# Probability and Statistics for Computer Science



"All models are wrong, but some models are useful"--- George Box

Credit: wikipedia

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#### Last time

- Stochastic Gradient Descent
- SUM DT Random For..

**\*** Naïve Bayesian Classifier

#### Objectives

- # Linear regression
  - \* The problem
  - \* The least square solution
  - \* The training and prediction
  - \* The R-squared for the evaluation of the fit.

#### Some popular topics in Ngram



## Regression models are Machine learning methods

- Regression models have been around for a while
- \* Dr. Kelvin Murphy's Machine Learning book has 3+ chapters on regression

### The regression problem

$x^{(1)} x^{(2)} x^{(d)} u^{[abe]}$
•.5 1 1 0
(1) (2) (d) P
to to
$x^{(1)} x^{(2)} \dots x^{(d)} y$
•.5 1 1 0.5
(1) (2) (d) 2P

#### Chicago social economic census

- \* The census included 77 communities in Chicago
- \* The census evaluated the average hardship index of the residents
- \* The census evaluated the following parameters for each community:
  - # PERCENT\_OF\_HOUSING\_CROWDED
  - # PERCENT\_HOUSEHOLD\_BELOW\_POVERTY
  - # PERCENT\_AGED\_16p\_UNEMPLOYED
  - # PERCENT\_AGED\_25p\_WITHOUT\_HIGH\_SCHOOL\_DIPLOMA
  - # PERCENT\_AGED\_UNDER\_18\_OR\_OVER\_64
  - # PER\_CAPITA\_INCOME

Given a new community and its parameters, can you predict its average hardship index with all these parameters?

### Wait, have we seen the linear regression before?



### It's about *Relationship* between data features

IDNO	BODYFAT	DENSITY	AGE	WEIGHT	HEIGHT
1	12.6	1.0708	23	154.25	67.75
2	6.9	1.0853	22	173.25	72.25
3	24.6	1.0414	22	154.00	66.25
4	10.9	1.0751	26	184.75	72.25
5	27.8	1.0340	24	184.25	71.25
6	20.6	1.0502	24	210.25	74.75
7	19.0	1.0549	26	181.00	69.75
8	12.8	1.0704	25	176.00	72.50
9	5.1	1.0900	25	191.00	74.00
10	12.0	1.0722	23	198.25	73.50

x : HIGHT, y: WEIGHT ▓

### Some terminology

- \* Suppose the dataset  $\{(\mathbf{x}, y)\}$  consists of N labeled items $(\mathbf{x}_i, y_i)$
- If we represent the dataset as a table
  - \* The d columns representing  $\{{f x}\}$  are called explanatory variables  ${f x}^{(j)}$
  - \* The numerical column y is called the dependent variable

	$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
)	1	3	0
$\int$	2	3	2
l	3	6	5

### Variables of the Chicago census

[1] "PERCENT\_OF\_HOUSING\_CROWDED"
[2]"PERCENT\_HOUSEHOLDS\_BELOW\_POVERTY"
[3] "PERCENT\_AGED\_16p\_UNEMPLOYED"
[4]"PERCENT\_AGED\_25p\_WITHOUT\_HIGH\_SCHOOL\_DI
PLOMA"
[5] "PERCENT\_AGED\_UNDER\_18\_OR\_OVER\_64"
[6]"PER\_CAPITA\_INCOME"
[7] "HardshipIndex"

Which is the dependent variable in the census example?

A. "PERCENT\_OF\_HOUSING\_CROWDED"
B. "PERCENT\_AGED\_25p\_WITHOUT\_HIGH\_SCHOOL\_DIPLOMA"
C. HardshipIndex"
D. "PERCENT\_AGED\_UNDER\_18\_OR\_OVER\_64"

#### Linear model

We begin by modeling y as a linear function of  $\mathbf{x}^{(j)}$ plus randomness  $y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \dots + \mathbf{x}^{(d)}\beta_d + \xi$ Where  $\xi$  is a zero-mean random variable that represents model error  $\overline{x} = [x'' \times x'' + x'']$ In vector notation:  $chicago = \mathbf{x}^{(1)}$   $d = \mathbf{6} \qquad 1$ ₩  $\mathbf{x}^{(2)}$ Y  $y = \mathbf{x}^T \boldsymbol{\beta} + \boldsymbol{\xi}$ 3 0 Where  $\beta$  is the d-dimensional 2 3 2 vector of coefficients that we train 3 6 5

#### Each data item gives an equation

\* The model: 
$$y = \mathbf{x}^T \boldsymbol{\beta} + \boldsymbol{\xi} = \mathbf{x}^{(1)} \boldsymbol{\beta}_1 + \mathbf{x}^{(2)} \boldsymbol{\beta}_2 + \boldsymbol{\xi}$$
  

$$N = 17$$

$$y_0 = \mathfrak{d} = \mathfrak{d} \times (\mathfrak{d} + \mathfrak{d} \, \mathfrak{d$$

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	3	0
2	3	2
3	6	5

#### Which together form a matrix equation

\* The model  $y = \mathbf{x}^T \boldsymbol{\beta} + \xi = \mathbf{x}^{(1)} \beta_1 + \mathbf{x}^{(2)} \beta_2 + \xi$ 



#### Which together form a matrix equation

\* The model  $y = \mathbf{x}^T \boldsymbol{\beta} + \xi = \mathbf{x}^{(1)} \beta_1 + \mathbf{x}^{(2)} \beta_2 + \xi$ 



$$\begin{bmatrix} 0\\2\\5 \end{bmatrix} = \begin{bmatrix} 1 & 3\\2 & 3\\3 & 6 \end{bmatrix} \begin{bmatrix} \beta_1\\\beta_2 \end{bmatrix} + \begin{bmatrix} \xi_1\\\xi_2\\\xi_3 \end{bmatrix}$$
$$\mathbf{y} = X \cdot \boldsymbol{\beta} + \mathbf{e}$$

#### Q. What's the dimension of matrix X?

A. N × d B. d × N C. N × N D. d × d

#### Training the model is to choose $\beta$

\* Given a training dataset  $\{(\mathbf{x}, y)\}$ , we want to fit a model  $y = \mathbf{x}^T \boldsymbol{\beta} + \xi$  $\mathcal{E}(\boldsymbol{j}) = \boldsymbol{o}$ 

\*\* Define 
$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$$
 and  $X = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix}$  and  $\mathbf{e} = \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_N \end{bmatrix}$ 

\* To train the model, we need to choose  $\beta$  that makes e small in the matrix equation  $y = X \cdot \beta + e$ 

#### Training using least squares

- \* In the least squares method, we aim to minimize  $||\mathbf{e}||^2$   $||\mathbf{x}||^2 = ||\mathbf{y} - X\beta||^2 = (\mathbf{y} - X\beta)^T (\mathbf{y} - X\beta)$ \* Differentiating with respect to  $\beta$  and setting to zero  $d||\mathbf{e}||^2 = X^T X\beta - X^T \mathbf{y} = 0$   $\mathbf{x}^T \mathbf{x} \ \mathbf{x}^T \mathbf{x} = \mathbf{x}^T \mathbf{y}$ 
  - \* If  $X^T X$  is invertible, the least squares estimate of the coefficient is:  $\lambda = \arg \min_{n} ||e||^{2}$

$$\widehat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y}$$

$$\mathbf{\dot{\beta}} = \mathbf{\dot{\lambda}} \mathbf{\dot{\beta}} + \mathbf{\dot{q}}$$

 $\begin{array}{c} \mathbf{x}^{\mathsf{T}}\mathbf{x} \\ \mathbf{x}^{\mathsf{T}} & \overset{\mathsf{T}}{\sim} & \mathcal{d} \mathbf{x} \, \mathcal{N} \\ \mathbf{x}^{\mathsf{T}} & \overset{\mathsf{T}}{\sim} & \mathcal{N} \mathbf{x} \, \mathcal{d} \end{array}$  $(x^{\top}x)^{\top}$  $=x^{T}x$ X(dxN) X(Nxd) (AB)T=OTAT = XX ~ dxd <sup>λ</sup>i symmetric. for XX,  $\lambda:$ ZO JUNXI prositive semidefinite

#### Derivation of least square solution

$$||e||^{2} = (y - x\beta)^{T} (y - x\beta)$$

$$= y^{T}y - \beta^{T}x^{T}y - \frac{y^{T}}{x}\beta + \beta^{T}x^{T}x\beta \quad (1)$$

$$||e||^{2} = (y - x\beta)^{T} (y - x\beta)$$

$$= y^{T}y - \beta^{T}x^{T}y - \frac{y^{T}}{x}\beta + \beta^{T}x^{T}x\beta \quad (1)$$

$$||e||^{2} = (A + A^{T})a \quad a, b \text{ are vectory}; A \text{ is a spore matrix}$$

$$= \frac{\partial(b^{T}a)}{\partial a} = b \Rightarrow \frac{\partial(y^{T}x\beta)}{\partial \beta} = x^{T}y \quad \Rightarrow \frac{\partial(\beta^{T}x^{T}x\beta)}{\partial \beta} = 2x^{T}x\beta$$

$$||e||^{2} \Rightarrow s \text{ calar} \quad (1) \text{ are scalar}$$

$$= \frac{\partial(b^{T}a)}{\partial a} = \frac{\partial(b^{T}a)^{T}}{\partial a} = \frac{\partial(a^{T}b)}{\partial a} = b \Rightarrow \frac{\partial(\beta^{T}x^{T}y)}{\partial \beta} = x^{T}y$$

$$||e||^{2} \Rightarrow s \text{ caler, all items in (i) are scalar}$$

$$= \frac{\partial||e||^{2}}{\partial \beta} = 0 - x^{T}y - x^{T}y + 2x^{T}x\beta = 0$$

$$\Rightarrow x^{T}x\beta = x^{T}y$$

$$||e||^{2} \Rightarrow \beta = (x^{T}x)^{-1}x^{T}y$$

$$||erre y \text{ is vector}|$$

#### Derivation of least square solution

 $X^T X \hat{\beta} - X^T \gamma = 0$  $\chi^T \gamma = \chi^T \chi \hat{\beta}$ X ~ dxN  $\Rightarrow \chi^{T}(\gamma - \chi \hat{\beta}) = 0$ e~ Nx1 (d×1) =) x<sup>T</sup>ê = 0  $(x^7 e)^T = o$ (12d) ⇒ é<sup>T</sup>×=0 J. u=0 (121) mul ane = ê x ŝ=o く 19: ê1 XB Uncorrelated !!

Least Square Loss Function

 $||e||^{2} = f(\beta) = \sum_{j=1}^{k} Q_{j}(\beta) = \sum_{j=1}^{k} (z_{j}\beta - y_{j})^{2}$  $Q_{j}(\beta) = (x_{j}^{T}\beta - y_{j})^{2}$ 

In the final project  $Q_{j}(\theta) = |z_{j}^{T}\theta - y_{j}|^{2}$  $\nabla Q_{j} = ? \qquad \frac{\partial Q_{j}}{\partial \theta} = ?$ 

#### Convex set and convex function

 If a set is convex, any line connecting two points in the set is completely included in the set





\* A convex function: the area above the curve is convex  $f(\lambda x + (1 - \lambda)y) < \lambda f(x) + (1 - \lambda)f(y)$ \* The least square
(a)
(a)
(b)

Credit: Dr. Kelvin Murphy

#### What's the dimension of matrix X<sup>T</sup>X?

A. N × d B. d × N C. N × N D. d × d  $d \rightarrow \forall ef$  features

#### Is this statement true?

If the matrix  $X^T X$  does NOT have zero valued eigenvalues, it is invertible.  $\lambda : (eigenvalue :)$  $\downarrow X^T X \downarrow 0$ 



#### Training using least squares example

\* Model: 
$$y = \mathbf{x}^T \boldsymbol{\beta} + \xi = \mathbf{x}^{(1)} \beta_1 + \mathbf{x}^{(2)} \beta_2 + \xi$$



#### Training data



$$\widehat{\boldsymbol{\beta}}_1 = 2 \\ \widehat{\boldsymbol{\beta}}_2 = -\frac{1}{3}$$

#### Prediction

If we train the model coefficients  $\widehat{oldsymbol{eta}}$  , we can predict  $y_0^p$ x.=0 from  $\mathbf{x}_0$  $y_0^p = \mathbf{x}_0^T \widehat{\boldsymbol{\beta}}$ In the model  $y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$  with  $\widehat{\boldsymbol{\beta}} = \begin{bmatrix} 2 \\ -\frac{1}{3} \end{bmatrix}$ \* The prediction for  $\mathbf{x}_0 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$  is  $y_0^p = \mathbf{z} \star [\mathbf{\beta}, \mathbf{z}] \star [\mathbf{\beta}, \mathbf{z}]$   $= \mathbf{z} \star [\mathbf{z}] + \mathbf{z} \star [\mathbf{z}]$ The prediction for  $\mathbf{x}_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$  is  $y_0^p$ 

#### A linear model with constant offset

The problem with the model  $y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$ when  $\chi'' = 0$ ,  $\chi'' = 0$ is: Let's add a constant offset  $\beta_0$  to the model  $y = \beta_0 + \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$   $\downarrow \not \beta_2 + \mathbf{x}^{\prime\prime} \cdot \not \beta_2 - \cdots$ 

## Training and prediction with constant offset

\* The model 
$$y = \beta_0 + \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi = \mathbf{x}^T \boldsymbol{\beta} + \xi$$



Training data:





### Comparing our example models

$y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi \qquad \qquad y = \beta_0 + \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$ $\mathbf{\beta} = (\mathbf{x}^{T}\mathbf{x}) \mathbf{x}^{T}\mathbf{\beta}$									ξ Be	
			$\hat{oldsymbol{eta}} =$	$\begin{bmatrix} 2\\ -\frac{1}{2} \end{bmatrix}$	1				$\widehat{oldsymbol{eta}}$ =	$=\begin{bmatrix} -3\\ 2\\ 1 \end{bmatrix}$
$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y	хŢÂ	L JJ	1	$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y	$\mathbf{x}^T \widehat{\boldsymbol{eta}}$	
1	3	0	1	-1	1	1	3	0	0	
2	3	2	3	-1	1	2	3	2	2	
3	6	5	4	١	1	3	6	5	5	

#### Variance of the linear regression model

\* The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$
  
$$\mathbf{y} = \mathbf{x} \hat{\boldsymbol{\beta}} + \mathbf{e} \quad \hat{\mathbf{e}} \perp \mathbf{x} \hat{\boldsymbol{\beta}}$$

\* The random error is uncorrelated to the least square solution of linear combination of explanatory variables.

$$\chi^T \gamma = \chi^T \chi \hat{\beta}$$

## Variance of the linear regression model: proof

\* The least squares estimate satisfies this property  $y = \chi (3 + 2)$   $var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$ 

Proof: 
$$Vur(\mathcal{Y}) = vur(\mathcal{X}\beta) + vur(e)$$
  
+  $2 uv(\mathcal{X}\beta, e)$ 

$$\begin{array}{c} X\beta + e\\ C V (X,\beta,e) = 0 \end{array}$$

## Variance of the linear regression model: proof

\* The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

#### **Proof:**

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])^T([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])$$

 $var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}]^T [X\hat{\beta} - \overline{X\hat{\beta}}] + 2[\mathbf{e} - \overline{\mathbf{e}}]^T [X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}]^T [\mathbf{e} - \overline{\mathbf{e}}])$ 

Because  $\overline{\mathbf{e}} = 0$  ;  $\mathbf{e}^T X \widehat{\boldsymbol{\beta}} = 0$  and  $\mathbf{e}^T \mathbf{1} = 0$  due to Least square minimized

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}]^T [X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}]^T [\mathbf{e} - \overline{\mathbf{e}}])$$
$$var[y] = var[X\hat{\beta}] + var[\mathbf{e}]$$

#### Evaluating models using R-squared

\* The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

\* This property gives us an evaluation metric called Rsquared

$$R^{2} = \frac{var(\{\mathbf{x}_{i}^{T}\widehat{\boldsymbol{\beta}}\})}{var(\{y_{i}\})} \quad \text{if } \mathcal{R} = 1$$

$$Var(\boldsymbol{e}) = 0$$

<sup>∗</sup> We have  $0 ≤ R^2 ≤ 1$  with a larger value meaning a better fit.

### Q: What is R-squared if there is only one explanatory variable in the model?

 $if X = N \times I \\ d = I$ R ~ r2 r is corr.

### Q: What is R-squared if there is only one explanatory variable in the model?

 $\hat{y} = r\hat{x} + \varepsilon$  $var(\hat{y}) = r^{2} var(\hat{x}) + var(\hat{z})$   $var(\hat{y}) = r^{2} var(\hat{x}) + var(\hat{z})$   $r^{2} = \frac{r^{2} var(\hat{x})}{var(\hat{y})}$   $var(\hat{y}) = r^{2}$   $var(\hat{y}) = r^{2}$ 1 r2

よ!(×)

## Q: What is R-squared if there is only one explanatory variable in the model?

#### R-squared would be **the correlation coefficient squared** (textbook pgs 43-44)

#### R-squared examples



### Linear regression model for the Chicago census data

Call: lm(formula = HardshipIndex ~ ., data = dat)

Residuals:

Min	1Q	Median	3Q	Max
-15.7157	-1.9230	0.1301	1.9810	8.6719

Coefficients:

	Estimate	Std. Error	t value Pr(> t )
(Intercept)	105.1394	37.3622	2.814 0.006346 **
PERCENT_OF_HOUSING_CROWDED	0.7189	0.2753	2.612 0.011014 *
PERCENT_HOUSEHOLDS_BELOW_POVERTY	0.6665	0.0781	8.534 1.90e-12 ***
PERCENT_AGED_16p_UNEMPLOYED	0.8023	0.1350	5.941 9.93e-08 ***
PERCENT_AGED_25p_WITHOUT_HIGH_SCHOOL_DIPLOMA	0.7751	0.1063	7.293 3.64e-10 ***
PERCENT_AGED_UNDER_18_OR_OVER_64	0.4807	0.1202	3.998 0.000156 ***
PER_CAPITA_INCOME	-11.8819	3.1888	-3.726 0.000391 ***
			77-7

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 3.9 on 70 degrees of freedom Multiple R-squared: 0.983, Adjusted R-squared: 0.9815 F-statistic: 673.9 on 6 and 70 DF, p-value: < 2.2e-16 dt=70 = N-d\* d\*=trof cry(controp + intercont

### Residual is normally distributed?

The Q-Q plot of the residuals is roughly normal

yo = X. B+ Ro { 50.3



### Prediction for another community

202)
2(

Predicted hardship index: 41.46038

Note: maximum of hardship index in the training data is 98, minimum is 1

## The clusters of the Chicago communities: clusters and hardship

#### **Clusters of community**



-15

-40

-20

0 tSNE1 Hardship index

50

25

20

## The clusters of the Chicago communities: per capital income and hardship

11.0

10.5 10.0 9.5

#### PER CAPITAL INCOME





#### Hardship index of communities



## The clusters of the Chicago communities: without diploma and hardship

#### PERCENT\_AGED\_25p\_WITHOUT \_HIGH\_SCHOOL\_DIPLOMA





### Assignments

#### Read Chapter 13 of the textbook

#### \*\* Next time: More on linear regression

### Additional References

- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. "Probability and Statistical Inference"
- \* Kelvin Murphy, "Machine learning, A Probabilistic perspective"

#### See you next time

See You!

