Computer experiments with big n: Has Gaussian process computation been tamed?

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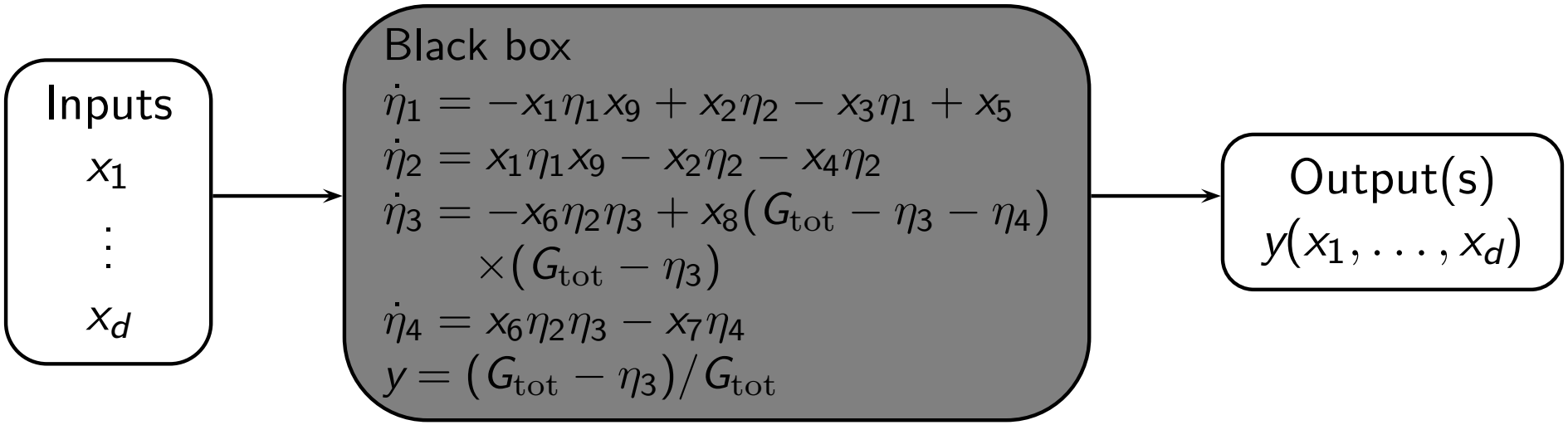
Outline

Computer Code



Standard Gaussian Process (GP) Model

- d-dimensional vector of inputs $\mathbf{x}$
- Output $y(\mathbf{x})$
- Treat $y(\mathbf{x})$ as a realization of

$$Y(\mathbf{x}) = \text{regression model} + Z(\mathbf{x})$$

- $Z(\mathbf{x})$ hence $Y(\mathbf{x})$ is a correlated process
- The correlation function $R(\mathbf{x}, \mathbf{x}') \equiv R(Y(\mathbf{x}), Y(\mathbf{x}'))$ is the workhorse of the GP model

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- Sacks et al. (1989)



All the methods discussed today use this model in some form.

What's the Problem?

Computational complexity

- Training data of n runs at $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}$
  - Key is the $n \times n$ correlation matrix

$$\mathbf{R} = R(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \quad \text{for } 1 \leq i, j \leq n$$

  - Maximum likelihood or Bayes MCMC needs $\mathbf{R}^{-1}$ and $\det(\mathbf{R})$, or the Cholesky decomposition
  - Computational time for one likelihood calculation is $O(n^3)$
  - Need 1000's or 10 000's likelihood calculations
- Prediction at N test points
  - Point prediction: $O(n)$ computation per prediction; $O(nN)$ for all test points
  - Predictive variance: $O(n^2)$ per prediction; $O(n^2 N)$ for all test points

Big n? Disclaimer

Dennis pointed out
big n to statisticians is not
so big. For GPs big is 1000's or 10 000's.

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- To illustrate methods, n will be really small: n
- Then some results for larger n

~~Student~~ Audience Participation

UBC Faculty of Science has an initiative in active learning

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Has Gaussian process computation been tamed?

A No

B Yes

C I don't know

D Nobody knows

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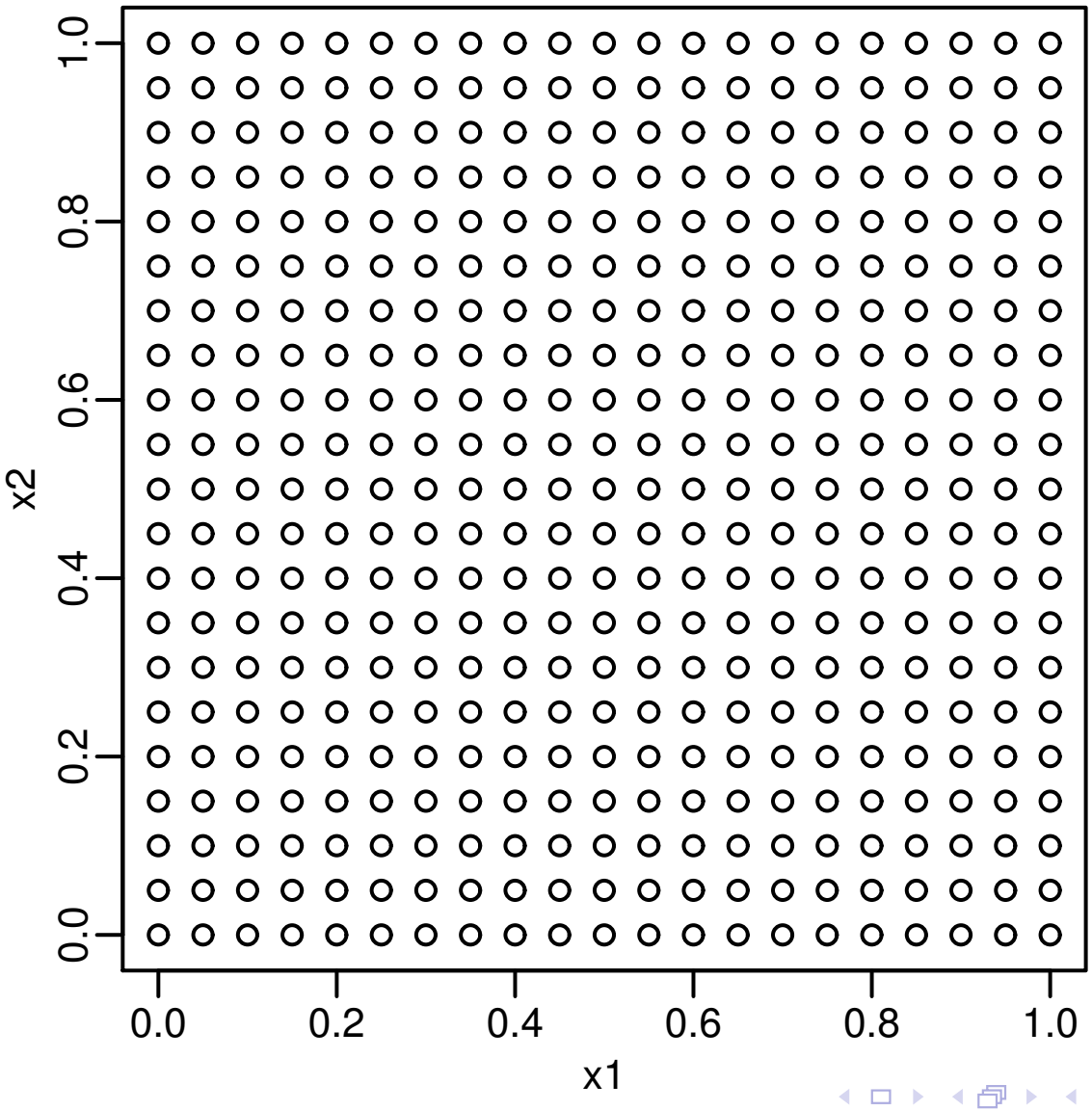
E Who cares? Isn't it dinner time yet?

Sparse Grid Designs for GPs

Same designs as Henry's talk

Grid Designs: Intuition

Design for $d = 2$ inputs on a 21×21 grid ($n = 441$)



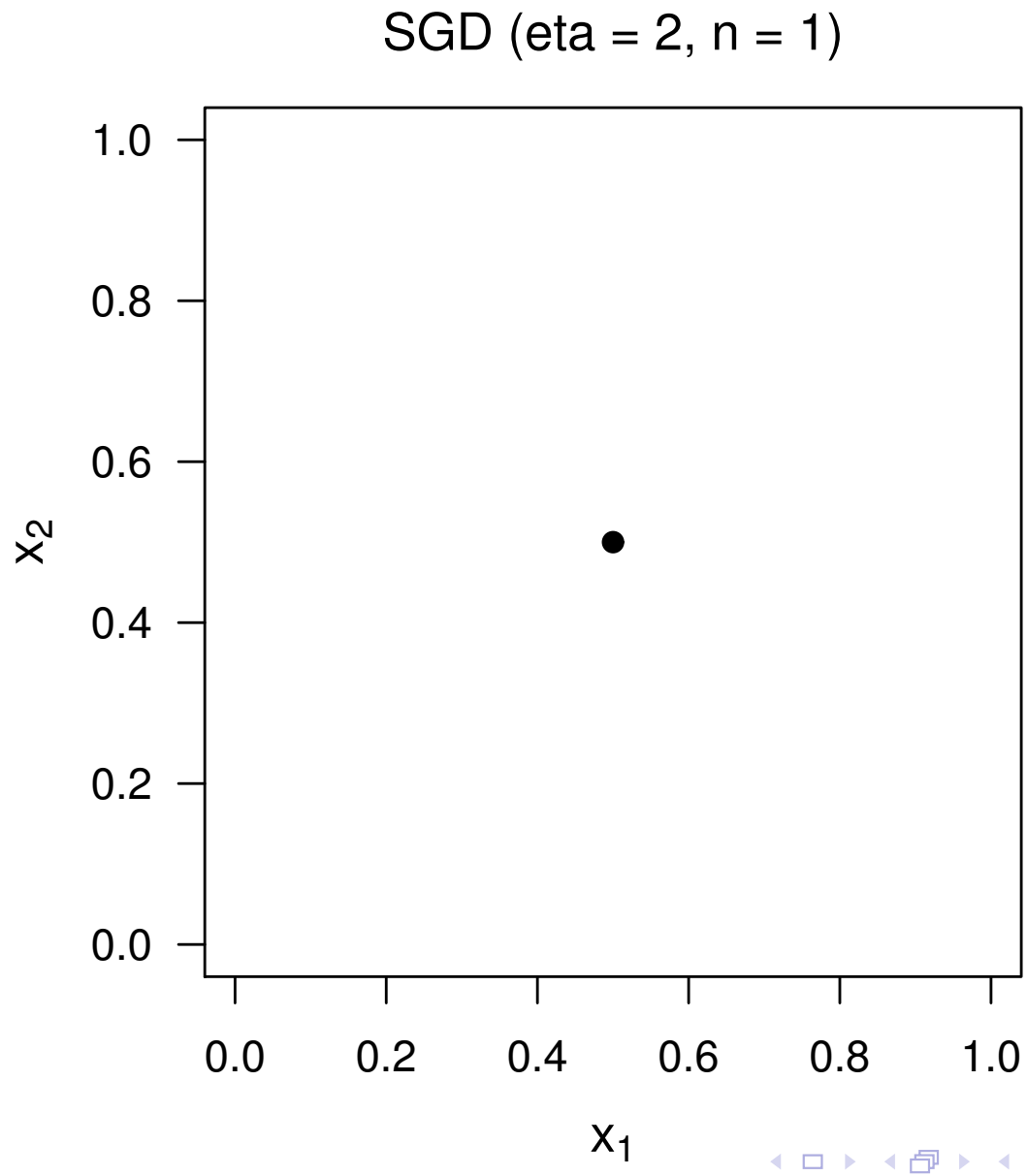
Grid Designs: Computational Complexity

- For the above 21×21 grid design

$$\underset{x_1 \text{ and } x_2}{\mathbf{R}_{441\times 441}} = \underset{x_1}{\mathbf{R}^{(1)}_{21\times 21}} \otimes \underset{x_2}{\mathbf{R}^{(2)}_{21\times 21}}$$

- $O(441^3)$ computation becomes $O(21^3) + O(21^3)$ computation
- In general, for $d = 2$ inputs $O(n^3)$ becomes $O(n^{3/2})$
- i.e., $O(n^{3/2})$ speed up
- For d inputs, $O(n^3)$ becomes $O(n^{3/d})$: even more relative speed-up
- But (dense) grid designs need too many computer-model runs, so ...

Sparse Grid Designs for GPs (SGDs, Plumlee, 2014)



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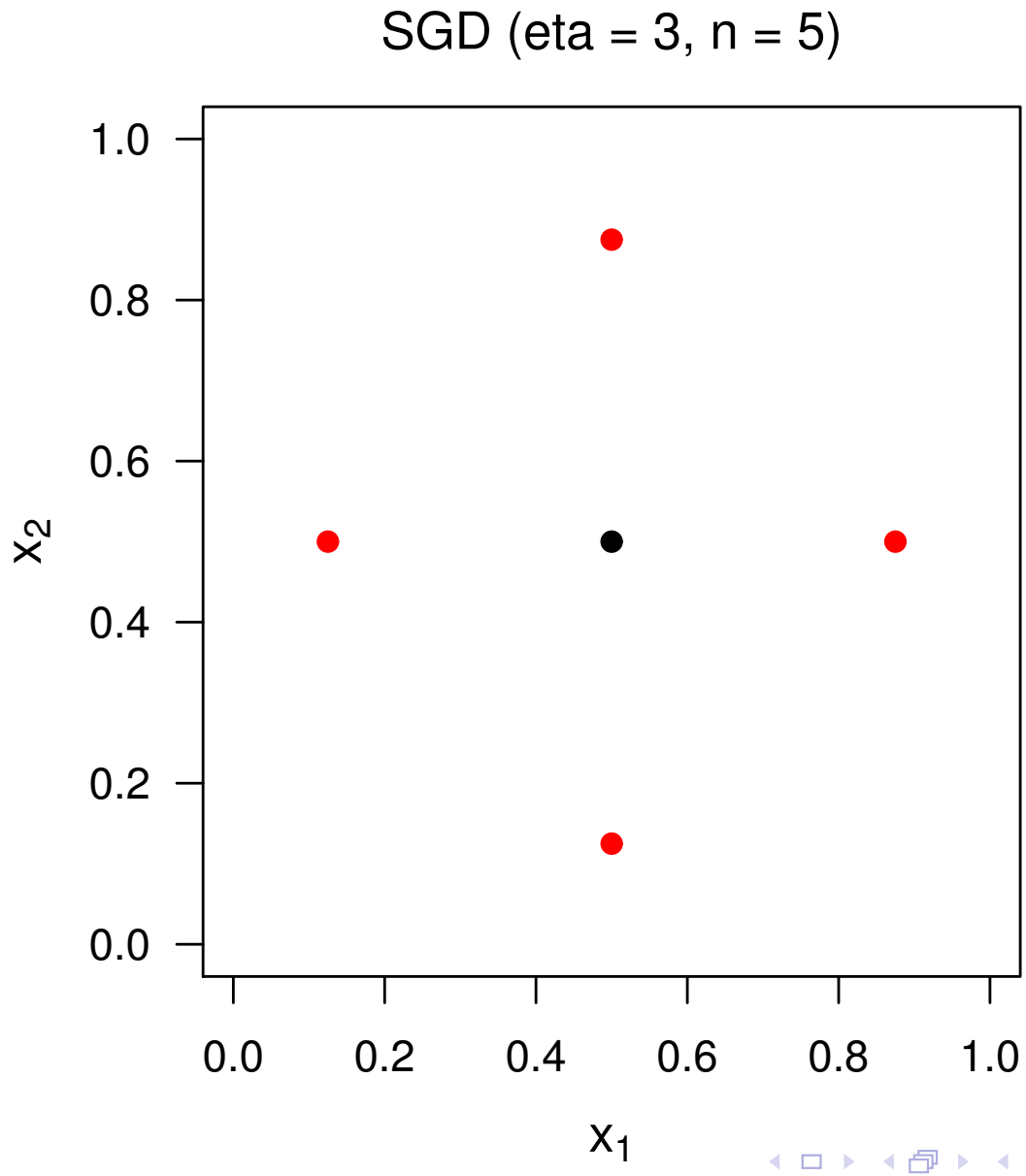

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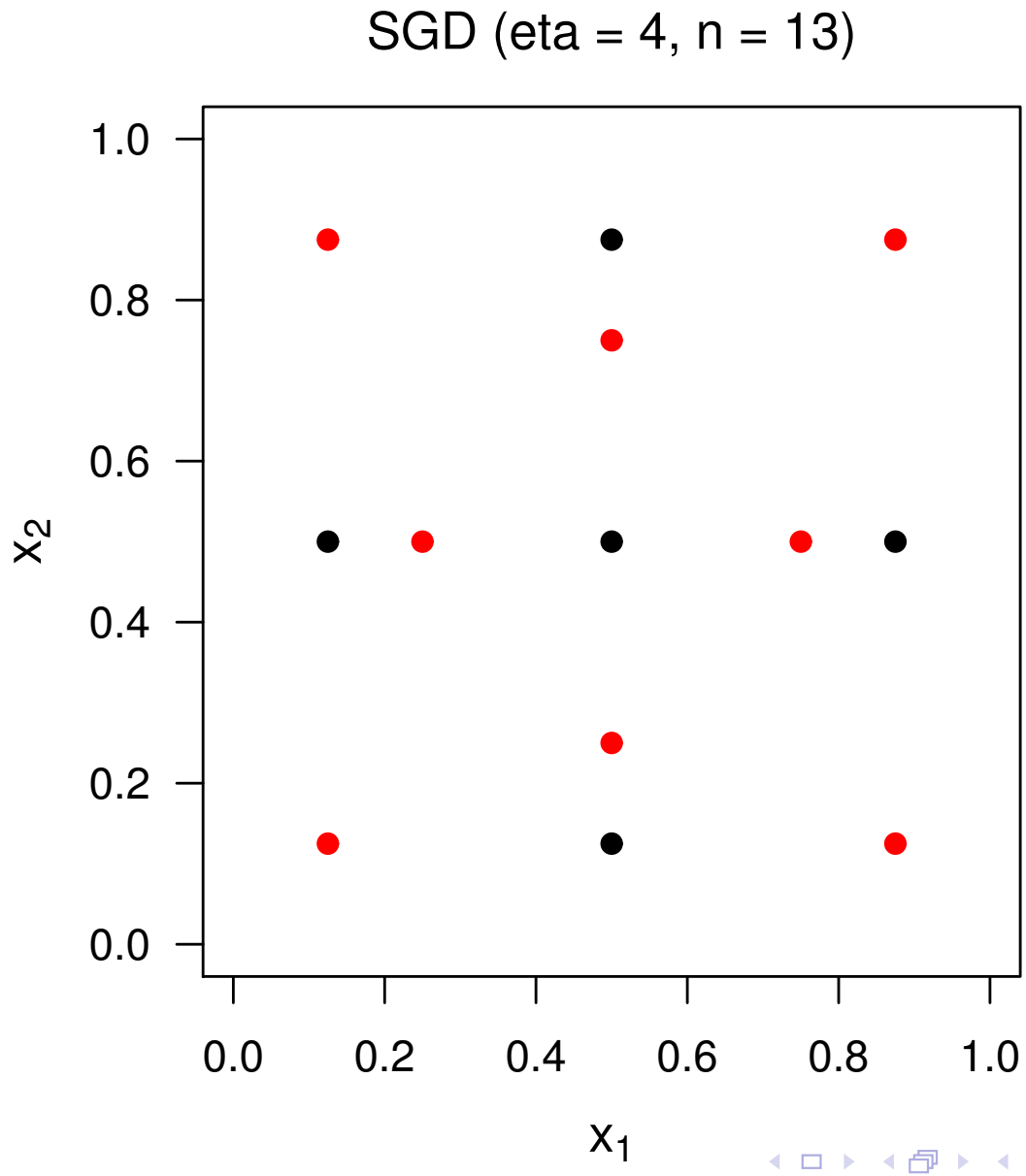

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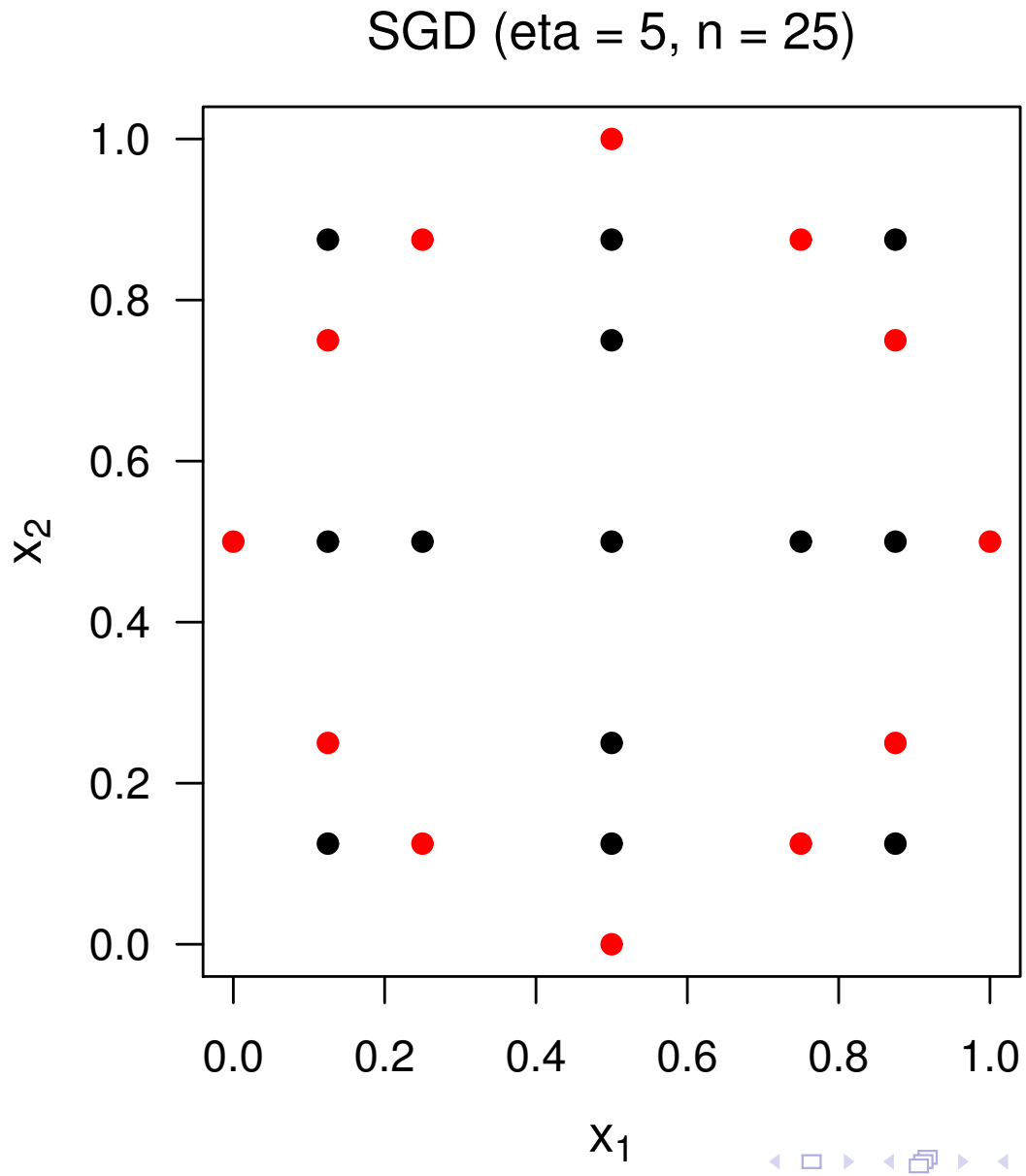

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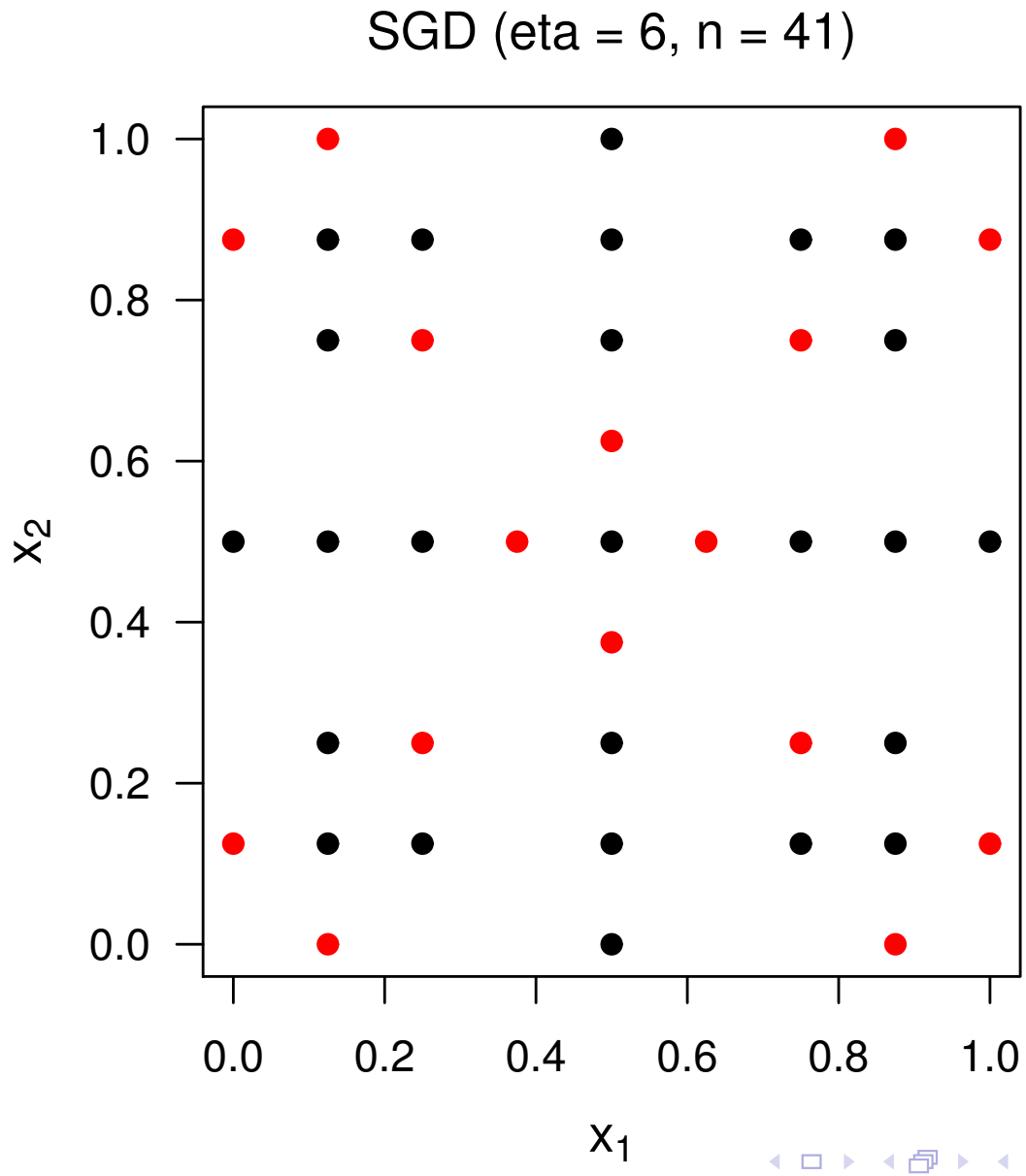
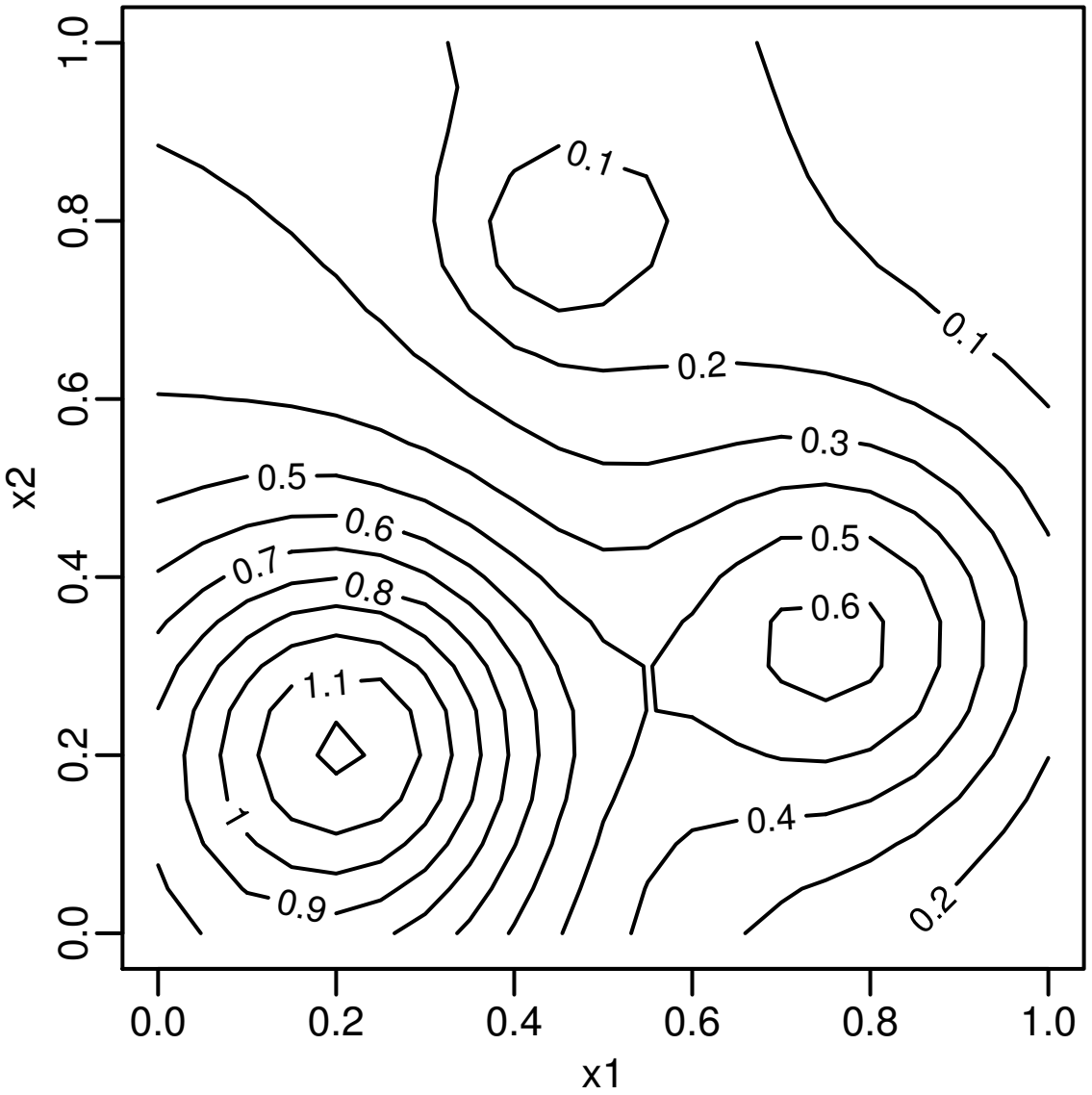
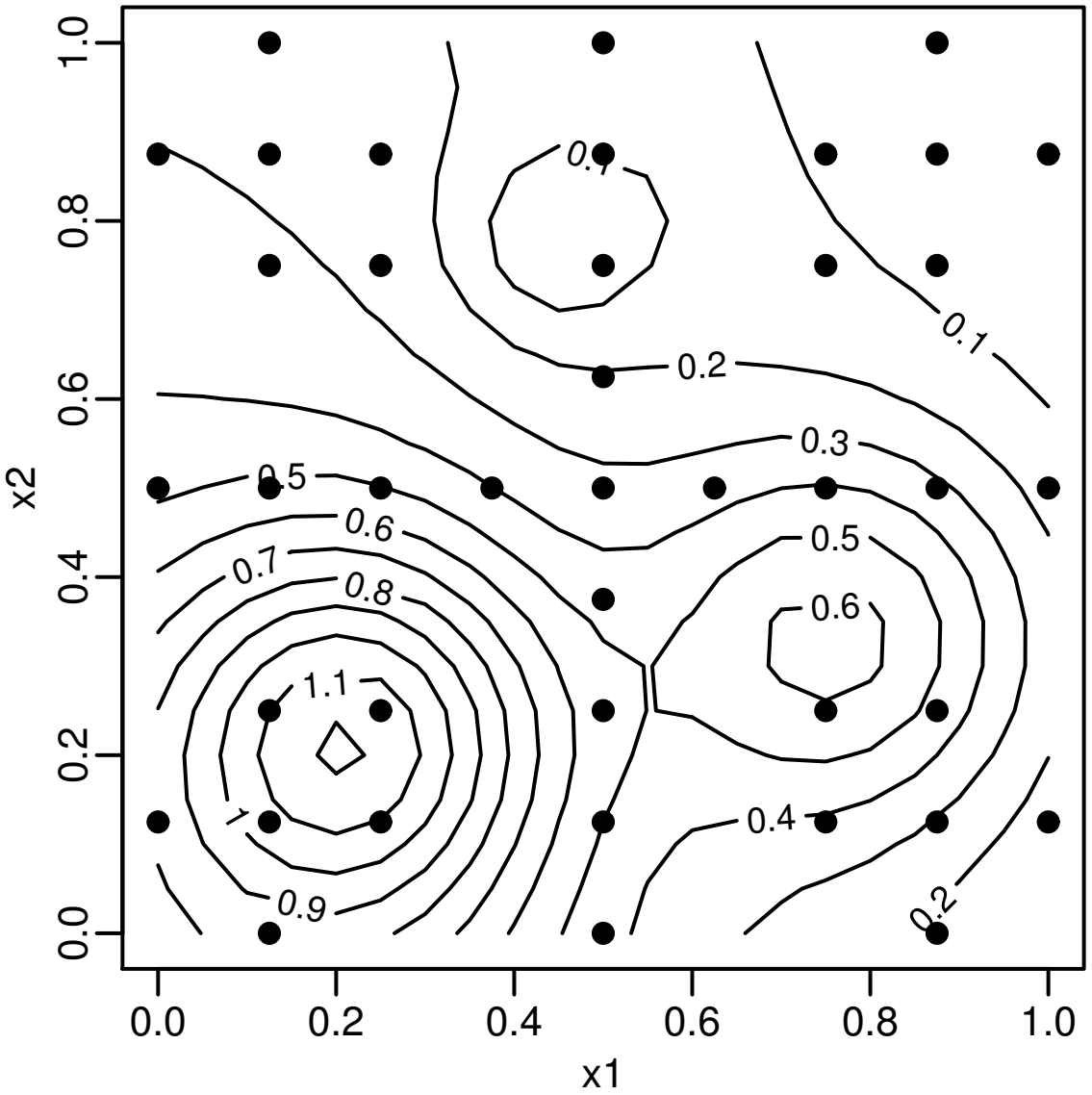


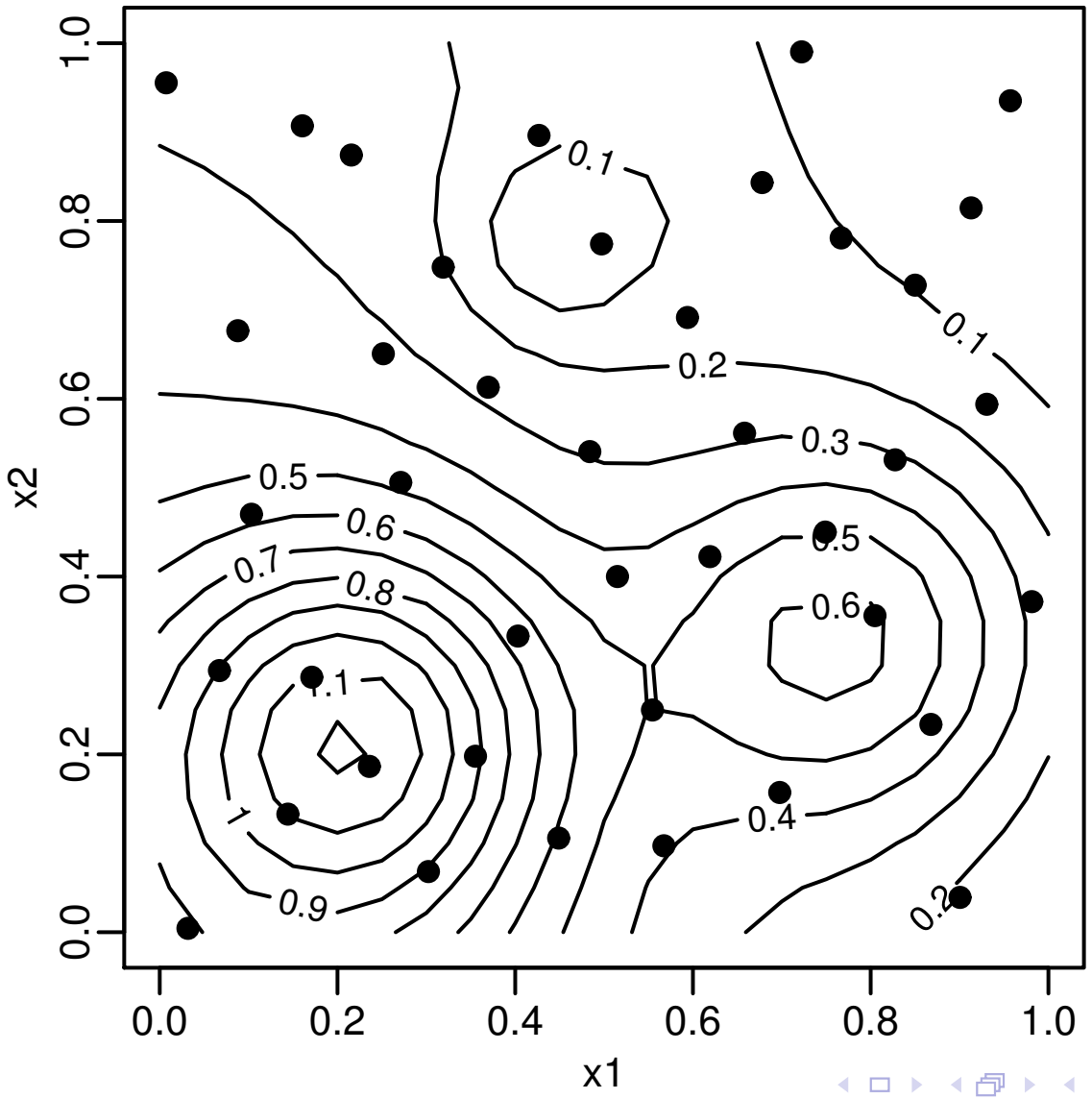
Franke's Function



Franke's Function and Sparse Grid Design ($n = 41$)



Franke's Function and Maximin Design ($n = 41$) for Comparison



Measures of Prediction Accuracy

- Prediction accuracy measured using "gold standard" hold-out test set
- $N = 1000$ or $10\,000$ random points $\mathbf{x}$ in the input space with y known
- Average error: Normalized root mean squared prediction error

$$\frac{\sqrt{\frac{1}{N}\sum_{\text{test points}}(y-\hat{y})^2}}{\text{test set standard deviation of } y}$$

- Worst error: Normalized max absolute prediction error

$$\frac{\max_{\text{test points}}|y-\hat{y}|}{\max_{\text{test points}}|y-\bar{y}|}$$

- Normalization: 0 = perfect, 1 = no better than predicting using $\bar{y}$

Franke's Function: Prediction Accuracy

(1000 test points from a random Latin hypercube)

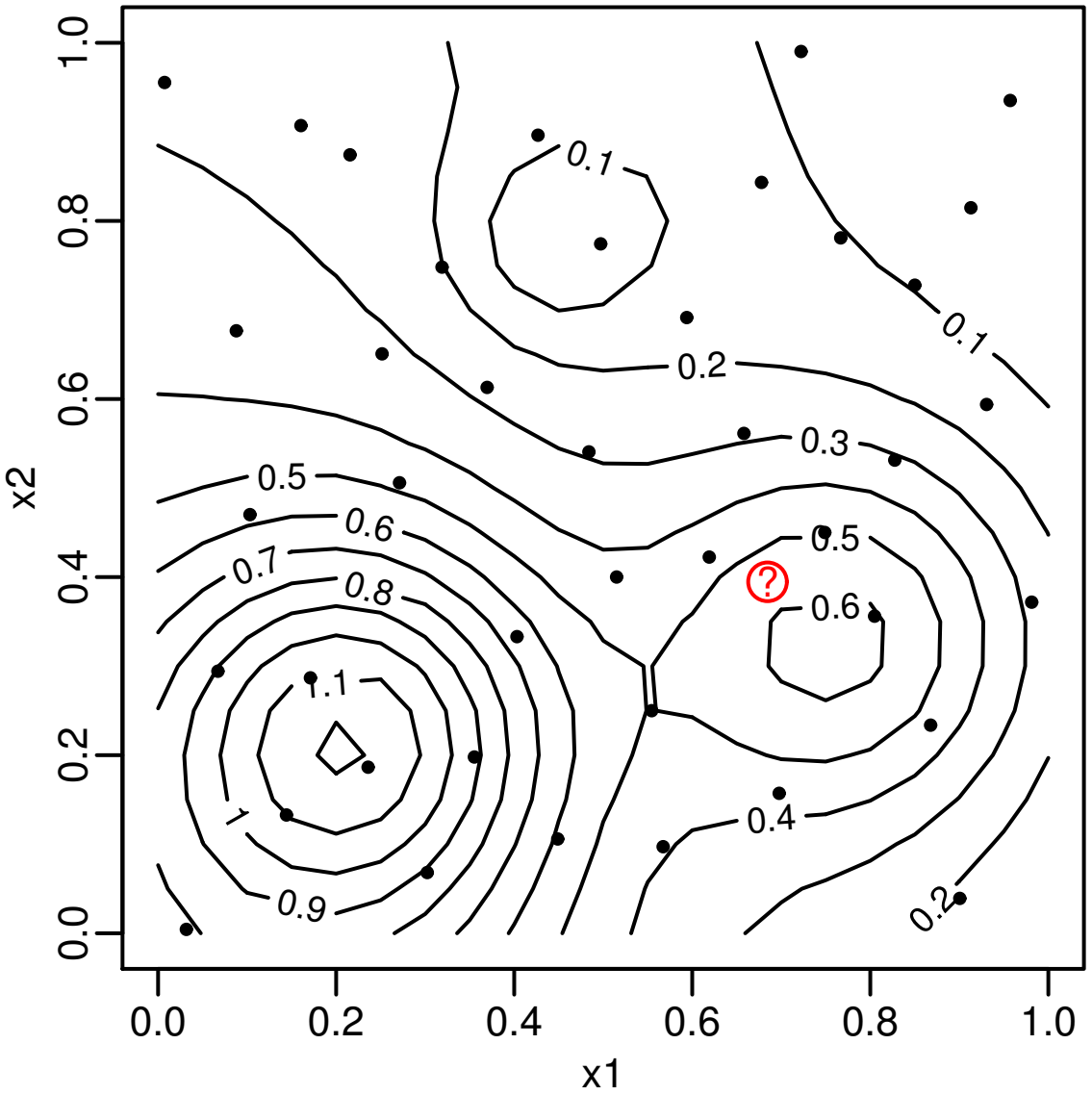
	Normalized	
Design	RMSPE	Max Error
Sparse grid	0.068	0.099
Maximin	0.047	0.110

Local Approximate Gaussian Processes (laGP, Gramacy and Apley, 2015; Gramacy, 2016)

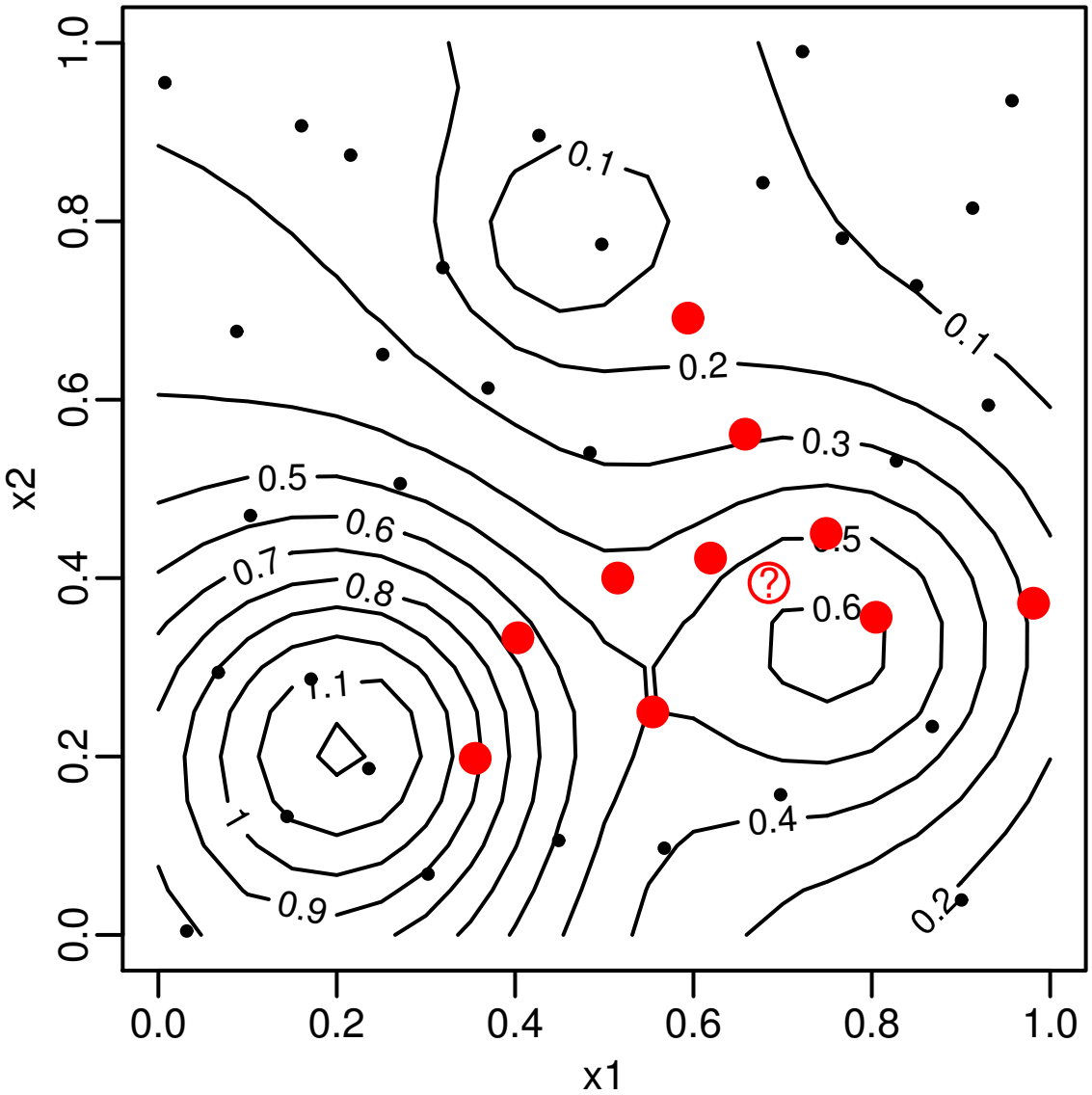
for each test point **do**
  Find $n_0 < n$ training neighbours of the test point
  Fit GP using only the n_0 neigbours of the test point
  Predict the test point using the GP
end for

- $O(n^3)$ training computation becomes $O(n_0^3)$, i.e., $(n/n_0)^3$ speed up
- Has to be repeated for each prediction

Franke's Function: Training Data and a Test Point



Franke's Function: 10 Local Training Points



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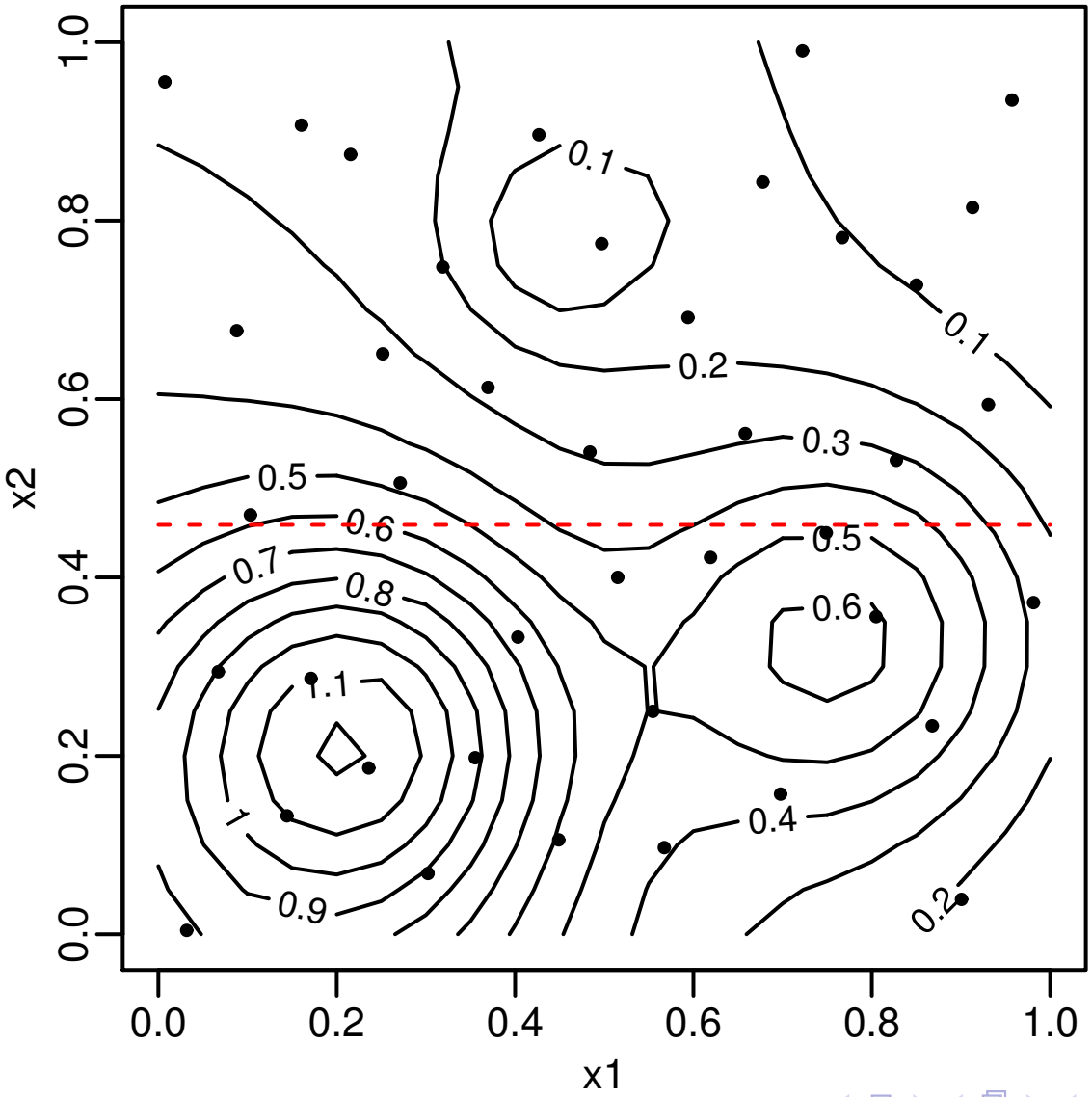
laGP	0.061	0.127

Treed GPs (tgp, Gramacy and Lee, 2008)

- Partition the input space with a binary tree
- For each leaf (terminal node) fit a GP using the leaf's data
- Actually builds many trees and averages them for prediction

Franke's Function: Treed GP

Tree with 2 leaves: $x_2 \leq 0.44$ and $x_2 > 0.44$



Franke's Function: Prediction Accuracy

(1000 test points from a random Latin hypercube)

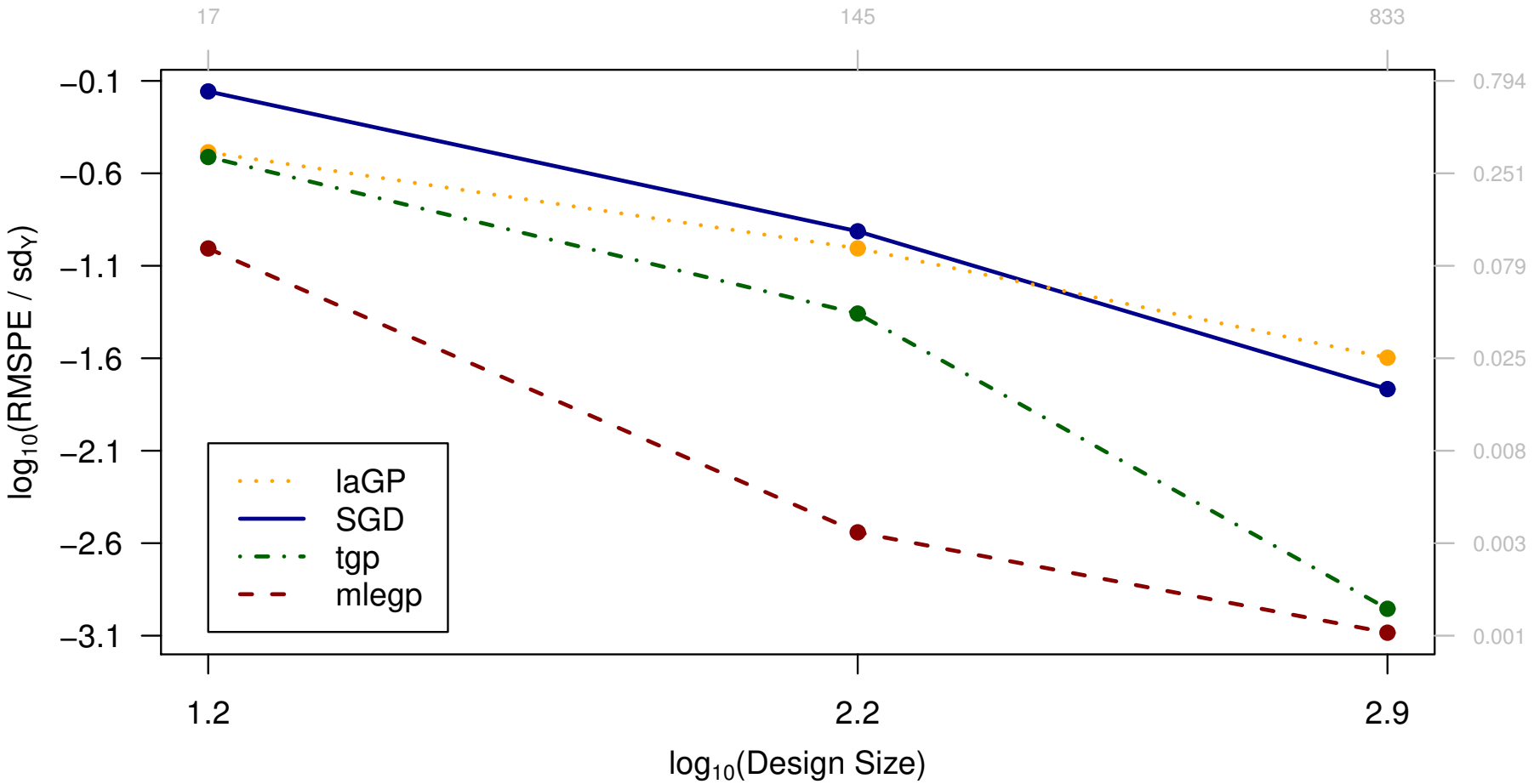
	Normalized	
Design	RMSPE	Max Error
Sparse grid	0.068	0.099
Maximin	0.047	0.110
laGP	0.061	0.127
Treed GP	0.259	0.425

Bigger n

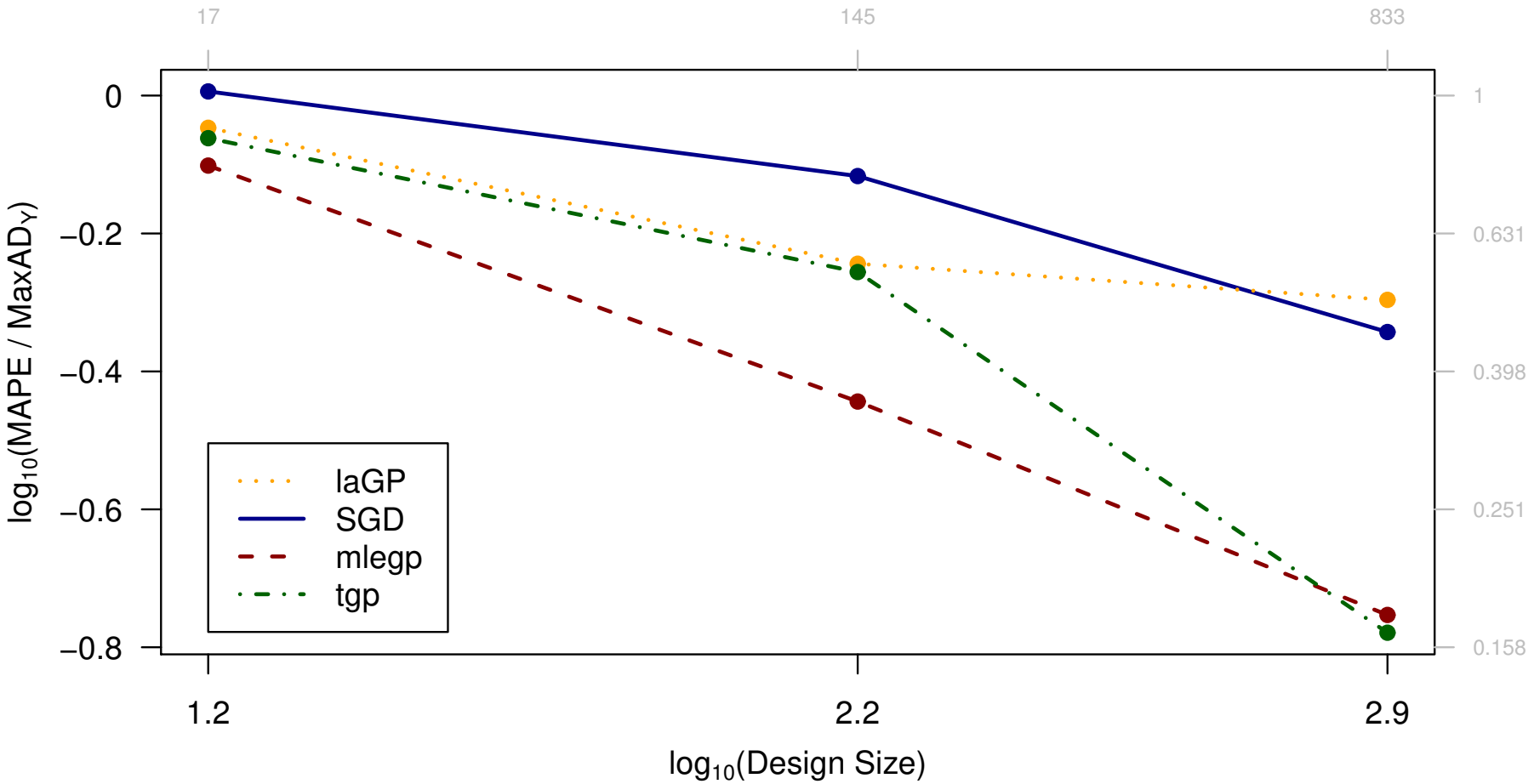
Two functions $y(\mathbf{x})$ with 8-dimensional $\mathbf{x}$

- Borehole function: easy to predict
- Corner peak function: difficult to predict (increases rapidly at the origin)

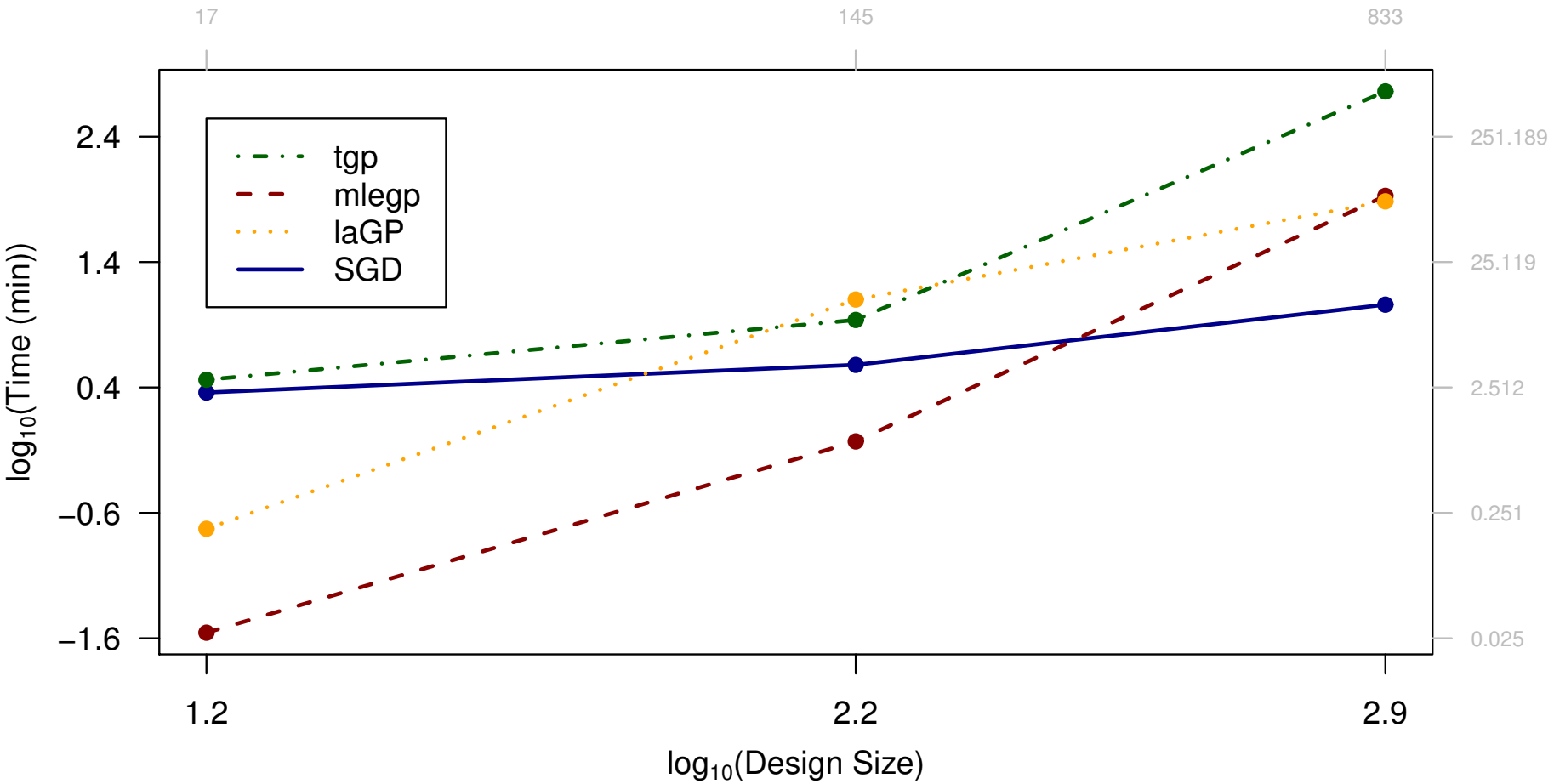
Borehole: Normalized RMS Prediction Error Versus n



Corner Peak: Normalized Max Absolute Error Versus n



Corner Peak: Computing Time Versus n



Other Methods

- Bayesian local kriging (Pronzato and Rendas, 2017): dynamically weighted combination of local GPs

- Compactly supported correlated functions (Kaufman, Bingham, Habib, Heitmann, and Frieman, 2011): induce sparse correlation matrix

Conclusion

Has Gaussian process computation been tamed?

A No

B Yes

C I don't know

D Nobody knows

E 3 hours to dinner

Unknowns

- Implementation of "standard" analysis is difficult for some local methods
- Any one of these methods is not one method:
  - How to choose a sparse grid?
  - How many points in a local region?
- Domain of practical problems?
  - Do these methods allow large enough n for a useful statistical model of a complex function?
  - Remember, we have to run the computer model n times

THANK YOU!

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