# A review of methods for Bayesian hierarchical clustering

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UCSD

# Background


Background
- Clustering
- Bayesian learning

Bayesian hierarchical clustering
- Coalescent models
- Diffusion models
- Inference

Adding interaction

Conclusion

# Unsupervised learning

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Finding low-dimensional representations of high-dimensional data

**Density estimation**

Estimating an underlying probability distribution given samples from the distribution

**Clustering**

Discovering natural groups in data

# Clustering

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$$\{1, 2, \ldots, N\} \rightarrow \{\{\ldots\}, \{\ldots\}, \ldots, \{\ldots\}\} \tag{1}$$

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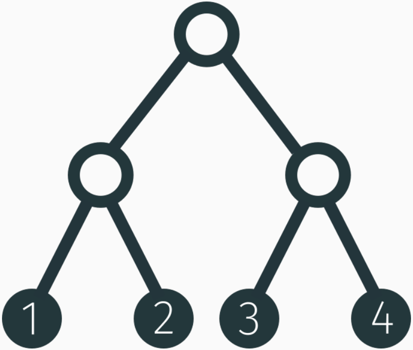
How do we pick $K$?

# Hierarchical clustering

In hierarchical clustering, data is recursively partitioned to form a tree (typically binary), also called a hierarchy.



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The tree is built by beginning with just singleton clusters (leaves) and iteratively merging them until we have one cluster (root)

**Divisive (top-down)**

The tree is built by beginning with a single cluster (root) and recursively partitioning it until we have just singleton clusters (leaves)

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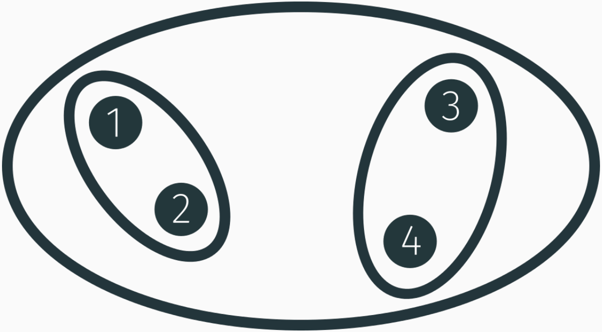


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# Agglomerative clustering examples

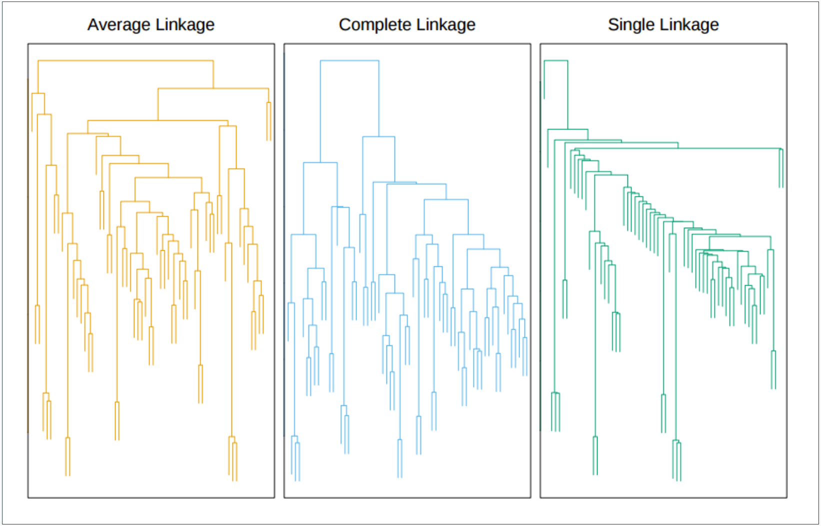


Figure 1: Trees produced by agglomerative clustering algorithms with different linkage criteria. Source: [1]

# Divisive clustering

In divisive clustering, we begin with the root cluster and recursively partition it until we are left with singleton leaf clusters.

## Approaches

- Use $k$-means recursively until only singleton clusters
- Define a similarity graph $G$ in terms of similarity function $s(x, x')$ and perform partitions by finding a minimum cut on $G$.

# Ambiguous data

Consider the two following scenarios where circles represent tight clusters of data.

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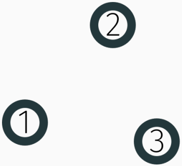
A single binary tree is not sufficient to describe either of these configurations.

# Multifurcating trees

Perhaps extending our binary trees to $k$-ary trees will help.

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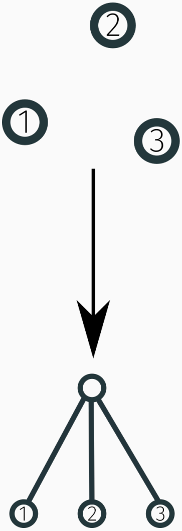


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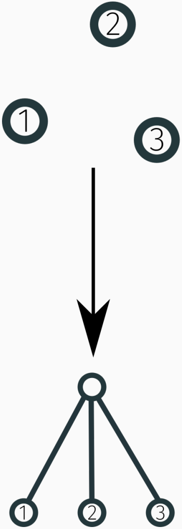


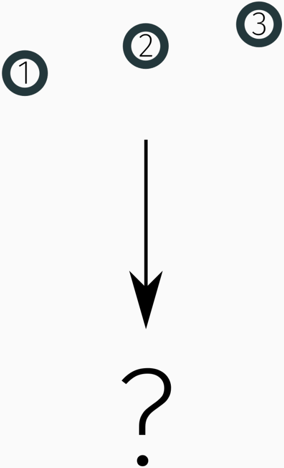

# Uncertainty in hierarchies

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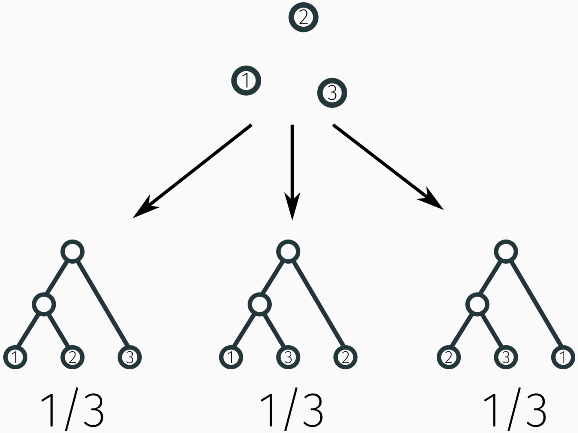

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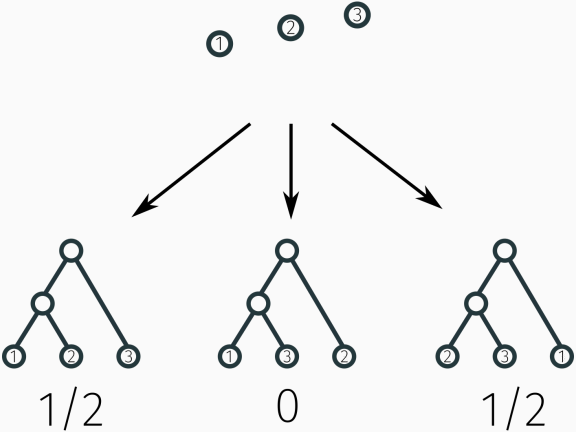

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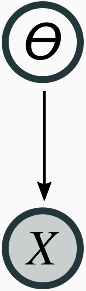

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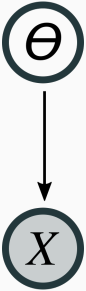


Our data $X$ is generated conditionally given a set of unobserved latent variables $\theta$.

# Distributions of interest

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$P(\theta)$ is called the prior distribution and $P(X|\theta)$ is called the likelihood model. They are specified beforehand.

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Otherwise, we usually approximate it with methods such as:

- Markov chain Monte Carlo (MCMC)
- Variational inference
- MAP estimation via EM

# Bayesian hierarchical clustering


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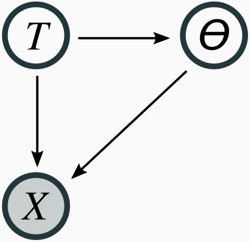


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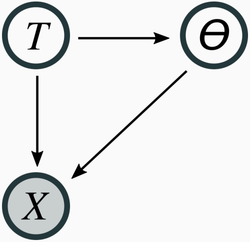
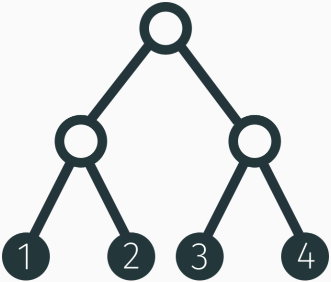



It is composed of data $X$ and latent variables $T$ and $\theta$.

- $T$ is a tree structure, sampled from a tree prior distribution $P(T)$.
- $\theta$ is a set of parameters, generated in a tree likelihood model $P(\theta | T)$.

# Tree priors

Most often we are interested in rooted binary trees with labeled leaves, also called cladograms.

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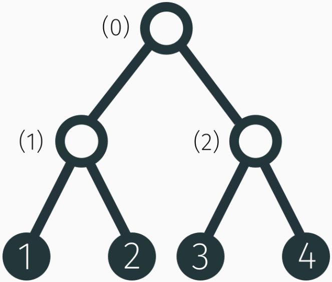


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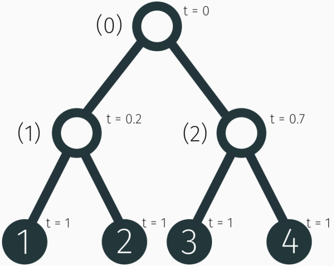


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- An ordering on the internal nodes
- Times associated with each node

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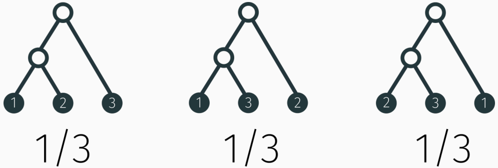

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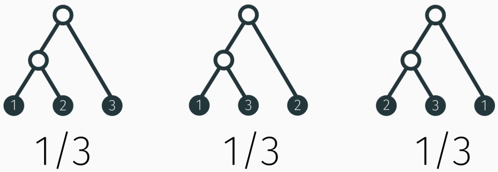


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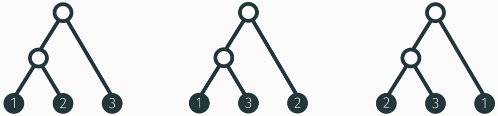


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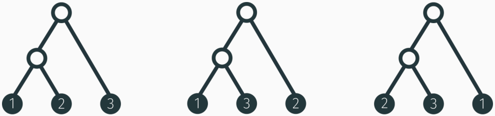


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**Coalescent models**

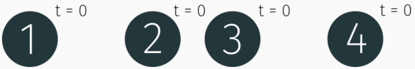
Trees are modeled in an agglomerative fashion, merging clusters until one is left

**Diffusion models**

Trees are modeled inductively, starting with a tree of size $1$ and growing it to a tree of size $N$.

# Coalescent models

Coalescent models begin with a set of $N$ data, or "individuals", at $t = 0$.



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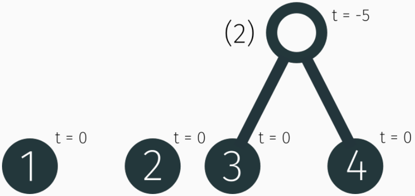


Every iteration, we:

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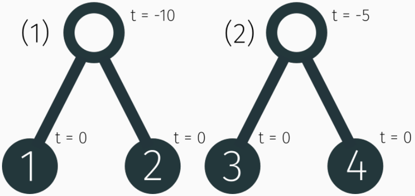


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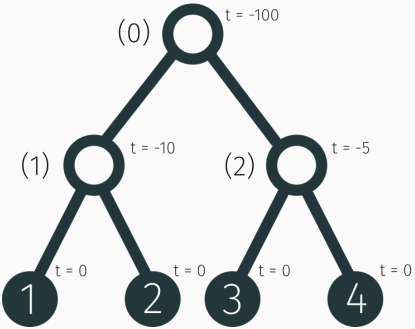


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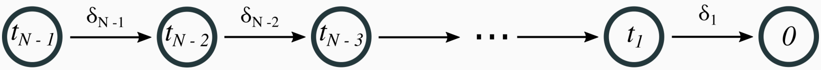

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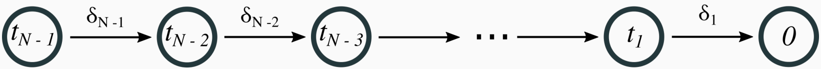


Let $\delta_i$ represent the elapsed time between coalescent event $i-1$ and $i$. We let

$$\delta_i \sim \mathrm{Exp}\left(\binom{N-i+1}{2}\right) \tag{4}$$

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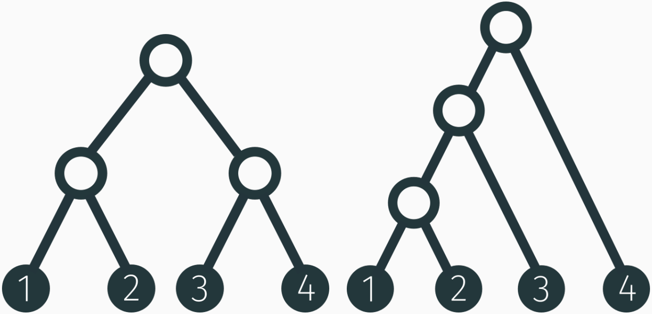
- What sort of trees does Kingman's coalescent favor?



# Diffusion models

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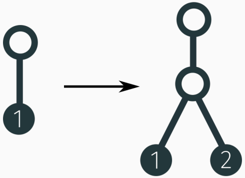

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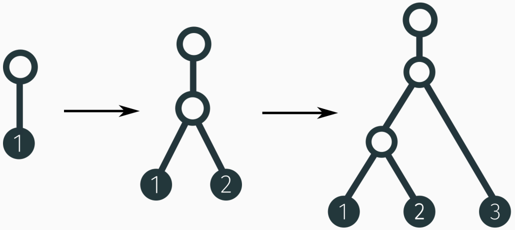

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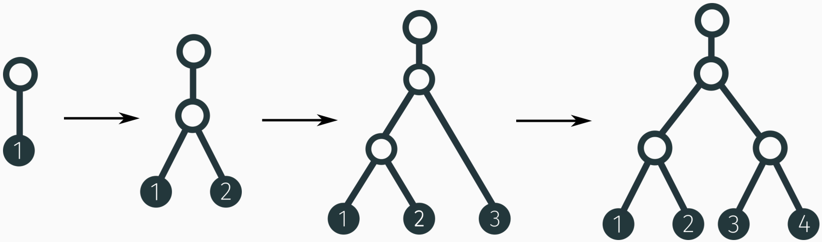

# Dirichlet diffusion tree

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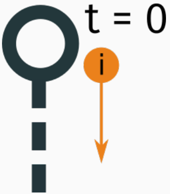
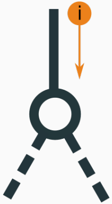



On each iteration, a particle labeled $i$ begins at the root and travels downwards.

**Case 1:** The particle reaches an internal node.



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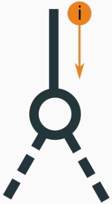


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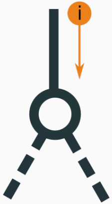


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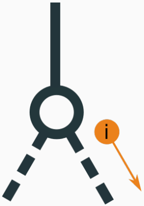

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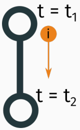
**Case 2:** The particle *diverges* on its current branch, creating an internal node and a leaf according to an acquisition function, $a(t)$.



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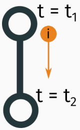


Let $m$ be the number of past particles that have traversed the current branch. The probability of diverging at time $dt$ is $a(t)dt/m$.

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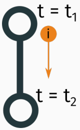


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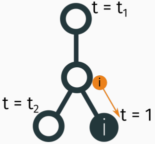

# Dirichlet diffusion tree

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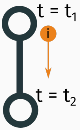


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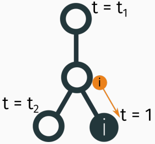


If $a(1) = \infty$, each particle is guaranteed to diverge before $t = 1$.

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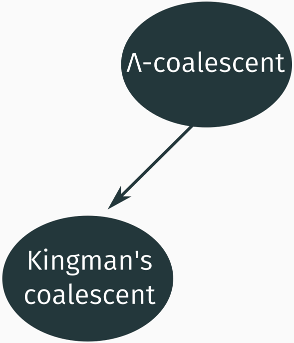

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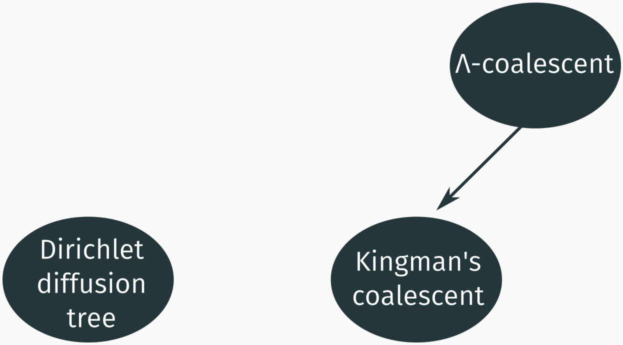

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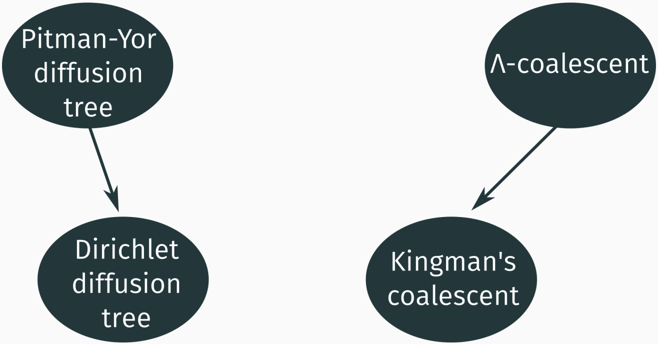

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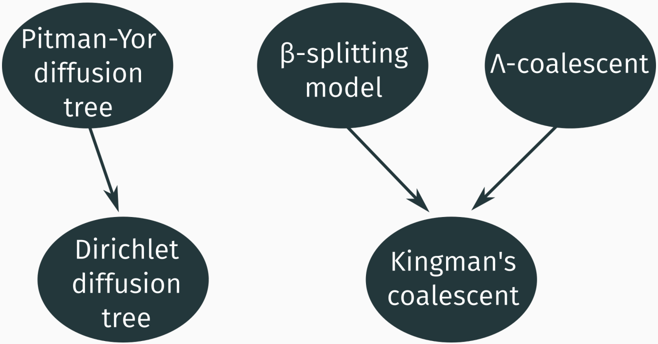

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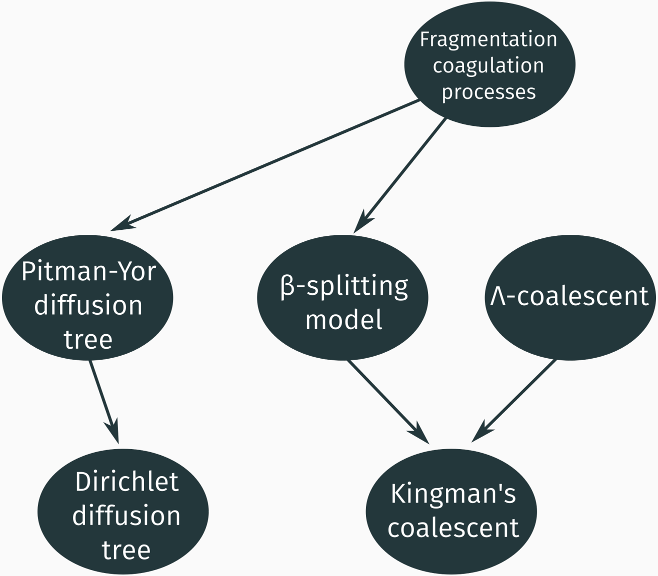

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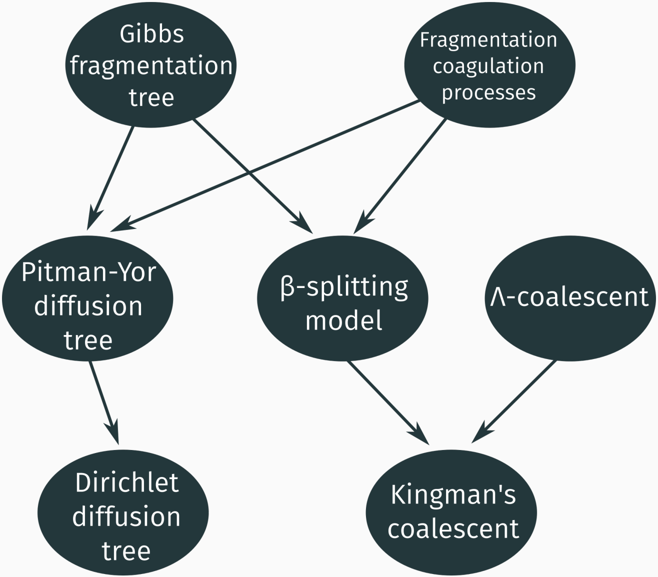

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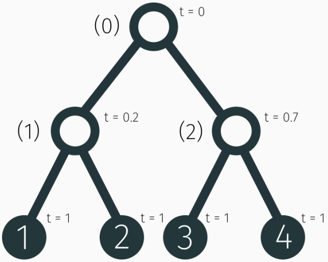

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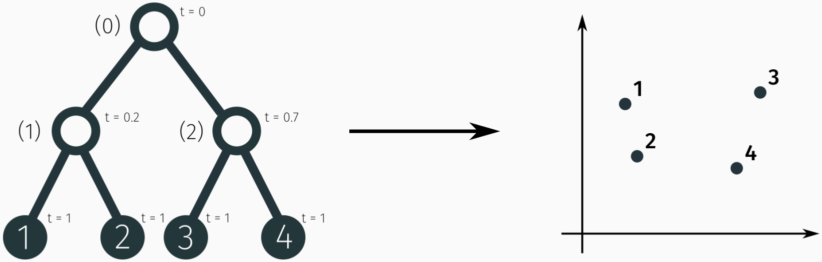

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For every internal node in the tree $n$ we associate a latent parameter $\theta_n$ which is in the same space as the data.

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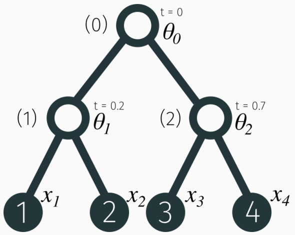


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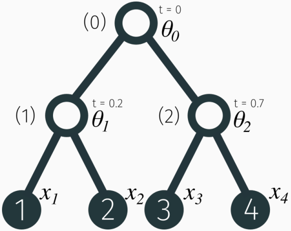


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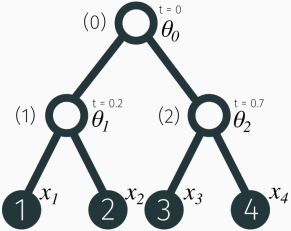


We then define:

- A prior distribution $P_0(\theta)$
- A transition kernel $T(\theta'|\theta)$

# Example likelihood models

The most common likelihood model is Brownian motion, also called Gaussian diffusion, which is

$$P_0(\theta) = \mathcal{N}(0, \sigma_0^2 I) \tag{5}$$

$$T(\theta'|\theta) = \mathcal{N}(\theta, \sigma^2(t - t')), \tag{6}$$

where $t$ and $t'$ are the times associated with nodes $\theta$ and $\theta'$ and $\sigma_0^2$ and $\sigma^2$ are hyperparameters.

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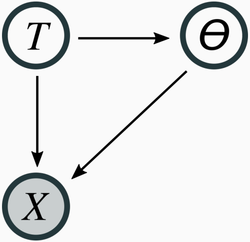
Other options are:

- Multinomial-Dirichlet diffusion: useful for categorical data
- Multinomial diffusion: useful for counts (such as bag-of-words)

Recall the latent variable model.



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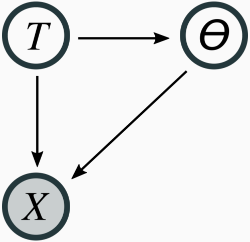


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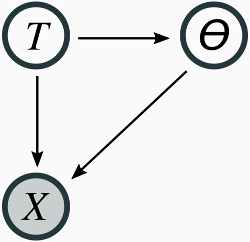


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We generally use approximate methods. In this report, we'll focus on a particular sampling method.

# Metropolis-Hastings

The Metropolis-Hastings (MH) algorithm is an MCMC method that uses samples from a distribution $p(x)$ to approximate it.

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## Metropolis-Hastings algorithm

- Given initial distribution $p_0(x)$ and proposal distribution $q(x'|x)$
- Instantiate $x_0$ by sampling $p_0(x)$.
- Repeat for $t = 1 \dots T$
    - Sample $x'$ from $q(x'|x_{t-1})$.
    - Calculate acceptance ratio

$$\alpha = \frac{p(x')q(x_t|x')}{p(x_t)q(x'|x_t)} \tag{7}$$

    - If $\alpha > 1$, accept the sample, setting $x_t = x'$
    - If $\alpha \leq 1$, accept $x'$ with probability $\alpha$ and reject otherwise, setting $x_t = x_{t-1}$.

# Sampling latent variables

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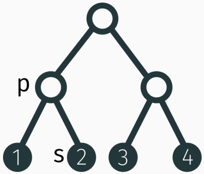

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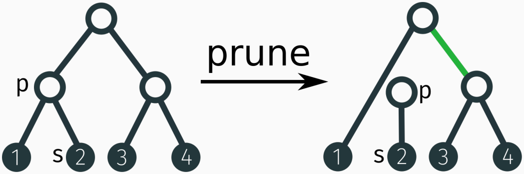

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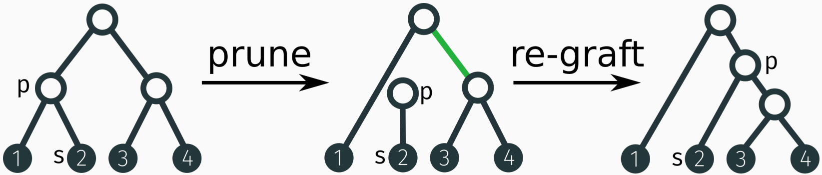

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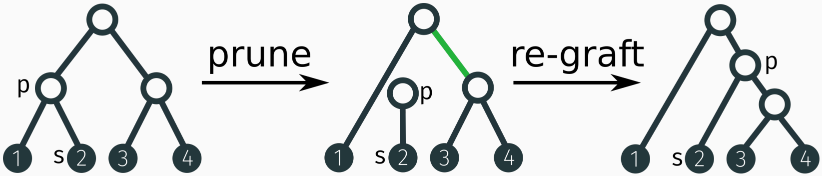



**Parameter proposal:** Gibbs sampling or marginalization

# Adding interaction

Background
- Clustering
- Bayesian learning

Bayesian hierarchical clustering
- Coalescent models
- Diffusion models
- Inference

Adding interaction

Conclusion

## Why interaction?

Recall the motivating example for Bayesian hierarchical clustering.

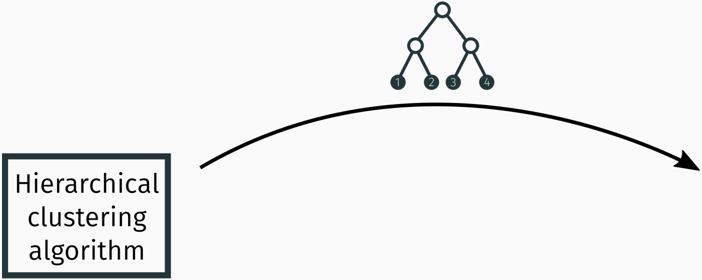

Could a user provide feedback and help decide which hierarchy makes the most sense?

- Interactive Bayesian Hierarchical Clustering - Vikram and Dasgupta (2016) [5]

# Interactive hierarchical clustering

Hierarchical clustering algorithm

# Interactive hierarchical clustering



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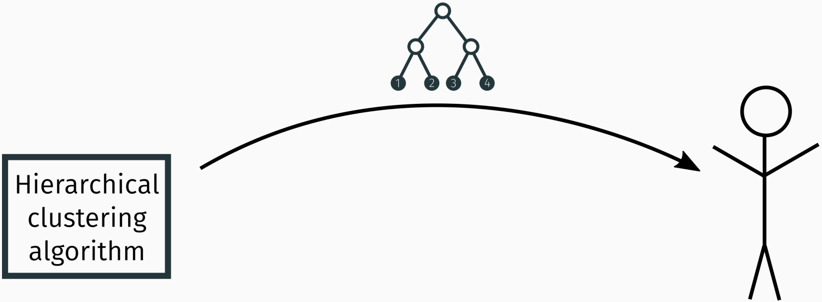

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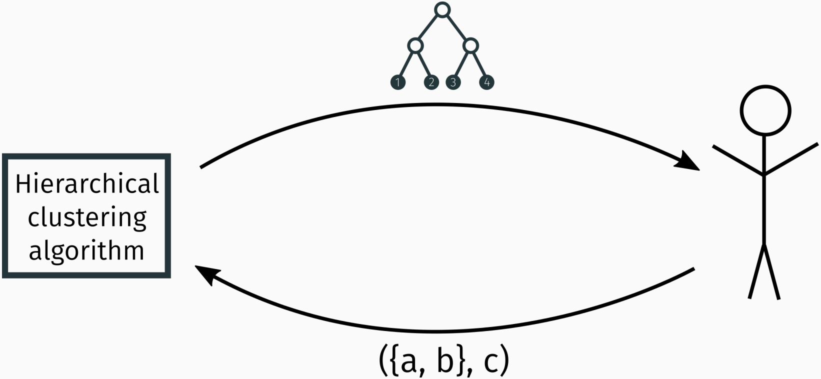

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To enforce constraints, we use a modified SPR move that avoids regraft branches that violate constraints.

**Intelligent subset queries**

We pick subsets of data that have high variance, which we can measure using samples.

# Results

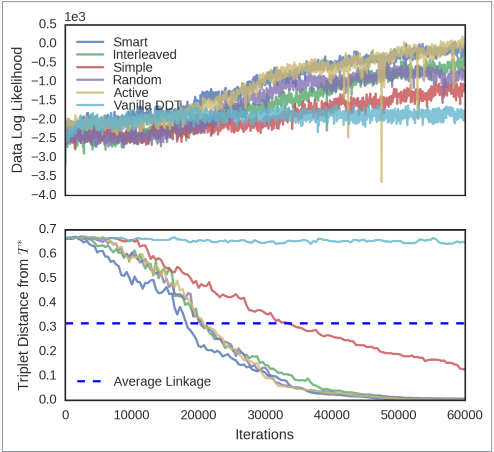


**Figure 2:** The results of interactive Bayesian hierarchical clustering on a dataset of zoo animals. Pictured are the data log likelihood and percentage of triplets satisfied for several subset querying methods. Source: [5]

# Conclusion

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- Bayesian hierarchical clustering (BHC) is a general framework in unsupervised learning that naturally handles ambiguity and uncertainty in data.
- BHC models can be decomposed into prior distributions on trees, and likelihood models. Tree priors can further be decomposed into coalescent and diffusion models.
- Inference in BHC can be performed with MCMC methods like Metropolis-Hastings using the subtree-prune and regraft move.
- BHC enables incorporating user interaction into hierarchical clustering.

# Future work

- How can we improve on interactive Bayesian hierarchical clustering? Robust constraints, more tree priors, other measures of variance

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- **What is the effect of interaction in Bayesian problems?** constrained posterior distributions, complexity of inference
- **How can we extend interactive methods to other domains?** metric learning, deep learning, embeddings

Questions?

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- Marginalizing out the time is easy, since it's generated independently. Node ordering is not so easy.
- The number of possible node orderings for a given unordered binary tree with $N$ leaves is

$$\frac{(N-1)!}{\prod_{i=1}^{N-1} m_i} \tag{8}$$

where $m_i$ is the number of internal nodes in the subtree indexed by $i$.

# TMC vs. Kingman's coalescent

Consider an ordered cladogram $\phi$ and an unordered cladogram $\psi$, both with $N$ leaves.

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- Kingman's coalescent and TMC favor balanced trees!

# The $\Lambda$-coalescent

- The $\Lambda$-coalescent generalizes Kingman's coalescent to both multifurcating trees and more complex distributions over times [6].

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- Rather than $\delta_i \sim \mathrm{Exp}\left(\binom{N-i+1}{2}\right)$, we have

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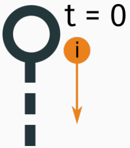
- When $\Lambda$ is the Dirac delta and $k = 2$, we have Kingman's coalescent.

# Pitman-Yor diffusion tree

The DDT has been extended to multifurcating trees with the Pitman-Yor diffusion tree (PYDT) [7].

The $i$-th particle behaves slightly differently, but starts in the same way.



# Pitman-Yor diffusion tree

**Case 1:** The particle reaches an internal node that has $b$ branches already.

# Pitman-Yor diffusion tree

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It picks the $k$-th branch with probability

$$\frac{m_k - \beta}{m + \alpha} \tag{11}$$

where $m_k$ is the number of past particles that have traversed the $k$-th branch, $m$ is the total number of particles that have traversed this subtree, and $\alpha$ and $\beta$ are hyperparameters.

# Pitman-Yor diffusion tree

**Case 2:** The particle reaches an internal node that has $b$ branches already.

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**Case 2:** The particle reaches an internal node that has $b$ branches already.


It creates a new branch with probability

$$\frac{\alpha + \beta b}{m + \alpha} \tag{12}$$

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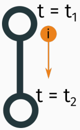

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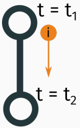


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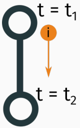


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$$\frac{a(t)\Gamma(m-\beta)dt}{\Gamma(m+1+\alpha)} \tag{13}$$

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We can easily enforce triplet constraints in Bayesian hierarchical clustering.

During inference, we use MH with a modified SPR proposal called the constrained-SPR proposal which will only select regraft branches that don't violate a set of triplet constraints.

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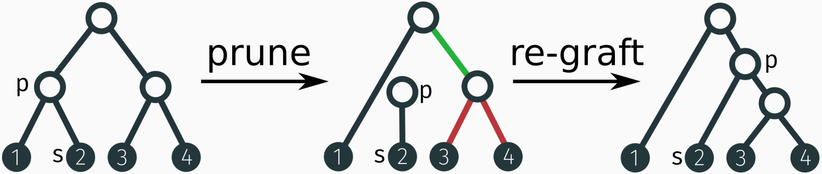

# Intelligent subset queries

The simplest way to select a subset of data to show the user is random selection, we can use the Bayesian framework to choose better subsets.

In BHC, we compute a posterior distribution over trees given data. Using the posterior, we can estimate the variance of various regions of the tree and show the user the region with the most variance.

**Definition: tree distance variance (TDV)**

Given a subset of data $S$ and tree samples $\mathcal{T} = T_1, \ldots, T_N$,

$$\mathrm{TDV}(S, \mathcal{T}) = \max_{i,j \in S} \mathrm{Var}_{T \in \mathcal{T}} \left[ \texttt{tree-dist}_{T|S}(i, j) \right] \tag{14}$$

where $\texttt{tree-dist}_T$ is the number of edges needed to get from leaf $i$ to leaf $j$ in tree $T$.

We now instantiate several random subsets and show the user the one with the highest TDV.