CSCI E-82

Advanced Machine Learning,
Data Mining & Artificial Intelligence
Lecture 4

Probability, Statistics, Regression Time Series Part I

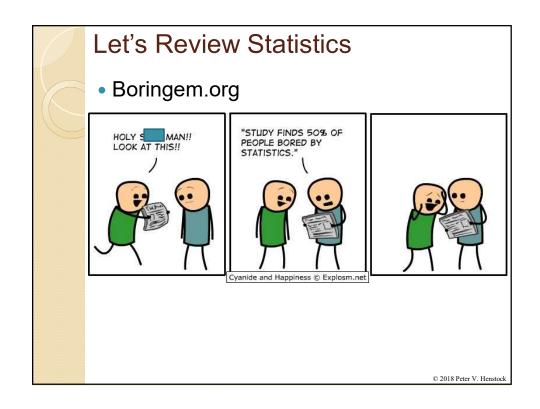
Peter V. Henstock Fall 2018

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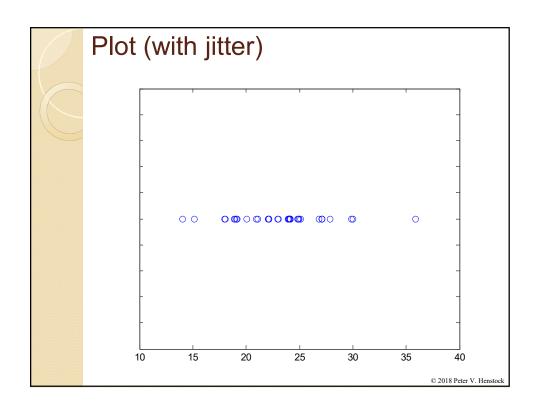
Administrivia

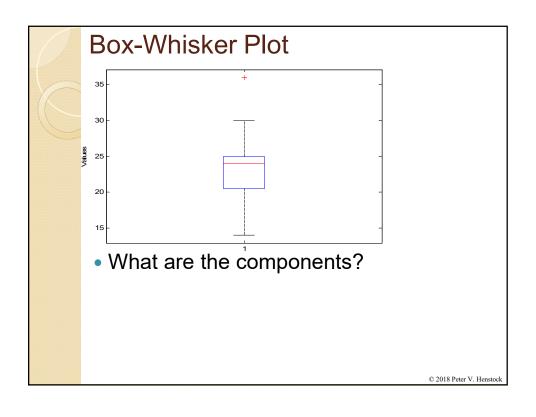
- HW2 how is it going?
- Topic Presentations
 - Accepting groups of 2 or 3
 - Sign up using the same Google spreadsheet
 - Welcome to keep your partner or switch
 - Please talk to your existing partner regardless
 - Goal: 15 minute presentation
 - Will schedule presentations shortly but you will have a week to prepare from them
 - Need to select a moderately narrow topic
 - I will review topics on the sheet.
 - · First sign-ups for a given topic win

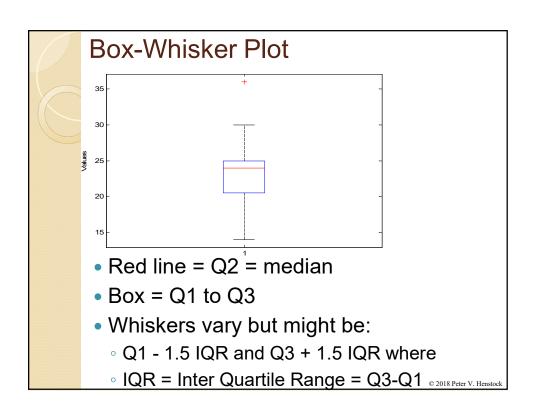
1D Data Statistics



Zoom Sign-in Times (min after hour) N=36			
14	23	27	
15	23	27	
18	23	27	
18	24	27	
19	24	28	
19	24	30	
19	24	30	
20	24	36	
21	24		
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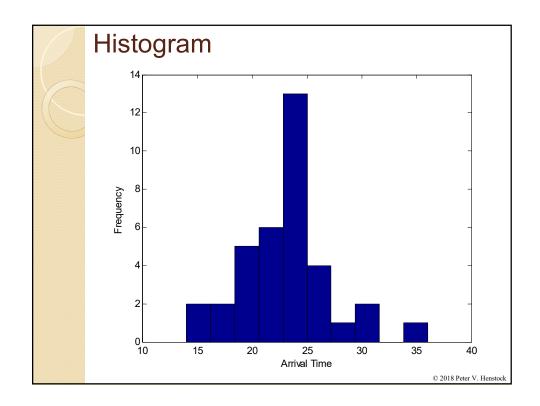
Sample Statistics & Robustness

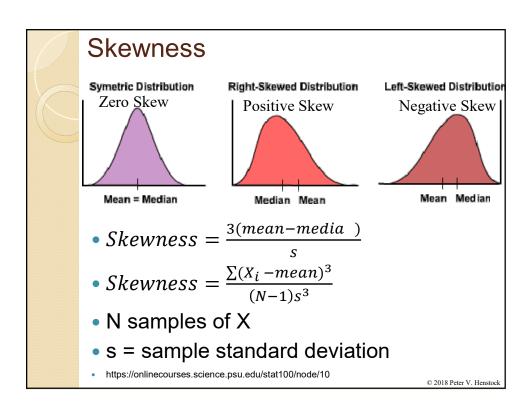
- Mean $\bar{\bar{x}} = \frac{1}{N} \sum_{i=0}^{N} x_i$
- Median =
 - ∘ x_i that is middle value of sorted X of odd N
 - $(x_i+x_{i+1})/2$ that is average of 2 central points
- Range = max(X) min(X)
- Sample variance $s^2 = \frac{\sum_{i=1}^{N} (x_i \bar{x})^2}{N-1}$
- Robustness = immunity to outliers
- Which of these are robust?

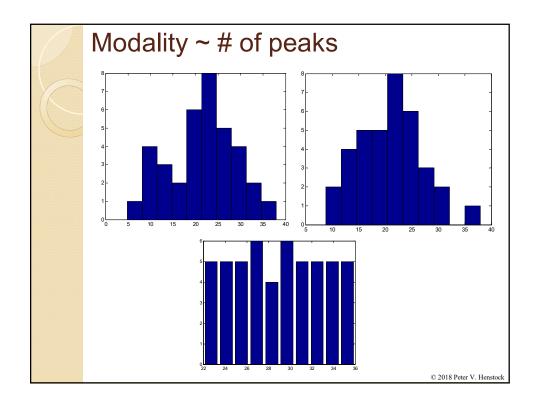
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Sample Statistics?

- Mean $\bar{\bar{x}} = \frac{1}{N} \sum_{i=0}^{N} x_i$
- Median =
 - \circ x_i that is middle value of sorted X of odd N
 - $(x_i+x_{i+1})/2$ that is average of 2 central points
- Range = max(X) min(X)
- Sample variance $s^2 = \frac{\sum_{i=1}^{N} (x_i \bar{x})^2}{N-1}$
- Why are these "sample" statistics?



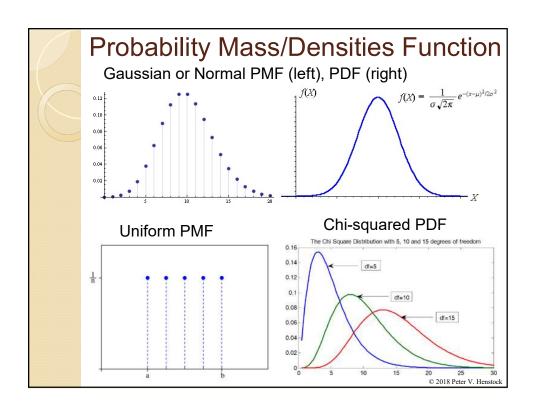




Distributions

Random Variable

- Variable that takes on a specific value
- Member of a group
- Group values are described according to a frequency distribution
- Types
 - Discrete
 - Continuous
- Frequently drawn from a distribution



Common density functions

Uniform(a,b)

$$f(x) = \frac{1}{b-a} \text{ for } x \in [a, b]$$

Bernoulli(p) for p in [0,1]

•
$$f(0) = 1-p = failure$$
 $f(1) = p = success$

$$f(1) = p = success$$

Binomial(n, p) = sum n Bernoulli trials

$$f(x) = \binom{n}{x} p^x p^{n-x} \quad x = 0, \dots n$$

• Normal (Gaussian) distribution $N(\mu, \sigma)$

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{(x-\mu)^2}{2\sigma^2})$$

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Other Discrete/Continuous densities

http://aleph0.clarku.edu/~djoyce/ma218/distributions.pdf

Distribution	Type	Mass/density function $f(x)$	Mean μ	Variance σ^2
Uniform(n)	D	1/n, for $x = 1, 2,, n$	(n+1)/2	$(n^2-1)/12$
$\operatorname{Uniform}(a,b)$	C	$\frac{1}{b-a}$, for $x \in [a,b]$	$\frac{a+b}{2}$	$\frac{(b-a)^2}{12}$
Bernoulli(p)	D	f(0) = 1 - p, f(1) = p	p	p(1 - p)
BINOMIAL (n, p)	D	$\binom{n}{x}p^x(1-p)^{n-x}$,	np	npq
GEOMETRIC(p)	D	for $x = 0, 1,, n$ $q^{x-1}p$, for $x = 1, 2,$	1/p	$(1-p)/p^2$
NEGATIVEBINOMIAL (p,r)	D	$\begin{pmatrix} \hat{x}-\hat{1} \\ r-1 \end{pmatrix} p^r q^{x-r},$	r/p	$r(1-p)/p^2$
${\bf HYPERGEOMETRIC}(N,M,n)$	D	for $x = r, r + 1,$ $\frac{\binom{M}{x}\binom{N-M}{n-x}}{\binom{N}{n}},$ for $x = 0, 1,, n$	np	np(1-p)
$Poisson(\lambda t)$	D	$\frac{1}{x!}(\lambda t)^x e^{-\lambda t}$, for $x=0,1,\ldots$	λt	λt
Exponential (λ)	C	$\lambda e^{-\lambda x}$, for $x \in [0, \infty)$	$1/\lambda$	$1/\lambda^2$
$\operatorname{Gamma}(\lambda,r)$	C	$\frac{1}{\Gamma(r)} \lambda^r x^{r-1} e^{-\lambda x}$	r/λ	r/λ^2
$Gamma(\alpha,\beta)$		$\frac{1}{\Gamma(r)} \lambda^r x^{r-1} e^{-\lambda x}$ $= \frac{x^{\alpha-1} e^{-x/\beta}}{\beta^{\alpha} \Gamma(\alpha)},$	$= \alpha \beta$	$=a\beta^2$
		for $x \in [0, \infty)$	[2018 Peter V. Henstock

Other Discrete/Continuous densities

http://aleph0.clarku.edu/~djoyce/ma218/distributions.pdf

$\text{Beta}(\alpha,\beta)$	C	$\frac{1}{\mathrm{B}(\alpha,\beta)} x^{\alpha-1} (1-x)^{\beta-1},$	$\frac{\alpha}{\alpha + \beta}$	$\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$
$Normal(\mu, \sigma^2)$	C	for $0 \le x \le 1$ $\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right),$	μ	σ^2
ChiSquared(ν)	C	for $x \in \mathbf{R}$ $\frac{x^{\nu/2-1}e^{x/2}}{2^{\nu/2}\Gamma(\nu/2)}, \text{ for } x \ge 0$	ν	2ν
$\mathrm{T}(u)$	C	$\frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\pi\nu}\Gamma(\frac{\nu}{2})(1+x^2/\nu)^{(\nu+1)/2}}$ for $x \in \mathbf{R}$	0	$\nu/(\nu-2)$
$\mathrm{F}(u_1, u_2)$	C	$ \frac{1}{B(\frac{\nu_1}{\nu_2}, \frac{\nu_2}{2})} \frac{(\frac{\nu_1}{\nu_2})^{\nu_1/2} x^{\nu_1/2 - 1}}{(1 + \frac{\nu_1}{\nu_2} x)^{(\nu_1 + \nu_2)/2}} $ for > 0	$\frac{\nu_2}{\nu_2 - 2}$	$\frac{2\nu_2^2(\nu_1+\nu_2-2)}{\nu_1(\nu_2-2)^2(\nu_2-4)}$

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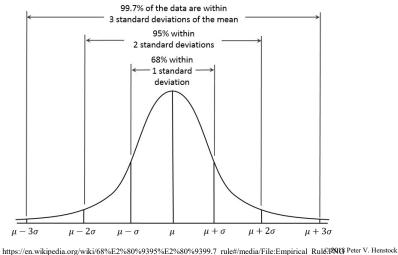
Properties of PMF/PDF

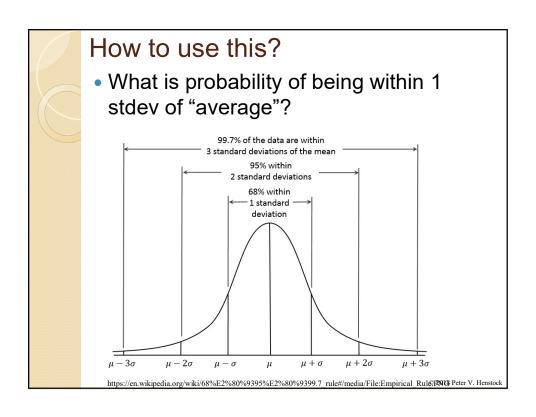
- prob(x) = p(x) = f(x) for discrete
- $p(x \in [a,b]) = \sum_{i=a}^{b} f(x_i)$ for discrete
- $p(x \in [a,b]) = \int_a^b f(x_i) dx$ for continuous

•
$$\sum_{-\infty}^{\infty} f(x_i) = 1$$
 $\int_{-\infty}^{\infty} f(x_i) dx = 1$

How to use this?

- Einstein had 160 IQ which is N(100,15)
- P(X >=160) = $\int_{160}^{\infty} f(x) dx$



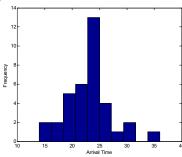


Statistics from PMF

- $Mean = \mu = \sum_{i=0}^{N} p_i x_i$
- $Var = \sigma^2 = \sum_{i=0}^{N} p_i (x_i \mu)^2$

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Why bother with PDF/PMFs?



- Provide an abstraction of actual sample histogram (normalized)
 - Avoids issues of outliers, etc.
- Data compression: N pts → parameters
- Enables statistical analyses

Randomness

Characteristic	Pseudo-Random Number Generators	True Random Number Generators	
Efficiency	Excellent	Poor	
Determinism	Determinstic	Nondeterministic	
Periodicity	Periodic	Aperiodic	

https://www.random.org/randomness/

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Normal Distribution

- If X and Y are random variables from a normal distribution, X+Y is also normal
- If you take many independent random variables from any single distribution, the sum approximates a normal distribution
 - Central Limit Theorem (with caveats)

Probabilities

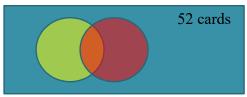
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Random Variable

- Variable that takes on a specific value
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- Types
 - Discrete
 - Continuous
- Frequently randomly drawn from a distribution

Probability Functions

- P(x) = probability of x occurring
 - Depends on the space of possibilities
- $P(x) = 1 P(\sim X)$



- P(spades) = ?
- P(~spades) = ?
- P(Red "Royalty")

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Joint Probabilities

- P(X,Y) = P(X and Y)
- P(X or Y) = P(X) + P(Y) P(X and Y)

$$P(X, Y)$$
 $P(X, Y)$ $P(X, Y)$

$$P(X) = \text{blue circle}$$
 $P(Y) = \text{red circle}$

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Joint Probabilities

- If X and Y are independent
 - \circ P(X,Y) = P(X)P(Y)
- Example 1
 - X = probability of flipping coin
 - Y = probability of rolling a die (dice)
- Example 2
 - X = probability of grass is wet
 - ∘ Y = probability of rain

What does this imply statistically?

A major airlines company received an anonymous bomb threat. To figure out ways of reducing the risk, a team was assembled. One of the members was a statistician. After careful thought and calculations, he handed a sealed bag to the airlines company and ordered them to put this bag in their plane during every journey. After a few journeys, the flight team were intrigued, and decided to open the bag. Inside, they found a bomb. They quickly confronted the statistician and asked for an explanation. He replied, "Well. Statistics show that there is a 1 in a 1,000,000 chance of a bomb being on a plane. But for 2 bombs to be on the same plane, the chances are only 1 in a 1,000,000,000,000."

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What does this imply statistically?

A major airlines company received an anonymous bomb threat. To figure out ways of reducing the risk, a team was assembled. One of the members was a statistician. After careful thought and calculations, he handed a sealed bag to the airlines company and ordered them to put this bag in their plane during every journey. After a few journeys, the flight team were intrigued, and decided to open the bag. Inside, they found a bomb. They quickly confronted the statistician and asked for an explanation. He replied, "Well. Statistics show that there is a 1 in a 1,000,000 chance of a bomb being on a plane. But for 2 bombs to be on the same plane, the chances are only 1 in a 1,000,000,000,000.

This is a joke. Neither the course staff nor Harvard endorses carrying bombs on planes

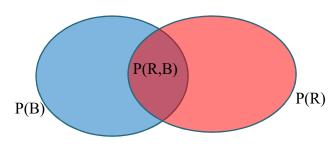
Conditional Probabilities

- P(X|Y) = Probability of X "given" Y
- P(X|Y) = P(X,Y) / P(Y)

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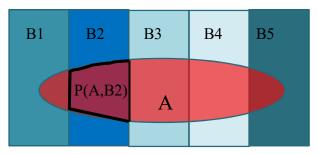
Conditional Probabilities

- P(X|Y) = Probability of X "given" Y
- P(X|Y) = P(X,Y) / P(Y)
- Probability in blue given it's in red?



Visual Idea

• $P(A) = \sum_{i=0}^{n} P(A | B_i) P(B_i)$



- Region overlap: P(B2, A)
- P(B2,A) = P(A|B2)P(B2)
- If we add up all intersections over B's:
 - $P(A) = \sum_{i=0}^{n} P(A \mid B_i) P(B_i)$

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Basic Rules for Probabilities

- Sum Rule:
 - \circ P(A U B) = P(A) + P(B) P(A \cap B)
- Product Rule:
 - \circ P(A \cap B) = P(A,B) = P(A|B)P(B) = P(B|A)P(A)
- Joint→Marginal
 - $P(A) = \sum_{i=0}^{n} P(A, B_i)$
 - $P(A) = \sum_{i=0}^{n} P(A \mid B_i) P(B_i)$

Chain Rule



What is the probability of this whole thing?

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Chain Rule

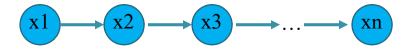


What is the probability of this whole thing?

P(x1, x2, ...xn)

How can we compute this using conditional probabilities? P(X1)*

Chain Rule



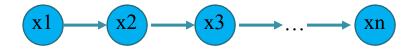
What is the probability of this whole thing?

P(x1, x2, ...xn)

How can we compute this using conditional probabilities? P(X1)*P(X2|X1)

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Chain Rule



What is the probability of this whole thing?

P(x1, x2, ...xn)

How can we compute this using conditional probabilities? P(X1)*P(X2|X1)*P(X3|X1,X2)...

. . .

Chain Rule



What is the probability of this whole thing?

P(x1, x2, ...xn)

How can we compute this using conditional probabilities? P(X1)*P(X2|X1)*P(X3|X1,X2)... ...P(Xn | X1..XN-1)

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Bayes Rule

Bayes Rule

Thomas Bayes 1702-1761 Presbyterian minister in UK



•
$$P(h|e) = \frac{P(e|h)P(h)}{P(e)}$$

Wikipedia

- Basis of classifiers
- Basis of network inferences
- Basis of structuring information or expert systems

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Bayes Rule

Thomas Bayes 1702-1761 Presbyterian minister in UK



Wikipedia

•
$$P(h|e) = \frac{P(e|h)P(h)}{P(e)}$$

•
$$P(h|e) = \frac{P(h,e)}{P(e)}$$
 $P(h,e) = P(e|h)P(h)$

Components of Bayes Rule

- $P(hyp|data) = \frac{P(data|hyp)P(hyp)}{P(data)}$
- p(data|hyp) = p(data, hyp) / p(hyp)
- What is p(hyp|data) if hyp and data are independent?

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Conditional Independence

- P(X,Y|Z) = P(X|Z)P(Y|Z)
 - ∘ "X is independent of Y given Z"
 - X and Y are conditionally independent
- Clearly an extension of the general independence
 - \circ P(A,B) = P(A)P(B)
- If X and Y are independent, can we say they are conditionally independent?

Conditional Independence Examples

- https://www.quora.com/What-areexamples-of-events-that-areindependent-but-not-conditionallyindependent-and-vice-versa
- Good examples to navigate:
 - [in]dependence
 - conditional [in]dependence
 - \circ P(x|y) if independent p(x) \rightarrow
 - $P(x|y) = P(x,y) / P(y) = P(x)P(y)/P(y) \rightarrow P(x)$

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Components of Bayes Rule

- $P(hyp|data) = \frac{P(data|hyp)P(hyp)}{P(data)}$
- P(hyp) = "Prior"
 - Prior probability of a hypothesis
- P(hyp|data) = "posterior"
 - Probability of hypothesis given data
- P(data|hyp) = "likelihood"
 - Probability of data fitting a given hypothesis
- P(data) = normalizing constant
 - Data is same across all hypotheses

2 Random Variables

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Two random variables

- Mean values are the same
- Standard deviations are the same
- Relationship:
 - Correlation Coefficient
 - Covariance

Covariance

- $Cov(X,Y) = \sigma(X,Y) = E[X-E(X)] E[Y-E(Y)]$
- Cov(X,Y) = $\frac{1}{N-1} \sum_{i=1}^{N} (X_i \bar{X})(Y_i \bar{Y})$
- Sample Covariance(X,Y)
 - $= \frac{1}{N-1} \sum_{i=1}^{N} (X_i \bar{X}) (Y_i \bar{Y})$

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Covariance

- $Cov(X,Y) = \sigma(X,Y) = E[X-E(X)] E[Y-E(Y)]$
- Cov(X,Y) = $\frac{1}{N-1} \sum_{i=1}^{N} (X_i \bar{X})(Y_i \bar{Y})$
- Sample Covariance(X,Y)

$$\circ = \frac{1}{N-1} \sum_{i=1}^{N} (X_i - \bar{X}) (Y_i - \bar{Y})$$

What is the Cov(X,X)?

Covariance

- $Cov(X,Y) = \sigma(X,Y) = E[X-E(X)] E[Y-E(Y)]$
- Cov(X,Y) = $\frac{1}{N-1} \sum_{i=1}^{N} (X_i \bar{X})(Y_i \bar{Y})$
- Sample Covariance(X,Y)

$$= \frac{1}{N-1} \sum_{i=1}^{N} (X_i - \bar{X}) (Y_i - \bar{Y})$$

- What is the Cov(X,X)?
- If X and Y are independent, what is Cov(X,Y)?

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Covariance Matrix

- Let $X = [X_1...X_n]^T$ be a column vector
- Covariance matrix is written with Σ
- $\Sigma_{ij} = \text{cov}(X_{i,}X_{j}) = \text{E}[(X_{i}-\mu_{i})(X_{j}-\mu_{j})]$

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1 - \mu_1)(X_1 - \mu_1)] & \mathrm{E}[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_1 - \mu_1)(X_n - \mu_n)] \\ \\ \mathrm{E}[(X_2 - \mu_2)(X_1 - \mu_1)] & \mathrm{E}[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_2 - \mu_2)(X_n - \mu_n)] \\ \\ \vdots & \vdots & \ddots & \vdots \\ \\ \mathrm{E}[(X_n - \mu_n)(X_1 - \mu_1)] & \mathrm{E}[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}$$

• $\Sigma = E(XX^T) - \mu\mu^T$

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Covariance Matrix

- Let $X = [X_1...X_n]^T$ be a column vector
- Covariance matrix is written with Σ
- $\Sigma_{ij} = \text{cov}(X_{i,}X_{j}) = \text{E}[(X_{i}-\mu_{i})(X_{j}-\mu_{j})]$

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1 - \mu_1)(X_1 - \mu_1)] & \mathrm{E}[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_1 - \mu_1)(X_n - \mu_n)] \\ \\ \mathrm{E}[(X_2 - \mu_2)(X_1 - \mu_1)] & \mathrm{E}[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_2 - \mu_2)(X_n - \mu_n)] \\ \\ \vdots & \vdots & \ddots & \vdots \\ \\ \mathrm{E}[(X_n - \mu_n)(X_1 - \mu_1)] & \mathrm{E}[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}$$

• If X1...Xn are all independent, what does the covariance matrix look like?

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Sample Covariance Matrix example

X	Υ
1	3
4	2
2	4
5	3
3	3
6	3

- Compute mean of X
- Compute mean of Y
- Sample cov of X, X
- Sample cov of Y, Y

Sample Covariance Matrix example

X	Υ
1	3
4	2
2	4
5	3
3	3
6	3

- Compute mean of X
 - \circ Sum(X)/6 = 3.5
- Compute mean of Y
- Sample cov of X, X
- Sample cov of Y, Y
- Sample cov of X, Y

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Sample Covariance Matrix example

X	Υ
1	3
4	2
2	4
5	3
3	3
6	3

- Compute mean of X
 - \circ Sum(X)/6 = 3.5
- Compute mean of Y
 - Sum(Y)/6 = 3
- Sample cov of X, X
- Sample cov of Y, Y
- Sample cov of X, Y

Sample Covariance Matrix example

X	Υ
1	3
4	2
2	4
5	3
3	3
6	3

- Compute mean of X
 - \circ Sum(X)/6 = 3.5
- Compute mean of Y
 - Sum(Y)/6 = 3
- Sample cov of X, X
 - [Σ (x-meanX)²] / (N-1)
- Sample cov of Y, Y
- Sample cov of X, Y

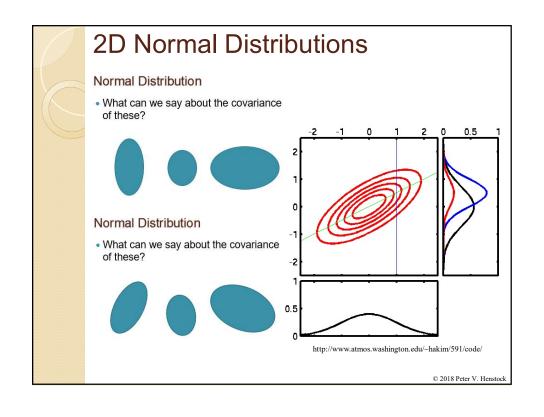
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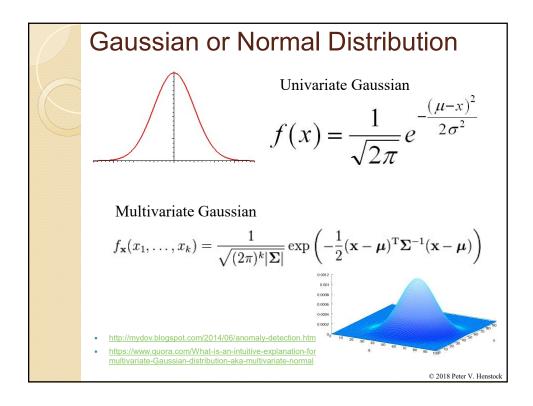
Sample Covariance Matrix example

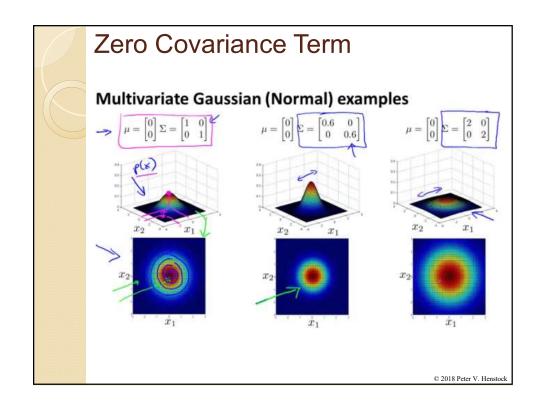
X	Υ
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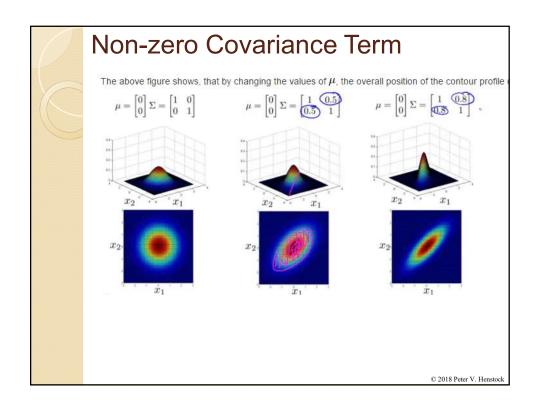
- Compute mean of X
 - \circ Sum(X)/6 = 3.5
- Compute mean of Y
 - \circ Sum(Y)/6 = 3
- Sample cov of X, X
 - \circ [Σ (xi-meanX)²] / (N-1) = 3.5
 - \circ [Σ (xi-3.5)²] / (6-1) = 3.5
- Sample cov of Y, Y
 - $[\Sigma (yi-meanY)^2] / (N-1) = 0.4$
- Sample cov of X, Y

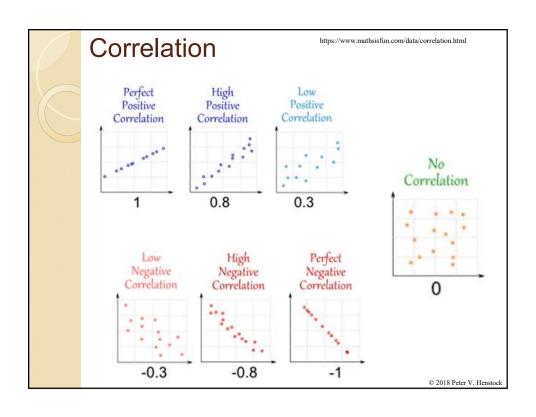
Sam	ple (Covariance Matrix example
X 1 4 2 5 3 6	3 2 4 3 3 3	 Compute mean of X Sum(X)/6 = 3.5 Compute mean of Y Sum(Y)/6 = 3 Sample cov of X, X [Σ (x-meanX)²] / (N-1) = 3.5 [Σ (x-3.5)²] / (6-1) = 3.5 Sample cov of Y, Y
		 [Σ (y-meanY)²] / (N-1) = 0.4 Sample cov of X, Y [Σ (x-meanX)(y-meanY)] / (N-1) = -0.4











Correlation coefficient

- $r = CorrCoef(X,Y) = cov(X,Y) / (s_X s_Y)$
 - Technically, the Pearson corr. Coef.

•
$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

- Range of values for correlation is [-1, 1]
- No units

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Regression

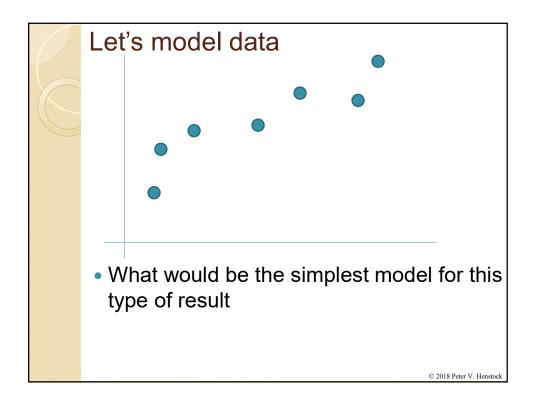
Sir Francis Galton

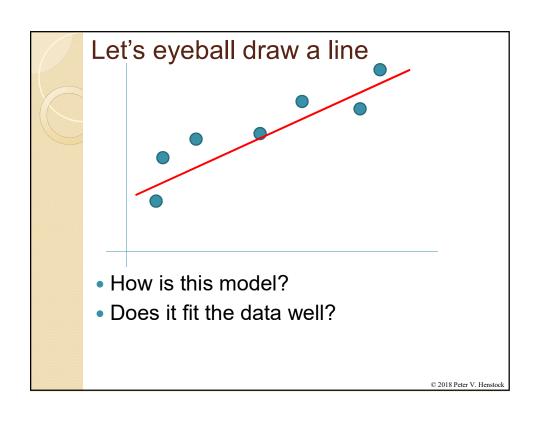
- 1822-1911 Victorian England
- Statistician & scientist
 - Regression
 - Standard deviation
 - Correlation
 - Psychometrics
 - Fingerprint classification
 - Weather map and scientific meteorology
- Coined terms in our lexicon:
 - Eugenics
 - Nature vs. Nurture

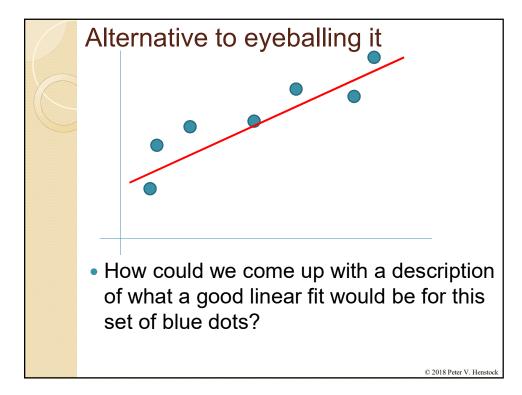
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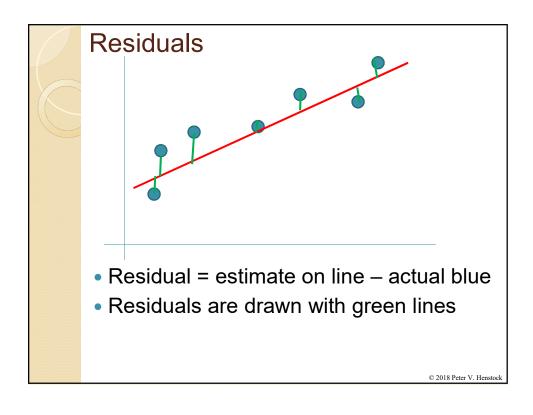
Types of Learning

- Supervised
 - Provide output labels/values & input features
- Unsupervised
 - Provide only input features
- Semi-supervised learning
- Reinforcement learning









Regression vs. PCA

 Is this regression line fit the same one as the principal component?

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Generative Model

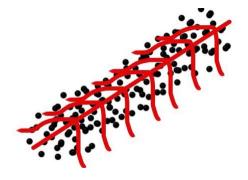
• What is it?

Generative Model

- What does generative mean?
 - Could try to model the residuals and come up some useful ideas on model
 - Instead we are going to create a model that assumes the points were distributed by a generating model
 - Specifically, we start with points on a line and randomly shift the points according to a distribution
- $y_i = w_0 + w_1 x_i + \varepsilon_i$
- ε_i ~ N(mean=0, stdev= σ)
- What does this have to do with residuals?

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Residuals



- Residuals come from a normal distribution centered on the line
- http://stats.stackexchange.com/questions/148803/how-does-linear-regressionuse-the-normal-distribution

Residuals → Best Fit Model

- How can we use the residuals to come up with a best fit line?
- What would be a good function to optimize?
- a) Σ residuals
- b) Σ |residuals|
- c) Σ [residuals]²
- d) Σ [yi residuals]²
- e) Σ [residuals / yi]²

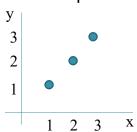
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Simple case

- Optimize the least squares function
- $SumsqError = \sum_{i=1}^{N} \epsilon_i^2$
- But $y_i = w_0 + w_1 x_i + \epsilon_i$ but we don't know the true weights so we estimate
- so $\epsilon_i = y_i \widehat{w_o} \widehat{w_1} x_i$
- SumsqError = $\sum_{i=1}^{N} (y_i \widehat{w_o} \widehat{w_1} x_i)^2$
- How can we minimize the error?
- How can we find the best $\widehat{w_0}$ and $\widehat{w_1}$?

Sanity check example

- Sumsq error = cost function = J
- Goal is to minimize J
- J = sum-square distance between
 - predicted y values of line given parameters
 - the actual y values
 - at each x point

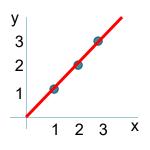


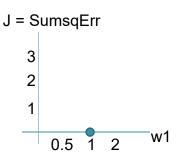
J = Sumsq Error

3
2
1
0.5 1 2 w1

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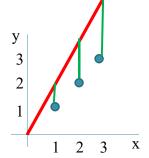
Figure out J for a few points

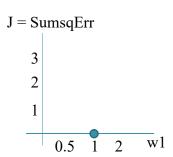




- Assume w0 = 0 (zero y-intercept)
- For w1 = 1:

Figure out J for a few points

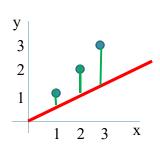


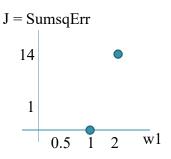


- Assume w0 = 0 (zero y-intercept)
- For w1 = 1: = 0
- For w1 = 2:

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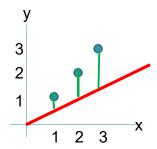
Figure out J for a few points

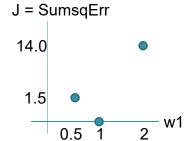




- Assume w0 = 0 (zero y-intercept)
- For w1 = 1: = 0
- For w1 = 2: = $(2-1)^2 + (4-2)^2 + (6-3)^2 = 14$
- For w1 = 0.5 =

Figure out J for a few points

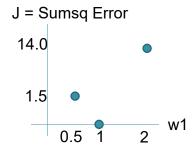




- Assume w0 = 0 (zero y-intercept)
- For w1 = 1: = 0
- For w1 = 2: = $(2-1)^2 + (4-2)^2 + (6-3)^2 = 14$
- For w1 = $0.5 = (1-1/2)^2 + (2-1)^2 + (1.5-1)^2$ = 1.5

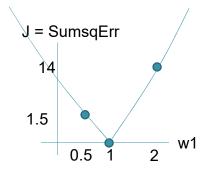
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Modeling the error



What shape is J vs. w1?

Parabola (badly drawn below)



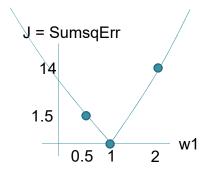
- Min value will be 0 in this case—why?
- How could we optimize the J as a function of w1?

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Derivative Formulation

What shape is J vs. w1?

Parabola (badly drawn below)



- Min value will be 0 in this case—why?
- How could we optimize the J as f(w1)?

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Take derivative and set to 0

- $\sum_{i=1}^{N} (y_i \widehat{w_o} \widehat{w_1} x_i)^2$
- Differentiate with respect to….?

Take derivative and set to 0

- $\sum_{i=1}^{N} (y_i \widehat{y}_i)^2 = \sum_{i=1}^{N} (y_i \widehat{w}_o \widehat{w}_1 x_i)^2$
- Differentiate with respect to the w_o & w_1

•
$$\frac{\partial y}{\partial w} \sum_{i=1}^{N} (y_i - \widehat{w_o} - \widehat{w_1} x_i)^2 =$$

•
$$2\sum_{i=1}^{N} y_i - 2N\widehat{w_o} - \widehat{w_1} \sum_{i=1}^{N} x_i)^2$$

•
$$\widehat{w_o} = \frac{1}{N} [\sum_{i=1}^{N} y_i - \widehat{w_1} \sum_{i=1}^{N} x_i]$$

•
$$\widehat{W}_{1} = \frac{\sum_{i=1}^{N} y_{i} x_{i} - \sum_{i=1}^{N} y_{i} \sum_{i=1}^{N} x_{i}}{N}$$

$$= \frac{\sum_{i=1}^{N} y_{i} x_{i} - \frac{\sum_{i=1}^{N} y_{i} \sum_{i=1}^{N} x_{i}}{N}}{\sum_{i=1}^{N} x_{i}^{2} - \frac{\left(\sum_{i=1}^{N} x_{i}\right)^{2}}{N}}$$
http://isites.harvard.edu/fs/docs/icb.topic51
5975.files/OLSDerivation.pdf

Which work for linear regression?

Ordinary Least Squares vs. MLE

- Previous derived a generative model that was based on least-squares
- Reasonable approach
- MLE = maximum likelihood estimation
- Different framework for optimizing
- Likelihood = P(Data | hyp)
- MLE = arg max P(Data | hyp)
 - Select the parameters that maximize this quantity as our estimates

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MLE Estimate

- Assume P(data_i | hyp) are independent
- MLE = argmax $\prod_{i=1}^{N} P(data_i \mid hyp)$
- What is this P(data_i | hyp) using our previous assumptions?
- argmax $\prod_{i=1}^{n} \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{1}{2\sigma^2}(Y_i \beta_0 \beta_1 X_i)^2}$
- What are we optimizing over in argmax?

MLE Optimizing

- Argmax $\prod_{i=1}^{n} \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{1}{2\sigma^2}(Y_i \beta_0 \beta_1 X_i)^2}$
- To make the math easy, take a log
- To optimize, take derivative with respect to the betas
- Result in this case will be identical to the least squares approach
 - MLE estimates equal to OLS in this case

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MLE Estimate

- Assume P(data_i | hyp) are independent
- MLE = argmax $\prod_{i=1}^{N} P(data_i \mid hyp)$
- What is this P(data_i | hyp) using our previous assumptions?

Multiple Linear Regression

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Multiple Linear Regression

- Previously had $y = w_0 + w_1 x_1$
- What if we had 3 or 10 variables?
- We can still use regression
- Here is a simple case:

$$Y = W_0 + W_1 X_1 + W_2 X_2 + ... W_k X_k = \sum W_i X_i = W^T X_i$$

Multiple Regression with Matrices

- Y = XW + e
- Y is Nx1 matrix
 - What do we usually call Y?

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Multiple Regression with Matrices

- Y = XW + e
- Y is N x 1 matrix
- X is N x (k+1) include a column of 1s
- W is (k+1) x 1
- What do we usually call Y?

Multiple Regression with Matrices

- Y = XW + e
- Y is N x 1 matrix
- X is N x (k+1) include a column of 1s
- W is (k+1) x 1
- What do we usually call Y?
- What do we usually call X?

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Multiple Regression with Matrices

- Y = XW + e
- Y is N x 1 matrix (column vector)
- X is N x (k+1) include a column of 1s
- W is (k+1) x1 matrix
- e is N x 1 column vector
- What do we usually call Y?
- What do we usually call X?
- What do we usually call W?

Multiple Regression with Matrices

- Y = XW + e
- Y is N x 1 matrix (column vector)
- X is N x (k+1) include a column of 1s
- W is (k+1) x 1 matrix
- e is N x 1 column vector
- What are the rows and column referring to for the X?

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Matrix Inverse

- For numbers:
 - Consider x * 1/x → 1
 - ∘ In a sense, 1/x is inverse of x
 - ∘ In a sense, x is inverse of 1/x
- For matrices
 - \circ A A⁻¹ = I and A⁻¹A = I
 - Fairly easy for 2x2 matrices
 - Possible for 3x3 matrices by hand
 - Challenging for anything larger so use any linear algebra software or python

Matrix Inverse

- Do all numbers have an inverse?
- Do all matrices have an inverse?

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Matrix Inverse

- Do all numbers have an inverse?
- Do all matrices have an inverse?
 - Officially, has to be a square matrix
 - (Note: there are pseudo inverses otherwise)
 - If it's square it also has to have "full rank"
 - · Can't have rows that are products of each other
 - Can't have zero rows
 - Can't have rows that are weighted sums of any other rows
 - Determinant cannot be 0

Least Squares Estimate

- SSE = $e^{T}e$
 - Is this an inner product or outer product?
- e = Y-XW
- SSE = $(Y-XW)^T(Y-XW)$
- SSE = $(Y^T-W^TX^T)(Y-XW)$
 - Note that (AB)^T = B^TA^T
- SSE = $(Y^TY W^TX^TY + W^TX^TXW Y^TXW)$
 - The 2nd and 4th term are equivalent
 - Not obvious from the matrix format
 - · True when you multiply them out

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Least Squares Estimate

- SSE = $e^{T}e$
 - Is this an inner product or outer product?
- e = Y-XW
- SSE = $(Y-XW)^T(Y-XW)$
- SSE = $(Y^T-W^TX^T)(Y-XW)$
 - ∘ Note that (AB)^T = B^TA^T
- $SSE=(Y^TY W^TX^TY + W^TX^TXW Y^TXW)$
 - ∘ The 2nd and 4th term are equivalent
- SSE = $(Y^TY 2Y^TXW + W^TX^TXW)$

Least Squares Estimate

- SSE = $(Y^TY 2Y^TXW + W^TX^TXW)$
- How to minimize this?
- Derivative wrt W and set to 0
- $d/dW \rightarrow 0 2X^{T}Y + 2X^{T}XW = 0$
 - Note that d/dW of U^TVW = V^TU
 - Last term with the W's on either side is a quadratic which yields 2 and removal of W^T
 - \circ X^TXW = X^TY \rightarrow W = (X^TX)-1X^TY
 - (X^TX)⁻¹X^T is the Moore-Penrose Pseudoinverse of X
- Why can't we just do an inverse of X?

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Observation

- From before:
 - $Y = W_0 + W_1 X_1 + W_2 X_2 + ... W_k X_k = \sum W_i X_i$
- What does x₁ actually look like?
- If we modified it to be 3x₁, what would happen to the overall equation?
- What if we used x_1^2 or cubed it to x_1^3 ?

Observation

• From before:

$$Y = W_0 + W_1 X_1 + W_2 X_2 + ... W_k X_k = \sum W_i X_i$$

- What does x₁ actually look like?
- If we modified it to be 3x₁, what would happen to the overall equation?
- What if we used x_1^2 or cubed it to x_1^3 ?
 - Obtain polynomial regression

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Full multiple linear regression

•
$$Y = W_0 + W_1X_1 + W_2X_2 + ... W_kX_k = \sum W_iX_i$$

- $Y = W_0 + W_1X_1 + W_2X_2 + ... W_kX_k + b_0X_1X_2 + b_1X_1X_3 + ... bzx_{k-1}x_k + c_0x_1x_2x_3 + ...$
- Y = sum of
 - Independent factors +
 - 2-way interactions +
 - 3-way interactions +
 - K-way interactions
- Can include squared, cubed, power terms

Hierarchy Principles

- Only found this is statistics and never machine learning
- Need to include all lower terms if you include a higher order term
- If you have x₁³
 - Need to include x₁² as well as x₁
- If you have x₁²x₂
 - Need to include x_1^2 , x_1x_2 , x_1 , x_2

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Further options

- Y = sqrt($X_1^5 X_2 X_3^3 X_4$)
- Can multiple linear regression work for this kind of model?
- What does Y look like?
- What is $\log(ab)$? $\rightarrow \log(a) + \log(b)$
- $\log(\operatorname{sqrt}(x))$? $\rightarrow 1/2\log(x)$

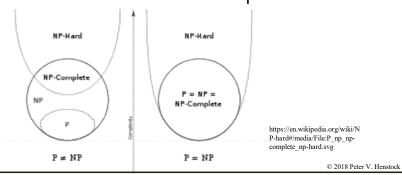
Big O notation

- Algorithms tend to be characterized by their approximate computational load
- Computation is a function of a parameter like n = size
- Sum of N numbers is O(N)
- Tree search is O(logN)
- We tend to round down so if the actual computation was O(5N³ + 4N + 17)
 - Use just O(N³)

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Complexity

- P = polynomial
- NP = nondeterministic polynomial time
- NP-complete = NP and NP-hard
- NP-hard =
 - o at least as hard as hardest problem in NP



Computational aspects

- Pseudoinverse
- Solution parameters = (X^TX)⁻¹X^Ty
- What is the computational requirement?
- Matrix addition?
- Matrix multiplication?
- Matrix inverse?

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Gradient Descent

Gradient Descent

- Problem:
 - You are placed on a hill in fog
- Goal:
 - Find the bottom of the hill
- Method
 - How would you do that?

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Gradient Descent

- Idea: you are placed on a hill in fog
 - Find the bottom of the hill

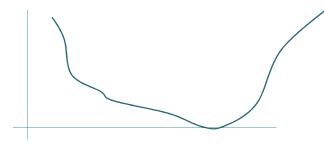
do {

- Figure out which way is "down"
- Move a certain distance in that direction

} until at lowest spot

What assumptions are we making?

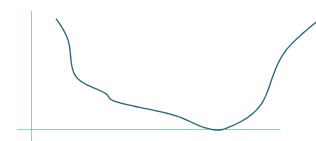




- Calculus tells us if that we have a function f then we need to do 2 things to find the minimum
 - 1)
 - 2)

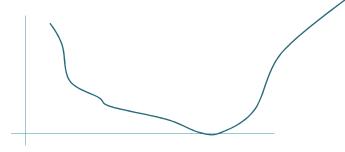
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Calculus Approach



- Calculus tells us if that we have a function f then we need to do 2 things to find the minimum
 - 1) Compute the derivative
 - 2) Check the concavity using 2nd derivative





- Calculus tells us if that we have a function f then we need to do 2 things to find the minimum
 - 1) Compute the derivative
 - 2) Check the concavity using 2nd derivative

How do we actually locate the minimum?

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General Gradient Descent

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \gamma_n \nabla F(\mathbf{x}_n), \ n \ge 0.$$

• For a partial derivative of 1 variable

$$\circ w_{n+1} = w_n - \alpha \frac{\partial}{\partial w_n} J(w_n)$$

- $\circ \alpha$ is the learning rate
- J() is the cost function
- Iteratively adjusting w_n with better estimates using the gradient of the cost function as the direction.



dJ > 0 Move left

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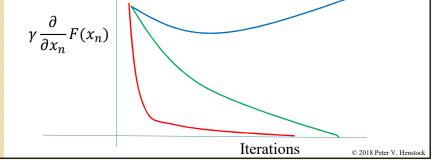
Diagnostics for Gradient Descent

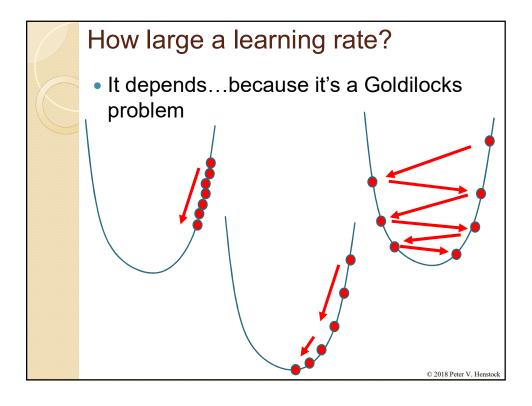
- What should the gradient look like as a function of time (iterations)?
- Hint:
 - When should gradient descent end?

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Diagnostics for Gradient Descent

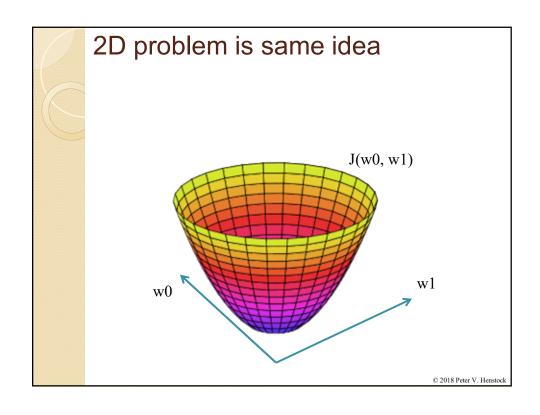
- What should the gradient look like as a function of time (iterations)?
- Hint:
 - When should gradient descent end?

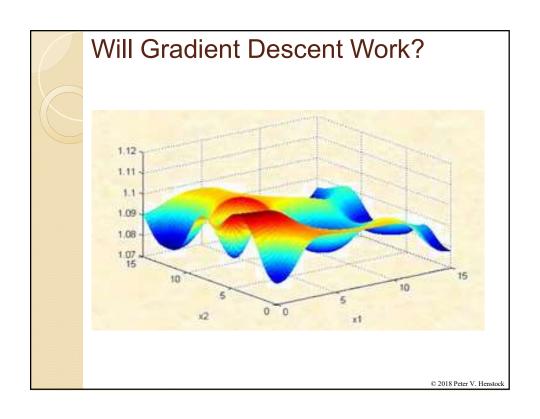




Gradient Descent

- Have an optimization function J we are trying to minimize
- Have 2 parameters w0 and w1
- Start with an initial guess of w0' and w1'
- Iteratively shift w0 and w1 in the direction to make J better until "done"





2D Gradient Descent

- For each loop
 - \circ $w_1 \leftarrow w_1 \alpha \partial J/\partial w_1$
 - $w_0 \leftarrow w_0 \alpha \partial J/\partial w_0$
- Note: J is a function of w₀ and w₁
 - Be sure to update both new values using the older values
 - Do not update w₁ and use the updated w₁ to update w₀

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2D Gradient Descent

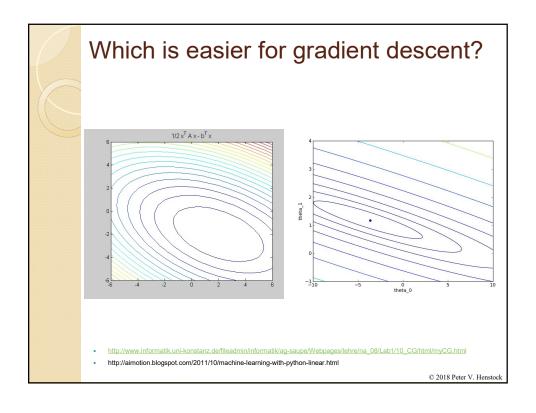
- For each loop
 - \circ $w_1 \leftarrow w_1 \alpha \partial J/\partial w_1$
 - $\circ \ \mathsf{w}_0 \leftarrow \mathsf{w}_0 \alpha \ \partial \mathsf{J}/\partial \mathsf{w}_0$
- $\partial J/\partial w_0 = 2\Sigma_i (w_1 x_i + w_0 y_i)$
- $\partial J/\partial w_1 = 2\Sigma_i (w_1x_i + w_0 y_i)x_i$

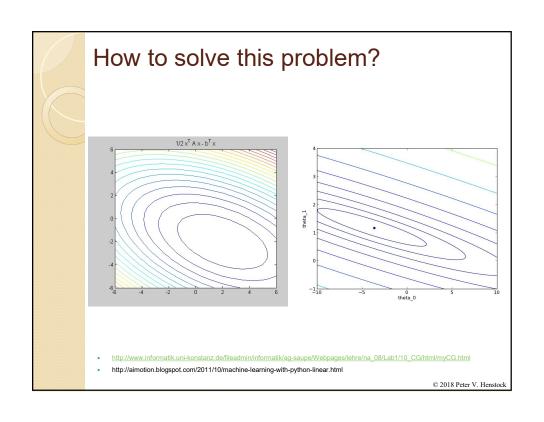
How to ensure achieved optimal?

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How to ensure achieved optimal?

- Start with multiple starting points
- Typically try a few different learning rates and plot the change of gradient to ensure things are going the right direction





Regression Diagnostics

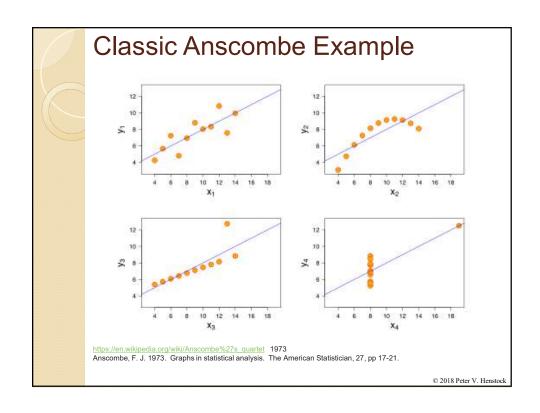
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Regression Process

- We load the data
- We perform a fit
- We're done!
- What could go wrong?

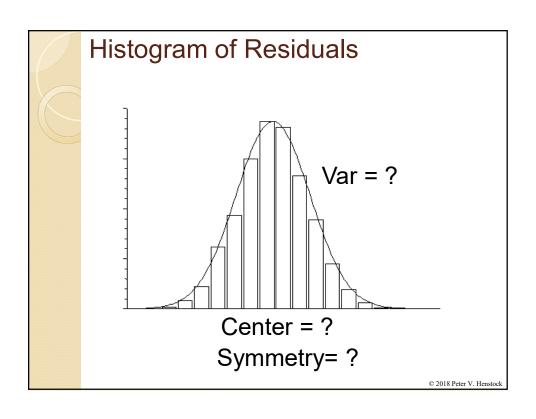
Regression Process

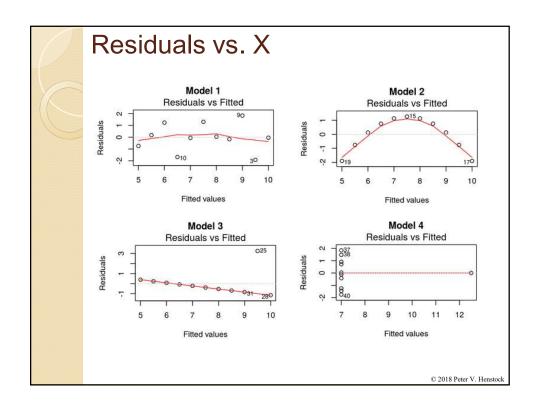
- We load the data
- We perform a fit
- We're done!
- What could go wrong?
- Assumptions:
 - iid errors = independent & identically distributed
 - Common variance
 - N(0, variance)
 - Y and X are related

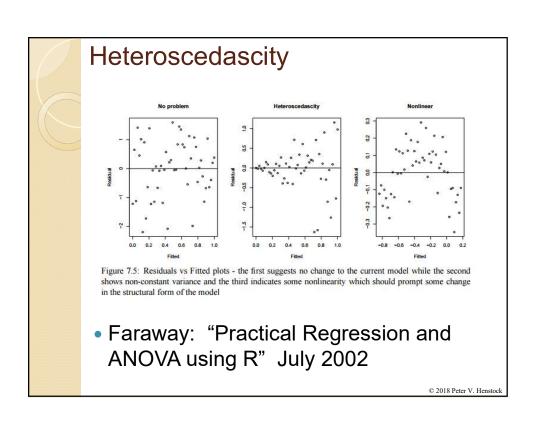


How can we diagnose the issues?

- Residuals should have a common variance
- Residuals should have a N(0, variance)
- Residuals should be iid

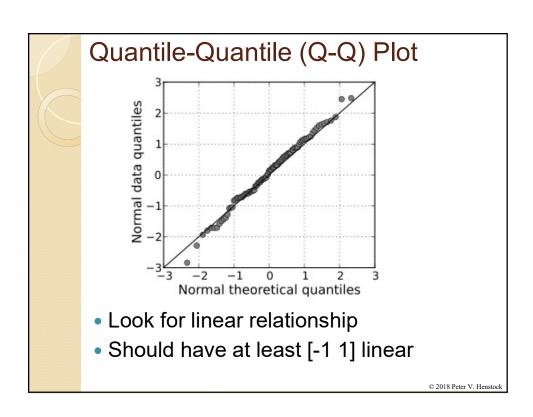






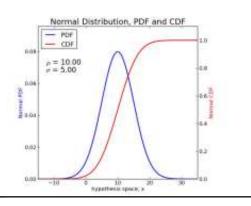
Data Transformations

- Common transformations include:
 - Log
 - Sqrt
 - Arcsin
- What do we apply these to?
 - Y?
 - X?



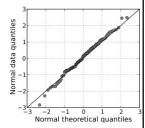
CMF = cumulative mass function

- Prob(a to b) = $\sum_{a}^{b} pmf$
- Cmf(x) = cumulative pmf = $\sum_{-\infty}^{x} pmf$
 - Maps from $x \rightarrow [0, 1]$ probability
- InvCmf(p) maps [0, 1] to an x-value

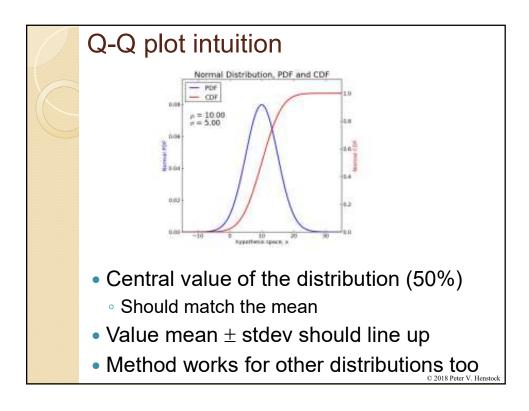


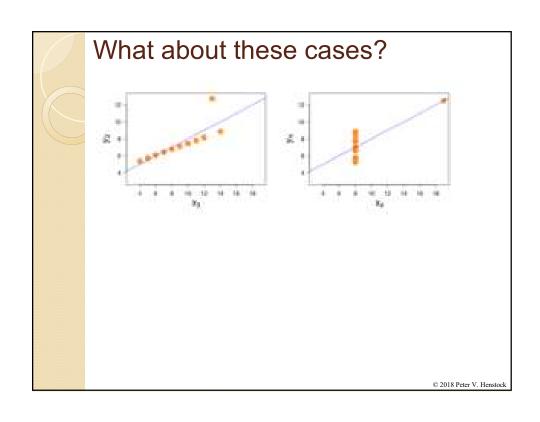
Quantile-Quantile (Q-Q) Plot

- Sort the residuals (y-axis)
 - Use Order Statistics



- Sample invnormal cdf evenly
 - · Sample at probabilities 1/(n+1), 2/(n+1)...n/n+1
 - Convert the probabilities back to x-values for the x-axis
- Plot the sampled invcdf vs. residuals





Leverage Points

- A single isolated point might have a lot of influence on the overall fit
- What characteristics might go into such a point?

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Leverage Points

- A single isolated point might have a lot of influence on the overall fit
- What characteristics might go into such a point?
- 1) Shifts the line
- 2) Isolated in x from other points

Leverage Points

- 1) Shifts the line
- 2) Isolated in x from other points

•
$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{j=1}^n (x_j - \bar{x})^2}$$

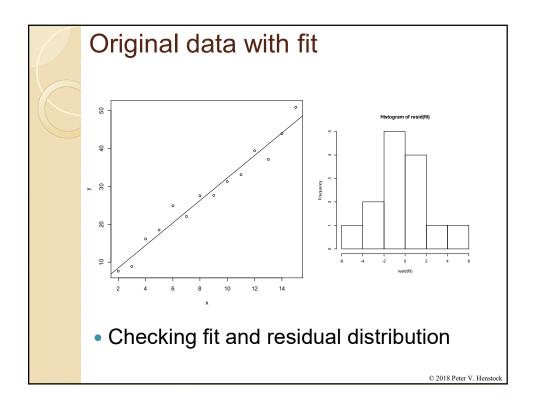
- High leverage point if > 4/n
- Bad leverage point: distorts line (outlier)
- Good leverage point: consistent with line

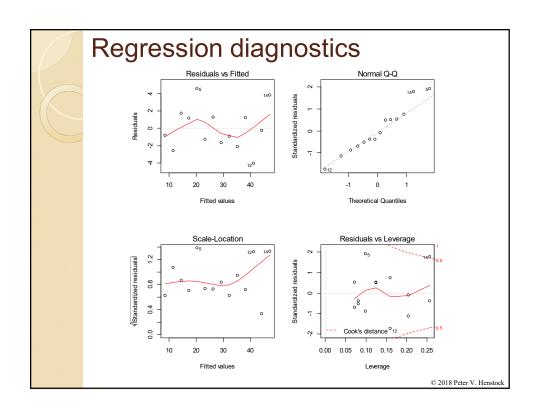
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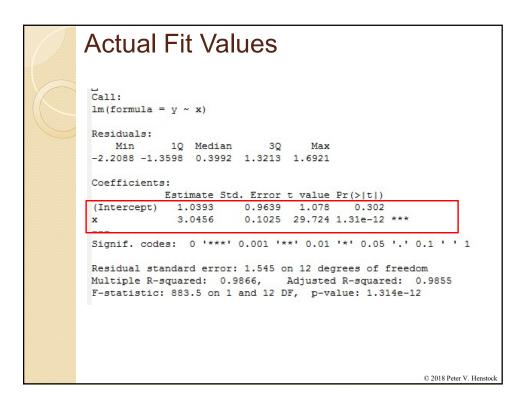
R Example for Regression

What does R do? x <- 2:15 y <- 1:length(x)*3 + 5 + rnorm(length(x))*2.5 plot(x,y) fit <- lm(y ~ x) summary(fit) hist(resid(fit)) plot(fit)</pre>

R call Call: lm(formula = y ~ x) Residuals: 1Q Median 3Q Max Min -2.2088 -1.3598 0.3992 1.3213 1.6921 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 1.0393 0.9639 1.078 0.302 x 3.0456 0.1025 29.724 1.31e-12 *** x Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 Residual standard error: 1.545 on 12 degrees of freedom Multiple R-squared: 0.9866, Adjusted R-squared: 0.9855 F-statistic: 883.5 on 1 and 12 DF, p-value: 1.314e-12 © 2018 Peter V. Henstock







Time Series Modeling Diagram Series Modeling http://www.artnet.com/artists/crt%c3%A9/complete-numbers-suite-set-of-10-HLI_PTOIsn_8aldkjAWWWv2 © 2018 Peter V. Henstock

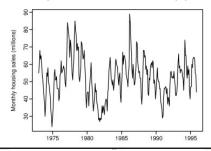
Why Do Time Series Analysis?

- Model of data
- Interpretation
- Forecasting
- Control
- Hypothesis testing
- Simulation

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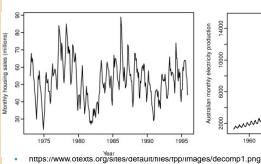
Time Series Modeling

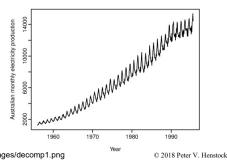
- Previously with regression:
 - \circ Y \sim f(X)
 - X samples are i.i.d.
 - Generative model: Y is f(x) + N(0,sigma)
- Why don't just use Y ~ f(t) ?

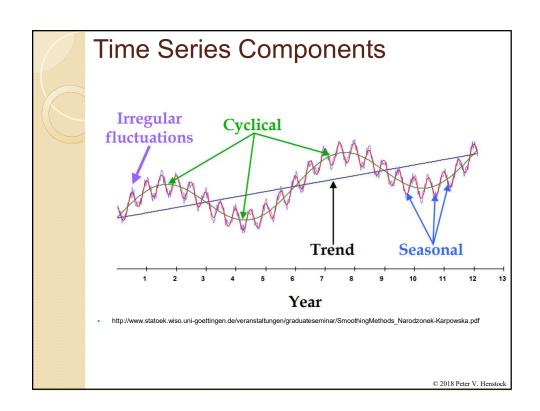


Signal vs. Noise Issue

- Regression model would probably smooth the data to provide a good trend
- Decomposition:
 - Could extract the trend and seasonality
 - Are they additive or multiplicative?
 - Then model the remainder which is what?







Smoothing

Moving Average: average over last m

$$x(n) = \frac{1}{m} \sum_{k=0}^{m-1} x(n-k)$$

Weighted Moving Average: avg over last m

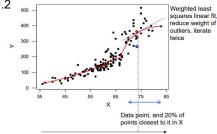
$$x(n) = \frac{1}{\sum_{k=0}^{m} w_k} \sum_{k=0}^{m} w_k x(n-k)$$

- Weights usually sum to 1
- Use this to heavily weight more recent
- Exponential Smoothing
 - Single: $s(n) = \alpha x(n) + (1-\alpha)s(n-1)$
 - Double: $s(n) = \alpha x(n) + (1-\alpha)[s(n-1) + b(n-1)]$
 - $b(n) = \beta[s(n)-s(n-1)] + (1-\beta) b(n-1)$

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Lowess smoothing

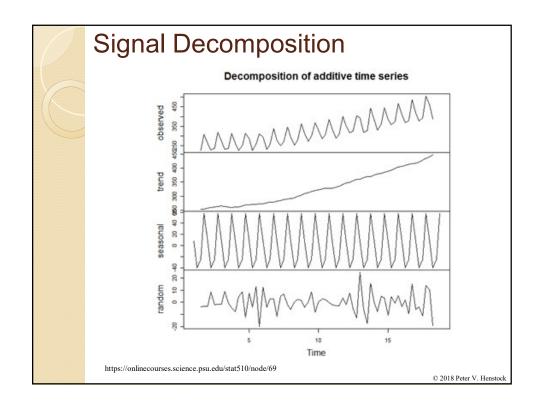
- Lowest (weighted) regression
- Non-parametric model
- http://sites.stat.psu.edu/~fxc11/Stat462 STABLE/Lect12 lowess.pdf
- Smoothing param 0.2
 = fraction of points
- Degree 1 = linear



Perform moving along the data points.

Weighted least squares linear fit Weight function

$$\min_{\beta_0,\beta_1} \sum_{j \in N_i} w_j (y_j - (\beta_0 + \beta_1 x_j))^2 \qquad w_i = \left(1 - \left(\frac{d(x_j, x_i)}{\max_{\ell \in N_i} d(x_\ell, x_i)}\right)^3\right)^3$$
F. Chiaromonte



In this lecture and next Remove the trend Figure out seasonality* Figure out frequency* Model the "random" * = next lecture

Time Series Framework

- Need a model to explain random signals
- Existing models may not be explainable by the Y~f(t) + noise
- Existing models may not be predictable
- But, we know something about Y
- Framework: random signals
 - Y(t) characterized by a distribution at each t

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Framework is Random Sequence

- x₁, x₂, ...x_n (Changed notation to x)
- Need to exploit the order of sequence
- As random, it cannot be predicted
- Deterministic process: known / predictable
- Stochastic or Random process:
 - System that generates all possible random sequences of which we have a realization x₁...x_n with the specific random values
 - Goal is to model the process
 - Model process as random since it's either random or we do not have a better model

Time Series Review

- Random Process
 - \circ w(k) = 0, 2, 0, -1, 2, -1, 2, 1, 0, 0, 1, 2, -1, -2
- AR Model
 - $\circ x(k) = \phi_1 x(k-1) + \phi_2 x(k-2) + ... + \phi_p x(k-p) + w(k)$
 - Let's use a 1st order model $\phi_1 = 0.9$
 - x(0) = 0
 - \circ x(1) = 0.9*0 + 2 = 2
 - \circ x(2) = 0.9*2 + 0 = 1.8
 - x(3) = 0.9*1.8 + -1 = 0.62

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Time Series Review

- Random Process
 - \circ w() = $\frac{0}{2}$, $\frac{2}{0}$, $\frac{1}{2}$, $\frac{1}{2}$
- MA Model (clearer notation)
 - $\circ x(k) = w(k) + \theta_1 w(k-1) + \theta_2 w(k-2) + ... + \theta_p w(k-p)$
 - Let's use a 2nd order model θ_1 = 0.7, θ_2 = 0.3
 - \circ Assume x(-1) = 0
 - $\cdot x(0) = 0$
 - x(1) = 2 + 0.7(0) = 2
 - x(2) = 0 + 0.7(2) + 0.3(0) = 1.4
 - x(3) = -1 + 0.7(0) + 0.3(2) = -0.4

Ergodic Process

- Time estimate converges to the true estimate as N → infinity
 - Ergodic mean
 - True if $1/N \Sigma x(k) = E[x(k)] = \mu \text{ as } N \rightarrow \text{infinity}$
- If we take a reasonably long sample,
 - Then we can infer the statistical properties of the whole sequence

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Strict Stationary

- If joint distribution of N observations is invariant to time shifts
- $F_{x(k1)}(x1) = F_{x(k1+T)}(x1)$
 - All have same distribution regardless of T

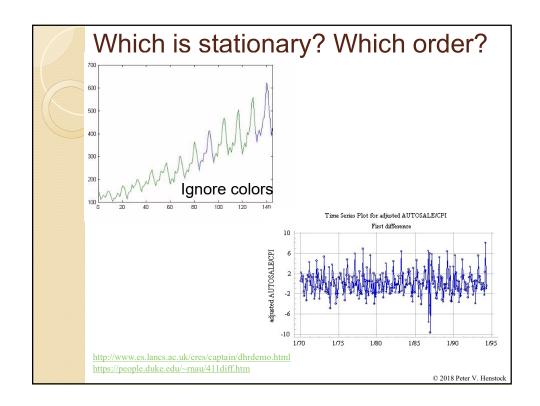
(Wide Sense or Weak) Stationarity

- Few real systems are strictly stationary
 - Joint distribution of all vectors of d dimensions remains the same for any fixed d
- Weaker definition is WSS
 - First order stationary: E[X(t)] is same for all t
 - Second order:
 - 1) First order stationary and
 - 2) Cov[X(t),X(t-lag)] is function of only lag

Note: Gaussian processes described by mean & cov

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Exploratory analysis Bankruptey cases filed in Colorado 4000 500 500 1000 500 1000



Mathematical idea of stationary

 $x(k) = A\cos(wk + u)$ where u is $U(0,\pi)$ Is this stationary?

How would we determine the answer?

Mathematical idea of stationary

 $x(k) = A\cos(wk + u)$ where u is $U(0,\pi)$ Is this stationary?

How would we determine the answer?

$$E(x|k) = ?$$

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Mathematical idea of stationary

 $x(k) = A\cos(wk + u)$ where u is $U(0,\pi)$ Is this stationary?

How would we determine the answer?

$$E(x|k) = \int_0^{\pi} [?] f(u) du$$
 where $f(u) = ?$

Mathematical idea of stationary

 $x(k) = A\cos(wk + u)$ where u is $U(0,\pi)$ Is this stationary?

How would we determine the answer?

$$E(\mathbf{x}|\mathbf{k}) = \int_0^{\pi} A\cos(\mathbf{w}\mathbf{k} + \mathbf{u}) f(u) du$$

$$E(\mathbf{x}|\mathbf{k}) = A \int_0^{\pi} \cos(\mathbf{w}\mathbf{k} + \mathbf{u}) \frac{1}{\pi} du = \frac{-2}{\pi} \sin(\mathbf{w}\mathbf{k})$$

So what can you conclude?

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Mathematical idea of stationary

 $x(k) = A\cos(wk + u)$ where u is $U(0,\pi)$ Is this stationary?

How would we determine the answer?

$$E(\mathbf{x}|\mathbf{k}) = \int_0^{\pi} A\cos(\mathbf{w}\mathbf{k} + \mathbf{u}) f(u) du$$

$$E(\mathbf{x}|\mathbf{k}) = \frac{A}{\pi} \int_0^{\pi} \cos(\mathbf{w}\mathbf{k} + \mathbf{u}) 1 du = \frac{-2A}{\pi} \sin(\mathbf{w}\mathbf{k})$$

$$E(\mathbf{x}|\mathbf{k}) \text{ depends on } \mathbf{k} \text{ so not stationary}$$

