CSC380: Principles of Data Science

Statistics 3

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Review: Maximum Likelihood Estimation

Suppose $x_i \sim p(x;\theta)$, the **joint probability** over N i.i.d $x_1, \ldots, x_N$

$$p(x_1, \ldots, x_N; \theta) = \prod_{i=1}^{N} p(x_i; \theta)$$

Maximum Likelihood Estimator (MLE) as the name suggests, maximizes the likelihood function.

$$\hat{\theta}^{\mathrm{MLE}} = \arg\max_{\theta} \mathcal{L}_N(\theta) = \prod_{i=1}^{N} p(x_i; \theta)$$

Log Likelihood Maximum

$$\hat{\theta}^{\mathrm{MLE}} = \arg\max_{\theta} \; \log \mathcal{L}_N(\theta) = \sum_{i=1}^{N} \log p(x_i; \theta)$$

Finding the MLE:

1. closed-form
2. iterative methods

Maximum Likelihood Estimator Properties

1) The MLE is a **consistent** estimator:

$$\lim_{n\to\infty} \hat{\theta}_n^{\mathrm{MLE}} \xrightarrow{P} \theta_*$$

Roughly, converges to the true value.

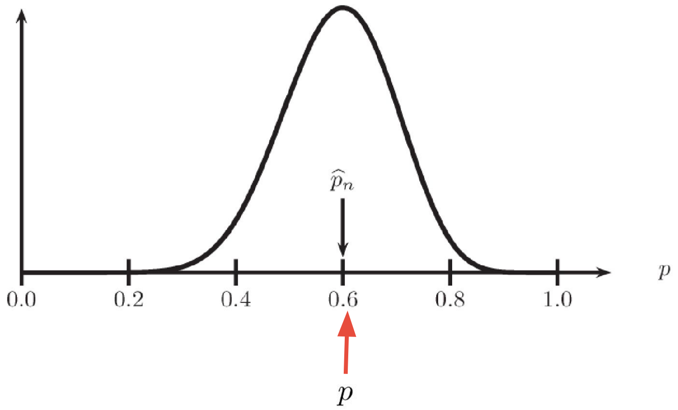
2) The MLE is **efficient**: roughly, has the lowest mean squared error among all consistent estimators.

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

3) The MLE is **Normal**: roughly, the estimator (which is a <u>random variable</u>) approaches a Normal distribution.

Maximum Likelihood Estimator Properties

3) The MLE is **Normal**: roughly, the estimator (which is a random variable) approaches a Normal distribution.



- We pick k different samples (each sample has N i.i.d observations)
- We pose a model with unknown parameter
- Get MLE estimation for the parameter (a total of k estimators)
- The distribution of k estimators is roughly normal distribution
    - Expectation
    - Variance

Q: for sample mean, what's E[X] and Var[X]?

Sample Mean: Expectation and Variance

Review: Bernoulli Expectation and Variance

Bernoulli *A.k.a. the* ***coinflip*** *distribution on* <u>*binary*</u> *RVs* $X \in \{0, 1\}$

$$p(X) = \pi^X (1-\pi)^{(1-X)}$$

$$\boxed{\mathbf{Var}[X] = \mathbf{E}[X^2] - (\mathbf{E}[X])^2}$$

Where π *is the probability of* ***success*** *(i.e., heads), and also the mean*

$$\mathbf{E}[X] = \pi \cdot 1 + (1-\pi) \cdot 0 = \pi$$

$$\mathbf{Var}[X] = \pi(1-\pi)$$

$$E[X^2] = \pi \cdot 1^2 + (1-\pi) \cdot 0^2 = \pi$$

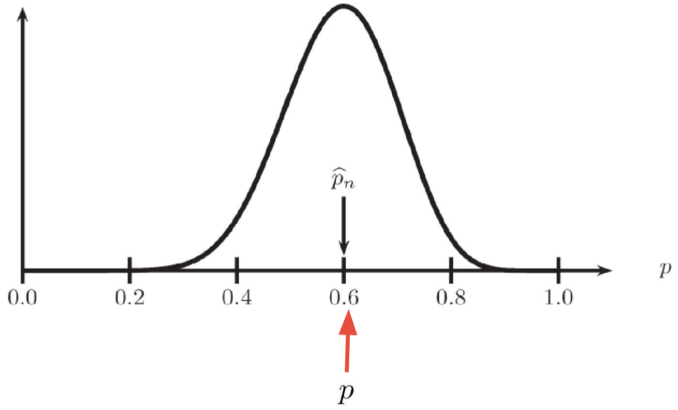
$$Var[X] = \pi - \pi^2$$

Expectation of the Sample Mean

Recall: An estimator $\hat{\theta}$ is a RV (Random Variable).

Example Let $X_1, \ldots, X_N \overset{\text{iid}}{\sim} \text{Bernoulli}(p)$
and estimate $\hat{p}$ be the *sample mean*,

$$\hat{p} = \frac{1}{N} \sum_i X_i$$



Question What is the expected value of $\hat{p}$?

Notation: $X := (X_1, \ldots, X_N)$

$$\mathbf{E}[\hat{p}(X)] = \mathbf{E}\left[\frac{1}{N}\sum_i X_i\right] \overset{(a)}{=} \frac{1}{N}\sum_i \mathbf{E}\left[X_i\right] \overset{(b)}{=} \frac{1}{N} Np = p$$

(a) Linearity of Expectation Operator

(b) Mean of Bernoulli RV = p

Conclusion *On average* $\hat{p} = p$ *(it is unbiased)*

Variance of the Sample Mean

Example Let $X_1, \ldots, X_N \overset{\text{iid}}{\sim} \text{Bernoulli}(p)$ and estimate $\hat{p}$ be the *sample mean.* Calculate the variance of $\hat{p}$:

quiz candidate

$$\mathbf{Var}(\hat{p}) = \mathbf{Var}\left(\frac{1}{N}\sum_i X_i\right) \overset{(a)}{=} \frac{1}{N^2}\mathbf{Var}\left(\sum_i X_i\right) \overset{(b)}{=} \frac{1}{N^2}\sum_i \mathbf{Var}\left(X_i\right)$$

$$\overset{(c)}{=} \frac{1}{N^2}\sum_i p(1-p) = \frac{1}{N}p(1-p) = \frac{1}{N}\mathbf{Var}(X)$$

(a) $\mathbf{Var}(cX) = c^2\mathbf{Var}(X)$ (b) Independent RVs (c) Var(X) = p(1-p) for Bernoulli

In General Variance of sample mean $\bar{X}$ for RV with variance σ^2;

STDEV of sample mean decreases as $1/\sqrt{N}$

$$\mathbf{Var}(\bar{X}) = \frac{\sigma^2}{N}$$

Decreases linearly with number of samples N

All Facts about Sample Mean

<u>Experiment</u> Flip a coin 100 times and observe 73 heads, 27 tails

- We don’t know the coin bias. By intuition, we guess coin bias is sample mean 0.73.
- We are told that maximum likelihood estimation is a method that can estimate the parameter of an assumed probability distribution.
- So we pose a model of bernoulli, and calculate the estimator that can maximum the log likelihood function.
- We find the maximum likelihood estimator is sample mean = our intuition!

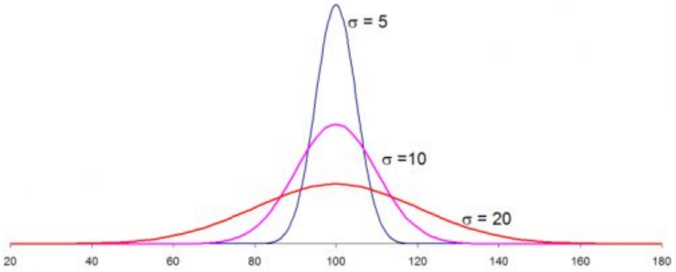
All Facts about Sample Mean

<u>Experiment</u> Flip a coin 100 times and observe 73 heads, 27 tails

- If we repeatedly flip a coin 100 times (N=100), say 1000 trails (1000 samples). We will get 1000 sample means. So sample mean is also a RV. It has a distribution.

- Pile 1000 sample means up, we get a distribution (roughly normal). The mean of the distribution (expectation) = true coin bias.

- If we flip a coin 10,000 times (N=10,000), repeat for 1000 trails (1000 samples). The variance of the distribution is very small. We can trust the sample mean more when estimating true coin bias



Sample Variance: Expectation

Unbiasedness of the Sample Variance?

Recall: Sample mean is an unbiased estimator for the true mean.
How about the sample variance?

Ex. Let $X_1, \ldots, X_N$ be drawn (iid) from any distribution with $\mathbf{Var}(X) = \sigma^2$ and,

$$\hat{\sigma}^2 = \frac{1}{N} \sum_i (X_i - \hat{\mu})^2$$

Then the sample variance is a **biased estimator**.

Source of bias: plug-in mean estimate

$$\mathbf{E}[\hat{\sigma}^2] = \frac{1}{N} \sum_i \mathbf{E}\left[(X_i - \hat{\mu})^2\right] = \text{boring algebra} = \frac{N-1}{N}\sigma^2$$

tends to underestimate

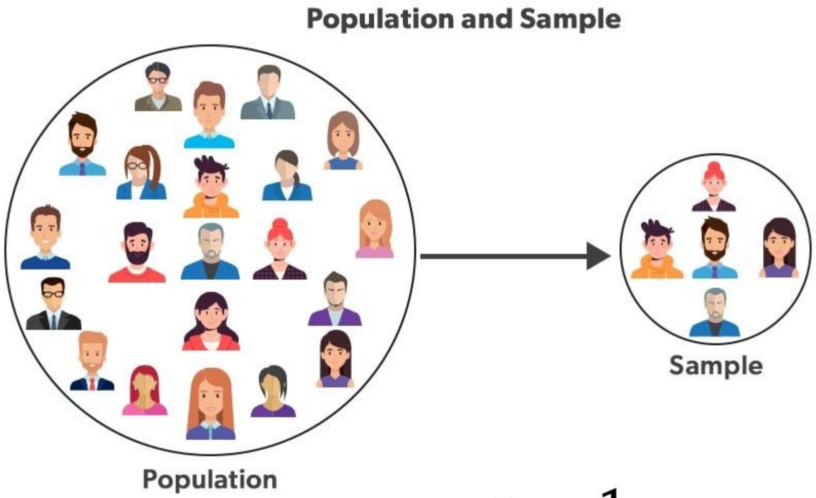
Q: is this estimator consistent or not?

Consistent!

Correcting bias yields unbiased variance estimator:

$$\hat{\sigma}^2_{\text{unbiased}} = \frac{N}{N-1}\hat{\sigma}^2 = \frac{1}{N-1} \sum_i (X_i - \hat{\mu})^2 \qquad E\left[\hat{\sigma}^2_{unbiased}\right] = \sigma^2$$

Sample Variance estimator vs MLE estimator



$\hat{\mu}, \hat{\sigma}$

Pose a Gaussian model with unknown parameters: μ, σ

$$\hat{\sigma}^2 = \frac{1}{n}\sum_i (x_i - \hat{\mu})^2$$ MLE: Biased

$$\hat{\sigma}^2_{unbiased} = \frac{1}{n-1}\sum_i (x_i - \hat{\mu})^2$$ Unbiased

$$\hat{\mu} = \frac{1}{n}\sum_i x_i$$

For parameter mean:
sample mean --- unbiased, consistent, efficient.

For parameter variance: biased or unbiased?

Numpy Background

- Often, you have a matrix of data: e.g., movie review score

User \ Movie	Inception	Jurassic park	Batman
A	5	2	3
B	1	4	2
C	4	3	3
D	1	2	3

Numpy arrays can be 2d

```
A = np.array([[1,2,3],[4,5,6]])
A[0,1]
⇒ 2
mean(A,0)
⇒ array([2.5, 3.5, 4.5])
mean(A,1)
⇒ array([2., 5.])
```

means $\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$

access A[0,1] means 1st row, 2nd column

computes average for each column

computes average for each row

var(A,0), var(A,1) works the same way!

More on Unbiased Estimator

<u>Task</u>: Compare the **<u>MSE</u>** (mean squared error) of the two variance estimators for N=5.

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

```
import numpy as np
import numpy.random as ra
X = ra.randn(10_000,5)   # 10k by 5 matrix of 𝒩(0,1) => 10k random trials
```

```
np.mean((var(X,1,ddof=0) - 1)**2)
⟹ 0.36310526687176103
```

ddof=0 uses 1/N

$$\hat{\sigma}^2 = \frac{1}{n}\sum_i (x_i - \hat{\mu})^2$$

```
np.mean((var(X,1,ddof=1) - 1)**2)
⟹ 0.5071783438808787
```

ddof=1 uses 1/(N-1)

$$\hat{\sigma}^2_{unbiased} = \frac{1}{n-1}\sum_i (x_i - \hat{\mu})^2$$

biased version is more accurate! (but recall that it will underestimate)

There is a trade off between bias and variance!!

Bias-Variance Tradeoff

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

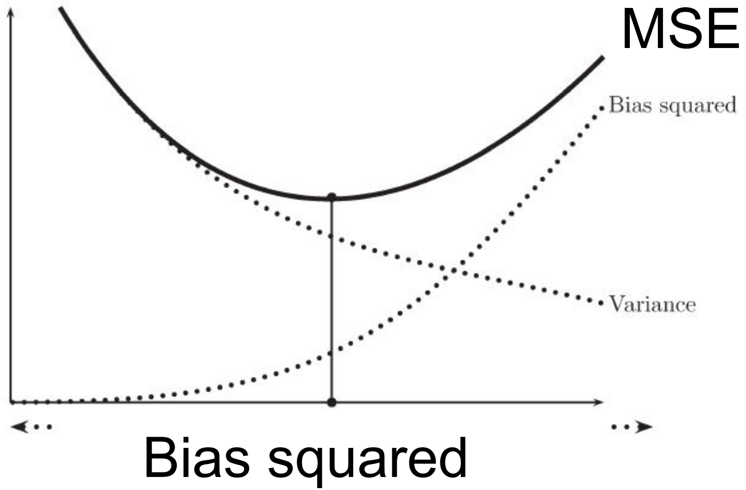
Evaluate the quality of estimate $\hat{\theta}$ using **mean squared error**,

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

- MSE for unbiased estimators is just,

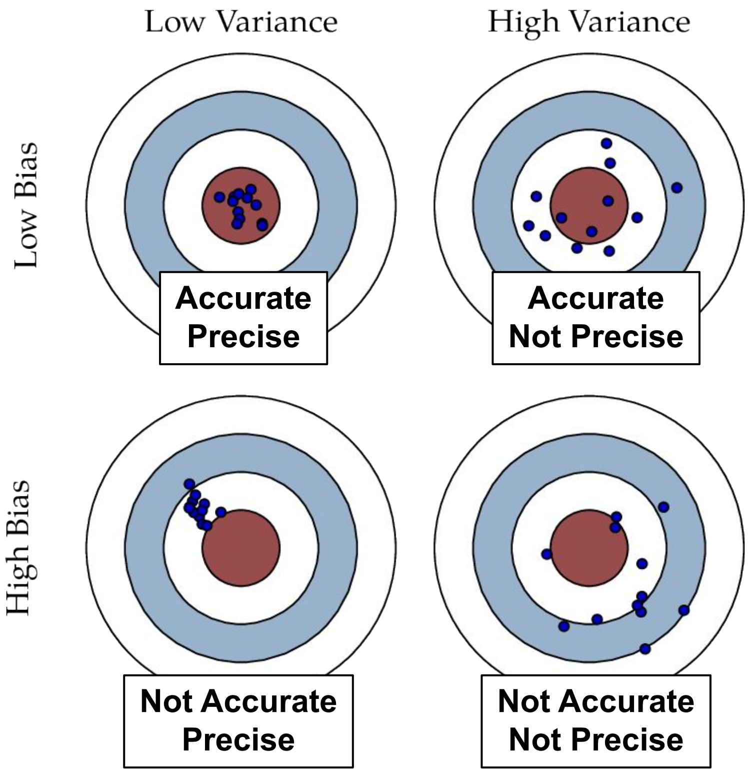
$$\mathrm{MSE}(\hat{\theta}) = \mathbf{Var}(\hat{\theta})$$

- Bias-variance is fundamental tradeoff in statistical estimation
- MSE increases as **square** of bias
- Biased estimator can be more accurate than an unbiased one.



Bias-Variance Tradeoff

Suppose an archer takes multiple shots at a target…



$$\mathrm{MSE}(\hat{\theta}) = \mathrm{bias}^2(\hat{\theta}) + \mathbf{Var}(\hat{\theta})$$

- Bias: distance from the center of target
- Variance: distance from the center of mutiple shots

MSE: MLE < Sample variance

- higher bias and lower var can be more efficient than lower bias and higher var.

Bias-Variance Decomposition

quiz candidate

$$
\begin{aligned}
\mathrm{MSE}(\hat{\theta}) &= \mathbf{E}\left[(\hat{\theta}(X) - \theta)^2\right] \\
&= \mathbf{E}\left[\left(\hat{\theta} - \mathbf{E}[\hat{\theta}] + \mathbf{E}[\hat{\theta}] - \theta\right)^2\right] \\
&= \mathbf{E}[(\hat{\theta} - \mathbf{E}[\hat{\theta}])^2] + 2(\mathbf{E}[\hat{\theta}] - \theta)\mathbf{E}[\hat{\theta} - \mathbf{E}[\hat{\theta}]] + \mathbf{E}\left[\left(\mathbf{E}[\hat{\theta}] - \theta\right)^2\right] \\
&= \left(\mathbf{E}[\hat{\theta}] - \theta\right)^2 + \mathbf{E}[(\hat{\theta} - \mathbf{E}[\hat{\theta}])^2] \\
&= \mathrm{bias}^2(\hat{\theta}) + \mathrm{Var}(\hat{\theta})
\end{aligned}
$$

Intuition Check

Compare the results of two coin flip experiments…

<u>Experiment 1</u> Flip 100 times and observe 73 heads, 27 tails

<u>Experiment 2</u> Flip 1,000 times and observe 730 heads, 270 tails

<u>Question</u> The MLE estimate of coin bias for both experiments is equivalent $\hat{\theta} = 0.73$. Which should we trust more? Why?

Answer: biases are the same (MLE use sample mean and therefore unbiased). Variance is smaller for experiment 2 (larger N). The estimator in Experiment 2 has smaller MSE.