Measuring the accuracy of likelihood-free inference

Aden Forrow & Ruth Baker

24 May, 2022

Outline

$$p(\theta|x^*) = \frac{p(x^*|\theta)p(\theta)}{p(x^*)}$$

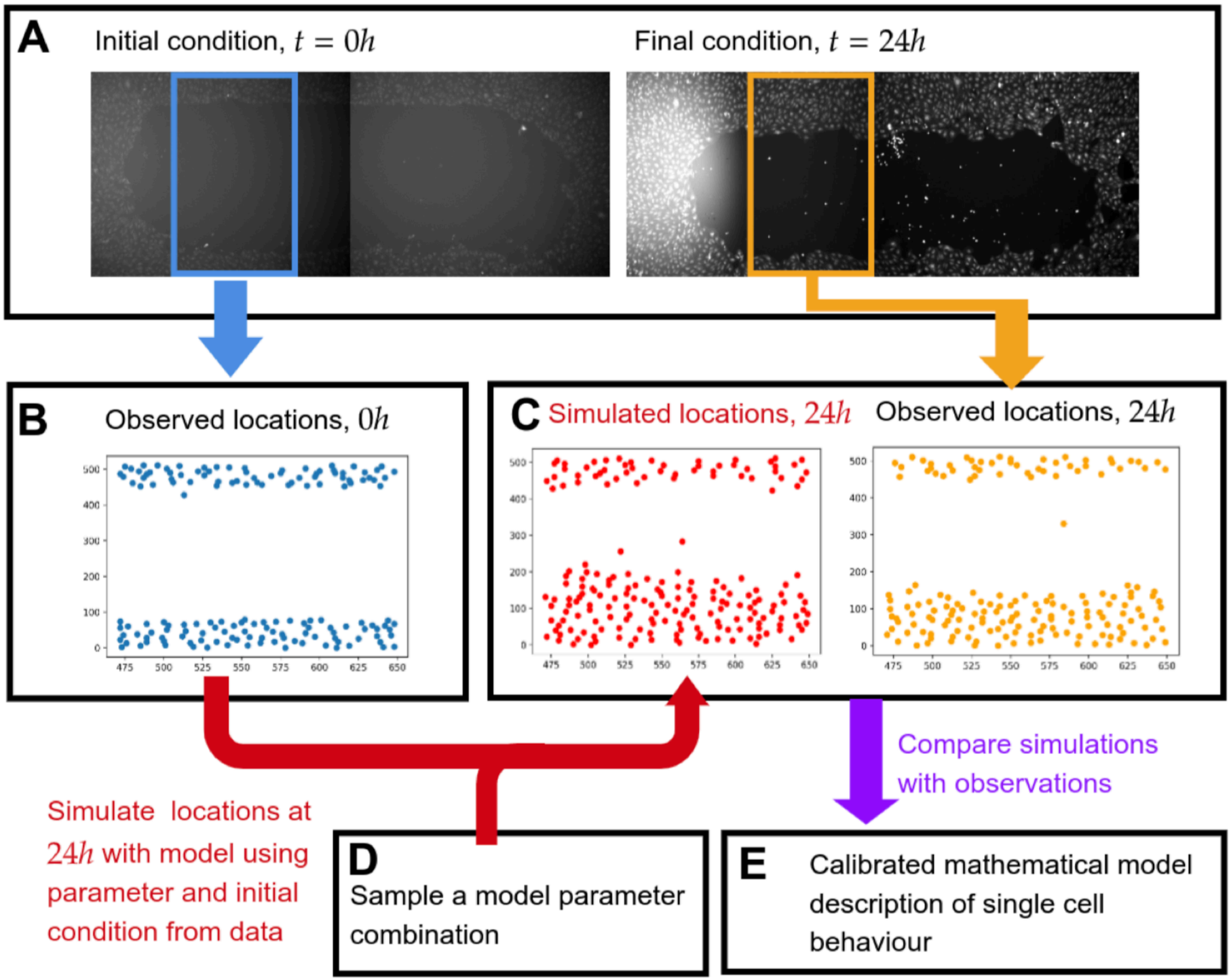
I Likelihood-free inference

- Bayesian inference without likelihoods
- ABC rejection sampling

II How well do algorithms work?

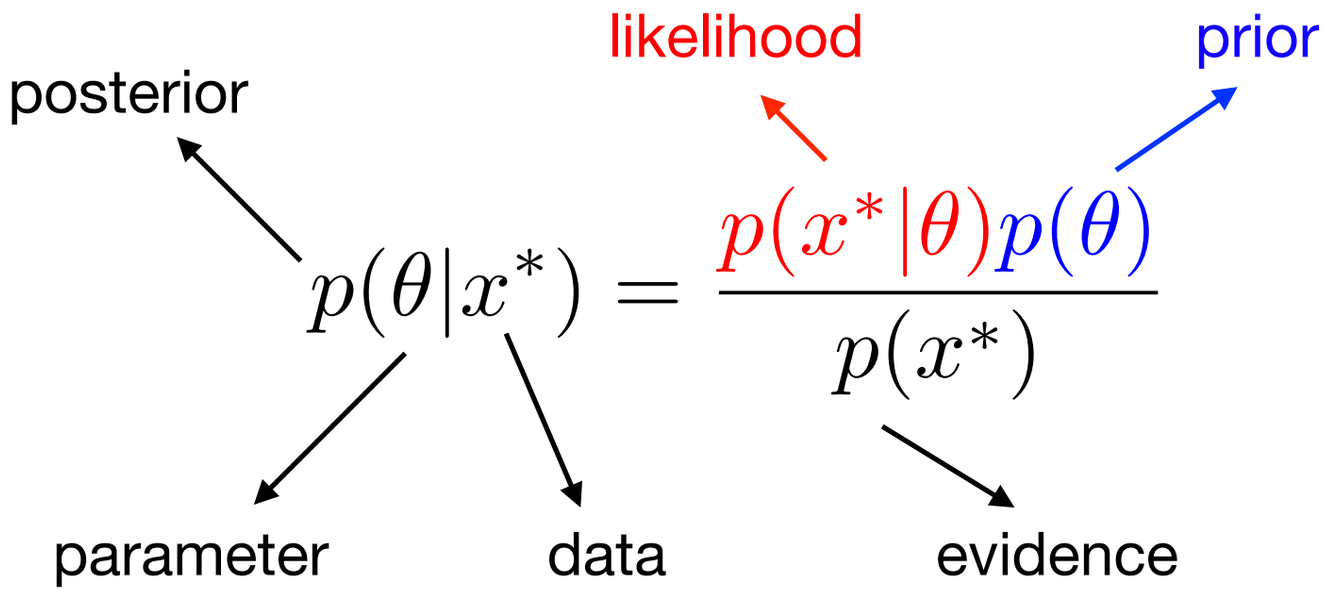
- Performance scores
  - Acceptance rate
  - Effective sample size
  - Error in expectations

III Comparing different scores



Martina-Perez et al., Efficient Bayesian inference for mechanistic modelling with high-throughput data, 2022

Bayesian inference



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Challenge 1: evidence can rarely be computed

Challenge 2: likelihood may be intractable → this talk

Likelihood-free inference

$$p(\theta|x^*) = \frac{p(x^*|\theta)p(\theta)}{p(x^*)}$$

For many models, we can't compute $p(x|\theta)$,

but we can simulate to draw samples $x \sim p(x|\theta)$.

ABC rejection sampling

“approximate Bayesian computation”

Step 1: sample parameters from prior

$$\theta_i \sim p(\theta)$$

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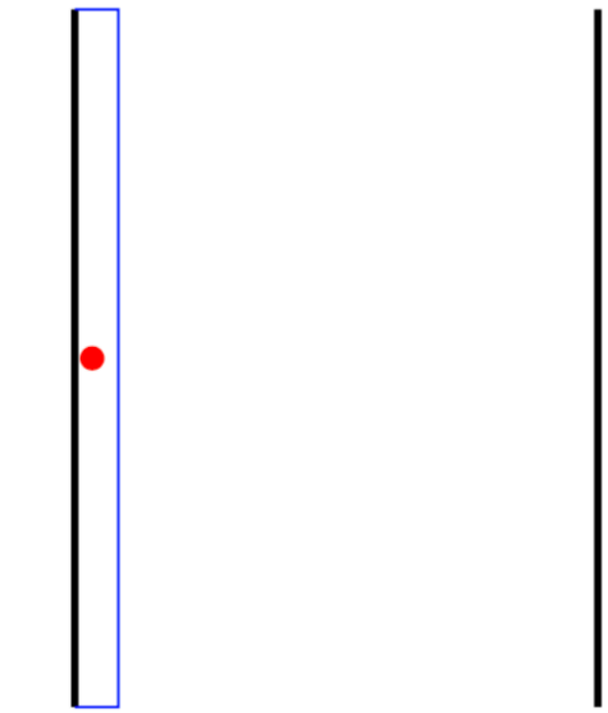
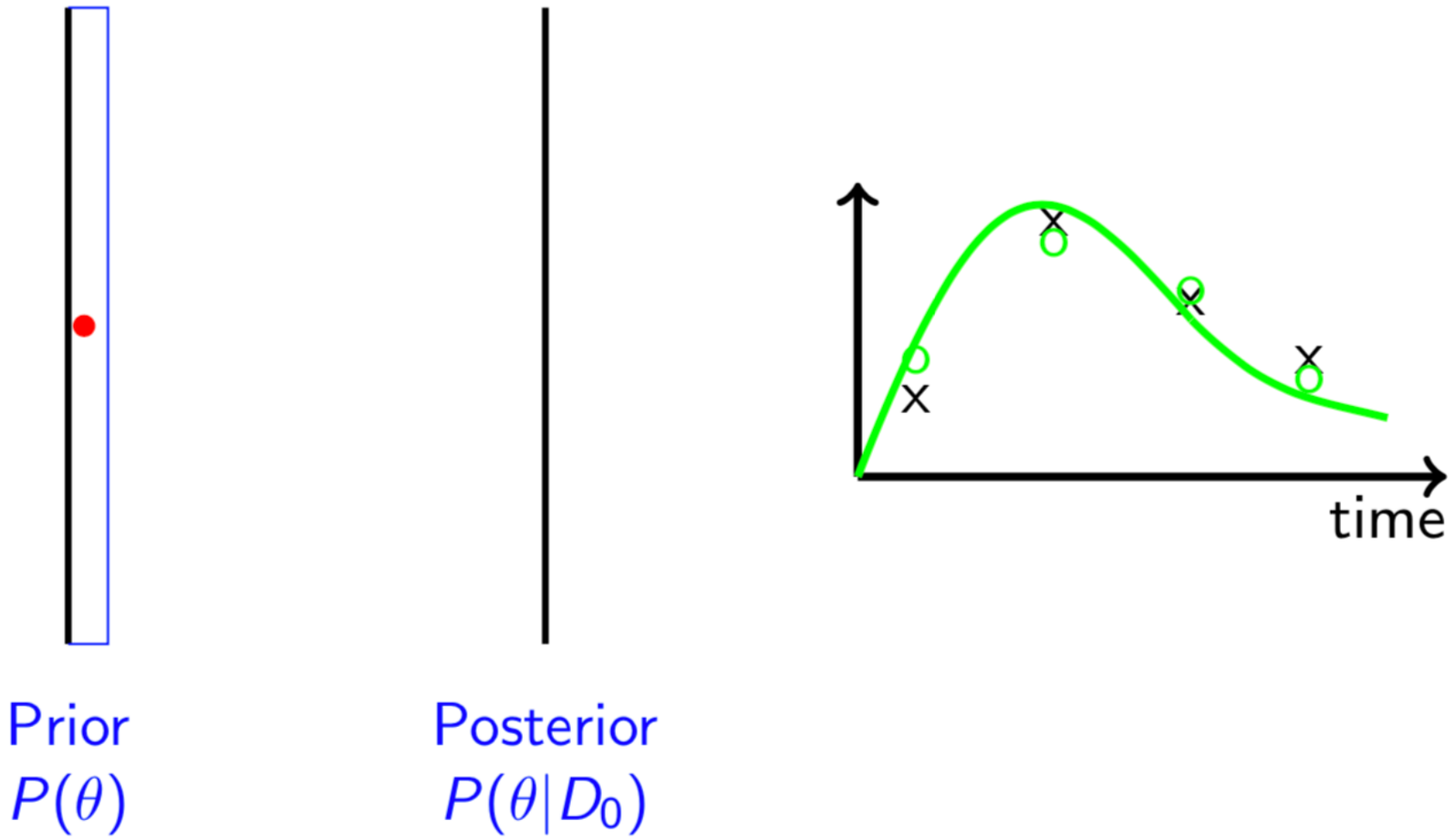


Prior
$P(\theta)$

Posterior
$P(\theta|D_0)$

Toni & Stumpf, Tutorial on ABC rejection and ABC SMC for parameter estimation and model selection, 2009

ABC rejection sampling



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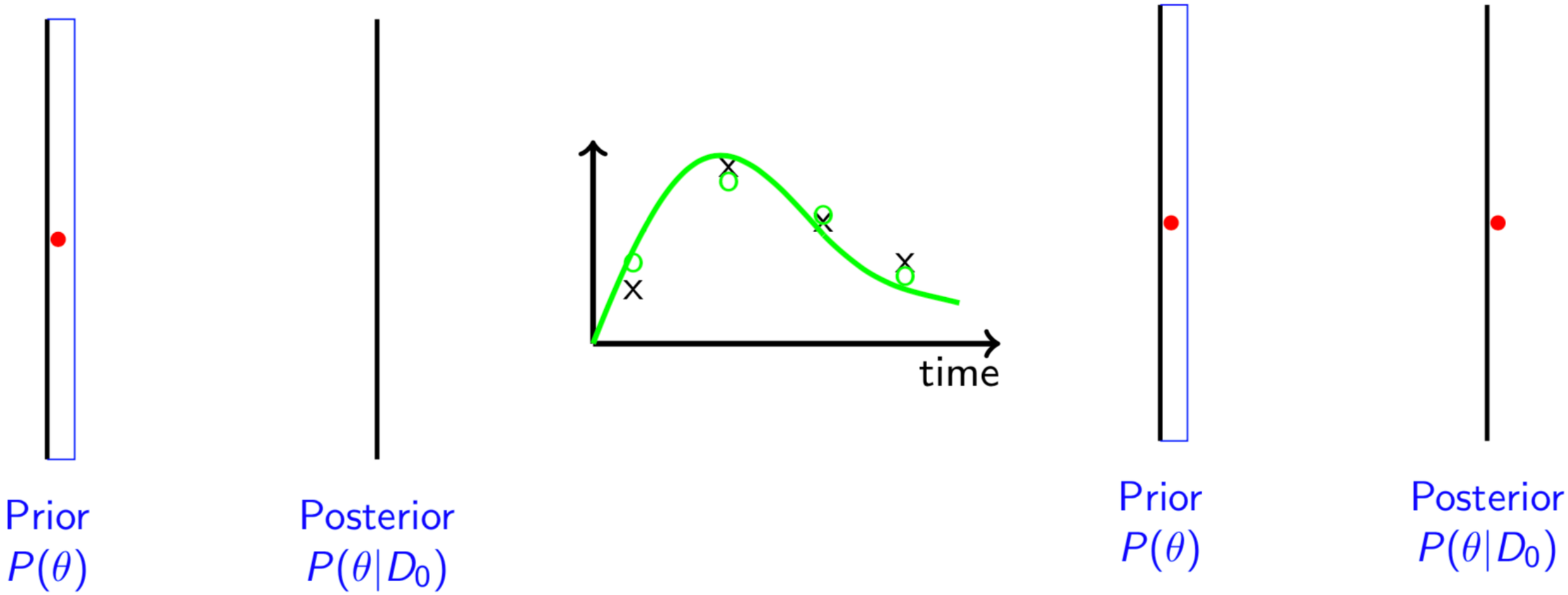

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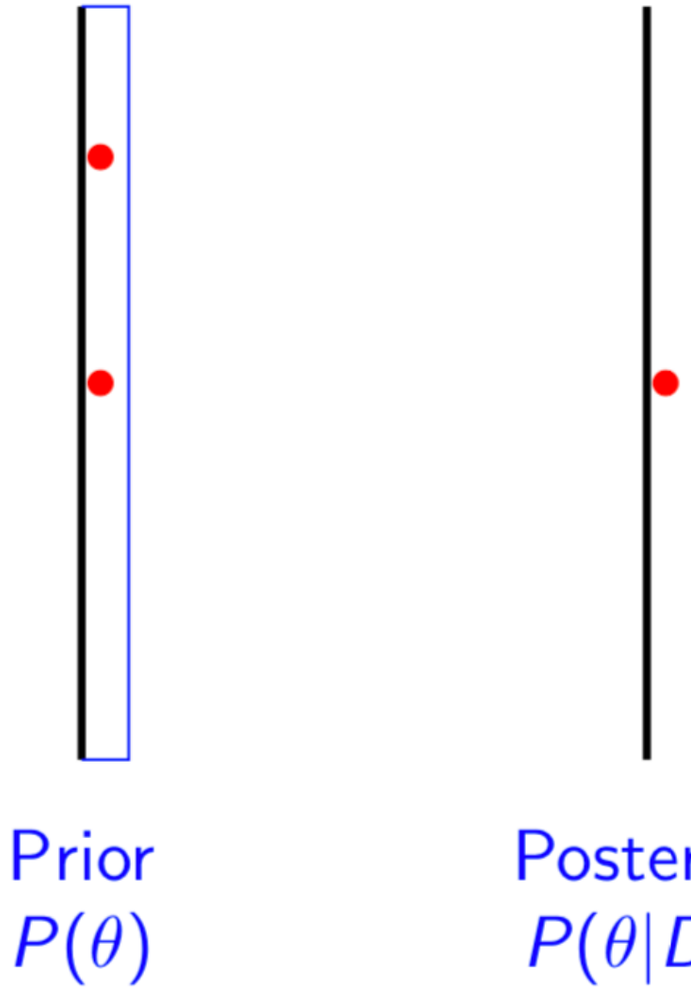

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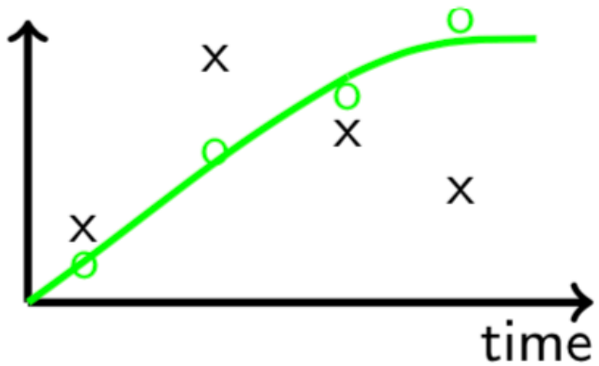

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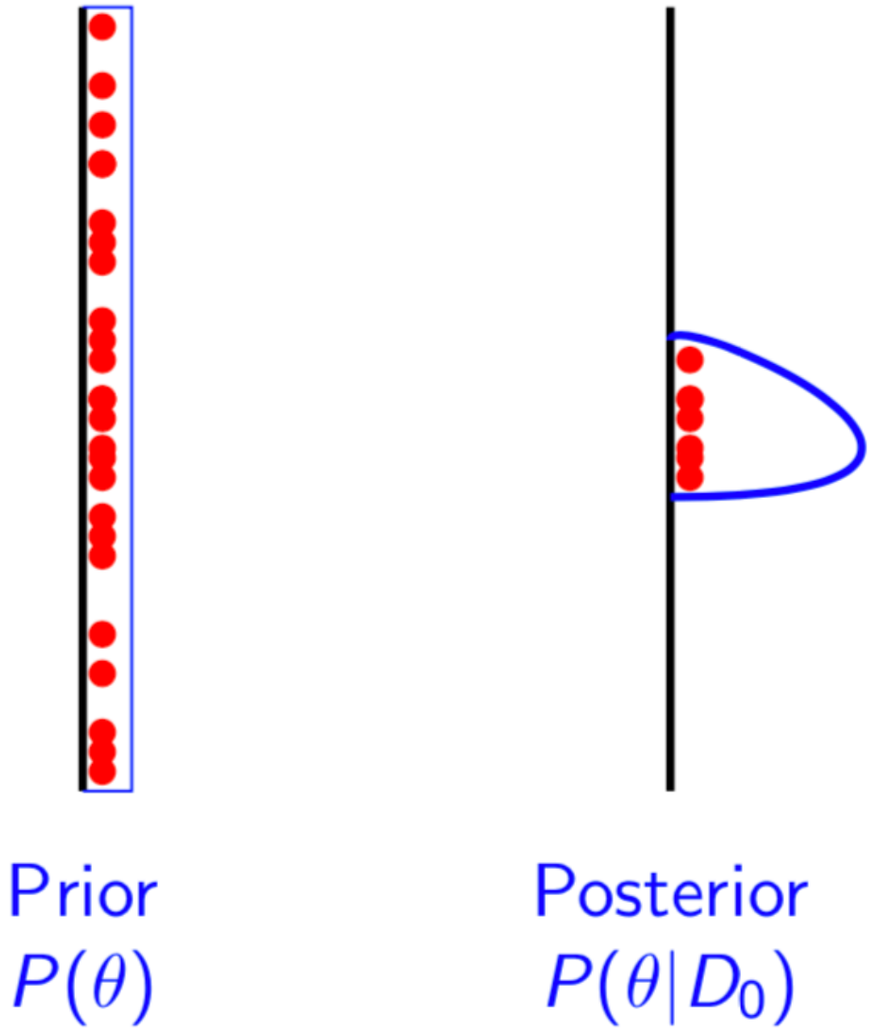

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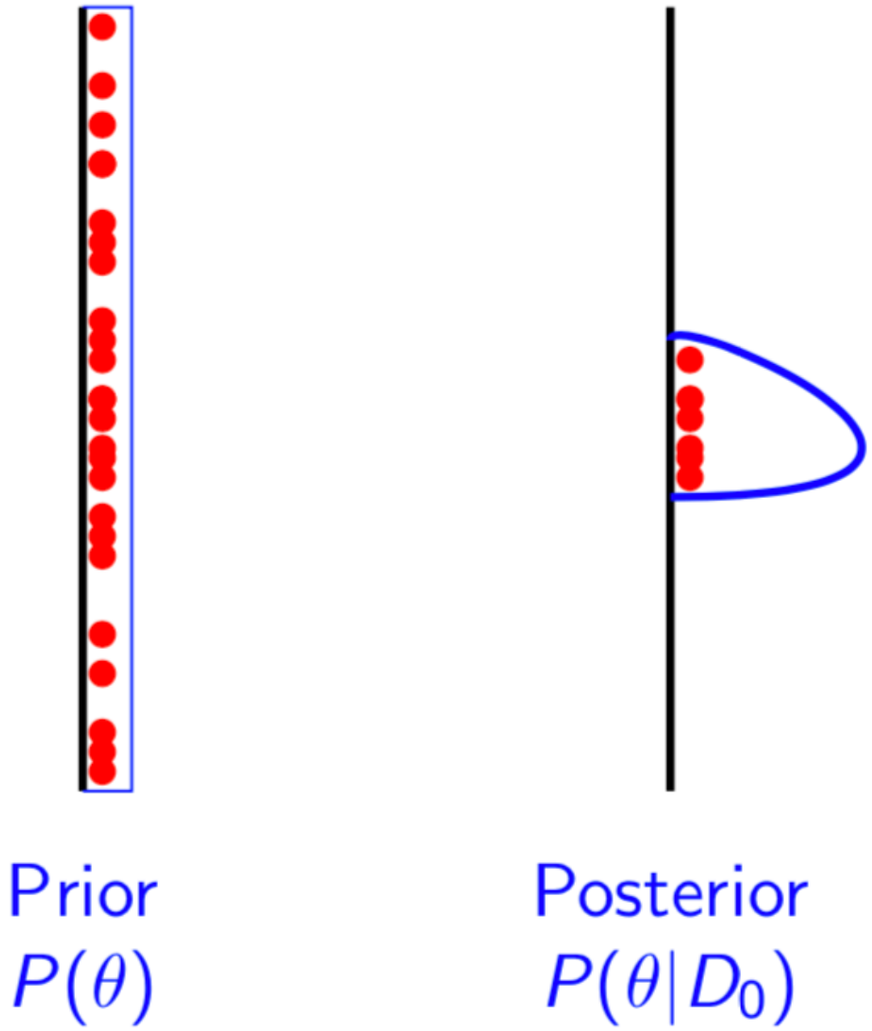

Many particles were rejected in the procedure, for which we have spent a lot of computational effort for simulation. ABC rejection is therefore computationally inefficient.

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With more accepted samples, our approximation should be better.

$\Longrightarrow$ *We want an algorithm with higher acceptance rate.*

Samples are more likely to be accepted where the likelihood is higher.

$\Longrightarrow$ *Sampling from the posterior should be better than sampling from the prior.*

Candidate scores for algorithms

1. Acceptance rate

$$\frac{N_{acc}}{N}$$

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$$\widehat{ESS} = \frac{\left(\sum_i w_i\right)^2}{\sum_i w_i^2}$$

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All of these are function expectations: $\mathbb{E}_{p(\theta|x^*)}[f(\theta)]$

Candidate scores for algorithms

1. Acceptance rate $\frac{N_{acc}}{N}$

2. Effective sample size $\widehat{ESS} = \frac{\left(\sum_i w_i\right)^2}{\sum_i w_i^2}$

3. Error in posterior expectations $\left|\left|\mathbb{E}_{\hat{p}(\theta|x^*)}[f(\theta)] - \mathbb{E}_{p(\theta|x^*)}[f(\theta)]\right|\right|^2$

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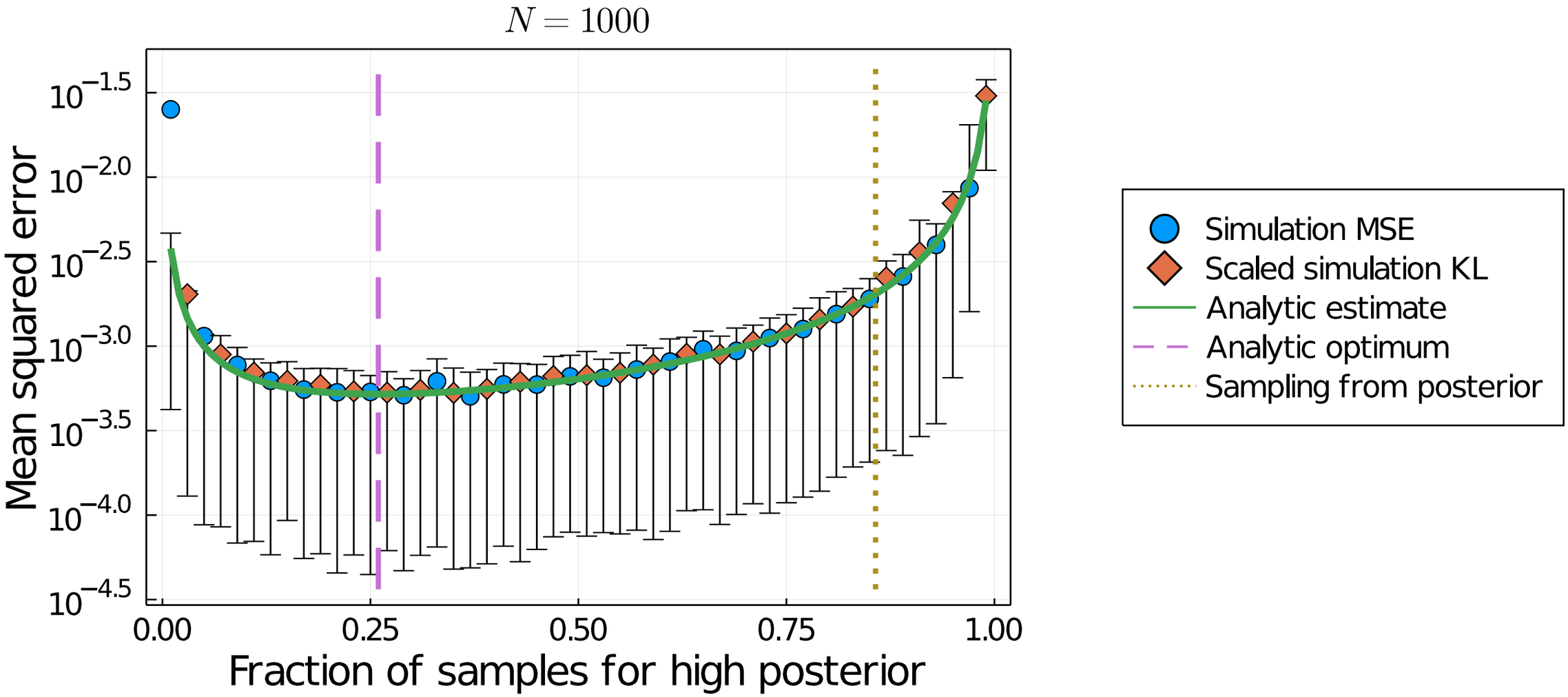
How do our scores depend on n_i?

Acceptance rate + ESS: always sample more where likelihood is higher.

Model selection with two hypotheses



Where did intuition go wrong?

Discrete parameter theory

i Variance calculation

ii Comparison of performance scores

Complications in practice

i Adaptive sampling

ii Continuous parameters

Expectation variance for discrete parameters

$$\mathbb{E}_{\hat{p}(\theta|x^*)}[f(\theta)] = \frac{\sum_i f(\theta_i)\hat{p}(x^*|\theta_i)p(\theta_i)}{\sum_i \hat{p}(x^*|\theta_i)p(\theta_i)} \equiv \frac{R}{S}$$

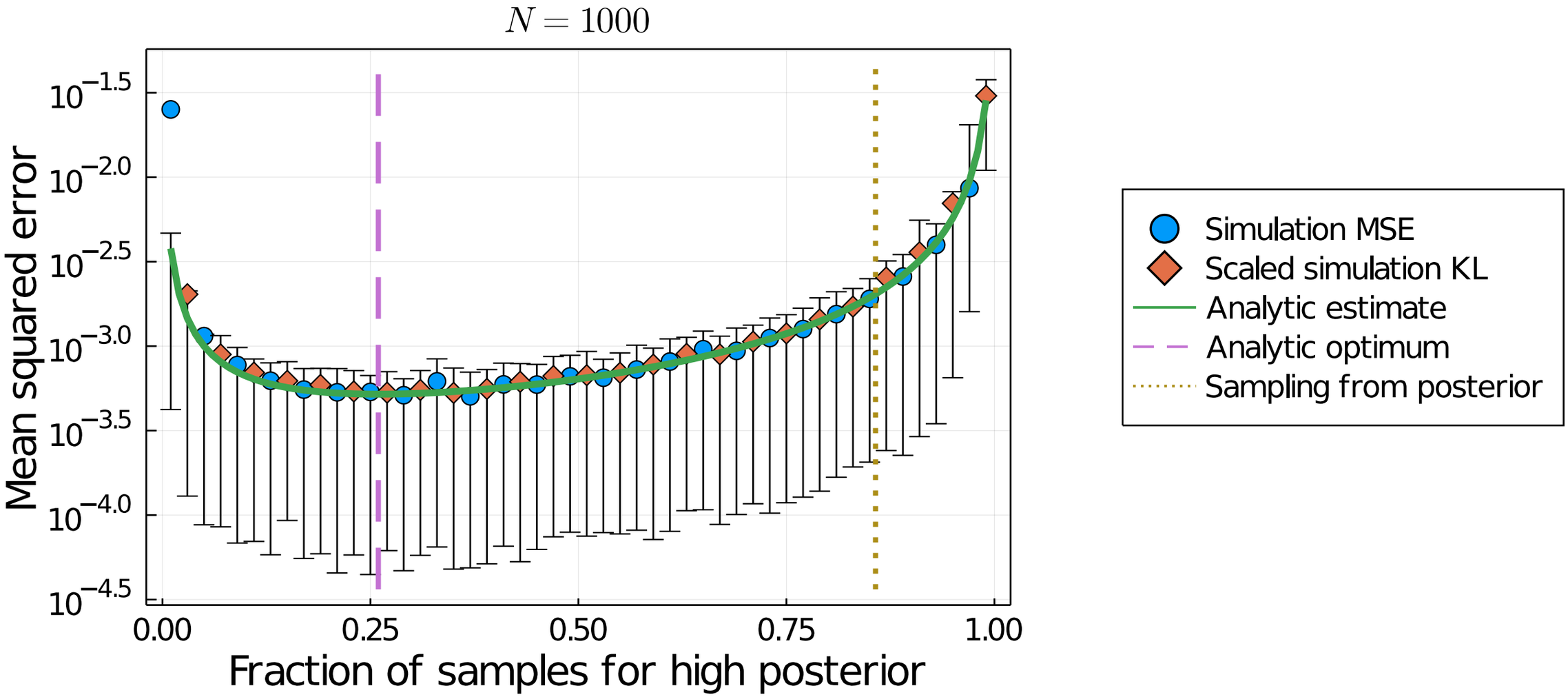
Delta method:

$$\mathrm{var}\left(\frac{R}{S}\right) \approx \frac{1}{\mu_S^2}\mathrm{var}(R) - 2\frac{\mu_R}{\mu_S^3}\mathrm{cov}(R,S) + \frac{\mu_R^2}{\mu_S^4}\mathrm{var}(S)$$

Expectation variance for discrete parameters

$$\mathrm{var}\left(\mathbb{E}_{\hat{p}(\theta|x^*)}\left[f(\theta)\right]\right) \approx p(x^*)^{-2} \sum_i p(\theta_i)^2 \frac{p(x^*|\theta_i)(1-p(x^*|\theta_i))}{n_i} \left(f(\theta_i) - \bar{f}\right)^2$$

Model selection with two hypotheses



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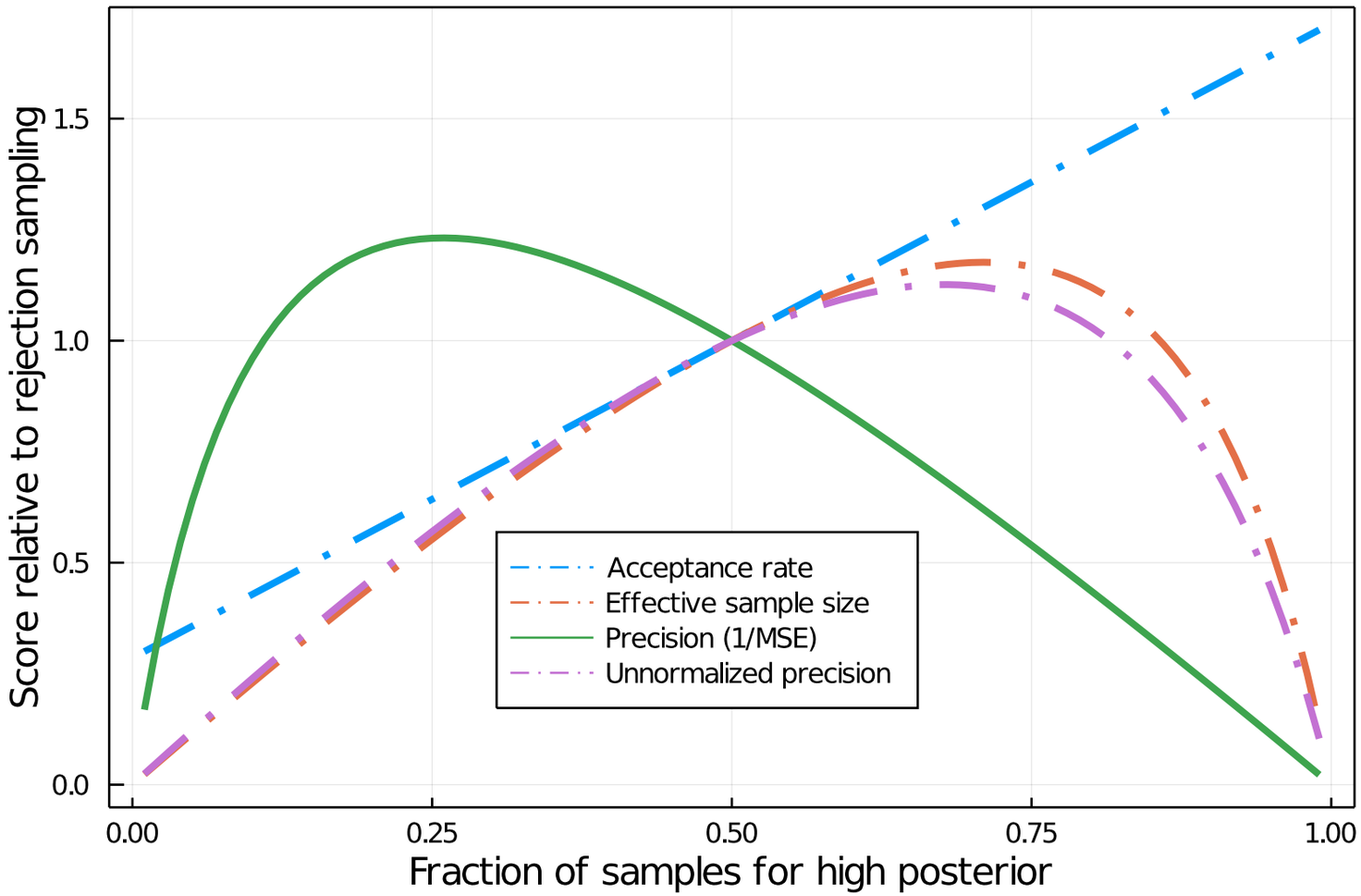

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Acceptance rate with rejection sampling

Expectation variance for discrete parameters

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$$n_i \propto p(\theta_i)(p(x^*|\theta_i)(1-p(x^*|\theta_i))^{1/2} \left| f(\theta_i) - \bar{f} \right|$$

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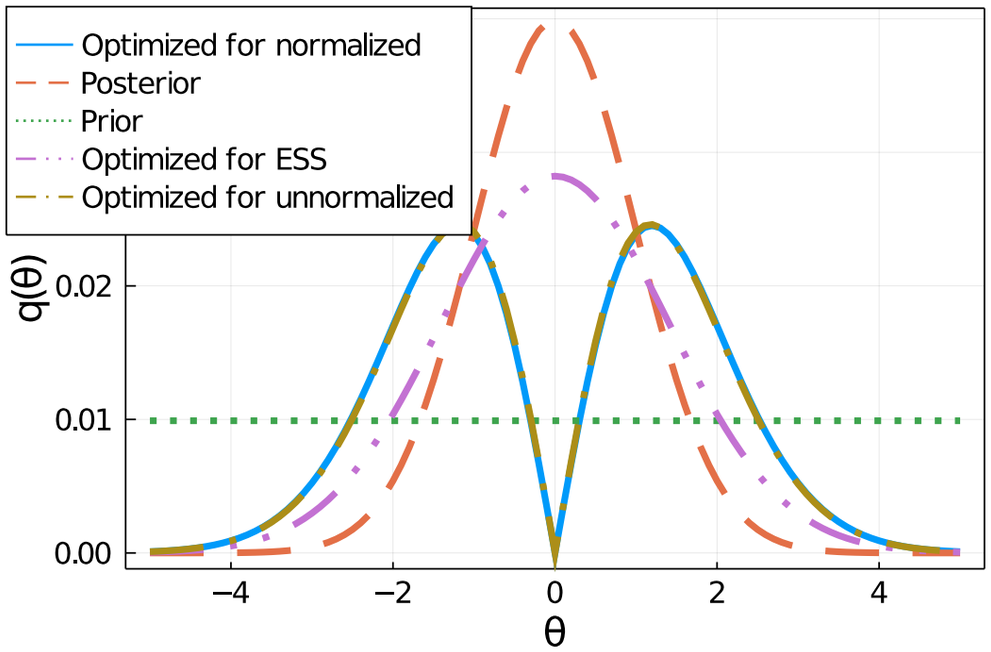
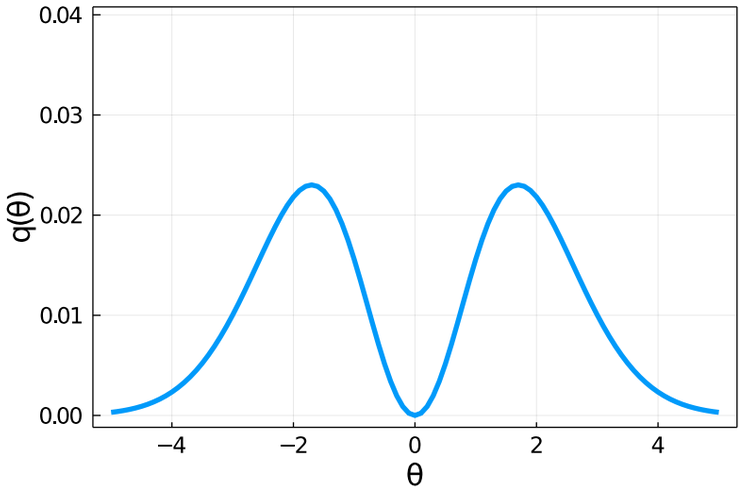
$$n_i \propto p(\theta_i)\left(p(x^*|\theta_i)(1-p(x^*|\theta_i)\right)^{1/2} \left|f(\theta_i) - \bar{f}\right|$$

$$n_1 \propto \left(p(x^*|\theta_2)(1-p(x^*|\theta_1))\right)^{1/2}$$

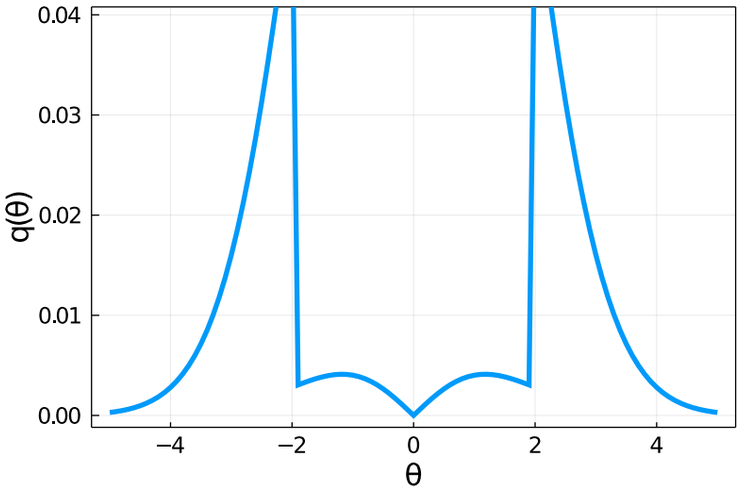
The optimal choice of simulations depends on *f*

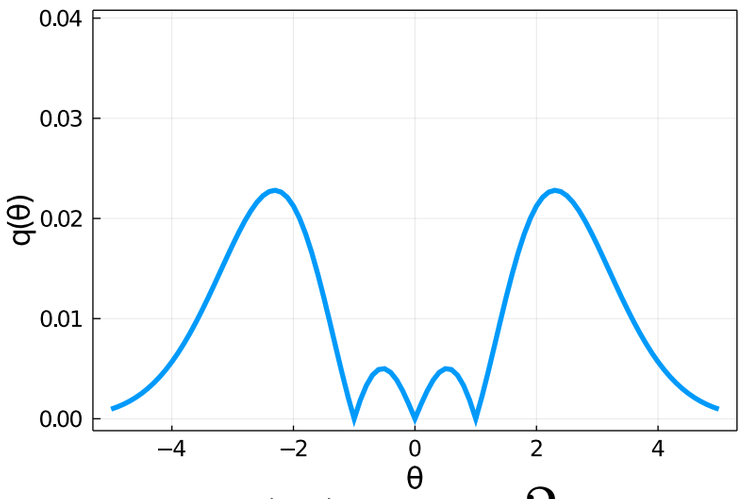


$f(\theta) = \theta$

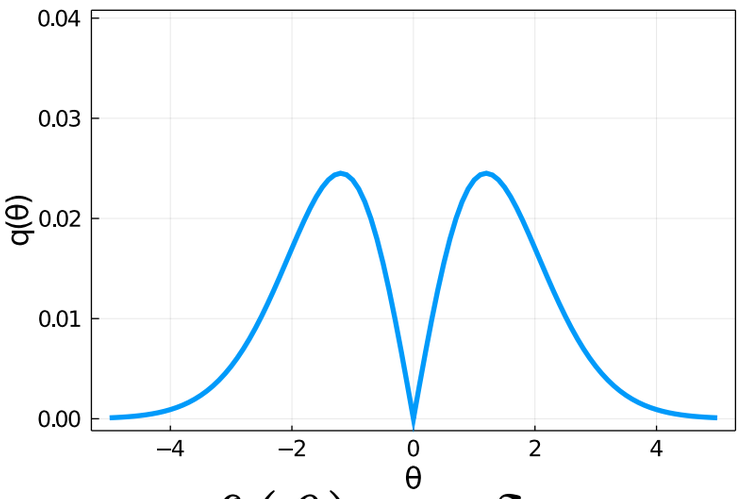


$f(\theta) = \mathbf{1}[|\theta| < 2]$



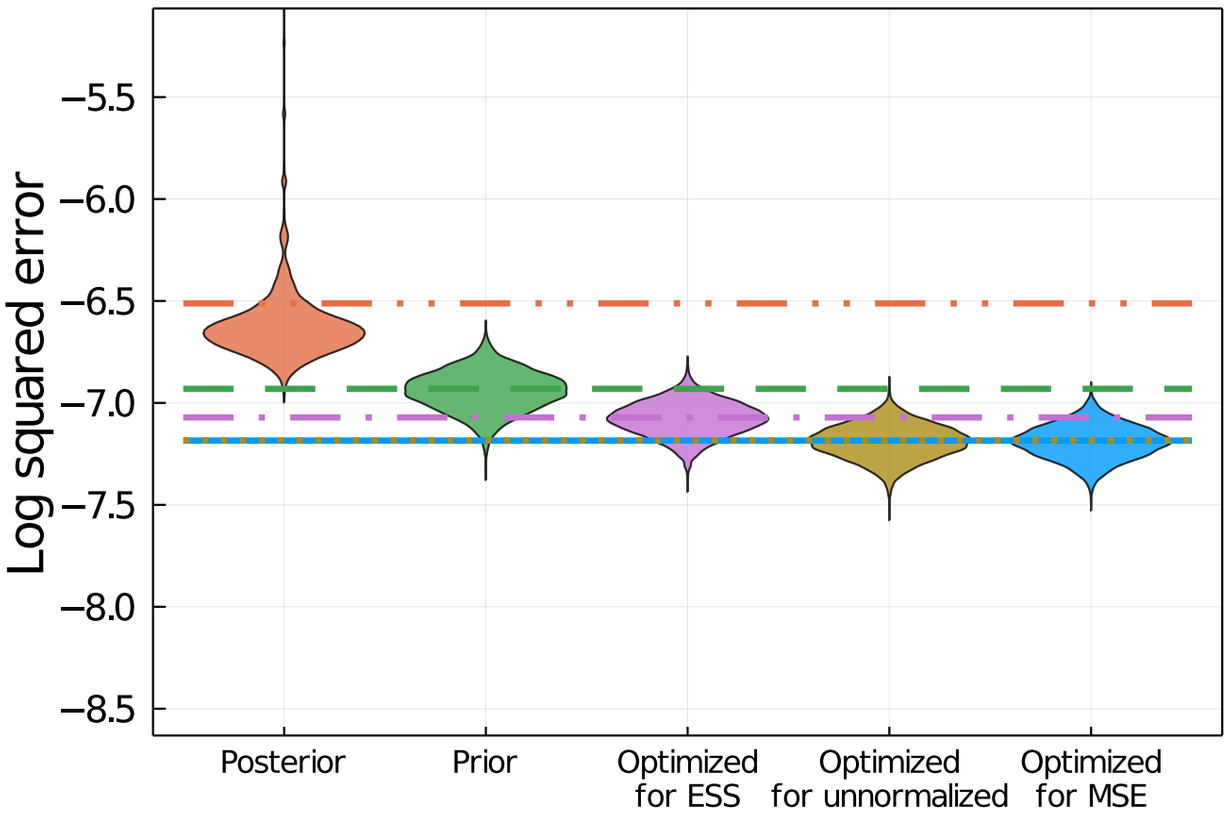


$f(\theta) = \theta^2$



$f(\theta) = \delta_{\theta,\theta'}$

Simulating from the posterior performs poorly



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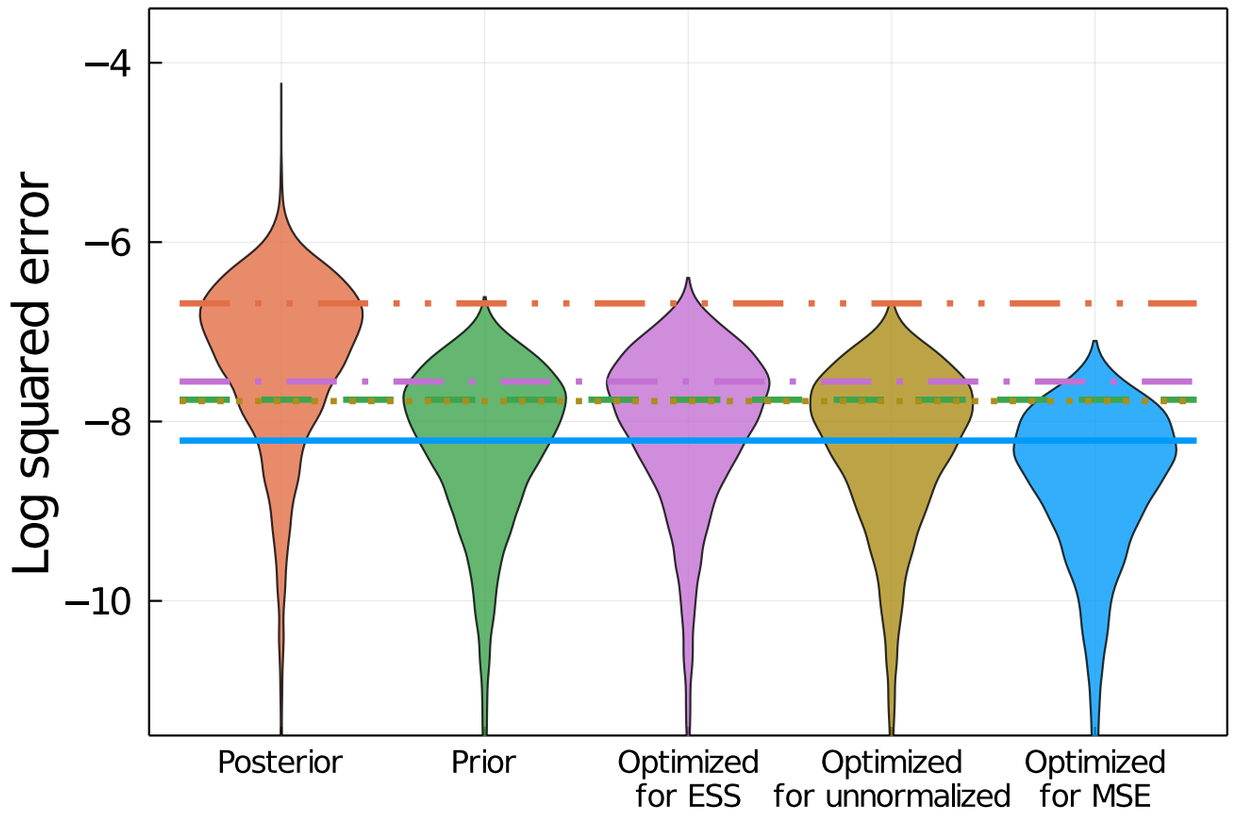

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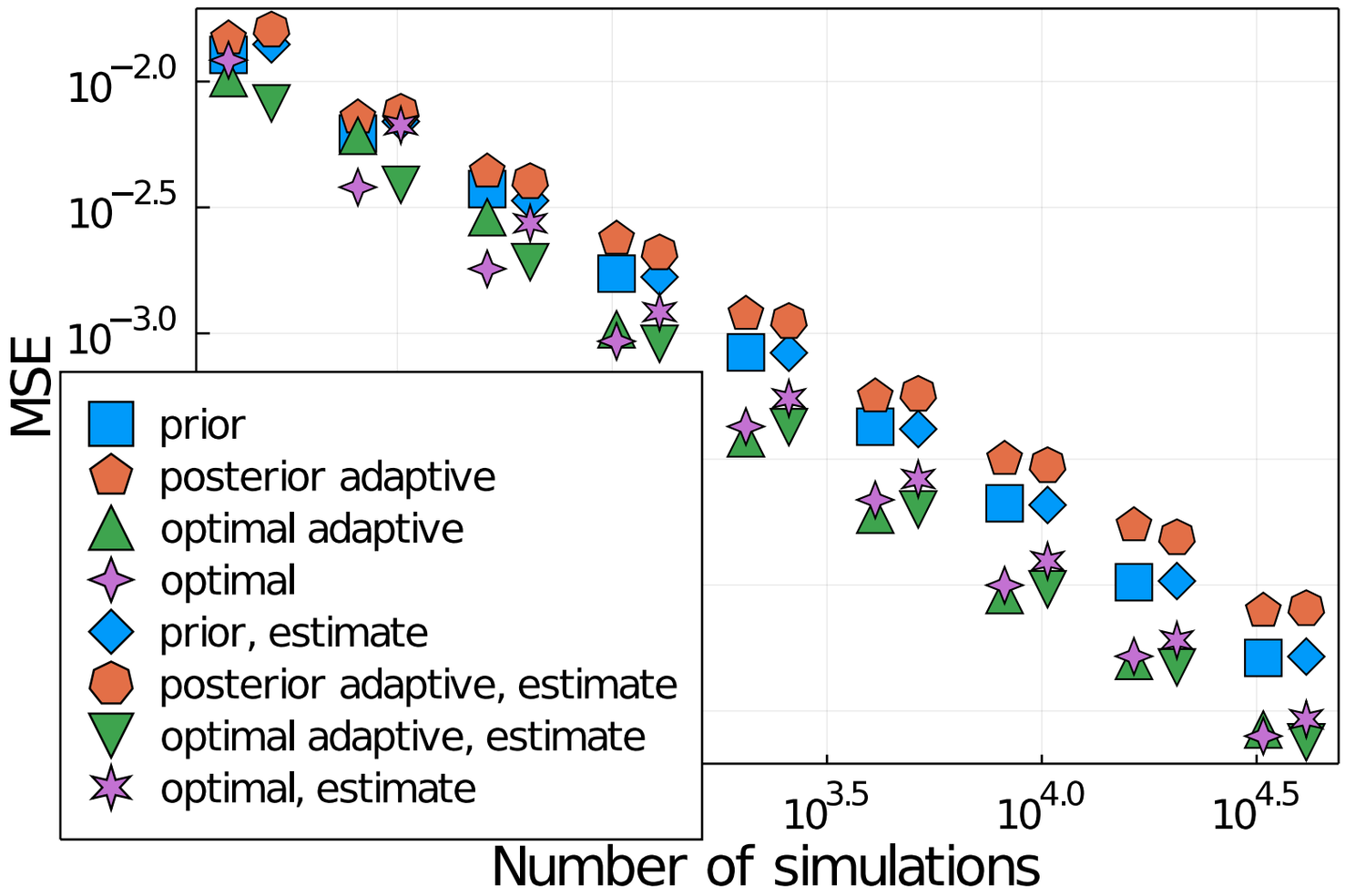
Adaptive sampling is straightforward

$$n_i \propto p(\theta_i)(p(x^*|\theta_i)(1-p(x^*|\theta_i))^{1/2}\left|f(\theta_i)-\bar{f}\right|$$



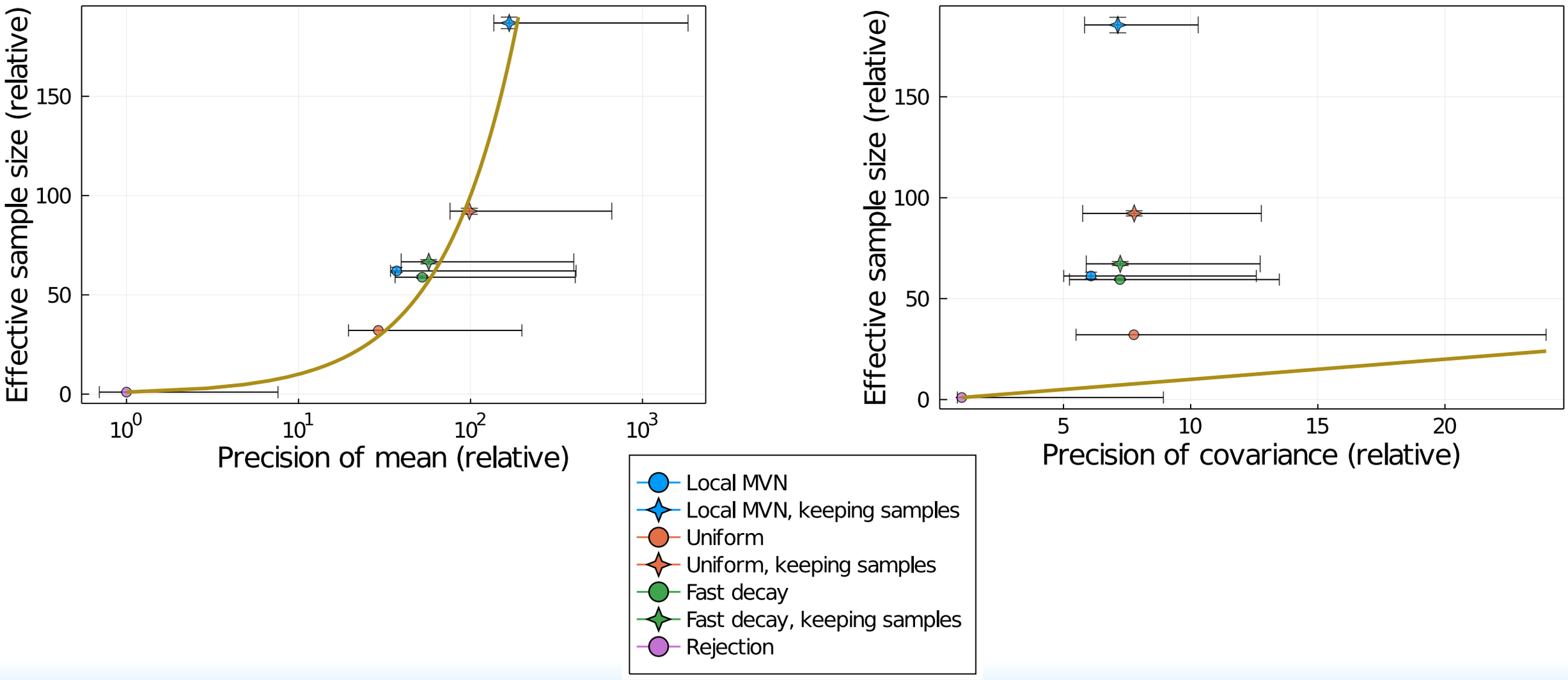
Results qualitatively translate to continuous parameters

Likelihood-free inference algorithms have two choices:

1. Which parameters to simulate from
2. How to approximate posterior from simulations

(2) is trivial for small discrete spaces, but not for continuous cases

Accuracy depends on target



Outline

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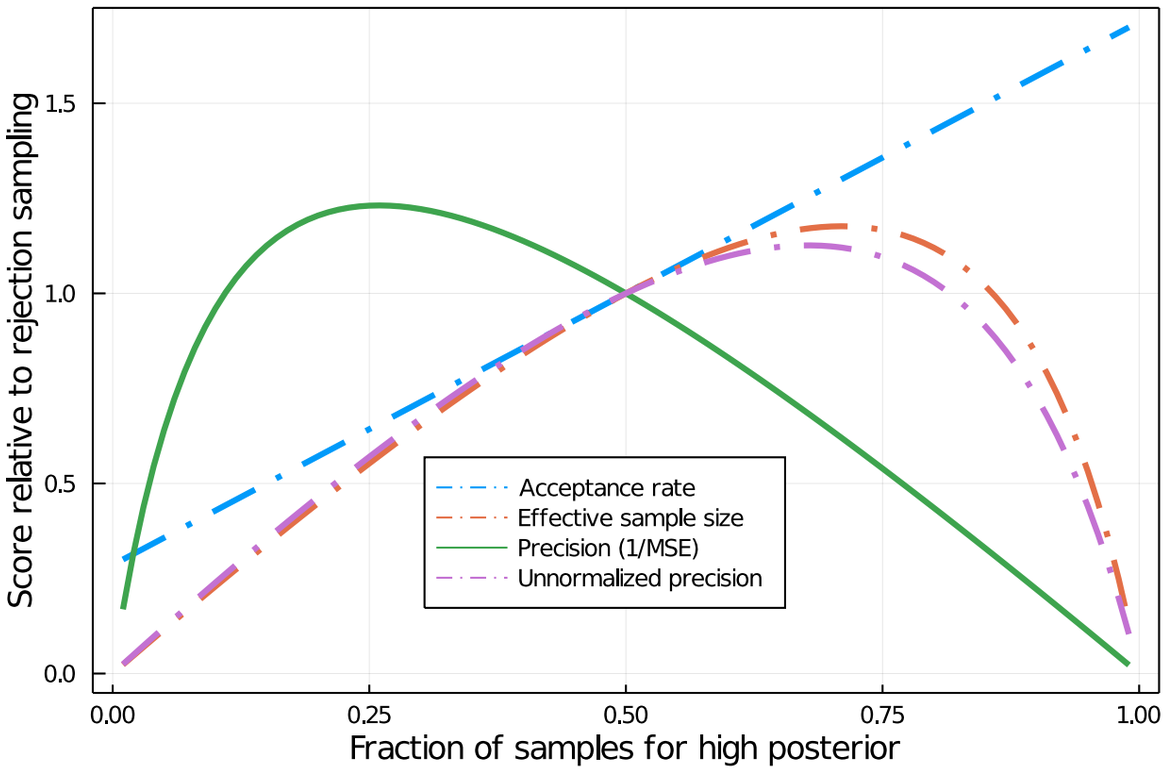
- ABC, ABC rejection

II How well do algorithms work?

- Performance scores

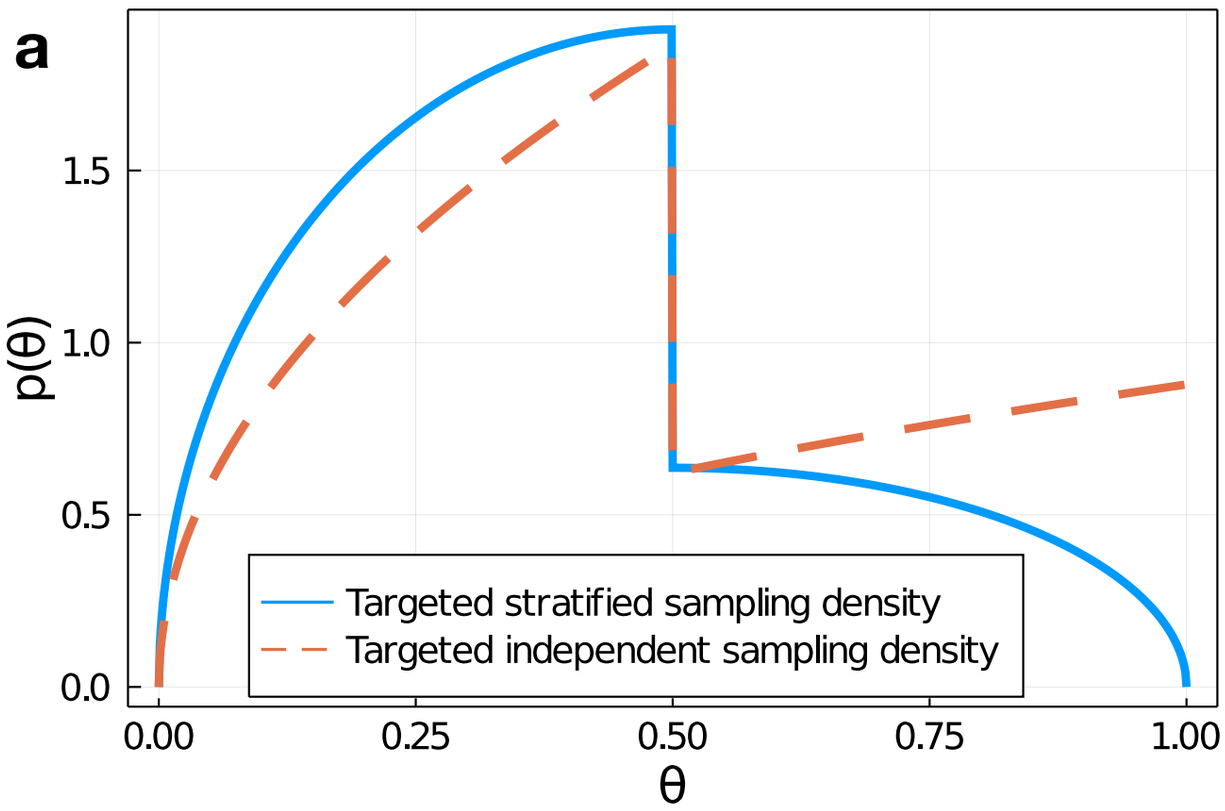
III Comparing different scores

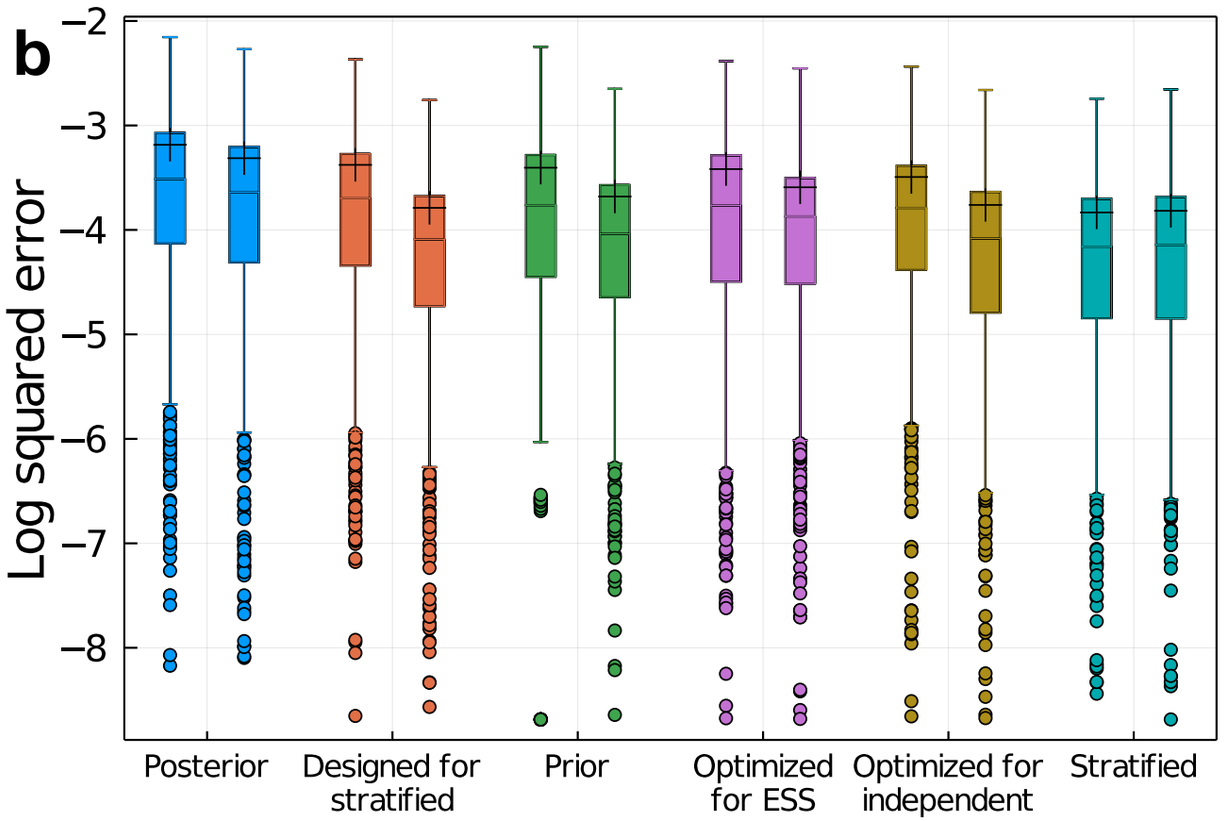
- How you measure performance matters
- ESS, and especially acceptance rate, are flawed heuristics
- If you know what you want to learn from your posterior, you can optimize your algorithm accordingly



Both sampling and estimation matter

$$\theta \in [0, 1] \qquad p(x^*|\theta) = \theta \qquad f(\theta) = \mathbf{1}[|\theta| > 0.5]$$





left: empirical average right: kernel regression

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“sequential Monte Carlo”: rather than sampling parameters from the prior, sample parameters from an adaptive approximation to the posterior

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We could instead take parameters from any round:

$$\{(\theta_i, w_i)\}_{all} = \{(\theta_{k,i}, \alpha_k w_{k,i}) | \Delta(x_{k,i}, x^*) < \epsilon_K,\ 1 \leq k \leq K\}$$

ESS is moderately informative about accuracy