

Bayesian Workflow

Dataset

- Data cleaning and preprocessing
- Identifying variables and visualizing data.
- Collating all available replicates.
- Choosing appropriate scaling and transformation. E.g., log-transform for microbial abundance.

ODE Model

- Choosing an appropriate ODE model.
- Identifying which variables are observed, which variables are latent.
- Making a simple least-squares fit.
- Identifying biologically plausible parameter regimes where the ODE should work.
- Choosing solvers. E.g., `scipy.odeint`, `pymc.ode.DifferentialEquation`, etc.
- Choosing physical constraints. E.g., minimum density.

Bayesian Model

- Selecting prior distributions for ODE parameters and initial conditions, informed by previous experiments, biological constraints, and other relevant considerations. E.g., Truncated Gaussian.
- Defining likelihood as a function of the ODE model and observed data. E.g., product of Gaussians for each time point for each variable and replicate.
- Choosing an error function.

Computing Posteriors

- Prior predictive checks
- Requirements: MAP vs complete posterior.
- Selecting tools/packages/programming languages.
- Choosing the type of computation: E.g., ABC, MCMC, HMC, VI, etc.
- Selecting samplers: E.g., NUTS for HMC, DRAM-MCMC for Metropolis samplers, etc.
- Hyperparameters: burn-in period, number of chains, traces, acceptance rates, etc.

Model validation

- Convergence tests: Gelman-Rubin, Geweke, IAT (and possible thinning), ESS, etc.
- Posterior parameter covariances and possible reparameterization.
- Posterior predictive checks.
- Inter-model comparison.