Supplementary Text for:

Laplacian eigenfunctions Learn Population Structure

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Theoretical ancestry-capturing vector for 2 populations

As part of **Simulation Study** A, we consider a population consisting of two discrete subpopulations, and we compare the results of PCA and LAPSTRUCT to a theoretically-derived ancestry-capturing vector. Here we provide the details on the theoretical ancestry-capturing vector for 2 populations. First note that the matrix C defined in Materials and Methods is orthogonal to the vector with all entries equal to 1, which we call the 1-vector. Therefore the top PC, which is normalized to have length 1, will be orthogonal to the 1-vector. Similarly, as described in Materials and Methods, the 0th eigenvector by the Laplacian approach is the 1-vector, so the 1st Laplacian eigenvector, which is normalized to have length 1, will be orthogonal to the 1-vector. Therefore, the optimal value, from the point of view of capturing ancestry, for the top PC and for the 1st Laplacian eigenvector would be a vector that is orthogonal to the 1-vector, that is of length 1, and that captures the ancestry perfectly, i.e. takes a constant value on population 1 and a different constant value on population 2. It is easy to verify that the only two vectors satisfying these properties are the vectors v and -v, where v is of length N and has entry $\frac{-N_2}{\sqrt{N_1N_2N}}$ for each individual in population 1 and entry $\frac{N_1}{\sqrt{N_1N_2N}}$ for each indvidual in population 2, where N_1 and N_2 are the total numbers of individuals from subpopulations 1 and 2, respectively, and $N = N_1 + N_2$.