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Pitman Yor Diffusion Trees for Bayesian Hierarchical Clustering

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IEEE Transactions on Pattern Analysis and Machine Intelligence,
Vol. 37, No. 2, February 2015

Presented by Robert McCartney and Jie Yuan

Pitman-Yor Diffusion Tree

Bayesian nonparametric prior over tree structures with arbitrary branching structure at each branch point to create an exchangeable distribution over data points

What?

- Nonparametric methods make no (or fewer) assumptions on the underlying probability distributions
- For instance, how many clusters are there?
- With k-means this is a parameter to the model
- Nonparametric methods want to let the data decide this

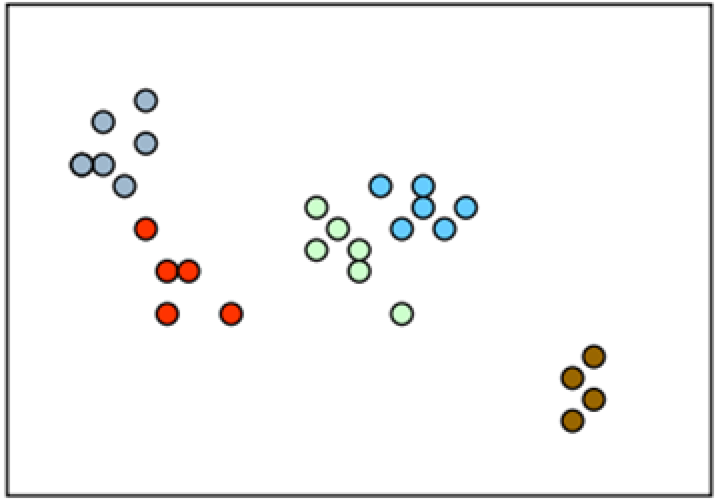


Figure from https://www.cs.cmu.edu/~kbe/dp_tutorial.pdf

Ok, go on..

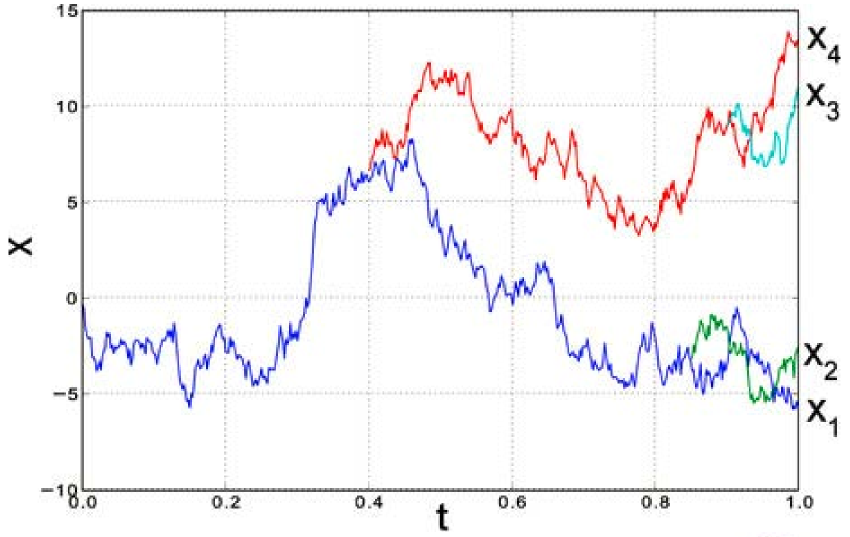
- Tree structures are used to hierarchically cluster the data
- They give interpretable results in data exploration stages
- They provide density estimations
- This is paper extends previous methods related to Dirichlet Diffusion Trees

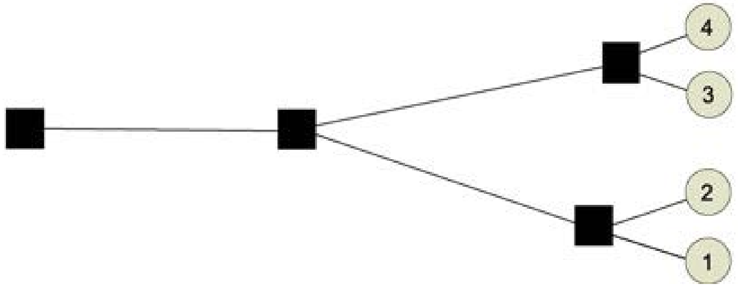
Dirichlet Diffusion Trees

- DDTs are like playing plinko
- Points start out following the path traced by previous points
- At each interval $\mathrm{dt} \in [0,1]$ the probability of diverging from current path with *m* datapoints having traveled it is:

$$\frac{a(t)dt}{m}, where\ a(t) = \frac{c}{1-t}$$

- Brownian motion with Gaussian distributions model the final destination of points

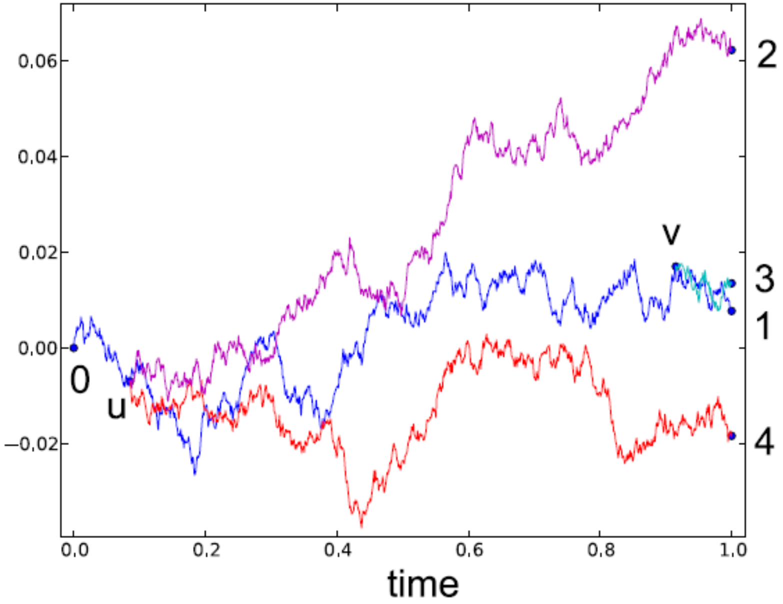


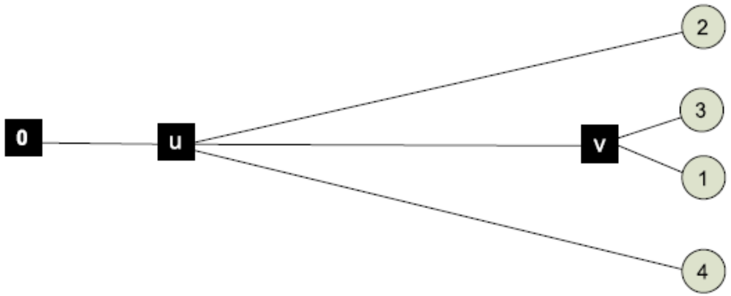


This paper - PYDT

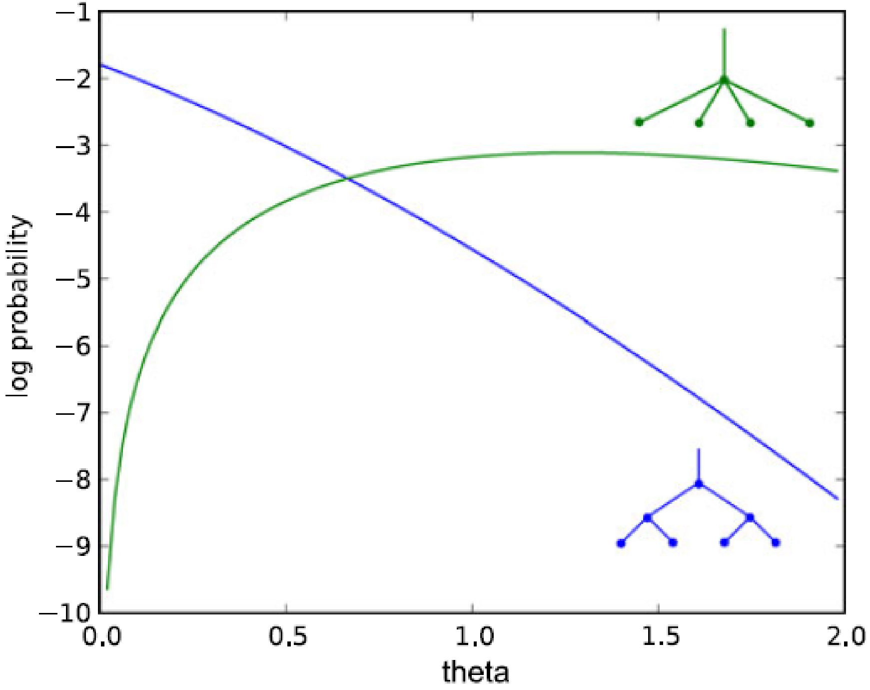
- <u>Arbitrary branching</u> means instead of binary there can be K branches
- Probability of following an existing path with n_k samples is $\frac{n_k - \alpha}{m+\theta}$ and diverging is $\frac{\theta + \alpha K}{m+\theta}$
- This sums to 1 since $\sum n_k = m$

- <u>Exchangeable distribution</u> means the probability of obtaining any given tree structure is invariant to reordering the data points
- This was proven in the paper





Recovering DDTs



- When $\theta = \alpha = 0$ this becomes a DDT
- θ determines branching behavior

You said no parameters

- The hyperparameters themselves $(\alpha, c, \theta, \sigma)$ are given prior distributions
- Markov Chain Monte Carlo is used to detach and reattach subtrees for thousands of iterations to maximize the tree’s marginal probability based off of the prior probabilities of the data
- Final tree is a density model of the joint distribution over the data and hyperparameters

Comparison to DDT

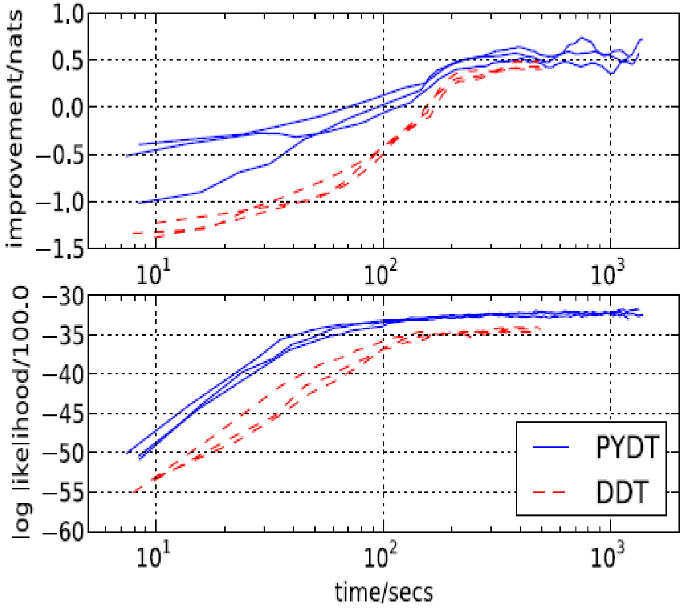


Fig. 11. Density modelling of the $D = 10, N = 200$ macaque skull measurement data set of [1]. *Top*: Improvement in test predictive likelihood compared to a kernel density estimate. *Bottom*: Marginal likelihood of current tree. The shared x-axis is computation time in seconds.

1. Moderate improvement in predictive performance

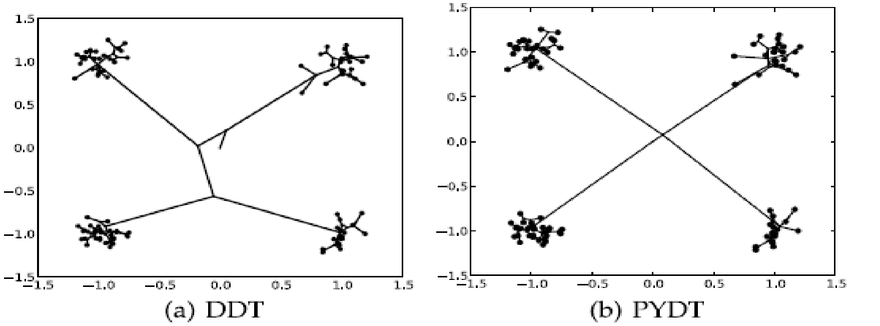


Fig. 10. Optimal trees learnt by the greedy EM algorithm for the DDT and PYDT on a synethic data set with $D = 2, N = 100$.

2. Improved interpretability through logical hierarchies

Questions

Backup slides

Dirichlet Process

Draw distribution G from DP(G0, alpha)
Draw observations x independently from G

xi|thetai ~ F(thetai)
thetai|G ~ G
G|alpha, H ~ DP(alpha, H)

(G(A1), … G(Ak) ~ Dir(alpha*H(A1), …
alpha*H(Ak))

Pitman Yor Diffusion Tree

Generalizes Dirichlet Diffusion Tree to allow arbitrary branching

probability of breaking from previous path is now a(t)Gamma(m-alpha)dt/Gamma(m+1+theta)

theta is concentration parameter (Dirichlet alpha)

When alpha = 0, Pitman Yor process reduces to CRP, but the more occupied tables, the more likely people will join new tables; tables with fewer people have less chance of getting more

At every branch point, go down existing path with prob (n_k - alpha)/(m + theta), but also diverge at branch point with prob (theta + alpha*K)/(m + theta) where K is existing #

Dirichlet Process (Chinese restaurant process)
- nonparametric selection of clusters given data

Dirichlet Diffusion Tree - generalization of
Dirichlet process (similar to CRP)

Pitman Yor Diffusion Tree (this paper) -
generalization of Dirichlet Diffusion Tree
(two parameter Chinese restaurant process vs

Chinese Restaurant Process

Each customer sits at a new table (K+1) with probability alpha/(alpha+n-1)

Customer sits at table k with probability n_k/(alpha+n-1)

each table represents a base distribution with some parameters

number of tables grows logarithmically with the data

http://blog.echen.me/2012/03/20/infinite-mixture-models-with-nonparametric-bayes-and-the-dirichlet-process/
http://www.gatsby.ucl.ac.uk/~ywteh/research/npbayes/dp.pdf