HT2015: SC4
Statistical Data Mining and Machine Learning

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Department of Statistics
Oxford

http://www.stats.ox.ac.uk/~sejdinov/sdmml.html

Course Information

- Course webpage: http://www.stats.ox.ac.uk/~sejdinov/sdmml.html
- Lecturer: Dino Sejdinovic
- TAs for Part C: Owen Thomas and Helmut Pitters
- TAs for MSc: Konstantina Palla and Maria Lomeli
- Sign up for course using sign up sheets.

Course Structure

Lectures

- 1400-1500 Mondays in Math Institute L4 (weeks 1-4,6-8), L3 (week 5).
- 1000-1100 Wednesdays in Math Institute L3.

Part C:

- 6 problem sheets.
- Due Mondays 10am (weeks 3-8) in 1 South Parks Road (SPR).
- Classes: Tuesdays (weeks 3-8) in 1 SPR Seminar Room.
- Group 1: 3-4pm, Group 2: 4-5pm

MSc:

- 4 problem sheets.
- Due Mondays 10am (weeks 3,5,7,9) in in 1 South Parks Road (SPR).
- Classes: Wednesdays (weeks 3,5,7,9) in 1 SPR Seminar Room.
- Group B: 3-4pm, Group A: 4-5pm.
- Practicals: Fridays, weeks 4 and 8 (assessed) in 1 SPR Computing Lab.
- Group B: 2-4pm, Group A: 4-6pm.

OxWaSP

Oxford-Warwick Centre for Doctoral Training in Next Generation Statistical Science

- Programme aims to produce Europe's future research leaders in statistical methodology and computational statistics for modern applications.
- 10 fully-funded (UK, EU) students a year (1 international).
- Website for prospective students.
- **Deadline: January 23, 2015**

Course Aims

1. Have ability to use the relevant R packages to analyse data, interpret results, and evaluate methods.
2. Have ability to identify and use appropriate methods and models for given data and task.
3. Understand the statistical theory framing machine learning and data mining.
4. Able to construct appropriate models and derive learning algorithms for given data and task.

What is Data Mining?

Oxford Dictionary

The practice of examining large pre-existing databases in order to **generate new information**.

Encyclopaedia Britannica

Also called **knowledge discovery** in databases, in computer science, the process of discovering **interesting and useful patterns and relationships** in large volumes of data.

What is Machine Learning?

Arthur Samuel, 1959

Field of study that gives computers the ability to **learn** without being explicitly programmed.

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Any computer program that **improves its performance** at some task **through experience**.

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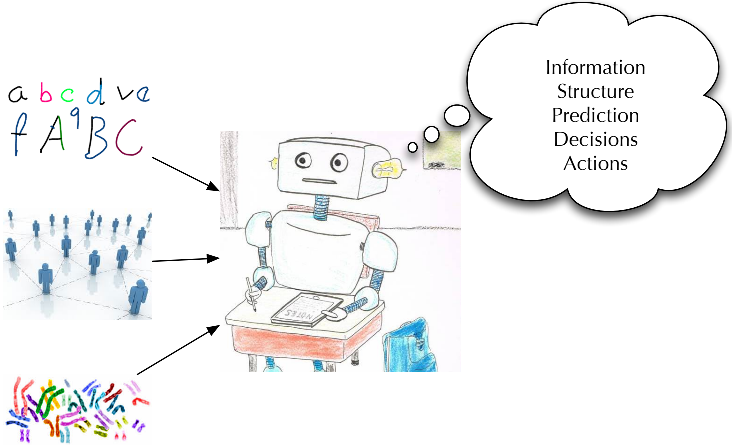
Kevin Murphy, 2012

To develop methods that can **automatically** detect **patterns in data**, and then to use the uncovered patterns to **predict** future data or other outcomes of interest.

What is Machine Learning?



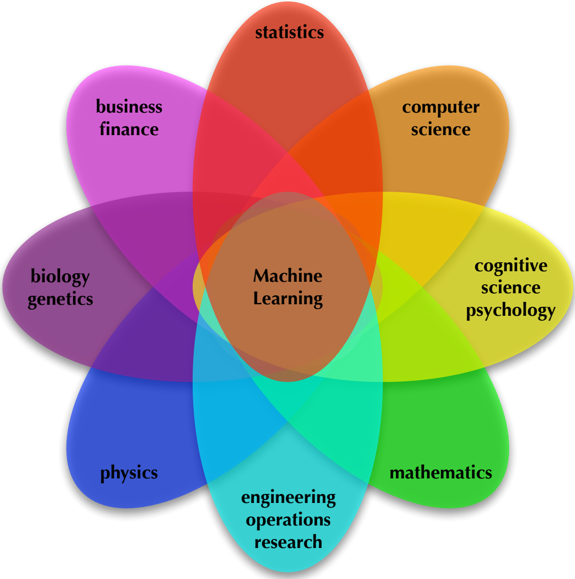
Information
Structure
Prediction
Decisions
Actions

data

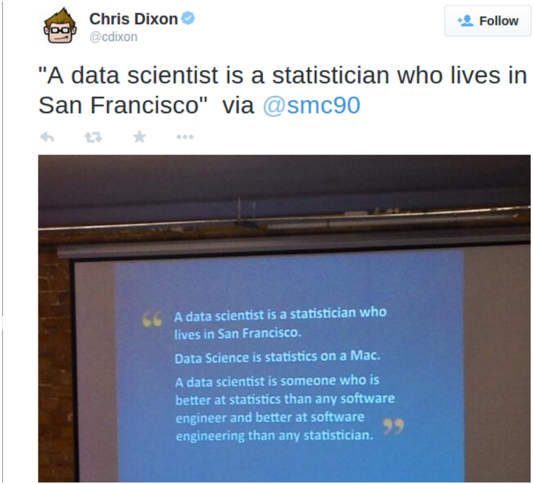
http://gureckislab.org

Larry Page about DeepMind's ML systems that can learn to play video games like humans

What is Machine Learning?



What is Data Science?



Chris Dixon
@cdixon

"A data scientist is a statistician who lives in San Francisco" via @smc90

"A data scientist is a statistician who lives in San Francisco.

Data Science is statistics on a Mac.

A data scientist is someone who is better at statistics than any software engineer and better at software engineering than any statistician."

'Data Scientists' Meld Statistics and Software WSJ article

Information Revolution

Traditional Problems in Applied Statistics

- Well formulated question that we would like to answer.
- Expensive data gathering and/or expensive computation.
- Create specially designed experiments to collect high quality data.

Information Revolution

- Improvements in data processing and data storage.
- Powerful, cheap, easy data capturing.
- Lots of (low quality) data with **potentially valuable** information inside.

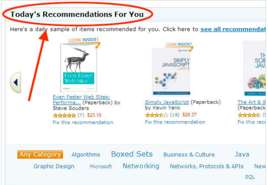
Statistics and Machine Learning in the age of Big Data

- ML becoming a thorough blending of computer science and statistics
- CS and Stats forced **back together**: unified framework of data, inferences, procedures, algorithms
  - statistics taking computation seriously
  - computing taking statistical risk seriously
- scale and granularity of data
- personalization, societal and business impact
- multidisciplinarity - and you are the interdisciplinary glue
- it's just getting started

Michael Jordan: On the Computational and Statistical Interface and "Big Data"

Applications of Machine Learning

spam filtering



Today's Recommendations For You

Here's a daily sample of items recommended for you. Click here to **see all recommendat**

Even Faster Web Sites: Performa... (Paperback) by Steve Souders
★★★★★ (7) $23.10
Fix this recommendation

Simply JavaScript (Paperback) by Kevin Yank
★★★½☆ (19) $26.37
Fix this recommendation

The Art & S
(Paperback
★★★★½ (5
Fix this reco

Any Category Algorithms Boxed Sets Business & Culture Java
Graphic Design Microsoft Networking Networks, Protocols & APIs New
SQL

recommendation systems

fraud detection

self-driving cars

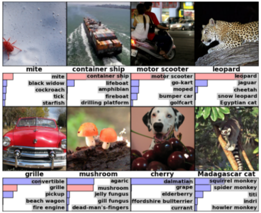


image recognition

stock market analysis

ImageNet: Krizhevsky et al, 2012

Applications of Machine Learning

- Automating employee access control
- Protecting animals
- Predicting emergency room wait times
- Identifying heart failure
- Predicting strokes and seizures
- Predicting hospital readmissions

Machine Learning is Eating the World: Forbes article

Types of Machine Learning

Supervised learning

- Data contains “labels”: every example is an input-output pair
- classification, regression
- Goal: **prediction on new examples**

Unsupervised learning

- Extract key features of the “unlabelled” data
- clustering, signal separation, density estimation
- Goal: **representation, hypothesis generation, visualization**

Types of Machine Learning

Semi-supervised Learning

A database of examples, only a small subset of which are labelled.

Multi-task Learning

A database of examples, each of which has multiple labels corresponding to different prediction tasks.

Reinforcement Learning

An agent acting in an environment, given rewards for performing appropriate actions, learns to maximize their reward.

Exploratory Data Analysis

Exploratory Data Analysis

Notation

- Data consists of p measurements (variables/attributes) on n examples (observations/cases)
- $\mathbf{X}$ is a $n \times p$-matrix with $\mathbf{X}_{ij} :=$ the j-th measurement for the i-th example

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1j} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2j} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{i1} & x_{i2} & \dots & x_{ij} & \dots & x_{ip} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nj} & \dots & x_{np} \end{bmatrix}$$

- Denote the ith data item by $x_i \in \mathbb{R}^p$. (This is transpose of ith row of $\mathbf{X}$)
- Assume $x_1, \dots, x_n$ are **independently and identically distributed** samples of a **random vector** X over $\mathbb{R}^p$.

Crabs Data ($n = 200$, $p = 5$)

Campbell (1974) studied rock crabs of the genus **leptograpsus**. One species, **L. variegatus**, had been split into two new species, previously grouped by colour: orange and blue. Preserved specimens lose their colour, so it was hoped that morphological differences would enable museum material to be classified.

Data are available on 50 specimens of each sex of each species, Each specimen has measurements on:

- the width of the frontal lobe `FL`,
- the rear width `RW`,
- the length along the carapace midline `CL`,
- the maximum width `CW` of the carapace, and
- the body depth `BD` in mm.

in addition to colour (species) and sex.

photo from: inaturalist.org

Crabs Data

```
## load package MASS containing the data
library(MASS)

## look at raw data
crabs

## create a combined species+sex field
crabs$spsex=paste(crabs$sp,crabs$sex,sep="")

## assign predictor and class variables
varnames<-c(’FL’,’RW’,’CL’,’CW’,’BD’)
Crabs <- crabs[,varnames]
Crabs.class <- factor(crabs$spsex)

## various plots
boxplot(Crabs)
...
```

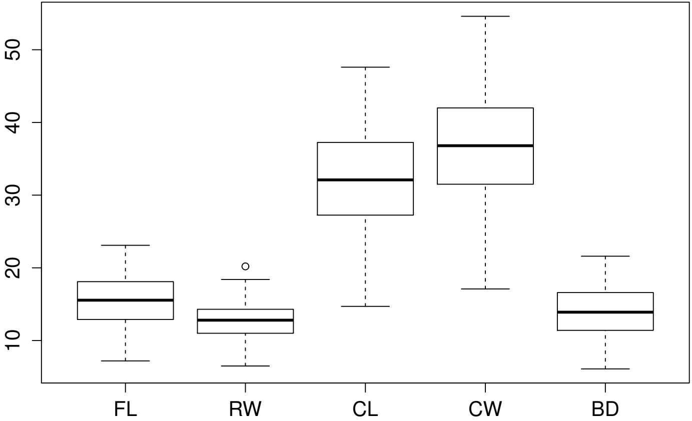
Crabs Data

```
## look at raw data
crabs
```

```
     sp sex  index FL   RW   CL   CW   BD
1    B   M     1  8.1  6.7 16.1 19.0  7.0
2    B   M     2  8.8  7.7 18.1 20.8  7.4
3    B   M     3  9.2  7.8 19.0 22.4  7.7
4    B   M     4  9.6  7.9 20.1 23.1  8.2
5    B   M     5  9.8  8.0 20.3 23.0  8.2
6    B   M     6 10.8  9.0 23.0 26.5  9.8
7    B   M     7 11.1  9.9 23.8 27.1  9.8
8    B   M     8 11.6  9.1 24.5 28.4 10.4
9    B   M     9 11.8  9.6 24.2 27.8  9.7
10   B   M    10 11.8 10.5 25.2 29.3 10.3
11   B   M    11 12.2 10.8 27.3 31.6 10.9
12   B   M    12 12.3 11.0 26.8 31.5 11.4
13   B   M    13 12.6 10.0 27.7 31.7 11.4
14   B   M    14 12.8 10.2 27.2 31.8 10.9
15   B   M    15 12.8 10.9 27.4 31.5 11.0
16   B   M    16 12.9 11.0 26.8 30.9 11.4
17   B   M    17 13.1 10.6 28.2 32.3 11.0
18   B   M    18 13.1 10.9 28.3 32.4 11.2
19   B   M    19 13.3 11.1 27.8 32.3 11.3
20   B   M    20 13.9 11.1 29.2 33.3 12.1
```

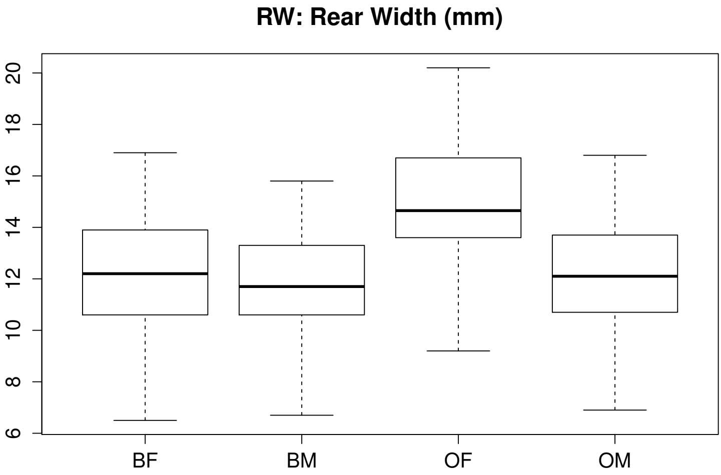
Univariate Boxplots

```
boxplot(Crabs)
```



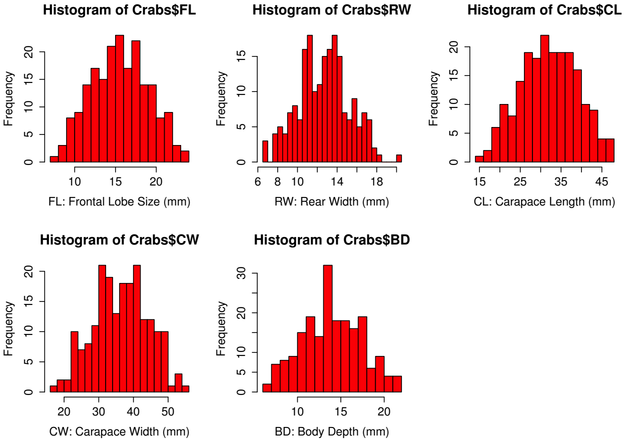
Univariate Boxplots

```
boxplot(RW~spsex,data=crabs); title('RW: Rear Width (mm)')
```



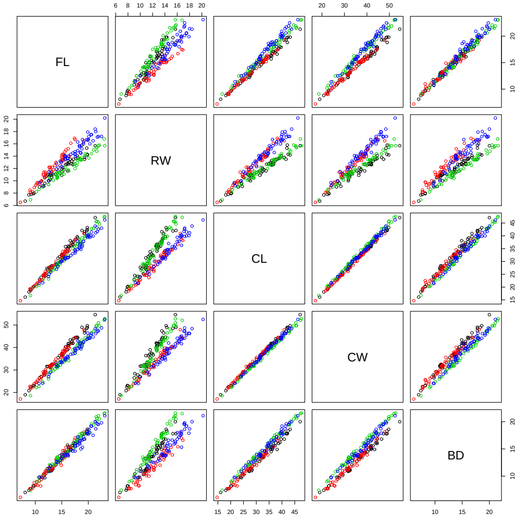
Univariate Histograms

```
par(mfrow=c(2,3))
hist(Crabs$FL,col='red',breaks=20,xlab='FL: Frontal Lobe Size (mm)')
hist(Crabs$RW,col='red',breaks=20,xlab='RW: Rear Width (mm)')
hist(Crabs$CL,col='red',breaks=20,xlab='CL: Carapace Length (mm)')
hist(Crabs$CW,col='red',breaks=20,xlab='CW: Carapace Width (mm)')
hist(Crabs$BD,col='red',breaks=20,xlab='BD: Body Depth (mm)')
```



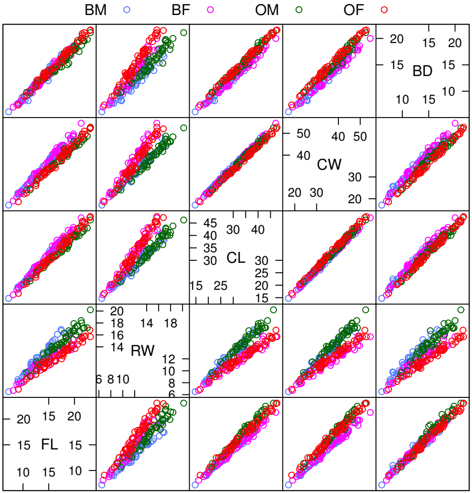
Simple Pairwise Scatterplots

```
pairs(Crabs,col=unclass(Crabs.class))
```



Simple Pairwise Scatterplots

```
require(lattice)
splom(~ Crabs, groups = unclass(Crabs.class), key = list( columns = 4,
  text = list(c("BM", "BF", "OM", "OF")),
  points = Rows(trellis.par.get("superpose.symbol"), 1:4) ) )
```



Visualization and Dimensionality Reduction

The summary plots are helpful, but do not help if the dimensionality p is high (a few dozens or even thousands). Visualizing higher-dimensional problems:

- We are constrained to view data in 2 or 3 dimensions
- Approach: look for 'interesting' projections of $\mathbf{X}$ into lower dimensions
- Hope that even though p is large, considering only carefully selected $k \ll p$ dimensions is just as informative.

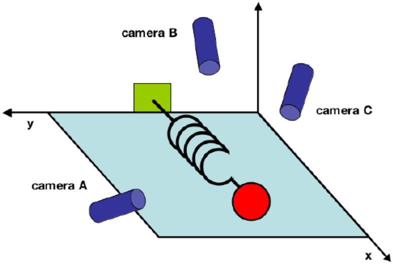
Dimensionality reduction

- For each data item $x_i \in \mathbb{R}^p$, find its lower dimensional representation $z_i \in \mathbb{R}^k$ with $k \ll p$.
- Map $x \mapsto z$ should preserve the **interesting statistical properties** in data.

Dimensionality Reduction

Dimensionality reduction

- deceptively many variables to measure, many of them redundant (large p)
- often, there is a simple but unknown underlying relationship hiding
- example: ball on a frictionless spring recorded by three different cameras
    - our imperfect measurements obfuscate the true underlying dynamics
    - are our coordinates meaningful or do they simply reflect the method of data gathering?



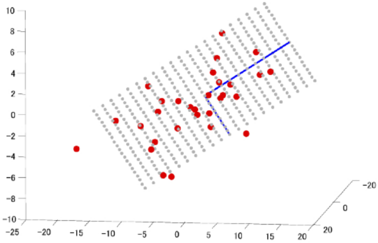
J. Shlens, A Tutorial on Principal Component Analysis, 2005

Principal Components Analysis (PCA)

- PCA considers interesting directions to be those with greatest **variance**.
- A **linear** dimensionality reduction technique: looks for a **new basis** to represent a noisy dataset.
- Workhorse for many different types of data analysis.
- Often the first thing to run on high-dimensional data.

Principal Components Analysis (PCA)

- For simplicity, we will assume from now on that our dataset is centred, i.e., we subtract the average $\bar{x}$ from each x_i.



PCA

Find an orthogonal basis $v_1, v_2, \ldots, v_p$ for the data space such that:

- The first principal component (PC) v_1 is the **direction of greatest variance** of data.
- The j-th PC v_j is the **direction orthogonal to** $v_1, v_2, \ldots, v_{j-1}$ **of greatest variance**, for $j = 2, \ldots, p$.

Principal Components Analysis (PCA)

- The k-dimensional representation of data item x_i is the vector of projections of x_i onto first k PCs:

$$z_i = V_{1:k}^\top x_i = \left[v_1^\top x_i, \ldots, v_k^\top x_i\right]^\top \in \mathbb{R}^k,$$

  where $V_{1:k} = [v_1, \ldots, v_k]$
- Reconstruction of x_i:

$$\hat{x}_i = V_{1:k} V_{1:k}^\top x_i.$$

- PCA gives the **optimal linear reconstruction** of the original data based on a k-dimensional compression (exercises).

Principal Components Analysis (PCA)

- Our data set is an i.i.d. sample $\{x_i\}_{i=1}^n$ of a random vector $X = \left[X^{(1)} \dots X^{(p)}\right]^\top$.
- For the 1^{st} PC, we seek a derived scalar variable of the form

$$Z^{(1)} = v_1^\top X = v_{11}X^{(1)} + v_{12}X^{(2)} + \cdots + v_{1p}X^{(p)}$$

  where $v_1 = [v_{11}, \dots, v_{1p}]^\top \in \mathbb{R}^p$ are chosen to maximise

$$\mathrm{Var}(Z^{(1)}).$$

- The 2^{nd} PC is chosen to be orthogonal with the 1^{st} and is computed in a similar way. It will have the largest variance in the remaining $p-1$ dimensions, etc.

Deriving the First Principal Component

- for any fixed v_1,

$$\mathrm{Var}(Z^{(1)}) = \mathrm{Var}(v_1^\top X) = v_1^\top \,\mathrm{Cov}(X) v_1.$$

- we do not know the **true** covariance matrix $\mathrm{Cov}(X)$, so need to replace with the sample covariance matrix, i.e.

$$S = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})^\top = \frac{1}{n-1}\sum_{i=1}^{n} x_i x_i^\top = \frac{1}{n-1}\mathbf{X}^\top\mathbf{X}.$$

- with no restriction on the norm of v_1, $\mathrm{Var}(Z^{(1)})$ grows without a bound: need constraint $v_1^\top v_1 = 1$, giving

$$\max_{v_1} \; v_1^\top S v_1$$

subject to: $v_1^\top v_1 = 1$.

Deriving the First Principal Component

- Lagrangian of the problem is given by:

$$\mathcal{L}\left(v_1, \lambda_1\right) = v_1^\top S v_1 - \lambda_1 \left(v_1^\top v_1 - 1\right).$$

- The corresponding vector of partial derivatives is

$$\frac{\partial \mathcal{L}(v_1, \lambda_1)}{\partial v_1} = 2Sv_1 - 2\lambda_1 v_1.$$

- Setting this to zero reveals the eigenvector equation $Sv_1 = \lambda_1 v_1$, i.e. v_1 must be an eigenvector of S and the dual variable λ_1 is the corresponding eigenvalue.
- Since $v_1^\top S v_1 = \lambda_1 v_1^\top v_1 = \lambda_1$, the first PC must be the eigenvector associated with the largest eigenvalue of S.

Properties of the Principal Components

- Derived scalar variable (projection to the j-th principal component) $Z^{(j)} = v_j^\top X$ has sample variance λ_j, for $j = 1, \ldots, p$
- S is a real symmetric matrix, so eigenvectors (principal components) are orthogonal.
- Projections to principal components are **uncorrelated**: $\mathrm{Cov}(Z^{(i)}, Z^{(j)}) \approx v_i^\top S v_j = \lambda_j v_i^\top v_j = 0$, for $i \neq j$.
- The **total sample variance** is given by $\sum_{i=1}^{p} S_{ii} = \lambda_1 + \ldots + \lambda_p$, so the **proportion of total variance explained** by the j^{th} PC is $\frac{\lambda_j}{\lambda_1+\lambda_2+\ldots+\lambda_p}$

R code

This is what we have had before:

```
> library(MASS)
> crabs$spsex=paste(crabs$sp,crabs$sex,sep="")
> varnames<-c(’FL’,’RW’,’CL’,’CW’,’BD’)
> Crabs <- crabs[,varnames]
> Crabs.class <- factor(crabs$spsex)
> pairs(Crabs,col=unclass(Crabs.class))
```

Now perform PCA with function `princomp`.
(Alternatively, solve for the PCs yourself using `eigen` or `svd`)

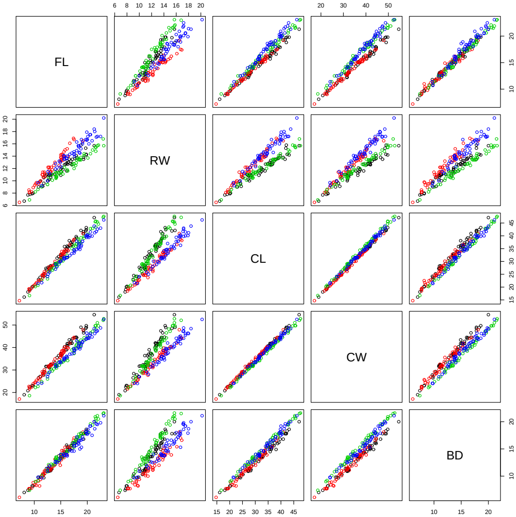
```
> Crabs.pca <- princomp(Crabs,cor=FALSE)
> summary(Crabs.pca)
> pairs(predict(Crabs.pca),col=unclass(Crabs.class))
```

Exploring PCA output

```
> Crabs.pca <- princomp(Crabs,cor=FALSE)
> summary(Crabs.pca)

Importance of components:
                          Comp.1      Comp.2      Comp.3       Comp.4       Comp.5
Standard deviation     11.8322521 1.135936870 0.997631086 0.3669098284 0.2784325016
Proportion of Variance  0.9824718 0.009055108 0.006984337 0.0009447218 0.0005440328
Cumulative Proportion   0.9824718 0.991526908 0.998511245 0.9994559672 1.0000000000

> loadings(Crabs.pca)

Loadings:
   Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
FL -0.289 -0.323  0.507  0.734  0.125
RW -0.197 -0.865 -0.414 -0.148 -0.141
CL -0.599  0.198  0.175 -0.144 -0.742
CW -0.662  0.288 -0.491  0.126  0.471
BD -0.284 -0.160  0.547 -0.634  0.439
```

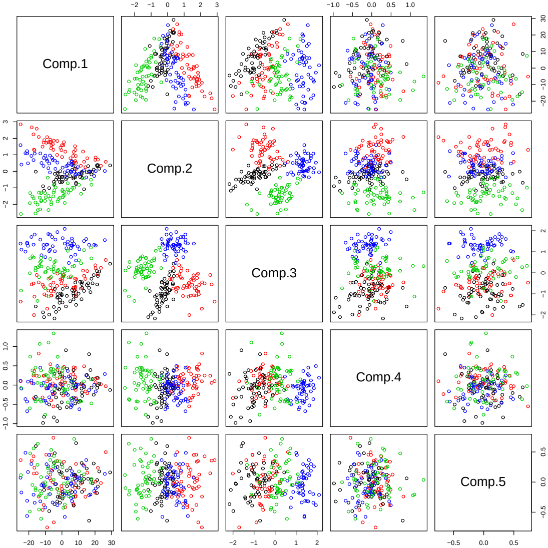
Raw Crabs Data

```
> pairs(Crabs,col=unclass(Crabs.class))
```



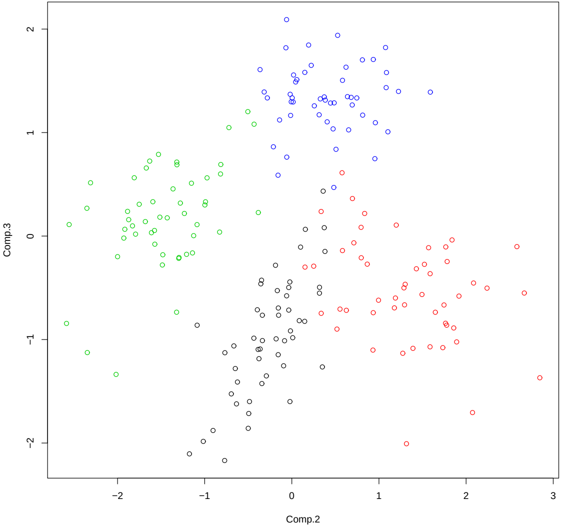
PCA of Crabs Data

```
> Crabs.pca <- princomp(Crabs,cor=FALSE)
> pairs(predict(Crabs.pca),col=unclass(Crabs.class))
```

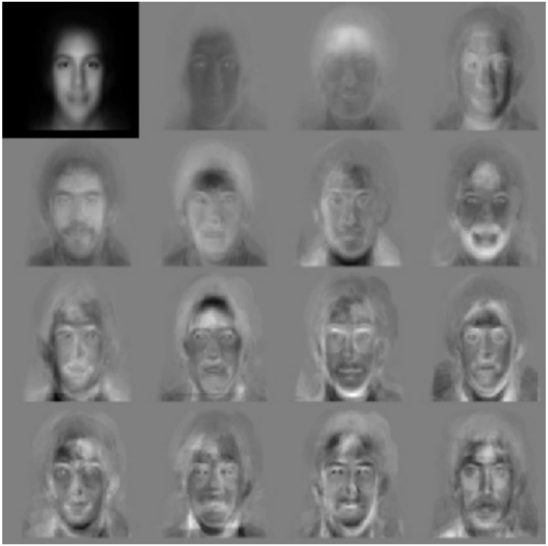


PC 2 vs PC 3

```
> Z<-predict(Crabs.pca)
> plot(Comp.3~Comp.2,data=Z,col=unclass(Crabs.class))
```

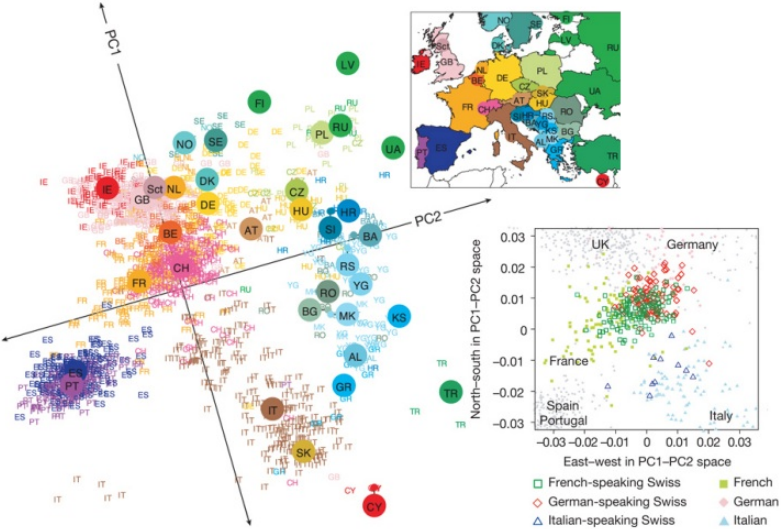


PCA on Face Images



http://vismod.media.mit.edu/vismod/demos/facerec/basic.html

PCA on European Genetic Variation



http://www.nature.com/nature/journal/v456/n7218/full/nature07331.html

Comments on the use of PCA

- PCA commonly used to project data X onto the first k PCs giving the k-dimensional view of the data that best preserves **the first two moments**.
- Although PCs are uncorrelated, scatterplots sometimes reveal structures in the data other than linear correlation.
- Emphasis on variance is where the weaknesses of PCA stem from:
    - Assuming large variances are meaningful (high signal-to-noise ratio)
    - The PCs depend heavily on the units measurement. Where the data matrix contains measurements of vastly differing orders of magnitude, the PC will be greatly biased in the direction of larger measurement. In these cases, it is recommended to calculate PCs from $\mathrm{Corr}(X)$ instead of $\mathrm{Cov}(X)$ (`cor=True` in the call of `princomp`).
    - Lack of robustness to outliers: variance is affected by outliers and so are PCs.