# STA 437/2005:
# Methods for Multivariate Data

## Week 1: Introduction and Preliminaries

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# What is this class about?

# Multivariate datasets

- Modern datasets are high-dimensional and highly unstructured.
- This means that we simultaneously observe many correlated features.
- Modelling them independently is both *wasteful* and statisticallly...
- The problem is that our intuition works well only in 1D-3D.

# This course

- Discuss some classical and more modern methods for multivariate datasets.
- Build math toolbox that gives deeper understanding for these methods.
- Aimed at advanced undergrad and master level graduate students.
- 2 hrs lecture + 1 hour tutorial to get more hands-on experience.
- We will use a lot of real analysis, probability, and linear algebra.
  - To large extend I am assuming you are comfortable with basic matrix algebra.

# Administrative details

# Course Information

Course Website: `https://pzwiernik.github.io/sta437/`

Main source of information is the course webpage; check regularly!

We will also use Quercus for **announcements & grades etc**.

- You received an announcement on Sunday.

We will use Piazza for **discussions**.

- Sign up via quercus or:
  `https://piazza.com/utoronto.ca/winter2024/sta414`
- Your grade **does not depend on your participation on Piazza**.
- We only allow questions that are related to the course materials/assignments/exams.

# Course Information

- This course have two *identical* sections:
  - Section 1: Wed 9-11am (tutorial Fri 9-10am)
  - Section 2: Wed 1-3pm (tutorial Fri 1-2pm)
- You are welcome to attend either one of the sections.
- Instructor office hours are Monday 2pm-3:30pm, UY 9040.
- TA office hours will be announced later.
- Questions during lectures/tutorials are always welcome!

# Course Information

- While cell phones and other electronics are not prohibited, talking, recording or taking pictures in class is prohibited without the consent of your instructor.
- Lecture slides and notes will be posted on the course webpage. Please do let me know about typos you notice and/or any suggestions you might have.
- For accessibility services: If you require additional academic accommodations, please contact UofT Accessibility Services as soon as possible, `studentlife.utoronto.ca/as`. No last minute arrangements will be considered.

# Literature

This course is not following any particular book.

Recommended readings will be given for each lecture. The following will be useful throughout the course:

- Mardia, Kent, Bibby (1979), *Multivariate Analysis*.
- Everitt, Hothorn (2011), *An Introduction to Applied Multivariate Analysis with R*.
- Holms, Huber (2023), *Modern Statistics for Modern Biology*.

Use Appendix A in [MKB] as reference for matrix algebra. Some other books

mentioned on the website.
There are lots of freely available, high-quality resources online.

# Requirements and Marking

Ask Xin how this goes.

- 10 quizes (in the end of the lecture)
  - Combination of pen & paper derivations and coding exercises
  - Equally weighted for a total of 30%
- Midterm
  - 26/27 February (tentative)
  - 2 hours
  - Worth 30% of course mark
- Final Exam (In-Person)
  - $\sim$ 2-3 hours
  - Date and time TBA
  - Worth 40% of course mark
- Exam questions are conceptual/theoretical; no coding.
- Everybody must take the final exam! No exceptions.

# More on tutorials

- The goal is to get a more hands-on experience with the presented methods.
- We will be using `R` but the TAs can also help in Python if needed.
- Extensions will be granted only in special situations, and you will need to fill out absence declaration form and **inform the instructor** or have documentation from the accessibility services.
- You will be using Python and Numpy on assignments.

# Related Courses

- STA314 and CSC311: Intro ML (overlap with clustering)
- STA414/2104: More advanced ML (overlap with graphical models)
- STA302: Linear regression and classical statistics
- CSC2515: Advanced CSC311
- CSC2532: Learning theory - Focus on mathematics of ML
- Various topics and seminar style courses offered at DoSS and DCS

# Provisional Calendar (tentative)

**I. Introduction and preliminaries**

week 1, Jan 8/9:

- Introduction, graphics, preliminaries.

**II. Multivariate Gaussian distribution and Multivariate Inference**

week 2, Jan 15/16:

- Multivariate Normal distribution
- Wishart distribution, Hotelling's T-squared test

**III. Dimensionality reduction techniques (based on geometry)**

week 3, Jan 22/23:

- SVD, Spectrum of a symmetric matrix
- Principal Component Analysis

# Provisional Calendar (cont'ed)

week 4, Jan 29/30:

- Canonical Correlation Analysis (CCA)
- UMAP

week 5, Feb 5/6:

- Quick primer in neural nerworks
- Autoencoders, Sparse Autoencoders

**IV. Advanced Classification and Clustering Methods**

week 6, Feb 12/13:

- Linear Discriminant Analysis, Gaussian mixtures, k-means
- hierarchical clustering

week 7: Reading week

# Provisional Calendar (cont'ed)

week 8, Feb 26/27:

- Midterm exam on Feb 27/28

**V. Dimensionality reduction techniques (based on probability)**

week 9, Mar 4/5:

- Probabilistic PCA
- Factor Analysis

week 10, Mar 11/12:

- Gaussian graphical models, Graphical LASSO
- Linear Structural Equation Models

week 11, Mar 18/19:

- Shrinkage estimation

**V. Tensor data**

# Introduction to multivariate statistics

# Multivariate data

- Many datasets consist of several variables measured on the same set of subjects: patients, samples, users, or organisms.
- Goal: investigation of connections or associations between the different variables measured.
- Usually the data are reported in a tabular data structure with one row for each subject and one column for each variable.

**Example**

Studying the expression of 25,000 gene (columns) on many samples (rows) of patient-derived cells, we notice that many of the genes act together, either that they are positively correlated or that they are anti-correlated. We would miss a lot of important information if we were to only study each gene separately.

# Example 1: Decathlon

The columns are a subset of gene expression measurements, they correspond to 156 genes that show differential expression between cell types:

```
> data("olympic", package = "ade4")
> athletes = setNames(olympic$tab,
+   c("m100", "long", "weight", "high", "m400", "m110", "disc", "pole", "javel", "m1500"))
> head(athletes)

   m100 long weight high  m400  m110  disc pole javel  m1500
1 11.25 7.43  15.48 2.27 48.90 15.13 49.28  4.7 61.32 268.95
2 10.87 7.45  14.97 1.97 47.71 14.46 44.36  5.1 61.76 273.02
3 11.18 7.44  14.20 1.97 48.29 14.81 43.66  5.2 64.16 263.20
4 10.62 7.38  15.02 2.03 49.06 14.72 44.80  4.9 64.04 285.11
5 11.02 7.43  12.92 1.97 47.44 14.40 41.20  5.2 57.46 256.64
6 10.83 7.72  13.58 2.12 48.34 14.18 43.06  4.9 52.18 274.07
```

# Example 2: Star Wars

The Star Wars dataset comes from the dplyr package. It describes 13 charac- teristics of 87 characters from the Star Wars universe.

```
> data("starwars", package = "dplyr")
> head(starwars[,c(1,2,3,5,6,7,8,11)])
```

| | name | height | mass | skin_color | eye_color | birth_year | sex | species |
|---|---|---|---|---|---|---|---|---|
| 1 | Luke Skywalker | 172 | 77 | fair | blue | 19.0 | male | Human |
| 2 | C-3PO | 167 | 75 | gold | yellow | 112.0 | none | Droid |
| 3 | R2-D2 | 96 | 32 | white, blue | red | 33.0 | none | Droid |
| 4 | Darth Vader | 202 | 136 | white | yellow | 41.9 | male | Human |
| 5 | Leia Organa | 150 | 49 | light | brown | 19.0 | female | Human |
| 6 | Owen Lars | 178 | 120 | light | blue | 52.0 | male | Human |

# Example 3: Pottery

Chemical analysis data on Romano-British pottery made in three different regions (kiln 1, kilns 2-3, and kilns 4-5):

```
> data("pottery", package = "HSAUR2")
> head(pottery)
```

| | Al2O3 | Fe2O3 | MgO | CaO | Na2O | K2O | TiO2 | MnO | BaO | kiln |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 18.8 | 9.52 | 2.00 | 0.79 | 0.40 | 3.20 | 1.01 | 0.077 | 0.015 | 1 |
| 2 | 16.9 | 7.33 | 1.65 | 0.84 | 0.40 | 3.05 | 0.99 | 0.067 | 0.018 | 1 |
| 3 | 18.2 | 7.64 | 1.82 | 0.77 | 0.40 | 3.07 | 0.98 | 0.087 | 0.014 | 1 |
| 4 | 16.9 | 7.29 | 1.56 | 0.76 | 0.40 | 3.05 | 1.00 | 0.063 | 0.019 | 1 |
| 5 | 17.8 | 7.24 | 1.83 | 0.92 | 0.43 | 3.12 | 0.93 | 0.061 | 0.019 | 1 |
| 6 | 18.8 | 7.45 | 2.06 | 0.87 | 0.25 | 3.26 | 0.98 | 0.072 | 0.017 | 1 |

Question: Do the chemical profiles of each pot suggest different types of pots and if any such types are related to kiln or region.

# Example 4: US pollution data

Air pollution in cities in the USA.

```
> data("USairpollution", package = "HSAUR2")
> head(USairpollution)
```

| | SO2 | temp | manu | popul | wind | precip | predays |
|---|---|---|---|---|---|---|---|
| Albany | 46 | 47.6 | 44 | 116 | 8.8 | 33.36 | 135 |
| Albuquerque | 11 | 56.8 | 46 | 244 | 8.9 | 7.77 | 58 |
| Atlanta | 24 | 61.5 | 368 | 497 | 9.1 | 48.34 | 115 |
| Baltimore | 47 | 55.0 | 625 | 905 | 9.6 | 41.31 | 111 |
| Buffalo | 11 | 47.1 | 391 | 463 | 12.4 | 36.11 | 166 |
| Charleston | 31 | 55.2 | 35 | 71 | 6.5 | 40.75 | 148 |

The following variables were obtained for 41 US cities:
`SO2`: SO2 content of air in micrograms per cubic metre;
`temp`: average annual temperature in degrees Fahrenheit;
`manu`: number of manufacturing enterprises employing 20 or more workers;
`popul`: population size (1970 census) in thousands;
`wind`: average annual wind speed in miles per hour;
`precip`: average annual precipitation in inches;
`predays`: average number of days with precipitation per year.

# Example 5: Academic salaries

The Salaries dataset comes from the carData package. It describes the 9- month academic salaries of 397 US college professors at a single institution in 2008-2009.

```
>         data(Salaries, package="carData")
> head(Salaries)

       rank discipline yrs.since.phd yrs.service  sex salary
1      Prof          B            19          18 Male 139750
2      Prof          B            20          16 Male 173200
3  AsstProf          B             4           3 Male  79750
4      Prof          B            45          39 Male 115000
5      Prof          B            40          41 Male 141500
6 AssocProf          B             6           6 Male  97000
```

# Example 6: A bigger example

Gene expression microarray dataset that reports the transcriptomes of 101 individual cells from mouse embryos at different time points in early development. 45101 genes are probed.

```
> if (!require("BiocManager", quietly = TRUE))
+     install.packages("BiocManager")
> BiocManager::install("Hiiragi2013")
> library("Hiiragi2013")
> data("x")
> dim(Biobase::exprs(x))

[1] 45101   101

> dfx = as.data.frame(Biobase::exprs(x))
```

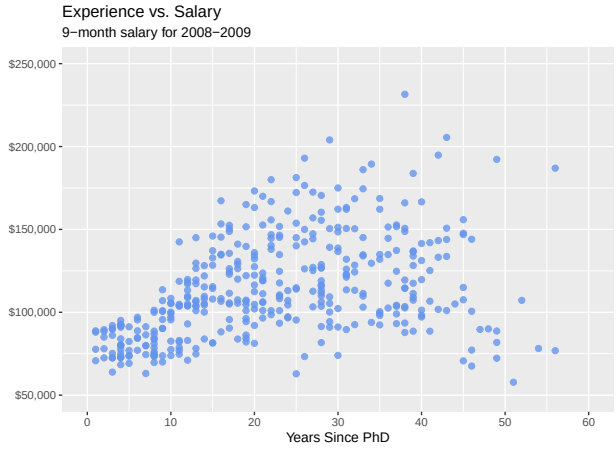
# Main challenges

- Having 25,000 dimensions of variation to consider at once is daunting; we will show how to reduce our data to a smaller number of most important dimensions without losing too much information.
- How to visualize multivariate data?
- Sometimes we do not want dimensionality reduction techniques and need to model a high-dimensional data sets directly. We will learn about high-dimensional statistics.

# Multivariate data visualization

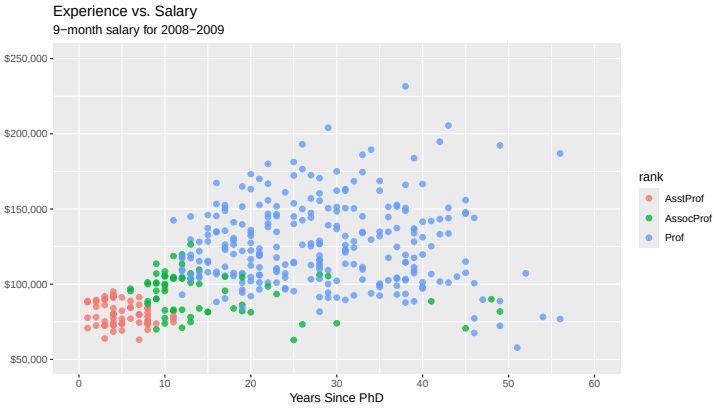
# Scatterplot for 2D datasets

The scatterplot is the standard for representing continuous bivariate data.



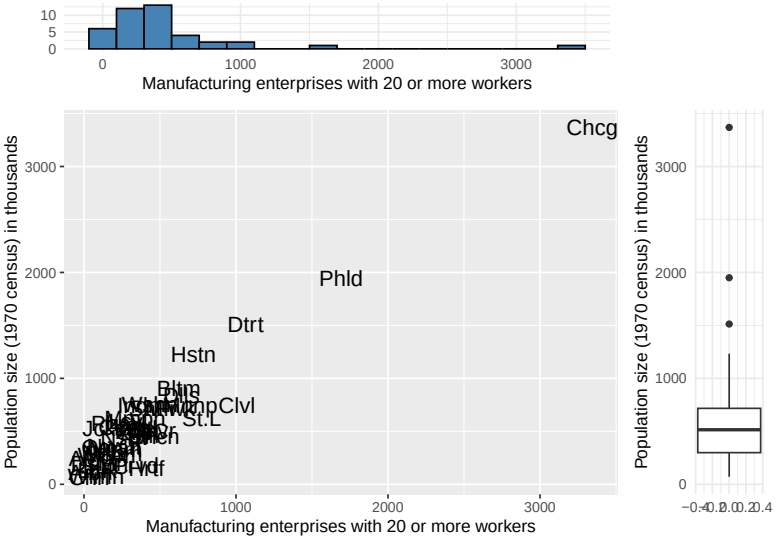
# Scatterplot for 2D datasets + categorical variable

The scatterplot is the standard for representing continuous bivariate data.




In the tutorial you will work more on this example and add more features to this plot.

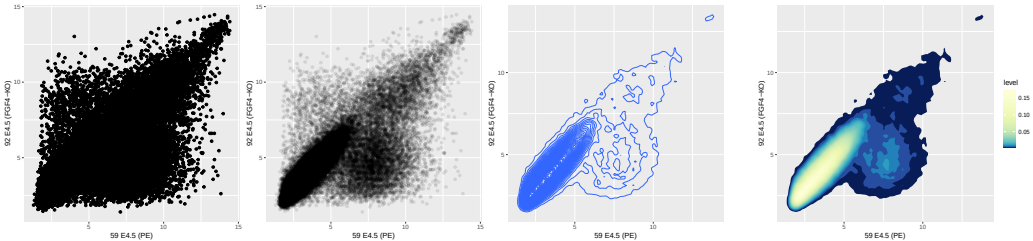
# Scatterplot with some marginal information



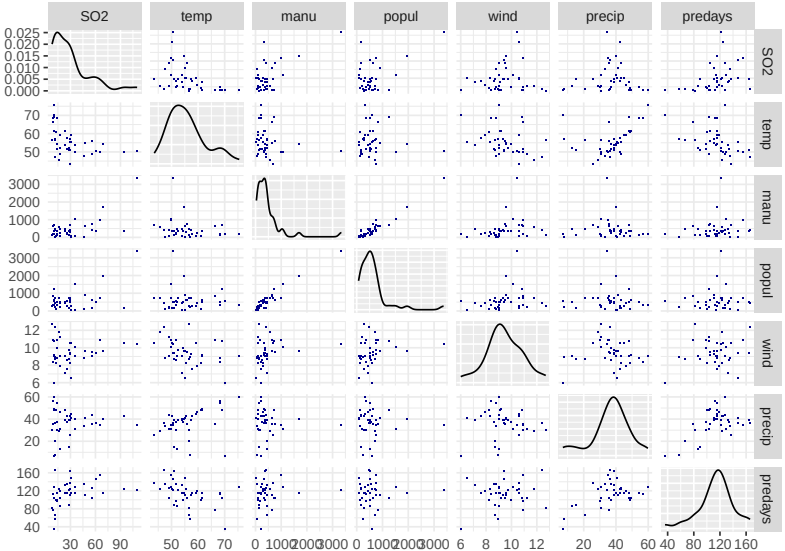
# 2D kernel density estimation

In our bigger gene expression dataset, take a look at differential expression between a wildtype and an FGF4-KO sample.

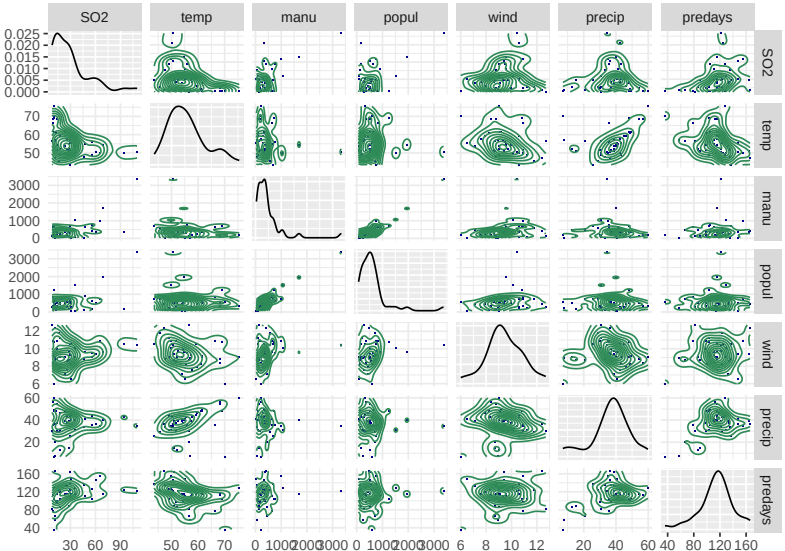
```
> scp <- ggplot(dfx, aes(x = `59 E4.5 (PE)`,y = `92 E4.5 (FGF4-KO)`))
> plot1 <- scp + geom_point()
> plot2 <- scp + geom_point(alpha = 0.1)
> plot3 <- scp + geom_density2d(h = 0.5, bins = 60)
> library("RColorBrewer")
> colorscale = scale_fill_gradientn(colors = rev(brewer.pal(9, "YlGnBu")),
+          values = c(0, exp(seq(-5, 0, length.out = 100))))
> plot4 <- scp + stat_density2d(h = 0.5, bins = 60,aes( fill = after_stat(level)), geom = "polygon") +  colorscale + coord_fixed()
```



# The scatterplot matrix and lattice plots



# The scatterplot matrix and lattice plots + 2D kernel density estimators



# Interactive graphics: Plotly

Plotly is a powerful library for creating interactive, web-based visualizations. It's available in several programming languages including R and Python. With Plotly, users can create interactive plots like scatter plots, bar charts, heatmaps, and 3D plots.

```
> library(ggplot2)
> library(plotly)
> p <- ggplot(mpg, aes(x=displ, y=hwy, color=class)) + geom_point(size=3) +
+ y = "Highway Mileage",color = "Car Class") + theme_bw()
> ggplotly(p)
```

Mousing over a point displays information about that point. Clicking on a legend point, removes that class from the plot. Clicking on it again returns it. Popup tools on the upper right of the plot allow you to zoom in and out of the image, pan, select, reset axes, and download the image as a png file.

# Notation and preliminaries (blackboard)

# Summary of this part

- Vectors, matrices, random vectors
- Interpretations for $A\mathbf{x}$ and $AB$
- Linearity of expectation, bilinearity of covariance