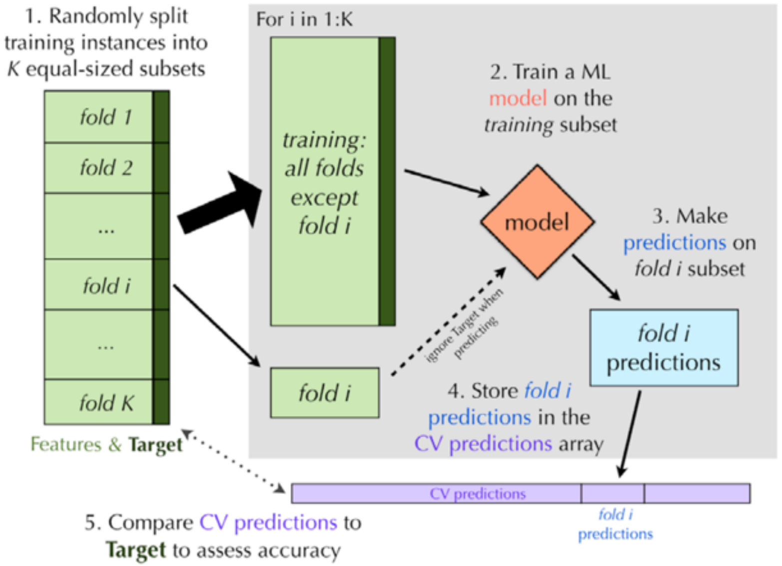
GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

REGRESSION & REGULARIZATION

LAST TIME:

I. BUMPY & PANDAS
II. VISUALIZATION
III. OVERFITTING & UNDERFITTING
IV. CROSS VALIDATION



QUESTIONS?

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WHAT WAS THE MOST INTERESTING THING YOU LEARNT?

WHAT WAS THE HARDEST TO GRASP?

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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The **simple linear regression** *model captures a linear relationship between a single input variable x and a response variable y:*

$$y = \alpha + \beta x + \varepsilon$$

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ε = **residual** *(the prediction error)*

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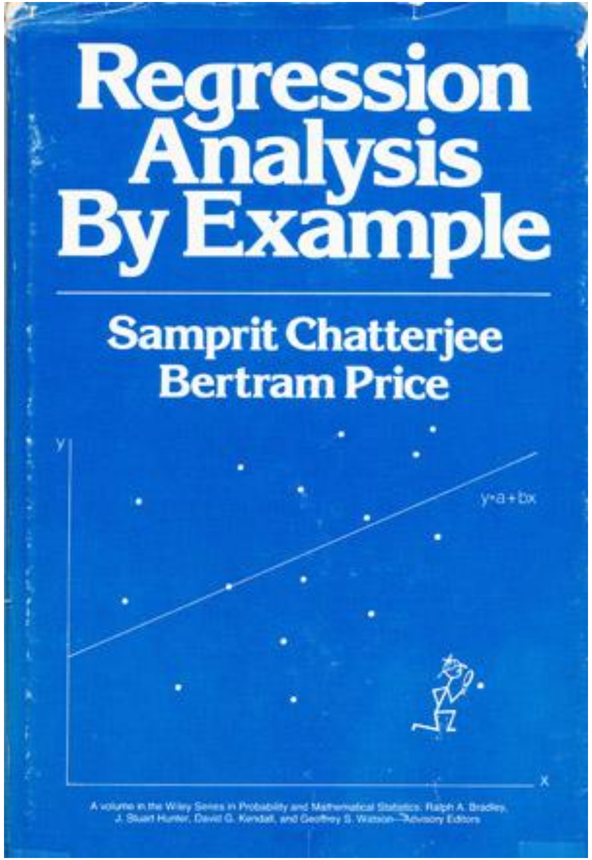
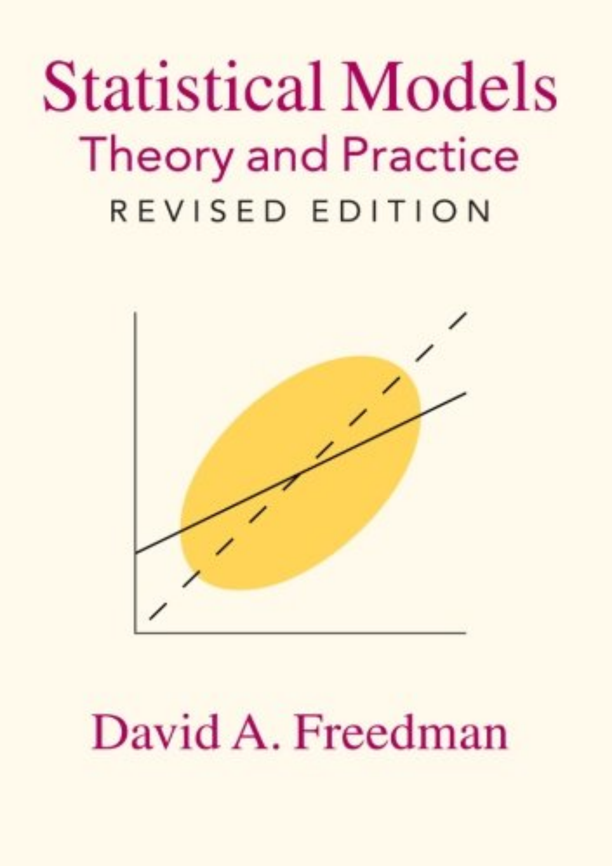
$$y = \alpha + \begin{bmatrix} \beta_1 & \beta_2 & \dots\beta_n \end{bmatrix} * \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix} + \varepsilon$$

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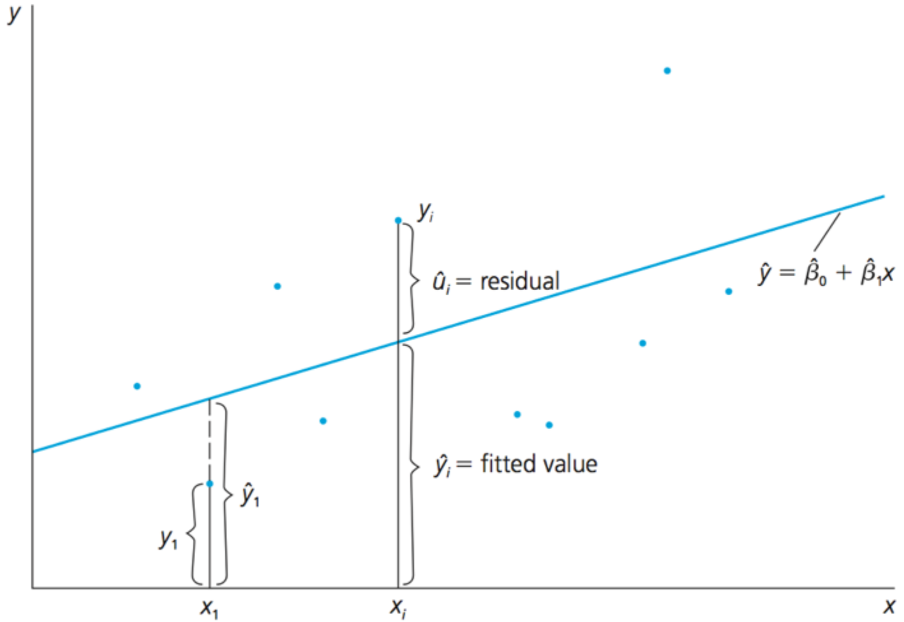
$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i.$$

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

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



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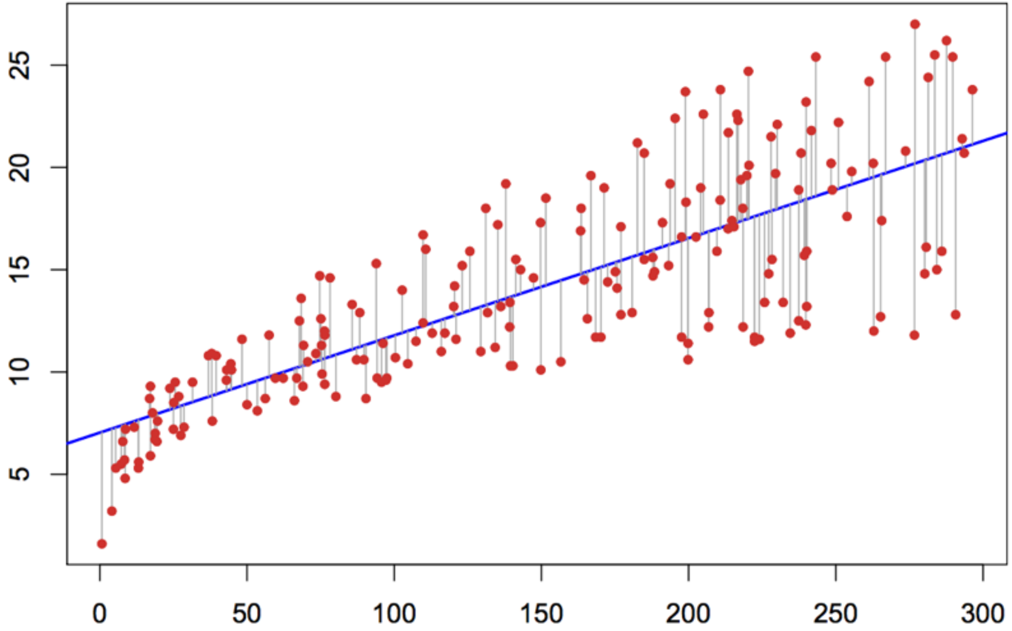

II: POLYNOMIAL REGRESSION

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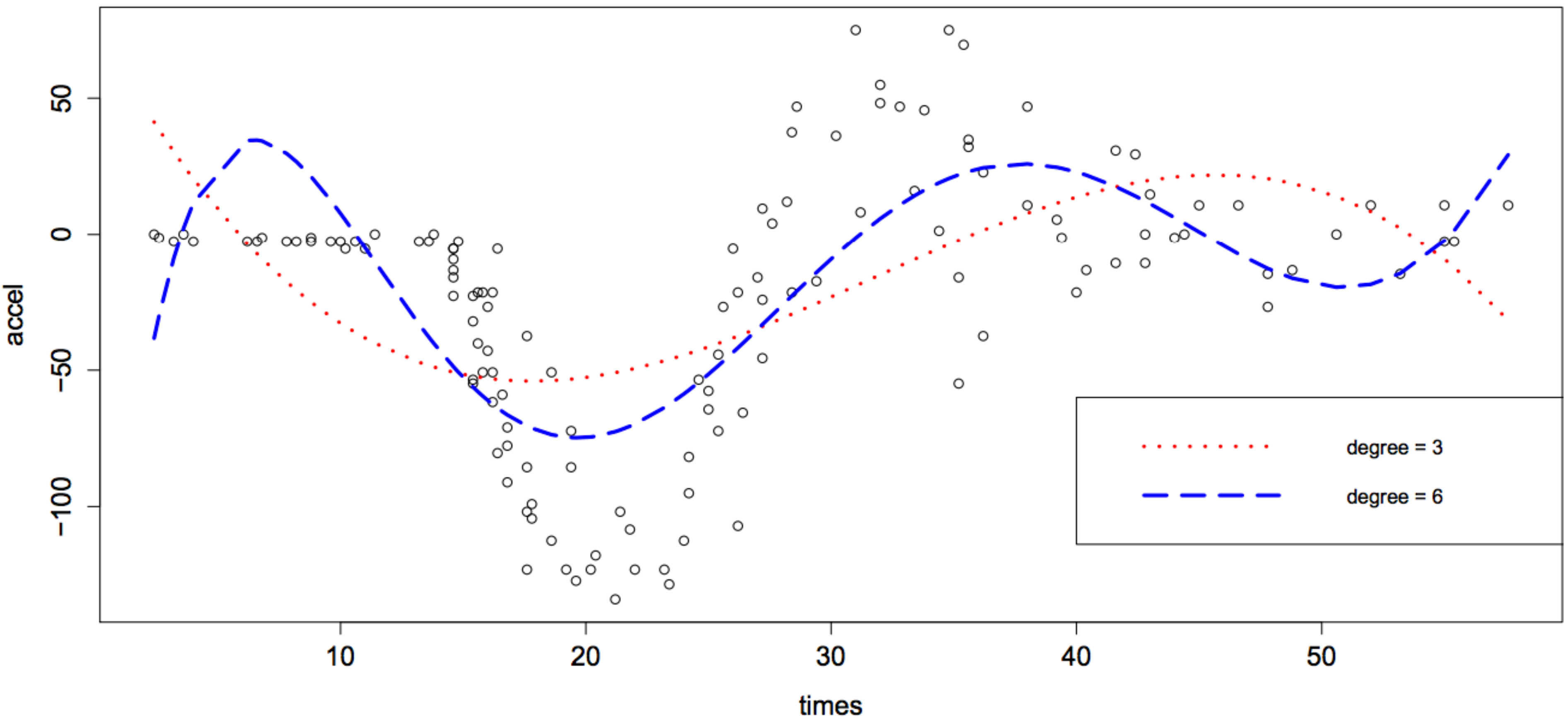
A: Yes, because it's linear in the β*'s!*

"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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When we talked about this in the context of classification, we said that it was a result of matching the training set too closely.

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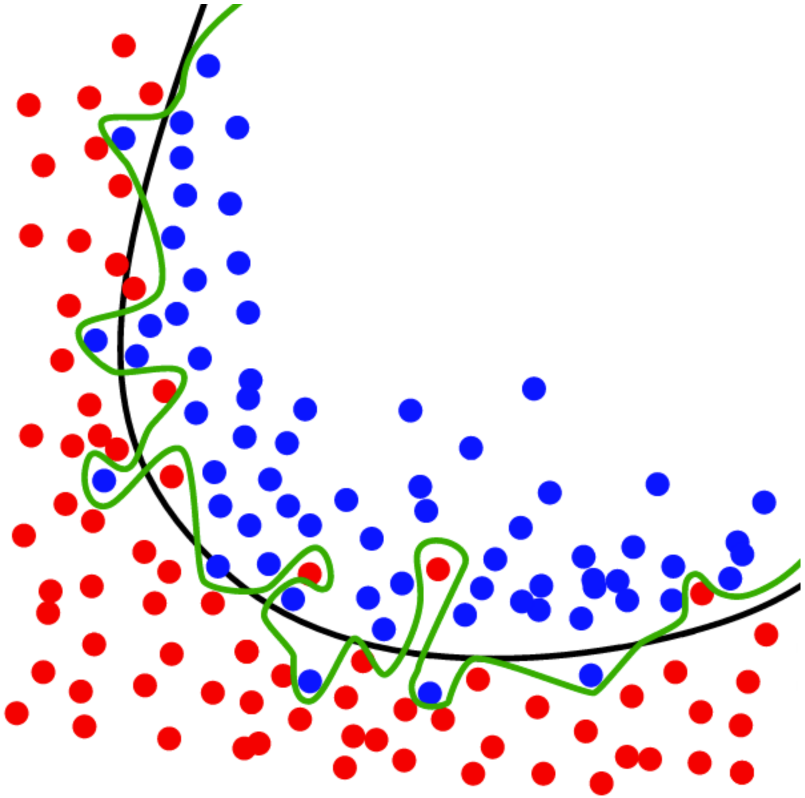
In other words, an overfit model matches the **noise** *in the dataset instead of the* **signal***.*

OVERFITTING EXAMPLE (CLASSIFICATION)



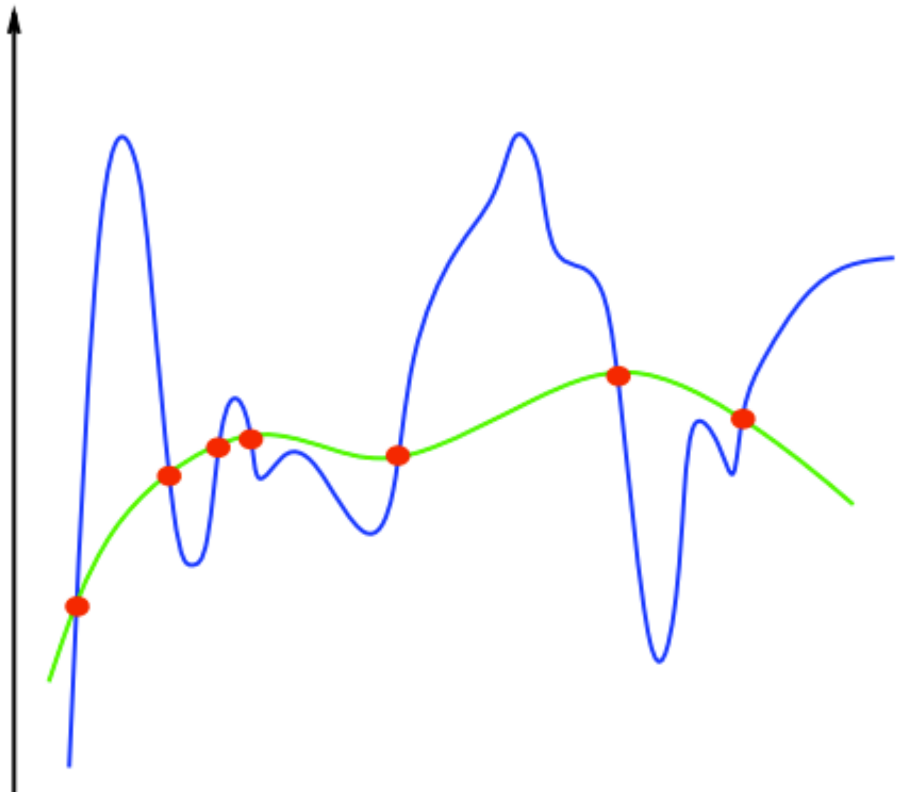
source: http://upload.wikimedia.org/wikipedia/commons/1/19/Overfitting.svg

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: $\Sigma \beta_i^2$

Q: How do we define the **complexity** *of a regression model?*

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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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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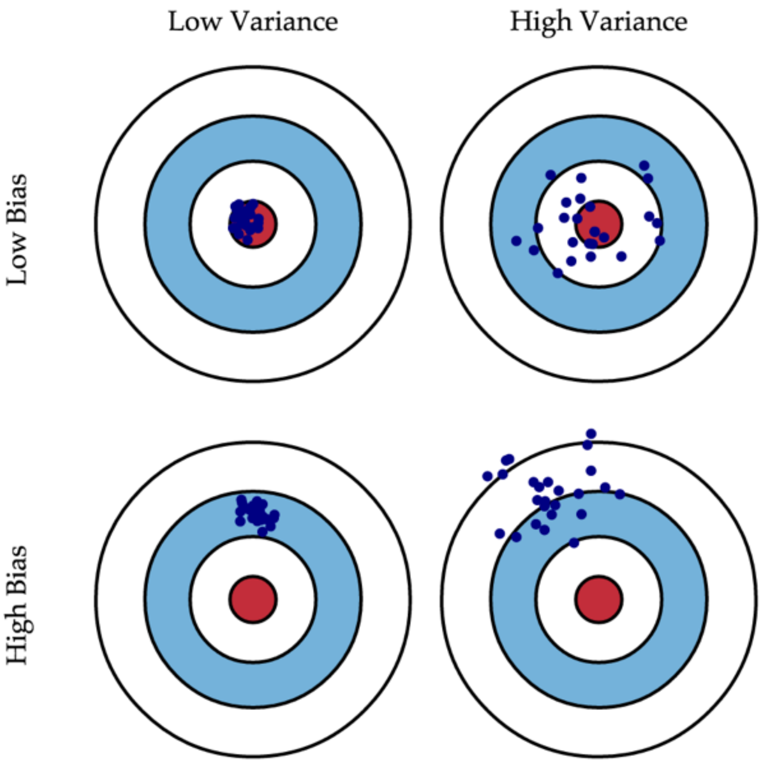
BIAS AND VARIANCE

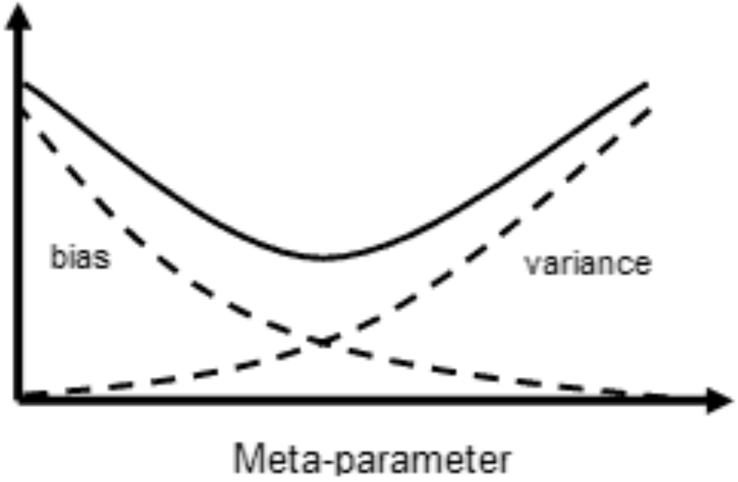


http://scott.fortmann-roe.com/docs/BiasVariance.html

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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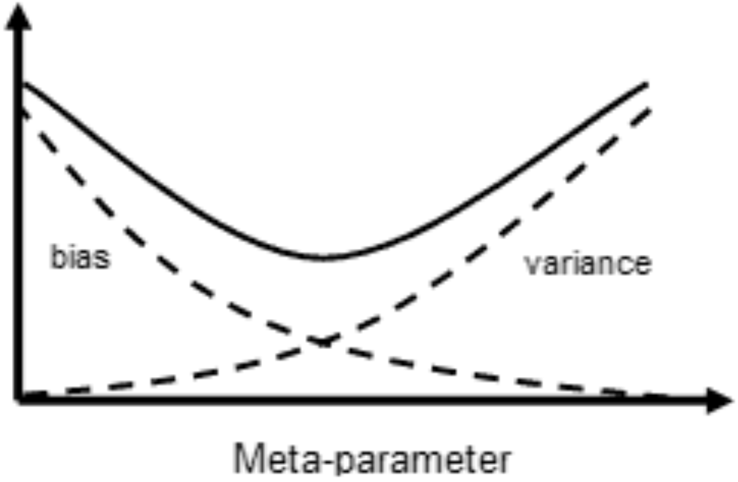


NOTE

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

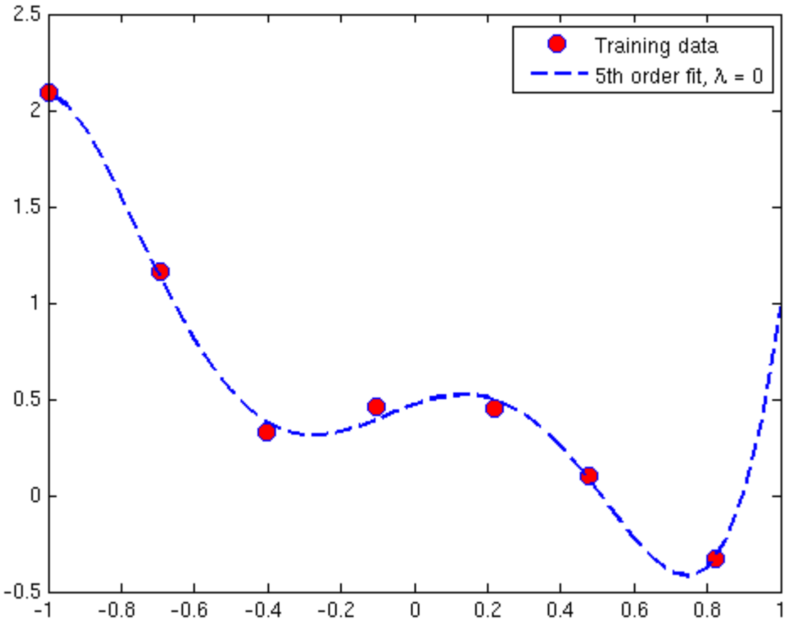
This tradeoff is regulated by a **hyperparameter** λ, *which we've already seen:*

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

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

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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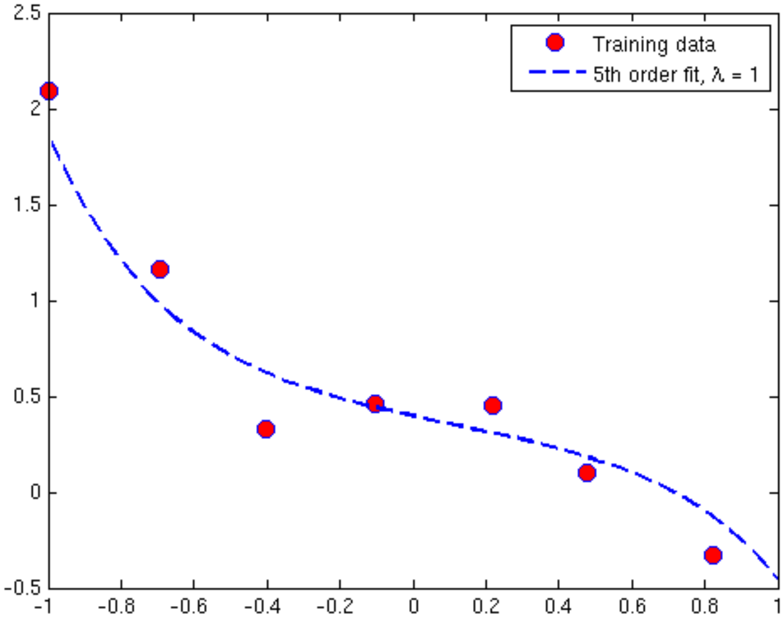

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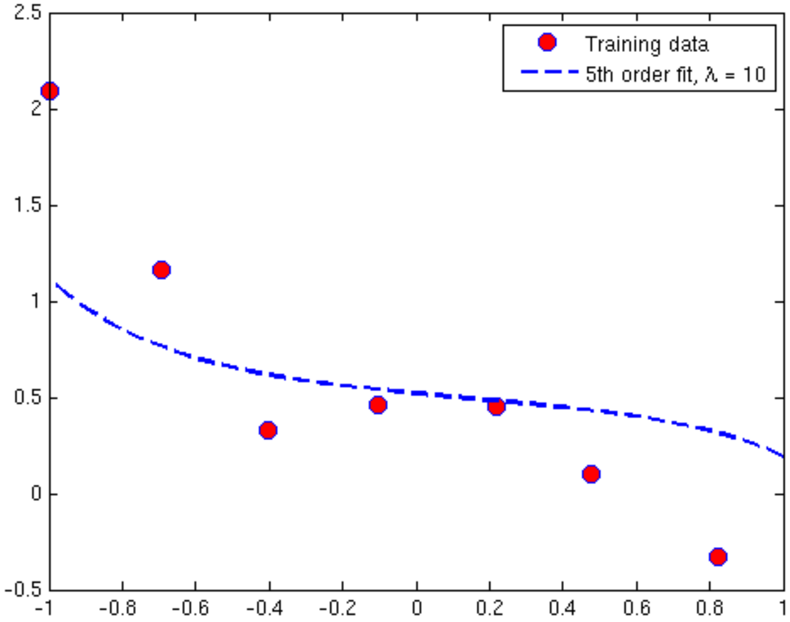

- Linear regression
- Multiple regression
- Polynomial regression
- The concept of minimizing some error or “cost” function
- Regularization

LAB: POLYNOMIAL REGRESSION & REGULARIZATION