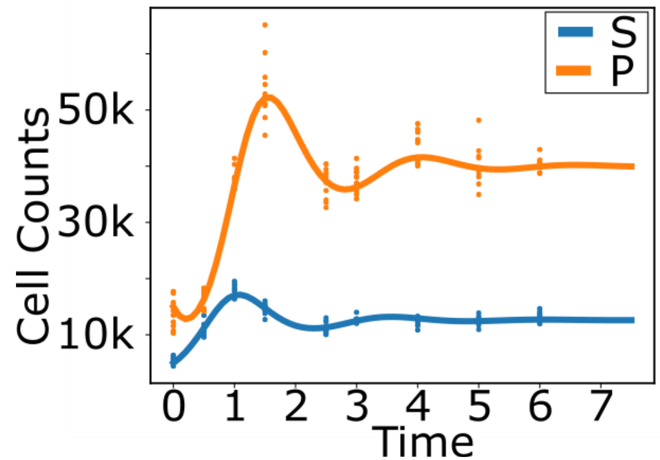
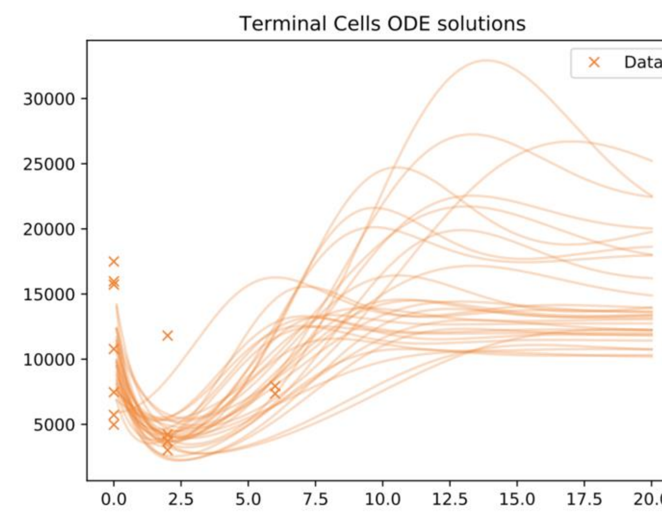
NSF-Simons Center for
Multiscale Cell Fate Research
UC Irvine

Bayesian Optimal Experimental Design: How to design informative experiments?

Luis M. Lomeli and Abdon Iniguez

- There are multiple variables that need to be adjusted when performing an experiment
- Maximize the information gain from an experiment by choosing a design varying:
  - Number of biological replicates, timing of the records and initial conditions
- We use a mechanistic model that captures important dynamics of hematopoiesis
- We use open source libraries in R and Python to solve ODEs and run Markov Chain Monte Carlo





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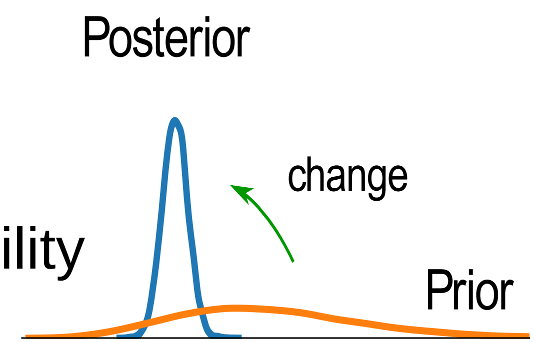

Quantify information gain

- Quantify uncertainty about the model parameters
- For each design *d,* calculate the KL-divergence utility

$$U(y,d) = \int_{\Theta} log\left(\frac{p(\Theta|y,d)}{p(\Theta)}\right) p(\Theta|y,d)d\Theta$$

- Compute the expected/median utility

$$u(d) = \mathbb{E}_{\Theta,y}\left[U(\Theta,y,d)\right] = \int_y \int_{\Theta} U(\Theta,y,d)p(y|\Theta,d)p(\Theta)d\Theta dy$$

- This is extremely computationally intensive since need to run tons of MCMC simulations
- Need to use HPC resources
- Also need to use Supercomputing tools to make MCMC faster and possibly more efficient