School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Bayesian Nonparametrics: Dirichlet Processes

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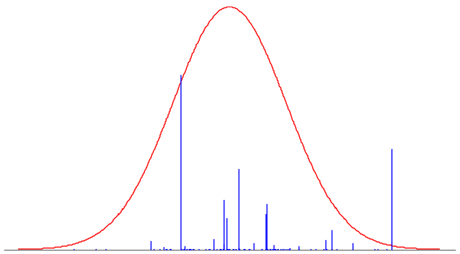
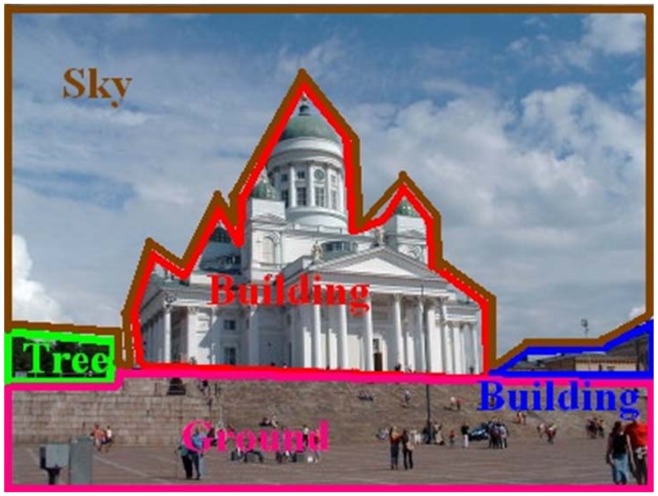
Lecture 19, March 26, 2014



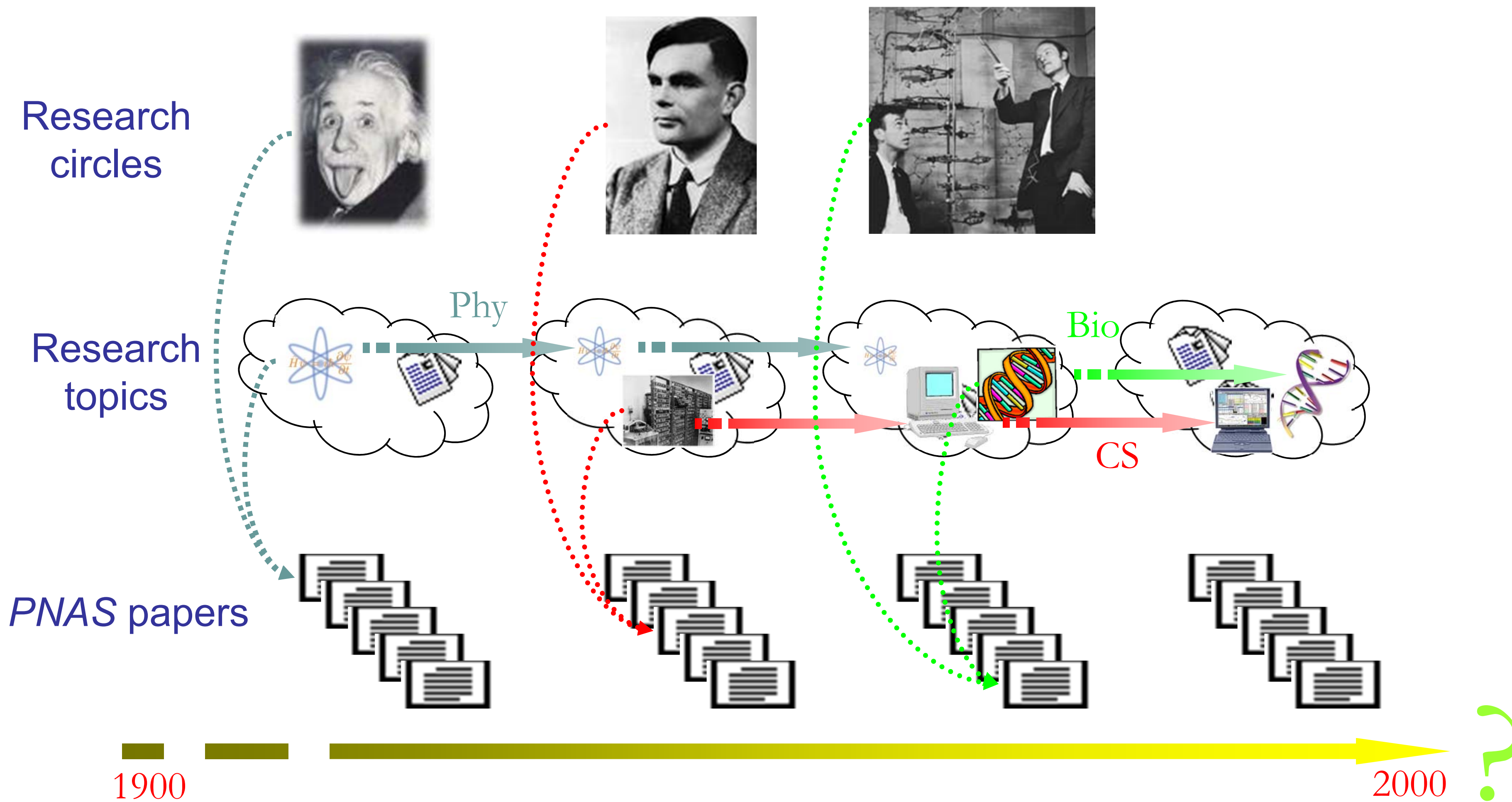
Acknowledgement: slides first drafted by Sinead Williamson

How Many Clusters?

How Many Segments?



How Many Topics?



Parametric vs nonparametric

Parametric model:

- Assumes all data can be represented using a fixed, finite number of parameters.
  - Mixture of *K* Gaussians, polynomial regression.

Nonparametric model:

- Number of parameters can grow with sample size.
- Number of parameters may be random.
  - Kernel density estimation.

Bayesian nonparametrics:

- Allow an *infinite* number of parameters *a priori.*
- A finite data set will only use a finite number of parameters.
- Other parameters are integrated out.

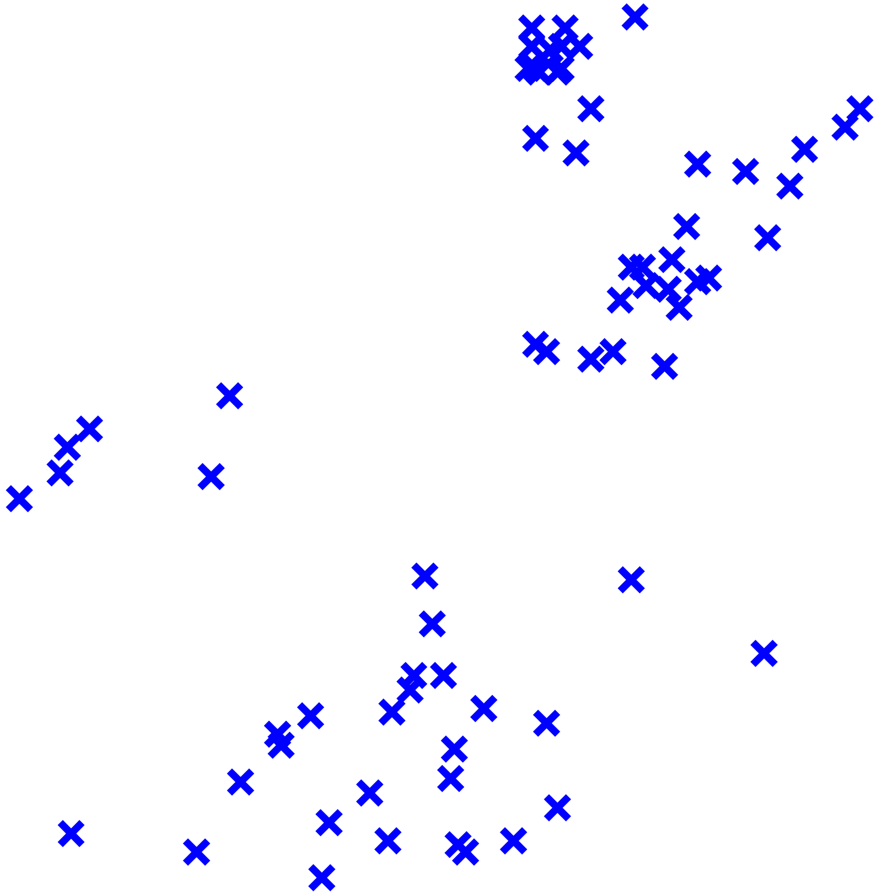
Clustered data

- How to model this data?

- Mixture of Gaussians:

$$p(x_1, \ldots, x_N | \pi, \{\mu_k\}, \{\Sigma_k\})$$
$$= \prod_{n=1}^{\infty} \sum_{k=1}^{K} \pi_k \mathcal{N}(x_k | \mu_k, \Sigma_k)$$

- Parametric model: Fixed finite number of parameters.



Bayesian finite mixture model

- How to choose the mixing weights and mixture parameters?
- Bayesian choice: Put a prior on them and integrate out:

$$p(x_1, \ldots, x_N)$$
$$= \int \int \int \left(\prod_{n=1}^{\infty} \sum_{k=1}^{K} \pi_k \mathcal{N}(x_k | \mu_k, \Sigma_k) \right)$$
$$p(\pi) p(\mu_{1:K}) p(\Sigma_{1:K}) d\pi d\mu_{1:K} d\Sigma_{1:K}$$

- Where possible, use conjugate priors
  - Gaussian/inverse Wishart for mixture parameters
  - What to choose for mixture weights?

The Dirichlet distribution

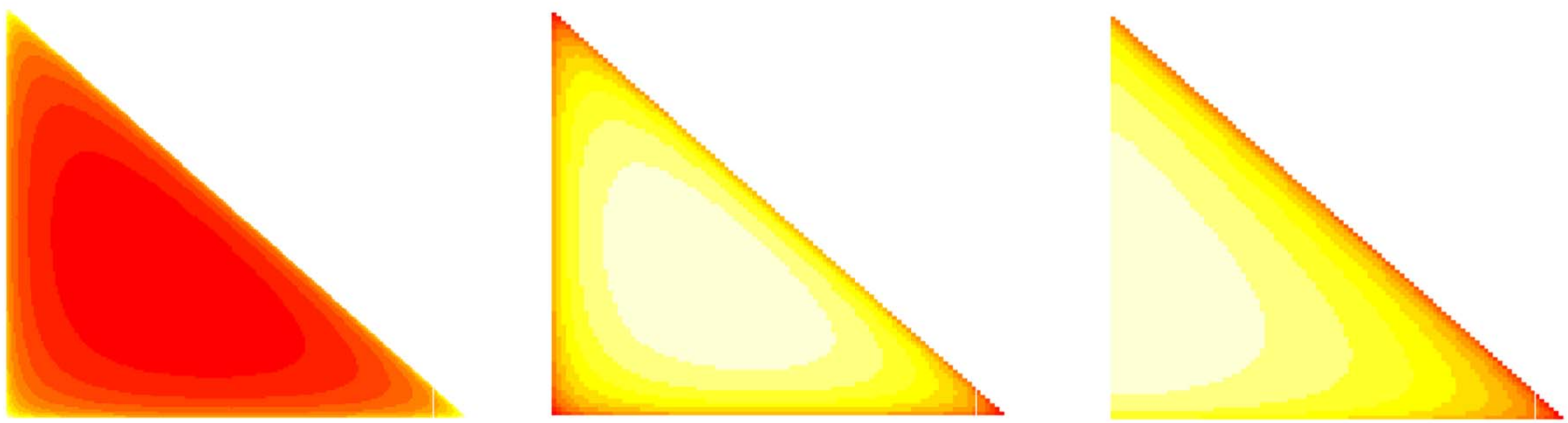
- The Dirichlet distribution is a distribution over the (*K-1*)-dimensional simplex.
- It is parametrized by a *K*-dimensional vector $(\alpha_1, \ldots, \alpha_K)$ such that $\alpha_k \geq 0, k = 1, \ldots, K$ and $\sum_k \alpha_k > 0$
- Its distribution is given by

$$\frac{\prod_{k=1}^{K} \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^{K} \alpha_k)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1}$$

Samples from the Dirichlet distribution

- If $\pi \sim \mathrm{Dirichlet}(\alpha_1, \ldots, \alpha_K)$ then $\pi_k \geq 0$ for all *k*, and $\sum_{k=1}^{K} \pi_k = 1.$

- Expectation: $\mathbb{E}\Big[(\pi_1, \ldots, \pi_K)\Big] = \frac{(\alpha_1, \ldots, \alpha_K)}{\sum_k \alpha_k}$



$\alpha = (0.01, 0.01, 0.01)$ $\alpha = (100, 100, 100)$ $\alpha = (5, 50, 100)$

Conjugacy to the multinomial

- If $\pi \sim \mathrm{Dirichlet}(\alpha_1, \ldots, \alpha_K)$ and $x_n \overset{iid}{\sim} \pi$

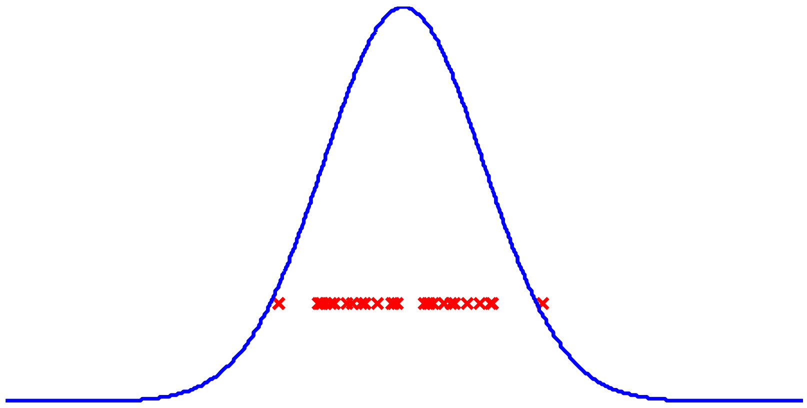
$$
\begin{aligned}
p(\pi | x_1, \ldots, x_n) \propto p(x_1, \ldots, x_n | \pi) p(\pi) \\
&= \left(\frac{\prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^K \alpha_k)} \prod_{k=1}^K \pi_k^{\alpha_k - 1} \right) \left(\frac{n!}{m_1! \ldots m_K!} \pi_1^{m_1} \ldots \pi_K^{m_K} \right) \\
&\propto \frac{\prod_{k=1}^K \Gamma(\alpha_k + m_k)}{\Gamma(\sum_{k=1}^K \alpha_k + m_k)} \prod_{k=1}^K \pi_k^{\alpha_k + m_k - 1} \\
&= \mathrm{Dirichlet}(\pi | \alpha_1 + m_1, \ldots, \alpha_K + m_K)
\end{aligned}
$$

Distributions over distributions

- The Dirichlet distribution is a distribution over positive vectors that sum to one.
- We can further associate each entry with a set of parameters
  - e.g. finite mixture model: each entry associated with a mean and covariance.
- In a Bayesian setting, we want these parameters to be *random.*
- We can combine the distribution over probability vectors with a distribution over parameters to get a **distribution over distributions over parameters.**

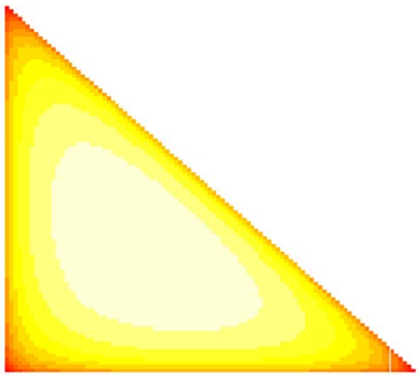
Example: finite mixture model

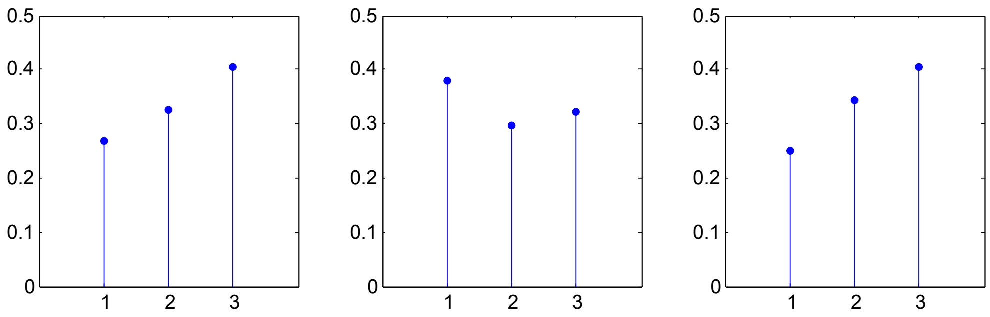
- Gaussian distribution: distribution over means.
  - Sample from a Gaussian is a real-valued number.



Example: finite mixture model

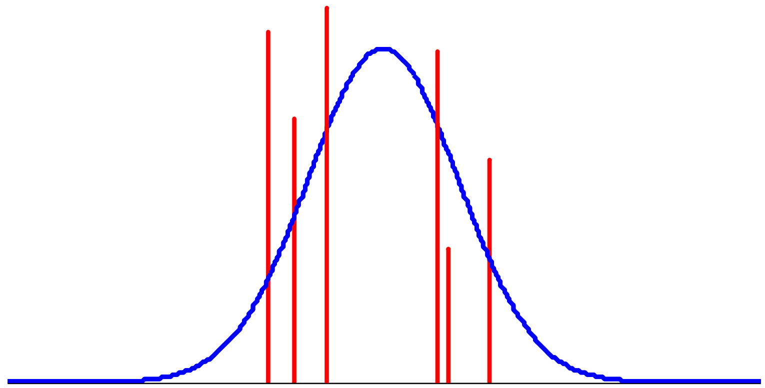
- Gaussian distribution: distribution over means.
  - Sample from a Gaussian is a real-valued number.
- Dirichlet distribution:
  - Sample from a Dirichlet distribution is a probability vector.





Example: finite mixture model

- Dirichlet Mixture Prior
  - Each element of a Dirichlet-distributed vector is associated with a parameter value drawn from some distribution.
  - Sample from a Dirichlet mixture prior is a probability distribution over parameters of a finite mixture model.



Properties of the Dirichlet distribution

- The coalesce rule:

$$(\pi_1 + \pi_2, \pi_3, \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1 + \alpha_2, \alpha_3, \ldots, \alpha_K)$$

- Relationship to gamma distribution: If $\eta_k \sim \text{Gamma}(\alpha_k, 1)$

$$\frac{(\eta_1, \ldots, \eta_K)}{\sum_k \eta_k} \sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_K)$$

- If $\eta_1 \sim \text{Gamma}(\alpha_1, 1)$ and $\eta_2 \sim \text{Gamma}(\alpha_2, 1)$ then

$$\eta_1 + \eta_2 \sim \text{Gamma}(\alpha_1 + \alpha_2, 1)$$

- Therefore, if $(\pi_1 \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_K)$ then

$$(\pi_1 + \pi_2, \pi_3, \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1 + \alpha_2, \alpha_3, \ldots, \alpha_K)$$

Properties of the Dirichlet distribution

- The "combination" rule:

- The beta distribution is a Dirichlet distribution on the 1-simplex.
- Let $(\pi_1 \ldots, \pi_K) \sim \mathrm{Dirichlet}(\alpha_1, \ldots, \alpha_K)$ and

  $\theta \sim \mathrm{Beta}(\alpha_1 b, \alpha_1(1-b)), 0 < b < 1.$
- Then

  $(\pi_1\theta, \pi_1(1-\theta), \pi_2, \ldots, \pi_K) \sim \mathrm{Dirichlet}(\alpha_1 b_1, \alpha_1(1-b_1), \alpha_2, \ldots, \alpha_K)$
- More generally, if $\theta \sim \mathrm{Dirichlet}(\alpha_1 b_1, \alpha_1 b_2, \ldots, \alpha_1 b_N), \sum_i b_i = 1.$ then

$$(\pi_1\theta_1, \ldots, \pi_1\theta_N, \pi_2, \ldots, \pi_K) \sim \mathrm{Dirichlet}(\alpha_1 b_1, \ldots, \alpha_1 b_N, \alpha_2, \ldots, \alpha_K)$$

Properties of the Dirichlet distribution

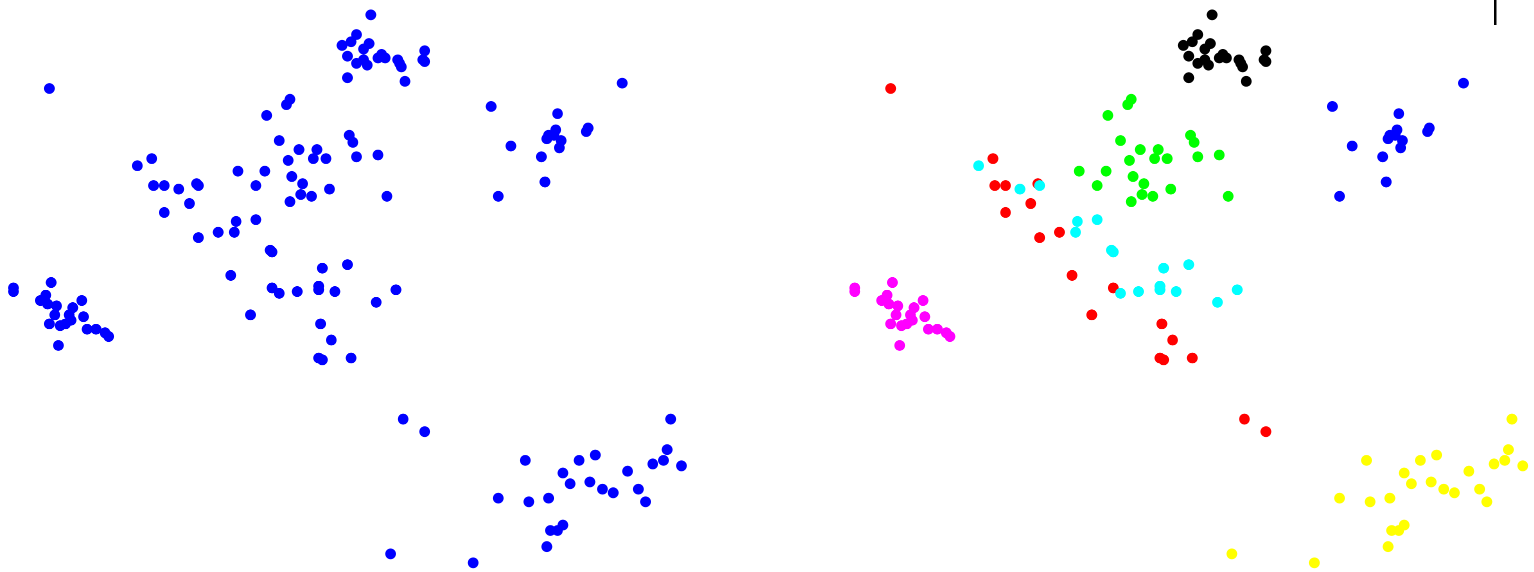
- The "Renormalization" rule:

If $(\pi_1 \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_K)$

then $\frac{(\pi_2, \ldots, \pi_K)}{\sum_{k=1}^{K} \pi_k} \sim ?$

$$\frac{(\pi_2, \ldots, \pi_K)}{\sum_{k=1}^{K} \pi_k} \sim \text{Dirichlet}(\alpha_2, \ldots, \alpha_K)$$

Choosing the number of clusters



- Mixture of Gaussians – but how many components?
- What if we see more data – may find new components?

Bayesian nonparametric mixture models

- Make sure we always have more clusters than we need.
- Solution – infinite clusters *a priori*!

$$p(x_n|\pi, \{\mu_k\}, \{\Sigma_k\}) = \sum_{k=1}^{\infty} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)$$

- A finite data set will always use a finite – but *random* – number of clusters.

- How to choose the prior?
- We want something *like* a Dirichlet prior – but with an infinite number of components. How such a distribution can be defined?

Constructing an appropriate prior

- Start off with $\pi^{(2)} = (\pi_1^{(2)}, \pi_2^{(2)}) \sim \text{Dirichlet}\left(\frac{\alpha}{2}, \frac{\alpha}{2}\right)$

- Split each component according to the splitting rule:

$$\theta_1^{(2)}, \theta_2^{(2)} \overset{iid}{\sim} \text{Beta}\left(\frac{\alpha}{2} \cdot \frac{1}{2}, \frac{\alpha}{2} \cdot \frac{1}{2}\right)$$

$$\pi^{(4)} = (\theta_1^{(2)}\pi_1^{(2)}, (1-\theta_1^{(2)})\pi_1^{(2)}, \theta_2^{(2)}\pi_2^{(2)}, (1-\theta_2^{(2)})\pi_2^{(2)})$$

$$\sim \text{Dirichlet}\left(\frac{\alpha}{4}, \frac{\alpha}{4}, \frac{\alpha}{4}, \frac{\alpha}{4}\right)$$

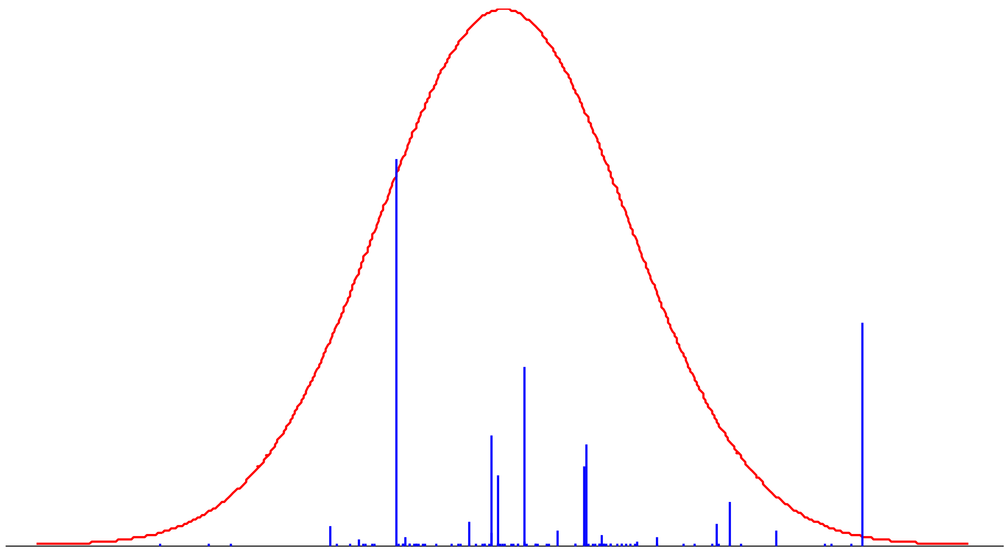
- Repeat to get $\pi^{(K)} \sim \text{Dirichlet}\left(\frac{\alpha}{K}, \dots, \frac{\alpha}{K}\right)$
- As $K \to \infty$, we get a vector with infinitely many components

The Dirichlet process

- Let *H* be a distribution on some space Ω – e.g. a Gaussian distribution on the real line.
- Let $\pi \sim \lim_{K\to\infty} \mathrm{Dirichlet}\left(\frac{\alpha}{K}, \ldots, \frac{\alpha}{K}\right)$
- For $k = 1, \ldots, \infty$ let $\theta_k \sim H.$
- Then $G := \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k}$ is an infinite distribution over Ω.
- We write $G \sim \mathrm{DP}(\alpha, H)$

Samples from the Dirichlet process

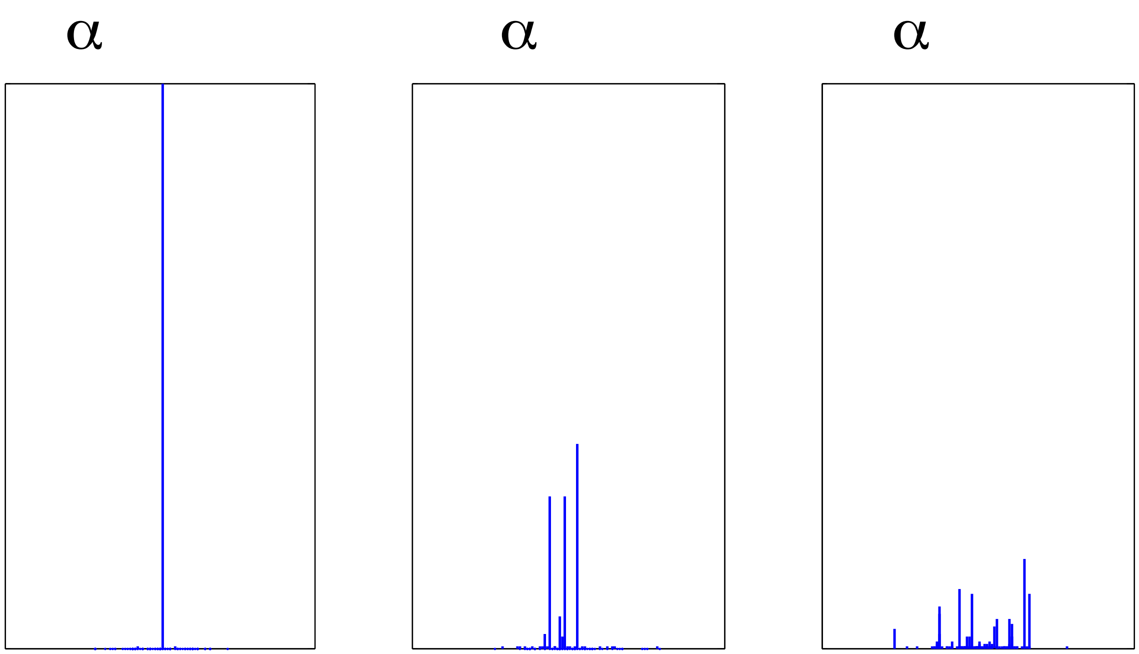
- Samples from the Dirichlet process are *discrete*.
- We call the point masses in the resulting distribution, *atoms*.



- The *base measure* H determines the *locations* of the atoms.

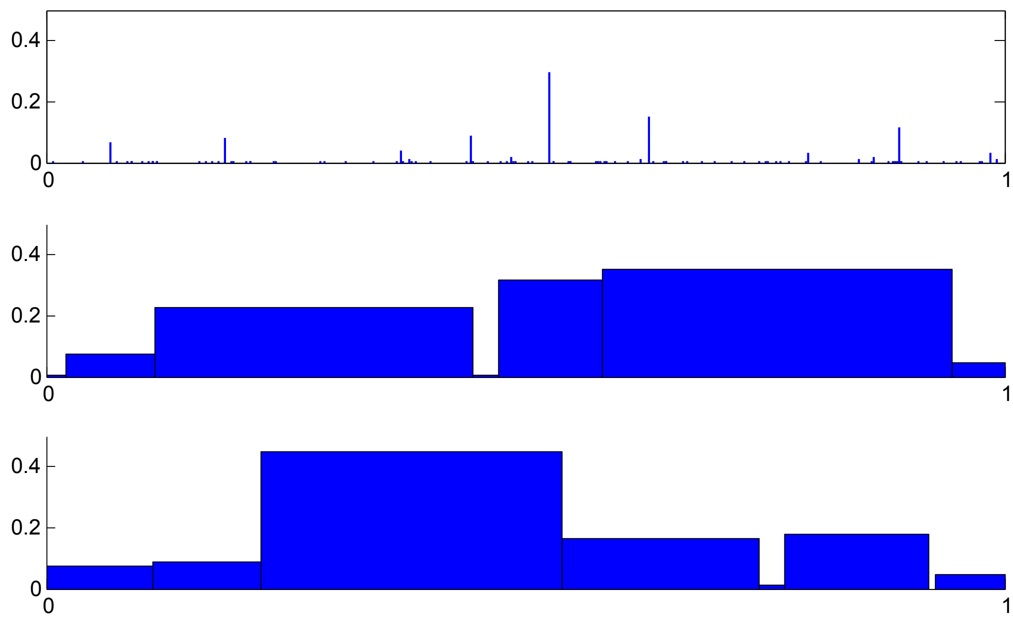
Samples from the Dirichlet process

- The *concentration parameter* α determines the distribution over atom sizes.
- Small values of α give *sparse* distributions.



Properties of the Dirichlet process

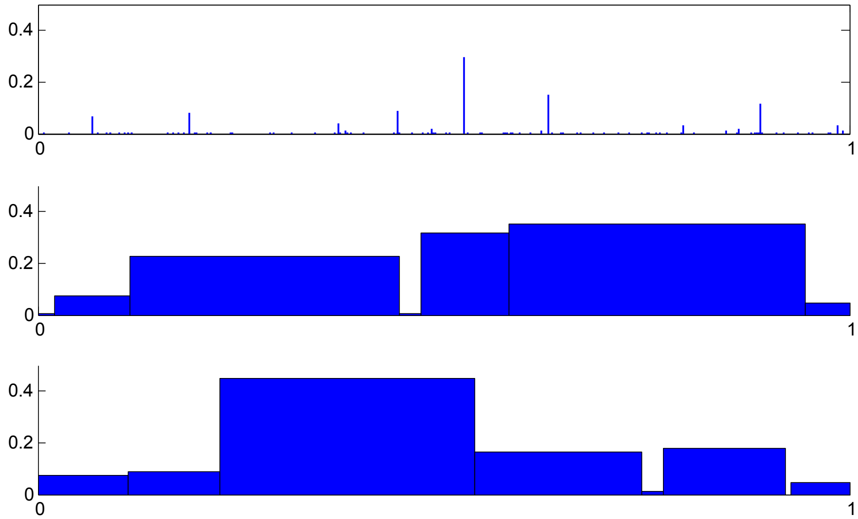
- For any partition $A_1, \ldots, A_K$ of Ω, the total mass assigned to each partition is distributed according to $Dir(\alpha H(A_1), \ldots, \alpha H(A_K))$



Definition: Finite marginals

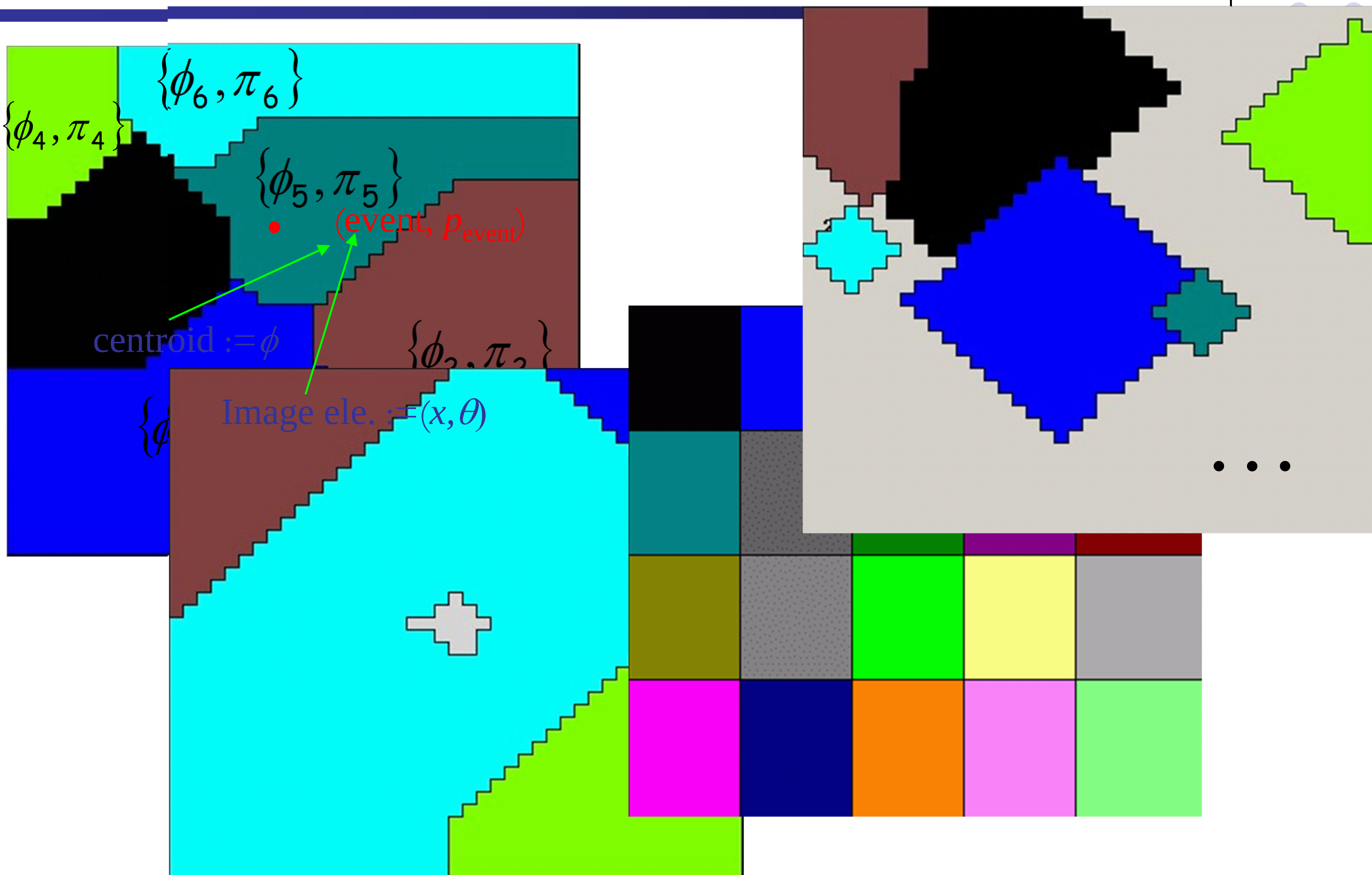
- A Dirichlet process is the unique distribution over probability distributions on some space Ω, such that for any finite partition $A_1, \ldots, A_K$ of Ω,

$$(P(A_1), \ldots, P(A_K)) \sim \text{Dirichlet}(\alpha H(A_1), \ldots, \alpha H(A_K)).$$

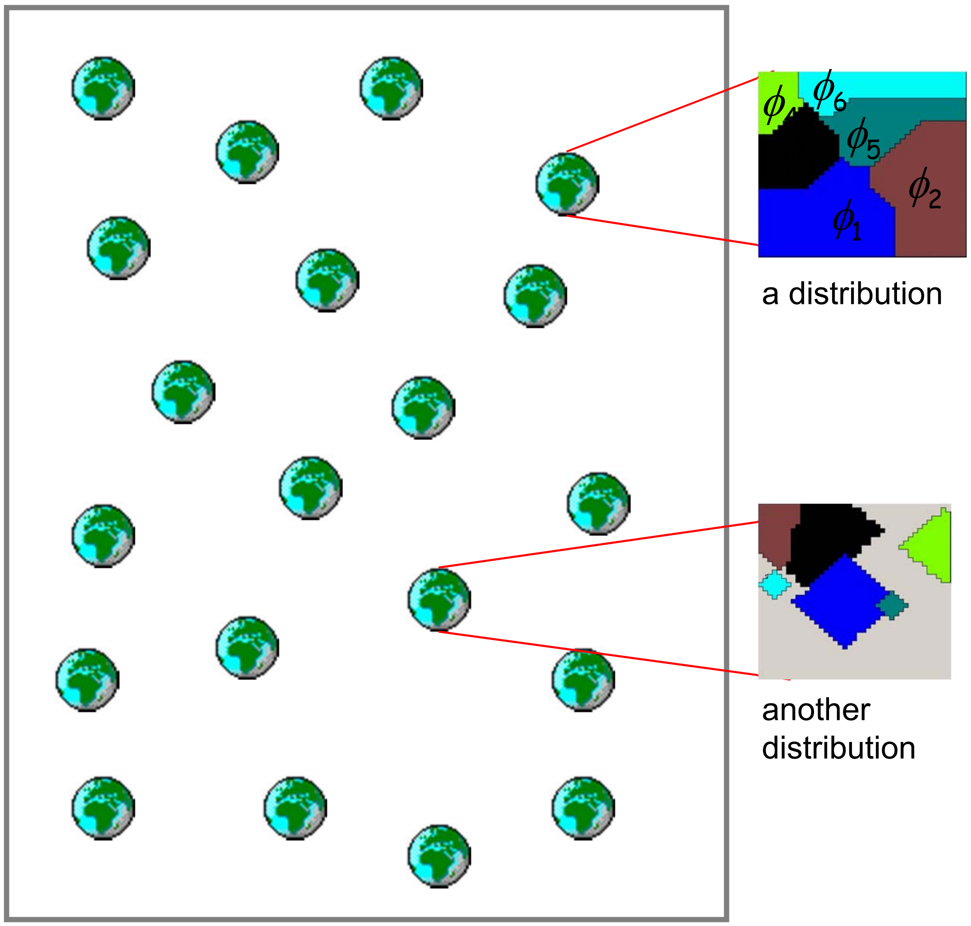


[Ferguson, 1973]

Random Partition of Probability Space



Dirichlet Process



- A *CDF*, G, on possible worlds of random partitions follows a Dirichlet Process if for any measurable finite partition $(\phi_1, \phi_2, .., \phi_m)$:

$$(G(\phi_1), G(\phi_2), \ldots, G(\phi_m)) \sim \text{Dirichlet}(\alpha G_0(\phi_1), \ldots., \alpha G0(\phi_m))$$

where G_0 is the base measure and α is the scale parameter

Thus a Dirichlet Process G defines a distribution of distribution

Conjugacy of the Dirichlet process

- Let $A_1,\dots,A_K$ be a partition of Ω, and let H be a measure on Ω. Let $P(A_k)$ be the mass assigned by $G \sim \mathrm{DP}(\alpha, H)$ to partition A_k. Then $(P(A_1),\dots,P(A_K)) \sim \mathrm{Dirichlet}(\alpha H(A_1),\dots,\alpha H(A_K))$.

- If we see an observation in the J^{th} segment (or fraction), then

$$(P(A_1),\dots,P(A_j),\dots,P(A_K)|X_1 \in A_j)$$
$$\sim \mathrm{Dirichlet}(\alpha H(A_1),\dots,\alpha H(A_j)+1,\dots,\alpha H(A_K)).$$

- This must be true for *all possible partitions of* Ω.
- This is only possible if the posterior of G, given an observation x, is given by

$$G|X_1 = x \sim \mathrm{DP}\left(\alpha+1, \frac{\alpha H + \delta_x}{\alpha+1}\right)$$

Predictive distribution

- The Dirichlet process clusters observations.
- A new data point can either join an existing cluster, or start a new cluster.
- Question: What is the predictive distribution for a new data point?
- Assume H is a continuous distribution on Ω. This means for every point θ in Ω, $H(\theta) = 0$.
  - *Therefore θ itself should not be treated as a data point, but parameter for modeling the observed data points*
- First data point:
  - Start a new cluster.
  - Sample a parameter θ_1 for that cluster.

Predictive distribution

- We have now split our parameter space in two: the singleton θ_1, and everything else.
- Let π_1 be the atom at θ_1.
- The combined mass of all the other atoms is $\pi_* = 1-\pi_1$.
- *A priori*, $(\pi_1, \pi_*) \sim \text{Dirichlet}(0, \alpha)$
- A posteriori, $(\pi_1, \pi_*)|X_1 = \theta_1 \sim \text{Dirichlet}(1, \alpha)$

Predictive distribution

- If we integrate out π_1 we get

$$
\begin{aligned}
P(X_2 = \theta_k | X_1 = \theta_1) &= \int P(X_2 = \theta_k | (\pi_1, \pi_*)) P((\pi_1, \pi_* | X_1 = \theta_1) d\pi_1 \\
&= \int \pi_k \text{Dirichlet}((\pi_1, 1 - \pi_1) | 1, \alpha) d\pi_1 \\
&= \mathbb{E}_{\text{Dirichlet}(1,\alpha)}[\pi_k] \\
&= \begin{cases} \frac{1}{1+\alpha} & \text{if } k = 1 \\ \frac{\alpha}{1+\alpha} & \text{for new } k. \end{cases}
\end{aligned}
$$

Predictive distribution

- Lets say we choose to start a new cluster, and sample a new parameter $\theta_2 \sim H$. Let π_2 be the size of the atom at θ_2.
- A posteriori, $(\pi_1, \pi_2, \pi_*)|X_1 = \theta_1, X_2 = \theta_2 \sim \text{Dirichlet}(1, \alpha)$.
- If we integrate out $\pi = (\pi_1, \pi_2, \pi_*)$ we get

$$
\begin{aligned}
P(X_3 = \theta_k | X_1 = \theta_1, X_2 = \theta_2) \\
&= \int P(X_3 = \theta_k|\pi) P(\pi|X_1 = \theta_1, X_2 = \theta_2) d\pi \\
&= \mathbb{E}_{\text{Dirichlet}(1,1,\alpha)}[\pi_k] \\
&= \begin{cases} \frac{1}{2+\alpha} & \text{if } k = 1 \\ \frac{1}{2+\alpha} & \text{if } k = 2 \\ \frac{\alpha}{2+\alpha} & \text{for new } k. \end{cases}
\end{aligned}
$$

Predictive distribution

- In general, if m_k is the number of times we have seen X_i=k, and K is the total number of observed values,

$$P(X_{n+1} = \theta_k | X_1, \ldots, X_n) = \int P(X_{n+1} = \theta_k | \pi) P(\pi | X_1, \ldots, X_n) d\pi$$
$$= \mathbb{E}_{\mathrm{Dirichlet}(m_1, \ldots, m_K, \alpha)} \left[\pi_k \right]$$
$$= \begin{cases} \frac{m_k}{n+\alpha} & \text{if } k \leq K \\ \frac{\alpha}{n+\alpha} & \text{for new cluster.} \end{cases}$$

- We tend to see observations that we have seen before – *rich-get-richer property.*
- We can always add new features – *nonparametric.*

A few useful metaphors for DP

DP – a Pólya urn Process

$$p = \frac{2}{5+\alpha}$$ ●

$$p = \frac{3}{5+\alpha}$$ ●

$$p = \frac{\alpha}{5+\alpha}$$

$G_0 := p($ ● ● ● $\ldots)$

Joint: $G($  $) \sim DP(\alpha G_0)$

Marginal: $$\phi_i \mid \phi_{-i}, \alpha, G_0 \sim \sum_{k=1}^{K} \frac{n_k}{i-1+\alpha} \delta_{\phi_k} + \frac{\alpha}{i-1+\alpha} G_0 .$$

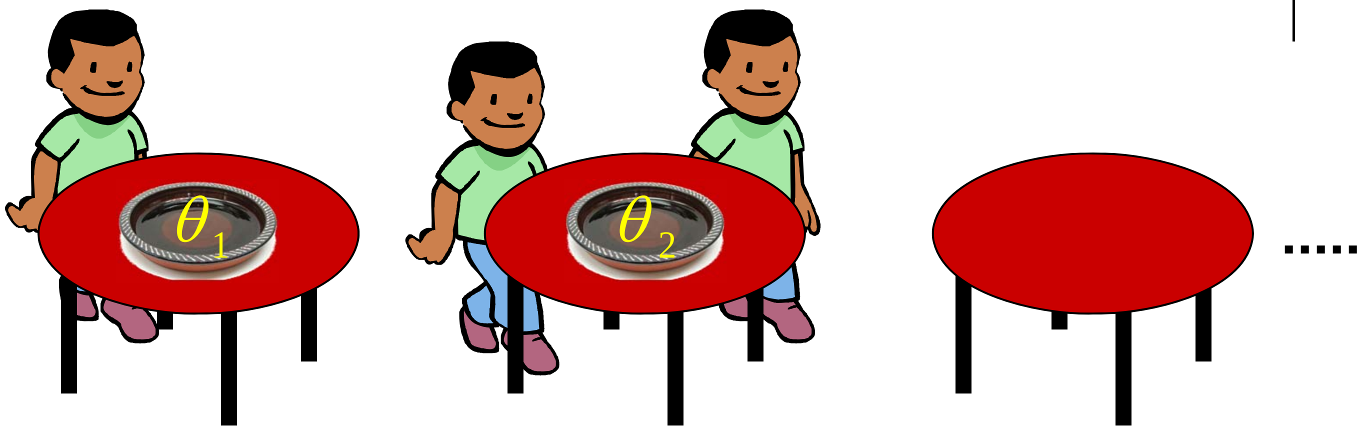
- Self-reinforcing property
- exchangeable partition of samples

Polya urn scheme

- The resulting distribution over data points can be thought of using the following urn scheme.
- An urn initially contains a black ball of mass α.
- For n=1,2,… sample a ball from the urn with probability proportional to its mass.
- If the ball is black, choose a previously unseen color, record that color, and return the black ball plus a unit-mass ball of the new color to the urn.
- If the ball is not black, record it's color and return it, plus another unit-mass ball of the same color, to the urn

[Blackwell and MacQueen,1973]

The Chinese Restaurant Process



$$P(c_i = k \mid \mathbf{c}_{-i}) =$$

1	0		0
$\frac{1}{1+\alpha}$	$\frac{\alpha}{1+\alpha}$		0
$\frac{1}{2+\alpha}$	$\frac{1}{2+\alpha}$		$\frac{\alpha}{2+\alpha}$
$\frac{1}{3+\alpha}$	$\frac{2}{3+\alpha}$		$\frac{\alpha}{3+\alpha}$
$\frac{m_1}{i+\alpha-1}$	$\frac{m_2}{i+\alpha-1}$	....	$\frac{\alpha}{i+\alpha-1}$

Exchangeability

- An interesting fact: the distribution over the clustering of the first *N* customers *does not depend on the order in which they arrived*.
- Homework: Prove to yourself that this is true.
- However, the customers are not independent – they tend to sit at popular tables.
- We say that distributions like this are *exchangeable*.
- De Finetti's theorem: If a sequence of observations is exchangeable, there must exist a distribution given which they are iid.
- The customers in the CRP are iid given the underlying Dirichlet process – by integrating out the DP, they become dependent.

The Stick-breaking Process

$$G \sim \mathrm{DP}(\alpha, G_0)$$

$$G = \sum_{k=1}^{\infty} \pi_k \delta(\theta_k)$$

$$\theta_k \sim G_0$$

Location

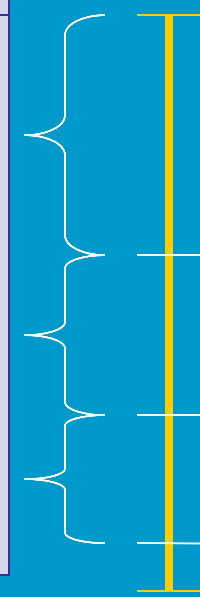
$$\sum_{k=1}^{\infty} \pi_k = 1$$

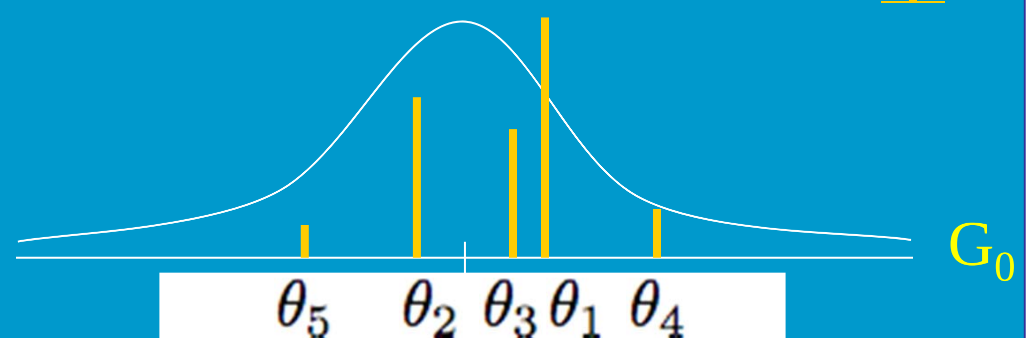
$$\pi_k = \beta_k \prod_{j=1}^{k-1} (1 - \beta_k)$$

Mass

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

$\prod_{j=1}^{k-1}(1-\beta_j)$	β_k	π_k
0	0.4	0.4
0.6	0.5	0.3
0.3	0.8	0.24





Stick breaking construction

- We can represent samples from the Dirichlet process exactly.
- Imagine a stick of length 1, representing total probability.
- For k=1,2,…
  - Sample a beta(1,α) random variable b_k.
  - Break off a fraction b_k of the stick. This is the k^{th} atom size
  - Sample a random location for this atom.
  - Recurse on the remaining stick.

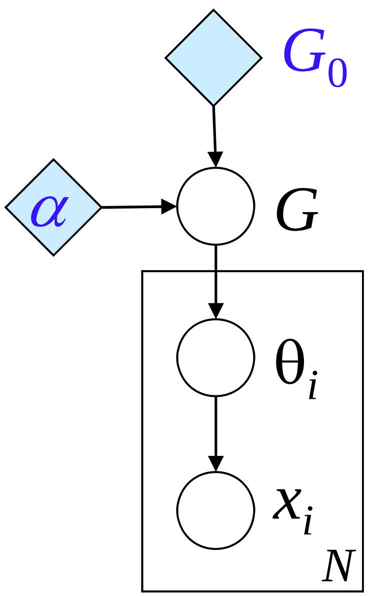
$$G := \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k}$$

$$\pi_k := b_k \prod_{j=1}^{k-1} (1 - b_k)$$

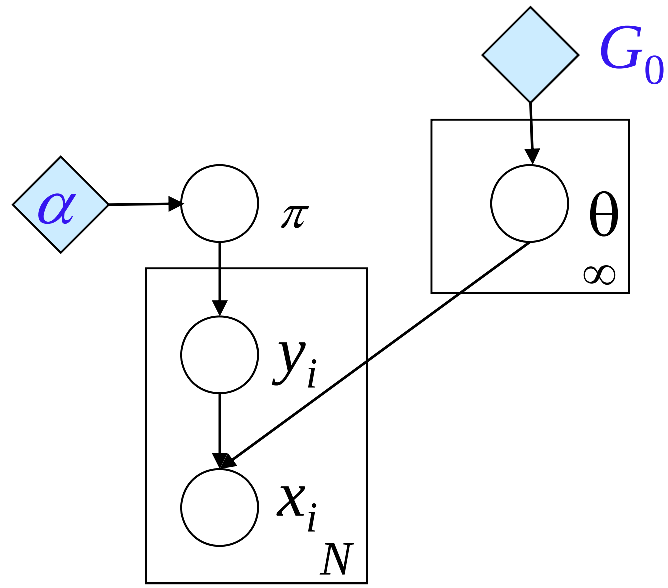
$$b_k \sim \text{Beta}(1, \alpha)$$

[Sethuraman, 1994]

Graphical Model Representations of DP



The Pólya urn construction



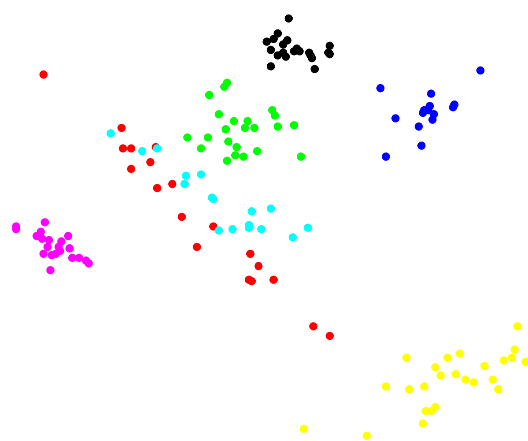
The Stick-breaking construction

Inference in the DP mixture model

$$G := \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k} \sim \mathrm{DP}(\alpha, H)$$

$$\phi_n \sim G$$

$$x_n \sim f(\phi_n)$$



Inference: Collapsed sampler

- We can integrate out G to get the CRP.
- Reminder: Observations in the CRP are exchangeable.
- Corollary: When sampling any data point, we can always rearrange the ordering so that it is the last data point.
- Let z_n be the cluster allocation of the nth data point.
- Let K be the total number of instantiated clusters.
- Then

$$p(z_n = k | x_n, z_{-n}, \phi_{1:K}) \propto \begin{cases} m_k f(x_n|\phi_k) & k \leq K \\ \alpha \int_\Omega f(x_n|\phi) H(d\phi) & k = K+1 \end{cases}$$

- If we use a conjugate prior for the likelihood, we can often integrate out the cluster parameters

Problems with the collapsed sampler

- We are only updating one data point at a time.
- Imagine two "true" clusters are merged into a single cluster – a single data point is unlikely to "break away".
- Getting to the true distribution involves going through low probability states ➔ mixing can be slow.
- If the likelihood is not conjugate, integrating out parameter values for new features can be difficult.
- Neal [2000] offers a variety of algorithms.
- Alternative: Instantiate the latent measure.

Inference: Blocked Gibbs sampler

- Rather than integrate out *G*, we can instantiate it.
- Problem: *G* is infinite-dimensional.
- Solution: Approximate it with a truncated stick-breaking process:

$$G^K := \sum_{k=1}^{K} \pi_k \delta_{\theta_k}$$

$$\pi_k = b_k \prod_{j=1}^{k-1} (1 - b_j)$$

$$b_k \sim \mathrm{Beta}(1, \alpha), k = 1, \ldots, K-1$$

$$b_K = 1$$

Inference: Blocked Gibbs sampler

- Sampling the cluster indicators:

$$p(z_n = k|\text{rest}) \propto \pi_k f(x_n|\theta_k)$$

- Sampling the stick breaking variables:
  - We can think of the stick breaking process as a sequence of binary decisions.
  - Choose $z_n = 1$ with probability b_1.
  - If $z_n \neq 1$, choose $z_n = 2$ with probability b_2.
  - *etc..*

$$b_k|\text{rest} \sim \text{Beta}\left(1 + m_k, \alpha + \sum_{j=k+1}^{K} m_j\right)$$

Inference: Slice sampler

- Problem with batch sampler: Fixed truncation introduces error.
- Idea:
  - Introduce *random truncation*.
  - If we marginalize over the random truncation, we recover the full model.
- Introduce a uniform random variable u_n for each data point.
- Sample indicator z_n according to

$$p(z_n = k | \text{rest}) = I(\pi_k > u_n) f(x_n | \theta_k)$$

- Only a **finite** number of possible values.

Inference: Slice sampler

- The conditional distribution for u_n is just:

$$u_n|\text{rest} \sim \text{Uniform}[0, \pi_{z_n}]$$

- Conditioned on the u_n and the z_n, the π_k can be sampled according to the block Gibbs sampler.

- Only need to represent a finite number K of components such that

$$1 - \sum_{k=1}^{K} \pi_k < min(u_n)$$

Summary: Bayesian Nonparametrics

- Examples: Dirichlet processes, stick-breaking processes …
- From finite, to infinite mixture, to more complex constructions (hierarchies, spatial/temporal sequences, …)
- Focus on the laws and behaviors of both the generative formalisms and resulting distributions
- Often offer explicit expression of distributions, and expose the structure of the distributions --- motivate various approximate schemes