Lecture II – Clustering – Part II: Non-parametric clustering

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1. Paradigms for clustering
2. Methods based on non-parametric density estimation
3. Model-based: Dirichlet process mixture models

What is clustering? Problem and Notation

- **Informal definition** **Clustering** = Finding groups in data
- **Notation**

$\mathcal{D}$	=	$\{x_1, x_2, \ldots x_n\}$ a **data set**
n	=	number of **data points**
K	=	number of **clusters** ($K << n$)
Δ	=	$\{C_1, C_2, \ldots, C_K\}$ a partition of $\mathcal{D}$ into disjoint subsets
$k(i)$	=	the **label** of point i
$L(\Delta)$	=	cost (loss) of Δ (to be minimized)

- **Second informal definition** **Clustering** = given n **data points**, separate them into K **clusters**
- Hard vs. soft clusterings
  - **Hard** clustering Δ: an item belongs to only 1 cluster
  - **Soft** clustering $\gamma = \{\gamma_{ki}\}_{k=1:K}^{i=1:n}$
    γ_{ki} = the **degree of membership** of point i to cluster k

$$\sum_k \gamma_{ki} = 1 \quad \text{for all } i$$

(usually associated with a probabilistic model)

Clustering Paradigms

Depend on type of data, type of clustering, type of cost (probabilistic or not), and constraints (about K, shape of clusters)

- Data = vectors $\{x_i\}$ in $\mathbb{R}^d$

Parametric (K known)	Cost based [hard]
	Model based [soft]
Non-parametric (K determined by algorithm)	Dirichlet process mixtures [soft]
	Information bottleneck [soft]
	Modes of distribution [hard]
	Gaussian blurring mean shift? [hard] Level sets of distribution [hard]

- Data = similarities between pairs of points $[S_{ij}]_{i,j=1:n}$, $S_{ij} = S_{ji} \geq 0$ **Similarity based clustering**

Graph partitioning	spectral clustering [hard, K fixed, cost based]
	typical cuts [hard non-parametric, cost based]
Affinity propagation	[hard/soft non-parametric]

Classification vs Clustering

	Classification	**Clustering**
Cost (or Loss) L	Expectd error	many! (probabilistic or not)
	Supervised	Unsupervised
Generalization	Performance on new data is what matters	Performance on current data is what matters
K	Known	Unknown
"Goal"	Prediction	Exploration Lots of data to explore!
Stage of field	Mature	Still young

Methods based on non-parametric density estimation

Idea The clusters are the isolated peaks in the (empirical) data density

- group points by the peak they are under
- some outliers possible
- $K = 1$ possible(no clusters)
- shape and number of clusters K determined by algorithm
- **structural parameters**
  - **smoothness** of the **density estimate**
  - what is a peak

Algorithms

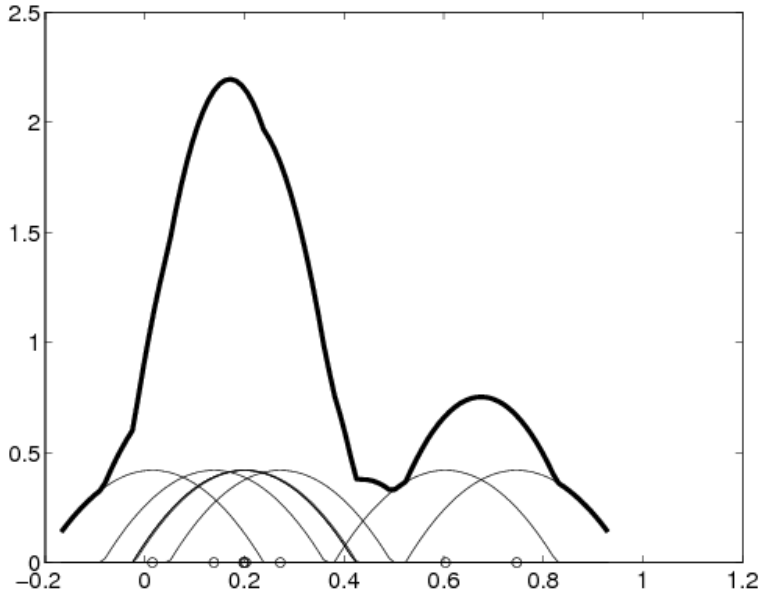
- peak finding algorithms Mean-shift algorithms
- level sets based algorithms
  - Nugent-Stuetzle, Support Vector clustering
- Information Bottleneck ?

Kernel density estimation

Input
- data $\mathcal{D} \subseteq \mathbb{R}^d$
- **Kernel** function $K(z)$
- parameter **kernel width** h (is a **smoothness parameter**)

Output $f(x)$ a **probability density** over $\mathbb{R}^d$

$$f(x) = \frac{1}{nh^d} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$



- f is sum of Gaussians centered on each x_i
- f is smoother (less variation) if h larger
- **caveat:** dimension d can't be too large

The kernel function

- Example $K(z) = \frac{1}{(2\pi)^{d/2}} e^{-||z||^2/2}$, $z \in \mathbb{R}^d$ is the Gaussian kernel
- In general
  - $K()$ should represent a density on $\mathbb{R}^d$, i.e $K(z) \geq 0$ for all z and $\int K(z)dz = 1$
  - $K()$ symmetric around 0, decreasing with $||z||$
- In our case, K must be differentiable

Mean shift algorithms

Idea find points with $\nabla f(x) = 0$

Assume $K(z) = e^{-||z||^2/2}/\sqrt{2\pi}$ Gaussian kernel

$$\nabla f(x) = -\frac{1}{nh^d} \sum_{i=1}^{n} K(\frac{x - x_i}{h})(x - x_i)/h$$

Local max of f is solution of implicit equation

$$x = \underbrace{\frac{\sum_{i=1}^{n} x_i K(\frac{x-x_i}{h})}{\sum_{i=1}^{n} K(\frac{x-x_i}{h})}}_{\text{the mean shift } m(x)}$$

Algorithm Simple Mean Shift

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, kernel $K(z)$, h

1. for $i = 1 : n$
   1. $x \leftarrow x_i$
   2. iterate $x \leftarrow m(x)$ until convergence to m_i
2. group points with same m_i in a cluster

Remarks

- mean shift iteration guaranteed to converge to a max of f
- computationally expensive
- a faster variant...

Algorithm Mean Shift (Comaniciu-Meer)

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, kernel $K(z)$, h

1. select q points $\{x_j\}_{j=1:q} = \mathcal{D}_q \subseteq \mathcal{D}$ that cover the data well
2. for $j \in \mathcal{D}_q$
   1. $x \leftarrow x_j$
   2. iterate $x \leftarrow m(x)$ until convergence to m_j
3. group points in $\mathcal{D}_q$ with same m_j in a cluster
4. assign points in $\mathcal{D} \setminus \mathcal{D}_q$ to the clusters by the **nearest-neighbor** method

$$k(i) = k(\operatorname*{argmin}_{j \in \mathcal{D}_q} ||x_i - x_j||)$$

[Supplement: Gaussian blurring mean shift]

Idea

- like **Simple Mean Shift** but points are shifted to new locations
- the density estimate f changes
- becomes concentrated around peaks very fast

Algorithm Gaussian Blurrring Mean Shift (GBMS)

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, Gaussian kernel $K(z)$, h

1. Iterate until STOP
   1. for $i = 1 : n$ compute $m(x_i)$
   2. for $i = 1 : n$, $x_i \leftarrow m(x_i)$

Remarks

- all x_i converge to a single point
  $\Rightarrow$ need to stop before convergence

Empirical stopping criterion ?

- define $e_i^t = ||x_i^t - x_i^{t-1}||$ the change in x_i at t
- define $H(e^t)$ the **entropy** of the **histogram** of $\{e_i^t\}$
- STOP when $\sum_{i=1}^n e_i^t/n <$`tol` OR $|H(e^t) - H(e^{t-1})| <$`tol`'

Convergence rate If true f Gaussian, convergence is **cubic**

$$||x_i^t - x^*|| \leq C||x_i^{t-1} - x^*||^3$$

very fast!!

The Nugent-Stuetzle algorithm

Algorithm Nugent-Stuetzle

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, kernel $K(z)$

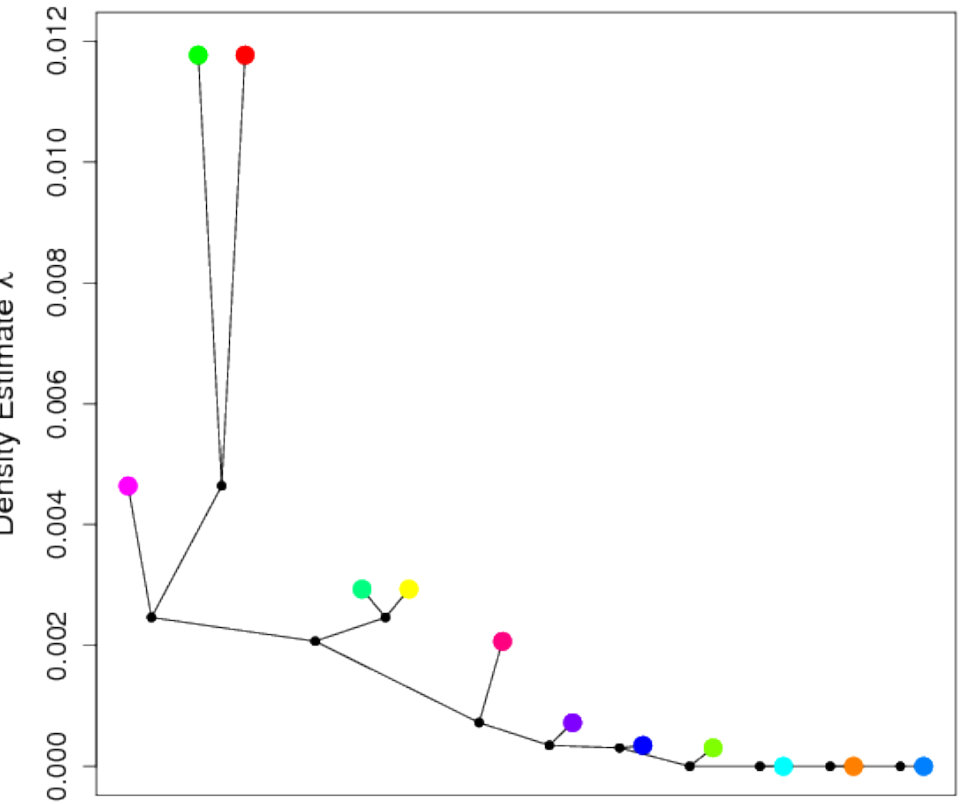
1. Compute KDE $f(x)$ for chosen h
2. for levels $0 < l_1 < l_2 < \ldots < l_r < \ldots < l_R \geq \sup_x f(x)$
   1. find **level set** $L_r = \{x \mid f(x) \geq l_r\}$ of f
   2. if L_r **disconnected** then each connected component is a cluster $\rightarrow (C_{r,1}, C_{r,2}, \ldots C_{r,K_r})$

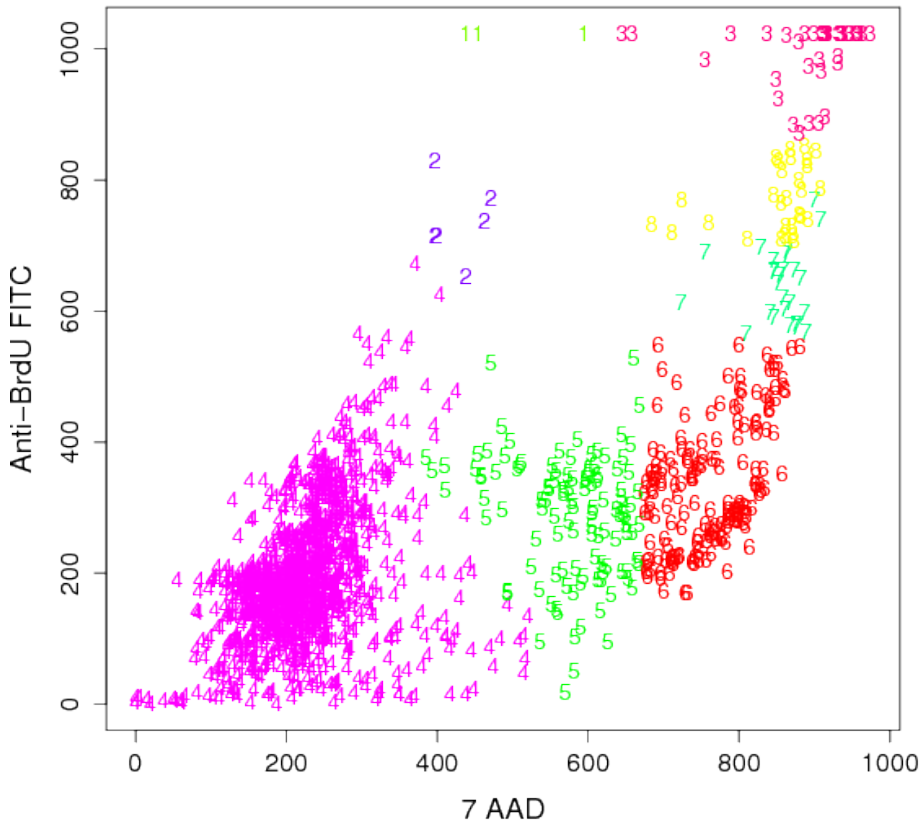
Output clusters $\{(C_{r,1}, C_{r,2}, \ldots C_{r,K_r})\}_{r=1:R}$

Remarks

- every cluster $C_{r,k} \subseteq$ some cluster $C_{r-1,k'}$
- therefore output is hierarchical clustering
- some levels can be pruned (if no change, i.e. $K_r = K_{r-1}$)
- algorithm can be made recursive, i.e. efficient
- finding level sets of f tractable only for $d = 1, 2$
- for larger d, $L_r = \{x_i \in \mathcal{D} \mid f(x_i) \geq l_r\}$
- to find connected components
  - for $i \neq j \in L_r$
    if $f(tx_i + (1-t)x_j) \geq l_r$ for $t \in [0, 1]$
    then $k(i) = k(j)$
- confidence intervals possile by resampling

Cluster tree with 13 leaves (8 clusters, 5 artifacts)





(from **?**)

Chaudhuri-Dasgupta Algorithm

- Uses k-**nearest neighbor** graphs (filtration)
- Parameters k (nearest neigbhors) and $\alpha \in [1, 2]$
- for $r \geq 0$, $G_r = (V_r, E_r)$ with
  - $x_i \in V_r$ iff **distance to k-nn of x_i** $\leq r$
  - $(x_i, x_j) \in E_r$ iff $||x_i - x_j|| \leq \alpha r$

Consistency Theorem For any ϵ (separation parameter) and δ (confidence), $\alpha \in [\sqrt{2}, 2]$ (graph density), if $k = C \log^2(1/\delta) \frac{d \log n}{\epsilon^2}$
for any two clusters C, C' in cluster tree, there exists a level r so that $C \cap \mathcal{D}, C' \cap \mathcal{D}$ are clusters at level r

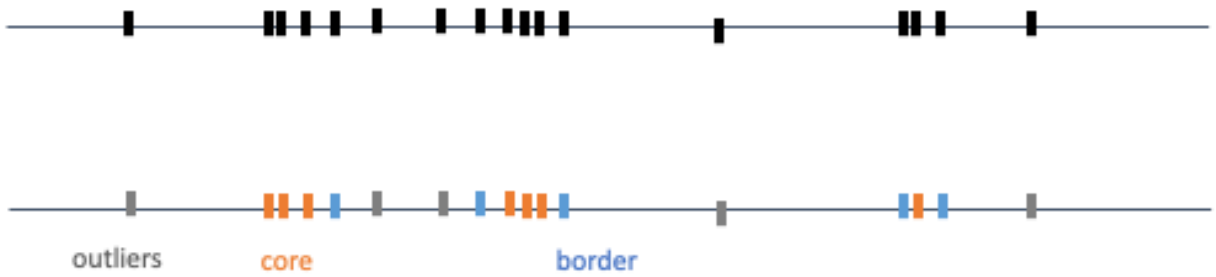
The K-nn density estimator

The K-nn density estimator

- Let $B_r(x)$ be the (closed) ball of radius r centered at x
- If $|B_r(x^i) \cap \mathcal{D}| = k$ then $\hat{p}(x^i) = \frac{1}{r^n \omega_n} \frac{k}{n}$ is an estimate of the density at x^i
  - $\omega_n = \pi^{n/2}/\Gamma(n/2+1)$ is the volume of the unit ball in $\mathbb{R}^n$
  - intuitively, the ball of radius r contains k/n probability mass
  - Note that the density $\hat{p}$ is not required to integrate to 1

DBScan

- Introduced with no proof, but widely used. Implicitly based on the K-nn estimator
- Parameters r radius, m minimum number points
- Definitions **core** $Q = \{x^i \in \mathcal{D}, \text{ with } B_r(x^i) \cap \mathcal{D}| \geq m\}$
- **border** $B = \{x^i \in \mathcal{D} \setminus Q, \text{ so that } x^i \in B_r(x^j), x^j \in Q\}$
- **outliers (noise)** $O = \mathcal{D} \setminus (Q \cup B)$



- Algorithm idea
- Construct directed graph $\mathcal{G}$ with edges (i, j) where $x^i \in Q, j \in B_r(x^i)$
- The graph edges between core points are undirected/symmetric, the other are from core to border
- Clusters are determined by the connected components of the graph restricted to Q.
- The border points are assigned to a cluster containing x^j so that $x^i \in B_r(x^j)$, $x^j \in Q$ Note that this assignment is not unique!

- Heuristic algorithm estimates r, m

[Supplement: Chaudhuri-Dasgupta Algorithm]

Consistency Theorem For any ϵ (separation parameter) and δ (confidence), $\alpha \in [\sqrt{2}, 2]$ (graph density), if $k = C \log^2(1/\delta) \frac{d \log n}{\epsilon^2}$
for any two clusters C, C' in cluster tree, there exists a level r so that $C \cap \mathcal{D}$, $C' \cap \mathcal{D}$ are clusters at level r

- r depends on $\lambda =$"bridge" between C, C' (and $\sigma > 0$ "tube" width)

$$r^d \omega_d \lambda = \frac{k}{n} + \ldots \textit{confidence term}$$

- it follows that the needed sample size n at level λ

$$n = \mathcal{O}\left(\frac{d}{\lambda \epsilon^2 (\sigma/2)^d \omega_d} \log \frac{d}{\lambda \epsilon^2 (\sigma/2)^d \omega_d} \right)$$

- this **sample complexity** n is almost tight
- for $\alpha < \sqrt{2}$ sample complexity is exponential in d

- New results **[Kent, B. P., Rinaldo, A. and Verstynen, T. 2013]**

- Remark: algorithm(s) can be applied in any metric space

[Supplement: Support Vector (SV) clustering]

Idea same as for Nugent-Stuetzle, but use **kernelized density estimator** instead of KDE

Algorithm SV

Input data $\mathcal{D}$, parameters q kernel width, $p \in (0,1)$ proportion of outliers

1. construct a 1-class SVM with parameters q, $C = 1/np$
   this is equivalent to enclosing the data in a sphere in feature space
   for any x its distance from center of sphere is

$$R^2(x) = K(x,x) - 2\sum_j \alpha_j K(x,x_j) + \sum_{i,j} K(x_i,x_j)$$

   for x_i support vector, $R(x_i) = R$ (same for all)
2. for all pairs $i,j = 1:n$
   - i,j in same cluster if segment $[i,j]$ is within sphere with radius R in feature space
   - practically, test if $R(tx_i + (1-t)x_j) < R$ for t on a grid over [0,1]

Remarks

- the **kernel** used by SV is $K(x, x') = e^{-q||x-x'||^2}$
- q controls boundary smoothness
- SV's lie on cluster boundaries, "margin error" points lie outside clusters (are outliers)
- SV theory $\frac{\text{margin errors}}{n} \rightarrow \frac{1}{nC} = p$ for large n
- hence p controls the proportion of outliers
- p, q together control K
  p larger, q smaller $\Rightarrow$ K smaller

The Dirichlet distribution

- $Z \in \{1 : r\}$ a discrete random variable, let $\theta_j = P_z(j)$, $j = 1, \ldots r$.
- **Multinomial distribution** Probability of i.i.d. sample of size N from P_z

$$P(z^{1,\ldots n}) = \prod_{j=1}^{r} \theta_j^{n_j}$$

where $n_j = \#$the value j is observed, $j = 1, \ldots r$

- $n_{1:r}$ are the **sufficient statistics** of the data.
- The **Dirichlet distribution** is defined over domain of $\theta_{1,\ldots r}$, with real parameters $N'_{1,\ldots r} > 0$ by

$$D(\theta_{1,\ldots r}; n'_{1,\ldots r}) = \frac{\Gamma(\sum_j n'_j)}{\prod_j \Gamma(n'_j)} \prod_j \theta_j^{n'_j - 1}$$

where $\Gamma(p) = \int_0^\infty t^{p-1} e^{-t} dt$.

Dirichlet process mixtures

- Model-based
- generalization of mixture models to
  - infinite K
  - Bayesian framework
- denote θ_k = parameters for component f_k
- assume $f_k(x) \equiv f(x, \theta_k) \in \{f(x, \theta)\}$
- assume prior distributions for parameters $g_0(\theta)$
- prior with hyperparameter $\alpha > 0$ on the number of clusters
- very flexible model

A sampling model for the data

- **Example: Gaussian mixtures**, $d = 1$, $\sigma_k = \sigma$ fixed
- $\theta = \mu$
- prior for μ is $Normal(0, \sigma_0^2 I_d)$
- Sampling process
  - for $i = 1 : n$ sample $x_i, k(i)$ as follows

    denote $\{1 : K\}$ the clusters after step $i - 1$
    define n_k the size of cluster k after step $i - 1$

    1. $$k(i) = \begin{cases} k & \text{w.p } \frac{n_k}{i-1+\alpha}, \ k = 1 : K \\ K+1 & \text{w.p } \frac{\alpha}{i-1+\alpha} \end{cases} \quad (1)$$
    2. if $k(i) = K + 1$ sample $\mu_i \equiv \mu_{K+1}$ from $Normal(0, \sigma_0^2)$
    3. sample x_i from $Normal(\mu_{k(i)}, \sigma^2)$
- can be shown that the distribution of $x_{1:n}$ is **interchangeable** (does not depend on data permutation)

The hyperparameters

- σ_0 controls spread of centers
  - should be large
- α controls number of cluster centers
  - α large $\Rightarrow$ many clusters
- cluster sizes non-uniform (larger clusters attract more new points)
- many single point clusters possible

General Dirichlet mixture model

- cluster densities $\{f(x, \theta)\}$
- parameters θ sampled from prior $g_0(\theta, \beta)$
- cluster membership $k(i)$ sampled as in (1)
- x_i sampled from $f(x, \theta_{k(i)})$
- **Model Hyperparameters** α, β

Clustering with Dirichlet mixtures

The clustering problem

- $\alpha, g_0, \beta, \{f\}$ given
- $\mathcal{D}$ given
- wanted $\theta_{1:n}$ (not all distinct!)
- note:
  - $\theta_{1:n}$ determines a hard clustering Δ
  - the posterior of $\theta_{1:n}$ given the data determines a soft clustering via $P(x_i \mid k) \propto \int f(x_i|\theta_k)g_k(\theta_k)d\theta_k$

Estimating $\theta_{1:n}$ cannot be solved in closed form
Usually solved by MCMC (Markov Chain Monte Carlo) sampling

Clustering with Dirichlet mixtures via MCMC

MCMC estimation for Dirichlet mixture

Input $\alpha, g_0, \beta, \{f\}, \mathcal{D}$

State cluster assignments $k(i)$, $i = 1 : n$,
parameters θ_k for all distinct k

terate

1. for $i = 1 : n$ (reassign data to clusters)
   1. remove i from its cluster (hence $\sum_k n_k = n - 1$)
   2. resample $k(i)$ by

$$k(i) = \begin{cases} \text{existing } k & \text{w.p } \propto \frac{n_k}{n-1+\alpha} f(x_i, \theta_k) \\ \text{new cluster} & \text{w.p } \frac{\alpha}{n-1+\alpha} \int f(x_i, \theta) g_0(\theta) d\theta \end{cases} \quad (2)$$

   3. if $k(i)$ is new label, sample a new $\theta_{k(i)} \propto g_0 f(x_i, \theta)$
2. for $k \in \{k(1 : n)\}$ (resample cluster parameters)
   1. sample θ_k from posterior $g_k(\theta) \propto g_0(\theta, \beta) \prod_{i \in C_k} f(x_i, \theta)$

g_k can be computed in closed form if g_0 is conjugate prior

Output a state with high posterior

Summary: Parametric vs. non-parametric

Parametric clustering

- Optimizes a cost L
- Most costs are NP-hard to optimize
- Assumes more detailed knowledge of cluster shapes
- Assumes K known (But there are wrapper methods to select K)
- Gets harder with larger K
- Older, more used and better studied

Non-parametric clustering

- Variety of paradigms
  - density-based methods have no cost function
  - (Max Likelihood: non-parametric mixture models)
  - Bayesian: Dirichlet Process Mixtures (samples from posterior of $k(1:n), \{\theta_k\}$ given $\mathcal{D}$)
- Do not depend critically on initialization
- K and outliers selected automatically, naturally
- Require hyperparameters (= smoothness parameters)

When to use

- Parametric
  - shape of clusters known
  - K not too large or known
  - clusters of comparable sizes
- Non-parametric (density based)
  - shape of clusters arbitrary
  - K large or many outliers
  - clusters sizes in large range (a few large clusters and many small ones)
  - dimension d small (except for **SV**)
  - lots of data
- Dirichlet Process mixtures
  - shape of clusters known
  - clusters sizes in large range

Notation

$||x - y||$ Euclidean distance for $x, y \in \mathbb{R}^d$, $||x - y|| = \sqrt{\sum_{j=1}^{d}(x_j - y_j)^2}$

Links

- Yee Whye Teh's tutorial on DP Mixtures http://mlg.eng.cam.ac.uk/tutorials/07/ywt.pdf
- Lecture on exponential family models http: