# Tree distances under random walks on tree spaces

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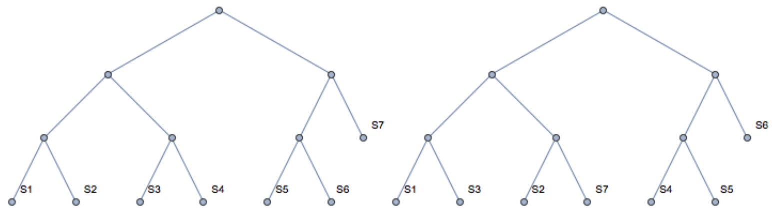
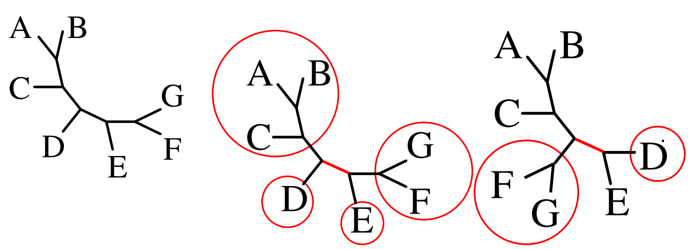
# Distances between phylogenetic trees

- Given two trees (rooted or unrooted) on the same set of leaves (taxa), to what extent to they differ?

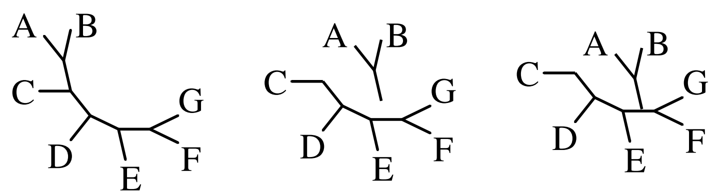



- Metrics on trees: Nearest Neighbor Interchange (NNI), Robinson-Foulds (RF) $\Delta$, Subtree-Prune-Regraft (SPR), Tree Bisection and Reconnection (TBR), Billera-Holmes-Vogtmann (BHV), ...

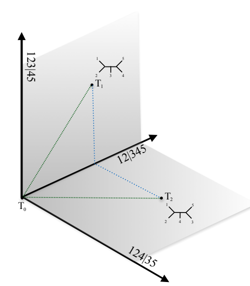
Nearest neighbor interchange move at edge between D and E:



Subtree-prune-regraft move at edge between subtree containing AB and the rest of the tree:



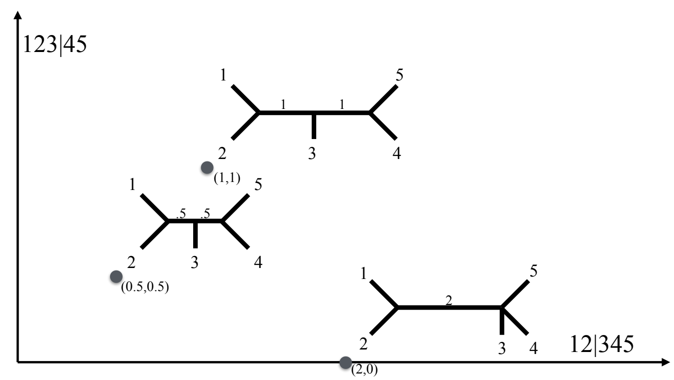
# Trees as Vectors




| | 1 \| 2345 | 2 \| 1345 | 3 \| 1245 | 4 \| 1235 | 5 \| 1234 | 12 \| 345 | 13 \| 245 | 14 \| 235 | 15 \| 234 | 23 \| 145 | 24 \| 135 | 25 \| 134 | 34 \| 125 | 35 \| 124 | 45 \| 123 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $T_0 = (1, 2, 3, 4, 5)$ | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $T_1 = ((1, 2), (3, (4, 5))$ | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| $T_2 = ((1, 2), (4, (3, 5))$ | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |

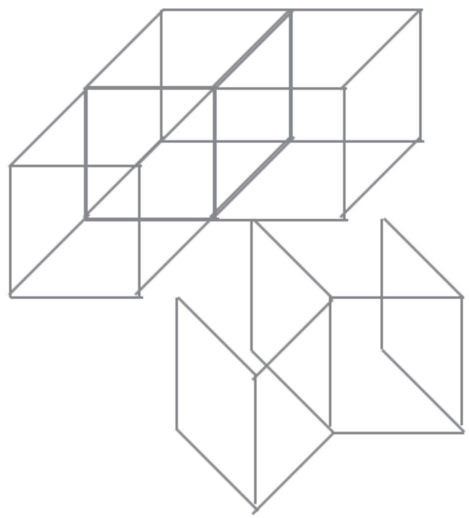
## Billeara-Holmes-Vogtmann space

- Trees on fixed *n* taxa, edge lengths positive reals
- Edges to leaves have fixed length 1
- Form a space with a metric which is locally Euclidean



## Billera-Holmes-Vogtmann treespace

- Adjacency of orthants: two orthants of dimension $k$ share a face of dimension $l$ if they have $l$ edges in common.
- Gives gluing of orthants to obtain space



## Geodesics in treespace

- Piecewise Euclidean segments in a sequence of orthants
- Many cells to consider
- First algorithms exponential
- Polynomial-time algorithm of order $O(n^4)$ of Owen-Provan (2011) uses incompatibility graph of edges to compute which edges to drop and introduce successively.
- Owen-Provan algorithm foundational for computing means, interpolations, variances, principal components, ...

## Random walks in tree spaces

Typical search algorithm:

- Generate a set of random trees
- Score them with respect to some optimality criterion
- Take the best or some of the best
- Perturb these trees with some local adjustments
- Take the best scoring and repeat.

## Random walks in tree spaces

Effectiveness of this process depends upon

- How well random walks visit regions of tree space
- How well hill-climbing works
- Length of process

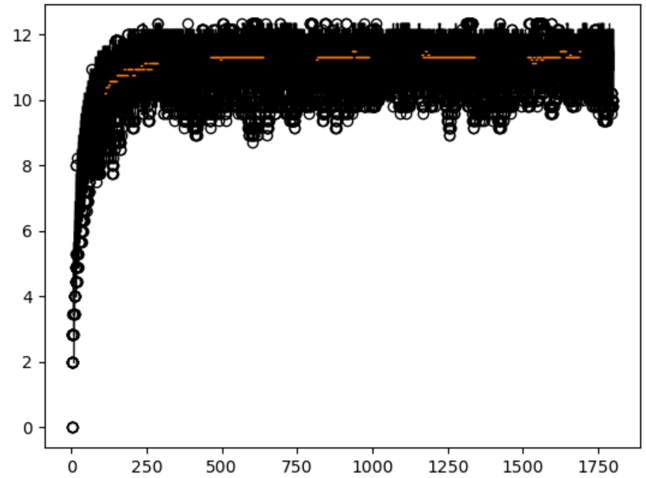
## Random walks in treespace

- Randomly generate an initial tree $T_0$.
- Select a location to perform a move (NNI, SPR) at random
- Apply move to get $T_{i+1}$
- Iterate to get sequence $\{T_0, T_1, T_2, \dots\}$

Look at BHV distances from $T_0$, gives sequence $d_i = d(T_0, T_i)$
Sequence of trees of generally increasing distance- how long until essentially $T_i$ is unrelated to $T_0$?

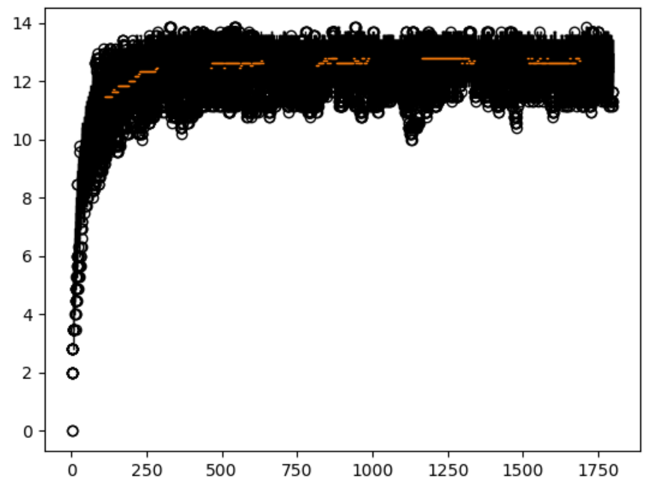
## Distances as walk lengthens

- Example: compute distance from an initial tree of size 40 under random NNI walks:



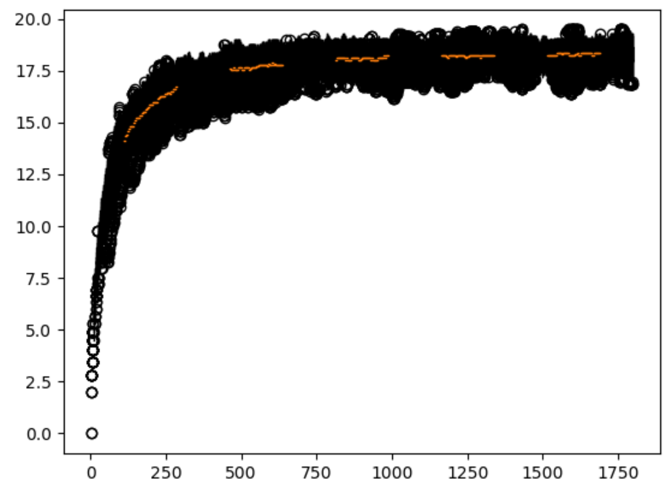
## Distances as walk lenghtens

- Example: compute distance from an initial tree of size 50 under random NNI walks:



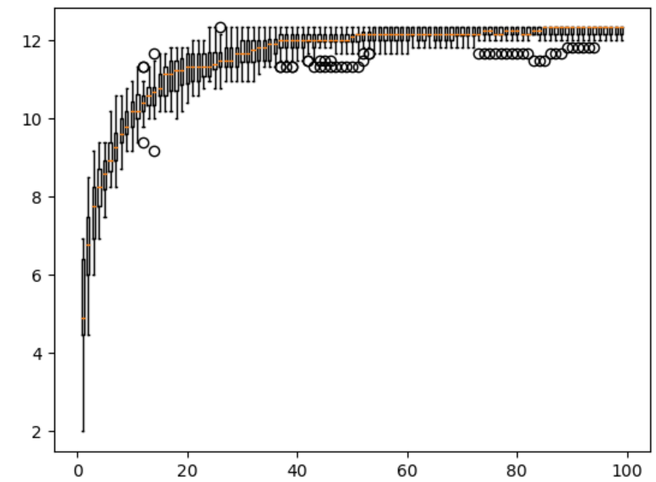
## Distances as walk lengthens

- Example: compute distance from an initial tree of size 100 under random NNI walks:



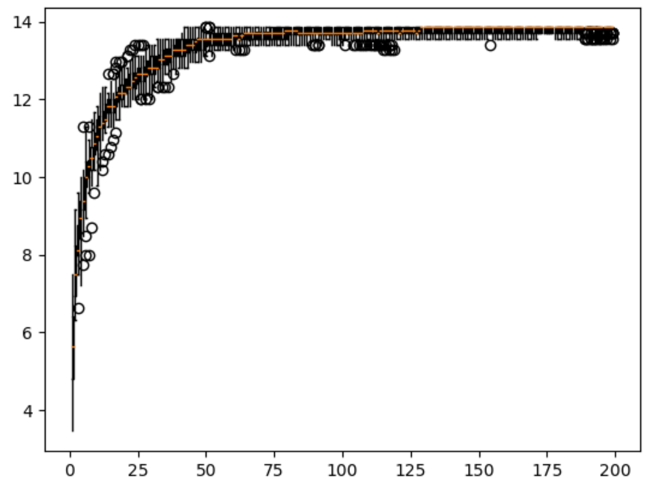
## Distances as walk lengthens

- Example: compute distance from an initial tree of size 40 under random SPR walks:



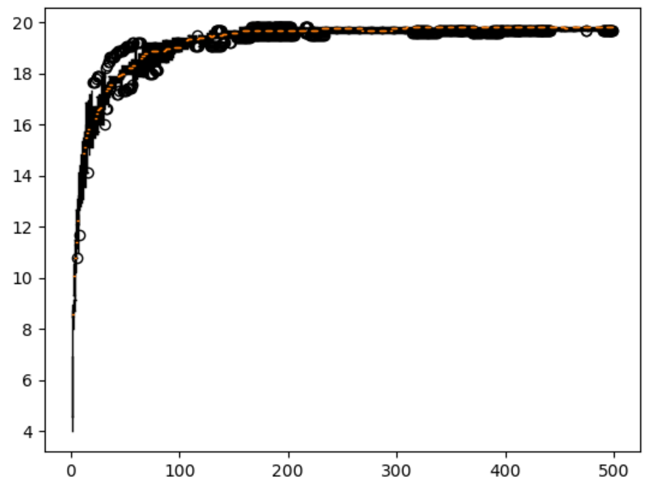
## Distances as walk lenghtens

- Example: compute distance from an initial tree of size 50 under random SPR walks:



## Distances as walk lengthens

- Example: compute distance from an initial tree of size 100 under random SPR walks:



## Walk for mixing

Observations:

- Diameter of treespace is $n$ for both NNI and SPR.
- Neighborhoods larger for SPR than NNI ($n^2$ vs. $n$.)
- These are for undirected random walks
- Walks used for searching are generally directed by optimality criterion

## Walk duration to lose initial information

Observations:

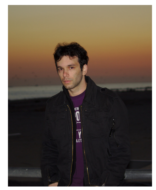
- Seems to grow about linearly with size of tree.
- Faster for SPR than NNI
- NNI can reverse earlier progress away from $T_0$ more readily than SPR
- Coupon-collecting arguments give $n \log n$ bound for all edges to be affected
- Don't need complete coupon collecting as random trees may have some common edges already.

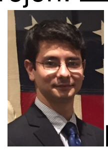
## Other results:

Observations:

- For weighted trees (edge lengths Poisson distributed, for example) similar behavior
- Random walks with weighted edges- selecting an edge equally or proportional to weight, similar behavior
- NNI moves mixing rate not known even for ordered trees (rotation moves)
- In edge length one case, time to a maximally distant tree (distance $2\sqrt{n-2}$) seems to grow as $n \log n$.

## Contributors

Alejandro Morejon: 

Roland Maio:  Haris Nadeem: 

Treespace Working Group:

sites.google.com/site/treespaceworkinggroup/