SAND2011-3283C

Evaluation of Mixed Continuous-Discrete Surrogate Approaches

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SIAM Conference on Optimization
Darmstadt, Germany
May 16-19, 2011

National Nuclear Security Administration

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Acknowledgements

- Genetha Gray, Sandia
- Bill Hart, Sandia
- Cindy Phillips, Sandia
- Ali Pinar, Sandia
- John Siirola, Sandia
- Jean-Paul Watson, Sandia
- David Woodruff, UC Davis

Mission needs motivate research in simulation-based analysis

http://safetycampus.files.wordpress.com/2008/12/forklift_accident_with_bomb.jpg

System Engineers

- Probability of Loss of Assured Safety if dropped?
- Adjust handling height?

↕

Analysts

- Use simulation with optimization and UQ tools?
- Most info from limited number of simulations?

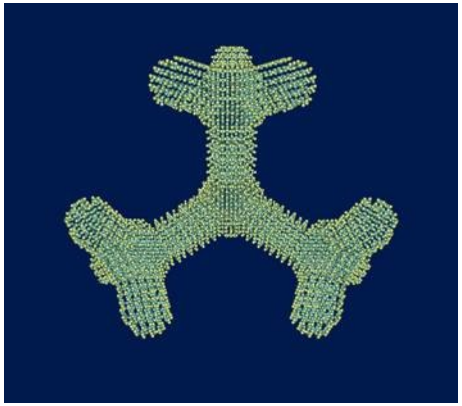
↕

Algorithm Developers

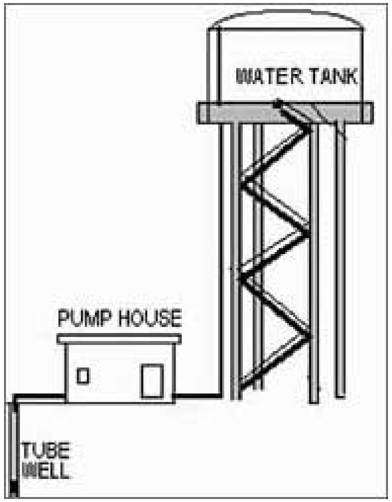
- New mathematics and statistics algorithms?
- Efficient implementations?

Categorical/discrete variables are finding their way into engineering and science simulations

System bolts
(Picture courtesy of J. Crowell)



Branched tetrapod nanocrystal generated by NREL "tetra" code
(Picture courtesy of P. Graf)

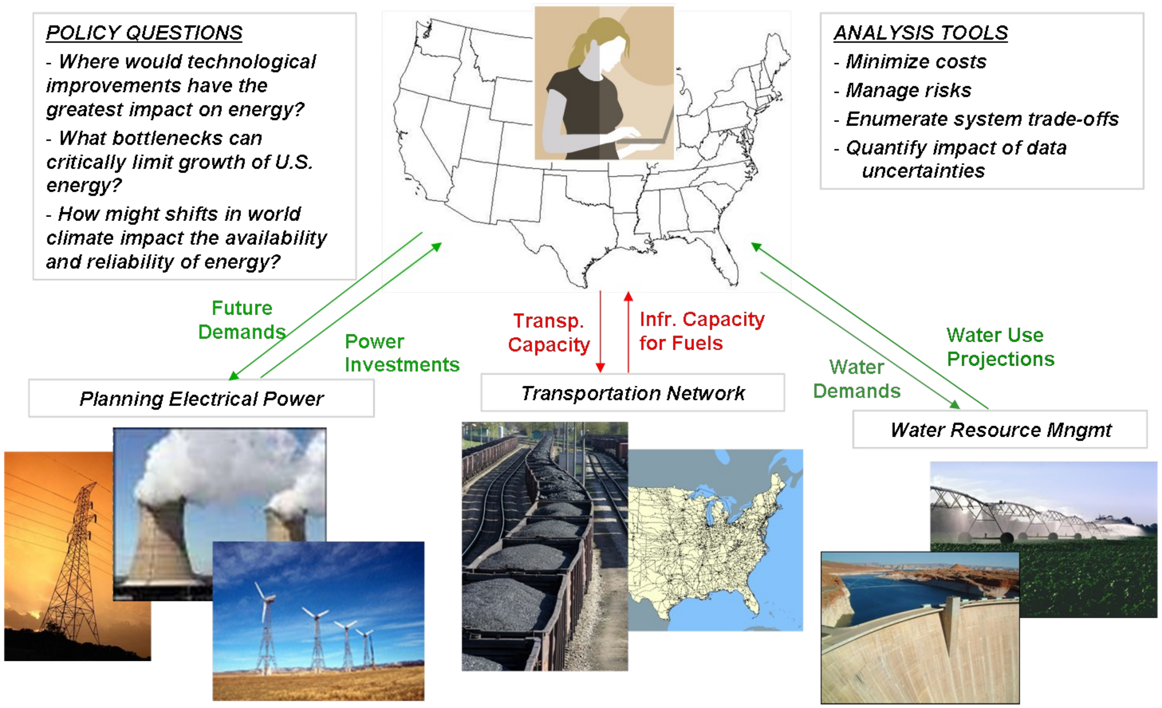


Water management system
(Picture courtesy of G. Gray)

- Modeling choices
  - Alternate plausible models
  - Choice between multiple materials
- Design choices
  - Material design
  - Operational settings

Key analysis characteristics
- Small number of variables
- Simulation based on computationally expensive equation solver

Additionally, large-scale "system of systems" simulations have many discrete variables



- Large-scale models decomposed into constitutive system models
- Black-box model of actor behavior, independent subsystems making choices based on input from others

Key analysis characteristics
- Large number of discrete and continuous variables
- Objective based on composition of heterogeneous models

Would like to use surrogate models to improve tractability of simulation-based analysis

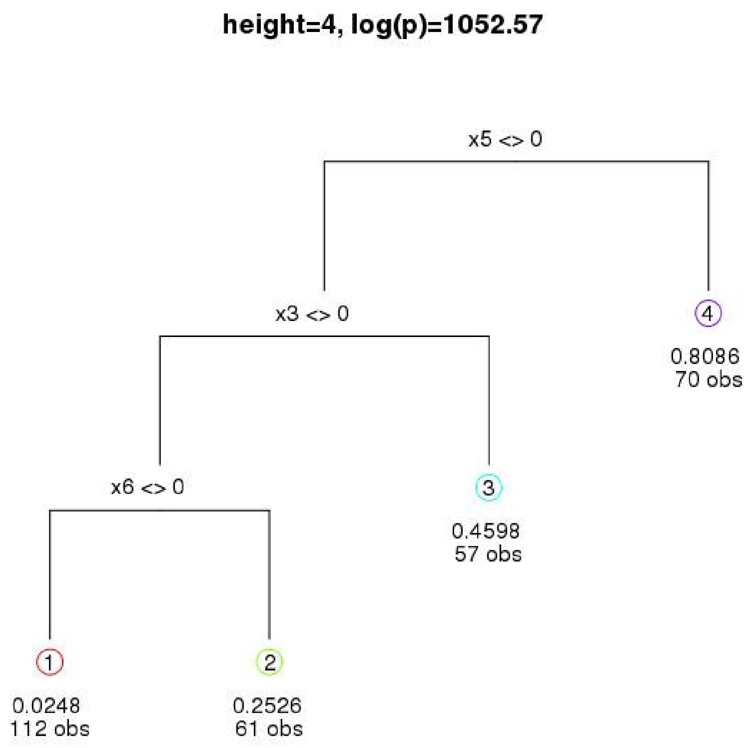
- Optimization and UQ methods are computationally expensive
- However, in mixed variable spaces...
  - Usual surrogate assumptions no longer hold
    - Continuous inputs
    - How output varies as input varies
  - Mixed variable surrogate approaches untested
  - Need a good testbed

Goal: Evaluate and compare mixed variable surrogate modeling approaches.

Approach 1: Categorical Regression

- Uses indicator functions for categorical variable levels
  - $Y=\beta_0 + \beta_1 X_1 + \beta_2 X_2$ where X_1 is continuous, X_2 is binary
    - $Y=\beta_0 + \beta_1 X_1$ for $X_2=0$, $Y=\beta_0 + \beta_1 X_1 + \beta_2$ for $X_2=1$
    - Results in 2 different models
- Computationally expensive
  - Need enough samples over continuous variables for *EACH* discrete combination for accurate regression function
  - Increase number of discrete variables + increase number of "levels" per variable => combinatorial explosion

Approach 2: Treed Gaussian Process (TGP)



- Gaussian process is a specified by mean and covariance
- TGP partitions space and constructs GP in each partition
- Mixed variable variant allows partitioning over categorical/discrete variables
  - Transforms each variable-level pair into binary variable
  - GP constructed at "leaf" nodes over only continuous variables

R. B. Gramacy and M. Taddy. "Categorical inputs, sensitivity analysis, optimization and importance tempering with tgp version 2, an R package for treed Gaussian process models." R manual available at http://cran.r-project.org/, 2009.

Approach 3: Adaptive COmponent Selection and Smoothing Operator (ACOSSO)

- Univariate smoothing spline estimate

$$\frac{1}{n}\sum_{i=1}^{n}[y_i - f(x_i)]^2 + \lambda\int_0^1 [f''(x)]^2 dx$$

Term which penalizes roughness

- ACOSSO Estimate: f is an additive function

$$f(x) = \sum_{j=1}^{q} f_j(x_j)$$

$$f_j(1) = c_1, f_j(2) = c_2, \ldots f_j(m_j) = c_{m_j}, \sum_{x=1}^{m_j} c_j(x) = 0$$

$$\frac{1}{n}\sum_{i=1}^{n}[y_i - f(\mathbf{x}_i)]^2 + \sum_{j=1}^{q}\lambda_j\int_0^1 [f_j''(x_j)]^2 dx$$

Term which penalizes trend

Term which penalizes categorical predictors

$$\frac{1}{n}\sum_{i=1}^{n}[y_i - f(\mathbf{x}_i)]^2 + \lambda\left(w_j \sum_{j=1}^{q}\left\{\left[\int_0^1 [f_j'(x_j)]dx_j\right]^2 + \int_0^1 [f_j''(x_j)]^2 dx_j\right\}^{1/2} + \sum_{j=q+1}^{p} w_j\left\{\sum_{x_j=1}^{m_j} f_j^2(x_j)\right\}^{1/2}\right)$$

C.B. Storlie, J.C. Helton,, B. J. Reich, and L.P. Swiler. "Analysis of Computationally Demanding Models with Qualitative and Quantitative Inputs." Draft manuscript.

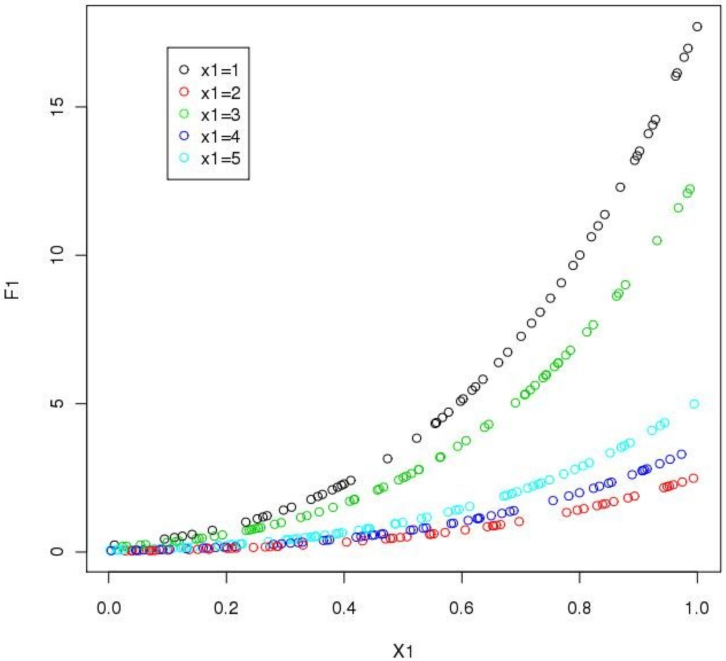
We established requirements for a testbed

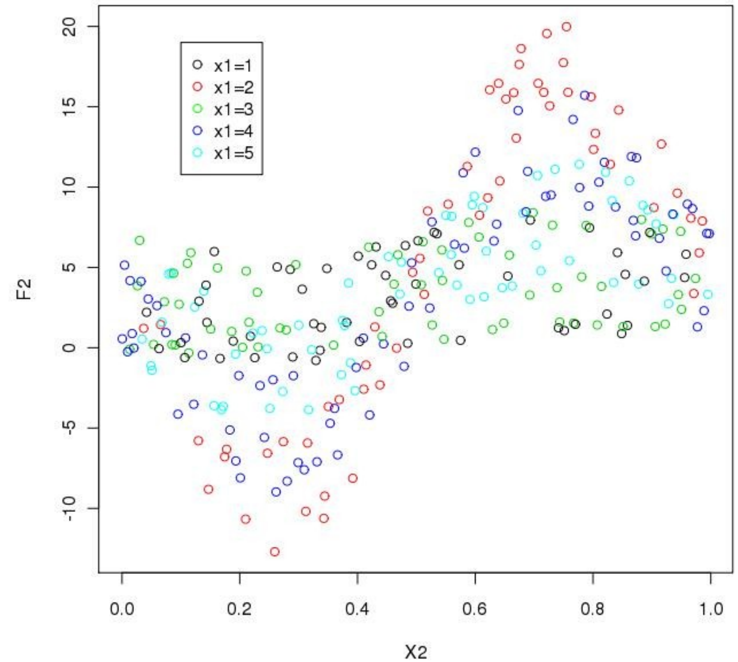
- Fast running evaluations
- Easy to compile, cross-platform compatibility
- Extendable
- File input/output
- Scalability of function in terms of number discrete variables and/or levels per variable
- Ability to control problem complexity

Testbed includes three defined functions

$$y = f_1(x) = \begin{cases} 3.5(x_2+0.5)^4 \text{ if } x_1 = 1 \\ 0.5(x_2+0.5)^4 \text{ if } x_1 = 2 \\ 2.5(x_2+0.5)^4 \text{ if } x_1 = 3 \\ 0.7(x_2+0.5)^4 \text{ if } x_1 = 4 \\ (x_2+0.5)^4 \text{ if } x_1 = 5 \end{cases}$$

$$y = f_2(x) = \begin{cases} \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) \text{ if } x_1 = 1 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 12\sin(2\pi x_3 - \pi) \text{ if } x_1 = 2 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 0.5\sin(2\pi x_3 - \pi) \text{ if } x_1 = 3 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 8\sin(2\pi x_3 - \pi) \text{ if } x_1 = 4 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 3.5\sin(2\pi x_3 - \pi) \text{ if } x_1 = 5 \end{cases}$$





$$y = f_3(x) = \sum_{i=1}^{n} (x_i - 1)^4$$

Scaled number of variables and number of levels per discrete variable.

Testbed also includes a random polynomial generator

- Generates a random polynomial
  - Degree between 2 and 6
  - Number of variables between 1 and 15
- Uses a system of linear equations to solve for the random coefficients, described in:
  - McDaniel, W. R. and B. E. Ankenman, “A Response Surface Test Bed.” Qual. Reliab. Engng. Int. 2000; 16: 363–372
- Can control the degree of nonlinearity, range of polynomial values, etc.

We applied the same evaluation process to all candidate surrogates using these test problems

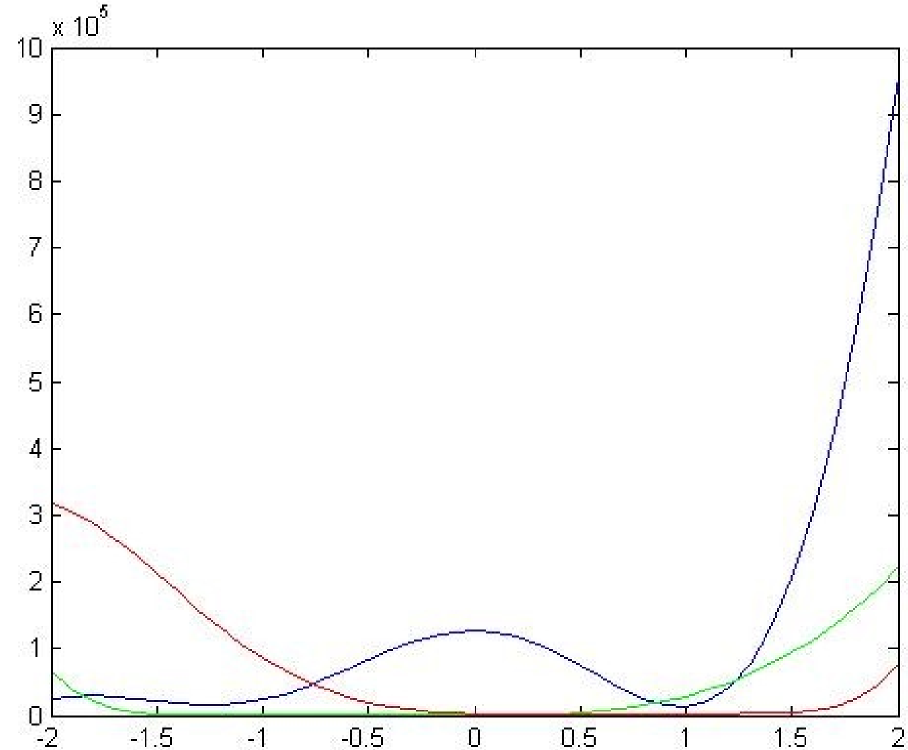
- Looked at surrogate performance over varying number of build points (LHS sample points)
- Used mean squared error (MSE) as a measure of goodness
  - Calculated over a grid (dimensioned based on the number of inputs)
- Categorical Regression run in DAKOTA
  - Generate a separate continuous surrogate for each combination of discrete variable values/levels
- TGP and ACOSSO run in R

Observations after first set of preliminary experiments were enlightening

- Categorical Regression performed very well on problems with small numbers of discrete variables/levels
- ACOSSO performed very well overall
- TGP performance was mixed
  - Ability to identify the splits
  - Not sufficient to aggregate across discrete levels
  - Adaptive methods may lead to improvement
- ACOSSO seemed to be the most scalable with respect to number of variables and discrete levels
- Need to further investigate the effects of parameter interactions

Results: Goldstein-Price Function

- Function of 2 variables that ranges over six orders of magnitude
- Y=(1+(x1+x2+1)2*(19-14x1+3x12-14x2+6x1x2+3x22)*(30+(2x1-3x2) 2*(18-32x1)+12x12+48x2-36x1x2+27x22))



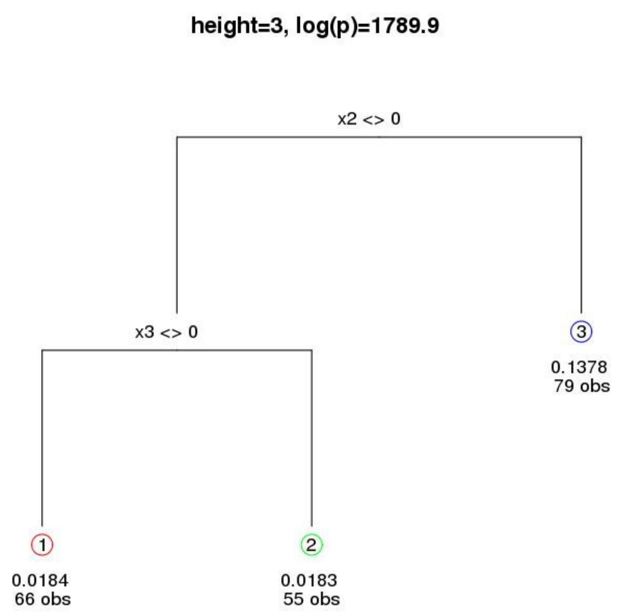
Results: Goldstein-Price Function

Actual Function		
Number Build Points	MSE TGP	MSE ACOSSO
50	3.87E+07	2.42E+07
100	3.89E+04	9.67E+06
150	2.50E+03	6.67E+06
200	9.51E+01	5.33E+06
250	4.39E+01	1.55E+06
300	2.20E+03	2.14E+04

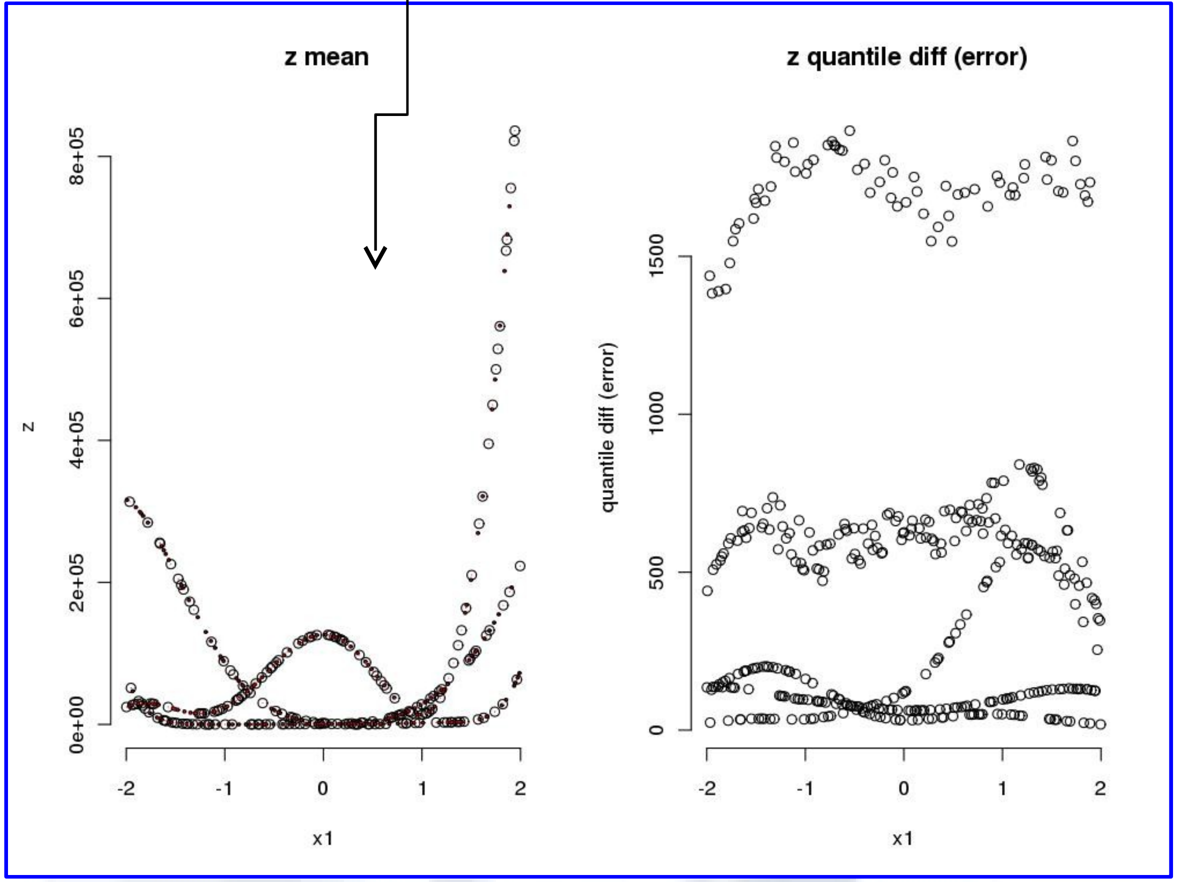
Log Scaled Function		
Number Build Points	MSE TGP	MSE ACOSSO
50	4.051E-01	1.164E-01
100	1.036E-02	5.991E-03
150	7.236E-03	8.764E-03
200	1.778E-04	3.718E-04
250	5.379E-03	1.803E-04
300	1.080E-02	3.208E-07

TGP performs better with the large range of output, because it can partition and create different GPs over different parts of the space. In log space, ACOSSO performs better.

Results: Goldstein-Price Function



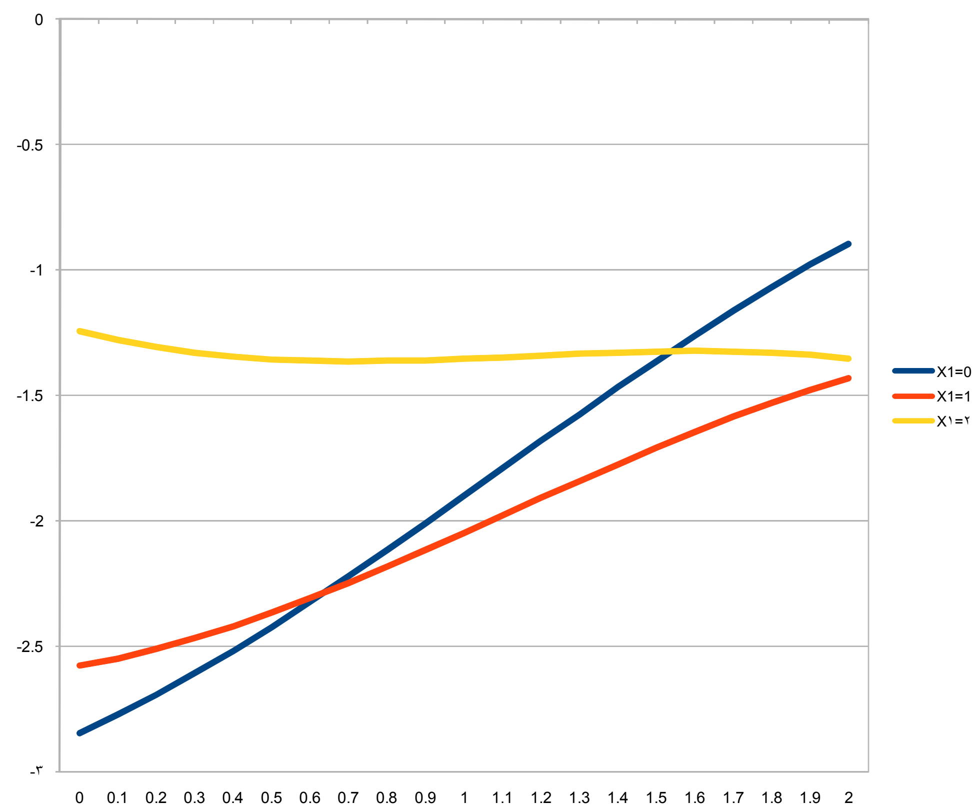
TGP predictions for the three discrete levels, as a function of the continuous one



TGP partitioning over levels of discrete variables

Results: 3rd-order Polynomial

- 10 terms, significant interaction
- We looked at two aspects: increasing the magnitude of the overall function (shifting it up or down from on the order of -2 below to -200K) and increasing the range (by multiplying by factors of 10)



Results: 3rd-order Polynomial

Shift Factor: 10		
Build Points	TGP:	ACOSSO
50	1.02E-08	8.97E-07
100	3.05E-11	1.61E-08
150	3.95E-12	1.46E-10
200	1.75E-12	1.11E-10
250	9.60E-13	2.81E-10
300	3.65E-12	8.75E-12

Shift Factor: 10000		
Build Points	TGP:	ACOSSO
50	1.02E-02	8.97E-01
100	3.76E-05	1.60E-02
150	3.41E-06	1.45E-04
200	1.47E-06	1.07E-04
250	1.07E-06	2.76E-04
300	3.72E-06	8.42E-06

Shift Factor: 1M		
Build Points	TGP:	ACOSSO
50	1.023E+02	8.965E+03
100	3.050E-01	1.610E+02
150	3.143E-02	1.480E+00
200	3.781E-02	1.119E+00
250	9.826E-03	2.411E+00
300	3.894E-02	9.024E-02

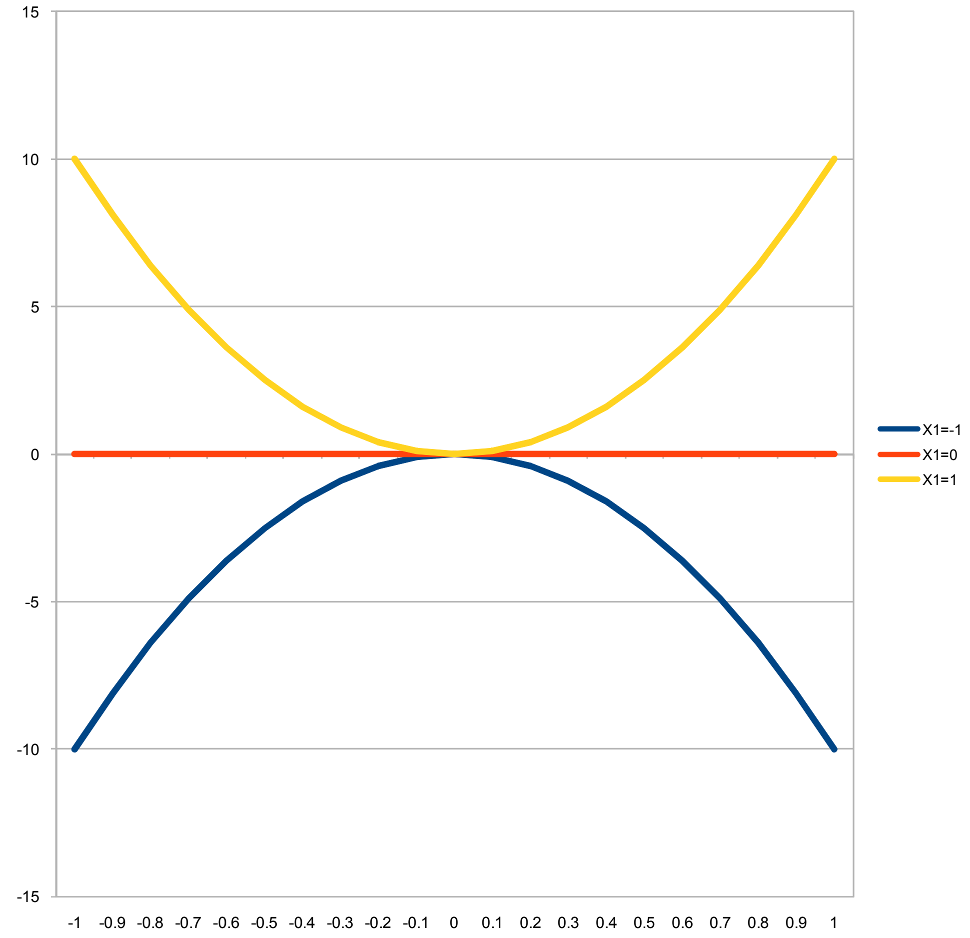
Scale Factor: 100		
Build Points	TGP	ACOSSO
50	6.03E-05	5.84E-03
100	1.99E-06	3.30E-04
150	4.29E-07	1.36E-06
200	3.56E-07	7.56E-07
250	7.71E-07	1.69E-06
300	3.28E-07	2.42E-07

Scale Factor: 100000		
Build Points	TGP	ACOSSO
50	6.03E+01	5.84E+03
100	1.99E+00	3.30E+02
150	4.26E-01	1.38E+00
200	7.43E-01	8.61E-01
250	5.29E-01	1.67E+00
300	2.59E-01	2.33E-01

TGP has better performance in all cases, regardless of whether the function is shifted or scaled, especially at with fewer build points. TGP performs better with larger function variations.

Results: Simple Function 10x1x2^2

- We thought this would be trivial
- The constant line at x1=0 proved to be pathological for TGP

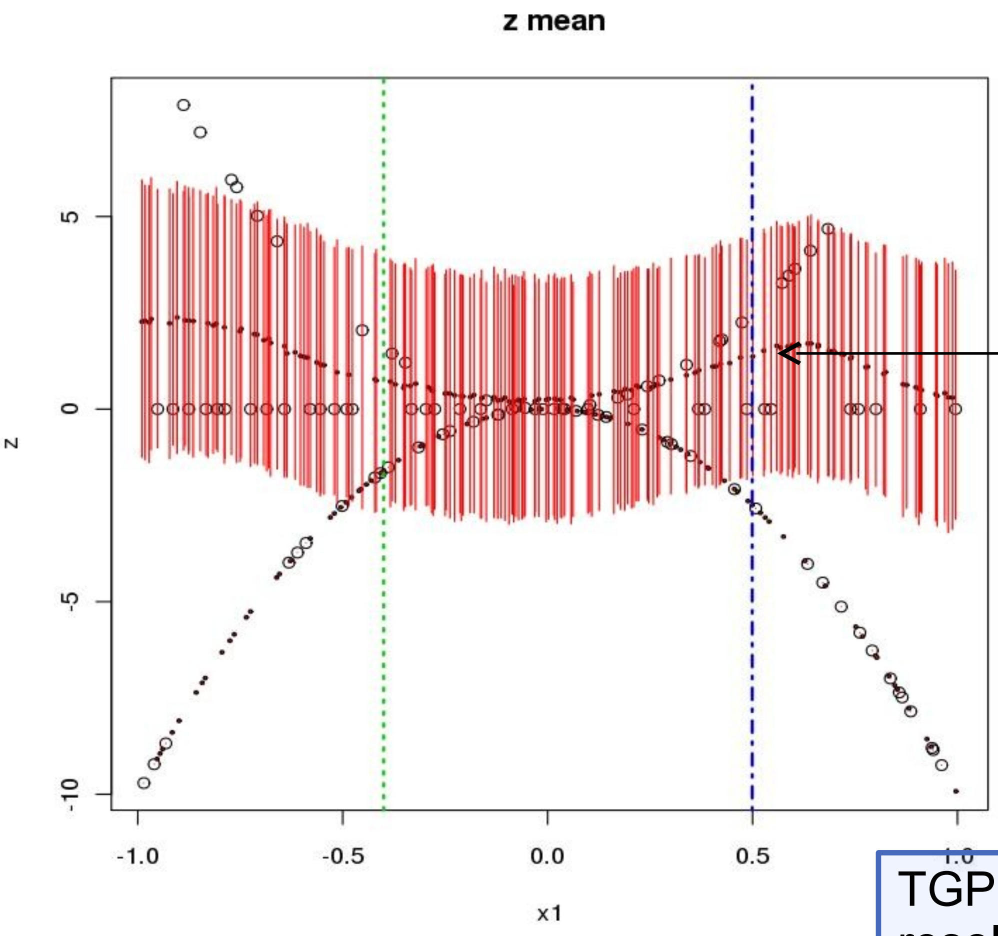


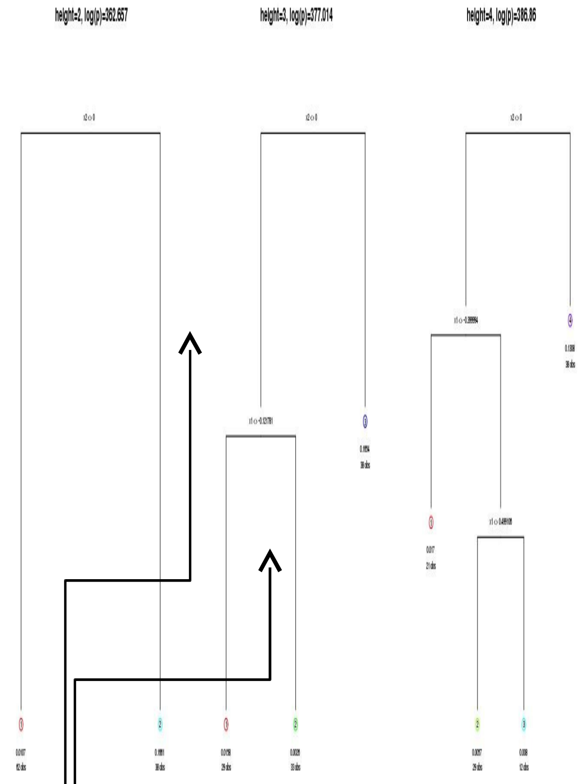
Results: Simple Function 10x1x2^2

- TGP has an option called “basemax” for mixed categorical/continuous variables.
- Basemax allows you to specify which variables are used to construct the GP at the leaves of the partitioned tree. Typically, basemax is used to specify the continuous variables: the tree can partition over categorical but the GP is only built on the continuous variables.
- In the case of this function, X2 is not predictive when X1=0. So, TGP fails in this case (constant MSE of around 4 regardless of number of build points)
- It can be remedied by not specifying basemax, but then the GP is built based on both the continuous and categorical variables, essentially treating the categorical as continuous. This usually is not the behavior we want.

Build Points	TGP	TGP with no basemax specified	ACOSSO
50	4.28E+00	5.97E-06	4.71E-05
100	4.20E+00	5.04E-08	2.80E-06
150	3.71E+00	1.55E-08	2.84E-05
200	3.45E+00	1.32E-08	3.62E-07
250	3.56E+00	1.91E-08	1.71E-07
300	3.88E+00	**	1.49E-07

Results: Simple Function 10x1x2^2

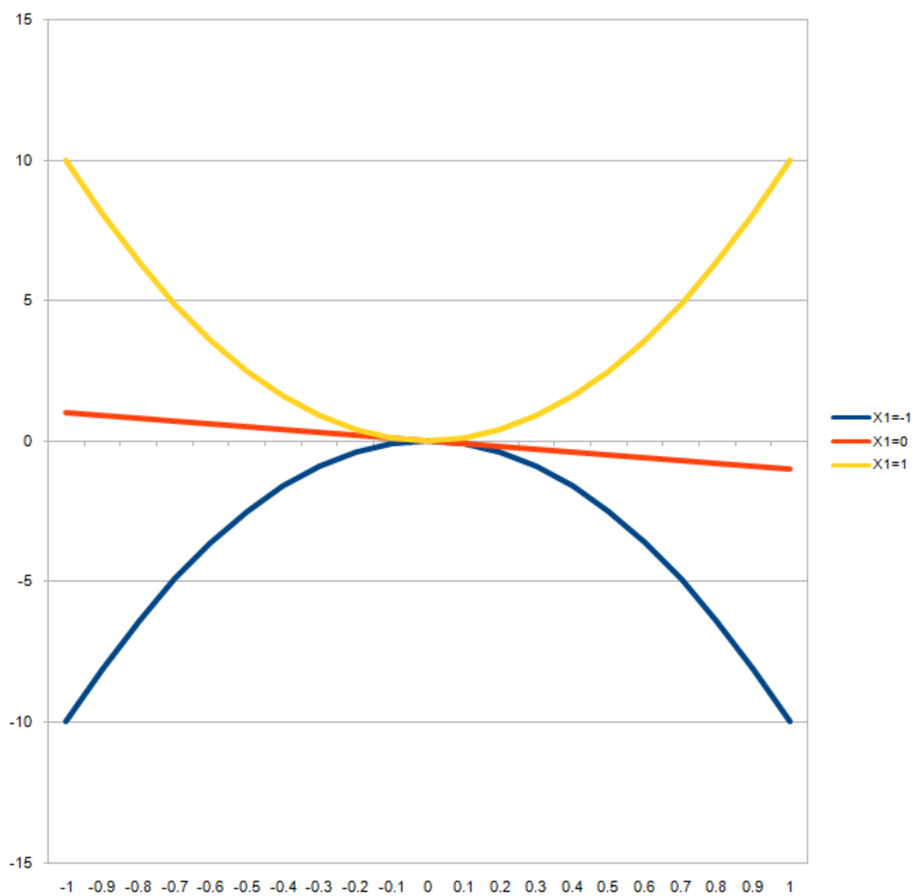


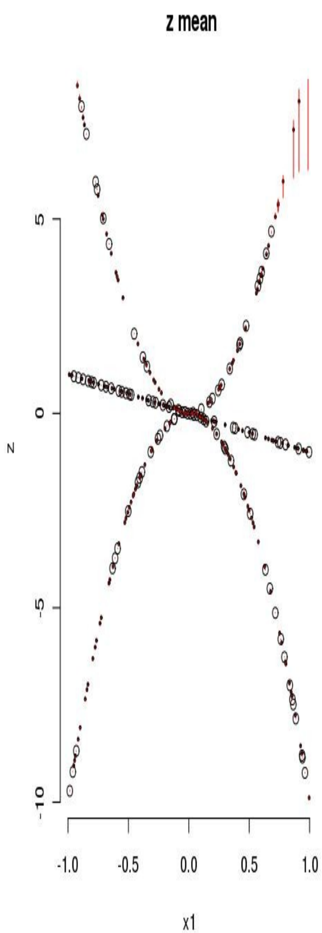


TGP gets the prediction for X1=-1, but cannot resolve the difference between X1=0 and X1=1. It does try to split over the continuous variable as well as the discrete, but this doesn't help.

Results: Variation on 10x1x2^2

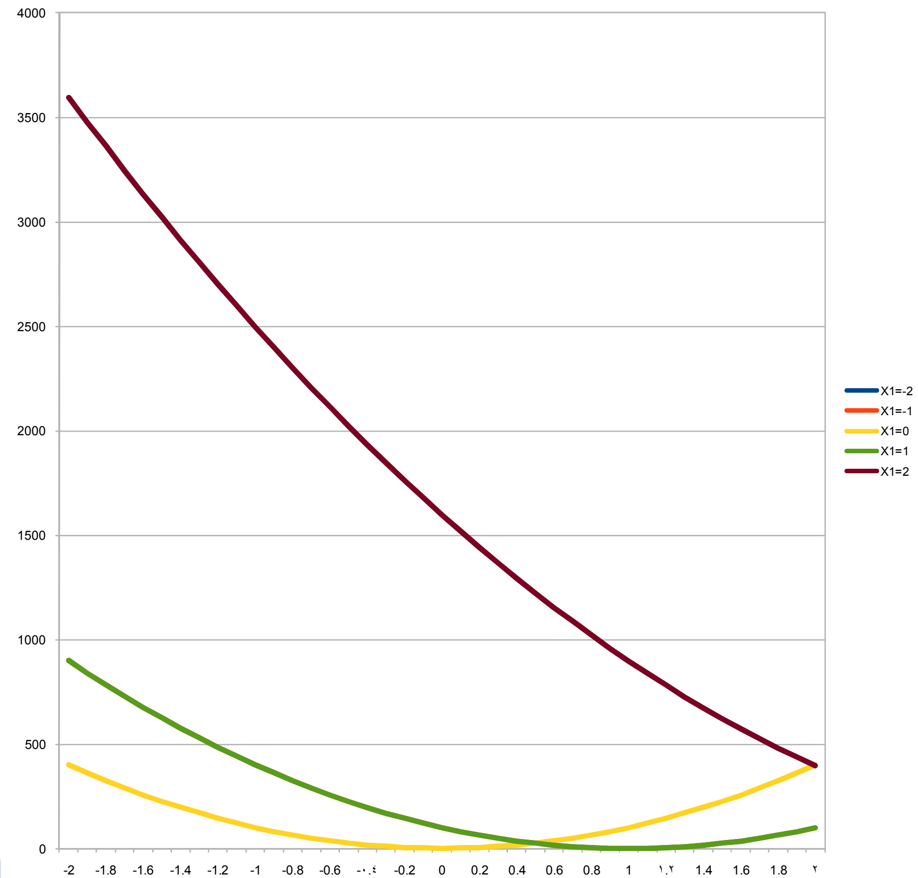
- Change line y=0 at x1=0 to y=-x2 at x1=0
- TGP has no problem in this case





Results: 4th-order Schittkowski function

- Y = 100(x2-x1^2)^2 + (1-x1^2)
- Shows both interactions and scale effects



Scale Factor: 100		
Build Points	TGP	ACOSSO
٥٠	٦.٠٣E-٠٥	٥.٨٤E-٠٣
١٠٠	١.٩٩E-٠٦	٣.٣٠E-٠٤
١٥٠	٤.٢٩E-٠٧	١.٣٦E-٠٦
٢٠٠	٣.٥٦E-٠٧	٧.٥٦E-٠٧
٢٥٠	٧.٧١E-٠٧	١.٦٩E-٠٦
٣٠٠	٣.٢٨E-٠٧	٢.٤٢E-٠٧
Scale Factor: 100000		
Build Points	TGP	ACOSSO
٥٠	٦.٠٣E+٠١	٥.٨٤E+٠٣
١٠٠	١.٩٩E+٠٠	٣.٣٠E+٠٢
١٥٠	٤.٢٦E-٠١	١.٣٨E+٠٠
٢٠٠	٧.٤٣E-٠١	٨.٦١E-٠١
٢٥٠	٥.٢٩E-٠١	١.٦٧E+٠٠
٣٠٠	٢.٥٩E-٠١	٢.٣٣E-٠١

Observations, the sequel

- Surrogate models are imperative for computational tractability of engineering analyses
- ACOSSO continues to have the most consistent performance
- TGP is best performer for problems with responses that vary over large orders of magnitude
- Indications are that TGP handles interactions better, but this still needs further exploration
- Still need to investigate
  - Degree of variable predictivity needed for TGP
  - Effects of degree/type of nonlinearity
  - Improving efficiency of TGP and ACOSSO implementations

References

- R.B. Gramacy and H. K. H. Lee. "Bayesian treed Gaussian process models with an application to computer modeling." *Journal of the American Statistical Association*, 103:1119-1130, 2008.
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- C.B. Storlie, J.C. Helton,, B. J. Reich, and L.P. Swiler. "Analysis of Computationally Demanding Models with Qualitative and Quantitative Inputs." Draft manuscript.

Backup Slides

Surrogate models improve computational tractability (Queipo, Haftka, Shyy, Goel, Vaidyanathan, and Tucker (2005))

- Response surface models
  - Draw data from simulation
  - Fit fast approximation to data
- Reduced-order models
  - Reduce the number of variables
  - Principal component analysis, proper orthogonal decomposition, dimensionality reduction
- Multi-fidelity models
  - Coarsen the discretization
  - Reduce the amount of geometric detail
  - Reduce the amount of physics included
- Stochastic expansion
  - Build global approximation as function of uncertain variables
  - Polynomial chaos, stochastic collocation

One of our favorite response surfaces is the Gaussian process

- Specified by mean and covariance
- Vanilla covariance function

$$C_{12}(\mathbf{x}^1, \mathbf{x}^2) = \sigma^2 \exp\{-\sum_{i=1}^{n} \rho_i^2 (\mathbf{x}_i^1 - \mathbf{x}_i^2)^2\}$$

  - σ and ρ_i found by maximizing likelihood function

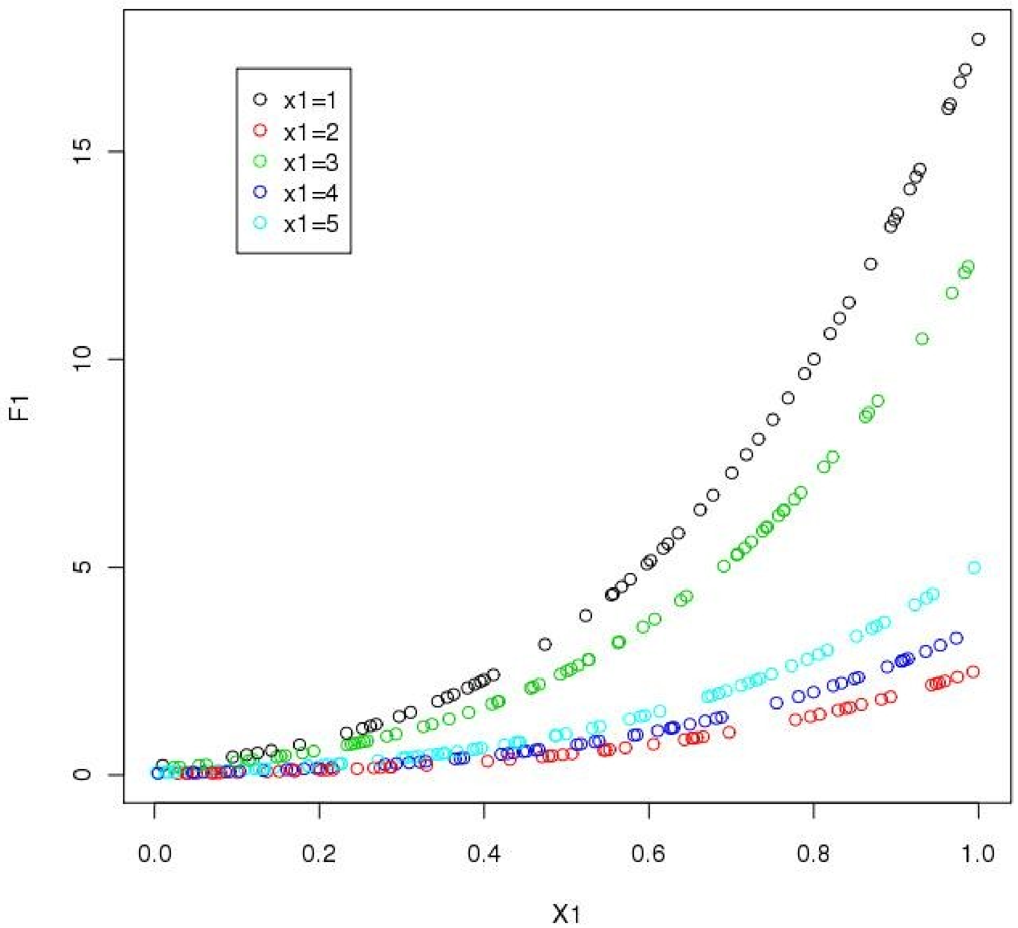
$$L = \frac{-n}{2}\log(2\pi) - \frac{1}{2}\log(\det(C)) - \frac{1}{2}\mathbf{z}^T C^{-1}\mathbf{z}$$

Key feature: Estimates both mean behavior and variance.

Approach 2: Treed Gaussian Process (TGP)

- Gaussian process is a random process specified by mean and covariance functions
- Mixed variable variant allows partitioning over categorical/discrete variables
  - Transforms each variable-level pair into binary variable
  - GP constructed at “leaf” nodes over only continuous variables
- Alternate approach has explicit representation of categorical variables in GP
  - P. Qian, H. Wu, and C.F.J. Wu. “Gaussian process models for computer experiments with qualitative and quantitative factors.” *Technometrics,* 50(3):383–396, 2008.
  - Recommend isotropic correlation structure

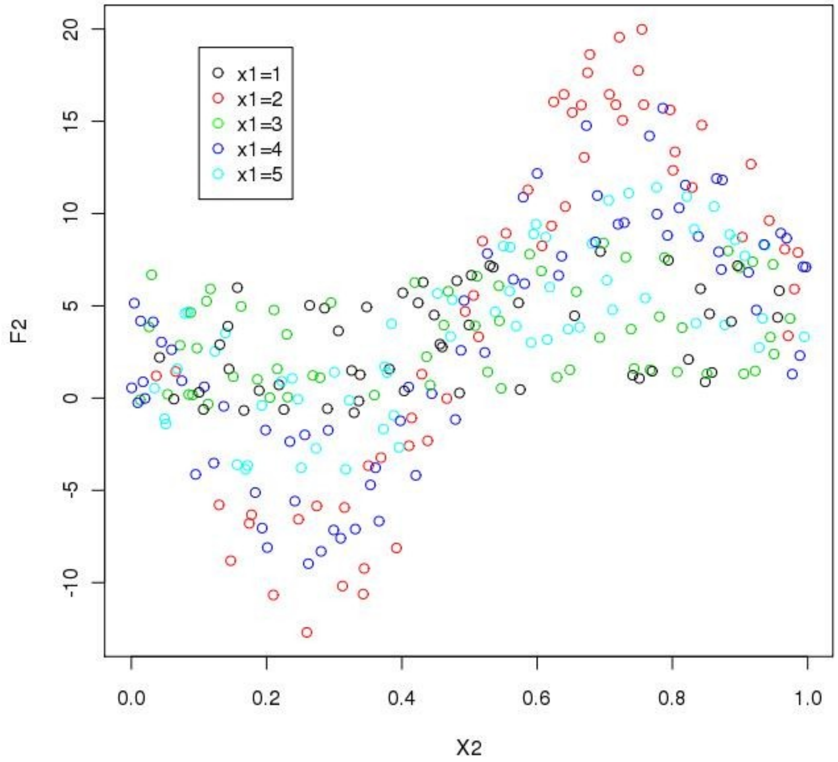
Testbed: Test Function 1



$$y = f_1(x) = \begin{cases} 3.5(x_2 + 0.5)^4 \text{ if } x_1 = 1 \\ 0.5(x_2 + 0.5)^4 \text{ if } x_1 = 2 \\ 2.5(x_2 + 0.5)^4 \text{ if } x_1 = 3 \\ 0.7(x_2 + 0.5)^4 \text{ if } x_1 = 4 \\ (x_2 + 0.5)^4 \text{ if } x_1 = 5 \end{cases}$$

Testbed: Test Function 2

$$y = f_2(x) = \begin{cases} \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) \text{ if } x_1 = 1 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 12\sin(2\pi x_3 - \pi) \text{ if } x_1 = 2 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 0.5\sin(2\pi x_3 - \pi) \text{ if } x_1 = 3 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 8\sin(2\pi x_3 - \pi) \text{ if } x_1 = 4 \\ \sin(2\pi x_3 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 3.5\sin(2\pi x_3 - \pi) \text{ if } x_1 = 5 \end{cases}$$

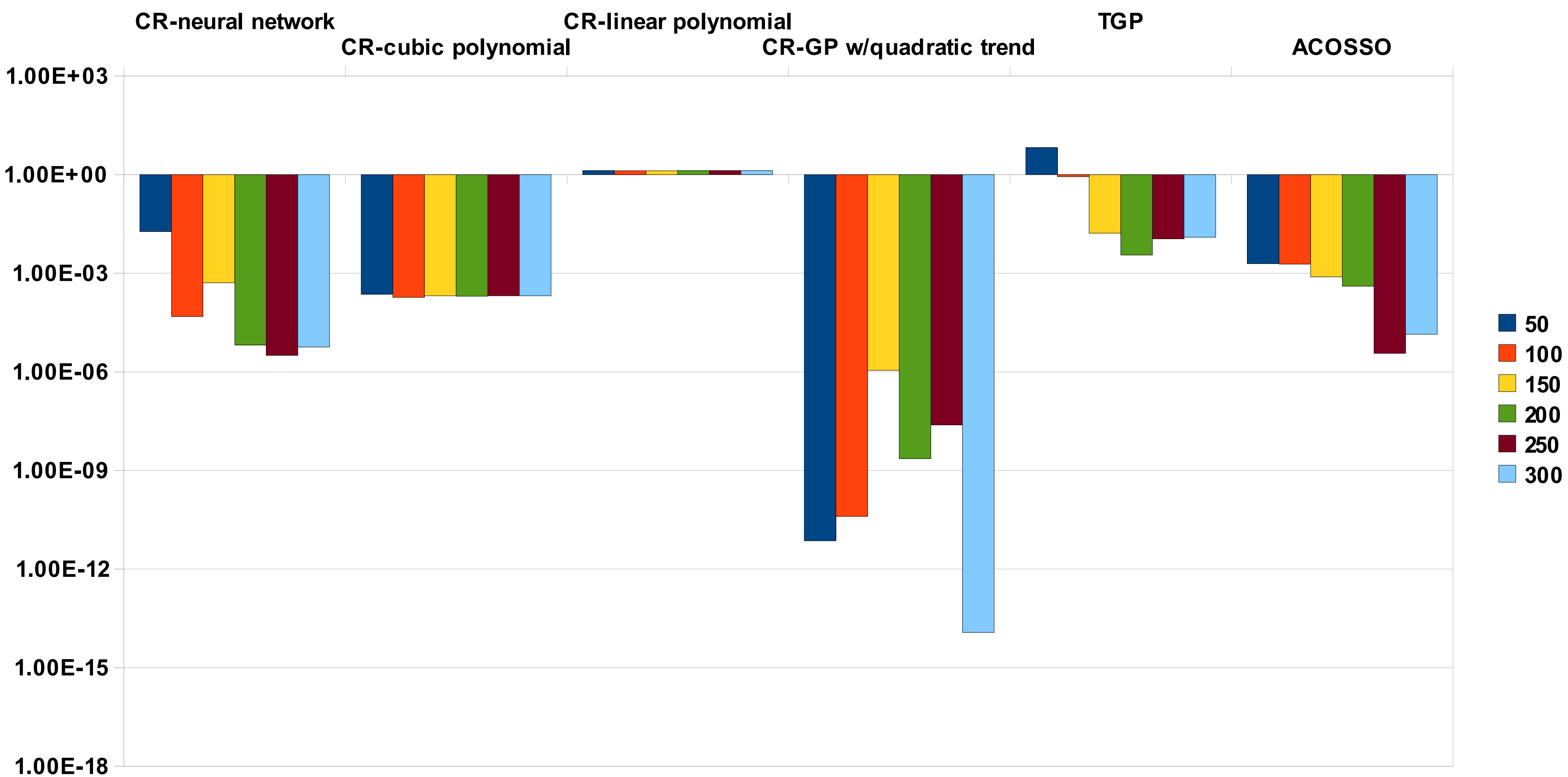


Testbed: Test Function 3

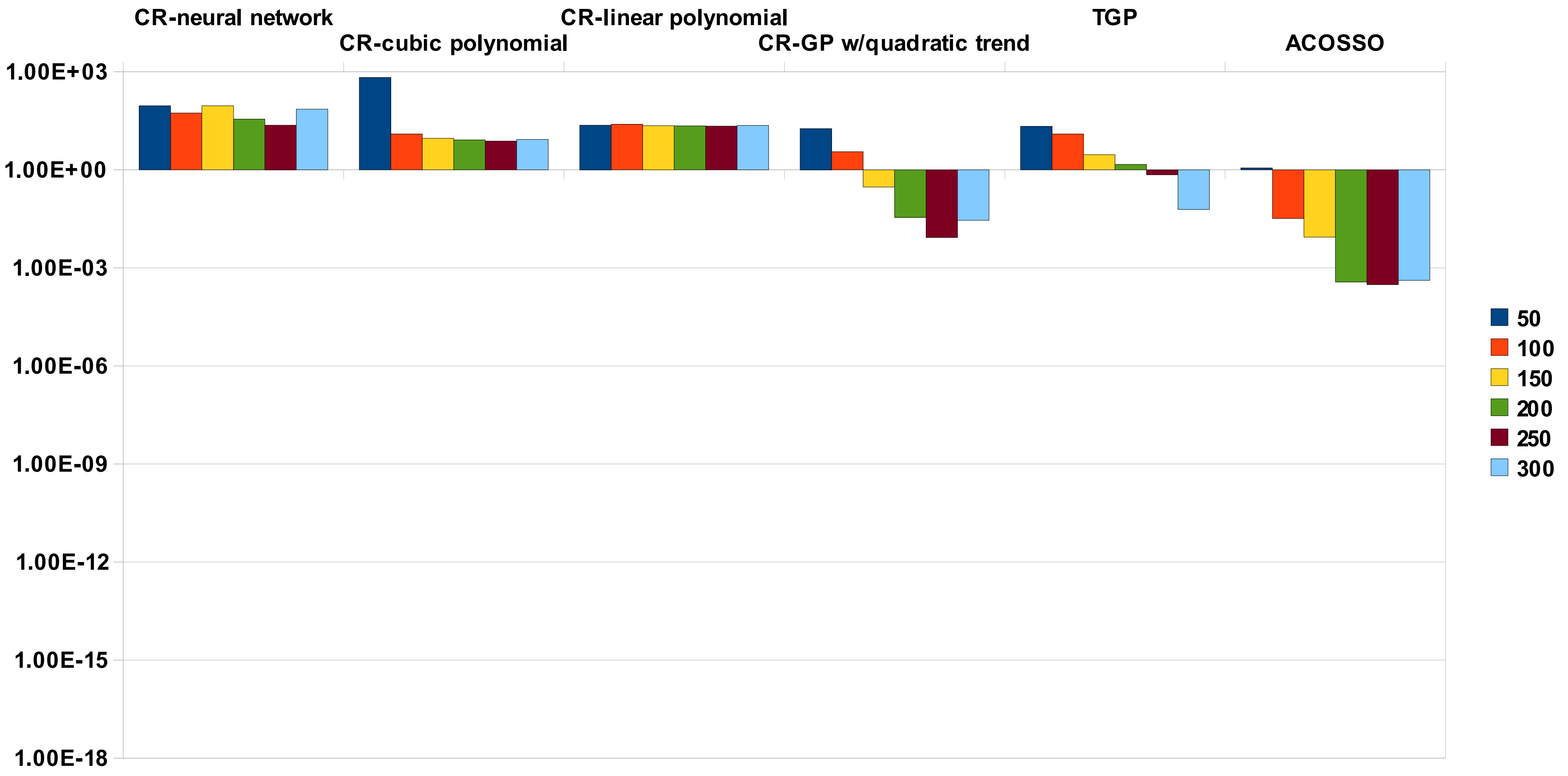
$$y = f_3(x) = \sum_{i=1}^{n} (x_i - 1)^4$$

- Initially started with 4 variables
  - 2 continuous on [0,2]
  - 2 discrete with values [0,1,2]
- Easy to scale up number of levels
  - Scaled number of levels to 5, with values [-1,0,1,2,3]
- Easy to scale up number of discrete variables
  - Scaled up to 5 discrete variables, with 3 and 5 levels
- Can also explore symmetry and function separability

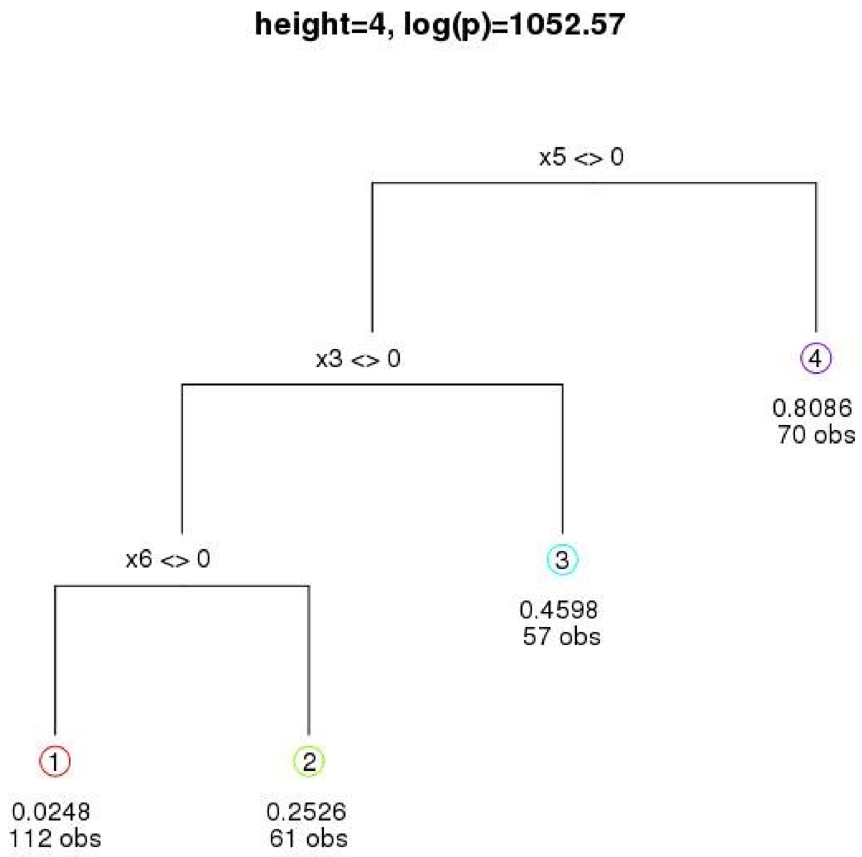
Test Function 1: Categorical regression works quite well, especially using GP



Test Function 2: All approaches have trouble resolving the categorical levels

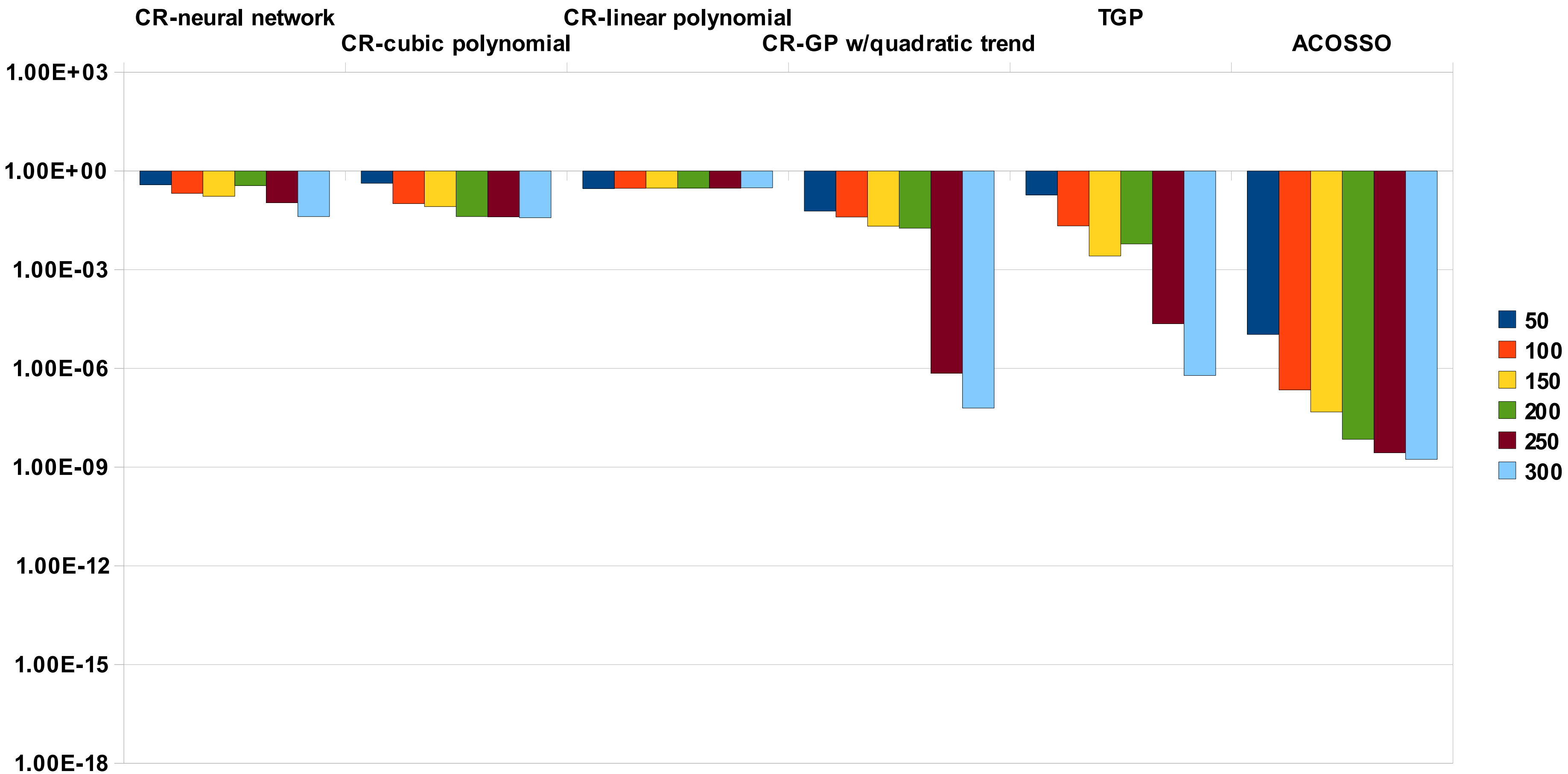


Aggregation of categorical levels in TGP may be a disadvantage



- TGP does not fully partition over all discrete variables
- Premise was that it would be sufficient to create surrogates over partitions which aggregrate the discrete variables
- Perhaps too coarse, resulting in inaccurate surrogates

Test Function 3: Categorical regression starts to degrade with slight increase in dimension



Test Function 3: TGP scales better with number of discrete variables than number of levels

- Scaling up discrete levels from 3 to 5
- Scaling up discrete variables from 2 to 5

Test Function 3	**SYMMETRIC - TGP**			
Discrete	2 [0-1-2]	2 [-1-0-1-2-3]	5 [0-1-2]	5 [-1-0-1-2-3]
Continuous	2 [0,2]	2 [0,2]	2 [0,2]	2 [0,2]
50	0.7217199	119.75	1.38	319.22
100	0.03391995	57.15	0.79	300.08
150	0.01617074	25.94	0.87	272.76
200	0.00631333	25.26	0.72	265.96
300	4.45E-05	17.91	0.52	231.41
500	1.74E-06	1.27	0.32	223.68

MSE decreases more quickly for more discrete variables vs. an increased number of levels per variable.

Test Function 3: Same trend holds for ACOSSO, though it still performs well

- Scaling up discrete levels from 3 to 5
- Scaling up discrete variables from 2 to 5

Test Function 3	SYMMETRIC - ACOSSO			
Discrete	2 [0-1-2]	2 [-1-0-1-2-3]	5 [0-1-2]	5 [-1-0-1-2-3]
Continuous	2 [0,2]	2 [0,2]	2 [0,2]	2 [0,2]
50	1.20E-04	8.15E-04	2.24E-04	2.56E-01
100	9.31E-06	1.55E-03	6.27E-06	4.06E-06
150	1.50E-06	1.34E-03	2.01E-06	2.56E-04
200	1.75E-07	3.20E-06	6.97E-07	1.99E-03
300	3.17E-07	4.68E-05	1.31E-07	5.24E-05
500	7.69E-08	3.08E-04	8.56E-08	2.14E-05

MSE decreases more quickly for more discrete variables vs. an increased number of levels per variable.

Test Function 3: Asymmetry has more adverse effects on TGP than ACOSSO

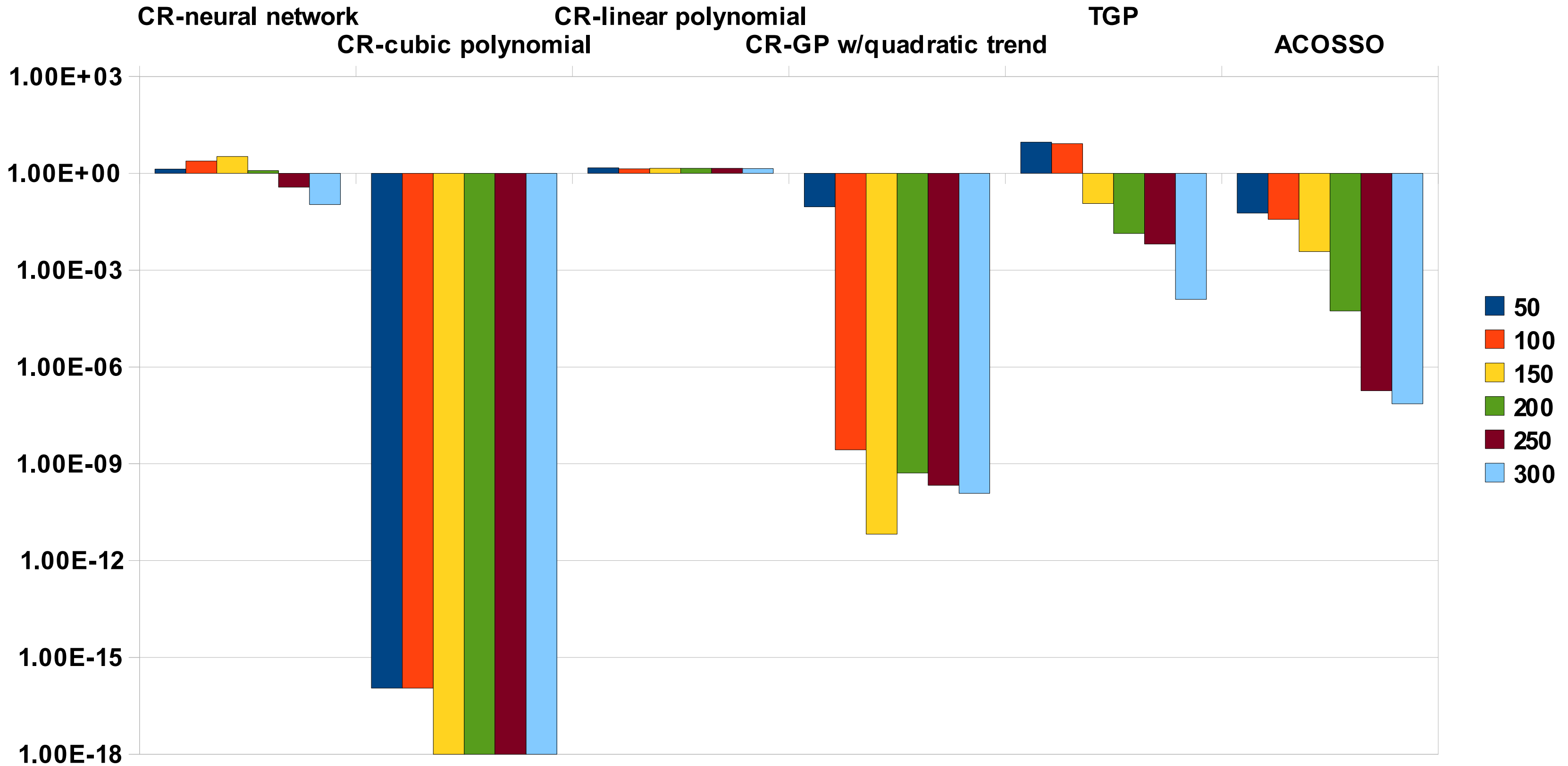
- Scaling up discrete levels from 3 to 5
- Scaling up discrete variables from 2 to 5
- Function is now asymmetric

Test Function 3	TGP		ACOSSO	
Discrete	2 [1-2-3]	2 [1-2-3-4-5]	2 [1-2-3]	2 [1-2-3-4-5]
Continuous	2 [0,2]	2 [0,2]	2 [0,2]	2 [0,2]
50	53.53	11843.35	3.67E-03	0.34
100	0.62	2444.52	1.96E-03	0.18
150	0.26	3402.73	3.27E-04	0.12
200	0.15	4494.97	9.94E-04	0.07
300	0.02	2382.42	3.55E-06	0.03
500	0.01	0.39	5.78E-04	0.06

Separability and lack of variable interactions, particularly between discrete and continuous, may be playing to the strengths of ACOSSO.

Polynomial Function: Categorical regression performs quite well, followed by ACOSSO

- 2nd order polynomial with 4 variables
  - 2 discrete variables at levels [20,50,80]
  - 2 continuous variables between 0 and 100



Polynomial Function: Complexity has more adverse effects on ACOSSO than TGP

- "Scaling" Problem Complexity
  - 2nd order polynomial with 14 terms
  - 3rd order polynomial with 24 terms
  - 4th order polynomial with 19 terms
- 10 discrete levels (instead of 3)

	Test Function Poly ٢		Test Function Poly 3		Test Function Poly ٤	
	TGP	**ACOSSO**	**TGP**	**ACOSSO**	**TGP**	**ACOSSO**
Discrete	2 [ten levels]	2 [ten levels]	2 [ten levels]	2 [ten levels]	2 [ten levels]	2 [ten levels]
Continuous	2[0,100]	2[0,100]	2[0,100]	2[0,100]	2[0,100]	2[0,100]
50	28.88	12.24	25.16	9.12	10.07	29.98
100	28.58	0.46	25.00	4.92	10.25	5.14
150	27.83	0.15	21.94	2.31	13.16	6.03
200	21.80	0.05	16.31	1.91	9.99	5.03
250	24.92	0.06	11.58	2.37	10.40	5.16
300	22.78	0.03	9.49	1.77	8.76	5.20

Possible increase in variable interactions and increased relative impact of continuous variables may be playing to the strengths of TGP.

Observations and Summary Thoughts

- Surrogate models are imperative for computational tractability of engineering analyses
- Categorical Regression performed very well on problems with small numbers of discrete variables/levels
- ACOSSO performs very well overall
- TGP performance is mixed
  - Functions 1, 2: performs well when it seems to get enough function evaluations (few hundred)
    - Ability to identify the splits
    - Not sufficient to aggregate across discrete levels
  - Functions 3, poly: performs poorly (i.e, high MSE)
    - Adaptive methods may lead to improvement

Observations and Summary Thoughts (2)

- Scalability
  - ACOSSO seems the most scalable
  - TGP suffers from too large an aggregation across discrete levels
  - Categorical regression is not scalable
  - Is there a difference between scalability across discrete variables vs. number of levels? Test function three suggests there might be
- Further work:
  - Amount of interaction between variables
  - Range/nonlinearity of function
  - Improving efficiency of TGP and ACOSSO implementations