

Addressing Uncertainty in the Choice of Covariance Function in Gaussian Process Modeling with Bayesian Model Averaging



Rob Williams

University of North Carolina at Chapel Hill

Research Objectives

Substantive problem:

Selecting covariance function for observed
 Gaussian process data e.g. spatial[1]

Methodological objective:

• Use Bayesian model averaging to account for uncertainty in correlation structure[2]

Gaussian Processes

Correlation between errors determined by Euclidean distance h between locations $s \in D$.

$$Z(s) = \underbrace{\mathbf{x}(s)'\boldsymbol{\beta}}_{\text{deterministic}} + \underbrace{\sigma^2\rho(h) + \tau^2\mathbf{1}(h=0)}_{\text{stochastic}}$$

Covariance functions evaluated in this study:

Exponential:
$$\rho(h) = \exp\left(-\frac{h}{\phi}\right)$$
Gaussian: $\rho(h) = \exp\left[-\left(\frac{h}{\phi}\right)^2\right]$
Spherical: $\rho(h) = \begin{cases} 1 - 1.5\frac{h}{\phi} + 0.5\left(\frac{h}{\phi}\right)^3, & \text{if } h < \phi \\ 0, & \text{otherwise} \end{cases}$

Bayesian Model Averaging

The posterior probability for any model l in the set of candidate models K is:

$$\pi(\mathcal{M}_l|y) = \frac{\pi(\mathcal{M}_l|y)\pi(\mathcal{M}_l)}{\sum_{m=1}^K \pi(\mathcal{M}_m|y)\pi(\mathcal{M}_m)}$$

The marginal posterior distribution of a parameter θ across K is:

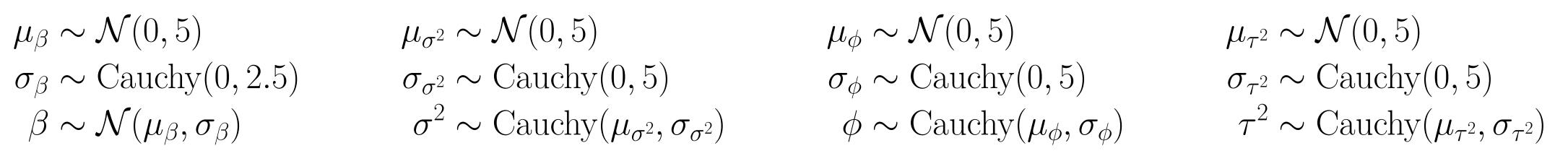
$$\pi(\theta|y) = \sum_{m=1}^{K} \pi(\theta|y, \mathcal{M}_l) \pi(\mathcal{M}_l|y)$$

Monte Carlo Simulation

10 simulated datasets are generated from a model with **exponential** covariance using each combination of the following parameters with the **geoR** package.

$$X_1 \sim \mathcal{N}(0, 1.25)$$
 $\sigma^2 \in \{15, 20, 25\}$
 $X_2 \sim \text{exponential}(4)$ $\phi \in \{10, 25, 50\}$
 $\boldsymbol{\beta} = [1.2, 3.5, -2.7]$ $\tau^2 \in \{5, 7.5, 10\}$

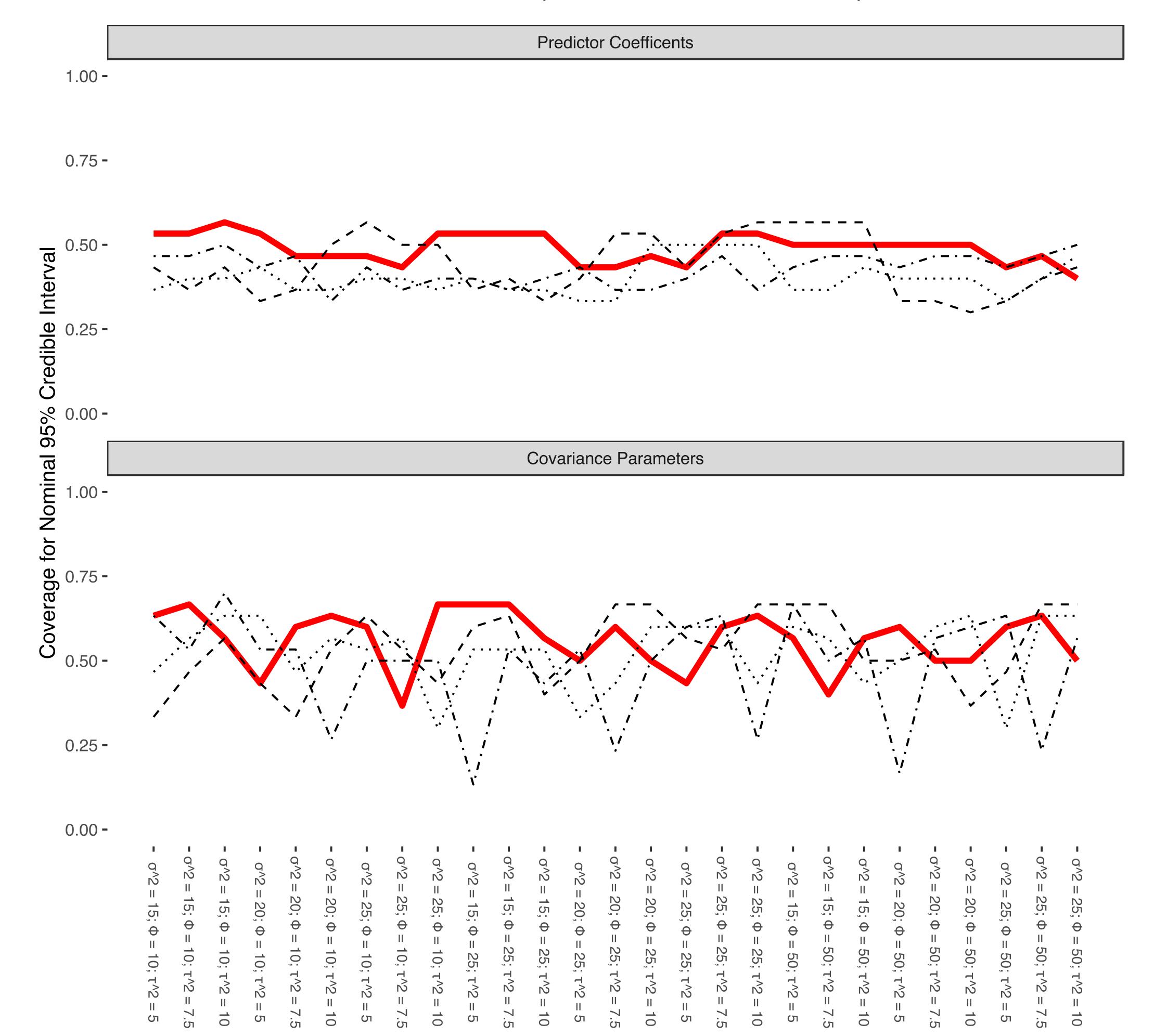
Model Parameters



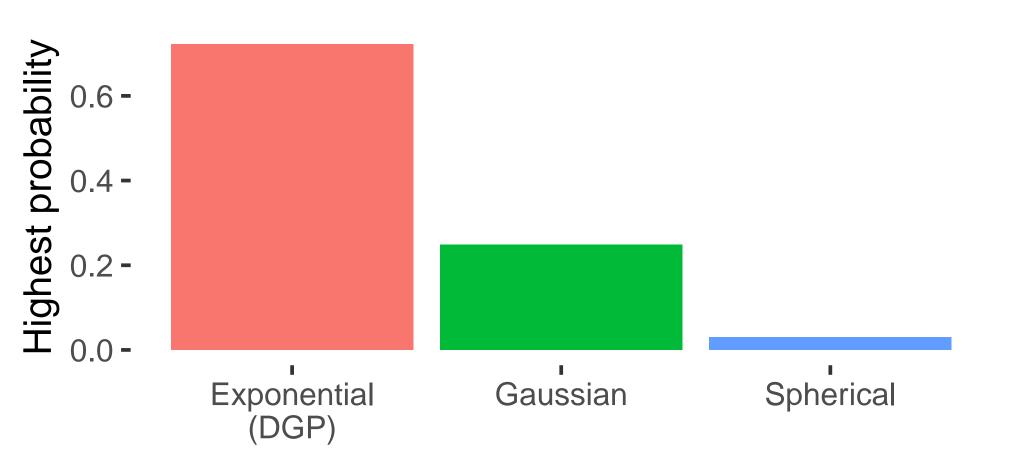
Models are estimated with Stan via rstan. Marginal likelihoods are estimated using the bridgesampling package. Posterior model probabilities are calculated with $\pi(\mathcal{M}_{\text{Exponential}}) = \pi(\mathcal{M}_{\text{Gaussian}}) = \pi(\mathcal{M}_{\text{Spherical}})$ and used to compute averaged point estimates and 95% credible intervals for all parameters in each simulation.

Monte Carlo Simulation Results

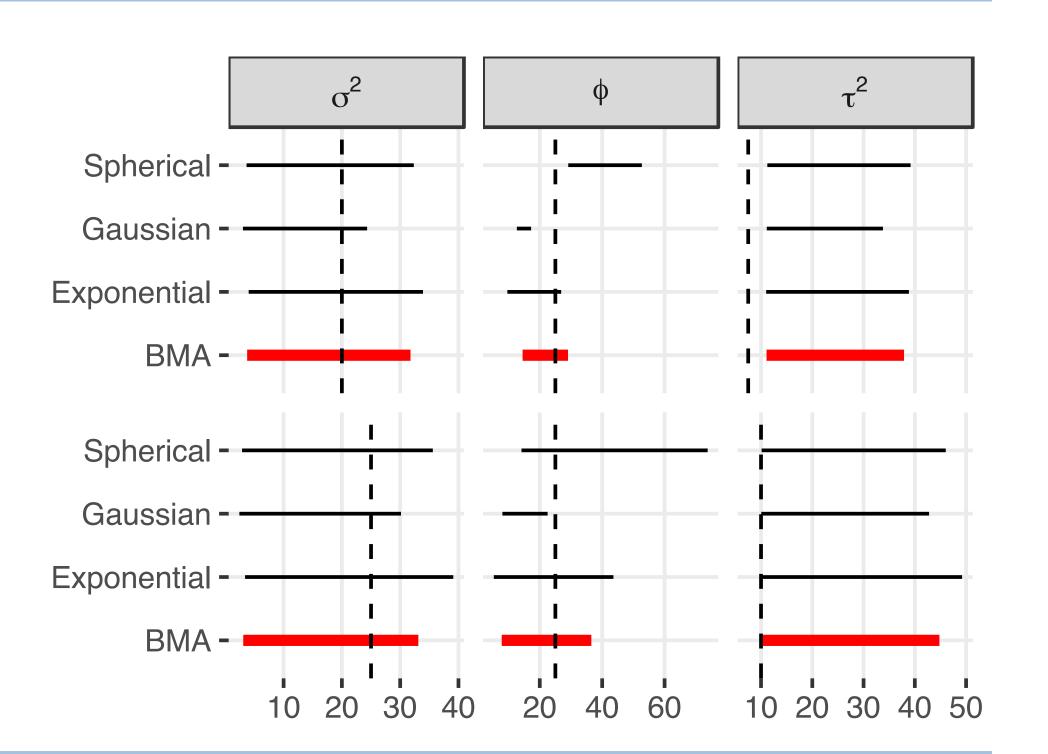




Most Likely Model



Representative Simulations



Conclusion

- BMA corrects for inclusion of ill-suited models.
- BMA is less biased, but also less efficient, at estimating covariance function parameters.

Next Steps

• Simulate data from additive and multiplicative combinations of covariance functions at a more fine-grained set of covariance function parameters.

Email: jrw@live.unc.edu
Web: jrw.web.unc.edu

References

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[2] Jacob M. Montgomery and Brendan Nyhan.
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