



Overview

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# Lecture 1 Introduction

## Probability Review

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STP598 Machine Learning and Deep Learning  
Fall 2021



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## Machine Learning and Deep Learning

- Instructor: Shiwei Lan <[slan@asu.edu](mailto:slan@asu.edu)>
  - Office: WXLR 544
  - Office hours: WF 11a - 12p @ <https://asu.zoom.us/j/8055899886>
- Teaching Assistants:
  - Shuyi Li <[shuyili3@asu.edu](mailto:shuyili3@asu.edu)>
  - Office hours: TBA



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- Course Schedule, Lecture Notes, etc.

<https://slan-teaching.github.io/STP598mldl/>

- Discussion and Questions

Slack channel [STP 598mldl](#)

- Homework and Grades on [Canvas](#)

- Coding Assignments on [Nbgrader](#)



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- Textbook:
  - **Required:** [ESL] Hastie, T., Tibshirani, R. Friedman, J. “[The Elements of Statistical Learning: Data Mining, Inference, and Prediction](#)”. Springer. ([free online PDF](#))
  - **Required:** [DL] Goodfellow, I., Bengio, Y. Courville, A. “[Deep Learning](#)” ([free online](#))
  - **Supplemental:** [DLP] Stevens, E., Antiga, L., Viehmann, T. “[Deep Learning with PyTorch](#)”. ([Link](#))
- Programming language:
  - [Python](#) is mandatory.
  - All homework reports must be submitted in either Word or PDF format, no other formats accepted.
  - R Markdown is recommended to generate PDF report.



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Statistical learning is the process of extracting statistical regularities from datasets. They are motivated from real world problems. A few examples:

- ▶ Email Spam (classification)
- ▶ Handwritten Digits (classification)
- ▶ DNA microarray (clustering)

# Examples

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A **compressive sensing** method is used to decompose a surveillance video image into background and moving objects. **Matrix decomposition and  $\ell_1$  penalization** are used in this method.



Examples from Jiang, Hong, Wei Deng, and Zuowei Shen. "Surveillance video processing using compressive sensing." arXiv preprint arXiv:1302.1942 (2013).

# Examples

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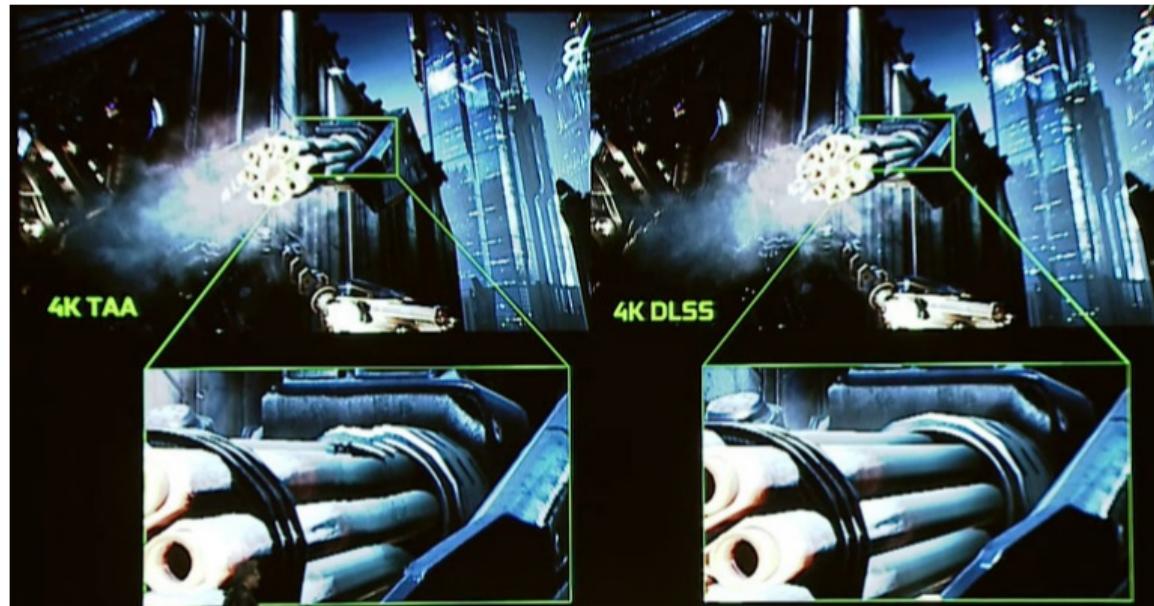
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**Single image super-resolution** is used for sharpening an image, or recovering a high-resolution image from a low-resolution one. Deep learning can be used to recognize the objects.



Example by NVIDIA using deep learning super-sampling in computer games.

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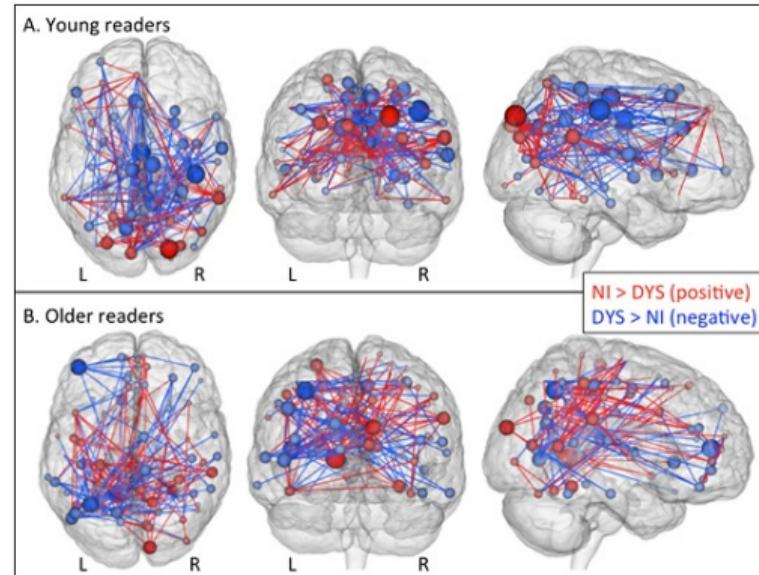
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Graphical models can be used to understand the network connectivity of multiple brain regions. This information can help diagnose diseases such as parkinson and dyslexia (difficulty reading).



Example from Finn, Emily S., et al. "Disruption of functional networks in dyslexia: a whole-brain, data-driven analysis of connectivity." Biological psychiatry 76.5 (2014): 397-404.

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**Auto piloting** is made possible by recognizing objects such as lines, cars, pedestrians, etc. in real time images. These are essentially classification problems, carried out through deep learning.



Example from Tesla: <https://www.tesla.com/autopilot>; And the video of accident that killed a woman in Tempe, Arizona.

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OpenAI Five is an AI system that plays Dota 2 against real human professionals. “... OpenAI Five sees the world as a list of 20,000 numbers which encode the visible game state, and chooses an action ...”. They lose to human professional team 0:2 in TI 2018.

 Bill Gates   
@BillGates

#AI bots just beat humans at the video game Dota 2. That's a big deal, because their victory required teamwork and collaboration – a huge milestone in advancing artificial intelligence. [b-gat.es/2KqAlzU](https://b-gat.es/2KqAlzU)

6:25 PM - Jun 26, 2018

14.9K  6,442 people are talking about this



OpenAI Five: <https://openai.com/five/>;

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The screenshot shows a web browser displaying a DeepMind blog post. The URL in the address bar is <https://deepmind.com/blog/article/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology>. The page title is "AlphaFold: a solution to a 50-year-old grand challenge in biology". The main content area features a large, colorful, geometric representation of a protein structure composed of many facets in shades of green, blue, purple, yellow, and red. Below the image, the text reads: "Proteins are essential to life, supporting practically all its functions. They are large complex molecules, made up of chains of amino acids, and what a protein does largely depends on its unique 3D structure. Figuring out what shapes proteins fold into is known as the "protein folding problem", and has stood as a grand challenge in biology for the past 50 years. In a major scientific advance, the latest version of our AI system AlphaFold has been recognised as a solution to this grand challenge by the organisers of the biennial Critical Assessment of protein Structure Prediction (CASP). This breakthrough demonstrates the impact AI can have on scientific discovery and its potential to dramatically accelerate progress in some of the most fundamental fields that explain and shape our world." At the bottom left, there is a link to "Read an update on our AlphaFold work [here](#)". On the left side of the page, there is a sidebar with a navigation menu including "About", "Research", "Impact", "Blog", "Safety & Ethics", and "Careers". There are also social media sharing icons for Twitter, Facebook, and LinkedIn, and a "SHARE" button.

AlphaFold: <https://deepmind.com/blog/article/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology>;

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- Probability: probability and random variables, distributions
- Statistics: estimators, likelihood, linear regressions
- Mathematics: linear algebra and calculus
- Programming and software:
  - program in [Python](#)
  - introduce Jupyter Notebook / R Markdown for homework
  - optimization basics



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# Learn pattern from data

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- Suppose we have a set of **training data**  $\mathcal{D}_n = \{x_i, y_i\}_{i=1}^n$ .
- Each  $x_i$  is a *p*-dimensional covariate vector that may represent
  - Gray scale of pixels in an image
  - Frequency of a particular word in an email
  - Concentration of a gene expression in blood
  - Brain electrical impulses
  - ...
- Each  $y_i$  is an outcome variable (or vector) that may represent
  - Cancer status (binary classification)
  - Type of object shown in the image (multicategory classification)
  - Surface temperature of a planet (regression)
  - Weight and volume of a tumor (multivariate regression)
  - ...
- **Goal:** learn patterns



# Supervised vs. Unsupervised Learning

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Oftentimes, there are two types of problems. And the goals are different:

- **Supervised learning**: data contains both “input” variables (covariates) and “output” variable(s). And we want to use the inputs to predict the values of the outputs.
- **Unsupervised learning**: data contains only the “input” variables, and we want to know what is the underlying mechanism that generates the data.



# Supervised Learning

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- Response variable or outcome  $Y$  (a random variable)
  - Regression:  $Y$  is quantitative/continuous:

$$y_i \in \mathbf{R}$$

- Classification:  $Y$  is categorical/discrete:

$$y_i \in C = \{0, 1\} \quad \text{or} \quad C = \{-1, +1\}$$

- Based on the training data  $\mathcal{D}_n = \{x_i, y_i\}_{i=1}^n$ , we aim to learn/estimate a function  $f$ , which describes the relationship between (variable)  $X$  and  $Y$ :

$$Y \leftarrow f(X)$$

- Goals:
  1. achieve small prediction error
  2. (and/or) assess the effect of each features on  $Y$



# Unsupervised Learning

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- No  $Y$ , just a set of features  $X \in \mathbb{R}^p$
- **Training data**  $\mathcal{D}_n = \{\mathbf{x}_i\}_{i=1}^n$  where each  $\mathbf{x}_i$  is a random draw of  $X$
- **Goal:** find patterns in the data (such as clusters), understand the data generating process of  $X$ , etc.
- Sometimes, it is difficult to measure the performance of an unsupervised learning method.
- The goal is fuzzy, but nevertheless it is an important problem.



# Types of Learning Problems

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- Supervised learning with **labeled** data: regression or classification
- Unsupervised learning with **unlabeled** data: clustering, network, graphical model
- There is also a **semi-supervised learning** that use a large set of unlabeled data to learn the distribution of independent variables and utilize that information for analyzing a smaller set of labeled data. However, we will not cover that in this course.



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- Supervised Learning:
  - Linear models and penalization
  - Classification, generalized linear regression
  - K nearest neighbor, tree, random forests
  - Support vector machine, neural networks
- Unsupervised Learning:
  - PCA, K-mean and hierarchical clustering
- Other Concepts / Topics
  - Bias-variance trade-off
  - Variable selection
  - Cross-validation
  - Deep neural networks



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- Normal distribution  $\mathcal{N}(\mu, \sigma^2)$ :

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

- Student's  $t$ -distribution with d.f.  $r$ :

$$f(x) = \frac{\Gamma(\frac{r+1}{2})}{\sqrt{\pi r} \Gamma(\frac{r}{2})} \left(1 + \frac{x^2}{r}\right)^{-\frac{r+1}{2}}$$

- $F$ -distribution with d.f.  $d_1$  and  $d_2$ :

$$f(x) = \frac{1}{B\left(\frac{d_1}{2}, \frac{d_2}{2}\right)} \left(\frac{d_1}{d_2}\right)^{\frac{d_1}{2}} x^{\frac{d_1}{2}-1} \left(1 + \frac{d_1}{d_2}x\right)^{-\frac{d_1+d_2}{2}}$$



# Relationships among distributions

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- $X \sim \mathcal{N}(0, 1) \rightarrow X^2 \sim \chi^2(1)$
  - $Z \sim \mathcal{N}(0, 1), X \sim \chi^2(r) \rightarrow \frac{Z}{\sqrt{X/r}} \sim t(r)$
  - $X_1 \sim \chi^2(a), X_2 \sim \chi^2(b) \rightarrow \frac{X_1/a}{X_2/b} \sim F(a, b)$
- ! Review the properties of Normal,  $\chi^2$ ,  $t$ , and  $F$ .



# Discrete distributions:

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- Bernoulli distribution  $\text{Bern}(p)$ :

$$f(k) = p^k(1-p)^{1-k}, \quad k \in \{0, 1\}$$

- Binomial distribution  $\mathcal{B}(n, p)$ :

$$f(k) = \binom{n}{k} p^k (1-p)^{n-k}, \quad k \in \{0, 1, \dots, n\}$$

- Poisson distribution with rate  $\lambda$ :

$$f(k) = \frac{\lambda^k e^{-\lambda}}{k!}$$



# Multivariate normal distribution

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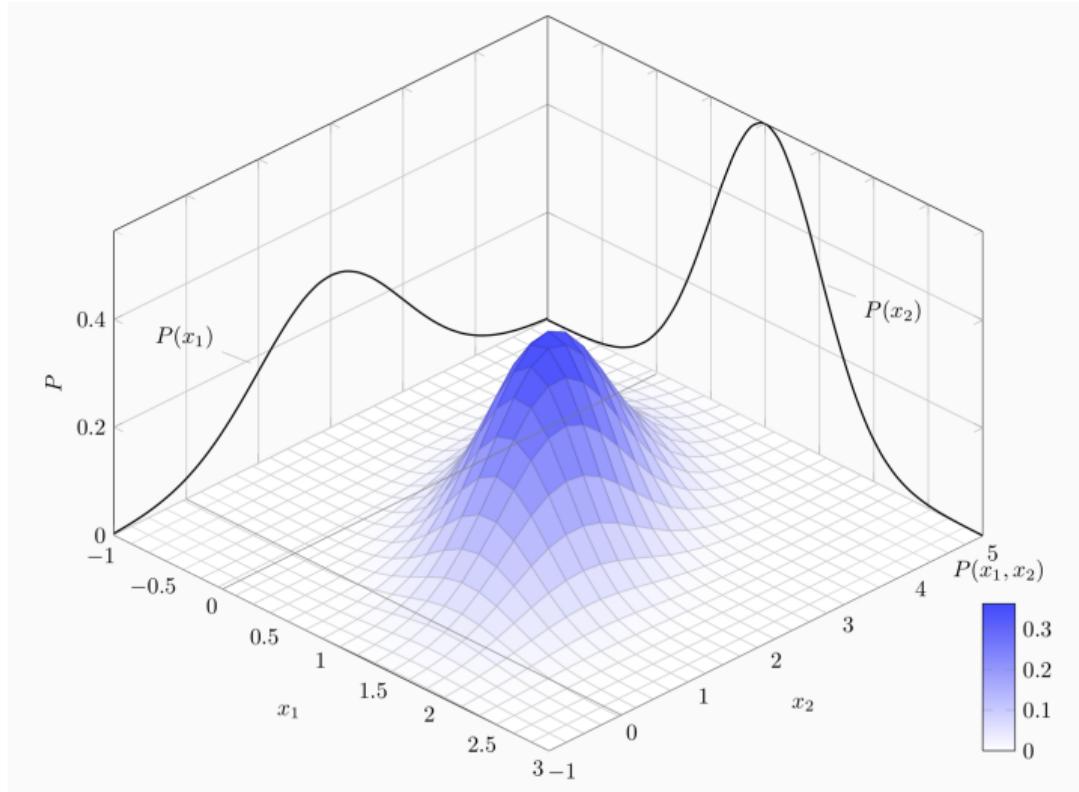
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- Normal (Gaussian) distribution is the most frequently used distribution in statistics
- By the central limit theory, sample means will converge to Gaussian as sample size increases
- In many cases, we will concern about two or many normally distributed random variables
- Lets consider two random variables  $X$  and  $Y$  that are **jointly normally distributed** with density function

$$f(x, y) = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \times \exp\left\{-\frac{1}{2(1-\rho^2)} \left[ \frac{(x - \mu_x)^2}{\sigma_x^2} + \frac{(y - \mu_y)^2}{\sigma_y^2} - \frac{2\rho(x - \mu_x)(y - \mu_y)}{\sigma_x\sigma_y} \right]\right\}$$

where  $\mu_x$  and  $\mu_y$  are the means,  $\sigma_x$  and  $\sigma_y$  are the standard deviations, and  $\rho$  is the **correlation coefficient**.

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- The sum of two random normal variables are also normally distributed.
- Suppose that  $X \sim \mathcal{N}(\mu_x, \sigma_x^2)$ ,  $Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$  and the correlation coefficient between  $X$  and  $Y$  is  $\rho$ , then the sum

$$X + Y \sim \mathcal{N}(\mu_x + \mu_y, \sigma_x^2 + \sigma_y^2 + 2\rho\sigma_x\sigma_y)$$

and the linear combination

$$aX + bY \sim \mathcal{N}(a\mu_x + b\mu_y, a^2\sigma_x^2 + b^2\sigma_y^2 + 2ab\rho\sigma_x\sigma_y)$$

- From the previous example, what is the probability that a randomly selected student has a combined score over 150, i.e.,  $P(X + Y > 150)$ ?
- Find  $P(2X + 3Y > 350)$ .
- Find that the student did better on Exam 1 than on Exam 2, i.e.,  $P(X - Y > 0)$ .

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- We usually represent a multivariate normal (MVN) distribution in a matrix form:
- Let  $X = (X_1, X_2, \dots, X_p)^T$  be a  $p$ -dimensional random vector that follows the distribution  $\mathcal{N}_p(\mu, \Sigma)$ , where the mean  $\mu_{p \times 1}$  is a  $p$ -dimensional vector, and the covariance  $\Sigma_{p \times p}$  is a  $p \times p$  dimensional symmetric and positive-definite matrix.
- The  $i$ -th element,  $\mu_i$ , and  $(i, j)$ -th element,  $\sigma_{ij}$  are defined as follows respectively

$$\mu_i = E(X_i), \quad \sigma_{ij} = \text{Cov}(X_i, X_j), \quad , i, j = 1, 2, \dots, p.$$

- In particular,  $\sigma_{ii} = \sigma_i^2 = \text{Var}(X_i)$ . And  $\sigma_{ij} = \sigma_i \sigma_j \rho_{ij}$ , where  $\rho_{ij}$  is the correlation between  $X_i$  and  $X_j$ . In this general case, we have correlation matrix  $\mathbf{P}_{p \times p}$  with  $\rho_{ij}$  as its  $(i, j)$ -th element.
- When  $p = 1$ ,  $\mathbf{P}_{p \times p} = \rho$  becomes correlation coefficient as mentioned before.



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- The pdf of  $X$  is

$$\frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

- Let  $Z$  be a  $q$ -dimensional vector of linear combinations of  $X$  such that  $Z = \mathbf{A}_{q \times p}X + \mathbf{b}_{q \times 1}$ , then  $Z$  follows a MVN distribution:

$$Z \sim \mathcal{N}(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top)$$

- A special case: if  $Z = \boldsymbol{\Sigma}^{-1/2}(X - \boldsymbol{\mu})$ , then entries in  $Z$  follow iid normal (We call this transformation *standardization*):

$$Z \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_{p \times p})$$

- For example, we could let  $Z = \mathbf{L}^{-1}(X - \boldsymbol{\mu})$  where  $\mathbf{L}$  is the Cholesky factor of  $\boldsymbol{\Sigma} = \mathbf{L}\mathbf{L}^\top$ , or  $Z = \mathbf{D}^{-1/2}\boldsymbol{\Gamma}^\top(X - \boldsymbol{\mu})$ , where we use the eigen-decomposition  $\boldsymbol{\Sigma} = \boldsymbol{\Gamma}\mathbf{D}\boldsymbol{\Gamma}^\top$ .



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- Conditional distribution of multivariate normal is also frequently used
- Let the random vector  $(X^T, Y^T)^T$  be jointly distributed as

$$\begin{pmatrix} X_{p \times 1} \\ Y_{q \times 1} \end{pmatrix} \sim \mathcal{N} \left( \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}, \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{xy}^T & \Sigma_{yy} \end{bmatrix} \right)$$

where  $\mu_x$  is  $p$ -dimensional,  $\mu_y$  is  $q$ -dimensional.  $\Sigma_{xx}$  is  $p \times p$  dimensional covariance matrix of  $X$ ,  $\Sigma_{yy}$  is  $q \times q$  dimensional covariance matrix of  $Y$ , and  $\Sigma_{xy}$  is  $p \times q$  dimensional (cross) covariance matrix between  $X$  and  $Y$  with  $(i, j)$ -th element  $\text{Cov}(X_i, Y_j)$ .

- The conditional distribution of  $X|Y = y$  is

$$X|Y = y \sim \mathcal{N} \left( \mu_x + \Sigma_{xy} \Sigma_{yy}^{-1} (y - \mu_y), \Sigma_{xx} - \Sigma_{xy} \Sigma_{yy}^{-1} \Sigma_{xy}^T \right)$$



# Probability Rules

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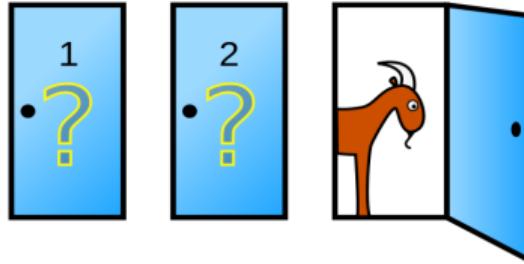
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- **Independent events** For two independent events  $A$  and  $B$ ,  
 $P(A \cap B) = P(A)P(B)$
- **Mutually exclusive events** For two mutually exclusive events  $A$  and  $B$ ,  
 $P(A \cap B) = 0 \implies P(A \cup B) = P(A) + P(B)$  “sum rule”
- **Conditional probability** The probability of  $A$  given  $B$ ,  
 $P(A|B) = P(A \cap B)/P(B) \implies P(A \cap B) = P(A|B)P(B)$  “multiplication rule”
- **Bayes (“inverse”) rule** The probability of  $A$  given  $B$  can be obtained

$$P(A|B) = \frac{P(A)P(B|A)}{P(B)} = \frac{P(A)P(B|A)}{P(A)P(B|A) + P(A^c)P(B|A^c)}$$

- posterior  $\propto$  prior  $\times$  likelihood

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The Monty Hall problem is a brain teaser, in the form of a probability puzzle, loosely based on the American television game show *Let's Make a Deal* and named after its original host, *Monty Hall*.

*Suppose you're on a game show, and you're given the choice of three doors: Behind one door is a car; behind the others, goats. You pick a door, say No. 1, and the host, who knows what's behind the doors, opens another door, say No. 3, which has a goat. He then says to you, "Do you want to pick door No. 2?"*

Is it to your advantage to switch your choice?

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# Python, Conda and Jupyter Notebook

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- **Python** is a free software environment for statistical machine learning and graphics.
  - <https://www.python.org>
- **Conda** is an open source package / environment management system for Python.
  - <https://anaconda.org>
- **Jupyter** Notebook is a Python package to integrate code, equations, visualizations in document.
  - <https://jupyter.org>
- **R Markdown** has also integrated Python. Check [link1](#) [link2](#).



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Notebook

The screenshot shows two Jupyter Notebooks side-by-side. The left notebook is titled 'Welcome to Python' and contains introductory text, a warning message about relying on the server, and a section on running Python code. It also includes a code cell with matplotlib imports. The right notebook is titled 'Exploring the Lorenz System' and describes the Lorenz system of differential equations. It shows the equations  $\dot{x} = \sigma(y - x)$ ,  $\dot{y} = \rho x - y - xz$ , and  $\dot{z} = -\beta z + xy$ . Below the text is an interactive IPython slider interface for parameters N, angle, max\_time, sigma, beta, and rho. At the bottom is a 3D plot of the Lorenz attractor, a complex, chaotic trajectory.

jupyter Welcome to Python

Welcome to the Python Notebook Server

This Notebook Server was created by

WARNING

Don't rely on this server!

Your server is hosted there

Run some Python code

To run the code below:

1. Click on the cell to select it
2. Press SHIFT+ENTER

A full tutorial for using the Python Notebook is available at

In [ ]:

```
%matplotlib inline

import pandas as pd
import numpy as np
import matplotlib
```

jupyter Lorenz Differential Equations (autosaved)

File Edit View Insert Cell Kernel Help

Cell Toolbar: None

Python 3

Exploring the Lorenz System

In this Notebook we explore the [Lorenz system](#) of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of complex behaviors as the parameters ( $\sigma$ ,  $\beta$ ,  $\rho$ ) are varied, including what are known as [chaotic solutions](#). The system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

In [7]:

```
interact(Lorenz, N=fixed(10), angle=(0.,360.),  
        sigma=(0.0,50.0),beta=(0.,5.), rho=(0.0,50.0))
```

angle: 306.2

max\_time: 12

$\sigma$ : 10

$\beta$ : 2.6

$\rho$ : 28