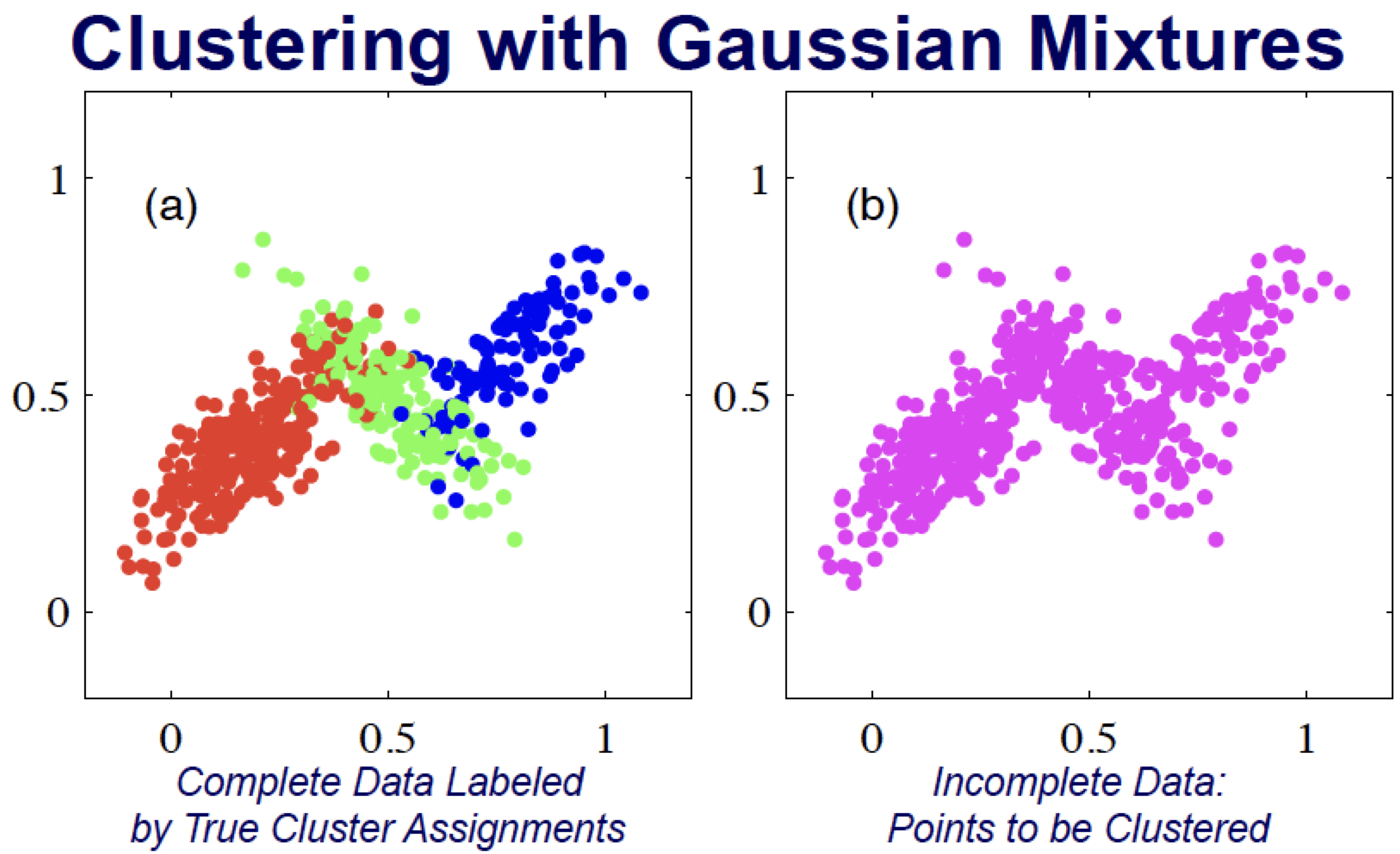
Dirichlet process

Dirichlet process: What's this good for?

- Principled, Bayesian method for fitting a mixture model with an unknown number of clusters

- Because it's Bayesian, can build hierarchies (e.g. HDPs) and integrate with other random variables in a principled way

Dirichlet process: What's this good for? Recall Clustering with GM



Dirichlet process: What's this good for? Recall Clustering with GM

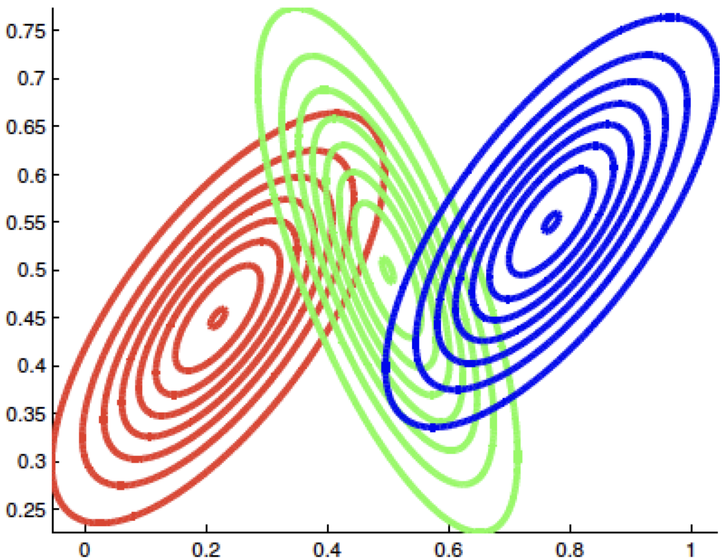
- Observed feature vectors: $x_i \in \mathbb{R}^d, \quad i = 1, 2, \ldots, N$
- Hidden cluster labels: $z_i \in \{1, 2, \ldots, K\}, \quad i = 1, 2, \ldots, N$
- Hidden mixture means: $\mu_k \in \mathbb{R}^d, \quad k = 1, 2, \ldots, K$
- Hidden mixture covariances: $\Sigma_k \in \mathbb{R}^{d \times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

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

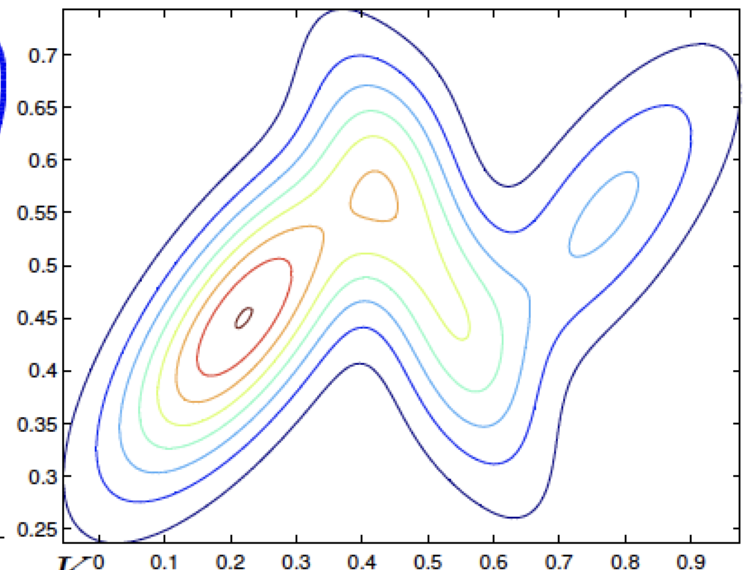
$$p(x_i \mid z_i, \pi, \mu, \Sigma) = \mathcal{N}(x_i \mid \mu_{z_i}, \Sigma_{z_i})$$

Dirichlet process: What's this good for? Recall Clustering with GM

Mixture of 3 Gaussian Distributions in 2D



Contour Plot of Joint Density, Marginalizing Cluster Assignments



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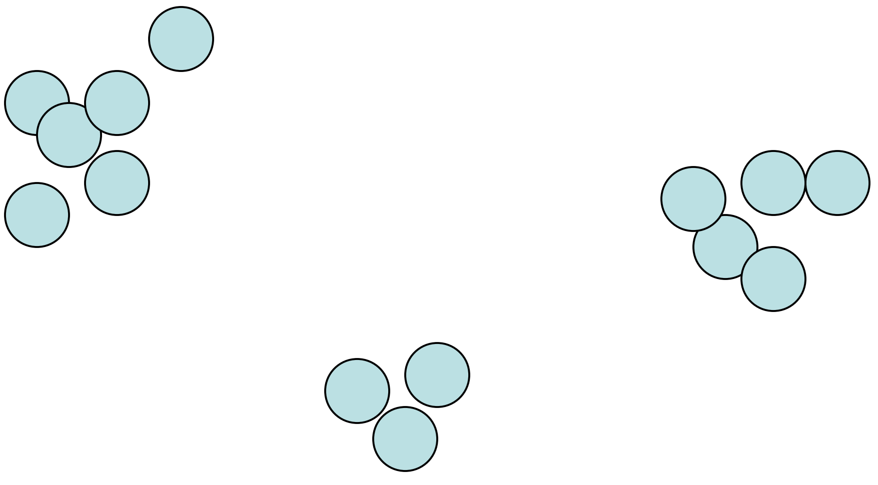
Aren't there other ways to count the number of clusters?

- Adhoc approaches (e.g., hierarchical clustering)
  - they do often yield a data-driven choice of K
  - but there is little understanding of how good these choices are
- Methods based on objective functions (M-estimators)
  - e.g., K-means, spectral clustering
  - do come with some frequentist guarantees
  - but it's hard to turn these into data-driven choices of K
- Parametric likelihood-based approaches
  - finite mixture models, Bayesian variants thereof
  - various model choice methods: hypothesis testing, cross-validation, bootstrap
    etc
  - but do the assumptions underlying the method really apply to this setting? (not often)
- Let's try something different...

Gaussian mixture model, revisited



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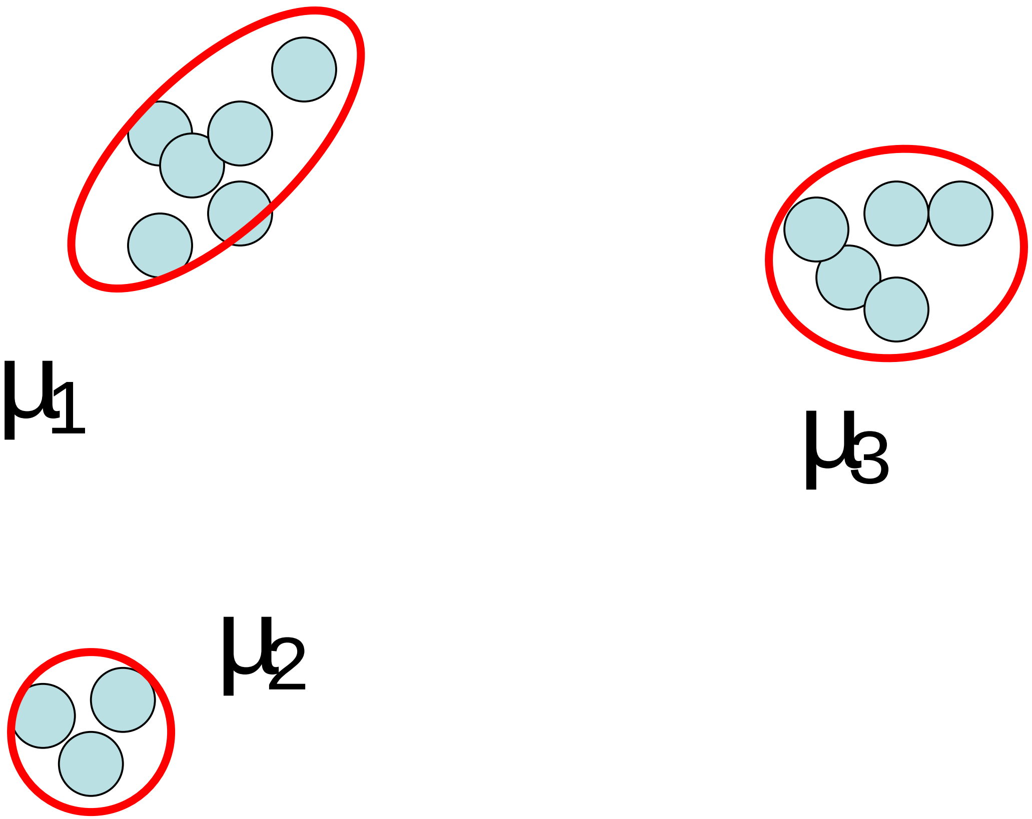

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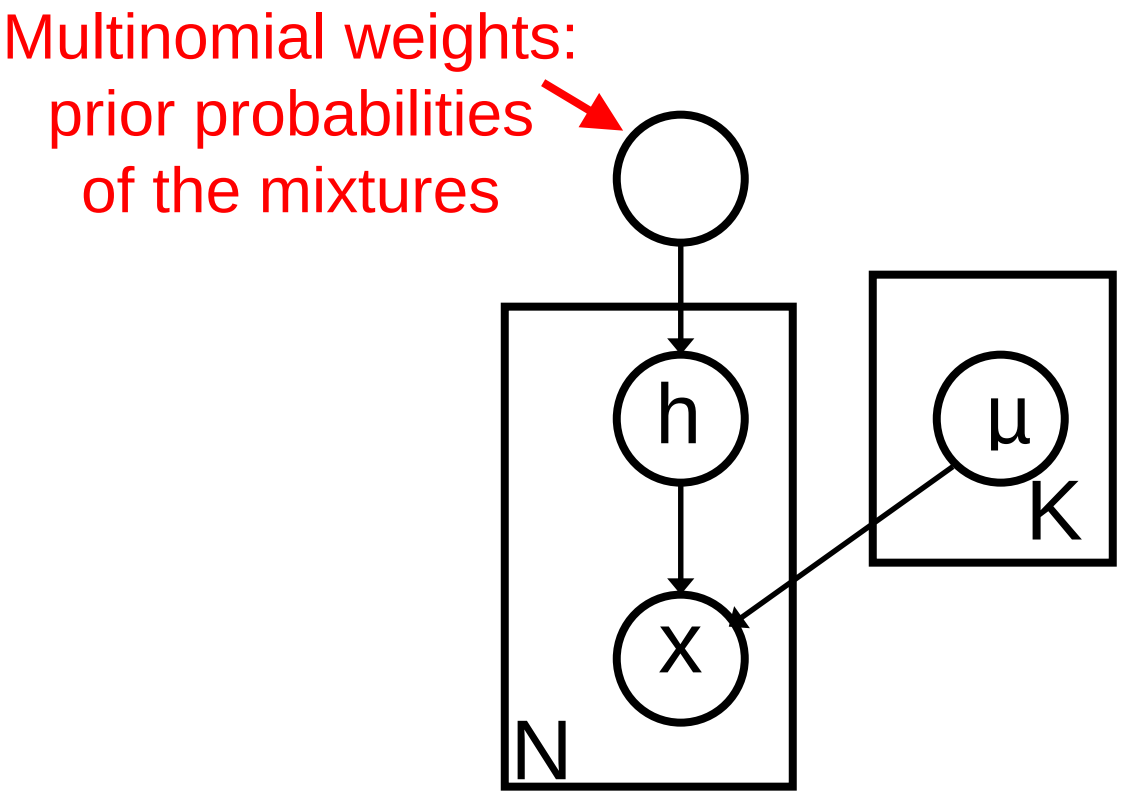
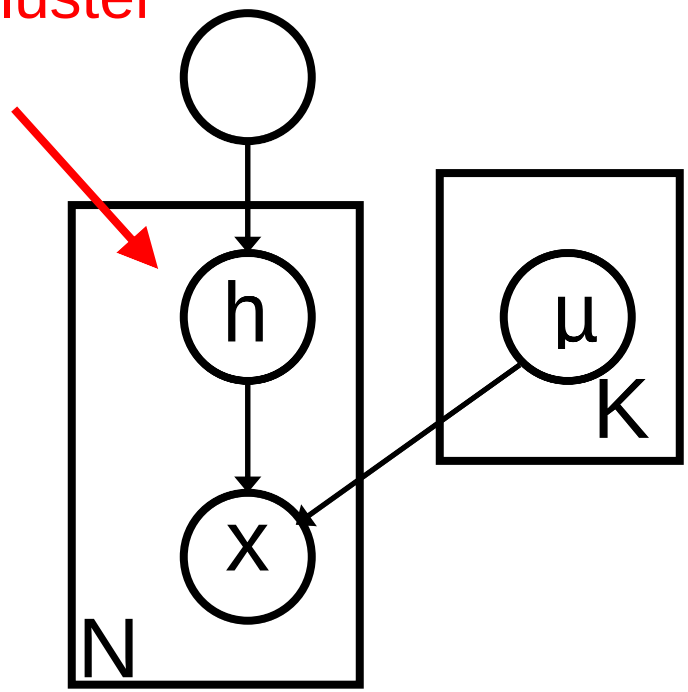
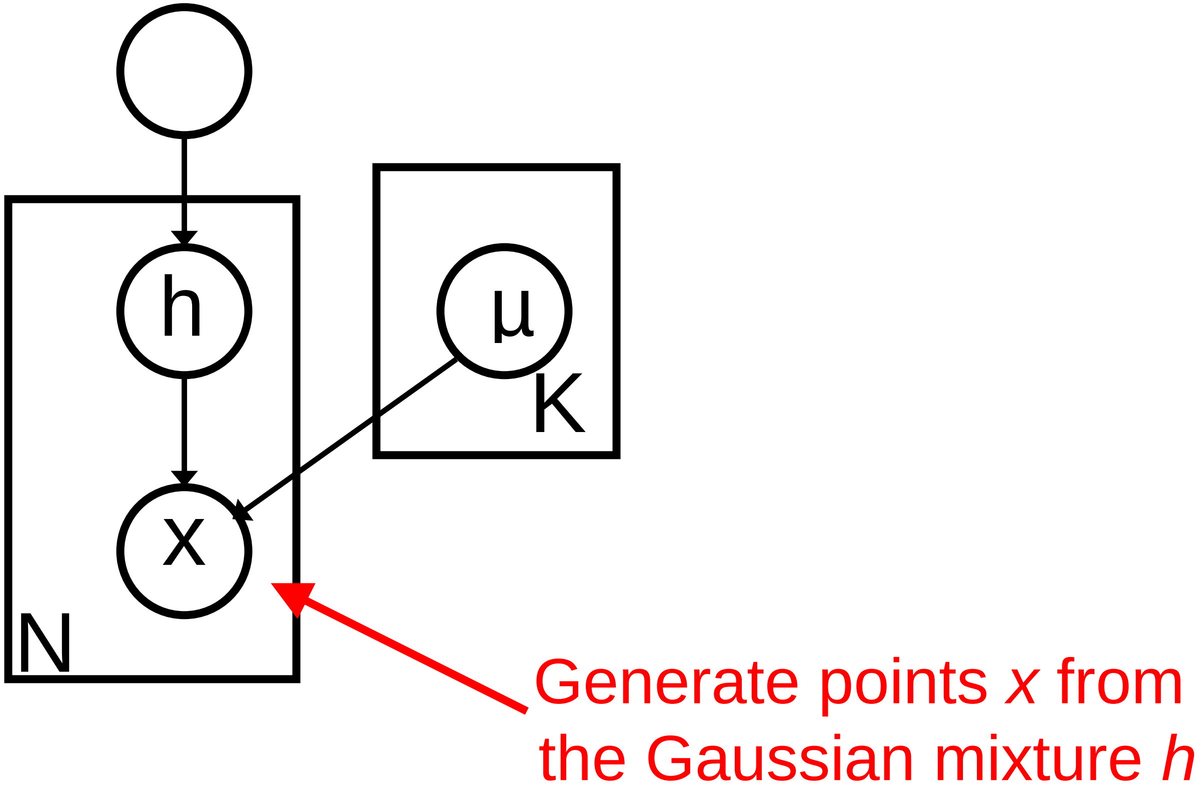


Gaussian mixture model, revisited

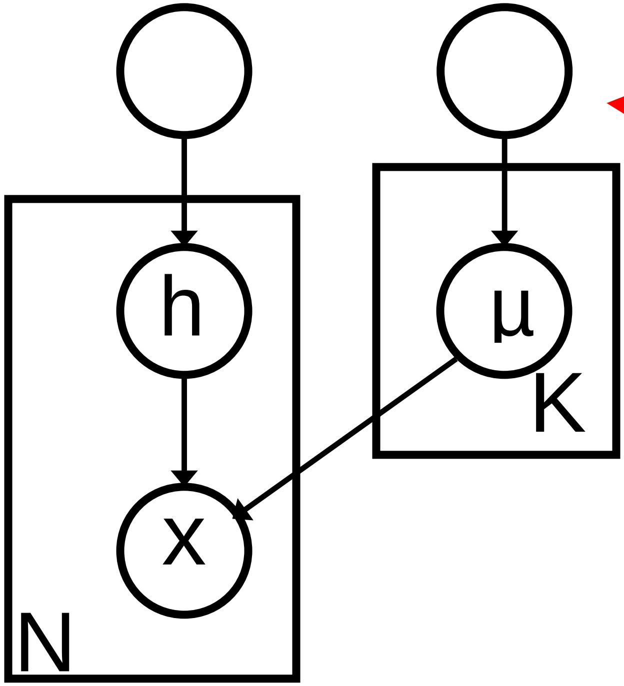
For each data point, choose cluster center *h*



Gaussian mixture model, revisited



Let us be more Bayesian…

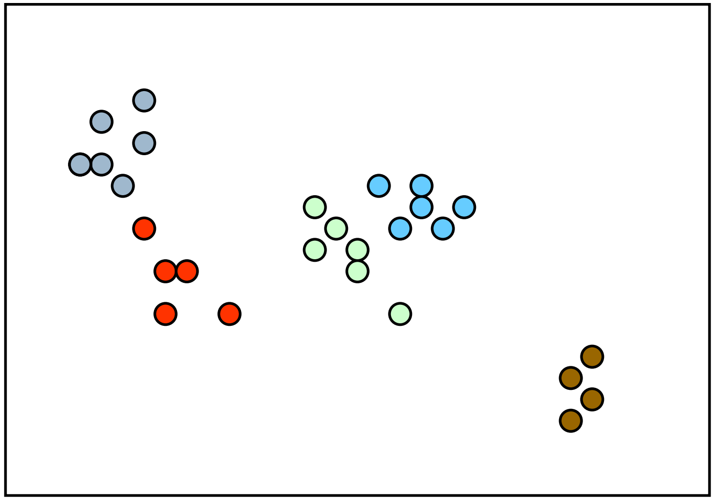


Put a prior over mixture parameters

For Gaussian mixtures, this is a normal inverse-Wishart density

Motivation

- We are given a data set, and are told that it was generated from a mixture of Gaussian distributions.



- Unfortunately, no one has any idea *how many* Gaussians produced the data.

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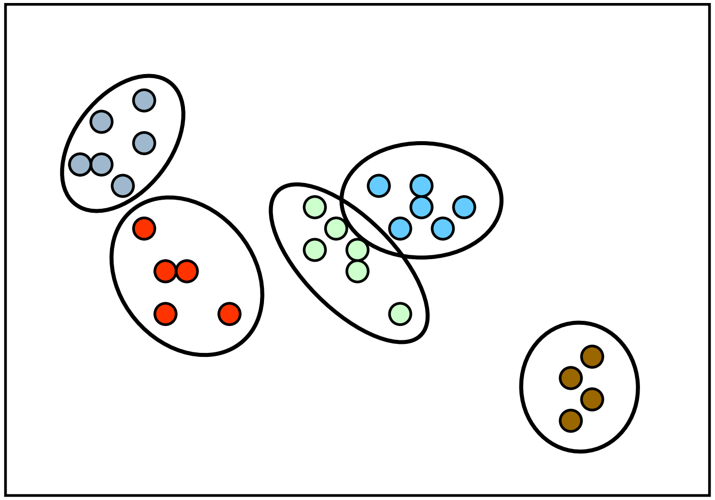

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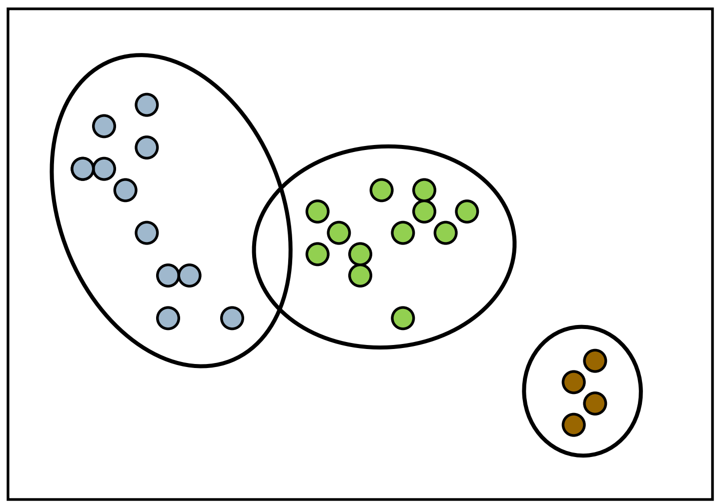


- Unfortunately, no one has any idea *how many* Gaussians produced the data.

The Dirichlet Distribution

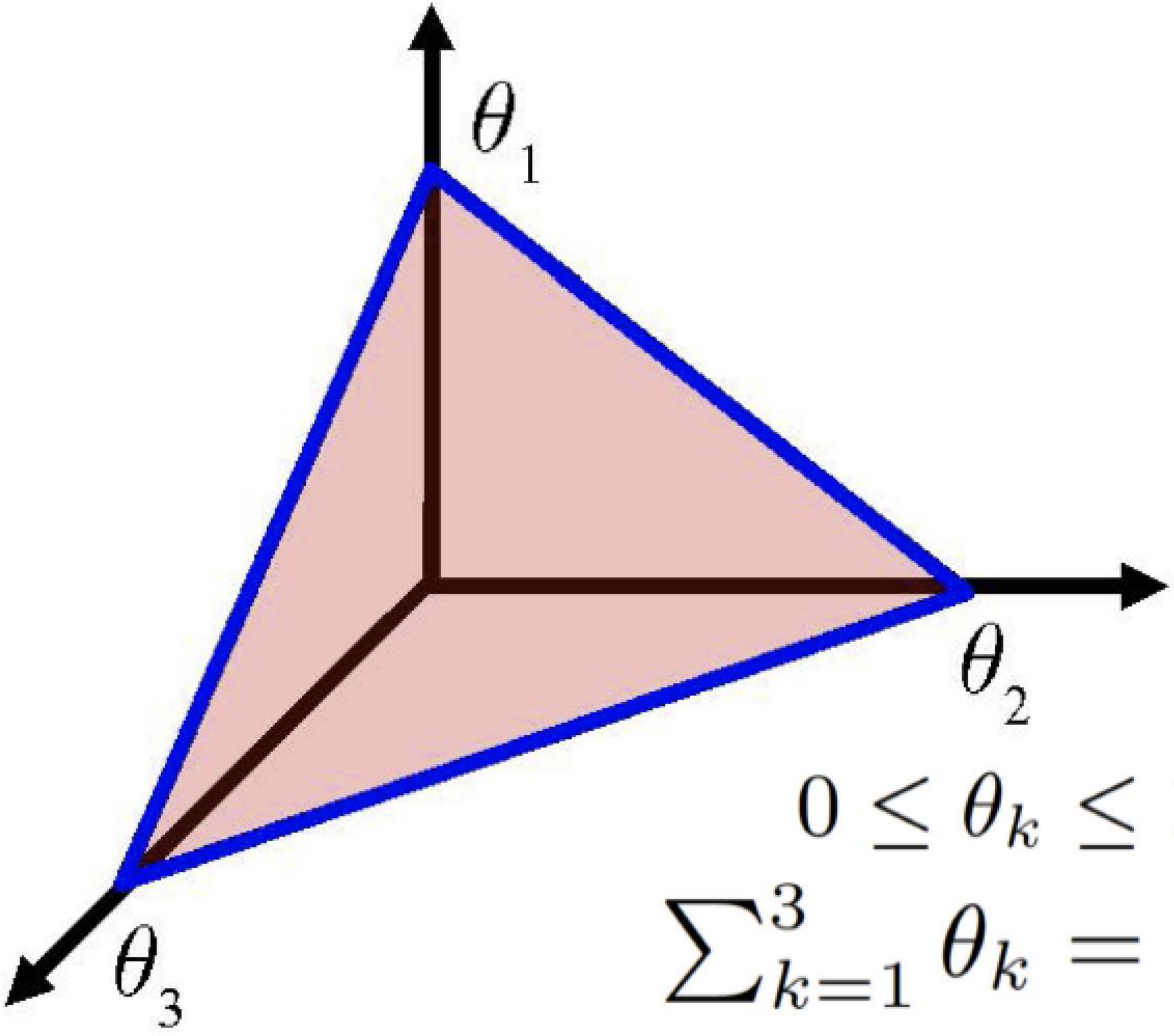
- Let $\Theta = \{\theta_1, \theta_2, \ldots, \theta_m\}$
- We write:

$$\Theta \sim \mathrm{Dirichlet}(\alpha_1, \alpha_2, \ldots, \alpha_m)$$

$$P(\theta_1, \theta_2, \ldots, \theta_m) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_{k=1}^{m} \theta_k^{\alpha_k - 1}$$

- Samples from the distribution lie in the *m-1* dimensional probability simplex

Multinomial Simplex



$$0 \le \theta_k \le 1$$

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

The Dirichlet Distribution

- Let $\boldsymbol{\Theta} = \{\theta_1, \theta_2, \ldots, \theta_m\}$
- We write:

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- Distribution over possible parameter vectors for a multinomial distribution, and is the conjugate prior for the multinomial.
- Beta distribution is the special case of a Dirichlet for 2 dimensions.
- Thus, it is in fact a "distribution over distributions."

Dirichlet Process

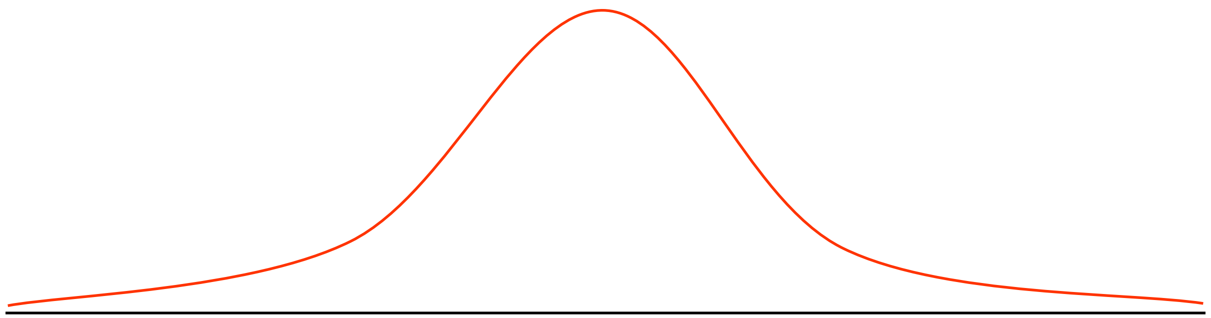
- A *Dirichlet Process* is also a distribution over distributions.
- Let G be Dirichlet Process distributed:

$$G \sim DP(\alpha, G_0)$$

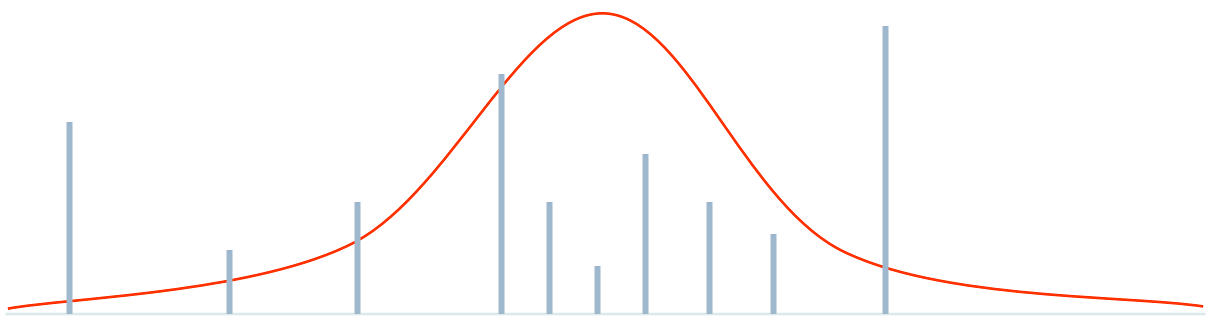
  - G_0 is a base distribution
  - α is a positive scaling parameter
- G is a random probability measure that has the same support as G_0

Dirichlet Process

- Consider Gaussian G_0

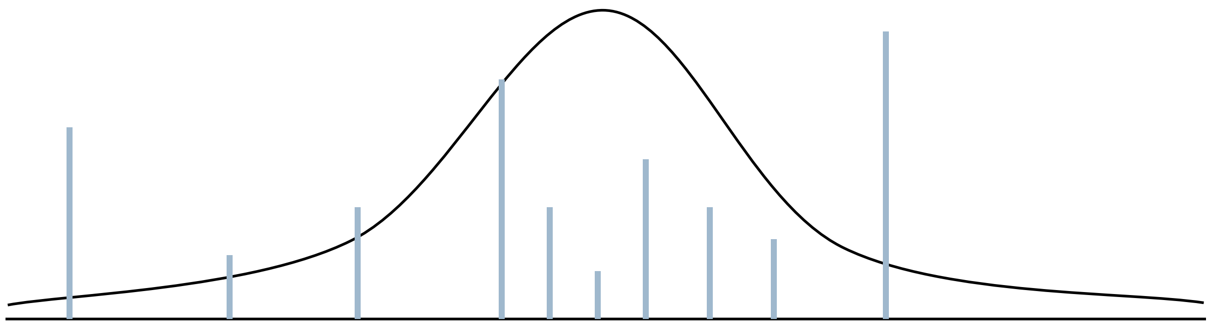


- $G \sim DP(\alpha, G_0)$



Dirichlet Process

- $G \sim DP(\alpha, G_0)$



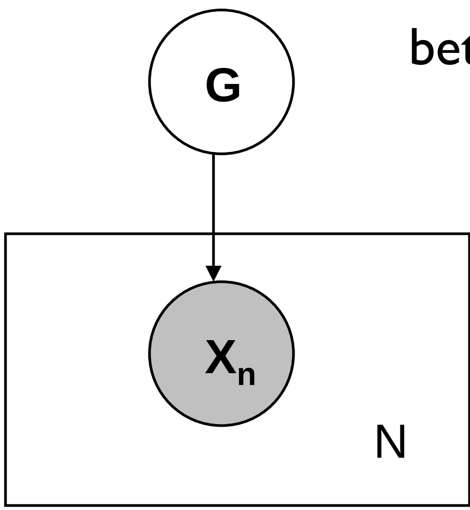
- G_0 is continuous, so the probability that any two samples are equal is precisely zero.
- However, G is a discrete distribution, made up of a countably infinite number of point masses [Blackwell]
  - Therefore, there is always a non-zero probability of two samples colliding

Samples from a Dirichlet Process

$G \sim DP(\alpha, G_0)$

$X_n \mid G \sim G$ for $n = \{1, \ldots, N\}$ (iid given G)

Marginalizing out G introduces dependencies between the X_n variables



$$P(X_1, \ldots, X_N) = \int P(G) \prod_{n=1}^{N} P(X_n|G)dG$$

Samples from a Dirichlet Process

$$P(X_1, \dots, X_N) = \int P(G) \prod_{n=1}^{N} P(X_n | G) dG$$

Assume we view these variables in a specific order, and are interested in the behavior of X_n given the previous n - 1 observations.

$$X_n | X_1, \dots, X_{n-1} = \begin{cases} X_i & \text{with probability } \frac{1}{n-1+\alpha} \\ \text{new draw from } G_0 & \text{with probability } \frac{\alpha}{n-1+\alpha} \end{cases}$$

Let there be K unique values for the variables:

$$X_k^* \text{ for } k \in \{1, \dots, K\}$$

Samples from a Dirichlet Process

$$X_n | X_1, \dots, X_{n-1} = \begin{cases} X_i & \text{with probability } \frac{1}{n-1+\alpha} \\ \text{new draw from } G_0 & \text{with probability } \frac{\alpha}{n-1+\alpha} \end{cases}$$

$$P(X_1, \dots, X_N) = P(X_1)P(X_2|X_1)\dots P(X_N|X_1, \dots, X_{N-1})$$

Chain rule

$$= \frac{\alpha^K \prod_{k=1}^{K} (\text{num}(X_k^*) - 1)!}{\alpha(1+\alpha)\dots(N-1+\alpha)} \prod_{k=1}^{K} G_0(X_k^*)$$

P(partition) **P(draws)**

Notice that the above formulation of the joint distribution does not depend on the order we consider the variables.

Samples from a Dirichlet Process

$$X_n | X_1, \ldots, X_{n-1} = \begin{cases} X_i & \text{with probability } \frac{1}{n-1+\alpha} \\ \text{new draw from } G_0 & \text{with probability } \frac{\alpha}{n-1+\alpha} \end{cases}$$

Let there be *K* unique values for the variables:

$$X_k^* \text{ for } k \in \{1, \ldots, K\}$$

Can rewrite as:

$$X_n | X_1, \ldots, X_{n-1} = \begin{cases} X_k^* & \text{with probability } \frac{\mathrm{num}_{n-1}(X_k^*)}{n-1+\alpha} \\ \text{new draw from } G_0 & \text{with probability } \frac{\alpha}{n-1+\alpha} \end{cases}$$

Blackwell-MacQueen Urn Scheme

$$G \sim DP(\alpha, G_0)$$

$$X_n \mid G \sim G$$

- Assume that G_0 is a distribution over colors, and that each X_n represents the color of a single ball placed in the urn.
- Start with an empty urn.
- On step *n*:
  - With probability proportional to α, draw $X_n \sim G_0$, and add a ball of that color to the urn.
  - With probability proportional to $n - 1$ (i.e., the number of balls currently in the urn), pick a ball at random from the urn. Record its color as X_n, and return the ball into the urn, along with a new one of the same color.

[Blackwell and Macqueen, 1973]

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