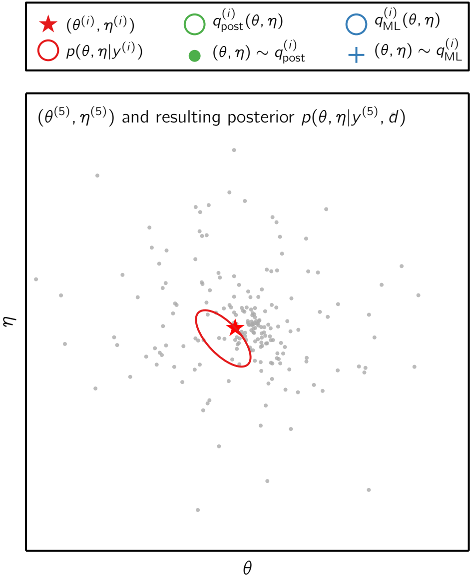
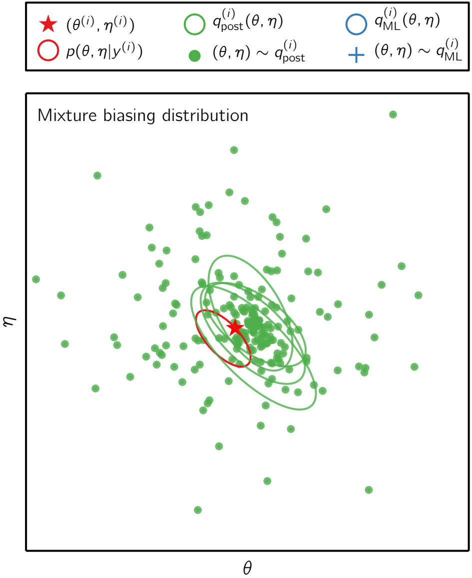
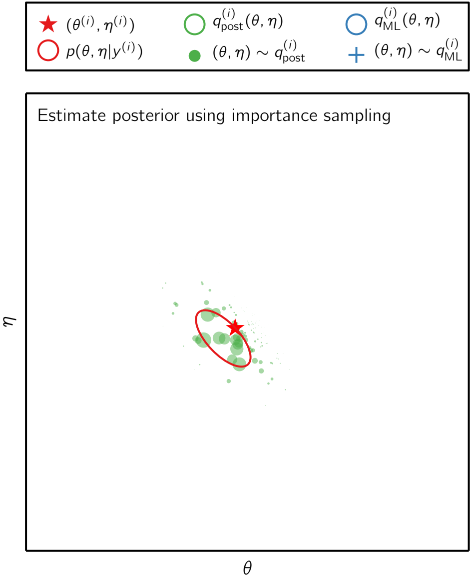
Layered multiple importance sampling



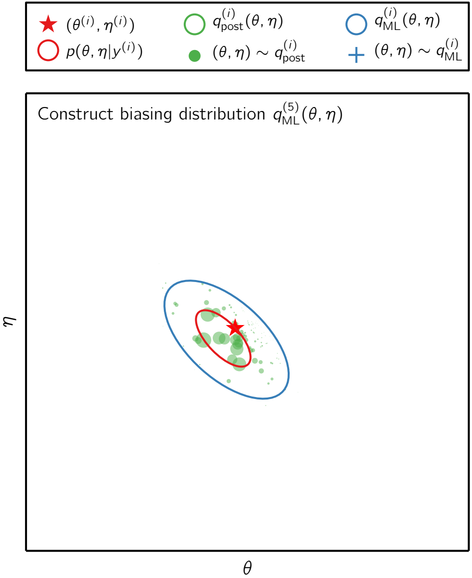
Layered multiple importance sampling

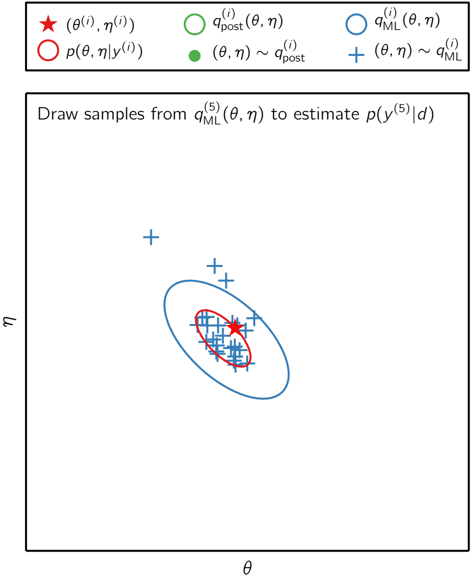


Layered multiple importance sampling

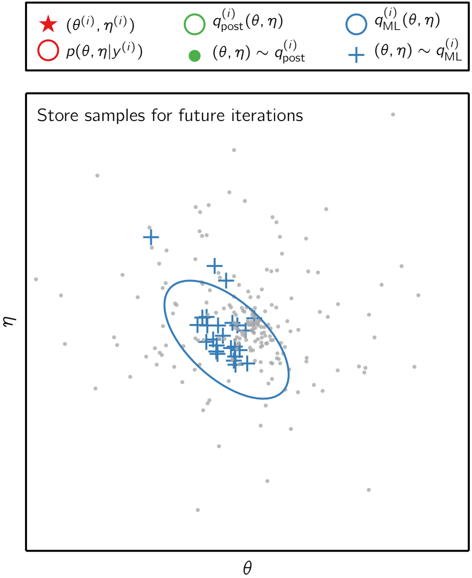


Layered multiple importance sampling

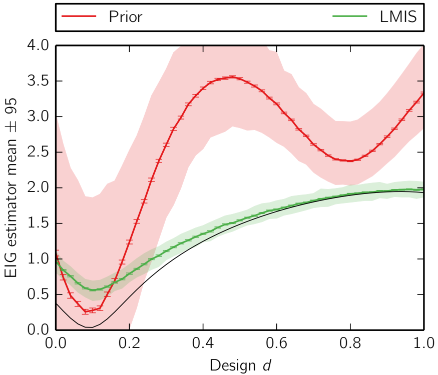



$(\theta^{(i)}, \eta^{(i)})$
$q_{\text{post}}^{(i)}(\theta, \eta)$
$q_{\text{ML}}^{(i)}(\theta, \eta)$
$p(\theta, \eta | y^{(i)})$
$(\theta, \eta) \sim q_{\text{post}}^{(i)}$
$(\theta, \eta) \sim q_{\text{ML}}^{(i)}$
Draw samples from $q_{\text{ML}}^{(5)}(\theta, \eta)$ to estimate $p(y^{(5)}|d)$
η
θ

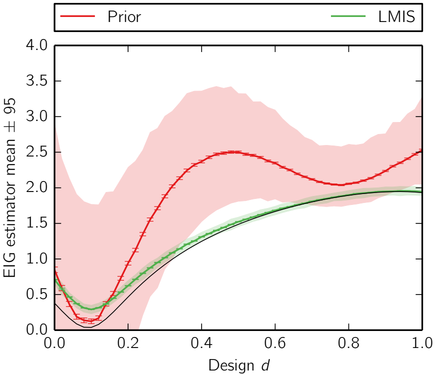
Layered multiple importance sampling



Numerical results: 4D linear–Gaussian example

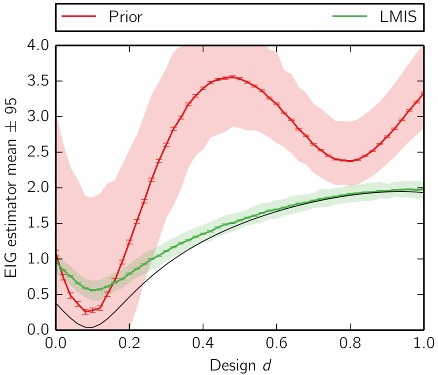


$N = M = 316$,
total 10^5 samples

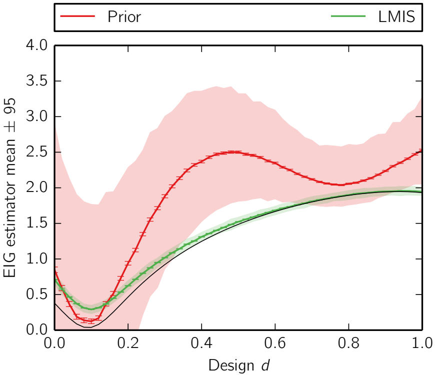


$(N = 1000,\ M = 100)$
$(N = 100,\ M = 1000)$
total 10^5 samples

Numerical results: 4D linear–Gaussian example



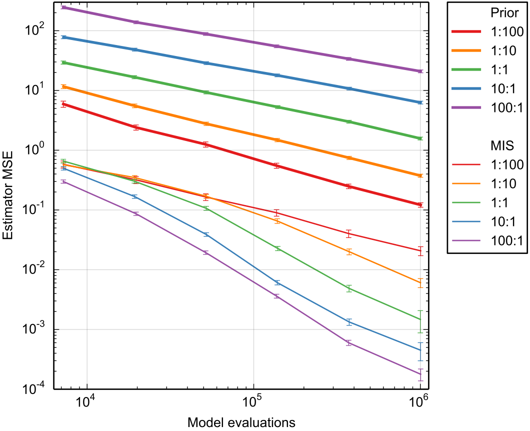
$N = M = 316$,
total 10^5 samples



($N = 1000,\ M = 100$)
($N = 100,\ M = 1000$)
total 10^5 samples

Q: What is a good ratio between N (# outer samples) and M (# inner samples)?

MSE vs. # model evaluations



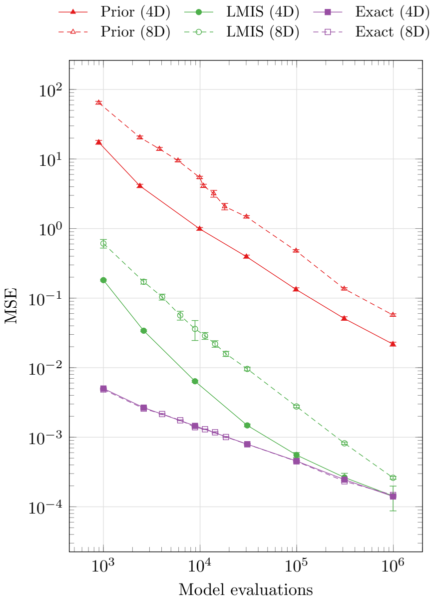
Prior strategy:

- Bias–variance tradeoff
- MSE here dominated by **bias**: use large M, small N
- Asymptotically optimal scaling is $M \sim N^{1/2}$

LMIS strategy: use large N, small M

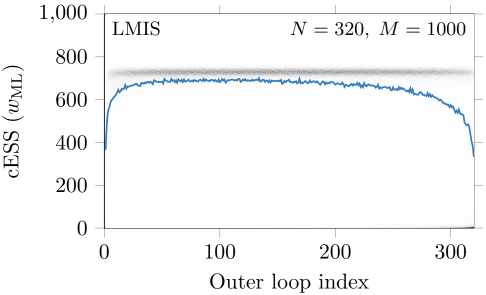
- Increasing N (outer) can improve quality of inner biasing distributions
- Seemingly no bias-variance tradeoff; just increase N
- Optimal scaling?

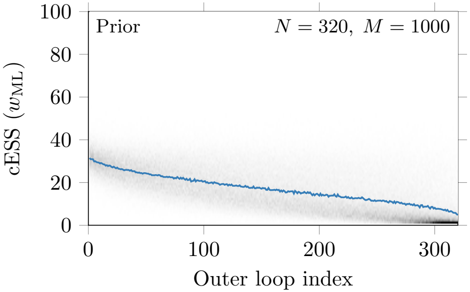
Convergence (MSE vs. # model evaluations)



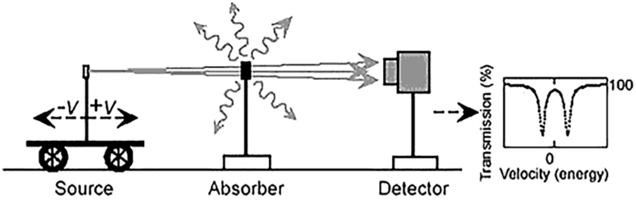
- Using $N/M = 100$ in LMIS, corresponding favorable ratio for prior

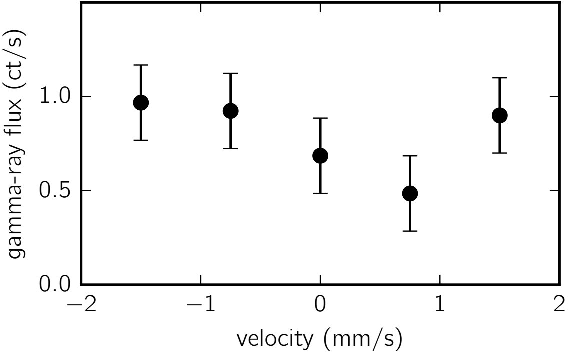
Incremental enrichment at work



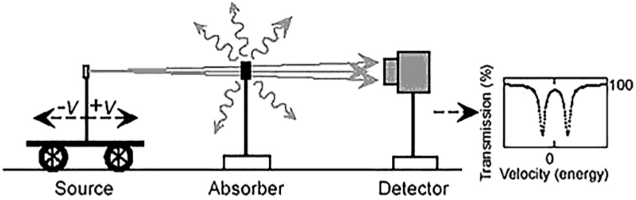


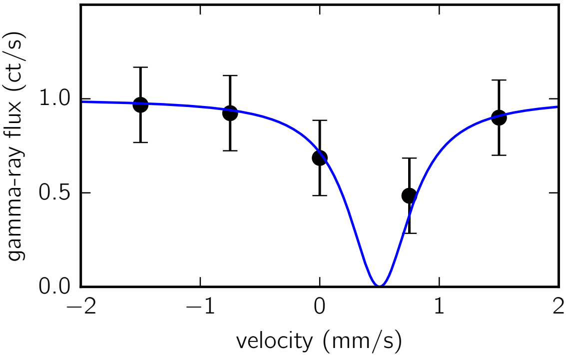
Nonlinear example: Mössbauer spectroscopy



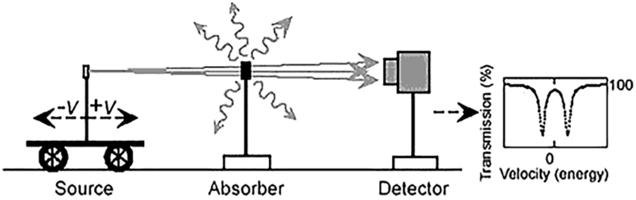


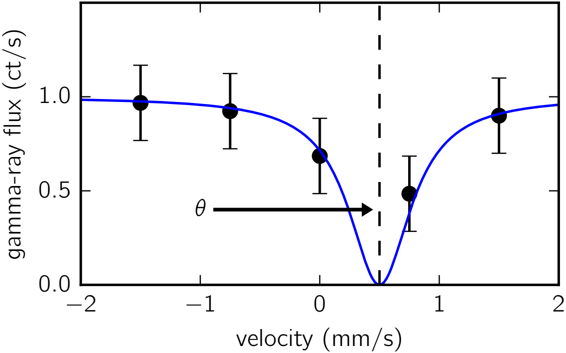
Nonlinear example: Mössbauer spectroscopy



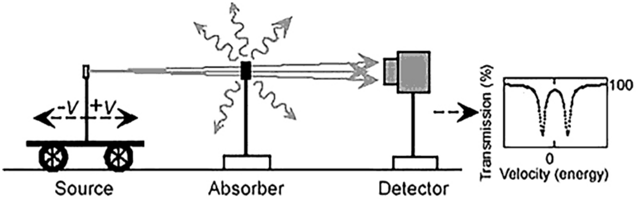


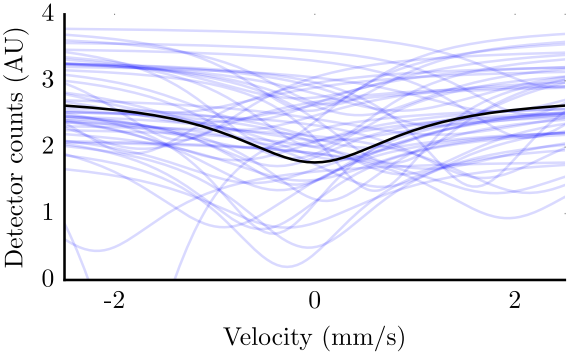
Nonlinear example: Mössbauer spectroscopy





Nonlinear example: Mössbauer spectroscopy

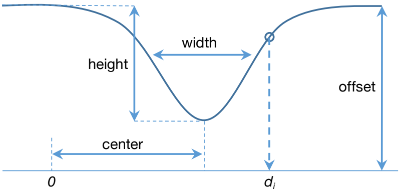


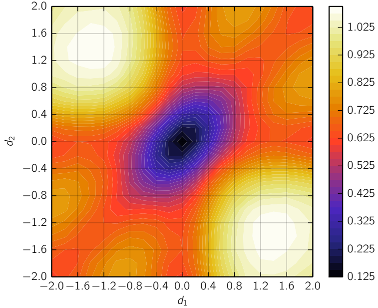


$$y_i = \text{offset} - \text{height}\frac{\text{width}^2}{\text{width}^2 + (\text{center} - d_i)^2} + \epsilon_i$$

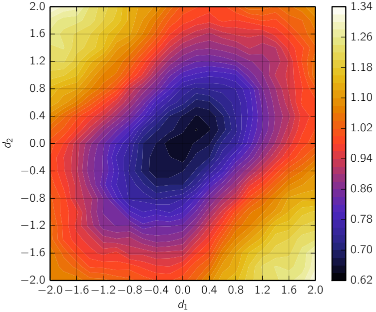
$\text{center} \sim \mathcal{N}(0, 1)$ $\quad$ $\exp(\text{height}) \sim \mathcal{N}(0, 0.3)$

$\exp(\text{width}) \sim \mathcal{N}(0, 0.3)$ $\quad$ $\exp(\text{offset}) \sim \mathcal{N}(1.0, 0.2)$





Expected utility for 'center' parameter
$\boldsymbol{d} = (0, d_1, d_2)$



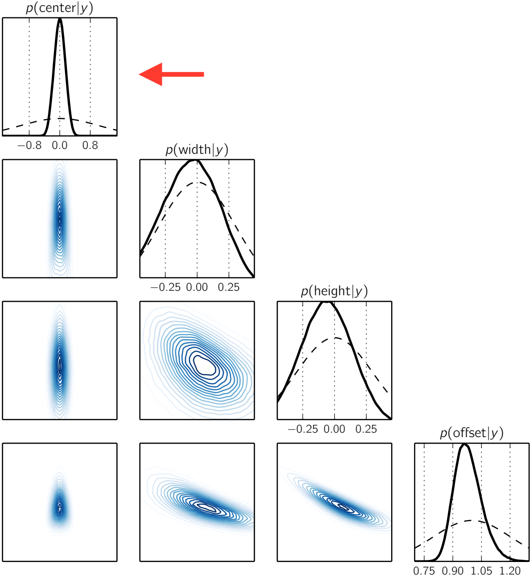
Expected utility for 'offset' parameter
$\boldsymbol{d} = (0, d_1, d_2)$

Posterior of optimal design for ‘center’

- Optimal design for ‘center’

$$\boldsymbol{d} = (-1.3, 0, 1.3)$$

- Non-Gaussian posteriors

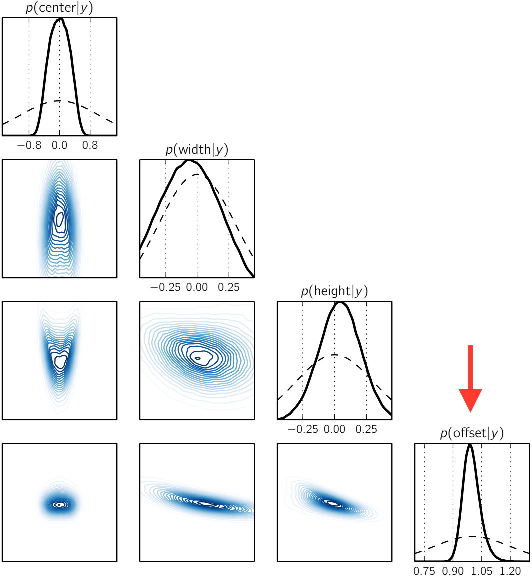


Posterior of optimal design for ‘offset’

- Optimal design for ‘offset’

$$\boldsymbol{d} = (-2, 0, 2)$$

- Non-Gaussian posteriors



Key extensions

- Focused design is a natural framework for incorporating models of **model inadequacy**
  - Stochastic representations of model inadequacy; hierarchical Bayesian models
  - Design experiments *robust* to model inadequacy
  - Design experiments to *elucidate* model inadequacy

Key extensions

- Focused design is a natural framework for incorporating models of **model inadequacy**
  - Stochastic representations of model inadequacy; hierarchical Bayesian models
  - Design experiments *robust* to model inadequacy
  - Design experiments to *elucidate* model inadequacy

- LMIS framework provides "hooks" for large-scale computation
  - Upper layer: estimate moments to devise a biasing distribution for the current posterior
    - Use and *reuse* Laplace approximations (cf. Beck *et al.* 2017)
    - Biasing distributions from different parametric families
  - Control variates for outer loop variance reduction
  - Hierarchies of model approximations

Future challenges/opportunities

- Model error or *misspecification* in Bayesian inference (broadly) and OED (specifically). **Robustness!**
- Richer or goal-oriented design criteria:
  - OED linked to downstream *optimization under uncertainty*
  - OED to better characterize material failure or rare events (from *indirect* data)
- Role of fast **approximate inference** in evaluating design criteria
- Optimal *sequential experimental design*, particularly in dynamic environments:
  - Dynamic programming; massive computational challenges