

Introduction to Data Science

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About you

- PhD / Masters / Undergraduate?
- What major?

About me

- □ Background in Physics: Stat/Bio/Astro
 - Astronomy surveys → Big Data
- Research interest
 Computational Statistics; Bayesian Inference;
 Statistical Learning; Scientific Databases;
- Office: Whitehead 212C

About the course

- Introduction to data science
- □ Basic methods used all the time
- Presentations + Codes
- Syllabus posted soon

Grades

- □ 30% Homework 1 & 2
- □ 50% Midterm 1 & 2
- □ 20% Project

Pre-requisites

- Linear algebra
- Intro to prob/stat?

Sections

- Use your laptop
 - Also in class...

Plan for the Timeline

- □ Homework 1 graded in time for dropping
- Midterm 1
- □ Homework 2
- □ Midterm 2 few weeks before end of semester
- □ Project presentations

Format of Lectures

- Alternating between
 - Presentations
 - Coding
- Everything is going to Blackboard

Homework

- Data Science problems
- Much like the examples

Unhomework

Same but not graded

Exams

- □ In class
- Coding

What's coming?

Supervised Unsupervised

	Supervised	Unsupervised
Discrete		
Continuous		

	Supervised	Unsupervised
Discrete	Classification	
Continuous		

	Supervised	Unsupervised
Discrete	Classification	
Continuous	Regression	

	Supervised	Unsupervised
Discrete	Classification	Clustering
Continuous	Regression	

	Supervised	Unsupervised
Discrete	Classification	Clustering
Continuous	Regression	Dimensionality Reduc'n

Topics

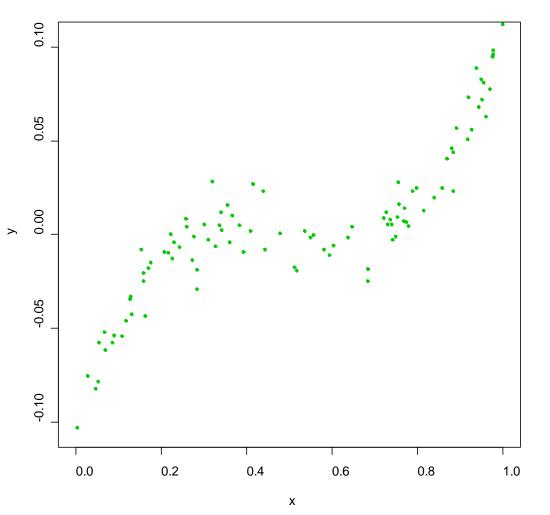
descriptive statistics – probabilistic density functions – normal distributions – regression – classification – nearest neighbors — bias-variance — Bayesian inference robustness – regularization – support vector machines – decisions trees – clustering – principal component analysis – expectation maximization – neural networks – spectral embedding – ...

Supervised Learning

Learning

- Model
 - Unknown function
 - Random noise

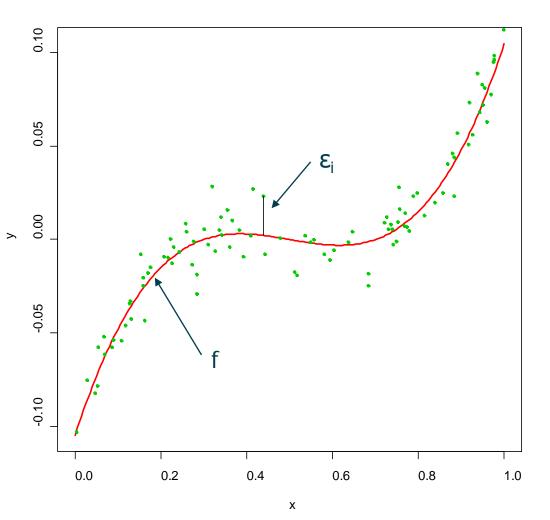
$$Y_i = f(\mathbf{X}_i) + \varepsilon_i$$



Learning

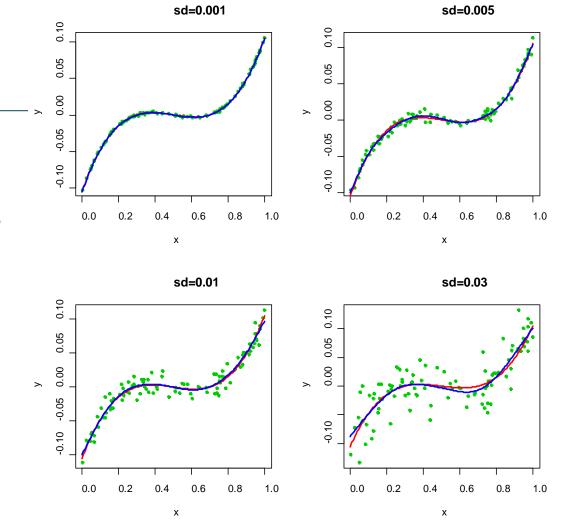
- Model
 - Unknown function
 - Random noise

$$Y_i = f(\mathbf{X}_i) + \varepsilon_i$$



Noise!

- Different scatter
- Different solutions



Why learn f(x)?

- Inference
 - Relation of variables to target
- Prediction
 - Estimate *y* for a new *x*

How to estimate f(x)?

- Using a training set with both
 - Input
 - Output

$$\{(\boldsymbol{x}_1,y_1),(\boldsymbol{x}_2,y_2),\ldots,(\boldsymbol{x}_n,y_n)\}$$

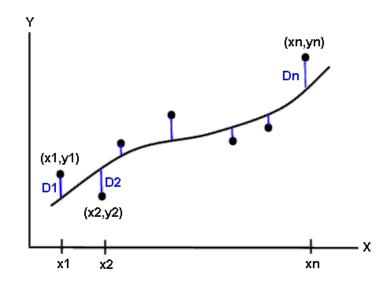
For example, assuming a linear model

$$f(\boldsymbol{x};\boldsymbol{\beta}) = \beta_0 + \beta_1 x_1 + \dots + \beta_d x_d$$

$$f(\boldsymbol{x}_i;\boldsymbol{\beta}) = \beta_0 + \beta_1 x_{i,1} + \dots + \beta_d x_{i,d}$$

How to estimate f(x)?

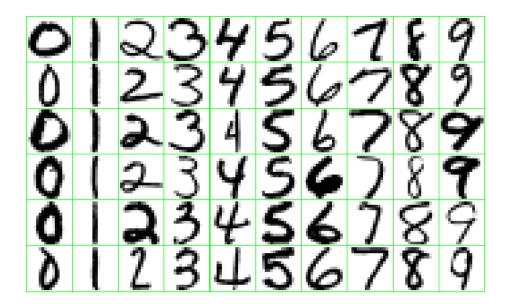
- One way is the method of least squares
 - Form differences of Y_i and $f(X_i)$
 - Minimize the sum of squares



Handwritten Numbers?

Which digit?

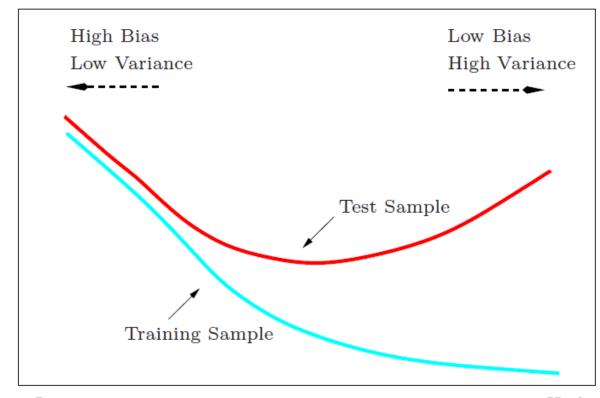
- Classification!
 - Training set



Complexity

Complicated models can better fit the data but harder to interpret and understand

- Too simple: underfitting
 - Bad fit on training & test sets
- Too complex: overfitting
 - Better on training but worse on test set



Low High
Model Complexity

Interpretation

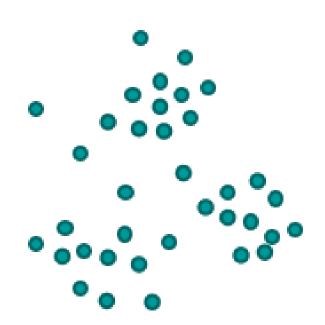
There is no true interpretation of anything; interpretation is a vehicle in the service of human comprehension. The value of interpretation is in enabling others to fruitfully think about an idea.

-Andreas Buja

Unsupervised Learning

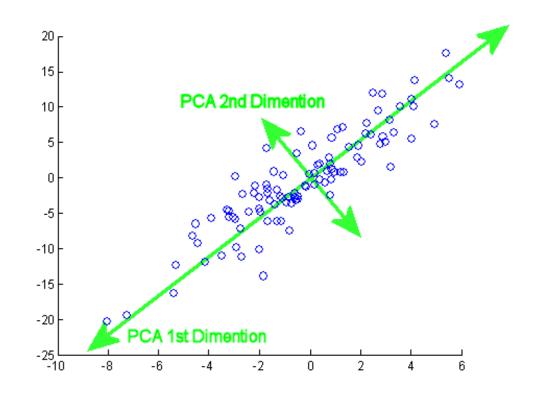
Clustering

- If no labels are provided
- We learn the clusters



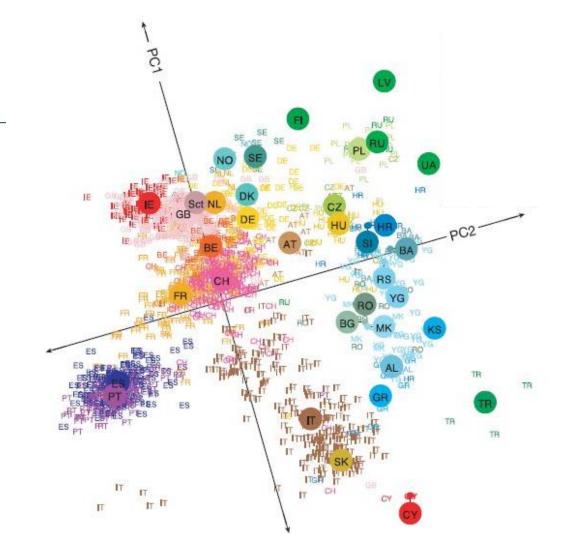
Principal Component Analysis

- Our model:
 - Direction of largest variation is relevant
 - The rest is "noise"



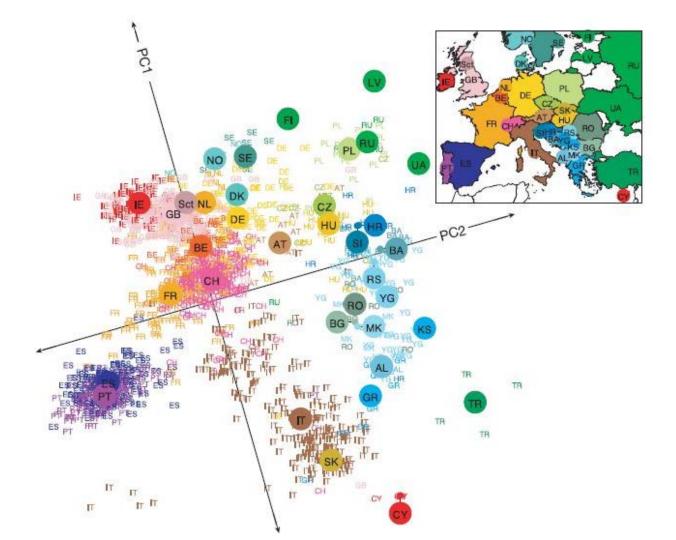
Genes

□ PCA



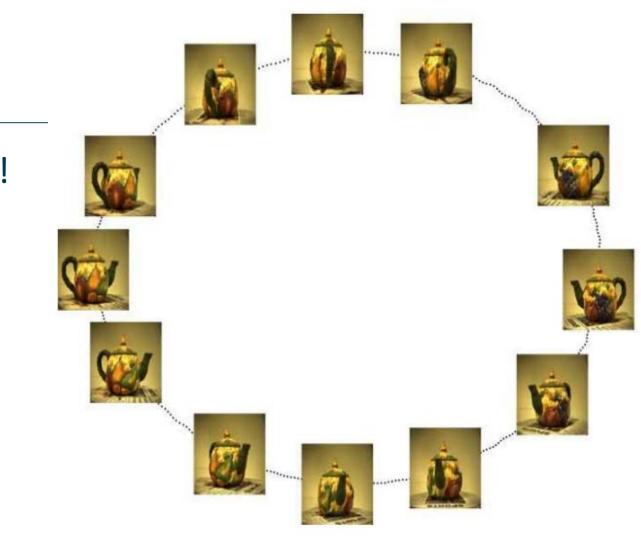
Genes

- □ PCA
- Мар



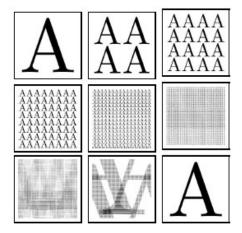
Nonlinear

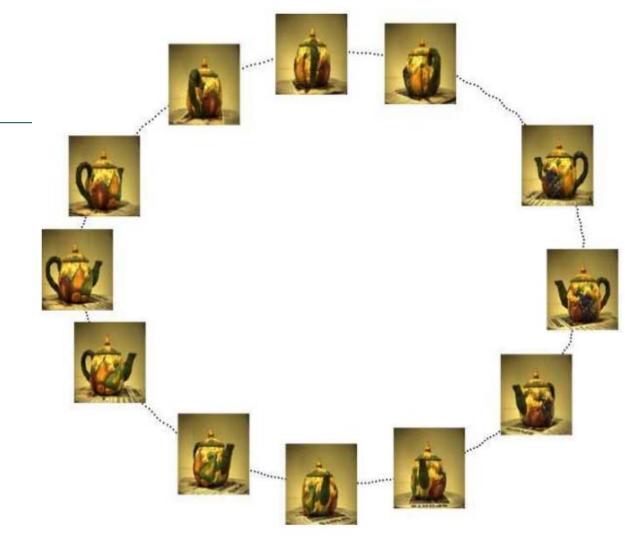
□ It's a rotation!



Nonlinear

- □ It's a rotation!
 - Even if pixels are shuffled!





More Parameters

■ How many?



More Parameters

■ How many?



Jupyter Notebook

Python

- General programming language
 - For scripting and prototyping
- Modules for everything
 - Including numerical & statistical packages

Jupyter

- Interactive analysis
 - Easy to use
 - Web interface
 - Smart rendering



