UVA CS 4501: Machine Learning

Lecture 3: Linear Regression

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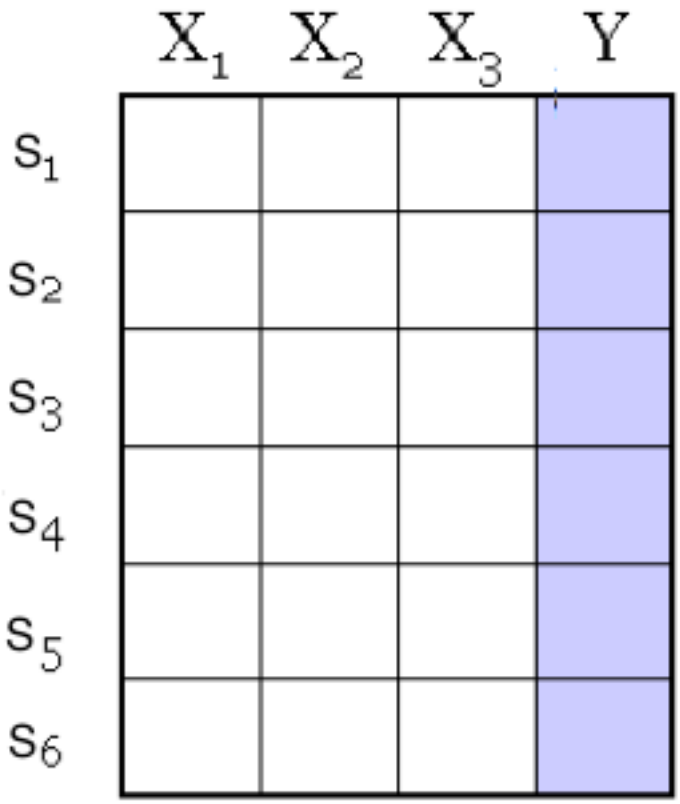
SUPERVISED LEARNING

$$f : X \longrightarrow Y$$

- Find function to map input space X to output space Y

- Generalisation: learn function / hypothesis from past data in order to "explain", "predict", "model" or "control" new data examples

KEY

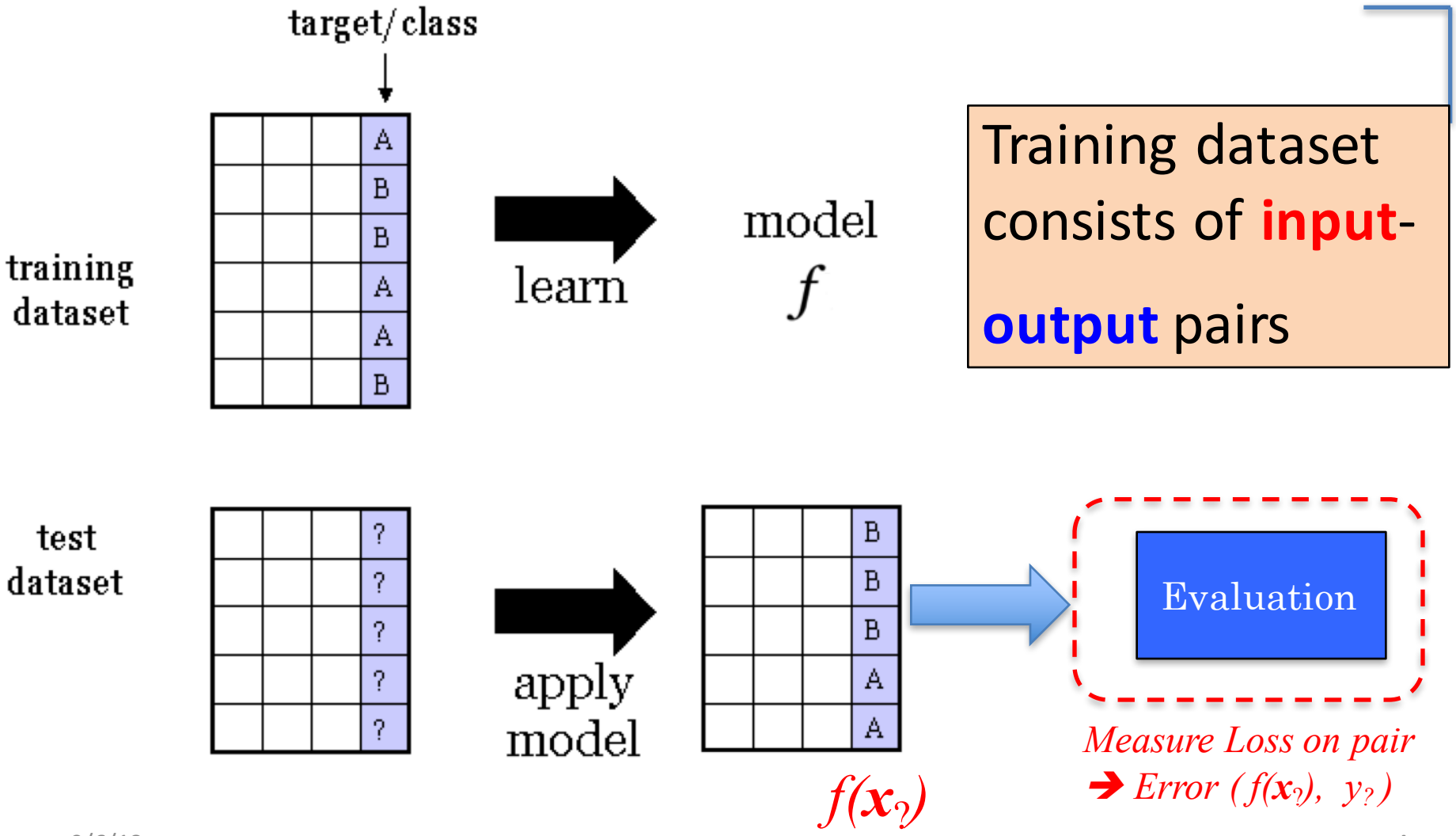


A Dataset

$$f : X \longrightarrow Y$$

- **Data***/points/instances/examples/samples/records*: [rows]
- **Features***/attributes/dimensions/independent variables/covariates/predictors/regressors*: [columns, except the last]
- **Target***/outcome/response/label/dependent variable*: special column to be predicted [last column]

SUPERVISED LEARNING



Notation

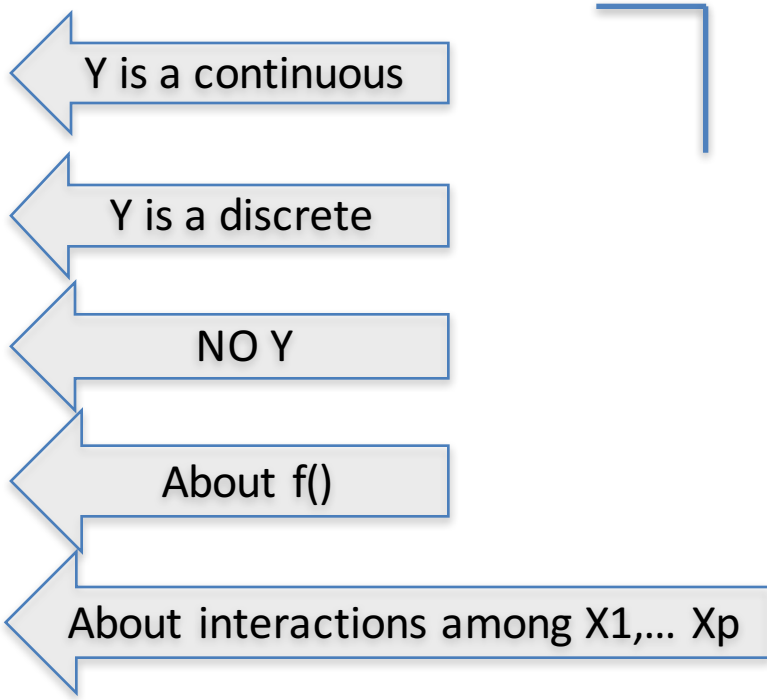
- Inputs
  - X, X_j (jth element of vector X) : random variables written in capital letter
  - p #inputs, N #observations
  - $\mathbf{X}$: matrix written in bold capital
  - Vectors are assumed to be column vectors
  - Discrete inputs often described by characteristic vector (dummy variables)

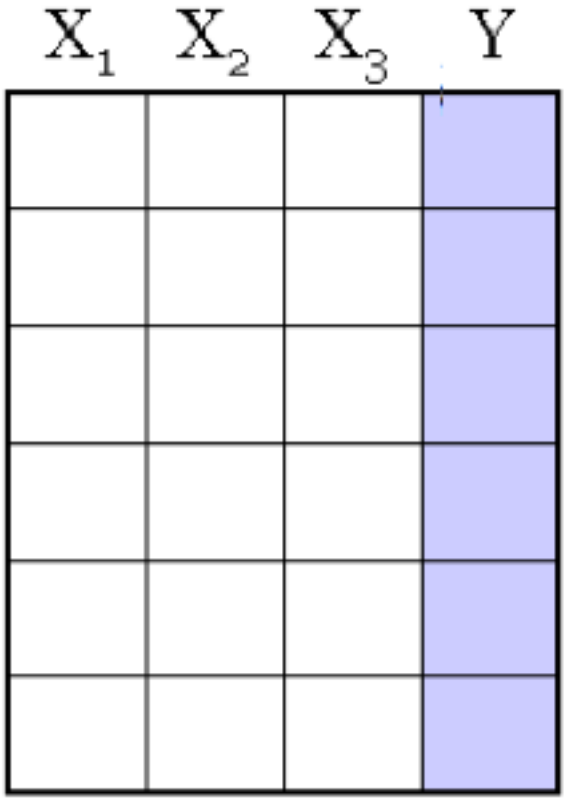
- Outputs
  - quantitative Y
  - qualitative C (for categorical)

- Observed variables written in lower case
  - The i-th observed value of X is $\boldsymbol{x}_i$ and can be a scalar or a vector

Where are we?
Five major sections of this course

- ❑ Regression (supervised)
- ❑ Classification (supervised)
- ❑ Unsupervised models
- ❑ Learning theory
- ❑ Graphical models





A Dataset for regression

$$f : X \longrightarrow Y$$

continuous valued variable

- **Data***/points/instances/examples/samples/records*: [rows]
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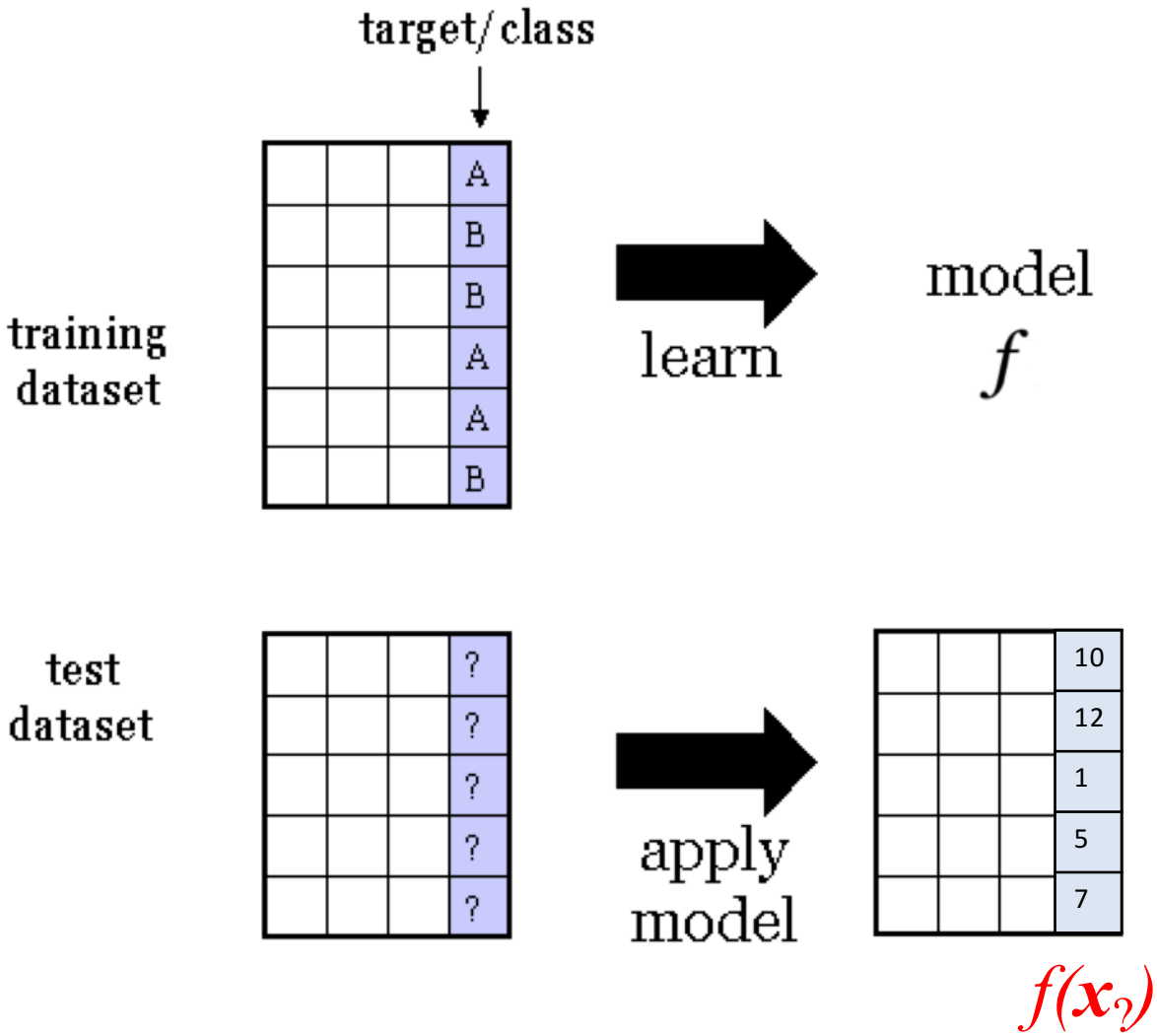
SUPERVISED Regression



Training dataset consists of **input-output** pairs

- When, target Y is a continuous target variable

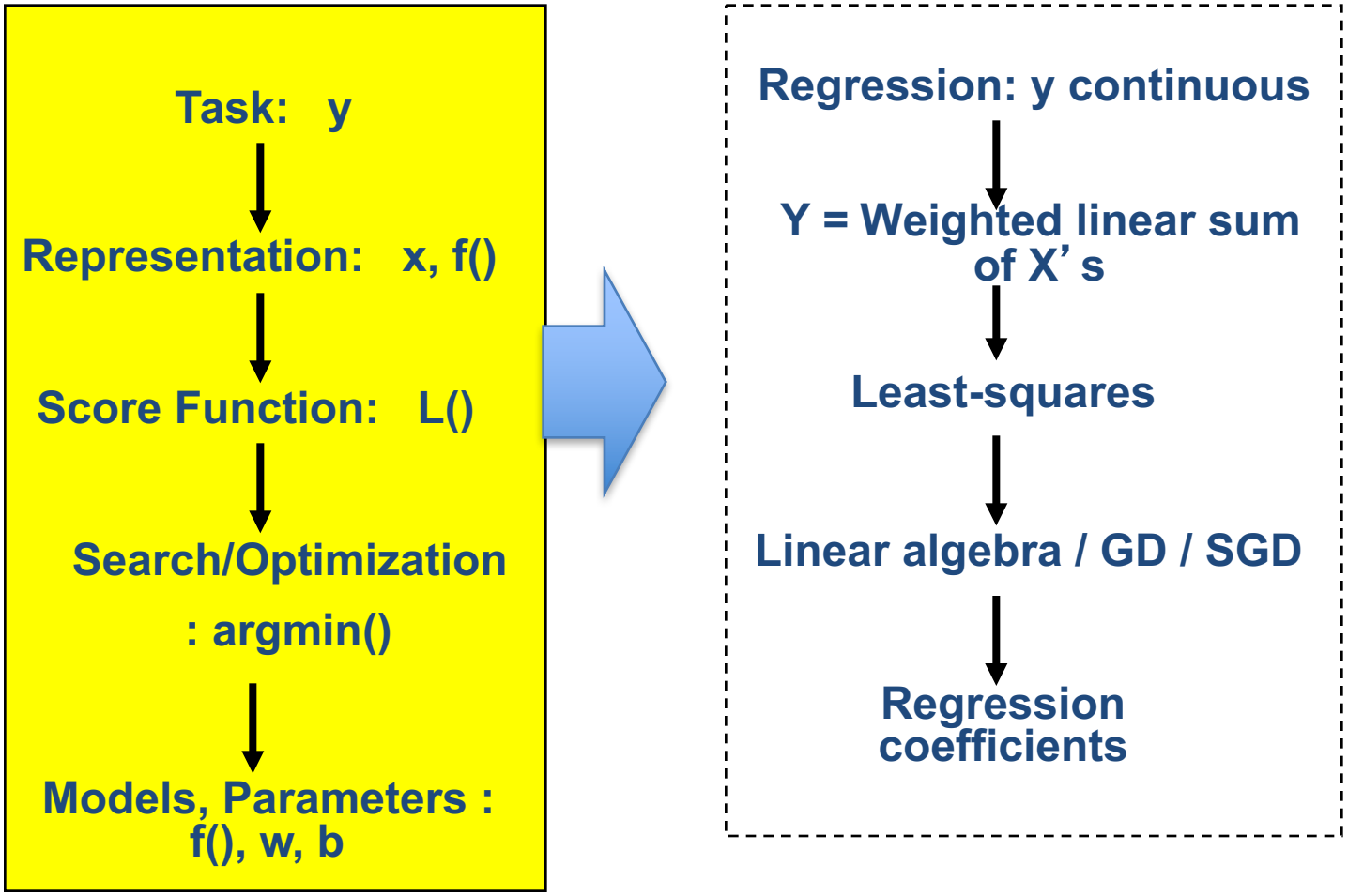
training dataset

$$\mathbf{X}_{train} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} \qquad \vec{y}_{train} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

test dataset

$$\mathbf{X}_{test} = \begin{bmatrix} -- & \mathbf{x}_{n+1}^T & -- \\ -- & \mathbf{x}_{n+2}^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_{n+m}^T & -- \end{bmatrix} \qquad \vec{y}_{test} = \begin{bmatrix} y_{n+1} \\ y_{n+2} \\ \vdots \\ y_{n+m} \end{bmatrix}$$

Multivariate Linear Regression Variations in a Nutshell



$$\hat{y} = f(x) = \theta^T x$$

Regression (supervised)

- Four ways to train / perform optimization for linear regression models
  - Normal Equation
  - Gradient Descent (GD)
  - Stochastic GD
  - Newton's method

} variations of $\arg\min_{\theta} L(\theta)$

- Supervised regression models
  - Linear regression (LR)
  - LR with non-linear basis functions
  - Locally weighted LR
  - LR with Regularizations

} variations of $f(x)$

→ variations of $L(\theta)$

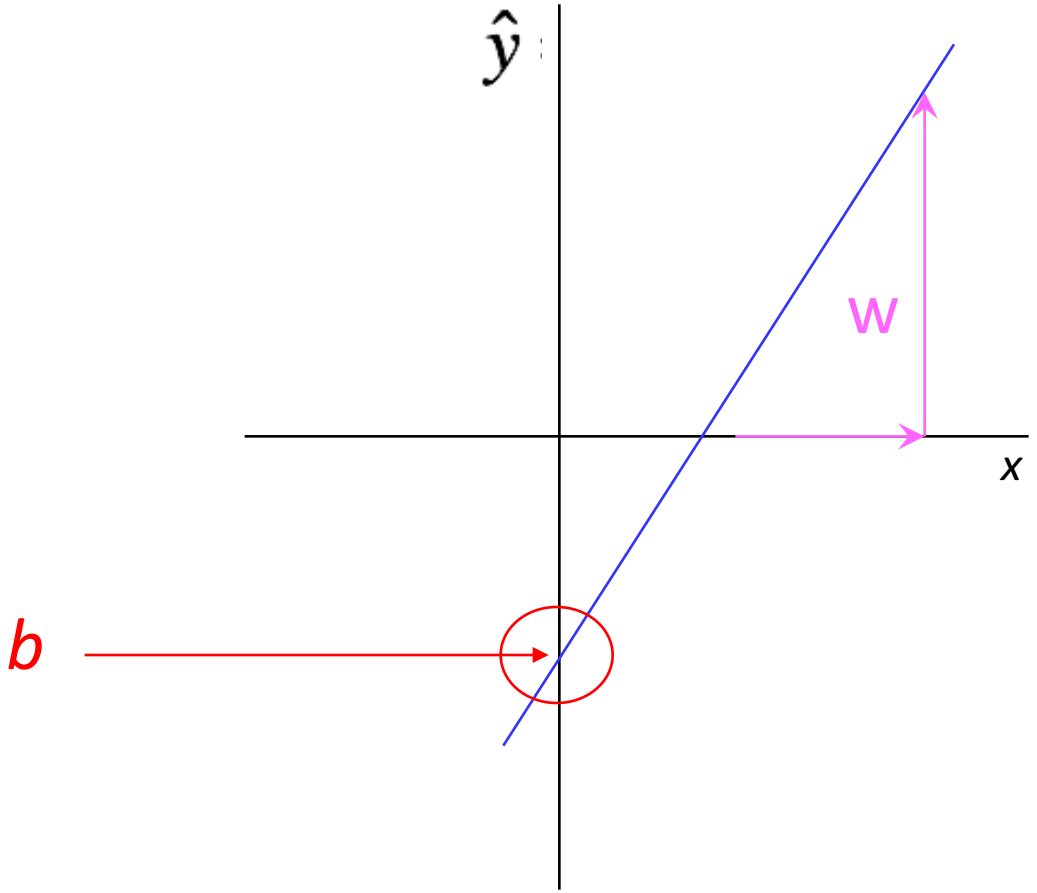
Today

- Linear regression (aka **least squares**)
- Learn to derive the least squares estimate by normal equation
- Evaluation with Cross-validation

Review: f(x) is Linear when X is 1D

- *f(x)=wx+b?*

A slope of 2 (i.e. w=2) means that every 1-unit change in X yields a 2-unit change in Y.



Review: f(x) is Linear when X is 1D

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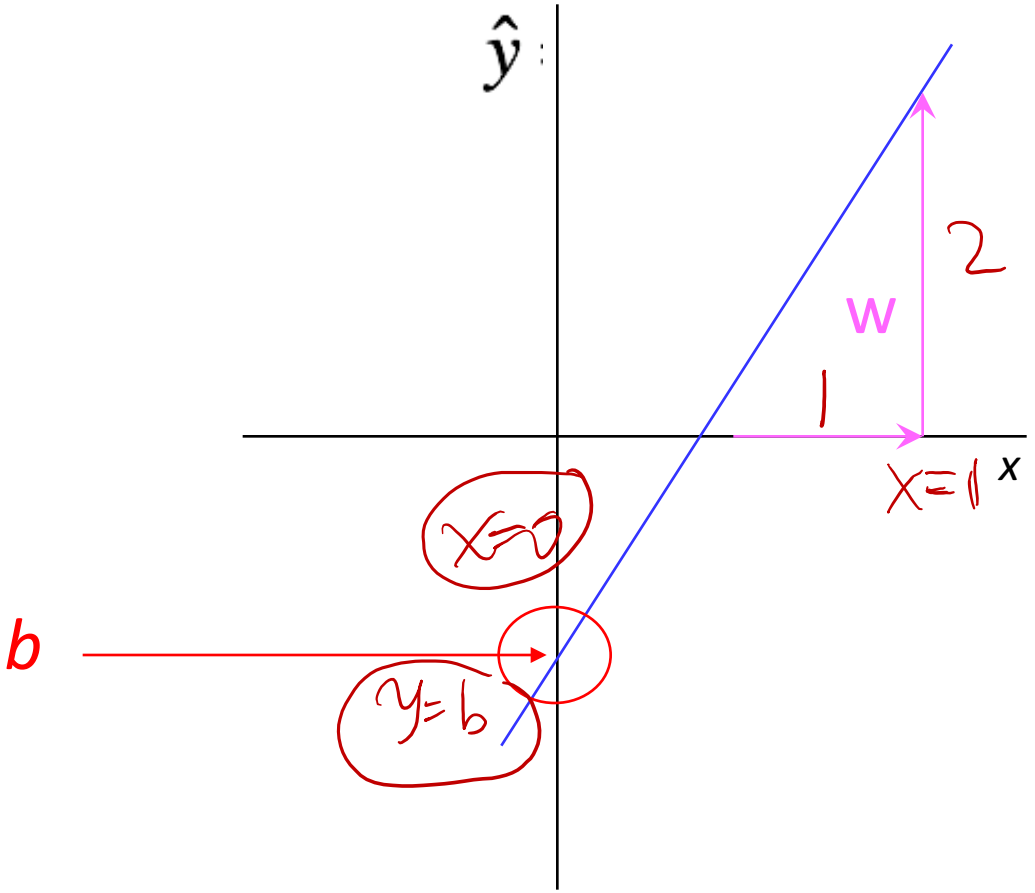
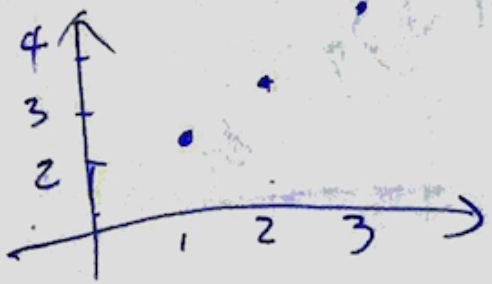


One concrete example

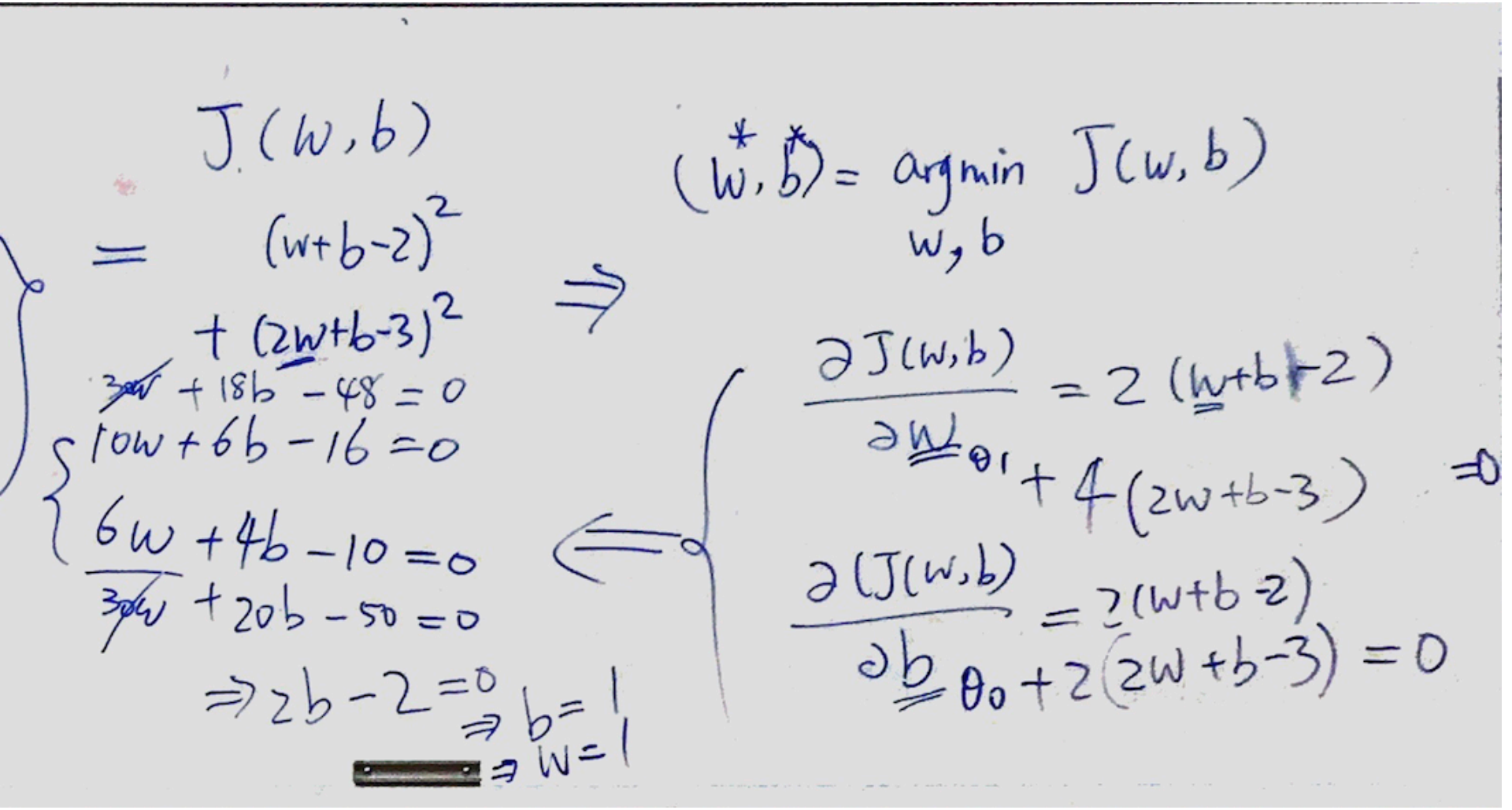
$p=1$

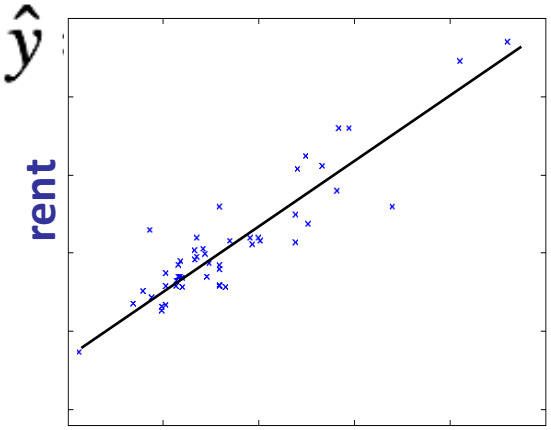
$n=3$

x_i	y_i	$f(x)=wx+b$	$(f(x)-y)^2$
1	2	$w+b$	$(w+b-2)^2$
2	3	$2w+b$	$(2w+b-3)^2$
3	4	$3w+b$	$(3w+b-4)^2$



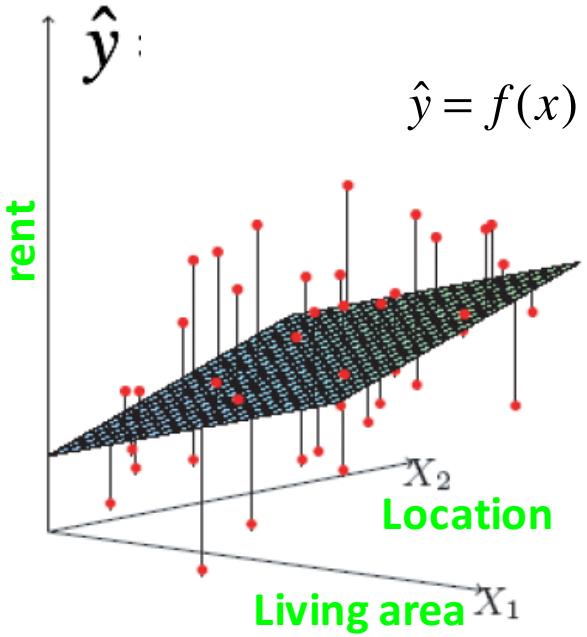
One concrete example





f(x)=wx+b

1D case ($\mathcal{X} = \mathbb{R}$): a line



$$\hat{y} = f(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

$\mathcal{X} = \mathbb{R}^2$: a plane

(Living area, Location) as X

Linear SUPERVISED Regression

$$f : X \longrightarrow Y$$

e.g. Linear Regression Models

$$\hat{y} = f(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

=> Features **x**:

e.g., Living area, distance to campus, # bedroom …

=> Target y:

e.g., Rent ➔ Continuous

Review: Special Uses for Matrix Multiplication

- Dot (or Inner) Product of two Vectors <x, y>

which is the sum of products of elements in similar positions for the two vectors

<x, y> = <y, x>

Where <x, y> = $x^T y \in \mathbb{R} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ x_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^{n} x_i y_i.$

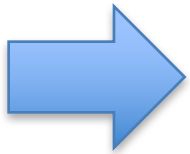
A new representation of f(x) (for each single data sample)

- Assume that each sample **x** is a column vector,
  - Here we assume a pseudo "feature" x_0=1 (this is the intercept term), and RE-define the feature vector to be:

$$\mathbf{x}^{\mathbf{T}}=[(x_0=1),\ x_1,\ x_2,\ \ldots\ ,x_p]$$

  - the parameter vector θ is also a column vector

$$\theta=\begin{bmatrix}\theta_0\\ \theta_1\\ \vdots\\ \theta_p\end{bmatrix}$$

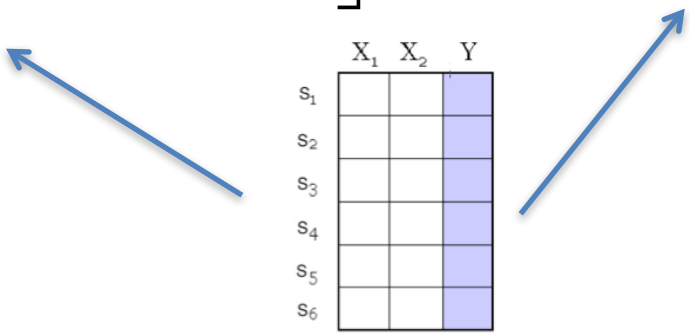


$$\hat{y}=f(\mathbf{x})=\mathbf{x}^T\theta=\theta^T\mathbf{x}$$

Training Set to Matrix Form

- Now represent the whole Training set (with n samples) as matrix form :

$$\mathbf{X} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} = \begin{bmatrix} x_{1,0} & x_{1,1} & \cdots & x_{1,p} \\ x_{2,0} & x_{2,1} & \cdots & x_{2,p} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n,0} & x_{n,1} & \cdots & x_{n,p} \end{bmatrix} \qquad \mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$



$$\vec{x}_1 = \begin{bmatrix} 1 \\ x_{1,1} \\ x_{1,2} \\ x_{1,3} \\ \vdots \\ x_{1,p} \end{bmatrix}$$

$$\vec{x}_1^{\,T} = \begin{bmatrix} 1, x_{1,1}, x_{1,2}, \cdots, x_{1,p} \end{bmatrix}$$

Regression Formulation f(x): from a single example to multiple examples in train set

- Represent as matrix form:
  - Predicted output

$$\hat{Y} = \mathbf{X}\theta = \begin{bmatrix} f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \vdots \\ f(\mathbf{x}_n) \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^T\theta \\ \mathbf{x}_2^T\theta \\ \vdots \\ \mathbf{x}_n^T\theta \end{bmatrix}$$

n x p p x 1 n x 1

  - Labels (the given output value)

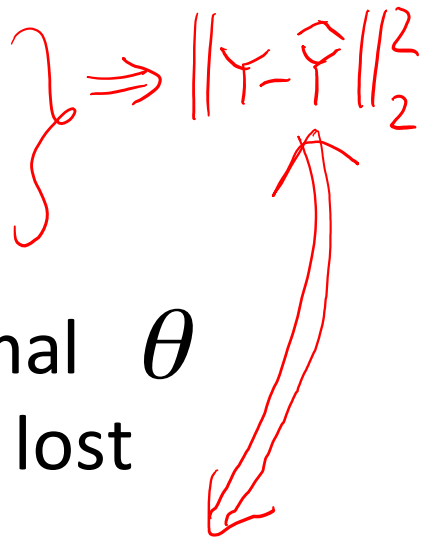
$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

n x 1

Now the loss function:

- Using matrix form, we get the following general representation of the linear regression function:

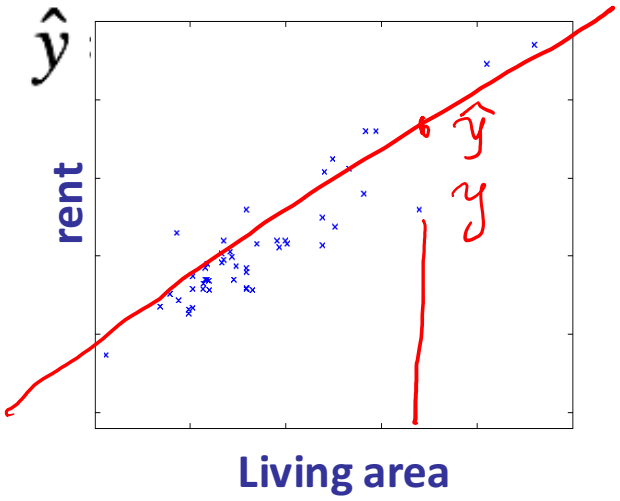
$$\hat{Y} = \mathbf{X}\theta$$



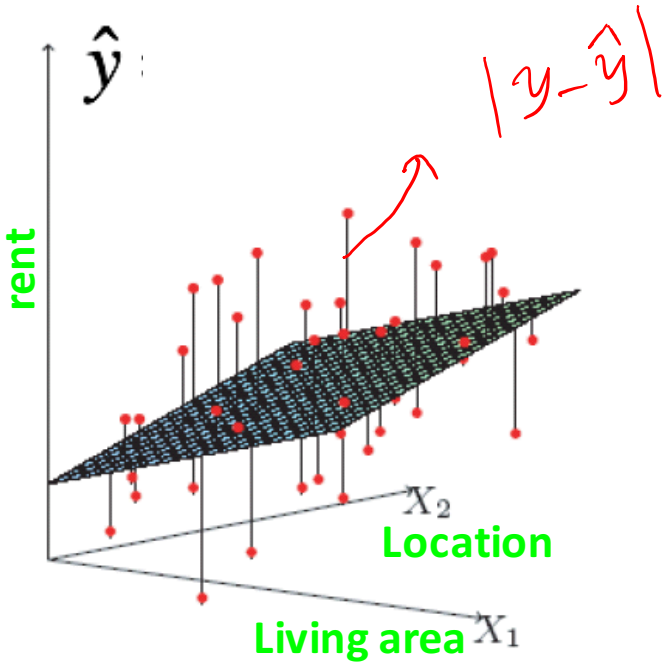
- Our goal is to pick the optimal θ that minimize the following lost function:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(f(\mathbf{x}_i) - y_i)^2$$

SSE: Sum of squared error



1D case ($\mathcal{X} = \mathbb{R}$): a line



$\mathcal{X} = \mathbb{R}^2$: a plane

Today

- Linear regression (aka **least squares**)
- Learn to derive the least squares estimate by Normal Equation
- Evaluation with Cross-validation

Method I: normal equations to minimize the loss

- Write the cost function in matrix form:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i^T\theta - y_i)^2$$
$$= \frac{1}{2}(X\theta - \vec{y})^T(X\theta - \vec{y})$$
$$= \frac{1}{2}\left(\theta^T X^T X\theta - \theta^T X^T\vec{y} - \vec{y}^T X\theta + \vec{y}^T\vec{y}\right)$$

$$\mathbf{X} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} \qquad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

To minimize $J(\theta)$, take derivative and set to zero:

$$\Rightarrow \boxed{X^T X\theta = X^T\vec{y}}$$

The normal equations

$$\Downarrow$$

$$\theta^* = \left(X^T X\right)^{-1} X^T\vec{y}$$

WHY ??

Review: Special Uses for Matrix Multiplication

- Sum the Squared Elements of a Vector

$$\mathbf{a} = \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix}$$

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i^T\theta - y_i)^2$$

$$\mathbf{a}^T = \begin{bmatrix} 5 & 2 & 8 \end{bmatrix}$$

$$\mathbf{a}^T\mathbf{a} = \begin{bmatrix} 5 & 2 & 8 \end{bmatrix}\begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix} = 5^2 + 2^2 + 8^2 = 93$$

Next : see White Board

$$a = \begin{bmatrix} \mathbf{x}_1^T\theta - y_1 \\ \mathbf{x}_2^T\theta - y_2 \\ \vdots \\ \mathbf{x}_n^T\theta - y_n \end{bmatrix} = X\theta - \vec{y}$$

$$\mathbf{a}^T\mathbf{a} = 2J(\theta) = \sum_{i=1}^{n} (\mathbf{x}_i^T\theta - y_i)^2$$

$$J(\theta)=\frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i^T\theta-y_i)^2$$

$$J(\theta)=\frac{1}{2}\sum_{i=1}^{n}(x_i^T\theta-y_i)^2$$

$$=\frac{1}{2}(X\theta-Y)^T(X\theta-Y)$$

$n\times p \quad p\times 1 \quad n\times 1$

$$=\frac{1}{2}(\theta^TX^T-Y^T)(X\theta-Y)$$

$$=\frac{1}{2}(\theta^TX^TX\theta+Y^TY-\theta^TX^TY-Y^TX\theta)$$

$$a^T b = b^T a$$

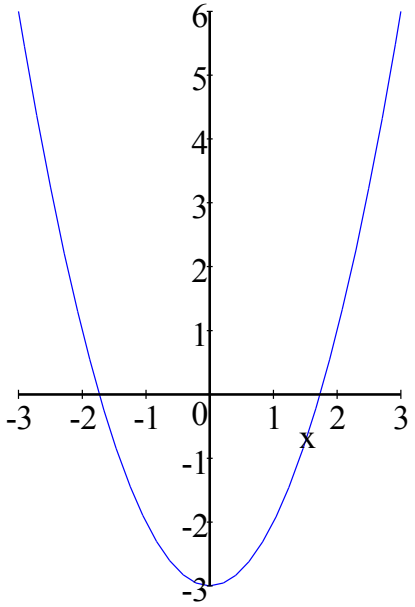
$$\Rightarrow \theta^T X^T y = y^T X \theta$$

$$\Rightarrow J(\theta) = \frac{1}{2}\left(\theta^T X^T X \theta - 2\theta^T X^T y + y^T y\right)$$

A convex function is minimized @ point whose

- ✓ derivative (slope) is zero
- ✓ gradient is zero vector (multivariate case)

Review: Derivative of a Quadratic Function



$$y = x^2 - 3$$

$$y' = 2x$$

$$y'' = 2$$

This convex function is minimized @ the unique point whose derivative (slope) is zero.

➔ If finding zeros of the derivative of this function, we can also find minima (or maxima) of that function.

Review (I): gradient of linear form

$$f(w) = w^T a = \begin{bmatrix} w_1, w_2, w_3 \end{bmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = w_1 + 2w_2 + 3w_3$$

➔ ***Denominator layout***

$$\frac{\partial f}{\partial w_1} = 1$$
$$\frac{\partial f}{\partial w_2} = 2$$
$$\frac{\partial f}{\partial w_3} = 3$$

$$\frac{\partial f}{\partial w} = \frac{\partial w^T a}{\partial w} = a = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

$$\frac{\partial (\theta^T X^T y)}{\partial \theta} = X^T y$$

Review (II): Gradient of Quadratic Form

- See L2-note Page 17, Page 23-24
- See white board

$$\frac{\partial(\theta^T X^T X\theta)}{\partial\theta} = \frac{\partial(\theta^T G\theta)}{\partial\theta} = 2G\theta = 2X^T X\theta$$

$$J(\theta) = (X\theta - y)^T (X\theta - y)\frac{1}{2}$$

$$= ((X\theta)^T - y^T)(X\theta - y)\frac{1}{2}$$

$$= (\theta^T X^T - y^T)(X\theta - y)\frac{1}{2}$$

$$= (\theta^T X^T X\theta - \theta^T X^T y - y^T X\theta + y^T y)\frac{1}{2}$$

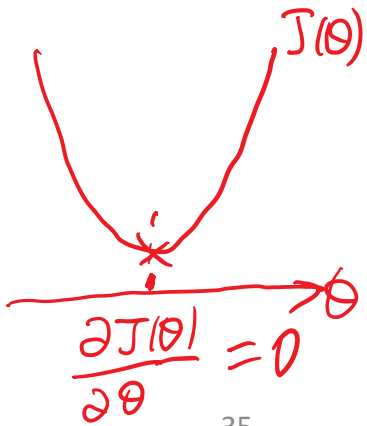
Since $\theta^T X^T y = y^T X\theta$

$\langle X\theta, y \rangle \quad \langle y, X\theta \rangle$

$$= (\theta^T X^T X\theta - 2\theta^T X^T y + y^T y)\frac{1}{2}$$

$\Rightarrow$ $J(\theta)$ quadratic func of θ;

1d case



See handout 4.1 + 4.3 ⇒ matrix calculus, partial deri ⇒ Gradient

$$\nabla_\theta (\theta^T X^T X \theta) = 2 X^T X \theta \quad (P24)$$

$$\nabla_\theta (-2 \theta^T X^T y) = -2 X^T y \quad (P24)$$

$$\nabla_\theta (y^T y) = 0$$

$$\Rightarrow \nabla_\theta J(\theta) = X^T X \theta - X^T y$$

Our loss function's Hessian is Positive Semi-definite

gram matrix is PSD

if X full rank, $X^T X$ PD ⇒ Invert

$$\Rightarrow \theta = \underbrace{(X^T X)^{-1}}_{PXP} \underbrace{X^T y}_{PX1} \Rightarrow PX1$$

Comments on the normal equation

- In most situations of practical interest, the number of data points n is larger than the dimensionality p of the input space and the matrix $\mathbf{X}$ is of full column rank. If this condition holds, then it is easy to verify that $X^T X$ is necessarily invertible.

$n >> p$

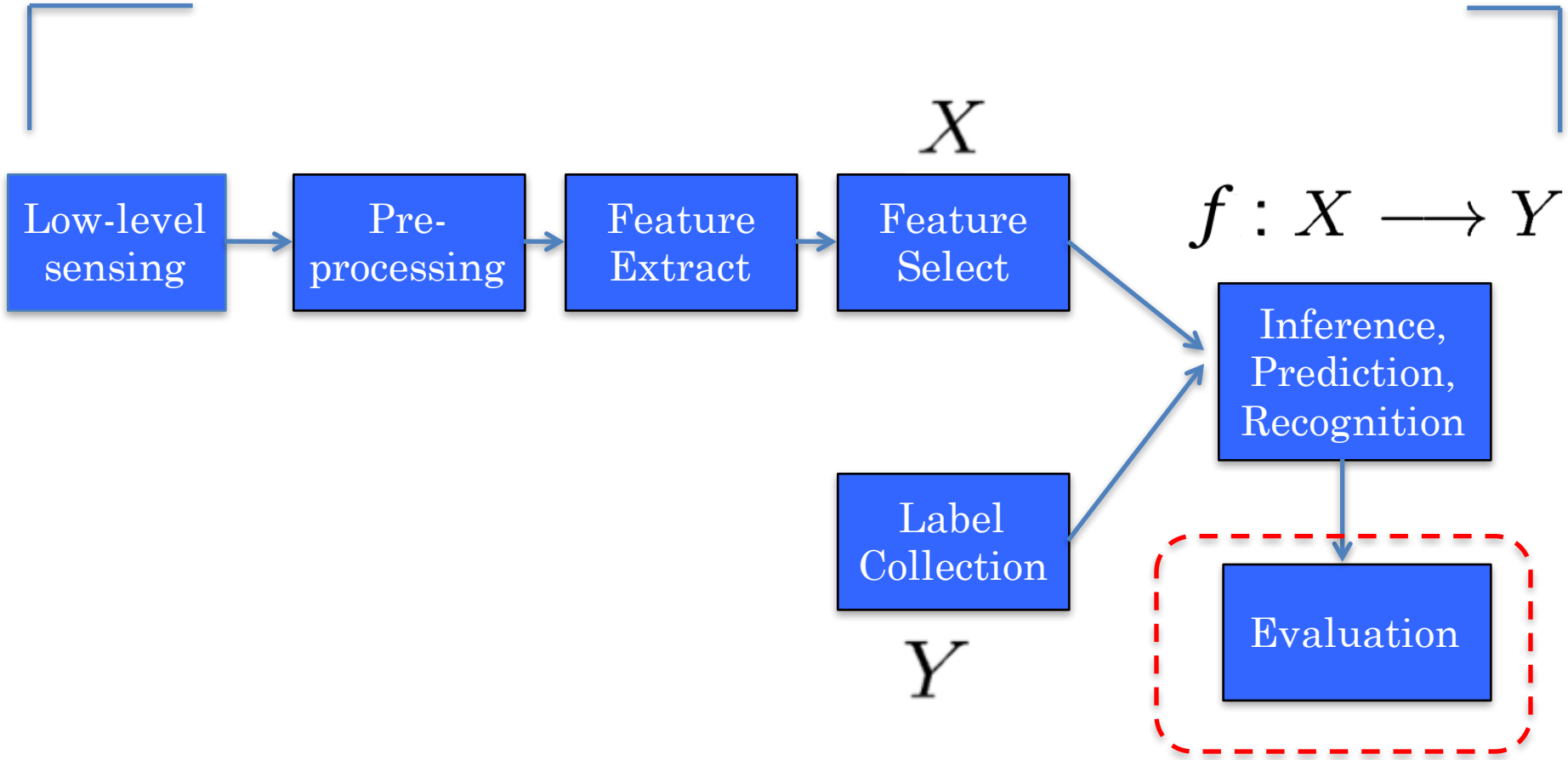
- The assumption that $X^T X$ is invertible implies that it is positive definite, thus the critical point we have found is a minimum.

- What if $\mathbf{X}$ has less than full column rank? → regularization (later).

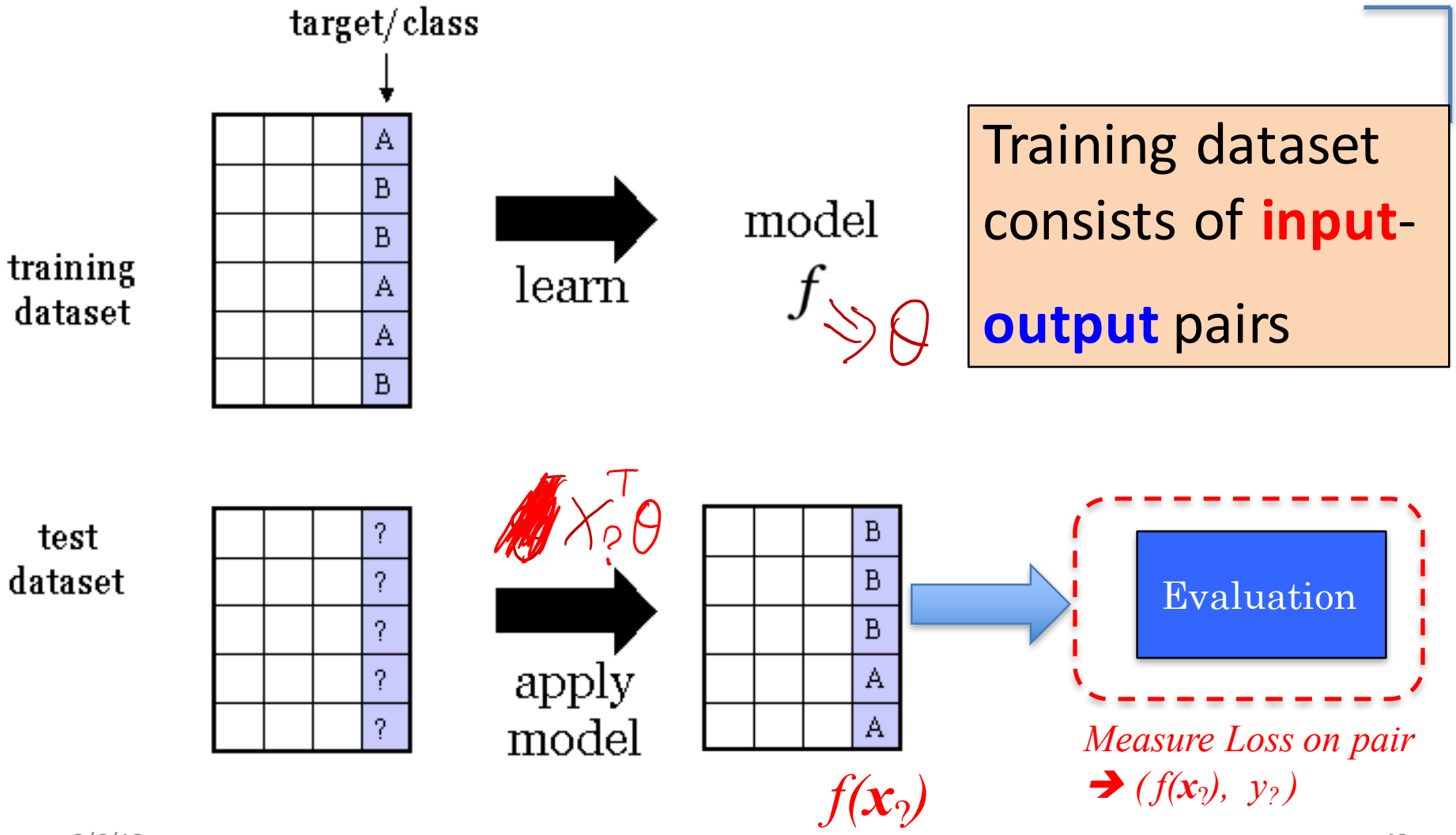
Today

- Linear regression (aka **least squares**)
- Learn to derive the least squares estimate by optimization
- Evaluation with Train/Test OR k-folds Cross-validation

TYPICAL MACHINE LEARNING SYSTEM



Evaluation Choice-I: Train and Test



Evaluation Choice-I:

e.g. for linear regression models

$$\mathbf{X}_{train} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} \qquad \vec{y}_{train} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

training dataset

$$\mathbf{X}_{test} = \begin{bmatrix} -- & \mathbf{x}_{n+1}^T & -- \\ -- & \mathbf{x}_{n+2}^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_{n+m}^T & -- \end{bmatrix} \qquad \vec{y}_{test} = \begin{bmatrix} y_{n+1} \\ y_{n+2} \\ \vdots \\ y_{n+m} \end{bmatrix}$$

test dataset

Evaluation Choice-I:

e.g. for linear regression models

- Training SSE (sum of squared error):

$$J_{train}(\theta) = \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i^T\theta - y_i)^2$$

- Minimize $J_{train}(\theta)$ ➔ *Normal Equation to get*

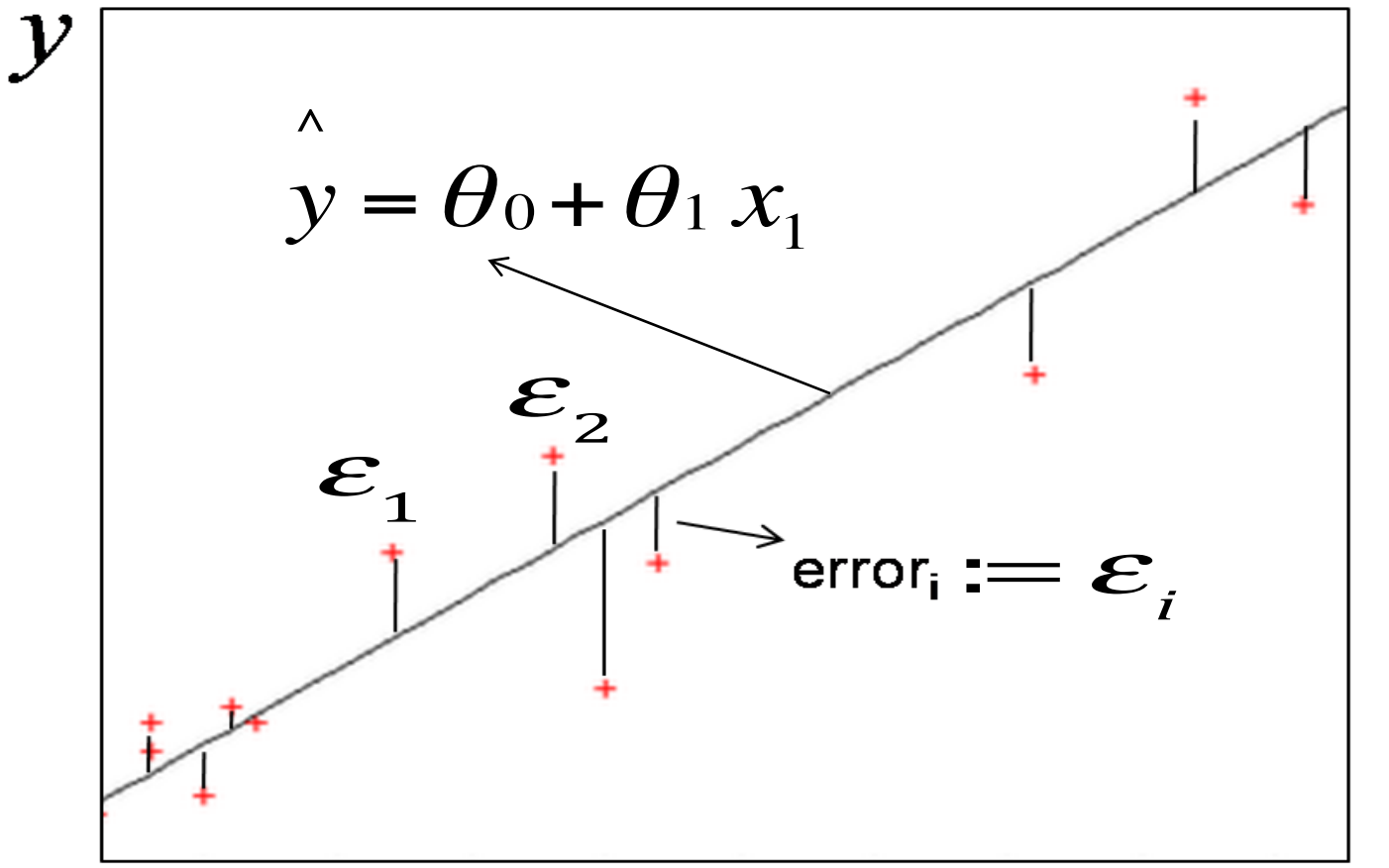
$$\theta^* = \text{argmin}\, J_{train}(\theta) = \left(X_{train}^T X_{train}\right)^{-1} X_{train}^T \vec{y}_{train}$$

Evaluation Choice-I: e.g. for Regression Models

- Testing MSE Error to report:

$$J_{test} = \frac{1}{m}\sum_{i=n+1}^{n+m}(\mathbf{x}_i^T\theta^* - y_i)^2 = \frac{1}{m}\sum_{i=n+1}^{n+m}\varepsilon_i^2$$

Linear regression (1D example)



$$\theta^* = \left(X^T X\right)^{-1} X^T \vec{y}$$

Evaluation Choice-II:
Cross Validation

- Problem: don't have enough data to set aside a test set
- Solution: Each data point is used both as train and test
- Common types:
  - -K-fold cross-validation (e.g. K=5, K=10)
  - -2-fold cross-validation
  - -Leave-one-out cross-validation (LOOCV, i.e., k=n_reference)

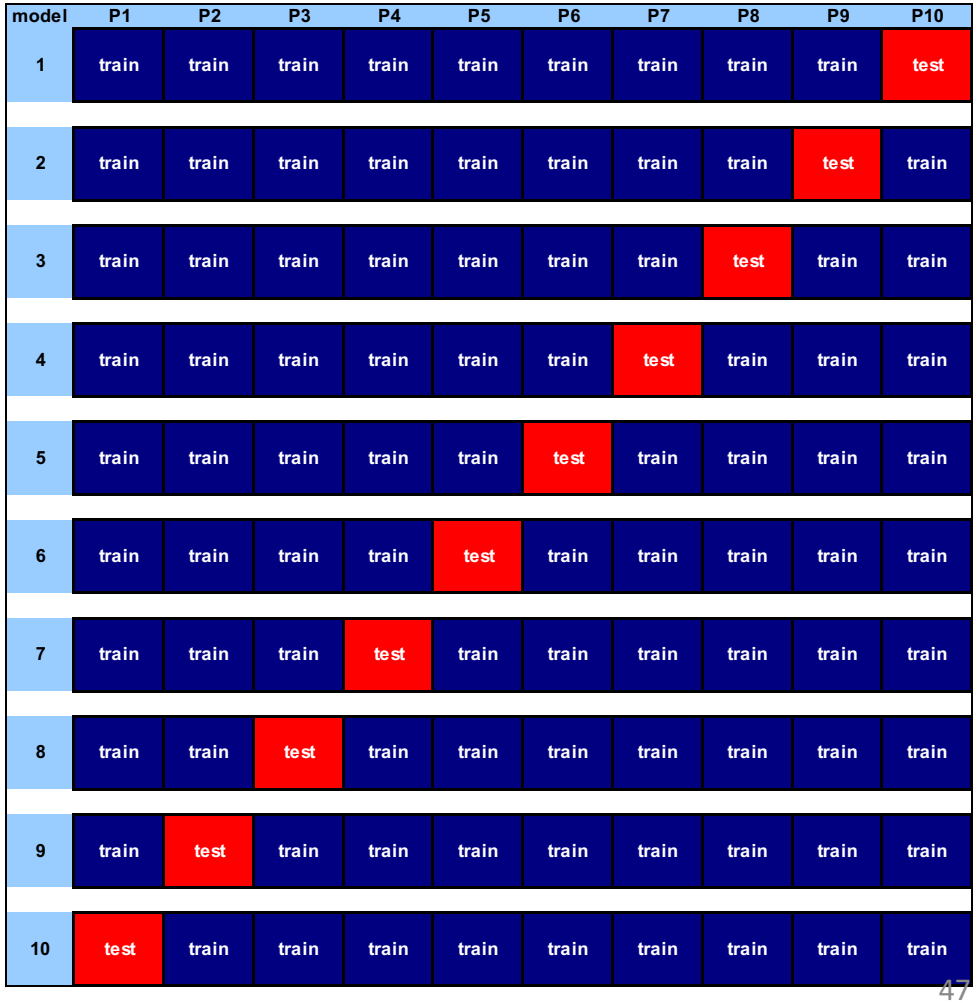
K-fold Cross Validation

- Basic idea:
  -Split the whole data to N pieces;
  -N-1 pieces for fit/train model; 1 for test;
  -Cycle through all N folds;
  -K=10 “folds” a common rule of thumb.

- The advantage:
  - all pieces are used for both training and validation;
  - each observation is used for validation exactly once.

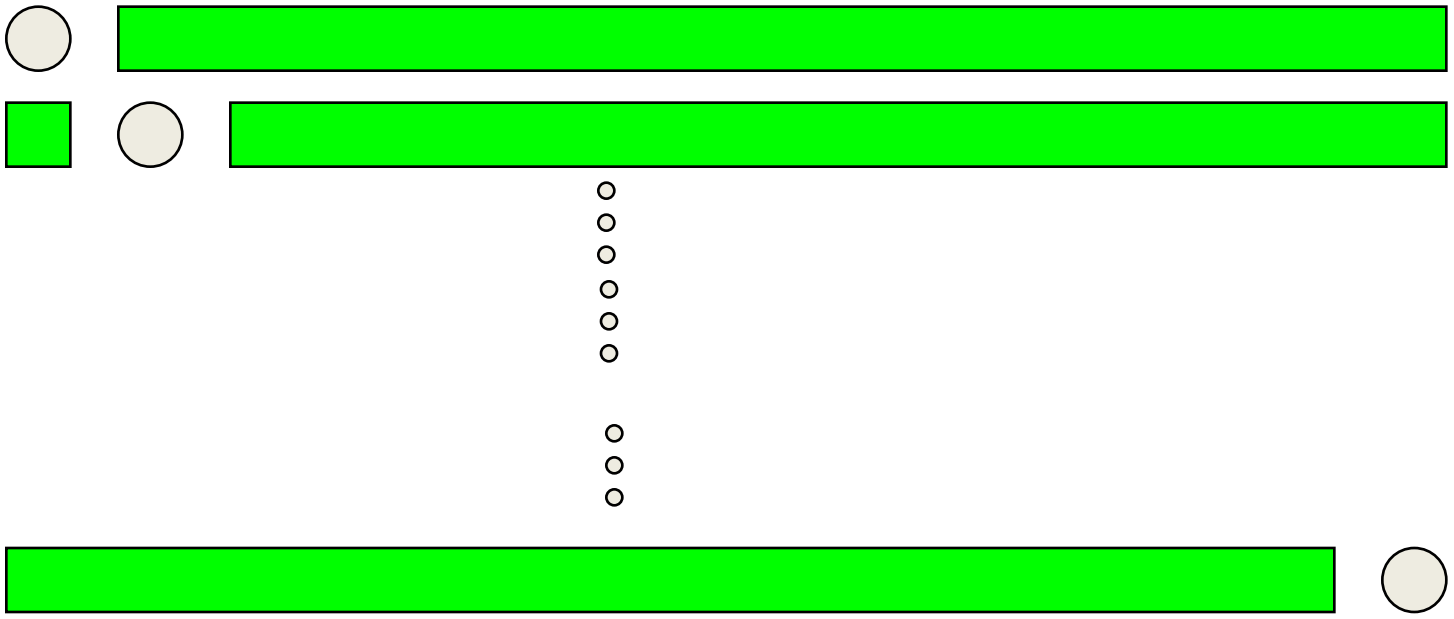
e.g. k=10 fold Cross Validation

- Divide data into 10 equal pieces
- 9 pieces as training set, the rest 1 as test set
- Collect the scores from the diagonal
- We normally use the mean of the scores



e.g. (k=n-1) Leave-one-out / LOOCV (n-fold cross validation)

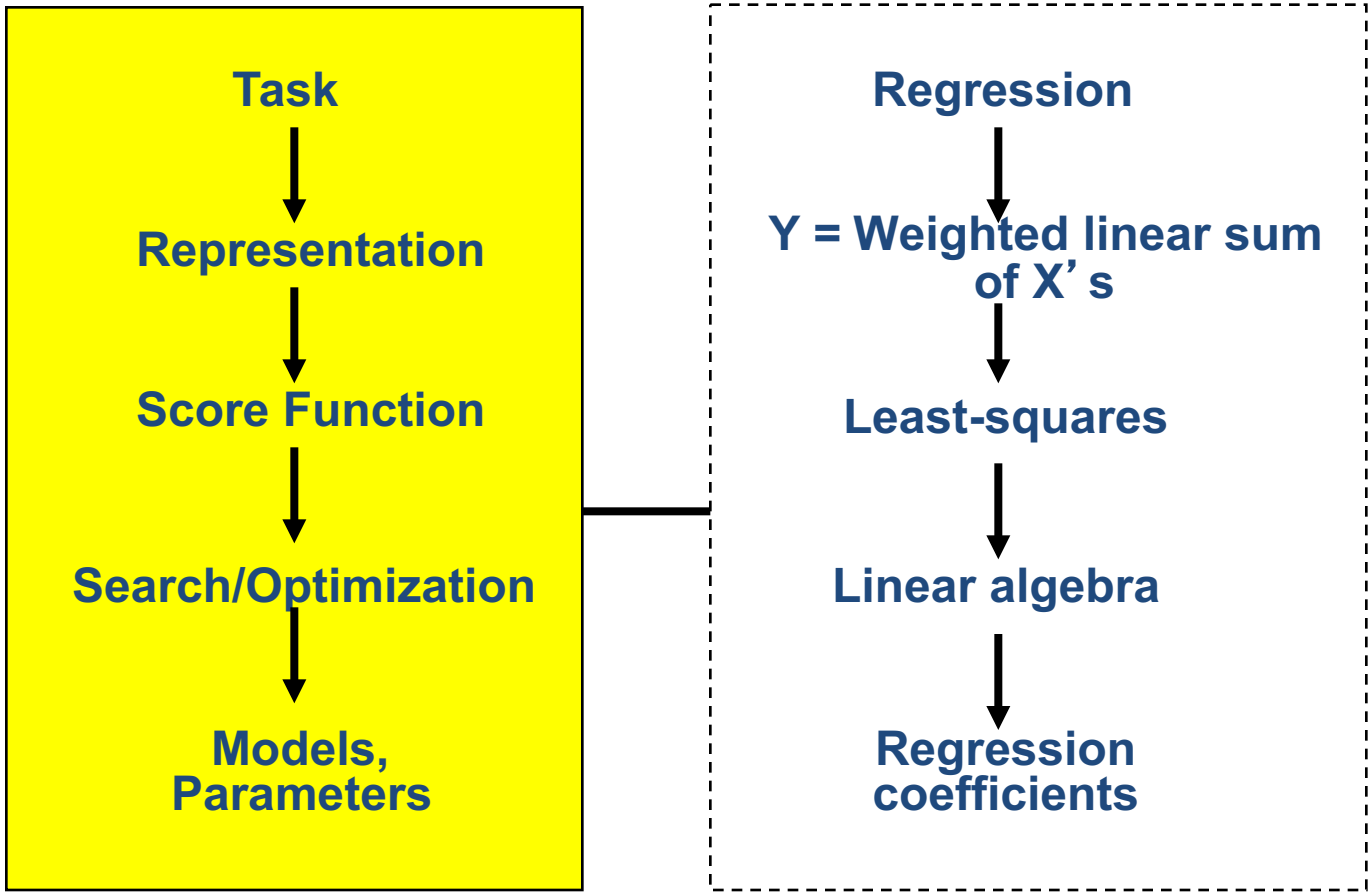
n is num. of data samples



Today Recap

- Linear regression (aka **least squares**)
- Learn to derive the least squares estimate by normal equation
- Evaluation with Train/Test OR k-folds Cross-validation

(1) Multivariate Linear Regression



$$\hat{y} = f(x) = \theta^T x$$

References

- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides

❑ http://www.cs.cmu.edu/~zkolter/course/15-884/linalg-review.pdf (please read)

❑ Prof. Alexander Gray's slides

EXTRA

Now: Taking Gradient of the J()

$$\Rightarrow \frac{\partial J(\theta)}{\partial \theta} = \frac{1}{2}\left(2X^T X\theta - 2X^T y\right) \overset{\text{Set}}{\underset{\text{to}}{=}} 0$$

$$\Rightarrow \quad X^T X\theta = X^T \vec{y}$$

The normal equations

$$\Downarrow$$

$$\theta^* = \left(X^T X\right)^{-1} X^T \vec{y}$$

$$\Rightarrow \theta = \underbrace{\underbrace{(X^T X)^{-1}}_{p\times n \; n\times p}}_{p\times p} \underbrace{\underbrace{X^T y}_{p\times n \; n\times 1}}_{p\times 1} \Rightarrow p\times 1$$

Extra: Convex function

- Intuitively, a convex function (1D case) has a single point at which the derivative goes to zero, and this point is a minimum.
- Intuitively, a function f (1D case) is convex on the range [a,b] if a function's second derivative is positive every-where in that range.

- Intuitively, if a multivariate function's Hessians is psd (positive semi-definite!), this (multivariate) function is Convex
  - Intuitively, we can think "Positive definite" matrices as analogy to positive numbers in matrix case

Extra: Loss J() is Convex

$$\Rightarrow J(\theta) = \frac{1}{2}(\theta^T X^T X \theta - 2\theta^T X^T y + y^T y)$$

$$\Rightarrow \text{Hessian}(J(\theta)) = X^T X$$

$X^T X$ → Gram matrix ⇓ [PSD]

⇓

$J(\theta)$ is Convex

If $\nabla J(\theta^*) = 0$, $J(\theta)$ is minimized @ θ^*

Extra: positive semi-definite!

L2-Note: Page 17

$A \in R^{n \times n}$, $\forall x \in R^n$

If $x^T A x \geq 0$

$1 \times n \quad n \times n \quad n \times 1$

$\Rightarrow$ A is positive semi-definite (PSD)

If $X^T A X > 0$

$\Rightarrow$ A is PD $\Rightarrow$ full rank / invertible

See proof on L2-Note: Page 18

Extra: Gram Matrix $G = X^T X$

is always positive semi-definite!

Because for any vector a

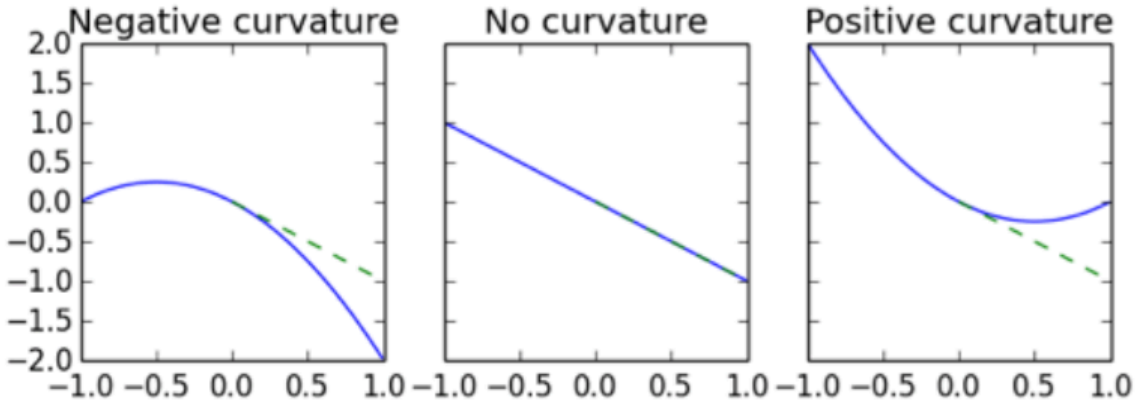
$$a^T X^T X a = | Xa |_2^2 \geq 0$$

Besides, when X is full rank, G is invertible

Extra: Hessian Matrix

Derivatives and Second Derivatives

Cost function	Gradient	Hessian
$J(\boldsymbol{\theta})$	$\boldsymbol{g} = \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$	$\boldsymbol{H}$
	$g_i = \frac{\partial}{\partial \theta_i} J(\boldsymbol{\theta})$	$H_{i,j} = \frac{\partial}{\partial \theta_j} g_i$

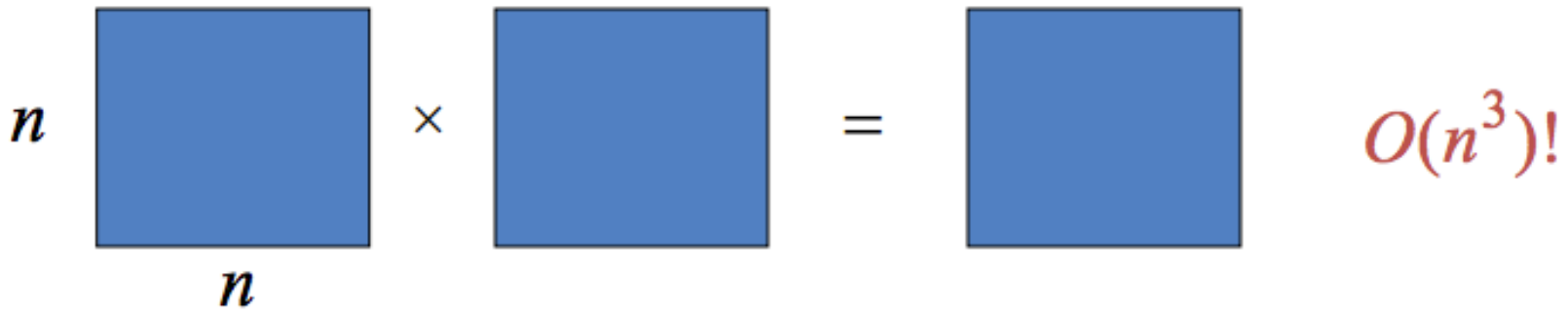


H PD for positive curvature

Extra: Scalability to big data?

- Traditional CS view: Polynomial time algorithm, Wow!
- Large-scale learning: Sometimes even O(n) is bad! => Many state-of-the-art solutions (e.g., low rank, sparse, hardware, sampling, randomized…)

Simple example: Matrix multiplication



From Wiki

The following complexity figures assume that arithmetic with individual elements has complexity $O(1)$, as is the case with fixed-preci
operations on a finite field.

Operation	Input	Output	Algorithm	Complexity
Matrix multiplication	Two $n \times n$ matrices	One $n \times n$ matrix	Schoolbook matrix multiplication	$O(n^3)$
			Strassen algorithm	$O(n^{2.807})$
			Coppersmith–Winograd algorithm	$O(n^{2.376})$
			Optimized CW-like algorithms[14][15][16]	$O(n^{2.373})$
Matrix multiplication	One $n \times m$ matrix & one $m \times p$ matrix	One $n \times p$ matrix	Schoolbook matrix multiplication	$O(nmp)$
Matrix inversion*	One $n \times n$ matrix	One $n \times n$ matrix	Gauss–Jordan elimination	$O(n^3)$
			Strassen algorithm	$O(n^{2.807})$
			Coppersmith–Winograd algorithm	$O(n^{2.376})$
			Optimized CW-like algorithms	$O(n^{2.373})$
Singular value decomposition	One $m \times n$ matrix	One $m \times m$ matrix, one $m \times n$ matrix, & one $n \times n$ matrix		$O(mn^2)$ ($m \leq n$)
		One $m \times r$ matrix, one $r \times r$ matrix, & one $n \times r$ matrix		
Determinant	One $n \times n$ matrix	One number	Laplace expansion	$O(n!)$
			Division-free algorithm[17]	$O(n^4)$
			LU decomposition	$O(n^3)$
			Bareiss algorithm	$O(n^3)$
			Fast matrix multiplication[18]	$O(n^{2.373})$
Back substitution	Triangular matrix	n solutions	Back substitution[19]	$O(n^2)$