Bayesian MARS UQ Research at the Center for Radiative Shock Hydrodynamics (CRASH)

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This work describes an extension of the Bayesian MARS emulator to include gradient information, when available.

Most uncertainty quantification tasks boil down to: “Estimate the sensitivity and/or variability in some quantity $y = f(x)$ resulting from uncertainty or variability in its dependencies.”

- Dimensionality of x and cost of $f(\cdot)$ may limit sampling density.
- **Emulators** (or response surfaces) “functionalize” the mapping $y = f(x)$ using a set of available samples, $y_i = f(x_i),\ i = 1 \ldots N$.
- An effective emulator
  1. is cheap to sample,
  2. provides accurate estimates of y at untried inputs, and
  3. gives an estimate of its own regression error.

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How can we use $\nabla_x f$?

Adjoint and/or automatic differentiation methods can possibly provide gradient information about $f(x)$. How can we use this information to improve the effectiveness of our emulators?

Inclusion of gradient information requires differentiation of the emulator's basis function.

Some examples:

1. Polynomial chaos: write the unknown as a multivariate polynomial expansion in x,

$$y \approx P(x) = \sum_i a_i \psi_i(x)$$

   and solve for the a_i's. Solution techniques vary, but gradient information is fairly straightforward to include.

2. Gaussian process regression: Model $f(x)$ as a multivariate random field specified by a mean and covariance function. Inclusion of gradient information requires differentiation of the mean and covariance function (Lockwood, Anitescu – Summer 2011 ANS meeting).

We apply the extension to the Multivariate Adaptive Regression Splines (MARS) emulator.

The gradient of a BMARS basis function is another BMARS function.

The gradient in direction x_n is:

$$\nabla_{x_n} B(x) = \sum_{k=1}^{K} o_{k,n} \beta_k \prod_{l=0}^{\mathbf{I}} (x_l - t_{k,l})_+^{o^*_{k,l}}$$

where

$$o^*_{k,l} = \begin{cases} o_{k,l} - 1 & l = n \\ o_{k,l} & l \neq n \end{cases} .$$

Thus, we can use the same machinery to evaluate B and ∇B. Our regression task is now to minimize the error in the fit:

$$B(x_i) \approx f(x_i),$$
$$\nabla_x B(x_i) \approx \nabla_x f(x_i).$$

The regression coefficients are solved for using a Bayesian least-squares approach.

The least squares problem is written as an over-constrained linear system:

$$\left(\mathbf{A}^T\mathbf{A} + \tau^2 I\right)\beta = \mathbf{A}^T b,$$
$$\mathbf{A} \in \mathbb{R}^{P\times K}, \quad b \in \mathbb{R}^P, \quad P > K, \quad \tau \in \mathbb{R}.$$

where

- the first I rows of matrix $\mathbf{A}$ contain the K unscaled splines $\hat{B}$ evaluated at each x_i;
- the next N blocks of I rows contain the unscaled gradients, $\dfrac{\partial \hat{B}}{\partial x_n}$, evaluated at each x_i;
- b contains the function and gradient response data;
- β are the regression coefficients; and
- τ is a Bayesian precision parameter.

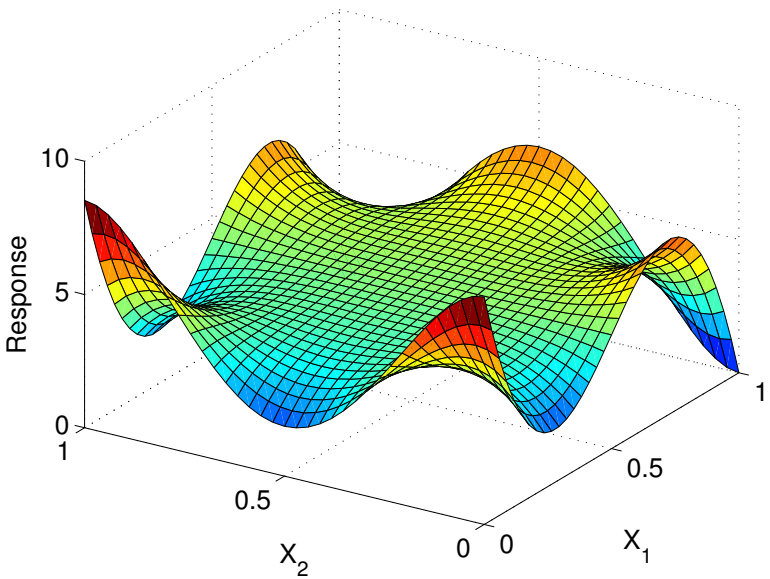
The regression coefficients are solved for using a Bayesian least-squares approach, ctd...

In explicit form (for $n = 1 \ldots N$):

$$\mathbf{A} = \begin{bmatrix} \hat{B}_1(x_1) & \hat{B}_2(x_1) & \ldots & \hat{B}_K(x_1) \\ \hat{B}_1(x_2) & \hat{B}_2(x_2) & \ldots & \hat{B}_K(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \hat{B}_1(x_I) & \hat{B}_2(x_I) & \ldots & \hat{B}_K(x_I) \\ \frac{d\hat{B}_1}{dx_n}(x_1) & \frac{d\hat{B}_2}{dx_n}(x_1) & \ldots & \frac{d\hat{B}_K}{dx_n}(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{d\hat{B}_1}{dx_n}(x_I) & \frac{d\hat{B}_2}{dx_n}(x_I) & \ldots & \frac{d\hat{B}_K}{dx_n}(x_I) \end{bmatrix}, \quad b = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_I) \\ \nabla_{x_n} f(x_1) \\ \vdots \\ \nabla_{x_n} f(x_I) \end{bmatrix}$$

We first test the algorithm on a set of test functions proposed by the original BMARS authors (Denison, et. al., 1998).

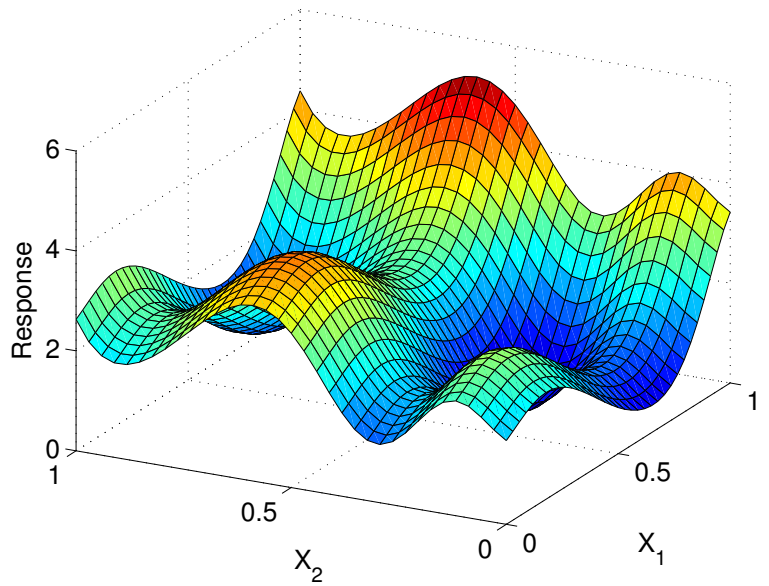
"Harmonic" Function



$$f(x_1,x_2) = 42.659\left[0.1+\hat{x}_1\left(0.05+\hat{x}_1^4-10\hat{x}_1^2\hat{x}_2^2+5\hat{x}_2^4\right)\right],$$

$$\hat{x}_n = x_n - .5$$

"Additive" Function



$$f(x_1,x_2) = 1.3356\Big\{1.5(1-x_1) + \exp(2x_1-1)\sin\left(3\pi(x_1-.6)^2\right) + \exp(3(x_2-.5))\sin\left(4\pi(x_2-.9)^2\right)\Big\}$$

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Using gradient information decreases regression error.

Our regression metric is the Fraction of Variance Unexplained (FVU):

$$\text{FVU} = \frac{\sum_i \left(B(x_i) - f(x_i)\right)^2}{\sum_i \left(f(x_i) - \bar{f}\right)^2},$$

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Case (# Samples)	**Training Data**		**Testing Data**	
Harmonic	BMARS	gBMARS	BMARS	gBMARS
5^2	8.761e-01	3.254e-02	9.821e-01	1.176e-01
10^2	2.464e-03	1.179e-03	8.407e-02	3.221e-03
15^2	1.926e-03	3.683e-04	3.594e-03	5.553e-04
Additive	BMARS	gBMARS	BMARS	gBMARS
5^2	1.020e-03	1.112e-03	3.432e-01	4.009e-02
10^2	6.644e-04	8.399e-04	1.297e-02	3.696e-03
15^2	7.373e-04	4.269e-04	3.577e-03	8.133e-04

- Training data: 5^2, 10^2, or 15^2 uniform samples on unit square
- Testing data: 10 000 uniform samples on unit square
- Reporting mean FVU of 5 repititions

We apply gBMARS to do UQ on a mock traveling wave reactor problem.

- A model problem for the CESAR Exascale center (ANL, TAMU, and others)
- Coupled 3-nuclide Bateman Eqs. and 1D diffusion (nonlinear):

$$\frac{\partial}{\partial t}N(r,t) = \mathbf{M}\big(\phi(r,t),p\big)N(r,t)$$
$$\mathbf{M}(N(r,t),p)\phi(r,t) - \Sigma_a^{\text{ext}}(t,p)\phi(r,t) = 0$$
$$\phi^T\Sigma_f - P_0 = 0$$

- Σ_a^{ext}: Engineering degree of freedom
- p: a vector of uncertain parameters (eg: cross-sections)

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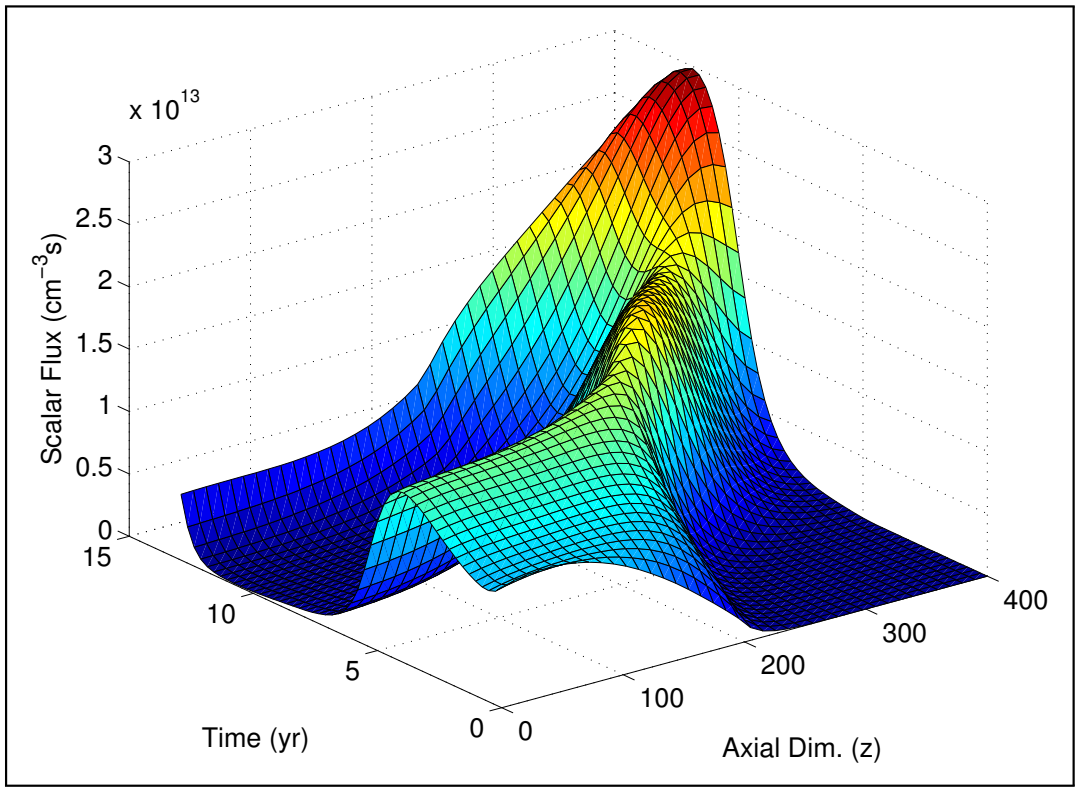
- Σ_a^{ext}: Engineering degree of freedom
- p: a vector of uncertain parameters (eg: cross-sections)
- Initial conditions: power concentrated at one end of reactor
- "Downstream" fertile material breeds and reaction moves through the slab

An adjoint framework provides gradient information.



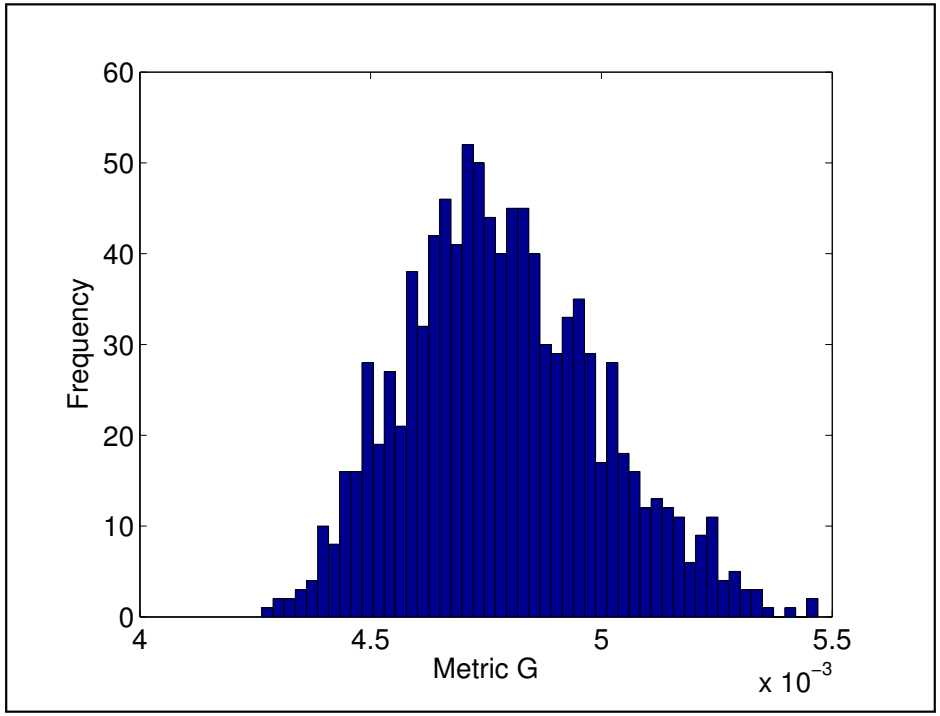
- We solve both the forward and adjoint problem.
- Define a neutron economy metric:

$$G = \frac{\text{Neutrons Used for Breeding}}{\text{Neutrons Lost to Leakage}}$$

- Adjoint problem gives sensitivity of G w.r.t parameters in p

Our UQ task is to estimate the mean, variance, and individual realizations of our neutron economy metric.

- Our 10 inputs are allowed to vary independently within 10% of their nominal value.
- We have 40 full forward/adjoint solution pairs (40 function/gradient evaluations) generated by LHS sampling of the inputs.
- We'll build and sample a BMARS model using 5, 10, 15, 20, 30, and 40 of these samples both with and without the gradient information.
- We also have 1000 forward LHS samples – we will verify the gBMARS predictions against these runs.



Distribution of our 1,000 "testing" runs.

Relative Error in Predicting the distribution mean

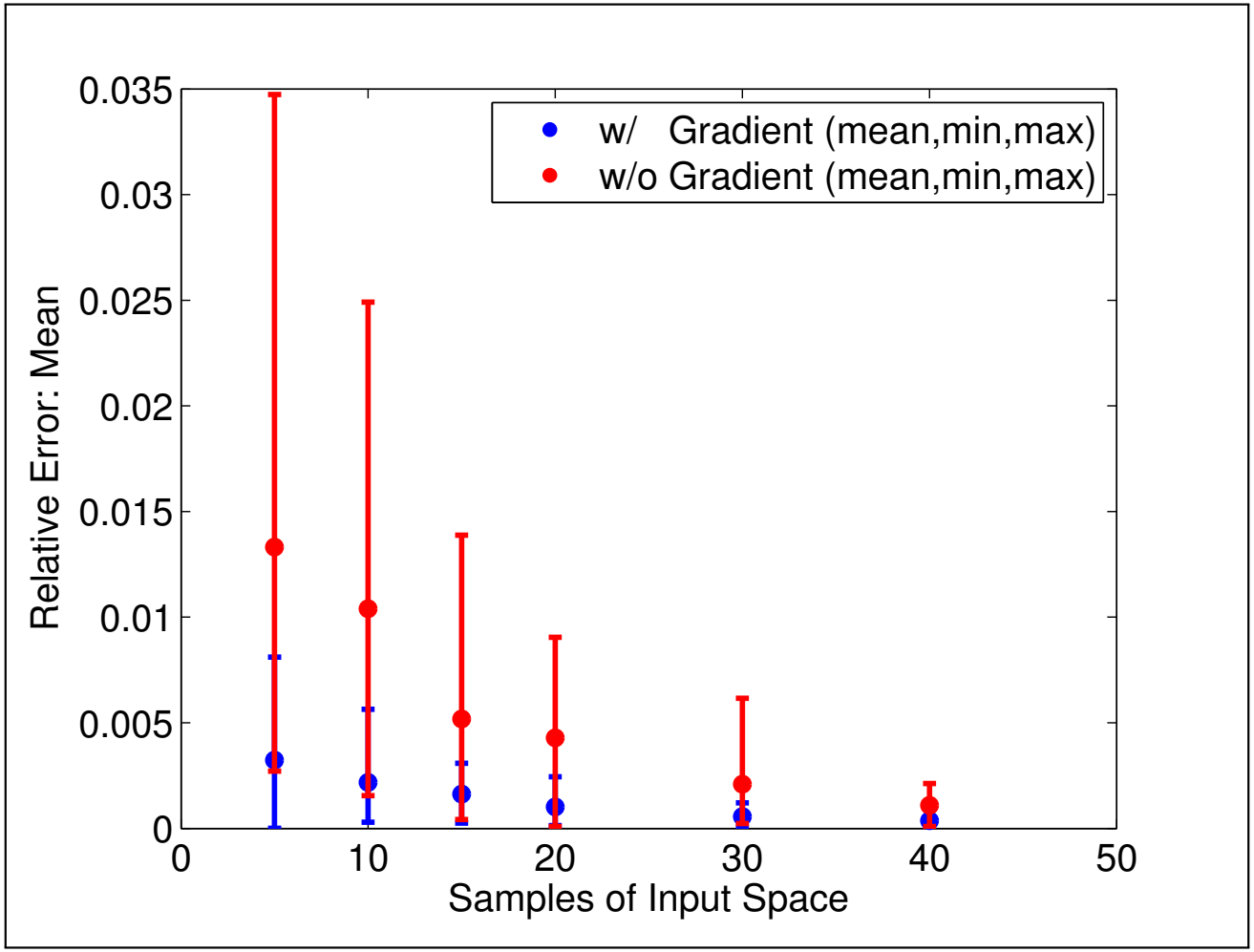


Figure: NOTE: 10 repetitions of each sample size

Relative Error in Predicting the distribution variance

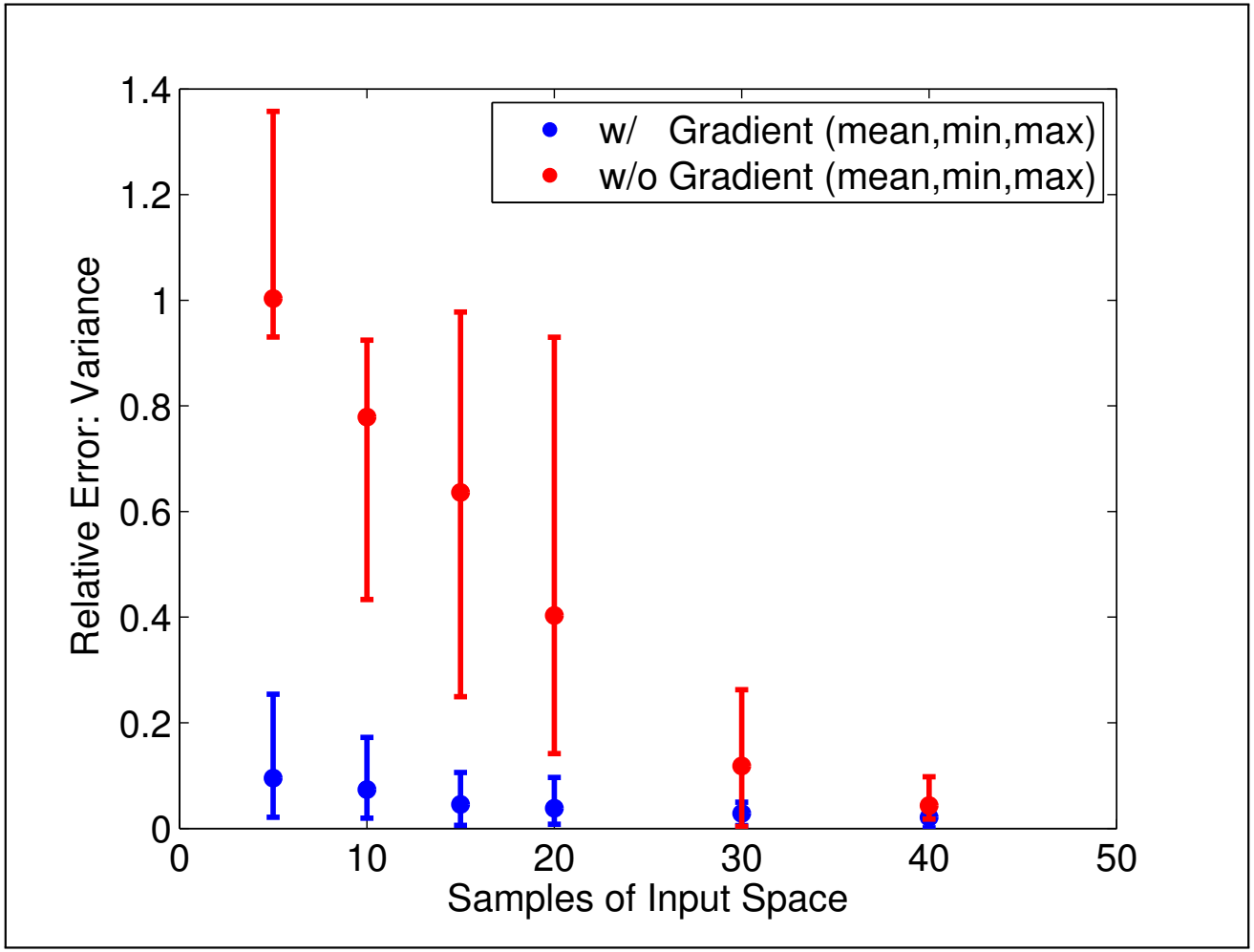
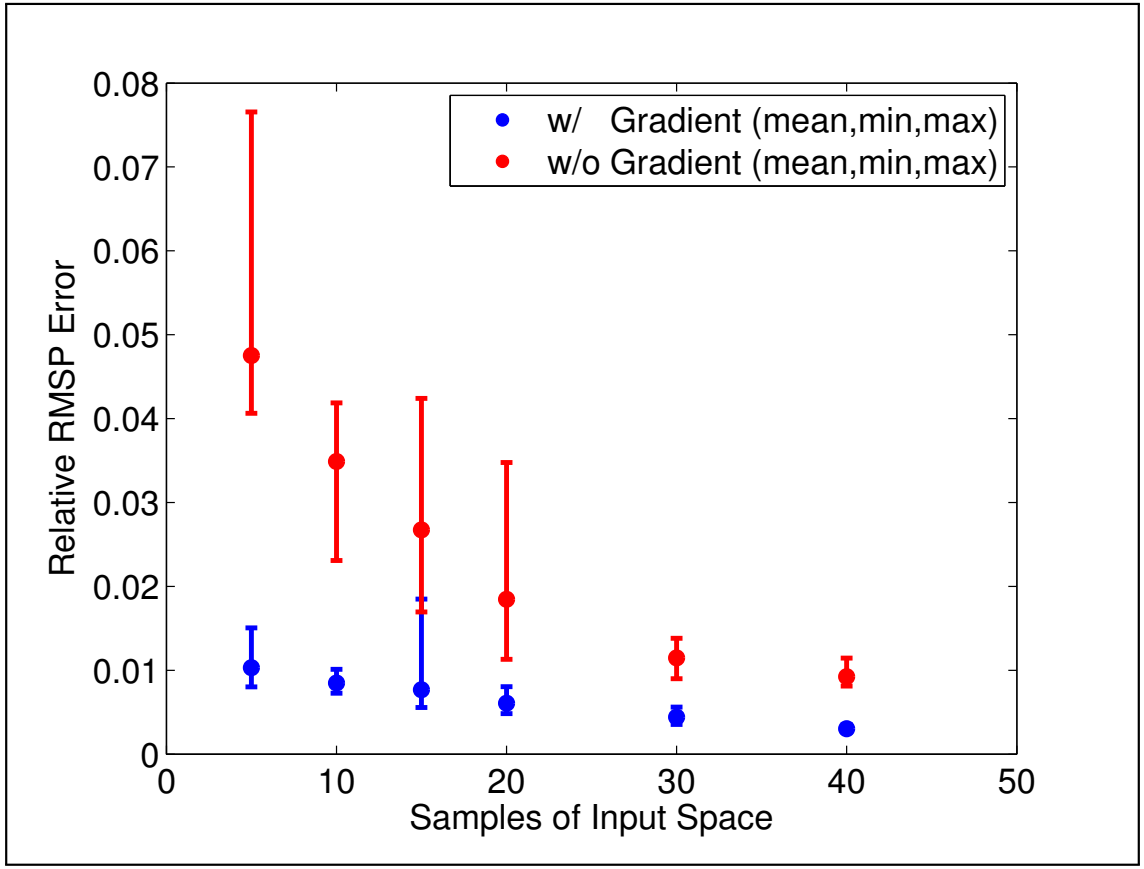


Figure: NOTE: 10 repetitions of each sample size

Root-Mean-Squared Predictive Error

$$\text{RMSPE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[B(x_i) - f(x_i)\right]^2}$$



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We demonstrate an extension of the BMARS algorithm to include gradient information for improved regression.

1. Gradient information is fairly straightforward to include in the BMARS emulator.
2. For both a suite of bivariate testing problems and a higher-dimensional reactor problem, the use of gradient information improved the regression of the underlying function and reduced the predictive variance.
3. Gradient information provided the greatest gains in:
   - 3.1 predicting both individual realizations and the variance of the metric distribution; and
   - 3.2 the cases of very sparse sampling of the input space.
4. Gradient enhanced emulators provide reasoning for a modeler to pay the extra cost of an adjoint or AD solve.

Questions?

Some gradient information produced using the INTLAB forward automatic differentiation package for MATLAB.