CSC380: Principles of Data Science

Statistics 1

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- Probability
- Statistics

- Data Visualization
- Predictive modeling
- Clustering

Outline

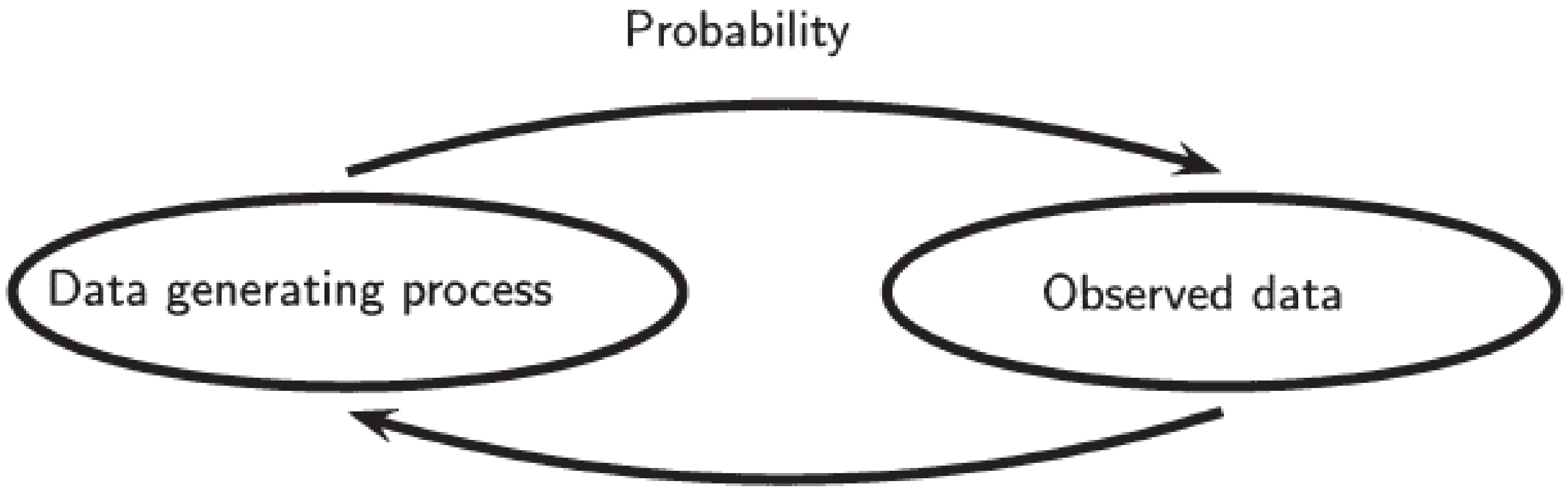
- Basic setup of parameter estimation
- Plug-in estimators
- Maximum-likelihood estimators

Probability and Statistics

Probability: ***Given a distribution****, compute probabilities of data/events.*

E.g., Given 5 fair coin flips, what is the probability of #heads ≥ 3?

e.g., data = outcome of coin flip



Inference / Estimation

E.g., We observed 5 flips of a coin H, T, T, T, T. How fair is the coin?

Statistics: ***Given data****, compute/infer the distribution or its properties.*

[Source: Wasserman, L. 2004]

Intuition Check

Suppose that we toss a coin 100 times. We don't know if the coin is fair or biased…

<u>Question 1</u> Suppose that we observe **<u>52</u>** heads and **<u>48</u>** tails. Is the coin fair? Why or why not?

Perhaps fair

<u>Question 2</u> Now suppose that out of 100 tosses we observed **<u>73</u>** heads and **<u>27</u>** tails. Is the coin fair? Why or why not?

Perhaps unfair

<u>Question 3</u> How might we estimate the bias of the coin with **<u>73</u>** heads and **<u>27</u>** tails?

Let's see..

Estimating Coin Bias

We can model each coin toss as a Bernoulli random variable,

$X \sim \text{Bernoulli}(p)$ => PMF

x=0	x=1
1-p	p

Recall that p is the coin bias (probability of heads) and that,

$$\mathbf{E}[X] = p$$

Suppose we observe N coin flips $x_1, \ldots, x_N$, estimate p using *sample mean*

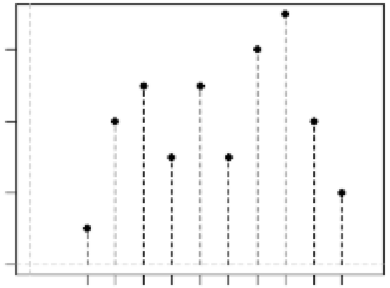
$$\hat{p} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

Why is this a good guess?

Law of large numbers $\Rightarrow \hat{p} \approx p$

Good & bad estimators

Example Estimate $\theta = \mu = \sum_x xf(x)$ for an unknown distribution



Say true $\theta = 3.5$

Our dataset X_1, X_2, X_3, X_4 are 3,6,5,-2.

Can try to estimate θ using *any function* of $X_1, \ldots, X_4$:

$\hat{\theta}_N$	$\frac{1}{4}\sum_{i=1}^{4} X_i$	$\frac{\min(X_1,..,X_4) + \max(X_1,..,X_4)}{2}$	$X_1 \cdot X_4$
	3	2	-6

Good & bad estimators

- Given an already-drawn sample, the quality of an estimator

e.g.

$$\frac{1}{4}\sum_{i=1}^{4} X_i \quad \text{or} \quad X_1 \cdot X_4$$

depends on the *representativeness* of the sample

Example Coin toss $X \sim \mathrm{Bernoulli}(p = 0.5)$

- If we are unlucky to observe 1, 1, 1, 1, then both estimators perform badly
- When we say "$\frac{1}{4}\sum_{i=1}^{4} X_i$ is a better estimator than $X_1 \cdot X_4$", what exactly do we mean?

Parameter Estimation: basic framework

We pose a model in the form of a probability distribution,
with unknown **parameters of interest** $\boldsymbol{\theta}$,

$$p_\theta$$

e.g. biased coin:
$\theta = p$
p_θ: Bernoulli(p)

Observe a sample of N *independent identically distributed (iid)* data points

$$x_1, \ldots, x_N \sim p_\theta,$$

e.g. one sample: 1, 0, 0, 0, 0
another draw of sample: 0, 1, 0, 1, 1

Find an **estimator** to estimate parameters of interest,

$$\hat{\theta}_N = r(x_1, \ldots, x_N)$$

e.g. sample mean

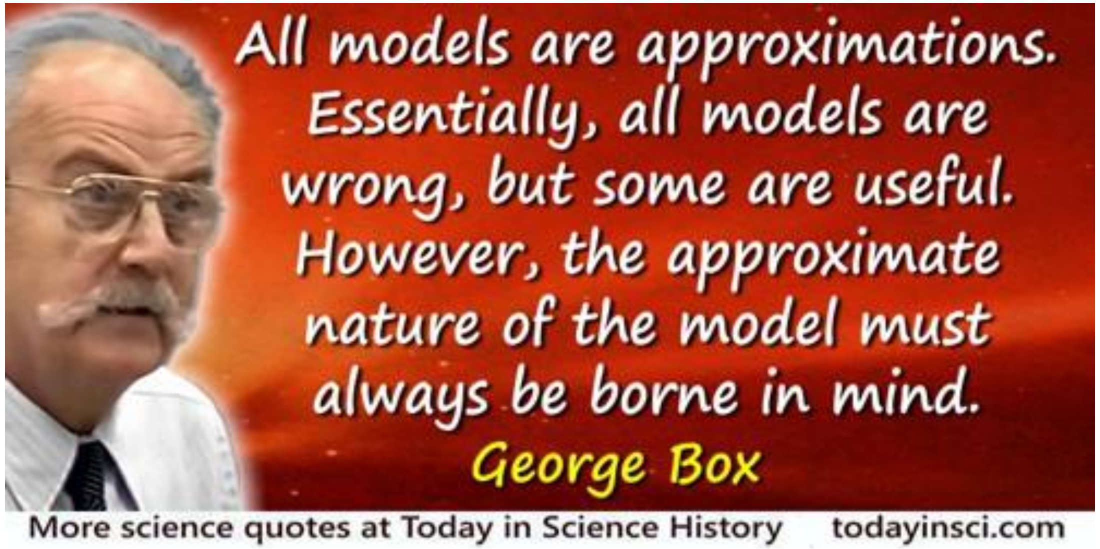
1/5 for the first dataset
3/5 for the second dataset

Note: θ fixed and unknown; $\hat{\theta}_N$ is a random variable

Parameter Estimation: basic framework

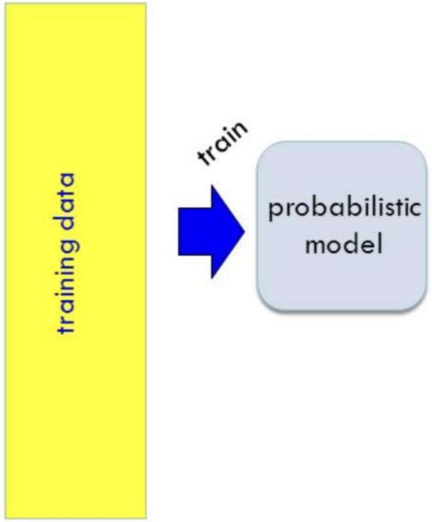
- We pose a model in the form of a probability distribution p_{θ}, with unknown **parameters of interest $\boldsymbol{\theta}$**

- Where do such models come from?
- Models are found by trial and errors in different applications



Bigger picture: Connection to Machine Learning

- Statistical inference is sometimes called “probabilistic machine learning”:
  1. Model how the data is generated by probabilistic models, but with parameters unspecified (modeling assumption / generative story)
  2. (Training) Learn the model parameter $\hat{\theta}$
  3. (Test) Make prediction / decision based on the learned model $P(z; \hat{\theta})$



In Statistics, we mostly stop at step 2

Machine Learning cares more about step 3: prediction & decision

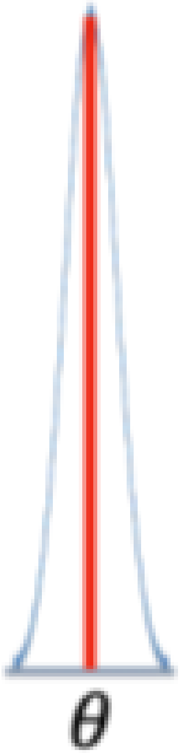
http://slideplayer.com/slide/4527958/

How good is an estimator

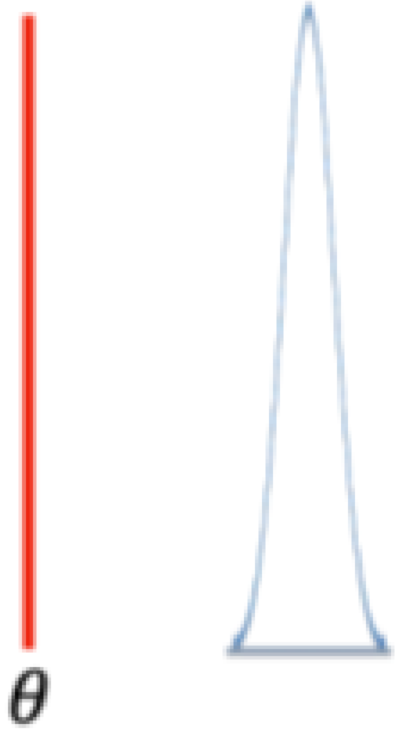
- We can get a sense of the quality of an estimator $\hat{\theta}_n$ by plotting its *probability distribution*

Recall: $\hat{\theta}_n$ *is a random variable*

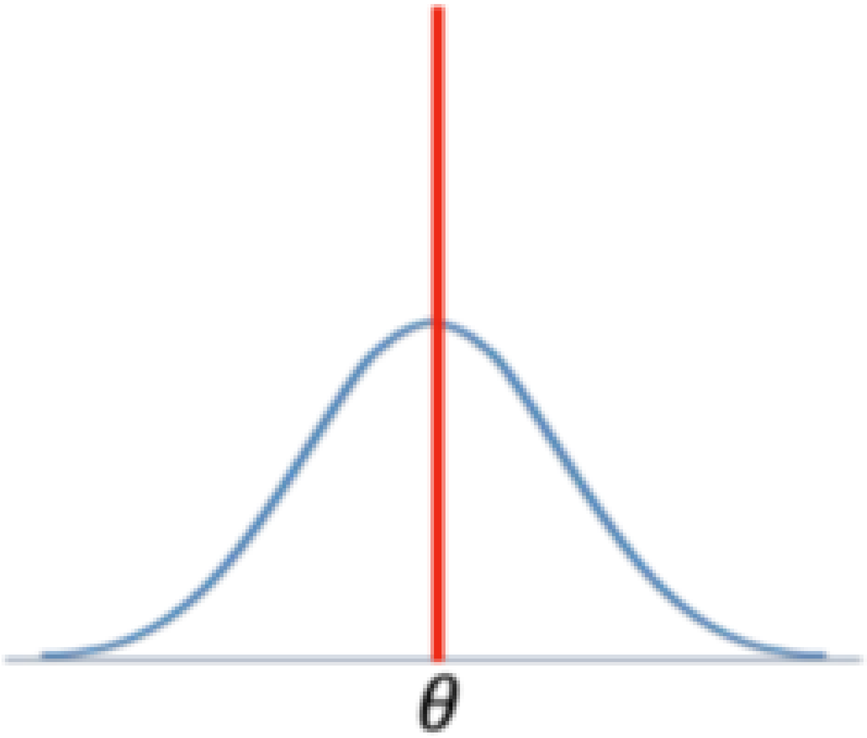
Distribution of $\hat{\theta}_n$



Good: have to be very unlucky to have a bad estimate



Bad



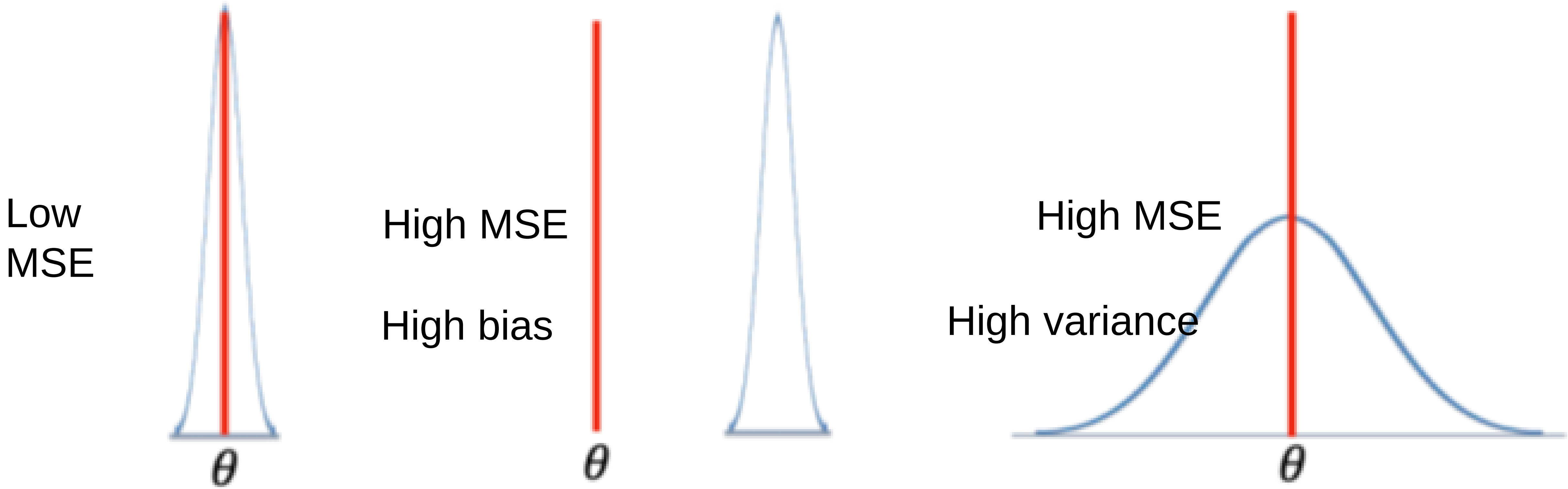
Bad

How good is an estimator

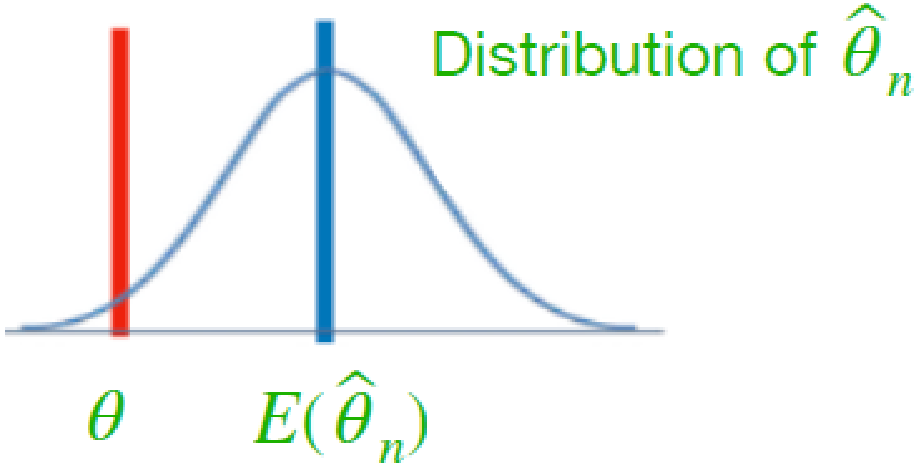
- Quantitatively, we can use the mean squared error (MSE) to measure the quality of an estimator

$$\mathrm{MSE} = \mathrm{E}\left[\left(\hat{\theta}_n - \theta\right)^2\right]$$

Distribution of $\hat{\theta}_n$



Bias



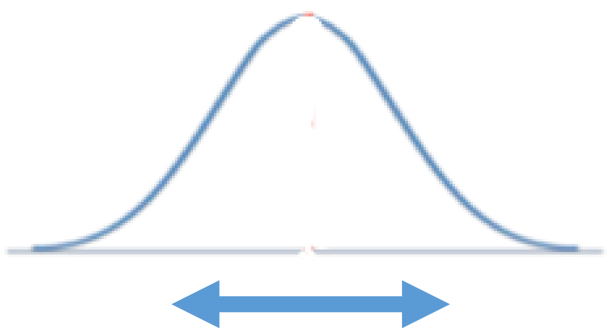
- Bias: expected overestimate of θ

- $\mathrm{Bias}(\hat{\theta}_n) = \mathrm{E}[\hat{\theta}_n] - \theta$
  also denoted as $\mu_{\hat{\theta}_n}$

- An estimator is *unbiased* if $\mathrm{Bias}(\hat{\theta}_n) = 0$

Variance

Distribution of $\hat{\theta}_n$



- Variance: how much $\hat{\theta}_n$ deviate from its mean

- $\mathrm{Var}\left(\hat{\theta}_n\right) = \mathrm{E}\left[(\hat{\theta}_n - \mathrm{E}\left[\hat{\theta}_n\right])^2\right]$

The bias-variance decomposition

Fact The MSE of an estimator $\hat{\theta}_n$ can be decomposed as:

$$\mathrm{MSE} = \mathrm{Bias}\left(\hat{\theta}_n\right)^2 + \mathrm{Var}\left(\hat{\theta}_n\right)$$

Justification

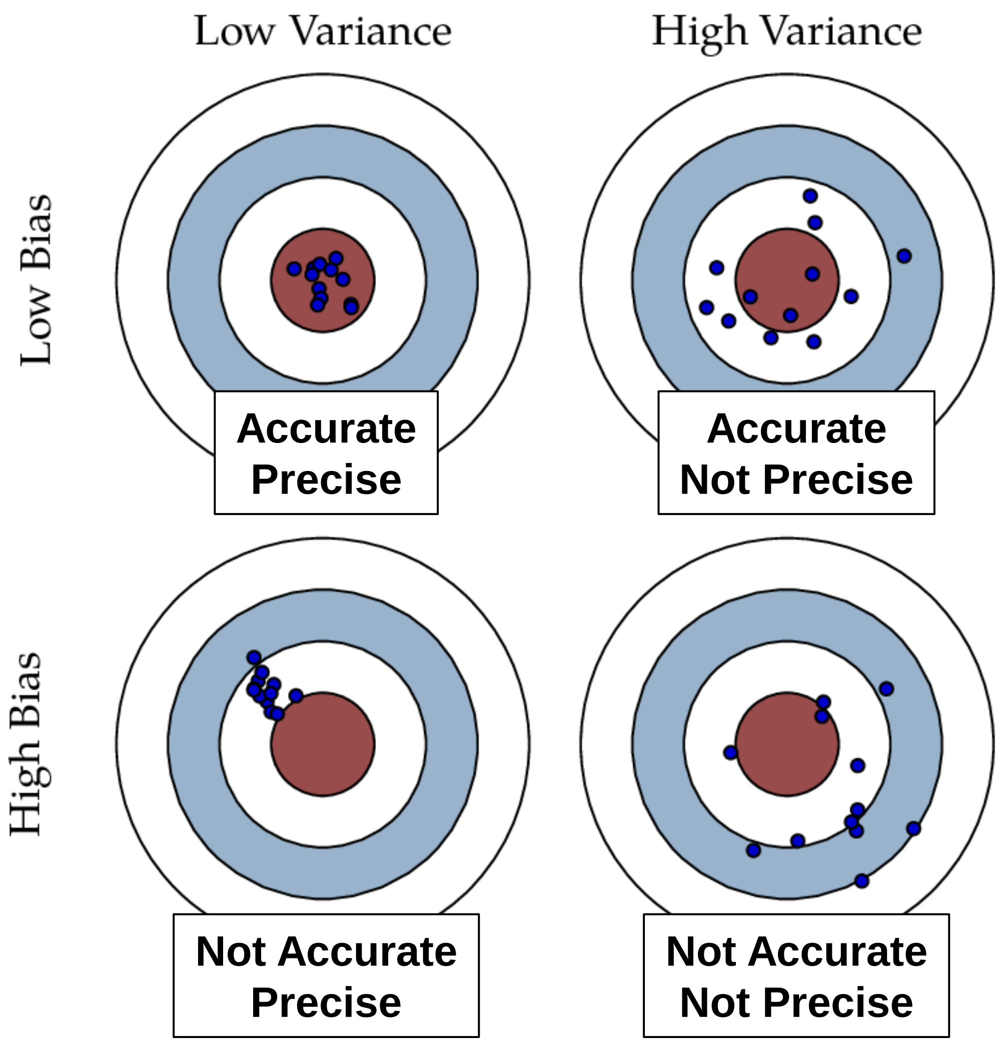
$\mu_{\hat{\theta}_n}$: the mean of $\hat{\theta}_n$

$$\mathrm{MSE} = \mathrm{E}\left[(\hat{\theta}_n - \mu_{\hat{\theta}_n} + \mu_{\hat{\theta}_n} - \theta)^2\right]$$

$$= \mathrm{E}\Big[\underbrace{(\hat{\theta}_n - \mu_{\hat{\theta}_n})^2}_{\text{Variance}} + \underbrace{(\mu_{\hat{\theta}_n} - \theta)^2}_{\text{Bias}} + \underbrace{2(\hat{\theta}_n - \mu_{\hat{\theta}_n})(\mu_{\hat{\theta}_n} - \theta)}_{\text{0 (why?)}}\Big]$$

Bias and Variance

Suppose an archer takes multiple shots at a target…



- Target = θ
- Each shot = an estimate $\hat{\theta}$

- Bias $\approx$ systematic error
- Variance $\approx$ random error

Coinflip

Example Observe n coin flips $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$

We use the sample mean $\bar{X}_n = \frac{1}{n}\sum_{i=1}^n X_i$ to estimate p. Find this estimator's bias, variance, MSE.

$$\mathrm{E}[\bar{X}_n] = \frac{1}{n}\sum_{i=1}^n \mathrm{E}[X_i] = p \Rightarrow \text{ Bias} = 0$$

$$\text{Var}[\bar{X}_n] = \frac{1}{n^2}\sum_{i=1}^n \text{Var}[X_i] = \frac{p(1-p)}{n}$$

$$p(1-p)$$

$$\text{MSE} = \text{Bias}^2 + \text{Variance} = \frac{p(1-p)}{n}$$

Coinflip: Laplace’s estimator

Example Observe n coin flips $X_1, \ldots, X_n \sim \mathrm{Bernoulli}(p)$

Consider another estimator $\hat{p}_B = \frac{1+\sum_i X_i}{2+n}$

e.g. 7 successes out of 10 trials,

sample mean $\bar{X}_n$: $\frac{7}{10} = 0.7$

new estimator $\hat{p}_B$: $\frac{8}{12} = 0.67$

This is called “Laplace’s Law of Succession” estimator

Laplace (1814) used it to estimate the probability of sun rising tomorrow

In-class exercise: bias & variance of Laplace's estimator

Example Observe n coin flips $X_1, \ldots, X_n \sim \mathrm{Bernoulli}(p)$

Consider another estimator $\hat{p}_B = \frac{1+\sum_i X_i}{2+n}$. Find the bias and variance of $\hat{p}_B$.

Solution

$$\mathrm{E}[\hat{p}_B] = \frac{1+\mathrm{E}[\sum_i X_i]}{2+n} = \frac{1+np}{2+n} \Rightarrow \ \mathrm{Bias} = \frac{1-2p}{2+n}$$

A biased estimator

$$\mathrm{Var}[\hat{p}_B] = \mathrm{Var}\left[\frac{\sum_i X_i}{2+n}\right] = \frac{1}{(2+n)^2}\sum_{i=1}^n \mathrm{Var}[X_i] = \frac{n\,p(1-p)}{(2+n)^2}$$

Smaller than that of sample mean

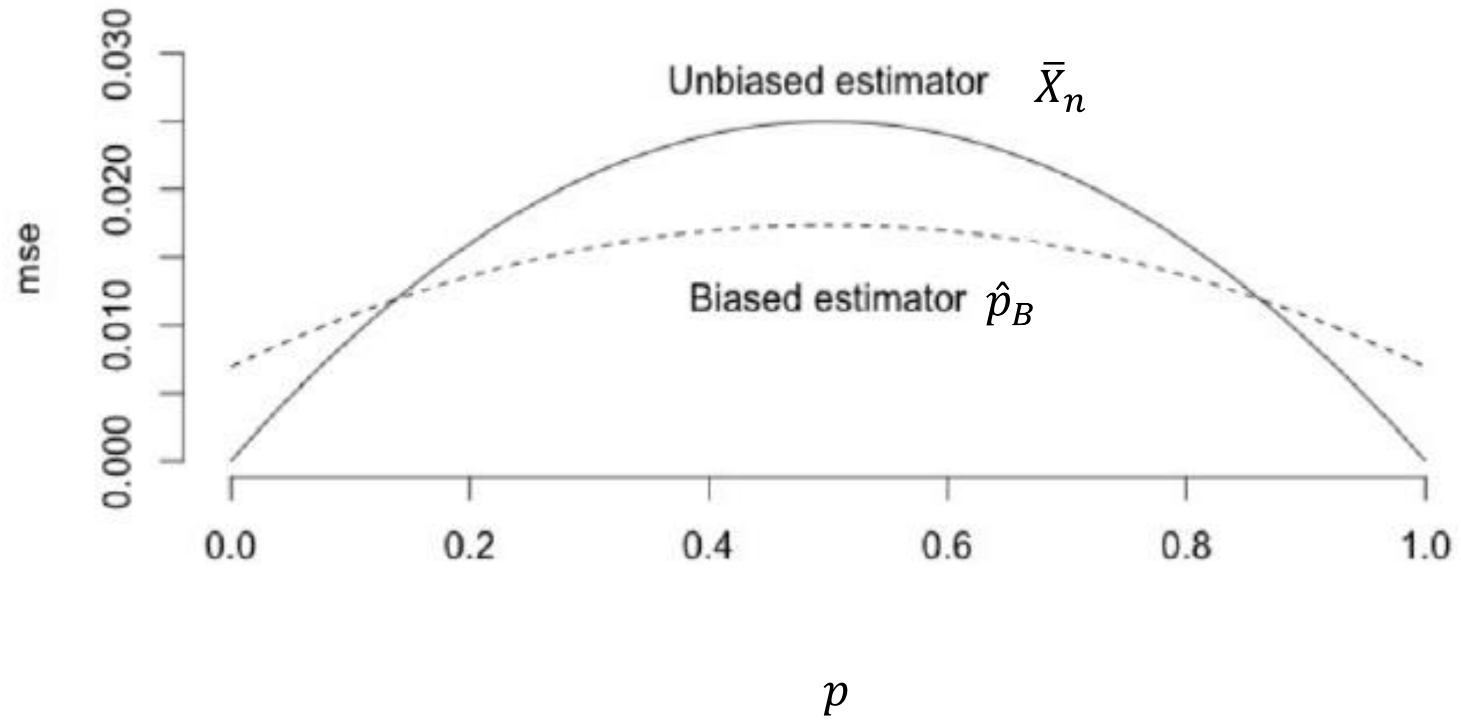
$$\text{MSE} = \mathrm{Bias}^2 + \mathrm{Variance} = \cdots$$

Comparison of two estimators

- Let's compare the two MSEs with n=10

- MSE of $\bar{X}_n$: $\frac{p(1-p)}{10}$

- MSE of $\hat{p}_B$: $\frac{1+6p-6p^2}{144}$



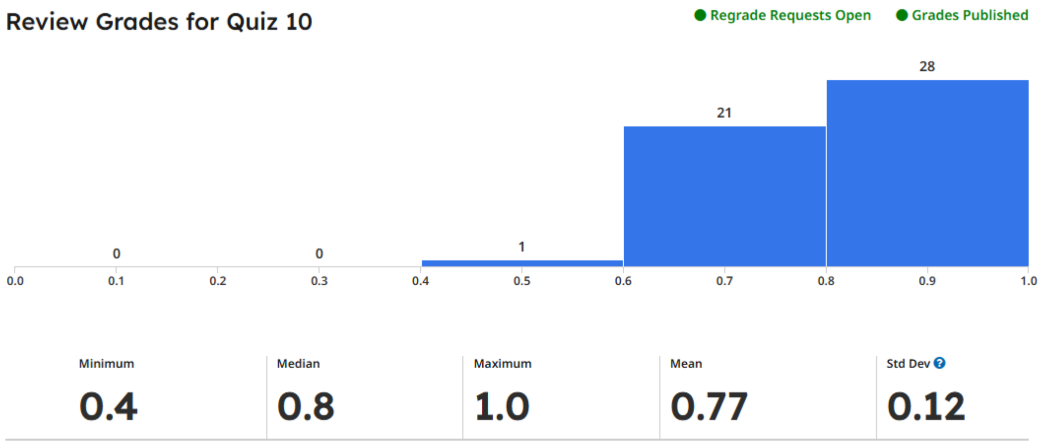
Is an unbiased estimator "better" than a biased one? It depends…

Announcements 4/23

- Project: If you analyze other interesting questions other than crimes, you are welcome to run them by me or the TAs.
  - We are generally happy to support the questions you are excited about!

- You're welcome to fill out SCS survey
  - 2nd lowest HW points will be dropped if we have >80% response rate

- Quiz 10 graded
  - if you don't see your grade on D2L let us know
- Quiz 11 next Monday



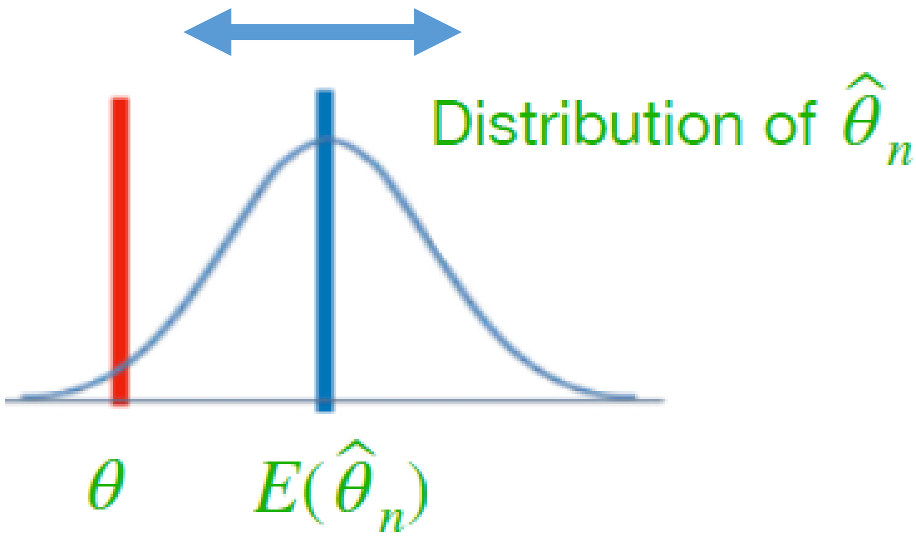
Recap 4/23

- The parameter estimation problem

$$\theta \;\rightarrow X_1, \dots, X_n \;\rightarrow \hat{\theta}_n$$

data generation process   estimator

- $\hat{\theta}_n$ is a random variable
- $\mathrm{Bias}(\hat{\theta}_n) = \mathrm{E}[\hat{\theta}_n] - \theta$



- $\mathrm{Var}(\hat{\theta}_n) = \mathrm{E}[(\hat{\theta}_n - \mathrm{E}[\hat{\theta}_n])^2]$
- $\mathrm{MSE} = \mathrm{Bias}(\hat{\theta}_n)^2 + \mathrm{Var}(\hat{\theta}_n)$
  - measures the overall quality of an estimator

Warmup question: coinflips

Example Observe n coin flips $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$

Consider a "blind" estimator $\hat{p} = \frac{1}{2}$.

What is $\hat{p}$'s bias and variance?

$$\text{Bias}(\hat{p}) = \text{E}[\hat{p}] - p = \frac{1}{2} - p$$

$$\text{Variance}(\hat{p}) = 0$$

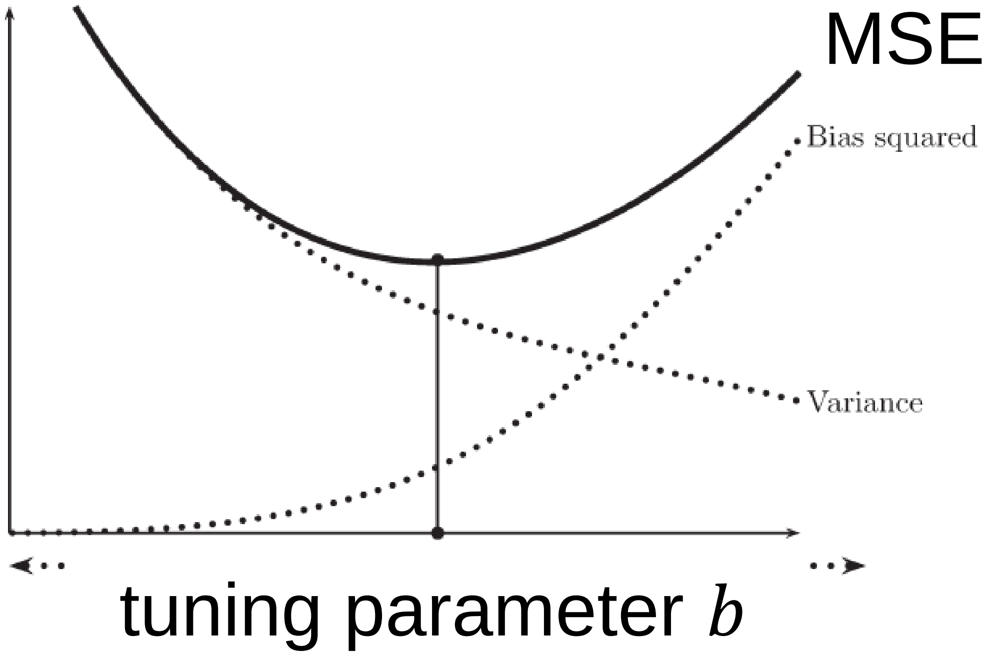
$$\text{MSE}(\hat{p}) = \text{Bias}(\hat{p})^2 + \text{Variance}(\hat{p}) = \left(\frac{1}{2} - p\right)^2$$

Bias-Variance Tradeoff

Consider a *family* of estimators $\hat{p}_b = \frac{b+\sum_i X_i}{2b+n}$ for coinflips

$b \uparrow \Rightarrow$ bias $\uparrow$, variance $\downarrow$

There is some ‘sweet spot’ in choosing b



This is known as bias-variance tradeoff

akin to bias-complexity tradeoff we saw in ML

Plug-in estimators

Plug-in estimators

Property of distribution: θ

Property of samples: $\hat{\theta}_N$

Mean: $\mu = \mathrm{E}[X] = \sum_x x f(x)$

Sample Mean: $\bar{X} = \frac{1}{N}\sum_{i=1}^{N} X_i$

Variance: $\sigma^2 = \mathrm{Var}[X] = \mathrm{E}[(X-\mu)^2]$

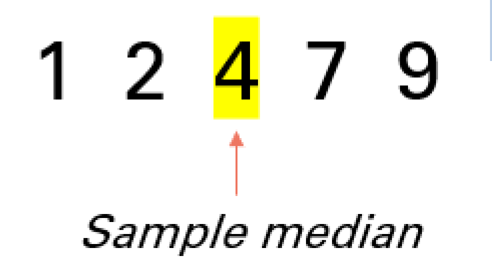
Sample Variance: $\widehat{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}(X_i - \mu)^2$?

$$\widehat{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}(X_i - \bar{X})^2$$

Correlation: $\rho(X,Y) = \frac{\mathrm{E}[(X-\mu_X)(Y-\mu_Y)]}{\sqrt{E[(X-\mu_X)^2]E[(Y-\mu_Y)^2]}}$

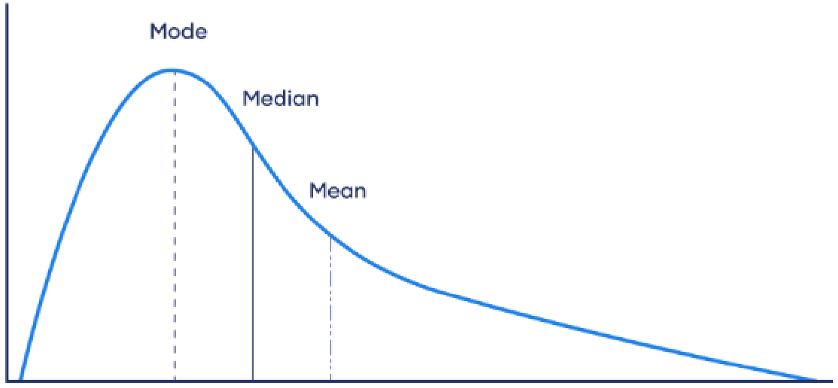
Sample Correlation: $\frac{\frac{1}{N}\sum_i (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(X_i-\bar{X})^2 \frac{1}{N}\sum_{i=1}^{N}(Y_i-\bar{Y})^2}}$

Plug-in estimators



What is the sample median estimating?

- Median of data distribution $F^{-1}\left(\frac{1}{2}\right)$



What is the sample mode estimating?

- Mode of data distribution $\operatorname{argmax}_x f(x)$

What is the sample minimum estimating?

- The minimum possible value that can be taken $\min\{x: f(x) > 0\}$

Sample variance estimator

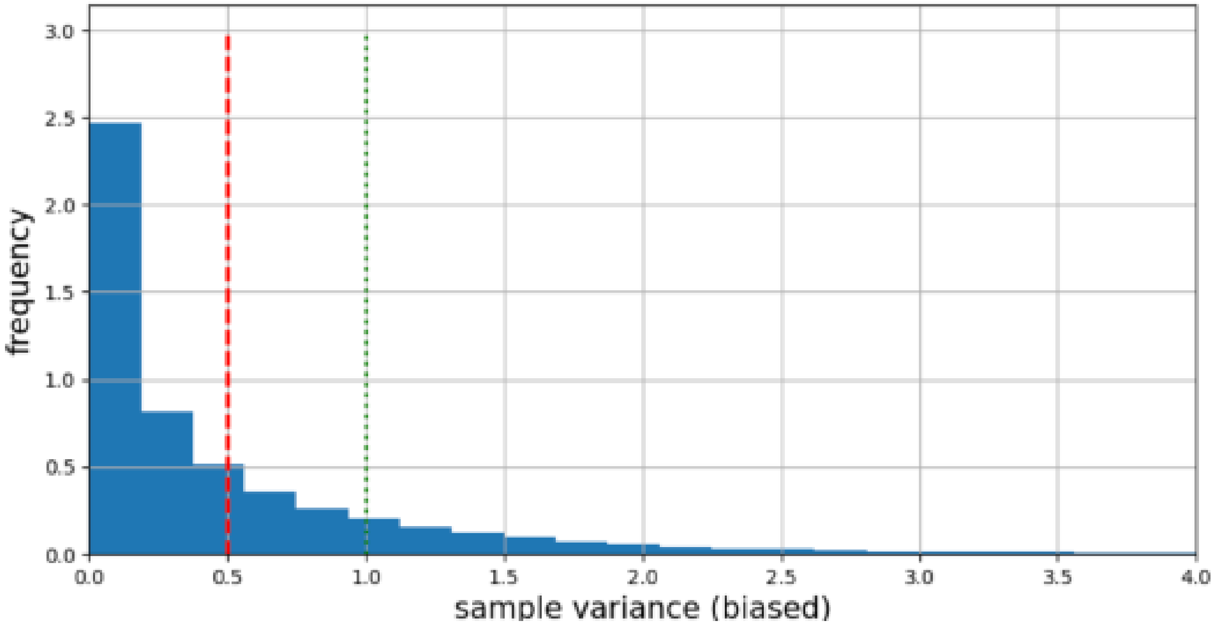
- Using $\widehat{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}(X_i - \bar{X})^2$ to estimate population variance σ^2, $N = 2$

```
n=2
s = 100000
X = np.random.normal(0,1,[n,s])
# ddof is 0(1) for dividing by n (n-1)
svar_b = np.var(X,axis=0,ddof=0)
mean_svar_b = np.mean(svar_b)
```

True σ^2: 1.0

$\widehat{\sigma^2}$'s mean: 0.5

$\widehat{\sigma^2}$ is a biased estimator of σ^2!



Sample variance estimator

- **Fact** $\mathrm{E}[\widehat{\sigma^2}] = \frac{N-1}{N}\sigma^2$ see reading for more details

- I.e. $\widehat{\sigma^2}$ has bias $\frac{N-1}{N}\sigma^2 - \sigma^2 = -\frac{1}{N}\sigma^2$
  - the bias can be significant if the sample size N is small

- How can we make it unbiased?

  Scale it: $\widehat{\sigma_1^2} = \frac{N}{N-1}\widehat{\sigma^2} = \frac{1}{N-1}\sum_{i=1}^{N}(X_i - \overline{X})^2$

Sample variance estimator

- Using $\widehat{\sigma_1^2} = \frac{1}{N-1}\sum_{i=1}^{N}(X_i - \bar{X})^2$ to estimate population variance σ^2, $N = 2$

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n=2
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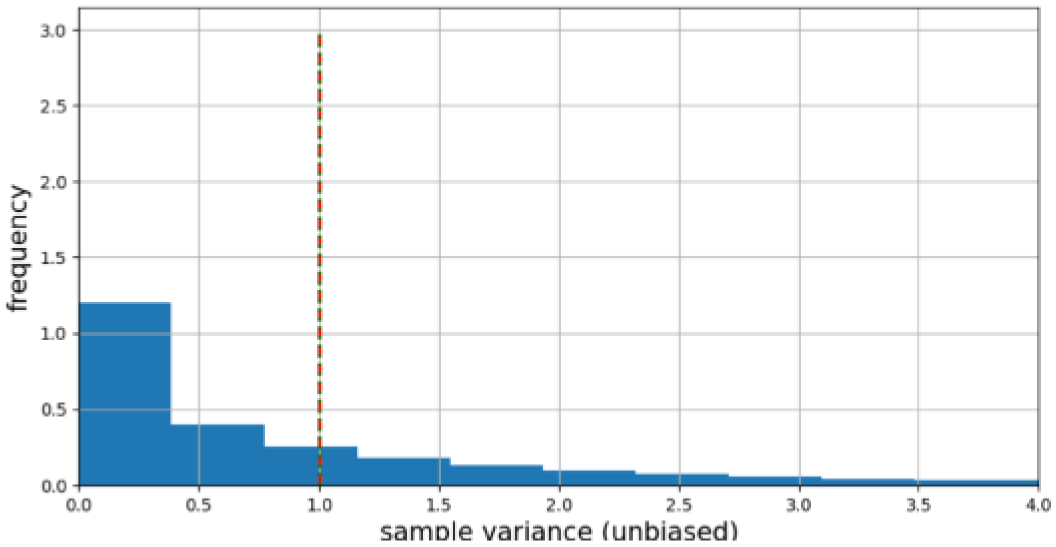
X = np.random.normal(0,1,[n,s])
# ddof is 0(1) for dividing by n (n-1)
svar_b = np.var(X,axis=0,ddof=1)
mean_svar_b = np.mean(svar_b)
```

True σ^2: 1.0

$\widehat{\sigma_1^2}$'s mean: 1.0

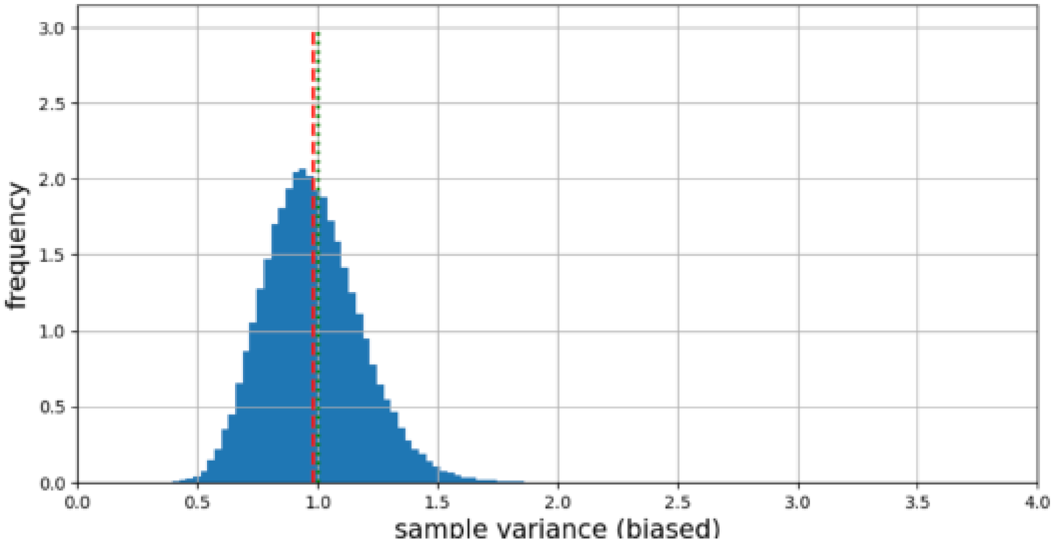
$\widehat{\sigma_1^2}$ is an unbiased estimator of σ^2



Sample variance estimator

- For large N, $\widehat{\sigma^2}$ has negligible bias, and is close to $\widehat{\sigma_1^2}$

```
n=50
s = 100000
X = np.random.normal(0,1,[n,s])
# ddof is 0(1) for dividing by n (n-1)
svar_b = np.var(X,axis=0,ddof=0)
mean_svar_b = np.mean(svar_b)
```



Maximum likelihood estimators

Likelihood

- Likelihood: joint probability of observing this sample given model parameter

Example 4 flips of a coin -> [H, T, H, H].

What is the likelihood of observing this sample if p = 0.75?

$$0.75^3 \; 0.25^1$$

Larger

What is the likelihood of observing this sample if p = 0.25?

$$0.25^3 \; 0.75^1$$

Larger likelihood seems to correspond to more plausible model

Maximum likelihood estimators (MLE)

- Likelihood function: joint PMF / PDF of the data as a function of unknown parameter θ
- Let $X_1, \dots, X_n$ be an iid sample with PMF / PDF $f(x;\theta)$

$$L(\theta) = \prod_{i=1}^{n} f(X_i;\theta)$$

How well θ "explains" data point X_i

- The maximum likelihood principle: find parameter θ that maximizes the likelihood
- Equivalently, we try to find θ that maximizes log-likelihood $\ln L(\theta)$

$$\ln L(\theta) = \sum_{i=1}^{n} \ln f(X_i;\theta)$$

Maximum likelihood estimator: coin flip

Example $X_1, \dots, X_n \sim \text{Bernoulli}(p)$. Find the MLE for p.

x=0	x=1
1-p	p

E.g. $1, 0, 1, 1,$

$L(p) = p \cdot (1-p) \cdot p \cdot p$

Solution $L(p) = \prod_{i=1}^{n} f(X_i; p) = p^{n_1}(1-p)^{n_0}$

here, n_0 and n_1 are the number of 0's and 1's in the sample

We would like to solve $\text{maximize}_{p\in[0,1]}\ p^{n_1}(1-p)^{n_0}$

Equivalently, $\text{maximize}_{p\in[0,1]} n_1 \ln p + n_0 \ln(1-p)$

Math Interlude: optimization problems

p: **Optimization variables**

$p \in [0,1]$: **constraint**

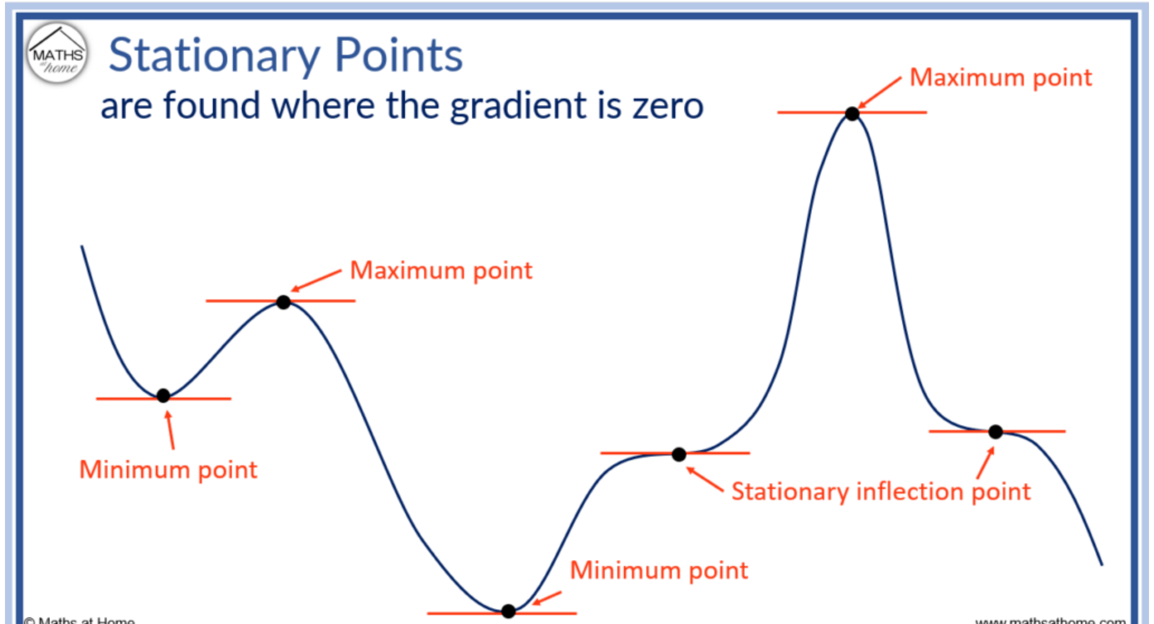
- Recall: $\text{maximize}_{p\in[0,1]} n_1 \ln p + n_0 \ln(1-p)$

is a constrained optimization problem

Note Setting the objective's derivative to zero and solve for p gives a *stationary point*, but

- It may be local maximum, or even *local minimum*
- It may fall out of constraint set

- We recommend always plotting the objective function to check



Maximum likelihood estimator: coin flip

$$\text{maximize}_{p\in[0,1]} n_1 \ln p + n_0 \ln(1-p)$$

- E.g. when $n_0 = 1, n_1 = 3$, we have:

- Its global maximizer indeed lie in its only stationary point

Stationary point can be found by

$$\frac{n_1}{p} - \frac{n_0}{1-p} = 0 \qquad \Rightarrow p = \frac{n_1}{n_1+n_0} = \frac{n_1}{n} = \text{sample mean}$$

Maximum likelihood for Fixed-variance Gaussians

Example Assume that UA students' heights (in centimeters) follow $N(\mu, 8^2)$, and we observe 4 students' heights:

163, 171, 179, 167

Find the maximum likelihood estimator for μ

Solution

Step 1: write down the log-likelihood function

$$\ln L(\mu) = \sum_{i=1}^{n} \ln f(x_i; \mu) \qquad f(x_i; \mu) = \frac{1}{\sqrt{2\pi 8^2}} \exp\left(-\frac{(x_i - \mu)^2}{2 \times 8^2}\right)$$

the sum has 4 terms -- e.g. the first term is $\ln \frac{1}{\sqrt{2\pi 8^2}} - \frac{(163-\mu)^2}{2\times 8^2}$

Maximum likelihood for Fixed-variance Gaussians

- **Step 2: simplify the log-likelihood function**

4 samples: 163, 171, 179, 167

$$\ln L(\mu) = \sum_{i=1}^{n} \left(\ln \frac{1}{\sqrt{2\pi 8^2}} - \frac{(x_i - \mu)^2}{2 \times 8^2} \right)$$

$$= -\frac{1}{128} \sum_{i=1}^{4} (x_i - \mu)^2 - 11.99$$

- **Step 3: find** μ that maximizes log-likelihood:

Recall Fact the μ that minimizes $\sum_{i=1}^{4} (x_i - \mu)^2$ is $\mu = \bar{x}$

the μ that maximizes $L(\mu)$ is $\bar{x} = \frac{163+171+179+167}{4} = 170$

Maximum likelihood for Fixed-variance Gaussians

Summary given the data we have, we estimate that UA students' heights follow $N(170, 8^2)$

How would you use it to predict an unseen UA student's height?

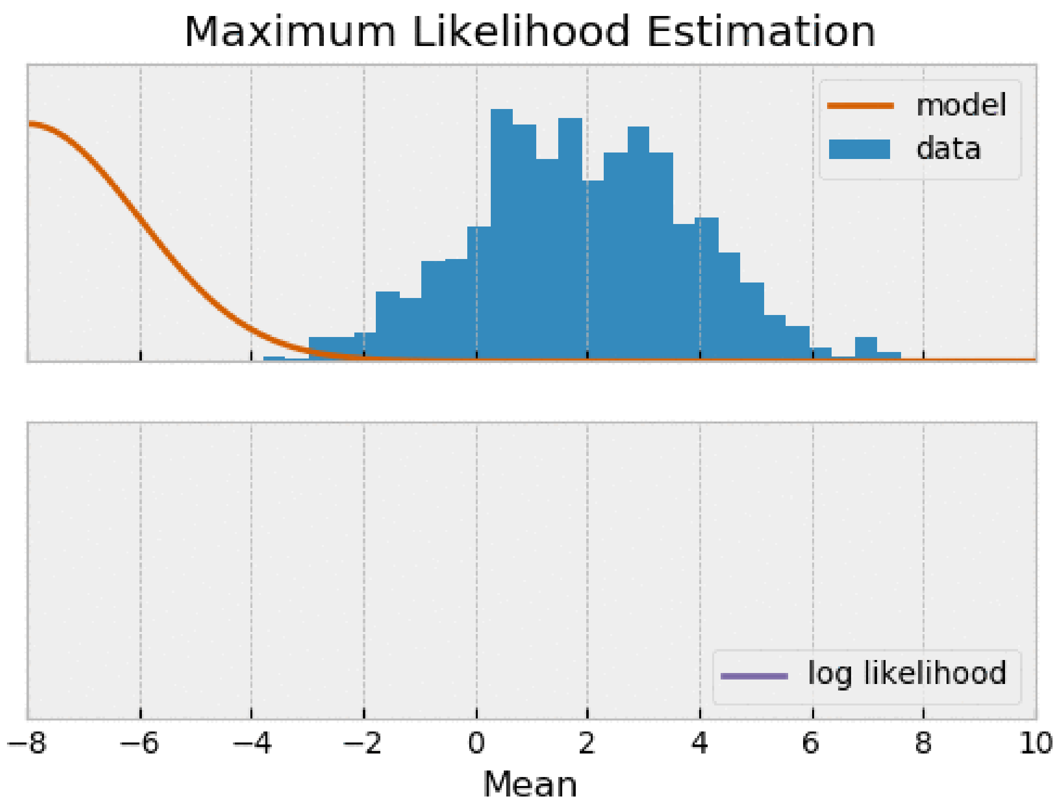
perhaps 170cm is a decent guess..

General Fact Fixed σ (e.g. $\sigma = 8$). Assume samples $x_1, \ldots, x_n$ are drawn from $N(\mu, \sigma^2)$. Then the MLE for μ is sample mean

$$\bar{x} = \frac{x_1 + \cdots + x_n}{n}$$

Maximum likelihood for Fixed-variance Gaussians

Among all $N(\mu, \sigma^2)$'s, $\mu = \bar{x}$ has the highest likelihood

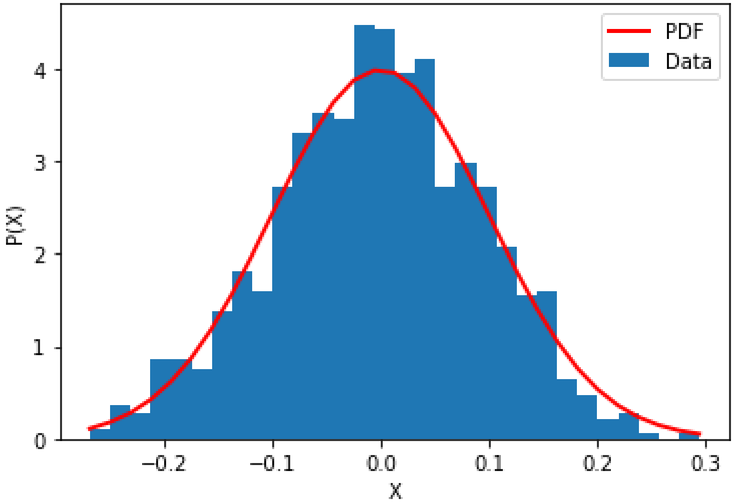


Maximum likelihood for General Gaussians

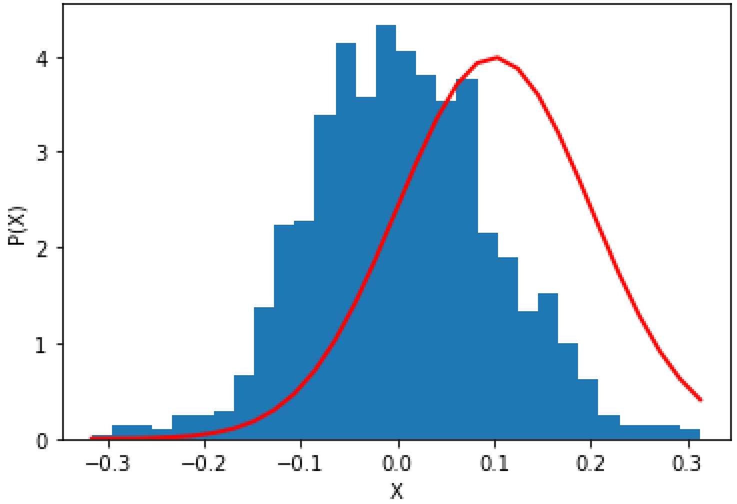
Suppose we observe n data points from a Gaussian model $N(\mu, \sigma^2)$
and wish to estimate **both $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$**

Say we only need to choose from the following three Gaussians…

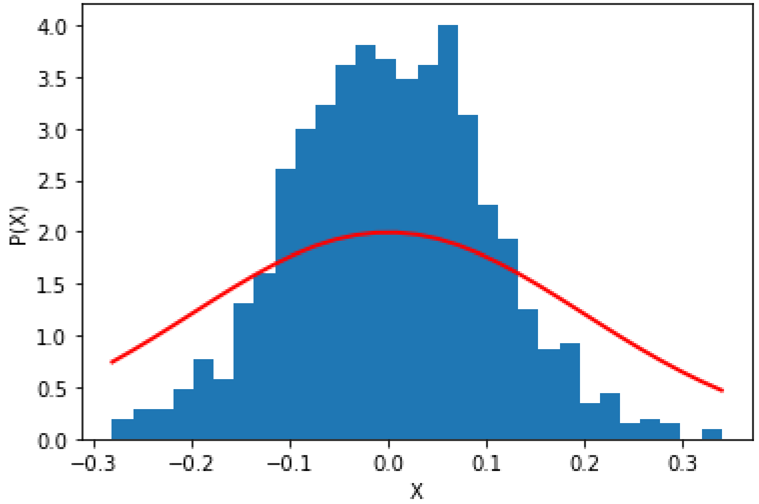
High Likelihood



Low Likelihood (mean)



Low Likelihood (variance)



Here, $L(\mu, \sigma^2) = \prod_{i=1}^{n} f(x_i; \mu, \sigma)$

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

Maximum likelihood for General Gaussians

Fact Assume samples $x_1, \ldots, x_n$ are drawn from $N(\mu, \sigma^2)$. Then the MLE for μ, σ is given by:

$$\mu = \bar{x} \text{ (sample mean)}$$

$$\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2} \text{ (sample standard deviation)}$$

Example Assume that UA students' weights (in kg) follow a Gaussian, and we observe 4 students' weights: 60, 65, 70, 75

The MLE $\mu = \frac{60+65+70+75}{4} = 67.5$,

MLE $\sigma = \cdots = 5.6$

Therefore our estimate of UA students' weights $\sim N(67.5, 5.6^2)$

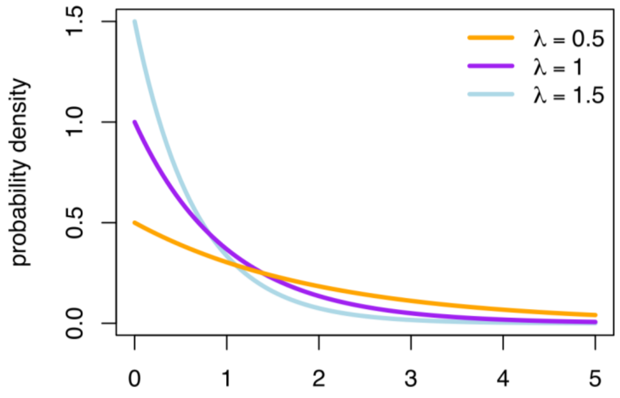
Maximum likelihood: in-class exercise

Wait time at the barbershop: Suppose you go to a barbershop every quarter. You want to be able to predict the waiting time. You have collected 4 data points (in minutes) from last year:

3, 2, 6, 5

Suppose we model the waiting time using an exponential distribution $\mathrm{Exponential}(\lambda)$:

$$f(x) = \lambda e^{-\lambda x}$$



- Find the maximum likelihood estimator for λ
- How would you use this to predict your next waiting time?

Maximum likelihood: in-class exercise

Step 1: write down the log-likelihood function

$$\ln L(\lambda) = \sum_{i=1}^{n} \ln f(x_i; \lambda)$$

$$f(x; \lambda) = \lambda e^{-\lambda x}$$

Step 2: simplify the log-likelihood function

$$\ln L(\lambda) = \sum_{i=1}^{n} (\ln \lambda - \lambda\, x_i) = n \ln \lambda - \lambda \sum_{i=1}^{n} x_i$$

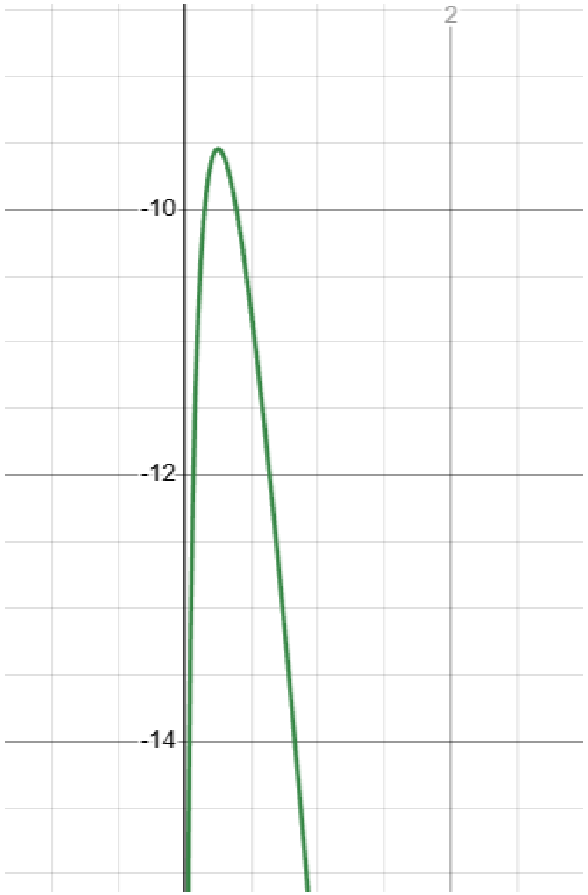
for our dataset, this is

Dataset: 3, 2, 6, 5

$$4 \ln \lambda - \lambda(3 + 2 + 6 + 5) = 4 \ln \lambda - 16\, \lambda$$

Maximum likelihood: in-class exercise

- **Step 3: maximize the log-likelihood function**



Maximize $L(\lambda) = 4 \ln \lambda - 16 \lambda$

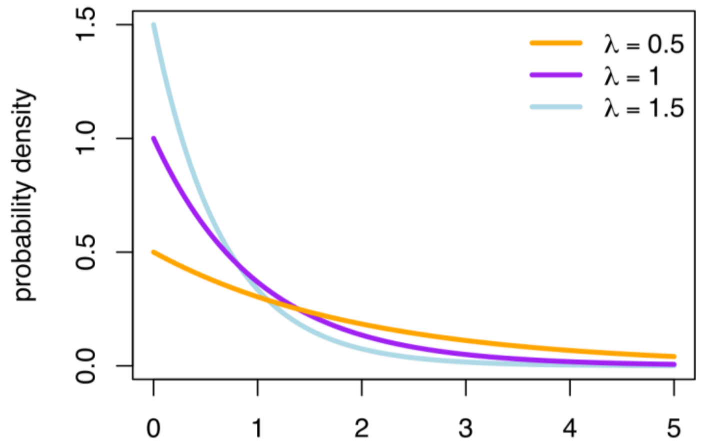
It has only one stationary point,
which corresponds to its maximum

can be found by solving $L'(\lambda) = 0$

$$\frac{4}{\lambda} - 16 = 0 \qquad \Rightarrow \lambda = \frac{1}{4}$$

Maximum likelihood: in-class exercise

Summary given the data, we estimate the waiting time to follow the $\text{Exponential}\left(\lambda = \frac{1}{4}\right)$ distribution



How would you use this to predict your next waiting time?

We can use the mean of our learned distribution:

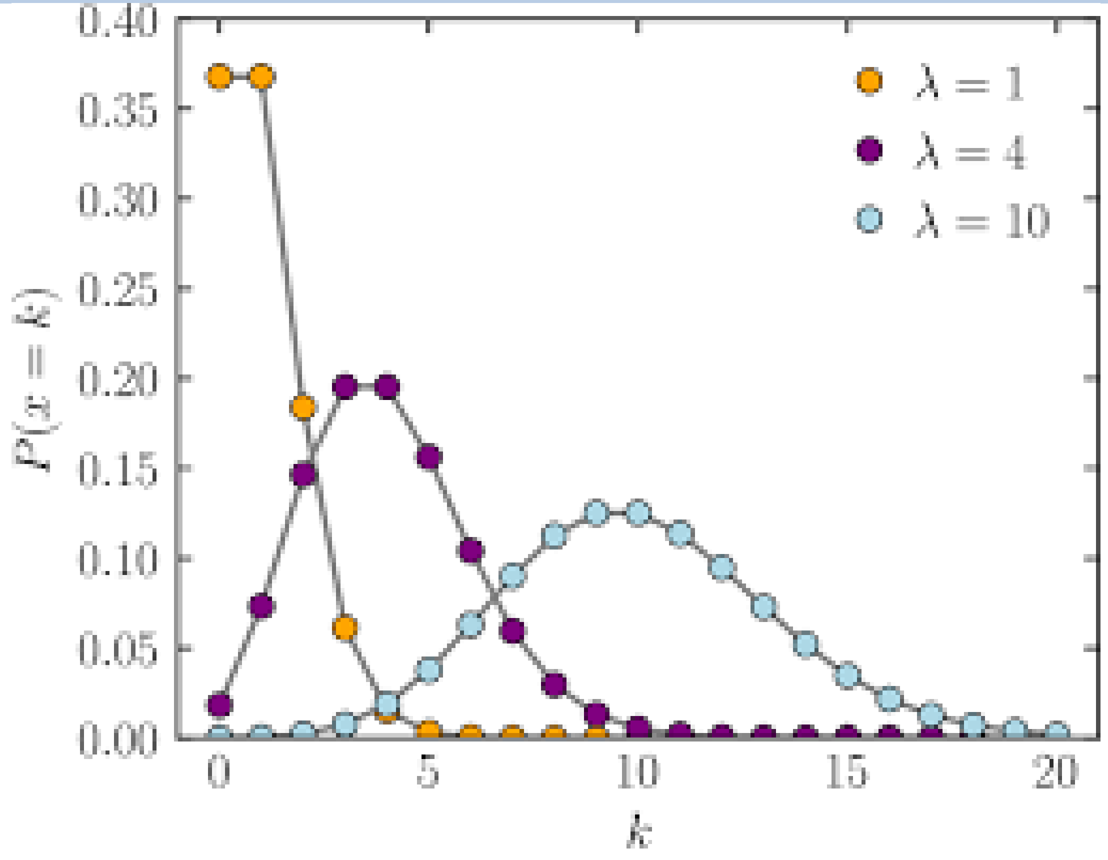
$$\frac{1}{\lambda} = 4 \text{ (minutes)}$$

Poisson distribution

$$P(X = x) = e^{-x}\frac{\lambda^x}{x!}, \qquad x = 0, 1, ..$$

Models:

- #meteorites greater than 1-meter diameter that strike Earth in a year
- #laser photons hitting a detector in a time interval
- #calls received in a call center in a time interval



Named after Poisson (1837)

Recherches sur la probabilité des jugements en matière criminelle et en matière civile

Backup