GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 6: REGRESSION & REGULARIZATION

Francesco Mosconi

DAT16 SF // August 17, 2015

DATA SCIENCE IN THE NEWS

DATA SCIENCE IN THE NEWS

WHY SECURITY DATA SCIENCE MATTERS AND HOW ITS DIFFERENT: PITFALLS AND PROMISES OF DATA SCIENCE BASED BREACH DETECTION AND THREAT INTELLIGENCE

black hat USA 2015

FROM FALSE POSITIVES TO ACTIONABLE ANALYSIS: BEHAVIORAL INTRUSION DETECTION MACHINE LEARNING AND THE SOC

THE APPLICATIONS OF DEEP LEARNING ON TRAFFIC IDENTIFICATION

https://www.blackhat.com/us-15/briefings.html

DATA SCIENCE IN THE NEWS

Why security data science matters and how it's different: pitfalls and promises of data science based breach detection and threat intelligence

Joshua Saxe, Invincea Labs

Work presented in this talk contains significant contributions from Alex Long, David Slater, Giacomo Bergamo, Konstantin Berlin, and Robert Gove

https://www.blackhat.com/docs/us-15/materials/us-15-Saxe-Why-Security-Data-Science-Matters-And-How-Its-Different.pdf

DATA SCIENCE IN THE NEWS

CLASSIFICATION OF ENCRYPTED WEB TRAFFIC USING MACHINE LEARNING ALGORITHMS

THESIS

William Charles Barto

AFIT-ENG-13-J-11

http://oai.dtic.mil/oai/oai?verb=getRecord&metadataPrefix=html&identifier=ADA585816

Cleaning MoMA's Artwork Collection Using Python

09 AUG 2015 on python, art, and cleaning

Use Python to Clean the Museum of Modern Art's Collection

Art is a messy business. Over centuries, artists have created everything from simple paintings to complex sculptures, and art historians have been cataloging everything they can along the way. The Museum of Modern Art, or MoMA for short, is considered one of the most influential museums in the world and recently released a dataset of all the artworks they've cataloged in their collection. This dataset contains basic information on metadata for each artwork and is part of MoMA's push to make art more accessible to everyone.

https://www.dataquest.io/blog/use-python-to-clean-moma-collection/

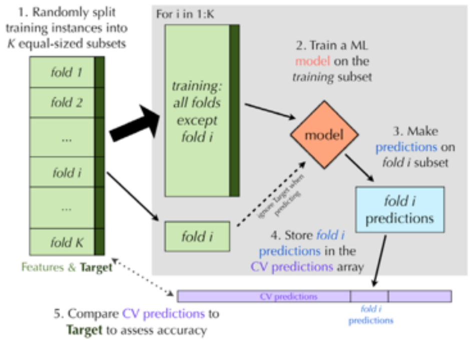
LAST TIME:

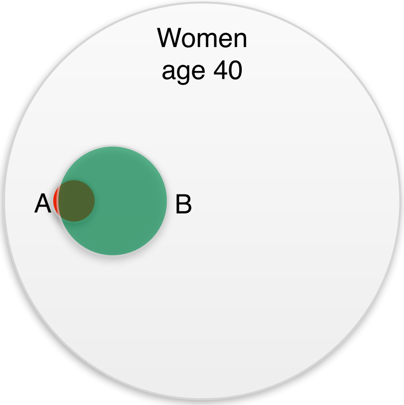
I. CROSS VALIDATION
II. INTRO TO PROBABILITY
III. NAÏVE BAYESIAN CLASSIFICATION

EXERCISES:

IV. NAÏVE BAYES CLASSIFICATION IN PYTHON

QUESTIONS?





QUESTIONS?

WHAT WAS THE MOST INTERESTING THING YOU LEARNT?

WHAT WAS THE HARDEST TO GRASP?

REVIEW GAME

AGENDA

I. LINEAR REGRESSION (INCL. MULTIPLE REGRESSION)
II. POLYNOMIAL REGRESSION
III. REGULARIZATION

LAB:
IV. IMPLEMENTING MULTIPLE REGRESSION & POLYNOMIAL REGRESSION IN PYTHON

KEY OBJECTIVES

- WHAT ARE LINEAR AND POLYNOMIAL REGRESSION
- WHICH PROBLEMS CAN BE TACKLED WITH REGRESSION TECHNIQUES
- HOW TO IMPLEMENT LINEAR AND POLYNOMIAL REGRESSION IN PYTHON
- WHAT IS REGULARIZATION
- HOW REGULARIZATION CAN HELP WHEN DATA IS NOISY
- HOW TO IMPLEMENT REGULARIZATION IN PYTHON

I. LINEAR REGRESSION

	Continuous	*Categorical*
Supervised	*???*	*???*
Unsupervised	*???*	*???*

	Continuous	Categorical
Supervised	*regression*	*classification*
Unsupervised	*dimension reduction*	*clustering*

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$\beta =$ regression coefficient *(the model "parameter")*

$\varepsilon =$ residual *(the prediction error)*

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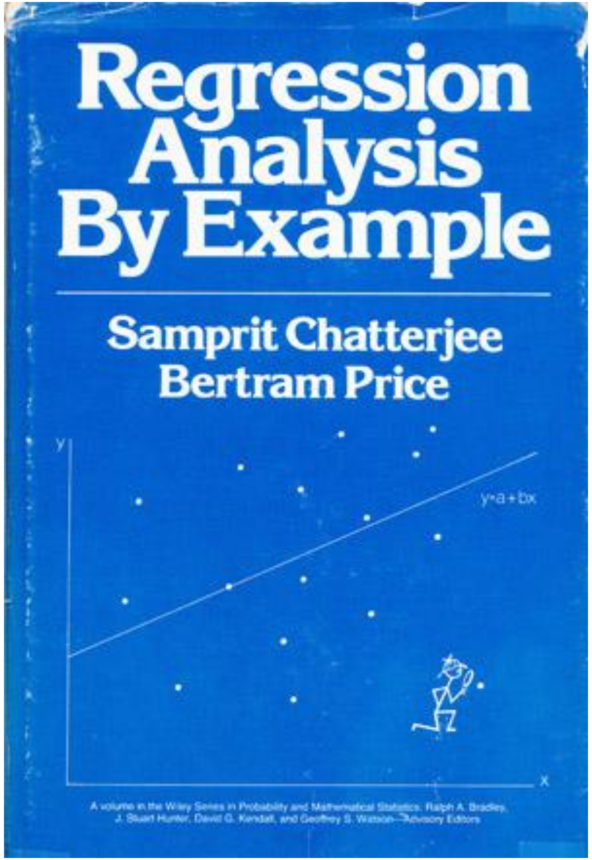
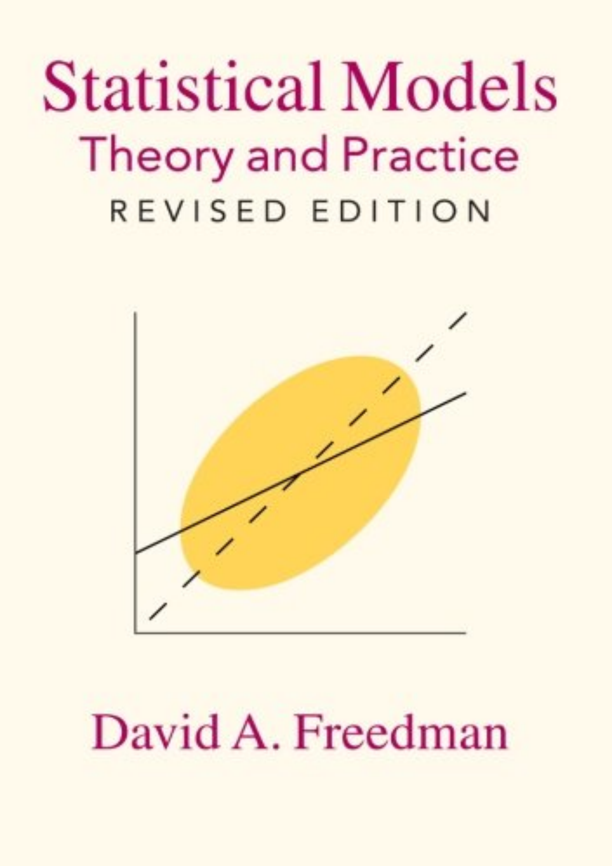
$$y = \alpha + \begin{bmatrix} \beta_1 & \beta_2 & \ldots\beta_n \end{bmatrix} * \begin{bmatrix} x_1 \\ x_2 \\ \ldots \\ x_n \end{bmatrix} + \varepsilon$$

Linear regression involves several technical assumptions and is often presented with lots of mathematical formality.

The math is not very important for our purposes, but you should check it out if you get serious about solving regression problems.


Regression Analysis By Example
Samprit Chatterjee
Bertram Price
y
y=a+bx
x
A volume in the Wiley Series in Probability and Mathematical Statistics. Ralph A. Bradley,
J. Stuart Hunter, David G. Kendall, and Geoffrey S. Watson—Advisory Editors


Statistical Models
Theory and Practice
REVISED EDITION
David A. Freedman

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But again, if you get serious about regression, you should learn how this works!

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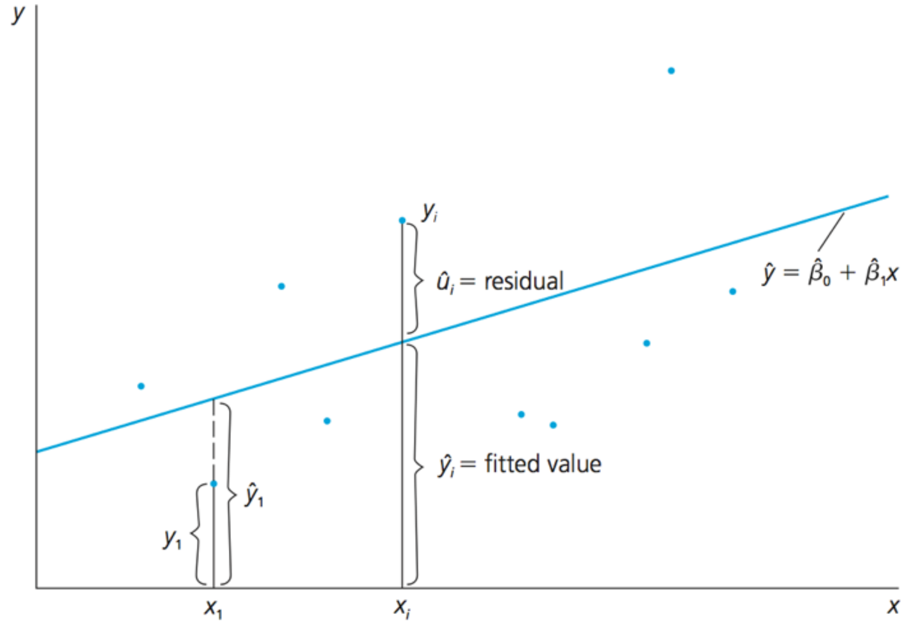
$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i.$$

$$\hat{u}_i = y_i - \hat{y}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i.$$

$$\sum_{i=1}^{n} \hat{u}_i^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2,$$



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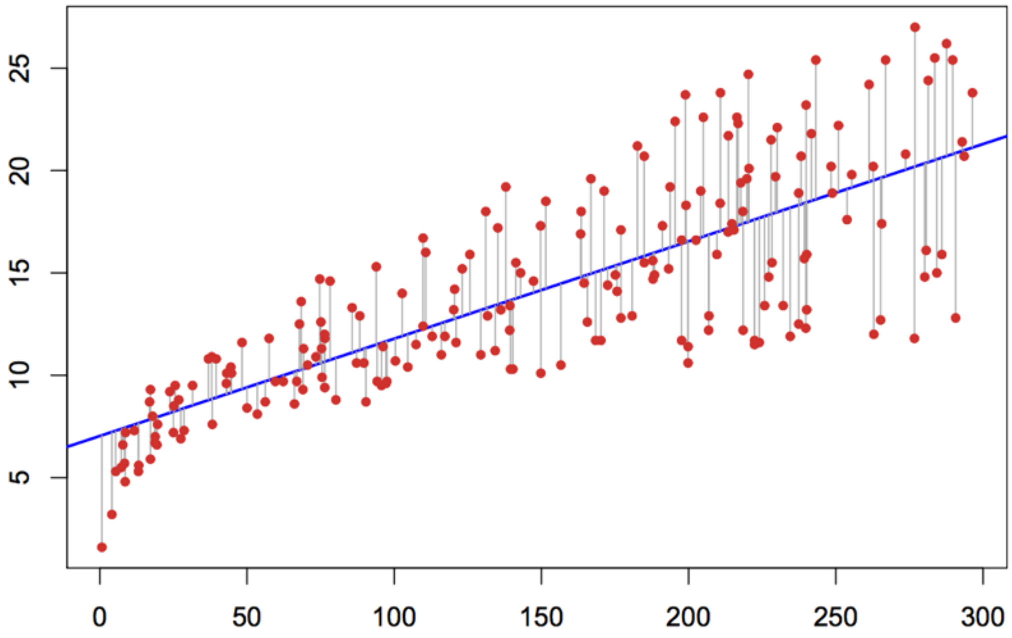

II: POLYNOMIAL REGRESSION

POLYNOMIAL REGRESSION

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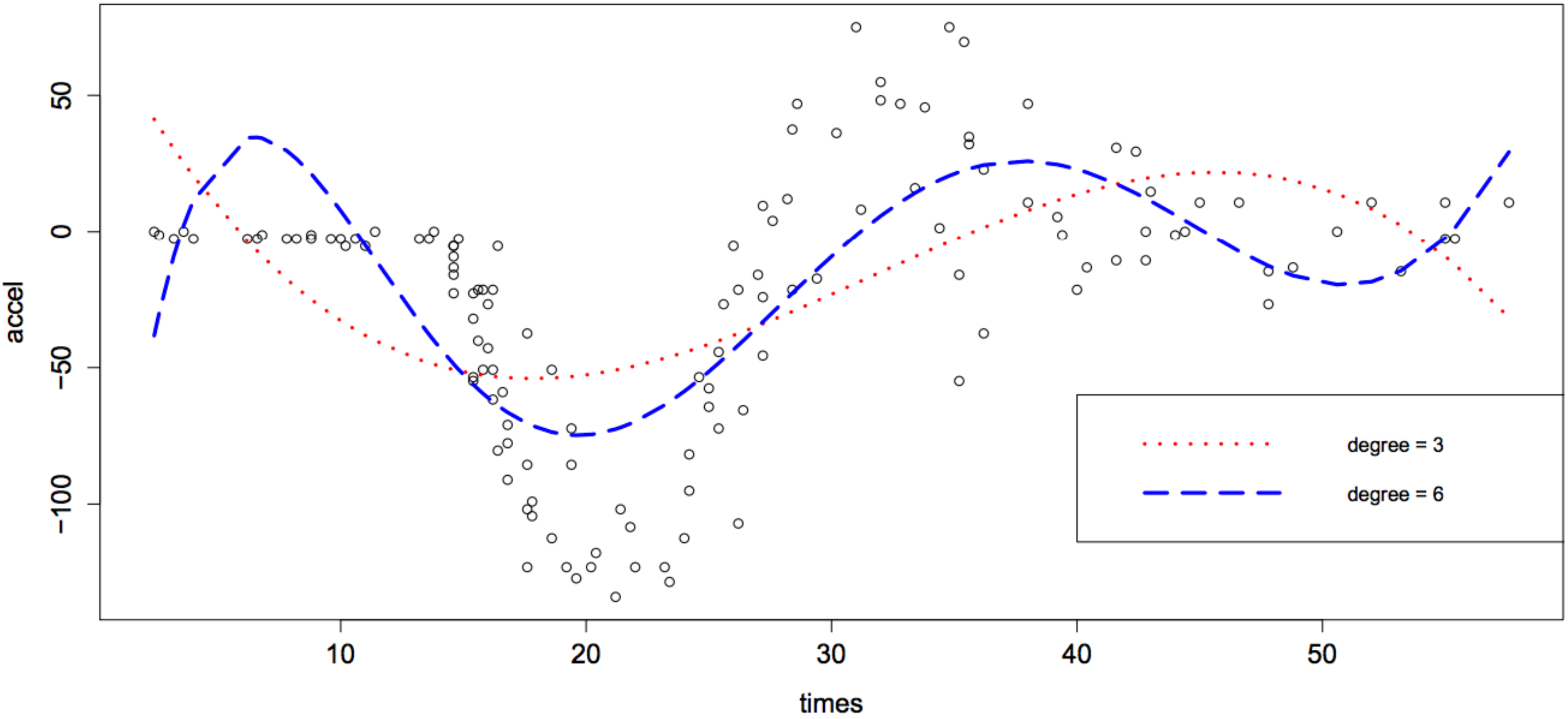
Q: This represents a nonlinear relationship. Is it still a linear model?

A: Yes, because it's linear in the β's!

"Although polynomial regression fits a nonlinear model to the data, as a statistical estimation problem it is linear, in the sense that the regression function E(y|x) is linear in the unknown parameters that are estimated from the data. For this reason, polynomial regression is considered to be a special case of multiple linear regression." -- *Wikipedia*

POLYNOMIAL REGRESSION



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But there is one problem with the model we've written down so far.

Q: Does anyone know what it is?

A: This model violates one of the assumptions of linear regression!

This model displays multicollinearity, *which means the predictor variables are highly correlated with each other.*

$$y = \alpha + \beta_1 x + \beta_2 x^2 + \ldots + \beta_n x^n + \varepsilon$$

Multicollinearity causes the linear regression model to break down, because it can't tell the predictor variables apart.

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OPTIONAL NOTE

These polynomial functions form an *orthogonal basis* of the function space.

So far, we've seen how polynomial regression allows us to fit complex nonlinear relationships, and even to avoid multicollinearity (by using basis functions).

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Q: Can a regression model be too complex?

III: REGULARIZATION

Recall our earlier discussion of overfitting.

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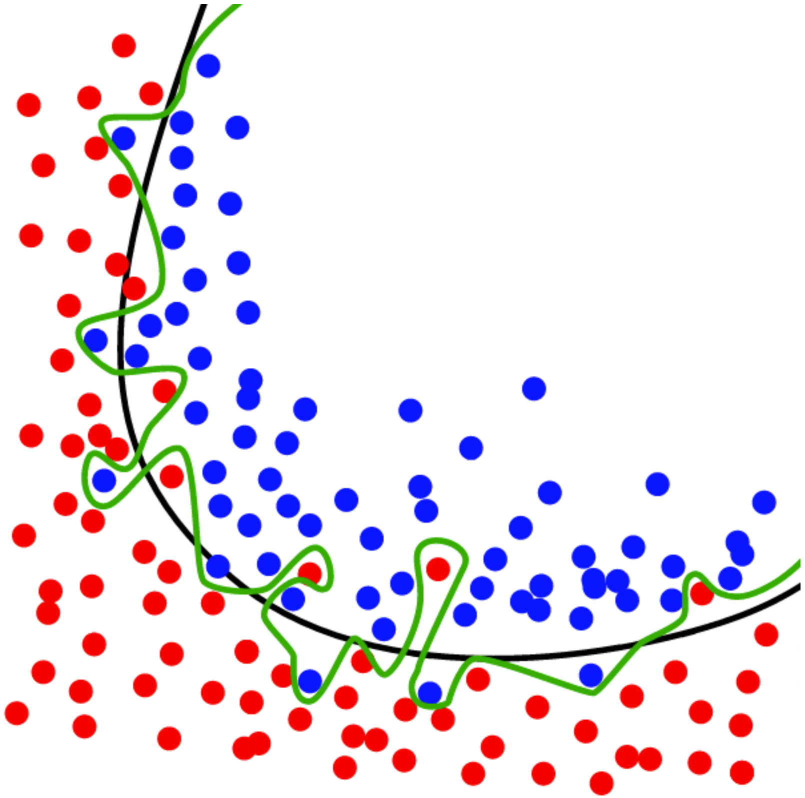
In other words, an overfit model matches the noise *in the dataset instead of the* signal.

OVERFITTING EXAMPLE (CLASSIFICATION)



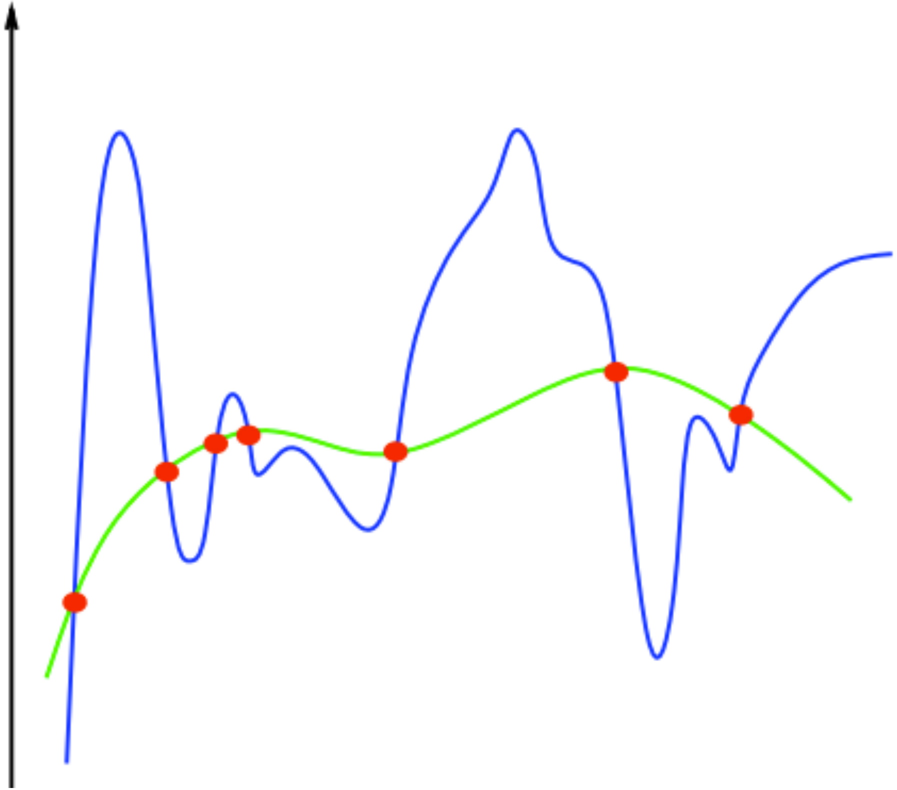
source: http://upload.wikimedia.org/wikipedia/commons/1/19/Overfitting.svg

The same thing can happen in regression.

It's possible to design a regression model that matches the noise in the data instead of the signal.

This happens when our model becomes too complex for the data to support.

OVERFITTING EXAMPLE (REGRESSION)



source: http://www.mit.edu/~9.520/spring12/slides/class02/class02.pdf

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Ex 1: $\Sigma |\beta_i|$

Ex 2: $\Sigma \beta_i^2$

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A: One method is to define complexity as a function of the size of the coefficients.

Ex 1: $\Sigma\,|\beta_i|$ *this is called the* L1-norm

Ex 2: $\Sigma\,\beta_i^2$ *this is called the* L2-norm

These measures of complexity lead to the following regularization *techniques:*

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L1 regularization: $y = \Sigma\, \beta_i x_i + \varepsilon \quad st. \quad \Sigma\, |\beta_i| < s$

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Regularization *refers to the method of preventing* overfitting *by explicitly controlling model* complexity.

These regularization problems can also be expressed as:

L1 regularization: $min(\|y - x\beta\|^2 + \lambda\|\beta\|)$

L2 regularization: $min(\|y - x\beta\|^2 + \lambda\|\beta\|^2)$

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L1 regularization (Lasso): $min(\|y - x\beta\|^2 + \lambda\|x\|)$

L2 regularization (Ridge): $min(\|y - x\beta\|^2 + \lambda\|x\|^2)$

This (Lagrangian) formulation reflects the fact that there is a cost associated with regularization.

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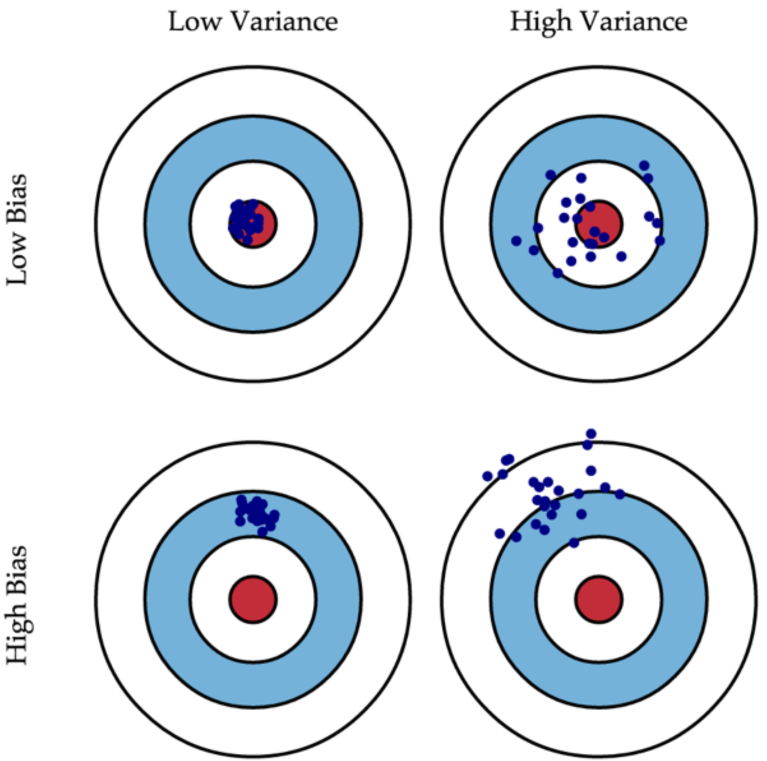
BIAS AND VARIANCE

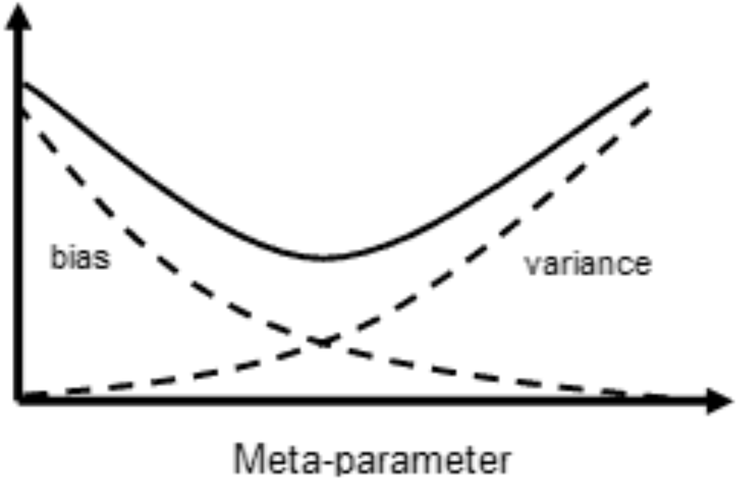


http://scott.fortmann-roe.com/docs/BiasVariance.html

Q: What are bias and variance?
A: Bias refers to predictions that are systematically inaccurate.
Variance refers to predictions that are generally inaccurate.

It turns out (after some math) that the generalization error in our model can be decomposed into a bias component and variance component.

This is another example of the bias-variance tradeoff.



source: http://www.isu.edu/chem/images/kalivasmeta.gif

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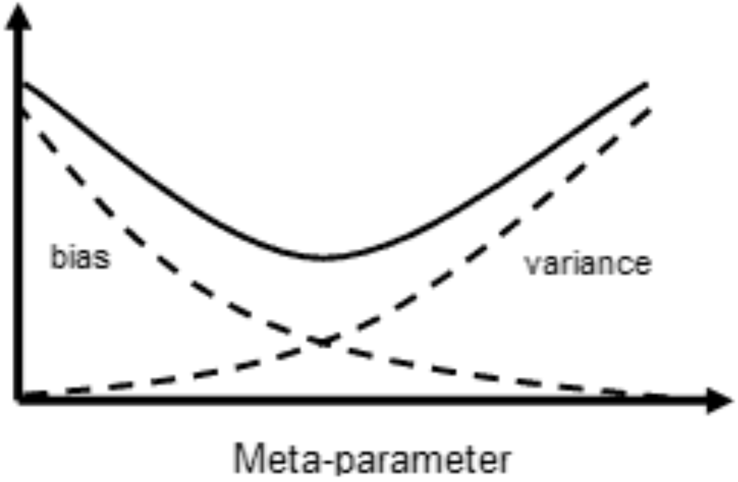


NOTE
The “meta-parameter” here is the lambda we saw above.

A more typical term is “hyperparameter”.

source: http://www.isu.edu/chem/images/kalivasmeta.gif

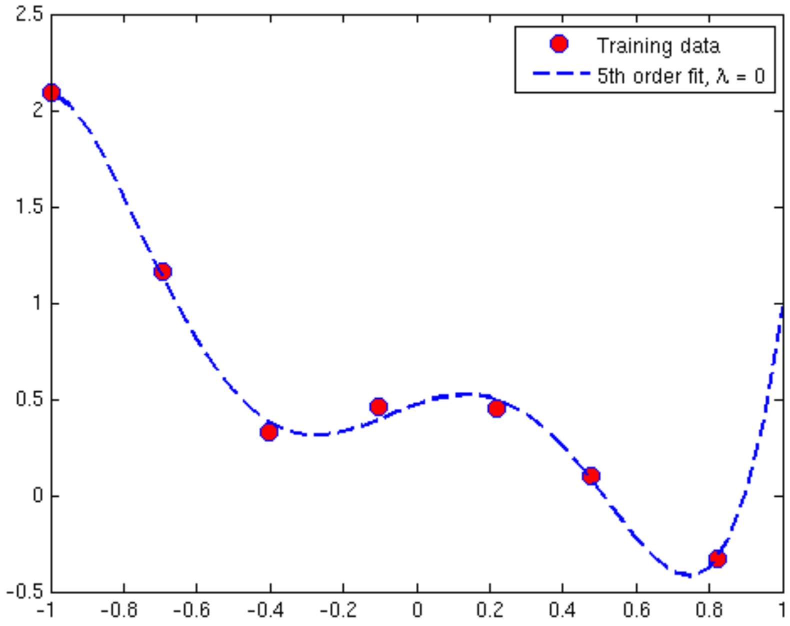
This tradeoff is regulated by a hyperparameter λ, *which we've already seen:*

L1 regularization*:* $y = \Sigma\, \beta_i x_i + \varepsilon$ *st.* $\Sigma\, |\beta_i| < \lambda$

L2 regularization*:* $y = \Sigma\, \beta_i x_i + \varepsilon$ *st.* $\Sigma\, \beta_i^2 < \lambda$

So regularization represents a method to trade away some variance for a little bias in our model, thus achieving a better overall fit.

L2 regularization: $\min(\|y - x\beta\|^2 + \lambda\|x\|^2)$



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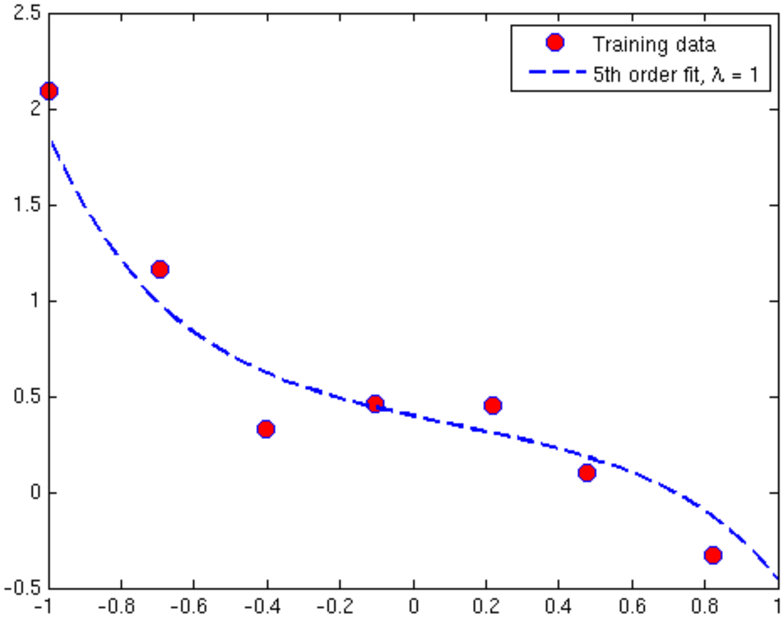

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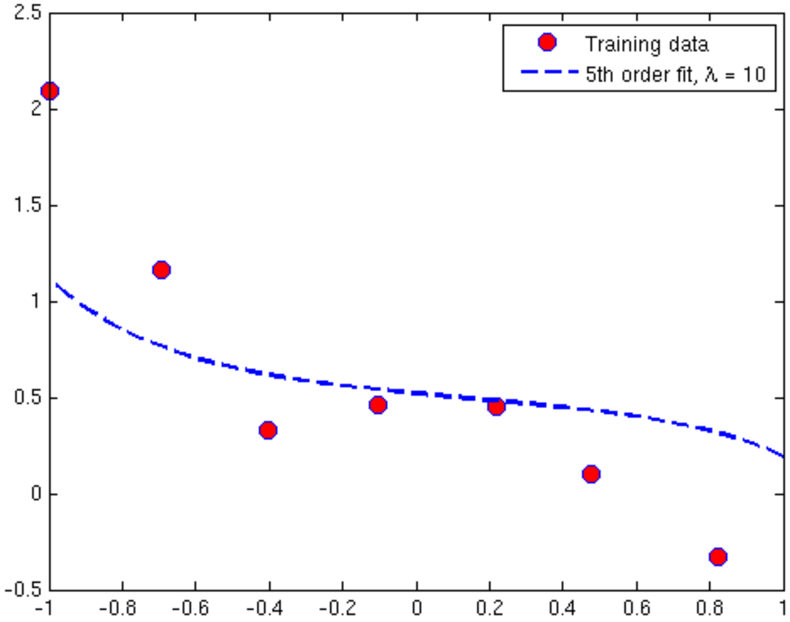

- Linear regression
- Multiple regression
- Polynomial regression
- The concept of minimizing some error or “cost” function
- Regularization

LAB: POLYNOMIAL REGRESSION & REGULARIZATION