Review for Quiz Chapter 2 (Probability) Chapter 3 (Estimation): Bias, Variance, Concentration Inequalities

CMPUT 267: Basics of Machine Learning

Logistics

- Quiz during class on Thursday
 - Join 10 minutes early on Zoom lecture
 - Or come to class physically
- Any questions/issues with Assignment 2?

Language of Probabilities

- Define random variables, and their distributions
 - Then can formally reason about them
- Express our beliefs about behaviour of these RVs, and relationships to other RVs
- Examples:
 - p(x) Gaussian means we believe X is Gaussian distributed
 - p(y | X = x) or written p(y | x) is Gaussian this means that conditioned on x,
 y is Gaussian; but p(y) might not be Gaussian
 - p(w) and p(w | Data)

PMFs and PDFs

0.3

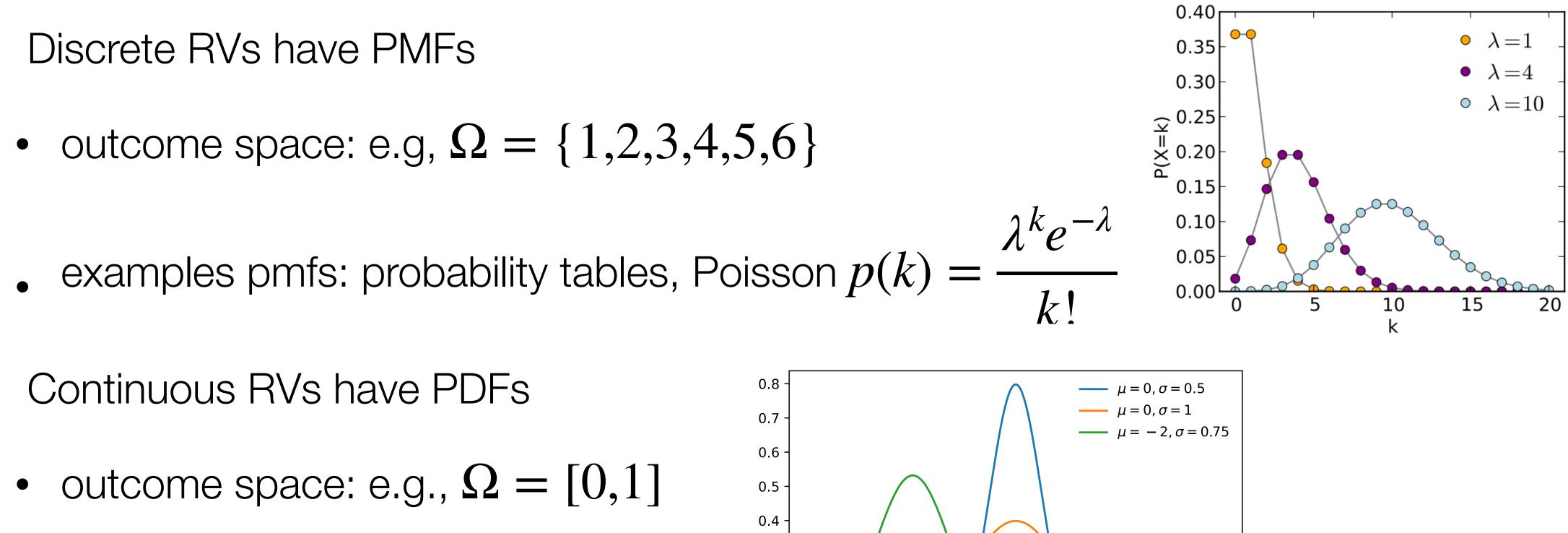
0.2

0.1

0.0

-4

- Discrete RVs have PMFs
 - outcome space: e.g, $\Omega = \{1, 2, 3, 4, 5, 6\}$
- Continuous RVs have PDFs \bullet
 - outcome space: e.g., $\Omega = [0,1]$
 - example pdf: Gaussian, Gamma



2

1

3

-2 -1

Ó

-3

A few questions

- Do PMFs p(x) have to output values between [0,1]?
- Do PDFs p(x) have to output values between [0,1]?
- What other condition(s) are put on a function p to make it a valid pmf or pdf?
- Is the following function a pdf or a pmf?

•
$$p(x) = \begin{cases} \frac{1}{b-a} & \text{if } a \le x \le b, \\ 0 & \text{otherwise.} \end{cases}$$

i.e.,
$$p(x) = \frac{1}{b-a}$$
 for $x \in [a, b]$

How would you define a uniform distribution for a discrete RV

- Imagine $x \in \{1, 2, 3, 4, 5\}$
- What is the uniform pmf for this outcome space?

•
$$p(x) = \begin{cases} \frac{1}{5} & \text{if } x \in \{1, 2, 3, 4, 5 \\ 0 & \text{otherwise.} \end{cases}$$

},

How do you answer this probabilistic question?

what is the probability that X is greater than 7?

$$\Pr(X > 7) = \int_{7}^{10} p(x)dx = \int_{7}^{10} \frac{1}{10}dx$$
$$= \frac{1}{10} \int_{7}^{10} dx = \frac{1}{10} x \Big|_{7}^{10}$$
$$= \frac{3}{10}$$

• For continuous RV X with a uniform distribution and outcome space [0,10],

Multivariate Setting

Conditional distribution, $p(y \mid x) =$

- Chain Rule $p(x, y) = p(y \mid x)p(x)$ • Bayes Rule $p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)}$
- Law of total probability $p(y) = \sum_{x \in Y} p(y) = \sum_{x \in Y} p(y)$ $x \in \mathcal{X}$
- \bullet

$$= \frac{p(x, y)}{p(x)}, \text{ Marginal } p(y) = \sum_{x \in \mathcal{X}} p(x, y)$$

$$p(x \mid y)p(y)$$

$$\sum_{x} p(y \mid x) p(x)$$

Question: How do you get the law of total probability from the chain rule?

$$\mathbb{E}[f(X)] = \begin{cases} \sum_{\chi} \\ \int_{\mathcal{X}} \\ \end{array}$$

Eg: $\mathscr{X} = \{1, 2, 3, 4, 5\}, f(x) = x^2, Y$ p(y) determined by p(x), e.g, p(Y = x)

Eg: $\mathscr{X} = \{-1, 0, 1\}, f(x) = |x|, Y$ p(Y = 1) = p(X = -1) + p(X =

Expectations

f(x)p(x) if X is discrete, f(x)p(x) dy if X is continuous.

$$X = f(X)$$
, map {1,2,3,4,5} \rightarrow {1,4,9,16,25}
= 4) = $p(X = 2)$

$$f(X), \max \{-1,0,1\} \to \{0,1\}$$

1), $\mathbb{E}[Y] = \sum_{y \in 0,1} yp(y) = \sum_{x \in \{-1,0,1\}} f(x)p(x)$

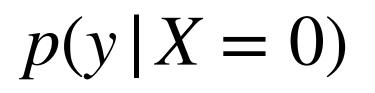
Definition: The expected value of Y conditional on X = x is $\mathbb{E}[Y \mid X = x] = \begin{cases} \sum_{y \in \mathscr{Y}} yp(y \mid x) & \text{if } Y \text{ is discrete,} \\ \int_{\mathscr{Y}} yp(y \mid x) \, dy & \text{if } Y \text{ is continuous.} \end{cases}$

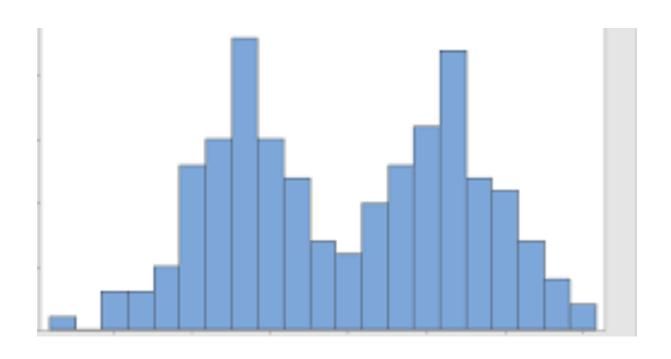
Conditional Expectations

Conditional Expectation Example

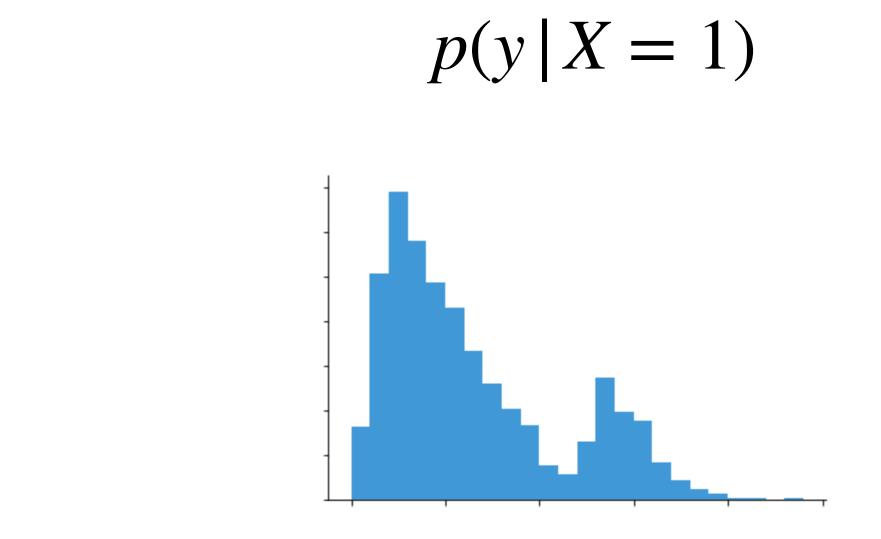
- X is the type of a book, 0 for fiction and 1 for non-fiction • p(X = 1) is the proportion of all books that are non-fiction
- Y is the number of pages
 - p(Y = 100) is the proportion of all books with 100 pages
- p(y | X = 0) is different from p(y | X = 1)
- $\mathbb{E}[Y|X=0]$ is different from $\mathbb{E}[Y|X=1]$
 - e.g. $\mathbb{E}[Y|X=0] = 70$ is different from $\mathbb{E}[Y|X=1] = 150$

Conditional Expectation Example (cont)





lacksquare



• $\mathbb{E}[Y|X=0]$ is the expectation over Y under distribution p(y|X=0)• $\mathbb{E}[Y|X=1]$ is the expectation over Y under distribution p(y|X=1)

What if Y is dollars earned?

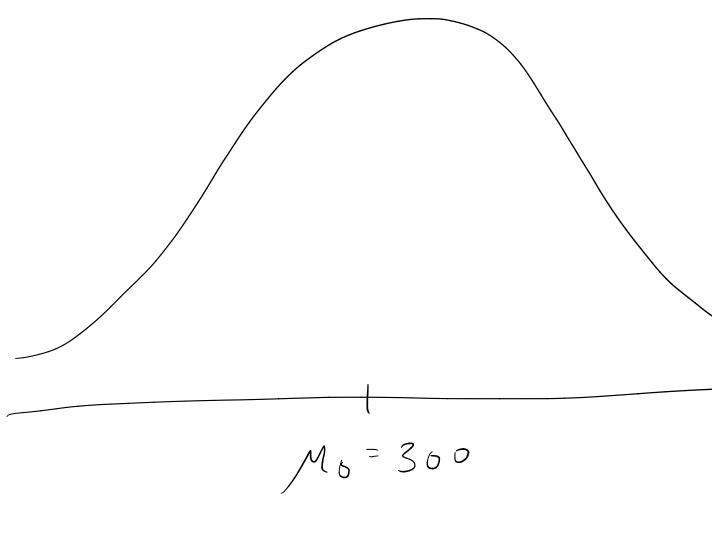
- Y is now a continuous RV
- What is p(y | x)?

What if Y is dollars earned?

- Y is now a continuous RV
- Notice that p(y|x) is defined by p(y|X=0) and p(y|X=1)

• What might be a reasonable choice for p(y | X = 0) and p(y | X = 1)?

What if Y is dollars earned? • Notice that p(y|x) is defined by p(y|X=0) and p(y|X=1) $P(Y | X = 0) = N(M_{0}, 6_{0}^{2}) \qquad P(Y | X = 1) = N(M_{1}, 6_{0}^{2})$ M = 100 $M_{6} = 300$ Fiction



Non-fiction

- Do you need to know p(x) to specify p(y | x)?

Exercise

• Come up with an example of X and Y, and give possible choice for $p(y \mid x)$

Properties of Expectations

- Linearity of expectation:
 - $\mathbb{E}[cX] = c\mathbb{E}[X]$ for all constant *c*
 - $\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$
- Products of expectations of independent random variables X, Y:
 - $\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y]$
- Law of Total Expectation:

• $\mathbb{E}\left[\mathbb{E}\left[Y \mid X\right]\right] = \mathbb{E}[Y]$

Properties of Expectations for X and Y independent

 $\mathbb{E}[XY] = \sum p(x, y)xy$ $x \in \mathcal{X} y \in \mathcal{Y}$ $= \sum p(y | x)p(x)xy$ $x \in \mathcal{X} y \in \mathcal{Y}$ $= \sum x p(x) \sum p(y | x) y$ $x \in \mathcal{X}$ $y \in \mathcal{Y}$ $= \sum x p(x) \mathbb{E}[Y|x]$ $x \in \mathcal{X}$ = $\sum xp(x)\mathbb{E}[Y]$ since X and Y independent $x \in \mathcal{X}$ $= \mathbb{E}[X]\mathbb{E}[Y]$

Variance

Definition: The **variance** of a random variable is

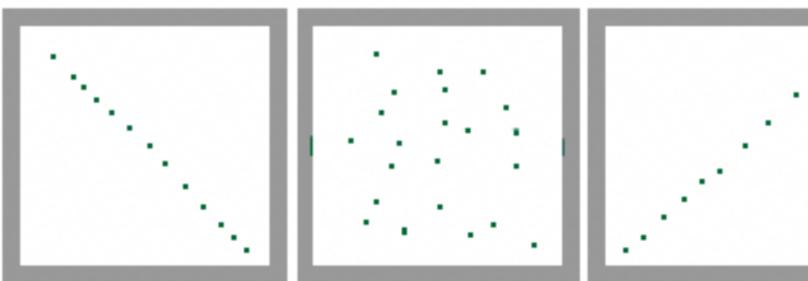
i.e., $\mathbb{E}[f(X)]$ where $f(x) = (x - \mathbb{E}[X])^2$. Equivalently,

 $\operatorname{Var}(X) = \mathbb{E}\left[(X - \mathbb{E}[X])^2 \right].$

 $Var(X) = \mathbb{E} \left[X^2 \right] - \left(\mathbb{E}[X] \right)^2$

Covariance

Definition: The **covariance** of two random variables is



Large Negative Covariance

- $Cov(X, Y) = \mathbb{E}\left[(X \mathbb{E}[X])(Y \mathbb{E}[Y])\right]$ $= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y].$

Near Zero Covariance

Large Positive Covariance

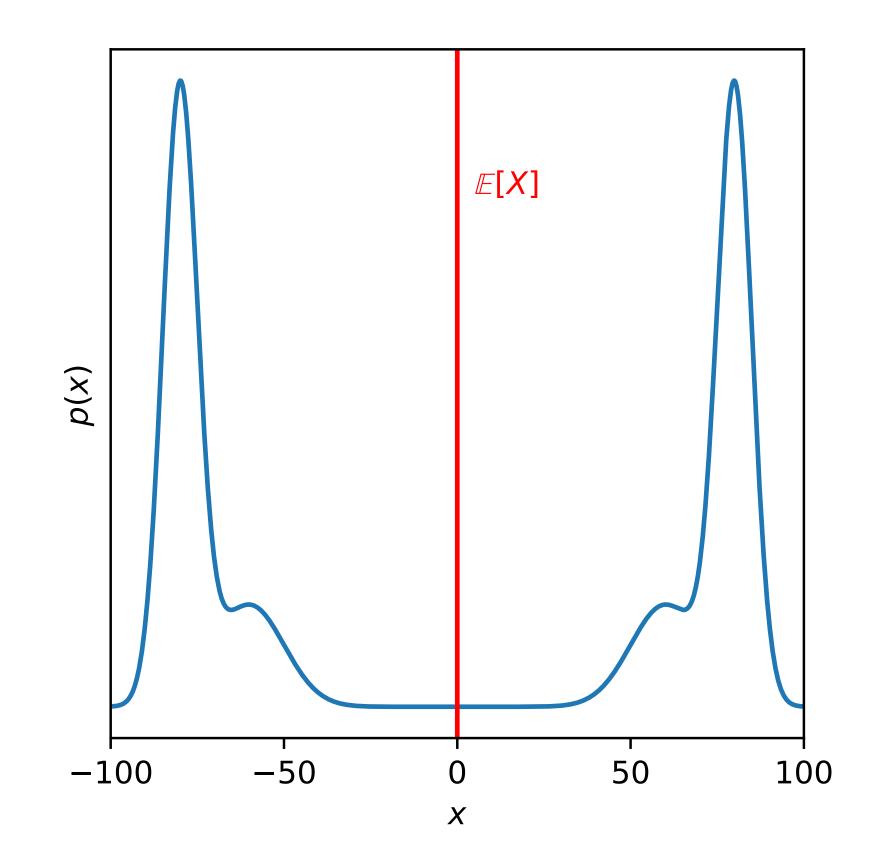
- Var[c] = 0 for constant c
- $Var[cX] = c^2 Var[X]$ for constant c
- $\operatorname{Var}[X + Y] = \operatorname{Var}[X] + \operatorname{Var}[Y] + 2\operatorname{Cov}[X, Y]$
- For independent X, Y, because Cov[X, Y] = 0Var[X + Y] = Var[X] + Var[Y]

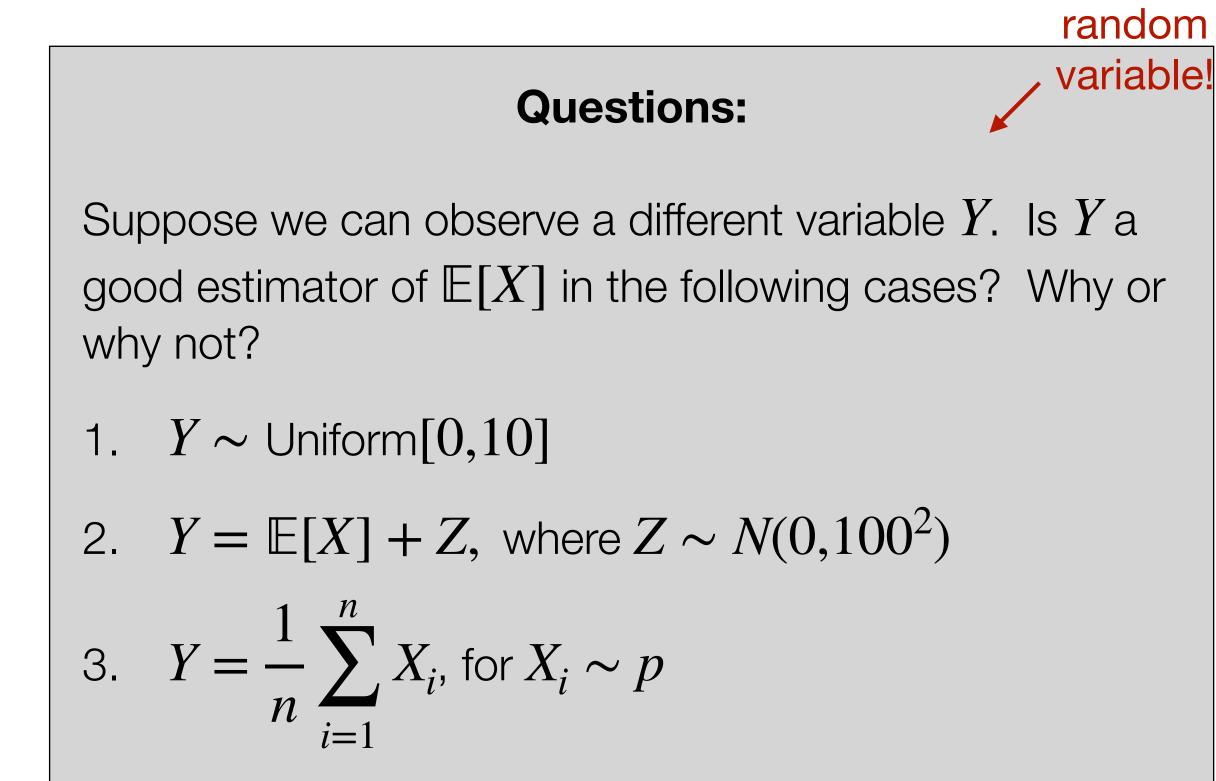
Properties of Variances

Estimators

Definition: An estimator is a procedure for estimating an unobserved quantity based on data.

Example: Estimating $\mathbb{E}[X]$ for r.v. $X \in \mathbb{R}$.





3.
$$Y = \frac{1}{n} \sum_{i=1}^{n} X_i$$
, for $X_i \sim p$



Independent and Identically Distributed (i.i.d.) Samples

- We usually won't try to estimate anything about a distribution based on only a single sample
- Usually, we use **multiple samples** from the **same distribution** ullet
 - *Multiple samples:* This gives us more information
 - Same distribution: We want to learn about a single population
- One additional condition: the samples must be **independent**

Definition: When a set of random variables are X_1, X_2, \ldots are all (independent and identically distributed), written

 X_1, X

- independent, and each has the same distribution $X \sim F$, we say they are i.i.d.

$$a_2, \ldots \overset{i.i.d.}{\sim} F.$$

Estimating Expected Value via the Sample Mean

 $\mathbb{E}[\bar{X}] = \mathbb{E} \left[\frac{1}{n} \sum_{i=1}^{n} X_i \right]$ $X_1, X_2, \ldots, X_n \stackrel{i.i.d}{\sim} F,$ $= \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[X_i]$ $=\frac{1}{n}\sum_{i=1}^{n}\mu$ $= \frac{1}{n} n \mu$

We want to estimate μ .

Example: We have n i.i.d. samples from the same distribution F, with $\mathbb{E}[X_i] = \mu$ and $\operatorname{Var}(X_i) = \sigma^2$ for each X_i . Let's use the sample mean $\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$ to estimate μ .

 $= \mu$.



Bias

Definition: The **bias** of an estimator *X* is its expected difference from the true value of the estimated quantity X: $\operatorname{Bias}(\hat{X}) = \mathbb{E}[\hat{X}] - \mathbb{E}[X]$

- Bias can be positive or negative or zero
- When $Bias(\hat{X}) = 0$, we say that the estimator \hat{X} is **unbiased**

Questions:

What is the **bias** of the following estimators of $\mathbb{E}[X]$?

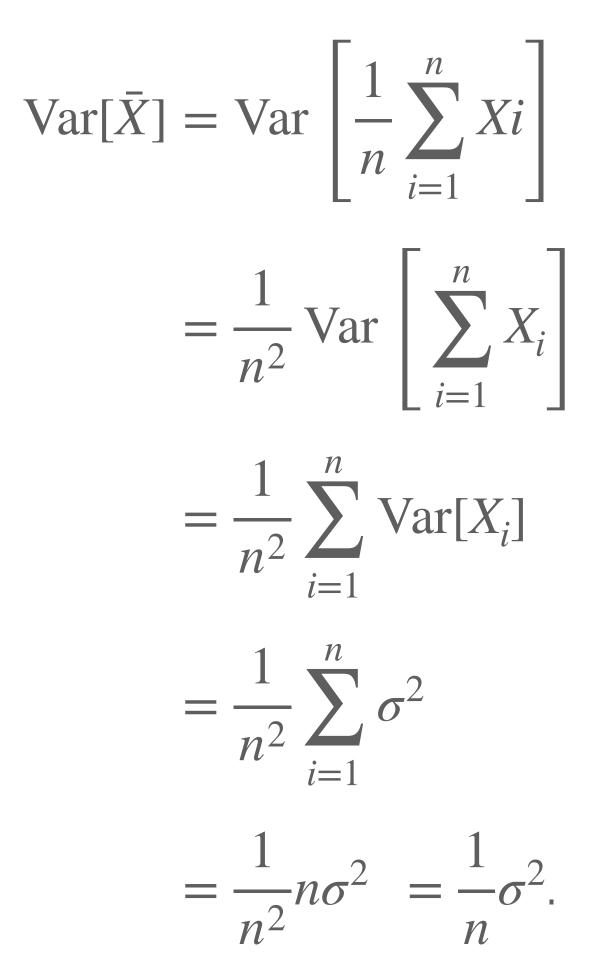
- 1. $Y \sim \text{Uniform}[0, 10]$
- 2. $Y = \mathbb{E}[X] + Z,$ where
 - $Z \sim \text{Uniform}[0,1]$
- 3. $Y = \mathbb{E}[X] + Z,$ where $Z \sim N(0, 100^2)$

4.
$$Y = \frac{1}{n} \sum_{i=1}^{n} X_i$$



Variance of the Estimator

- Intuitively, more samples should make the estimator "closer" to the estimated quantity
- We can formalize this intuition partly by characterizing the variance $Var[\hat{X}]$ of the estimator itself.
 - The variance of the estimator should decrease as the number of samples increases
- **Example:** \overline{X} for estimating μ :
 - The variance of the estimator shrinks linearly as the number of samples grows.



Mean-Squared Error

- **Bias:** whether an estimator is correct in expectation
- Consistency: whether an estimator is correct in the limit of infinite data
- Convergence rate: how fast the estimator approaches its own mean
 - For an **unbiased** estimator, this is also how fast its **error bounds** shrink
- We don't necessarily care about an estimator's being unbiased.
 - Often, what we care about is our estimator's accuracy in expectation

Definition: Mean squared error of an



estimator
$$\hat{X}$$
 of a quantity X :

$$\mathbb{E}\left[(\hat{X} - \mathbb{E}[X])^2\right]$$

different!

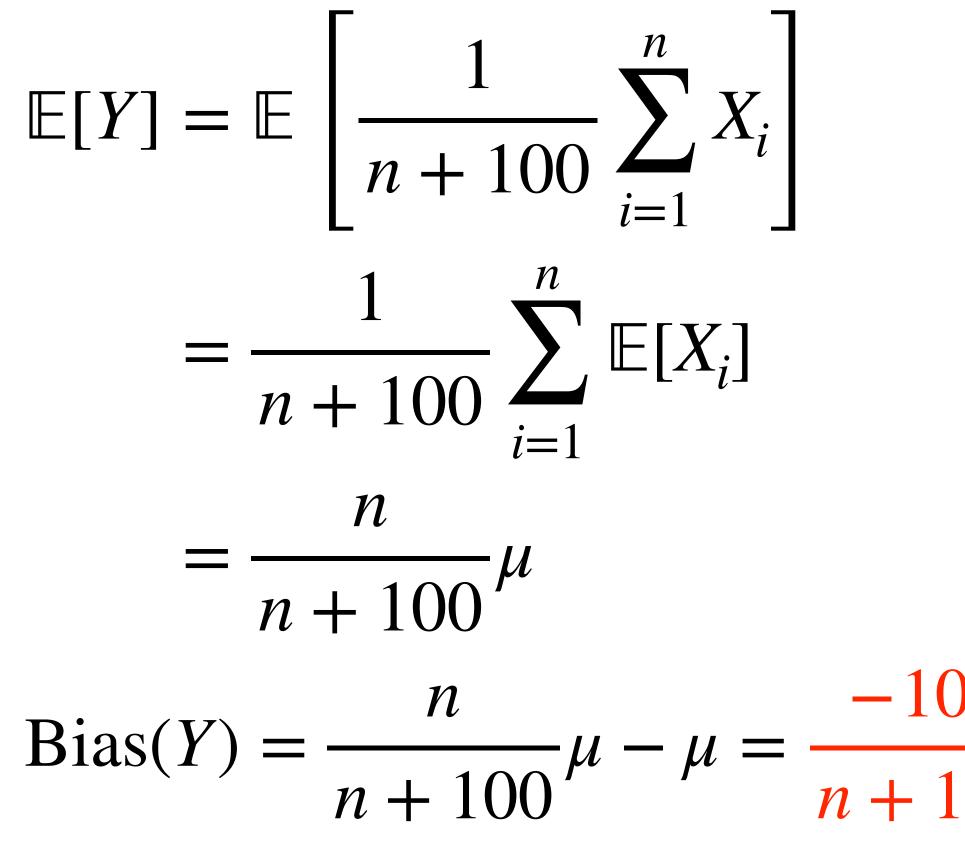
Bias-Variance Tradeoff

$MSE(\hat{X}) = Var[\hat{X}] + Bias(\hat{X})^2$

- If we can decrease bias without increasing variance, error goes down
- If we can decrease variance without increasing bias, error goes down
- Question: Would we ever want to increase bias?
- YES. If we can increase (squared) bias in a way that decreases variance more, then error goes down!
 - Interpretation: Biasing the estimator toward values that are more likely to be true (based on prior information)

Downward-biased Mean Estimation **Example:** Let's estimate μ given i.i.d X_1, \ldots, X_n with $\mathbb{E}[X_i] = \mu$ using: $Y = \frac{1}{n+100} \sum_{i=1}^n X_i$ This estimator has **low variance**: $\operatorname{Var}(Y) = \operatorname{Var} \left| \frac{1}{n+100} \sum_{i=1}^{n} X_i \right|$ $= \frac{1}{n+100} \sum_{i=1}^{n} \mathbb{E}[X_i]$ $= \frac{1}{(n+100)^2} \operatorname{Var} \left| \sum_{i=1}^{n} X_i \right|$ $= \frac{1}{(n+100)^2} \sum_{i=1}^{n} \text{Var}[X_i]$ $= \frac{1}{n+100} \mu$ Bias(Y) = $\frac{n}{n+100}\mu - \mu = \frac{-100}{n+100}\mu$ $=\frac{n}{(n+100)^2}\sigma^2$

This estimator is **biased**:



Estimating µ Near 0

Example: Suppose that $\sigma = 1$, n = 10, and $\mu = 0.1$

 $\operatorname{Bias}(\bar{X}) = 0$

$$MSE(\bar{X}) = Var(\bar{X}) + Bias(\bar{X})^{2}$$
$$= Var(\bar{X}) \quad Var(\bar{X}) = \frac{\sigma^{2}}{n}$$
$$= \frac{1}{10}$$

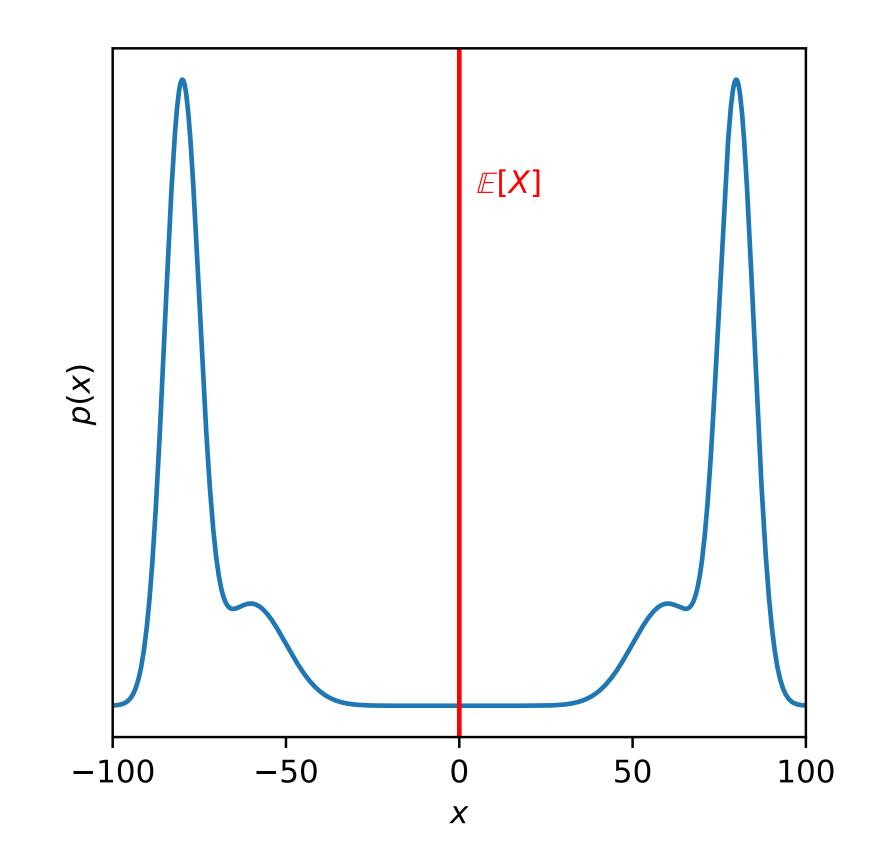
 $MSE(Y) = Var(Y) + Bias(Y)^2$

$$= \frac{n}{(n+100)^2} \sigma^2 + \left(\frac{100}{n+100}\mu\right)^2$$
$$= \frac{10}{110^2} + \left(\frac{100}{110}0.1\right)^2$$
$$\approx 9 \times 10^{-4}$$



Exercise: What is the variance of these estimators?

Example: Estimating $\mathbb{E}[X]$ for r.v. $X \in \mathbb{R}$.



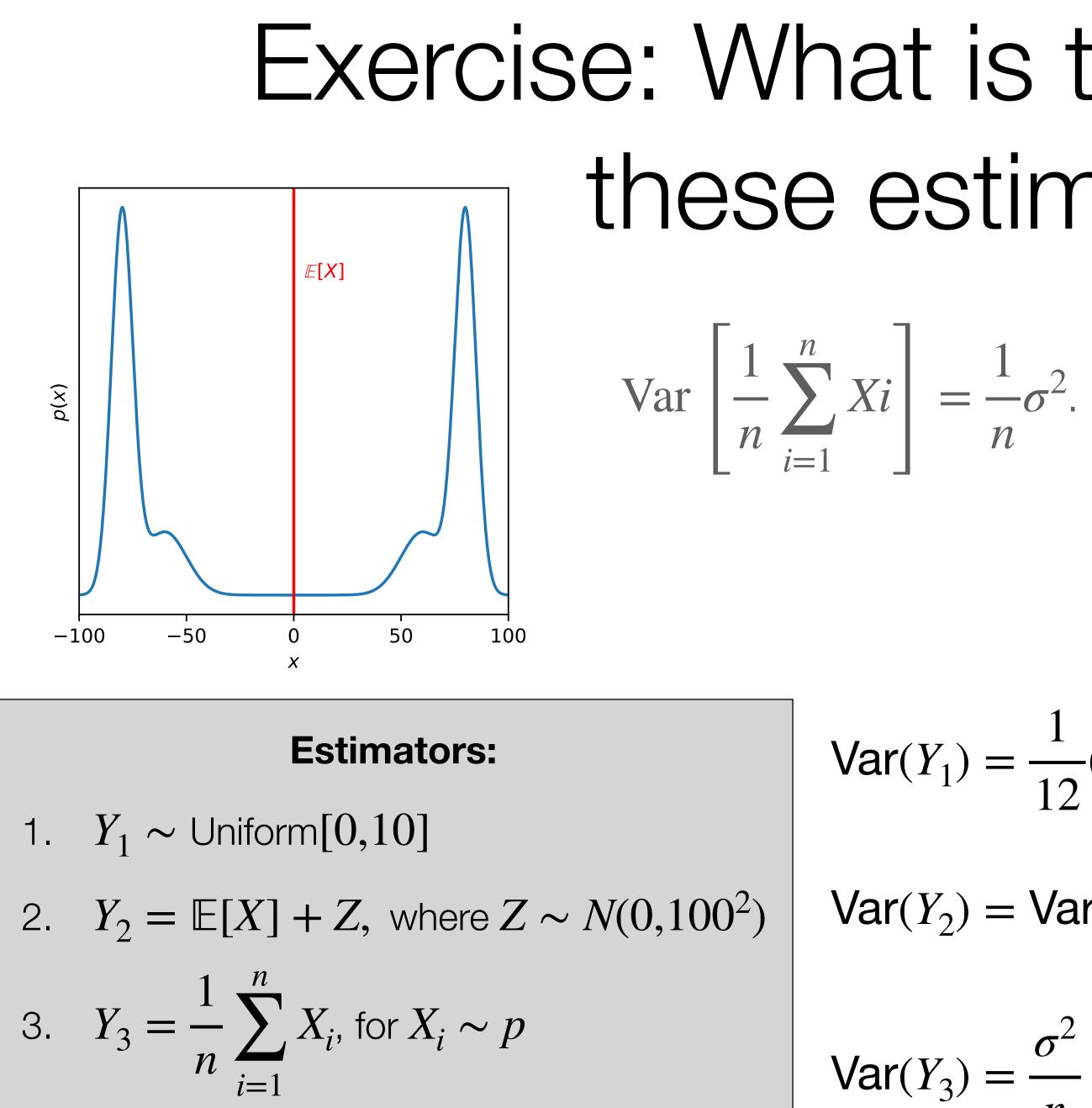
Questions:

Suppose we can observe a different variable Y. Is Y a good estimator of $\mathbb{E}[X]$ in the following cases? Why or why not?

- 1. $Y \sim \text{Uniform}[0, 10]$
- 2. $Y = \mathbb{E}[X] + Z$, where $Z \sim N(0, 100^2)$

3.
$$Y = \frac{1}{n} \sum_{i=1}^{n} X_i$$
, for $X_i \sim p$





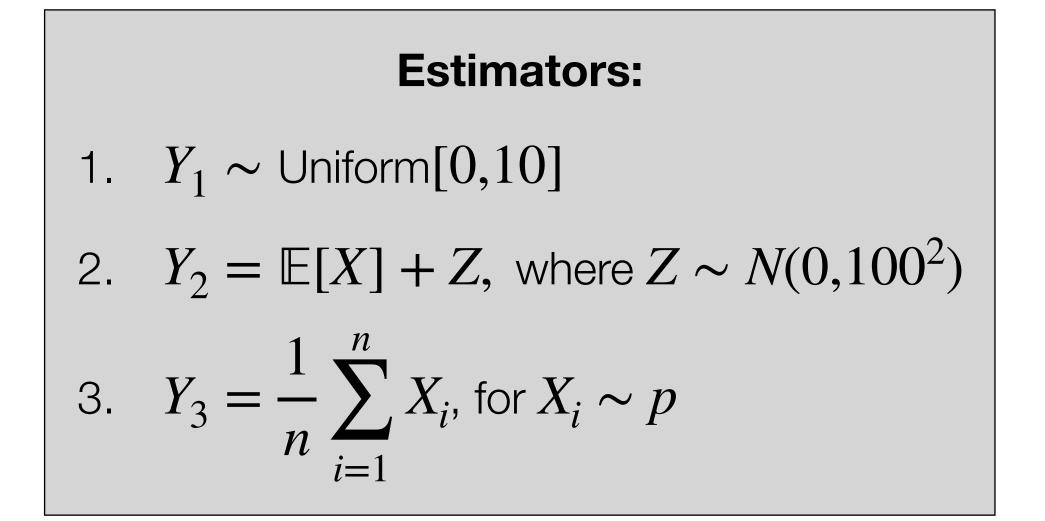
Exercise: What is the variance of these estimators?

$$Y_1) = \frac{1}{12}(10-0)^2 = \frac{100}{12} = 8.\overline{3}$$

 $Var(Y_2) = Var(\mathbb{E}[X] + Z) = ?$

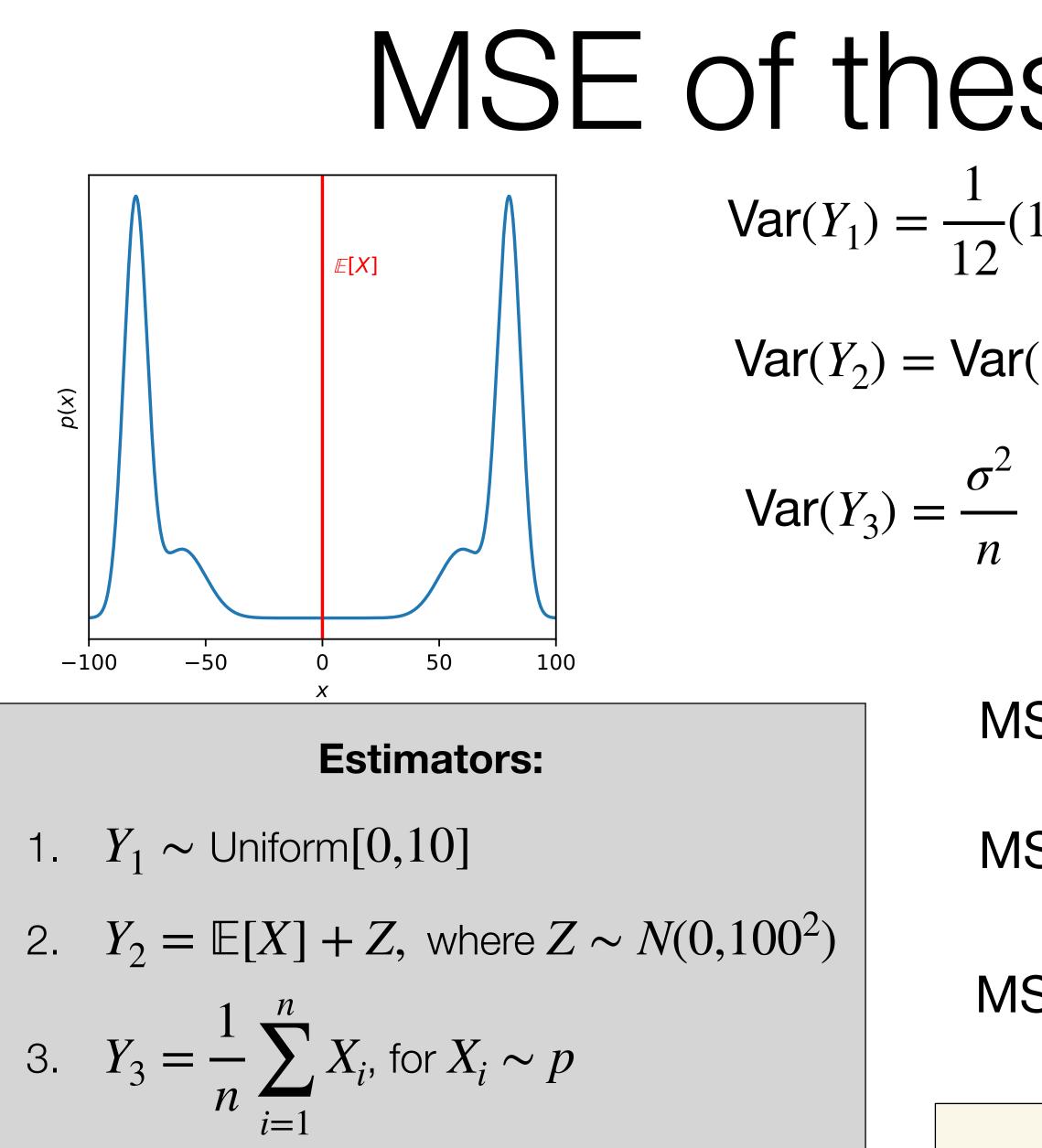
 $\operatorname{Var}(Y_3) = \frac{\sigma^2}{2}$

Exercise: What is the variance of these estimators?



 $Var(Y_2) = Var(\mathbb{E}[X] + Z)$ = Var(Z) $= 100^2$

 \triangleright Var(c + Y) = Var(Y)



Se estimators
$$(10-0)^2 = \frac{100}{12} = 8.\overline{3}$$
 Bias $(Y_1) = \mathbb{E}[Y_1] - \mathbb{E}[X]$

 $Var(Y_2) = Var(\mathbb{E}[X] + Z) = 100^2$ $Bias(Y_2) = \mathbb{E}[Y_2] - \mathbb{E}[X] = 0$

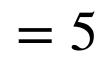
 $\mathsf{Bias}(Y_3) = 0$

 $MSE(Y_1) = 5^2 + 8.\overline{3} = 33.\overline{3}$

 $MSE(Y_2) = 0 + 100^2 = 10000$

$$\mathsf{ISE}(Y_3) = 0 + \frac{\sigma^2}{n}$$

 $MSE(\hat{X}) = Var[\hat{X}] + Bias(\hat{X})^2$



Concentration Inequalities

- We would like to be able to claim Pr for some $\delta, \epsilon > 0$
- $\operatorname{Var}[\bar{X}] = \frac{1}{n} \sigma^2$ means that with "enough" data, $\operatorname{Pr}\left(\left|\bar{X} \mu\right| < \epsilon\right) > 1 \delta$ for any $\delta, \epsilon > 0$ that we pick

• **Question:** What is
$$\Pr\left(\left|\bar{X} - \mu\right| < \right)$$

$$\left(\left|\bar{X}-\mu\right| < \epsilon\right) > 1 - \delta$$

• Suppose we have n = 10 samples, and we know $\sigma^2 = 81$; so $Var[\bar{X}] = 8.1$.

Knowing the Variance Is Not Enough

Knowing $\operatorname{Var}[\overline{X}] = 8.1$ is **not enough** to compute $\Pr(|\overline{X} - \mu| < 2)!$ **Examples:**

$$p(\bar{x}) = \begin{cases} 0.9 & \text{if } \bar{x} = \mu \\ 0.05 & \text{if } \bar{x} = \mu \pm 9 \end{cases} \Longrightarrow$$
$$p(\bar{x}) = \begin{cases} 0.999 & \text{if } \bar{x} = \mu \\ 0.0005 & \text{if } \bar{x} = \mu \pm 90 \end{cases} \Longrightarrow$$
$$p(\bar{x}) = \begin{cases} 0.1 & \text{if } \bar{x} = \mu \\ 0.45 & \text{if } \bar{x} = \mu \pm 3 \end{cases} \Longrightarrow$$

- Var[\bar{X}] = 8.1 and Pr($|\bar{X} \mu| < 2$) = 0.9
- Var $[\bar{X}] = 8.1$ and Pr $(|\bar{X} \mu| < 2) = 0.999$
- $Var[\bar{X}] = 8.1$ and $Pr(|\bar{X} \mu| < 2) = 0.1$

Hoeffding's Inequality

Theorem: Hoeffding's Inequality Suppose that X_1, \ldots, X_n are distributed i.i.d, with $a \leq X_i \leq b$. Then for any $\epsilon > 0$, $\Pr\left(\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \ge \epsilon\right)$ Equivalently, $\Pr\left(\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \le (k)\right)$

$$b(x) \le 2 \exp\left(-\frac{2n\epsilon^2}{(b-a)^2}\right).$$
$$b(x) = b - a \sqrt{\frac{\ln(2/\delta)}{2n}} \ge 1 - \delta$$

Chebyshev's Inequality

Theorem: Chebyshev's Inequality Suppose that X_1, \ldots, X_n are distributed i.i.d. with variance σ^2 . Then for any $\epsilon > 0$, $\Pr\left(\left|\bar{X}-\mathbb{E}\right|\right)$ Equivalently, $\Pr \left| \bar{X} - \mathbb{E}[\bar{X}] \right| \leq \sqrt{2}$

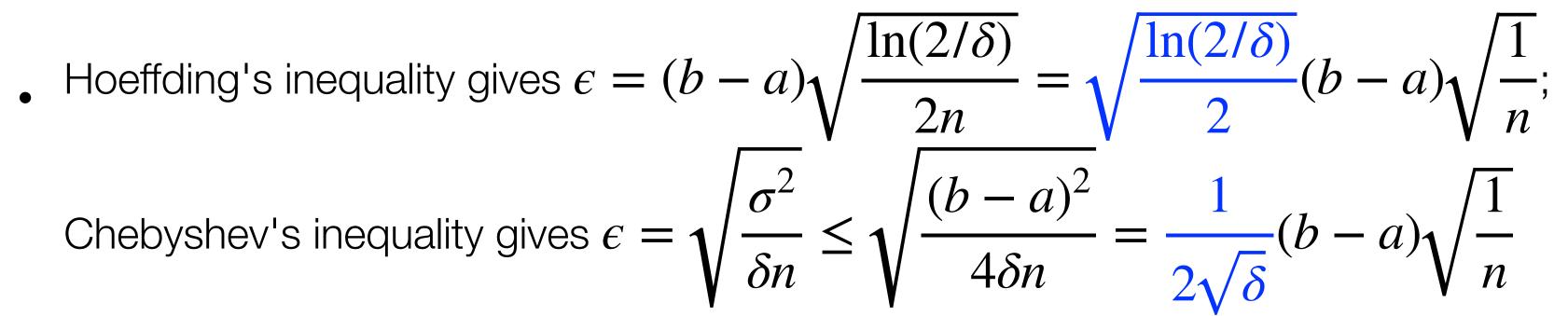
$$\left| \frac{\bar{X}}{\bar{X}} \right| \ge \epsilon \right) \le \frac{\sigma^2}{n\epsilon^2}$$
$$\left| \frac{\sigma^2}{\delta n} \right| \ge 1 - \delta.$$

When to Use Chebyshev, When to Use Hoeffding?

- If $a \le X_i \le b$, then $\operatorname{Var}[X_i] \le \frac{1}{4}(b-a)^2$
- Chebyshev's inequality gives $\epsilon = \sqrt{\frac{\sigma^2}{\delta n}} \le \sqrt{\frac{(b-a)^2}{4\delta n}} = \frac{1}{2\sqrt{\delta}}(b-a)\sqrt{\frac{1}{n}}$
- variables

* whenever
$$\sqrt{\frac{\ln(2/\delta)}{2}} < \frac{1}{2\sqrt{\delta}} \iff$$

• Chebyshev's inequality can be applied even for unbounded variables



Hoeffding's inequality gives a tighter bound*, but it can only be used on bounded random

 $\delta < \sim 0.232$

Sample Complexity

Definition:

The sample complexity of an estimator is the number of samples required to guarantee an error of at most ϵ with probability $1 - \delta$, for given δ and ϵ .

- We want sample complexity to be small lacksquare
- Sample complexity is determined by:
 - 1. The **estimator** itself
 - Smarter estimators can sometimes improve sample complexity
 - 2. Properties of the data generating process
 - lacksquare
 - lacksquarecorrect value

If the data are high-variance, we need more samples for an accurate estimate But we can reduce the sample complexity if we can bias our estimate toward the

Sample Complexity

Definition:

of at most ϵ with probability $1 - \delta$, for given δ and ϵ .

For $\delta = 0.05$, **Chebyshev** gives

$$\epsilon = \sqrt{\frac{\sigma^2}{\delta n}} = \frac{1}{\sqrt{0.05}} \frac{\sigma}{\sqrt{n}}$$
$$\iff \epsilon = 4.47 \frac{\sigma}{\sqrt{n}}$$
$$\iff \sqrt{n} = 4.47 \frac{\sigma}{\epsilon}$$
$$\iff n = 19.98 \frac{\sigma^2}{\epsilon^2}$$

The sample complexity of an estimator is the number of samples required to guarantee an expected error

With Gaussian assumption and $\delta = 0.05$,

$$\epsilon = 1.96 \frac{\sigma}{\sqrt{n}}$$

$$\iff \sqrt{n} = 1.96 \frac{\sigma}{\epsilon}$$

$$\iff n = 3.84 \frac{\sigma^2}{\epsilon^2}$$



Exercise: Sample Complexity for a Biased Estimator

- around it's mean
- But if it is biased, then the mean of the estimator \neq the true mean
- we introduce

The concentration inequalities only tell us how the estimator concentrates

• We can reduce the sample complexity (by reducing variance and/or by making stronger assumptions), but need to be careful about how much bias

Consistency of Downward-biased Mean Estimation
Example:
$$Y = \frac{1}{n+100} \sum_{i=1}^{n} X_i$$

This estimator is **biased**:
 $Bias(Y) = \frac{n}{n+100} \mu - \mu = \frac{-100}{n+100} \mu$ Var $(Y) = \frac{n}{(n+100)^2} \sigma^2$

Does this estimator have lower sample complexity than the sample average?

Is this estimator consistent? (Namely, in the limit of samples, does it approach the true mean?) (In other words, does it's bias go to zero?)

DN

Summary

- Concentration inequalities let us bound the probability of a given estimator being at least ϵ from the estimated quantity
- Sample complexity is the number of samples needed to attain a desired error bound ϵ at a desired probability $1-\delta$
- The mean squared error of an estimator decomposes into bias (squared) and variance
- Using a **biased** estimator can have **lower error** than an unbiased estimator
 - Bias the estimator based on some prior information
 - But this only helps if the prior information is correct, cannot reduce error by adding in arbitrary bias