Module 3: Bayesian Nonparametrics

Gaussian Processes cont'd

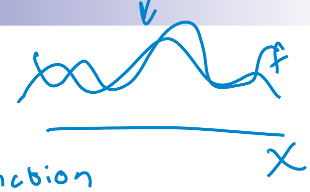
STAT/BIOSTAT 527, University of Washington

Emily Fox

May 2nd, 2013

Gaussian Processes

GP is a dist of this



- Distribution on functions
  - $f \sim GP(m, \kappa)$
    - m: mean function
    - κ: covariance function = kernel function

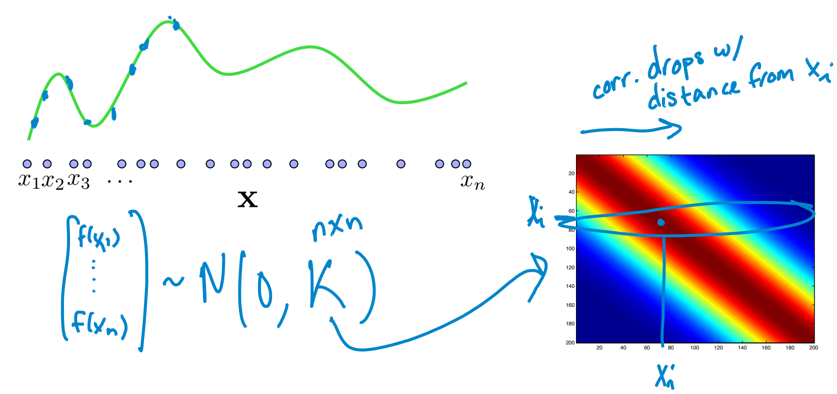
  ⇕ iff ∀n and any $x_1, \ldots, x_n$

  - $p(f(x_1), \ldots, f(x_n)) \sim N_n(\mu, K)$
    - $\mu = [m(x_1), \ldots, m(x_n)]$
    - $K_{ij} = \kappa(x_i, x_j)$ Gram matrix

- Idea: If x_i, x_j are similar according to the kernel, then $f(x_i)$ is similar to $f(x_j)$ similar outputs captured by K

Induced Multivariate Gaussian

- Evaluating the GP-distributed function at any set of locations, we have



Relating GPs to Splines

- Recall smoothing spline objective

$$\min_f \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \int f''(x)^2 dx$$

- Consider the following model

$$f(x) = \beta_0 + \beta_1 x + r(x)$$

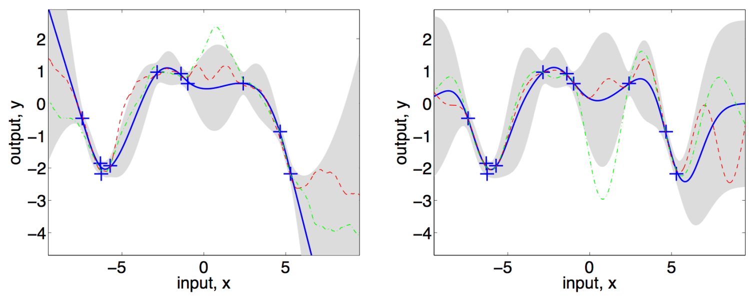
where

- One can show that the MAP estimate of *f*(*x*) is a ***cubic smoothing spline*** when $p(\beta_j) \propto 1$

- Penalty parameter λ is now given by σ_y^2 / σ_f^2

Relating GPs to Splines

- The spline kernel leads to a smooth posterior mode/mean, but posterior samples are not smooth.
  - Again, as in lasso, regularizers do not always make good priors



(a), spline covariance (b), squared exponential cov.

Figure from Rasmussen and Williams 2006

- See Rasmussen and Williams 2006 for more details

GP Regression Recap

	Linear Basis Expansion	Gaussian Process
Prior	$\beta \sim N(0, \alpha^{-1} I_M)$ $f(x) = \sum_{m=1}^{M} \beta_m \phi_m(x)$	$f \sim \mathrm{GP}(0, \kappa(x, x'))$
Distribution on $x_1, \ldots, x_n$	$f \sim N(0, \alpha^{-1} \Phi \Phi^T)$	$f \sim N(0, K)$
Choices	• *Choose M* • *Choose bases*	• *Choose* $\kappa(x, x')$ • *Choose covariance hyperparameters*

GP Regression Recap

Linear Basis Expansion	**GP regression**	**Splines**	**Kernels**
$\{\phi_m(x)\}$	$\kappa(x, x')$		
↓	↓		
f	f		
↓	↓		
y	y		

Effective Degrees of Freedom

- For the training set, the fit is given by

$$\hat{f} = K(K + \sigma_y^2 I_n)^{-1} y$$

- Since *K* is a positive definite Gram matrix, it has eigendecomp

$$K = \sum_{i=1}^{n} \lambda_i u_i u_i^T$$

- Using this, one can show that $K(K + \sigma_y^2 I_n)^{-1}$ has eigenvals

$$\frac{\lambda_i}{\lambda_i + \sigma_y^2}$$

- Therefore, the effective degrees of freedom is

$$\nu = tr\left(K(K+\sigma_y^2 I_n)^{-1}\right) = \sum_i \frac{\lambda_i}{\lambda_i + \sigma_y^2}$$

↓ fcn of how quickly eigvals decay

- Remember that this specifies how "wiggly" the curve is

Choice of Covariance Function

- Definitions
  - ***Stationary*** kernel – only depends on $x - x'$
  - ***Isotropic*** kernel – furthermore only depends on $||x - x'||$
- Examples
  - ***Squared exponential*** – $\kappa_{SE}(r) = e^{-\frac{r}{2\ell^2}}$
    - Kernel is infinitely differentiable → GP has mean square derivatives of all orders → resulting functions are very smooth
  - ***Matern*** – $\kappa_{Matern}(r) = \frac{2^{1-\nu}}{\Gamma(\nu)}\left(\frac{\sqrt{2\nu r}}{\ell}\right)^{\nu} K_v\left(\frac{\sqrt{2\nu r}}{\ell}\right)$
    - When $\nu \to \infty$: squared exponential
    - When $\nu = \frac{1}{2}$: exponential kernel $\kappa_{exp}(r) = e^{-\frac{r}{\ell}}$
      ** equal to Brownian motion in 1D **

Sample Paths using Matern Kernel

- Can produce very rough sample paths

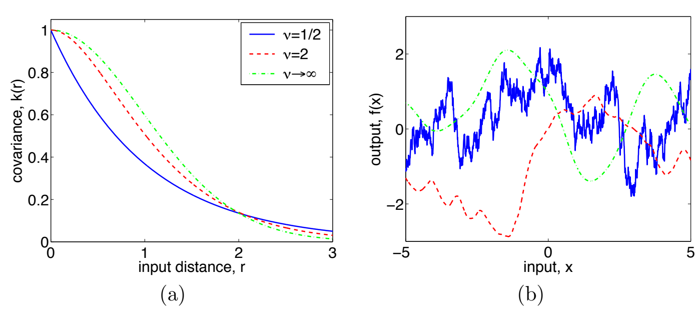
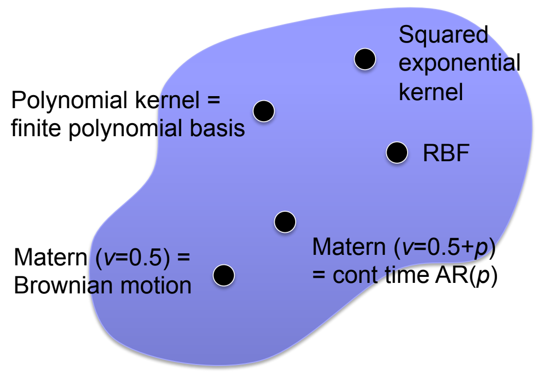


Figure from Rasmussen and Williams 2006

Family of Gaussian Processes



Module 3: Bayesian Nonparametrics

Finite Mixture Models

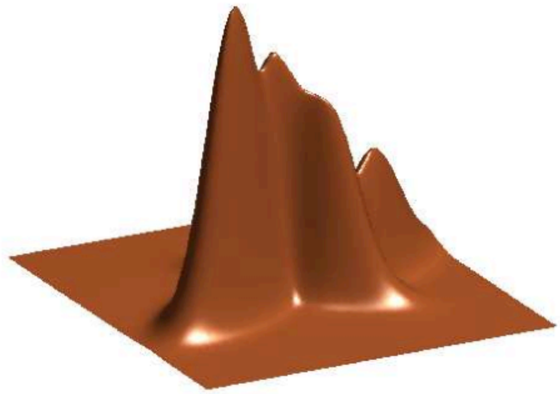
STAT/BIOSTAT 527, University of Washington

Emily Fox

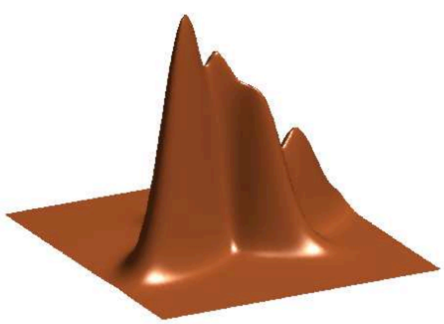
May 2nd, 2013

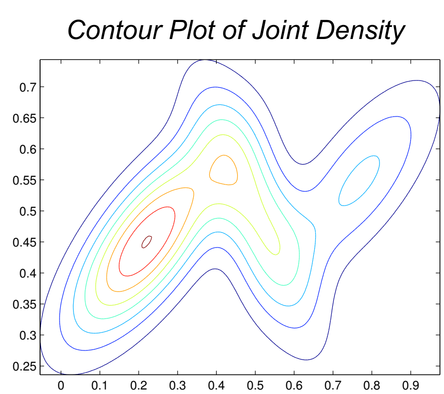
Density Estimation

- Estimate a density based on $x_1, \ldots, x_N$



Density Estimation

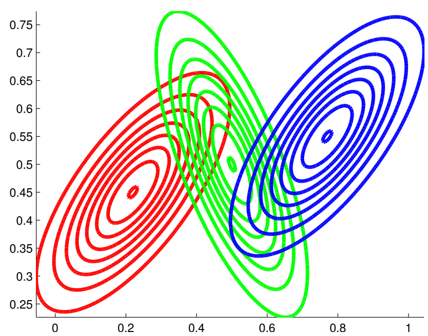




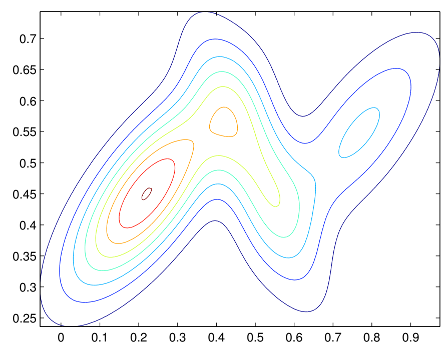
Density as Mixture of Gaussians

- Approximate density with a mixture of Gaussians

Mixture of 3 Gaussians



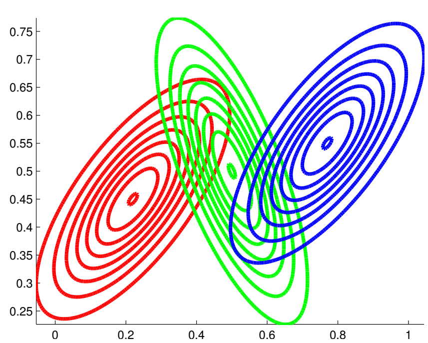
Contour Plot of Joint Density



Density as Mixture of Gaussians

- Approximate density with a mixture of Gaussians

Mixture of 3 Gaussians

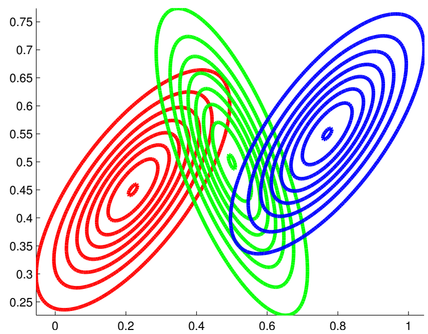


$$p(x_i \mid \pi, \mu, \Sigma) =$$

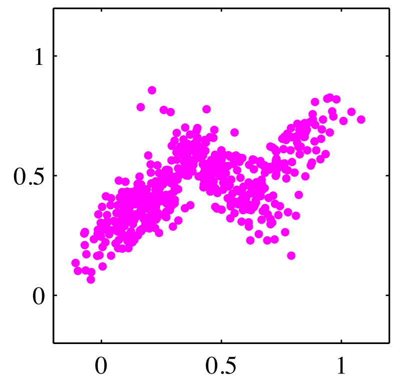
Density as Mixture of Gaussians

- Approximate with density with a mixture of Gaussians

Mixture of 3 Gaussians



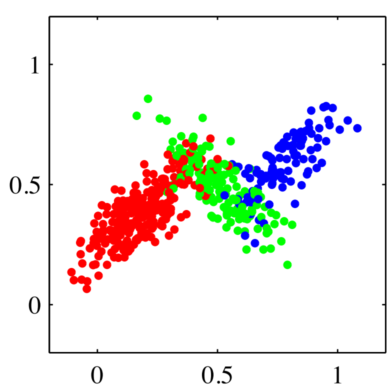
Our actual observations



C. Bishop, Pattern Recognition & Machine Learning

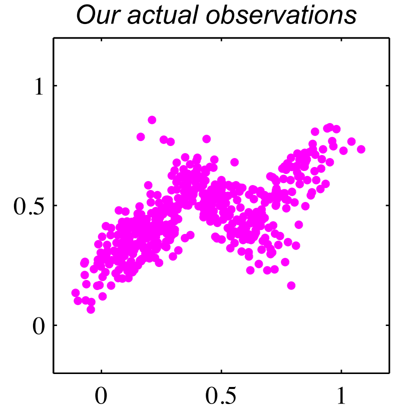
Clustering our Observations

- Imagine we have an assignment of each x_i to a Gaussian



Complete data labeled by true cluster assignments

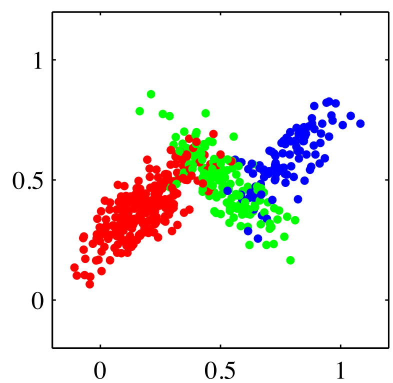
Our actual observations



C. Bishop, Pattern Recognition & Machine Learning

Clustering our Observations

- Imagine we have an assignment of each x_i to a Gaussian



Complete data labeled by true cluster assignments

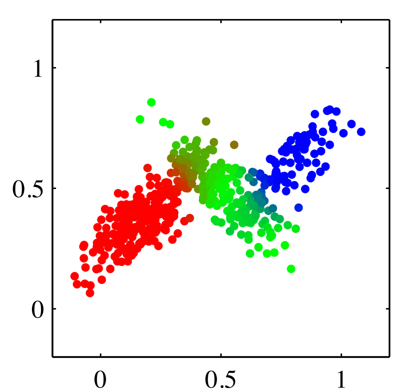
- Introduce latent cluster indicator variable z_i
- Then we have

$$p(x_i \mid z_i, \pi, \mu, \Sigma) =$$

C. Bishop, Pattern Recognition & Machine Learning

Clustering our Observations

- We must infer the cluster assignments from the observations



Soft assignments to clusters

- Posterior probabilities of assignments to each cluster *given* model parameters:

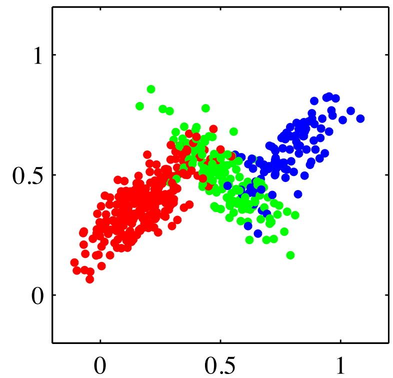
$$r_{ik} = p(z_i = k \mid x_i, \pi, \theta) =$$

C. Bishop, Pattern Recognition & Machine Learning

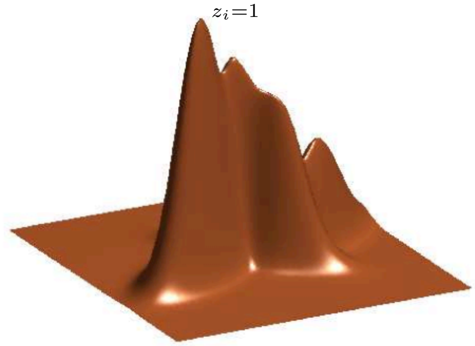
Summary of GMM Concept

- Estimate a density based on $x_1, \ldots, x_N$

$$p(x_i \mid \pi, \mu, \Sigma) = \sum_{z_i=1}^{K} \pi_{z_i} \mathcal{N}(x_i \mid \mu_{z_i}, \Sigma_{z_i})$$



Complete data labeled by true cluster assignments



Surface Plot of Joint Density, Marginalizing Cluster Assignments

Summary of GMM Components

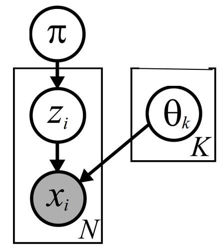
- Observations $x_i \in \mathbb{R}^d, \quad i = 1, 2, \ldots, N$
- Hidden cluster labels $z_i \in \{1, 2, \ldots, K\}, \quad i = 1, 2, \ldots, N$
- Hidden mixture means $\mu_k \in \mathbb{R}^d, \quad k = 1, 2, \ldots, K$
- Hidden mixture covariances $\Sigma_k \in \mathbb{R}^{d \times d}, \quad k = 1, 2, \ldots, K$
- Hidden mixture probabilities $\pi_k, \quad \sum_{k=1}^{K} \pi_k = 1$

Gaussian mixture marginal and conditional likelihood :

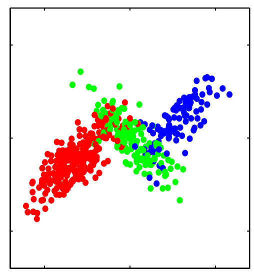
$$p(x_i \mid \pi, \mu, \Sigma) = \sum_{z_i=1}^{K} \pi_{z_i} \mathcal{N}(x_i \mid \mu_{z_i}, \Sigma_{z_i})$$

$$p(x_i \mid z_i, \pi, \mu, \Sigma) = \mathcal{N}(x_i \mid \mu_{z_i}, \Sigma_{z_i})$$

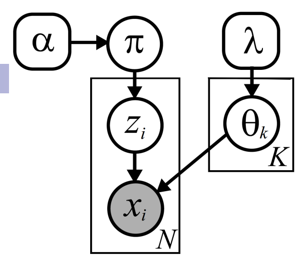
Generative Model



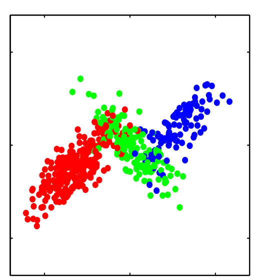
- We can think of *sampling* observations from the model
- For the GMM, define model parameters
  - Cluster means and covariances
  - Cluster weights
- For each observation *i*,
  - Sample a cluster assignment
  - Sample the observation from the selected Gaussian



A Bayesian GMM

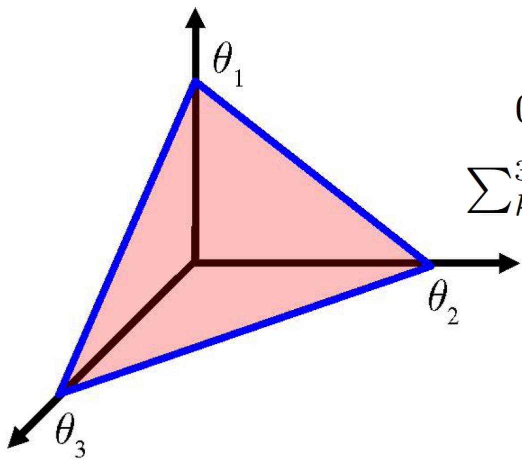


- In a Bayesian approach, we place priors on the model parameters
- Conjugate priors are a computationally convenient choice
- Conjugate prior for θ_k
  - Known variance: Gaussian prior on mean
  - Unknown mean & variance: *normal inverse-Wishart*
- Conjugate prior for π ???



The Simplex in 3D

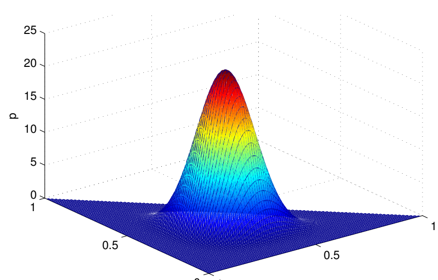
- The simplex defines the hyperplane of vectors that sum to 1



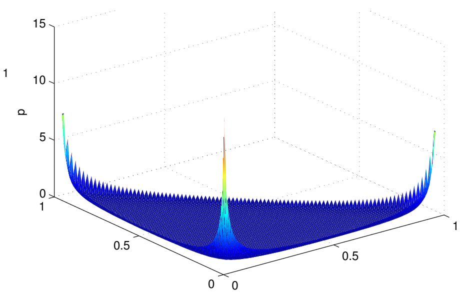
$$0 \leq \theta_k \leq 1$$
$$\sum_{k=1}^{3} \theta_k = 1$$

Dirichlet Distributions

- The Dirichlet distribution is defined on the simplex



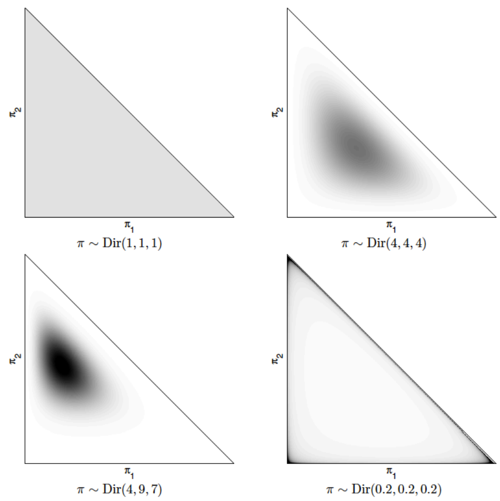
$$p(\pi \mid \alpha) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1}$$



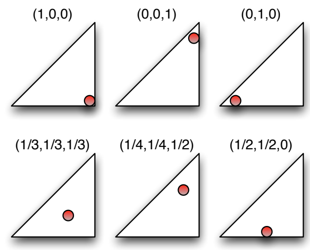
Moments: $\mathbb{E}_\alpha[\pi_k] = \frac{\alpha_k}{\alpha_0}$

$$\text{Var}_\alpha[\pi_k] = \frac{K-1}{K^2(\alpha_0+1)}$$

Dirichlet Probability Densities



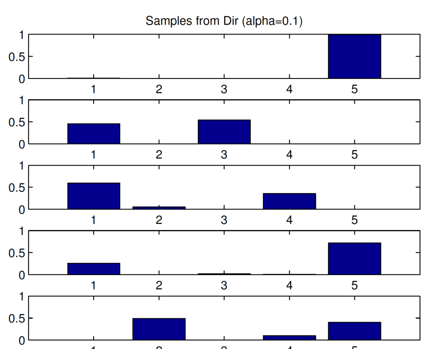
$$\pi \sim \mathrm{Dir}(\alpha_1, \ldots, \alpha_K)$$



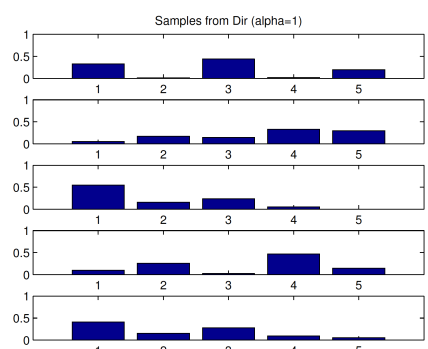
Dirichlet Samples

$$\mathbb{E}_\alpha[\pi_k] = \frac{\alpha_k}{\alpha_0}$$

- Samples are ***sparse*** for small values of α_i

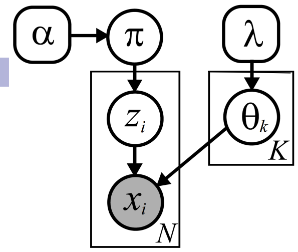


$\mathrm{Dir}(\pi \mid 0.1, 0.1, 0.1, 0.1, 0.1)$

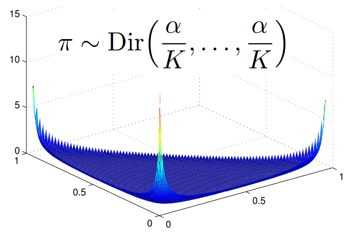


$\mathrm{Dir}(\pi \mid 1.0, 1.0, 1.0, 1.0, 1.0)$

Model Summary



- Prior on model parameters
  - E.g., symmetric Dirichlet for π

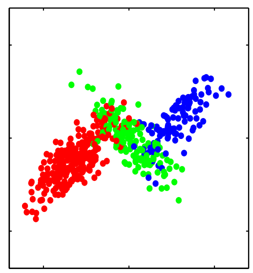


  - Normal inverse Wishart prior for θ_k

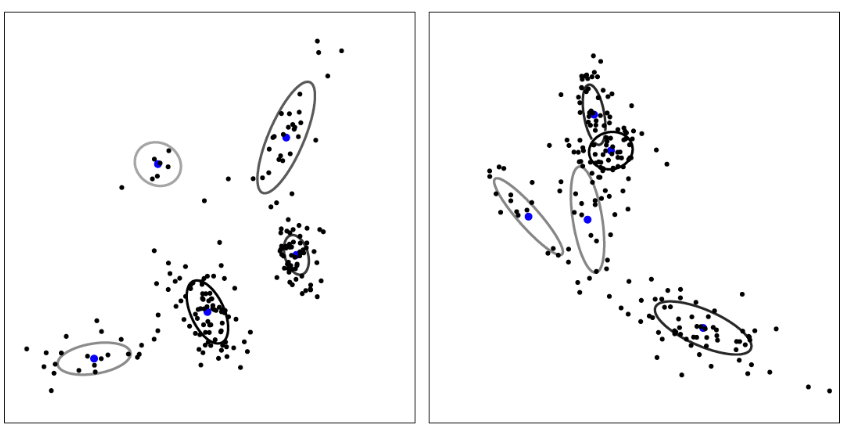
- Sample observations as

$$z_i \sim \pi$$

$$x_i \mid z_i \sim N(\mu_{z_i}, \Sigma_{z_i})$$



Samples Generated from GMM



Posterior Computations

- From our observations, we want to infer model params
- MAP estimation can be done using expectation maximization (EM) algorithm:

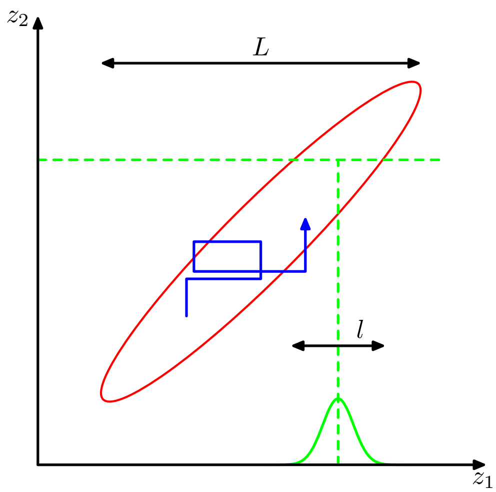
$$\hat{\theta}^{MAP} = \arg\max_{\theta} p(\theta \mid x)$$

- What if we want a full characterization of the posterior?
  - Maintain a measure of uncertainty
  - Estimators other than posterior mode (different loss functions)
  - Predictive distributions for future observations
- Often no closed-form characterization (e.g., mixture models)
- Alternatives:
  - Markov chain Monte Carlo (MCMC) providing samples from posterior
  - Variational approximations to posterior

Gibb Sampling

- Let *z* indicate the set of ***all variables in the model***: e.g., cluster indicators and parameters
- Want draws:
- Construct Markov chain whose steady state distribution is
- Simplest case:

Gibbs Sampler for a 2D Gaussian



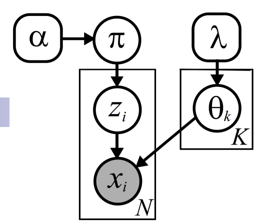
General Gibbs Sampler

$$z_i^{(t)} \sim p(z_i \mid z_{\setminus i}^{(t-1)}) \qquad i = i(t)$$
$$z_j^{(t)} = z_j^{(t-1)} \qquad j \neq i(t)$$

Under mild conditions, converges assuming all variables are resampled infinitely often (order can be fixed or random)

C. Bishop, Pattern Recognition & Machine Learning

Example – GMM



- Recall model
  - Observations: $x_1, \ldots, x_N$
  - Cluster indicators: $z_1, \ldots, z_N$
  - Parameters: π, θ_k

$$\pi = [\pi_1, \ldots, \pi_K]$$
$$\theta_k = \{\mu_k, \Sigma_k\}$$

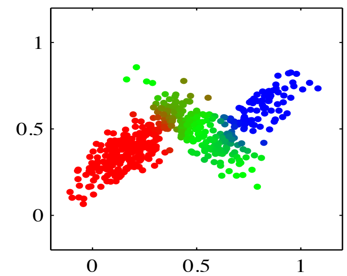
  - Generative model:

$$\pi \sim \mathrm{Dir}(\alpha_1, \ldots, \alpha_K) \qquad z_i \sim \pi$$
$$\{\mu_k, \Sigma_k\} \sim \mathrm{NIW}(\lambda) \qquad x_i \mid z_i, \{\theta_k\} \sim N(\mu_{z_i}, \Sigma_{z_i})$$

- Iteratively sample

Complete Conditional $p(z_i \mid \pi, \{\theta_k\}, \{x_i\})$

- We have
$$z_i \sim \pi$$
$$x_i \mid z_i, \{\theta_k\} \sim N(\mu_{z_i}, \Sigma_{z_i})$$
- As before, we can compute the "responsibility" of each cluster to the observation
$$r_{ik} = p(z_i = k \mid x_i, \pi, \theta) = \frac{\pi_k p(x_i \mid \theta_k)}{\sum_{\ell=1}^K \pi_\ell p(x_i \mid \theta_\ell)}$$
- Sample each cluster indicator as



Complete Conditional $p(\pi \mid \{z_i\})$

- Recall conjugate Dirichlet prior
$$\pi \sim \text{Dir}(\alpha_1, \dots, \alpha_K) \qquad p(\pi \mid \alpha) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_k \pi_k^{\alpha_k - 1}$$
- Dirichlet posterior
  - Assume we condition on cluster indicators $z_i \sim \pi$
  - Count occurrences of $z_i = k$
  - Then,
$$p(\pi \mid \alpha, z_1, \dots, z_N) \propto$$
  - Conjugacy: This **posterior** has same form as **prior**

Complete Conditional $p(\theta_k \mid \{z_i\}, \{x_i\})$

- Recall NIW prior…Let's consider 1D example → N-IG

$$\mu_k \mid \sigma_k^2 \sim N(0, \gamma\sigma_k^2) \quad \sigma_k^2 \sim \text{IG}\left(\frac{\nu_0}{2}, \frac{\nu_0 S_0}{2}\right)$$

- Normal inverse gamma posterior
  - Consider observation indices *i* such that $z_i = k$
  - For these observations, $x_i \mid z_i = k \sim N(\mu_k, \Sigma_k)$
  - Then,

$$\mu_k \mid \sigma_k^2, \{z_i\}, \{x_i\} \sim N\left(\frac{1}{N_k + \gamma^{-1}} \sum_{i:z_i=k} x_i, \frac{1}{N_k + \gamma^{-1}} \sigma_k^2\right)$$

$$\sigma_k^2 \mid \{z_i\}, \{x_i\} \sim \text{IG}\left(\frac{\nu_0 + N_k}{2}, \frac{\nu_0 S_0 + \sum_{i:z_i=k} x_i^2 - (N_k + \gamma^{-1})^{-1}(\sum_{i:z_i=k} x_i)^2}{2}\right)$$

  - Conjugacy: This **posterior** has same form as **prior**

Standard Finite Mixture Sampler

Given mixture weights $\pi^{(t-1)}$ and cluster parameters $\{\theta_k^{(t-1)}\}_{k=1}^K$ from the previous iteration, sample a new set of mixture parameters as follows:

1. Independently assign each of the N data points x_i to one of the K clusters by sampling the indicator variables $z = \{z_i\}_{i=1}^N$ from the following multinomial distributions:

$$z_i^{(t)} \sim \frac{1}{Z_i} \sum_{k=1}^K \pi_k^{(t-1)} f(x_i \mid \theta_k^{(t-1)}) \, \delta(z_i, k) \qquad Z_i = \sum_{k=1}^K \pi_k^{(t-1)} f(x_i \mid \theta_k^{(t-1)})$$

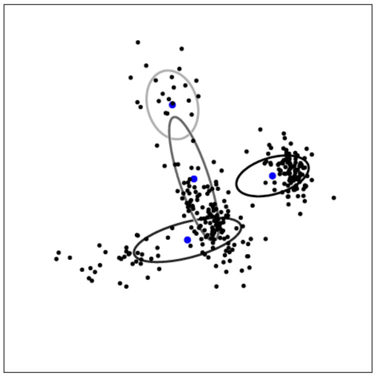
2. Sample new mixture weights according to the following Dirichlet distribution:

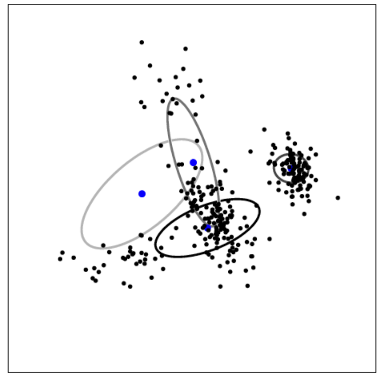
$$\pi^{(t)} \sim \text{Dir}(N_1 + \alpha/K, \ldots, N_K + \alpha/K) \qquad N_k = \sum_{i=1}^N \delta(z_i^{(t)}, k)$$

3. For each of the K clusters, independently sample new parameters from the conditional distribution implied by those observations currently assigned to that cluster:

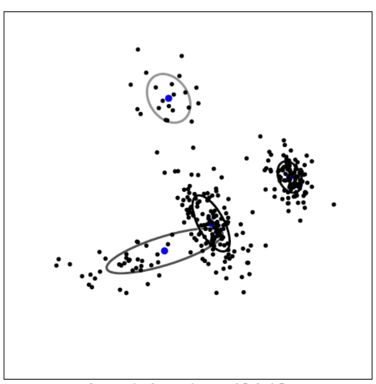
$$\theta_k^{(t)} \sim p(\theta_k \mid \{x_i \mid z_i^{(t)} = k\}, \lambda)$$

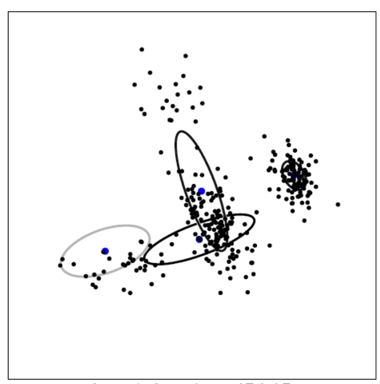
Standard Sampler: 2 Iterations


$\log p(x \mid \pi, \theta) = -539.17$

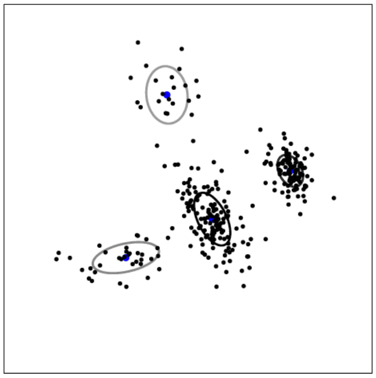

$\log p(x \mid \pi, \theta) = -497.77$

Standard Sampler: 10 Iterations

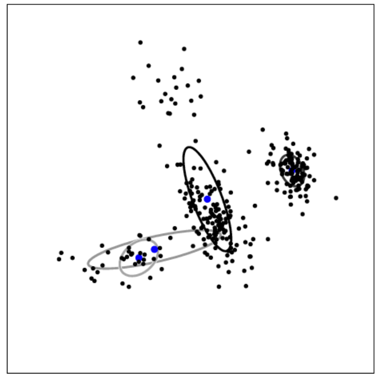

$\log p(x \mid \pi, \theta) = -404.18$


$\log p(x \mid \pi, \theta) = -454.15$

Standard Sampler: 50 Iterations



log p(x | π, θ) = –397.40



log p(x | π, θ) = –442.89

Acknowledgements

Slides based on parts of the lecture notes of Erik Sudderth for "Applied Bayesian Nonparametrics" at Brown University