

Description of Additional Supplementary Files

Supplementary Data 1: Model parameter results for *uaDf5*.

Using the code included with this study, the maximum-likelihood parameters of the model described in this study were estimated for the mtDNA genotype *uaDf5* using the Source Data provided. Maximum-likelihood results were then obtained for 100 bootstrap data sets, generated using the maximum-likelihood values under the empirical data. These results, together with the log likelihood values that are maximized in our inference procedure, are included. (*uaDf5*)

Supplementary Data 2: Model parameter results for *mptDf2*.

Similar to Supplementary Data 1 but for genotype *mptDf2*. Maximum-likelihood model parameters were estimated using the Source Data and for 100 bootstrap data sets generated using the maximum-likelihood values under the empirical data. Included with the results are the log likelihood values that are maximized in our inference procedure.

Supplementary Data 3: Model parameter results for *mpt4*.

Similar to Supplementary Data 1 but for genotype *mpt4*. Maximum-likelihood model parameters were estimated using the Source Data and for 100 bootstrap data sets generated using the maximum-likelihood values under the empirical data. Included with the results are the log likelihood values that are maximized in our inference procedure.

Supplementary Data 4: Model parameter results for *mpt2*.

Similar to Supplementary Data 1 but for genotype *mpt2*. Maximum-likelihood model parameters were estimated using the Source Data and for 100 bootstrap data sets generated using the maximum-likelihood values under the empirical data. Included with the results are the log likelihood values that are maximized in our inference procedure.

Supplementary Data 5: Model parameter results for *mptDf3*.

Similar to Supplementary Data 1 but for genotype *mptDf3*. Maximum-likelihood model parameters were estimated using the Source Data and for 100 bootstrap data sets generated using the maximum-likelihood values under the empirical data. Included with the results are the log likelihood values that are maximized in our inference procedure.

Supplementary Code 1: Guidance on running the code provided in this study.

The guidance for running this code is available in the file README.md at <https://github.com/bgitschlag/MiSelf>, and is reproduced below.

This document provides guidance on modeling evolutionary dynamics of selfish mitochondrial genomes, using the MiSelf Python script, included with this study as Supplementary Code 1 (see file Supplementary_Code_1.py).

The MiSelf script (Supplementary Code 1) is prepared to be run from the terminal, from a working directory that contains the sub-directory /Source_data, which will require three input data files (example input data can be downloaded from <https://github.com/bgitschlag/MiSelf>):

1. INTRA-ORGANISMAL SELECTION DATA. The files are called as './Source_data/{genotype}_intra_organismal_source_data.csv'. Each data file should consist of a three-column table with column labels 'Replicate', 'Parent' (for parents), and 'Adult progeny' (for progeny). Each row consists of one biological replicate parent-progeny lineage. Data should be expressed as float values between 0 and 1, representing raw mutant (heteroplasmic) frequency measurements.

2. INTER-ORGANISMAL SELECTION DATA. The files are called as './Source_data/{genotype}_organismal_source_data.csv'. Each data file should consist of a table with columns indexing biological replicates (one competed population per replicate, see Gitschlag et al. 2024 Methods) and labeled sequentially as 'Rep 1' to 'Rep n' where n is the number of replicate populations. Rows index generational time points which are numbered sequentially in the column 'Generation'. Inter-organismal selection data are expressed as log-ratios, $\text{LN}(\text{het}/\text{hom})$, where het and hom are heteroplasmic and homoplasmic (wildtype) fractions of the population, respectively. As part of the original experiment, non-competed control populations were run in parallel, and their population-wide mutant frequency measurements are used as estimates for the mean homoplasmic (wildtype) fraction of the competed populations (see Gitschlag et al. 2024 Methods).

3. MUTANT FREQUENCY MEASUREMENTS. The file is called as './Source_data/mutant_frequency_samples_source_data.csv'. This file should consist of a single table with genotype names as column labels. Genotypes and biological replicates are indexed by column and row, respectively.

Customizable settings (such as sample sizes and model input parameters for simulated data) can be found in lines 20-55 of the code file.