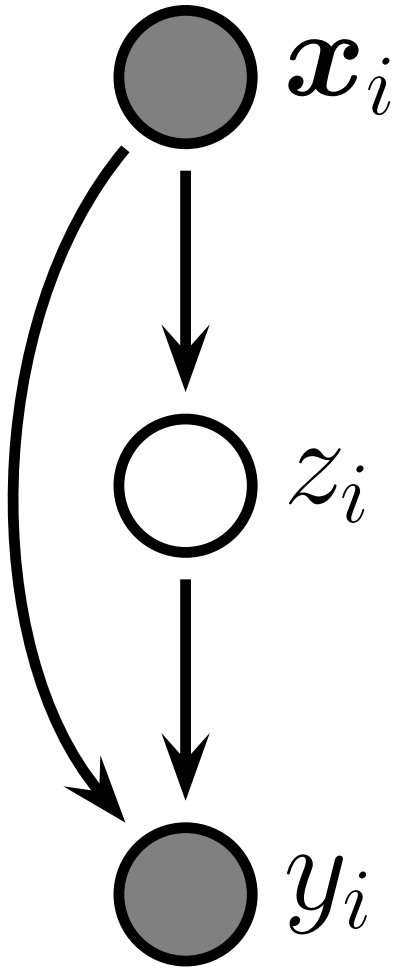
$$p\left(y|\mathbf{x},\theta\right) = \sum_{k=1}^{K} p\left(z=k|\mathbf{x},\theta\right) p\left(y|\mathbf{x},z=k,\theta\right).$$

- Different components can model the distribution in different regions (they are 'experts' at making predictions in their own regions).

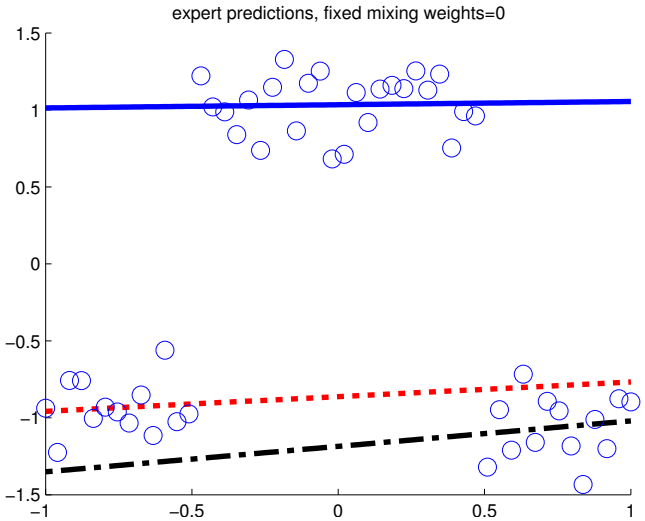
Model (II)

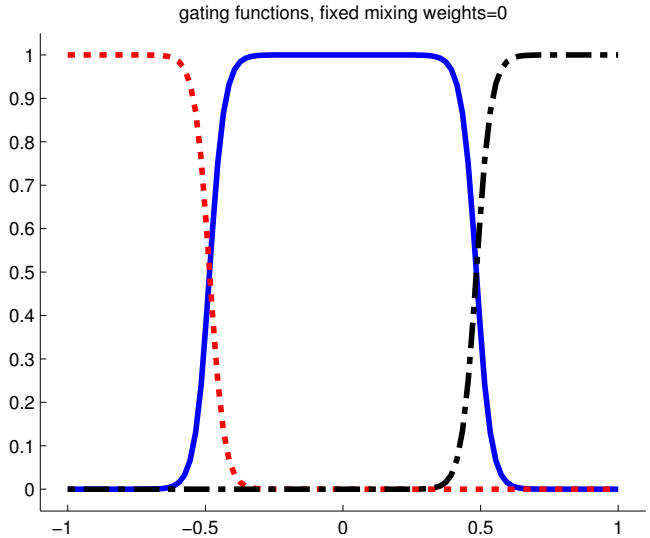
- The gating functions determine which components are dominant in which region.
- The gating functions $\pi_k(\mathbf{x})$ must satisfy the constraints for mixing coefficients,
  - $0 \leqslant \pi_k(\mathbf{x}) \leqslant 1$.
  - $\sum_k \pi_k(\mathbf{x}) = 1$.

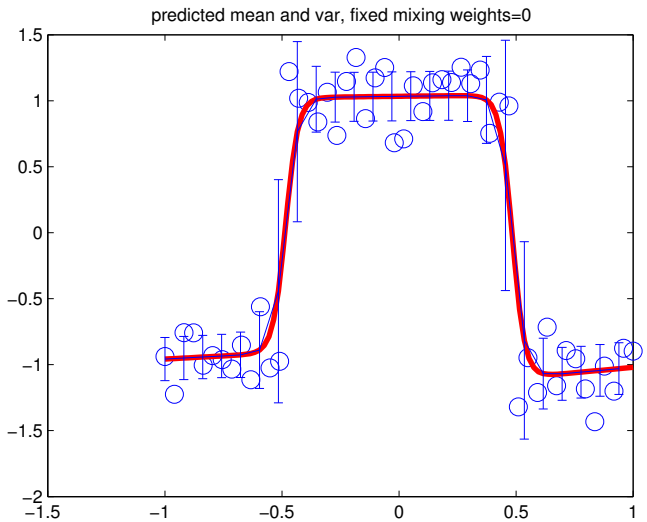
Graphical model



Linear models as experts



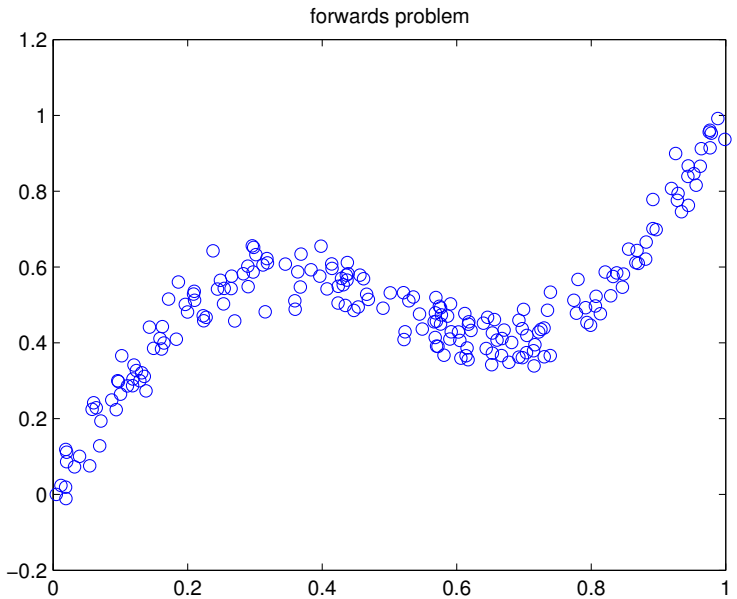




Some data fit with three separate regression lines; the gating functions for three different “experts” and the conditionally weighted average of the three expert predictions.

Application to inverse problems (I)

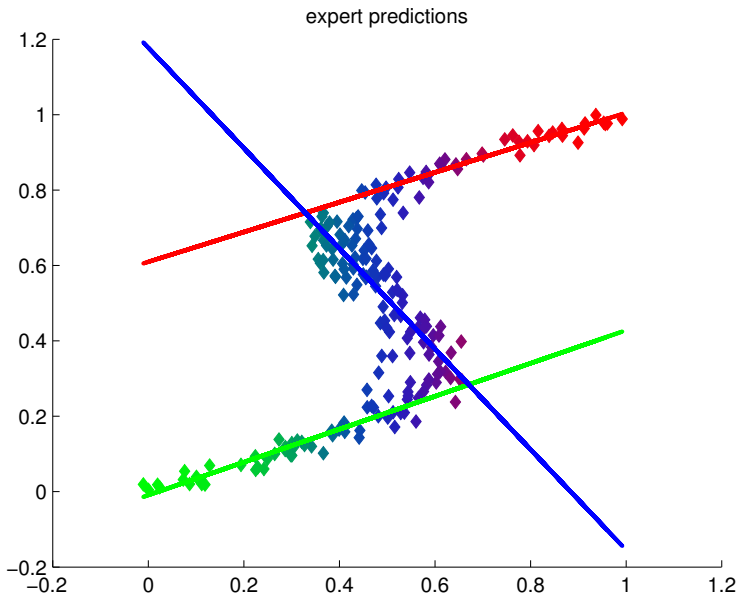
- Mixtures of experts are useful in solving **inverse problems**.
- These are problems where we have to invert a many-to-one mapping.
- This figure shows an example of a function $y = f(x)$: for every value x along the horizontal axis, there is a unique response y.



- This is sometimes called the **forwards model**.

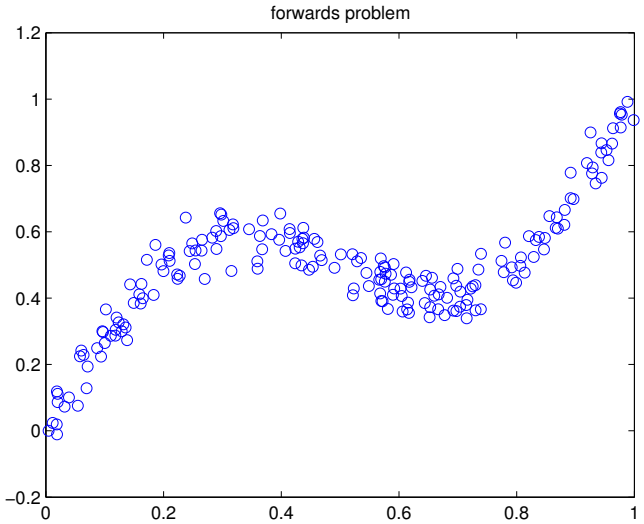
Application to inverse problems (II)

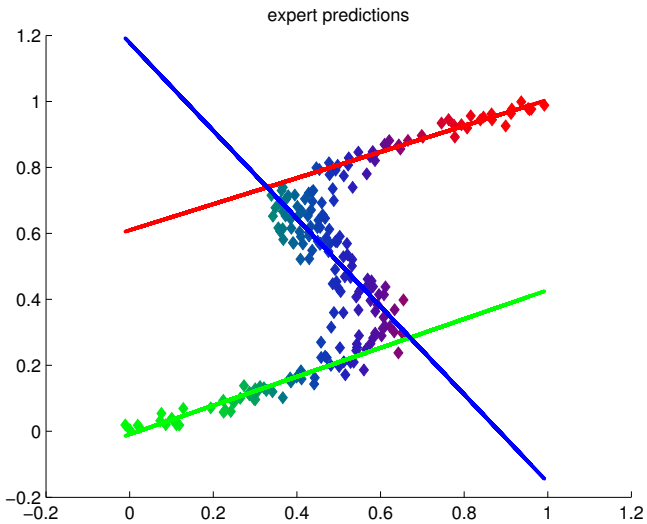
- Now consider the problem of computing $x = f^{-1}(y)$.
- The corresponding inverse model is shown in the following figure

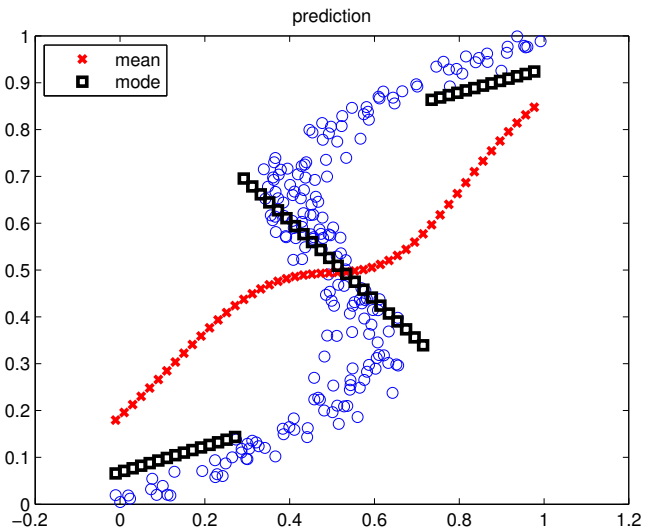


- The figure is obtained by simply interchanging the x and y axes.
- For some values along the horizontal axis, there are multiple possible outputs, so the inverse is not uniquely defined. For example, if $y = 0.6$, then x could be 0.2 or 0.8.
- Consequently, the predictive distribution, $p(x|y, \theta)$, is multimodal.
- Mixtures of experts are useful in solving **inverse problems**.

Fit of a mixture of linear experts to the data







- The posterior mean does not yield good predictions.
- However, the posterior mode, where the mode is input dependent, provides a reasonable approximation

Contents

First mixture of Gaussian processes

- The first mixture of GPs was proposed by Volker Tresp in 2001 (Tresp, 2001).
- There are $\{f_k^{\mu}(\mathbf{x})\}_{k=1}^K$ Gaussian process regression models used as experts.
- There are $\{f_k^{z}(\mathbf{x})\}_{k=1}^K$ used to compute the gating function $\pi_k(\mathbf{x})$.
- In particular, if there are K components and $\pi_i(\mathbf{x}) = p(z = i|\mathbf{x})$, then

$$p(z = i|\mathbf{x}) = \frac{\exp(f_i^z(\mathbf{x}))}{\sum_{j=1}^K \exp(f_j^z(\mathbf{x}))}$$

First mixture of Gaussian processes

- Furthermore, Tresp (2001) considers heteroscedastic GPs for the experts, such that

$$p_k(y|\mathbf{x}) = \mathcal{N}(y|f_k^{\mu}(\mathbf{x}), \exp(2f_k^{\sigma}(\mathbf{x}))).$$

- The ME is then given as

$$p(y|\mathbf{x}) = \sum_{k=1}^{K} p(z=k|\mathbf{x})\mathcal{N}(y|f_k^{\mu}(\mathbf{x}), \exp(2f_k^{\sigma}(\mathbf{x}))).$$

- The conditional expected value for y given $\mathbf{x}$ follows as

$$\mathbb{E}[y|\mathbf{x}] = \sum_{k=1}^{K} p(z=k|\mathbf{x}) f_k^{\mu}(\mathbf{x}).$$

Inference using the EM algorithm

- Tresp (2001) proposes an Expectation-Maximization (EM) algorithm for inference over the gating function and the experts.

- The negative log of the likelihood, including the log of the priors over the different Gaussian processes is given as

$$
\begin{aligned}
&-\sum_{n=1}^{N}\log\sum_{k=1}^{K}p\left(z=k|\mathbf{x}_n\right)\mathcal{N}\left(y_n|f_k^{\mu}\left(\mathbf{x}_n\right),\exp\left(2f_k^{\sigma}\left(\mathbf{x}_n\right)\right)\right)\\
&+\frac{1}{2}\sum_{i=1}^{K}\left(\mathbf{f}_i^{z,k}\right)^{\top}\left(\boldsymbol{\Sigma}_i^{z,k}\right)^{-1}\mathbf{f}_i^{z,k}+\frac{1}{2}\sum_{i=1}^{K}\left(\mathbf{f}_i^{\mu,k}\right)^{\top}\left(\boldsymbol{\Sigma}_i^{\mu,k}\right)^{-1}\mathbf{f}_i^{\mu,k}\\
&+\frac{1}{2}\sum_{i=1}^{K}\left(\mathbf{f}_i^{\sigma,k}\right)^{\top}\left(\boldsymbol{\Sigma}_i^{\sigma,k}\right)^{-1}\mathbf{f}_i^{\sigma,k},
\end{aligned}
$$

where $\mathbf{f}_i^{\mu,k}=\left(f_i^{\mu}\left(\mathbf{x}_1\right),\ldots,f_i^{\mu}\left(\mathbf{x}_N\right)\right)^{\top}$.

E step

- In the E step, we compute the posterior distribution $p(z = k|y_k, \mathbf{x}_k)$.

- It follows the same expression that we use for the responsabilities in a Gaussian mixture model, this is

$$\hat{p}\left(z = i|\mathbf{x}_n, y_n\right) = \frac{p\left(z = i|\mathbf{x}_n\right)\mathcal{N}\left(y_n|\hat{f}_i^{\mu}\left(\mathbf{x}_n\right), \exp\left(2\hat{f}_i^{\sigma}\left(\mathbf{x}_n\right)\right)\right)}{\sum_{j=1}^{K} p\left(z = j|\mathbf{x}_n\right)\mathcal{N}\left(y_n|\hat{f}_j^{\mu}\left(\mathbf{x}_n\right), \exp\left(2\hat{f}_j^{\sigma}\left(\mathbf{x}_n\right)\right)\right)}$$

M step

- In the M step, the Gaussian processes at the data points are updated.

- We obtain

$$\hat{\mathbf{f}}_i^{\mu,k} = \boldsymbol{\Sigma}_i^{\mu,k} \left(\boldsymbol{\Sigma}_i^{\mu,k} + \boldsymbol{\Psi}_i^{\mu,k} \right)^{-1} \mathbf{y}^k,$$

  where $\boldsymbol{\Psi}_i^{\mu,k}$ is a diagonal matrix with entries

$$\left(\boldsymbol{\Psi}_i^{\mu,k} \right)_{m,m} = \exp \left(2 \hat{f}_i^{\sigma} \left(\mathbf{x}_n \right) \right) / \hat{p} \left(z = i | x_n, y_n \right).$$

- To update the other Gaussian processes iterative Fisher scoring steps have to be used (Tresp, 2001).

Infinite mixture of Gaussian process experts

- Rasmussen and Ghahramani (2001) proposed a mixture of Gaussian process experts where the gating network is based on a Dirichlet process.
- To make the gating network input dependent, they use a kernel function to compute a parameter (the occupation number) in the Dirichlet process.
- The authors use Gibbs sampling for inference.

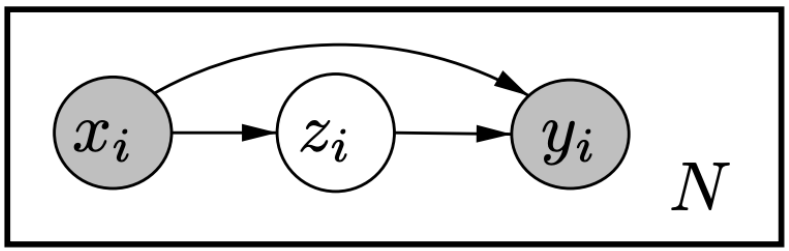
Gating function: discriminative vs generative

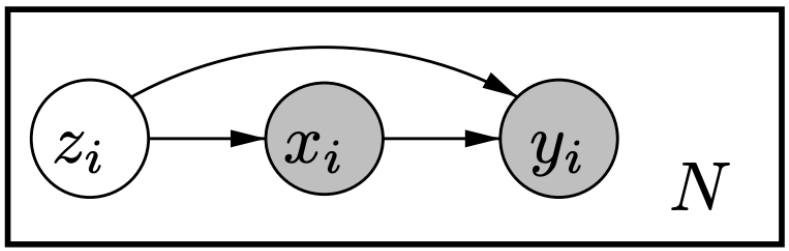
- In the mixture of experts, we have modeled the gating function as $p(z = k|\mathbf{x})$, e.g. as a conditional distribution.
- In ML, these types of models are usually referred to as discriminative.
- Alternatively, we can model both $p(z = k)$ and $p(\mathbf{x}|z = k)$, and compute the posterior distribution $p(z = k|\mathbf{x})$ to use as the gating function,

$$p(z = k|\mathbf{x}) = \frac{p(z = k)p(\mathbf{x}|z = k)}{\sum_j p(z = j)p(\mathbf{x}|z = j)}.$$

- The distribution of input locations is now given by a mixture model, with components for each expert.
- Conditioned on the input locations, the posterior responsibilities for each mixture component behave like a gating network.
- This approach is known as generative.

Gating function: discriminative vs generative





Advantages generative approach: deals with partially specified data and infer inverse functional mappings (from **x** to y).

Variational Mixture of GP Experts: experts

- Yuan and Neubauer (2009) proposed to use variational inference for a finite mixture of Gaussian process experts.

- A local Gaussian process expert is specified by the following linear model given the expert indicator $t = l$ (where $l = 1 : L$)

$$P\left(y|\mathbf{x}, t = l, \mathbf{v}_l, \boldsymbol{\theta}_l, \mathcal{I}_l, \gamma_l\right) = \mathcal{N}\left(y|\mathbf{v}_l^\top \boldsymbol{\phi}_l(\mathbf{x}), \gamma_l^{-1}\right),$$

where $\phi_l(\mathbf{x}) = \left[k_l\left(\mathbf{x}, \mathbf{x}_{\mathcal{I}_{l_1}}\right), k_l\left(\mathbf{x}, \mathbf{x}_{\mathcal{I}_{l_2}}\right), \ldots, k_l\left(\mathbf{x}, \mathbf{x}_{\mathcal{I}_{l_M}}\right)\right]^\top$ and $\{\mathcal{I}_{l_j}\}_{j=1}^M$ refer to indexes of the elements of the active set $\mathcal{I}_l$.

- The prior for $\mathbf{v}_l$ is given as $\mathcal{N}\left(\mathbf{v}_l|\mathbf{0}, \mathbf{U}_l^{-1}\right)$, where $\mathbf{U}_l = \mathbf{K}_l + \sigma_{hl}^2\mathbf{I}$ and $\mathbf{K}_l$ is the kernel matrix computed from the elements in the active set.

- $\boldsymbol{\theta}_l$ refers to the hyperparameters of the kernel.

Variational Mixture of GP Experts: experts

- The combination of $\mathcal{N}\left(y|\mathbf{v}_l^\top \phi_l(\mathbf{x}), \gamma_l^{-1}\right)$ and $\mathcal{N}\left(\mathbf{v}_l|\mathbf{0}, \mathbf{U}_l^{-1}\right)$ is equivalent to the subset of regressors approximation for sparse GPs.

- The prior of γ_l is set as a Gamma distribution.

Variational Mixture of GP Experts: gating function

- The gating functions are modeled as GMMs (generative approach)

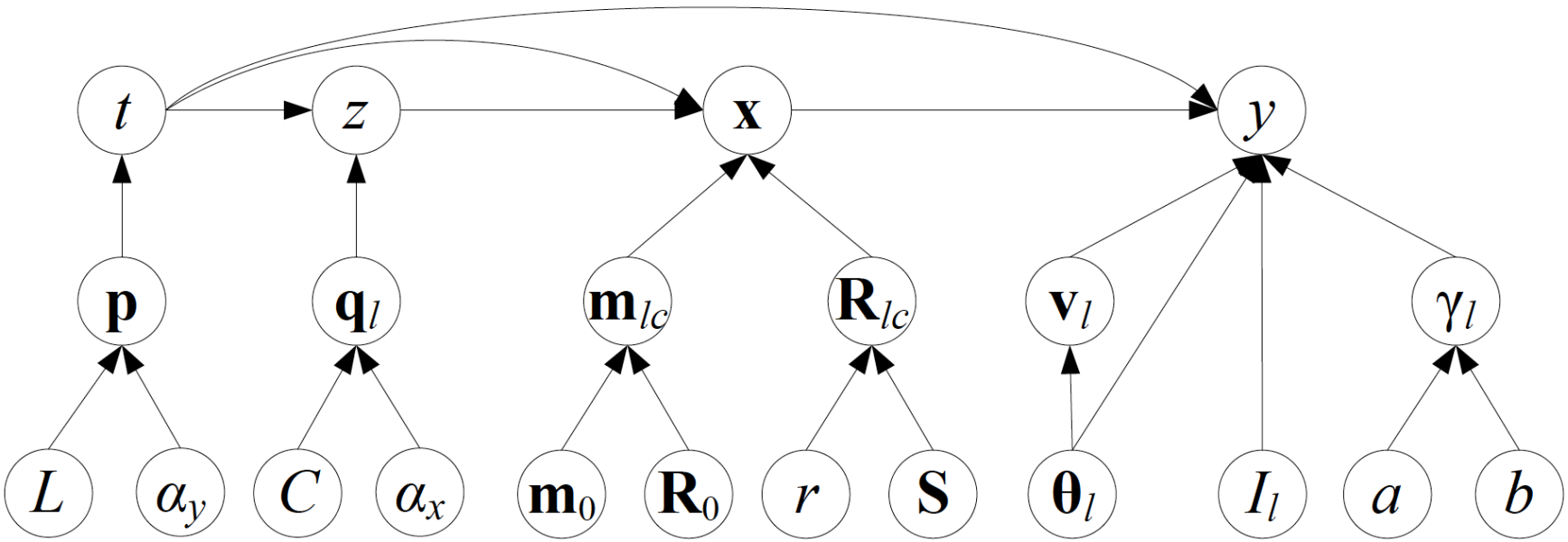
$$
\begin{aligned}
p(\mathbf{x}|t=l) &= \sum_{c=1}^{C} p(z=c|t=l,\mathbf{q}_l)\mathcal{N}(\mathbf{x}|\mathbf{m}_{lc},\mathbf{R}_{lc}^{-1}) \\
&= \sum_{c=1}^{C} q_{lc}\mathcal{N}(\mathbf{x}|\mathbf{m}_{lc},\mathbf{R}_{lc}^{-1}) \\
p(\mathbf{t}|\mathbf{p}) &= \mathrm{Cat}(\mathbf{t}|\mathbf{p}), \\
p(\mathbf{p}) &= \mathrm{Dir}\left(\mathbf{p}|\frac{\alpha_y}{L},\cdots,\frac{\alpha_y}{L}\right).
\end{aligned}
$$

- Additionally, the following priors are used

$$
\begin{aligned}
p(\mathbf{q}_l) &= \mathrm{Dir}\left(\mathbf{q}_l|\frac{\alpha_x}{C},\cdots,\frac{\alpha_x}{C}\right) \\
p(\mathbf{m}_{lc}) &= \mathcal{N}\left(\mathbf{m}_{lc}|\mathbf{m}_0,\mathbf{R}_0^{-1}\right) \\
p(\mathbf{R}_{lc}) &= \mathcal{W}\left(\mathbf{R}_{lc}|r,\mathbf{S}\right),
\end{aligned}
$$

where $\mathcal{W}(\cdot)$ is a Wishart distribution.

Variational Mixture of GP Experts: graphical model



Variational Mixture of GP Experts: mean field

- The authors use mean-field variational inference to compute the posterior distribution over the parameters $\mathbf{\Psi}$, expert indicators $\mathbf{T} = \{t_{1:N}\}$, and cluster indicators $\mathbf{Z} = \{z_{1:N}\}$.

- They use $\mathbf{\Omega} = \{\mathbf{\Psi}, \mathbf{T}, \mathbf{Z}\}$.

- The approximated posterior has the form

$$Q(\mathbf{\Omega}) = \prod_{l,c} Q(\mathbf{m}_{lc})\, Q(\mathbf{R}_{lc}) \prod_{l} Q(\mathbf{q}_l)\, Q(\mathbf{v}_l)\, Q(\gamma_l)\, Q(\mathbf{p}) \prod_{n} Q(t_n, z_n)\,.$$

- Expressions for all the posterior distributions above can be computed in closed form.

Variational inference for the infinite mixtures of GPs

- Sun and Xu (2011) proposed to use variational inference for computing posterior distributions in the model proposed by Rasmussen and Ghahramani (2001)

- They use a generative model for the gating functions similarly to Yuan and Neubauer (2009).

Variational inference for the infinite mixtures of GPs

- In practice, the model is pretty similar to the one proposed by Yuan and Neubauer (2009).
- The differences are:
  - Instead of using a GMM, they use a single Gaussian distribution for $p(\mathbf{x}|t = l)$. So instead of

$$p(\mathbf{x}|t = l) = \sum_{c=1}^{C} p(z = c|t = l, \mathbf{q}_l)\mathcal{N}(\mathbf{x}|\mathbf{m}_{lc}, \mathbf{R}_{lc}^{-1}),$$

    they use

$$p(\mathbf{x}|t = l) = \mathcal{N}(\mathbf{x}|\mathbf{m}_l, \mathbf{R}_l^{-1}).$$

  - Instead of using a Dirichlet distribution for $p(\mathbf{p})$, they use a Dirichlet process

$$p(\mathbf{p}) \sim DP(\alpha, H),$$

    where the base measure H is a Normal-Wishart distribution, similar to Yuan and Neubauer (2009).

Variational inference for the infinite mixtures of GPs

- Sun and Xu (2011) use the stick breaking construction for the Dirichlet process.
- They use mean field variational inference for computing the posterior distributions.
- The posterior distributions for the terms β_l in the stick breaking construction are approximated as in Blei and Jordan (2005).

Contents

Linear operators

- Since differentiation is a linear operator, the derivative of a Gaussian process is another Gaussian process.
- We can use GPs to either make predictions about derivatives, or to make inference based on derivative information.
- We can make inference based on the joint Gaussian distribution of function values and partial derivatives.

Kernel functions and inference

- The covariance between function values and partial derivatives and the covariance between partial derivatives are given as

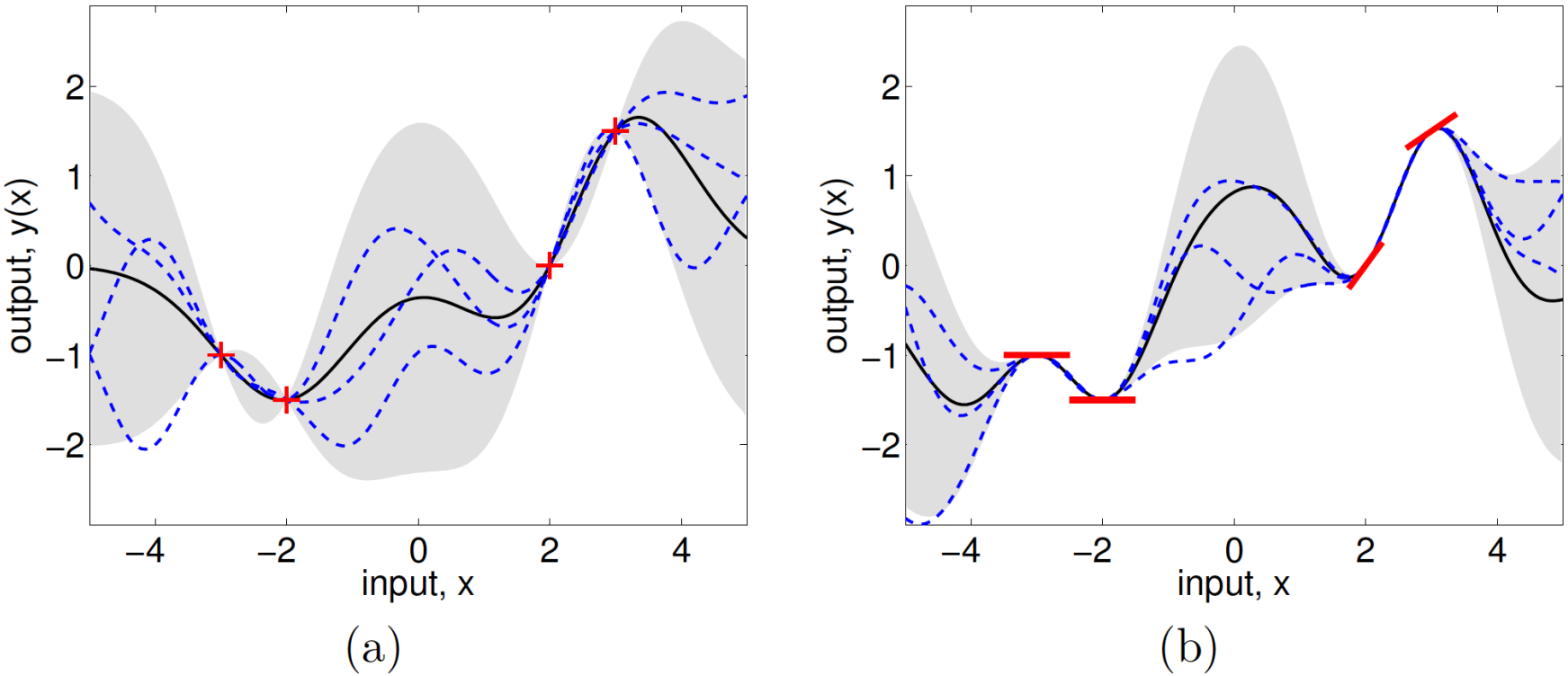
$$\operatorname{cov}\left(f_i, \frac{\partial f_j}{\partial x_{dj}}\right) = \frac{\partial k\left(\mathbf{x}_i, \mathbf{x}_j\right)}{\partial x_{dj}}, \quad \operatorname{cov}\left(\frac{\partial f_i}{\partial x_{di}}, \frac{\partial f_j}{\partial x_{ej}}\right) = \frac{\partial^2 k\left(\mathbf{x}_i, \mathbf{x}_j\right)}{\partial x_{di} \partial x_{ej}}$$

- Observed function values and derivatives may often have different noise levels

- We add a diagonal contribution with differing hyperparameters, one for the function and one for the derivative.

- Inference and predictions are done as usual.

Function and derivative evaluations



In panel (a) we show four data points in a one dimensional noise-free regression problem, together with three functions sampled from the posterior and the 95% confidence region in light grey. In panel (b) the same observations have been augmented by noise-free derivative information, indicated by small tangent segments at the data points. The covariance function is the squared exponential with unit process variance and unit length-scale. (Rasmussen and Williams, 2006)

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