# Lecture 6

## Linear Regression

Luigi Freda

ALCOR Lab
DIAG
University of Rome "La Sapienza"

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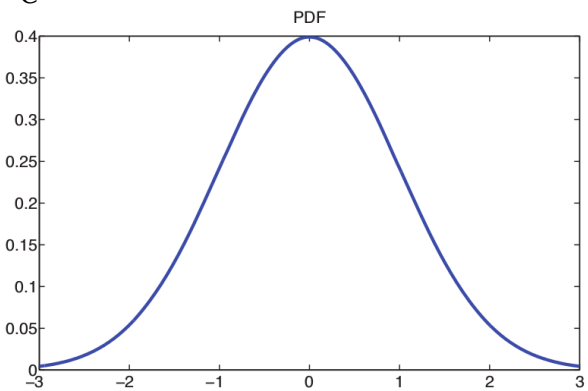
# Outline

# Outline

**Linear Regression**

$$y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + \epsilon = \sum_{j=1}^{D} w_j x_j + \epsilon$$




- $y \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^D$
- $\mathbf{w} \in \mathbb{R}^D$ is the **weight vector**
- $\epsilon \sim \mathcal{N}(0, \sigma^2)$ is the **residual error**

This entails

$$p(y|\mathbf{x}, \theta) = \mathcal{N}(\mu(\mathbf{x}), \sigma^2) = \mathcal{N}(\mathbf{w}^T\mathbf{x}, \sigma^2)$$

- $\mu(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = [w_0, \tilde{\mathbf{w}}^T\tilde{\mathbf{x}}]^T$ where $\mathbf{x} = [1, \tilde{\mathbf{x}}]^T$
- $\boldsymbol{\theta} = (\mathbf{w}, \sigma^2)$ are the **model parameters**

**Polynomial Regression**

if we replace $\mathbf{x}$ by a non-linear function $\phi(\mathbf{x})$

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

we now have

$$p(y|\mathbf{x}, \theta) = \mathcal{N}(\mathbf{w}^T \phi(\mathbf{x}), \sigma^2)$$

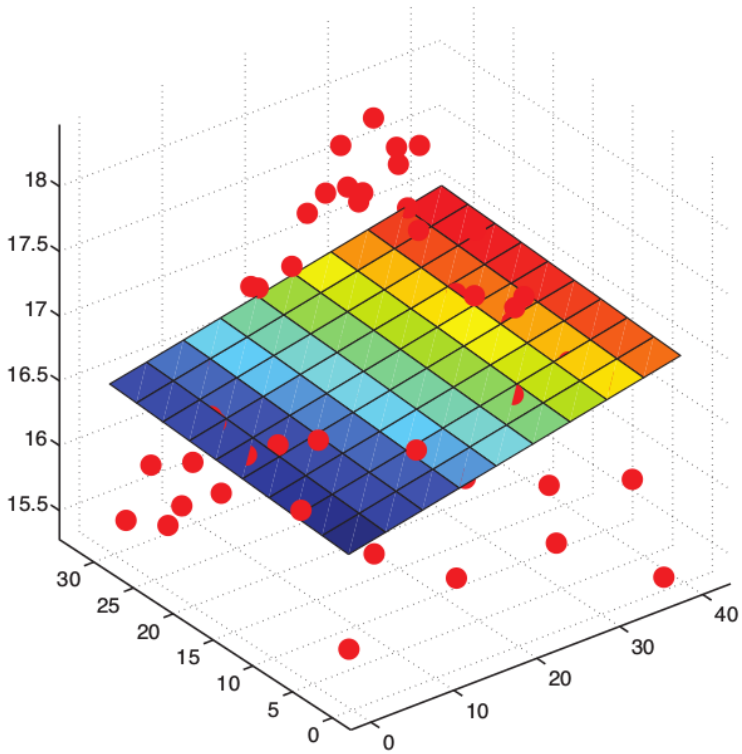
- $\mu(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$ (**basis function expansion**)
- if $x \in \mathbb{R}$ we can use $\phi(x) = [1, x, x^2, ..., x^d]$ which is the vector of **polynomial basis functions**
- in general if $\mathbf{x} \in \mathbb{R}^D$ we can use a **multivariate polynomial expansion** $\mathbf{w}^T \phi(\mathbf{x}) = \sum w_{i_1 i_2 \ldots i_D} \prod_{j=1}^{D} x_j^{i_j}$ up to a certain degree $d$
- $\boldsymbol{\theta} = (\mathbf{w}, \sigma^2)$ are the **model parameters**

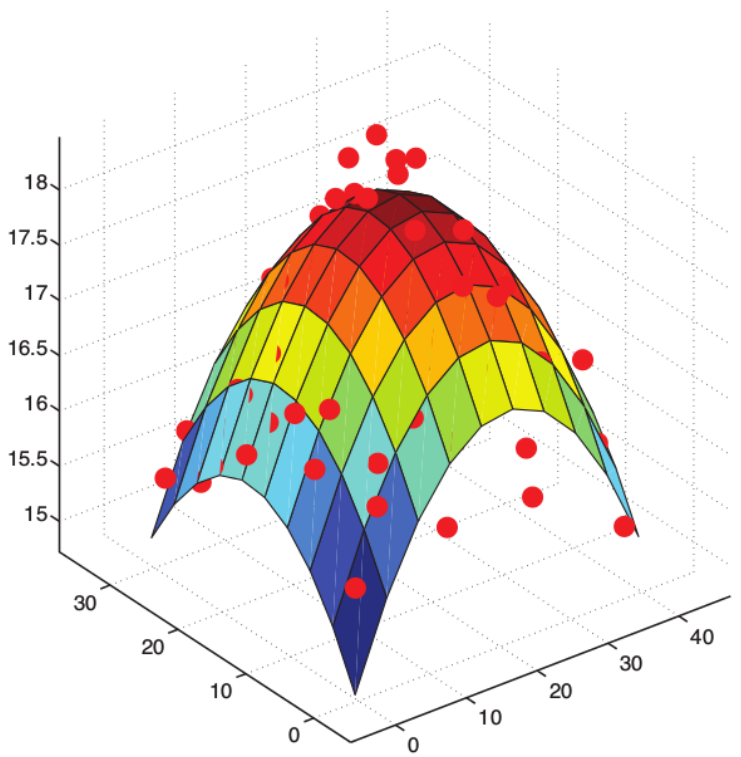
N.B.: note that the model is still linear in the parameters $\mathbf{w}$

# Linear Regression

## 2D Data

vertical axis is the temperature, horizontal axes are location within a room




- *left*: fitted function is a plane $\hat{f}(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2$
- *right*: fitted function is quadratic $\hat{f}(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2$

# Outline

# MLE - Least Squares

- the MLE of a parameter $\boldsymbol{\theta}$ is computed as

$$\hat{\boldsymbol{\theta}}_{MLE} \triangleq \underset{\theta}{\text{argmax}}\ p(\mathcal{D}|\boldsymbol{\theta})$$

- given a dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$ of iid samples, the **log-likelihood** can be computed as

$$l(\boldsymbol{\theta}) \triangleq \log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \boldsymbol{\theta})$$

- maximizing the log-likelihood is equivalent to minimize the **Negative Log-Likelihood** (NLL)

$$\text{NLL}(\boldsymbol{\theta}) \triangleq -\sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \boldsymbol{\theta})$$

# MLE - Least Squares

- inserting the linear regression model into the log-likelihood returns

$$l(\boldsymbol{\theta}) = \sum_{i=1}^{N} \log \left[ \left( \frac{1}{2\pi\sigma^2} \right)^{\frac{1}{2}} \exp \left( -\frac{1}{2\sigma^2} (y_i - \mathbf{w}^T \mathbf{x}_i)^2 \right) \right] =$$

$$= -\frac{\text{RSS}(\mathbf{w})}{2\sigma^2} - \frac{N}{2} \log(2\pi\sigma^2)$$

  where RSS stands for **Residual Sum of Squares**

$$\text{RSS}(\mathbf{w}) \triangleq \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

  aka **Sum of Squared Errors** (SSE), i.e SSE = RSS

- the Mean Squared Error (MSE) is MSE $\triangleq$ SSE$/N$

# MLE - Least Squares

- the log-likelihood is

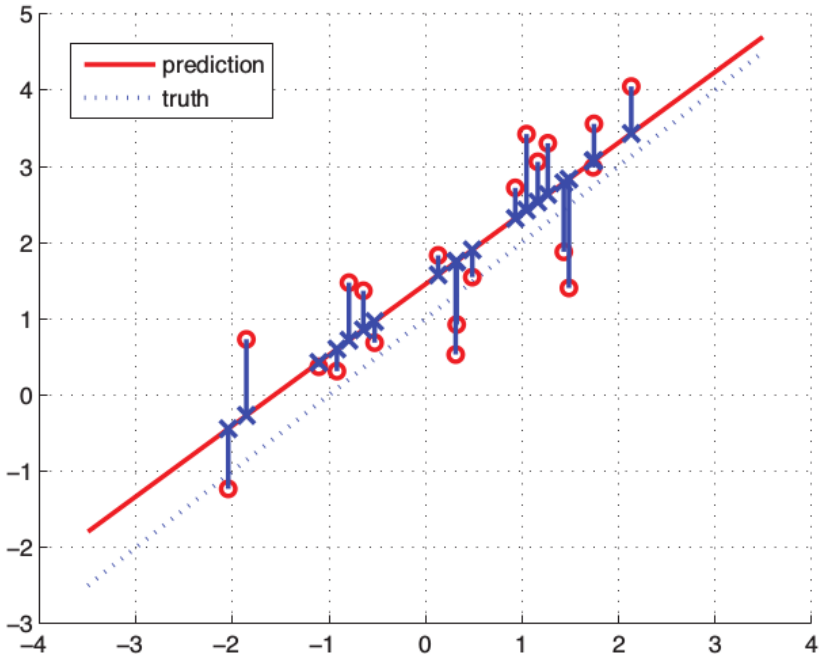
$$l(\boldsymbol{\theta}) = -\frac{\text{RSS}(\mathbf{w})}{2\sigma^2} - \frac{N}{2}\log(2\pi\sigma^2)$$

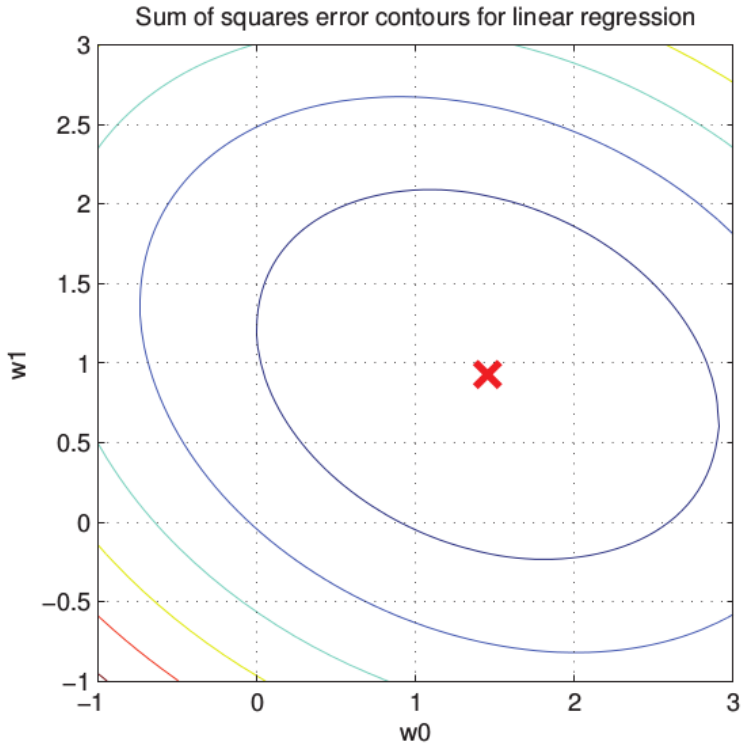
- if we define the **residual errors** $\epsilon_i \triangleq y_i - \mathbf{w}^T\mathbf{x}_i$, one has

$$\text{RSS}(\mathbf{w}) = \|\boldsymbol{\epsilon}\|_2^2 = \sum_{i=1}^{N} \epsilon_i^2$$

- the MLE for $\mathbf{w}$ minimizes the RSS, and for this reason the method is called **least squares**

# MLE - Least Squares




- *left*: red circles are training points; blue crosses are approximations
- in least squares we try to minimize the sum of squared distances from each training point to its approximation (i.e. the sum of the lengths of the little vertical blue lines)
- *right*: contours of the RSS error; the surface is a **bowl** with a **unique minimum**

# Outline

# Derivation of the MLE

- the NLL can be rewritten as

$$\text{NLL}(\mathbf{w}) = \frac{1}{2}\|\mathbf{y}-\mathbf{X}\mathbf{w}\|^2 = \frac{1}{2}(\mathbf{y}-\mathbf{X}\mathbf{w})^T(\mathbf{y}-\mathbf{X}\mathbf{w}) = \frac{1}{2}\mathbf{w}^T(\mathbf{X}^T\mathbf{X})\mathbf{w}-\mathbf{w}^T(\mathbf{X}^T\mathbf{y})+\frac{1}{2}\mathbf{y}^T\mathbf{y}$$

  where $\mathbf{y} = [y_1, ..., y_N]^T \in \mathbb{R}^N$, $\mathbf{X} \in \mathbb{R}^{N\times D}$ is the design matrix

- in order to minimize the NLL we have to compute its gradient

$$\mathbf{g}(\mathbf{w}) = (\mathbf{X}^T\mathbf{X})\mathbf{w} - (\mathbf{X}^T\mathbf{y})$$

  and equating it to zero we get the **normal equation**

$$\mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$$

- the corresponding solution is called the **Ordinary Least Squares** (OLS)

$$\hat{\mathbf{w}}_{OLS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- considering that $\mathbf{X}^T\mathbf{X} = \sum_{i=1}^N \mathbf{x}_i\mathbf{x}_i^T$ and $\mathbf{X}^T\mathbf{y} = \sum_i \mathbf{x}_i y_i$, one has

$$\hat{\mathbf{w}}_{OLS} = (\sum_{i=1}^N \mathbf{x}_i\mathbf{x}_i^T)^{-1}\sum_i \mathbf{x}_i y_i$$

# Outline

# Geometric Interpretation

## Least Squares

- let's consider the optimization problem we solve

$$\hat{\mathbf{w}}_{OLS} = \underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2$$

- this optimization problem is equivalent to solve the **normal equation**

$$\mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$$

- these equations have an elegant geometric interpretation

- the columns of $\mathbf{X} = [\tilde{\mathbf{x}}_1, ..., \tilde{\mathbf{x}}_D] \in \mathbb{R}^{N \times D}$ define a linear subspace in $\mathbb{R}^N$
- N.B.: the columns $\tilde{\mathbf{x}}_j \in \mathbb{R}^N$ of $\mathbf{X}$ are different from the rows $\mathbf{x}_i \in \mathbb{R}^D$ of $\mathbf{X}$
- the vector $\mathbf{y}$ lives in $\mathbb{R}^N$
- the least squares problem above is equivalent to

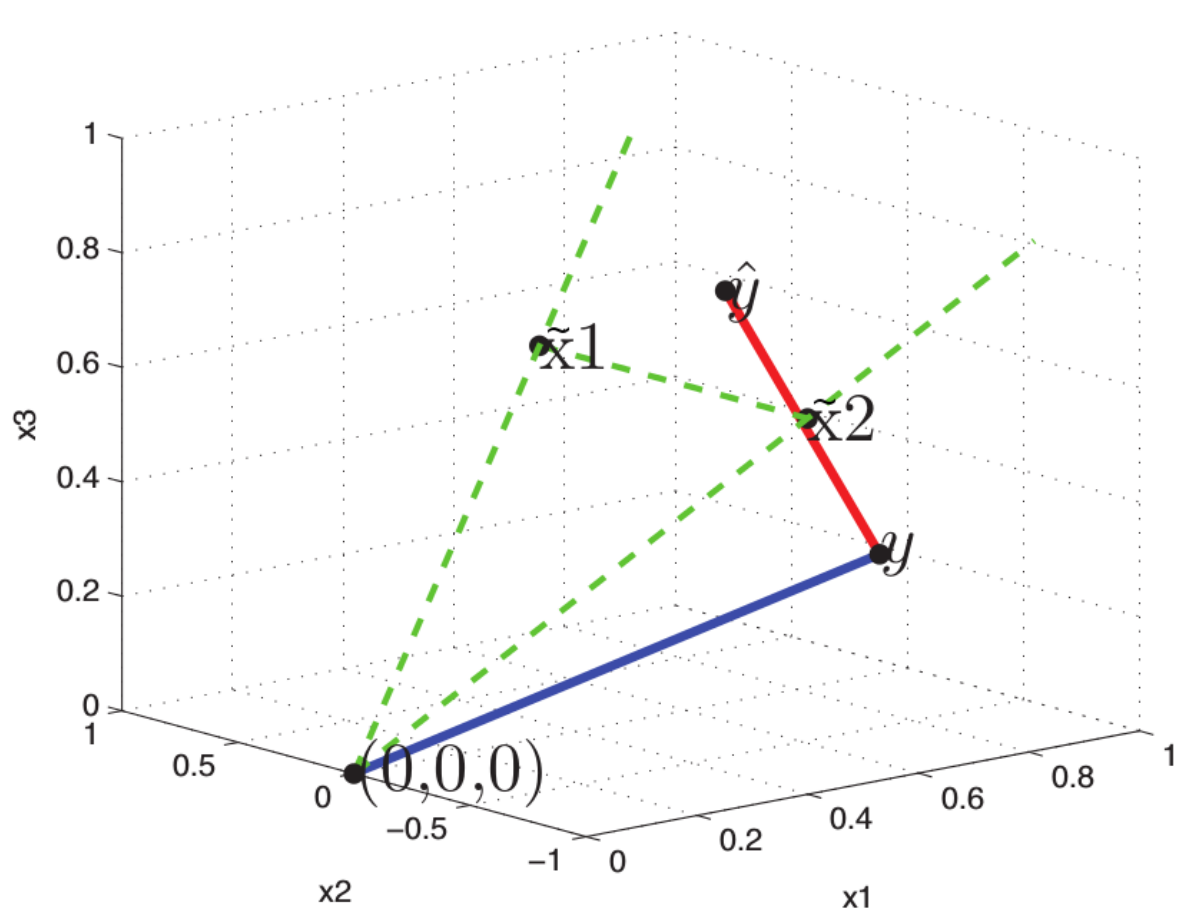
$$\underset{\hat{\mathbf{y}} \in \text{span}(\{\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_D\})}{\operatorname{argmin}} \frac{1}{2}\|\mathbf{y} - \hat{\mathbf{y}}\|^2 \qquad (\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = w_1\tilde{\mathbf{x}}_1 + ... + w_D\tilde{\mathbf{x}}_D)$$

# Geometric Interpretation

## Least Squares

- let's assume $N = 3$ and $D = 2$

$$\mathbf{X} = \begin{bmatrix} 1 & 2 \\ 1 & -2 \\ 1 & 2 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 8.89 \\ 0.61 \\ 1.77 \end{bmatrix}$$

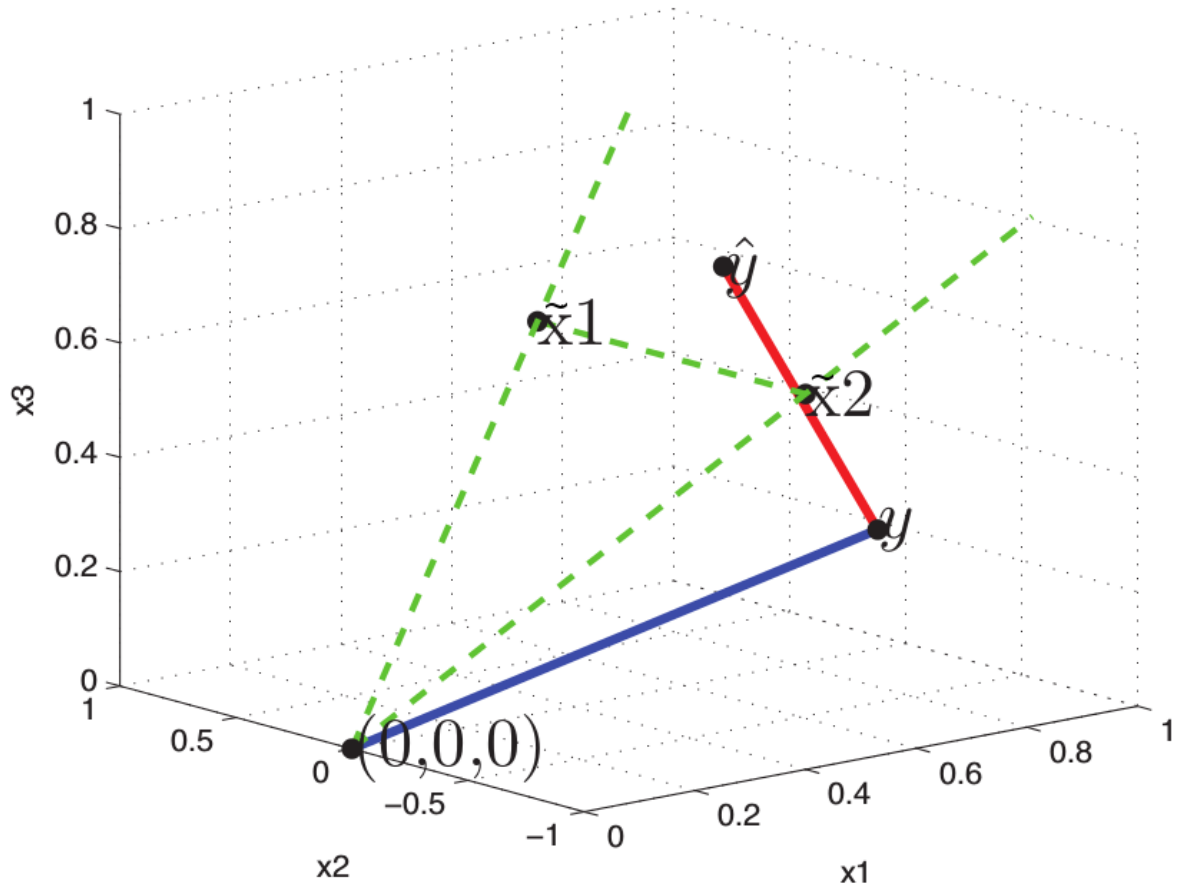


# Geometric Interpretation

## Least Squares

- we seek a vector $\hat{\mathbf{y}} \in \mathbb{R}^N$ that lies in the linear subspace defined by the columns of $\mathbf{X}$ and is close as possible to $\mathbf{y} \in \mathbb{R}^N$

$$\underset{\hat{\mathbf{y}} \in \text{span}(\{\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_D\})}{\text{argmin}} \quad \frac{1}{2}\|\mathbf{y} - \hat{\mathbf{y}}\|^2 \qquad (\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = w_1\tilde{\mathbf{x}}_1 + \ldots + w_D\tilde{\mathbf{x}}_D)$$

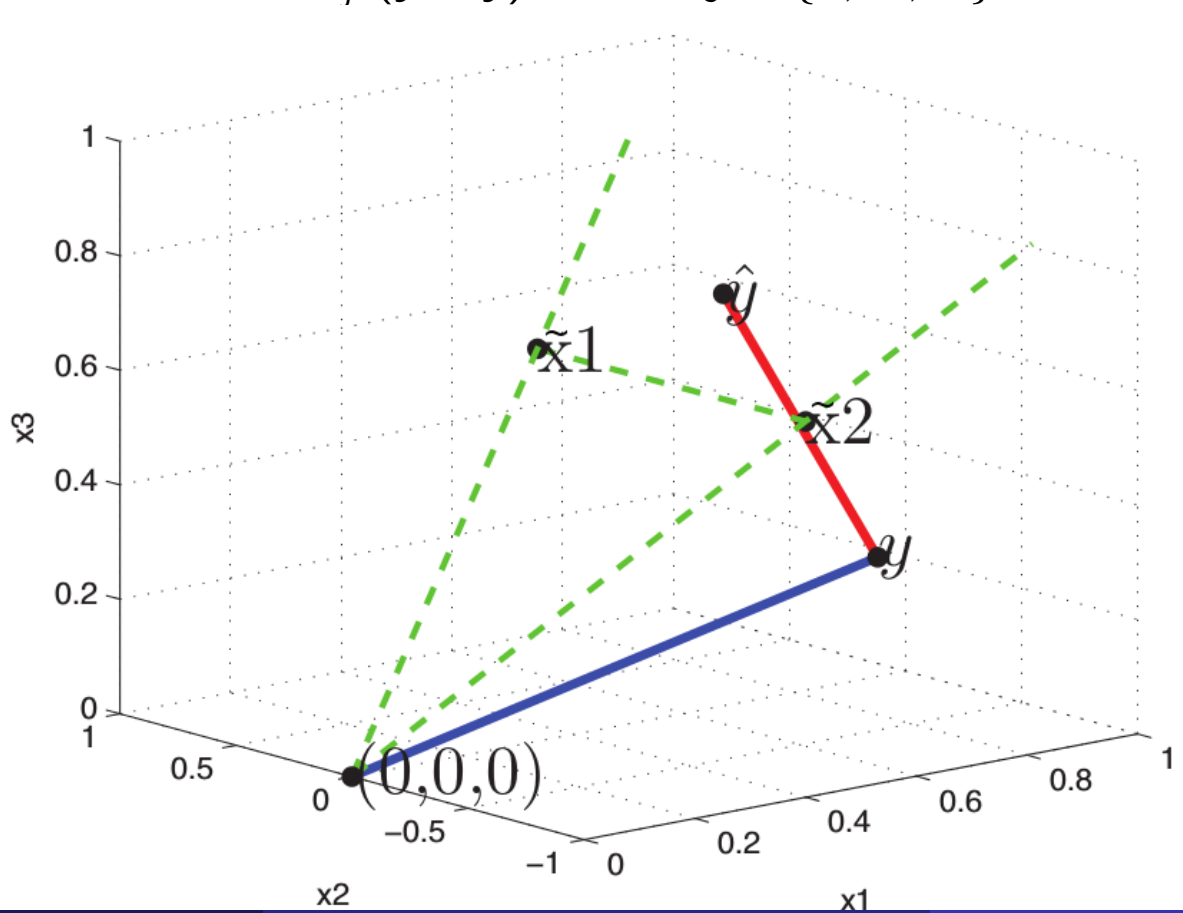


# Geometric Interpretation

## Least Squares

- if we want to minimize the residual $\underset{\hat{\mathbf{y}} \in \text{span}(\{\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_D\})}{\text{argmin}} \frac{1}{2}\|\mathbf{y} - \hat{\mathbf{y}}\|^2$ then we also want the residual vector $\mathbf{y} - \hat{\mathbf{y}}$ to be orthogonal to the linear space (hyperplane) defined by the columns of $\mathbf{X}$

$$\tilde{\mathbf{x}}_j^T(\hat{\mathbf{y}} - \mathbf{y}) = 0 \text{ for } j \in \{1, \ldots, D\}$$

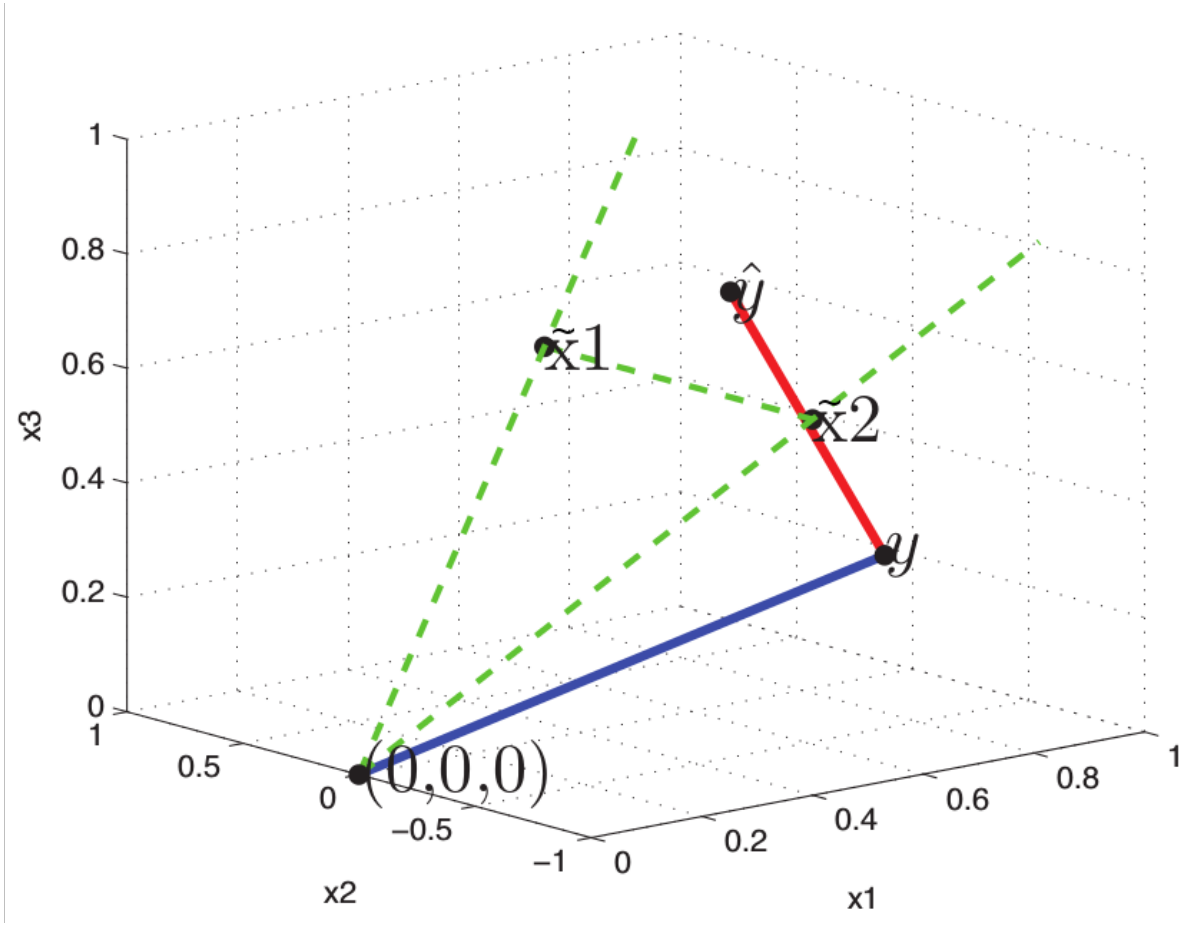


# Geometric Interpretation

## Least Squares

- hence, solving $\underset{\hat{\mathbf{y}} \in \text{span}(\{\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_D\})}{\text{argmin}} \frac{1}{2}\|\mathbf{y} - \hat{\mathbf{y}}\|^2$ is equivalent to solve the normal equation

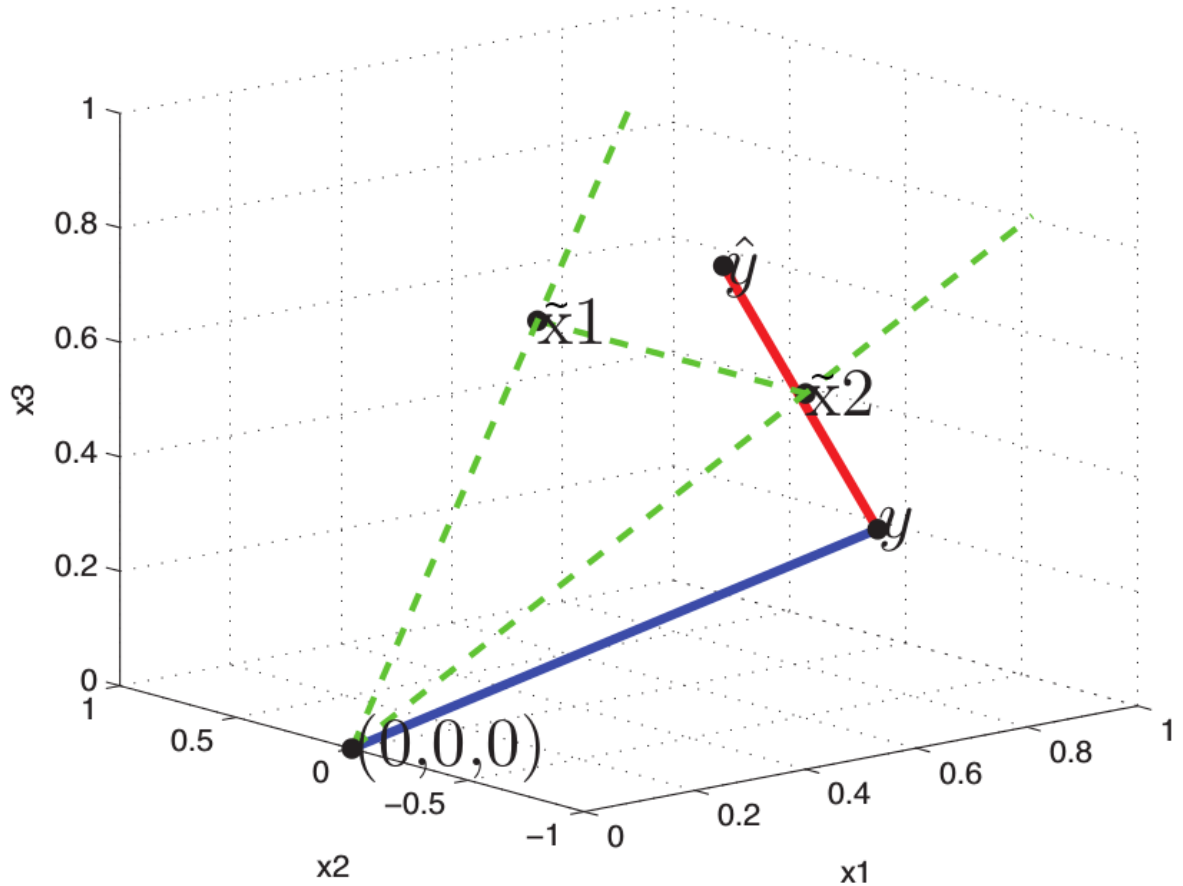
$$\tilde{\mathbf{x}}_j^T(\hat{\mathbf{y}} - \mathbf{y}) = 0 \text{ for } j \in \{1, \ldots, D\} \implies \mathbf{X}^T(\hat{\mathbf{y}} - \mathbf{y}) = \mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$$



# Geometric Interpretation

## Least Squares

- solving $\mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$ returns $\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
- we can get the **orthogonal projection** $\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
- the projection matrix $\mathbf{P} \triangleq \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is called the **hat matrix**, since it "puts the hat" on $\mathbf{y}$

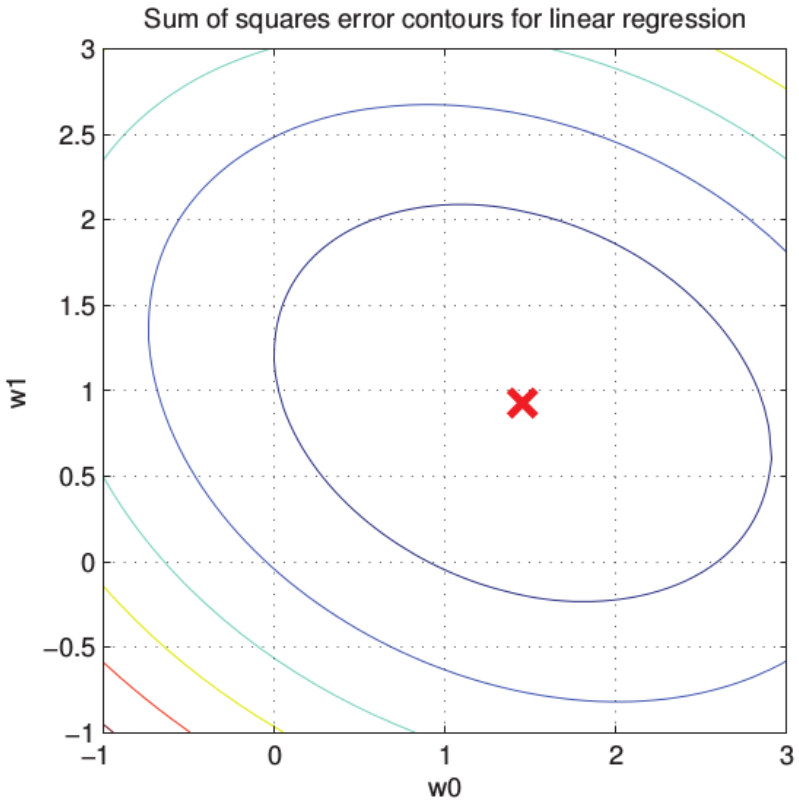


# Outline

# Convexity

## Intro

- when solving least squares, we noted that the NLL had a bowl shape with a **unique minimum**
- the technical term for functions like this is **convex**
- convex functions play a very important role in machine learning



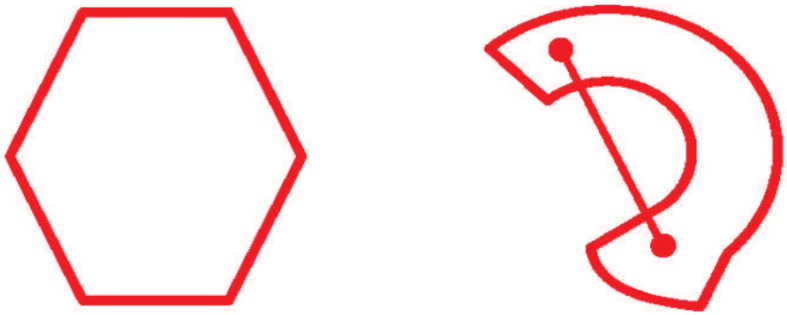
# Outline

- a set $\mathcal{S}$ is **convex** if for any $\boldsymbol{\theta}, \boldsymbol{\theta}' \in \mathcal{S}$ we have

$$\lambda\boldsymbol{\theta} + (1-\lambda)\boldsymbol{\theta}' \in \mathcal{S} \quad \forall\lambda \in [0,1]$$

that is, if we draw a line from $\boldsymbol{\theta}$ to $\boldsymbol{\theta}'$, all points on the line lie inside the set $\mathcal{S}$

- for instance in this figure



we have a convex set on the left and a nonconvex set on the right

# Outline

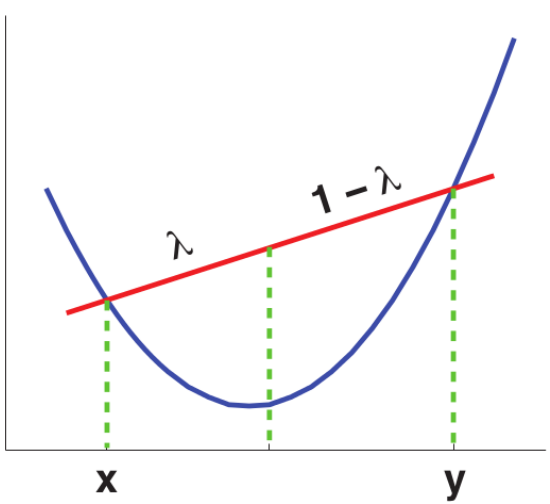
# Convexity

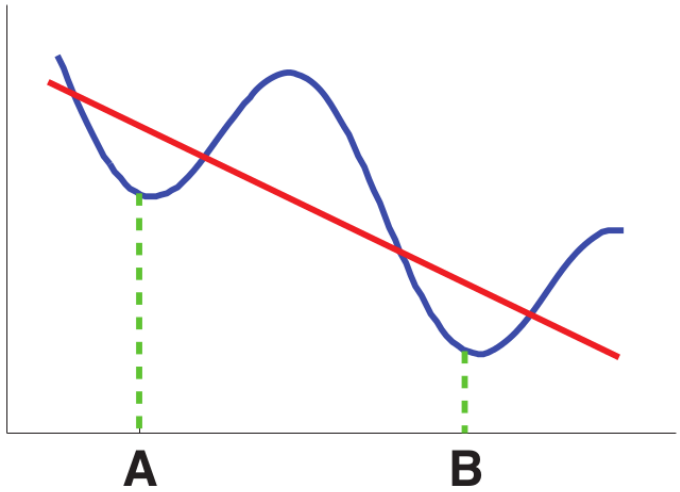
## Convex Function Definition

- a function $f(\boldsymbol{\theta})$ is **convex** if it is defined on a convex set and if, for any $\boldsymbol{\theta}, \boldsymbol{\theta}' \in \mathcal{S}$, and for any $\lambda \in [0, 1]$, we have

$$f(\lambda\boldsymbol{\theta} + (1-\lambda)\boldsymbol{\theta}') \leq \lambda f(\boldsymbol{\theta}) + (1-\lambda) f(\boldsymbol{\theta}')$$

- a function $f(\boldsymbol{\theta})$ is **strictly convex** if the inequality is strict
- a function $f(\boldsymbol{\theta})$ is **concave** if $-f(\boldsymbol{\theta})$ is convex
- for instance, in the following figure



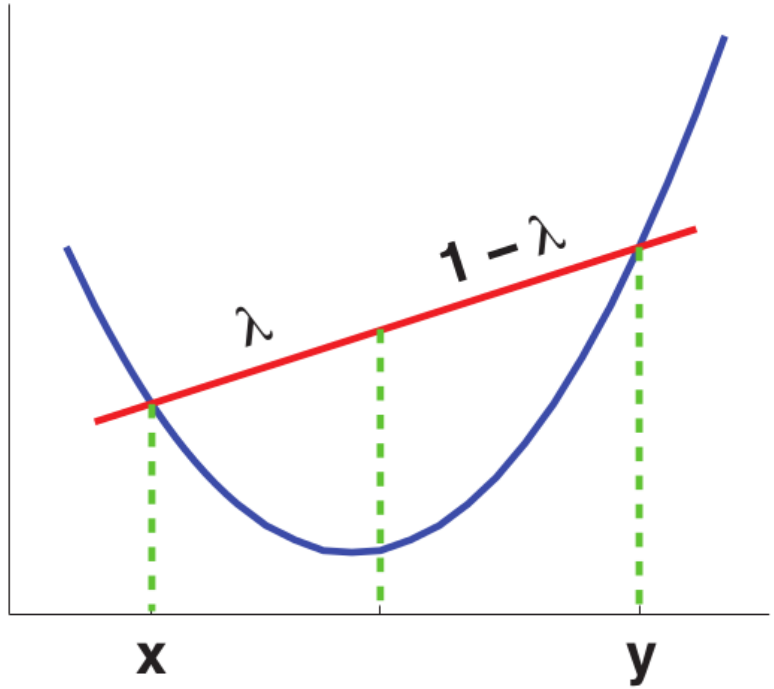




the function on the left is convex and the function on the right is neither concave nor convex

# Convexity

## Convex Function Definition

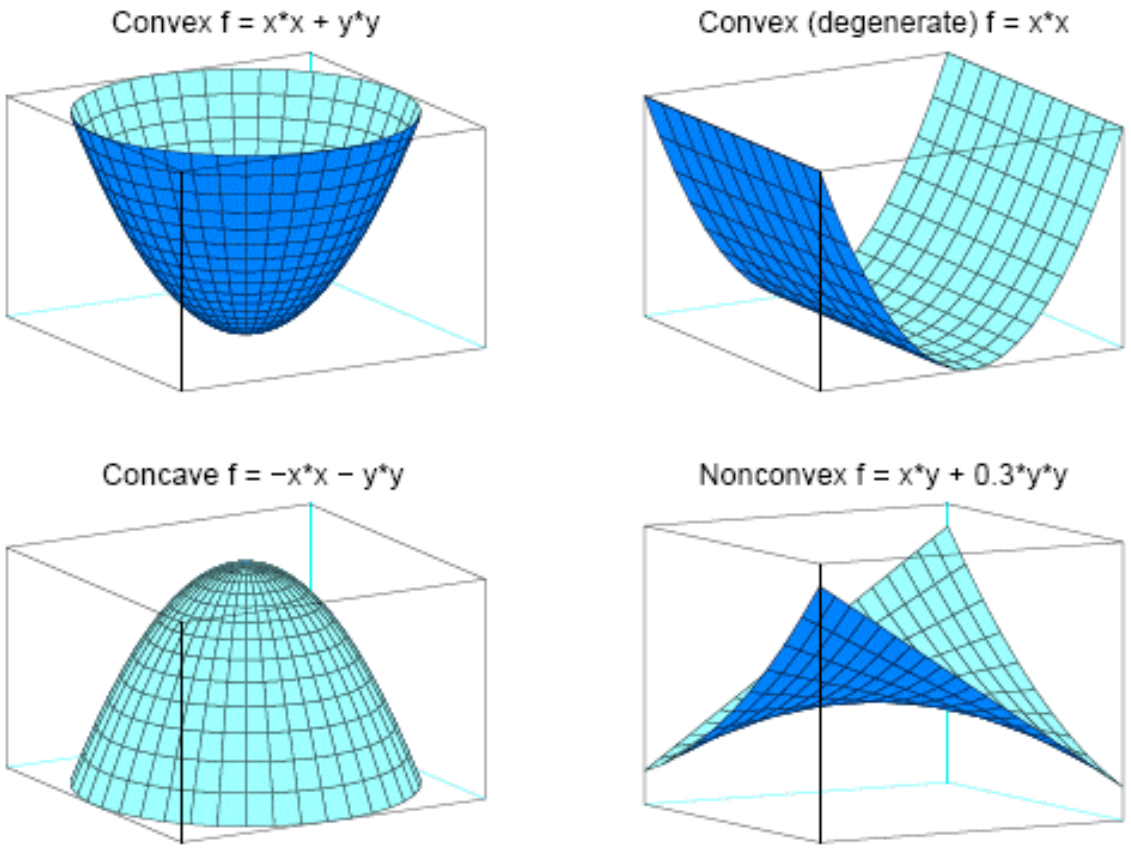
- examples of scalar convex functions include $\theta^2$, $e^\theta$ and $\theta \log \theta$ (for $\theta > 0$)
- examples of concave functions include $\log \theta$ and $\sqrt{\theta}$




- intuitively, a (strictly) convex function has a *bowl shape*, and hence has a **unique global minimum** $\theta^*$ corresponding to the bottom of the bowl
- in the scalar case, a convex function has its second derivative positive everywhere, i.e. $\frac{d}{d\theta^2} f(\theta) > 0$

# Convexity

## Convex Function Examples




- convex(concave) functions have a unique global minimum(maximum)

# Outline

## Theorem 1

*a twice-continuously differentiable, multivariate function $f(\boldsymbol{\theta}) \in \mathbb{R}$ is convex* **iff** *its Hessian is positive definite for all $\boldsymbol{\theta}$*

- the **Hessian matrix** $\mathbf{H} = \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2}$ of a function $f(\boldsymbol{\theta}) \in \mathbb{R}$ is defined as follows (element-wise)

$$\mathbf{H}_{jk} = \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_j \partial \theta_k}$$

- the Hessian is symmetric since $\frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_j \partial \theta_k} = \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_k \partial \theta_j}$ (Schwartz's theorem)
- recall that a matrix $\mathbf{H}$ is **positive definite** iff $\mathbf{v}^T \mathbf{H} \mathbf{v} > 0$ for any $\mathbf{v} \neq 0$
- a convex function has a bowl shape

- a convex function can be approximated about its unique global minimum $\boldsymbol{\theta}^*$ with a bowl shaped quadratic function (paraboloid in 3D)

$$f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}^*) + \frac{\partial f}{\partial \boldsymbol{\theta}}\bigg|_{\boldsymbol{\theta}^*} (\boldsymbol{\theta} - \boldsymbol{\theta}^*) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)^T \mathbf{H}(\boldsymbol{\theta}^*)(\boldsymbol{\theta} - \boldsymbol{\theta}^*) =$$

$$= f(\boldsymbol{\theta}^*) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)^T \mathbf{H}(\boldsymbol{\theta}^*)(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$$

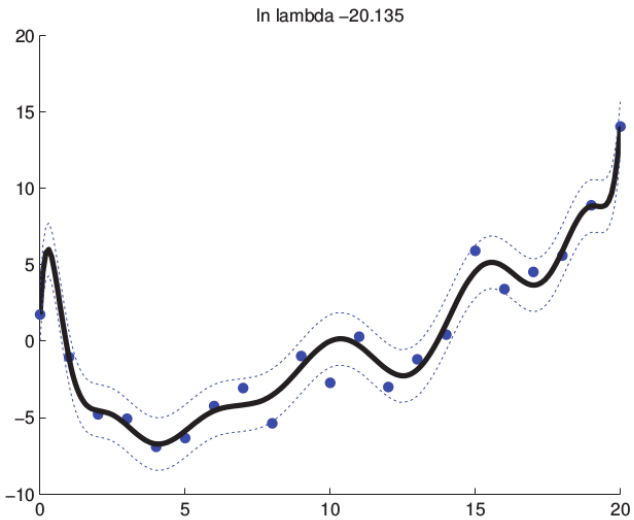
where we used the fact that at the minimum $\boldsymbol{\theta}^*$ one has $\frac{\partial f}{\partial \boldsymbol{\theta}}|_{\boldsymbol{\theta}^*} = 0$ and we know that $\mathbf{H}(\boldsymbol{\theta}^*) > 0$

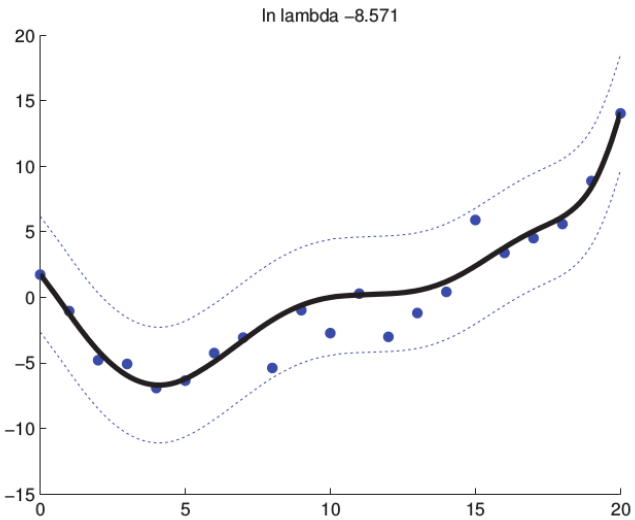
# Outline

# Ridge Regression

## MLE Issues

- one problem with ML estimation is that it can result in **overfitting**
- the reason that the MLE can overfit is that it is picking the parameter values that are the best for modeling the **training data**
- but if the data is **noisy**, such parameters often result in complex functions
- as a simple example, suppose we fit a degree 14 polynomial to N = 21 data points using least squares. The resulting curve is very "wiggly"
- in this case, overfitting equals interpolating noise
- if we change the data a little bit our estimate of **w** will change a lot (unstable estimation)



# Ridge Regression

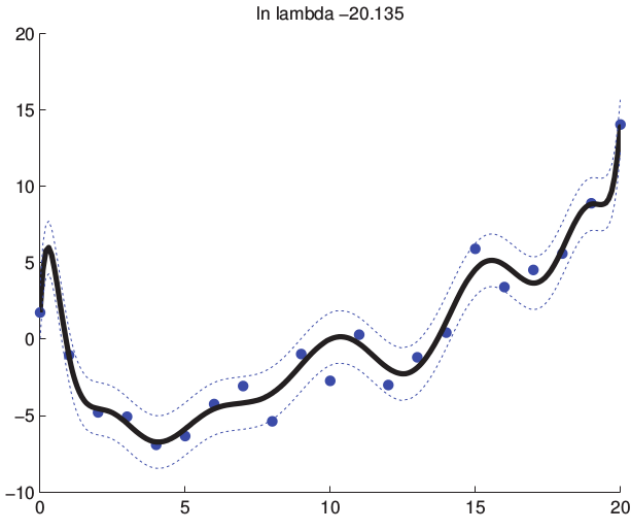
## Basic Idea

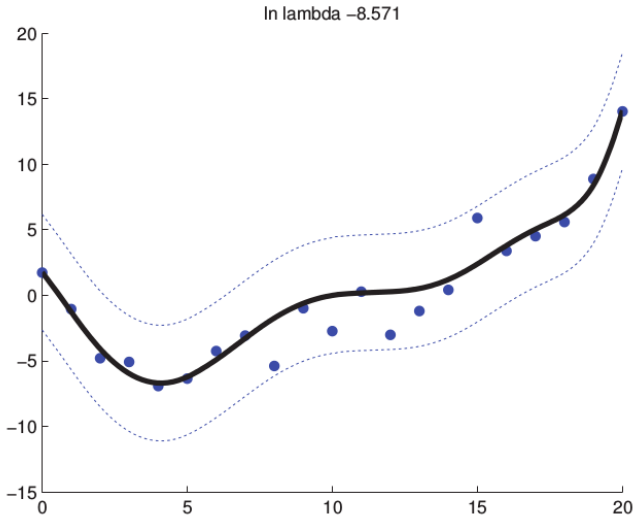
- the corresponding least squares coefficients $\mathbf{w}$ (excluding $w_0$ ) are as follows

$$6.560, -36.934, -109.255, 543.452, 1022.561, -3046.224, -3768.013,$$

$$8524.540, 6607.897, -12640.058, -5530.188, 9479.730, 1774.639, -2821.526$$

- there are many large positive and negative numbers
- these variations balance out exactly to make the curve "wiggle" in just the right way so that it almost perfectly interpolates the data



# Outline

# Ridge Regression

- we can encourage the parameters to be small, thus resulting in a smoother curve, by using a zero-mean Gaussian prior

$$p(\mathbf{w}) = \prod_j \mathcal{N}(w_j|\mathbf{0}, \tau^2)$$

where the precision $1/\tau^2$ controls the strength of the prior

- the corresponding MAP estimation problem becomes

$$\hat{\mathbf{w}}_{MAP} = \underset{\mathbf{w}}{\text{argmax}}\, p(\mathbf{w}|\mathcal{D}) = \underset{\mathbf{w}}{\text{argmax}}\, p(\mathcal{D}|\mathbf{w})p(\mathbf{w}) = \underset{\mathbf{w}}{\text{argmax}}\, \log p(\mathcal{D}|\mathbf{w}) + \log p(\mathbf{w}) =$$

$$= \underset{\mathbf{w}}{\text{argmax}} \sum_{i=1}^{N} \log \mathcal{N}(y_i|w_0 + \mathbf{w}^T\mathbf{x}_i, \sigma^2) + \sum_{i=1}^{D} \log \mathcal{N}(w_j|\mathbf{0}, \tau^2)$$

- it is simple to show that this is equivalent to minimize

$$J(\mathbf{w}) = \frac{1}{N}\sum_{i=1}^{N}(y_i - (w_0 + \mathbf{w}^T\mathbf{x}_i)^2) + \lambda\|\mathbf{w}\|_2^2 = \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_2^2$$

where $\lambda \triangleq \sigma^2/\tau^2$ and $\|\mathbf{w}\|_2^2 = \mathbf{w}^T\mathbf{w}$

- the first term is the MSE/NLL as usual, and the second term with $\lambda > 0$ is a **complexity penalty**

# Ridge Regression

- minimization problem

$$J(\mathbf{w}) = \frac{1}{N}\sum_{i=1}^{N}(y_i - (w_0 + \mathbf{w}^T\mathbf{x}_i)^2) + \lambda\|\mathbf{w}\|_2^2 = \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_2^2$$

- the solution is

$$\hat{\mathbf{w}}_{ridge} = (\lambda\mathbf{I}_D + \mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

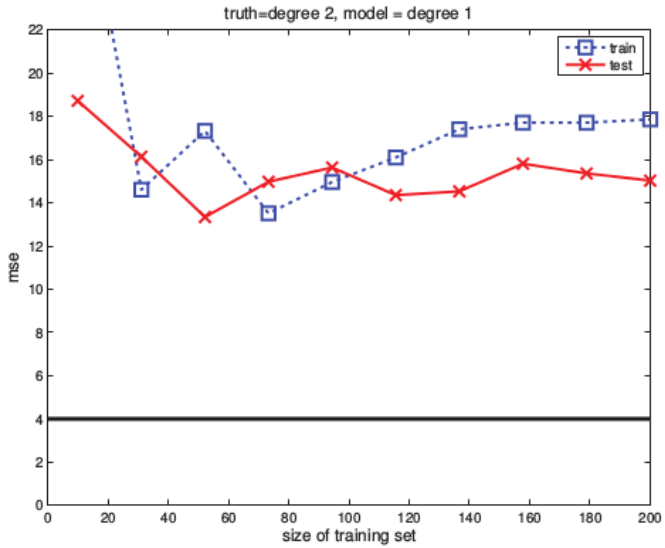
- this technique is known as **ridge regression**

# Outline

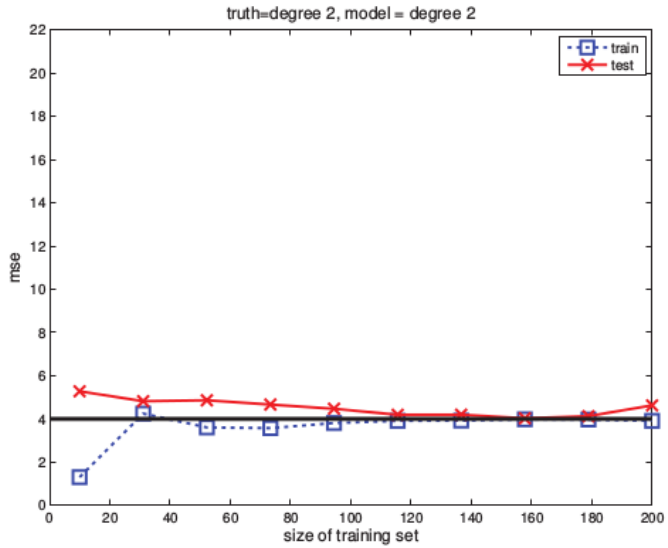
# Regularization Effects of Big Data

- **regularization** is the most common way to avoid **overfitting**
- another effective approach — which is not always available — is to use **lots of data**
- intuitively, the more training data we have, the better we will be able to learn
- let's consider a **polynomial regression** and let's plot the Mean Squared Error (MSE) incurred on the test set achieved by models of different degrees vs $N = |\mathcal{D}|$
- a plot of error vs training set size is known as a **learning curve**

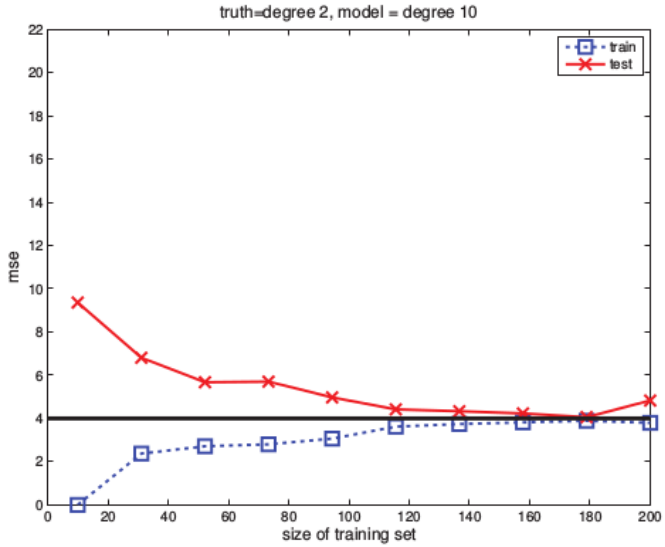
# Regularization Effects of Big Data



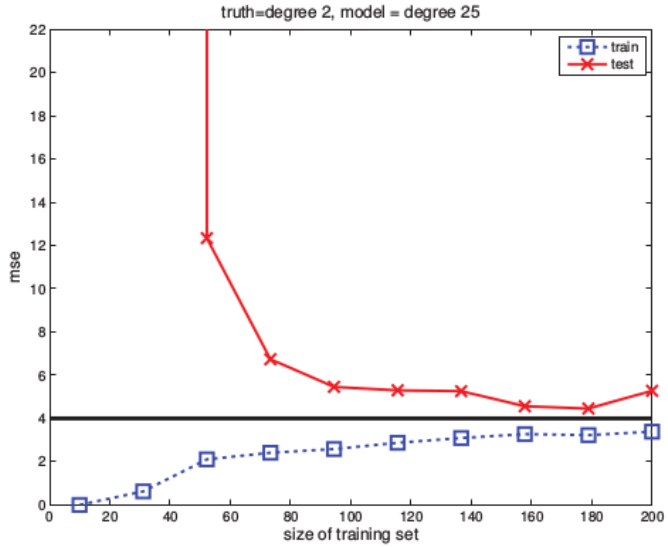

(a)




(b)



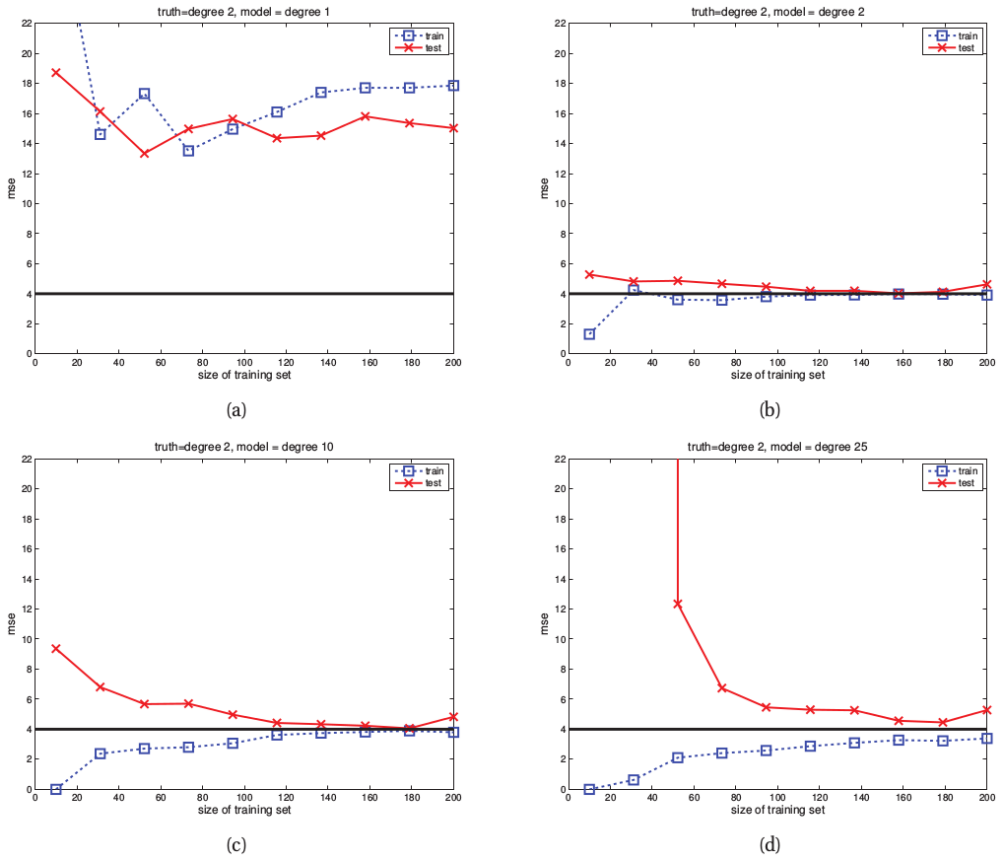

(c)




(d)

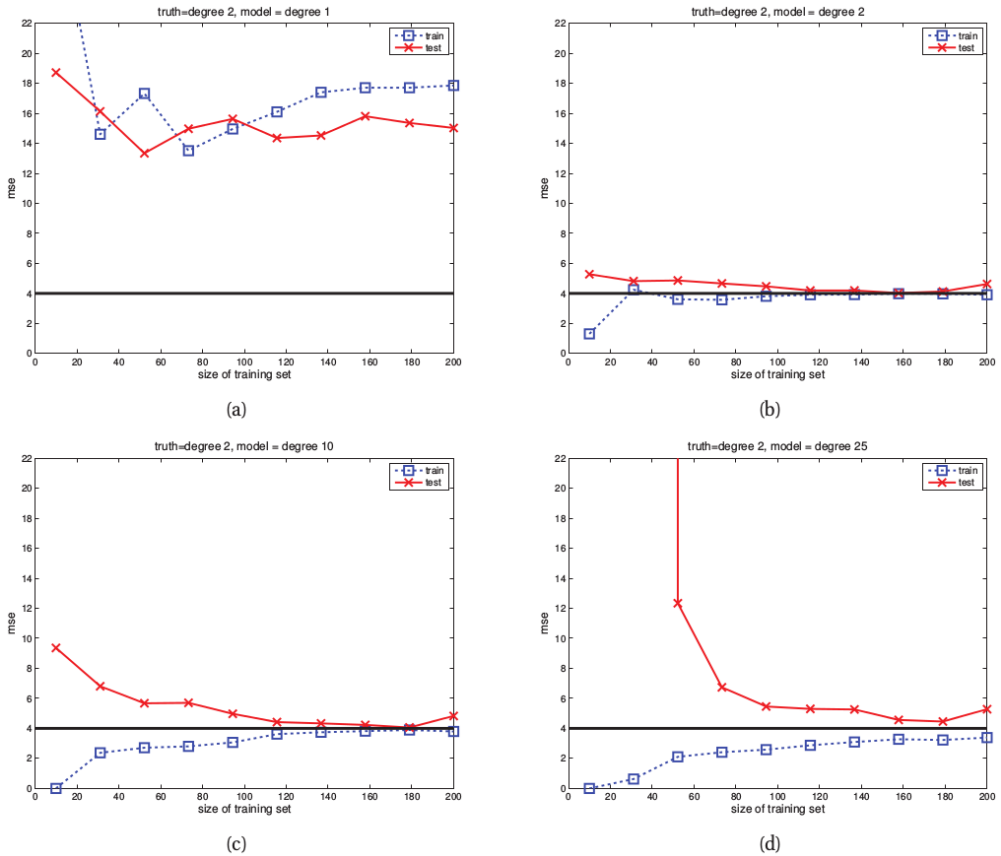
# Regularization Effects of Big Data

- the truth is a degree 2 polynomial
- we try fitting polynomials of degrees 1, 2, 10 and 25 to this data (respectively models $\mathcal{M}_1$,$\mathcal{M}_2$,$\mathcal{M}_{10}$ and $\mathcal{M}_{25}$)



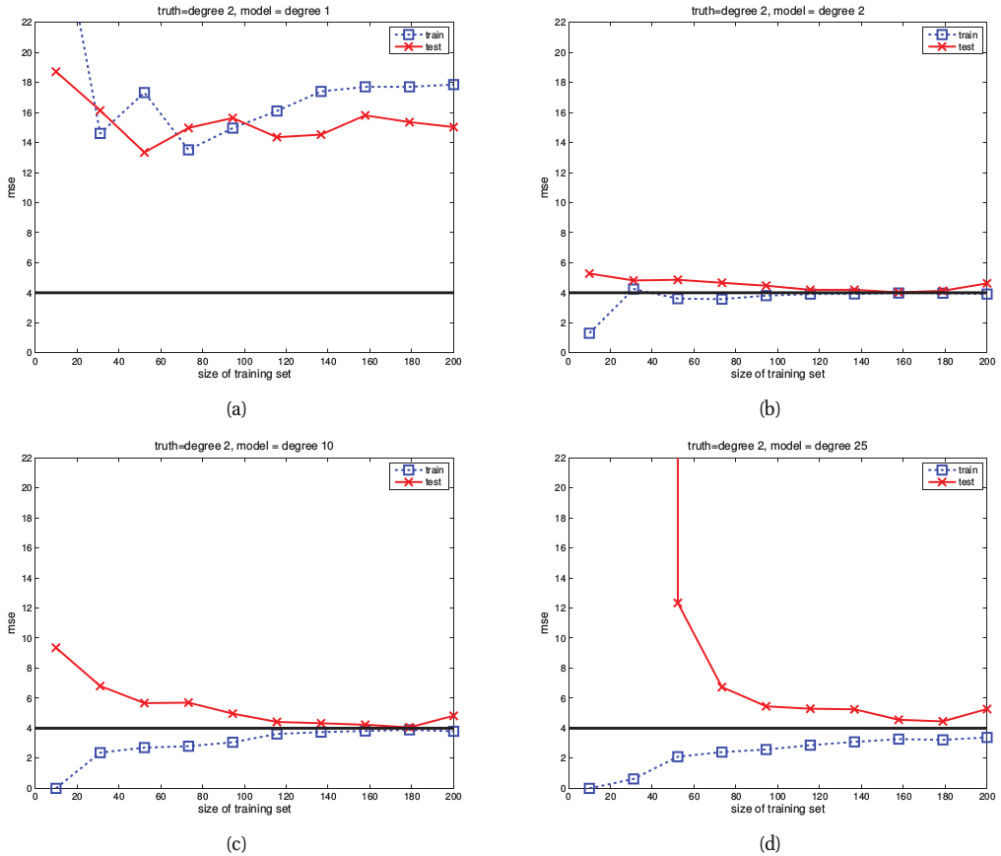
# Regularization Effects of Big Data

- the level of the plateau for the test error consists of two terms
  1. **noise floor**: an irreducible component that all models incur, due to the intrinsic variability of the generating process
  2. **structural error**: a component that depends on the discrepancy between the generating process (the "truth") and the model



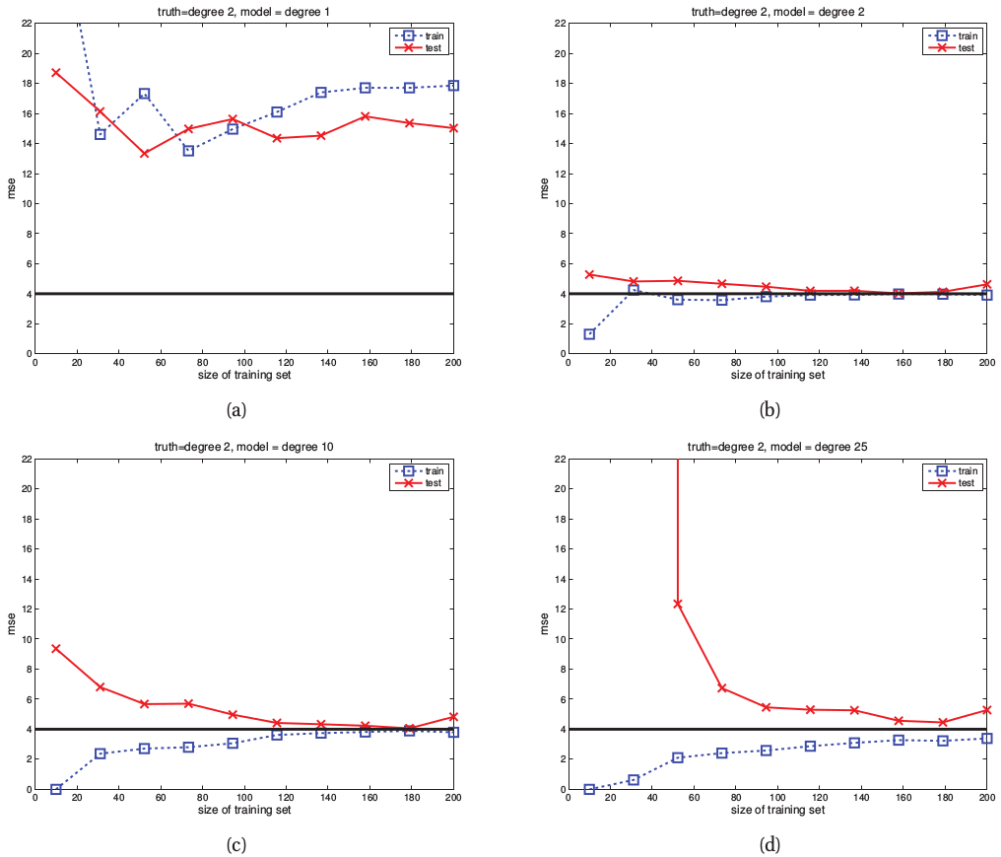
# Regularization Effects of Big Data

- the structural error for models $\mathcal{M}_2$, $\mathcal{M}_{10}$ and $\mathcal{M}_{25}$ is zero, since both are able to capture the true generating process
- the structural error for $\mathcal{M}_1$ is substantial, which is evident from the fact that the plateau occurs high above the noise floor



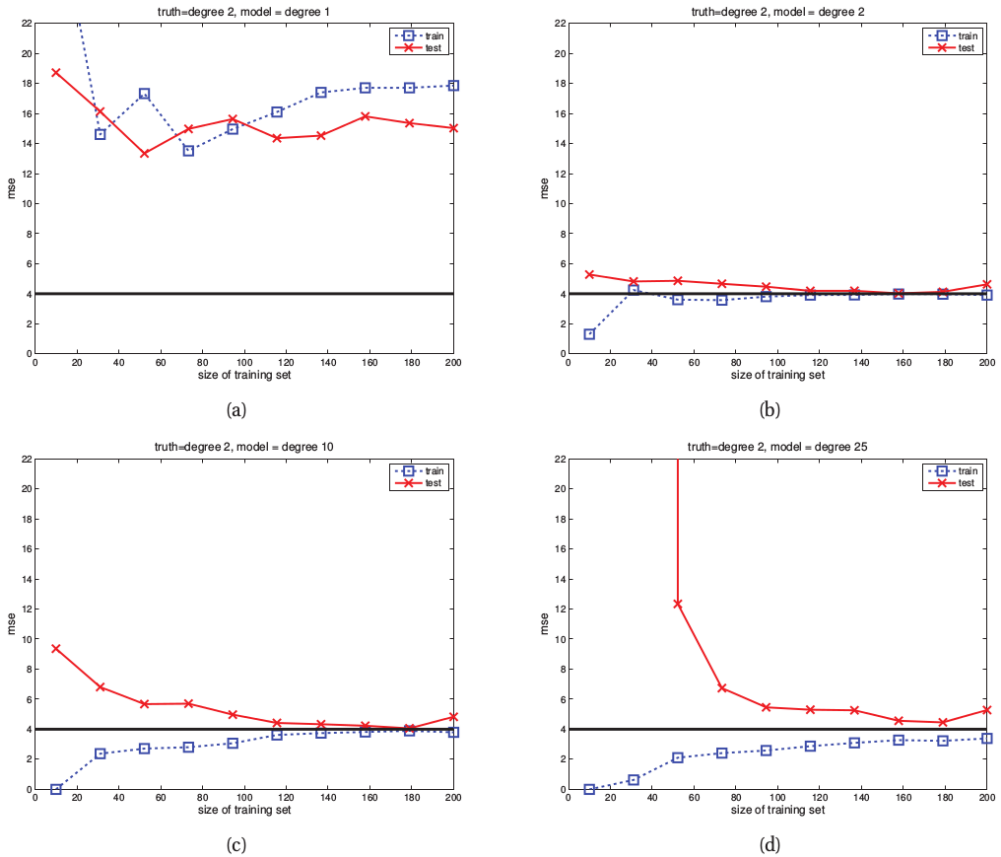
# Regularization Effects of Big Data

- for any model that is expressive enough to capture the truth (i.e., one with small structural error), the **test error** will go to the **noise floor** as $N \to \infty$
- the error will typically go to zero faster for simpler models (fewer parameters to estimate)



# Regularization Effects of Big Data

- for finite training sets, there will be some discrepancy between the parameters that we estimate and the best parameters that we could estimate given the particular model class
- this discrepancy is called **approximation error**, and goes to zero as $N \to \infty$ , but it goes to zero faster for simpler models



# Regularization Effects of Big Data

- in domains with lots of data, **simple methods** can work surprisingly well
- however, there are still reasons to study more **sophisticated learning methods**, because there will always be problems for which we have **little data**
- for example, even in such a data-rich domain as web search, as soon as we want to start **personalizing the results**, the amount of data available for any given user starts to look small again (relative to the complexity of the problem)

# Credits

- Kevin Murphy's book