Geostatistical modeling with graphs

w/ many of my invaluable co-authors

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Spanning tree-based multivariate spatial model

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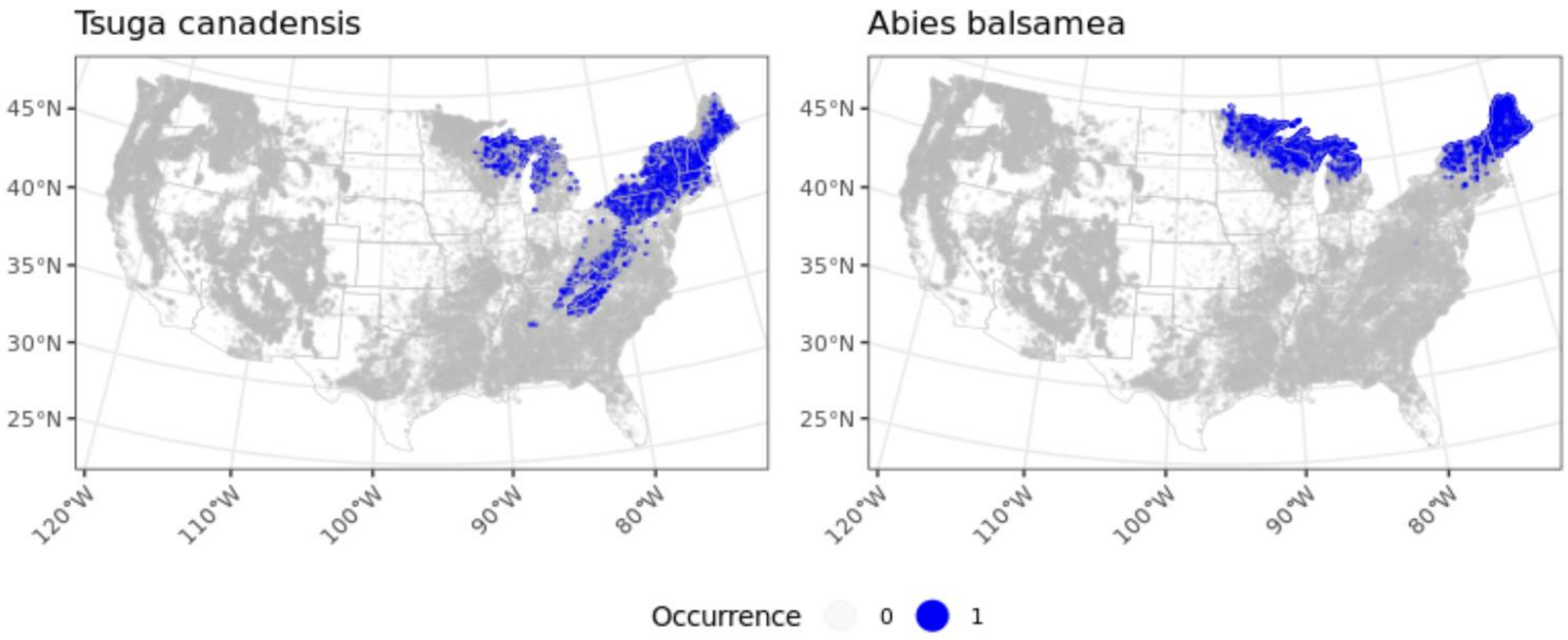
Motivation

- Spatial distribution of particle size curves (88 particle sizes, 3340 samples)
- Tree species co-occurrence analysis (96 species, 78804 samples)
- Air quality monitoring, spatial transcriptomics, spatial proteomics, etc.
- We want a **scalable** and **interpretable** method for highly multivariate ($q > 30$) and large ($n > 10000$) geostatistical data.

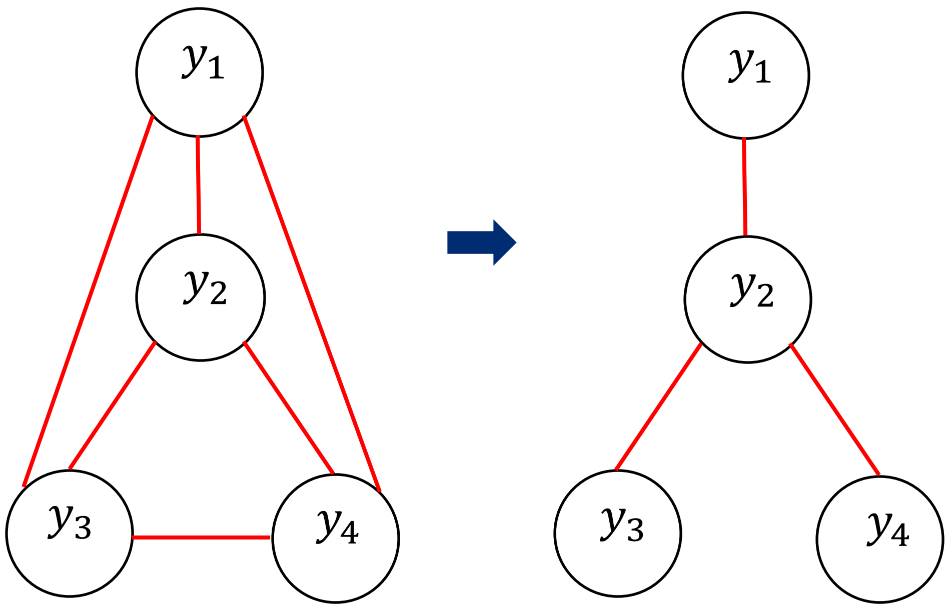


Existing multivariate methods

- Spatial factor model (+ NNGP)
  - Finley et al. (2015), Tikhonov et al. (2020), Doser et al. (2022)
  - Difficult to interpret (a latent process w is a linear combination of independent latent processes...🤯)
  - Difficult to fix or assign priors to hyperparameters
  - Choosing the ‘right’ number of factors is another area of research
- Parsimonious cross-covariance matrix function (+ NNGP)
  - Bevilacqua et al. (2015), Peruzzi (2024)
  - Computational burden and dimension increases quadratically (or more) with q
- “treed” DAG
  - Peruzzi and Dunson (2022)
  - Multiresolution/ recursive scheme scales poorly with q
- Process-level conditional independence using a graphical model
  - Dey et al. (2022)
  - Exhaustive stochastic exploration over sparse graph space is infeasible

Spanning tree-based approach

- Construct a multivariate process exploiting variable-level conditional independence relationships implied by a data generating inter-variable graph.
- Consider a minimum spanning tree as the backbone of the inter-variable graph.
- **Spanning trees** are economical to handle
    - Span all q variables
    - Include only $q-1$ edges

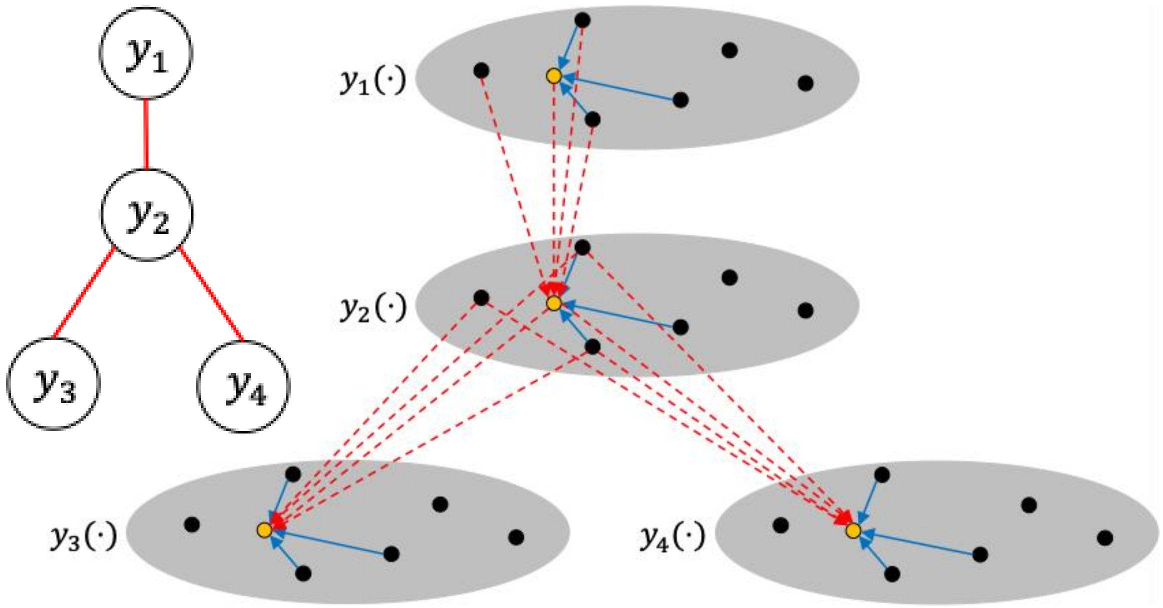


Spanning tree-based approach

- The spanning tree T on variables + a sparse DAG on locations
- For $\boldsymbol{y}(s) = \left(y_1(s), \dots, y_q(s)\right)^T$,

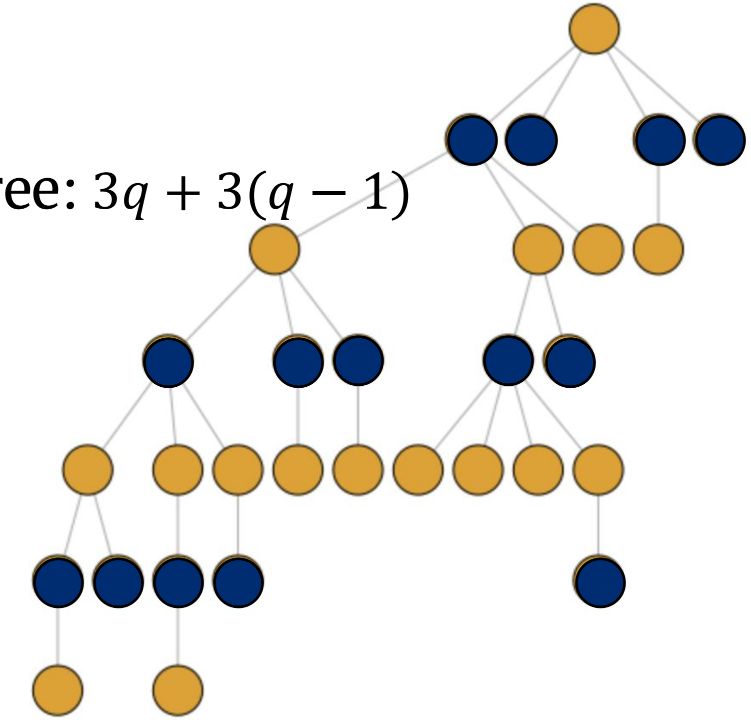
$$\tilde{f}(\boldsymbol{y}(s)) = f\left(y_1(s) \middle| y_1(N(s))\right) \prod_{(j,k) \in E_T} f\left(y_k(s) \middle| y_k(N(s)), y_j(s), y_j(N_u(s))\right)$$

  - Variable k is independent to other variables conditional on variable j connected by T
  - Different sets of neighbors from the parent variable
  - Useful when data are misaligned



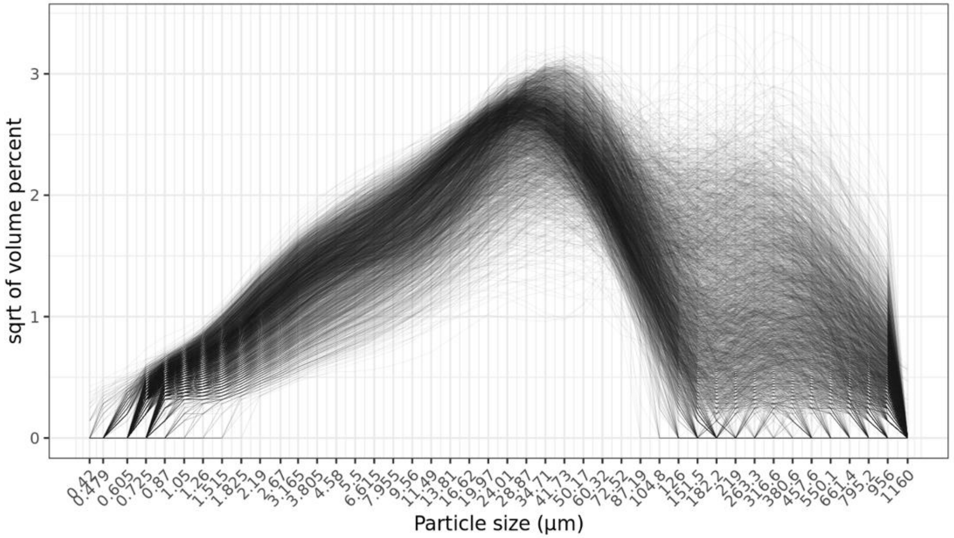
Properties

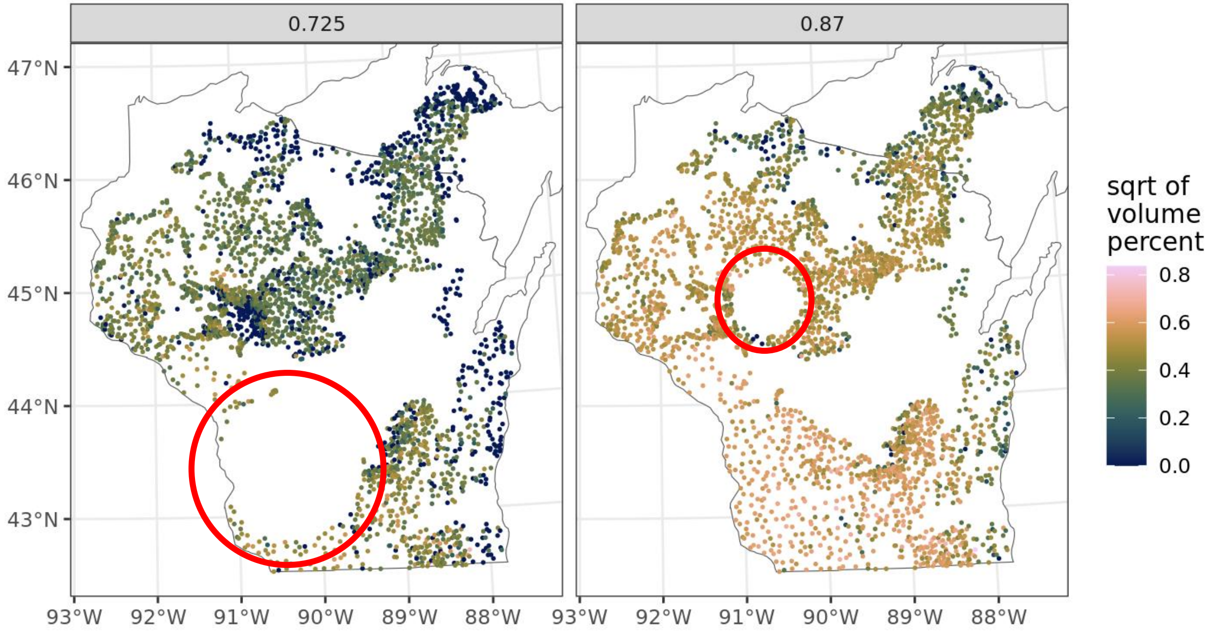
- Any variable can serve as the root; No arbitrary variable ordering.
- Resulting multivariate process preserves process-level conditional independence specified by T.
- Sufficient to ensure validity of a **bivariate** cross-covariance function for each pair of variables connected by T.
    - Substantial dimension reduction when q is large.
    - Multivariate Matérn: $3q + 3q(q-1)/2$ vs. Spanning tree: $3q + 3(q-1)$
- Parallelization using graph coloring
    - Only 2 colors because of a tree structure
    - All variables in yellow updated in parallel,
    - then all variables in blue in parallel



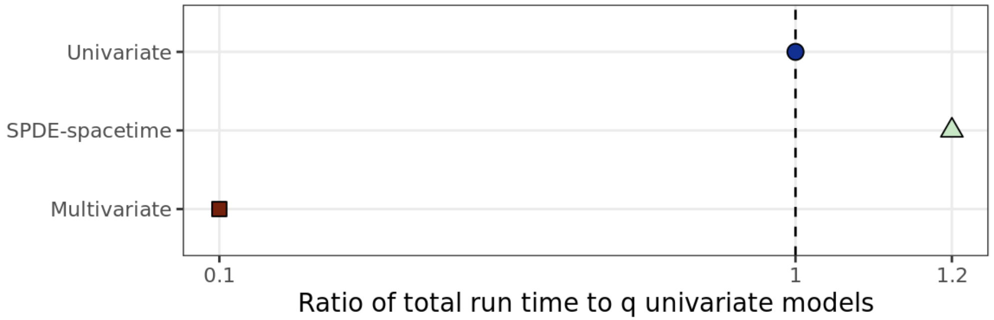
Particle size curves

- $n = 3340$ soil samples around Wisconsin and Michigan
- A curve representing sqrt of the volume of particles across $q = 44$ different sizes at each location
- Misalignment at every other particle size
- Aim to predict a curve at a new location
- Choice of T: path graph

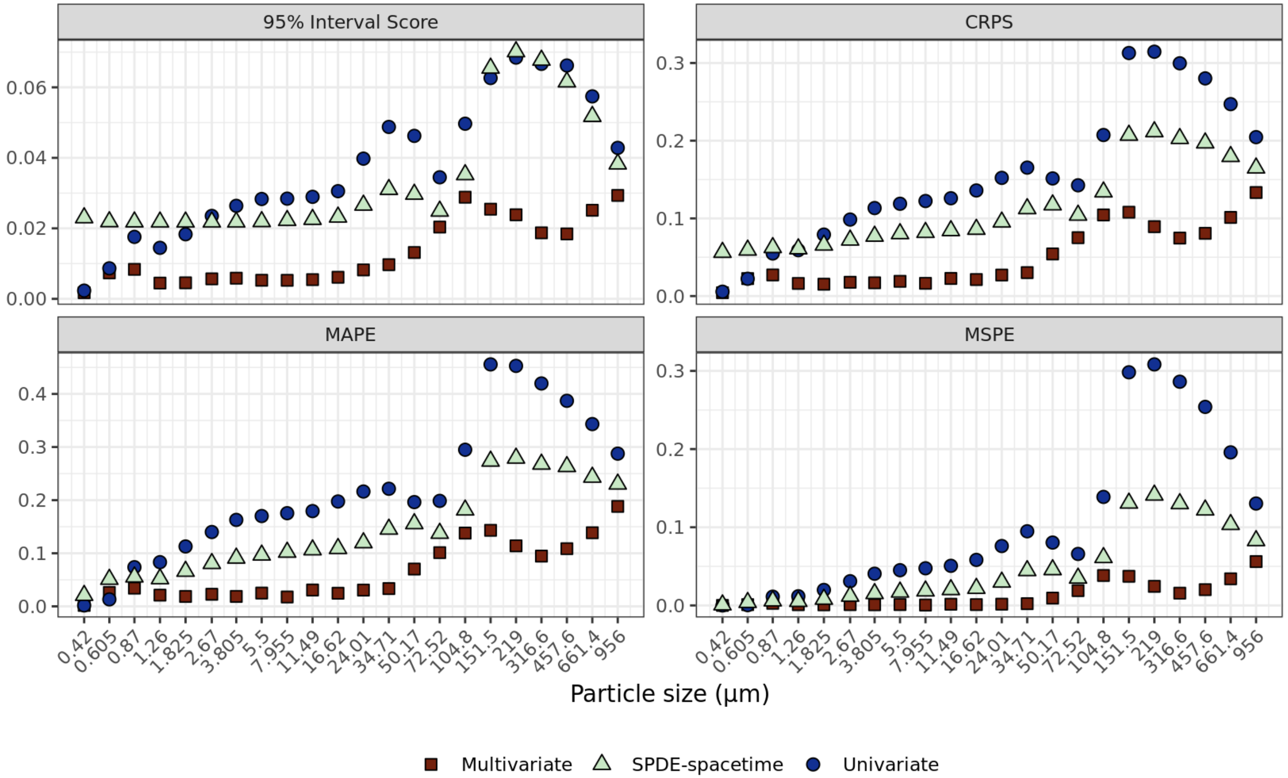


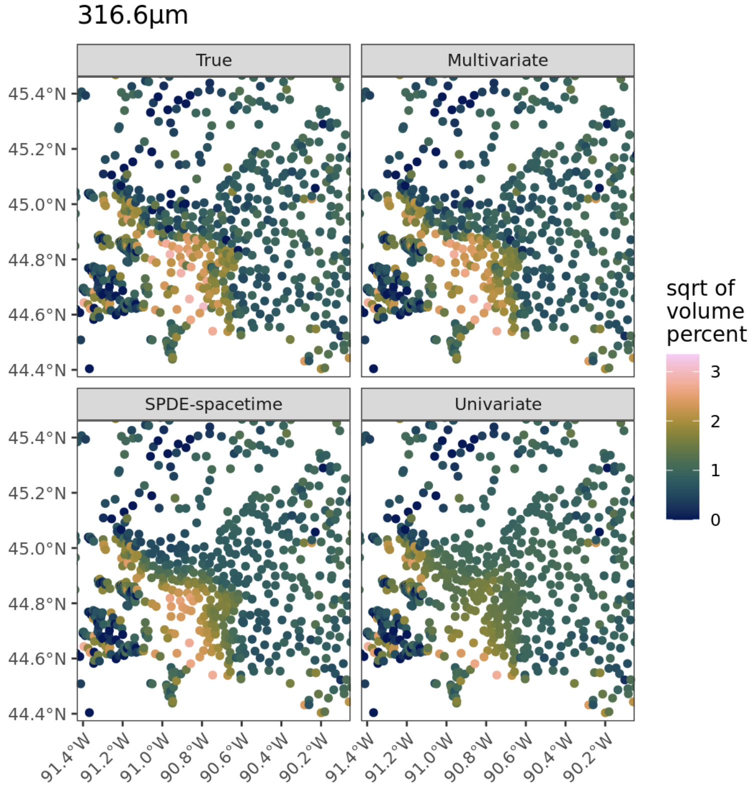


Particle size curves



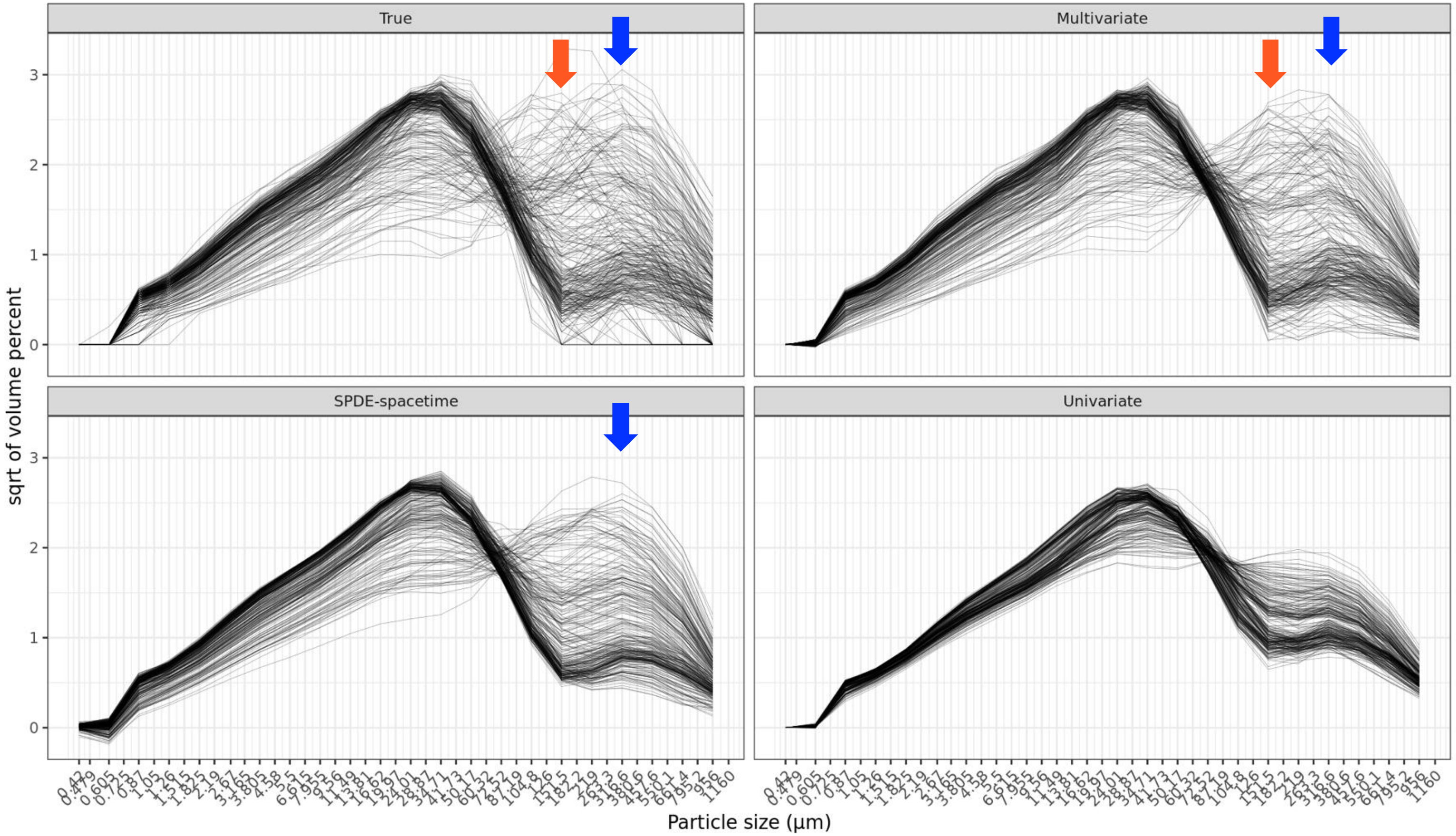
- Reduction in computation time
- Gain in prediction accuracy for misaligned locations
  - Silt dominating area; competitors underestimate volume of coarse particles





Particle size curves

- Separable spacetime model and independent univariate model struggle to find hotspots rich with medium or large sand.



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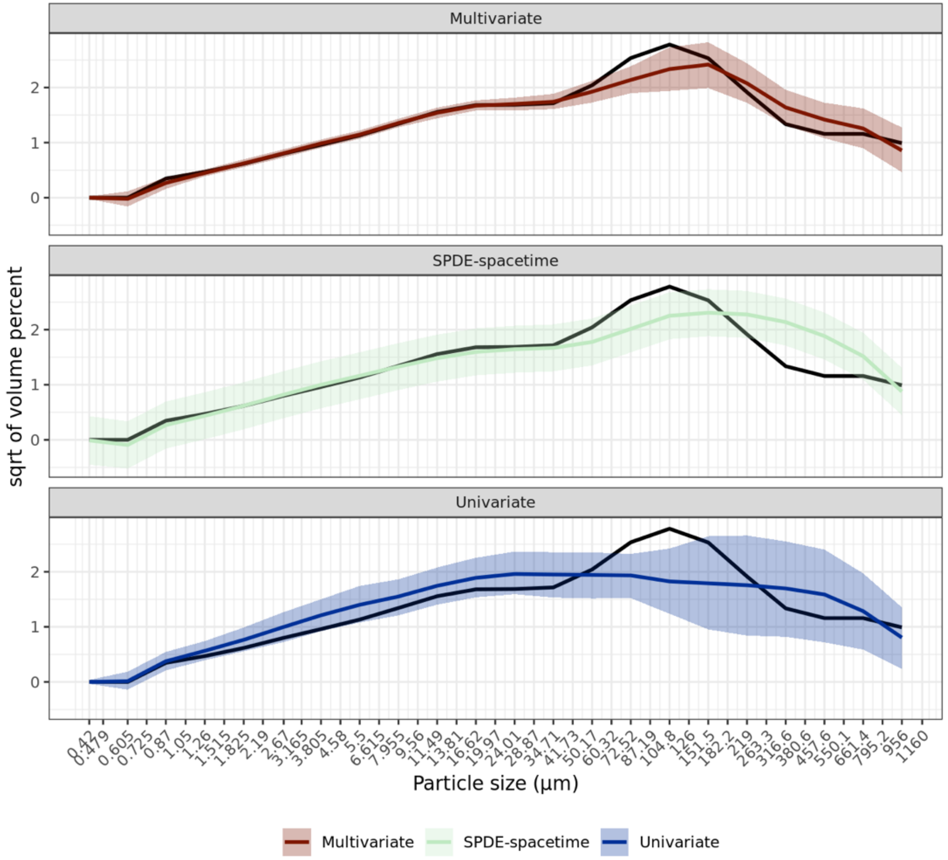
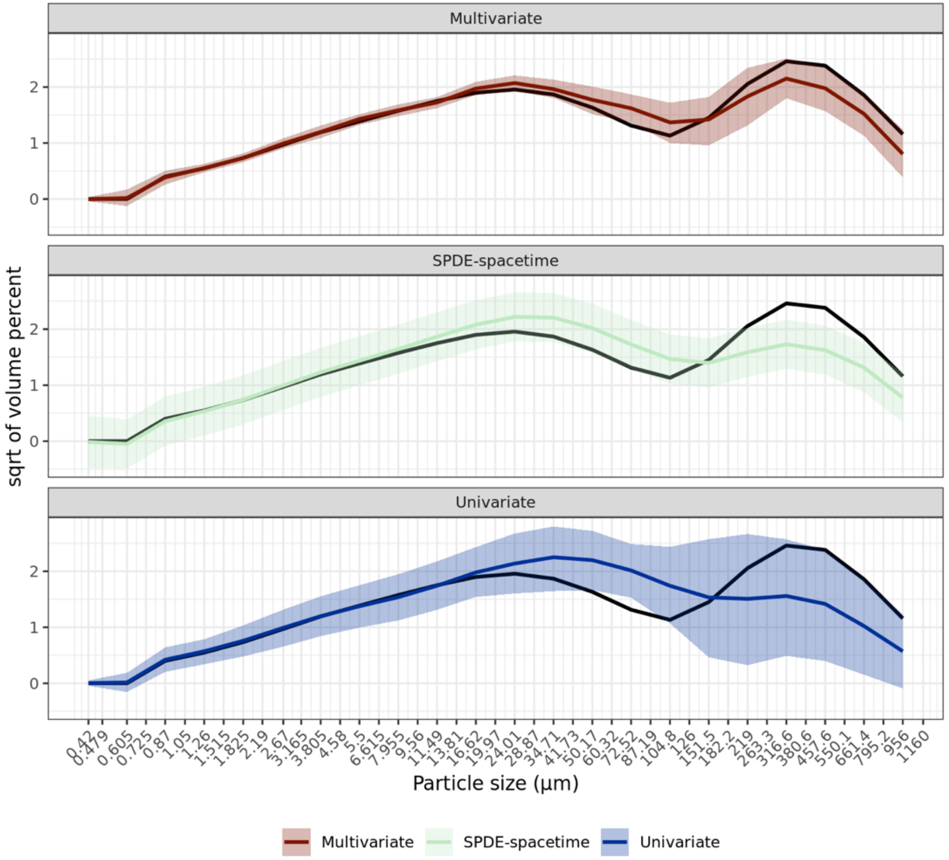
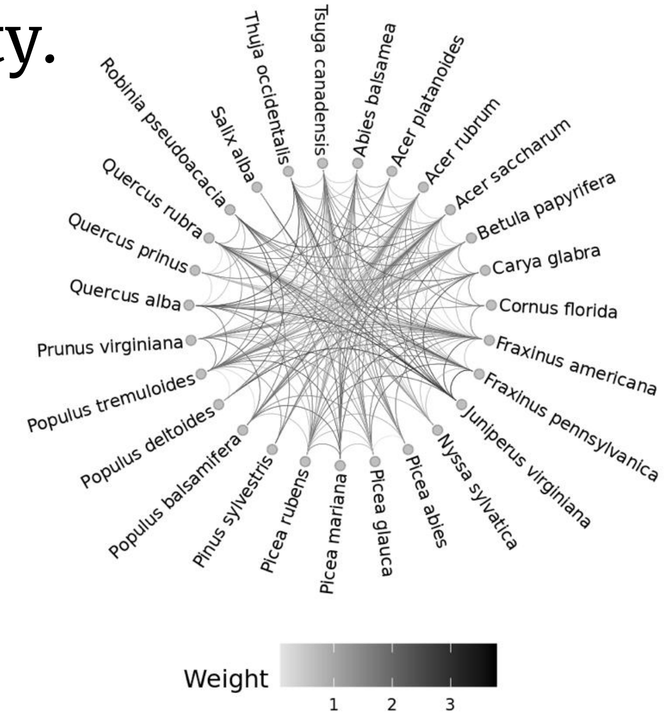
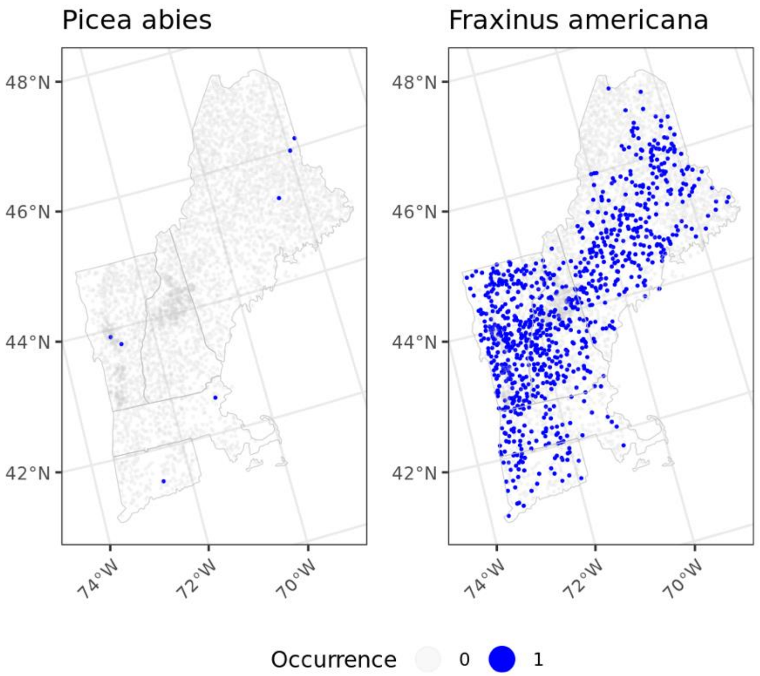




Tree species co-occurrence

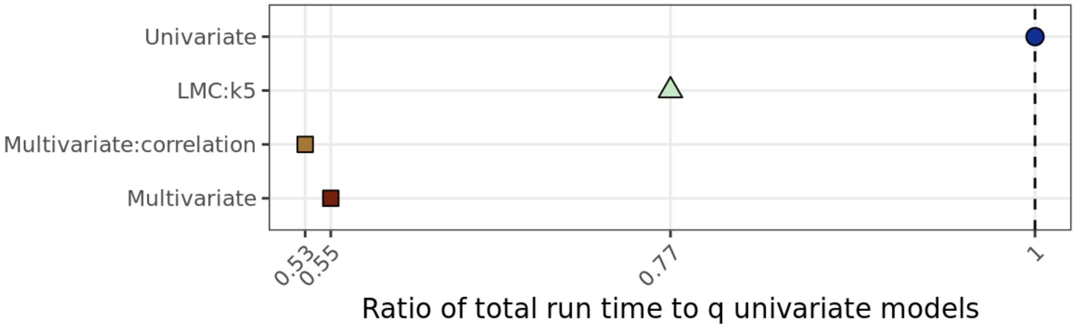
- $q = 27$ tree species occurrence data at $n = 3663$ locations around New England
- Inter-variable graph created based on field knowledge whose weights are defined by closeness in a space of trees' resistance to drought and wood density.

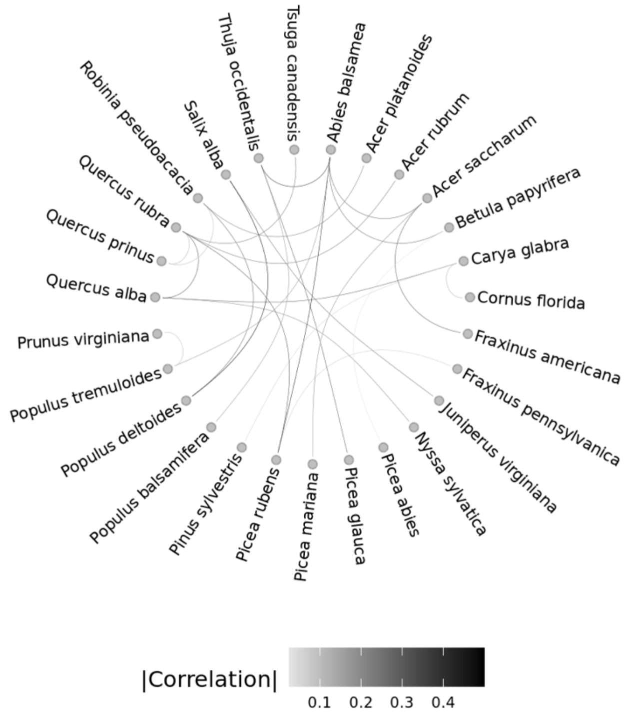




Tree species co-occurrence

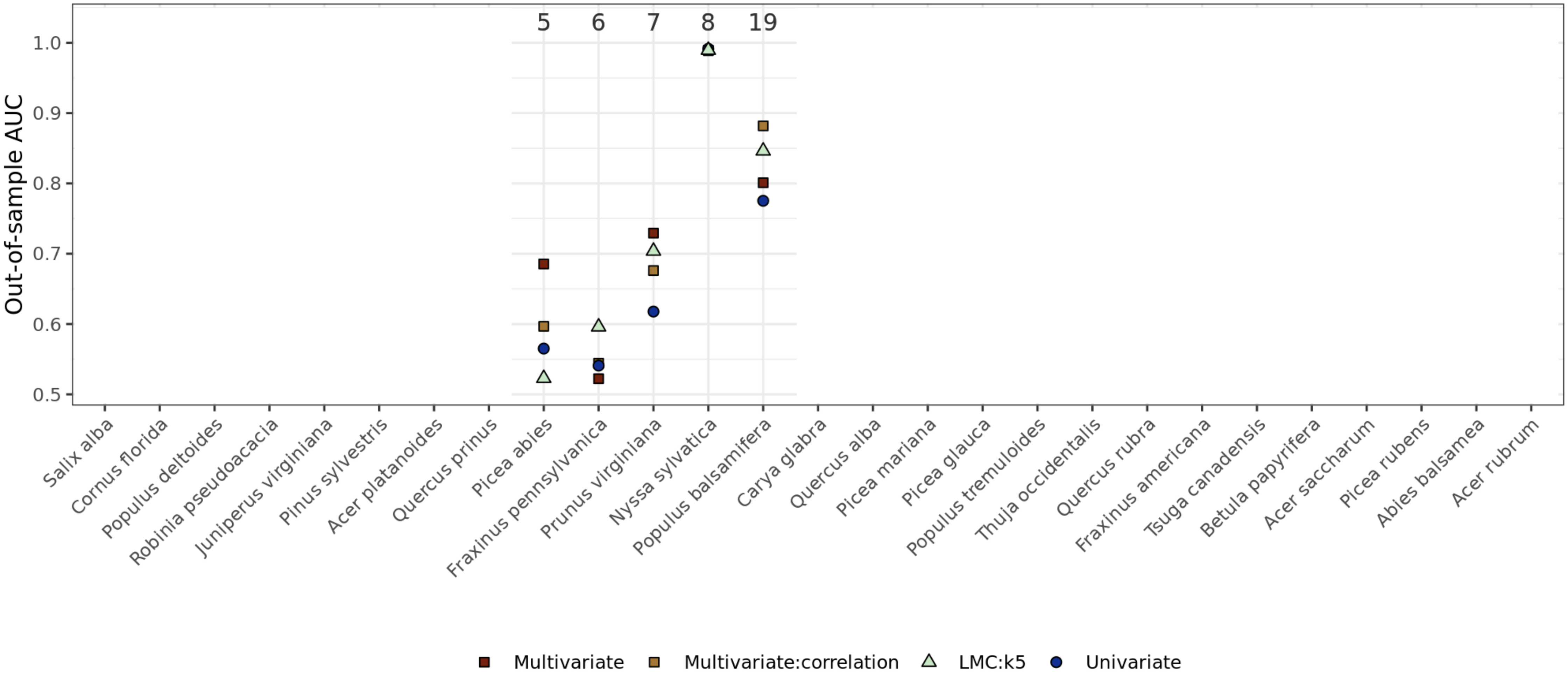
- Choice of T: minimum spanning tree with
  - negative weights
  - negative absolute correlations
- Reduction in computation time





Tree species co-occurrence

- Gain in prediction accuracy for moderately rare species



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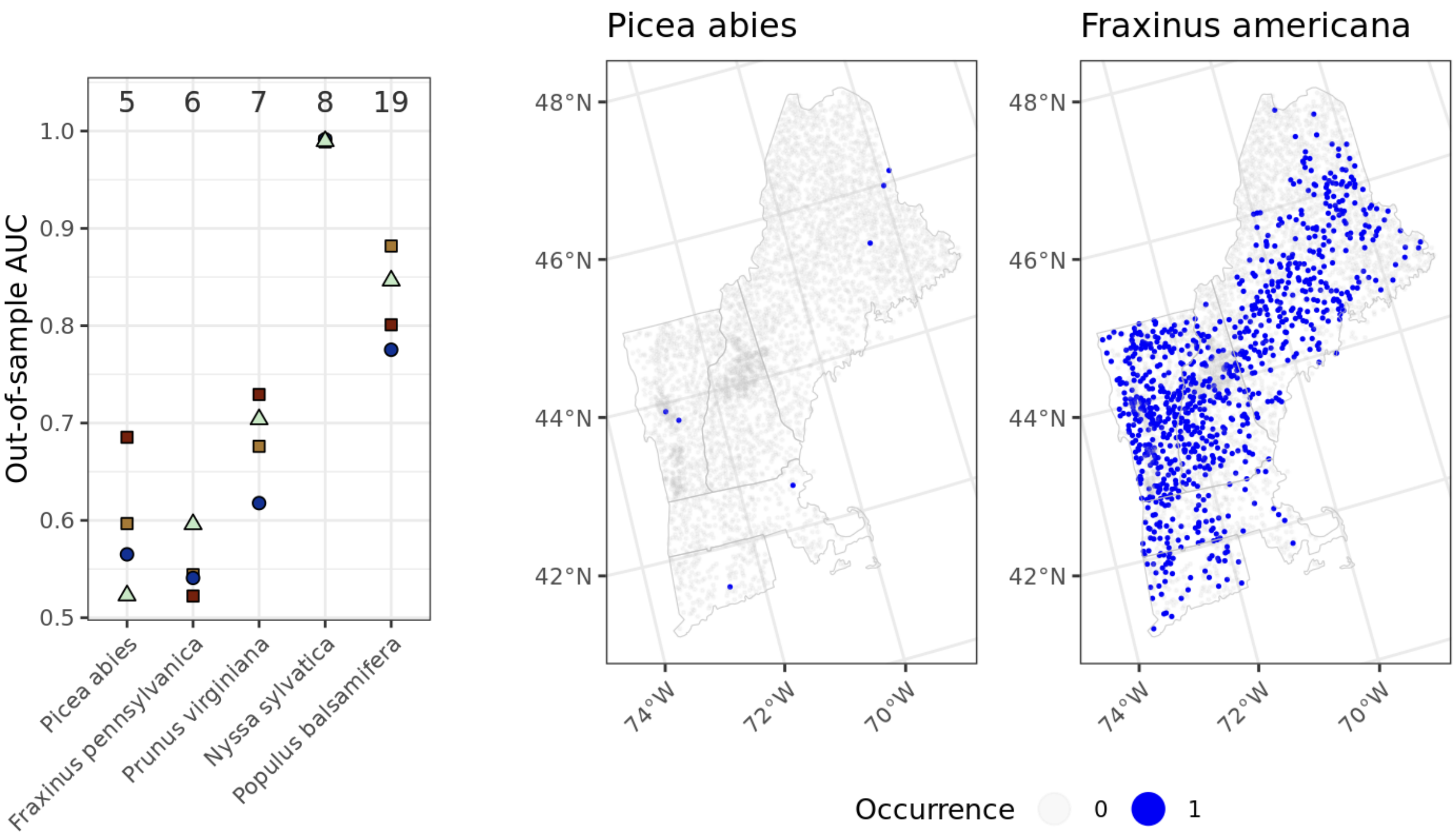

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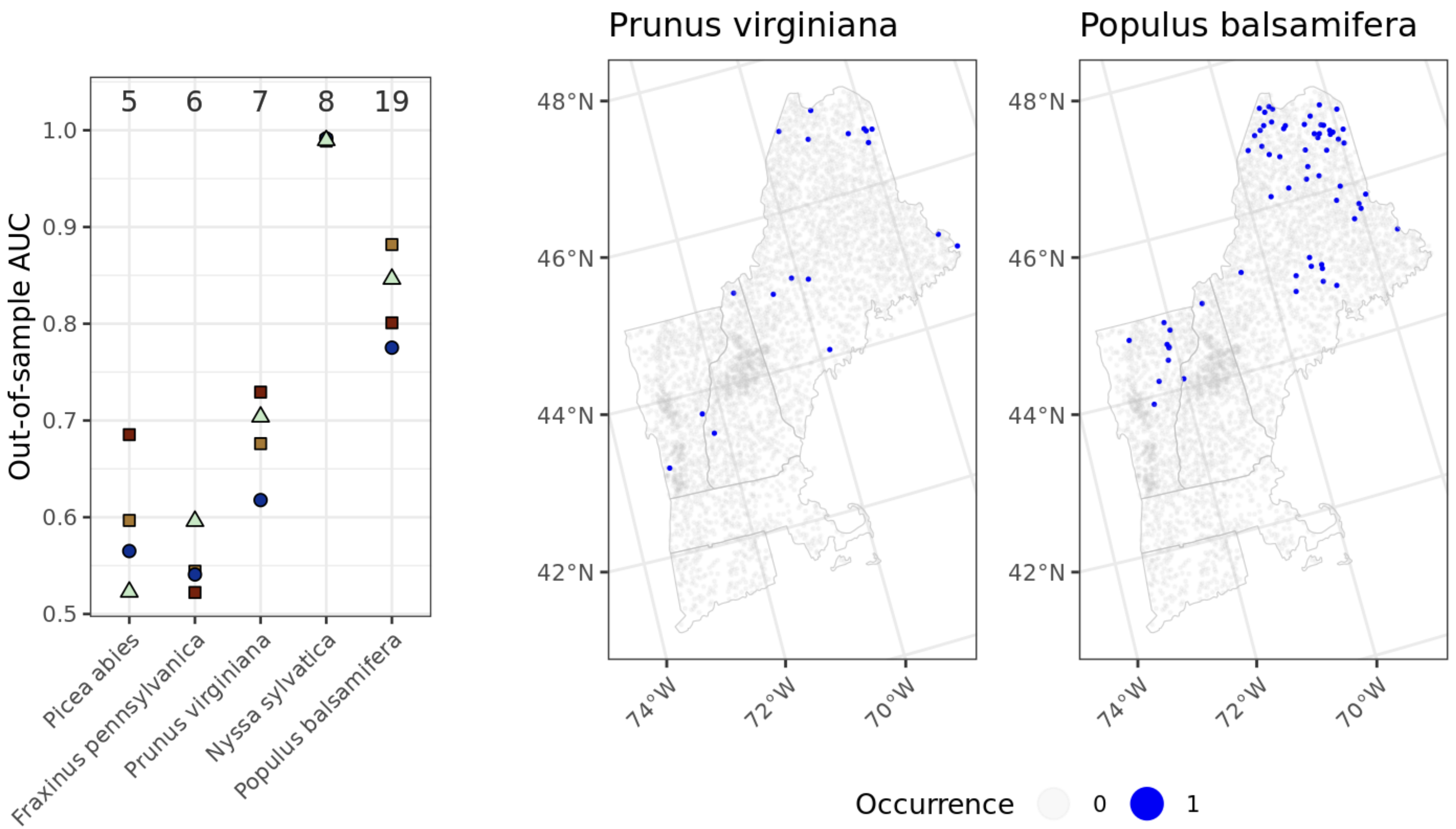

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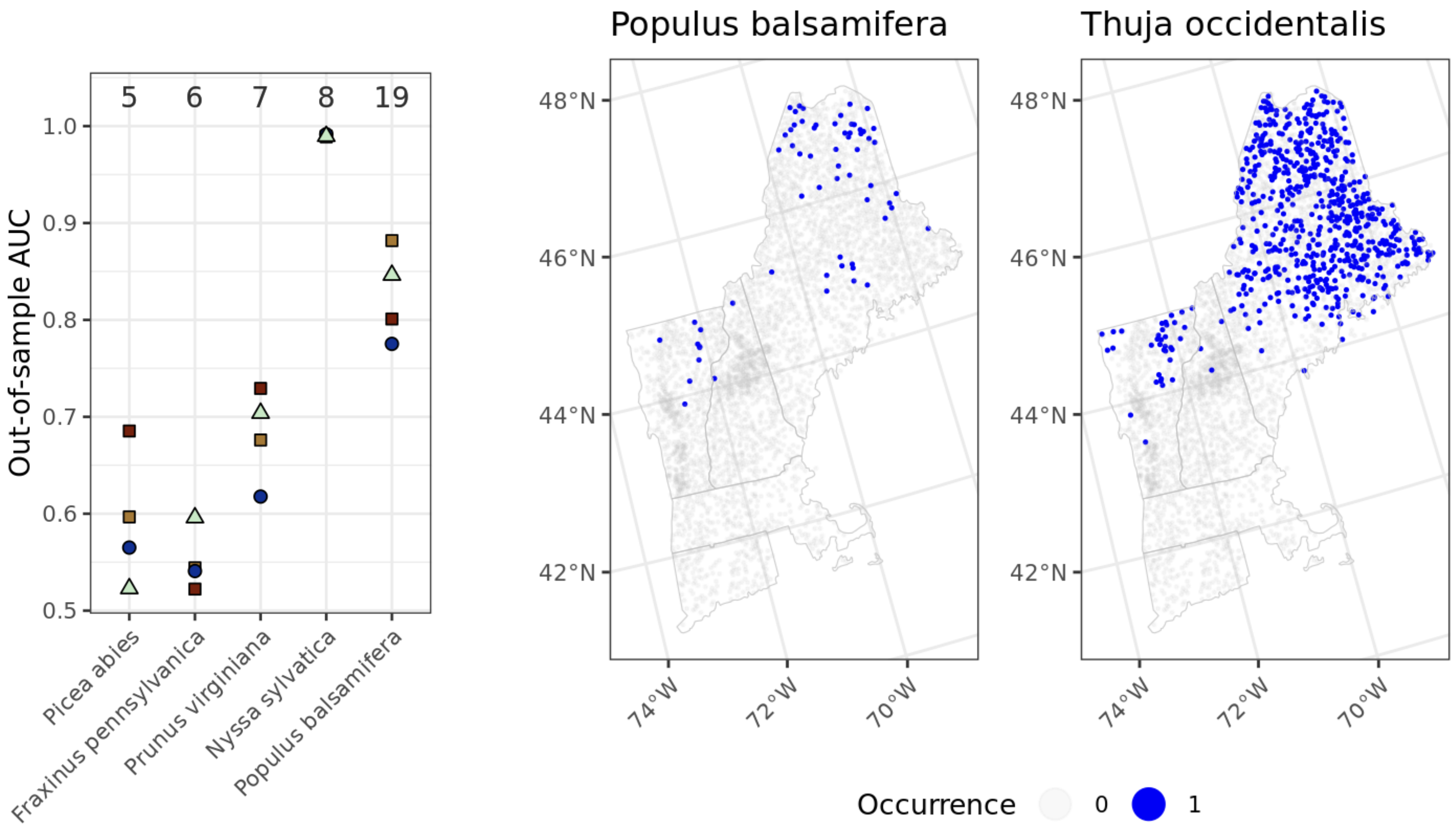
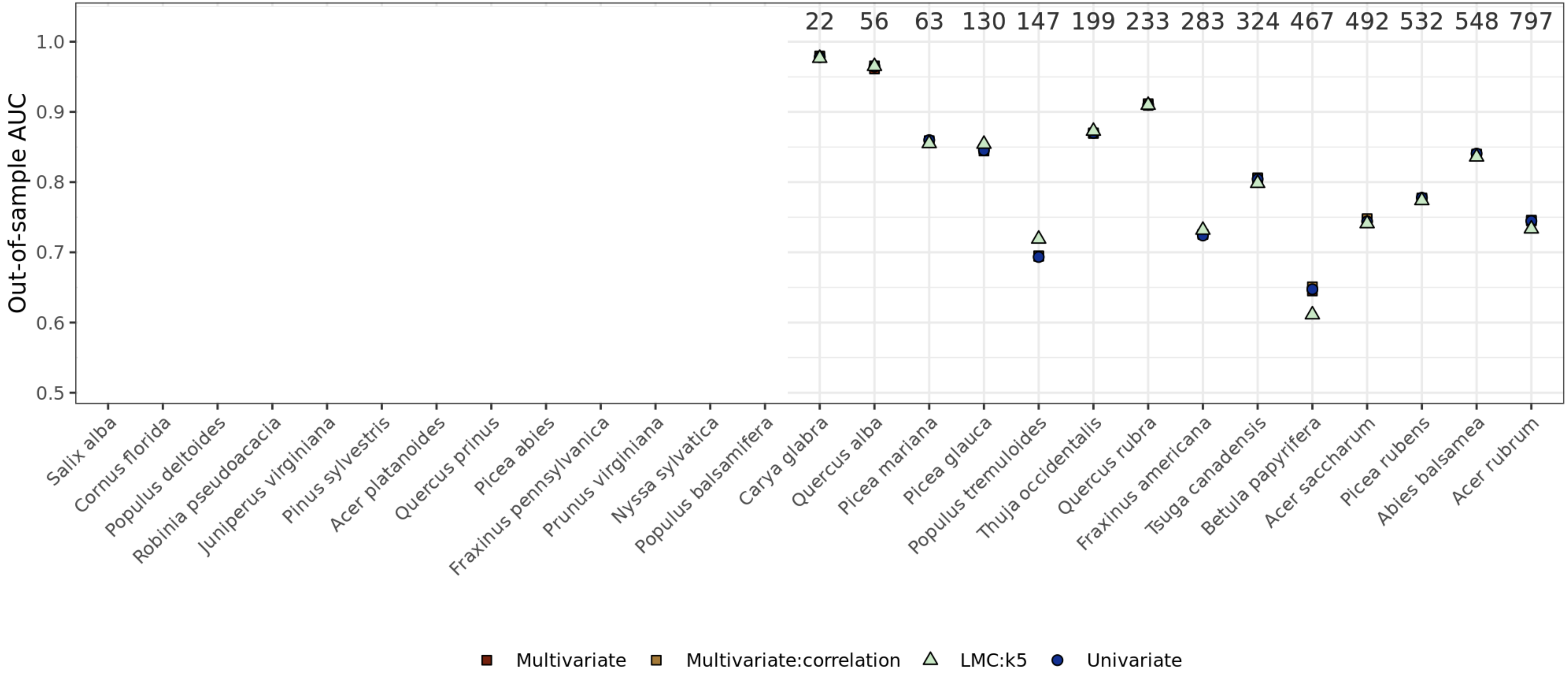


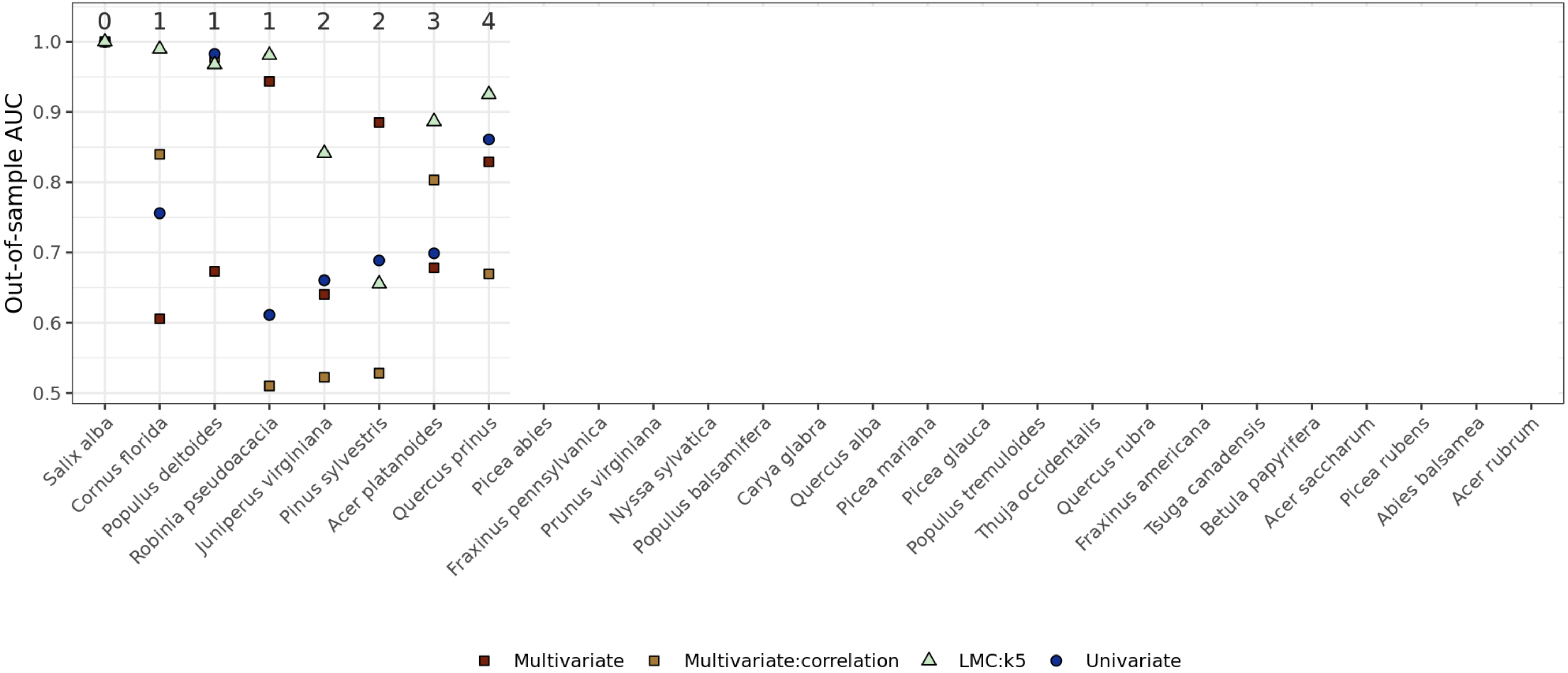
Tree species co-occurrence

- Similar prediction performance for frequently observed species



Tree species co-occurrence

- Factor model helps the most for extremely rare species



Future direction

- Using a minimum spanning tree can be too restrictive; combine results over multiple minimum spanning trees
- Choice of a minimum spanning tree can be arbitrary when graph structure is not intrinsic among variables; alternative ways to infer inter-variable relationships?
- With fixed covariance parameters, MCMC can be avoided (predictive stacking; Zhang et al. 2023).

Happy to hear your insight/suggestions/feedback!

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Reference

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