GENERAL ASSEMBLY

# INTRO TO DATA SCIENCE:
## REGRESSION AND REGULARIZATION

I. LINEAR REGRESSION

II. POLYNOMIAL REGRESSION

III. REGULARIZATION

EXERCISES:

III. IMPLEMENTING MULTIPLE REGRESSION & POLYNOMIAL REGRESSION 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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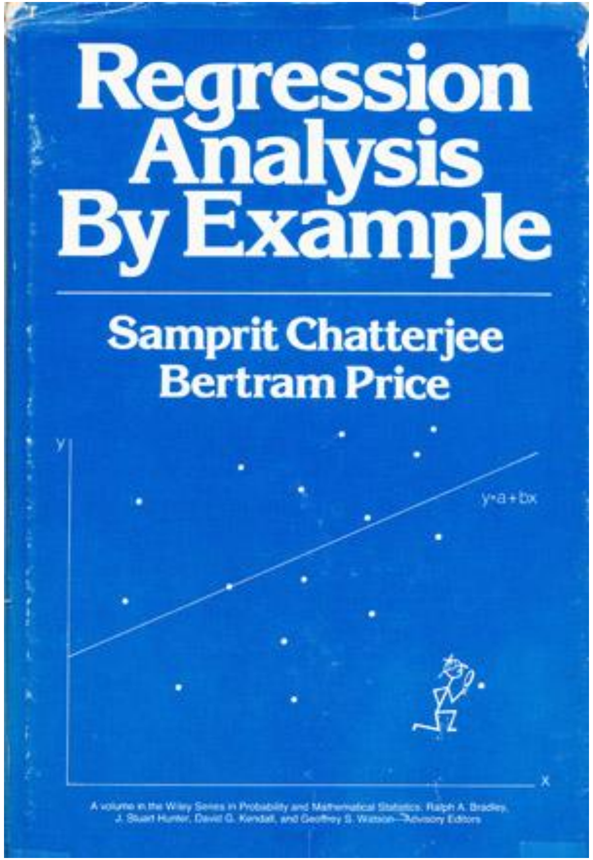
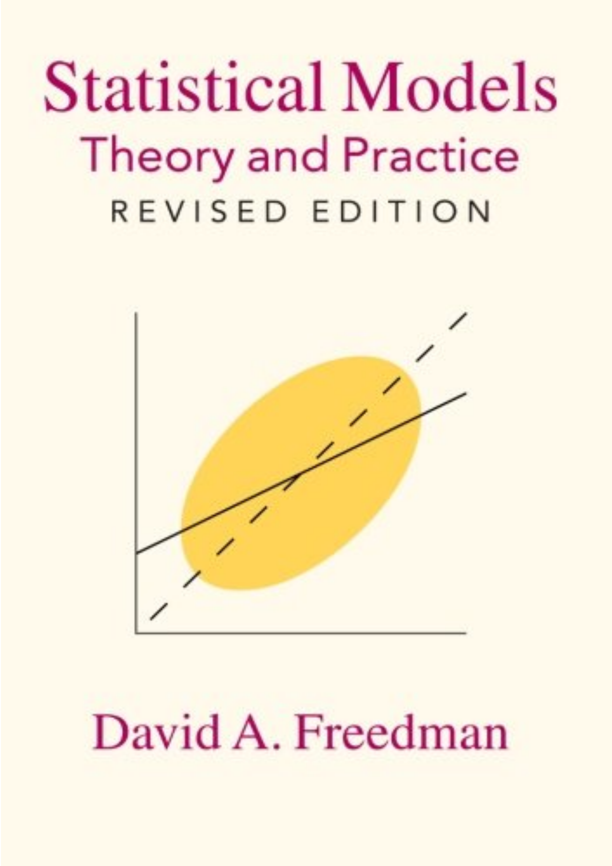
$$y = \alpha + \beta_1 x_1 + \ldots + \beta_n x_n + \varepsilon$$

*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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*In practice, any respectable piece of software will do this for you.*

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

# II: POLYNOMIAL REGRESSION

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*A: Yes, because it's linear in the $\beta$'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*

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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.*

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

```
> x <- seq(1, 10, 0.1)
> cor(x^9, x^10)
[1] 0.9987608
```

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**NOTE**

This results in a *singularity*. We will see an example of this in just a minute!

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**OPTIONAL NOTE**

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

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*Q: Can a regression model be too complex?*

# III: REGULARIZATION

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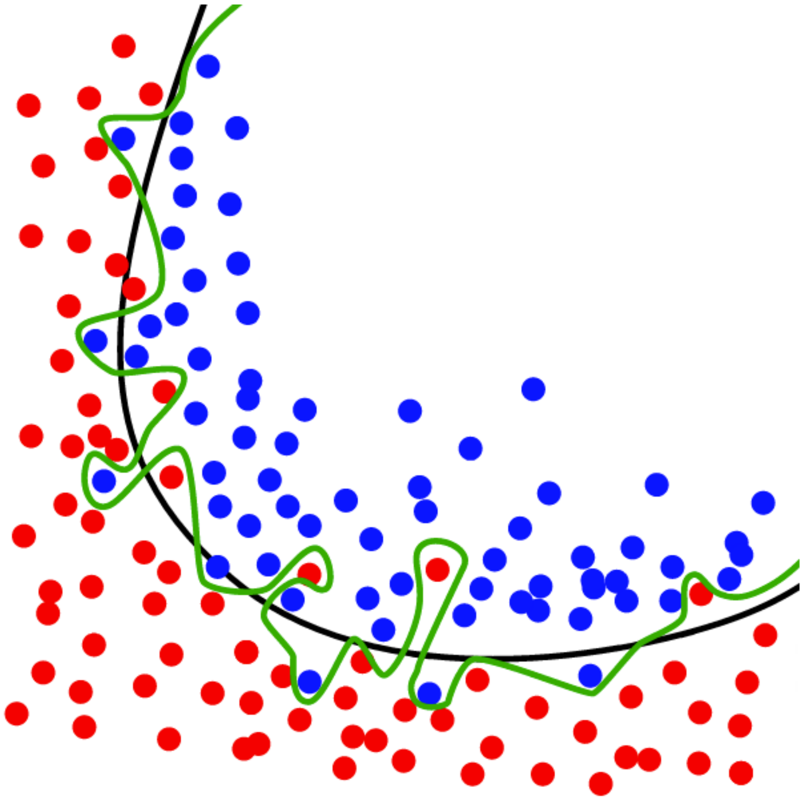
*When we talked about this in the context of classification, we said that it was a result of matching the training set too closely.*

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

# OVERFITTING EXAMPLE (CLASSIFICATION)

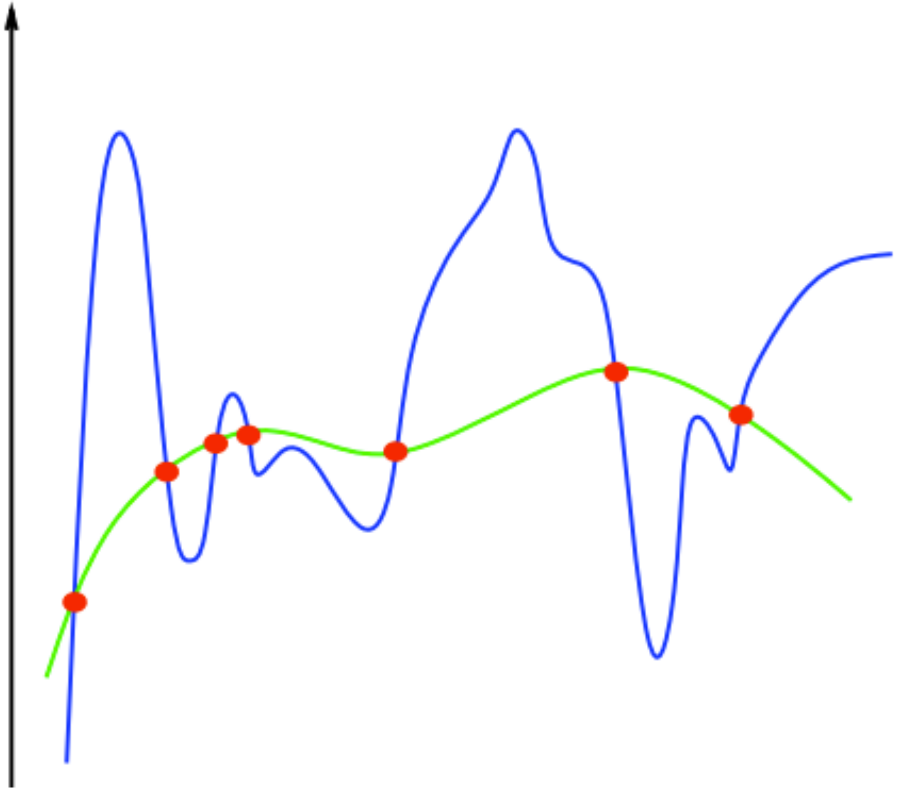


*source: http://upload.wikimedia.org/wikipedia/commons/1/19/Overfitting.svg*

*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.*



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

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*Ex 1:* $\Sigma |\beta_i|$

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*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**

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

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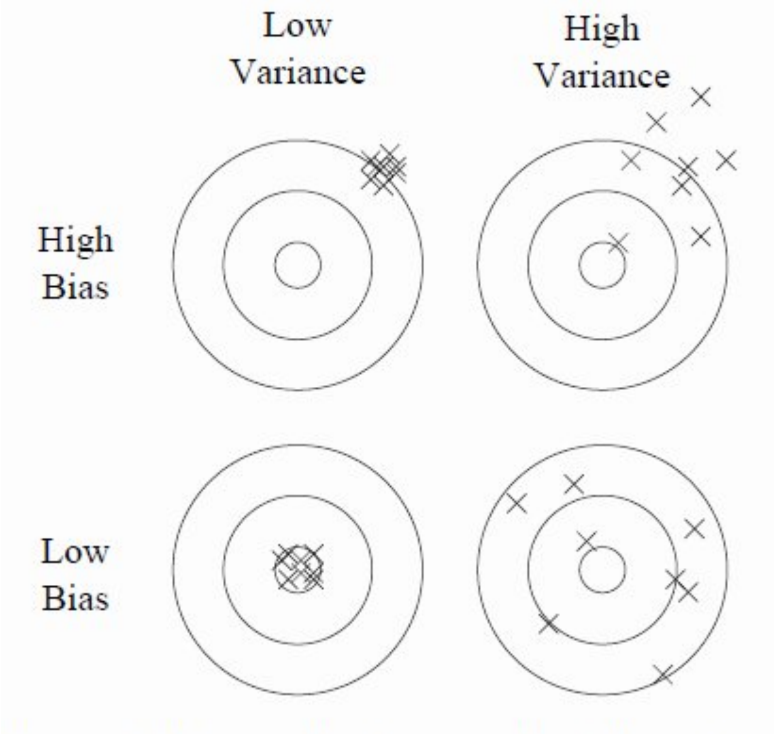



Figure 1: Bias and variance in dart-throwing.

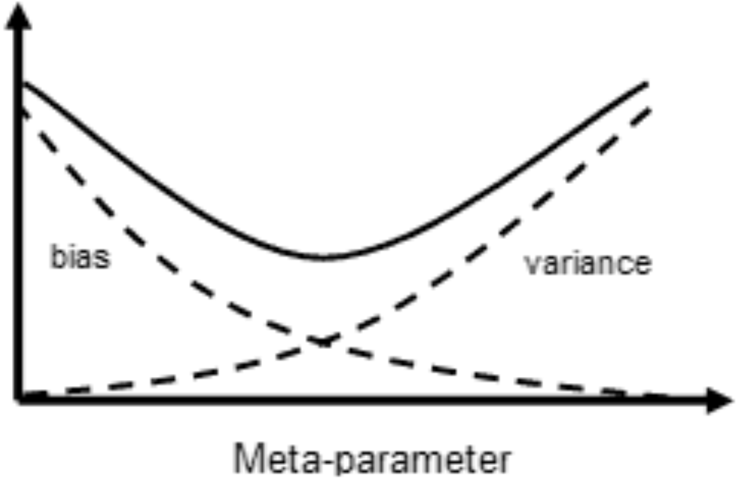
*source: http://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf*

*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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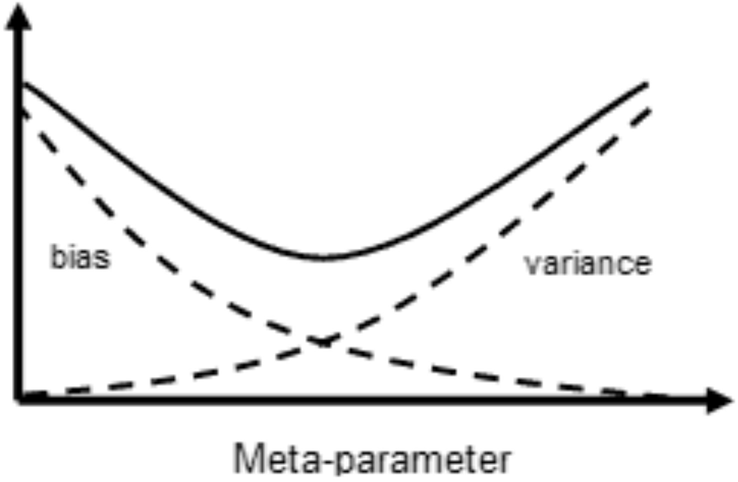


**NOTE**

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** $\lambda$*, which we've already seen:*

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

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

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

# EX: POLYNOMIAL REGRESSION & REGULARIZATION