DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 12 | Part 1

Parametric Density Estimation

Bayes Classifier

- Recall the **Bayes Classifier:** predict

$$\begin{cases} 1, & \text{if } \mathbb{P}(Y = 1 \mid \vec{X} = \vec{x}) > \mathbb{P}(Y = 0 \mid \vec{X} = \vec{x}), \\ 0, & \text{otherwise.} \end{cases}$$

- Equivalently, using **Bayes' rule**:

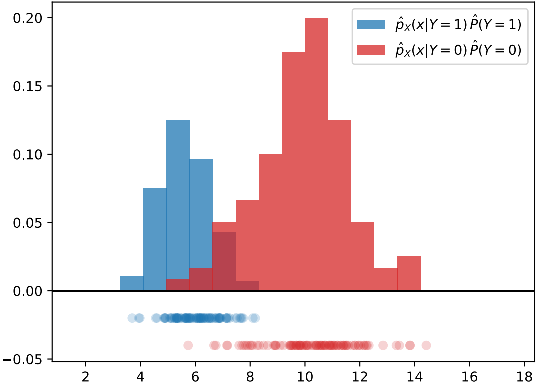
$$\begin{cases} 1, & \text{if } p_X(x \mid Y = 1)\mathbb{P}(Y = 1) > p_X(x \mid Y = 0)\mathbb{P}(Y = 0), \\ 0, & \text{otherwise.} \end{cases}$$

Estimating Densities

- We rarely know the true distribution.
- We must **estimate** it from data.
- When $\vec{X}$ is continuous, we estimate **density**.

Last Time: Histogram Estimators

- **Histograms** provide one way of estimating densities.



Histogram Drawbacks

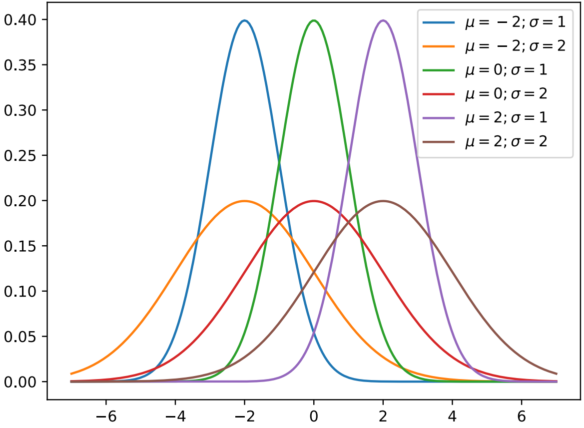
- We saw that histograms need massive amounts of data in high dimensions.
- The **Curse of Dimensionality**.

Observation

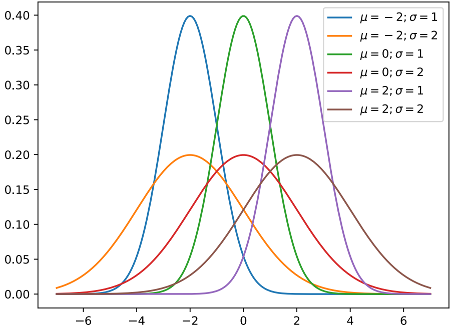
- Histogram estimators assume nothing about the **shape** of the true density.
- This makes them very flexible, but also data-hungry.
- **Idea:** Assume that the true, underlying density has a certain form.

Example: Gaussians

- Often assume that the true distribution is **Gaussian** (aka, **Normal**).



Example: Gaussians



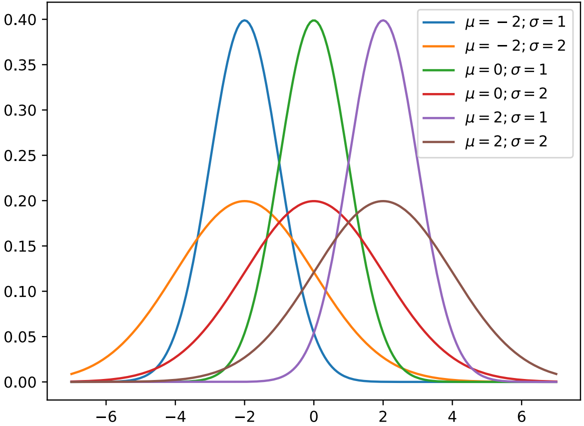
- **Recall:** the pdf of the Gaussian distribution:

$$p(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

- μ and σ are **parameters**
  - μ controls center
  - σ controls width

Gaussian

- **Central Limit Theorem**: sums of independent random variables are Gaussian
- **Examples:** test scores, heights, measurement errors, ...



Parametric Distributions

- A **parametric distribution** is **totally determined** by a finite number of **parameters**.

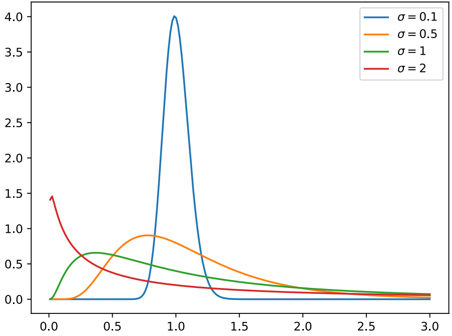
- **Example:** knowing μ and σ tells you everything about a Gaussian distribution.

Other Parametric Distributions

- There are many parametric distributions.
- **Discrete**: Bernoulli, Multinomial, Poisson, ...
- **Continuous**: Log-normal, Gamma, Pareto, ...

Example: Lognormal

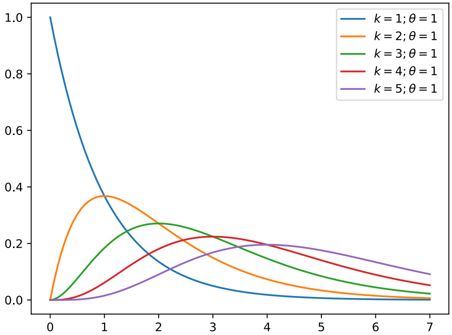
- Product of many independent positive random numbers.
- **Example:** length of comments in an internet forum



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

Example: Gamma

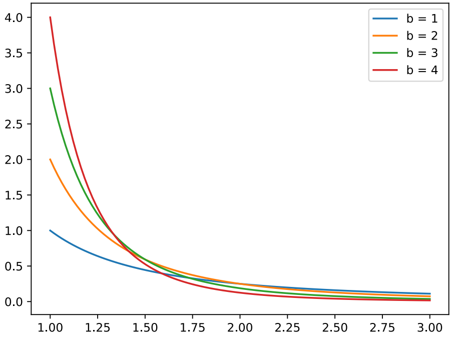
- **Examples:** wait times, size of rainfalls, insurance claims, ...



$$p(x; k, \theta) = \frac{1}{\Gamma(k)\theta^k} x^{k-1} e^{-x/\theta}$$

Example: Pareto

- **Examples:** distribution of wealth, size of meteorites, ...



$$p(x; x_m, \alpha) = \frac{\alpha x_m^\alpha}{x^{\alpha+1}}$$

Parametric Density Estimation

- In **parametric density estimation**, we assume data comes from some parametric density.
  - E.g., Gaussian, Log-Normal, Pareto, etc.

- But we don't know the parameters.

- Use data to **estimate** the parameters.

Non-Parametric Density Estimation

- Contrast this with estimating density with histograms.
- There were no parameters controlling the shape of the density.
- Histograms are **non-parametric** density estimators.

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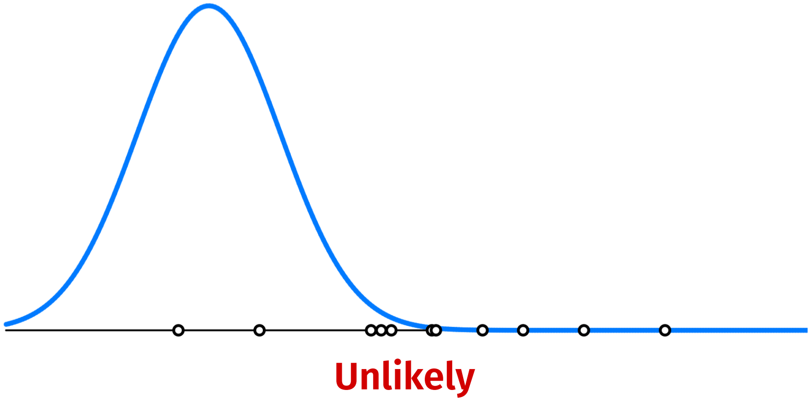
Probabilistic Modeling & Machine Learning

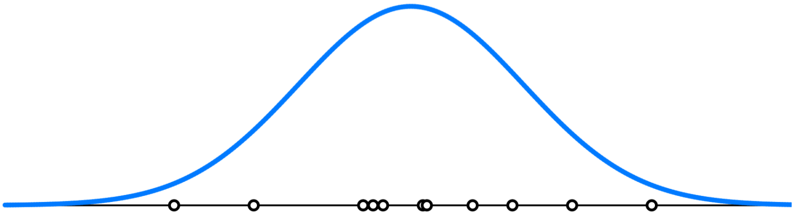
Lecture 12 | Part 2

Maximum Likelihood Estimation

Parametric Density Estimation

- Suppose we have data $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}$.
- Assume it came from a parametric distribution.
  - Say, a Gaussian.
- What were the parameter values used to generate the data?
- Using data to guess μ and σ is called **estimating** the parameters.


Unlikely



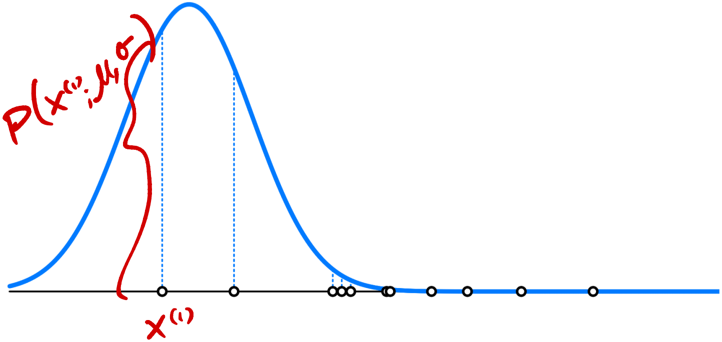
Likely

Intuition

- Some parameter choices seem **more likely** than others.
- That is, there is a greater chance that the data could have been generated by them.
- How can we quantify this?

Intuition

- Let p be the Guassian probability density function.
- $p(x^{(i)}; \mu, \sigma)$ quantifies how likely it is to see $x^{(i)}$ if parameters μ and σ are used.



Exercise

Assume that $x^{(1)}, \ldots, x^{(n)}$ are all sampled independently from a density with parameters μ, σ.

Think of $p(x^{(i)}; \mu, \sigma)$ as the "chance" of seeing $x^{(i)}$ under parameters μ and σ.

What is the chance of seeing $x^{(1)}$ *and* $x^{(2)}$ *and* $x^{(3)}$ *and* … *and* $x^{(n)}$?

Intuition

- $p(x^{(1)}; \mu, \sigma) \times p(x^{(2)}; \mu, \sigma) \times \cdots \times p(x^{(n)}; \mu, \sigma)$ quantifies likelihood of seeing $x^{(1)}, \ldots, x^{(n)}$ simultaneously.
- In fact, it is the **joint density** of the data.
- But instead think of this as a function of μ and σ.

Likelihood

- The **likelihood** of μ and σ with respect to data $x^{(1)}, \dots, x^{(n)}$ is:

$$\begin{aligned}\mathcal{L}(\mu, \sigma; x^{(1)}, \dots, x^{(n)}) &= p(x^{(1)}; \mu, \sigma) \times p(x^{(2)}; \mu, \sigma) \times \cdots \times p(x^{(n)}; \mu, \sigma) \\ &= \prod_{i=1}^{n} p(x^{(i)}; \mu, \sigma)\end{aligned}$$

Likelihood

- The likelihood function takes in parameters μ and σ and returns a real number.
- **Interpretation:** likelihood that data was generated by this choice of μ and σ.
- **Goal:** find μ and σ that **maximize** the likelihood.

http://dsc140a.com/static/vis/mle/

Maximizing Likelihood

- To maximize $\mathcal{L}(\mu, \sigma)$, we might take derivatives $\frac{\partial \mathcal{L}}{\partial \mu}$ and $\frac{\partial \mathcal{L}}{\partial \sigma}$, set to 0, solve.
- But the likelihood is often difficult to work with.

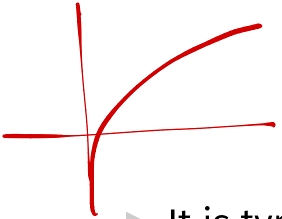
Example: Gaussian

- Assume that p is the Gaussian pdf.

$$p(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

- Then the likelihood function is:

$$\mathcal{L}(\mu, \sigma) = \prod_{i=1}^{n} \left(\frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x^{(i)}-\mu)^2}{2\sigma^2}} \right)$$



ln a > ln b

a > b

Log Likelihood

- It is typically easier to work with the **log likelihood** instead.

$$\tilde{\mathcal{L}}(\mu, \sigma) = \ln \mathcal{L}(\mu, \sigma)$$

- **Fact:** Because $\ln x$ is **monotonically increasing**, a maximizer of $\ln \mathcal{L}$ also maximizes $\mathcal{L}$

Procedure: Gaussian

1. Write the log likelihood function $\tilde{\mathcal{L}}$.
2. Take derivatives $\partial\tilde{\mathcal{L}}/\partial\mu$ and $\partial\tilde{\mathcal{L}}/\partial\sigma$
3. Set to zero and solve for μ and σ.

$$\ln\left(p(x^{(1)}) \cdot p(x^{(2)}) \cdot p(x^{(3)})\right) = \ln p(x^{(1)}) + \ln p(x^{(2)}) + \ln p(x^{(3)})$$

Recall: Log Properties

- If a and b are positive: $\ln(a \times b) = \ln a + \ln b$
- If a and b are positive: $\ln(a/b) = \ln a - \ln b$
- If a is positive: $\ln a^p = p \ln a$

Step 1: Write Log Likelihood

- Write the log likelihood function for the Normal distribution.

$$p(x^{(i)};\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}$$

$$\mathcal{L}(\mu,\sigma) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}$$

$$\tilde{\mathcal{L}}(\mu,\sigma) = \ln \mathcal{L}(\mu,\sigma) = \ln \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}$$

$$\ell$$

Step 1: Write Log Likelihood

- Write the log likelihood function for the Normal distribution.

$$\ln \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}} = \sum_{i=1}^{n} \ln\left[\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}\right]$$

$$= \sum_{i=1}^{n}\left[\ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right) + \ln\left(e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}\right)\right]$$

$$= \sum_{i=1}^{n}\left[-\ln\sigma - \ln\sqrt{2\pi} - (x^{(i)}-\mu)^2/2\sigma^2\right]$$

Step 2: Differentiate

- We have: $\tilde{\mathcal{L}} = \sum_{i=1}^{n} \left[-\ln \sigma - \ln \sqrt{2\pi} - \frac{(x^{(i)}-\mu)^2}{2\sigma^2} \right]$
- Compute $\partial \tilde{\mathcal{L}} / \partial \mu$:

$$\frac{\partial}{\partial \mu} \sum_{i=1}^{n} \left[-\ln \sigma - \ln \sqrt{2\pi} - \frac{(x^{(i)}-\mu)^2}{2\sigma^2} \right]$$

$$= \sum_{i=1}^{n} \left[\underbrace{\frac{\partial}{\partial \mu}(-\ln \sigma)}_{0} - \underbrace{\frac{\partial}{\partial \mu}(\ln \sqrt{2\pi})}_{0} - \frac{1}{2\sigma^2} \frac{\partial}{\partial \mu} (x^{(i)} - \mu)^2 \right]$$

$$= \sum_{i=1}^{n} -\frac{2}{2\sigma^2} (x^{(i)} - \mu)(-1) = \frac{1}{\sigma^2} \sum_{i=1}^{n} (x^{(i)} - \mu)$$

Step 2: Differentiate

$$\frac{d}{dx} \ln x = \frac{1}{x}$$

- We have: $\tilde{\mathcal{L}} = \sum_{i=1}^{n} \left[-\ln \sigma - \ln \sqrt{2\pi} - \frac{(x^{(i)} - \mu)^2}{2\sigma^2} \right]$
- Compute $\partial \tilde{\mathcal{L}} / \partial \sigma$:

Step 3: Solve

- We have $\partial\tilde{L}/\partial\mu = \frac{1}{\sigma^2}\sum_{i=1}^{n}(x^{(i)} - \mu)$
- Solve $\partial\tilde{L}/\partial\mu = 0$ for μ.

$$\frac{1}{\sigma^2}\sum_{i=1}^{n}(x^{(i)} - \mu) = 0$$

$$\Rightarrow \sum_{i=1}^{n}(x^{(i)} - \mu) = 0 \Rightarrow \sum_{i=1}^{n} x^{(i)} - \underbrace{\sum_{i=1}^{n}\mu}_{n\mu} = 0$$

$$\Rightarrow \sum_{i=1}^{n} x^{(i)} - n\mu = 0 \Rightarrow \mu_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x^{(i)}$$

Step 3: Solve

- We have $\partial\tilde{L}/\partial\sigma = \sum_{i=1}^{n}\left[-\frac{1}{\sigma} + \frac{(x^{(i)}-\mu)^2}{\sigma^3}\right]$
- Solve $\partial\tilde{L}/\partial\sigma = 0$ for σ.

$$\sum_{i=1}^{n}\left[\frac{-1}{\sigma} + \frac{(x^{(i)}-\mu)^2}{\sigma^3}\right] = 0$$

$$\sigma_{MLE} = \sqrt{\frac{1}{n}\sum(x^{(i)}-\mu_{MLE})^2}$$

$$\Rightarrow \sum \frac{-1}{\sigma} + \frac{1}{\sigma^3}\sum(x^{(i)}-\mu)^2 = 0$$

$$\Rightarrow \frac{-n}{\sigma} + \frac{1}{\sigma^3}\sum(x^{(i)}-\mu)^2 = 0$$

$$\Rightarrow -n + \frac{1}{\sigma^2}\sum(x^{(i)}-\mu)^2 = 0$$

$$\Rightarrow \sigma = \sqrt{\frac{1}{n}\sum_i(x^{(i)}-\mu)^2}$$

MLEs for Gaussian Distribution

- We have found the **maximum likelihood estimates** for the Gaussian distribution:

$$\mu_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x^{(i)} \qquad \sigma_{\text{MLE}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(x^{(i)} - \mu_{\text{MLE}}\right)^2}$$

“Fitting” a Guassian

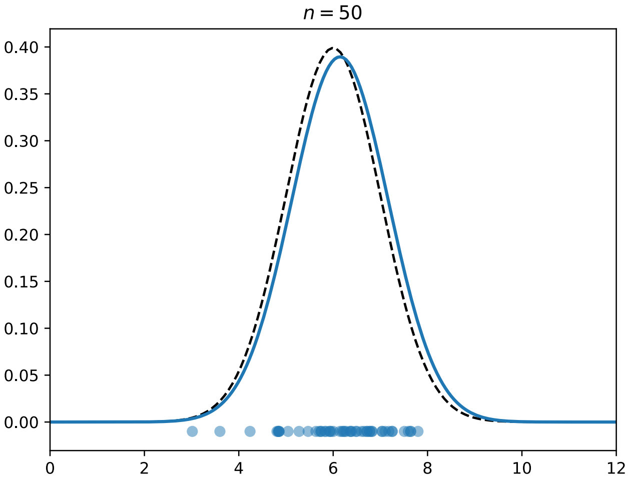
- Suppose we wish to “fit” a Gaussian to data $x^{(1)}, \dots, x^{(n)}$.

- The **maximum likelihood** approach:
  1. Compute:

$$\mu_{\text{MLE}} = \frac{1}{n} \sum_{i=1}^{n} x^{(i)} \qquad \sigma_{\text{MLE}} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - \mu_{\text{MLE}})^2}$$

  2. Use these as parameters of the Gaussian.

Example



In General

- **Maximum Likelihood Estimation** (MLE) can be used for a variety of densities.

- Suppose density p has parameters $\theta_1, \ldots, \theta_k$

1. Write log likelihood function:

$$\ln \mathcal{L}(\theta_1, \ldots, \theta_k) = \sum_{i=1}^{n} \ln p(x^{(1)}, \ldots, x^{(n)}; \theta_1, \ldots, \theta_k)$$

2. Compute derivatives: $\partial\tilde{\mathcal{L}}/\partial\theta_1, \partial\tilde{\mathcal{L}}/\partial\theta_2, \ldots, \partial\tilde{\mathcal{L}}/\partial\theta_k$

3. Set derivates to zero, solve for $\theta_1, \ldots, \theta_k$.

In Practice

- The MLE for a parameter only needs to be derived once.
- Many textbooks, statistics packages, and Wikipedia list the MLE parameter estimators.

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Probabilistic Modeling & Machine Learning

Lecture 12 | Part 3

Parametric vs. Non-Parametric Density Estimation

Making Predictions

- We observe a data set $\{(x^{(i)}, y_i)\}$ of flipper lengths and penguin species (0 or 1).

- **Task**: Given the flipper length of a new penguin, what is its species?

- Bayes' classifier: predict

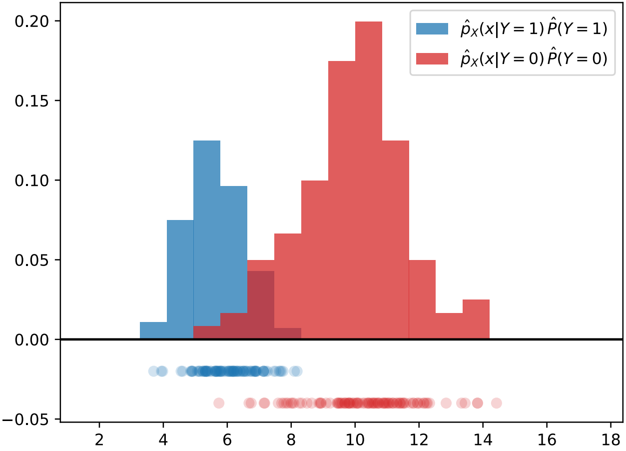
$$\begin{cases} 1, & \text{if } p_X(x \mid Y = 1)\mathbb{P}(Y = 1) > p_X(x \mid Y = 0)\mathbb{P}(Y = 0), \\ 0, & \text{otherwise.} \end{cases}$$

Estimating Densities

- We must estimate $p_X(x \mid Y = 0)$ and $p_X(x \mid Y = 1)$.
- Approach 1: Non-parametric (histograms)
- Approach 2: Parametric

Approach 1: Non-Parametric

- Estimate $p_X(x \mid Y = 0)$ and $p_X(x \mid Y = 1)$ with histograms.

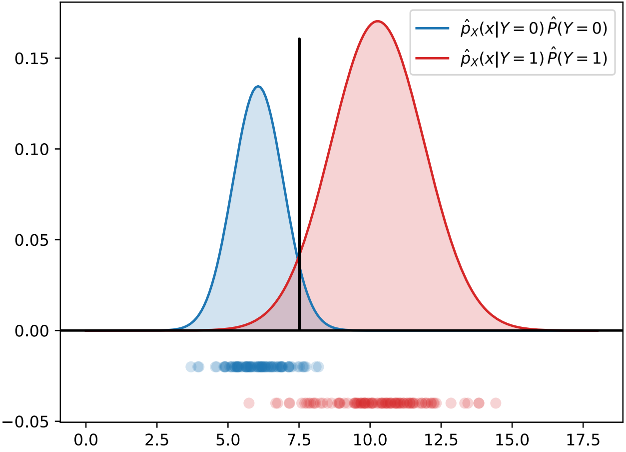


Approach 2: Parametric

- Must choose a parametric distribution.
- Plotting a histogram, data looks roughly normal.
- We will fit Gaussians.

Approach 2: Parametric

- Estimate $p_X(x \mid Y = 0)$ and $p_X(x \mid Y = 1)$ by fitting Gaussians with MLE.

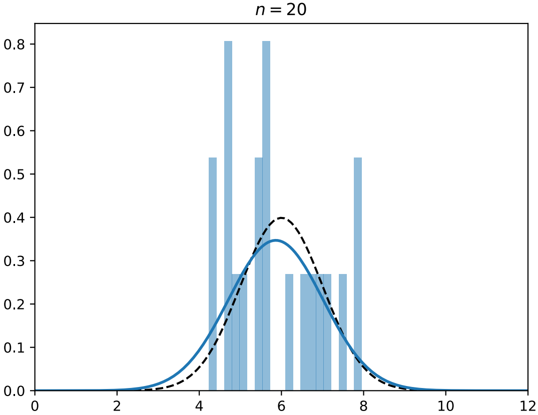


Data Requirements

- Suppose the underlying distribution that produced the data actually was a Gaussian.
  - Or close to one.

- The parametric approach will require less data than the non-parametric.

Data Requirements



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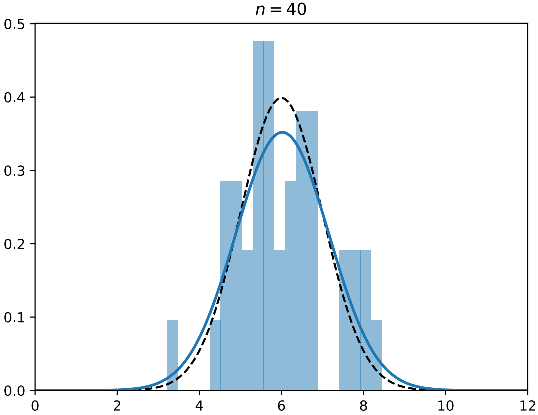

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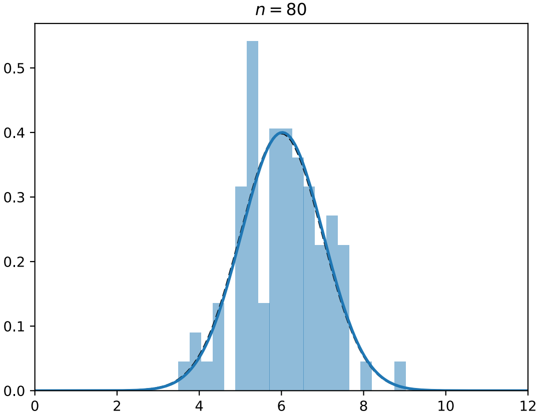

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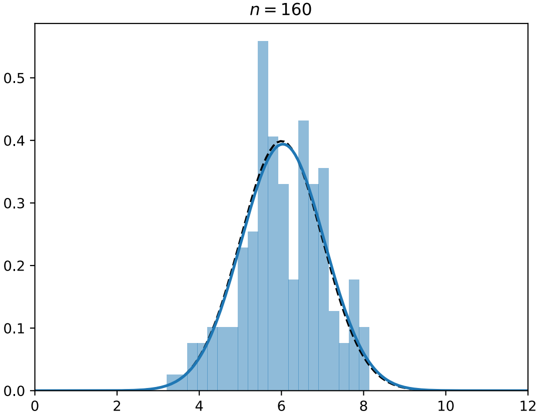

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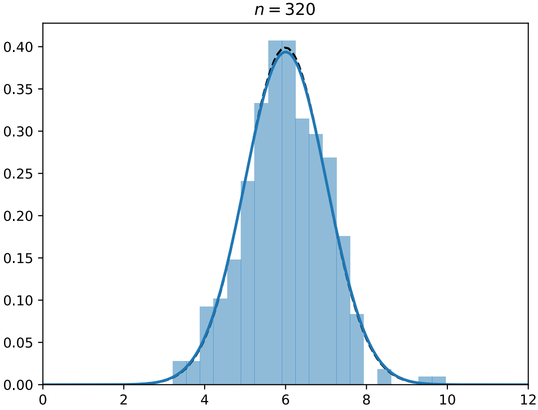

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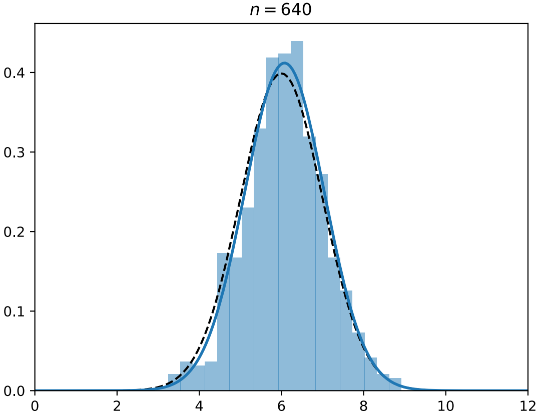

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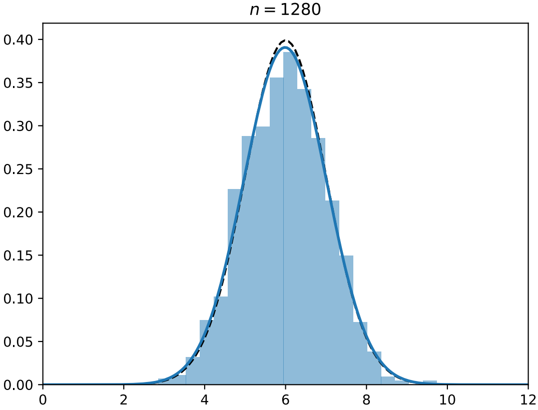
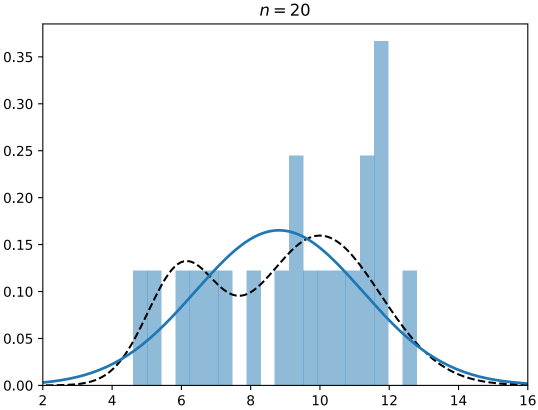


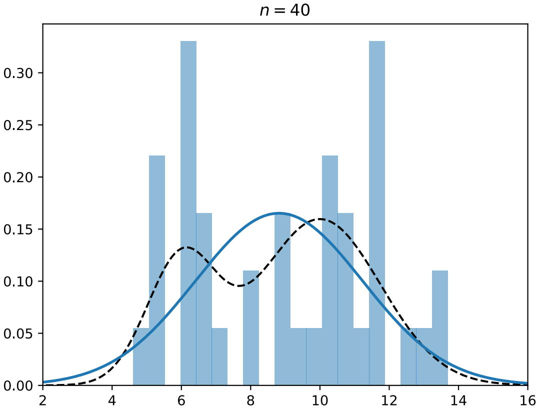
Mis-specification

- However, suppose the underlying distribution is **not** Gaussian.
- No amount of data will allow the parametric approach to get close.
  - The model has been **mis-specified**.
- But the non-parametric approach will be close, eventually.

Parametric vs. Non-Parametric



Parametric vs. Non-Parametric



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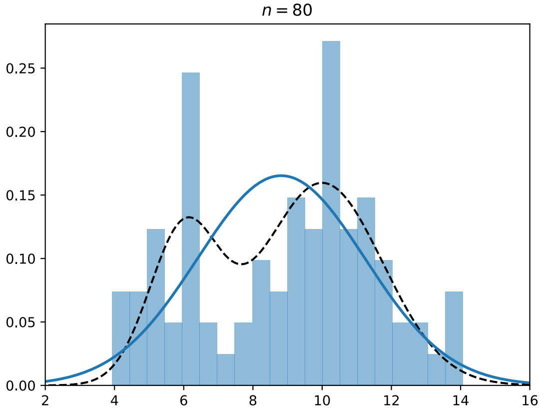
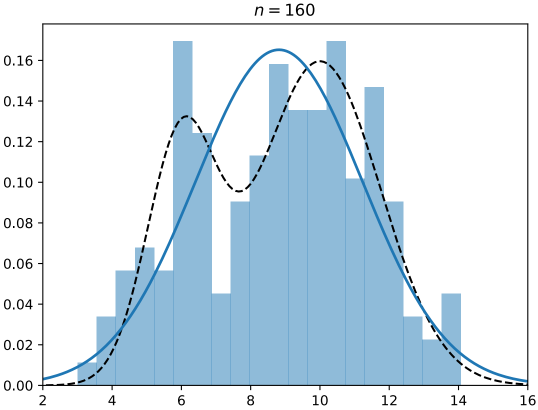


Parametric vs. Non-Parametric



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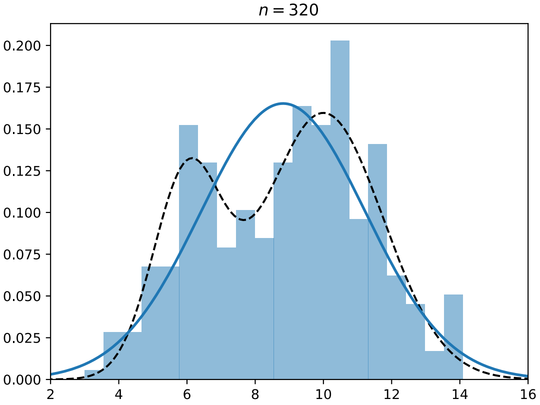

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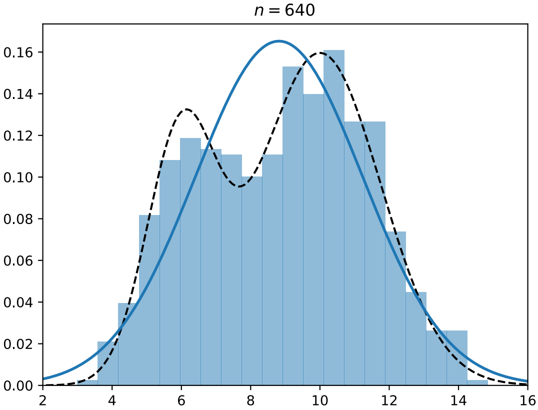
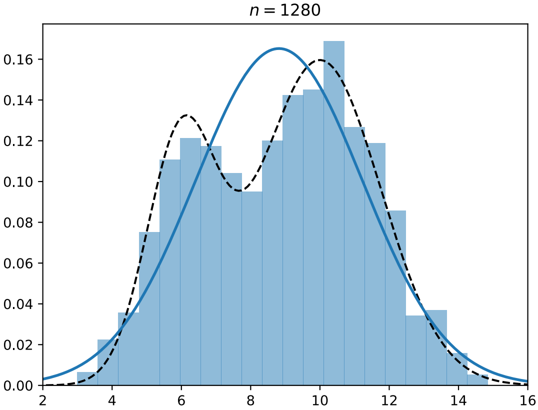


Parametric vs. Non-Parametric



High Dimensions

- Non-parametric approaches can fit arbitrary densities, but they require lots of data.
  - Especially in high dimensions!

- Parametric approaches require less data, provided that they are correctly specified.

- **Next time:** parametric density estimation in high dimensions.