Small Variance Asymptotics for Non-parametric Bayesian Clustering

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- We start with a hard non-parameteric clustering algorithm.
- We then extend this algorithm to a hierarchical structure using Hierarchical Dirichlet process.
- Finally, we generalize the clustering algorithm, to use bregman divergence instead of just euclidean distance.

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Definition

(Ferguson) We say G is Dirichlet Process distributed with base distribution H and concentration parameter α, written as $G \sim DP(\alpha, H)$ if $(G(A_1), \ldots, G(A_r)) \sim Dir(\alpha H(A_1), \ldots, \alpha H(A_r))$ for every finite measurable partition $A_1, \ldots, A_r$ of Θ which is support of H

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- Constructions like Blackwell-MacQueen urn scheme and Stick breaking process ensure existence of DP.

Posterior of DP

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- Using conjugacy: $(G(A_1), \ldots, G(A_r) | \theta_1, \ldots \theta_n) \sim Dir(\alpha H(A_1) + n_1, \ldots, \alpha H(A_r) + n_r)$

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- We have seen CRP and stick breaking process in class.

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- Let $k \to \infty$ to get infinite mixture model

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- Proceed in cyclic manner until convergence.

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- However one subtle difference is that if the distance to closest mean is is greater than $\lambda(\alpha)$, then the probabilities corresponding to each of the existing cluster falls to zero and we start a new cluster.

Underlying Objective function

1. We will show in report that the hard clustering algorithm minimizes the objective function:

$$min_{\{l_j\}_{j=1}^{k}} \sum_{c=1}^{k} \sum_{x \in l_c} ||x - \mu_c||^2 + \lambda k$$

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2. This is similar to the K-means algorithm, only value of k is not fixed and the objective penalizes large k.

Hard Clustering Algorithm

- Input: $x_1, ..., x_n, \lambda$: cluster penalty parameter.
- Output: Clustering of points in $l_1, ..., l_k$ and no. of cluster k.

1. Initialize $k = 1, l_1 = x_1, ..., x_n, \mu_1 = \frac{\sum x_i}{n}$ and $z_i = 1$ for each point.
2. Repeat until convergence:
    - For each point x_i,
      - Compute distance from all means i.e. $d_{ic} = ||x_i - \mu_c||^2$ for all c.
      - if $min_c d_{ic} > \lambda$, set $k = k + 1, z_i = k, \mu_k = x_i$.
      - Else, set $z_i = min_c d_{ic}$
    - Assign points x_i with $z_i = c$ to the cluster l_c.
    - For each cluster c, $\mu_c = \frac{\sum_{x_j \in l_c} x_j}{|l_c|}$.

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$$G_0|\gamma, H \sim DP(\gamma, H) \qquad G_j|\alpha, G_0 \sim DP(\alpha, G_0)$$
$$\phi_{ji}|G_j \sim G_j \qquad x_{ji}|\phi_{ji} \sim F(\phi_{ji})$$

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- There is a metaphor called *Chinese Restaurant Franchise* that gives an alternative view of HDP.

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where k, g is total number of local and global clusters respectively. λ_l, λ_g are regularization parameters, l_p is the set points assigned to cluster p and $\mu_p = \frac{1}{|l_p|} \sum_{x_{ij} \in l_p} x_{ij}$

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Definitions

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(Bregman, 1967) Let $\phi : S \to \mathbb{R}$ be a strictly convex function defined on convex set S such that ϕ is differentiable on interior of S. The bregman divergence is defined as $d_\phi = \phi(\boldsymbol{x}) - \phi(\boldsymbol{y}) - \langle \boldsymbol{x} - \boldsymbol{y}, \nabla\phi(\boldsymbol{y}) \rangle$

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Definition

(Rockfellar 1970) Let ψ be a **proper**, **closed**, convex function with $\Theta = \mathit{interior}(\mathit{domain}(\psi))$. The pair (Θ, ψ) is called a convex function of legendre type if following are satisfied

- Θ is nonempty
- ψ is strictly convex and differentiable on Θ
- $\forall \theta_b \in bd(\Theta), \lim_{\theta \to \theta_b} ||\nabla \psi(\theta)|| \to \infty, \theta \in \Theta$

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Theorem

(Rockfellar) Let ψ be proper, closed strictly convex function with conjugate function ψ^*. Let $\Theta = int(dom(\psi))$ and $\Theta^* = int(dom(\psi^*))$. If (θ, ψ) is a convex function of legendre type then

Legendre Dual

Theorem (cntd..)

- (θ^*, ψ^*) *is a convex function of legendre type.*
- (θ^*, ψ^*) *and* (θ, ψ) *are called legendre duals of each other.*
- *The gradient function* $\nabla\psi$ *is a one to one function from open convex set* Θ *onto the open convex set* Θ^**.*
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Using theorem and lemma, (Θ, ψ) and $(int(dom(\phi)), \phi)$ are legendre dual of each other.
More importantly, $\nabla\psi^{-1}(\boldsymbol{\mu}) = \theta(\boldsymbol{\mu}) = \nabla\phi(\boldsymbol{\mu}) \quad (1)$
$\implies \phi(\boldsymbol{\mu}) = \langle\theta(\boldsymbol{\mu}), \boldsymbol{\mu}\rangle - \psi(\theta(\boldsymbol{\mu})) \quad (2)$

Relation with Exponential Family

Theorem

Let $p_{\psi,\theta}(\mathbf{x})$ be pdf of regular exponential family family distribution. Let ϕ be the conjugate of ψ. Let θ be natural parameter and $\boldsymbol{\mu}$ be expectation parameter. Let d_ϕ be the bregman divergence derived from ϕ. Then $p_{\psi,\theta}(\mathbf{x})$ can be uniquely expressed as
$p_{\psi,\theta}(\mathbf{x}) = exp(-d_\phi(\mathbf{x}, \boldsymbol{\mu}))b_\phi(\mathbf{x})$ where $b_\phi(\mathbf{x}) = exp(\phi(\mathbf{x}))h(\mathbf{x})$

Proof.

$$\begin{aligned}
p_{\psi,\theta}(\mathbf{x}) &= h(x)exp(\langle \mathbf{x}, \theta\rangle - \psi(\theta)) \\
&= h(x)exp(\phi(\boldsymbol{\mu}) + \langle \mathbf{x} - \boldsymbol{\mu}, \nabla\phi(\boldsymbol{\mu})\rangle) \\
&= h(x)exp(-(\phi(\mathbf{x}) - \phi(\boldsymbol{\mu}) - \langle \mathbf{x} - \boldsymbol{\mu}, \nabla\phi(\boldsymbol{\mu})\rangle) + \phi(\mathbf{x})) \\
&= exp(-d_\phi(\mathbf{x}, \boldsymbol{\mu}))b_\phi(\mathbf{x}) \text{ where } b_\phi(\mathbf{x}) = exp(\phi(\mathbf{x}))h(\mathbf{x})
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Bijection

Theorem

(Banerjee et al) There is a bijection between regular exponential families and regular bregman divergences

Examples

- For 1-d Gaussian distribution $p(x|\mu) = \frac{1}{\sqrt{2\pi}} exp(-\frac{(x-\mu)^2}{2})$, the corresponding bregman divergence is $(x-\mu)^2$

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We can use this idea in the previous DP-means and HDP-means to obtain a new algorithm for hard clustering by replacing euclidean distance with above bregman divergence.

Bregman DP means

- **Input** $x_1, x_2, ...x_n, \lambda$
- **Initialize** $\mu_1 = \frac{1}{n}\sum_{i=1}^{n} x_n$
- **Assignment** For each x_i,
  - Compute bregman divergence of the x_i with current cluster centers.
  - If $\underset{c}{min}\ d_\phi(\boldsymbol{x}, \boldsymbol{\mu}_c) < \lambda$, then assign it to cluster $\underset{c}{argmin}\ d_\phi(\boldsymbol{x}, \boldsymbol{\mu})$
  - Else, define a new cluster with its mean as x_i and assign x_i to this cluster.
- **Mean Update** For each cluster, set its means $\mu_c = \frac{1}{|l_j|}\sum_{\boldsymbol{x} \in l_j} \boldsymbol{x}$ where l_j is the set of points in j^{th} cluster

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The corresponding algorithm for Hierarchical Dirichlet process is similar, where we replace euclidean distance with the above defined bregman divergence

Evaluation metrics

1. NMI
2. Custom Validation

NMI

$$\mathbb{NMI}(Y, C) = \frac{2 \times \mathbb{I}(Y; C)}{\mathbb{H}(Y) + \mathbb{H}(C)}$$

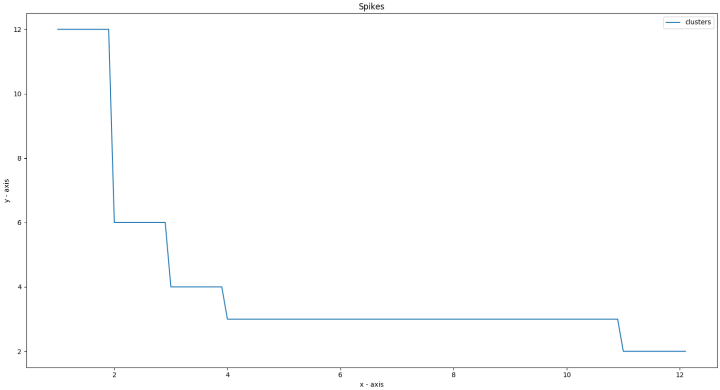
where:

1. Y := class labels
2. C := cluster labels
3. $\mathbb{H}(.)$:= Entropy
4. $\mathbb{I}(Y; C)$:= Mutual Information b/w Y and C
   $\mathbb{I}(Y; C) := \mathbb{H}(Y) - \mathbb{H}(Y|C)$

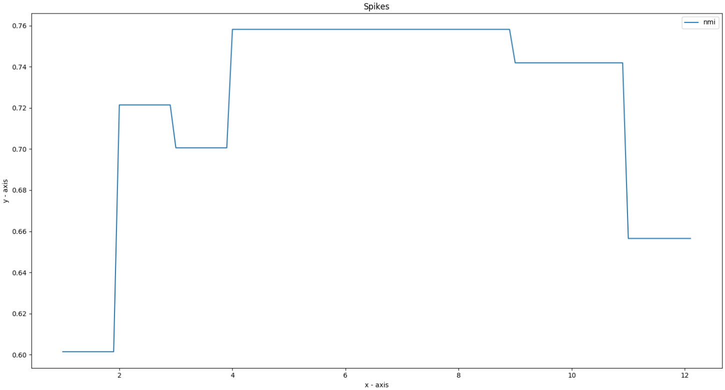
Custom Validation

- For each generated cluster label, we find the original cluster label that it maps to.
- We then find the accuracy of this mapping w.r.t. the clustering.

DP Means: No. of Clusters

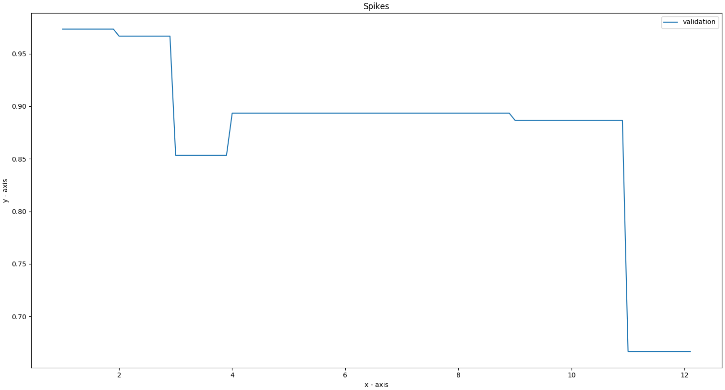


DP Means: NMI

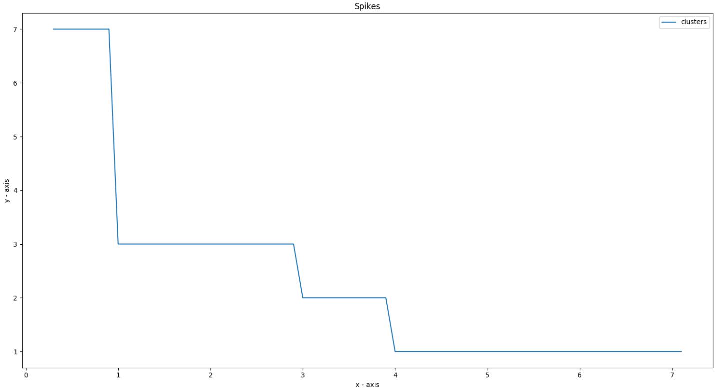


Spikes
nmi
0.76
0.74
0.72
0.70
0.68
0.66
0.64
0.62
0.60
y - axis
2
4
6
8
10
12
x - axis

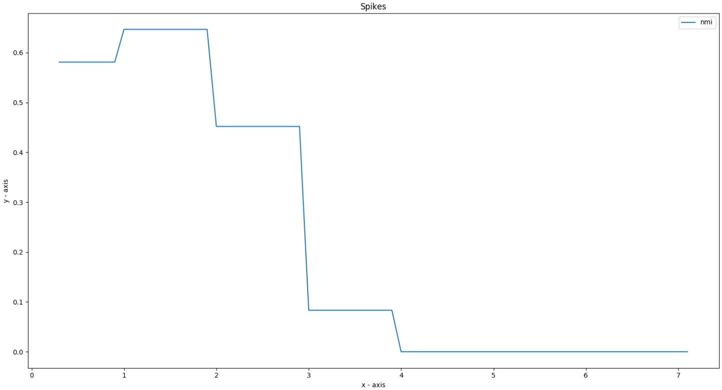
DP Means: Custom Validation



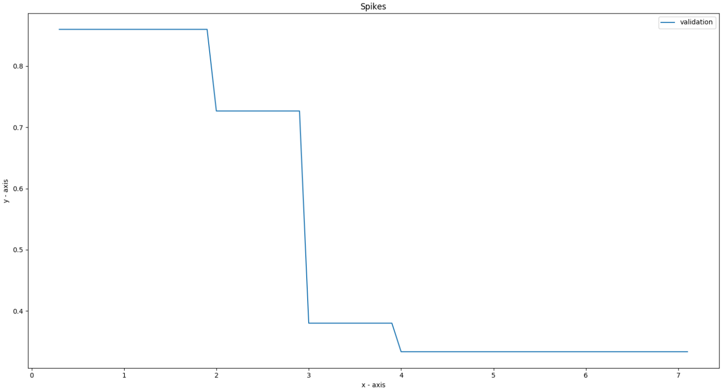
DP Means with Bregman Divergence: No. of Clusters



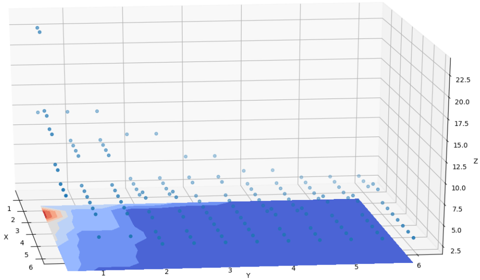
DP Means with Bregman Divergence: NMI



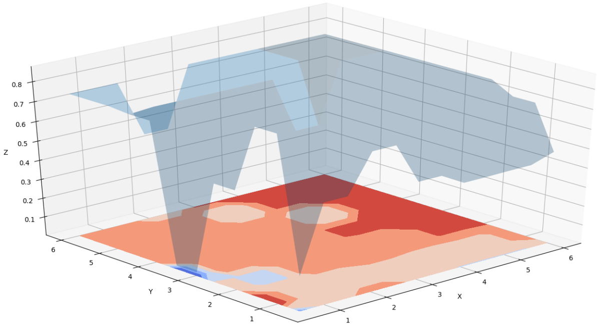
DP Means with Bregman Divergence: Custom Validation



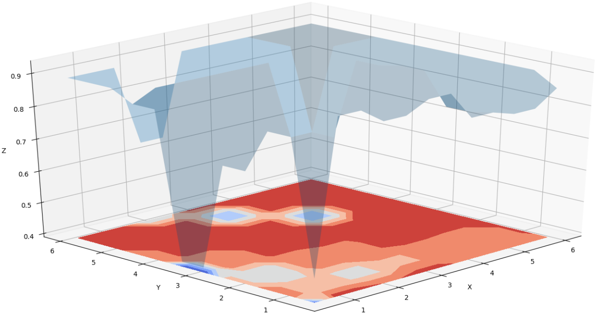
Hierarchical DP: No. of Clusters



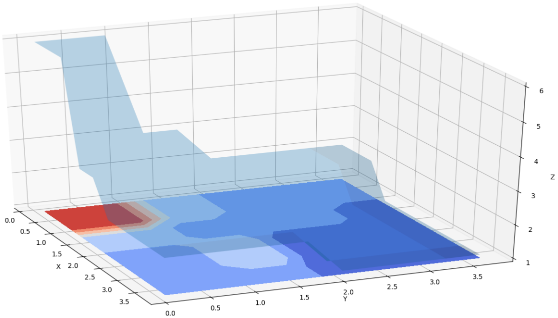
Hierarchical DP: NMI



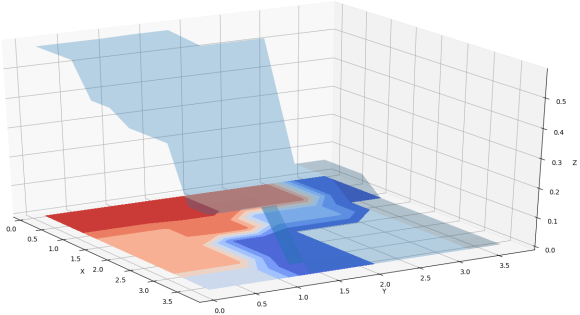
Hierarchical DP: Custom Validation



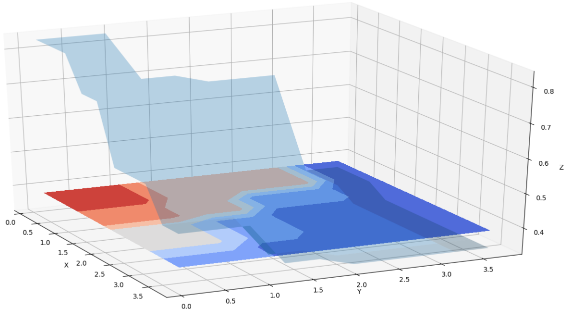
Hierarchical DP with Bregman Divergence: No. of Clusters



Hierarchical DP with Bregman Divergence: NMI



Hierarchical DP with Bregman Divergence: Custom Validation



Things learnt from Project

- Never (ever) code a ML model in C++ (unless absolutely required) :p
- Learnt the concepts of Dirichlet and Hierarchical Dirichlet Prior
- Learnt about Bregman Divergences
- Learnt how small variance asymptotics can be useful

Thank You ☺