Tree distances under random walks on tree spaces

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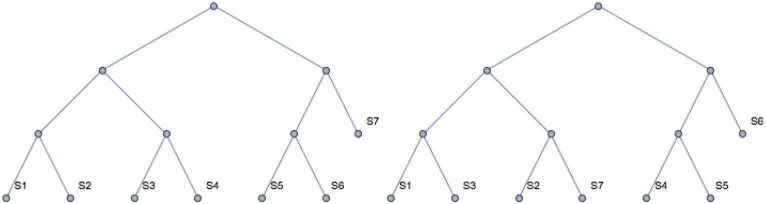
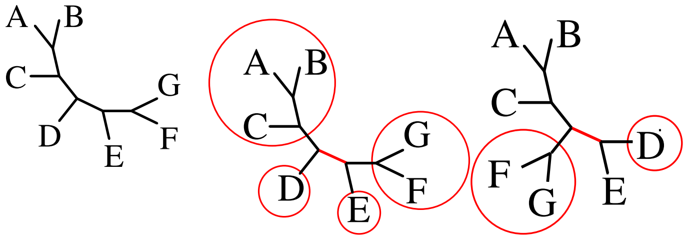
Distances between phylogenetic trees

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

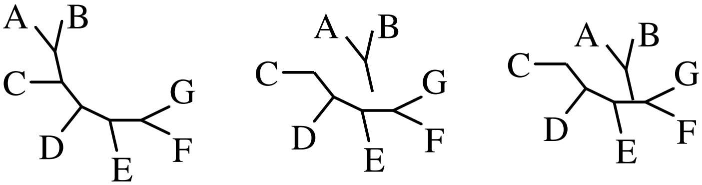


- Metrics on trees: Nearest Neighbor Interchange (NNI), Robinson-Foulds (RF) Δ, Subtree-Prune-Regraft (SPR), Tree Bisection and Reconnection (TBR), Billera-Holmes-Vogtmann (BHV), ...

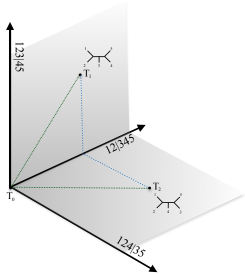
Nearest neighbor interchange move at edge between D and E:



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



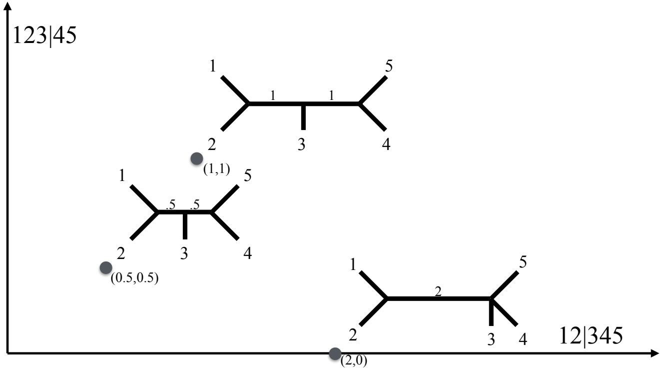
Trees as Vectors



	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

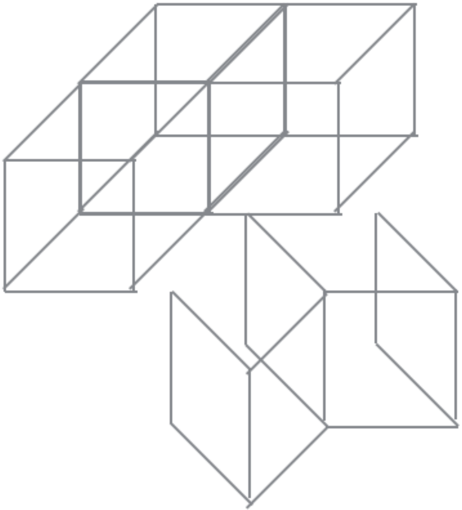
Billeara-Holmes-Vogtmann space

- 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

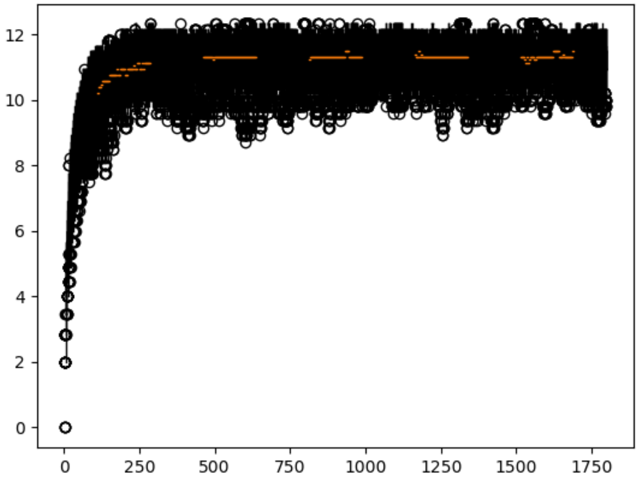
Random walks in treespace

- 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?

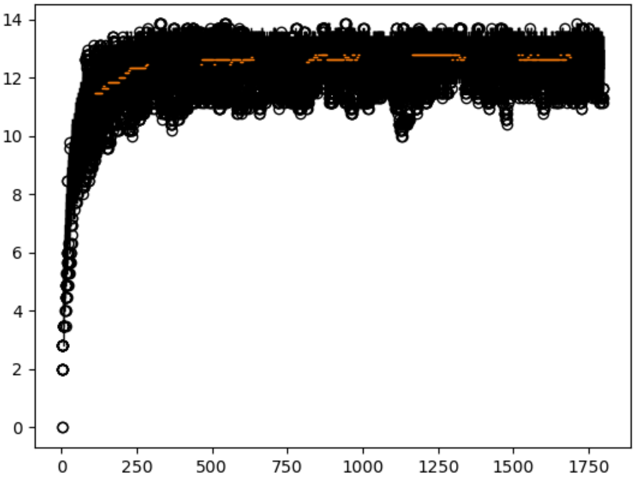
Distances as walk lengthens

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



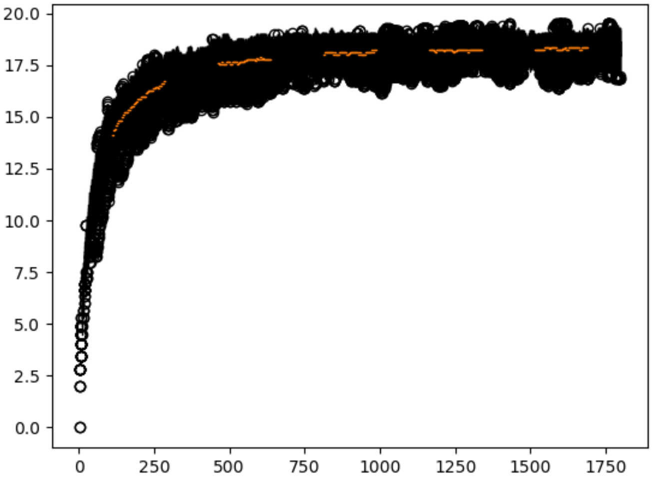
Distances as walk lenghtens

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



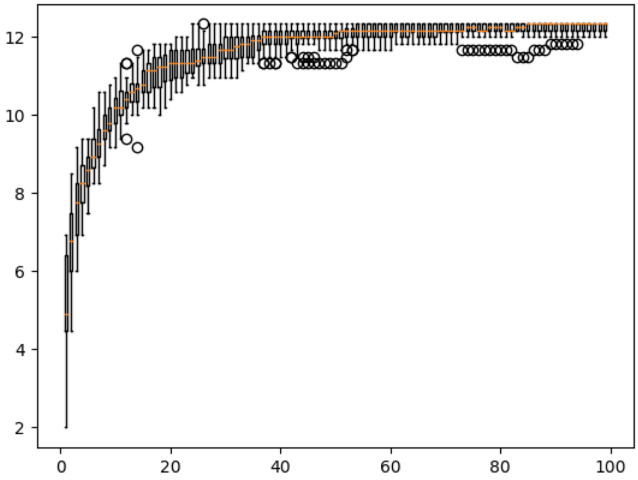
Distances as walk lengthens

- 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

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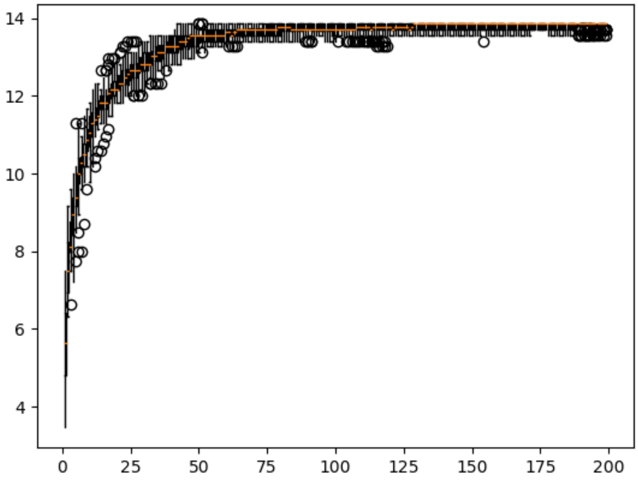

Distances as walk lengthens

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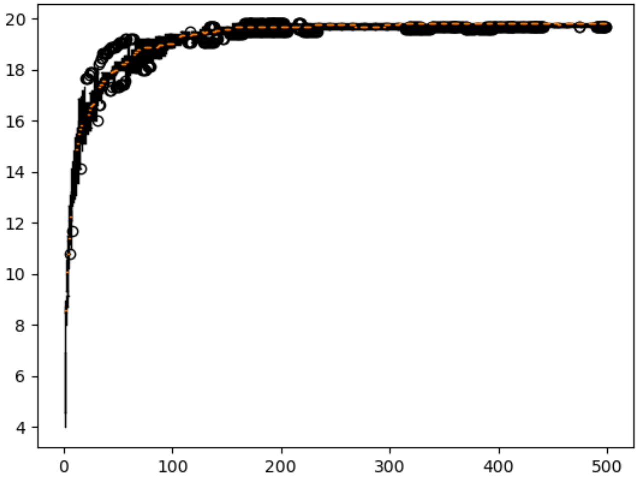


Walk for mixing

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:

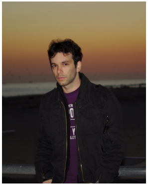
- Seems to grow about linearly with size of tree.
- Faster for SPR than NNI
- NNI can reverse earlier progress away from T_0 more readily than SPR
- Coupon-collecting arguments give $n \log n$ bound for all edges to be affected
- Don't need complete coupon collecting as random trees may have some common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

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sites.google.com/site/treespaceworkinggroup/