Outline

- Basis function expansion to capture non-linear relationships
- Understanding the bias-variance tradeoff
- How does overfitting occur

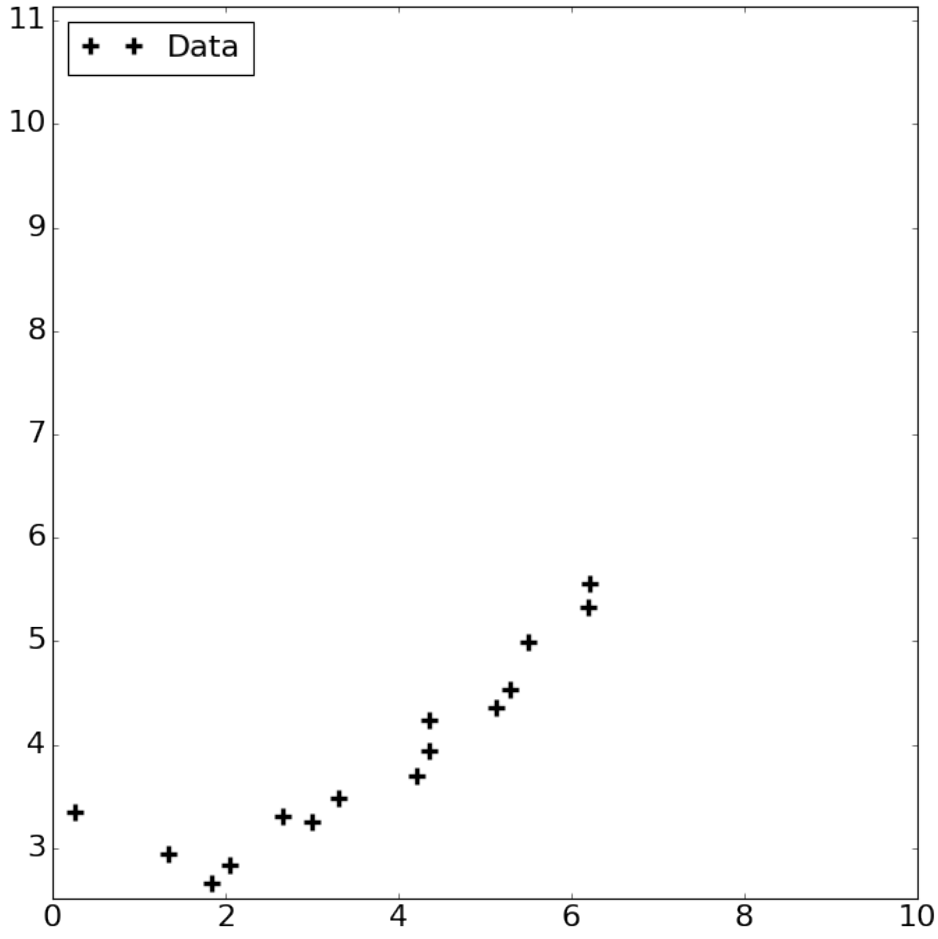
Outline

Basis Function Expansion

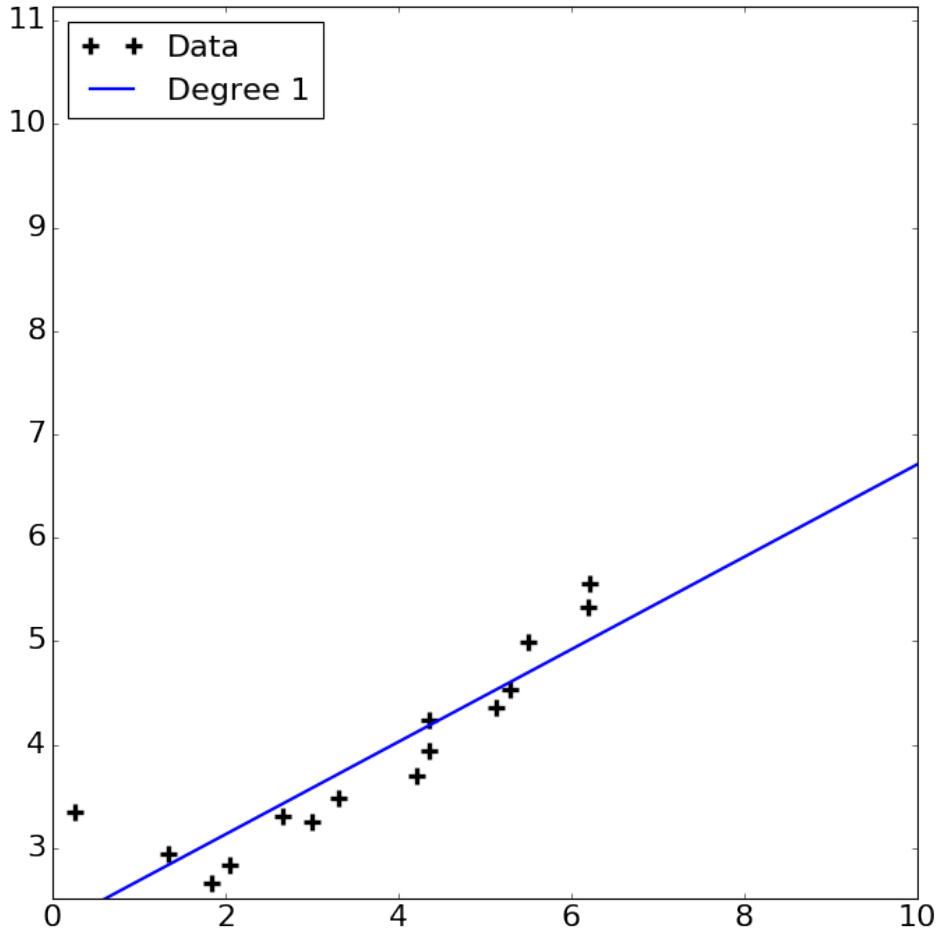
Overfitting and the Bias-Variance Tradeoff

Sources of Overfitting

Linear Regression : Polynomial Basis Expansion



Linear Regression : Polynomial Basis Expansion



Linear Regression : Polynomial Basis Expansion

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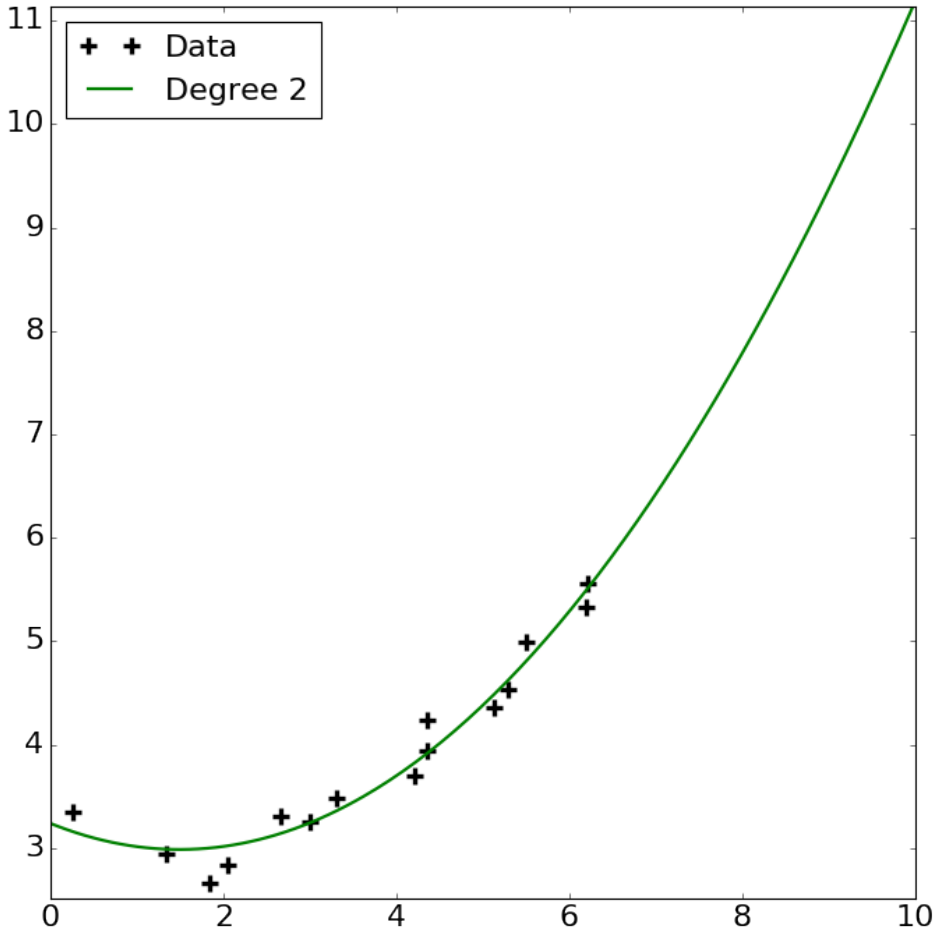

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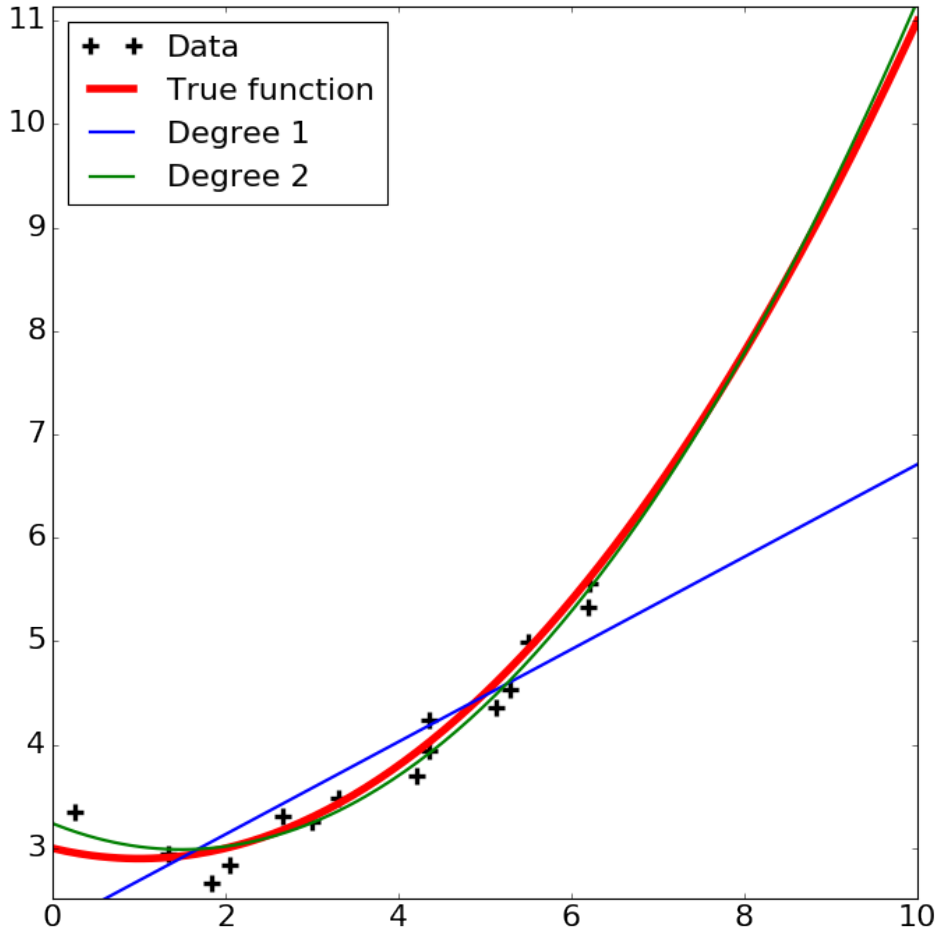
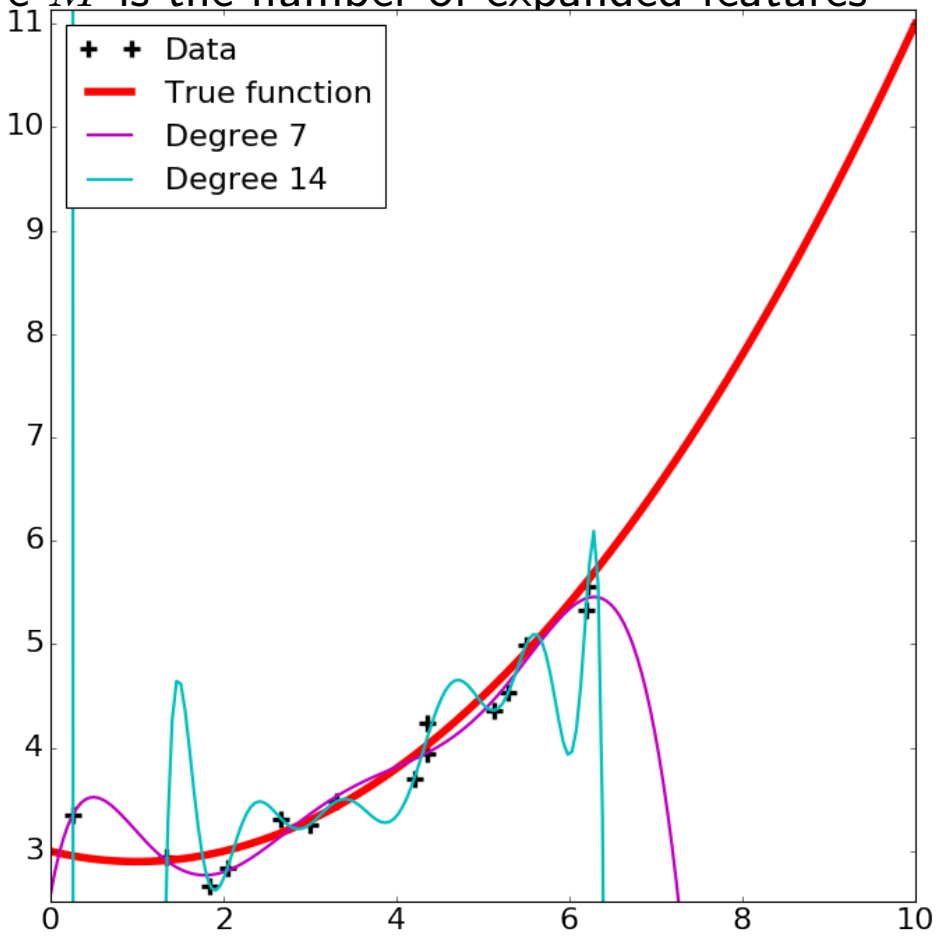


Linear Regression : Polynomial Basis Expansion

$\boldsymbol{\phi}(x) = [1, x, x^2, \cdots, x^d]$

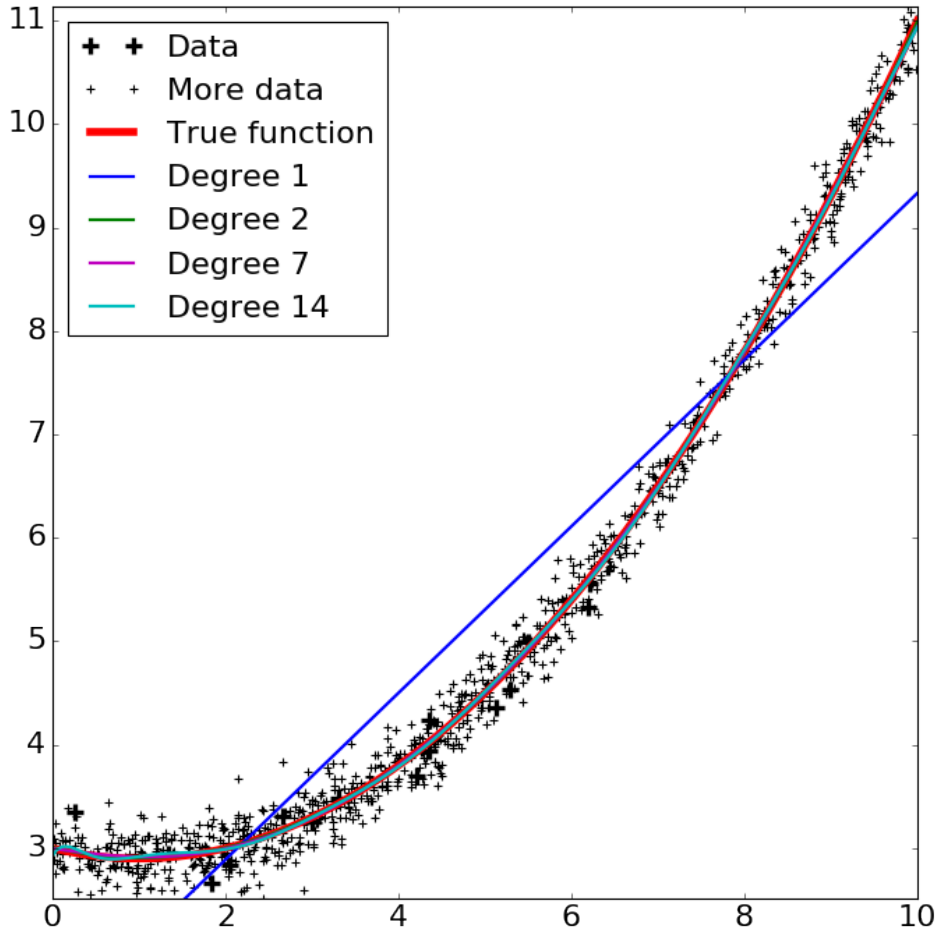
Model $y = \mathbf{w}^\mathsf{T}\boldsymbol{\phi}(x) + \epsilon$

Here $\mathbf{w} \in \mathbb{R}^M$, where M is the number of expanded features



Linear Regression : Polynomial Basis Expansion

Getting more data can avoid overfitting!



Polynomial Basis Expansion in Higher Dimensions

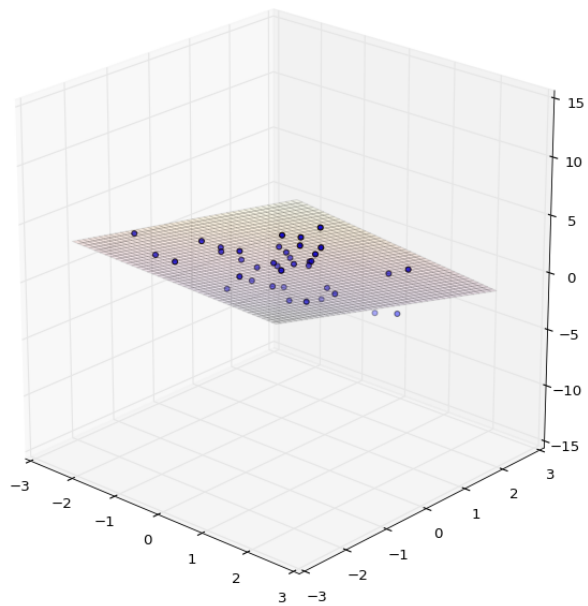
Basis expansion can be performed in higher dimensions

We're still fitting linear models, but using more features

$$y = \mathbf{w} \cdot \boldsymbol{\phi}(\mathbf{x}) + \epsilon$$

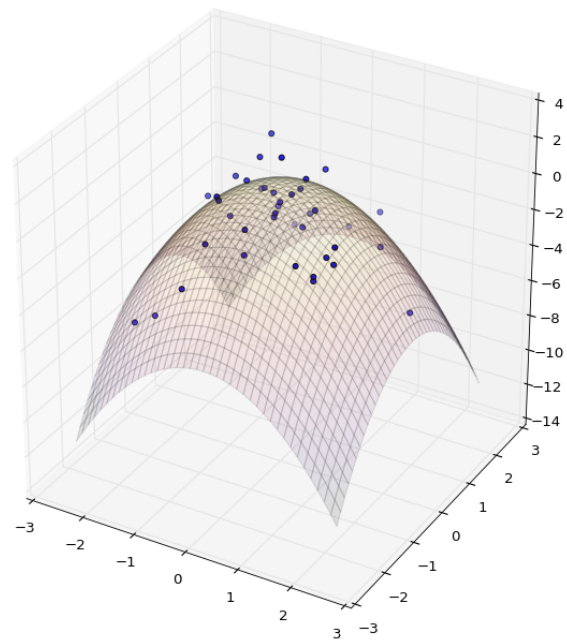
Linear Model

$\phi(\mathbf{x}) = [1, x_1, x_2]$



Quadratic Model

$\phi(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2, x_1 x_2]$



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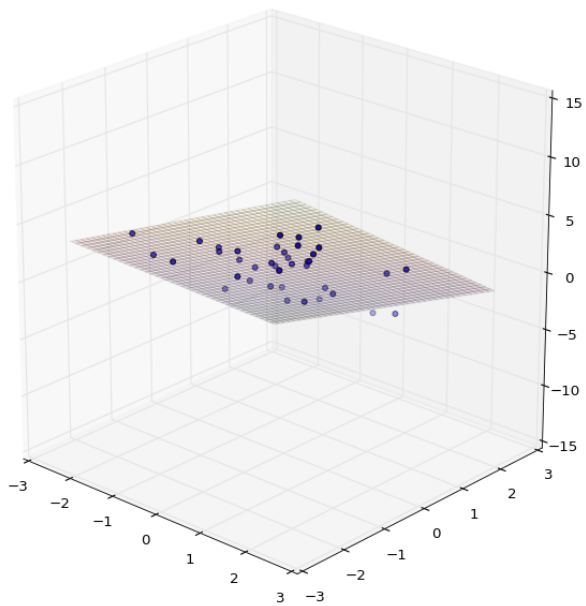

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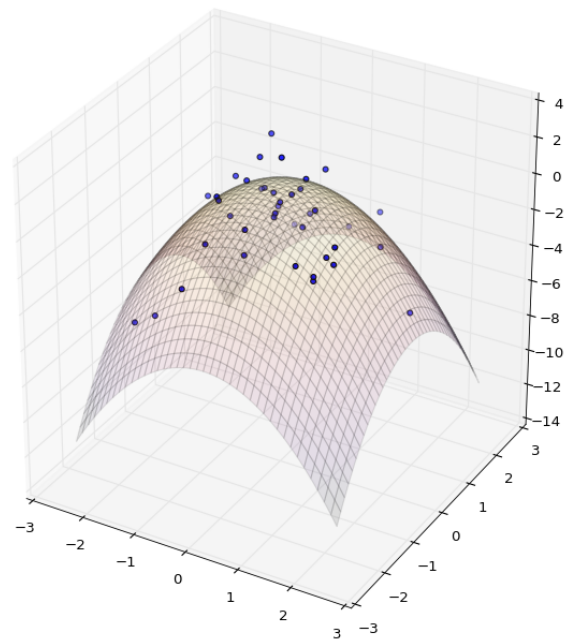


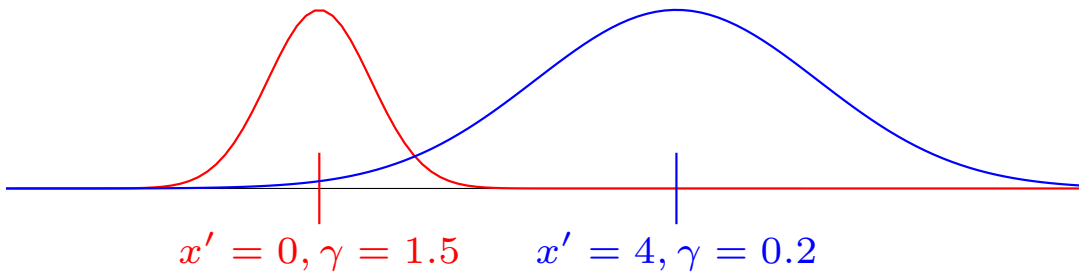
Using degree d polynomials in D dimensions results in $\approx D^d$ features!

Basis Expansion Using Kernels

We can use kernels as features

A Radial Basis Function (RBF) kernel with width parameter γ is defined as

$$\kappa(\mathbf{x}', \mathbf{x}) = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$$



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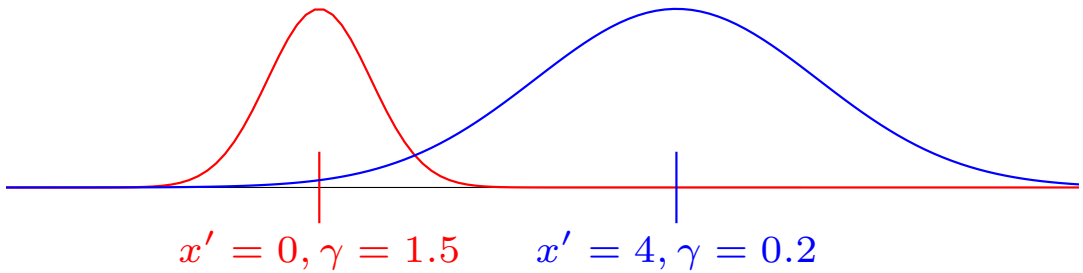

A kernel computes the dot product $\kappa(\mathbf{x}', \mathbf{x}) : \mathcal{X} \times \mathcal{X} \to \mathbb{R} = \phi(\mathbf{x}') \cdot \phi(\mathbf{x})$ of some expansion ϕ, see e.g. Sec. 5.7.2 in GBC.

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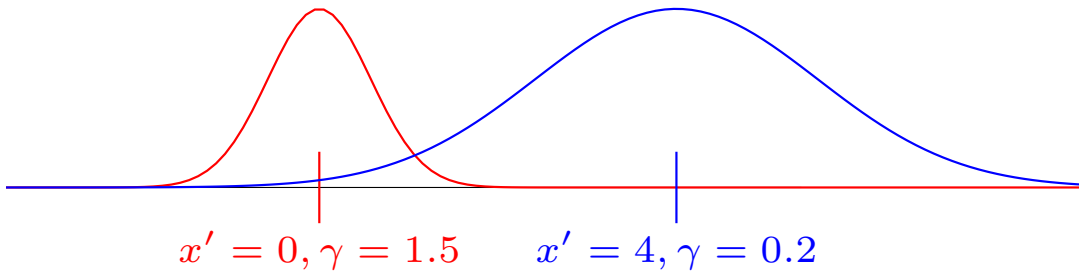

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Other kernels:

- Polynomial kernel: $\kappa(\mathbf{x}', \mathbf{x}) = (\mathbf{x}^\mathsf{T} \cdot \mathbf{x}' + c)^d$
- String kernels
- Graph kernels

Basis Expansion Using Kernels

- RBF kernel: $\kappa(\mathbf{x}', \mathbf{x}) = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$
- Choose centres $\mu_1, \mu_2, \ldots, \mu_M$
- Feature map: $\phi(\mathbf{x}) = [1, \kappa(\mu_1, \mathbf{x}), \ldots, \kappa(\mu_M, \mathbf{x})]$

$$y = w_0 + w_1 \kappa(\mu_1, \mathbf{x}) + \cdots + w_M \kappa(\mu_M, \mathbf{x}) + \epsilon = \mathbf{w} \cdot \boldsymbol{\phi}(\mathbf{x}) + \epsilon$$

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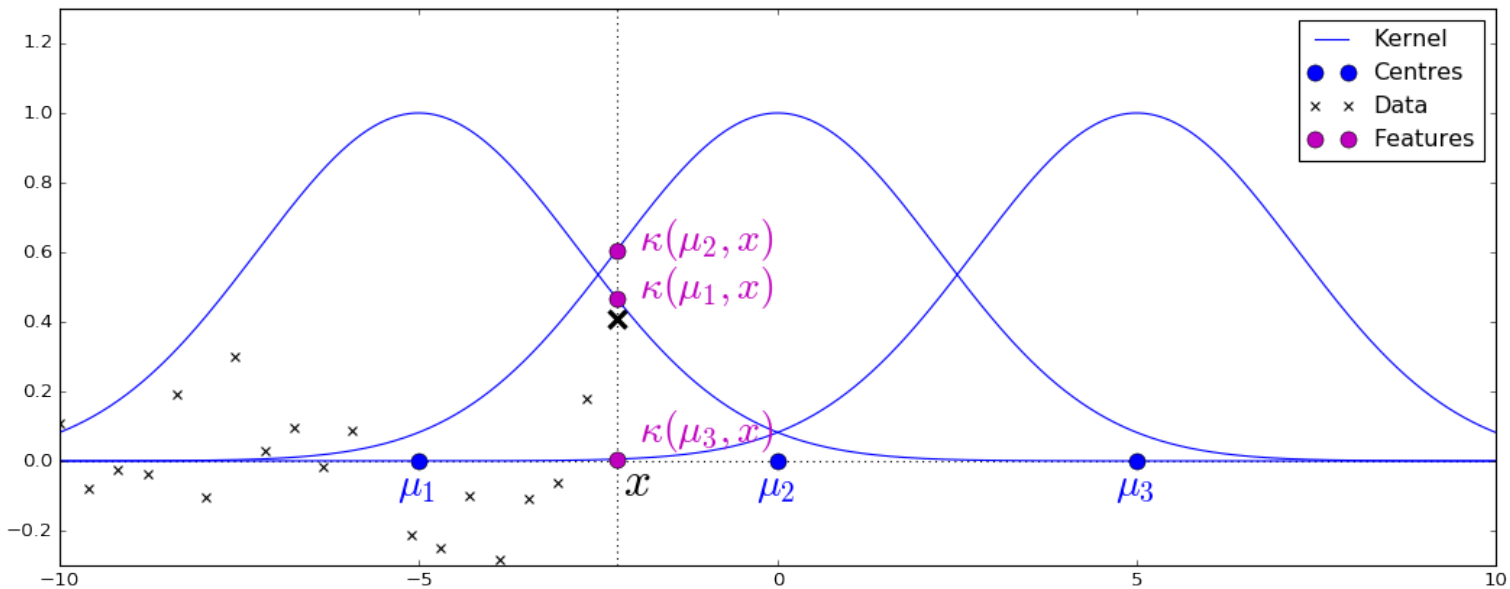
- How do we choose the centres?



Basis Expansion Using Kernels

One reasonable choice is to choose data points themselves as centres for kernels

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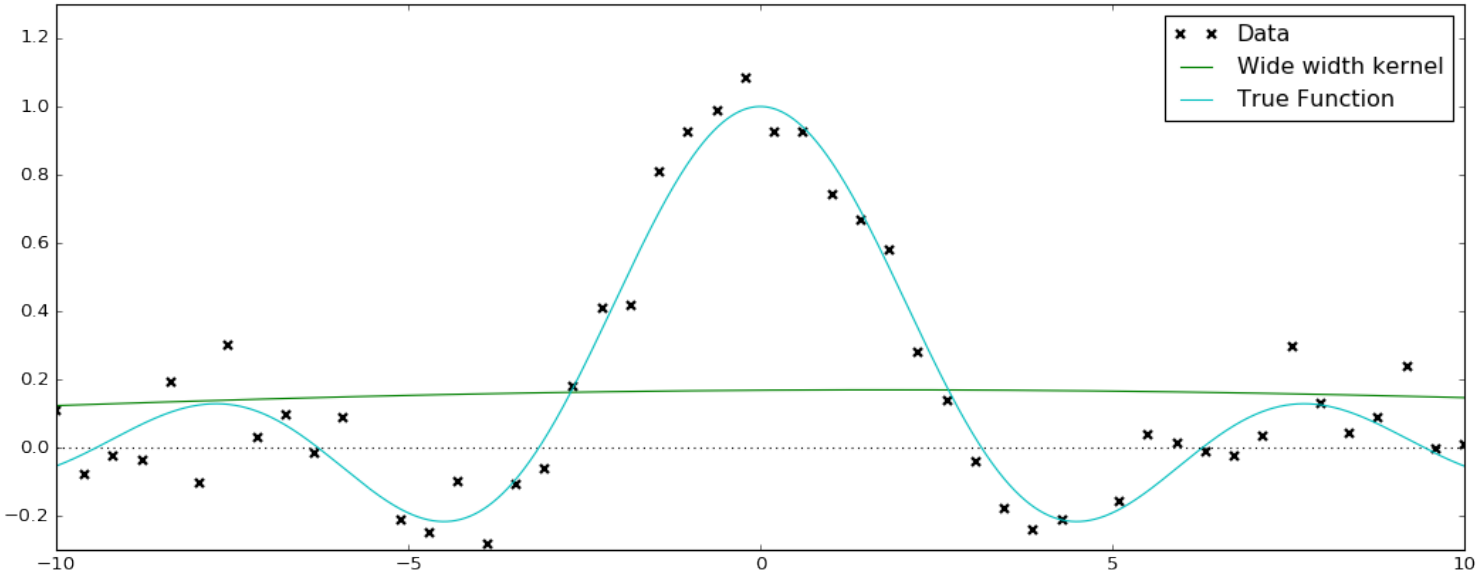
Need to choose width parameter γ for the RBF kernel

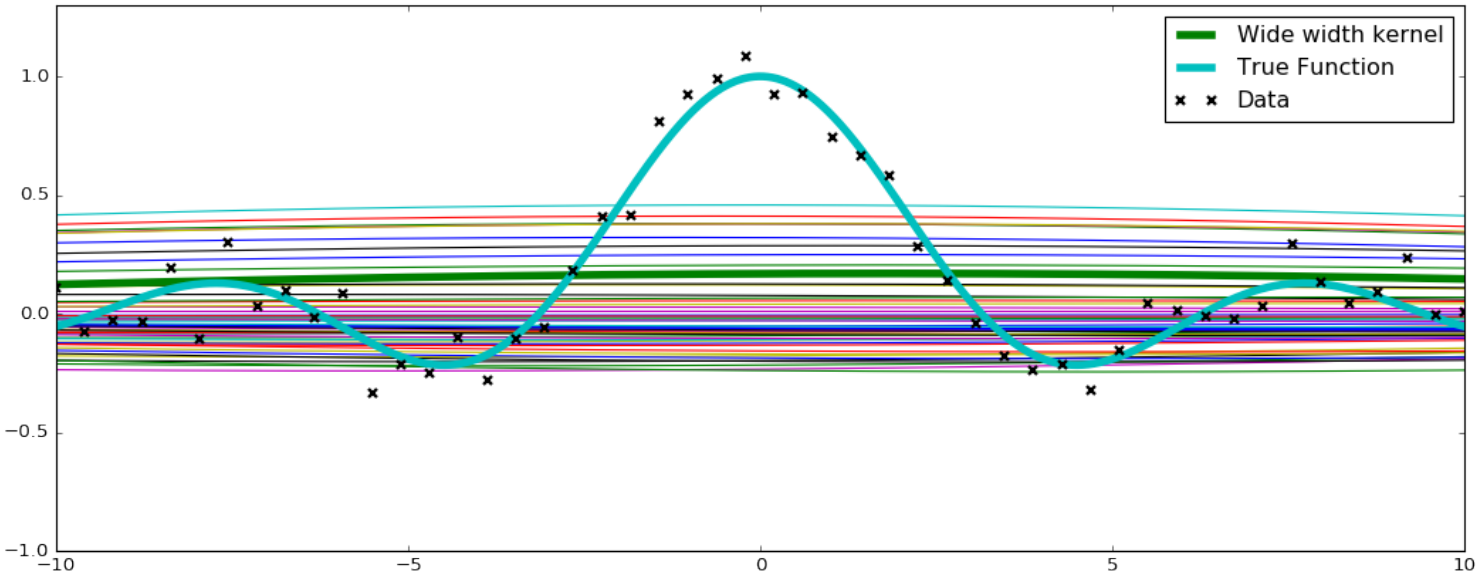
$$\kappa(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$$

As with the choice of degree in polynomial basis expansion, depending on the width of the kernel, overfitting or underfitting may occur

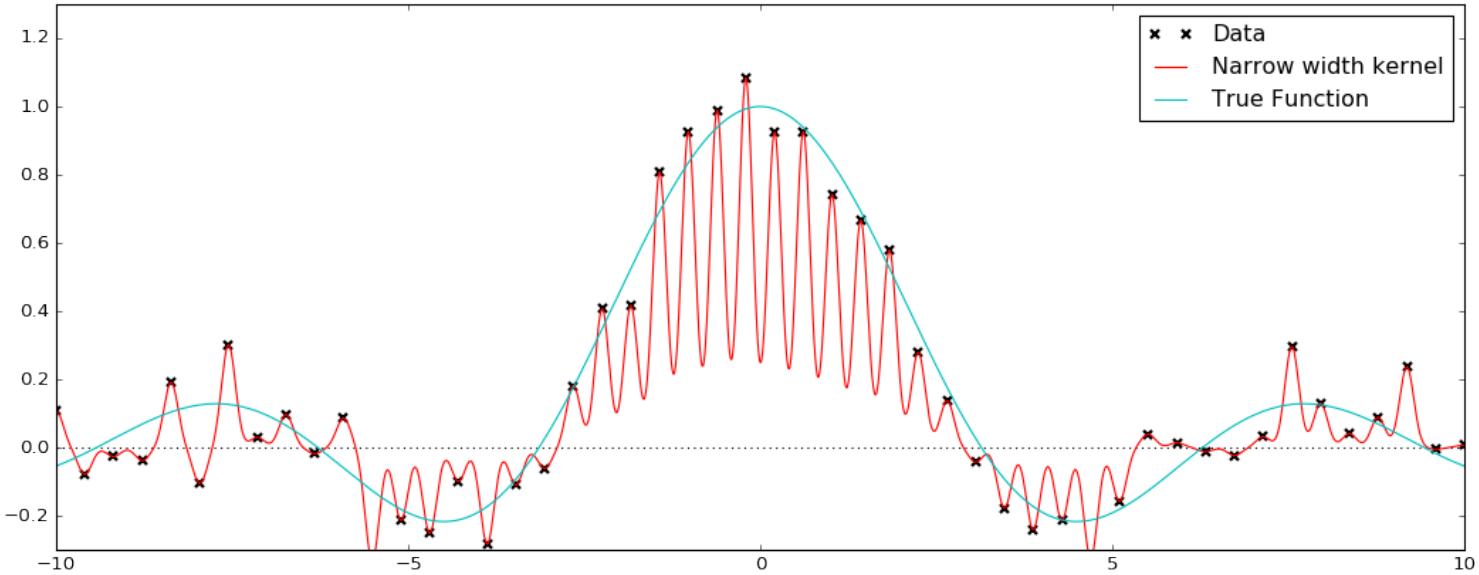
- Overfitting occurs if the width is too small, *i.e.*, γ very large
- Underfitting occurs if the width is too large, *i.e.*, γ very small

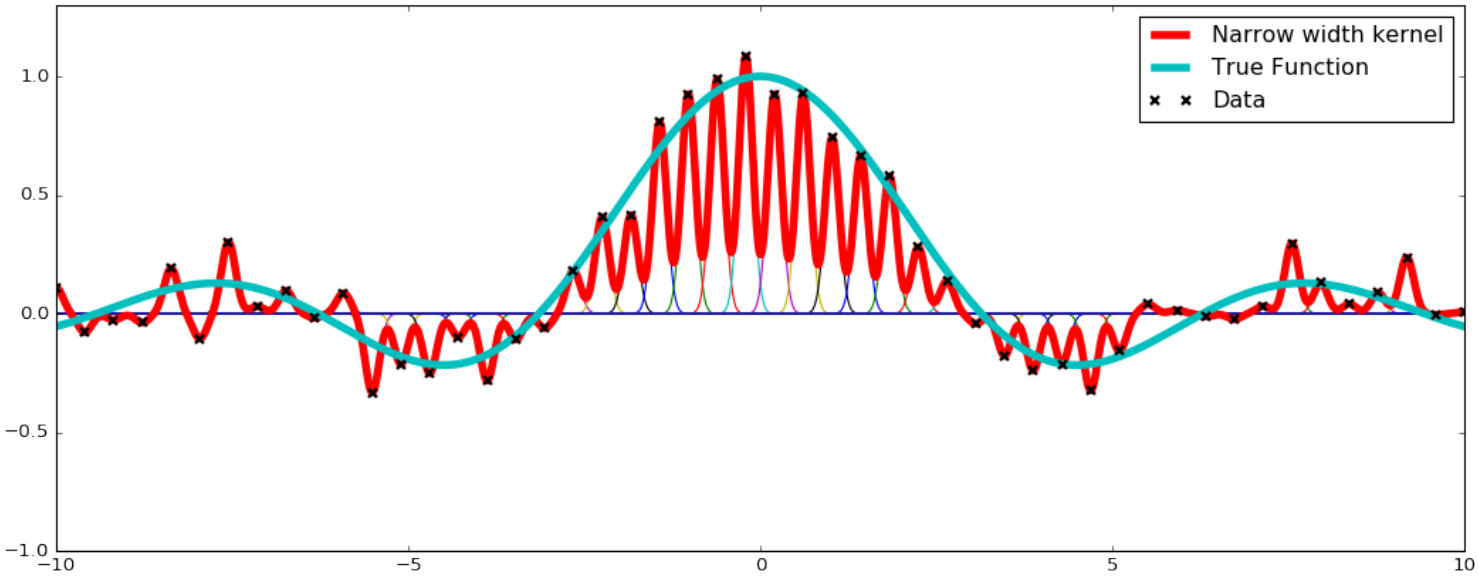
When the kernel width is too large



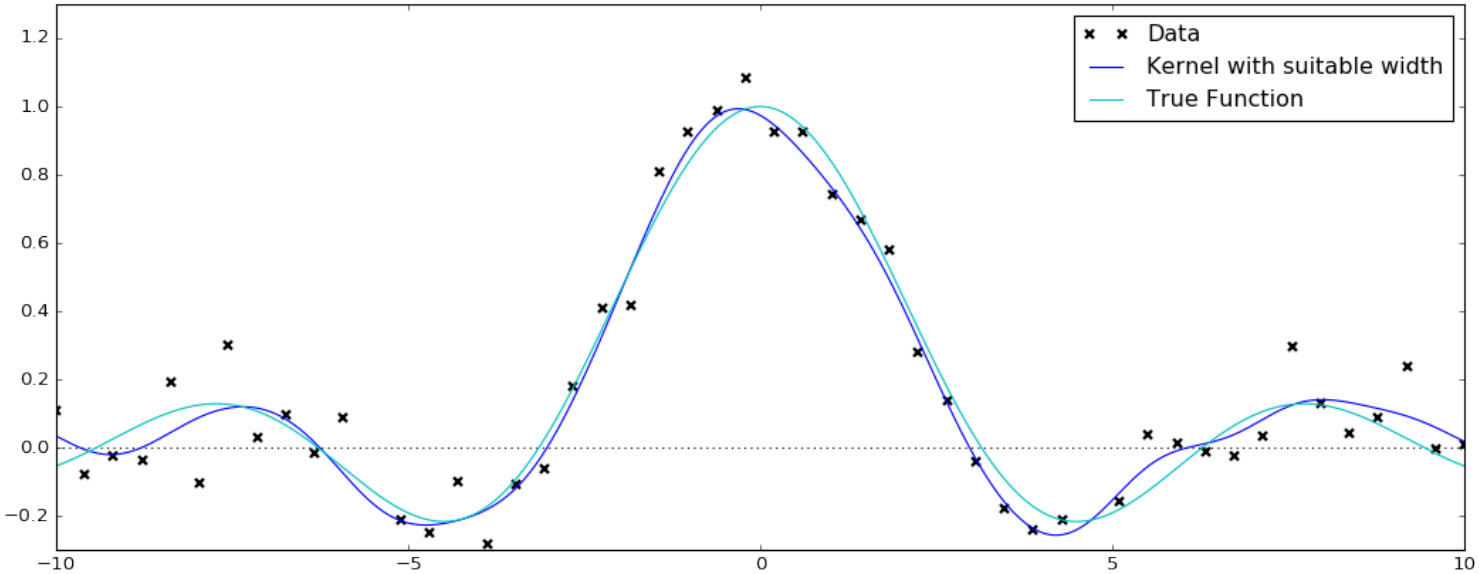


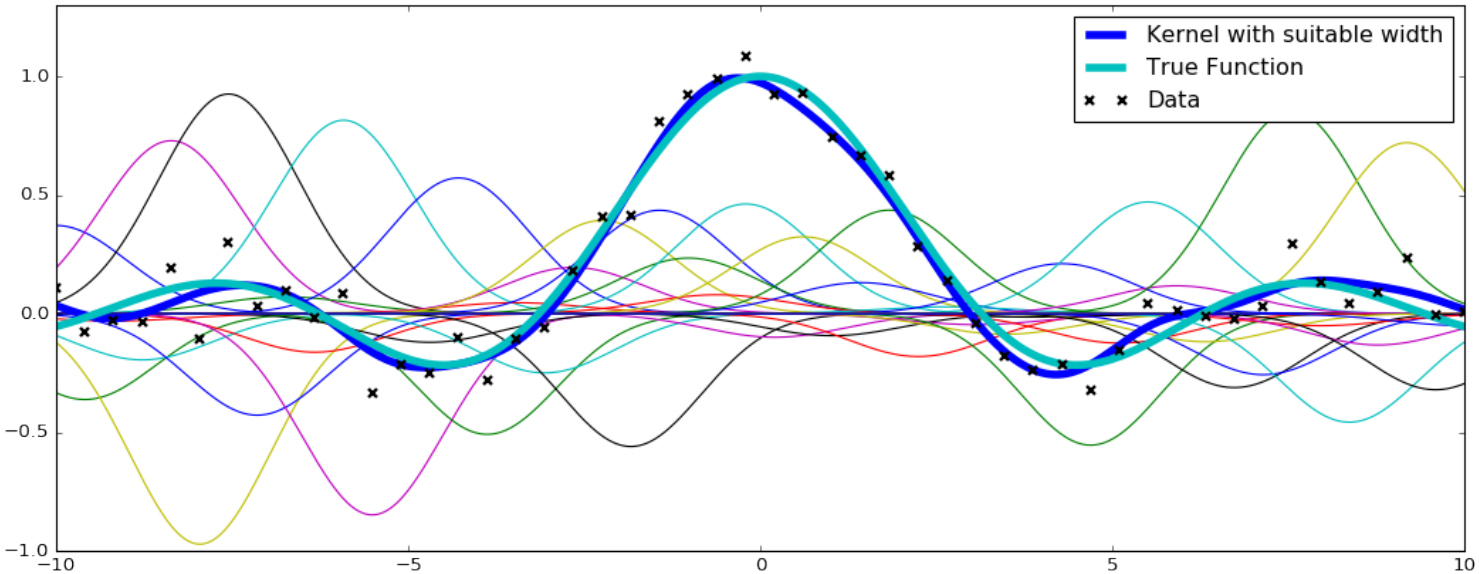
When the kernel width is too small



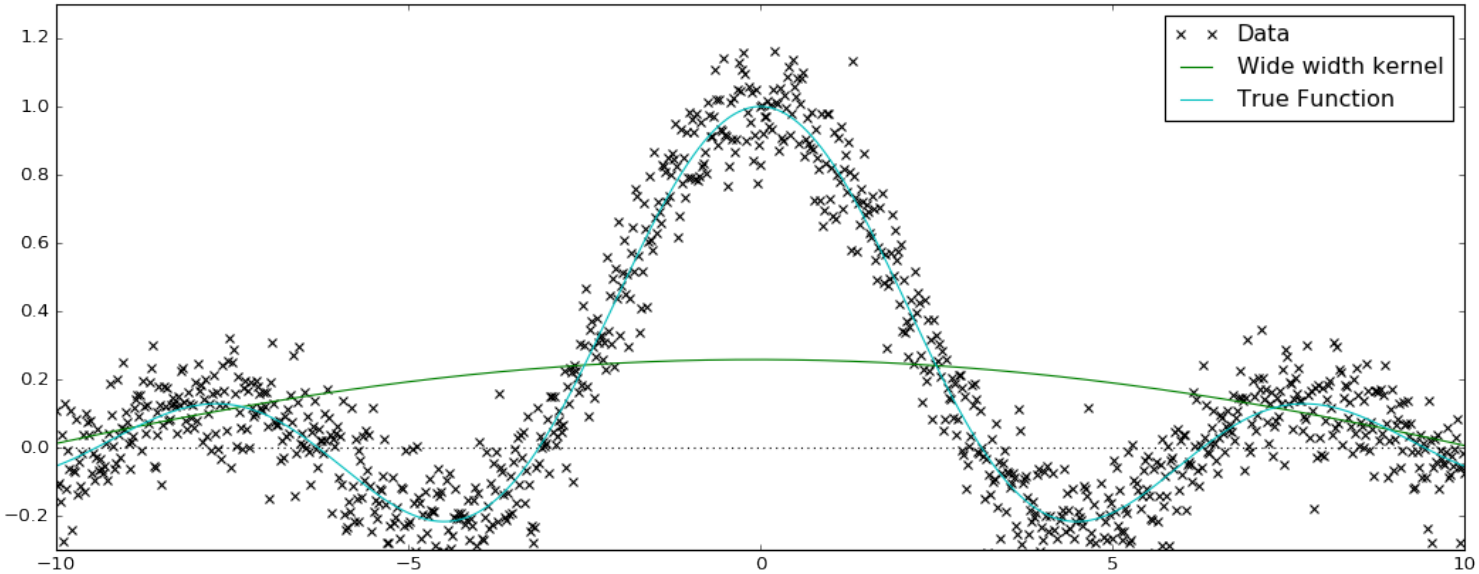


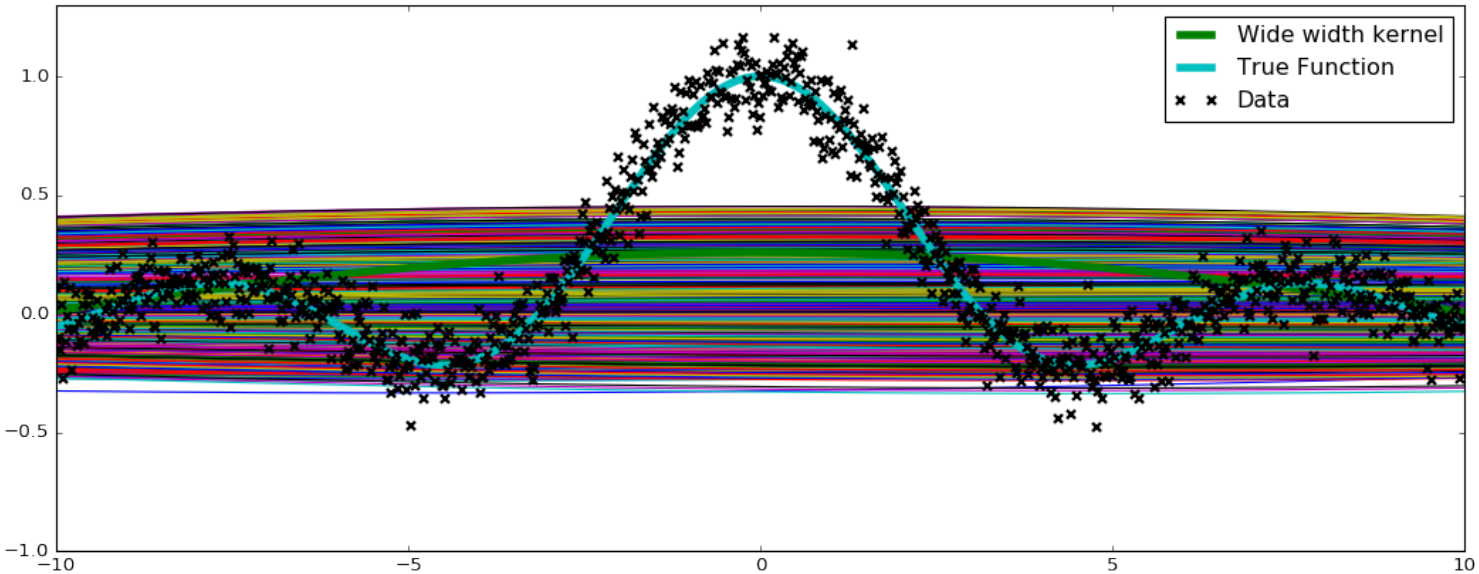
When the kernel width is chosen suitably





Big Data: When the kernel width is too large





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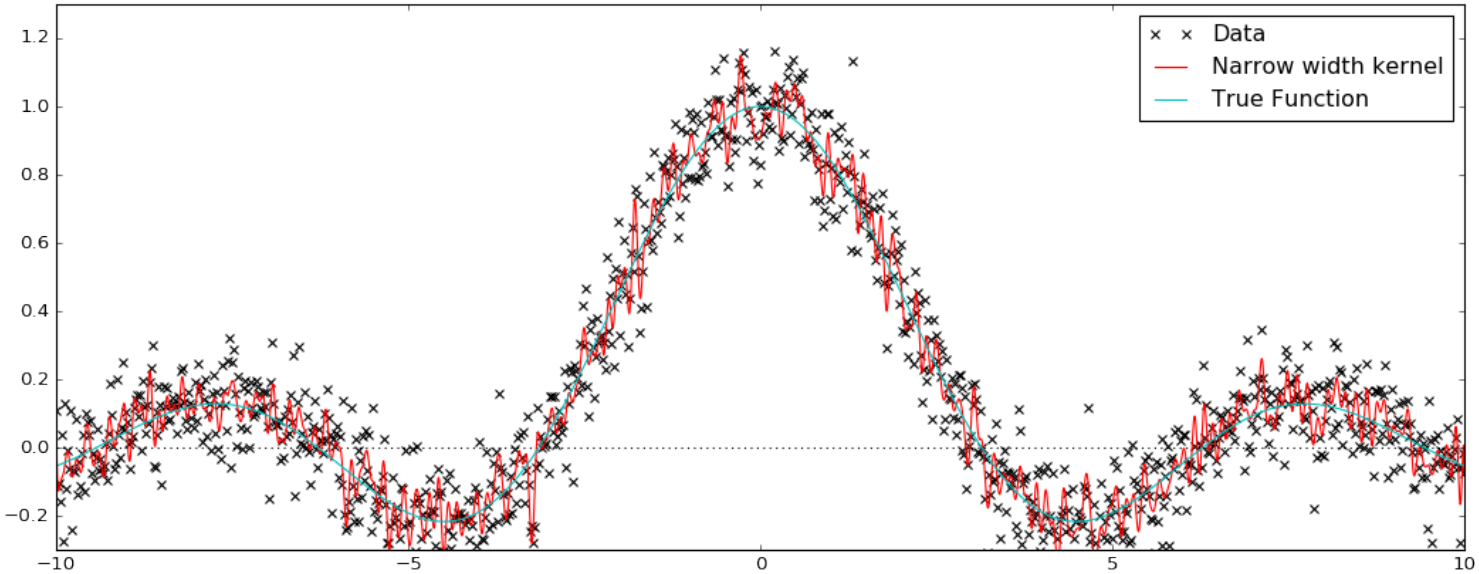

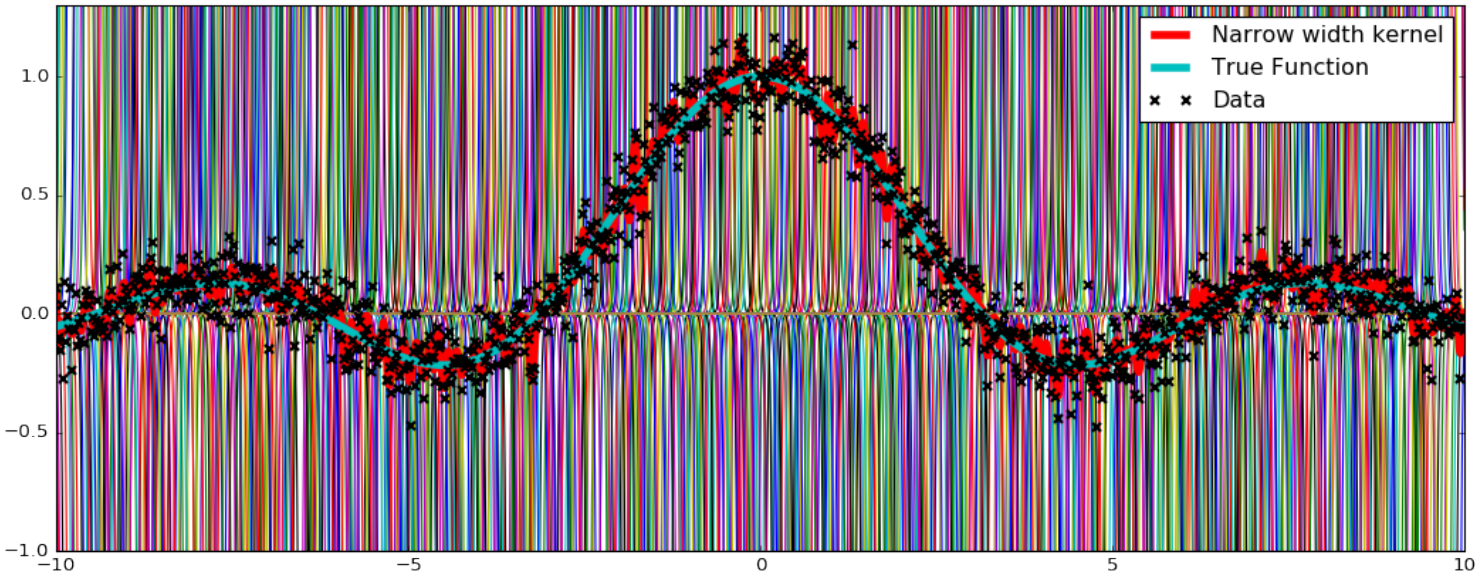

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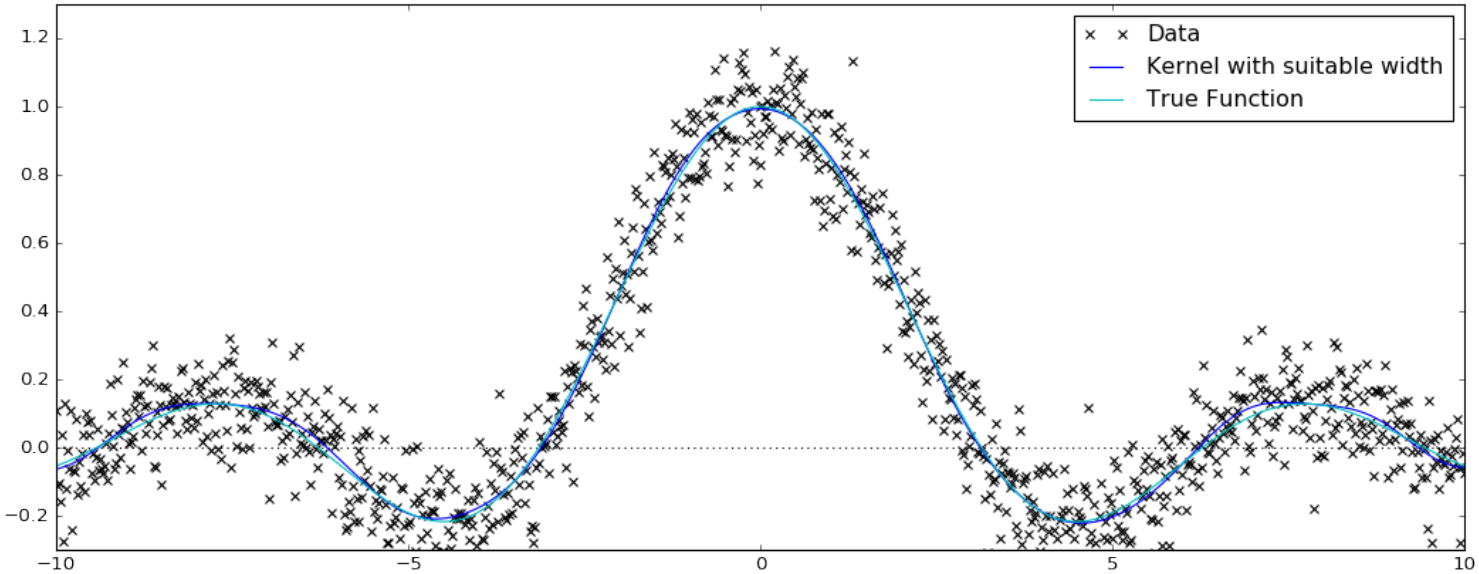

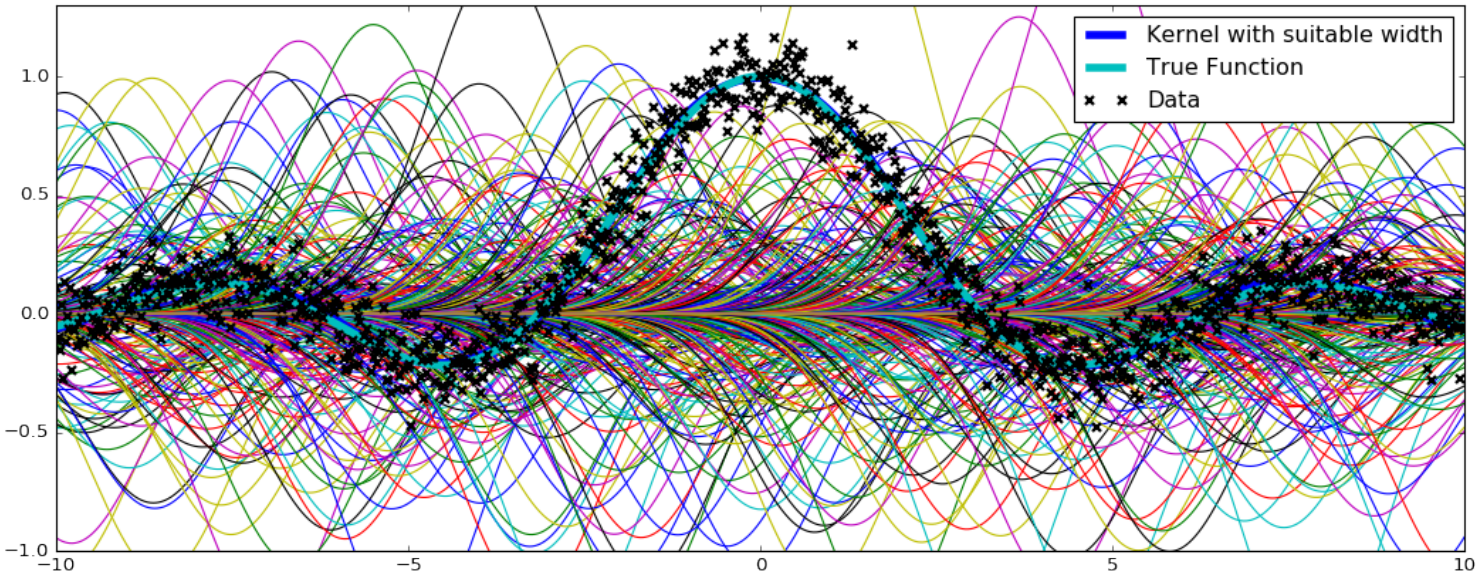

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- When the data lies in a high-dimensional space we may encounter the curse of dimensionality
  - If the width is too large then we may underfit
  - Might need exponentially large (in the dimension) sample for using modest width kernels
  - Connection to Problem 1 on Sheet 1

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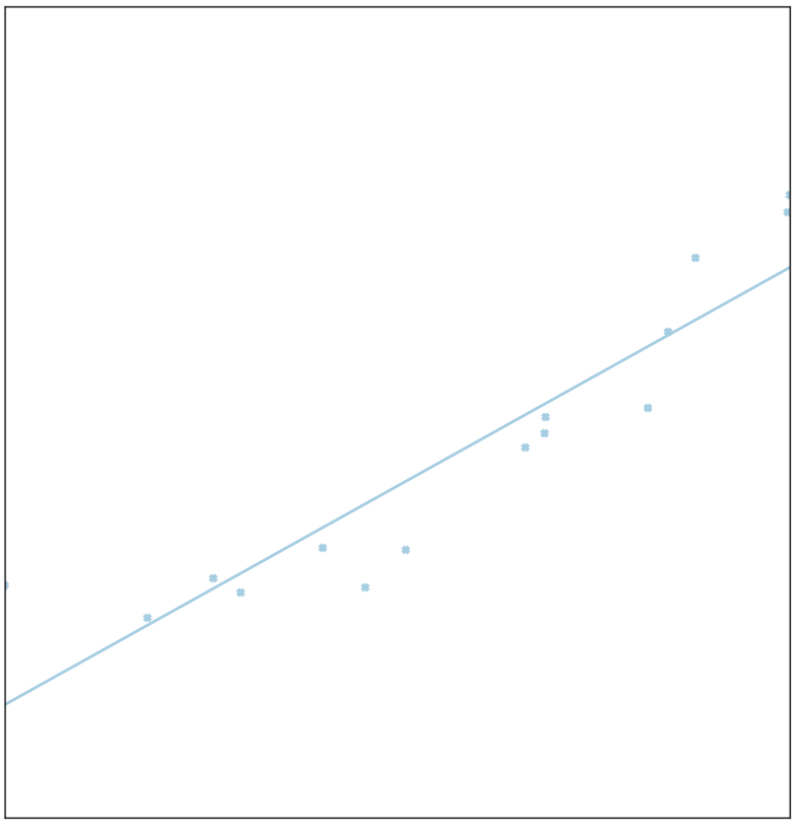
Basis Function Expansion

Overfitting and the Bias-Variance Tradeoff

Sources of Overfitting

The Bias Variance Tradeoff

High Bias



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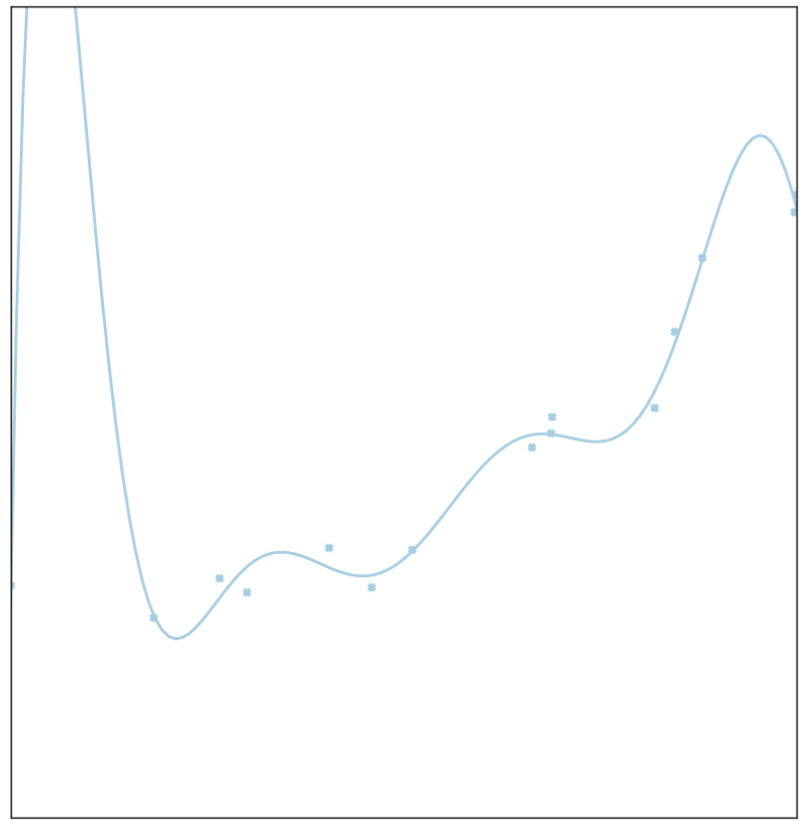

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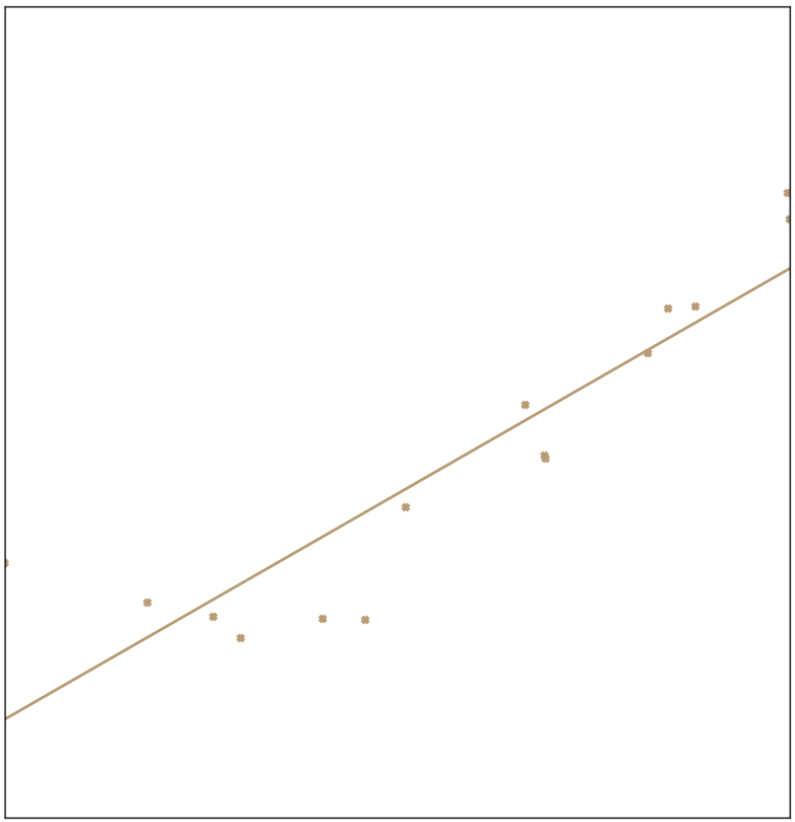

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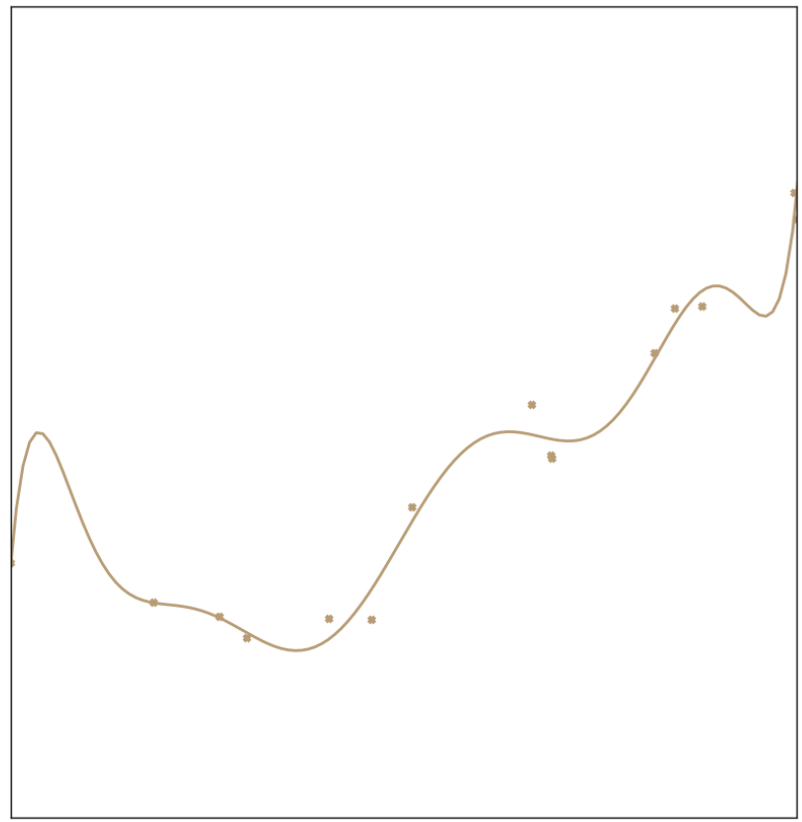

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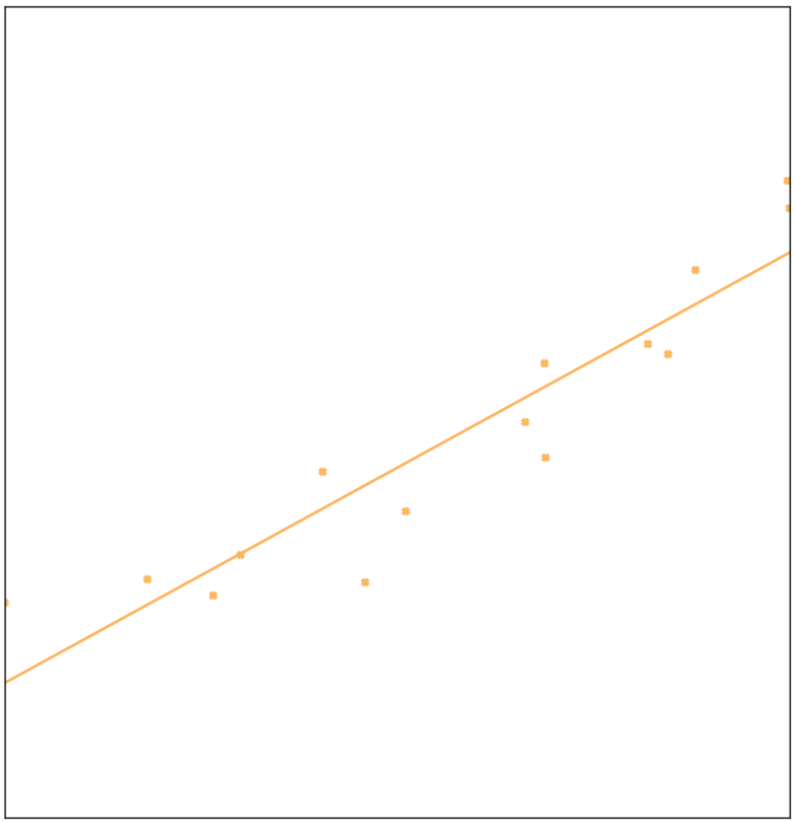

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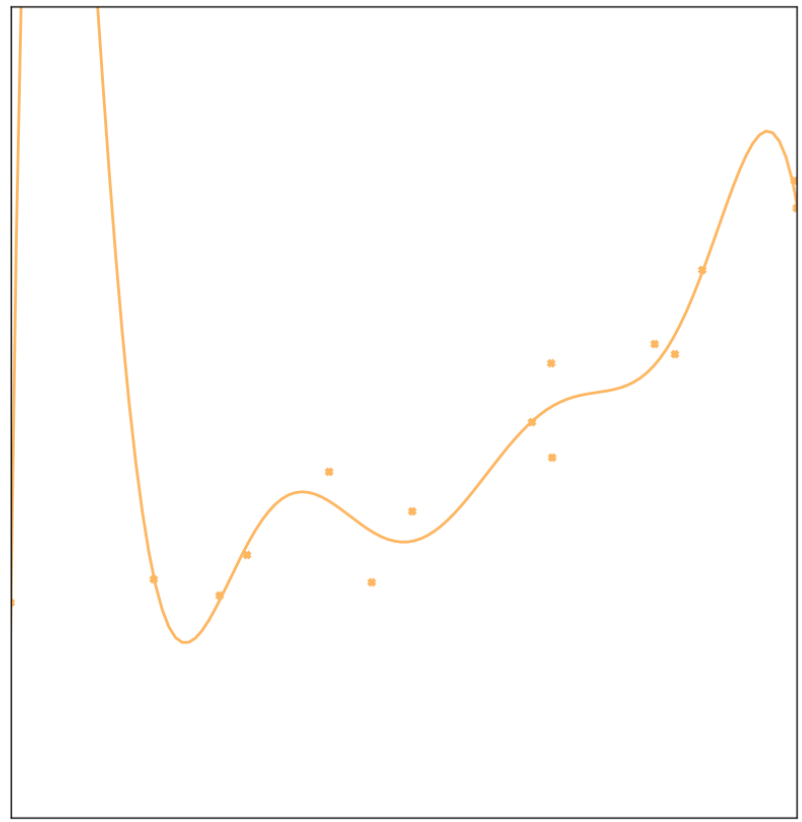

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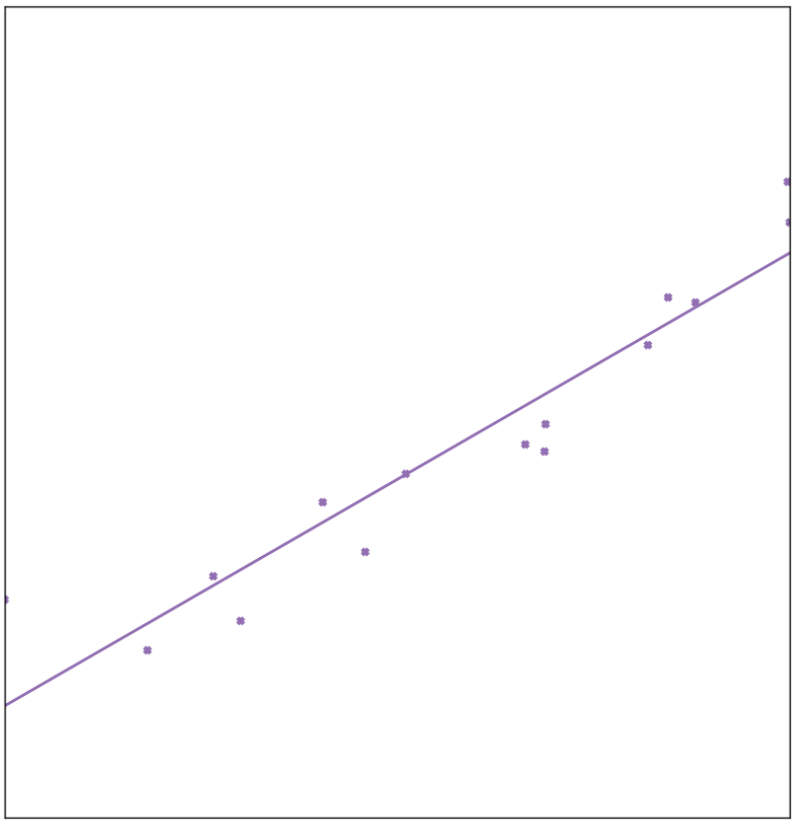

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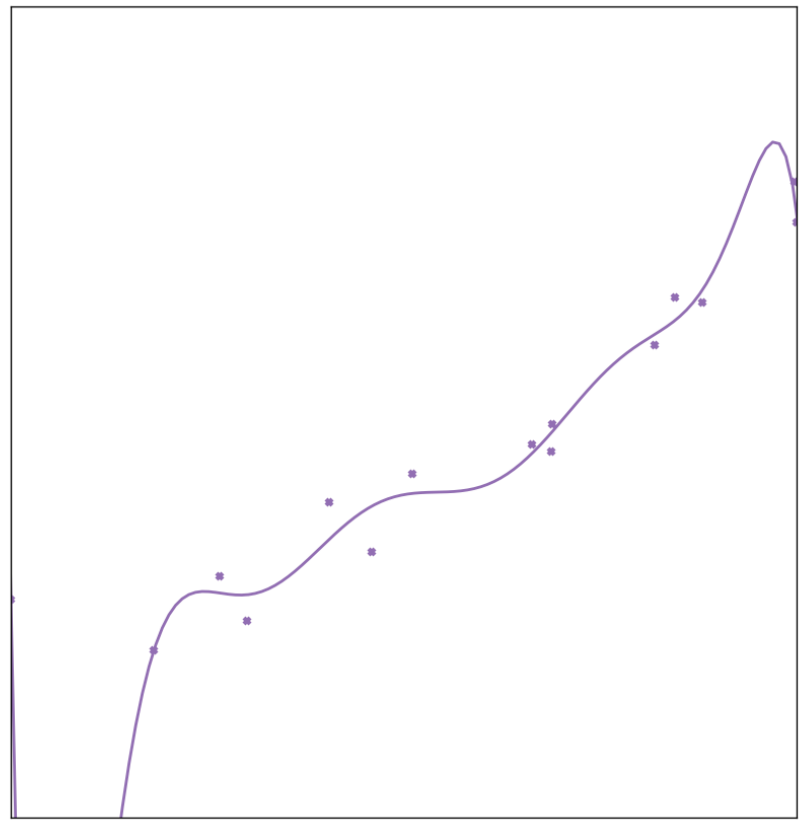

The Bias Variance Tradeoff

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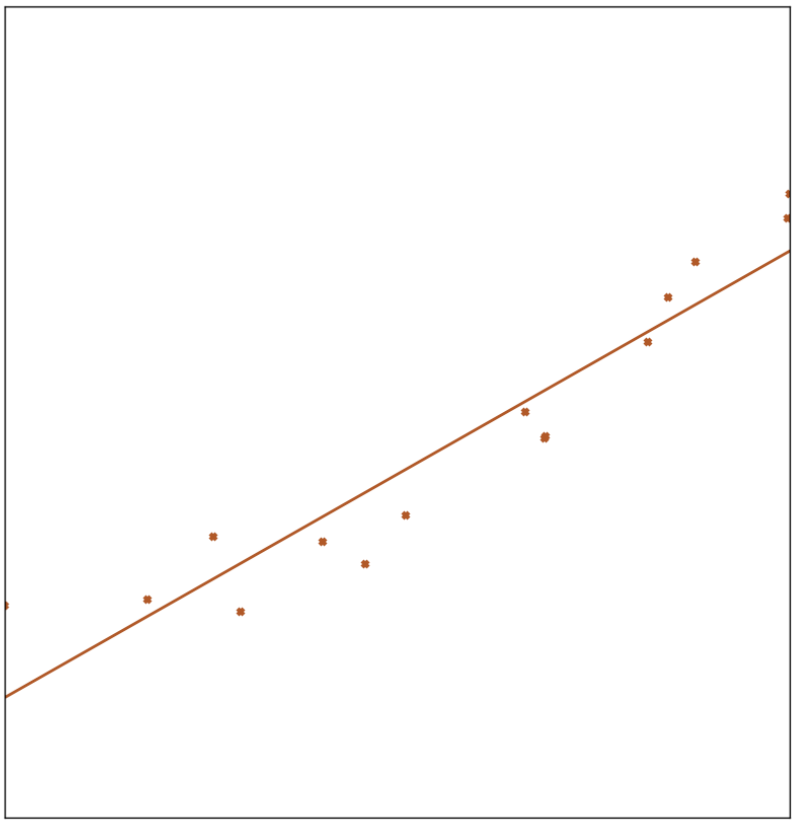

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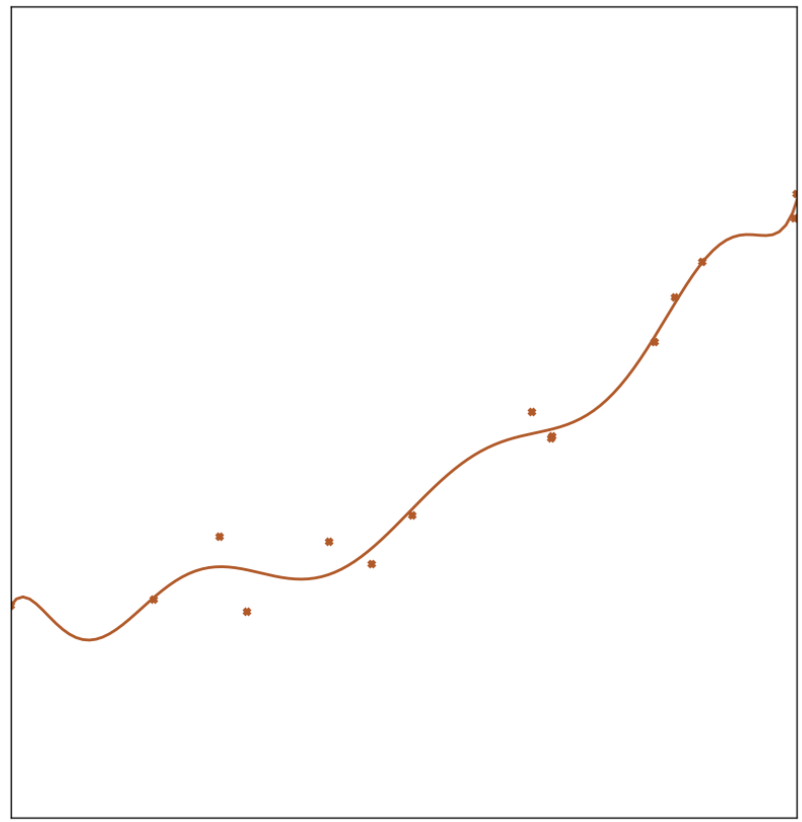
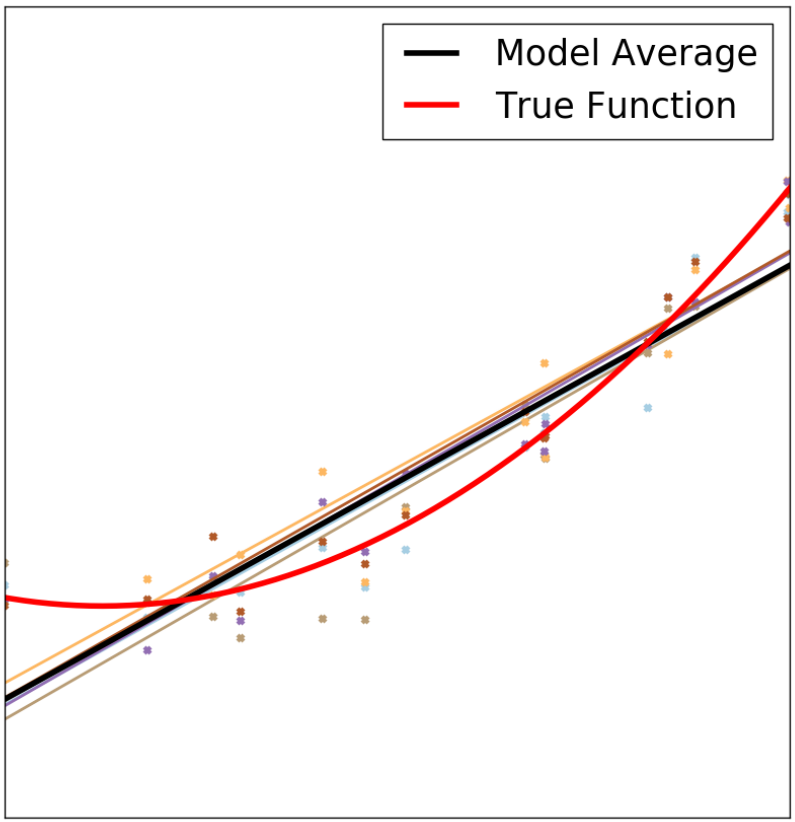


The Bias Variance Tradeoff

High Bias



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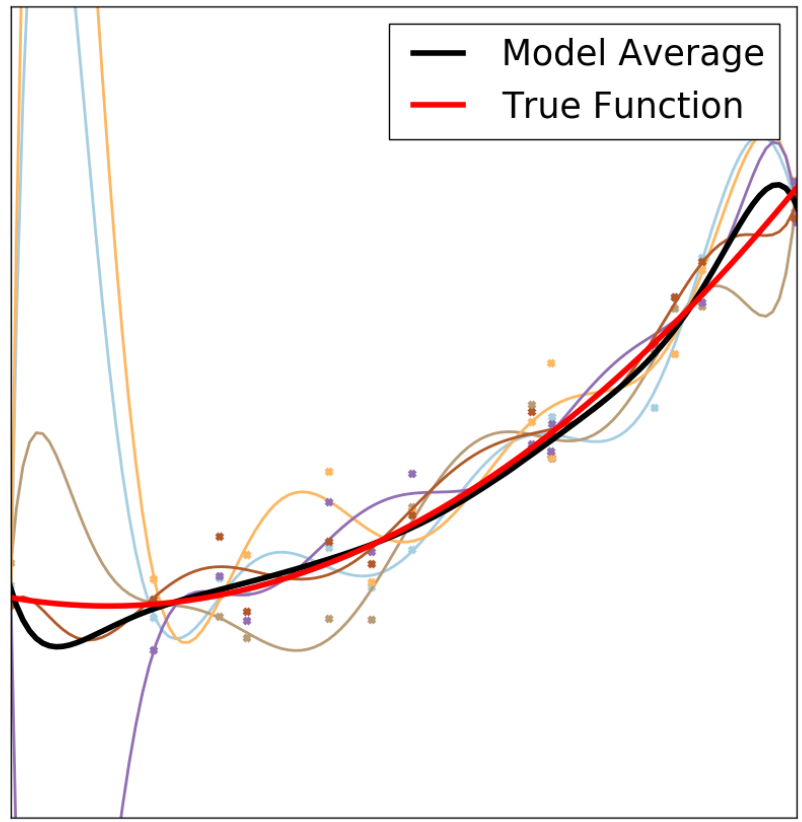

The Bias Variance Tradeoff

- Having high bias means that we are underfitting
- Having high variance means that we are overfitting
- The terms bias and variance in this context are precisely defined statistical notions
- See Problem Sheet 2, Q3 for precise calculations in one particular context
- See Sec. 5.4 in the GBC book for a much more detailed description

Learning Curves

Suppose we've trained a model and used it to make predictions

But in reality, the predictions are often poor

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  - Should we simplify the model (lower degree polynomials, larger width kernels, etc.) to reduce the number of parameters?
- Should we try and obtain more data?
  - Often there is a computational and monetary cost to using more data

Learning Curves

Split the data into a training set and testing set

Train on increasing sizes of data

Plot the training error and test error as a function of training data size

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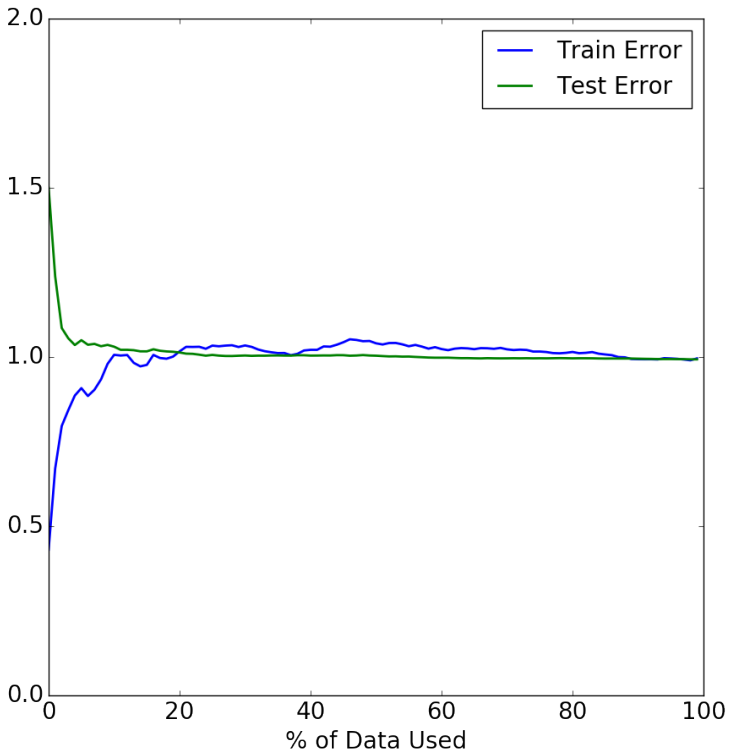

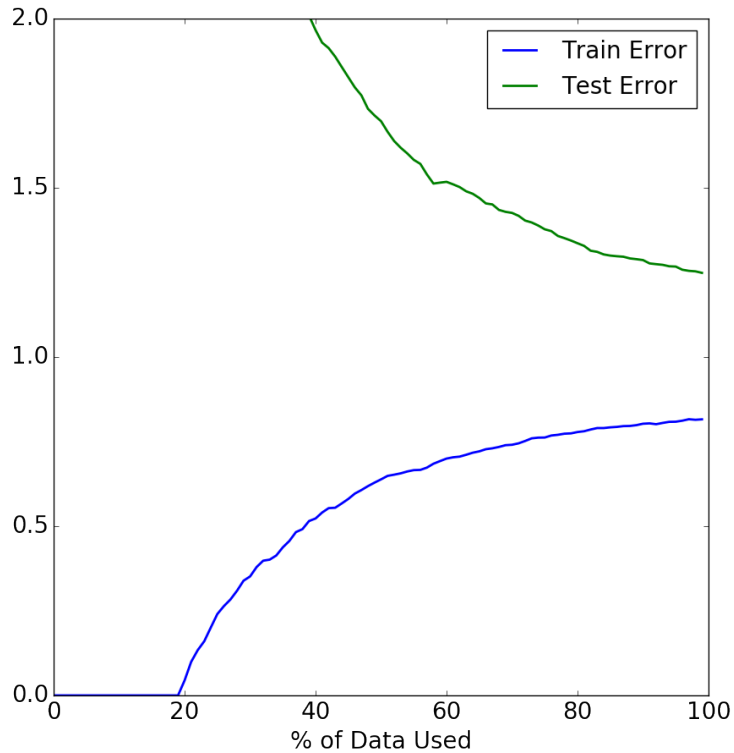

More data is not useful

More data would be useful

Outline

Basis Function Expansion

Overfitting and the Bias-Variance Tradeoff

Sources of Overfitting

Overfitting: How does it occur?

Overfitting: How does it occur?

When dealing with high-dimensional data (which may be caused by basis expansion) even for a linear model we have many parameters

With $D = 100$ input variables and using degree 10 polynomial basis expansion we have $\sim 10^{20}$ parameters!

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Enrico Fermi to Freeman Dyson

"I remember my friend Johnny von Neumann used to say, with four parameters I can fit an elephant, and with five I can make him wiggle his trunk."

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Suppose we have $D = 100$ and $N = 100$ so that $\mathbf{X}$ is 100×100

Suppose every entry of $\mathbf{X}$ is drawn from $\mathcal{N}(0, 1)$

And let $y_i \sim x_{i,1} + \mathcal{N}(0, \sigma^2)$, for $\sigma = 0.2$

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