Local Sensitivity Derivative Enhanced Monte Carlo

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February 26, 2013

Key Questions

- How do we ensure the accuracy and reliability of our simulations?
- How do we quantify the impact of model parameter uncertainty on model outputs?

Forward Propagation of Uncertainty

Key Challenges

- Curse of dimensionality: Number of samples needed increases exponentially with stochastic dimensions
- High cost per sample
- Smoothness of response function in stochastic space

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Monte Carlo method

- Slow convergence : $\frac{C}{N_s^{\frac{1}{2}}}$, but independent of dimension
- Faster MC methods using efficient surrogates

Surrogate based MC acceleration

- Random parameters: ξ, mean: μ_ξ, QoI: $Q(\mathbf{u}, \xi)$
- Sensitivity Derivative Enhanced Monte Carlo Method (SDEMC) [Cao et al., 2004]. Taylor Series about mean:

$$Q_1(\mathbf{u}, \xi) = Q(\mathbf{u}, \mu_\xi) + Q^{'}(\mathbf{u}, \mu_\xi)(\xi - \mu_\xi)$$

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- Use enhanced estimator:

$$\frac{1}{N_{ss}} \sum_{j=1}^{N_{ss}} Q_1(\mathbf{u}, \xi_j) + \frac{1}{N_{ts}} \sum_{i=1}^{N_{ts}} [Q(\mathbf{u}, \xi_i) - Q_1(\mathbf{u}, \xi_i)]$$

- Decreases the overall variance and improves the convergence constant
- Can we construct better surrogates and improve the rate?

- Associate each sample $\{\xi_i\}_{i=1}^{N_s}$ with a Voronoi cell $\{R_i\}_{i=1}^{N_s}$

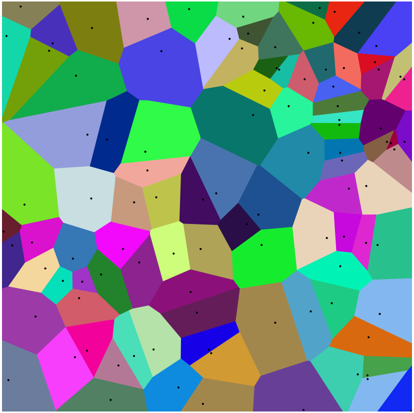
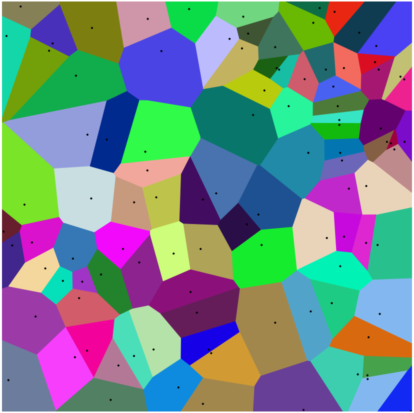


Figure : 2-d Voronoi diagram

LSDEMC Surrogate Construction

- Associate each sample $\{\xi_i\}_{i=1}^{N_s}$ with a Voronoi cell $\{R_i\}_{i=1}^{N_s}$
- Draw another set of samples $\{\xi_j\}_{j=1}^{N_{ss}}$ where $N_{ss} >> N_s$



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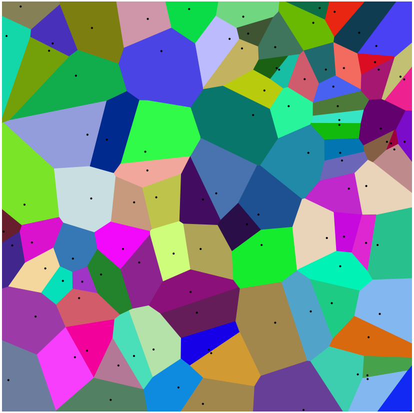

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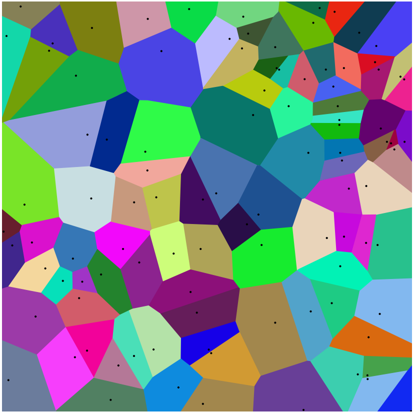
- Surrogate construction cost: $\mathcal{O}(N_s N_{ss}) \leq \mathcal{O}\left(N_s N_{\text{dofs}}^k\right)$



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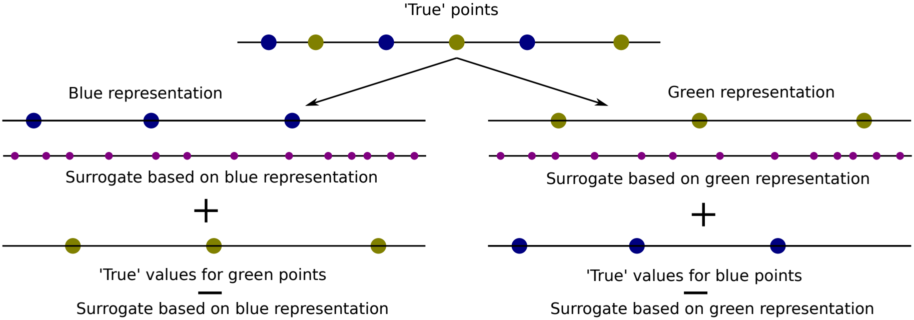
Bias Correction



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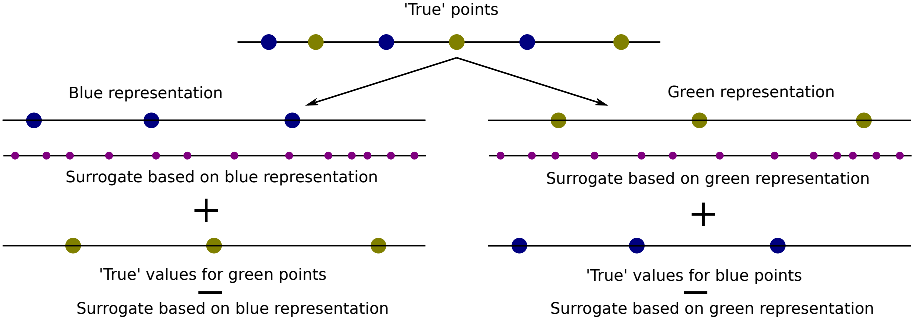

Estimator for the mean

$$\frac{1}{N_R}\sum_{r=1}^{N_R}\left(\frac{1}{N_{ss}}\sum_{l=1}^{N_{ss}} Q_{r,1}(\xi_l) + \frac{1}{N_s - \frac{N_s}{N_R}}\sum_{c=1}^{N_s - \frac{N_s}{N_R}} \left(Q(\xi_c) - Q_{r,1}(\xi_c)\right)\right)$$

Numerical Experiments

Test problem

- $Q(\xi) = e^{\sum_{i=1}^{d} \xi_i}$
- $\xi_i \equiv \mathcal{N}\left(\frac{\mu_{input}}{d}, \frac{\sigma^2_{input}}{d}\right)$
- $N_{ss} = N_s^2,\ N_R = 2$

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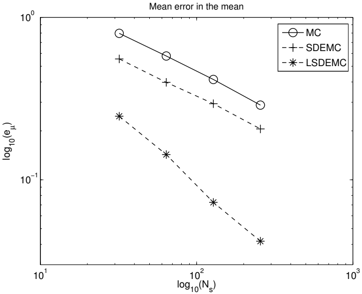

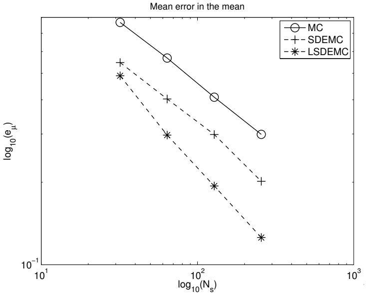

Error Analysis

Asymptotic Distribution

- Convergence rate: $N_s^{-\frac{1}{2}-\frac{f(d)}{d}}$ $\lim_{d\to\infty}\frac{f(d)}{d}=0$

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Let ξ^i be the nearest sample to point 0

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- Voronoi Cells $\to$ Surrogate $\to$ Expectation
- What is the asymptotic size of the Voronoi cells ?

Let ξ^i be the nearest sample to point 0

$$\text{In 1-d, } E(\xi^i) = \frac{1}{N_s p(0)} + \mathcal{O}\left(\frac{1}{N_s^2}\right)$$

$$\text{In higher dimensions, } E(\boldsymbol{\xi}^j) = \frac{1}{N_s^{\frac{1}{d}} p(\mathbf{0})} + \mathcal{O}\left(\frac{1}{N_s^{\frac{2}{d}}}\right)$$

Limitations of LSDEMC

Curse of Dimensionality

- Voronoi cells become larger with dimension, Taylor series approximation worse
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Curse of Dimensionality

- Voronoi cells become larger with dimension, Taylor series approximation worse
- But a d dimensional problem does not need to be d dimensional everywhere
- For example: $e^{\sum_{i=1}^{d} \xi_i}$ we only care about one 'dimension' $\sum_{i=1}^{d} \xi_i$

Local Dimension Reduction

- Euclidean norm not necessarily the best choice

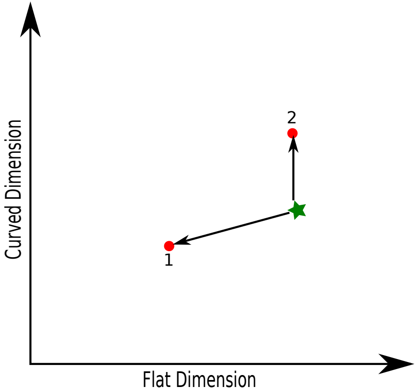

Figure : Euclidean Norm cannot distinguish the curved dimension from the flat dimension

Local Dimension Reduction

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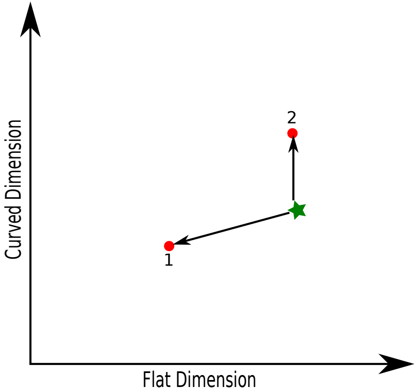
- Need to weight the distances in each direction by the curvature



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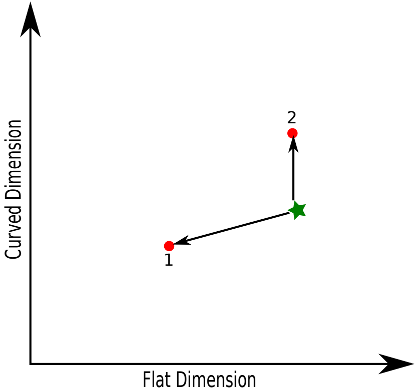
Local Dimension Reduction

- Euclidean norm not necessarily the best choice
- Need to weight the distances in each direction by the curvature
- Second order term in Taylor series: approximates the surrogate error, incorporates curvature



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Local Sensitivity Hessian Enhanced Monte Carlo

- Same algorithm as LSDEMC, but metric for Voronoi cell construction: $|(\xi_{ss} - \xi_s)^T H^s (\xi_{ss} - \xi_s)|$
- Rank of H^s gives local dimensionality
- If function is of globally lower dimension, should converge with the rate associated with that lower dimension

Numerical Experiments

Test problem 1

- $Q(\xi) = \left(\sum_{i=1}^{d} \xi_i \right)^2$
- $\xi_i \equiv \mathcal{N}\left(\frac{\mu_{input}}{d}, \frac{\sigma^2_{input}}{d} \right)$
- d varied from 4 to 256
- $N_s = 32$, $N_{ss} = 4N_s$, $N_R = 2$

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Absolute Error			
d	MC	LSDEMC	LSHEMC
4	0.1992	0.1050	0.0477
16	0.1916	0.2189	0.0384
256	0.2002	0.4548	0.0383

Numerical Experiments

Test problem 2

- $Q(\xi) = e^{\sum_{i=1}^{d} \xi_i} + e^{-\xi_1 + \sum_{i=2}^{d} \xi_i}$
- d varied from 4 to 64
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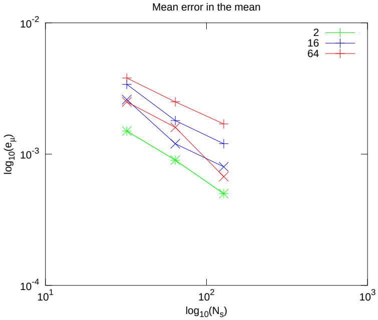

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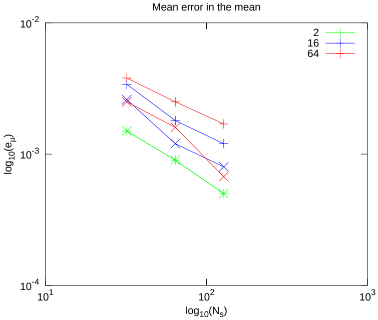
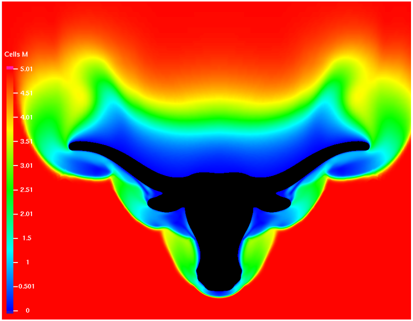
Convergence Rate			
d	MC	LSDEMC	LSHEMC
4	0.48	0.79	0.79
16	0.51	0.75	0.85
64	0.55	0.58	0.94



Where we stand

- Improved Monte Carlo convergence + Automatic Dimension Reduction
- Adjoints provide inexpensive sensitivies for surrogates, and can provide Hessians
- Can full Hessian construction be avoided ?

Questions ?



Thank You

This work was supported in part by DOE Award DE-SC0009297, as part of the DiaMonD Multifaceted Mathematics Integrated Capability Center.

Bibliography I

Cao, Y., Hussaini, M. Y., and Zang, T. A. (2004).
Exploitation of sensitivity derivatives for improving sampling methods.
AIAA journal, 42(4):815–822.