Lecture 10:
Modeling Data Surrogate Based Modeling, Hybrid Piecewise Polynomial Modeling, and Random Forest

COSC 526: Introduction to Data Mining
Spring 2020

THE UNIVERSITY OF TENNESSEE
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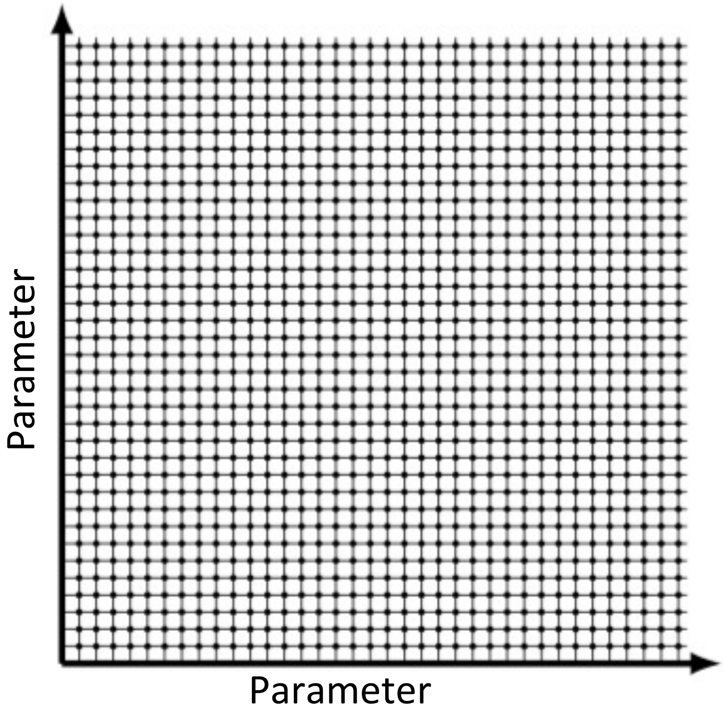
Exhaustive Search

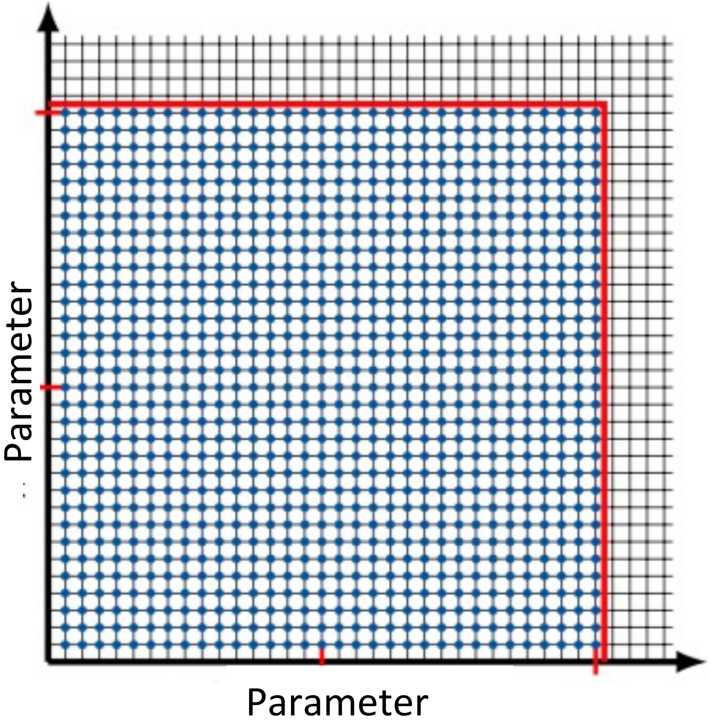
Exhaustive Search



Step 1: Reduce to finite search space

P. K. Lakkimsetti, A Framework for Automatic Optimization of MapReduce Programs Based on Job Parameter Configurations, M. Thesis, Kansas State University, 2011.

Exhaustive Search



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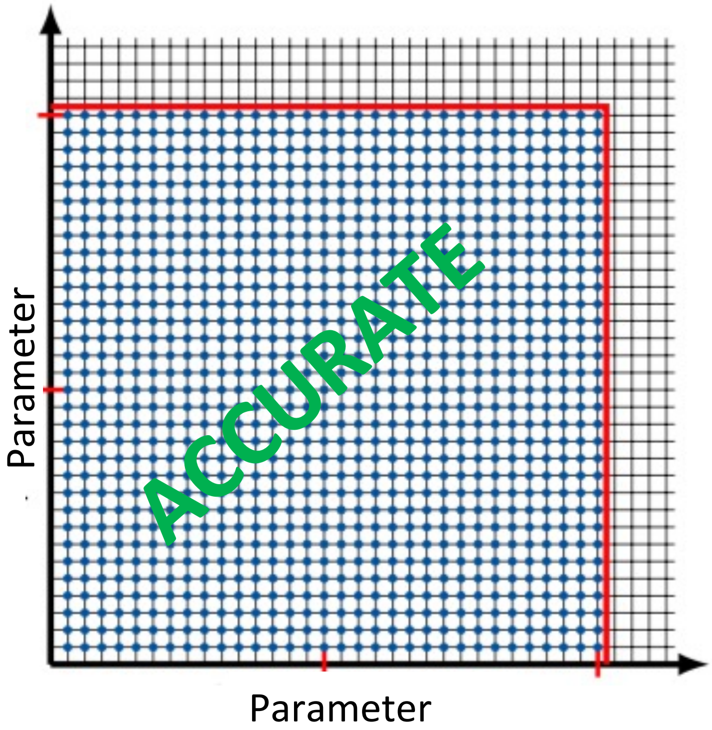

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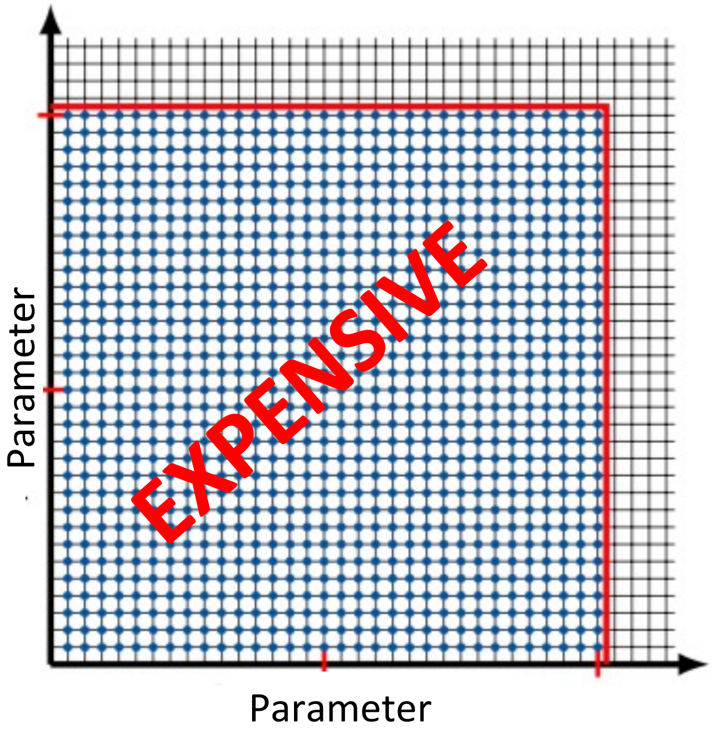
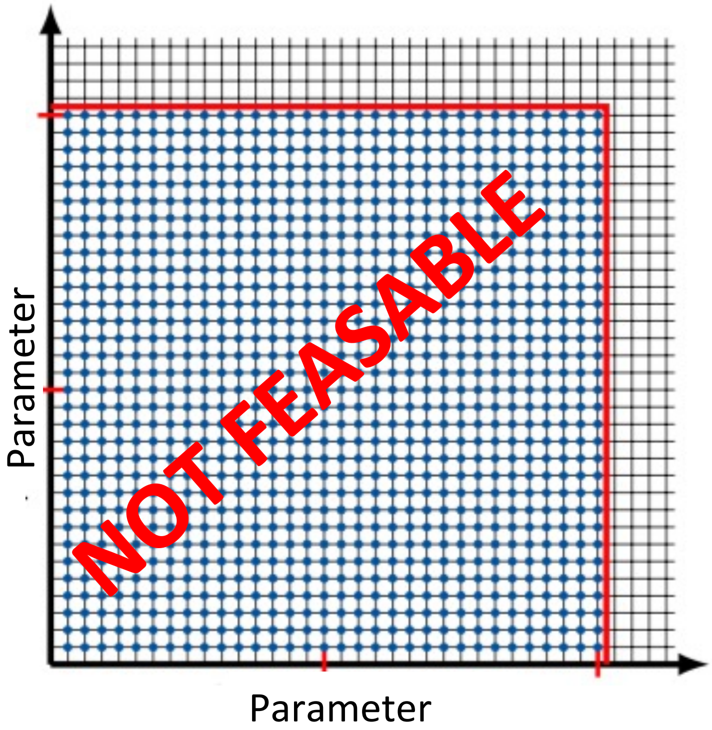


Step 2: Sample all these points **EXPENSIVE**

- Sample the entire population of the United States to leaner what each individual eats

Exhaustive Search



Step 2: Sample all these points **NOT FEASABLE**

- Satellites do not collect all the points across the globe

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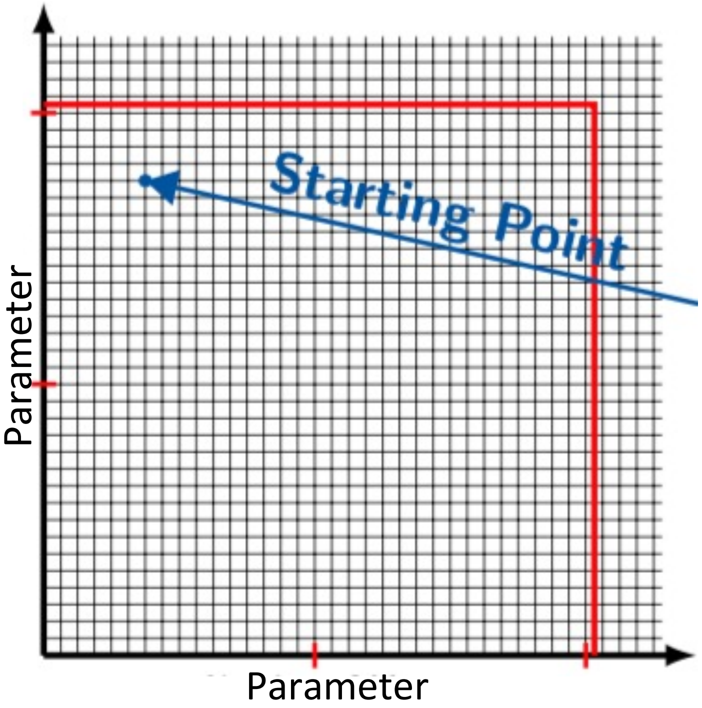
Local Search

Local Searching Algorithms



Methods: Grid Hill [1] and Simulated Annealing [2]

Step 1: Reduce to finite search space

Step 2: Randomly choose starting point and sample neighbors

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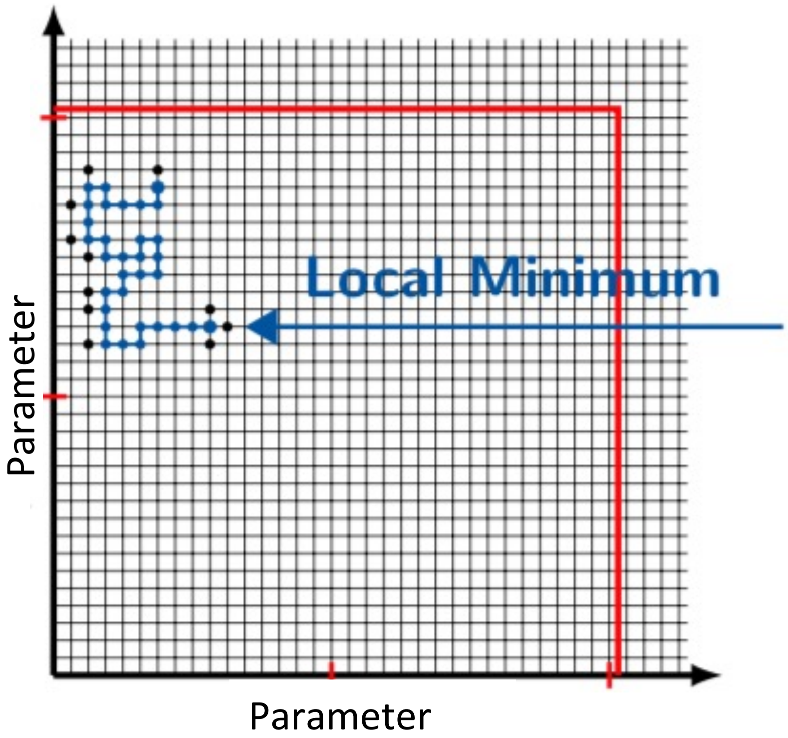
[2] D. Wu, A Profiling and Performance Analysis Based Self-tuning System for Optimization..., M. Thesis, Vanderbilt, 2013.

Local Searching Algorithms



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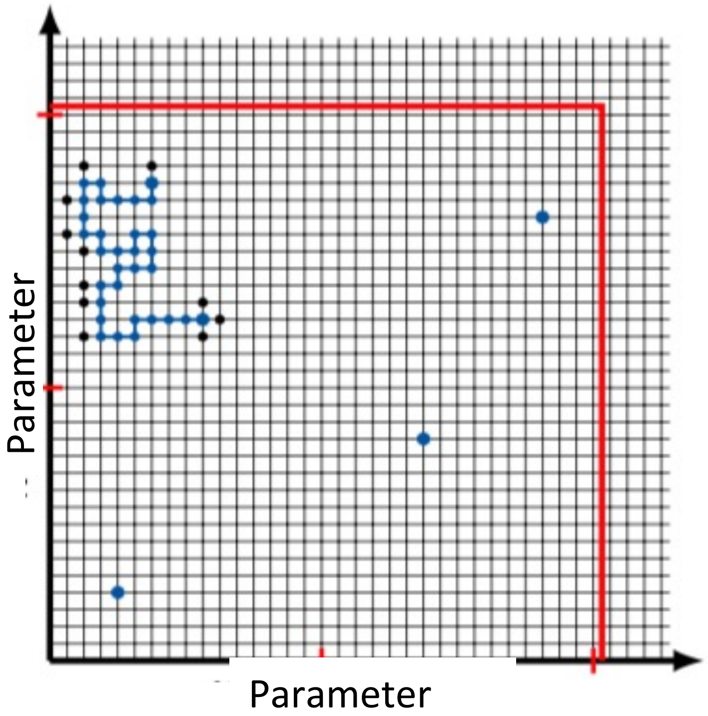

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Step 3: Repeat Step 2 with new starting point(s)

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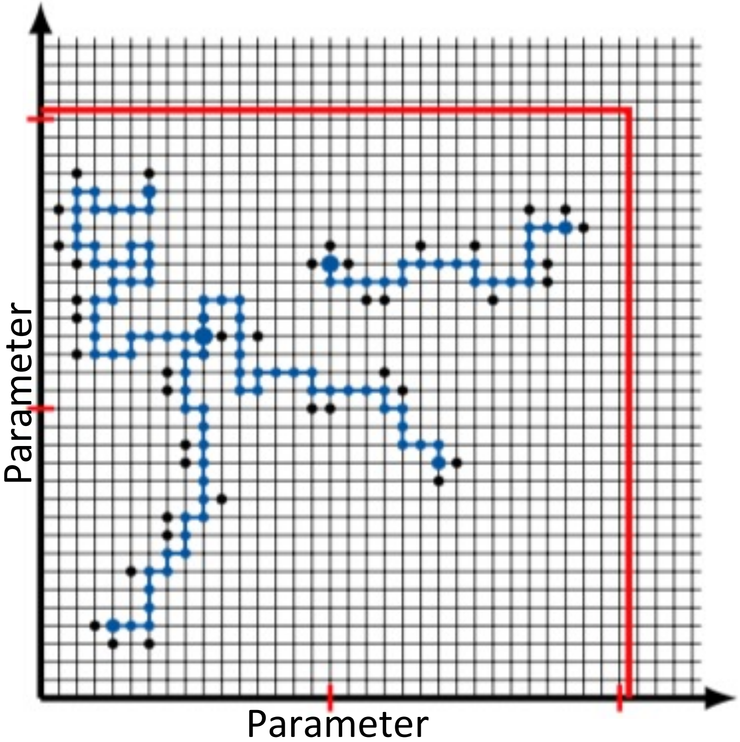

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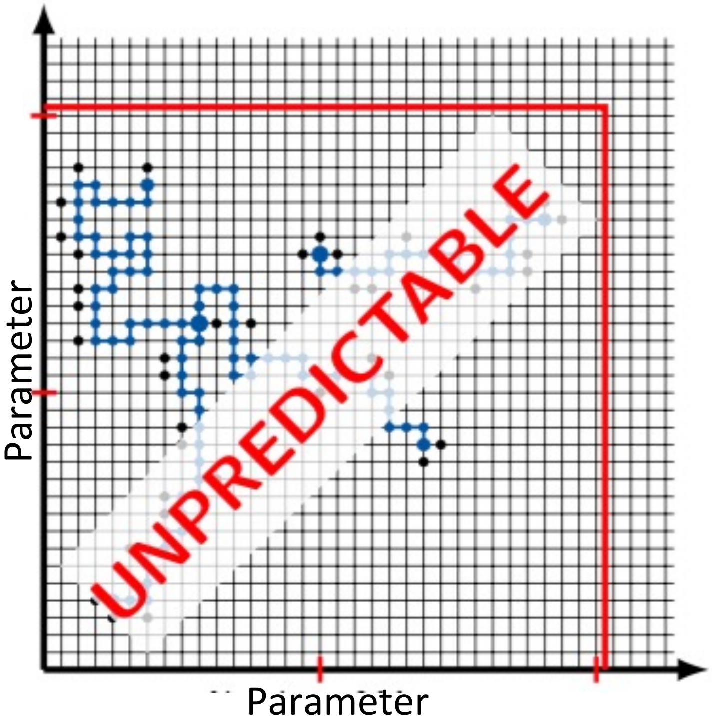

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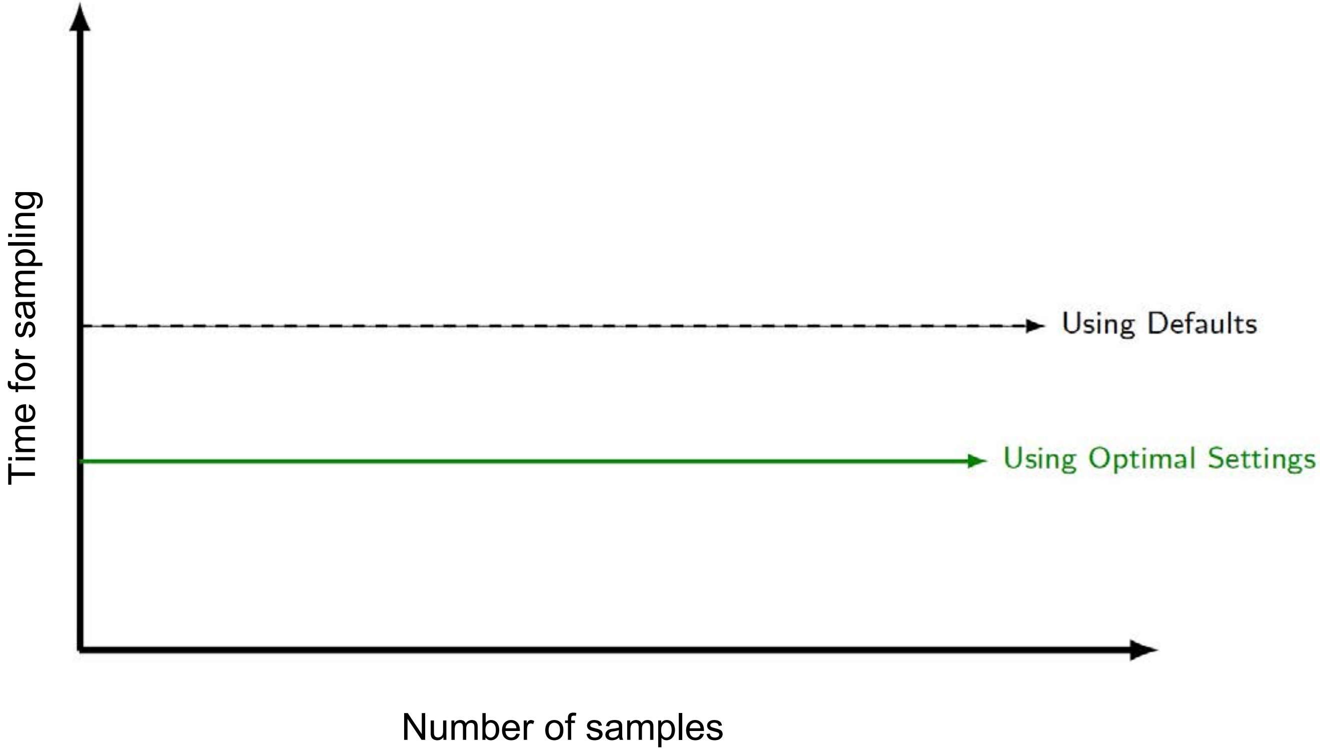
Exhaustive and Local Searches

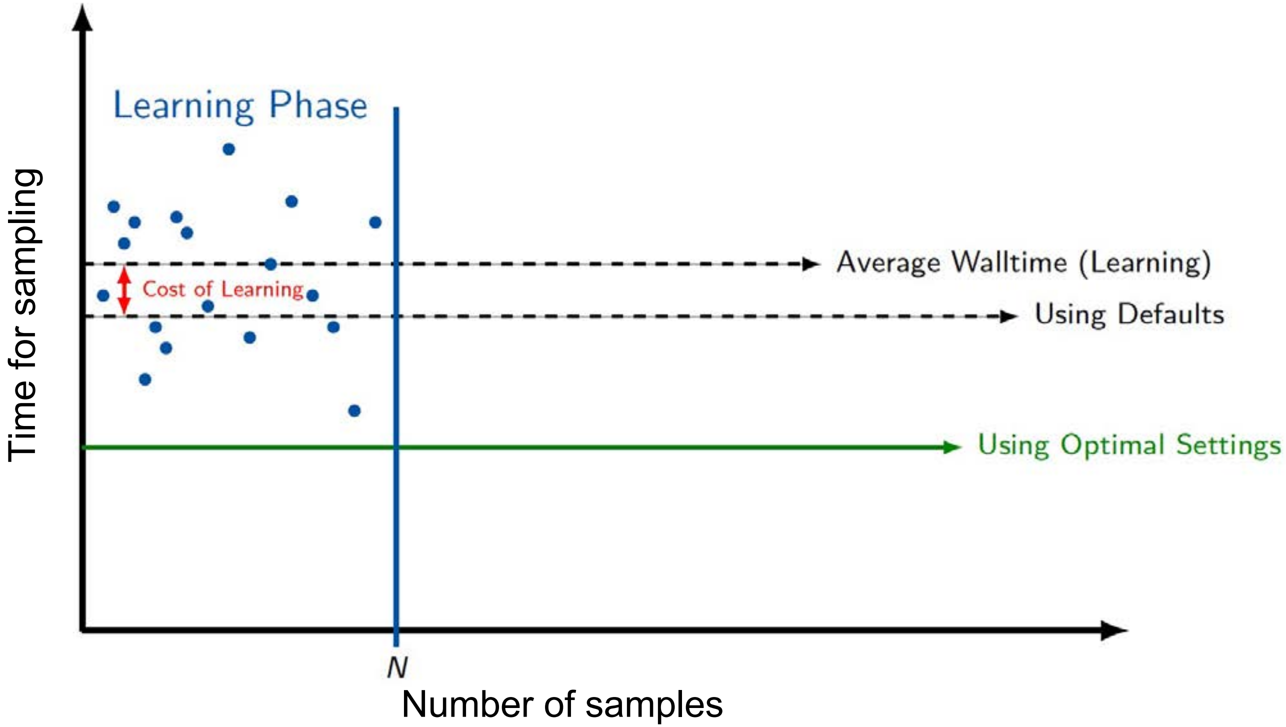
- Exhaustive sampling is too expensive
- Local search algorithms (LSAs) sample fewer points but are unpredictable

Cost of Sampling

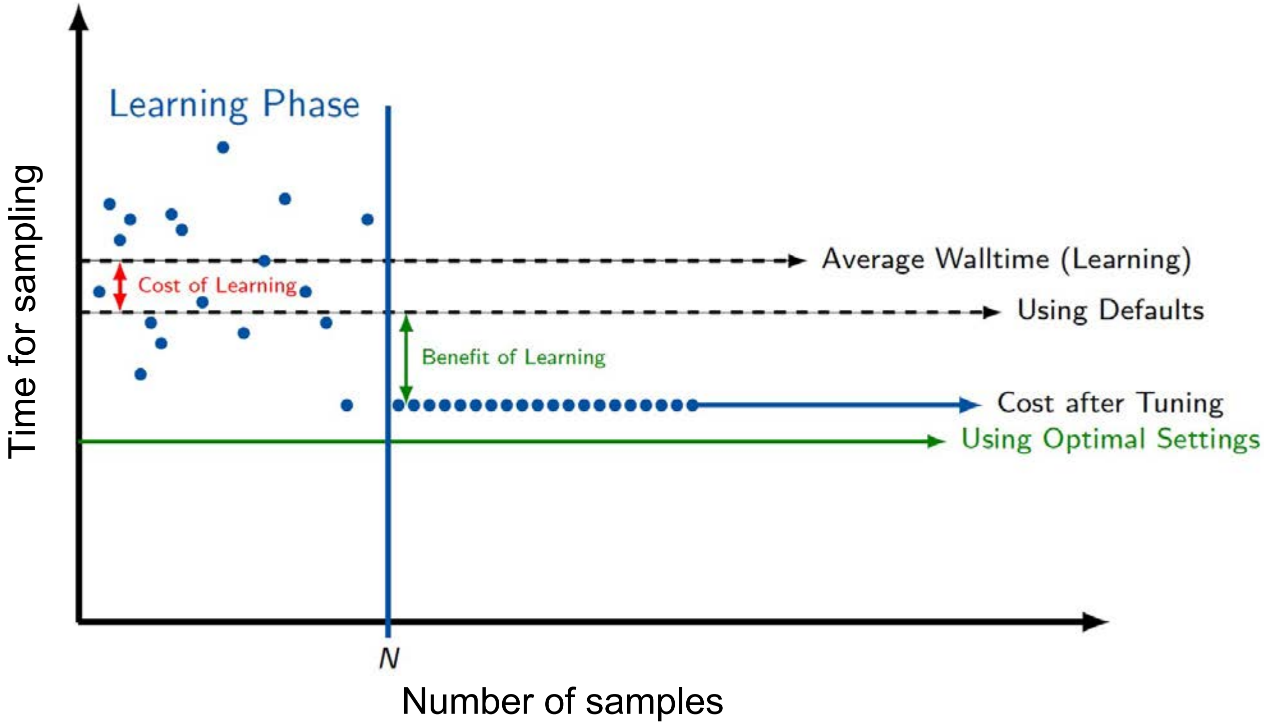
Amortizing the Cost of Sampling



Amortizing the Cost of Sampling



Amortizing the Cost of Sampling



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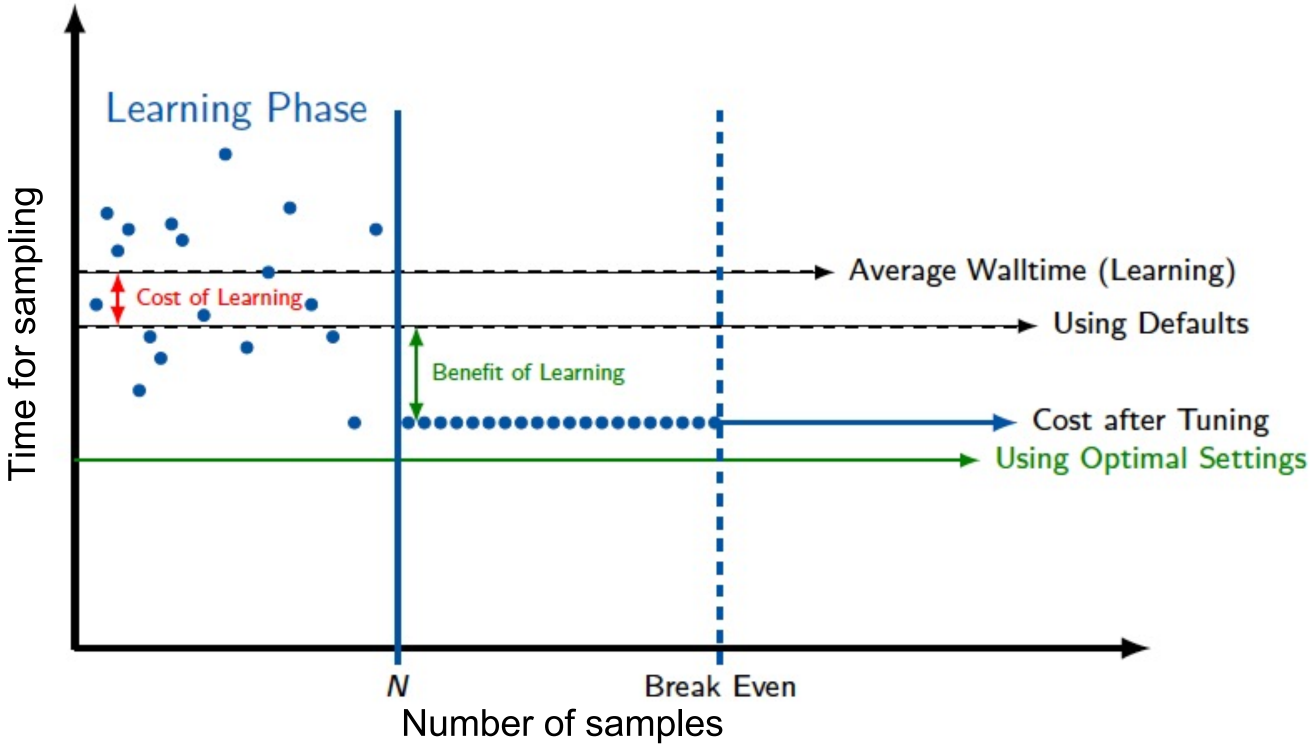
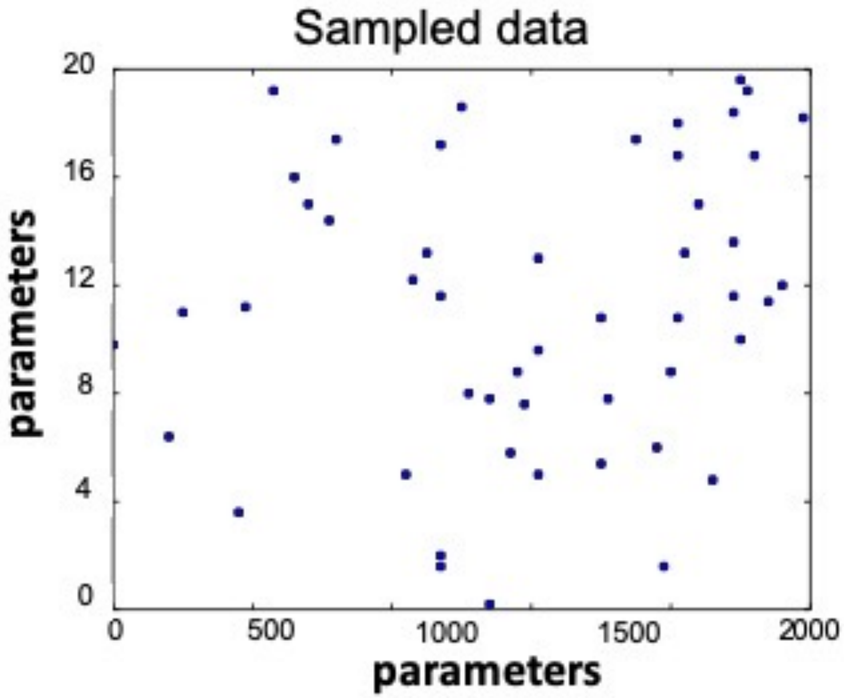


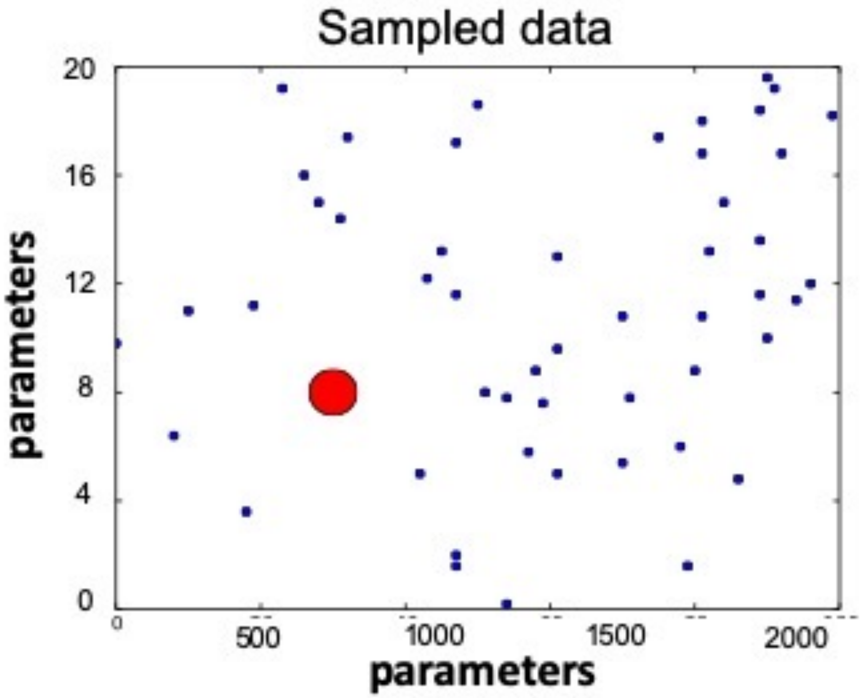
Amortizing the Cost of Sampling

- How do we focus the learning phase to maximize the return on our investment?

k Nearest Neighbors or kNN

k Nearest Neighbors Model

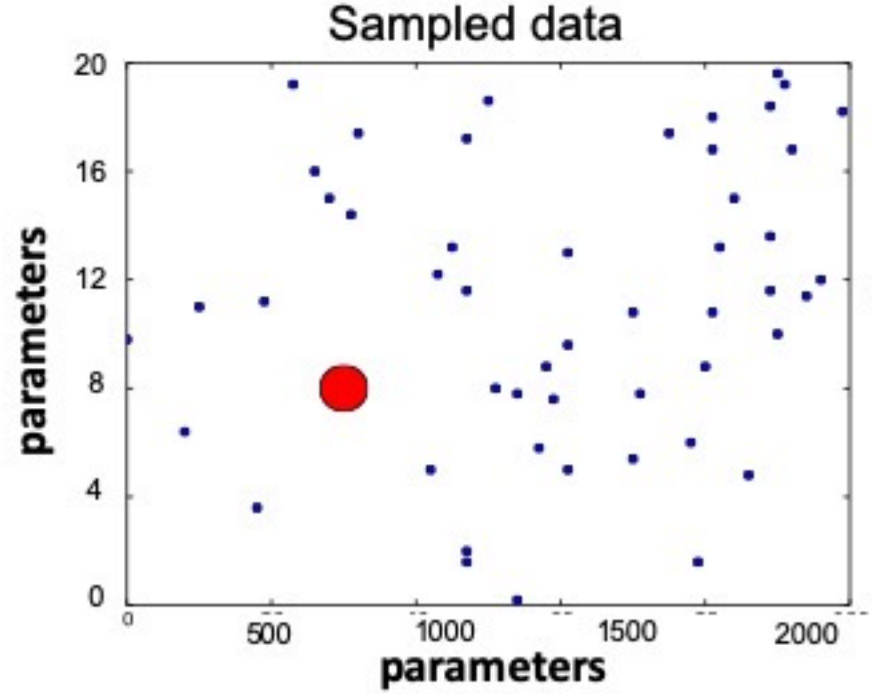


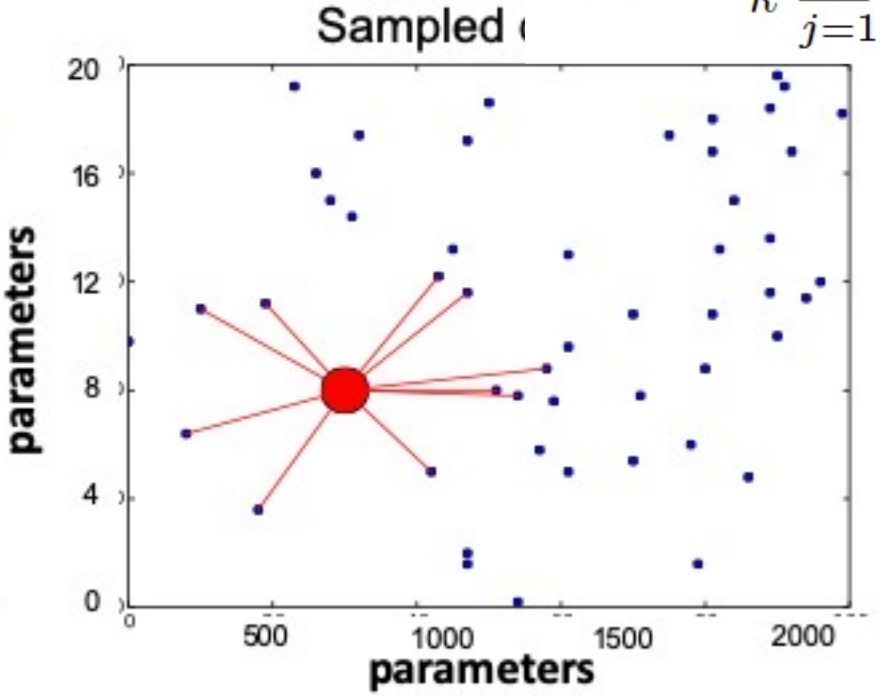


k Nearest Neighbors Model

Polynomial with degree zero

$$z(\vec{x}) := \frac{1}{k}\sum_{j=1}^{k} z_{i_j}$$





kNN

KNN:

→ Use **local data**

→ Compute k and distance kernel using cross validation automatically

→ Compute weighted means with the kernel (***many values***)

0	0	0	0

0	0	0	0	0

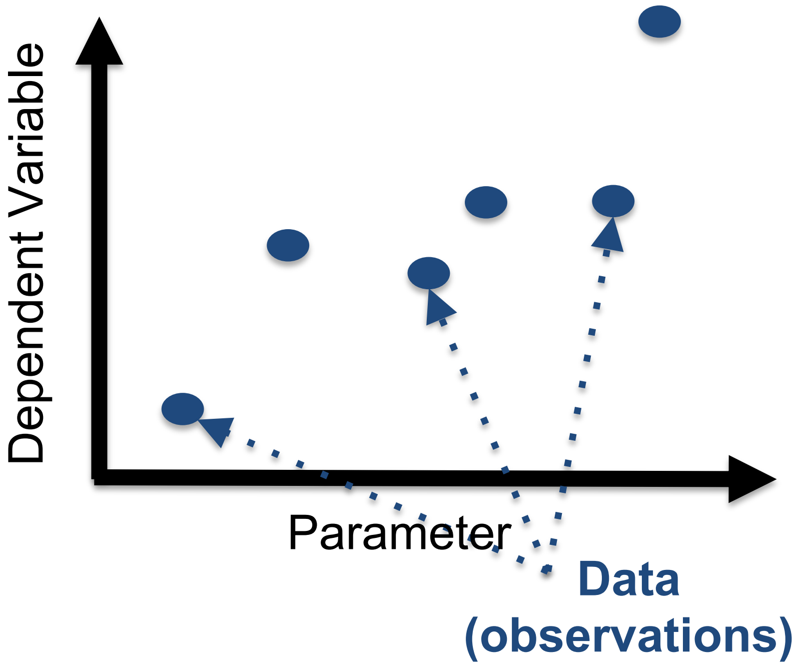
D. Rorabaugh, M. Guevara, R. Llamas, J. Kitson, R. Vargas, and **M. Taufer**. SOMOSPIE: A Modular SOil MOisture SPatial Inference Engine based on Data Driven Decisions. eScinece 2019.

Surrogate-Based Modeling

Using Surrogate-Based Modeling

- The surrogate model may predict optimal configurations that were never sampled in the learning phase
- We can explicitly determine the number of points required to build a surrogate model

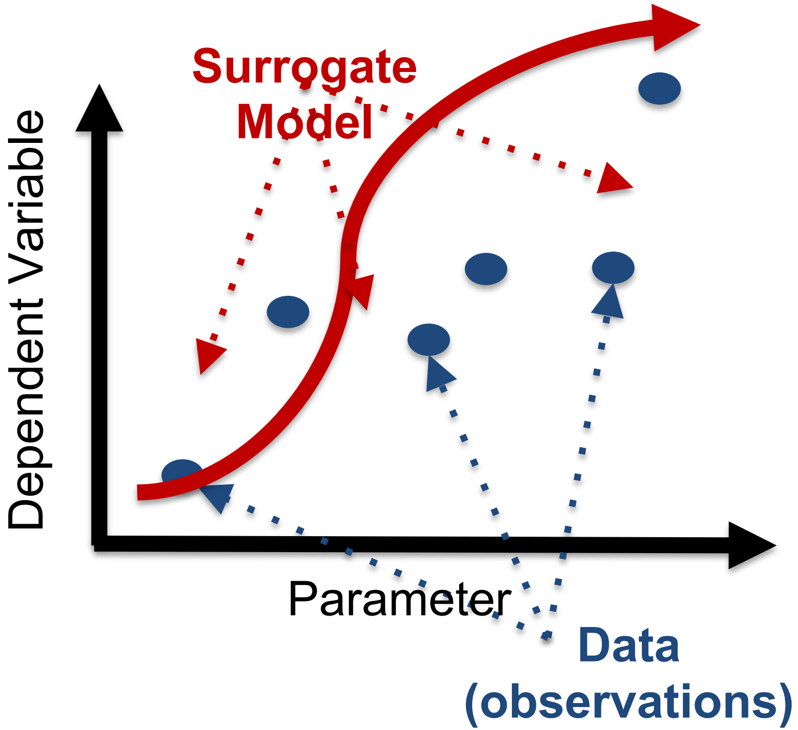
Surrogate-Based Modeling



- Data → **all** sampled data to create a **single global model**
- Model → fit a **polynomial** to data (continuous and differentiable)
- Best for→ finding underlying **global trends** when they exist

Image source: Johnston, R., Taufer

Surrogate-Based Modeling



- Data → **all** sampled data to create a **single global model**
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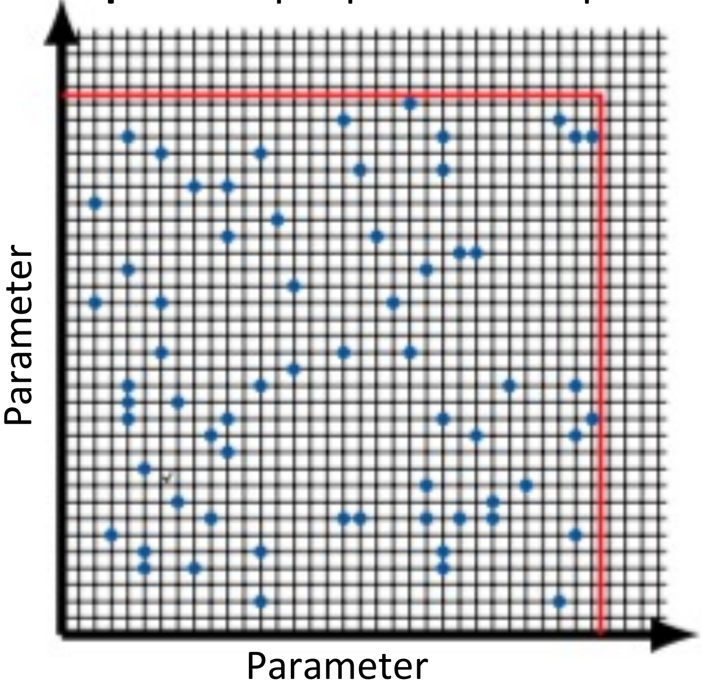
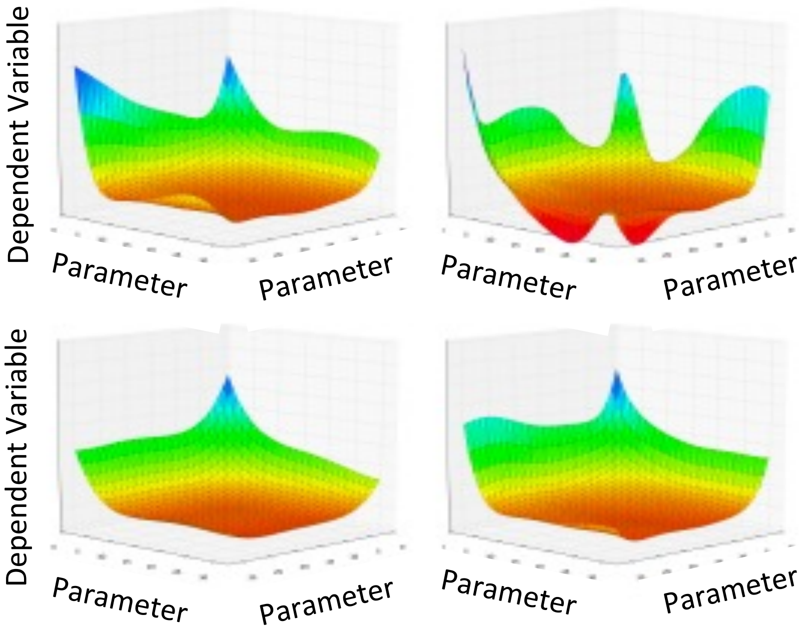
Image source: Johnston, R., Taufer

Surrogate-Based Modeling

Step 1: Sample parameter space

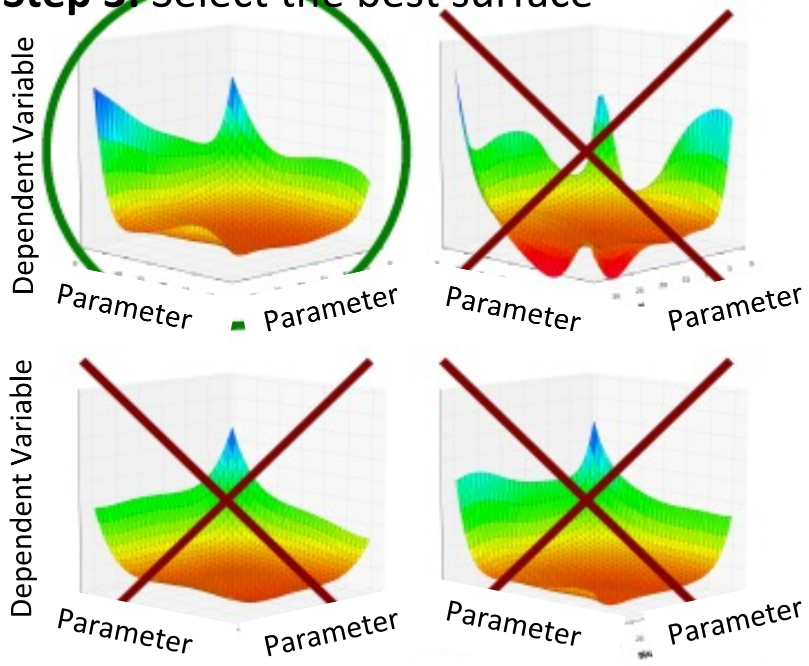


Step 2: Build candidate surfaces

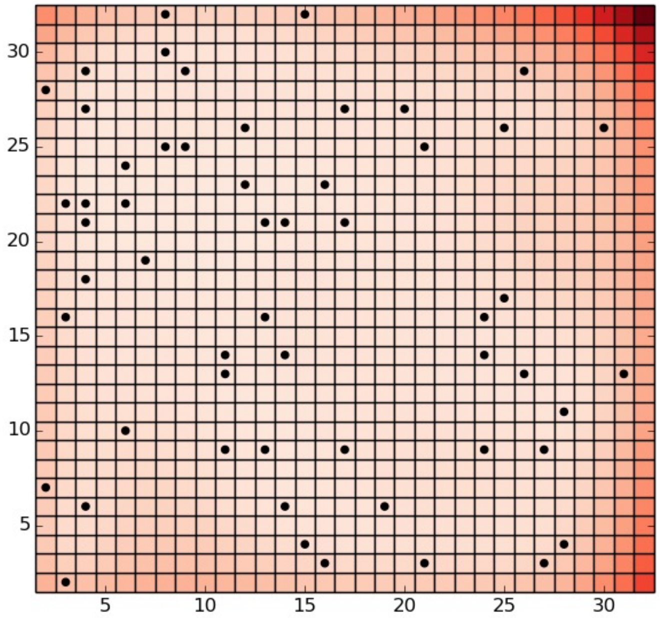


Surrogate-Based Modeling

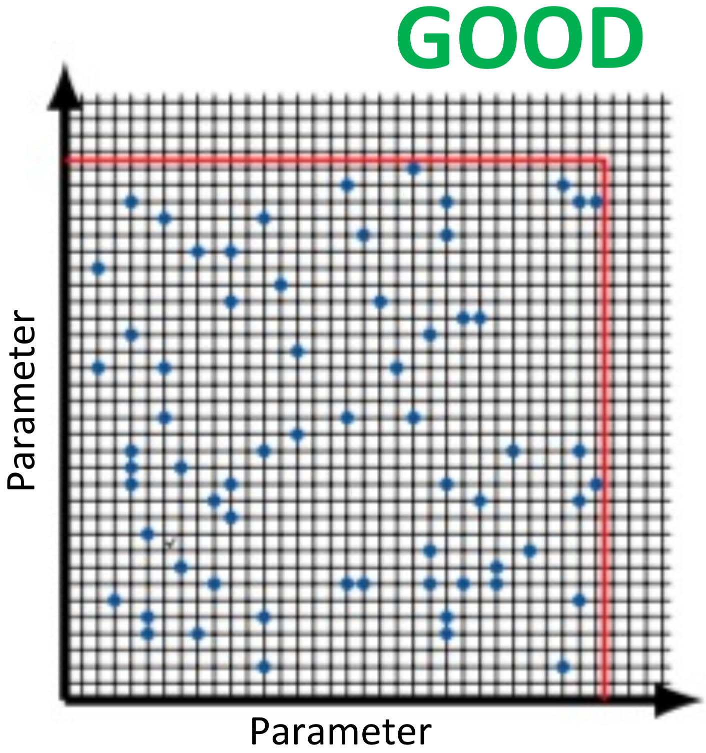
Step 3: Select the best surface

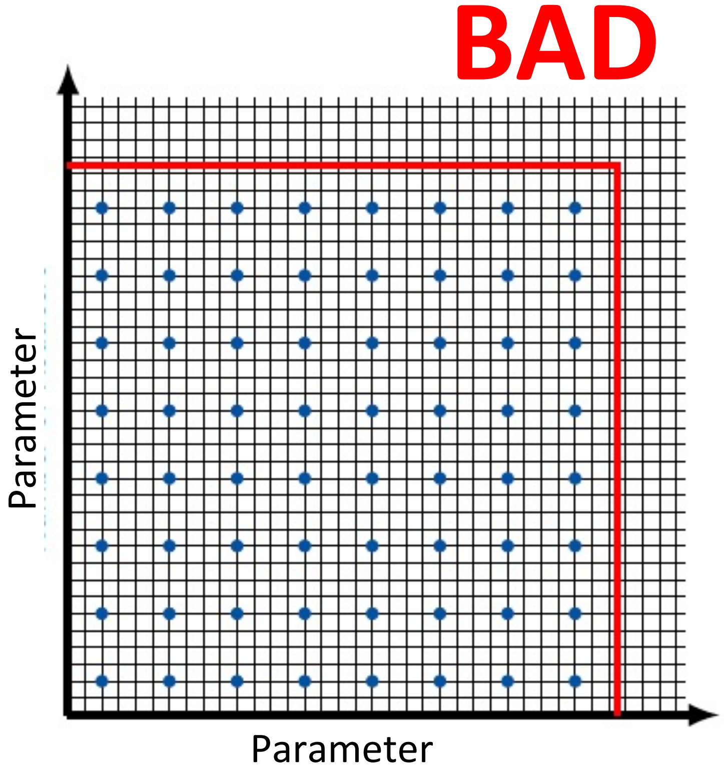


Step 4: Apply confidence interval



Step 1: Random sampling





Step 2: Building candidate surfaces

What kind of surfaces do we build?

- We represent our **surface** by a multivariate **polynomials**
- The candidate surfaces look like: **Z = B X**

- $z_1(x,y) = \beta_1 + \beta_2 x + \beta_3 y$ Degree 1
- $z_2(x,y) = \beta_1 + \beta_2 x + \beta_3 y + \beta_4 x^2 + \beta_5 xy + \beta_6 y^2$ Degree 2
- $z_3(x,y) = z_2(x,y) + \beta_7 x^3 + \beta_8 x^2 y + \beta_9 xy^2 + \beta_{10} y^3$ Degree 3

Step 2: Building candidate surfaces

Why build a polynomial surface?

- Polynomials are easy to describe and represent in memory
- Polynomials can generate quite complex surfaces
- Polynomials easily generalize to any number of variables

Step 2: Building candidate surfaces

- We construct best fit polynomial surfaces of degree *d* for each reasonable value of d, i.e. d = {1, 2, …, M} where M is small enough that the matrix X^TX is invertible

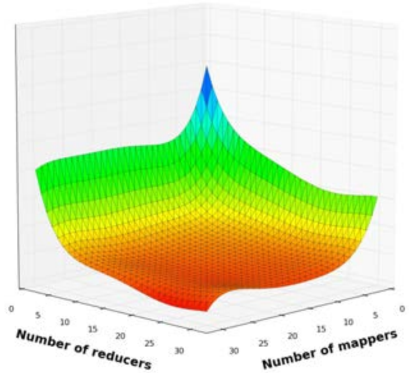
Step 2: Building candidate surfaces

How many points do we need to sample?

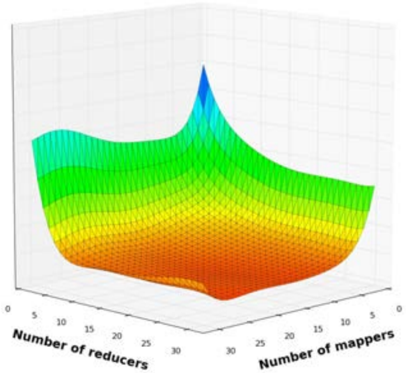
- To build the surface, we determine the coefficients B by solving the matrix equation:

  $X B = Z \dashrightarrow \mathbf{X^T X\ B = X^T Z}$

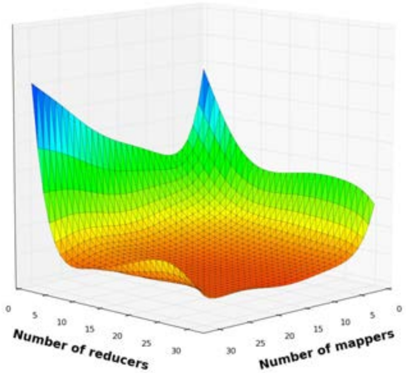
- If $\mathbf{X^T X}$ is not invertible, then there is not a unique solution for B
- If the number of samples taken is smaller than the number of terms in our polynomial, then $X^T X$ is not invertible
- To build a surface of degree d with *v* variables we need at least $\binom{d+v}{v}$



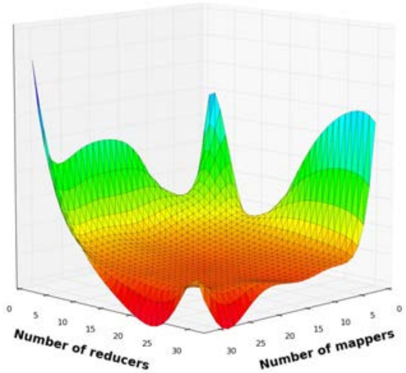
Degree 5



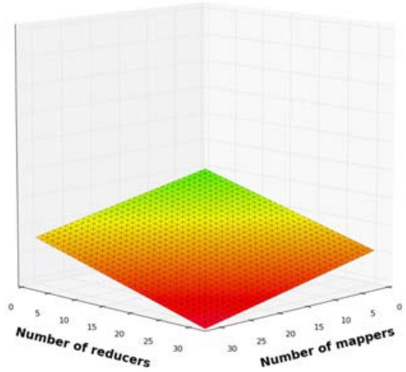
Degree 6



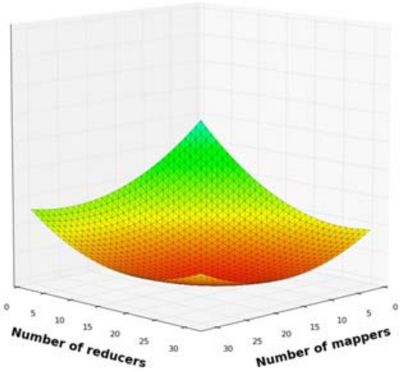
Degree 7



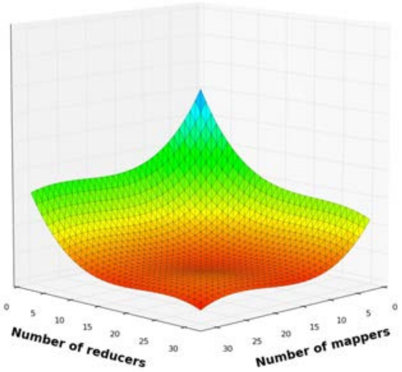
Degree 8



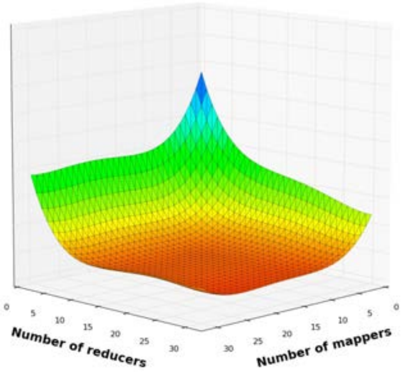
Degree 1



Degree 2

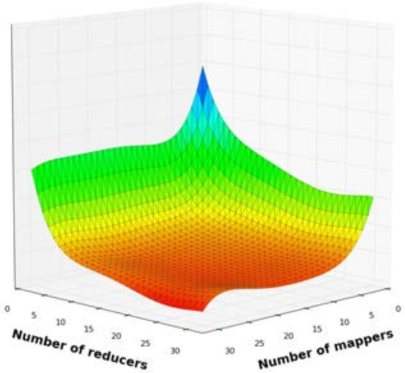


Degree 3

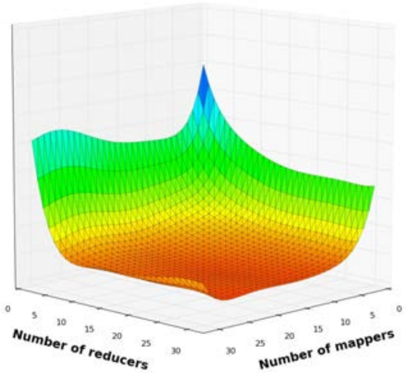


Degree 4

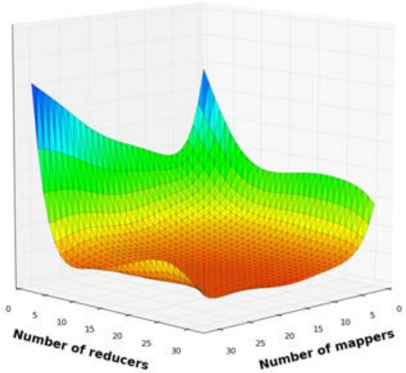
Which Model is Best?



Degree 5



Degree 6



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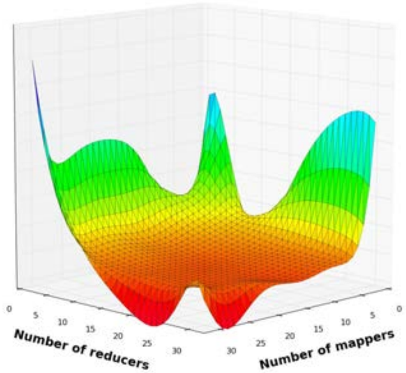
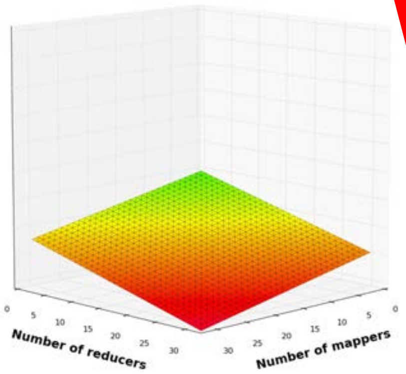
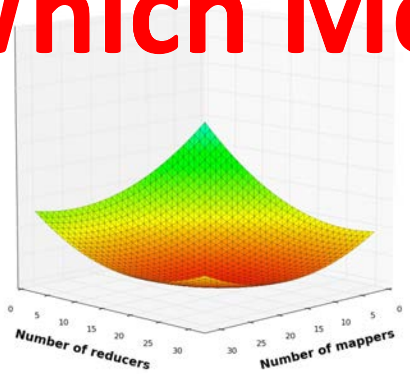


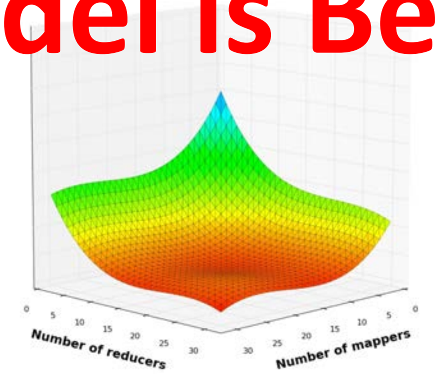
Degree 8



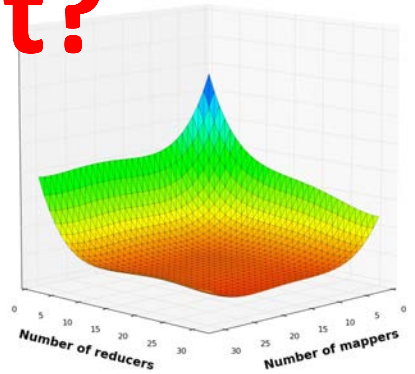
Degree 1



Degree 2



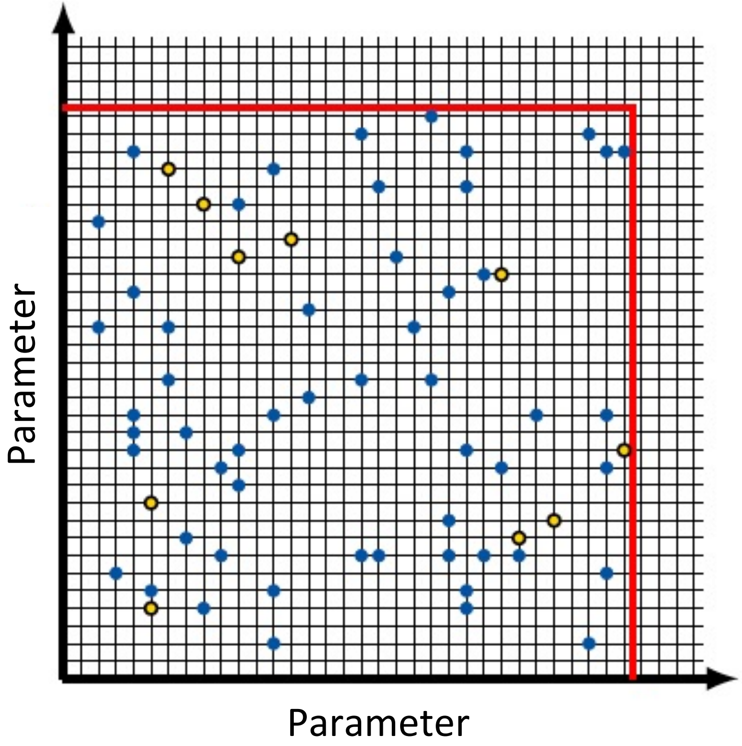
Degree 3



Degree 4

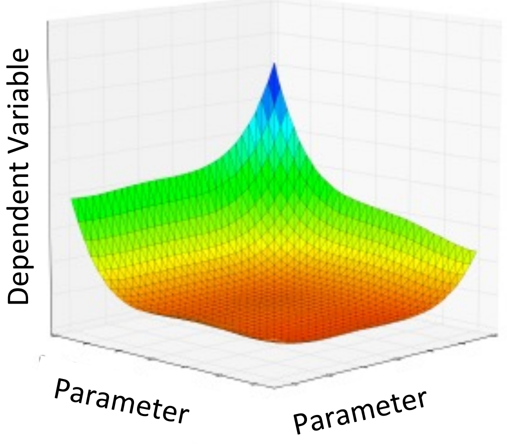
Step 3: Selecting the best surface using k-fold cross validation

- Partition samples into k sets of equal size
- k -1 sets are used for learning; one is use for testing
- Build best fit polynomial surface from learning set
- Use polynomial surface to predict unknown variables in testing set
- Use points in the testing set to compute SSE



Partition 1

- Learning Sets(k -1)
- Testing Set (1)

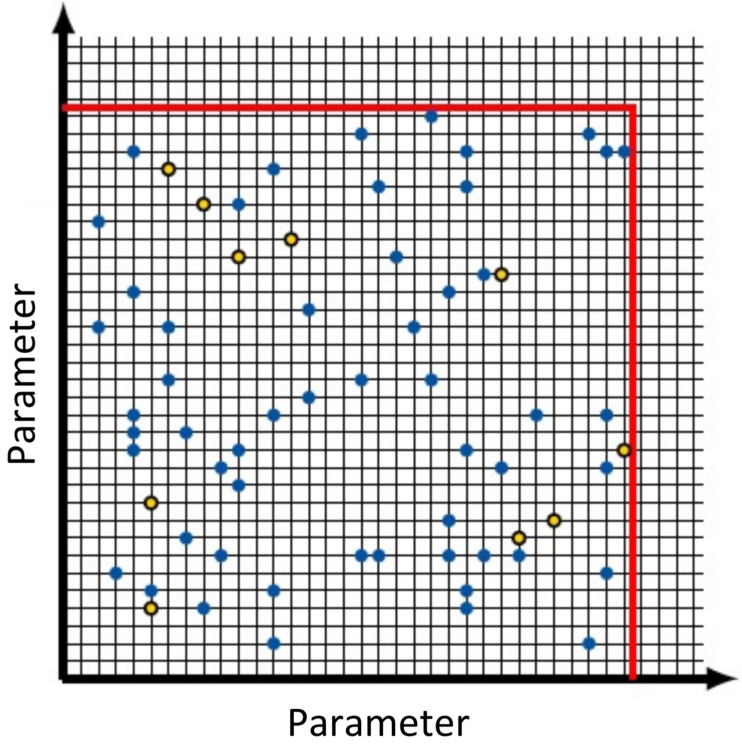


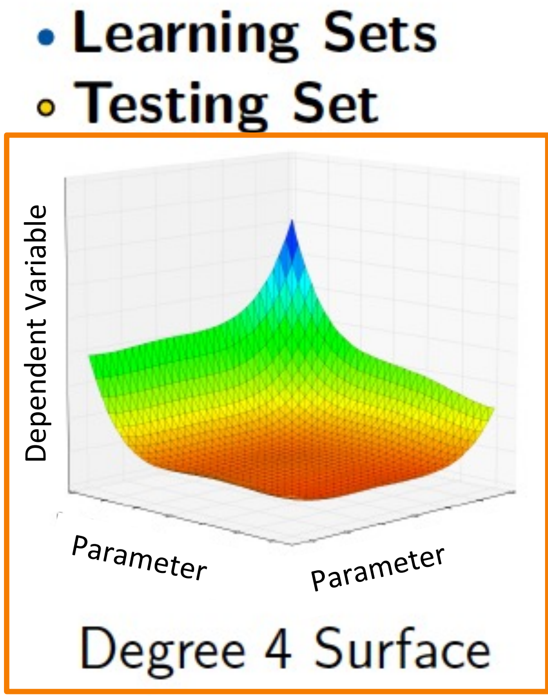
Degree 4 Surface

Step 3: Selecting the best surface using k-fold cross validation

Partition 1

- Partition samples into k sets of equal size
- k -1 sets are used for learning; one is use for testing
- **Build best fit polynomial surface from learning set**
- Use polynomial surface to predict unknown variables in testing set
- Use points in the testing set to compute SSE



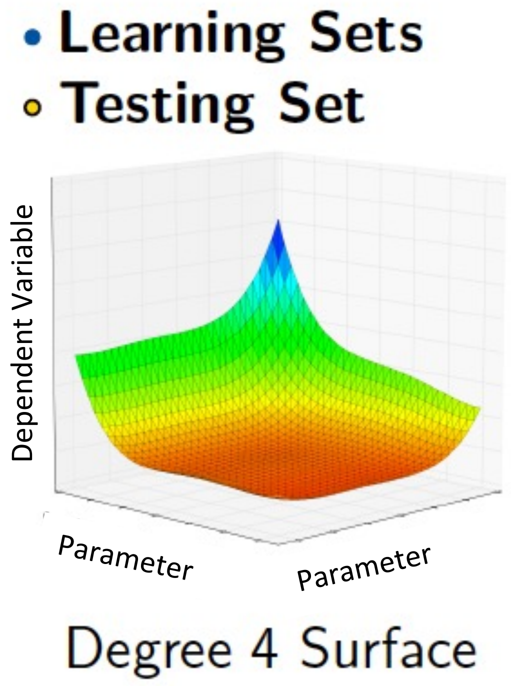


Step 3: Selecting the best surface using k-fold cross validation

Partition 1

- Partition samples into k sets of equal size
- k -1 sets are used for learning; one is use for testing
- Build best fit polynomial surface from learning set
- **Use polynomial surface to predict unknown variables in testing set**
- **Use points in the testing set to compute SSE**

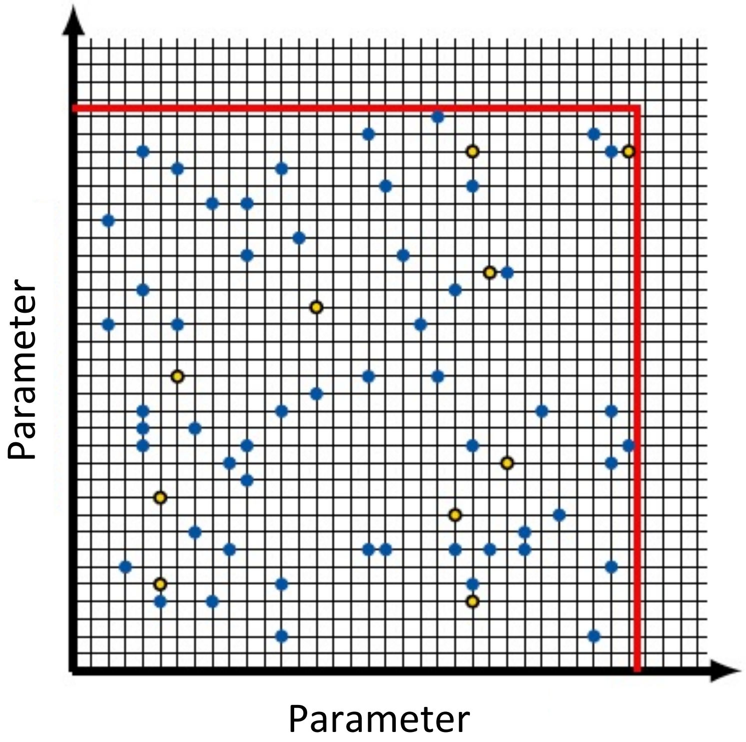
Compute SSE:
Observed variables
in testing points
vs
predicted variable
(using surface)
in testing pints

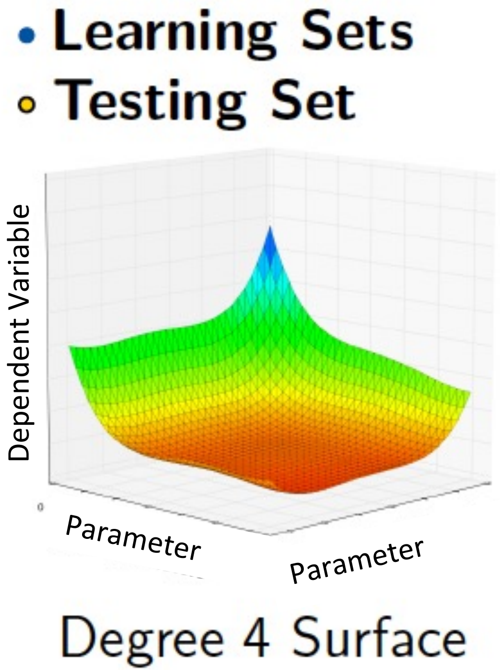


Step 3: Selecting the best surface using k-fold cross validation

Partition 2

- Partition samples into k sets of equal size
- k -1 sets are used for learning; one is use for testing
- Build best fit polynomial surface from learning set
- Use polynomial surface to predict unknown variables in testing set
- Use points in the testing set to compute SSE





Step 3: Selecting the best surface using k-fold cross validation

Partition 3

- Partition samples into k sets of equal size
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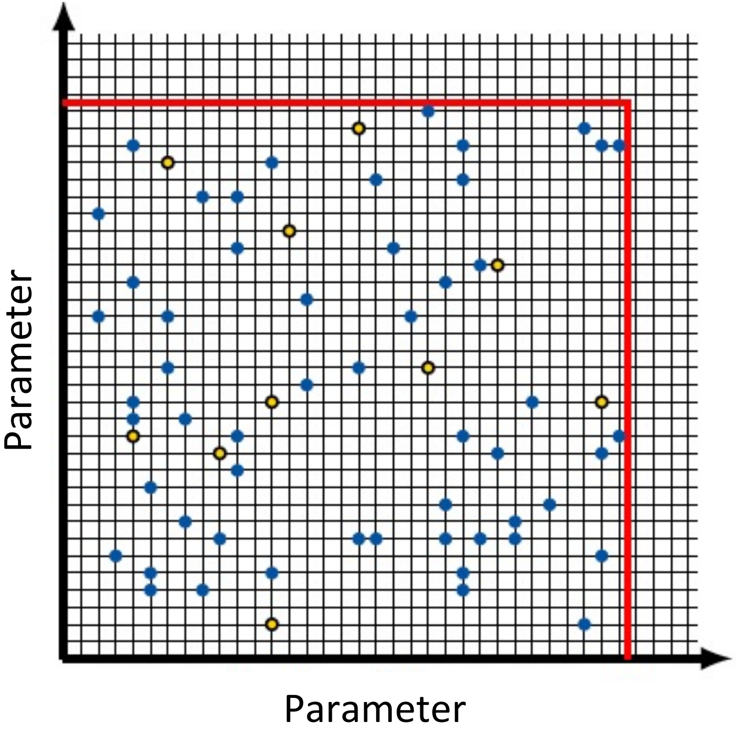
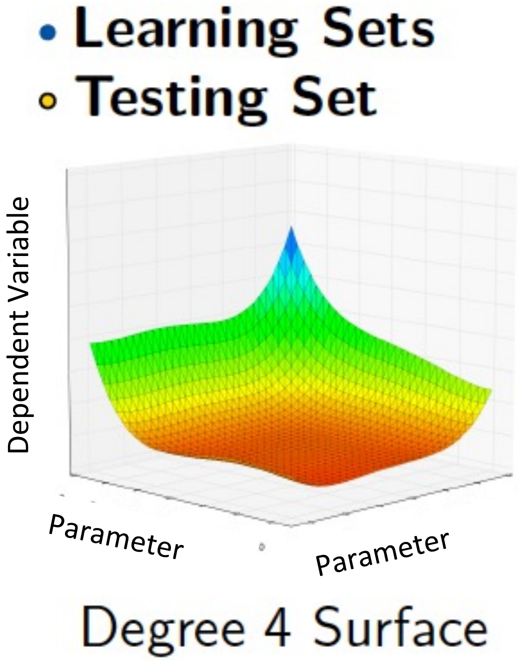
- Build best fit polynomial surface from learning set
- Use polynomial surface to predict unknown variables in testing set
- Use points in the testing set to compute SSE





Step 3: Selecting the best surface using k-fold cross validation

Partition 4

- Partition samples into k sets of equal size
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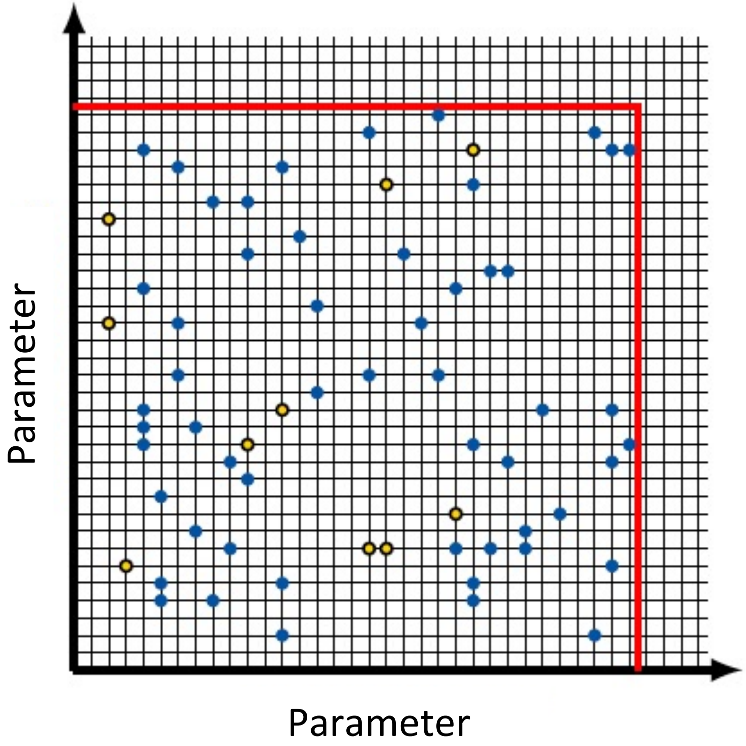
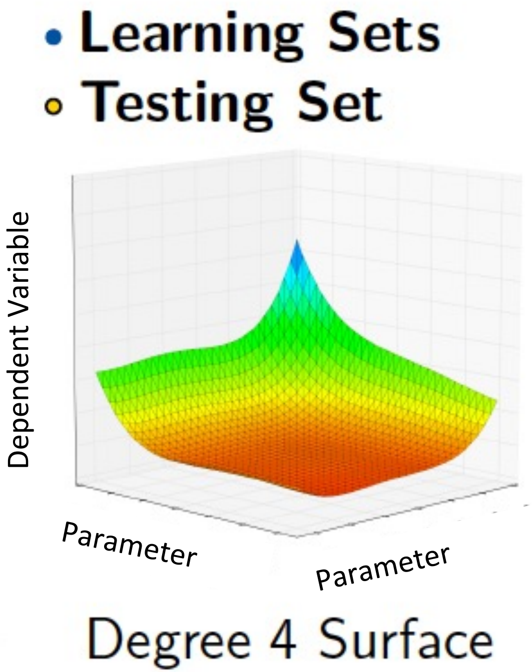
- Use polynomial surface to predict unknown variables in testing set
- Use points in the testing set to compute SSE

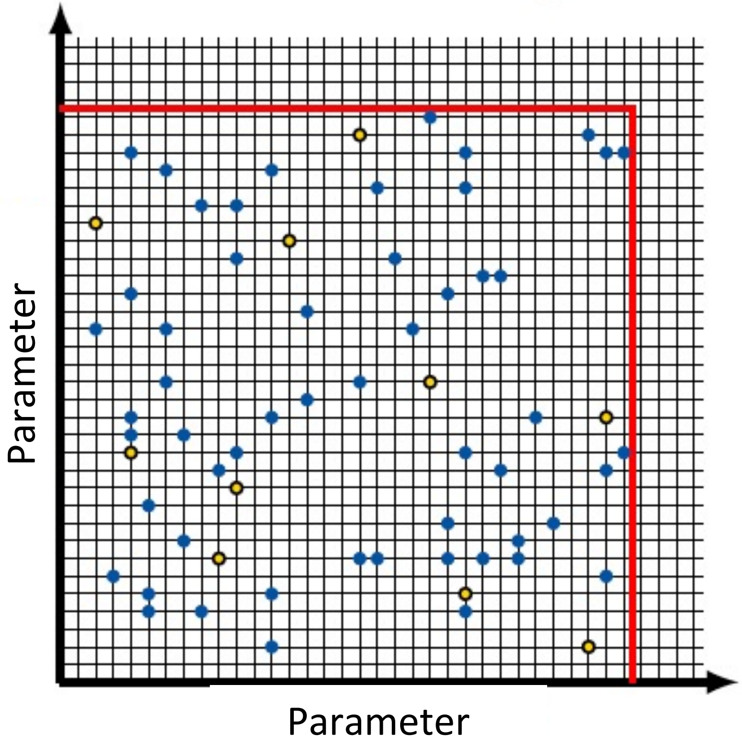


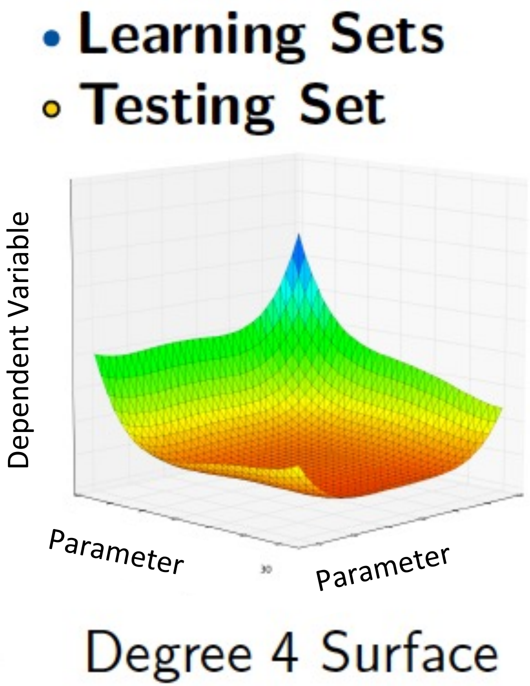


Step 3: Selecting the best surface using k-fold cross validation

Partition 5

- Partition samples into k sets of equal size
- k -1 sets are used for learning; one is use for testing
- Build best fit polynomial surface from learning set
- Use polynomial surface to predict unknown variables in testing set
- Use points in the testing set to compute SSE





Step 3: Selecting the best surface using k-fold cross validation

- Partition samples into k sets of equal size
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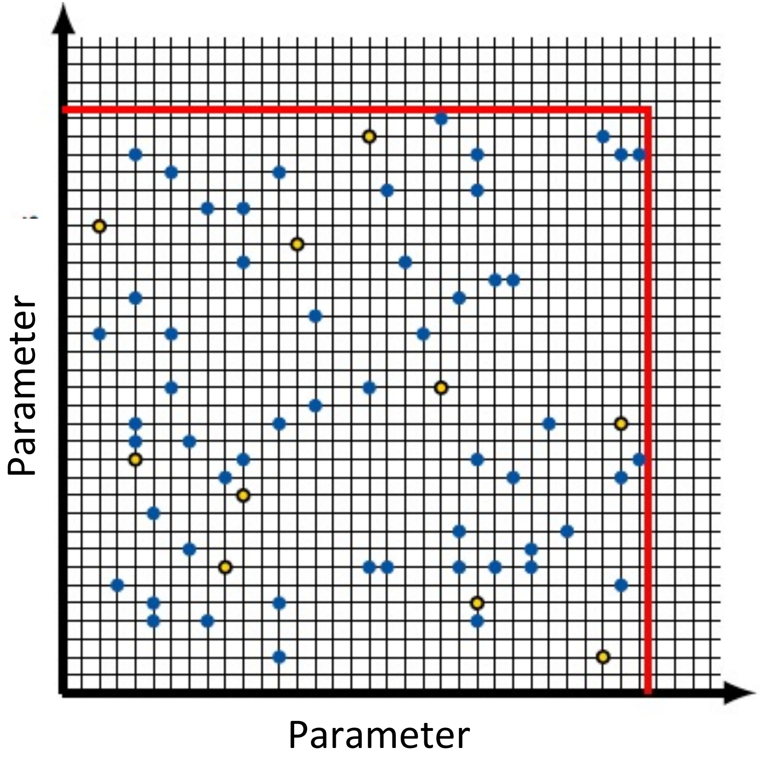

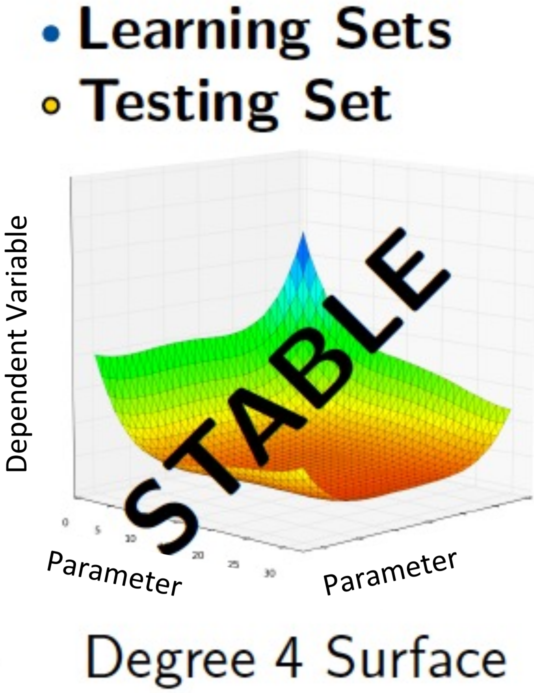

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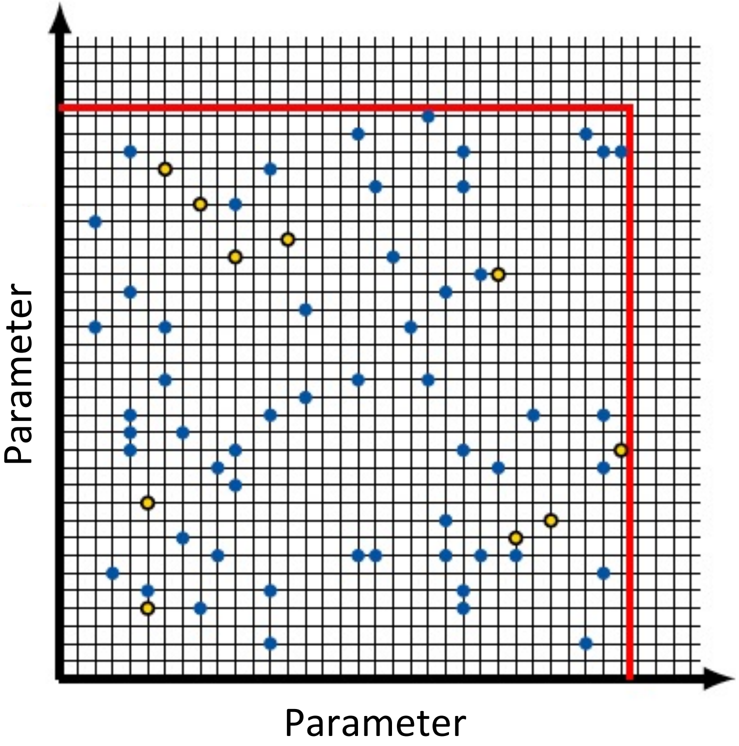

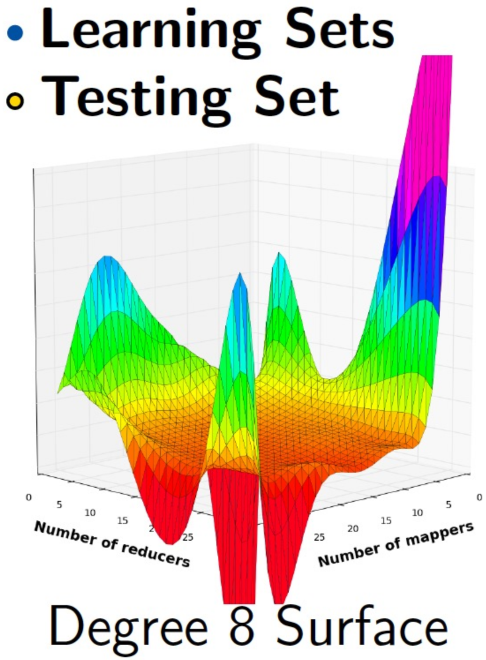

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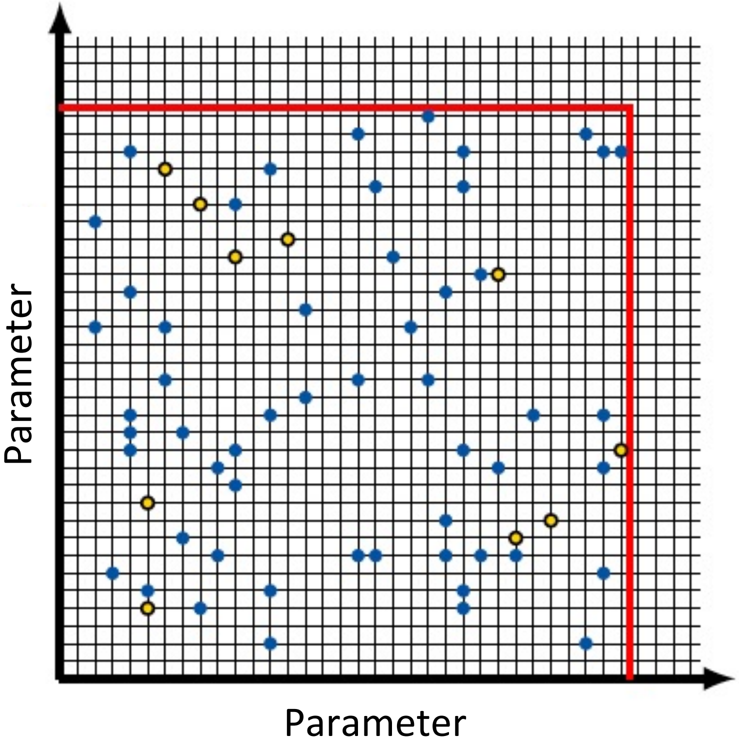

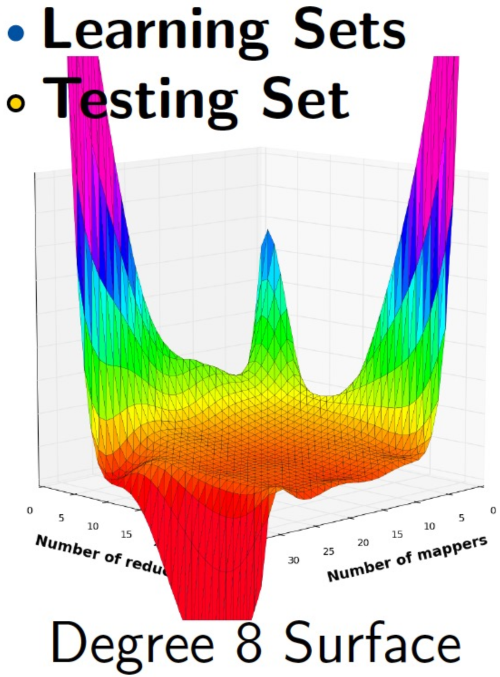

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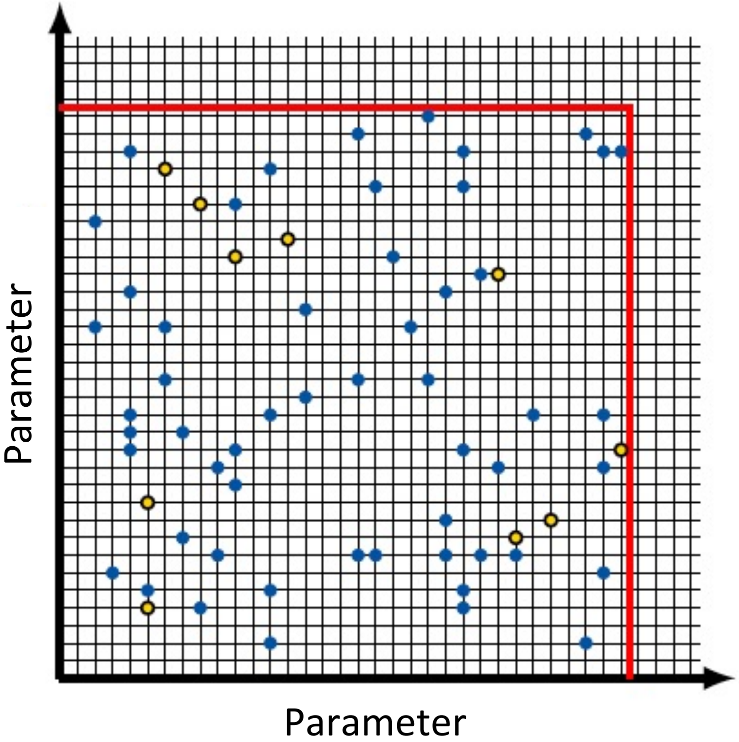
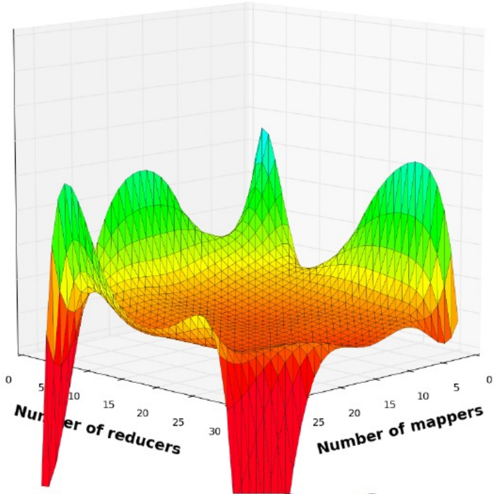


- Learning Sets
- Testing Set



Degree 8 Surface

Step 3: Selecting the best surface using k-fold cross validation

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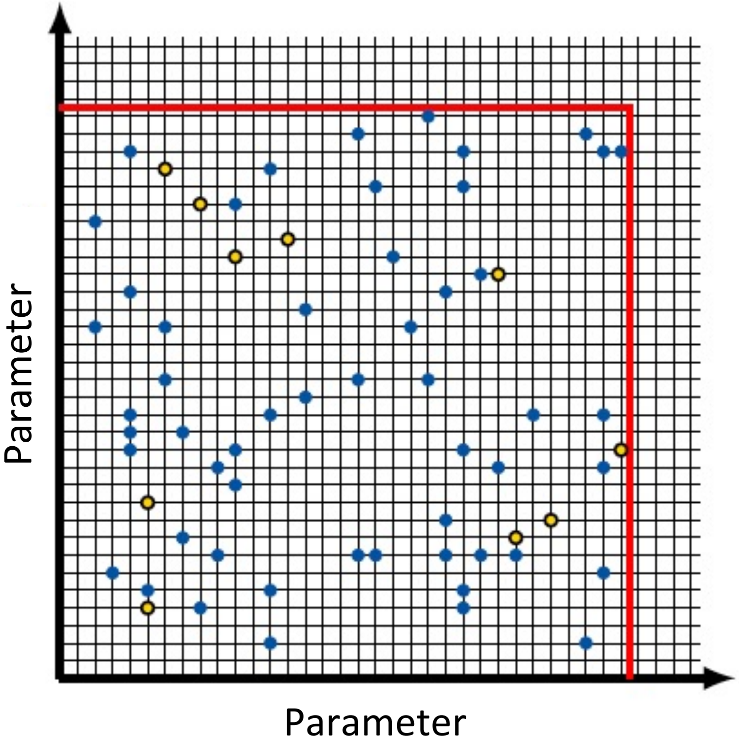

- Learning Sets
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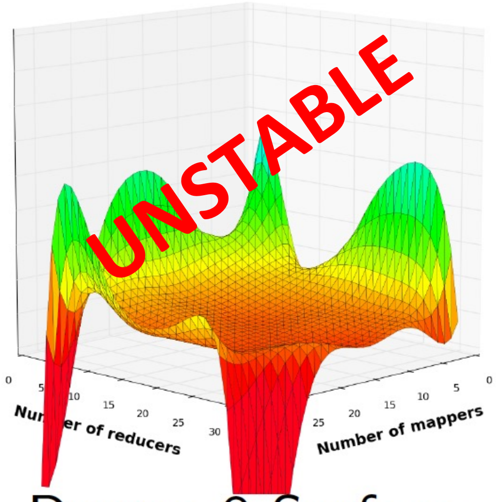
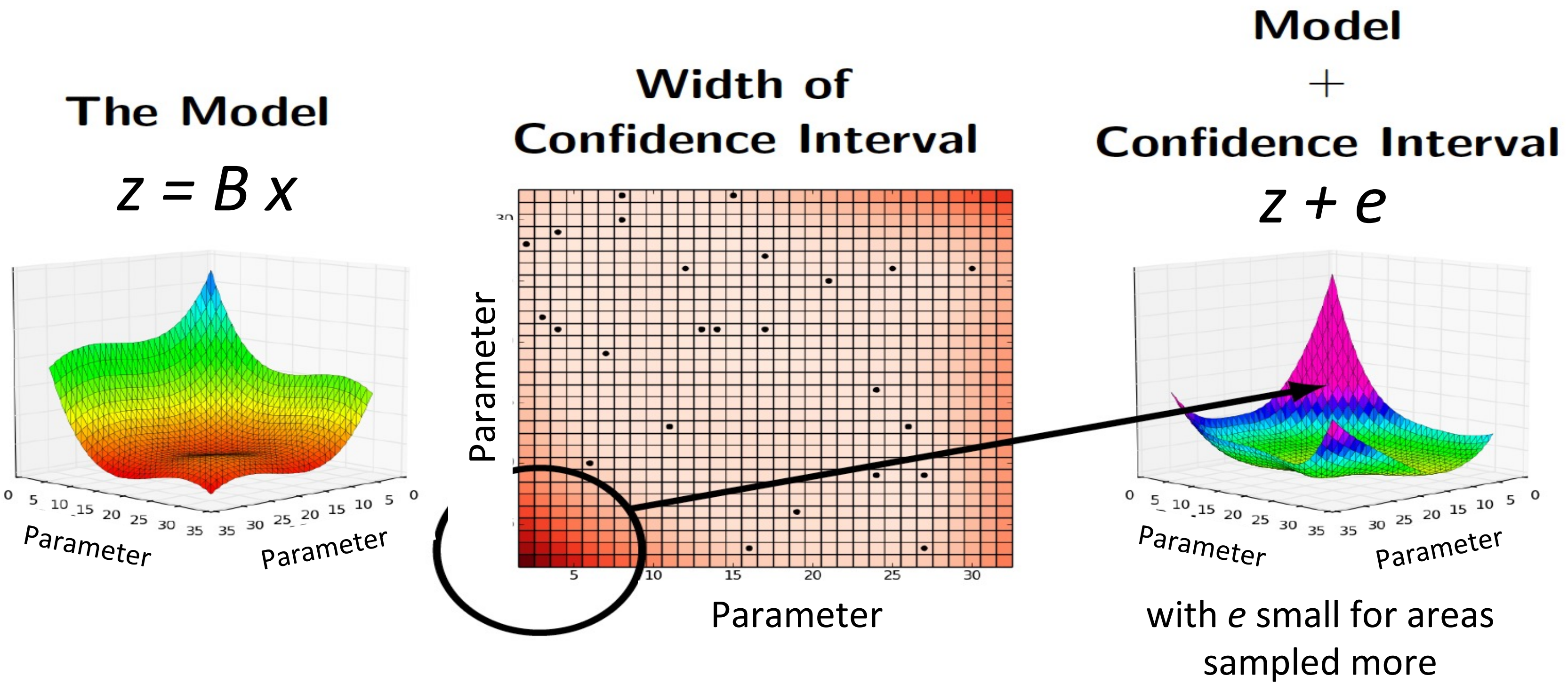


Degree 8 Surface

Step 4: Applying a confidence interval



KNN and SBM

KNN:

→ Use **local data**

→ Compute k and distance kernel using cross validation automatically

→ Compute weighted means with the kernel (***many values***)

0 0 0 0

0 0 0 0 0

Surrogate based model (SBM):

→ Use **all sampled data**

→ Use regression to generate one single polynomial model (***single polynomial model***)

4 4 4 4

4 4 4 4 4

D. Rorabaugh, M. Guevara, R. Llamas, J. Kitson, R. Vargas, and **M. Taufer**. SOMOSPIE: A Modular SOil MOisture SPatial Inference Engine based on Data Driven Decisions. eScinece 2019.

Hybrid Piecewise Polynomial Modeling

HYbrid Piecewise POlynomial modeling (HYPPO)

k Nearest Neighbors

- Use **local** data
- Compute the average
  (*many simple local models*)

Surrogate-Based Modeling

- Use **all** sampled data
- Construct **one** **polynomial**
  (*single complex global model*)

Hybrid modeling ⍰ HYPPO

- Use **local** data
- Construct many **polynomials**
  (*many complex local models*)

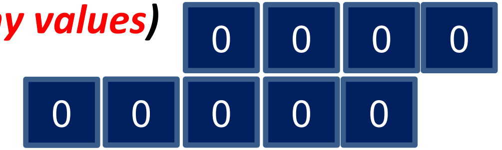
KNN, SBM, and HYPPO

KNN:

→ Use **local data**

→ Compute k and distance kernel using cross validation automatically

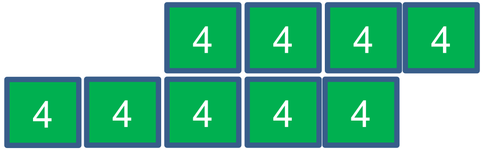
→ Compute weighted means with the kernel (***many values***)



Surrogate based model (SBM):

→ Use **all sampled data**

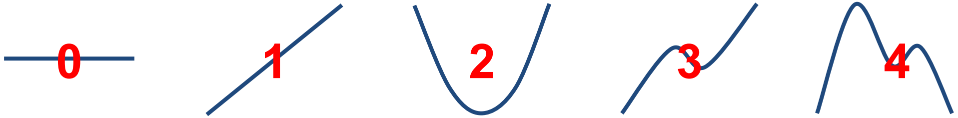
→ Use regression to generate one single polynomial model (***single polynomial model***)



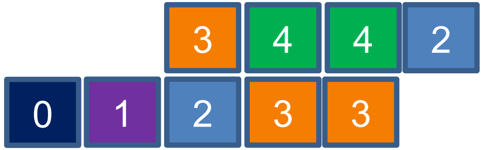
HYPPO (Hybrid Piecewise Polynomial Modeling):

→ Use **local data**

→ Determine local polynomial degree using cross validation



→ Use regression to generate local polynomial model (***many polynomial models***)



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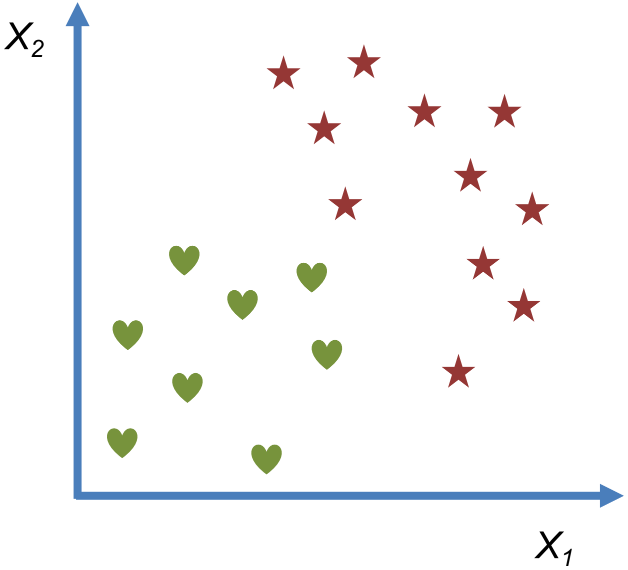
BIG ORANGE BIG IDEAS

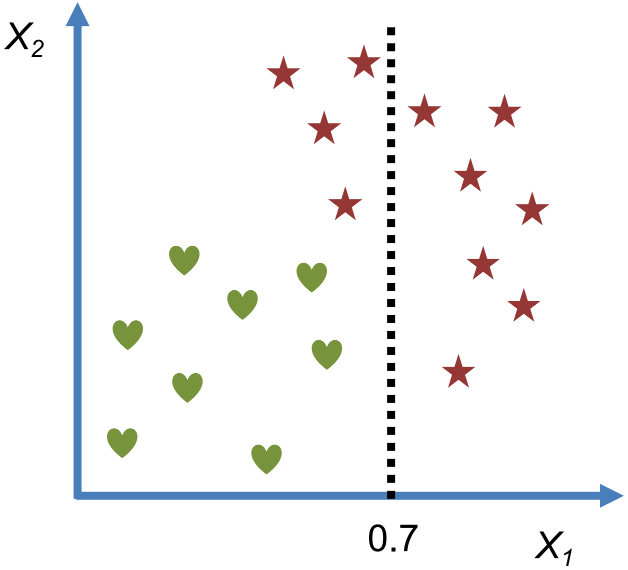
Random Forest

Divide and Conquer



- Information gain is used to decide how to divide the dataset for classification
- The data is recursively divided until subdivision are all one class

Divide and Conquer



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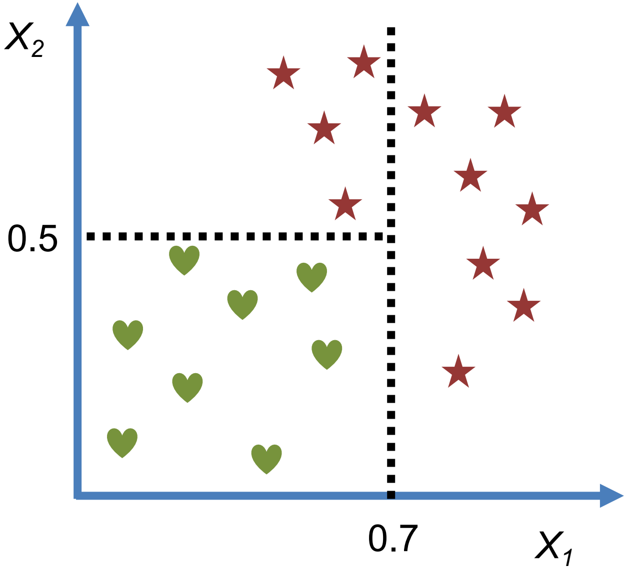

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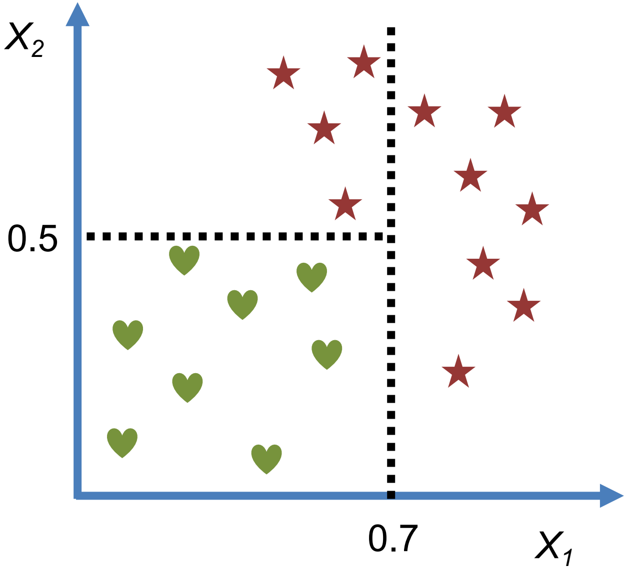
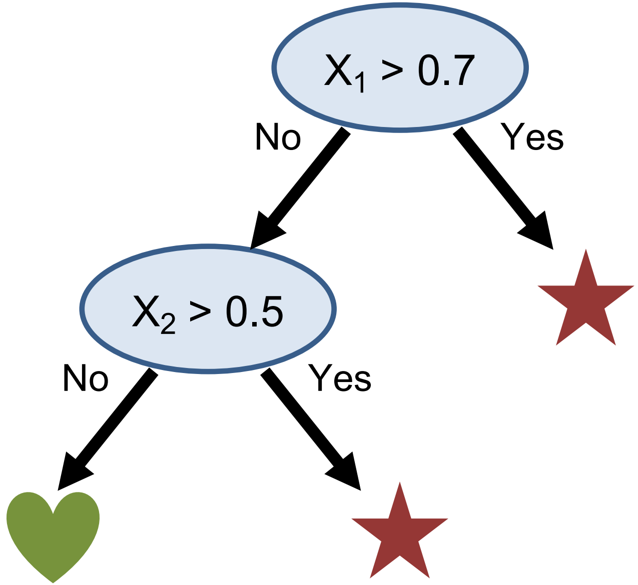
Divide and Conquer





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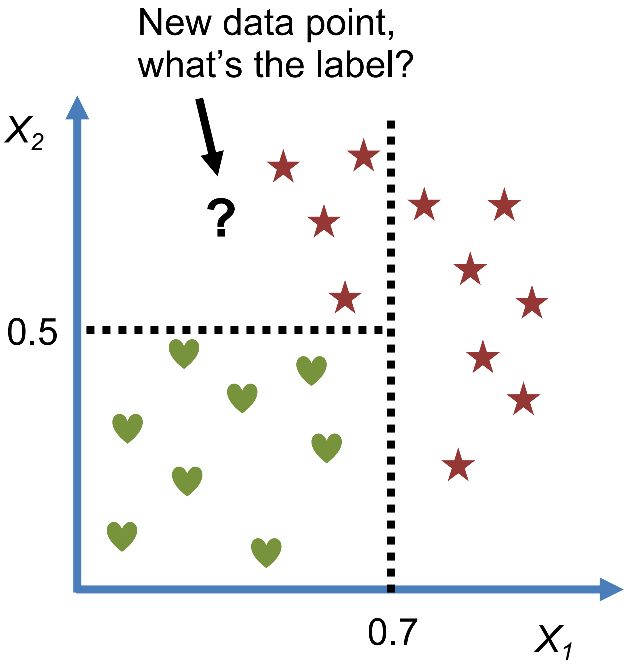

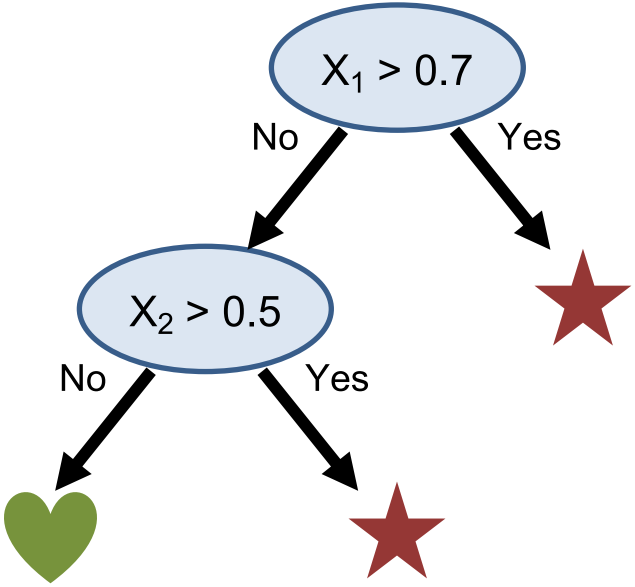

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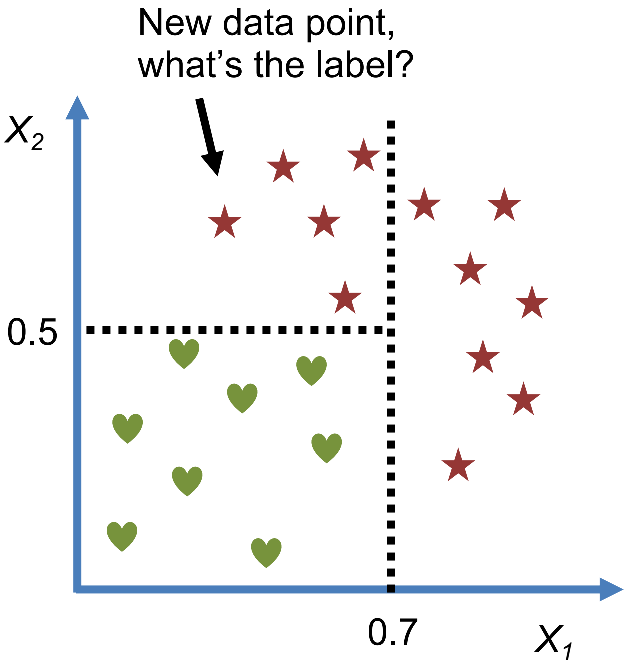
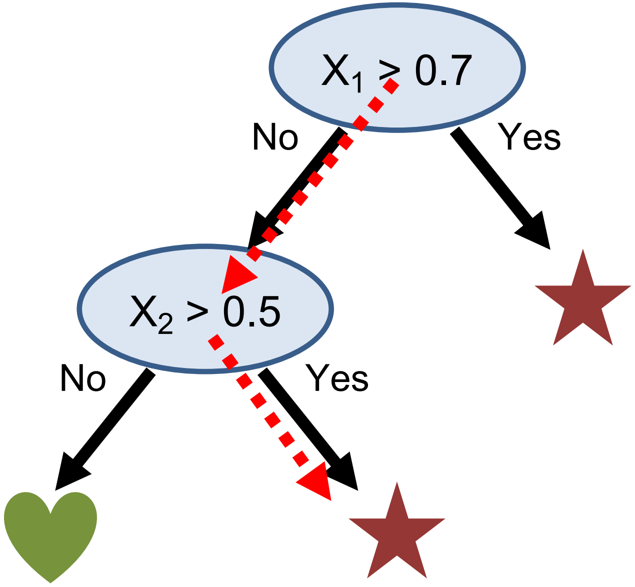
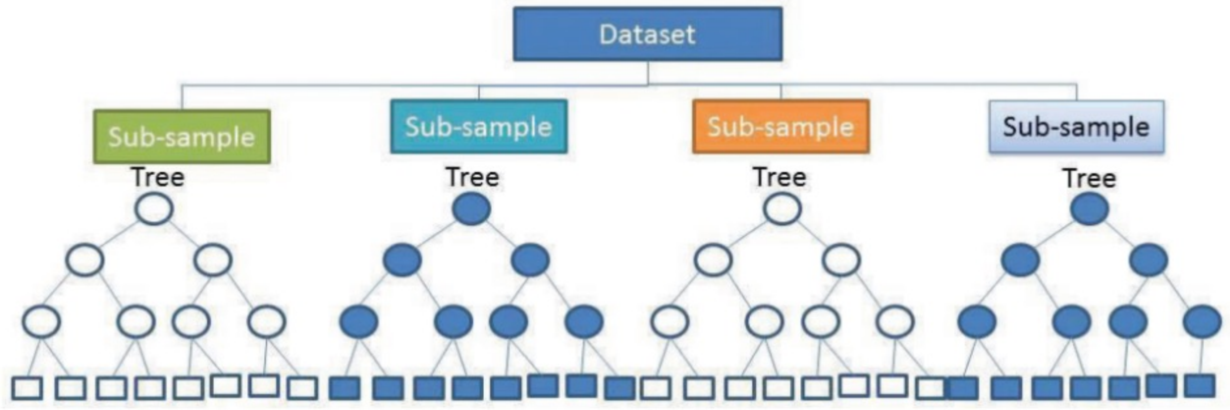




Random Forests: Ensembles of Trees

- The prediction of many trees is better than the prediction of any one tree



- Each tree is built with a random sample of data rows and data features
- Each tree makes a prediction and the most popular prediction is returned

Reading

Reading

- T. Johnston, M. Alsulmi, P. Cicotti and M. Taufer. Performance Tuning of MapReduce Jobs Using Surrogate-Based Modeling. In *Proceedings of the International Conference on Computational Science (ICCS)*, pp. 49 – 59. Reykjavik, Iceland. June 1 – 3, 2015.
- T. Johnston, C. Zannin, and M. Taufer. HYPPO: A Hybrid, Piecewise Polynomial Modeling Technique for Non-Smooth Surfaces. In *Proceedings of the 28th IEEEE International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD)*, pp. 1 – 8. Los Angeles, CA, USA. October 26 – 28, 2016.
- Breiman, L. Random Forests. *Machine Learning* **45,** 5–32 (2001). https://doi.org/10.1023/A:1010933404324

Live Chat

Live Chat

- GTC 2015 Keynote with Jeff Dean, Google

  https://video.ibm.com/recorded/60071572