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Title:	Computationally Efficient Use of Derivatives in Emulation of Complex Computational Models
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Computationally Efficient Use of Derivatives in Emulation of Complex Computational Models

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LA-UR-12-

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Abstract

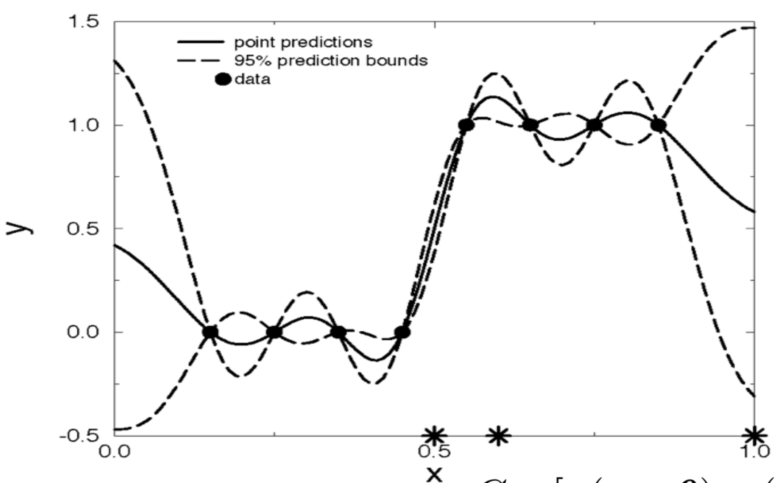
We will investigate the use of derivative information in complex computer model emulation when the correlation function is of the compactly supported Bohman class. To this end, a Gaussian process model similar to that used by Kaufman et al. (2011) is extended to a situation where first partial derivatives in each dimension are calculated at each input site (i.e. using gradients). A simulation study in the ten-dimensional case is conducted to assess the utility of the Bohman correlation function against strictly positive correlation functions when a high degree of sparsity is induced.

Outline

- Emulation of computational models
- Incorporation of derivative information
- Compactly supported covariance functions
- Simulation Study
- Results
- Conclusions

Emulator

- Use training runs to develop a statistical surrogate model for the complex code (i.e., the *emulator*)
  - Deterministic code is interpolated with zero uncertainty
- Kriging Predictor $\hat{\eta}(\boldsymbol{x};\boldsymbol{\theta}) = \boldsymbol{f}'(\boldsymbol{x})\hat{\boldsymbol{\beta}} + \boldsymbol{r}'(\boldsymbol{x};\boldsymbol{\theta})\boldsymbol{R}^{-1}(\boldsymbol{\theta})(\boldsymbol{\eta} - \boldsymbol{F}\hat{\boldsymbol{\beta}})$



correlations between prediction site **x** and training runs $\mathbf{x}_1,\ldots,\mathbf{x}_m$

outputs evaluated at training runs $\mathbf{x}_1,\ldots,\mathbf{x}_m$

Regression functions evaluated at prediction site **x** and parameters

pairwise correlations between training runs $\mathbf{x}_1,\ldots,\mathbf{x}_m$

- Kriging Variance

$$Cov[\eta(\boldsymbol{x}_1,\boldsymbol{\theta}),\eta(\boldsymbol{x}_2,\boldsymbol{\theta})|\boldsymbol{\eta}] = \sigma^2 \left(R(\boldsymbol{x}_1,\boldsymbol{x}_2;\boldsymbol{\theta}) - \boldsymbol{r}'(\boldsymbol{x}_1,\boldsymbol{\theta})\boldsymbol{R}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{x}_2,\boldsymbol{\theta}) + \boldsymbol{h}'(\boldsymbol{x}_1,\boldsymbol{\theta})(\boldsymbol{F}'\boldsymbol{R}^{-1}(\boldsymbol{\theta})\boldsymbol{F})^{-1}\boldsymbol{h}(\boldsymbol{x}_2;\boldsymbol{\theta})\right)$$

$$\boldsymbol{h}(\boldsymbol{x};\boldsymbol{\theta}) = \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{F}'\boldsymbol{R}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{x};\boldsymbol{\theta})$$

  - Full Bayes inference for σ^2, θ

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Incorporating Derivatives

- Morris, Mitchell and Ylvisaker (*Technometrics*, 1993)

$$\begin{pmatrix} \eta(\boldsymbol{t}) \\ \frac{\partial \eta(\boldsymbol{t})}{\partial t_i} \end{pmatrix} \sim GP\,, \quad \text{mean} \begin{pmatrix} \mu(\boldsymbol{t}) \\ \frac{\partial \mu(\boldsymbol{t})}{\partial t_i} \end{pmatrix} ; \quad \text{covariance} \begin{pmatrix} C(\boldsymbol{t},\boldsymbol{s}) & \frac{\partial C(\boldsymbol{t},\boldsymbol{s})}{\partial s_i} \\ \frac{\partial C(\boldsymbol{t},\boldsymbol{s})}{\partial t_i} & \frac{\partial^2 C(\boldsymbol{t},\boldsymbol{s})}{\partial t_i \partial s_i} \end{pmatrix}$$

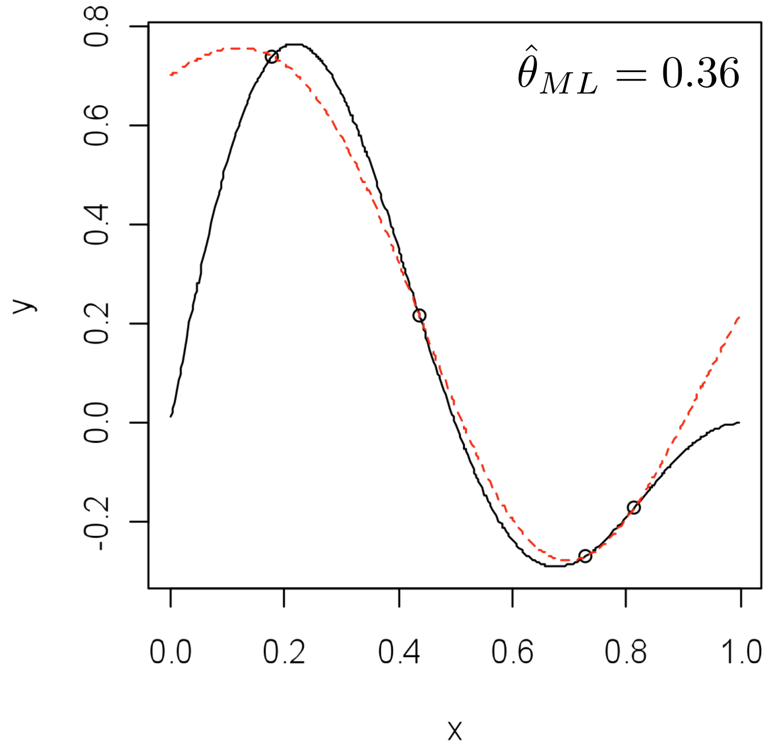
- Computational efficiency eventually required

Size of Covariance Matrix

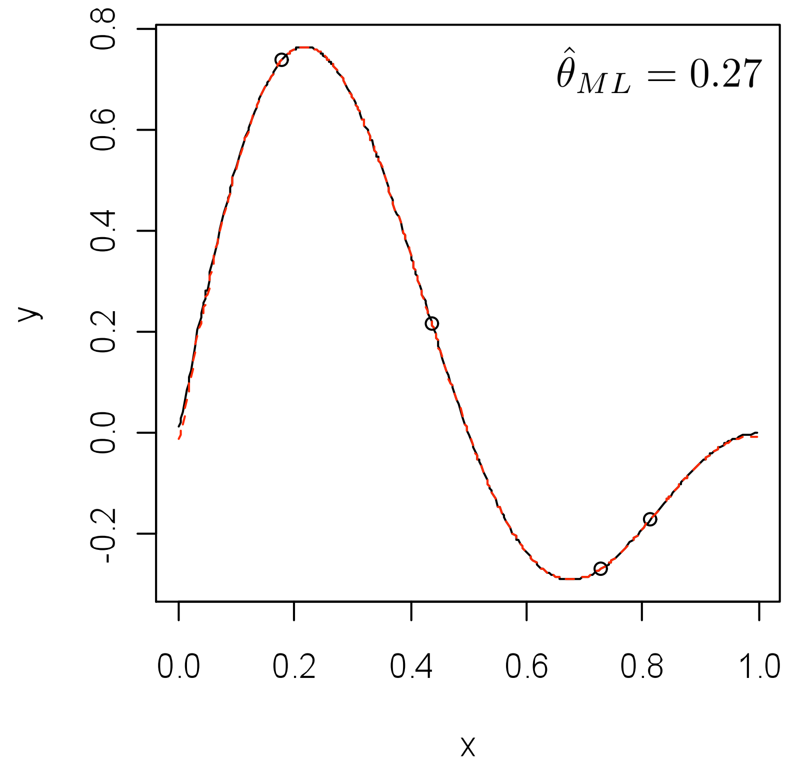
Sample Size	Input Dimension (D)				
	1	5	10	20	50
1.5D	3	45	165	630	3825
5D	10	150	550	2100	12750
10D	20	300	1100	4200	25500

Small Sample Sizes Enhanced With Derivatives

Gaussian Correlation
No Derivatives



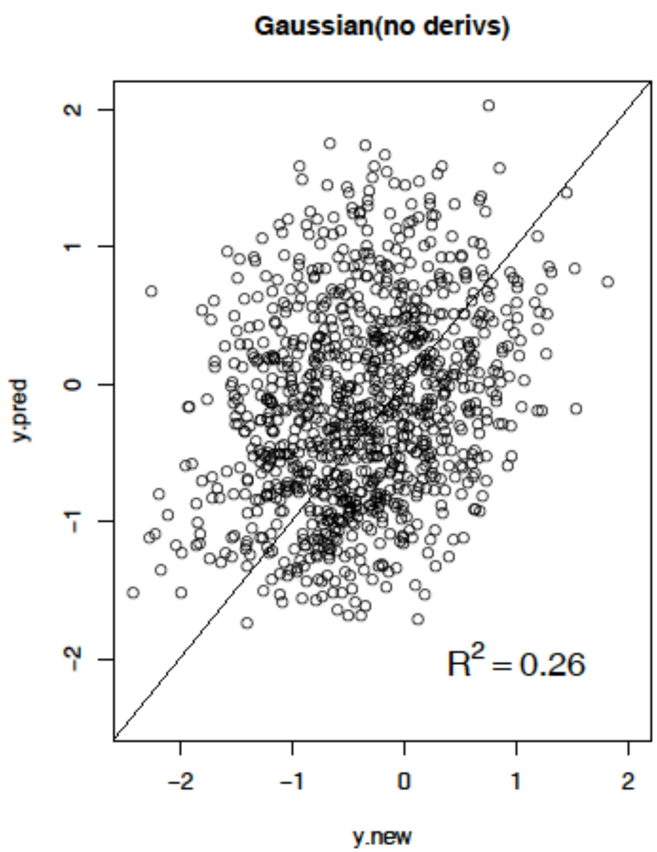
Gaussian Correlation
First Derivatives

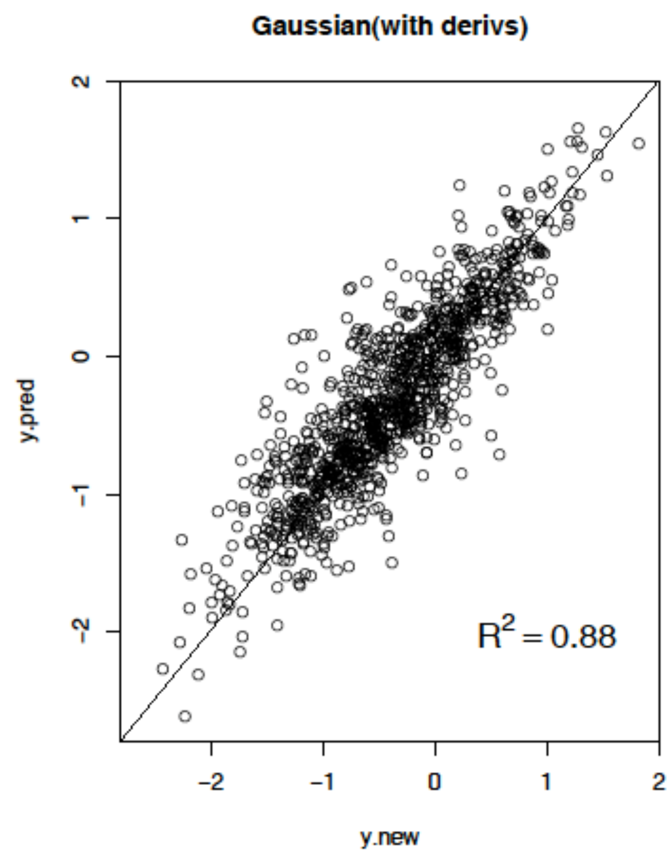


$$R(x_1, x_2) = \exp\left\{-[|x_1 - x_2|/\theta]^2\right\}$$

Benefits of Derivatives in Higher Dimensions

- D = 8, N = 2D = 16
- True function generated from GP with Gaussian correlation





Compactly Supported Covariance

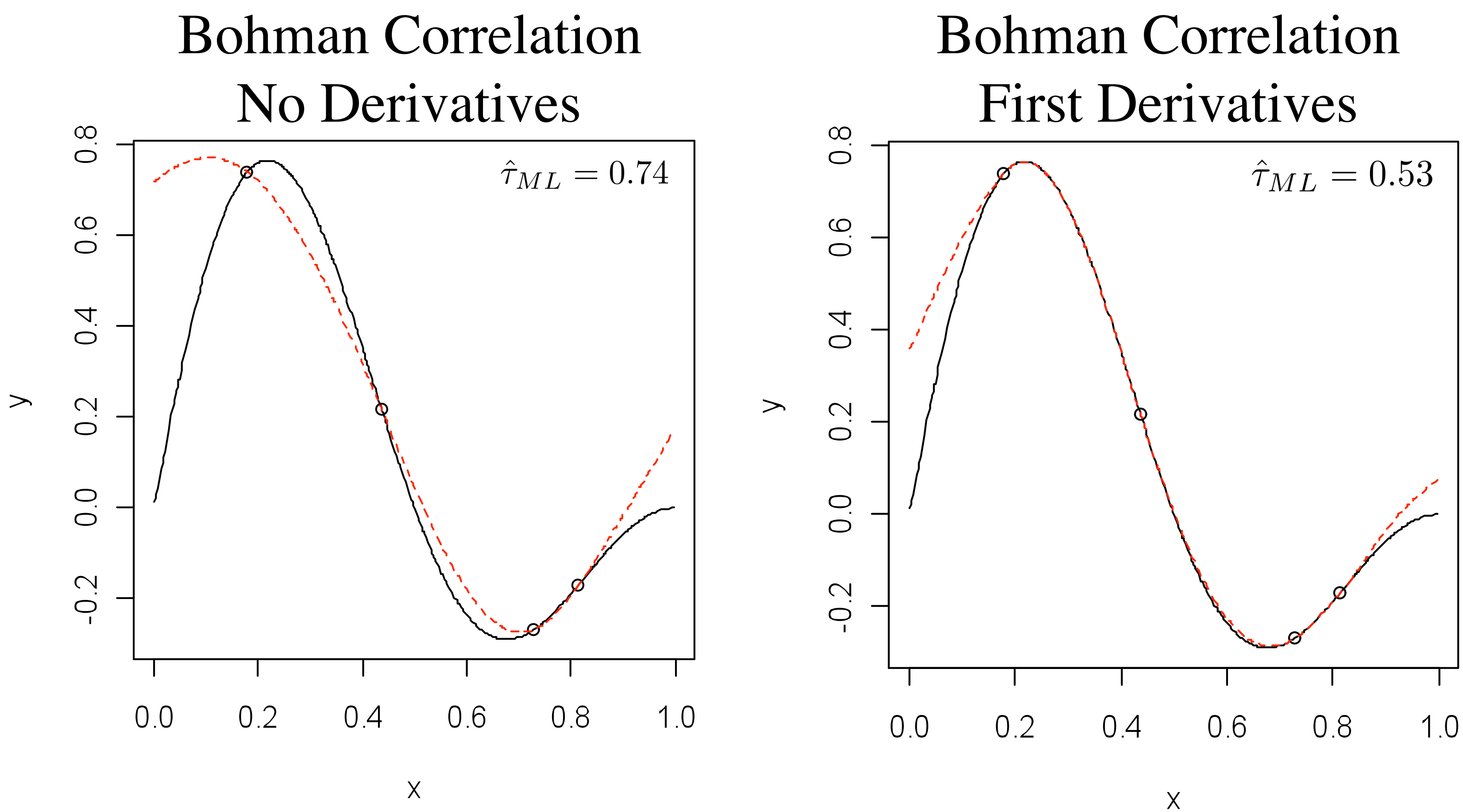
- Kaufman, *et al.* (2011)
  - 20,000 simulator evaluations
  - Use low order regression models and compactly supported covariance function to achieve a good fit with sparse covariance matrix
  - Increased sparsity resulted in less prediction efficiency, especially for more difficult functions, but improvement with sample size
  - Sparsity resulted in improved coverage properties but gains declined with sample size

- Bohman correlation function

$$R(t;\tau) = \begin{cases} (1 - t/\tau)\cos(\pi t/\tau) + \sin(\pi t/\tau)/\pi\,, & t < \tau \\ 0\,, & t \geq \tau \end{cases}$$

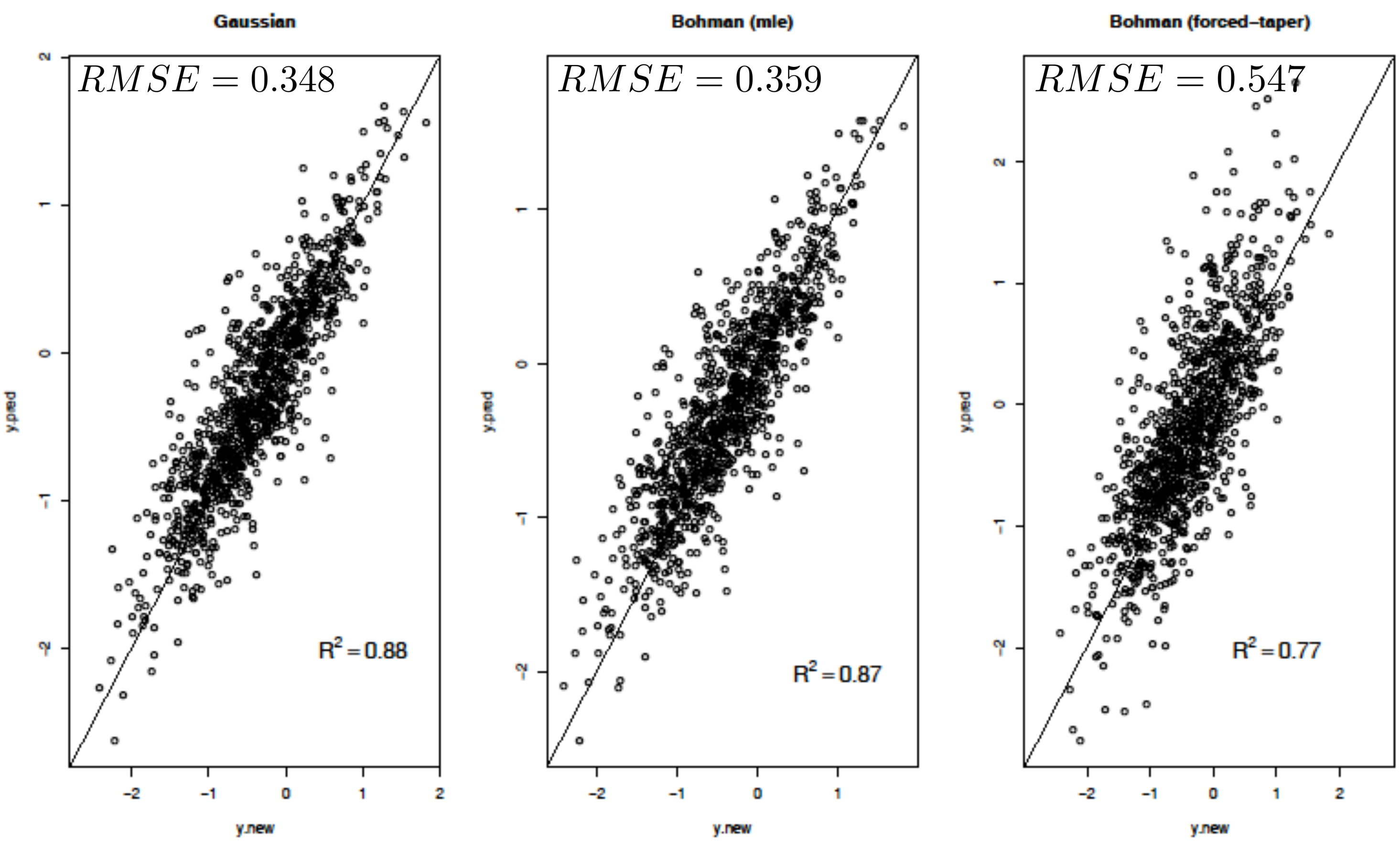
  - Prior restriction: $\boldsymbol{\tau} \in \mathcal{R}^D \;:\; \tau_j \geq 0 \text{ for all } D\,, \sum_{j=1}^{D} \tau_j \leq C\,,\, C > 0$

Advantage of Derivatives Persists with Sparsity



Benefits of Derivatives Even With High Sparsity

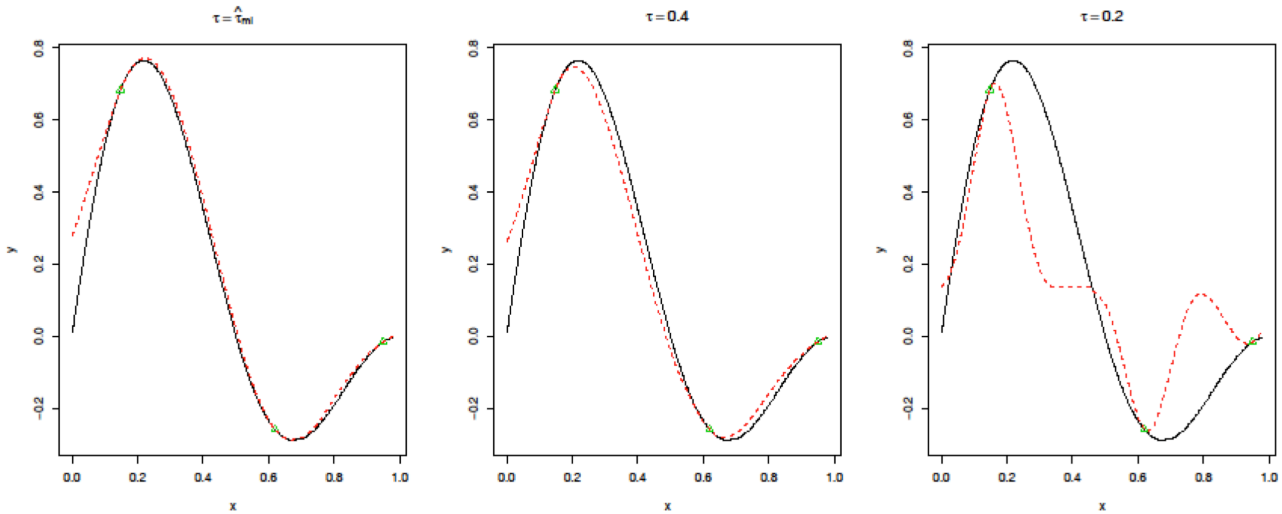
- D = 8, N = 2D = 16
- True function generated from GP with Gaussian correlation



90% sparsity

Inclusion of Regression Model

- Regression often necessary to allow for covariance sparsity



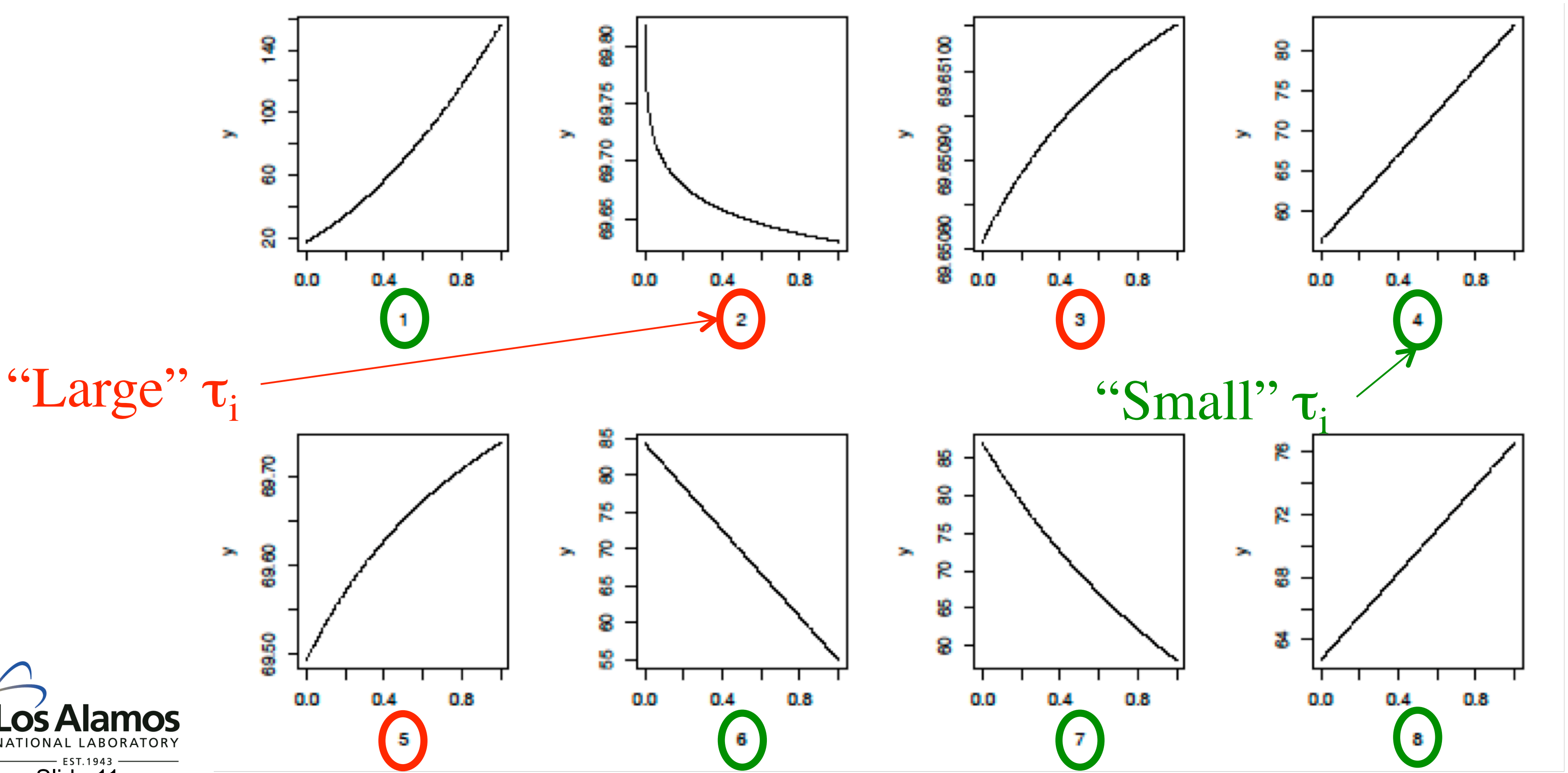
- Advantages are seen in higher dimensional input spaces

RMS Errors
D = 8

Degree of Regression Model	Unconstrained Bohman	Constrained Bohman (~90% sparsity)
0	0.3591	0.7464
1	0.3668	0.9553
2	0.4548	0.5474
3	0.4766	0.5611

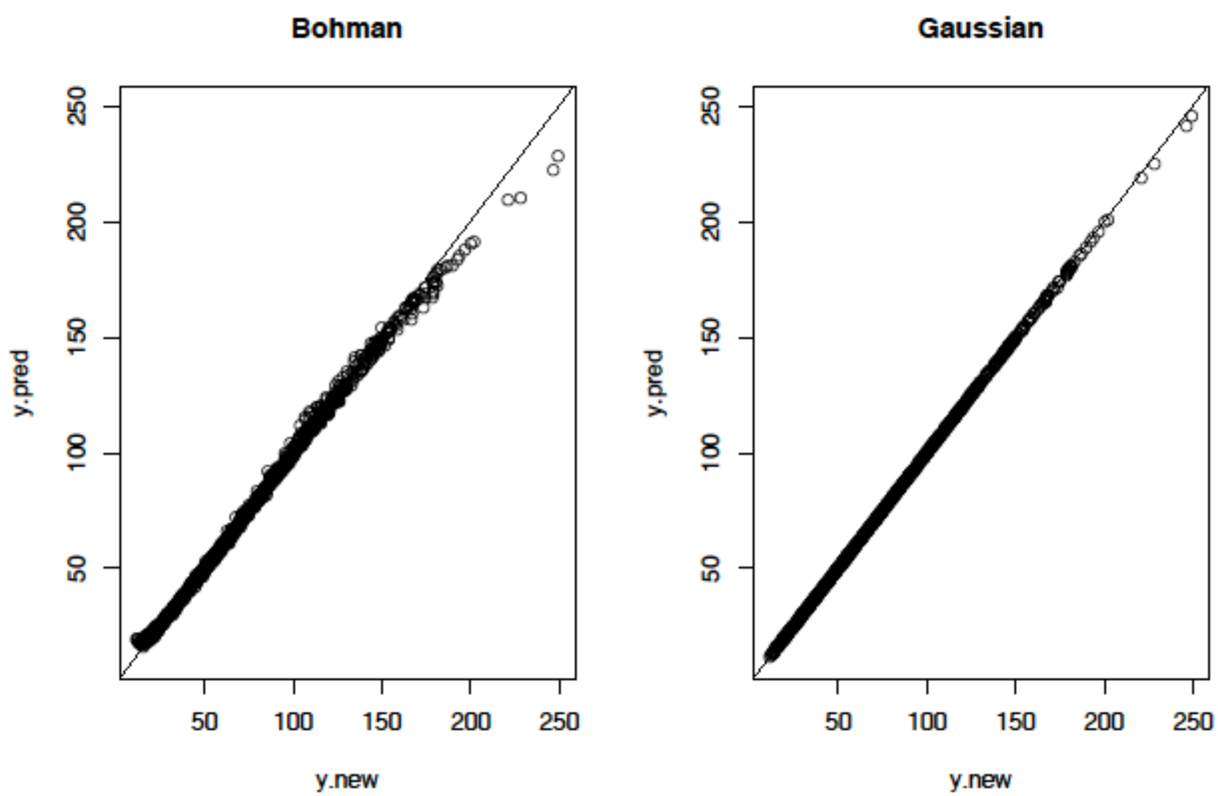
Regression Helps Induce Sparsity

- Borehole: Morris (1993) with inputs scaled to unit cube, $[0,1]^8$
- Sparsity constraint results in larger correlation length τ in dimensions not modeled well by regression



Sparsity and Predictive Capability

- Sparsity is pushed towards 99% but still produces an R^2 of 0.999
  - Dense correlation matrices (e.g. from Gaussian or Matern) may be ill-conditioned in this situation



Sparsity and Computing

- Sparsity depends on tapering parameters and design (which depends on dimension, sample size)
  - We used maximin Latin hypercube designs
- Computation time depends on sparse matrix algorithms used
  - In R 'spam' uses Yale sparse format
- Times using 'spam' in R are below
  - Predicting 1000 new values
  - Algorithms are even faster above ~95% sparsity

N = 2D	Sparse	Dense	N = 3.5D	Sparse	Dense
D = 10	0.05 / 1.34	0.06 / 2.17		0.06 / 1.52	0.11 / 2.24
D = 20	0.24 / 3.31	0.58 / 5.31		0.55 / 4.51	1.85 / 8.65
D = 30	1.69 / 9.09	4.45 / 15.4		6.17 / 18.5	16.1 / 36.2

Likelihood evaluation

Prediction

Simulation Study

- Generate a GP with specified covariance structure (Gaussian assumed here) and get response values and partial derivative information
- Two input dimensions (D = 10 and D = 20)
- Two complexity levels ("Full" and "KL group 3")
- Seven modeling choices:
  - True correlation model (Gaussian)
  - Bohman at two levels of sparsity (~90% and ~95%) and four levels of regression modeling (none, linear, quadratic, quadratic + some cubic terms)
- Five replications of each factor-level combination

KL Expansion

- Decomposition of process into eigenvalues and eigenfunctions

$$\eta(\boldsymbol{x},\omega) = \mu(\boldsymbol{x}) + \sum_{j=1}^{\infty} \sqrt{\lambda_j}\,\phi_j(\boldsymbol{x})\,Z_j(\omega)$$

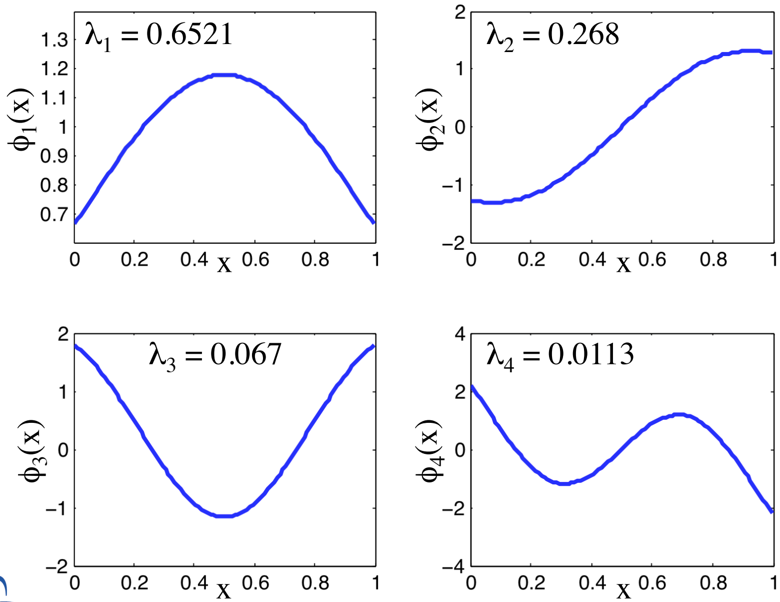
N(0,1)

$$\int_D C(\boldsymbol{u},\boldsymbol{v})\,\phi(\boldsymbol{v})\,d\boldsymbol{v} = \lambda\,\phi(\boldsymbol{u})$$

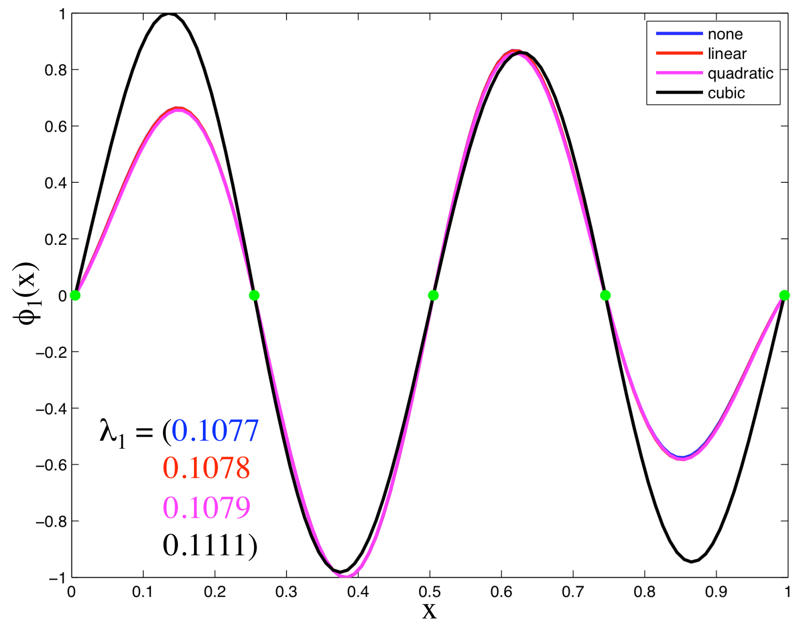
Fredholm integral equation of the second kind

- Solutions via Galerkin approximation (low-D)

Gaussian correlation



Bohman correlation



GP Simulation

- Simulate from zero-mean Gaussian process with product Gaussian correlation function
  - Complexity and sparsity specified (Loeppky, *et al.* (2010))
  - Output and derivatives desired
- Use 1-d KL expansion
  - Decomposition by dimension

eigenvalues	eigenfunctions
$\lambda_{1,1}, \ldots, \lambda_{1,m_1}$	$\phi_{1,1}(x_1), \ldots, \phi_{1,m_1}(x_1)$
$\vdots$	$\vdots$
$\lambda_{D,1}, \ldots, \lambda_{D,m_D}$	$\phi_{D,1}(x_D), \ldots, \phi_{D,m_D}(x_D)$

  - Eigenfunctions are tensor products of 1-d eigenfunctions

Group	Eigenfunction	Terms
first	$\prod_{j=1}^{D} \phi_{j,1}(x_j)$	1
second	replace $\phi_{i,1}(x_i)$ with $\phi_{i,2}(x_i)$	D
third	replace $\phi_{i_1,1}(x_{i_1})$ and $\phi_{i_2,1}(x_{i_2})$ with $\phi_{i_1,2}(x_{i_1})$ and $\phi_{i_2,2}(x_{i_2})$	$\binom{D}{2}$

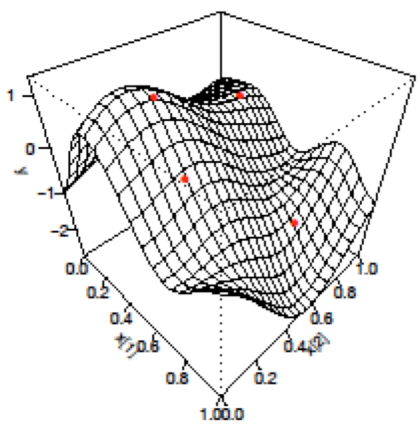
  - Partial derivatives are easily calculated

$$\text{replace } \phi_{i,j}(x_i) \text{ with } \frac{\partial \phi_{i,j}(x_i)}{\partial x_i}$$

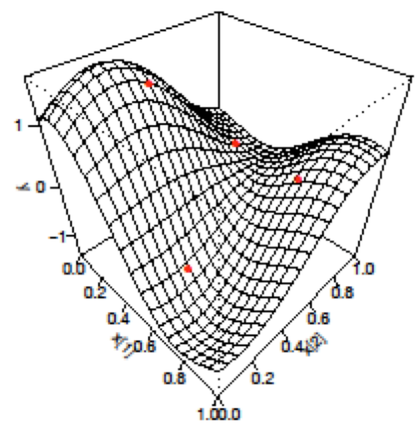
Response Surfaces for Simulation Study

- D = 10 dimensional input space
- More complex functions obtained with use of more second order eigenfunctions

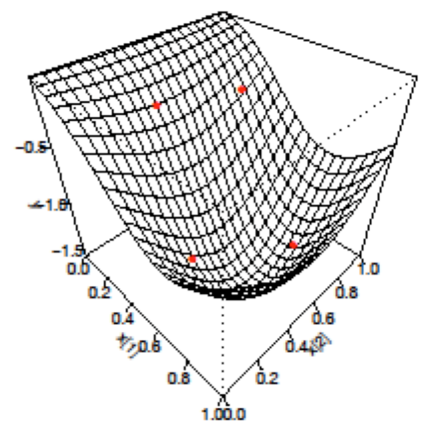
"Full"
Replace 3 $\phi_{.,1}$ with $\phi_{.,2}$



"Group 3"
Replace 2 $\phi_{.,1}$ with $\phi_{.,2}$



Replace 1 $\phi_{.,1}$ with $\phi_{.,2}$



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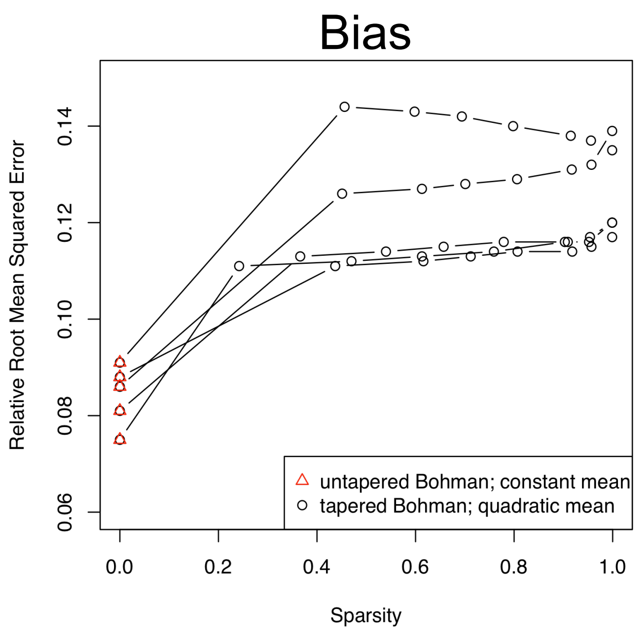
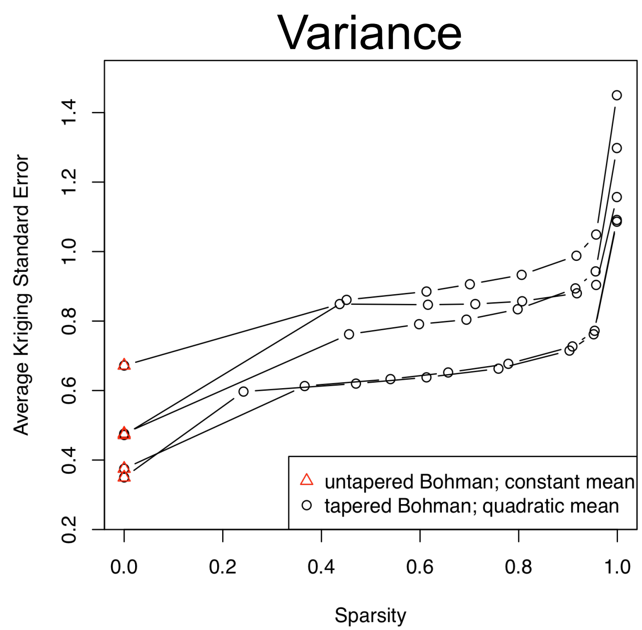
Results: Effects of Sparsity

Surfaces drawn from GP with Gaussian correlation function
(D = 10; N = 20)

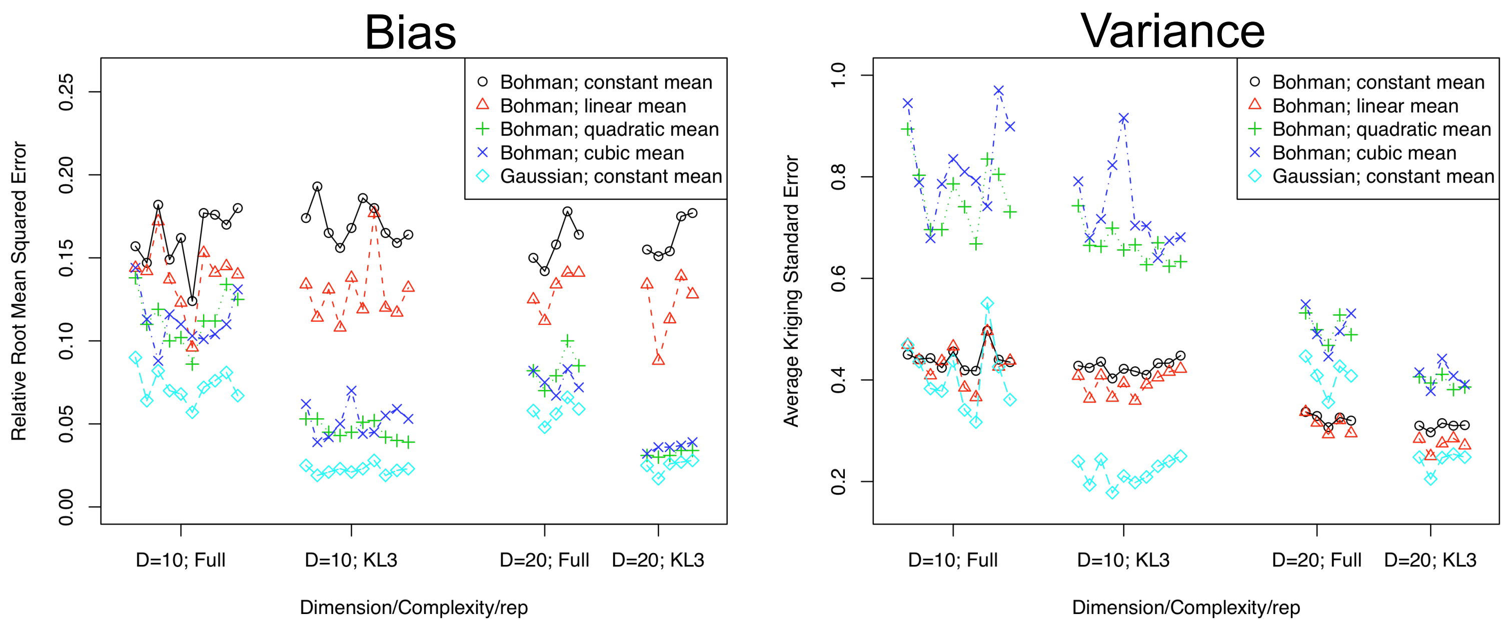




- Results using just model outputs (ignoring first partials)
  - ✧ untapered Bohman, constant mean
  - ✧ Relative RMSE: 0.165 (> RMSE with derivatives at all sparsity levels)
  - ✧ ARMPSE: 0.75 (comparable to avg. ARMPSE with derivatives at ~95% sparsity)

Results: Accuracy and Precision of Emulators

Surfaces drawn from GP with Gaussian correlation function
Full and KL3 complexity
(D = 10; N = 20 and D=20; N=40)
Bohman correlation tapered to 90+% sparsity



- RMSE values lower for higher order regression models with tapering
- ARMPSE values higher for higher order regression models with tapering

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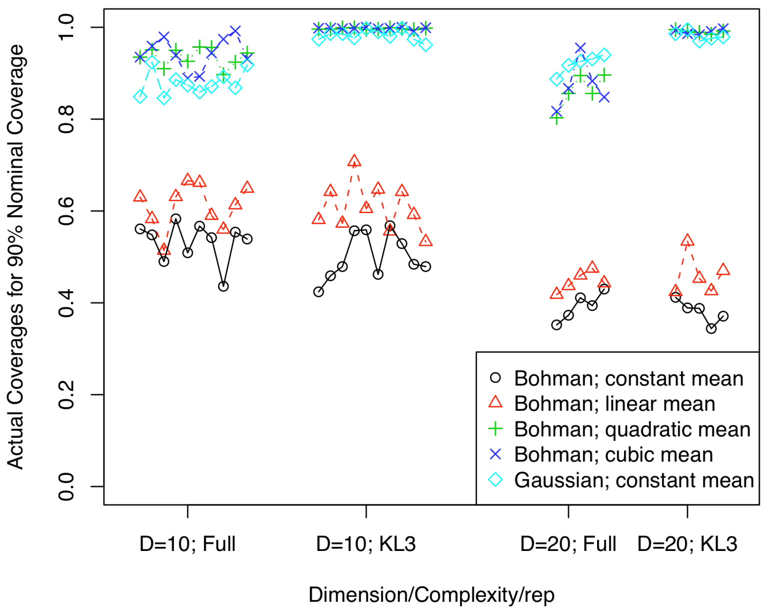
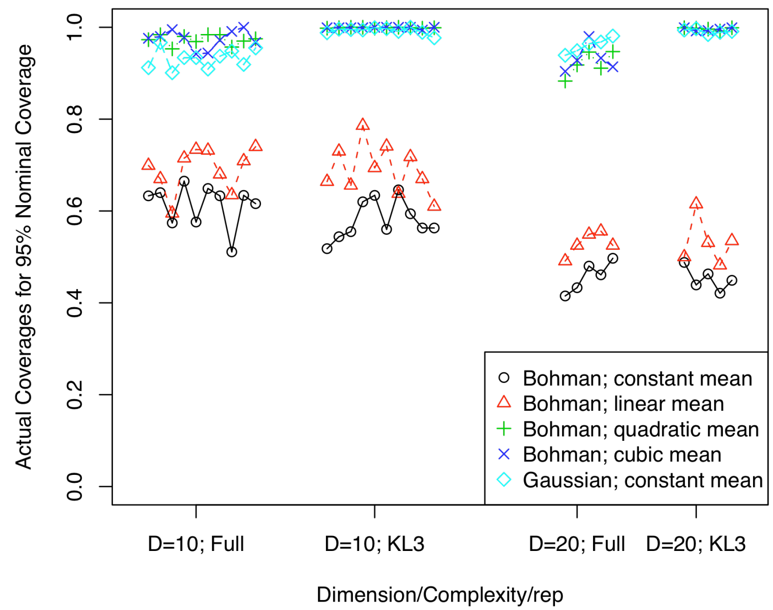
Results: Frequentist Coverage

Surfaces drawn from GP with Gaussian correlation function
Full and KL3 complexity
(D = 10; N = 20 and D=20; N=40)
Bohman correlation tapered to 90+% sparsity





- Actual coverages low for inadequate regression models with tapering
- Higher kriging SE required with tapering versus true correlation model to achieve nominal coverage

Compromise

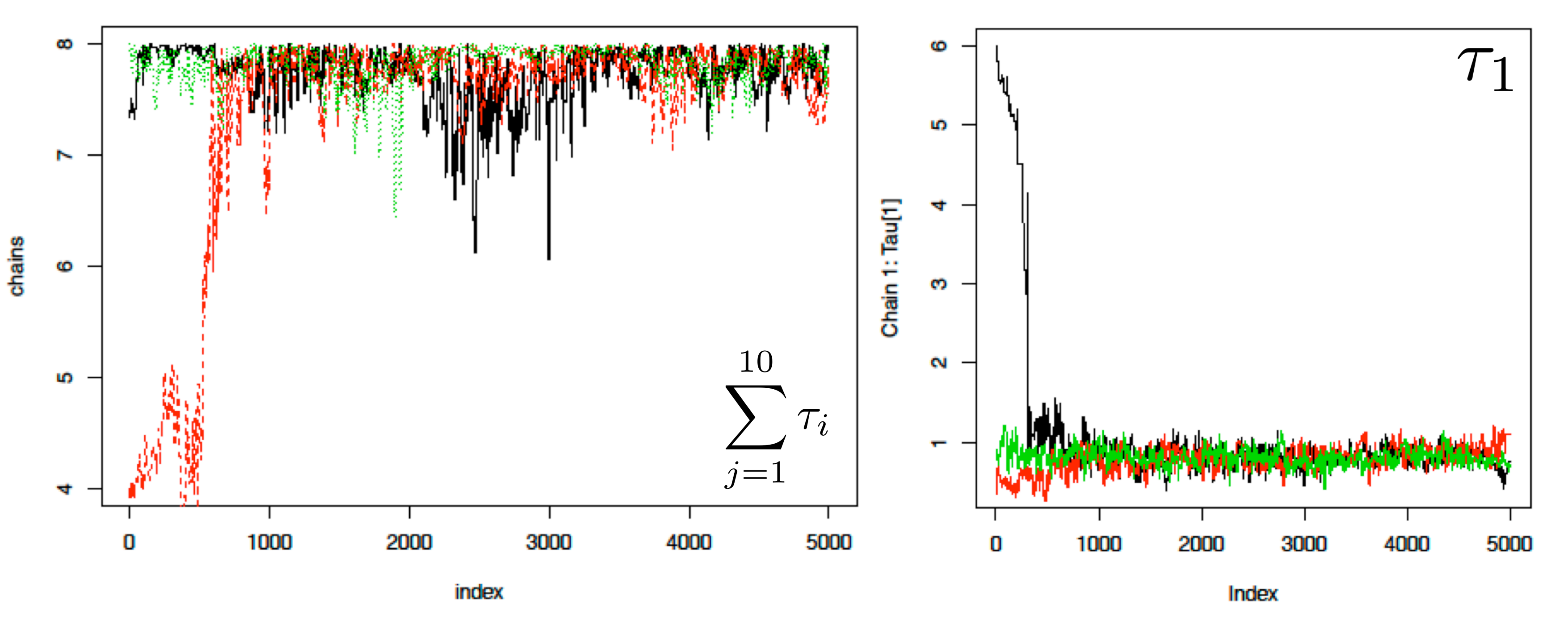
- Trade-off between computation time and predictive capability
  - Sparsity restriction complicates the ability to model deviations from smooth global trend and can lead to increased prediction variances and, to a lesser extent (depending on regression model), increased prediction biases relative to "ideal" emulator
- In the extreme case of ~100% sparsity, the surrogate is essentially regression with derivatives, but the prediction intervals become useless
- In the case of <100% sparsity, the full Bayesian approach (with informative prior) can be used to get improved prediction intervals relative to use of plug-in parameter estimates

MCMC: Metropolis Within Gibbs

- Gibbs updates of regression parameters
- Metropolis sampling of τ vector
  - Optimal τ vector may lie on a boundary of the simplex defined by the sparsity constraint
- Start at the center of the simplex: $C/2 = \sum_{j=1}^{D} \tau_j/2$
  - Multivariate normal proposal distribution
  - weak proposal covariance matrix
- Every 100 iterations tune covariance to the sample covariance of the parameters
  - Do this 50-100 times
  - Multiply covariance matrix obtained at end of burn-in by $(2.38^2)/D$ (this is for optimal acceptance when target is multivariate normal)
  - Proceed with Metropolis updates of entire τ vector
- Generate predictions using a thinned sample of the parameters

MCMC Worst Case Scenario

- Adaptive MCMC performs well across a variety of scenarios, including when starting values are poor (in the wrong corner of the prior simplex, as below).



Conclusions

- Using compactly-supported covariance can speed up computation time
  - Allows use of derivative information in situations when computations would be prohibitively expensive with dense covariance matrices
- Using compactly-supported covariance may compromise predictive capability relative to “ideal” covariance
  - Higher prediction variances required to achieve nominal coverage when >90% sparsity is required for computational efficiency
  - Depending on complexity of underlying response, larger than nominal prediction bias may be introduced with forced sparsity
- Using only outputs requires 3-4 times more runs to achieve similar prediction quality with regression and 90% sparsity
  - 5-8 times more runs with dense correlation function

Future work

- Test the method against surfaces generated by real simulator codes that produce first partial derivatives, especially as the input dimension grows
- Better understand the equivalent sample size of using gradients vs. not using gradients

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Thanks!