# AWC Anual Meeting: Convergence and curvature of phylogenetic Markov chains

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21st October 2015

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# Motivation

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### Answer

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**Answer**

*I don't know*

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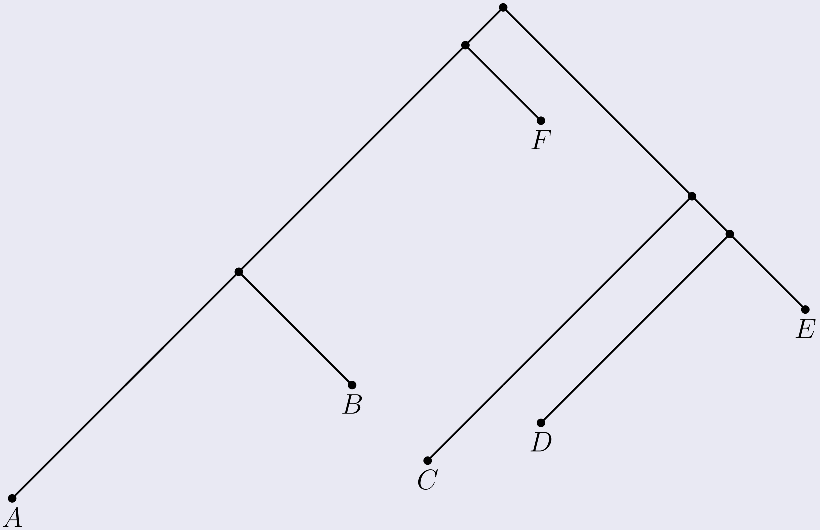
**Answer**

*I don't know geometry well.*

# Discrete time-trees

## Definition (Ranked tree topology)



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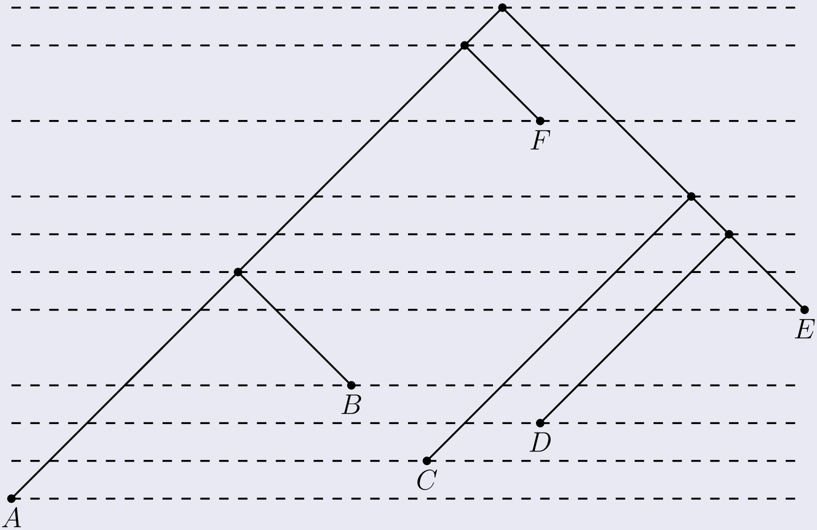

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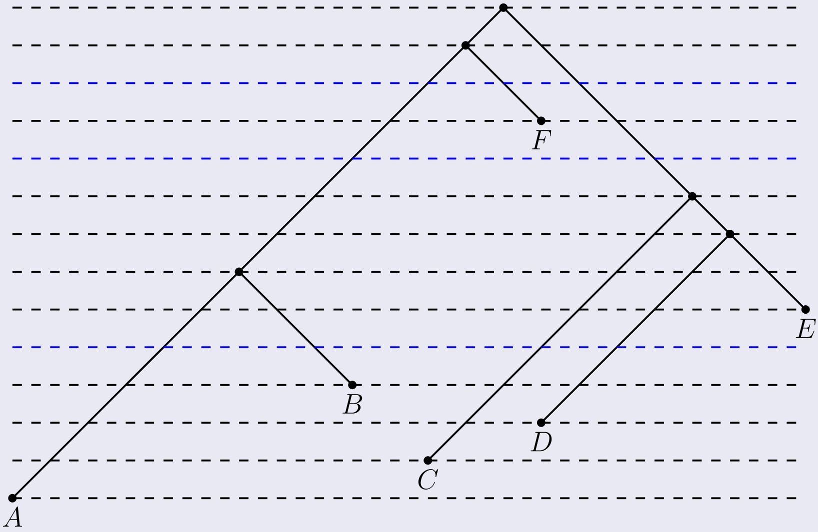
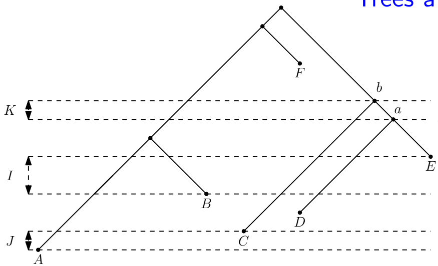
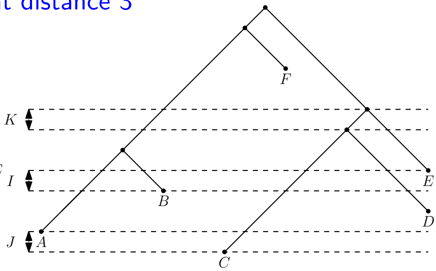


# Discrete time-tree space

## Trees at distance 3



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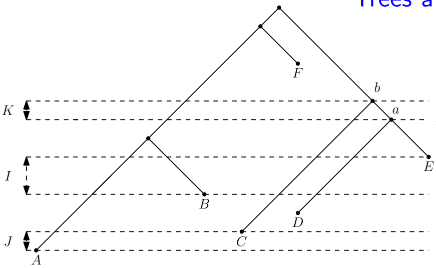
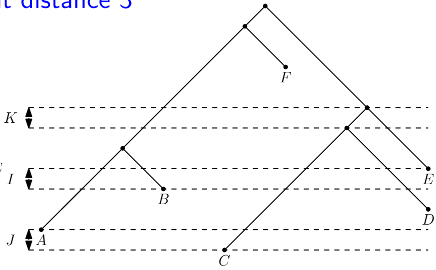
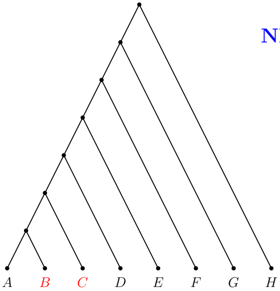
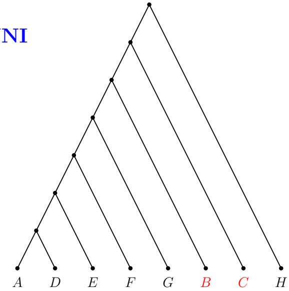



## NNI vs rNNI



# 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 $\chi_m$ 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*

$$
\begin{aligned}
\kappa(T,R) &\geq \frac{-n^2+2n}{3.5n^2-15n+16} \geq -2/5 && \textit{in } \mathrm{rSPR} \textit{ space,} \\
\kappa(T,R) &\geq -\frac{4}{n-1} && \textit{in } \mathrm{DtT} \textit{ space,} \\
\kappa(T,R) &\geq -\frac{4}{n-2} && \textit{in } \mathrm{NNI} \textit{ space,} \\
\kappa(T,R) &\geq -\frac{8}{n-1} && \textit{in } \mathrm{rNNI} \textit{ space.}
\end{aligned}
$$

*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*

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

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

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

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

*The bounds are tight.*

# Life is good, at infinity

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

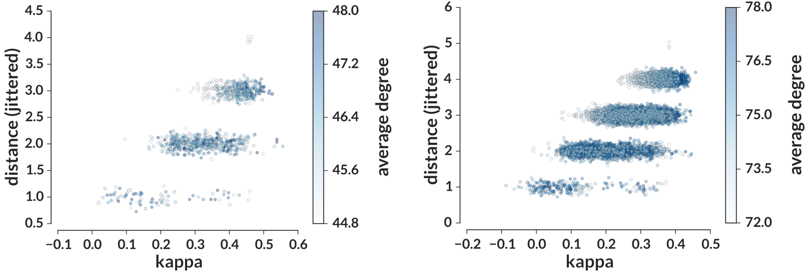
*Let* $\{T_n \mid n \in \mathbb{N}\}$ *and* $\{S_n \mid n \in \mathbb{N}\}$ *be two sequences of phylogenetic trees such that* $d(T_n, R_n) = 1$ *for all* $n$*. Then*

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

*for the uniform random walk on the SPR graph**, *the NNI graph, the* $\tau$*-graph, and the discrete* $\tau$*-space.*

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

# Whidden and Matsen [2015]




(a) 6 taxa (b) 7 taxa

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

# 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

Alex Gavryushkin
`https://github.com/gavruskin/tTauCurvature`