Supplemental Sampling Details

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This appendix outlines the details of the sampling discussed in Section 3.1 of the main text. The parameters to update are:

- Correlation scale parameters for the emulator and discrepancy: β , γ
- Precision parameters for the emulator and discrepancy: κ , κ_{δ}
- Calibration parameters: $\boldsymbol{\theta}$
- Likelihood parameters: $\boldsymbol{\omega}_o$
- Link-transformed latent mean values: $g(\mu(\mathbf{x}))$

1 Sampling β , γ , κ , κ_{δ} , θ

We use single-site Metropolis-Hastings to update the correlation scale parameters β and γ , the precision parameters κ and κ_{δ} , and θ . We use a log-normal proposal distribution for all but θ as they have support on positive reals. For θ , a normal proposal distribution is used. The scale of the proposal distribution is tuned to have an acceptance rate near 30% using trial runs of the sampler. The normal proposal for θ with bounded support can lead to a large number of rejections if the posterior for θ is concentrated near a boundary of the prior support; however, the tuning largely mitigates this problem.

2 Sampling $g(\mu(\mathbf{x}))$

We sample $g(\mu(\mathbf{x}))$ using elliptical slice sampling proposed by (Murray et al., 2010). The proposed latent mean vector are generated from a mixture of the current state, $g(\mu(\mathbf{x}))$, and a draw from the Gaussian process prior, $\boldsymbol{\nu}$. Possible proposed vectors lie on an ellipse between the draw from the prior and the current value, with the angle θ along the ellipse determining how close the proposed vector is to the current vector. For $\theta = 0$, the proposal is equal to the current vector while for $\theta = \pi$, the proposal is equal to $\boldsymbol{\nu}$. Slice sampling is used to determine the angle parameter by iteratively shrinking the interval on the ellipse that θ can be drawn from until a vector is accepted. Demonstration of detailed balance for the method and other details can be found in Murray et al. (2010). Pseudocode for the sampling is found in Algorithm 1. We have found that initializing the sampler for a value of $g(\mu(\mathbf{x}))$ at empirical mean of all replicates at \mathbf{x} worked well, possibly adding a small constant to ensure the sampler was initialized on the proper support.

Algorithm 1 EllipicalSliceSampler($\mathbf{g} = g(\mu(\mathbf{x}))$) 1: Draw $\boldsymbol{\nu}$ from the Gaussian process prior N(0, Σ) 2: Draw a random uniform $u \sim \text{Uniform}(0, 1)$ 3: Obtain log-likelihood acceptance threshold: thresh = $logL(\mathbf{g}) + log(u)$ 4: Draw an angle $\theta \sim \text{Uniform}(0, 2\pi)$ 5: Set $\theta_{min} = \theta - 2\pi, \theta_{max} = \theta$ 6: repeat Propose $\mathbf{g}^* = \mathbf{g}\cos(\theta) + \boldsymbol{\nu}\sin(\theta)$ 7:8: Calculate log-likelihood for the proposal: $ll = logL(\mathbf{g}^*)$ 9: if ll >thresh then Accept \mathbf{g}^* 10: 11: else if $\theta > 0$ then 12:13:Set $\theta_{max} = \theta$ else 14:Set $\theta_{min} = \theta$ 15:Draw an angle $\theta \sim \text{Uniform}(\theta_{min}, \theta_{max})$ 16:17: **until** Accept \mathbf{g}^* 18: return g^*

References

Murray, I., Adams, R. P., and MacKay, D. J. (2010), Elliptical slice sampling., in *AISTATS*, Vol. 13, pp. 541–548.