

Uncertainty prop. using Monte Carlo estimators

- we can get global approximations for $E[f]$ + $\text{Var}[f]$ by

$$E[f]_{MC} \approx \frac{1}{M} \sum_{i=1}^M f(\vec{x}; \vec{\theta}^i) = \bar{f}$$

$$\text{Var}[f]_{MC} \approx \frac{1}{M-1} \sum_{i=1}^M (f(\vec{x}; \vec{\theta}^i) - \bar{f})^2$$

$$= \underbrace{E[f^2]}_{\text{approx by MC}} - \bar{f}^2$$

where $\vec{\theta}^i \sim p(\vec{\theta})$ come from some PDF on $\vec{\theta}$.

ISSUE: This converges with rate $O(1/\sqrt{M})$

Bayesian Framework

- If we solve a Bayesian inverse problem first, we can use $\pi(\vec{\theta} | \vec{y})$ to generate credible + prediction intervals for \vec{y} .

- Let $y_i = f(x_i; \vec{\theta}) + \epsilon_i$, $\epsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_\epsilon^2)$, $i=1, \dots, N_y$, $y_i \in \mathbb{R}$

• We have likelihood

$$P(\vec{y} | \vec{\theta}, \sigma_\epsilon^2) = \frac{1}{(2\pi\sigma_\epsilon^2)^{N_y/2}} \exp\left(-\frac{1}{2\sigma_\epsilon^2} \sum_{i=1}^{N_y} (y_i - f(x_i; \vec{\theta}))^2\right)$$

- The posterior predictive distribution is

$$\pi^*(y^* | \vec{y}_{\text{prev}}) = \int_{\mathbb{R}} \int_{\mathbb{R}^p} P(y^* | \vec{\theta}, \sigma_\epsilon^2) \underbrace{\pi(\vec{\theta}, \sigma_\epsilon^2 | \vec{y}_{\text{prev}})}_{\text{Posterior}} d\vec{\theta} d\sigma_\epsilon^2$$

Algorithm

i) Specify M_{pred} Samples

ii) For $i=1, \dots, M_{\text{pred}}$

1) Draw $\vec{\theta}^i$ from posterior chain (use previous chain)

2) Sample $\epsilon^i \sim N(0, \sigma_\epsilon^2)$, where

a) σ_ϵ^2 is fixed

b) Draw σ_ϵ^2 from chain

3) Generate $\vec{y}^* = f(x^*; \vec{\theta}^i) + \epsilon^i$

iii) Sort \vec{y}^* + construct quantile