JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING

Introduction to Data Science

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Dept of Computer Science
Dept of Physics & Astronomy

About you

- PhD / Masters / Undergraduate?
- What major?

About me

- Background in Physics: Stat/Bio/Astro
  - Astronomy surveys $\rightarrow$ Big Data
- Research interest

  Computational Statistics; Bayesian Inference;

  Statistical Learning; Scientific Databases;
- Office: Wyman Park N437

About the course

- Introduction to data science
- Basic methods
- Methods & coding
- Syllabus on Canvas

Grades

- 60% Weekly homework
- 40% Midterm 1 & 2

Format of Lectures

- Alternating between
  - Methodology
  - Coding
- Everything is going to Canvas

Homework

- Data Science problems
- Much like the examples

Unhomework

- Not graded

Exams & Homework

- Exams are 75 mins as if in class
- HW assignments from Thu to Wed
- Mostly coding

What’s coming?

Statistical Learning

Supervised	Unsupervised

Statistical Learning

	Supervised	Unsupervised
Discrete		
Continuous		

Statistical Learning

	Supervised	Unsupervised
Discrete	Classification	
Continuous		

Statistical Learning

	Supervised	Unsupervised
Discrete	Classification	
Continuous	Regression	

Statistical Learning

	Supervised	Unsupervised
Discrete	Classification	Clustering
Continuous	Regression	

Statistical Learning

	Supervised	Unsupervised
Discrete	Classification	Clustering
Continuous	Regression	Dimensionality Reduc’n

Topics

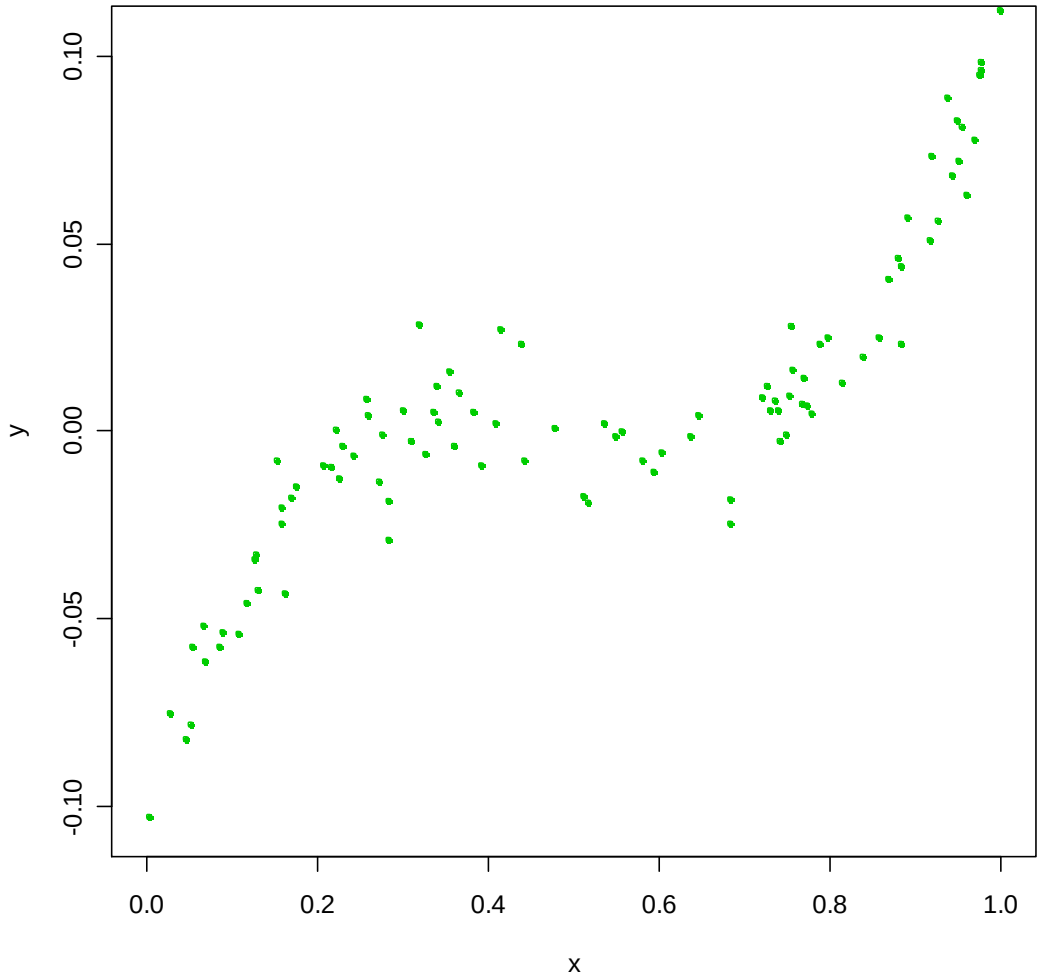
descriptive statistics – probabilistic density functions – regression – regularization – principal component analysis – classification – nearest neighbors – Bayesian inference – decisions trees – random forest – support vector machines – clustering – expectation maximization – spectral clustering and embedding – databases – robustness – neural networks…

Supervised Learning

Learning

- Model
  - Unknown function
  - Random noise

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



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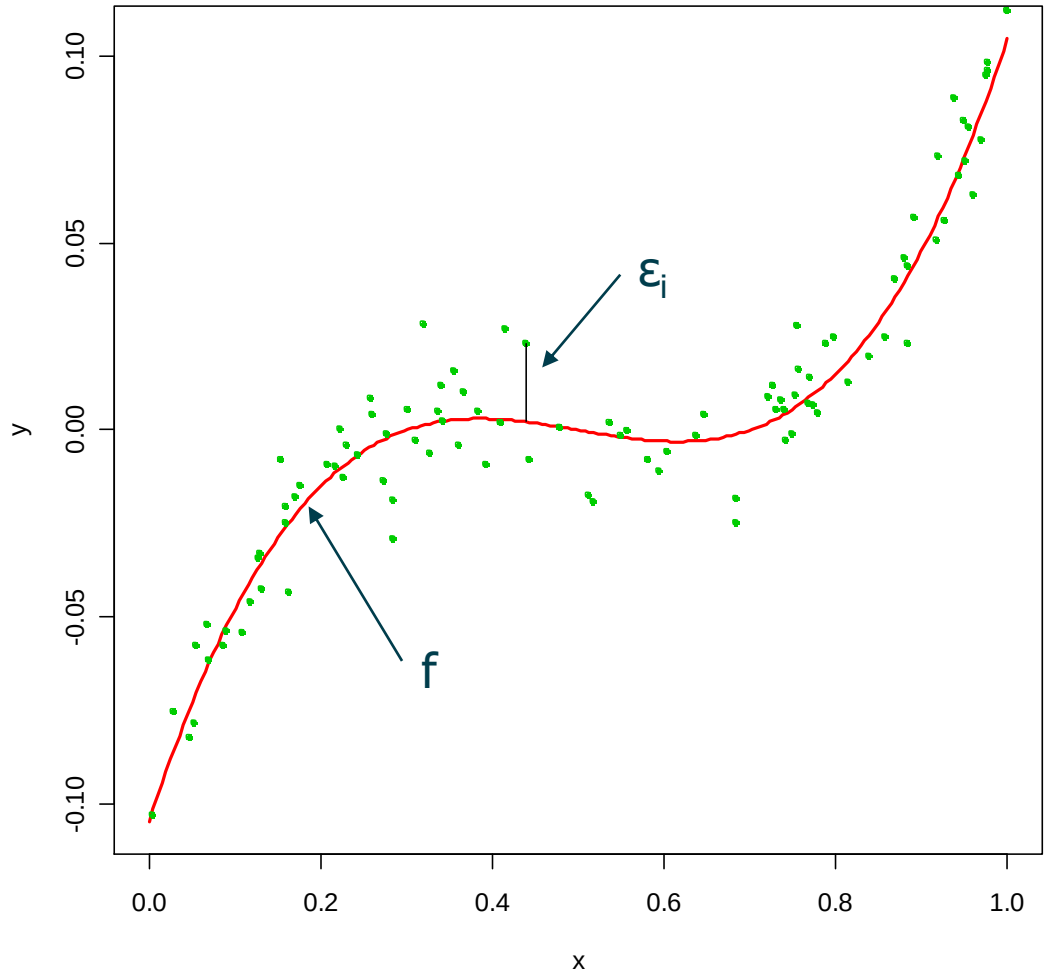
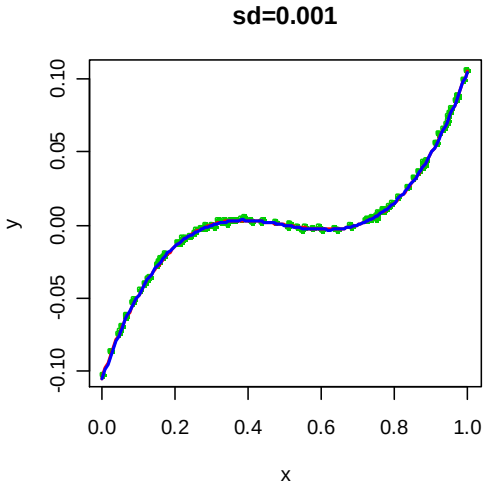
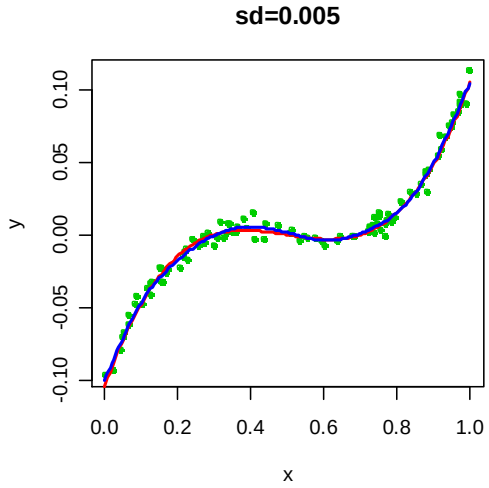
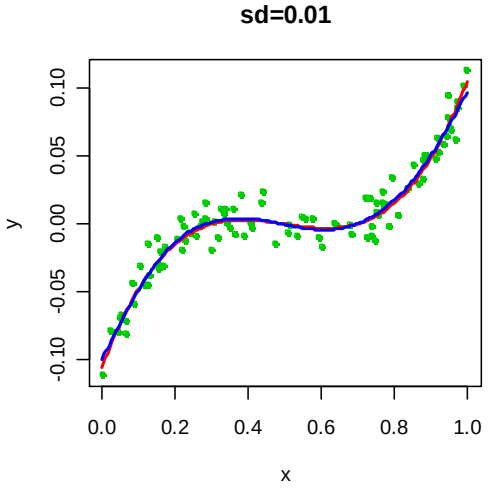


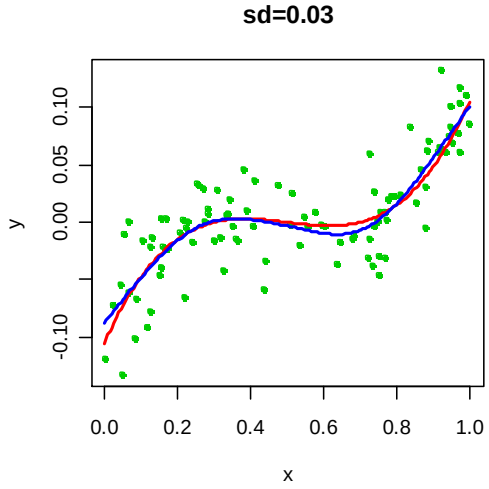
Noise!

- Different scatter
- Different solutions









Why learn $f(x)$?

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

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

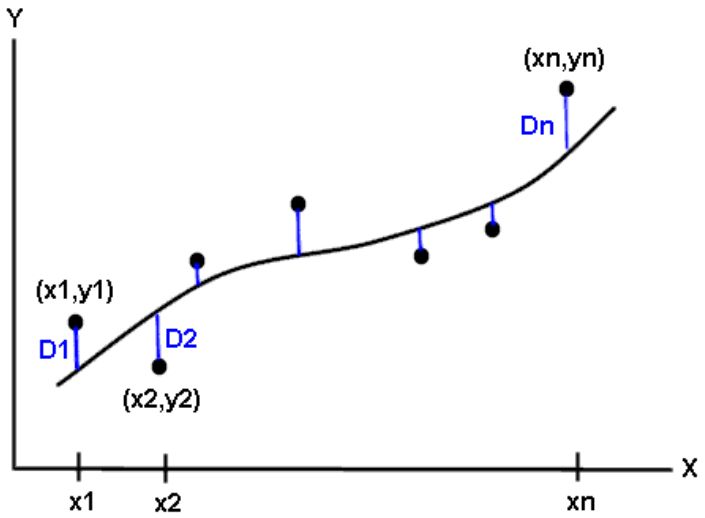
- For example, assuming a linear model

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

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

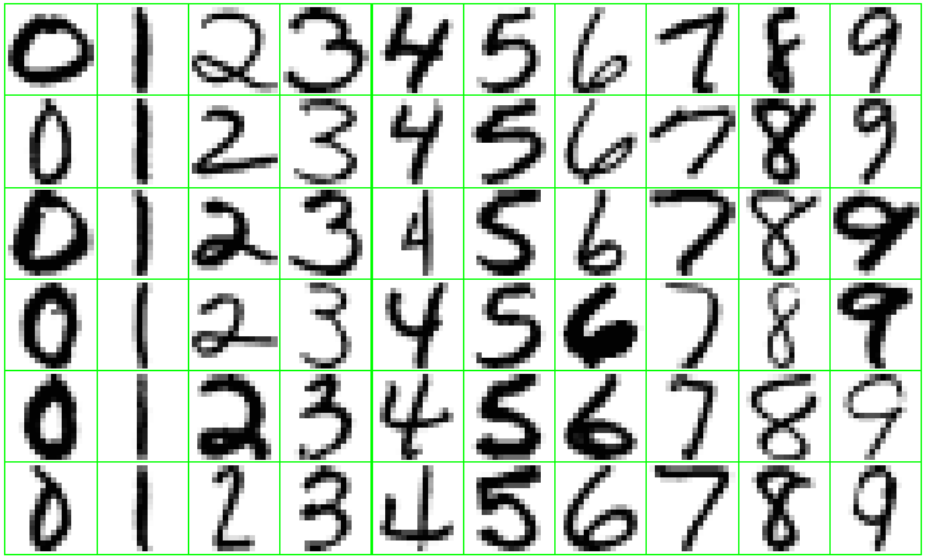
How to estimate $f(x)$?

- One way is the method of least squares
  - Form differences of Y_i and $f(\boldsymbol{X}_i)$
  - Minimize the sum of squares



Handwritten Numbers?

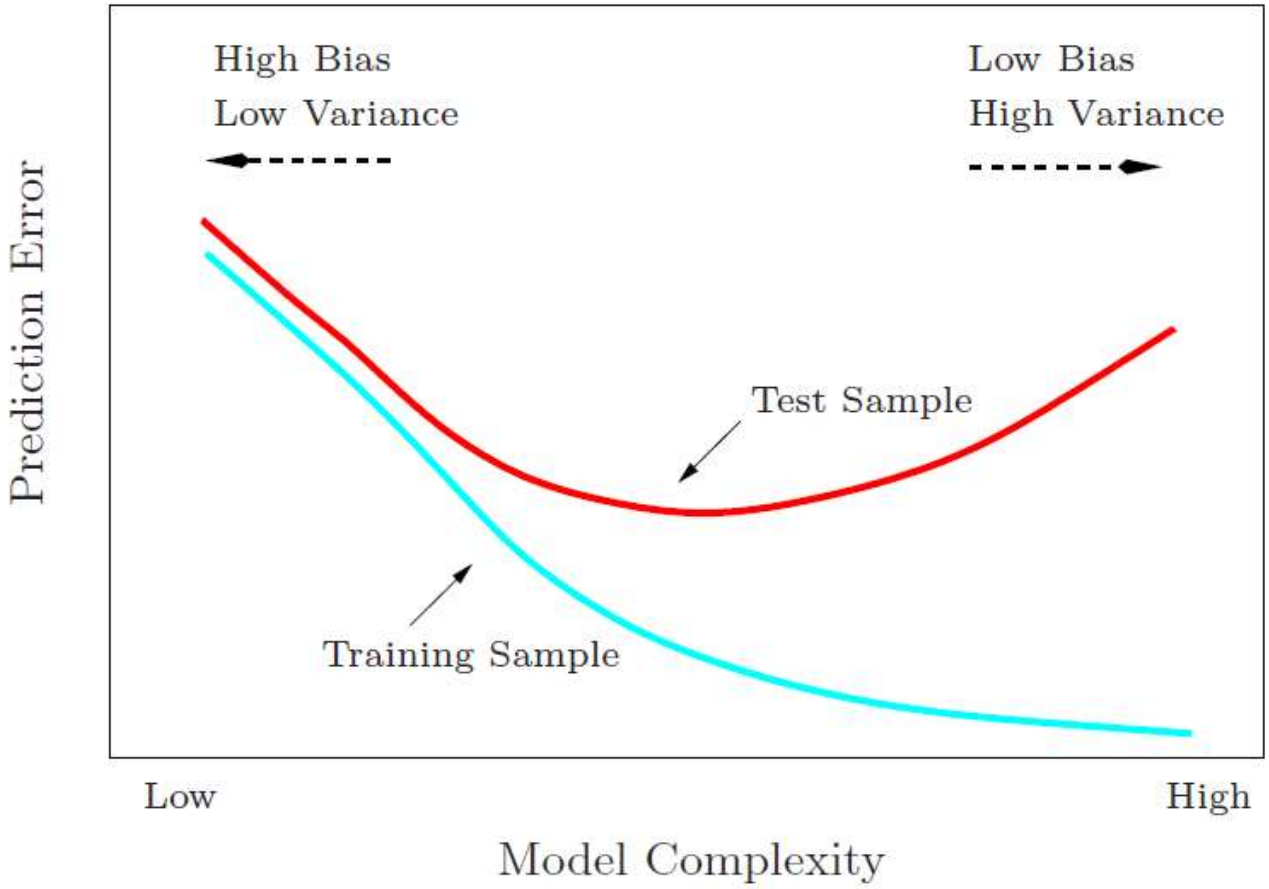
- Which digit?
- Classification!
  - Training set



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


High Bias
Low Variance
Low Bias
High Variance
Prediction Error
Test Sample
Training Sample
Low
High
Model Complexity

Interpretation

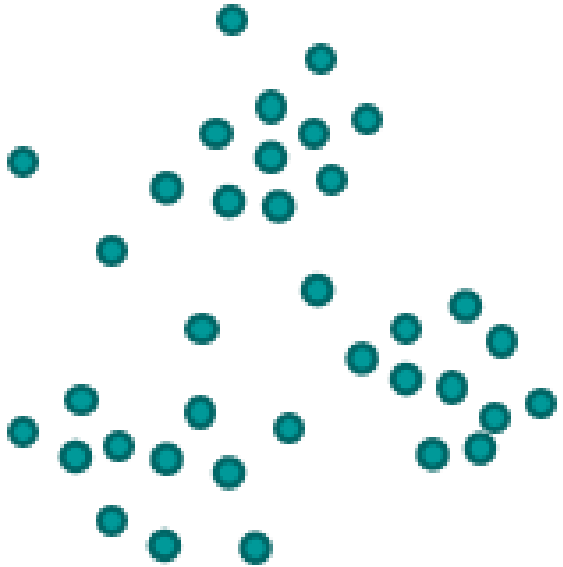
There is no true interpretation of anything; interpretation is a vehicle in the service of human comprehension. The value of interpretation is in enabling others to fruitfully think about an idea.

–Andreas Buja

Unsupervised Learning

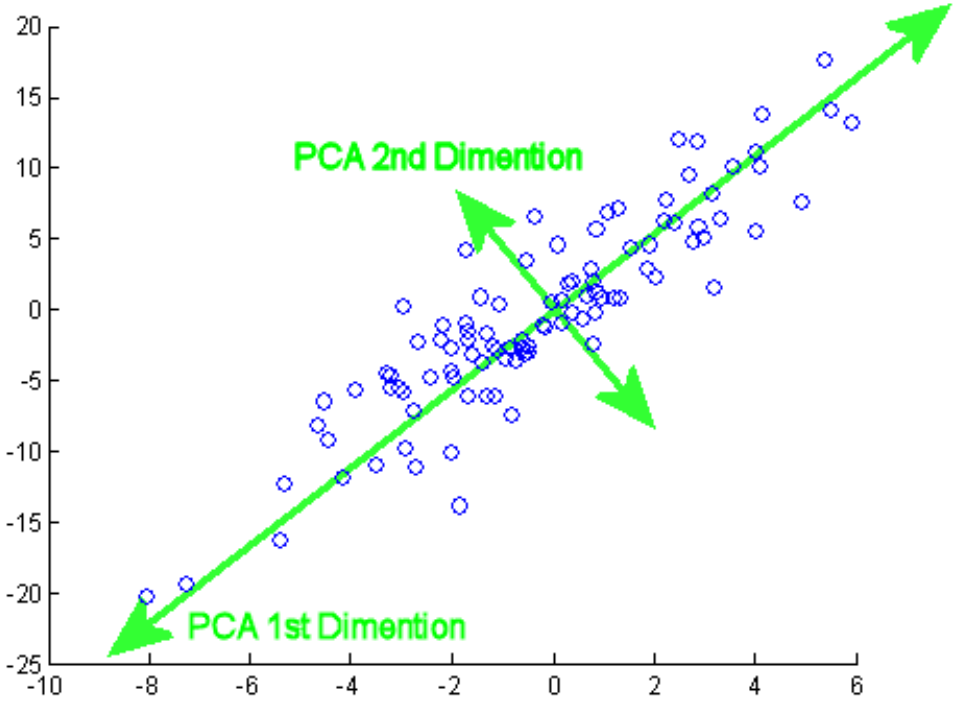
Clustering

- If no labels are provided
- We learn the clusters



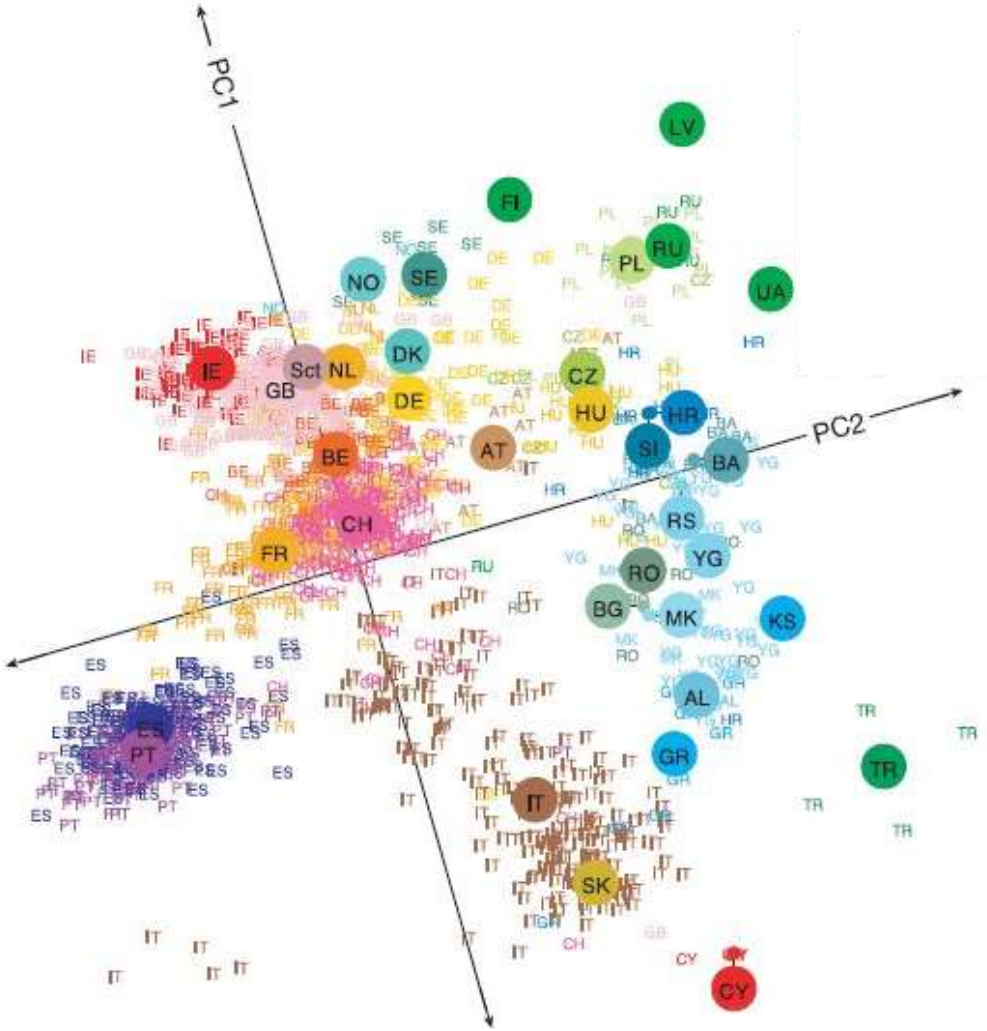
Principal Component Analysis

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



Genes

- PCA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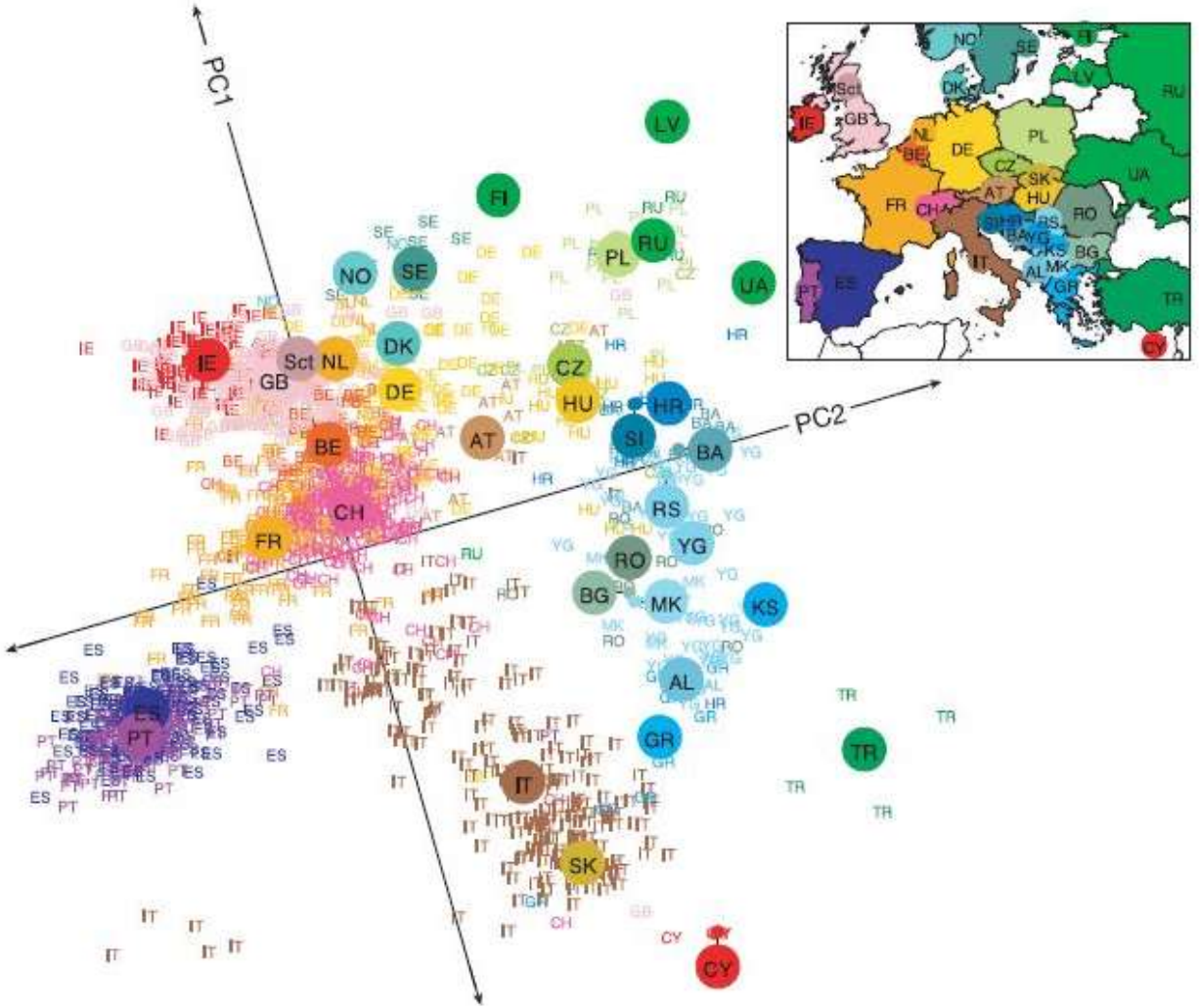
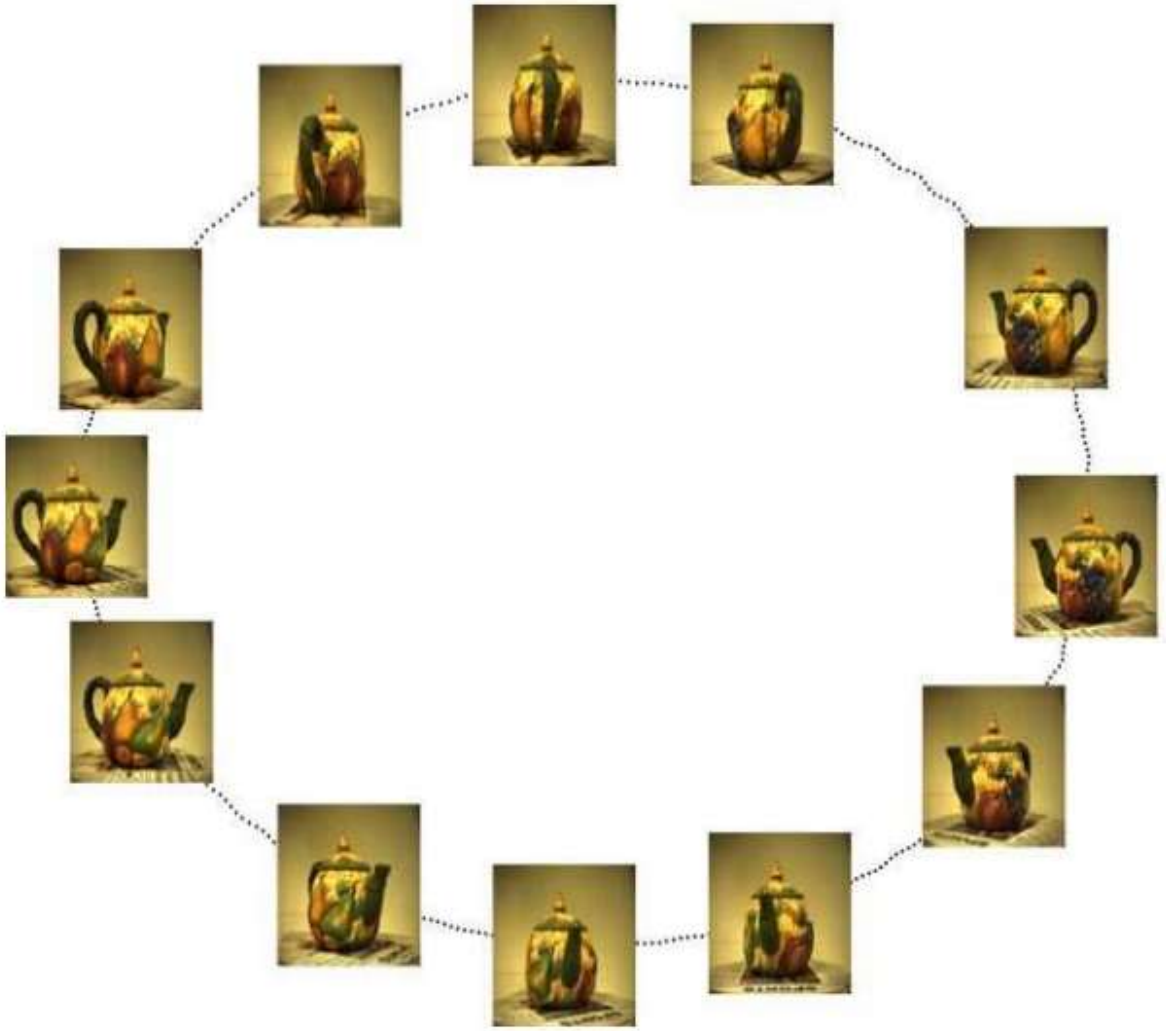
Genes

- PCA
- Map



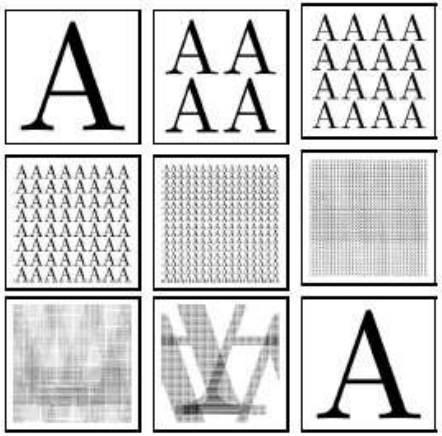
Nonlinear

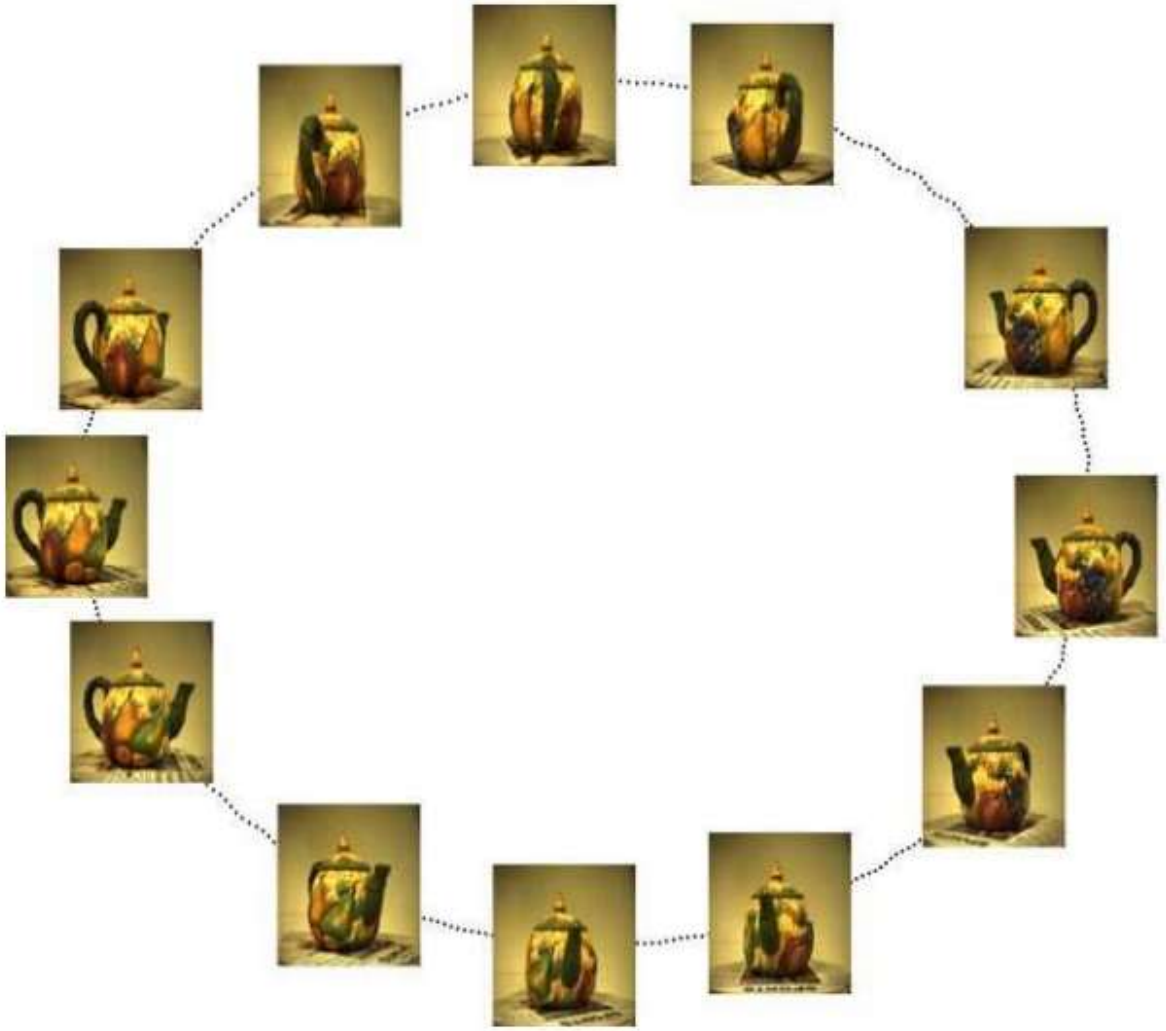
- It’s a rotation!



Nonlinear

- It’s a rotation!
  - Even if pixels are shuffled!





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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