## MATH 567: Mathematical Techniques in Data Science Overview

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- Course website: http://www.math.udel.edu/~dguillot/ (Just google "Dominique Guillot")
- Slides will be posted in advance (will do my best).
- Textbook: An Introduction to Statistical Learning
by James, Witten, Hastie, and Tibshirani (50-75\$).
Free pdf: http://www-bcf.usc.edu/ gareth/ISL/.
- Watch for reading material on the course website (mandatory).
- We will have a lab most Wednesdays (mandatory, some will count for credits). Bring your laptop. People who are auditing the class are expected to participate.
- Teamwork is encouraged. Keep in mind, however, that you will be alone during the exams (a large part of them will involve programming/numerical work).


## Supervised vs unsupervised learning

Statistical learning: learn from a (usually large, but possibly small) number of observations.
Supervised learning: outcome variable to guide the learning process

- Set of input variables (predictors, independent variables).
- Set of output variables (response, dependent variables).
- Want to use the input to predict the output.
- Data is labelled.

Unsupervised learning: we observe only the features and have no measurements of the outcome.

- Only have features.
- Data is unlabelled.
- Want to detect structure, patterns, etc.

Note: output can be continuous (regression) or discrete (classification).

## Examples

- Handwritten digits

$$
\begin{aligned}
& 00000000000000000000 \\
& 1111111111111111111111 \\
& 222222222222222222232 \\
& 33333333333333343333 \\
& 44444444444444444444 \\
& 55555555555555555555 \\
& 66666666666666666666 \\
& 77777777777777777547 \\
& 88888888888889888884 \\
& 19999999499994999994
\end{aligned}
$$

- You are provided a dataset containing images ( $16 \times 16$ grayscale images say) of digits.
- Each image contains a single digit.
- Each image is labelled with the corresponding digit.
- Can think of each image as a vector in $X \in \mathbb{R}^{256}$ and the label as a scalar $Y \in\{0, \ldots, 9\}$.
- Idea: with a large enough sample, we should be able to learn to identify/predict digits.

Gene expression data: rows $=$ genes, columns $=$ sample.


- DNA microarrays measure the expression of a gene in a cell.
- Nucleotide sequences for a few thousand genes are printed on a glass slide.
- Each "spot" contains millions of identical molecules which will bind a specific DNA sequence.
- A target sample and a reference sample are labeled with red and green dyes, and each are hybridized with the DNA on the slide.
- Through fluoroscopy, the $\log$ (red/green) intensities of RNA hybridizing at each site is measured.

Question: do certain genes show very high (or low) expression for certain cancer samples?

## Examples (cont.)

## Inferring the climate of the past:

- We have about 150 years of instrumental temperature data.
- Many things on Earth (proxies) record temperature indirectly (e.g. tree rings width, ice cores, sediments, corals, etc.).
- Want to infer the climate of the past from overlapping measurements.

- Information from 4601 email messages, in a study to screen email for "spam" (i.e., junk email).
- Data donated by George Forman from Hewlett-Packard laboratories.

$$
\begin{aligned}
& \text { TABLE 1.1. Averge perentage of words or characters in an email measage } \\
& \begin{array}{l}
\text { equal to the indeated word or charater. We haze chasen } \\
\text { showing the hergest difference betuken apasa and ena il. }
\end{array}
\end{aligned}
$$

$$
\begin{aligned}
& \begin{array}{lllllllllllll} 
& \text { paril } & 1.27 & 1.27 & 0.44 & 0.90 & 0.52 & 0.01 & 0.07 & 0.43 & 0.11 & 0.51 & 0.13 \\
\hline 0.42 & 0.01 & 0.28 \\
\hline
\end{array} \\
& \text { ESL, Table } 1.1
\end{aligned}
$$

- Each message is labelled as spam/email.
- Want to predict the label using characteristics such as word counts.
- Which words or characters are good predictors?

Note: labelling data can be very tedious/expensive. Not always available.

## Examples (cont.)

## Clustering:



- Unsupervised problem.
- Work only with features/independent variables.
- Want to label points according to a measure of their similarity.

In modern problems:

- Dimension $p$ is often very large.
- Sample size $n$ is often very small compared to $p$.

In classical statistics:

- It is often assumed a lot of samples are available.
- Most results are asymptotic $(n \rightarrow \infty)$.
- Generally not the right setup for modern problems.

How do we deal with the $p \gg n$ case?

## The $p \gg n$ case: sparsity

- A modern approach to deal with the $p \gg n$ case is to assume some form of sparsity inside the problem.


## Examples:

- Predict if a person has a disease $Y=0,1$ given its gene expression data $X \in \mathbb{R}^{p}$ with $p$ large. Probably only a few genes are useful to make the prediction.
- The spam data: many of the English words are probably not useful to predict spam. A small (but unknown) set of words should be enough (e.g. "win", "free", "!!!", "money", etc.).
- Climate reconstructions: large number of grid points, few annual observations. Can exploit conditional independence relations within the data.


## The curse of dimensionality

- Consider a hypercube with sides of length $c$ along the axes in a unit hypercube. Its volume is $c^{p}$. To capture a fraction $r$ of the unit hypercube:

$$
c^{p}=r
$$

Thus, $c=r^{1 / p}$.

- A small sample of points in the hypercube will not cover a lot of the space.
- If $p=10$, in order to capture $10 \%$ of the volume, we need $c \approx 0.8$ !



ESL, Figure 2.6 .

## The $p \gg n$ case: sparsity

A linear regression problem: suppose we try to use linear regression to estimate $Y$ (response) using $X$ (predictors)

$$
Y=\beta_{1} X_{1}+\cdots+\beta_{p} X_{p}+\epsilon
$$

- Classical statistical theory guarantees (under certain hypotheses) that we can recover the regression coefficients $\beta$ if $n$ is large enough (consistency).
- In modern problems $n / p$ is often small.
- What if we assume only a small percentage of the "true" coefficients are nonzero?
- Obtain consistency results when $p, n \rightarrow \infty$ with $n / p=$ constant .
- How do we identify the "right" subset of predictors?
- We can't examine all the $\binom{p}{k}$ possibilities! For example, $\binom{1000}{25} \approx 2.7 \times 10^{49!}$

We will use $\mathbf{R}$ to program, analyse data, etc. during the semester.


- Free. Open-source.
- Interpreted.
- A LOT of statistical packages.

If you have used Python or Matlab before:
http://mathesaurus. sourcef orge.net/octave-r.html http://mathesaurus.sourceforge.net/r-numpy .html

Get started with R :

- Download R at:
https://cran.r-project.org/
- Download RStudio (free version):
https://www.rstudio.com/products/rstudio/download/
- Install the packages ISLR and MASS. (Tools/Install packages... in RStudio)
- Tutorial:
http://tryr.codeschool.com
Do (at least) the first 3 parts before the class on Wednesday. Reading: Chapter 1 of the book.

