




1 autoStreamTree: Genomic variant data fitted to 2 geospatial networks

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DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

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Submitted: 06 November 2023

Published: unpublished

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8 Summary

9 Landscape genetics is a statistical framework that parses genetic variation within the con-
10 text of spatial covariates, but current analytical methods typically fail to accommodate the
11 unique topologies and autocorrelations inherent to network-configured habitats (e.g., streams
12 or rivers). We developed autoStreamTree to analyze and visualize genome-wide variation
13 across dendritic networks (i.e., riverscapes). autoStreamTree is an open source workflow
14 (<https://github.com/tkchafin/autostreamtree>) that automatically extracts a minimal graph
15 representation of a geospatial network from a provided shapefile, then ‘fits’ the components of
16 genetic variation using a least-squares algorithm. To facilitate downstream population genomic
17 analyses, genomic variation can be represented per-locus, per-SNP, or via microhaplotypes (i.e.,
18 phased data). We demonstrate the workflow by quantifying genetic variation in an empirical
19 demonstration involving Speckled Dace (*Rhinichthys osculus*).

Statement of need

20 Network approaches, particularly those graph-theoretic in nature, are increasingly being used
21 to capture functional ecological or evolutionary processes (e.g., dispersal, gene flow) within/
22 among habitat patches ([Peterson et al., 2013](#)). In some cases (e.g., riverscapes) topological
23 patterns are explicitly mirrored by the physical habitat, such that the network structure itself
24 places constraints upon processes such as individual movement ([Campbell Grant et al., 2007](#)).
25 It is no surprise then, that the importance of network properties such as topological complexity
26 are increasingly implicated as driving evolutionary dynamics in dendritic habitats ([Chiu et al.,](#)
27 [2020](#); [Thomaz et al., 2016](#)).

28 Despite this, quantitative frameworks for modelling the relationships between evolutionary
29 and ecological processes (e.g., through spatio-genetic associations) are predominantly focused
30 on landscapes, and as such often involving mechanistic assumptions which translate poorly
31 to networks. We address this limitation by providing a novel package, autoStreamTree, that
32 facilitates network modeling of genome-scale data. It first computes a graph representation
33 from spatial databases, then analyses individual or population-level genetic data to ‘fit’ distance
34 components at the stream- or reach- level within the spatial network. Doing so within a network
35 context allows the explicit coupling of genetic variation with other network characteristics (e.g.,
36 environmental covariates), in turn promoting a downstream statistical process which can be
37 leveraged to understand how those features drive evolutionary processes (e.g., dispersal/ gene
38 flow). We demonstrate the utility of this approach with a case study in a small stream-dwelling
39 fish in western North America.
40

Program Description

Workflow and user interface

autoStreamTree employs the Python networkx library (Hagberg et al., 2008) to parse geospatial input (i.e., large stream networks) into a graph structure with stream segments as edges, sampling locations as endpoints, and river junctions as nodes. Sample data comprise a tab-delimited table of latitude/longitude coordinates, genome-wide variant data in VCF format, and (optionally) a tab-delimited population map. The data structure 'graph' on which downstream computations are performed is built as follows: 1) Sample points are 'snapped' to nearest river network nodes (i.e., defining endpoints); 2) Shortest paths are identified between each set of endpoints (Dijkstra, 1959); and 3) A minimal network of original geometries, with contiguous edges derived by joining individual segments with junctions (nodes) retained that fulfill shortest paths.

Pairwise genetic distances from VCF-formatted genotypes (Danecek et al., 2011) are derived among individuals, sites, or populations (via a priori user-specifications). Options for sequence- and frequency-based statistics are provided (-d/--dist). Mantel tests are available to quantify correlations among genetic/ hydrologic distance matrices. The primary workflow is a least-squares procedure analogous to that used to compute branch lengths within a neighbor-joining phylogenetic tree (Kalinowski et al., 2008). The procedure fits components of the genetic matrix to k -segments in a network, such that fitted distance values (r) for each segment separating two populations will sum to the observed pairwise matrix value. This provides a distance (r_k) for each of k -segments as the genetic distance 'explained' by that segment.

Workflow steps are controlled through the command-line interface (-r/--run), with results as plain text tables, and plots via the seaborn package (Waskom, 2021). Fitted distances are added as annotations to an exported geodatabase.

Features

Additional layers of control are provided to minimize pre-processing steps. Users may define individual/ site aggregates: 1) Through a tab-delimited classification file; 2) By automatically deriving group membership geographically; or 3) Using an automated DBSCAN clustering method in scikit-learn (Pedregosa et al., 2011).

Users may also provide pre-computed genetic distance matrices either directly at individual or locus levels. Built-in options are provided to concatenate single-nucleotide polymorphisms (SNPs) either globally, or per contig/scaffold. Individual-level statistics include uncorrected p -distances (i.e., proportion of nucleotide differences/alignment length), aggregated by site- or at population-level (e.g., as median, arithmetic mean, or adjusted harmonic mean (Rossman, 1990)), or computed as distances via several frequency-based methods (e.g., Chord distance (Cavalli-Sforza & Edwards, 1967); F_{ST} (Weir & Cockerham, 1984)). autoStreamTree can also be computed per-locus by specifying -r RUNLOCI, and with -c LOC in the case of phased data to treat linked SNPs to microhaplotypes.

Demonstration

Empirical case study

To demonstrate autoStreamTree, we employed existing SNP data for Speckled Dace (*Rhinichthys osculus*) (Mussmann, 2018). Data represent 13,219 SNPs from $N=762$ individuals across 78 localities in the Colorado River ecosystem.

Stream networks were parsed directly as a minimal sub-graph from RiverATLAS, which contains various local-scale environmental/ hydrological features as annotations (i.e., physiography,

climate, land-cover, geology, anthropogenic effects) (Linke et al., 2019). Genetic distances were computed globally and per-locus among sites as linearized F_{ST} (Weir & Cockerham, 1984) ($=F_{ST}/1-F_{ST}$). To compare with Kalinowski et al. (2008), we used unweighted least-squares, iterative negative distance correction, and replicated analyses using linearized F_{ST} independently recalculated in Adegnet (Jombart, 2008).

We examined variation in per-locus fitted distances as a function of environmental and anthropogenic covariates, carried over as annotations to RiverATLAS. We reduced $N=281$ hydro-environmental RiverATLAS attributes using forward-selection in adeSpatial (Dray et al., 2018), after first removing variables showing significant pairwise correlations. Remaining selected variables were employed in partial-redundancy analysis (pRDA; to 'partial-out' hydrologic distance), with outliers as stream segments/SNPs with loadings ± 3 standard deviations from the mean.

Results and comparison

Runtimes are reported for a 2021 Macbook Pro, 16GB memory, 3.2GHz M1 CPU. Time required to calculate/extract a minimal sub-graph containing 118 dissolved edges from RiverATLAS (North America shapefile totaling 986,463 original vertices) was 35min. Computing pairwise hydrologic distances required an additional 3sec. Pairwise population genetic distances were computed in ~24min (linearized F_{ST}), with Mantel test and distance fitting requiring 11sec and 10sec, respectively. Re-running the entire pipeline per-locus (i.e., -r RUNLOC) took 3h 34min. Fitted- F_{ST} for autoStreamTree (Figure 1) matched that re-calculated using the Kalinowski et al. (2008) method (adjusted $R^2 = 0.9955$; $p < 2.2e-16$). However, due to runtime constraints and manual pre-processing for the latter, per-locus distances were not attempted. The pRDA selected four variables, with 221 SNPs and 9 edges as outliers (Figure 1).

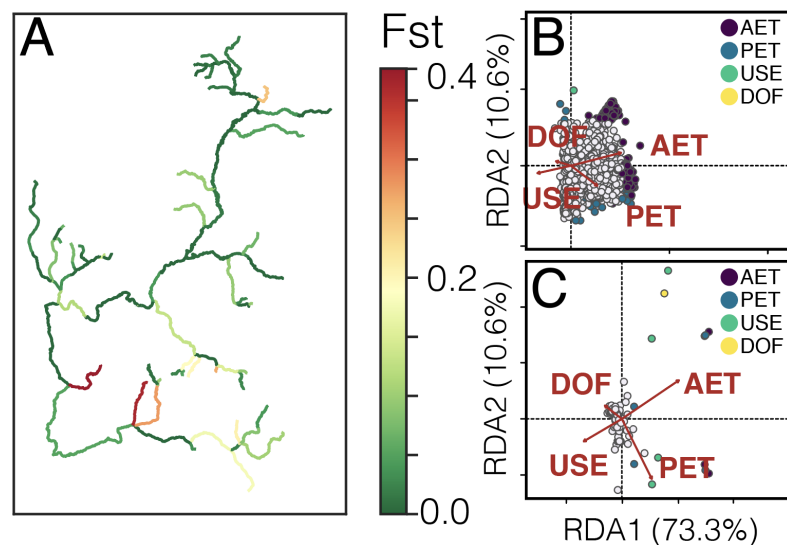


Figure 1: autoStreamTree output. Shown are F_{ST} distances fitted onto original stream network (A), variation in per-locus fitted- F_{ST} distances via pRDA (controlling for stream length) scaled by loci (B), and by stream segment (C). Outliers highlighted according to most closely correlated explanatory axis and abbreviated as: AET (actual evapotranspiration), PET (predicted evapotranspiration), DOF (degree of fragmentation), and USE (proportion of water for anthropogenic use).

Conclusion

The utility of autoStreamTree was demonstrated with a population genomic dataset as a demonstrative case study. The benefits of the automated approach are underscored by locus-wise microhaplotype versus SNP analysis, which in turn feeds into a quantitative framework that allows 'outlier' loci exhibiting environmental/ spatial associations within the autocorrelative structure of the network to be detected. This may potentially imply adaptive variation (although not evaluated herein). In addition, the approach is portable to other data types – indeed, any distance matrix that can be appropriately modeled additively can be supplied, and the process is generalizable to any manner of spatial network.

Acknowledgements

Links to non-Service websites do not imply any official U.S. Fish & Wildlife Service endorsement of the opinions or ideas expressed therein or guarantee the validity of the information provided. The findings, conclusions, and opinions expressed in this article represent those of the authors, and do not necessarily represent the views of the U.S. Fish & Wildlife Service.

This work was supported by University of Arkansas via Doctoral Fellowships (TKC/SMM) and endowments (MED: 21st Chair Century Global Change Biology; MRD: Bruker Life Sciences Professorship). TKC is currently supported by the Scottish Government's Rural and Environment Science and Analytical Services Division (RESAS). Data and scripts associated with this work can be found on the Open Science Framework (doi: 10.17605/OSF.IO/4UXFJ).

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