

Machine Learning for Networks: Regression

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	ML task	Linear Regression	Logistic Regression	Tree-based learning	Neural Networks	k -Nearest Neighbors
Supervised	Regression Classification	x	x	x	x	
Unsupervised	Clustering Dimensionality reduction Anomaly detection			x	x	x
	Recommender Systems				x	

- Supervised Learning Models
- Linear Regression
- Train / Test / Cross-Validation

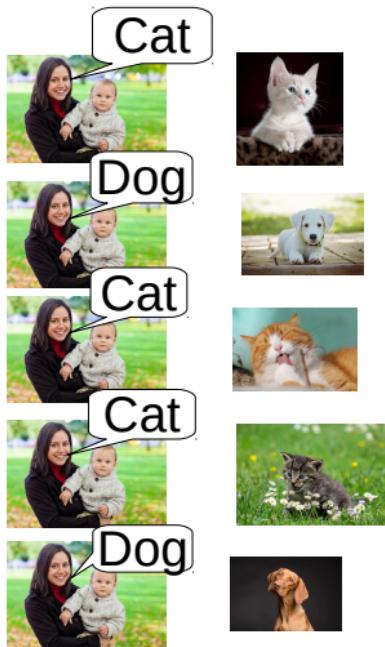
Section 1

Introduction to Supervised Learning

How humans learn

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TRAINING (learning)



Some think instead that we learn in a different [Tho20]

TRAINING (learning)



INFERENCE (prediction)



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TRAINING (learning)



INFERENCE (prediction)



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TRAINING (learning)

Training dataset



TRAINING (learning)

Training dataset

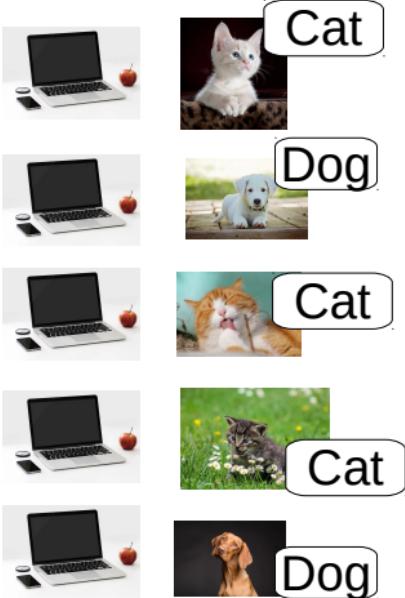


INFERENCE (prediction)



TRAINING (learning)

Training dataset

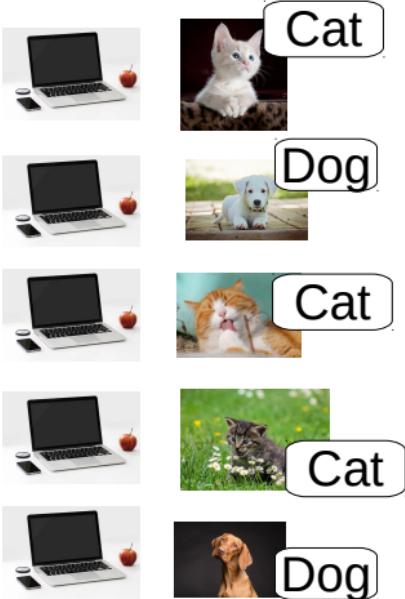


INFERENCE (prediction)



TRAINING (learning)

Training dataset



INFERENCE (prediction)



Deep Neural Network better than humans to classify several image datasets.

Cambridge English Dictionary:

the process of getting an understanding of something by studying it or by experience

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What can we learn in a network, by just observing traffic (encrypted)?

- Anomaly/attack
- Application protocols hidden in encrypted traffic
- Quality of Experience (QoE)
- Malfunctioning of a device
- ...

- **Problem [KEB19]:**

Infer video chunk resolution

only observing network information, e.g., throughput, packet size, inter-arrival times, etc.

Traffic is encrypted.

- **Motivation:**

Network operators can have insights on QoE without *Deep Packet Inspection*

Features (or Columns):

- Throughput mean (bps)
Throughput st.dev. (bps)
Packet size mean (B)
Packet size st.dev.
Inter-arrival mean (ms), etc.

Label (or target):

- Resolution of downloaded video chunks (360p, 720p)
- (it indicates the number of vertical pixels)

Features (or Columns):

- Throughput mean (bps)
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Inter-arrival mean (ms), etc.

Label (or target):

- Resolution of downloaded video chunks (360p, 720p)
- (it indicates the number of vertical pixels)

Model:

- A function $h(\text{features}) = \text{label}$
- If label $\in \mathbb{R}$: **regression** model
- If label discrete: **classification** model

Example

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		Features (or Independent variables)					True Label	
	Sample	TP mean	TP st.dev.	Pkt size mean	Pkt std. dev.	Int-Arriv mean	$y^{(i)}$ (Resolution)	
Our dataset	$\mathbf{x}^{(1)^T} =$ \vdots $\mathbf{x}^{(M)^T} =$	2 Mbps ⋮ 2 Mbps	1 Kbps ⋮ 1.1 Kbps	1 KB ⋮ 1.3 KB	300 B ⋮ 400 B	30 ms ⋮ 20 ms	475 ⋮ 720	
New samples	$\mathbf{x}^{(M+1)^T} =$ \vdots	2 Mbps ⋮	1 Kbps ⋮	1 KB ⋮	300 B ⋮	30 ms ⋮	? ⋮	

Example

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		Features (or Independent variables)					True Label	Pred Label	
	Sample	TP mean	TP st.dev.	Pkt size mean	Pkt std. dev.	Int-Arriv mean	$y^{(i)}$ (Resolution)	$\hat{y}^{(i)} = h(\mathbf{x}^{(i)})$	
Our dataset	$\mathbf{x}^{(1)^T} =$ ⋮ $\mathbf{x}^{(M)^T} =$	2 Mbps	1 Kbps	1 KB	300 B	30 ms	475	482	⋮
	$\mathbf{x}^{(M+1)^T} =$ ⋮	2 Mbps	1.1 Kbps	1.3 KB	400 B	20 ms	720	693	⋮
New samples							?	1078	⋮

- Model: function h used to predict

Example

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Our dataset	$\mathbf{x}^{(1)^T} =$ ⋮ $\mathbf{x}^{(M)^T} =$	2 Mbps	1 Kbps	1 KB	300 B	30 ms	475	482	1083
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
New samples	$\mathbf{x}^{(M+1)^T} =$ ⋮	2 Mbps	1 Kbps	1 KB	300 B	30 ms	720	693	323
	⋮	⋮	⋮	⋮	⋮	⋮	?	1078	376

- Model: function h used to predict

Which of the two models would you trust more to predict?

Example

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- Model: function h used to predict

Which of the two models would you trust more to predict?

- h is “good” if $h(\mathbf{x}^{(i)}) \simeq y^{(i)}$ for the new samples.

Example

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- Model: function h used to predict

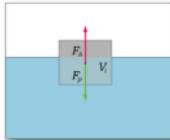
Which of the two models would you trust more to predict?

- h is “good” if $h(\mathbf{x}^{(i)}) \simeq y^{(i)}$ for the new samples.
- But we do not know $y^{(i)}$ for the new samples.
- We can just evaluate how $h(\cdot)$ performs in our dataset.

Famous examples of models “by hand”

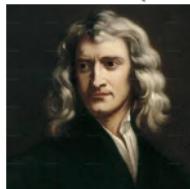
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Archimedes (III cent. BC)



weight of displaced fluid = weight of object in vacuum – weight of object in fluid

Newton (XVII cent.)



$$\mathbf{F} = m\mathbf{a}$$

Maxwell (XVII cent.)



$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$$

They created a model $h(\cdot)$ relating a target to some features, **based on observation.**

Generalization

For **any** object with m and \mathbf{a} , we know the force \mathbf{F} it produces.

Pictures: Wikipedia

- Convention

$$\mathbf{x}^{(i)T} = (x_1^{(i)}, \dots, x_N^{(i)}) \in \mathbb{R}^{N+1}$$

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- Linear Model

$$\begin{aligned} h_{\theta}(\mathbf{x}^{(i)}) &= \theta^T \cdot \mathbf{x}^{(i)} = \sum_{j=0}^N \theta_j \cdot x_j^{(i)} \\ &= \theta_0 + \theta_{\text{TP mean}} \cdot x_{\text{TP mean}}^{(i)} \\ &\quad + \theta_{\text{TP st.dev.}} \cdot x_{\text{TP st.dev.}}^{(i)} + \dots \end{aligned}$$

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- Neural Network (NN):

$h_{\theta}(\cdot)$ is the output of a NN with weights θ .

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Loss: $J = \frac{1}{M} \sum_{i=1}^M \left(\underbrace{y^{(i)} - h_{\theta}(\mathbf{x}^{(i)})}_{\text{Residual } \varepsilon^{(i)}} \right)^2$

- Quadratic Model

$$\begin{aligned} h_{\theta}(\mathbf{x}^{(i)}) &= \theta_0 + \theta_1 x_1^{(i)} + \dots + \theta_N x_N^{(i)} \\ &\quad + \theta_{N+1} \cdot x_1^{(i)2} + \dots + \theta_N \cdot x_{N+N}^{(i)2} \\ &\quad + \theta_{2N+1} \cdot x_1^{(i)} \cdot x_2^{(i)} + \theta_{2N+1} \cdot x_1^{(i)} \cdot x_N^{(i)} \\ &\quad + \dots \end{aligned}$$

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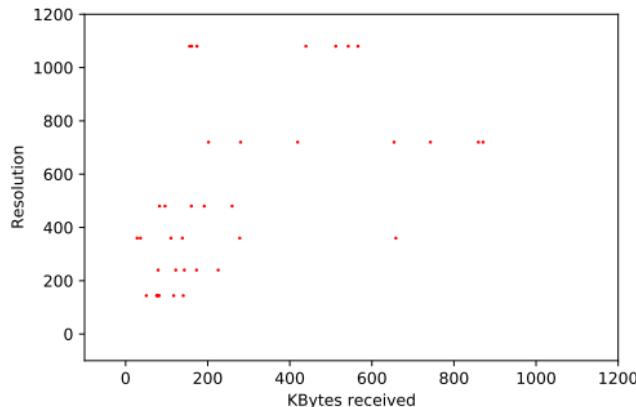
Training

Find $\theta^* \triangleq \arg \min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$

Example of univariate model

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Predict the video resolution just based on KB received in 100ms time slot.
Are you able to find a simple model $h(\text{KBytesReceived})$ “by hand”?



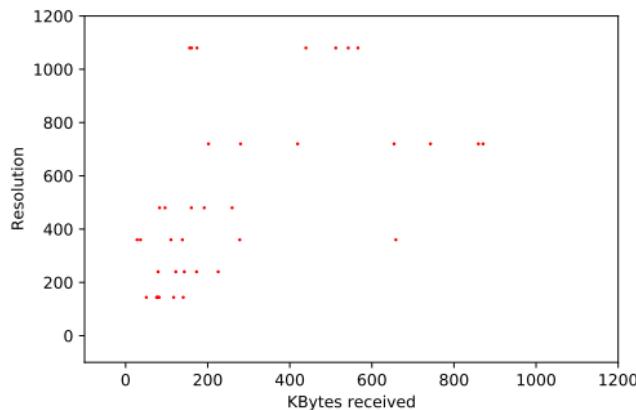
KBytesReceived	avg_qual
10.086	0
16.218	0
16.187	0
13.187	0
36.199	360
16.832	0
17.040	0
16.522	0
77.605	144
16.475	0
16.344	0
75.432	144
11.361	0
11.507	0
17.902	0
278.065	360
19.808	0
27.840	360

[Source of data [[GGA⁺19](#)]]

Example of univariate model

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Predict the video resolution just based on KB received in 100ms time slot.
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Generalization

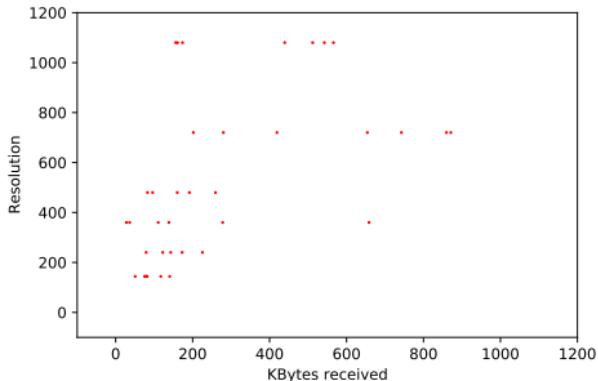
If we see that a new connection with 500 KB / 100ms, what is the predicted video resolution?

[Source of data [GGA⁺19]]

KBytesReceived	avg_qual
10.086	0
16.218	0
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27.840	360

Training a Linear Model: Example

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Find θ_0, θ_1 such that $h_{\theta}(\mathbf{x}^{(i)}) \simeq \theta_0 + \theta_1 \cdot x_1^{(i)}$.

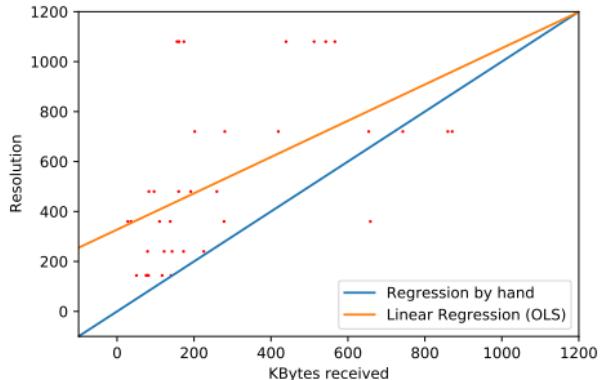
- Regression “by hand”

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Source of data [GGA⁺19]

Training a Linear Model: Example

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Find θ_0, θ_1 such that $h_{\theta}(\mathbf{x}^{(i)}) \simeq \theta_0 + \theta_1 \cdot x_1^{(i)}$.

- Regression “by hand”
- Ordinary Least Square (OLS) regression

$$\theta^* = \arg \min_{\theta} J \quad \theta_0^* = 351.8 \quad \theta_1^* = 0.7.$$

KBytesReceived	avg_qual
10.086	0
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16.187	0
13.187	0
36.199	360
16.832	0
17.040	0
16.522	0
77.605	144
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Source of data [GGA⁺19]

Bi-variate linear model

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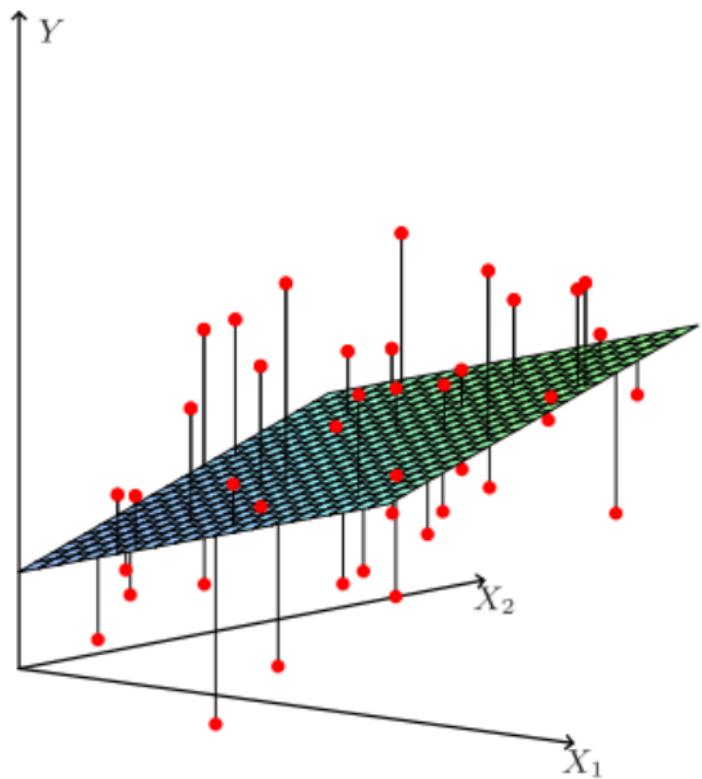


Figure 3.1 of [HTF09]

- Matrix of samples: $\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)T} \\ \vdots \\ \mathbf{x}^{(M)T} \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \dots & x_N^{(1)} \\ \dots & \dots & \dots & \dots & \dots \\ 1 & x_1^{(M)} & x_2^{(M)} & \dots & x_N^{(M)} \end{bmatrix}$
- Vector of true labels: $\mathbf{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(M)} \end{bmatrix}$
- Vector of model parameters: $\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_N \end{bmatrix}$
- Vector of predicted labels: $\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}^{(1)} \\ \vdots \\ \hat{y}^{(M)} \end{bmatrix} = \begin{bmatrix} h_{\boldsymbol{\theta}}(\mathbf{x}^{(1)}) \\ \vdots \\ h_{\boldsymbol{\theta}}(\mathbf{x}^{(M)}) \end{bmatrix}$

Examples of loss function

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For regression

- Mean Square Error (MSE)

$$J(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = \frac{1}{M} \sum_{i=1}^M \left(\underbrace{y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})}_{\text{Residual } \varepsilon^{(i)}} \right)^2$$

- Root Mean Square Error (RMSE)

$$J(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = \sqrt{\frac{1}{M} \sum_{i=1}^M (y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}))^2}$$

- ...

For classification:

- Misclassification Rate

$$J(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = \frac{1}{M} \sum_{i=1}^M I_{y^{(i)} \neq h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})}$$

- ...

Training

Find $\theta^* \triangleq \arg \min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$

Solution algorithm:

- Linear regression: matrix inversion
- Neural network: backpropagation
- ...

Note that

- θ^* depends on the observed data (\mathbf{X}, \mathbf{y}) .
- If we observed other data $(\mathbf{X}', \mathbf{y}')$ we would get another θ^* .
- ...

Section 2

Ordinary Least Squares

For any sample $\mathbf{x}^{(i)}$, a linear model is:

$$h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) = \theta_0 \cdot 1 + \theta_1 \cdot x_1^{(i)} + \cdots + \theta_N \cdot x_N^{(i)} = \mathbf{x}^{(i)T} \cdot \boldsymbol{\theta}$$

Assume the loss function below:

$$\text{MSE} = J(\boldsymbol{\theta}, \mathbf{X}, \hat{\mathbf{y}}) = \frac{1}{M} \sum_{i=1}^M \left(y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) \right)^2$$

The model $h_{\boldsymbol{\theta}^*}$ that minimizes MSE is called **Ordinary Least Squares** (OLS) model.

Theorem: Normal equation

The optimal parameter vector is

$$\boldsymbol{\theta}^* = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y} \quad (1)$$

(provided that $(\mathbf{X}^T \cdot \mathbf{X})^{-1}$ is invertible)

NB: Given a certain training set (\mathbf{X}, \mathbf{y}) , we can immediately find the optimal $\boldsymbol{\theta}^*$.

Training a Linear Regression Model (I)

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For any sample $\mathbf{x}^{(i)}$, the prediction is (This proof is similar to §3.2 of [HTF09].):

$$h_{\theta}(\mathbf{x}^{(i)}) = \theta_0 \cdot 1 + \theta_1 \cdot x_1^{(i)} + \cdots + \theta_N \cdot x_N^{(i)} = \mathbf{x}^{(i)T} \cdot \boldsymbol{\theta}$$

The loss function is:

$$\begin{aligned} J(\boldsymbol{\theta}, \mathbf{X}, \hat{\mathbf{y}}) &= \frac{1}{M} \sum_{i=1}^M \left(y^{(i)} - h_{\theta}(\mathbf{x}^{(i)}) \right)^2 = \frac{1}{M} \sum_{i=1}^M \left(y^{(i)} - \mathbf{x}^{(i)T} \cdot \boldsymbol{\theta} \right)^2 \\ &= \frac{1}{M} (\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\theta})^T \cdot (\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\theta}) \end{aligned}$$

To minimize the function, we set the gradient to 0:

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}, \mathbf{X}, \hat{\mathbf{y}}) = \mathbf{0}$$

Chain rule of derivation:

$$\frac{2}{M} (\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\theta}) \cdot \nabla_{\boldsymbol{\theta}} (\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\theta}) = \mathbf{0} \quad -\mathbf{y} \cdot \mathbf{X} + \mathbf{X} \cdot \boldsymbol{\theta} \cdot \mathbf{X} = \mathbf{0} \quad (4)$$

(2)

$$\frac{2}{M} (\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\theta}) \cdot (-\mathbf{X}) = \mathbf{0} \quad (3)$$

Training a Linear Regression Model (II)

Let us isolate θ :

$$\mathbf{X} \cdot \theta \cdot \mathbf{X} = \mathbf{y} \cdot \mathbf{X} \quad (5)$$

$$\mathbf{X}^T \cdot \mathbf{X} \cdot \theta \cdot \mathbf{X} = \mathbf{X}^T \cdot \mathbf{y} \cdot \mathbf{X} \quad (6)$$

Multiply on the left by $(\mathbf{X}^T \cdot \mathbf{X})^{-1}$
(Assuming it exists):

$$\theta \cdot \mathbf{X} = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y} \cdot \mathbf{X} \quad (7)$$

Multiply on the right by \mathbf{X}^T

$$\theta \cdot \mathbf{X} \cdot \mathbf{X}^T = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y} \cdot \mathbf{X} \cdot \mathbf{X}^T \quad (8)$$

Multiply on the right by^a $(\mathbf{X} \cdot \mathbf{X}^T)^{-1}$:

$$\theta = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y} \quad (9)$$

^aBy the property of transpose matrices, if $(\mathbf{X}^T \cdot \mathbf{X})^{-1}$ exists, then $(\mathbf{X} \cdot \mathbf{X}^T)^{-1}$ exists as well.

Interpreting regression results: sign

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You want to predict Resolution based on KBytesReceived:

$$\hat{y}^{(i)} = \theta_0 + \theta_{\text{KBytesReceived}} \cdot x_{\text{KBytesReceived}}^{(i)}$$

KBytesReceived	Resolution
36.199	360
77.605	144
75.432	144
278.065	360

Running the OLS model we get:

	coef	P> t
const	351.7606	0.000
KBytesReceived	0.7115	0.001

The model is

$$\hat{y}^{(i)} = 351.76 + 0.71 \cdot x_{\text{KBytesReceived}}^{(i)}$$

Does the **sign** makes sense?
Positive/negative dependency.

p-value for feature j : probability to obtain that coefficient θ_j just by chance, i.e., under the hypothesis that there is no dependence between j and the label.

p-values: *significance* of a coefficient.

	coef	P> t
const	351.7606	0.000
KBytesReceived	0.7115	0.001

Hypothesis testing:

- **Null hypothesis:** No dependency between KBytesReceived and the target.

p-values: *significance* of a coefficient.

	coef	P> t
const	351.7606	0.000
KBytesReceived	0.7115	0.001

Hypothesis testing:

- **Null hypothesis:** No dependency between KBytesReceived and the target.

- Performing OLS, under the null hp

$$\mathbb{P} \left[|\hat{\theta}_{\text{KBytesReceived}}^*| \geq 0.71 \right] = 0.001$$

- Would you *accept* or *reject* the null hp?

p-values: *significance* of a coefficient.

	coef	P> t
const	351.7606	0.000
KBytesReceived	0.7115	0.001

Hypothesis testing:

- **Null hypothesis:** No dependency between KBytesReceived and the target.

- Performing OLS, under the null hp

$$\mathbb{P}\left[|\hat{\theta}_{\text{KBytesReceived}}^*| \geq 0.71\right] = 0.001$$

- Would you *accept* or *reject* the null hp?

- Accept $\Rightarrow 0.71$ is not significant
 - Reject $\Rightarrow 0.71$ is significant.

p -values: *significance* of a coefficient.

	coef	P> t
const	351.7606	0.000
KBytesReceived	0.7115	0.001

Hypothesis testing:

- **Null hypothesis:** No dependency between KBytesReceived and the target.

- Performing OLS, under the null hp

$$\mathbb{P}\left[|\hat{\theta}_{\text{KBytesReceived}}^*| \geq 0.71\right] = 0.001$$

- Would you *accept* or *reject* the null hp?

- Accept $\Rightarrow 0.71$ is not significant
- Reject $\Rightarrow 0.71$ is significant.

Usually:

- p -value $\leq 5\% \Rightarrow$ reject null hp \Rightarrow Coeff significant
- o.w. Coeff not significant

Interpreting regression results

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Predict Resolution based on
PacketsSent, KBytesReceived and
BufferHealth:

$$\hat{y}^{(i)} = \theta_0 + \theta_1 \cdot x_1^{(i)} + \theta_2 \cdot x_2^{(i)} + \theta_3 \cdot x_3^{(i)}$$

PacketsSent	KBytesReceived	BufferHealth	Resolution
6	36.199	10.241165	360
10	77.605	4.446780	144
14	75.432	3.989780	144
33	278.065	3.700462	360
6	27.840	4.512780	360
58	658.375	9.454706	360
14	77.429	4.606780	144
33	201.903	5.301853	720
18	172.740	3.638107	240
23	181.476	5.314732	240

Training the OLS model:

	coef	P> t
const	282.8794	0.017
PacketsSent	-0.5551	0.925
KBytesReceived	0.5986	0.194
BufferHealth	18.3779	0.343

The model is

$$\hat{y}^{(i)} = 282.9 - 0.56 \cdot x_1^{(i)} + 0.60 \cdot x_2^{(i)} + 18.34 \cdot x_3^{(i)}$$

Interpretation:

- Fixing all features
- 1KB more received (in the 100 ms window) \Rightarrow resolution \nearrow by 0.60p
- \iff increase of 1MB \Rightarrow resolution \nearrow of 600p.

Interpreting regression results

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		coef	P> t
	const	282.8794	0.017
	PacketsSent	-0.5551	0.925
	KBytesReceived	0.5986	0.194
	BufferHealth	18.3779	0.343

$$\hat{y}^{(i)} = 282.9 - 0.56 \cdot x_1^{(i)} + 0.60 \cdot x_2^{(i)} + 18.34 \cdot x_3^{(i)}$$

Do the **signs** make sense?

		coef	P> t
	const	282.8794	0.017
	PacketsSent	-0.5551	0.925
	KBytesReceived	0.5986	0.194
	BufferHealth	18.3779	0.343

$$\hat{y}^{(i)} = 282.9 - 0.56 \cdot x_1^{(i)} + 0.60 \cdot x_2^{(i)} + 18.34 \cdot x_3^{(i)}$$

Do the **signs** make sense?

Are coefficients **significant**?

Theorem

Assume that

- for any sample \mathbf{x} , the target is a random variable (r.v.):

$$\hat{y} = \mathbf{x}^T \cdot \boldsymbol{\beta} + \epsilon \quad (10)$$

- $\boldsymbol{\beta}$: some “true” parameter vector
- ϵ : noise, Gaussian r.v. $\epsilon \sim N(0, \sigma^2)$
- σ^2 : variance of the residuals

- The true label $y^{(i)}$ is a realization of \hat{y} .

Then

- the coefficients $\hat{\theta}_j^*$ we get from linear regression are also Gaussian r.v. They are **unbiased**, i.e.,

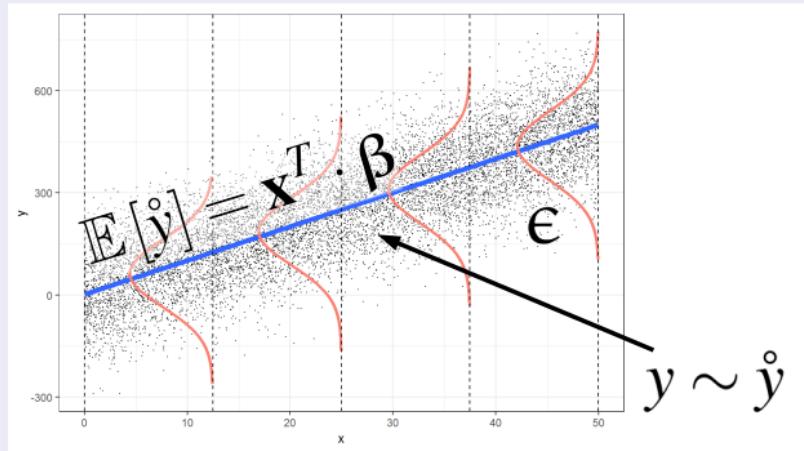
$$\mathbb{E} \left[\hat{\theta}_j^* \right] = \beta_j$$

How is the p -value computed (II)

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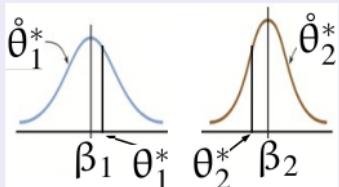
Theorem

Assume that



Picture from [LR19], Ch. I

Then



How is the p -value computed (III)

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Proof of the previous claim.¹

- Let's write (10) in vectorial form. Given a dataset $\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)\top} \\ \vdots \\ \mathbf{x}^{(M)\top} \end{bmatrix}$, the target vector is:

$$\hat{\mathbf{y}} = \mathbf{X} \cdot \boldsymbol{\beta} + \boldsymbol{\epsilon}$$

It is a Gaussian r.v., since it is a constant matrix $\mathbf{X} \cdot \boldsymbol{\beta}$ plus a random vector $\boldsymbol{\epsilon}$.

- The parameter vector we get from OLS regression is:

$$\hat{\boldsymbol{\theta}}^* = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \hat{\mathbf{y}}$$

It is a Gauss.r.v., since it is a constant matrix $(\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T$ multiplied by the Gauss.r.v. $\hat{\mathbf{y}}$.

- The mean is

$$\mathbb{E}[\hat{\boldsymbol{\theta}}^*] = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbb{E}[\hat{\mathbf{y}}] = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{X} \cdot \boldsymbol{\beta} = \boldsymbol{\beta}$$

and thus $\mathbb{E}[\hat{\theta}_j^*] = \beta_j$

- We can also compute the variance of $\hat{\boldsymbol{\theta}}^*$.²

¹To know more, check Sec. 3.8 of [HTF09], [these videos](#) and [this video](#).

²

How is the p -value computed (IV)

- Compute

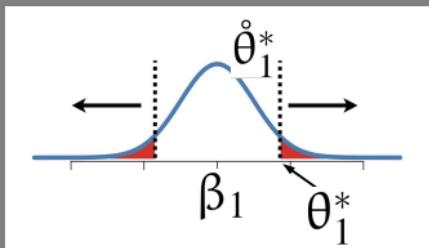
$$\boldsymbol{\theta}^* = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

- $\boldsymbol{\theta}^*$ is a realization of the Gauss.r.v.

$$\hat{\boldsymbol{\theta}}^* = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \hat{\mathbf{y}}$$

- For any feature j :

- θ_j^* realization of $\hat{\theta}_j^*$, such that $\mathbb{E} [\hat{\theta}_j^*] = \beta_j$
- Assume true parameter $\beta_j = 0$.
- Compute the variance $\text{Var}(\hat{\theta}_j^*)$.
- Draw the probability density of $\hat{\theta}_j^*$.



p-value
$\mathbb{P} [\hat{\theta}_j^* \geq \theta_j^*]$

Significance degradation

Adding features can degrade significance

	coef	P> t
const	351.7606	0.000
KBytesReceived	0.7115	0.001

	coef	P> t
const	282.8794	0.017
PacketsSent	-0.5551	0.925
KBytesReceived	0.5986	0.194
BufferHealth	18.3779	0.343

Theorem: prediction and true value averages

In an OLS regression, the average of the predictions equals the average of the true values of the target:

$$\bar{\hat{y}} = \bar{y}$$

where:

$$\bar{\hat{y}} \triangleq \frac{1}{M} \sum_{i=1}^M \hat{y}^{(i)} \quad \bar{y} \triangleq \frac{1}{M} \sum_{i=1}^M y^{(i)}$$

Proof

Normal equation:

$$\theta^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Theorem: prediction and true value averages

In an OLS regression, the average of the predictions equals the average of the true values of the target:

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Proof

Normal equation:

$$\theta^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Multiplying on the left by $\mathbf{X}^T \mathbf{X}$:

$$\mathbf{X}^T \mathbf{X} \cdot \underbrace{\theta^*}_{\mathbf{y}} = \mathbf{X}^T \mathbf{y}$$

Theorem: prediction and true value averages

In an OLS regression, the average of the predictions equals the average of the true values of the target:

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Proof

Normal equation:

$$\theta^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Multiplying on the left by $\mathbf{X}^T \mathbf{X}$:

$$\mathbf{X}^T \underbrace{\mathbf{X} \cdot \theta^*}_{\hat{y}} = \mathbf{X}^T \mathbf{y}$$

Theorem: prediction and true value averages

In an OLS regression, the average of the predictions equals the average of the true values of the target:

$$\bar{\hat{y}} = \bar{y}$$

where:

$$\bar{\hat{y}} \triangleq \frac{1}{M} \sum_{i=1}^M \hat{y}^{(i)} \quad \bar{y} \triangleq \frac{1}{M} \sum_{i=1}^M y^{(i)}$$

Proof

Normal equation:

$$\theta^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Multiplying on the left by $\mathbf{X}^T \mathbf{X}$:

$$\mathbf{X}^T \mathbf{X} \cdot \underbrace{\theta^*}_{\hat{y}} = \mathbf{X}^T \mathbf{y} \implies \mathbf{X}^T \hat{y} = \mathbf{X}^T \mathbf{y}$$

Theorem: prediction and true value averages

In an OLS regression, the average of the predictions equals the average of the true values of the target:

$$\bar{\hat{y}} = \bar{y}$$

where:

$$\bar{\hat{y}} \triangleq \frac{1}{M} \sum_{i=1}^M \hat{y}^{(i)} \quad \bar{y} \triangleq \frac{1}{M} \sum_{i=1}^M y^{(i)}$$

Proof

Normal equation:

$$\theta^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

The first element is:

$$[1 \dots 1] \cdot \hat{\mathbf{y}} = [1 \dots 1] \cdot \mathbf{y}$$

Multiplying on the left by $\mathbf{X}^T \mathbf{X}$:

$$\mathbf{X}^T \underbrace{\mathbf{X} \cdot \theta^*}_{\hat{\mathbf{y}}} = \mathbf{X}^T \mathbf{y} \implies \mathbf{X}^T \hat{\mathbf{y}} = \mathbf{X}^T \mathbf{y}$$

$$\hat{y} = \theta_0 + \underbrace{\theta_1 x_1 + \cdots + \theta_N x_N}_{\text{dependency}}$$

- θ_0 does not capture (x, y) dependency
- θ_0 just “aligns” predictions to meet the label average.

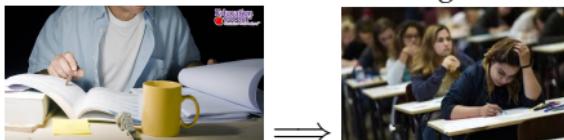
Section 3

Validation of a model

- Supervised learning: we construct a model $h(\mathbf{x})$ based on observed $(\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots)$ for the purpose of approximating y for new samples \mathbf{x} .
- **Generalization:**^a when the constructed model $h(\mathbf{x})$ is good at approximating labels y of **new** samples \mathbf{x} :

$$h(\mathbf{x}) \simeq y$$

- How do we test if the model *generalizes*.



- Student analogy
 - He/she checks the answers during **training**
 - Answers are hidden during the **test**

^aSec. 3.1 of [GBD92].

Training and test sets

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BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
4.446780	0.007103	true	q144p	144
3.989780	0.006509	true	q144p	144
3.700462	0.005897	true	q360p	360
4.512780	0.007156	true	q360p	360
9.454706	0.016805	true	q360p	360
4.606780	0.008046	true	q144p	144
5.301853	0.007990	true	q720p	720
3.638107	0.005493	true	q240p	240
5.314732	0.007147	true	q240p	240
8.554780	0.007118	true	q480p	480
4.189780	0.007516	true	q360p	360
3.633641	0.005897	true	q480p	480
1.495841	0.002473	true	q720p	720
8.802211	0.014076	true	q1080p	1080
4.611142	0.009263	true	q144p	144
5.590378	0.009113	true	q480p	480
4.940168	0.008851	true	q1080p	1080
4.940168	0.008851	true	q1080p	1080
9.239532	0.016335	true	q720p	720

X y

Training and test sets

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BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
4.446780	0.007103	true	q144p	144
3.989780	0.006509	true	q144p	144
3.700462	0.005897	true	q360p	360
4.512780	0.007156	true	q360p	360
9.454780	0.016805	true	q360p	360
4.606780	0.008046	true	q144p	144
5.301850	0.007990	true	q720p	720
3.638107	0.005193	true	q240p	240
5.314732	0.009400	true	q240p	240
8.554780	0.011688	true	q480p	480
4.189780	0.007516	true	q360p	360
3.633641	0.005897	true	q480p	480
1.495841	0.002473	true	q720p	720
8.802211	0.014076	true	q1080p	1080
4.611142	0.009263	true	q144p	144
5.590378	0.009113	true	q480p	480
4.940168	0.008851	true	q1080p	1080
4.940168	0.008451	true	q1080p	1080
9.239532	0.015355	true	q720p	720

X train Y train

X test Y test

Training and test sets

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BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
4.446780	0.007103	true	q144p	144
3.989780	0.006509	true	q144p	144
3.700462	0.005897	true	q360p	360
4.512780	0.007156	true	q360p	360
9.454750	0.016805	true	q360p	360
4.606780	0.008046	true	q144p	144
5.301957	0.007990	true	q720p	720
3.638107	0.005393	true	q240p	240
5.314732	0.009400	true	q240p	240
8.554780	0.011688	true	q480p	480
4.189780	0.007516	true	q360p	360
3.633641	0.005897	true	q480p	480
1.495841	0.002473	true	q720p	720
8.802211	0.014076	true	q1080p	1080
4.611142	0.009263	true	q144p	144
5.590378	0.009113	true	q480p	480
4.940168	0.008851	true	q1080p	1080
4.940168	0.008451	true	q1080p	1080
9.239532	0.016335	true	q720p	720

X train Y train



X test Y test

Training and test sets

36 / 54

Train using only the **training set** ($\mathbf{X}, \hat{\mathbf{y}}$):

BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
4.446780	0.007103	true	q144p	144
3.989780	0.006509	true	q144p	144
3.700462	0.005897	true	q360p	360
4.512780	0.007156	true	q360p	360
9.454750	0.016805	true	q360p	360
4.606780	0.008046	true	q144p	144
5.301957	0.007990	true	q720p	720
3.638107	0.005393	true	q240p	240
5.314732	0.009400	true	q240p	240
8.554780	0.011688	true	q480p	480
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1.495841	0.002473	true	q720p	720
8.802211	0.014076	true	q1080p	1080
4.611142	0.009263	true	q144p	144
5.590378	0.009113	true	q480p	480
4.940168	0.008851	true	q1080p	1080
4.940168	0.008451	true	q1080p	1080
9.239532	0.016335	true	q720p	720

X train Y train
X test Y test

$$\boldsymbol{\theta}^* \triangleq \arg \min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}, \mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}})$$

The trained model is

$$h_{\boldsymbol{\theta}^*}(\cdot)$$

Evaluate the quality of the trained model via:

$$J(\boldsymbol{\theta}^*, \mathbf{X}_{\text{test}}, \mathbf{y}_{\text{test}})$$

(Test error or generalization error^a or out-of-sample error)

The J used during training and test may be different.

Which method is better?

BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
4.446780	0.007103	true	q144p	144
3.989780	0.006509	true	q144p	144
3.700462	0.005897	true	q360p	360
4.512780	0.007156	true	q360p	360
9.454706	0.016805	true	q360p	360
4.606780	0.008046	true	q144p	144
5.301853	0.007990	true	q720p	720
3.638107	0.005493	true	q240p	240
5.314732	0.009400	true	q240p	240
8.554780	0.011688	true	q480p	480
4.189780	0.007516	true	q360p	360
3.633641	0.005897	true	q480p	480
1.495641	0.002473	true	q720p	720
8.802211	0.014076	true	q1080p	1080
4.611142	0.009263	true	q144p	144
5.590378	0.009113	true	q480p	480
4.940168	0.008851	true	q1080p	1080
4.940168	0.008851	true	q1080p	1080
9.239532	0.016335	true	q720p	720

BufferHealth	BufferProgress	BufferValid	label	label_num
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9.454706	0.016805	true	q360p	360
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4.611142	0.009263	true	q144p	144
5.590378	0.009113	true	q480p	480
4.940168	0.008851	true	q1080p	1080
4.940168	0.008851	true	q1080p	1080
9.239532	0.016335	true	q720p	720

What if the data provider first experimented with all low resolutions and finally with all the highest?



Go to notebook 02.regression/a.regression.ipynb

Section 4

Instability of a model (Variance)

$$\text{Var}(j) = \frac{1}{M-1} \sum_{i=1}^M (x_j^{(i)} - \mu_j)^2$$

- Suppose $x_j^{(i)} = c$ for all samples i
- $\mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & c & \dots & x_N^{(1)} \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 1 & x_1^{(M)} & \dots & c & \dots & x_N^{(M)} \end{bmatrix}$
- Not full rank
- $\Rightarrow (\mathbf{X}^T \mathbf{X})^{-1}$ does not exist
- $\theta^* = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$ impossible

- Two features j_1, j_1 (columns of \mathbf{X}) are **collinear** if they are proportional

$$\begin{bmatrix} x_{j_1}^{(1)} \\ \vdots \\ x_{j_1}^{(N)} \end{bmatrix} = \alpha \begin{bmatrix} x_{j_2}^{(1)} \\ \vdots \\ x_{j_2}^{(N)} \end{bmatrix}$$

In this case, column j_2 **adds no information** about prediction.

- $\Rightarrow \mathbf{X}$ has no full rank
- $\Rightarrow (\mathbf{X}^T \cdot \mathbf{X})$ is not invertible
- \Rightarrow not unique.
- \Rightarrow The normal equation

$$\boldsymbol{\theta}^* = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

cannot be computed.

- In real world, perfect collinearity is rare, but

$$\begin{bmatrix} x_{j_1}^{(1)} \\ \vdots \\ x_{j_1}^{(N)} \end{bmatrix} \simeq \alpha \begin{bmatrix} x_{j_2}^{(1)} \\ \vdots \\ x_{j_2}^{(N)} \end{bmatrix}$$

and the computer is able to compute the normal equation, but ...

- For any model h_θ :

$$\begin{aligned} h_\theta(\mathbf{x}) &= \theta_{j_1}x_{j_1} + \theta_{j_2}x_{j_2} + \sum_{j \notin \{j_1, j_2\}} \theta_j x_j \\ &\simeq (\alpha\theta_{j_1} + \theta_{j_2})x_{j_2} + \sum_{j \notin \{j_1, j_2\}} \theta_j x_j \end{aligned}$$

- Infinite pairs of $(\theta_{j_1}, \theta_{j_2})$ would be almost equivalent
 - Ex.

- How does OLS choose among such pairs? Randomly
- Small differences of $\mathbf{X} \Rightarrow$ big differences in $(\theta_{j_1}^*, \theta_{j_2}^*)$
- \Rightarrow Variance

- If j -th feature is a linear combination of others

$$\mathbf{X}_j = \alpha_1 \mathbf{X}_{j_1} + \alpha_2 \mathbf{X}_{j_2} + \dots$$

- $\mathbf{X} = [\mathbf{1} | \mathbf{X}_1 | \dots | \mathbf{X}_N]$ no full rank
- The normal equation

$$\boldsymbol{\theta}^* = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

cannot be computed.

- How to discover Multi-collinearity? ...

- Humans are good at generalizing knowledge ...
- ... because their perception models have low variance

Instability

A model is **unstable** if, by perturbing a bit the training dataset, the model changes completely [Wiknd].

Suppose $\tilde{\mathbf{X}}, \tilde{\mathbf{y}}$ is a slightly perturbed version of \mathbf{X}, \mathbf{y} . If a model is unstable:

$$\tilde{\theta}^* = \arg \min_{\theta} J(\theta, \tilde{\mathbf{X}}, \tilde{\mathbf{y}})$$

completely different than

$$\theta^* = \arg \min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

- Instability \Rightarrow high sensitivity to training data.
(§5 of [BK11])



A good learner would learn the same



Go to notebook 02regression/.a.regression.ipynb

Section 5

Cross-validation

How can we be sure that, if we change train/test split the error does not change?
⇒ **Cross-validation.**

Algorithm 1 K -fold validation

- 1: Divide the dataset in K subsets
 - 2: **for** $i = 1$ to K **do**
 - 3: Keep subset i for test
 - 4: Train on all the others
 - 5: Compute test error
 - 6: **end for**
 - 7: Error = average of test errors
-

BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
4.446780	0.007103	true	q144p	144
3.989780	0.006509	true	q144p	144
3.700462	0.005897	true	q360p	360
4.512780	0.007156	true	q360p	360
9.454706	0.016805	true	q360p	360
4.606780	0.008046	true	q144p	144
5.301853	0.007990	true	q720p	720
3.638107	0.005493	true	q240p	240
5.314732	0.009400	true	q240p	240
8.554780	0.011688	true	q480p	480
4.189780	0.007516	true	q360p	360
3.633641	0.005897	true	q480p	480
1.495841	0.002473	true	q720p	720
8.802211	0.014076	true	q1080p	1080
4.611142	0.009263	true	q144p	144
5.590378	0.009113	true	q480p	480
4.940168	0.008851	true	q1080p	1080
4.940168	0.008851	true	q1080p	1080
9.239532	0.016335	true	q720p	720

TRAINING SET

TEST SET



Go to notebook 02.regression/a.regression.ipynb

In this lesson

- Supervised Learning
- First Model in Python
(Linear Regression)
- Feature selection
- Validation: Train/Test; Cross-validation

Regression (continued)

- Polynomial Regression
- Model Variance / Complexity
- Regularization
- Scaling
- Feature Selection

Classification

- Logistic Regression
- Classification Performance
- Class imbalance

- Dealing with Multi-collinearity [DEB⁺13]
- Variance Inflation Factor for testing Multi-collinearity: pag. 101-102 of [JWHT13]
- Cross-validation from [machinelearningmastery](#)

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