ETHZ Computational Biology Seminar: Convergence and curvature of phylogenetic Markov chains

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(joint work with Alexei Drummond,
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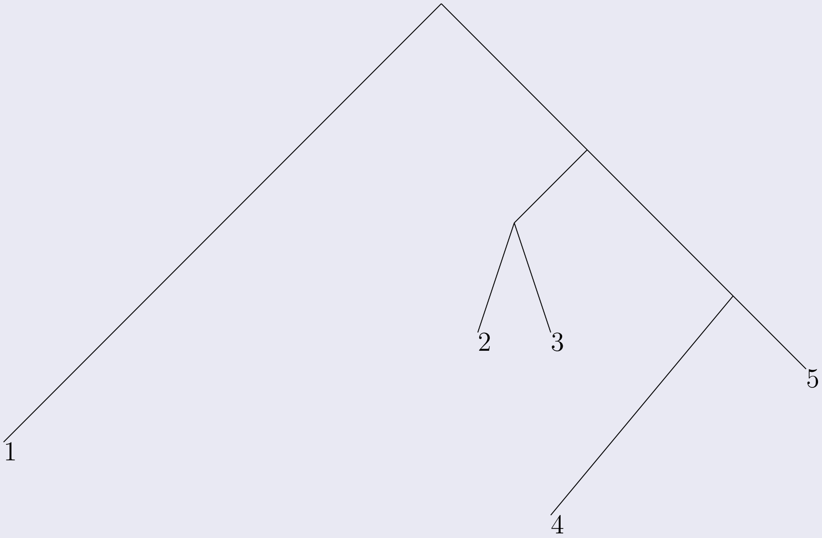
THE UNIVERSITY OF AUCKLAND
NEW ZEALAND

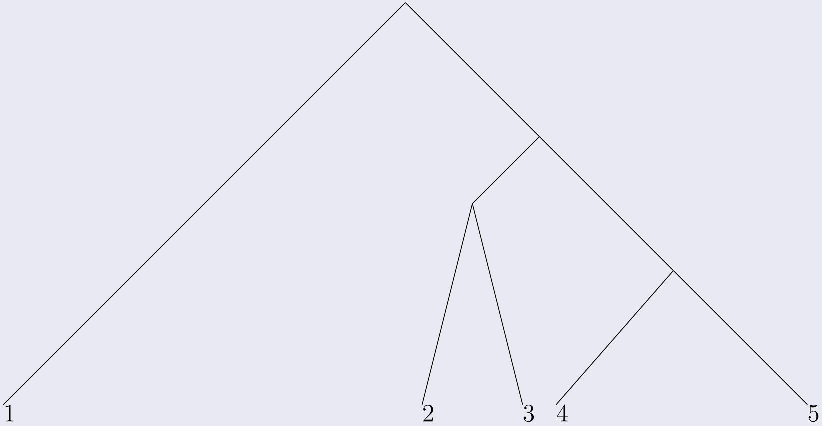
Rooted phylogenetic tree

Definition



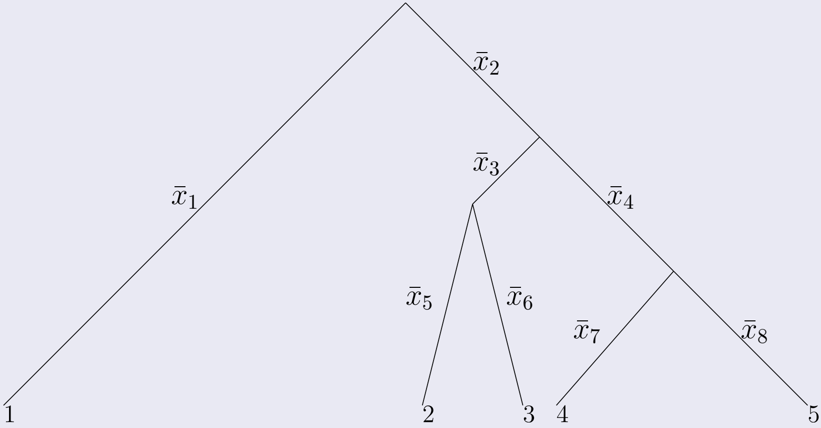
Equidistant (ultrametric) phylogenetic tree

Definition



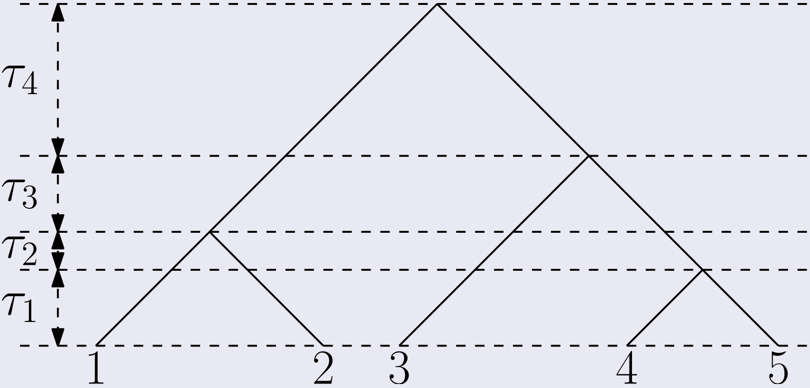
Equidistant phylogenetic tree with parameters

Definition

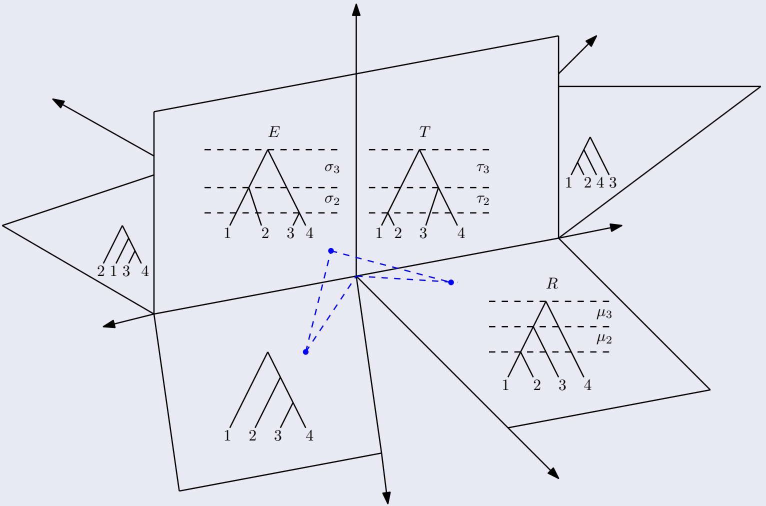


τ-parameterisation

Definition

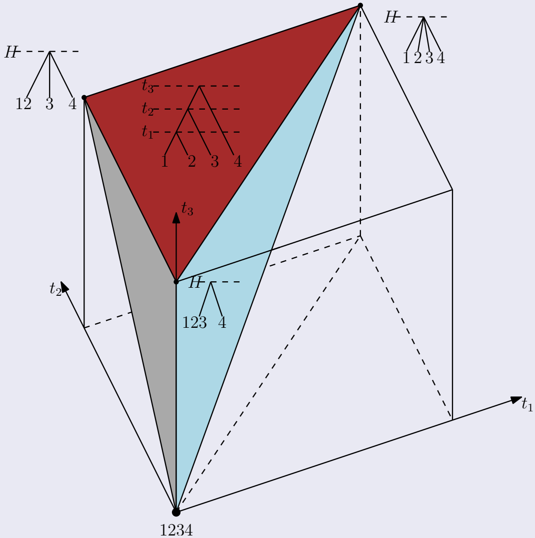


Definition



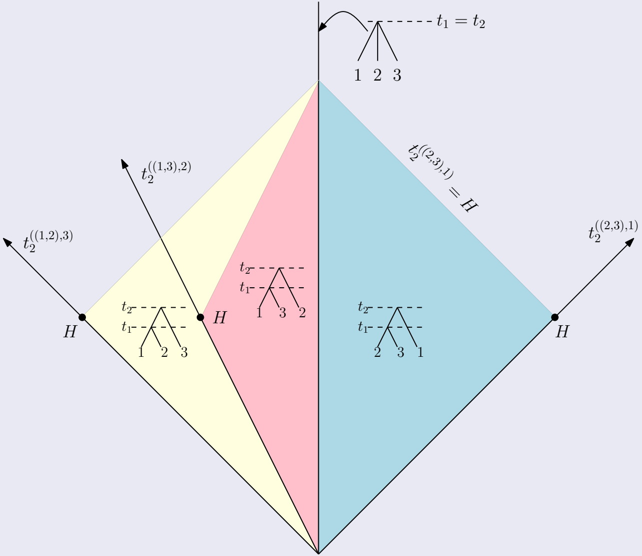
t-parameterisation

Definition



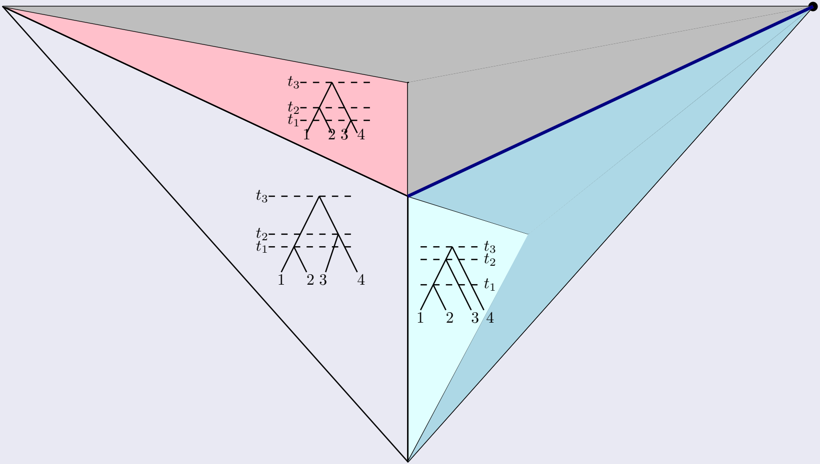
t-space

Definition



t-space

Definition



Motivation

1. Bayesian MCMC: Mixing rate, access time, efficient proposals.
2. Summarising posterior: No need to introduce several random variables on different probability spaces, no need to fit inconsistent data together.
3. Interesting algorithmic/data structures problems: How to solve NP-complete problems on real computers for real data (Chris and Erick can compute SPR-distance).
4. Interesting geometries: "Every new example of a non-trivial simplicial complex of non-positive curvature is a big deal."

Nice metric spaces

Definition

A metric space is called *nice* if most statisticians would like it.

Examples of nice metric spaces include real line, Euclidean space, and its nice subspaces.
Examples of not nice metric spaces include all non-measurable subsets of a Euclidean space, all nowhere dense subsets of a Euclidean space, and most importantly the spaces where it is hard to define a random variable.

Theorem (Billera, Holmes, and Vogtmann [2001])

The space of phylogenetic trees is a nice space.

Theorem (G and Drummond [2015])

The space of equidistant phylogenetic trees is a nice space.

Parameterisation matters!

Theorem (G and Drummond [2015])

t*-space is not so nice.*

Parameterisation matters!

Theorem (G and Drummond [2015])

t-*space is not so nice.*

More formally

Definition

A geodesic metric space is called *nice* if it is a convex path-connected subspace of a computable metric space with unique geodesics of the same dimension.

Theorem (G and Drummond [2015])

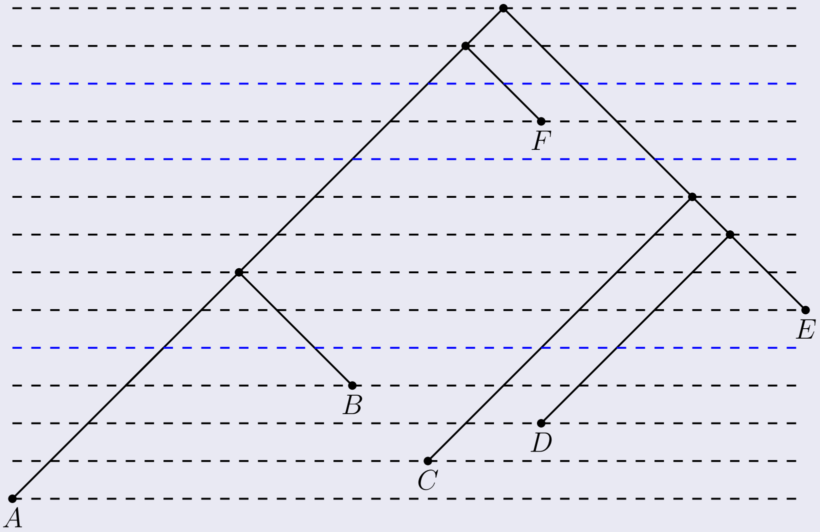
τ-*space is an efficiently computable cubical complex with unique geodesics.*

Theorem (G and Drummond [2015])

t-*space is a simplicial complex with unique geodesics.*

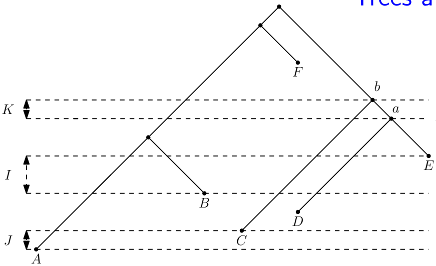
Discrete time-trees

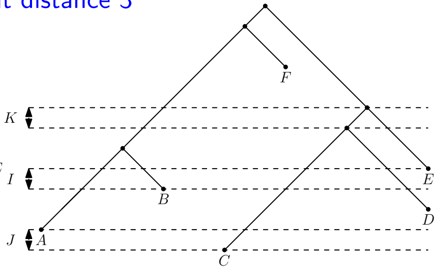
Definition (Discrete time-tree)



Discrete time-tree space

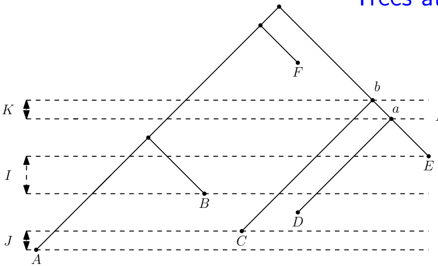
Trees at distance 3

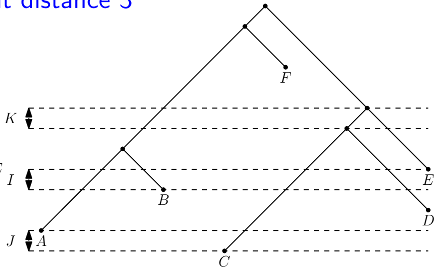




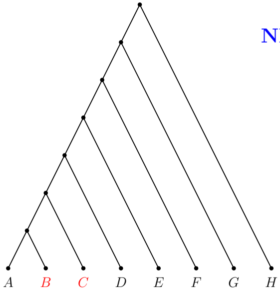
Discrete time-tree space

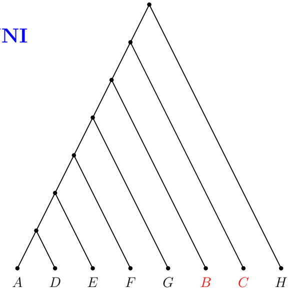
Trees at distance 3





NNI vs rNNI





Ricci-Ollivier curvature

Definition (Ollivier [2009])

Let $(\mathcal{T}, d)$ be a metric (tree) space with a random walk

$$m = (m_T)_{T \in \mathcal{T}}.$$

Let $T, R \in \mathcal{T}$ be two distinct points (trees). The Ricci-Ollivier curvature of $(\mathcal{T}, d, m)$ along $\overrightarrow{TR}$ is

$$\kappa_m(T, R) = 1 - \frac{W(m_T, m_R)}{d(T, R)},$$

where $W(\cdot\,, \cdot)$ is the earth mover's distance.

In a nutshell

Negative VS positive

$$\kappa_m(T,R) \leq 0 \iff W(m_T, m_R) \geq d(T,R)$$

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Take-home message

Negative curvature is bad.

Curvature of Markov chains on graphs

Theorem (Ollivier [2009])

If $(\mathcal{T}, d)$ is a geodesic space then curvature is a local property.

Definition

Let $(\mathcal{T}, d)$ be a graph with a Markov chain m.Then the *curvature of the Markov chain m* on the graph $\mathcal{T}$ is the greatest number χ_m such that

$$\chi_m \leq \kappa_m(T, R) \text{ for adjacent } T \text{ and } R.$$

Trivial observation

Under a distance-one random walk, the following is true for any finite metric d and any pair of points T, R:

$$\frac{-2}{d(T,R)} \leq \kappa(T,R) \leq \frac{2}{d(T,R)}.$$

Random walks

For now, we consider three simplest random walks on various phylogenetic tree spaces.

- Metropolis-Hastings random walk: Choose a tree from the one neighbourhood and accept it with probability $\min(1, \frac{|N_1(T_{old})|}{|N_1(T_{new})|})$.
- Uniform random walk.
- Uniform p-lazy random walk, where p is the laziness probability.

Lower bounds

Theorem (G, Whidden, Matsen [2015])

Let T and R be adjacent trees. Then both the asymptotic curvature of the space with p-lazy uniform random walk and the curvature of the space with uniform random walk are at least

$$\kappa(T,R) \geq \frac{-n^2+2n}{3.5n^2-15n+16} \geq -2/5 \qquad \textit{in } \mathrm{r}SPR \textit{ space},$$

$$\kappa(T,R) \geq -\frac{4}{n-1} \qquad \textit{in } \mathrm{DtT} \textit{ space},$$

$$\kappa(T,R) \geq -\frac{4}{n-2} \qquad \textit{in } \mathrm{NNI} \textit{ space},$$

$$\kappa(T,R) \geq -\frac{8}{n-1} \qquad \textit{in } \mathrm{rNNI} \textit{ space}.$$

The bounds are tight.

Upper bounds

Theorem (G, Whidden, and Matsen [2015])

Let T and R be adjacent trees. Then the curvature of the following spaces with uniform random walk satisfy

$$\kappa(T,R) \leq \frac{6n-17}{3n^2-13n+14} \qquad \textit{in } \mathrm{rSPR} \textit{ space,}$$

$$\kappa(T,R) \leq \frac{1}{2(n-1)} \qquad \textit{in } \mathrm{DtT} \textit{ space,}$$

$$\kappa(T,R) \leq \frac{1}{2(n-2)} \qquad \textit{in } \mathrm{NNI} \textit{ space, and}$$

$$\kappa(T,R) \leq \frac{1}{n-1} \qquad \textit{in } \mathrm{rNNI} \textit{ space.}$$

The bounds are tight.

Life is good, at infinity

Theorem (G, Whidden, and Matsen [2015])

Let $\{T_n \mid n \in \mathbb{N}\}$ *and* $\{S_n \mid n \in \mathbb{N}\}$ *be two sequences of phylogenetic trees such that* $d(T_n, R_n) = 1$ *for all* n*. Then*

$$\lim_{n\to\infty} \kappa_n(T_n, S_n) = 0$$

*for the uniform random walk on the SPR graph**, *the* NNI *graph, the* rNNI*-graph, and the* DtT*-graph.*

*For the SPR graph, we have to bound the size of the subtree which is getting moved.

Whidden and Matsen [2015]

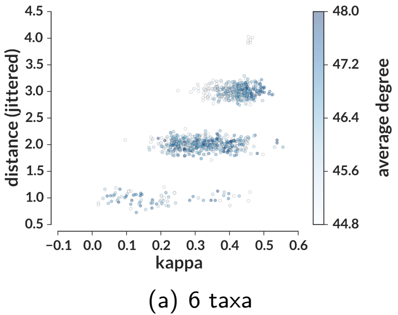

Figure: Scatter plot of $\kappa(\mathrm{MH}; T_1, T_2)$ values versus $d_{SPR}(T_1, T_2)$ for the rSPR graph. Colour displays the average degree of T_1 and T_2. Distance values randomly perturbed ("jittered") a small amount to avoid superimposed points.

Take-home message

$$1.001^{10000} = 21916.68\ldots$$

BUT

$$0.999^{10000} = 0.000045\ldots$$

Take-home message

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BUT

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- The curvature of basic random walks is normally positive.
- Although the spaces flatten out when the number of taxa n grows, there always are negatively curved pieces.
- Importantly, the number of those pieces grows with n.

Thank you for your attention!

- Yann Ollivier
  Ricci curvature of Markov chains on metric spaces
  J. Functional Analysis, 256, 3, 810–864, 2009
- Alex Gavryushkin and Alexei Drummond
  The space of ultrametric phylogenetic trees
  arXiv preprint arXiv:1410.3544, 2014
- Chris Whidden and Frederick A. Matsen IV
  Quantifying MCMC exploration of phylogenetic tree space
  Systematic Biology, doi:10.1093/sysbio/syv006, 2015
- Chris Whidden and Frederick A. Matsen IV
  Ricci-Ollivier curvature of two random walks on rooted phylogenetic subtree-prune-regraft graph
  To appear in the proceedings of the *Thirteenth Workshop on Analytic Algorithmics and Combinatorics*, 2015
- Alex Gavryushkin, Chris Whidden, and Frederick A. Matsen IV
  Random walks over discrete time-trees
  To appear on the *arXiv*, 2015
- `https://github.com/gavruskin/tauGeodesic`
- `https://github.com/gavruskin/tTauCurvature`