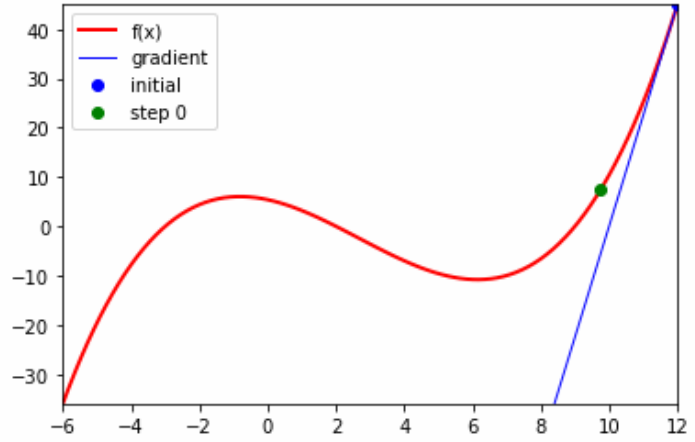
Note) Slides and example codes are available:
https://github.com/mint-lab/prog_meets_math

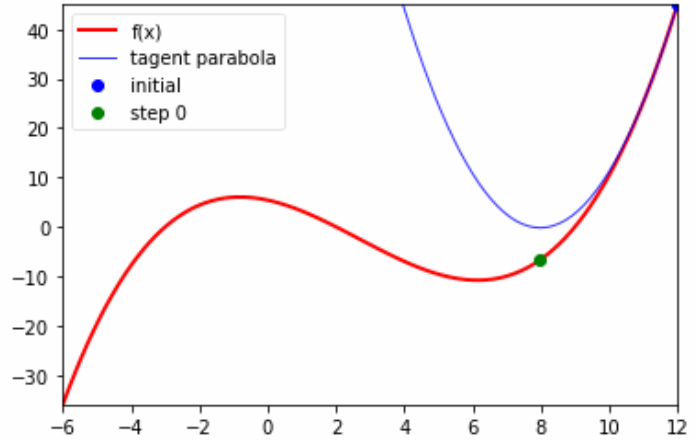
Programming meets Mathematics: Probability

Sunglok Choi, Assistant Professor, Ph.D.
Computer Science and Engineering Department, SEOULTECH
sunglok@seoultech.ac.kr | https://mint-lab.github.io/

Programming meets Mathematics

- ~~Calculus~~ **Differentiation**
- ~~Linear Algebra~~ **Vector and Matrix**
- ~~Optimization~~ **Nonlinear Optimization** (as local optimization)
  - Gradient descent: Selecting the search direction **with the 1st derivative**
    - Possible problems: Too small and large step size
  - Newton's method: Selecting the search direction and step **with the 1st and 2nd derivatives**
    - Possible problems: The maxima problem, the saddle point problem
  - scipy.optimize: A magic wand **without derivatives**
- **Probability**
- **Information Theory**

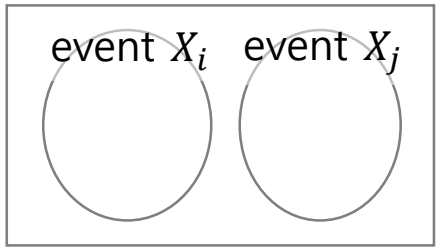




Probability

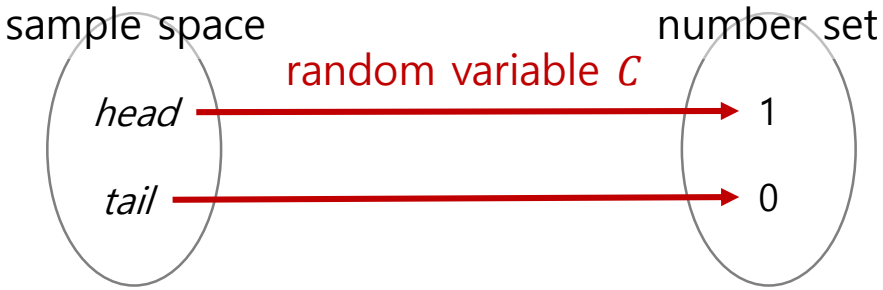
- **Why probability?**
  - Uncertain observation (∵ noise and error)
  - Incomplete data (∵ unobservable or missing elements)
  - Imperfect knowledge and rules/models (∵ over-simplified or incorrect)
- **Probability**
  - A numerical description of how likely an event is to occur or how likely a proposition is true
  - Notation: $P(X)$ or $Pr(X)$ for the probability of an event X
  - Axioms
    1. For any event X, $0 \leq P(X)$
    2. Probability of the sample space S is $P(S) = 1$
    3. If X_1, X_2, … are disjoint events, then $P(X_1 \cup X_2 \cup \cdots) = P(X_1) + P(X_2) + \cdots$

       (mutually exclusive; $P(X_i \cap X_j) = 0$)



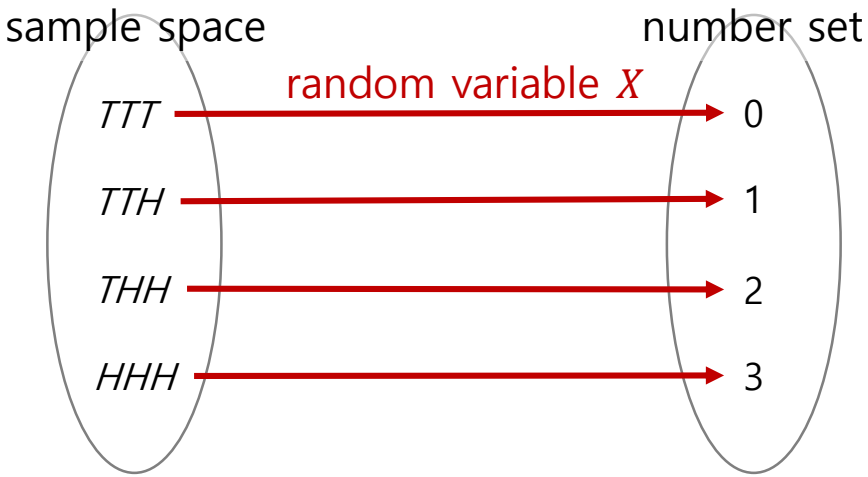
Probability

- **Random variable**
  - Roughly, a mapping from a sample space to a measurable number set (usually $\mathbb{R}$ or $\mathbb{N}$)
  - e.g. Event D: Rolling a dice (sample space: 1, 2, 3, 4, 5, and 6)
    - The probability of an event of rolling a dice: $P(D)$
    - The probability of getting 3 after rolling a dice: $P(D = 3)$
  - e.g. Event H: Measure height of a student (sample space: $\mathbb{R}$)
    - The probability of a student's height is more than 180: $P(H > 180)$
  - e.g. Event C: Tossing a coin (sample space: *head* and *tail*)
    - The probability of getting *head* after tossing a coin: $P(C = 1)$



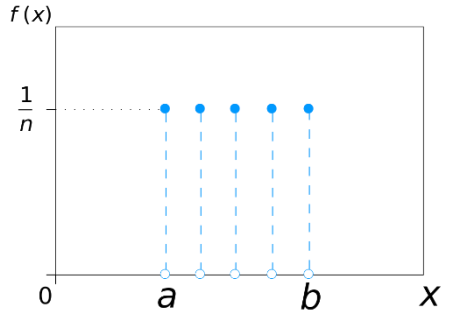
Probability

- **Random variable**
  - Roughly, a mapping from a sample space to a measurable number set (usually $\mathbb{R}$ or $\mathbb{N}$)
  - e.g. Event X: Tossing three coins together (sample space: *TTT*, *TTH*, *THH*, *HHH*)
    - The probability of getting two *head* after tossing the coins: $P(X = 2)$ if X is the number of heads



Probability

- **Probability distribution**
  - Probability **mass** function (pmf) for **discrete** random variable
    - $P(X = x_i) = p(X = x_i)$ (Note: In short, $p_X(x_i)$)
      - Each point has a probability value.
    - From the axioms
      - $p_X(x_i) \geq 0$
      - $\sum_{x_i \in S_X} p_X(x_i) = 1$



  - Probability **density** function (pdf) for **continuous** random variables
    - $P(a \leq X \leq b) = \int_a^b f(X = x)dx$ (Note: In short, $f_X(x)$)
      - The area is a probability value, not a point.
    - From the axioms
      - $f_X(x_i) \geq 0$
      - $\int_{-\infty}^{\infty} f_X(x)\, dx = 1$

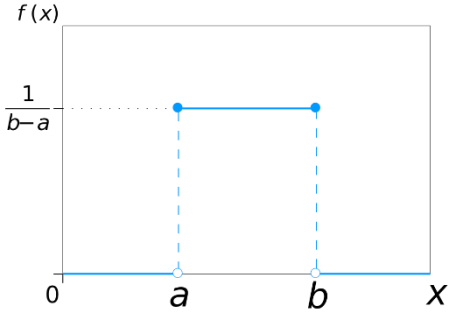


Image: Wikipedia (discrete uniform dist. and continuous uniform dist.)

Probability

- **Probability distribution**
  - **Cumulative** distribution function (cdf)
    - $F_X(x) = P(X \leq x) \quad \rightarrow \quad P(a < X \leq b) = F_X(b) - F_X(a)$
    - For a discrete random variable, $F_X(x) = \sum_{x_i \leq x} p_X(x_i)$
    - For a continuous random variable, $F_X(x) = \int_{-\infty}^{x} f_X(t)\, dt$
    - Properties: Non-decreasing, right-continuous, reaching 1 at the right end

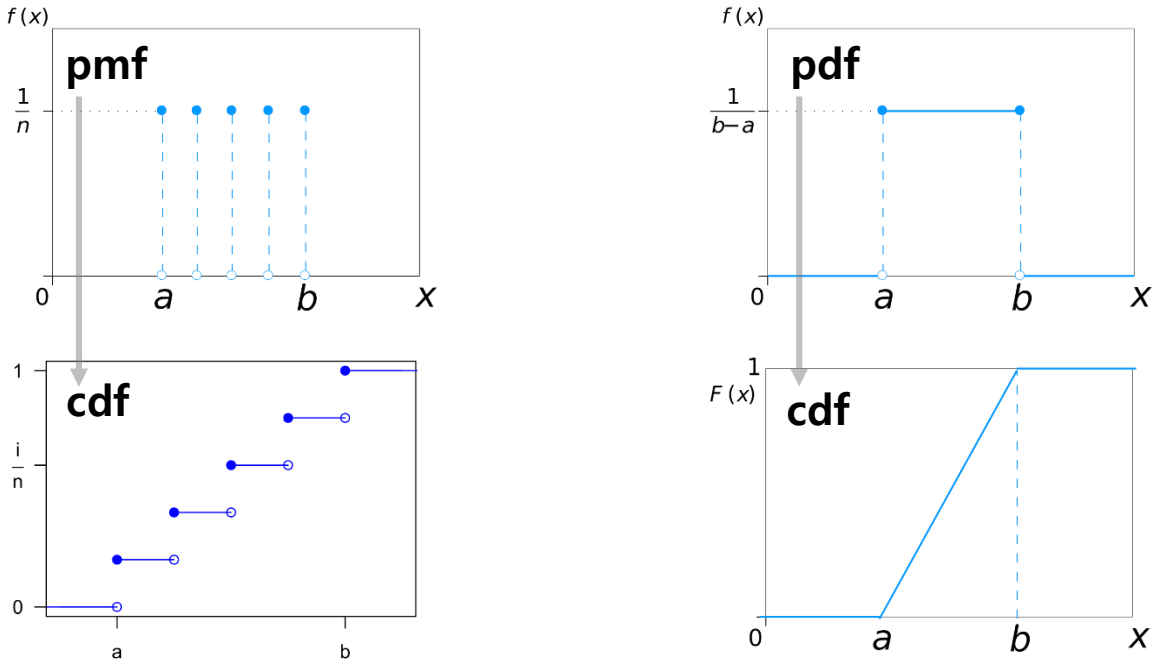
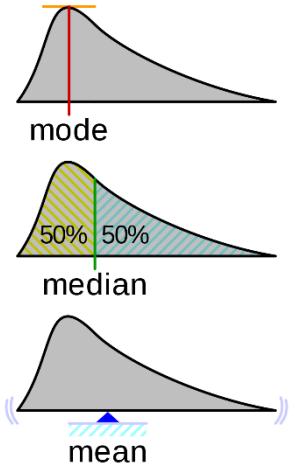


Image: Wikipedia (discrete uniform dist. and continuous uniform dist.)

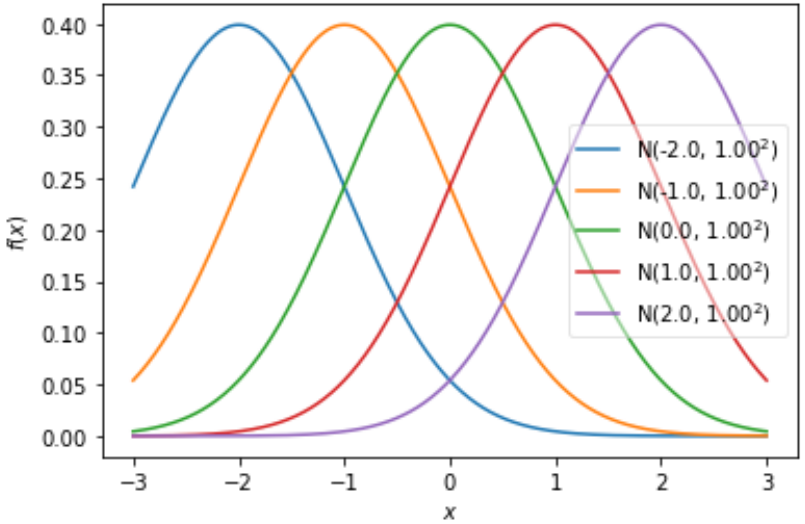
Probability

- **Probability distribution** [see more distributions]
  - e.g. Normal distribution (a.k.a. Gaussian distribution)

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



  - Notation: $N(\mu, \sigma^2)$
  - Parameters: mean μ (~ location), variance σ^2 (~ squared width)
    - Note) mean = median = mode = μ
  - Shapes (Note: $N(0,1)$ - Standard normal distribution)



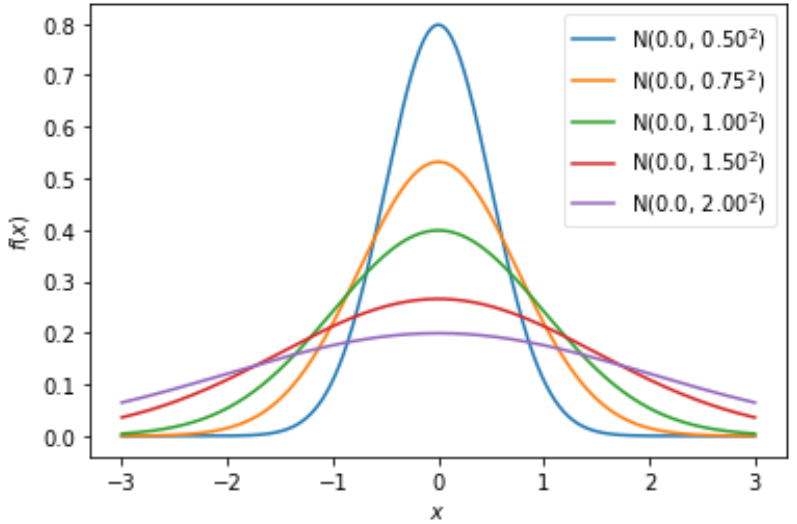


Image: Wikipedia

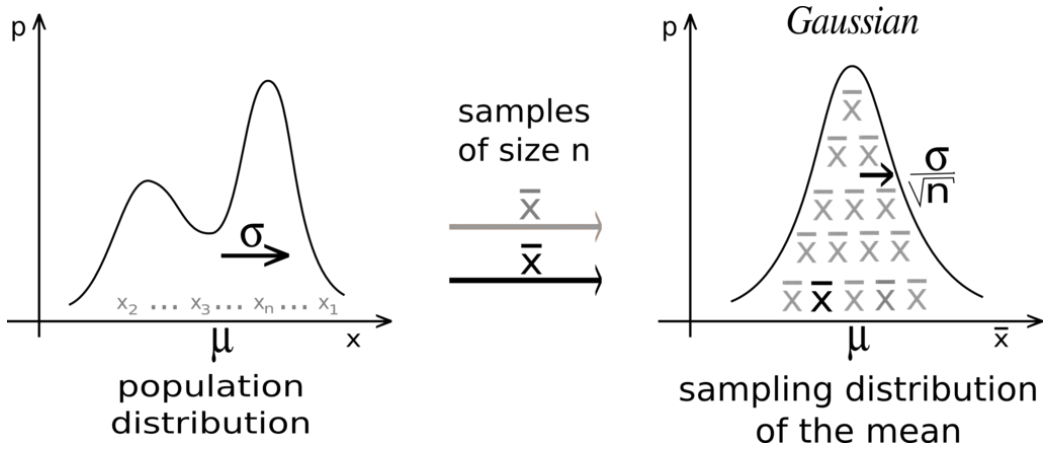
Probability

- **Probability distribution** [see more distributions]
  - e.g. Normal distribution (a.k.a. Gaussian distribution)
    - Example) Visualize the normal distribution with varying parameters

```
import numpy as np
import matplotlib.pyplot as plt

xs = np.linspace(-3, 3, 1000)
mu_set = [0]                          # [0] or [-2, -1, 0, 1, 2]
sigma_set = [0.5, 0.75, 1, 1.5, 2] # [1] or [0.5, 0.75, 1, 1.5, 2]

for mu in mu_set:
    for sigma in sigma_set:
        pdf = 1 / sigma / np.sqrt(2*np.pi) * np.exp(-0.5*((xs - mu)/sigma)**2)
        plt.plot(xs, pdf, label=f'N({mu:.1f}, ${sigma:.2f}^2$)')

plt.xlabel('$x$')
plt.ylabel('$f(x)$')
plt.legend(framealpha=0.5)
plt.show()
```

Probability

- **Probability distribution** [see more distributions]
  - e.g. Normal distribution (a.k.a. Gaussian distribution)
    - Why important? The central limit theorem (CLT)



- Example) Validating CLT (1/2)
  - Rolling a dice (discrete uniform dist.)
    - n: the number of samples
    - 10,000 trials

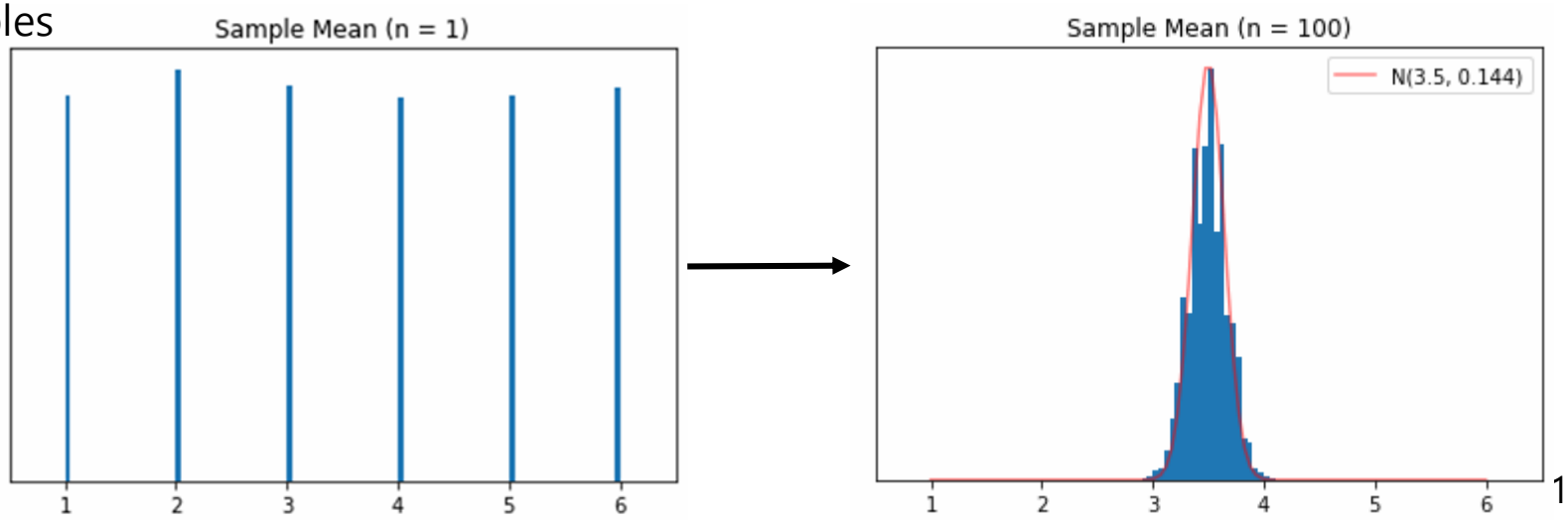


Image: Wikipedia

Probability

- **Probability distribution** [see more distributions]
  - e.g. Normal distribution (a.k.a. Gaussian distribution)
    - Example) Validating CLT (2/2)

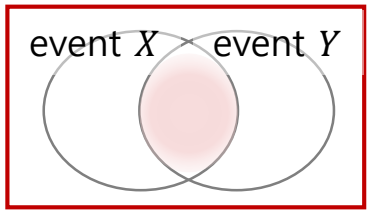
```
import numpy as np
import matplotlib.pyplot as plt

hist_pts = 10000
hist_bins = 100
dice_range = (1, 6)
n = 100 # Please decrease and increase `n`

# Acquire multiple sample means
samples = []
for i in range(hist_pts):
    samples.append(np.mean(np.random.randint(dice_range[0], dice_range[1]+1, n)))

# Visualize the distribution of sample means
plt.title(f'Sample Mean (n = {n})')
plt.hist(samples, bins=hist_bins, range=dice_range, density=True, align='mid')
plt.xlim(dice_range[0]-0.5, dice_range[1]+0.5)
plt.yticks([])
plt.show()
```

Central Limit Theorem

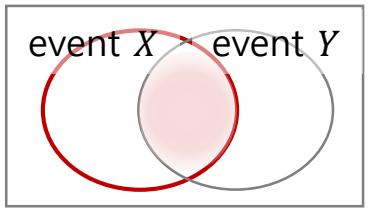
Image: The Hankyoreh.

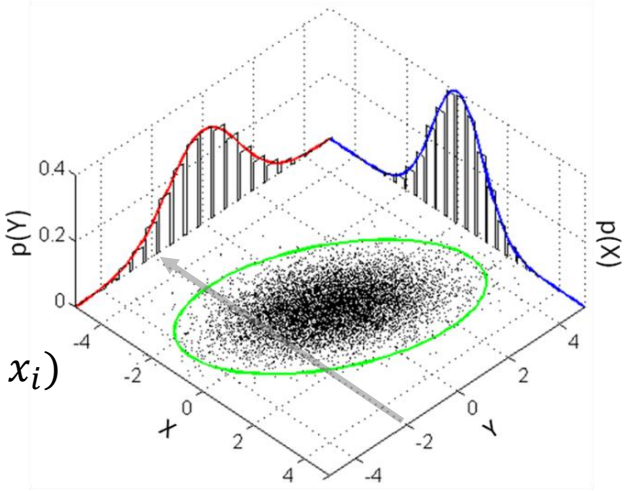
Probability

- **Joint probability**
  - How likely would X and Y happen together? $P(X,Y)$ or $P(X \cap Y)$
  - Note) Independence: $P(X,Y) = P(X)\,P(Y)$

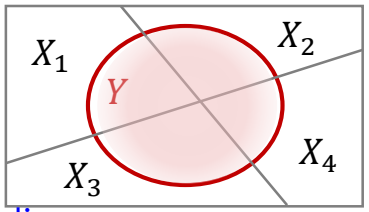


- **Conditional probability**
  - Given X, how likely would Y happen? $P(Y|X) = \frac{P(Y,X)}{P(X)}$
  - Note) Independence: $P(Y|X) = P(Y)$
  - Chain rule: $P(Y,X) = P(Y|X)\,P(X) \;\rightarrow\; P(X_3,X_2,X_1) = P(X_3|X_2,X_1)\,P(X_2|X_1)\,P(X_1)$
  - Bayes' theorem: $P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)}$ (posterior, likelihood, prior, and marginalization)





- **Marginal probability**
  - Regardless of what happens to X, how likely would Y happen? $P(Y) = \sum_{x_i \in S_X} P(Y, X = x_i)$
  - Law of total probability: $P(Y) = \sum_i P(Y,X_i) = \sum_i P(Y|X_i)P(X_i)$



if $\{X_i | i = 1,2,\dots\}$ is a set of pairwise disjoint events whose union is the entire sample space.

Image: Wikipedia

Probability

- **Bayes' theorem**
  - $P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)}$ (posterior, likelihood, prior, and marginalization)
  - Alias: Bayes' law, Bayes' rule, and Bayesian theorem
  - Example) Pancreatic cancer rate (췌장암 in Korean)
    - Patients with the cancer have a certain symptom: 100%
    - Occurrence rate of the cancer: 1 / 100,000
    - Occurrence rate of the same symptom for healthy persons: 10 / 100,000
    - **If you have the symptom, what is the probability that you have the cancer?**

Probability

- **Bayes' theorem**
  - $P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)}$ (posterior, likelihood, prior, and marginalization)
  - Alias: Bayes' law, Bayes' rule, and Bayesian theorem
  - Example) Pancreatic cancer rate (췌장암 in Korean)
    - Patients with the cancer have a certain symptom: 100% → $P(X|Y) = 1$
    - Occurrence rate of the cancer: 1 / 100,000 → $P(Y) = 0.00001$, $P(\neg Y) = 0.99999$
    - Occurrence rate of the same symptom for healthy persons: 10 / 100,000 → $P(X|\neg Y) = 0.0001$
    - **If you have the symptom, what is the probability that you have the cancer?**

      X $P(Y|X)$ Y

      - From the law of total probability, $P(X) = P(X|Y)P(Y) + P(X|\neg Y)P(\neg Y)$
      - Therefore, $P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)} = \frac{1}{11} \approx 9.1\%$

Symptom \ Cancer	Yes (Y)	No ($\neg Y$)	Total
Yes (X)	**1**	**10**	11
No ($\neg X$)	**0**	99989	99989
Total	**1**	**99999**	**100000**

If you know the joint probability distribution, you can derive anything you want.

Probability

- **Expectation**
  - A generalization of weighted average
    - Alias: Mean, average, the **first moment**

$$E[X] = \sum_{i=1}^{n} x_i \, P(x_i) \quad \text{or} \quad E[X] = \int_{\mathbb{R}} x \, f(x) dx$$

    - Note) Arithmetic mean ($\frac{\sum_{i=1}^{n} x_i}{n}$) is the expectation under uniform distribution.
  - Properties
    - Linearity: $E[X + Y] = E[X] + E[Y]$ and $E[aX] = aE[X]$
    - Non-multiplicativity: $E[XY] \neq E[X] \, E[Y]$
      - Note) If X and Y are independent, $E[XY] = E[X] \, E[Y]$

Probability

- **Variance**
  - The expectation of the squared deviation of X from its mean
    - Alias: The **second central moment**

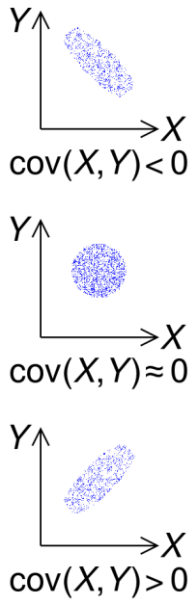
$$Var(X) = E[(X - \mu)^2]$$

  - Calculation: $Var(X) = E[X^2] - E[X]^2 = E[X^2] - \mu^2$
  - Properties
    - $Var(X) \geq 0$: Non-negative
    - $Var(X + a) = Var(X)$: Invariant to a location parameter
    - $Var(aX) = a^2 Var(X)$: Squared scale
    - $Var(aX + bY) = a^2 Var(X) + b^2 Var(Y) + 2ab\ \mathrm{cov}(X, Y)$

Probability

- **Variance**
  - The expectation of the squared deviation of X from its mean
    - Alias: The **second central moment**

$$Var(X) = E[(X - \mu)^2]$$



- Note) **Covariance**
  - The joint variability of two or more random variables

$$\text{cov}(X, Y) = E[(X - E[X])(Y - E[Y])]$$

  - A single variable: $\text{cov}(X, X) = E[(X - E[X])(X - E[X])] = Var(X)$

- Note) **Correlation**
  - The normalized covariance (range: [0, 1])
    - Alias: Dependence

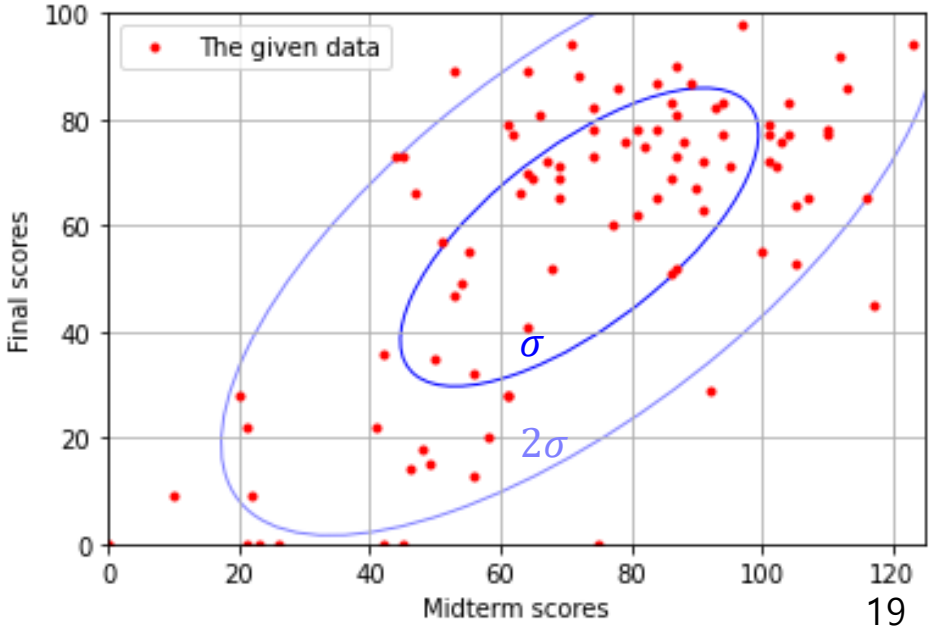
$$\text{corr}(X, Y) = \frac{cov(X, Y)}{\sigma_X \, \sigma_Y}$$

Image: Wikipedia

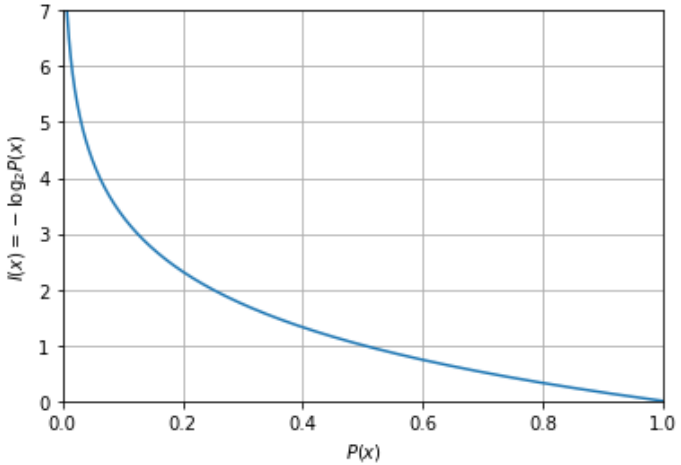
Probability

- **Variance**, **Covariance**, and **Correlation**
  - Example) Correlation of the midterm and final exam scores

```
# Load score data
class_kr = np.loadtxt('data/class_score_kr.csv', delimiter=',')
class_en = np.loadtxt('data/class_score_en.csv', delimiter=',')
scores = np.vstack((class_kr, class_en))

# Calculate the variance, covariance, and correlation
midtm = [func(scores[:,0]) for func in [np.mean, np.var, np.std]] # [72.07, 751.26, 27.41]
final = [func(scores[:,1]) for func in [np.mean, np.var, np.std]] # [57.81, 790.18, 28.11]

cov_all = np.cov(scores.T, ddof=0) # [[751.26, 534.94],
print(cov_all)                     #  [534.94, 790.18]]

cor_all = np.corrcoef(scores.T)    # [[  1.  ,   0.69],
print(cor_all)                     #  [  0.69,   1.  ]]
```



~~Information Theory~~ Cross Entropy



- **(Shannon) Information** of an event X

$$I(x) = -\log_2 P(x)$$

  - An alternative way of expressing probability
    - Alias: Surprisal, information content
  - As the concept of *surprisal*, Shannon information is roughly the level of surprise if the event is true (~ more surprises, less probable, more informative)
    - e.g. What is the most significant news if the news is correct?
      1) Tomorrow the sun will rise in the east.
      2) Tomorrow it will rain.
      3) Tomorrow the sun will rise in the west.
  - In the view of compression or communication, Shannon information is the length of a message necessary for an optimal coding of the random variable
    - e.g. Shannon information of tossing two coins: Each probability $P(x) = \frac{1}{4} \rightarrow I(x) = 2$ (2-bit coding)
    - e.g. Shannon information of rolling a dice: Each probability $P(x) = \frac{1}{6} \rightarrow I(x) = 2.585$ (3-bit coding)

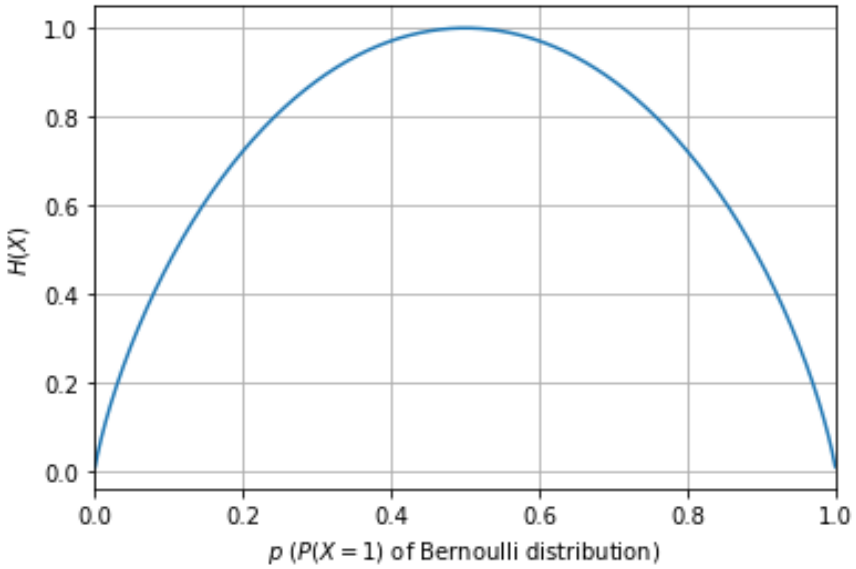
Cross Entropy

- **(Shannon) Entropy** of a random variable X

$$H(X) = E_X[-\log P(X)] = -\sum_{i=1}^{n} P(x_i) \log P(x_i)$$

  - The expectation of Shannon information (or surprise or the number of bits with an optimal coding) inherent in the variable's all possible outcomes
  - Example) Entropy of tossing an **unfair** coin (*head* = 1, *tail* = 0)
    - Bernoulli distribution: $p(X = k) = \begin{cases} p & \text{if } k = 1 \\ 1 - p & \text{otherwise} \end{cases}$

```
p = np.linspace(0, 1, 1000)
entropy = -p*np.log2(p) - (1-p)*np.log2(1-p)
```



Cross Entropy

- **(Shannon) Entropy** of a random variable X
  - Example) Entropy of rolling an **unfair** dice
    - Non-uniform distribution

      $P_X(1) = P_X(2) = 0.4$ and $P_X(3) = P_X(4) = P_X(5) = P_X(6) = 0.05$

```
p = np.array([0.4, 0.4, 0.05, 0.05, 0.05, 0.05])
entropy = sum(-p*np.log2(p)) # 1.922...
```

    - Q) How to encode them to achieve the average 2-bit message?
    - A)

X	**Code**
1	0
2	10
3	11 00
4	11 01
5	11 10
6	11 11

Cross Entropy

- **Cross entropy** of the distribution q relative to a distribution p (over the same underlying sample space)

$$H(p,q) = E_p[-\log q] = -\sum_{x \in S_X} p(x) \log q(x)$$

  - The average number of bits if a coding scheme is optimized for probability distribution q instead of the true distribution p
  - Cross entropy roughly represents difference of two probability distributions similar to the Kullback–Leibler divergence.
  - Example) Cross entropy of rolling an **unfair** dice

```
p  = np.array([1/6, 1/6, 1/6, 1/6, 1/6, 1/6])
entropy  = sum(-p*np.log2(p))  # 2.585...

q1 = np.array([0.4, 0.4, 0.05, 0.05, 0.05, 0.05])
entropy1 = sum(-p*np.log2(q1)) # 3.322...

q2 = np.array([0.2, 0.2, 0.2, 0.2, 0.1, 0.1])
entropy2 = sum(-p*np.log2(q2)) # 2.655...

q3 = np.array([0.6, 0.2, 0.1, 0.05, 0.04, 0.01])
entropy3 = sum(-p*np.log2(q3)) # 3.665...
```

Summary

- **Probability**
  - Why probability? What is probability?
  - **Random variable** ~ Mapping from events to numbers
  - Probability distribution
    - Representation: pmf (for discrete; ~ histogram), pdf (for continuous), cdf (for both)
    - e.g. Normal distribution (and the central limit theorem)
  - Joint probability, conditional probability, and marginal probability
    - Chain rule, Bayes' theorem, and law of total probability
  - Expectation, variance, covariance (~ variance of two or more variables), and correlation (~ normalized covariance)
- ~~Information Theory~~ **Cross Entropy**
  - Shannon information ~ The level of surprise (another representation of probability), but related to optimal coding
  - Entropy ~ The expectation of Shannon information
  - Cross entropy ~ Difference of two probability distributions