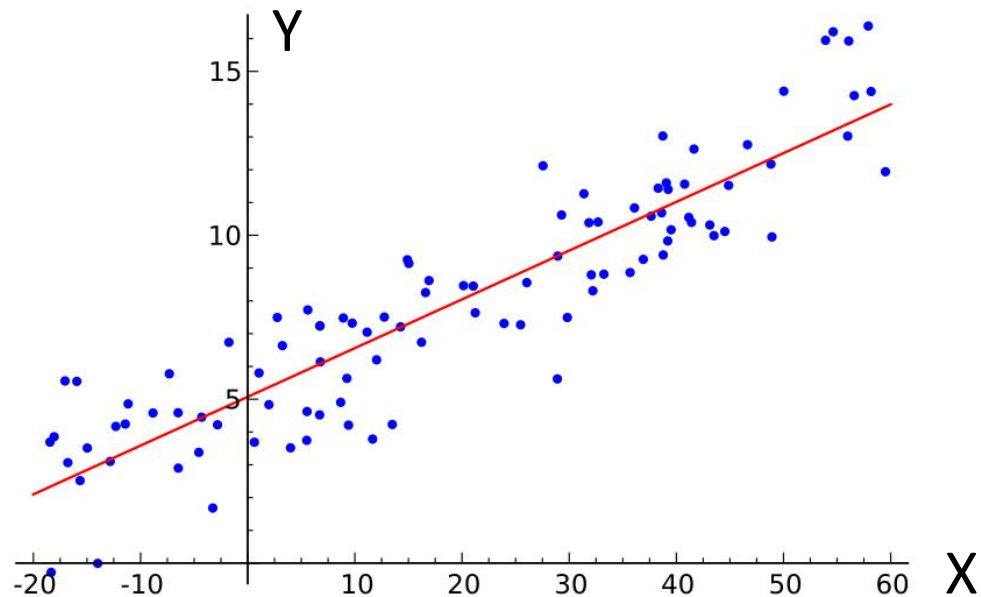


Linear Regression and the Bias Variance Tradeoff

Lecture by Shangsong Liang
Sun Yat-sen University

Thanks to Joseph E. Gonzalez, Tom Mitchell

Simple Linear Regression



Response
Variable

Covariate

Linear Model: $Y = mX + b$

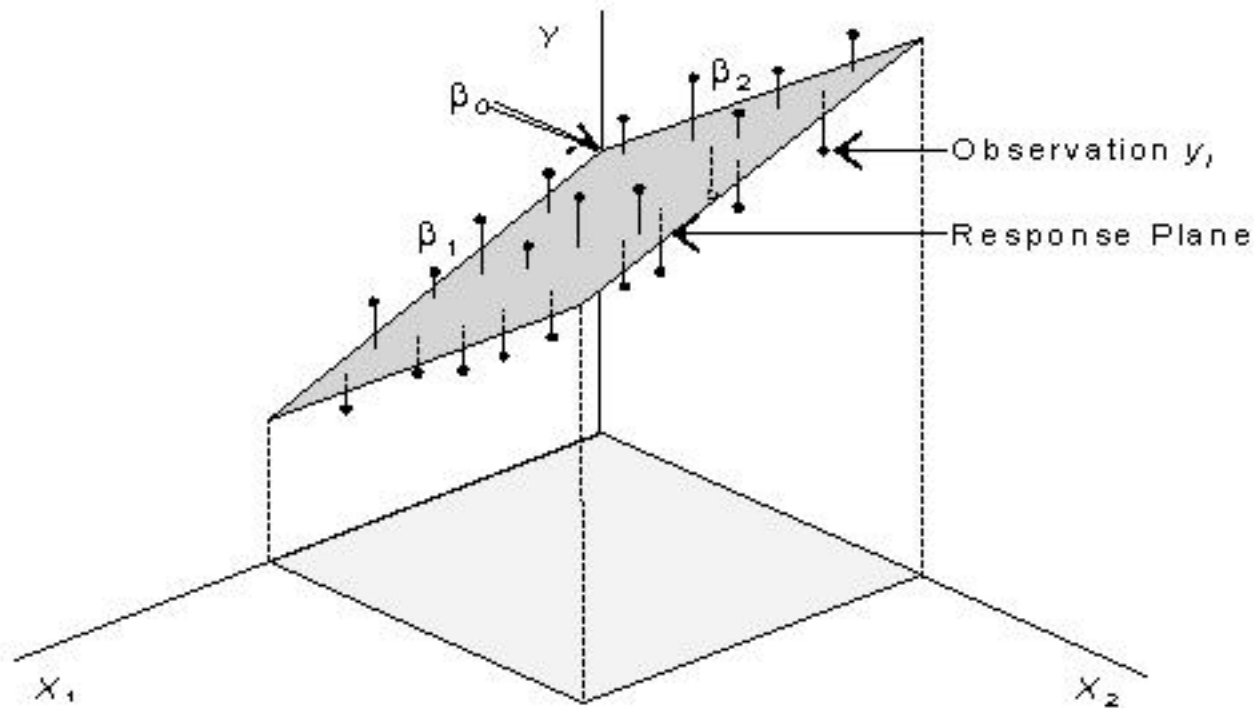
Slope

Intercept (bias)

Motivation

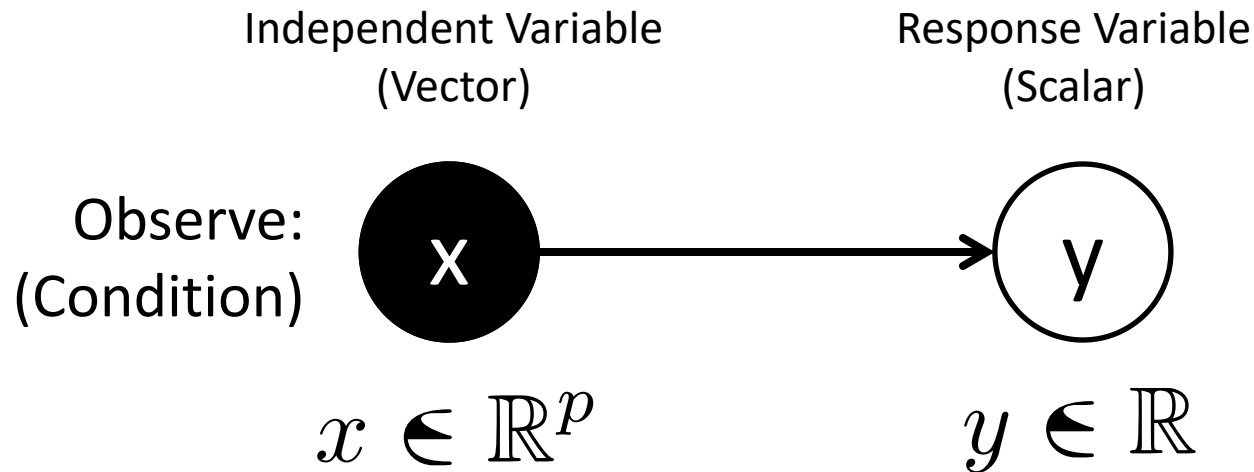
- One of the most widely used techniques
- Fundamental to many larger models
 - Generalized Linear Models
 - Collaborative filtering
- Easy to interpret
- Efficient to solve

Multiple Linear Regression



The Regression Model

- For a *single* data point (x, y) :



- Joint Probability:

$$p(x, y) = p(x)p(y|x)$$

Discriminative
Model

END
DUALITY
GAP

SUPPORT
VECTOR
MACHINES

BAYSIANS
AGAINST
DISCRIMINATION

PEOPLE
vs
PROFIT

Public
Option
or
Market

ANANE
ANEA

The Linear Model

Scalar Response

Vector of Parameters

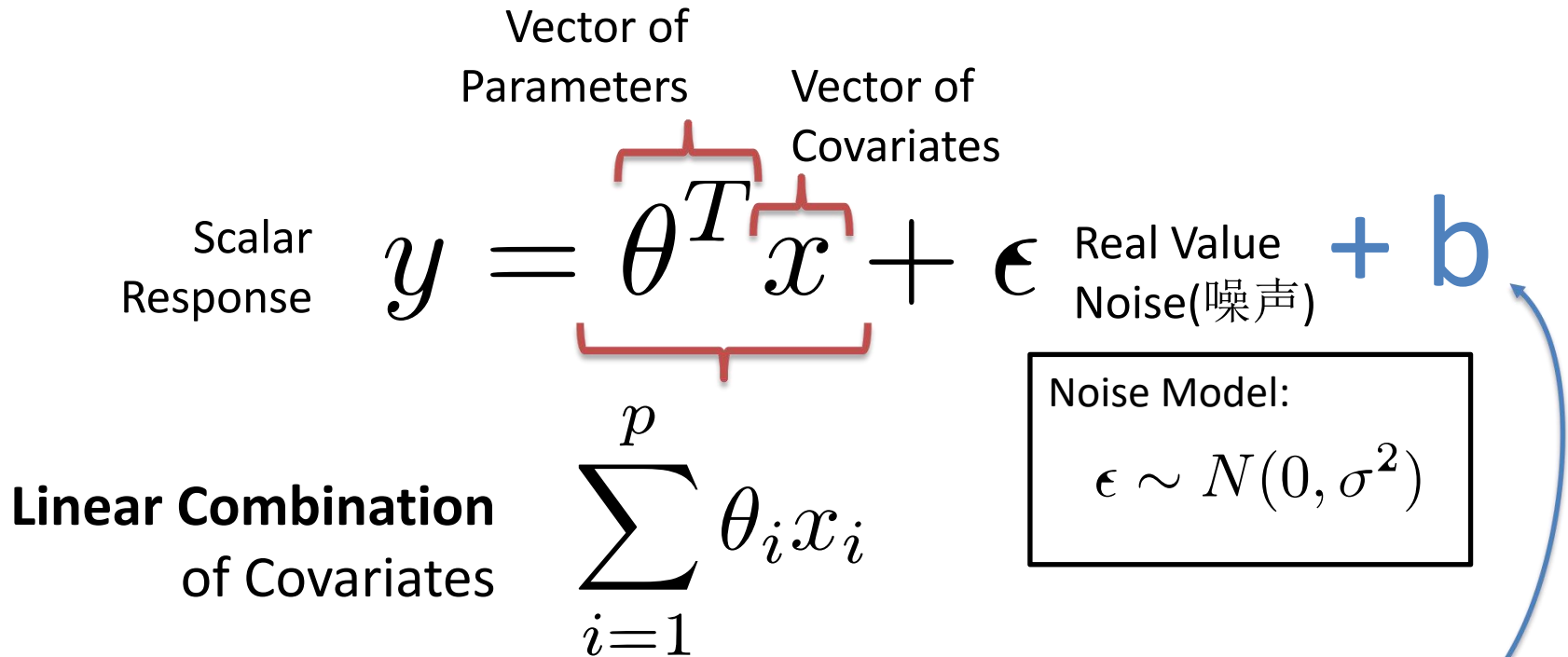
Vector of Covariates

Real Value Noise(噪声)

Linear Combination of Covariates

$$y = \theta^T x + \epsilon + b$$

Noise Model:

$$\epsilon \sim N(0, \sigma^2)$$


What about bias(偏置)/intercept term?

Define: $x_{p+1} = 1$

Then redefine $p := p+1$ for notational simplicity

Conditional Likelihood $p(y|x)$

- Conditioned on x :

$$y = \overbrace{\theta^T x}^{\text{Constant}} + \epsilon \sim N(0, \sigma^2)$$

Normal Distribution
Mean Variance

- Conditional distribution of Y :

$$Y \sim N(\theta^T x, \sigma^2)$$

$$p(y|x) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{(y - \theta^T x)^2}{2\sigma^2} \right)$$

Parameters and Random Variables

Parameters

$$y \sim N(\theta^T x, \sigma^2)$$

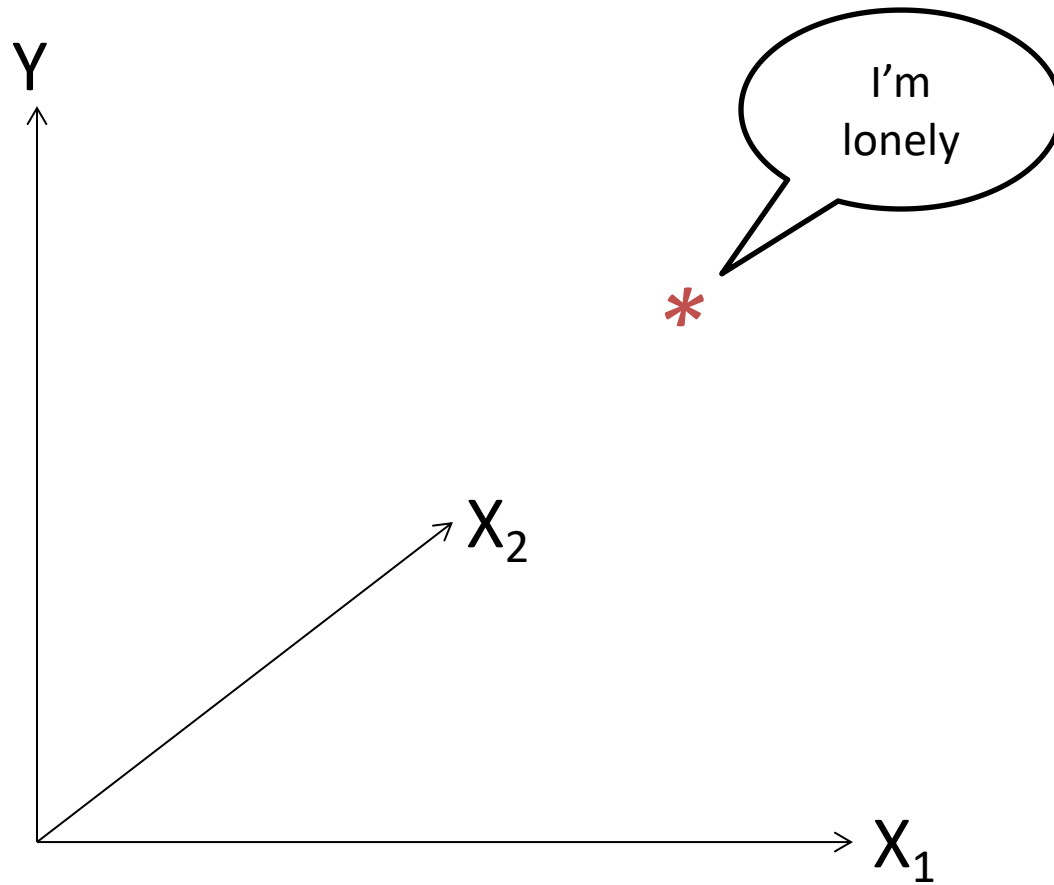
- Conditional distribution of y :
 - Bayesian(贝叶斯): parameters as random variables

$$p(y|x, \theta, \sigma^2)$$

- Frequentist: parameters as (unknown) constants

$$p_{\theta, \sigma^2}(y|x)$$

So far ...



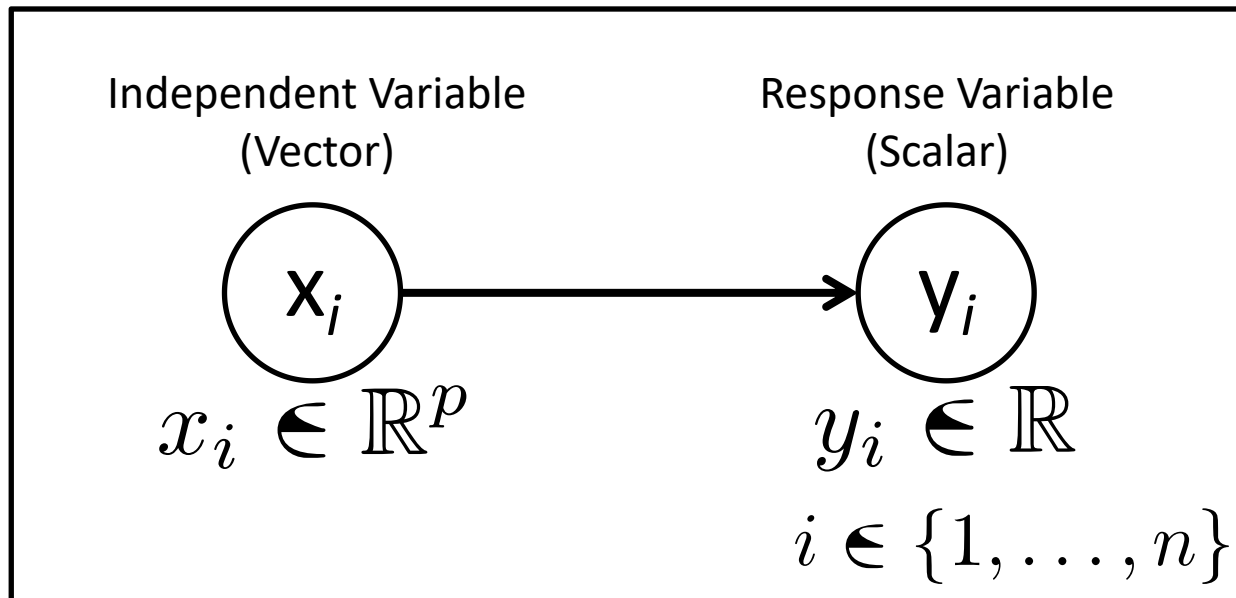
Independent and Identically Distributed (iid) Data

- For n data points:

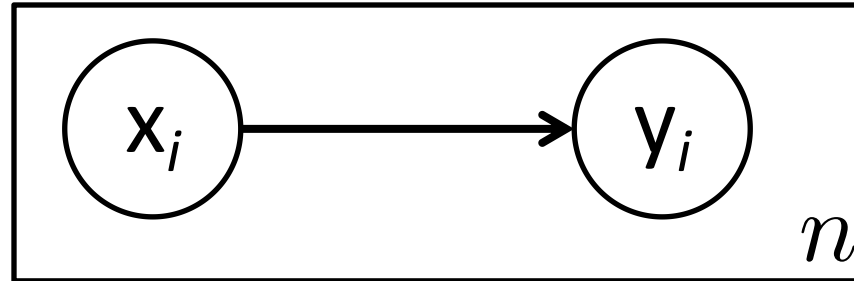
$$\begin{aligned}\mathcal{D} &= \{(x_1, y_1), \dots, (x_n, y_n)\} \\ &= \{(x_i, y_i)\}_{i=1}^n\end{aligned}$$

Plate Diagram

graphical model



Joint Probability



- For n data points **independent and identically distributed (iid)**(独立同分布):

$$\begin{aligned} p(\mathcal{D}) &= \prod_{i=1}^n p(x_i, y_i) \\ &= \prod_{i=1}^n p(x_i) p(y_i | x_i) \end{aligned}$$

Rewriting with Matrix Notation

- Represent data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ as:

Covariate (Design)
Matrix

Response
Vector

$$X = \begin{matrix} \underbrace{\quad}_{n} \left[\begin{array}{c} \text{--- } x_1 \text{ ---} \\ \text{--- } x_2 \text{ ---} \\ \vdots \\ \text{--- } x_n \text{ ---} \end{array} \right] \in \mathbb{R}^{np} \\ \underbrace{\quad}_{p} \end{matrix}$$

Assume X
has rank p
(not degenerate)

$$Y = \begin{matrix} \underbrace{\quad}_{n} \left[\begin{array}{c} y_1 \\ y_2 \\ \vdots \\ y_n \end{array} \right] \in \mathbb{R}^n \\ \underbrace{\quad}_{1} \end{matrix}$$

Rewriting with Matrix Notation

- Rewriting the model using matrix operations:

$$Y = X\theta + \epsilon$$

Diagram illustrating the dimensions of the variables in the equation $Y = X\theta + \epsilon$:

- Y : A vertical vector of size n by 1 .
- X : A matrix of size n by p .
- θ : A vertical vector of size p by 1 .
- ϵ : A vertical vector of size n by 1 .

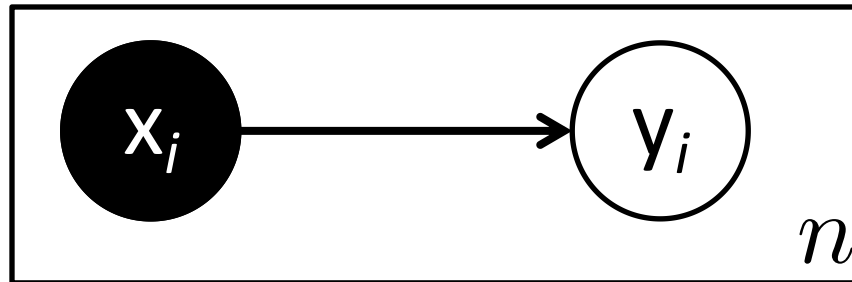
Estimating the Model

- Given data how can we estimate θ ?

$$Y = X\theta + \epsilon$$

- Construct maximum likelihood estimator (MLE最大似然):
 - Derive the log-likelihood
 - Find θ_{MLE} that maximizes log-likelihood
 - Analytically: Take derivative and set = 0
 - Iteratively: (Stochastic) gradient descent

Joint Probability



- For n data points:

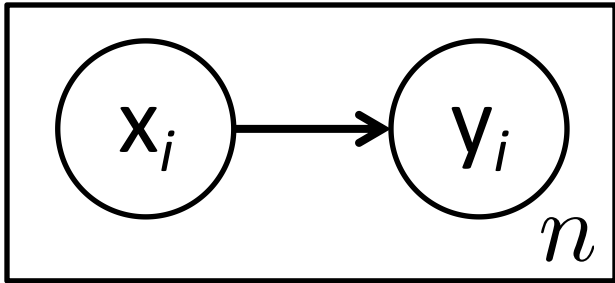
$$p(\mathcal{D}) = \prod_{i=1}^n p(x_i, y_i)$$

$$= \prod_{i=1}^n \cancel{p(x_i)} p(y_i | x_i)$$

“常数”

Discriminative Model

Defining the Likelihood



$$p_{\theta}(y|x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y - \theta^T x)^2}{2\sigma^2}\right)$$

$$\begin{aligned}\mathcal{L}(\theta|\mathcal{D}) &= \prod_{i=1}^n p_{\theta}(y_i|x_i) \\ &= \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y_i - \theta^T x_i)^2}{2\sigma^2}\right) \\ &= \frac{1}{\sigma^n (2\pi)^{\frac{n}{2}}} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \theta^T x_i)^2\right)\end{aligned}$$

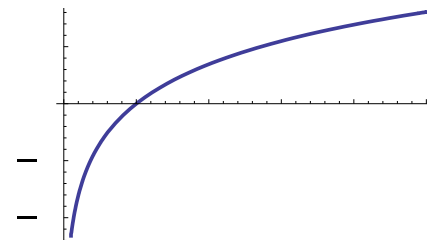
Maximizing the Likelihood

- Want to compute:

$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta \in \mathbb{R}^p} \mathcal{L}(\theta | \mathcal{D})$$

- To simplify the calculations we take the log:

$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta \in \mathbb{R}^p} \log \mathcal{L}(\theta | \mathcal{D})$$



which does not affect the maximization because log is a monotone function.

$$\mathcal{L}(\theta|\mathcal{D}) = \frac{1}{\sigma^n (2\pi)^{\frac{n}{2}}} \exp \left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \theta^T x_i)^2 \right)$$

- Take the log:

$$\log \mathcal{L}(\theta|\mathcal{D}) = -\log(\sigma^n (2\pi)^{\frac{n}{2}}) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \theta^T x_i)^2$$

- Removing constant terms with respect to θ :

$$\log \mathcal{L}(\theta) = - \sum_{i=1}^n (y_i - \theta^T x_i)^2$$

Monotone Function
(Easy to maximize)

$$\log \mathcal{L}(\theta) = - \sum_{i=1}^n (y_i - \theta^T x_i)^2$$

- Want to compute:


$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta \in \mathbb{R}^p} \log \mathcal{L}(\theta | \mathcal{D})$$

- Plugging in log-likelihood:

$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta \in \mathbb{R}^p} - \sum_{i=1}^n (y_i - \theta^T x_i)^2$$

$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta \in \mathbb{R}^p} - \sum_{i=1}^n (y_i - \theta^T x_i)^2$$

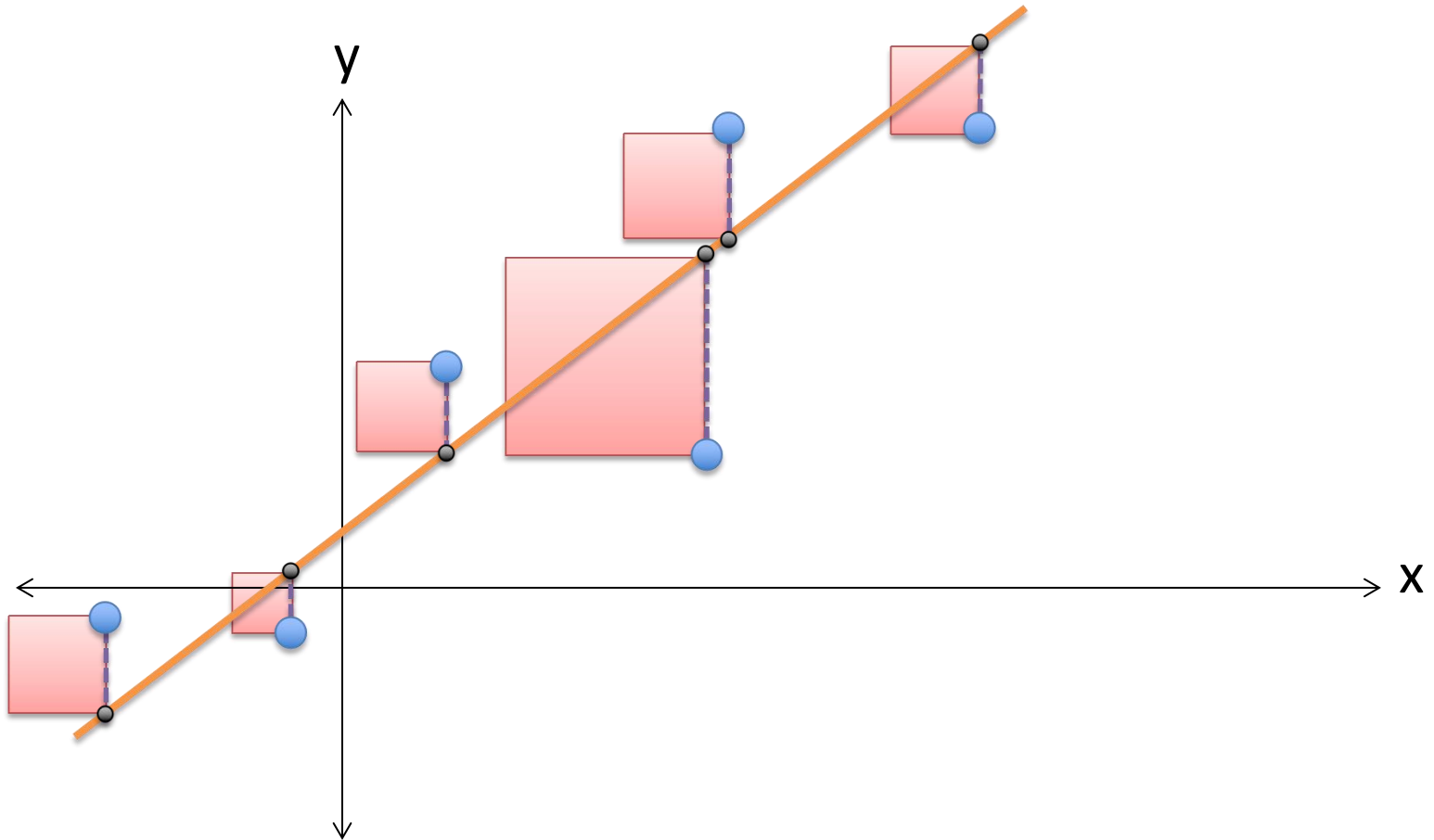
- Dropping the sign and flipping from maximization to minimization:

$$\hat{\theta}_{\text{MLE}} = \arg \min_{\theta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \theta^T x_i)^2$$


Minimize Sum (Error)²

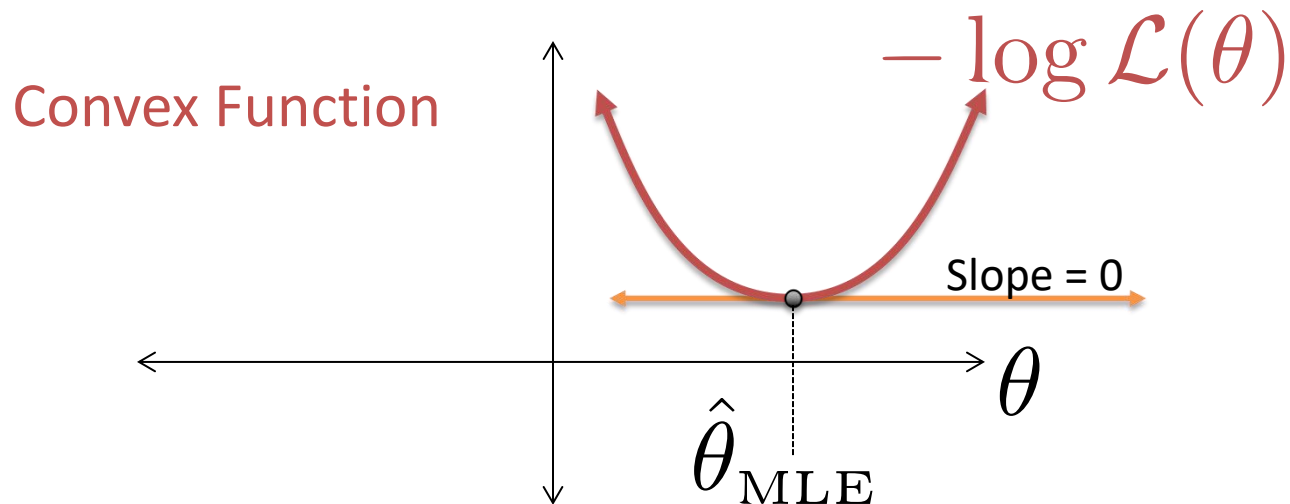
- Gaussian Noise Model → Squared Loss
 - Least Squares Regression

Pictorial Interpretation of Squared Error



Maximizing the Likelihood (Minimizing the Squared Error)

$$\hat{\theta}_{\text{MLE}} = \arg \min_{\theta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \theta^T x_i)^2$$



- Take the gradient and set it equal to zero

Minimizing the Squared Error

$$\hat{\theta}_{\text{MLE}} = \arg \min_{\theta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \theta^T x_i)^2$$

- Taking the gradient

$$-\nabla_{\theta} \log \mathcal{L}(\theta) = \nabla_{\theta} \sum_{i=1}^n (y_i - \theta^T x_i)^2$$

Chain Rule \rightarrow

$$\begin{aligned} &= -2 \sum_{i=1}^n (y_i - \theta^T x_i) x_i \\ &= -2 \sum_{i=1}^n y_i x_i + 2 \sum_{i=1}^n (\theta^T x_i) x_i \end{aligned}$$

- Rewriting the gradient in matrix form:

$$\begin{aligned} -\nabla_{\theta} \log \mathcal{L}(\theta) &= -2 \sum_{i=1}^n y_i x_i + 2 \sum_{i=1}^n (\theta^T x_i) x_i \\ &= -2X^T Y + 2X^T X \theta \end{aligned}$$

- To make sure the log-likelihood is convex compute the second derivative (Hessian)

$$-\nabla^2 \log \mathcal{L}(\theta) = 2X^T X$$

- If X is full rank then $X^T X$ is positive definite and therefore θ_{MLE} is the minimum
 - Address the degenerate cases with regularization

$$-\nabla_{\theta} \log \mathcal{L}(\theta) = -2X^T y + 2X^T X \theta = 0$$

- Setting gradient equal to 0 and solve for θ_{MLE} :

$$(X^T X) \hat{\theta}_{\text{MLE}} = X^T Y$$

$$\hat{\theta}_{\text{MLE}} = (X^T X)^{-1} X^T Y$$

Normal
Equations
(Write on
board)

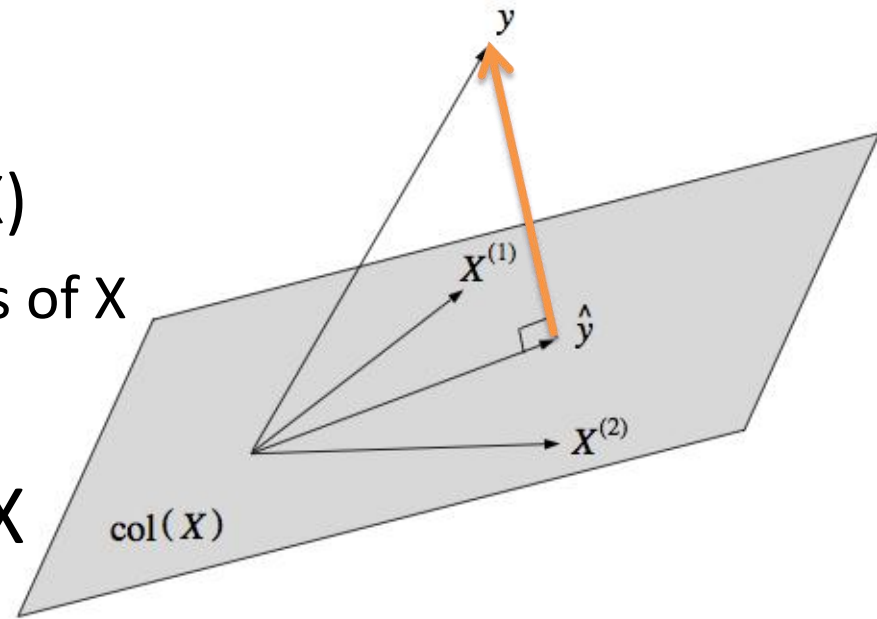
$$\begin{matrix} n \\ p \end{matrix} \begin{matrix} \text{vector} \end{matrix} = \left(\begin{matrix} n & p \\ \text{matrix} \end{matrix} \right)^{-1} \left(\begin{matrix} n & 1 \\ \text{matrix} \end{matrix} \right)$$

Geometric Interpretation


- View the MLE as finding a projection on $\text{col}(X)$
 - Define the estimator:

$$\hat{Y} = X\theta$$

- Observe that \hat{Y} is in $\text{col}(X)$
 - linear combination of cols of X
 - Want to \hat{Y} closest to Y
- Implies $(Y - \hat{Y})$ normal to X

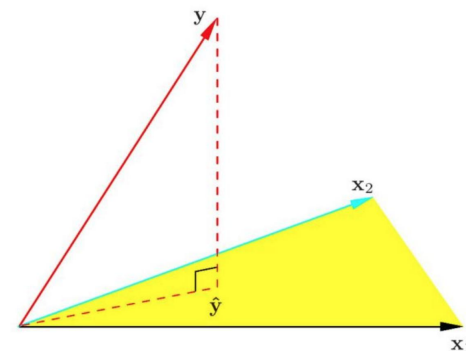


$$X^T(Y - \hat{Y}) = X^T(Y - X\theta) = 0$$



$$\Rightarrow X^T X \theta = X^T Y$$

Geometric Interpretation



假设我们通过一个特征来估计 y ，依然有 5 条数据， $X = \begin{bmatrix} 1 & x_{11} \\ 1 & x_{21} \\ 1 & x_{31} \\ 1 & x_{41} \\ 1 & x_{51} \end{bmatrix}$ ， X 的两条列向量

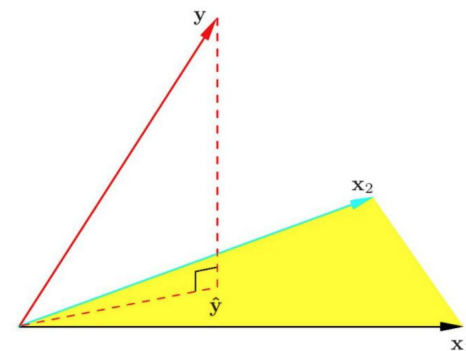
$x_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ 和 $x_2 = \begin{bmatrix} x_{11} \\ x_{21} \\ x_{31} \\ x_{41} \\ x_{51} \end{bmatrix}$ 通过权重 $w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$ 张成了 2 维的子空间，也就是一个平面，我们

通过获得数据知道向量 y 。因为误差， y 不在 x_1 和 x_2 张成的平面上，怎么样才能找到最好的 w 呢？一种答案是找到 y 在 x_1 和 x_2 张成的平面上投影 $\hat{y} = X\hat{w}$ ，如上图所示， \hat{w} 就是最好的 w 。

由投影的性质可知 $y - \hat{y}$ 垂直于 x_1 和 x_2 ，用人话说就是从 \hat{y} 的终点到 y 的终点是一条垂直于 x_1 和 x_2 的向量，可得

Geometric Interpretation

$$\begin{aligned}(y - \hat{y})^T x_1 &= (y - X\hat{w})^T x_1 = 0 \\ (y - \hat{y})^T x_2 &= (y - X\hat{w})^T x_2 = 0\end{aligned}$$



把上式合并，可得

$$\begin{aligned}(y - X\hat{w})^T X &= 0 \\ X^T(y - X\hat{w}) &= 0 \\ X^T y - X^T X\hat{w} &= 0 \\ X^T X\hat{w} &= X^T y \\ \hat{w} &= (X^T X)^{-1} X^T y\end{aligned}$$

最小二乘法和投影矩阵是两种完全不同的思路，却得到了相同结论，究其原因，投影使 \hat{y} 与 y 的欧式距离最短，这与最小二乘法让误差项平方和最小的思想不谋而合，岂不妙哉？

Connection to Pseudo-Inverse

$$\hat{\theta}_{\text{MLE}} = \underbrace{(X^T X)^{-1} X^T}_{\substack{\text{Moore-Penrose} \\ \text{Pseudoinverse}}} X^\dagger Y$$

- Generalization of the inverse:
 - Consider the case when X is square and invertible:

$$X^\dagger = (X^T X)^{-1} X^T = X^{-1} (X^T)^{-1} X^T = X^{-1}$$

- Which implies $\theta_{\text{MLE}} = X^{-1} Y$ the solution to $X \theta = Y$ when X is square and invertible

Computing the MLE

$$\hat{\theta}_{\text{MLE}} = (X^T X)^{-1} X^T Y$$

- **Not** typically solved by inverting $X^T X$
- Solved using direct methods:

- Cholesky factorization:

- Up to a factor of 2 faster

- QR factorization:

- More numerically stable

or use the
built-in solver
in your math library.

R: `solve(Xt %*% X, Xt %*% y)`

- Solved using various iterative methods:
 - Krylov subspace methods
 - (Stochastic) Gradient Descent

Cholesky Factorization

$$\text{solve } \hat{\theta}_{\text{MLE}} \quad \underbrace{(X^T X)}_C \hat{\theta}_{\text{MLE}} = \underbrace{X^T Y}_d$$

- Compute symm. matrix $C = X^T X$ $O(np^2)$
- Compute vector $d = X^T Y$ $O(np)$
- Cholesky Factorization $LL^T = C$ $O(p^3)$
 - L is lower triangular
- Forward subs. to solve: $Lz = d$ $O(p^2)$
- Backward subs. to solve: $L^T \hat{\theta}_{\text{MLE}} = z$ $O(p^2)$

Connections to graphical model inference:

http://ssg.mit.edu/~willsky/publ_pdfs/185_pub_MLR.pdf and <http://yaroslavvb.blogspot.com/2011/02/junction-trees-in-numerical-analysis.html> with illustrations

Solving Triangular System

$A_{11}x_1$	$A_{12}x_2$	$A_{13}x_3$	$A_{14}x_4$
	A_{22}	A_{23}	A_{24}
		A_{33}	A_{34}
			A_{44}

 $*$

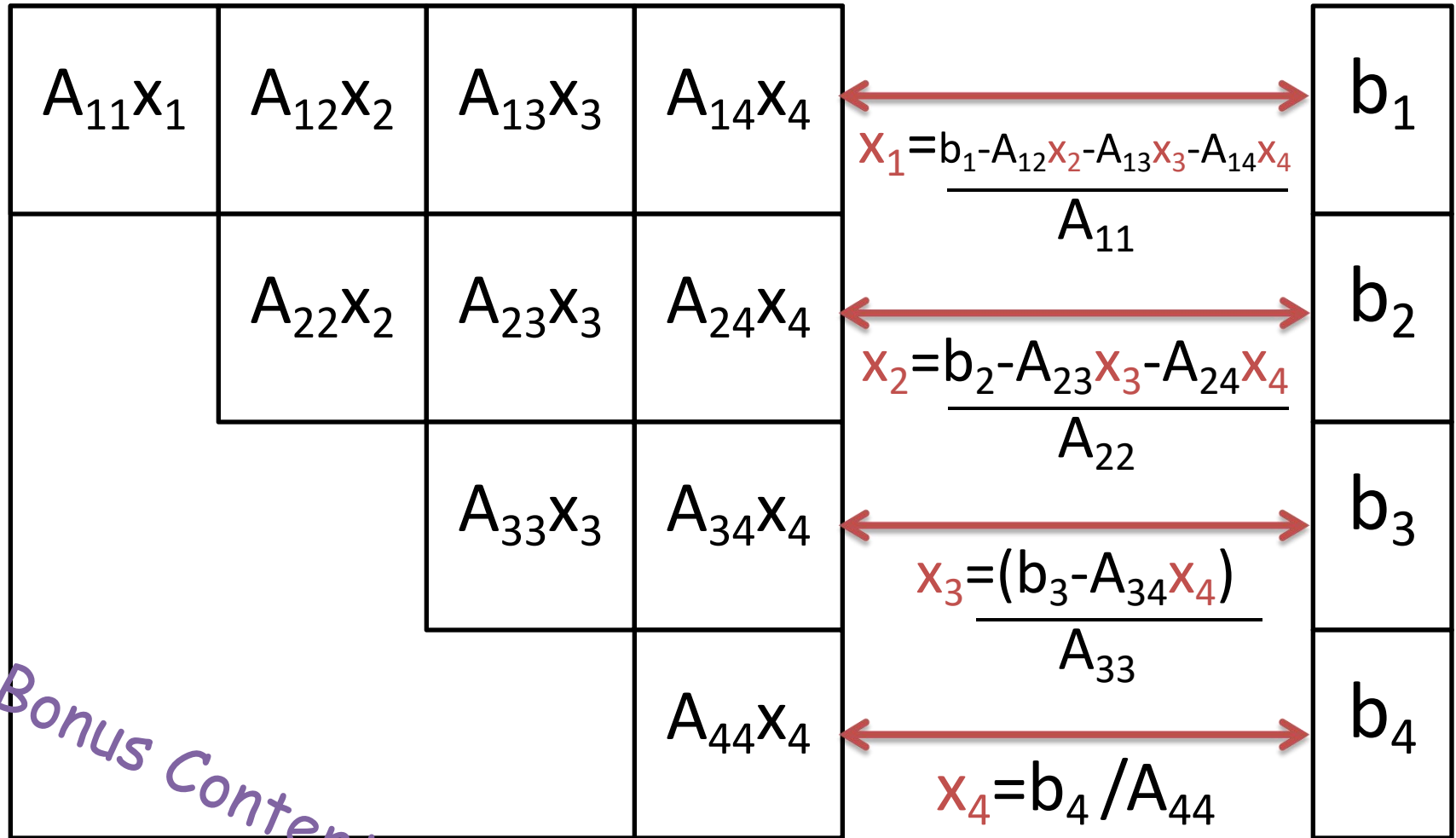
x_1
x_2
x_3
x_4

 $=$

b_1
b_2
b_3
b_4

Bonus Content

Solving Triangular System

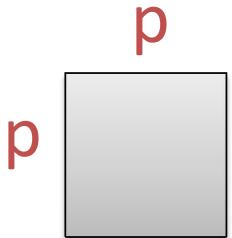



Bonus Content

Distributed Direct Solution (Map-Reduce)

$$\hat{\theta}_{\text{MLE}} = (X^T X)^{-1} X^T Y$$

- Distribution computations of sums:

 $C = X^T X = \sum_{i=1}^n x_i x_i^T$ $O(np^2)$

 $d = X^T y = \sum_{i=1}^n x_i y_i$ $O(np)$

- Solve system $C \theta_{\text{MLE}} = d$ on master. $O(p^3)$

Gradient Descent:

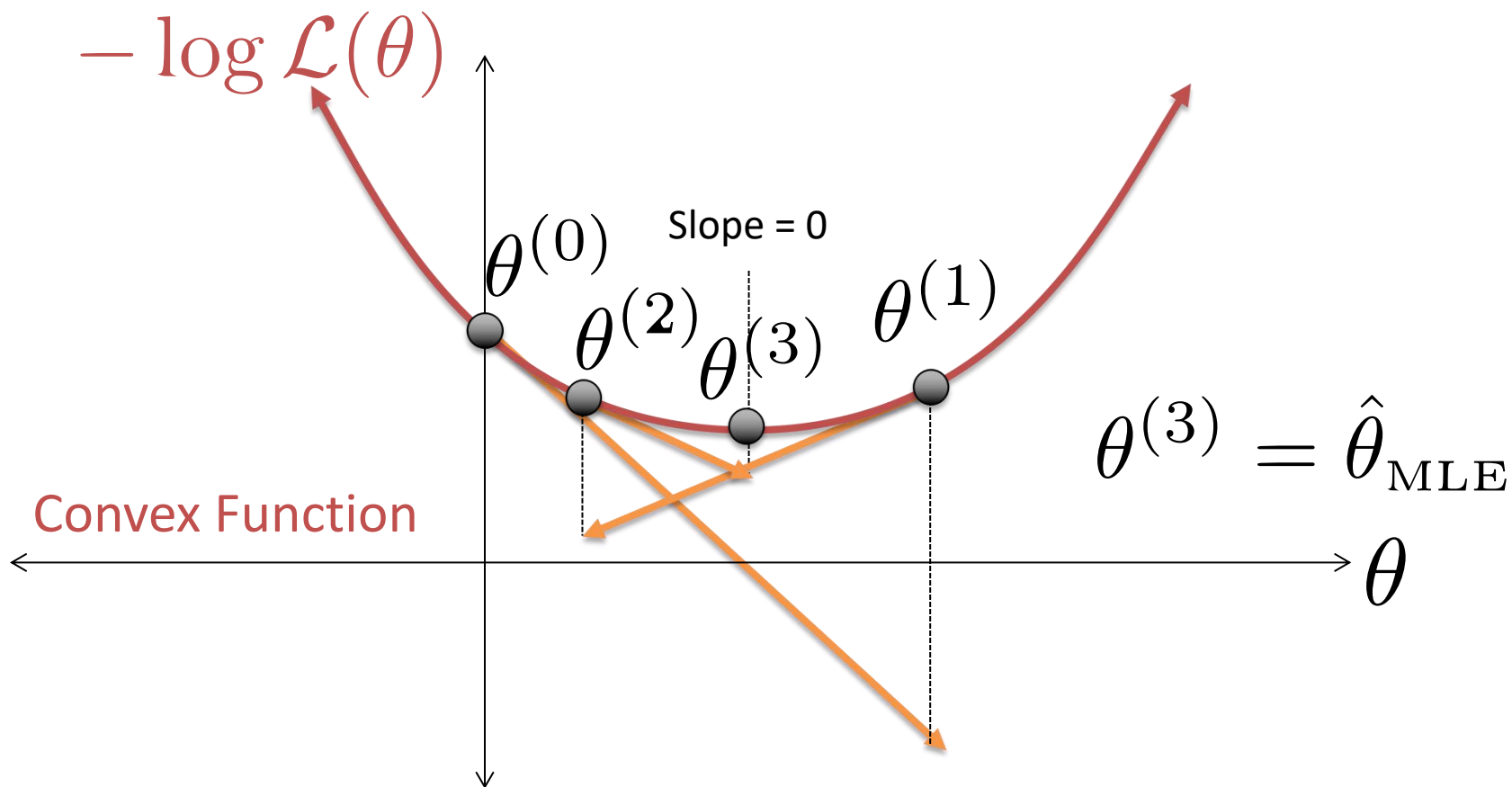
What if p is large? (e.g., $n/2$)

- The cost of $O(np^2) = O(n^3)$ could be prohibitive
- Solution: Iterative Methods
 - Gradient Descent:

For τ from 0 until *convergence*

$$\theta^{(\tau+1)} = \theta^{(\tau)} - \underset{\text{Learning rate}}{\rho(\tau)} \nabla \log \mathcal{L}(\theta^{(\tau)} | D)$$

Gradient Descent Illustrated:



Gradient Descent:

What if p is large? (e.g., $n/2$)

- The cost of $O(np^2) = O(n^3)$ could be prohibitive
- Solution: Iterative Methods
 - Gradient Descent:

For τ from 0 until *convergence*

$$\begin{aligned}\theta^{(\tau+1)} &= \theta^{(\tau)} - \rho(\tau) \nabla \log \mathcal{L}(\theta^{(\tau)} | D) \\ &= \theta^{(\tau)} + \rho(\tau) \underbrace{\frac{1}{n} \sum_{i=1}^n (y_i - \theta^{(\tau)T} x_i) x_i}_{\text{Estimate of the Gradient}} \quad O(np)\end{aligned}$$

- Can we do better?

Estimate of the Gradient

Stochastic Gradient Descent

- Construct noisy estimate of the gradient:

For τ from 0 until *convergence*

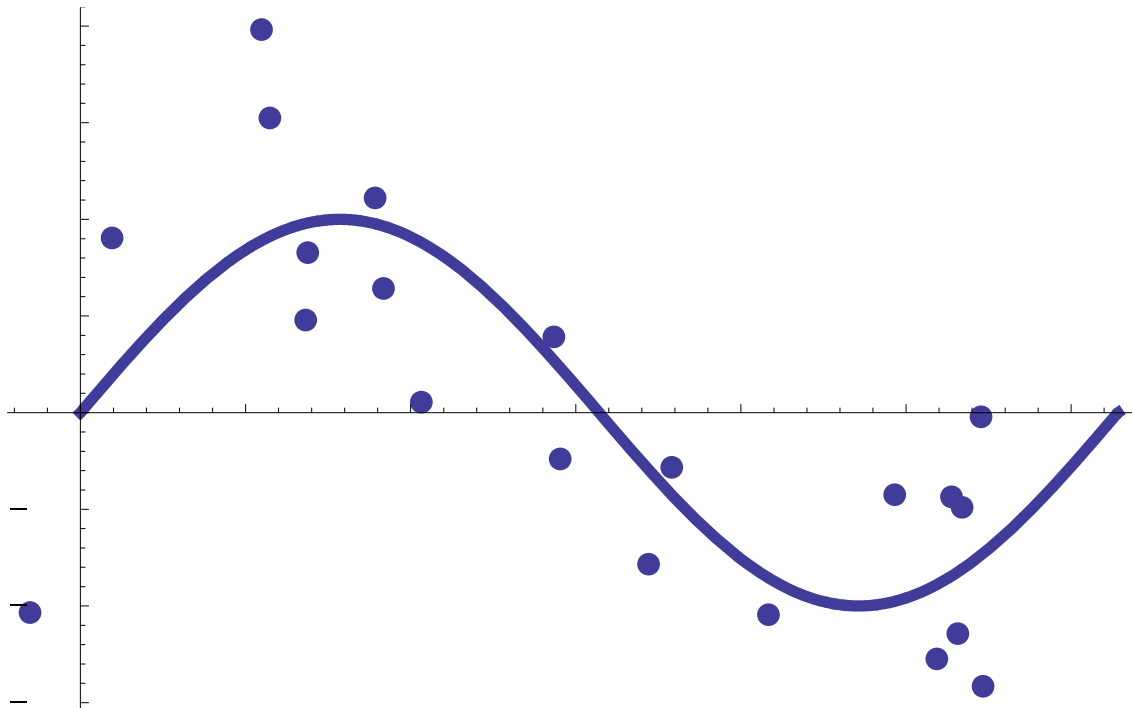
1) *pick a random i*

2) $\theta^{(\tau+1)} = \theta^{(\tau)} + \rho(\tau)(y_i - \theta^{(\tau)T}x_i)x_i$ $O(p)$

- Sensitive to choice of $\rho(\tau)$ typically ($\rho(\tau)=1/\tau$)
- Also known as Least-Mean-Squares (LMS)
- Applies to streaming data $O(p)$ storage

Fitting Non-linear Data

- What if Y has a non-linear response?



- Can we still use a linear model?

Transforming the Feature Space

- Transform features x_i

$$x_i = (X_{i,1}, X_{i,2}, \dots, X_{i,p})$$

- By applying non-linear transformation ϕ :

$$\phi : \mathbb{R}^p \rightarrow \mathbb{R}^k$$

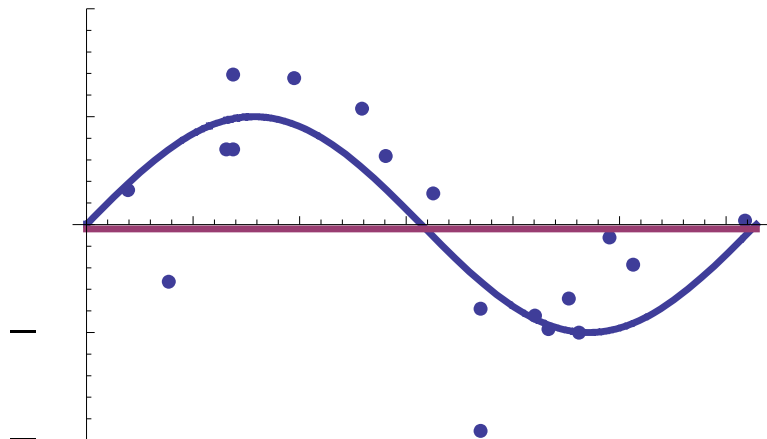
- Example:

$$\phi(x) = \{1, x, x^2, \dots, x^k\}$$

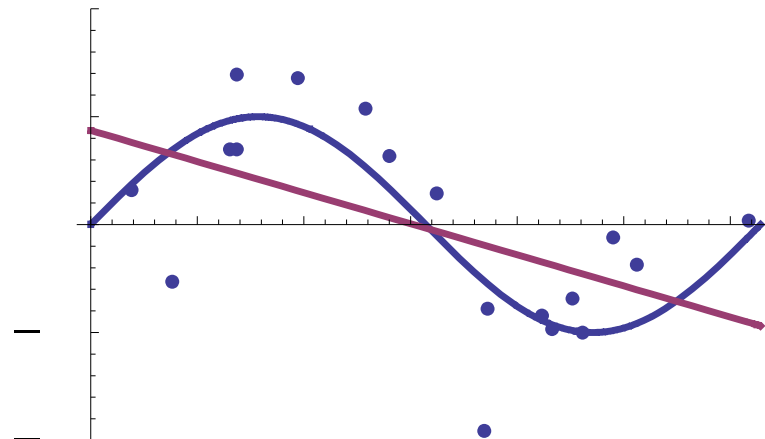
- others: splines, radial basis functions, ...
- Expert engineered features (modeling)

Under-fitting

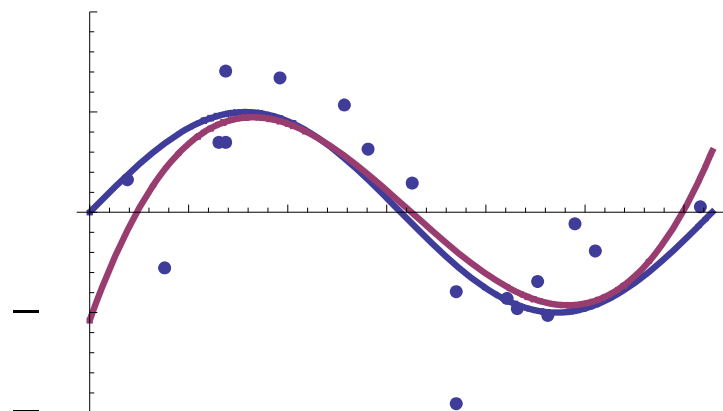
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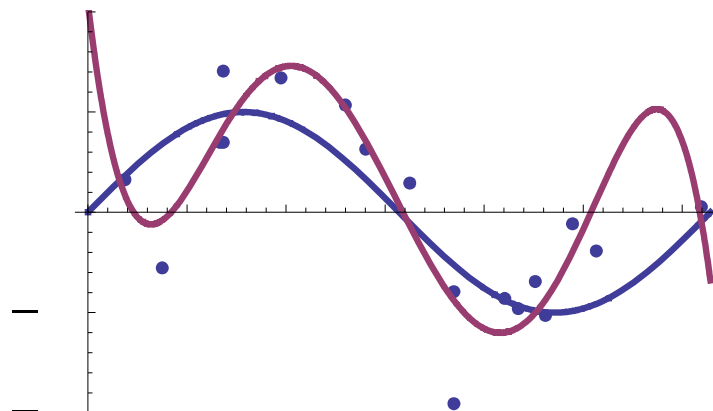
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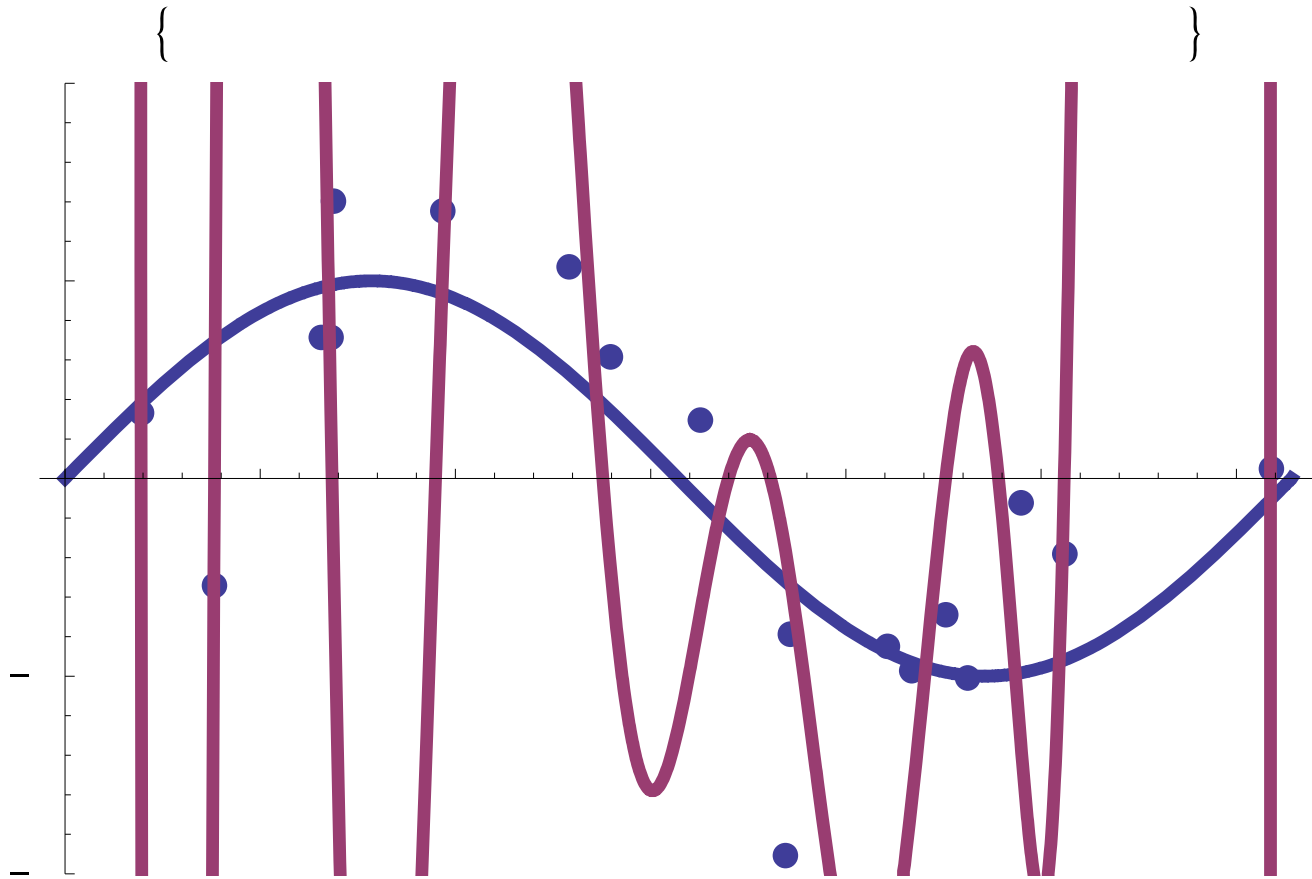


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Over-fitting

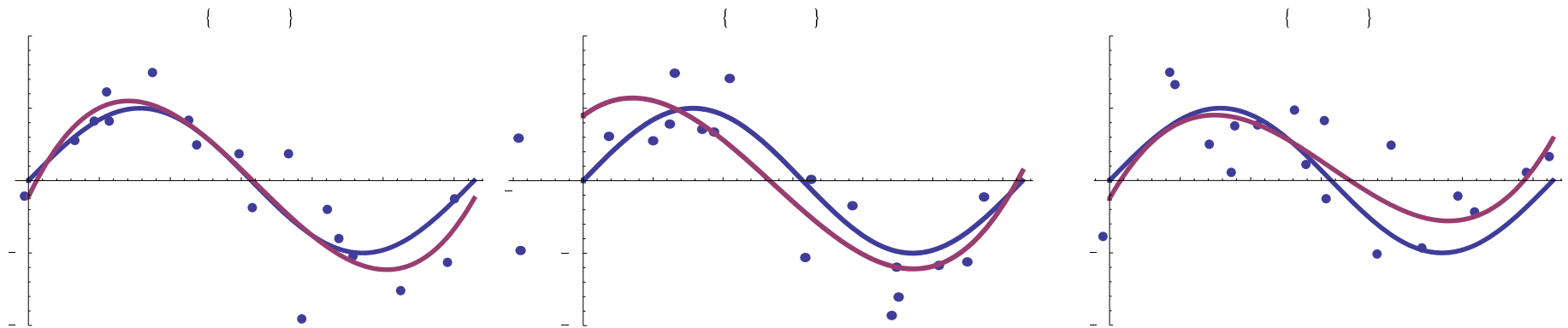
Really Over-fitting!



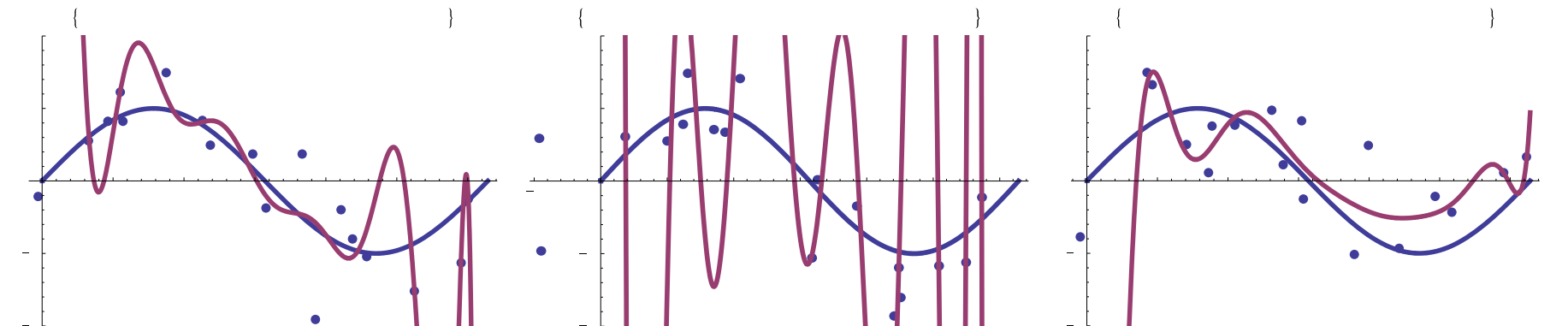
- Errors on training data are small
- But errors on new points are likely to be large

What if I train on different data?

Low Variability:



High Variability



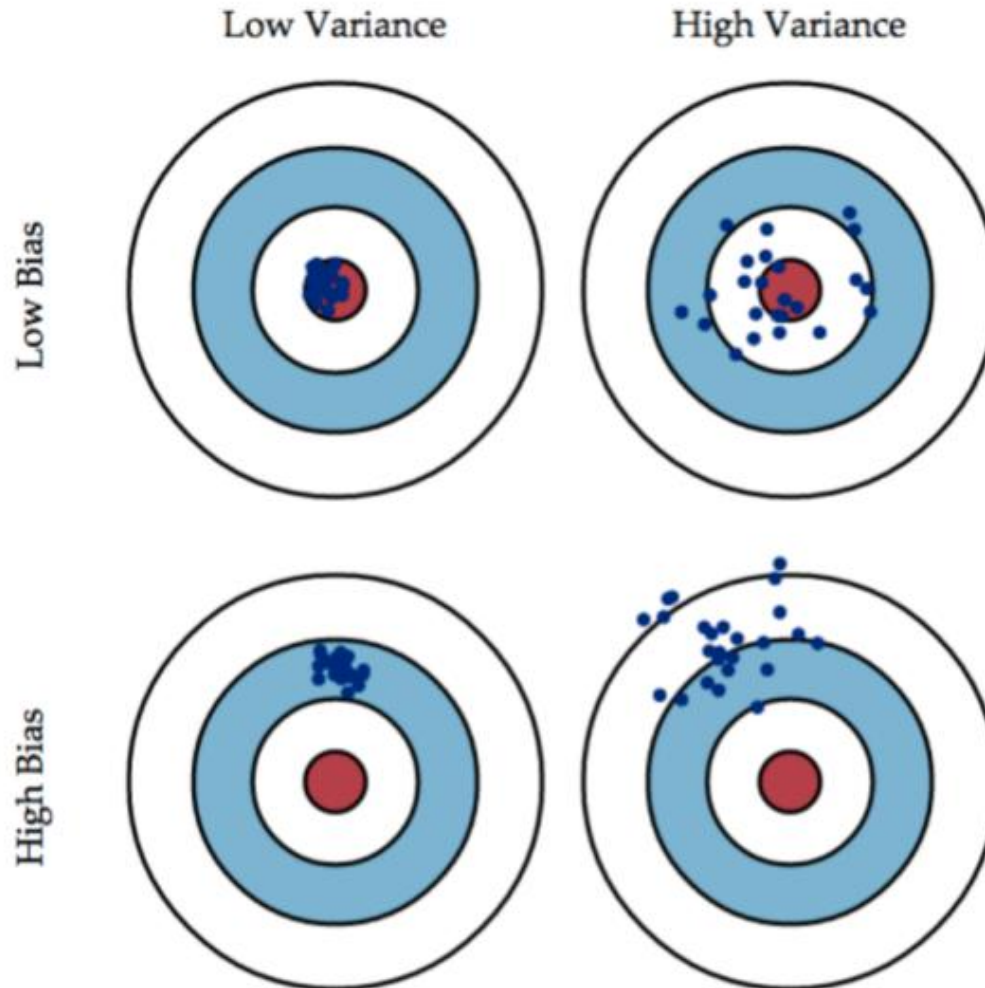
Bias-Variance Tradeoff

- So far we have minimized the error (loss) with respect to **training data**
 - Low training error does not imply good expected performance: **over-fitting**
- We would like to reason about the **expected loss (Prediction Risk)** over:
 - Training Data: $\{(y_1, x_1), \dots, (y_n, x_n)\}$
 - Test point: (y_*, x_*)
- We will decompose the expected loss into:

$$\mathbf{E}_{D, (y_*, x_*)} \left[(y_* - f(x_* | D))^2 \right] = \text{Noise} + \text{Bias}^2 + \text{Variance}$$

Bias-Variance Tradeoff

- Bias (偏差)、Error (误差)、Variance (方差)



- Define (unobserved) the true model (h):

$$y_* = h(x_*) + \epsilon_*$$

Assume 0 mean noise
[bias goes in $h(x_*)$]

- Completed the squares with: $h(x_*) = h_*$

$$\mathbf{E}_{D, (y_*, x_*)} [(y_* - f(x_* | D))^2] \quad \text{Expected Loss}$$

$$= \mathbf{E}_{D, (y_*, x_*)} [(y_* \underbrace{- h(x_*)}_a + \underbrace{h(x_*) - f(x_* | D)}_b)^2]$$

$$(a + b)^2 = a^2 + b^2 + 2ab$$

$$= \mathbf{E}_{\epsilon_*} [(y_* - h(x_*))^2] + \mathbf{E}_D [(h(x_*) - f(x_* | D))^2] \\ + 2\mathbf{E}_{D, (y_*, x_*)} [y_* h_* - y_* f_* - h_* h_* + h_* f_*]$$

- Define (unobserved) the true model (h):

$$y_* = h(x_*) + \epsilon_*$$

- Completed the squares with: $h(x_*) = h_*$

$$\mathbf{E}_{D, (y_*, x_*)} [(y_* - f(x_*|D))^2] \quad \text{Expected Loss}$$

$$= \mathbf{E}_{D, (y_*, x_*)} [(y_* - h(x_*) + h(x_*) - f(x_*|D))^2]$$

$$= \mathbf{E}_{\epsilon_*} [(y_* - h(x_*))^2] + \mathbf{E}_D [(h(x_*) - f(x_*|D))^2]$$

$$+ 2\mathbf{E}_{D, (y_*, x_*)} [y_* h_* - y_* f_* - h_* h_* + h_* f_*]$$

Substitute defn. $y_* = h_* + \epsilon_*$

$$\mathbf{E} [(h_* + \epsilon_*)h_* - (h_* + \epsilon_*)f_* - h_* h_* + h_* f_*] =$$

$$\cancel{h_* h_*} + \mathbf{E}[\epsilon_*] h_* - h_* \mathbf{E}[f_*] - \mathbf{E}[\epsilon_*] f_* - \cancel{h_* h_*} + h_* \mathbf{E}[f_*]$$

- Define (unobserved) the true model (h):

$$y_* = h(x_*) + \epsilon_*$$

- Completed the squares with: $h(x_*) = h_*$

$$\mathbf{E}_{D, (y_*, x_*)} [(y_* - f(x_*|D))^2] \quad \text{Expected Loss}$$

$$= \mathbf{E}_{D, (y_*, x_*)} [(y_* - h(x_*) + h(x_*) - f(x_*|D))^2]$$

$$= \underbrace{\mathbf{E}_{\epsilon_*} [(y_* - h(x_*))^2]}_{\text{Noise Term}} + \underbrace{\mathbf{E}_D [(h(x_*) - f(x_*|D))^2]}_{\text{Model Estimation Error}}$$

Noise Term
(out of our control)



Model Estimation Error
(we want to minimize this)

Expand

- Minimum error is governed by the noise.

- Expanding on the model estimation error:

$$\mathbf{E}_D [(h(x_*) - f(x_*|D))^2]$$

- Completing the squares with $\mathbf{E} [f(x_*|D)] = \bar{f}_*$

$$\begin{aligned} & \mathbf{E}_D [(h(x_*) - f(x_*|D))^2] \\ &= \mathbf{E} [(h(x_*) - \mathbf{E} [f(x_*|D)] + \mathbf{E} [f(x_*|D)] - f(x_*|D))^2] \\ &= \mathbf{E} [(h(x_*) - \mathbf{E} [f(x_*|D)])^2] + \mathbf{E} [(f(x_*|D) - \mathbf{E} [f(x_*|D)])^2] \\ & \quad + 2\mathbf{E} [h_* \bar{f}_* - h_* f_* - \bar{f}_* f_* + \bar{f}_*^2] \\ & \qquad \qquad \qquad = h_* \bar{f}_* - h_* \mathbf{E} [f_*] - \bar{f}_* \mathbf{E} [f_*] + \bar{f}_*^2 = \\ & \qquad \qquad \qquad h_* \bar{f}_* - h_* \bar{f}_* - \bar{f}_* \bar{f}_* + \bar{f}_*^2 = 0 \end{aligned}$$

- Expanding on the model estimation error:

$$\mathbf{E}_D [(h(x_*) - f(x_*|D))^2]$$

- Completing the squares with $\mathbf{E} [f(x_*|D)] = \bar{f}_*$

$$\begin{aligned} & \mathbf{E}_D [(h(x_*) - f(x_*|D))^2] \\ &= \underbrace{\mathbf{E} [(h(x_*) - \mathbf{E} [f(x_*|D)])^2]}_{(h(x_*) - \mathbf{E} [f(x_*|D)])^2} + \mathbf{E} [(f(x_*|D) - \mathbf{E} [f(x_*|D)])^2] \end{aligned}$$

- Expanding on the model estimation error:

$$\mathbf{E}_D [(h(x_*) - f(x_*|D))^2]$$

- Completing the squares with $\mathbf{E} [f(x_*|D)] = \bar{f}_*$

$$\begin{aligned} \mathbf{E}_D [(h(x_*) - f(x_*|D))^2] \\ = \underbrace{(h(x_*) - \mathbf{E} [f(x_*|D)])^2}_{(\text{Bias})^2} + \underbrace{\mathbf{E} [(f(x_*|D) - \mathbf{E} [f(x_*|D)])^2]}_{\text{Variance}} \end{aligned}$$

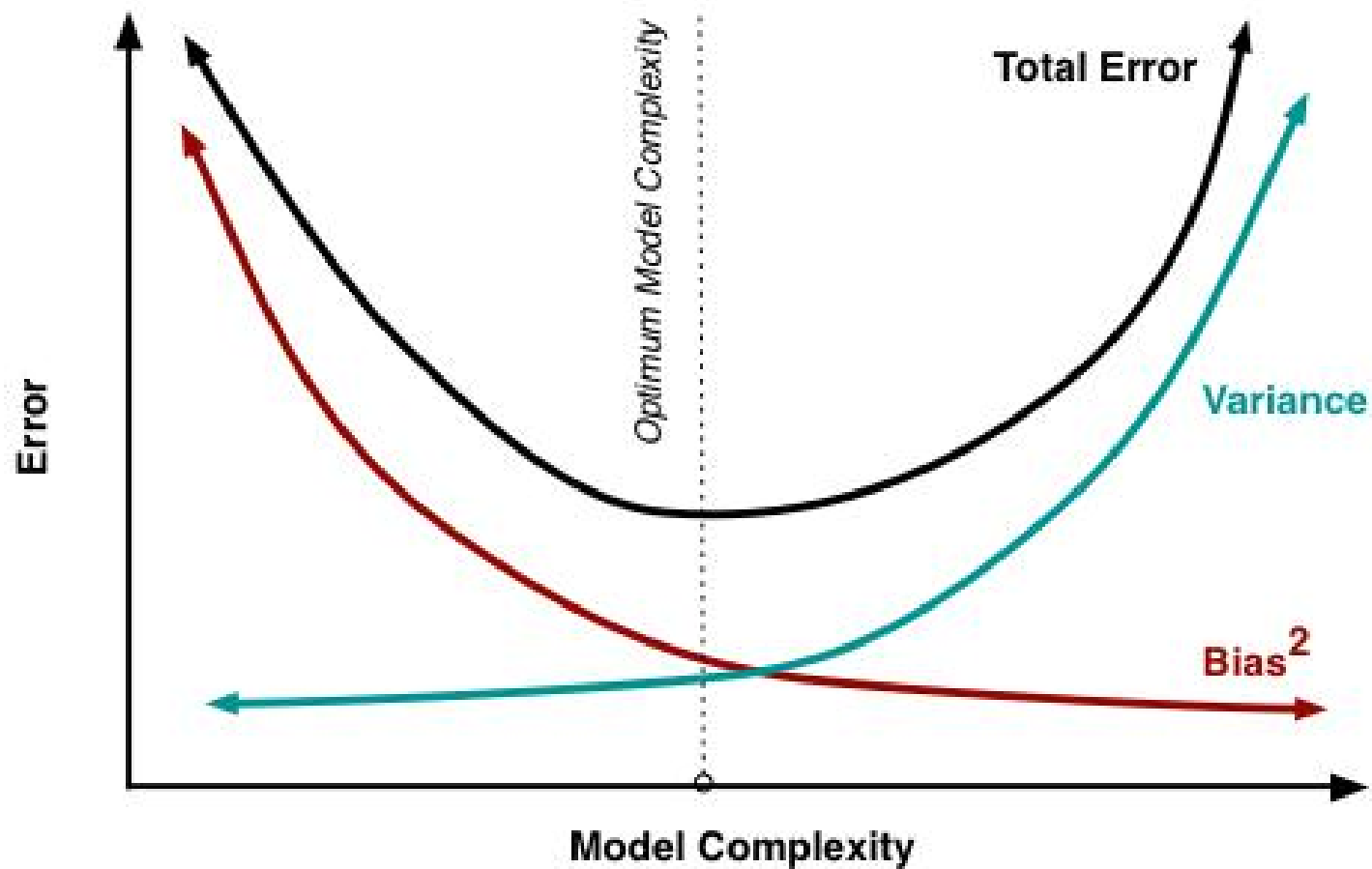
- Tradeoff between bias and variance:
 - **Simple Models:** High Bias, Low Variance
 - **Complex Models:** Low Bias, High Variance

Summary of Bias Variance Tradeoff

$$\begin{aligned}\mathbf{E}_{D, (y_*, x_*)} [(y_* - f(x_*|D))^2] &= \text{Expected Loss} \\ &\quad \mathbf{E}_{\epsilon_*} [(y_* - h(x_*))^2] \quad \text{Noise} \\ &\quad + (h(x_*) - \mathbf{E}_D [f(x_*|D)])^2 \quad (\text{Bias})^2 \\ &\quad + \mathbf{E}_D [(f(x_*|D) - \mathbf{E}_D [f(x_*|D)])^2] \quad \text{Variance}\end{aligned}$$

- Choice of models balances bias and variance.
 - Over-fitting → Variance is too High
 - Under-fitting → Bias is too High

Bias Variance Plot



Analyze bias of $f(x_*|D) = x_*^T \hat{\theta}_{\text{MLE}}$

- Assume a true model is linear: $h(x_*) = x_*^T \theta$

$$\text{bias} = h(x_*) - \mathbf{E}_D [f(x_*|D)]$$

$$= x_*^T \theta - \mathbf{E}_D [x_*^T \hat{\theta}_{\text{MLE}}]$$

$$= x_*^T \theta - \mathbf{E}_D [x_*^T (X^T X)^{-1} X^T Y]$$

$$= x_*^T \theta - \mathbf{E}_D [x_*^T (X^T X)^{-1} X^T (X\theta + \epsilon)]$$

$$= x_*^T \theta - \mathbf{E}_D [x_*^T (X^T X)^{-1} X^T X\theta + x_*^T (X^T X)^{-1} X^T \epsilon]$$

$$= x_*^T \theta - \mathbf{E}_D [x_*^T \theta + x_*^T (X^T X)^{-1} X^T \epsilon]$$

$$= x_*^T \theta - x_*^T \theta + x_*^T (X^T X)^{-1} X^T \mathbf{E}_D [\epsilon]$$

$$= x_*^T \theta - x_*^T \theta = 0$$

$\hat{\theta}_{\text{MLE}}$ is unbiased!

Substitute MLE

Plug in definition of Y

Expand and cancel

Assumption:

$$\mathbf{E}_D [\epsilon] = 0$$

Analyze Variance of $f(x_*|D) = x_*^T \hat{\theta}_{\text{MLE}}$

- Assume a true model is linear: $h(x_*) = x_*^T \theta$

$$\text{Var.} = \mathbf{E} \left[(f(x_*|D) - \mathbf{E}_D [f(x_*|D)])^2 \right]$$

$$= \mathbf{E} \left[(x_*^T \hat{\theta}_{\text{MLE}} - x_*^T \theta)^2 \right] \quad \leftarrow \text{Substitute MLE + unbiased result}$$

$$= \mathbf{E} \left[(x_*^T (X^T X)^{-1} X^T Y - x_*^T \theta)^2 \right] \quad \leftarrow \text{Plug in definition of } Y$$

$$= \mathbf{E} \left[(x_*^T (X^T X)^{-1} X^T (X\theta + \epsilon) - x_*^T \theta)^2 \right]$$

$$= \mathbf{E} \left[(x_*^T \theta + x_*^T (X^T X)^{-1} X^T \epsilon - x_*^T \theta)^2 \right]$$

$$= \mathbf{E} \left[(x_*^T (X^T X)^{-1} X^T \epsilon)^2 \right]$$

- Use property of scalar: $a^2 = a a^T$

Expand and cancel

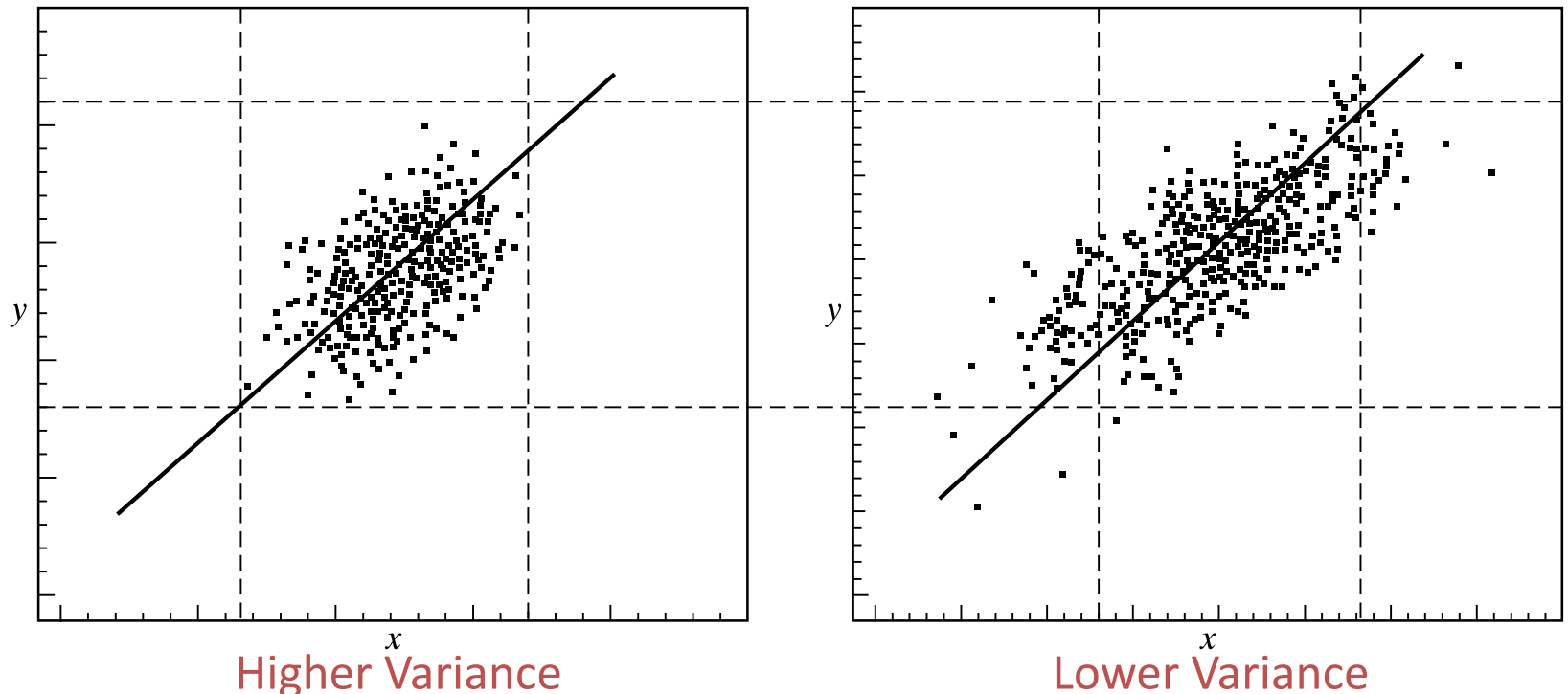
Analyze Variance of $f(x_*|D) = x_*^T \hat{\theta}_{\text{MLE}}$

- Use property of scalar: $a^2 = a a^T$

$$\begin{aligned}\text{Var.} &= \mathbf{E} [(f(x_*|D) - \mathbf{E}_D [f(x_*|D)])^2] \\&= \mathbf{E} [(x_*^T (X^T X)^{-1} X^T \epsilon)^2] \\&= \mathbf{E} [(x_*^T (X^T X)^{-1} X^T \epsilon)(x_*^T (X^T X)^{-1} X^T \epsilon)^T] \\&= \mathbf{E} [x_*^T (X^T X)^{-1} X^T \epsilon \epsilon^T (x_*^T (X^T X)^{-1} X^T)^T] \\&= x_*^T (X^T X)^{-1} X^T \mathbf{E} [\epsilon \epsilon^T] (x_*^T (X^T X)^{-1} X^T)^T \\&= x_*^T (X^T X)^{-1} X^T \sigma_\epsilon^2 I (x_*^T (X^T X)^{-1} X^T)^T \\&= \sigma_\epsilon^2 x_*^T (X^T X)^{-1} X^T X (x_*^T (X^T X)^{-1})^T \\&= \sigma_\epsilon^2 x_*^T (x_*^T (X^T X)^{-1})^T \\&= \sigma_\epsilon^2 x_*^T (X^T X)^{-1} x_*\end{aligned}$$

Consequence of Variance Calculation

$$\begin{aligned}\text{Var.} &= \mathbf{E} \left[(f(x_*|D) - \mathbf{E}_D [f(x_*|D)])^2 \right] \\ &= \sigma_\epsilon^2 x_*^T (X^T X)^{-1} x_*\end{aligned}$$



Analyze Variance of $f(x_*|D) = x_*^T \hat{\theta}_{\text{MLE}}$

- Assume a true model is linear: $h(x_*) = x_*^T \theta$

$$\text{Var.} = \mathbf{Var} [f(x_*|D) - \mathbf{E}_D [f(x_*|D)]]$$

$$= \mathbf{Var} [x_*^T \hat{\theta}_{\text{MLE}} - x_*^T \theta] \quad \leftarrow \text{Substitute MLE + unbiased result}$$

$$= \mathbf{Var} [x_*^T (X^T X)^{-1} X^T Y - x_*^T \theta] \quad \leftarrow \text{Plug in definition of } Y$$

$$= \mathbf{Var} [x_*^T (X^T X)^{-1} X^T (X\theta + \epsilon) - x_*^T \theta]$$

$$= \mathbf{Var} [x_*^T \theta + x_*^T (X^T X)^{-1} X^T \epsilon - x_*^T \theta]$$

$$= \mathbf{Var} [x_*^T (X^T X)^{-1} X^T \epsilon]$$

- Next: use matrix variance identity

Expand and cancel

Analyze Variance of $f(x_*|D) = x_*^T \hat{\theta}_{\text{MLE}}$

- Define: $A = x_*^T (X^T X)^{-1} X^T$

$$\text{Var.} = \mathbf{Var} [x_*^T (X^T X)^{-1} X^T \epsilon] = \mathbf{Var} [A\epsilon]$$

- Use matrix variance identity: $\mathbf{Var} [A\epsilon] = A\Sigma_\epsilon A^T$

$$\text{Var.} = A\Sigma_\epsilon A^T = \sigma_\epsilon^2 AA^T$$

$$= \sigma_\epsilon^2 x_*^T (X^T X)^{-1} X^T (x_*^T (X^T X)^{-1} X^T)^T$$

$$= \sigma_\epsilon^2 x_*^T (X^T X)^{-1} X^T X (x_*^T (X^T X)^{-1})^T$$

$$= \sigma_\epsilon^2 x_*^T (x_*^T (X^T X)^{-1})^T$$

$$= \sigma_\epsilon^2 x_*^T (X^T X)^{-1} x_*$$

- If we assume x is iid $N(0, 1)$: $\mathbf{E}_{X, x_*} [\text{Var.}] = \sigma_\epsilon^2 \frac{p}{n}$

Deriving the final identity

- Assume x_i and x_* are $N(0,1)$

$$\begin{aligned}\mathbf{E}_{X, x_*} [\text{Var.}] &= \sigma_\epsilon^2 \mathbf{E}_{X, x_*} [x_*^T (X^T X)^{-1} x_*] \\&= \sigma_\epsilon^2 \mathbf{E}_{X, x_*} [\text{tr}(x_* x_*^T (X^T X)^{-1})] \\&= \sigma_\epsilon^2 \text{tr}(\mathbf{E}_{X, x_*} [x_* x_*^T (X^T X)^{-1}]) \\&= \sigma_\epsilon^2 \text{tr}(\mathbf{E}_{x_*} [x_* x_*^T] \mathbf{E}_X [(X^T X)^{-1}]) \\&= \frac{\sigma_\epsilon^2}{n} \text{tr}(\mathbf{E}_{x_*} [x_* x_*^T]) \\&= \frac{\sigma_\epsilon^2}{n} p\end{aligned}$$

Summary

- Least-Square Regression is Unbiased:

$$\mathbf{E}_D \left[x_*^T \hat{\theta}_{\text{MLE}} \right] = x_*^T \theta$$

- Variance depends on:

$$\begin{aligned} \mathbf{E} \left[(f(x_*|D) - \mathbf{E} [f(x_*|D)])^2 \right] &= \sigma_\epsilon^2 x_*^T (X^T X)^{-1} x_* \\ &\approx \sigma_\epsilon^2 \frac{p}{n} \end{aligned}$$

- Number of data-points n
- Dimensionality p
- Not on observations Y

Gauss-Markov Theorem

- The linear model:

$$f(x_*) = x_*^T \hat{\theta}_{\text{MLE}} = x_*^T (X^T X)^{-1} X^T Y$$

has the **minimum variance** among all **unbiased** linear estimators

– Note that this is linear in Y

- **BLUE: Best Linear Unbiased Estimator**

Summary

- Introduced the Least-Square regression model
 - Maximum Likelihood: Gaussian Noise
 - Loss Function: Squared Error
 - Geometric Interpretation: Minimizing Projection
- Derived the normal equations:
 - Walked through process of constructing MLE
 - Discussed efficient computation of the MLE
- Introduced basis functions for non-linearity
 - Demonstrated issues with over-fitting
- Derived the classic bias-variance tradeoff
 - Applied to least-squares model



SUPPORT
VECTOR
MACHINES

REPEAL
POWER
LAWS

END
DUALITY
GAP

Map Reduce
Map Reuse
Map Recycle
Combiner Data Partitioning

BAYSIANS
AGAINST
DISCRIMINATION

FREE
VARIABLES!

BAN
GENETIC
ALGORITHMS

Logistic Regression

Classification

- **Learn:** $h: \mathbf{X} \rightarrow Y$
 - \mathbf{X} – features
 - Y – target classes
- Suppose you know $P(Y | \mathbf{X})$ exactly, how should you classify?
 - Bayes classifier:
$$y^* = h_{bayes}(x) = \arg \max_y P(Y = y | X = x)$$
- Why?

Generative vs. Discriminative Classifiers - Intuition

- Generative classifier, e.g., Naïve Bayes:
 - Assume some functional form for **$P(\mathbf{X}|\mathbf{Y})$** , **$P(\mathbf{Y})$**
 - Estimate parameters of $P(\mathbf{X}|\mathbf{Y})$, $P(\mathbf{Y})$ directly from training data
 - Use Bayes rule to calculate $P(\mathbf{Y}|\mathbf{X}=\mathbf{x})$
 - This is ‘generative’ model
 - Indirect computation of $P(\mathbf{Y}|\mathbf{X})$ through Bayes rule
 - But, can generate a sample of the data, $P(\mathbf{X}) = \sum_y P(y)P(\mathbf{X} | y)$
- Discriminative classifier, e.g., Logistic Regression:
 - Assume some functional form for **$P(\mathbf{Y}|\mathbf{X})$**
 - Estimate parameters of $P(\mathbf{Y}|\mathbf{X})$ directly from training data
 - This is the ‘discriminative’ model
 - Directly learn $P(\mathbf{Y}|\mathbf{X})$
 - But cannot sample data, because $P(\mathbf{X})$ is not available

The Naïve Bayes Classifier

- Given:
 - Prior $P(Y)$
 - n conditionally independent features X given the class Y
 - For each X_i , we have likelihood $P(X_i | Y)$

- Decision rule:

$$y^* = h_{NB}(x) = \arg \max_y P(y)P(x_1, \dots, x_n | y)$$

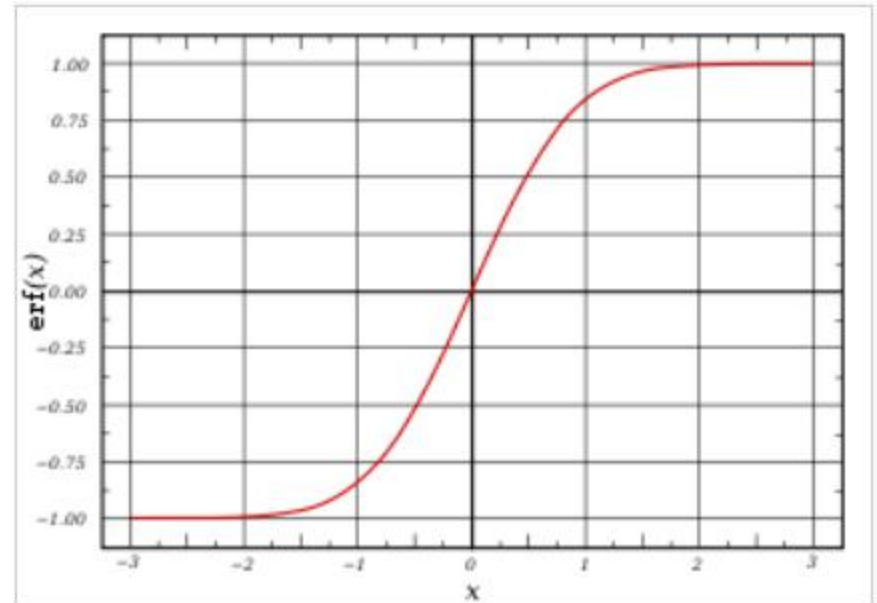
$$= \arg \max_y P(y) \prod_i P(x_i | y)$$

- If assumption holds, NB is optimal classifier!

Logistic Regression

- Let X be the data instance, and Y be the class label:
Learn $P(Y|X)$ directly
 - Let $W = (W_1, W_2, \dots, W_n)$, $X = (X_1, X_2, \dots, X_n)$, $\mathbf{W}\mathbf{X}$ is the dot product
 - Sigmoid function:

$$P(Y = 1 | \mathbf{X}) = \frac{1}{1 + e^{-\mathbf{W}\mathbf{X}}}$$



Logistic Regression

- In logistic regression, we learn the conditional distribution $P(y|x)$
- Let $p_y(x;w)$ be our estimate of $P(y|x)$, where w is a vector of adjustable parameters.
- Assume there are two classes, $y = 0$ and $y = 1$ and

$$p_1(\mathbf{x}; \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w}\mathbf{x}}} \quad p_0(\mathbf{x}; \mathbf{w}) = 1 - \frac{1}{1 + e^{-\mathbf{w}\mathbf{x}}}$$

- This is equivalent to

$$\log \frac{p_1(\mathbf{x}; \mathbf{w})}{p_0(\mathbf{x}; \mathbf{w})} = \mathbf{w}\mathbf{x}$$

- That is, the log odds of class 1 to class 0 is a linear function of x
- Q: How to find \mathbf{w} ?

Constructing a Learning Algorithm

- The conditional data likelihood is the probability of the observed Y values in the training data, conditioned on their corresponding X values. We choose parameters \mathbf{w} that satisfy

$$\mathbf{w} = \arg \max_{\mathbf{w}} \prod_l P(y^l | \mathbf{x}^l, \mathbf{w})$$

- where $\mathbf{w} = \langle w_0, w_1, \dots, w_n \rangle$ is the vector of parameters to be estimated, y^l denotes the observed value of Y in the l th training example, and \mathbf{x}^l denotes the observed value of \mathbf{X} in the l th training example

Constructing a Learning Algorithm

- Equivalently, we can work with the log of the conditional likelihood:

$$\mathbf{w} = \arg \max_{\mathbf{w}} \sum_l \ln P(y^l | \mathbf{x}^l, \mathbf{w})$$

- This conditional data log likelihood, which we will denote $l(\mathbf{w})$ can be written as

$$l(\mathbf{w}) = \sum_l y^l \ln P(y^l = 1 | \mathbf{x}^l, \mathbf{w}) + (1 - y^l) \ln P(y^l = 0 | \mathbf{x}^l, \mathbf{w})$$

- Note here we are utilizing the fact that Y can take only values 0 or 1, so only one of the two terms in the expression will be non-zero for any given y^l

Computing the Likelihood

- We can re-express the log of the conditional likelihood as:

$$\begin{aligned} l(\mathbf{w}) &= \sum_l y^l \ln P(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}) + (1 - y^l) \ln P(y^l = 0 \mid \mathbf{x}^l, \mathbf{w}) \\ &= \sum_l y^l \ln \frac{P(y^l = 1 \mid \mathbf{x}^l, \mathbf{w})}{P(y^l = 0 \mid \mathbf{x}^l, \mathbf{w})} + \ln P(y^l = 0 \mid \mathbf{x}^l, \mathbf{w}) \\ &= \sum_l y^l (w_0 + \sum_{i=1}^n w_i x_i^l) - \ln(1 + \exp(w_0 + \sum_{i=1}^n w_i x_i^l)) \end{aligned}$$

Fitting LR by Gradient Ascent

- Unfortunately, there is no closed form solution to maximizing $l(\mathbf{w})$ with respect to \mathbf{w} .
Therefore, one common approach is to use gradient ascent
- The i th component of the vector gradient has the form

$$\frac{\partial}{\partial w_i} l(\mathbf{w}) = \sum_l x_i^l (y^l - \hat{P}(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}))$$

Logistic Regression
prediction

Fitting LR by Gradient Ascent

- Given this formula for the derivative of each w_i , we can use standard gradient ascent to optimize the weights \mathbf{w} . Beginning with initial weights of zero, we repeatedly update the weights in the direction of the gradient, changing the i th weight according to

$$w_i \leftarrow w_i + \eta \sum_l x_i^l (y^l - \hat{P}(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}))$$

Regularization in Logistic Regression

- Overfitting the training data is a problem that can arise in Logistic Regression, especially when data has very high dimensions and is sparse.
- One approach to reducing overfitting is regularization, in which we create a modified “penalized log likelihood function,” which penalizes large values of \mathbf{w} .

$$\mathbf{w} = \arg \max_{\mathbf{w}} \sum_l \ln P(y^l | \mathbf{x}^l, \mathbf{w}) - \frac{\lambda}{2} \|\mathbf{w}\|^2$$

Regularization in Logistic Regression

- The derivative of this penalized log likelihood function is similar to our earlier derivative, with one additional penalty term

$$\frac{\partial}{\partial w_i} l(\mathbf{w}) = \sum_l x_i^l (y^l - \hat{P}(y^l = 1 | \mathbf{x}^l, \mathbf{w})) - \lambda w_i$$

- which gives us the modified gradient descent rule

$$w_i \leftarrow w_i + \eta \sum_l x_i^l (y^l - \hat{P}(y^l = 1 | \mathbf{x}^l, \mathbf{w})) - \eta \lambda w_i$$

Summary of Logistic Regression

- Learns the Conditional Probability Distribution $P(y|x)$
- Local Search.
 - Begins with initial weight vector.
 - Modifies it iteratively to maximize an objective function.
 - The objective function is the conditional log likelihood of the data – so the algorithm seeks the probability distribution $P(y|x)$ that is most likely given the data.

What you should know LR

- In general, NB and LR make different assumptions
 - NB: Features independent given class \rightarrow assumption on $P(X|Y)$
 - LR: Functional form of $P(Y|X)$, no assumption on $P(X|Y)$
- LR is a linear classifier
 - decision rule is a hyperplane
- LR optimized by conditional likelihood
 - no closed-form solution
 - concave \rightarrow global optimum with gradient ascent