JOHNS HOPKINS
WHITING SCHOOL of ENGINEERING

Introduction to Data Science

Tamás Budavári
Dept of Applied Mathematics & Statistics
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 – used all the time
- Presentations + Codes
- Syllabus posted soon

Grades

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

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

Zoom

- Recurring invite was sent to everyone
- Video recordings will be made available for 7 days
- No other recordings are allowed

Exams & HW on Gradescope

- Exams are 75 mins as if in class
- HW assignments – 1 week
- Mostly coding

Microsoft Teams

- Team for everybody is already online
- Communicate with peers and TAs

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

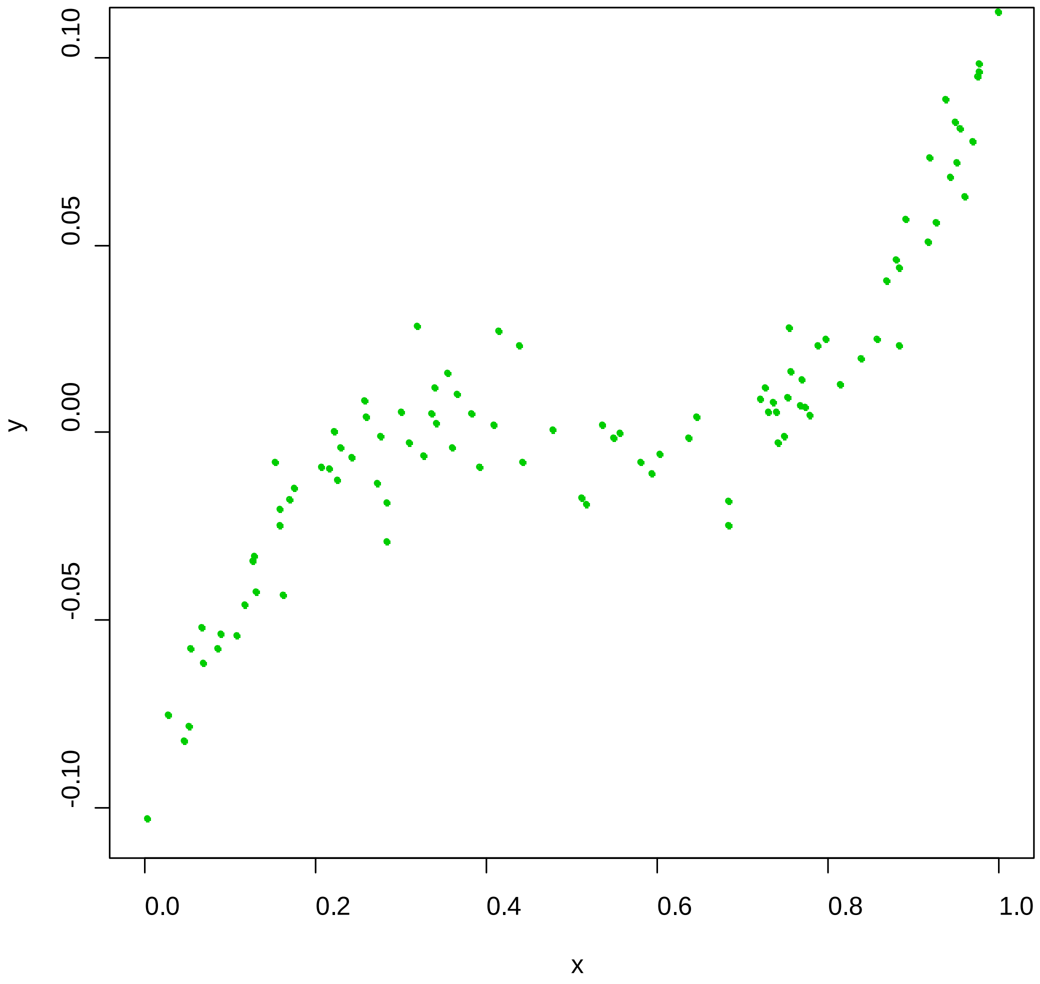
descriptive statistics – probabilistic density functions – regression – regularization – principal component analysis – classification – nearest neighbors – Bayesian inference – decisions trees – random forest – support vector machines – clustering – expectation maximization – spectral clustering and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

Supervised Learning

Learning

- Model
  - Unknown function
  - Random noise

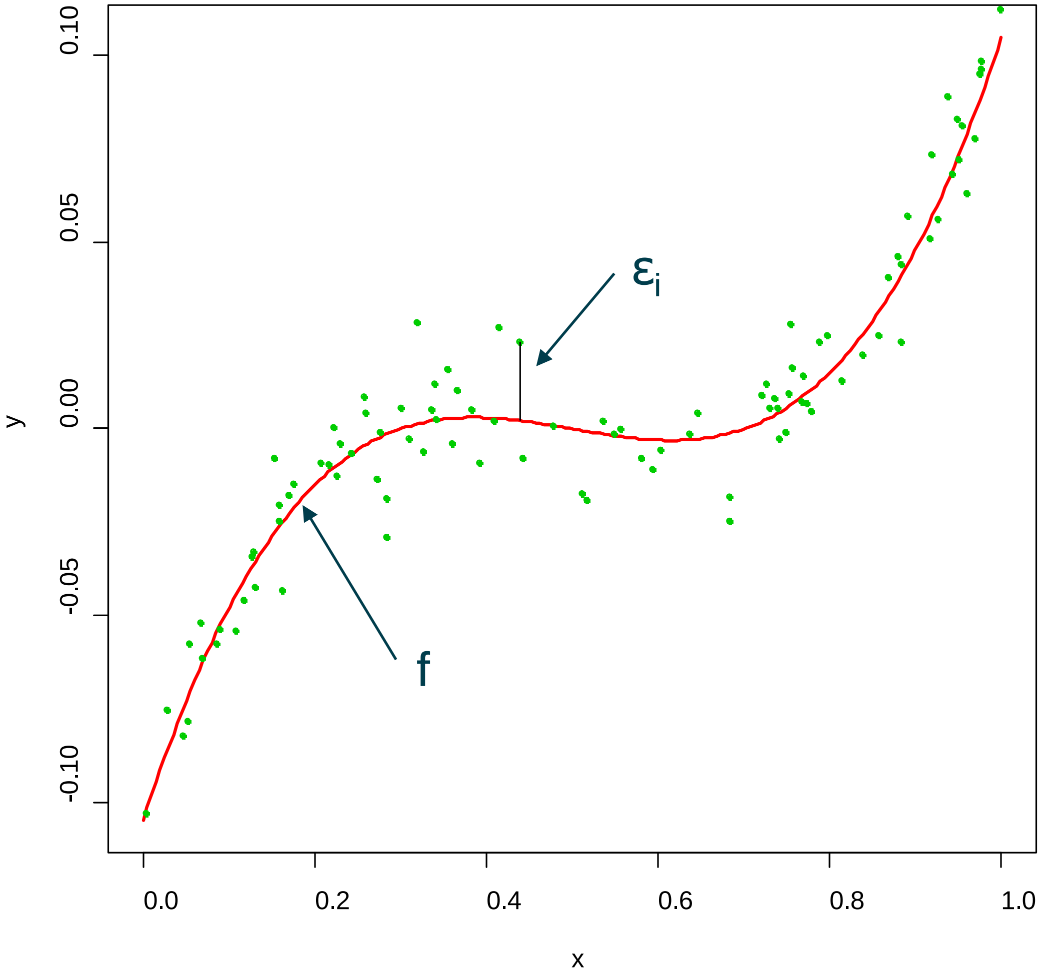
$$Y_i = f(\mathbf{X}_i) + \varepsilon_i$$



Learning

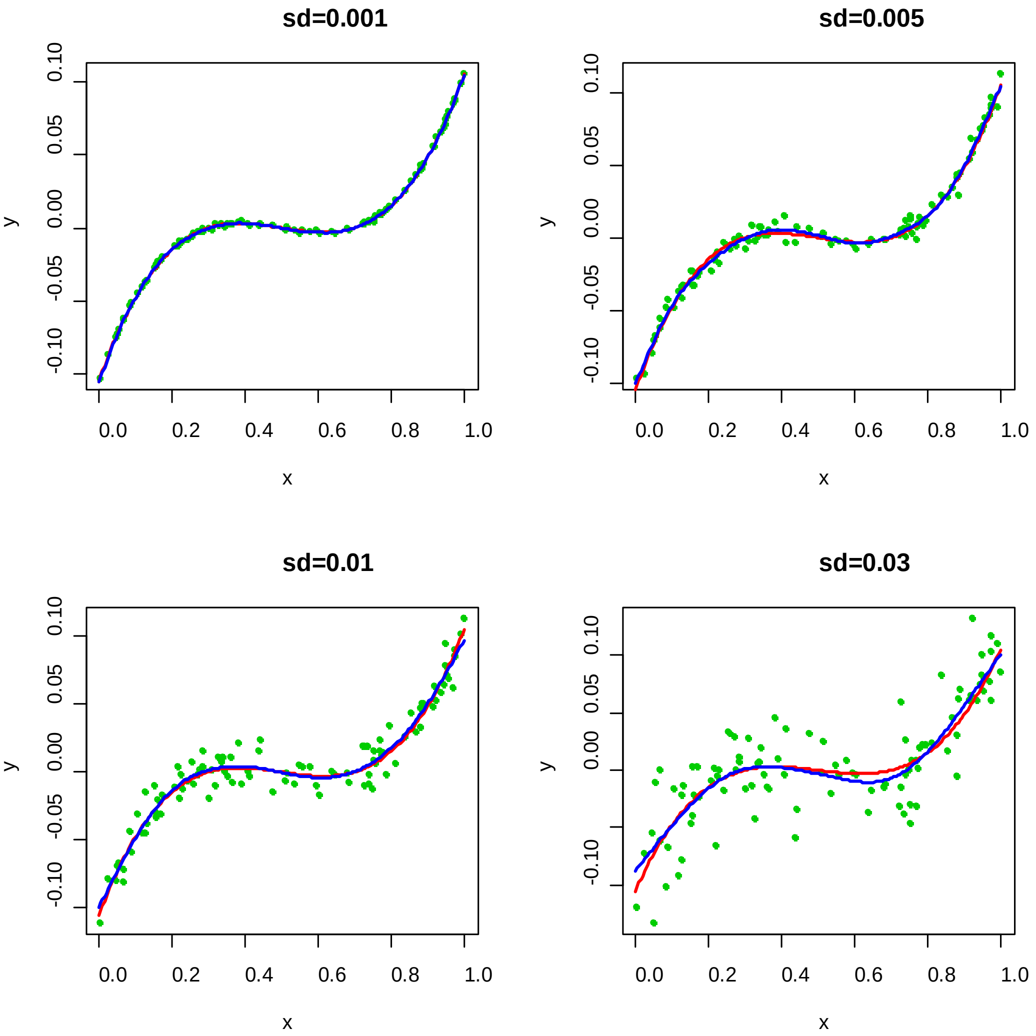
- Model
  - Unknown function
  - Random noise

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



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

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

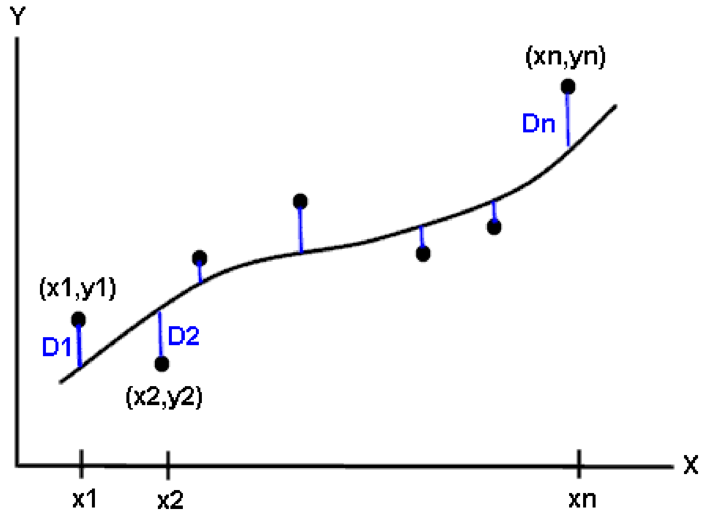
- For example, assuming a linear model

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

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

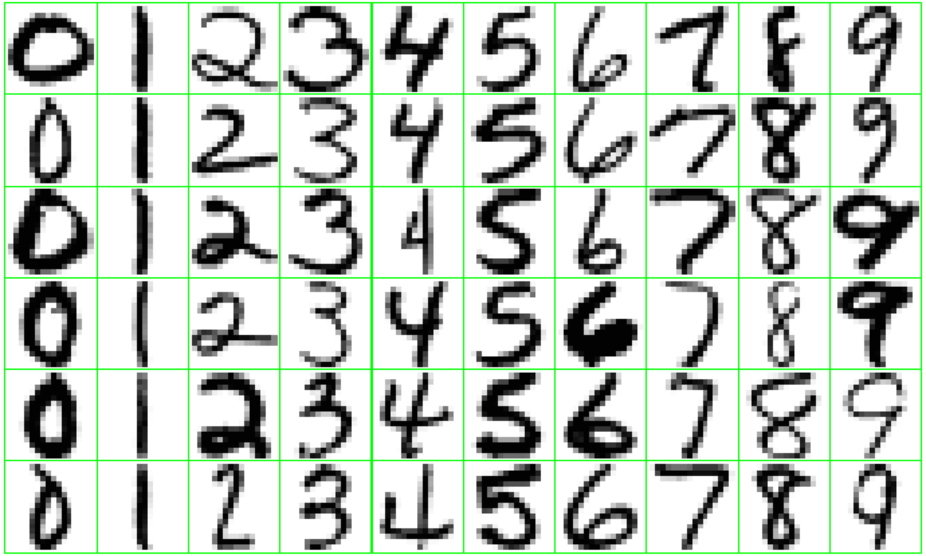
How to estimate $f(x)$?

- 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?

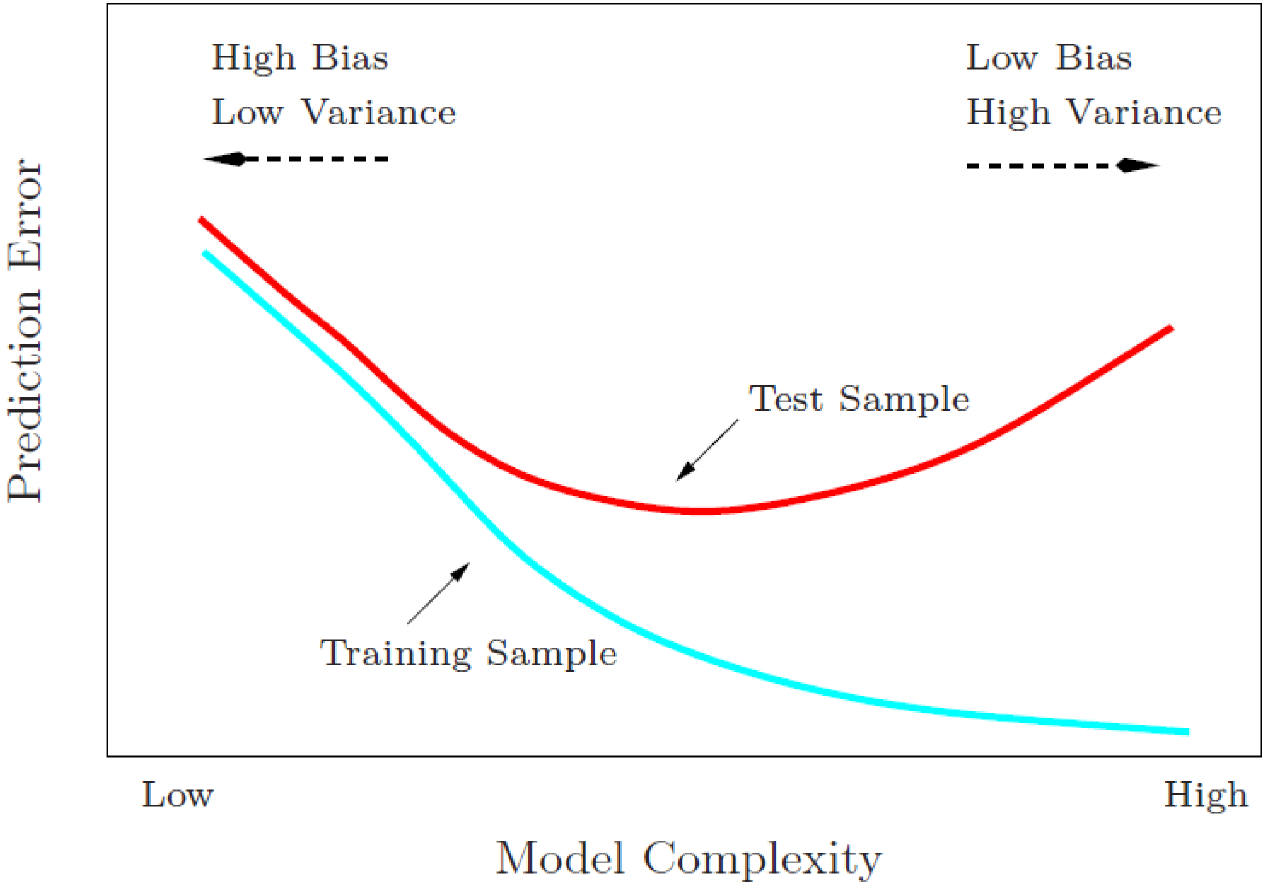
- Which digit?
- Classification!
  - Training set



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
Test Sample
Training Sample
Prediction Error
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

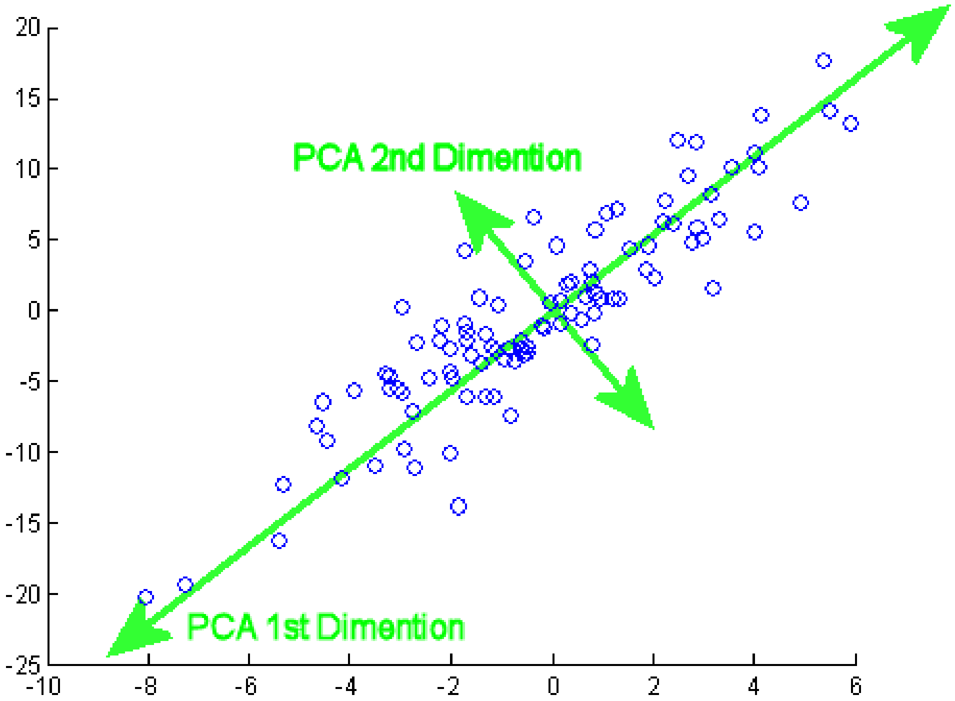
Unsupervised Learning

Clustering

- If no labels are provided
- We learn the clusters

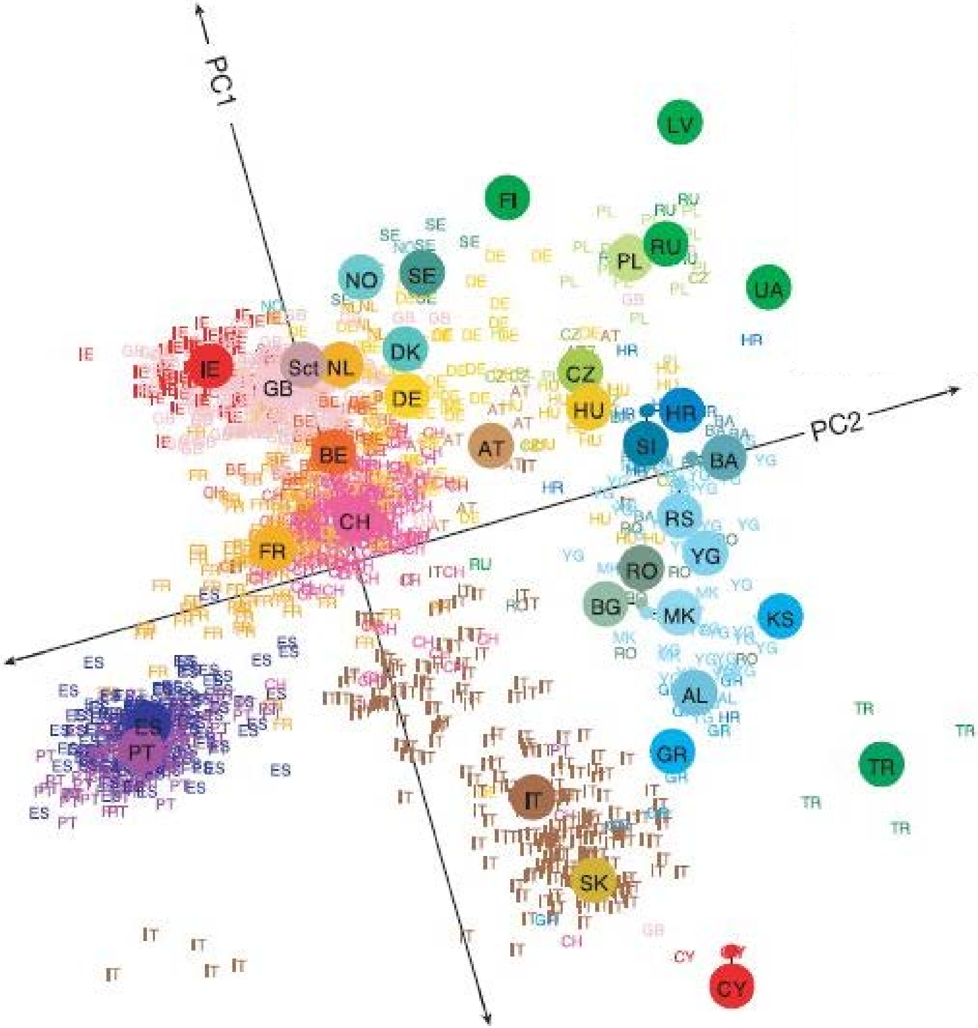
Principal Component Analysis

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



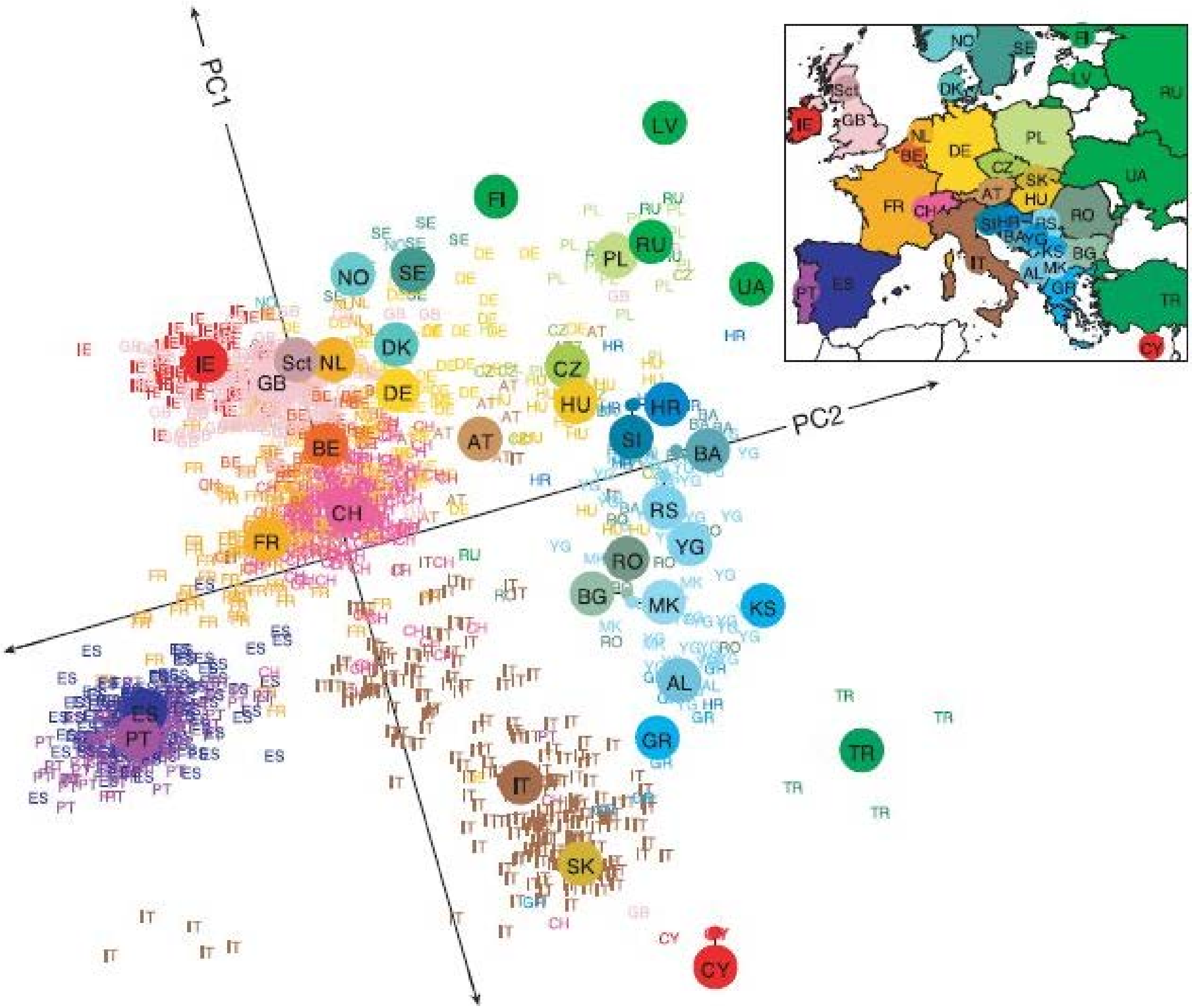
Genes

- PCA


PC1
PC2
LV
FI
UA
RU
PL
NO
SE
DK
CZ
IE
Sct
NL
GB
DE
HU
HR
SI
BA
BE
AT
RS
CH
FR
YG
RO
BG
MK
KS
AL
ES
PT
GR
TR
IT
SK
CY

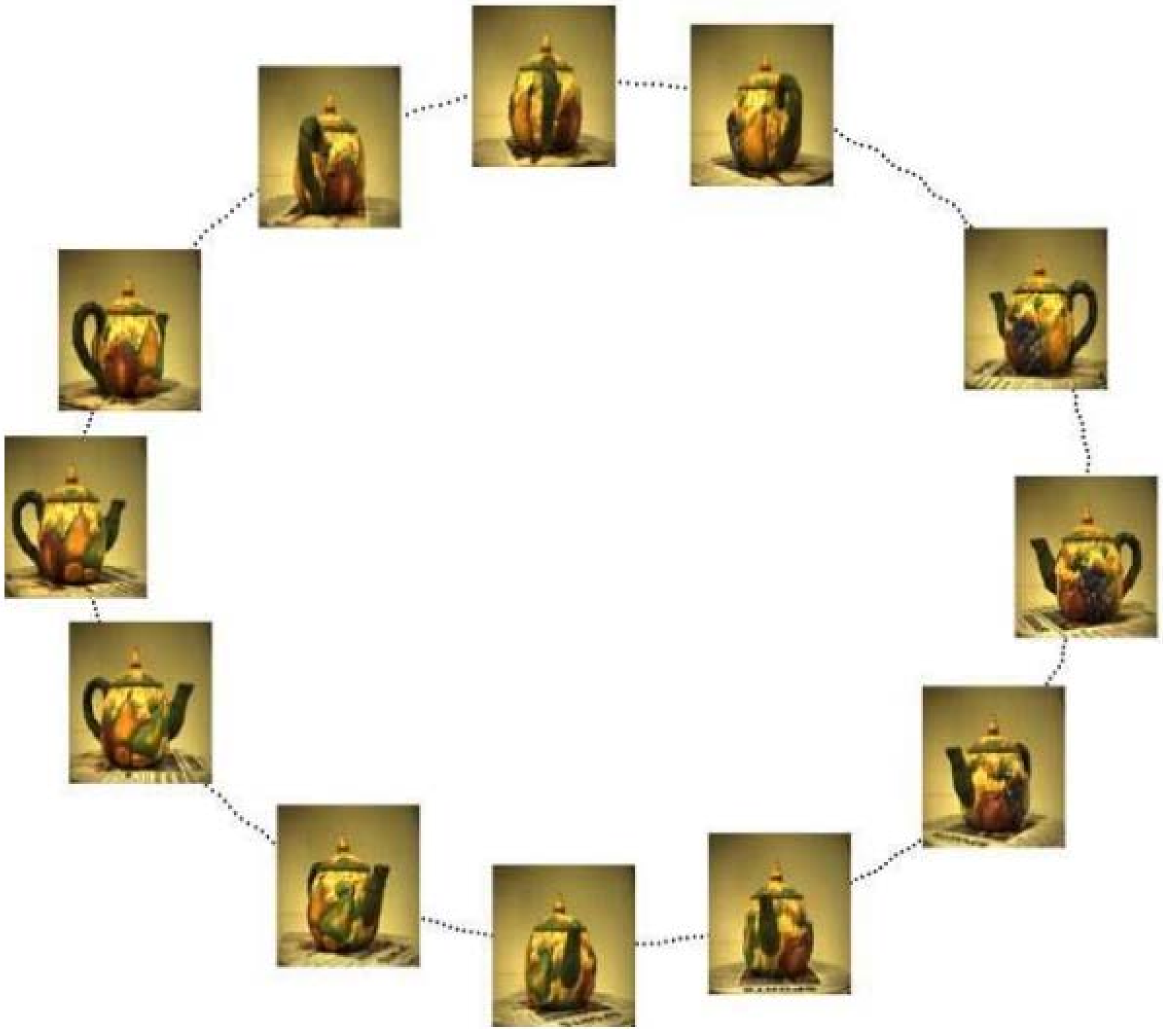
Genes

- PCA
- Map



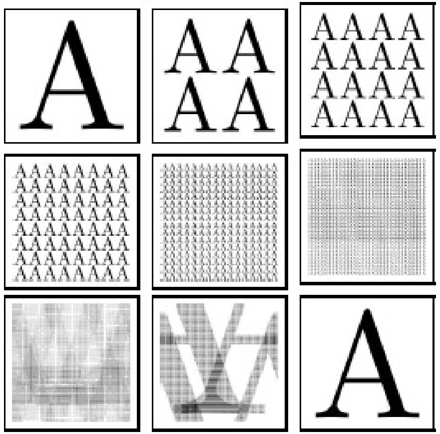
Nonlinear

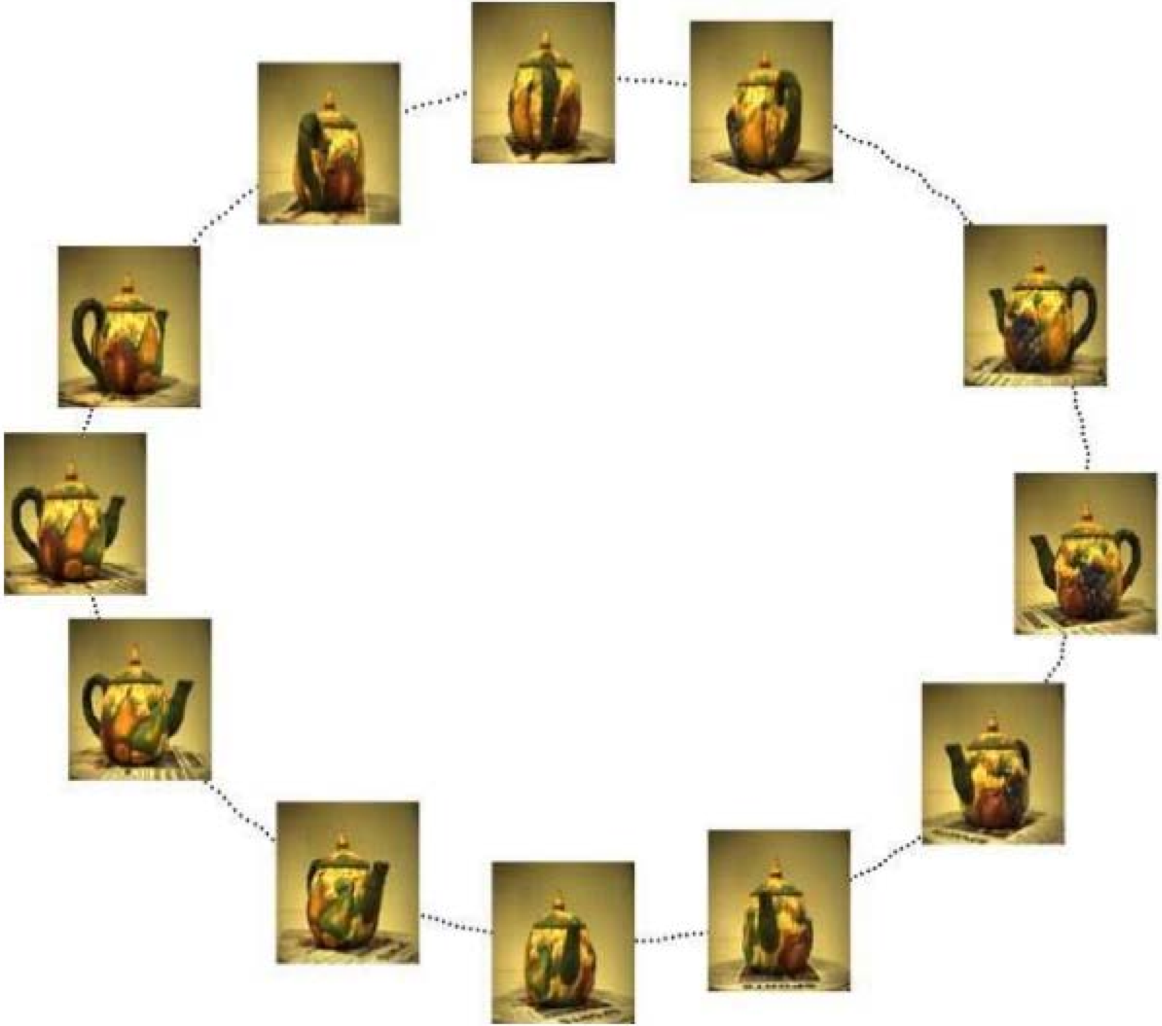
- It’s a rotation!



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

JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING