Binary Density Estimation

CPSC 440/550: Advanced Machine Learning

`cs.ubc.ca/~dsuth/440/23w2`

University of British Columbia, on unceded Musqueam land

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Motivation: COVID-19 prevalence

- What percentage of UBC students have COVID-19 right now?
- "Brute force" approach:
  - Line up every single student, test them all, count the portion that test positive.
- Statistical apporach:
  - Grab an "independent and identically distributed" (iid) sample of students
  - Estimate the proportion that have it, based on the sample

General problem: binary density estimation

- This is a special case of density estimation with binary data:
  - Input: n iid samples of binary values $x^{(1)}, x^{(2)}, \ldots, x^{(n)} \in \{0, 1\}$
  - Output: a probability model for a random variable X: here, just $\Pr(X = 1)$
- As a picture:

$\mathbf{X} \in \mathbb{R}^{n \times 1}$ contains our sample data

X is a random variable over $\{0, 1\}$ from the distribution

$$\mathbf{X} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \xrightarrow{\text{density estimator}} \Pr(X = 1) = 0.4$$

- We'll start by discussing major concepts for this very simple case
  - We'll slowly build to more complicated cases
  - Beyond binary data, more than one variable, conditional versions, deep versions, etc

Other applications of binary density estimation

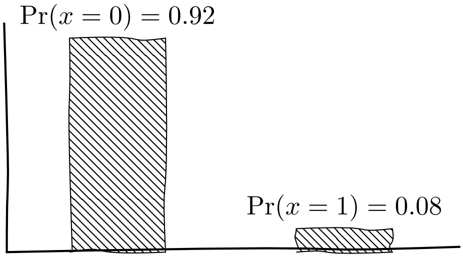
- Some other questions we might ask:
  1. What's the probability this medical treatment works?
  2. What's the probability that if you plant 10 seeds, at least one will germinate?
  3. How many lottery tickets should you expect to buy before you win?

- In the first example, we're computing $\Pr(X = 1)$ like before
- For the other two, we're using the model to compute some other quantity
  - We call all three "inference" with this model

Model definition: Bernoulli distribution

- We're going to start by using a parameterized probability model
  - i.e. a model with some parameters we can learn

- For binary variables, we usually use the Bernoulli distribution
- x is Bernoulli with parameter θ, or $x \sim \text{Bern}(\theta)$, if $\Pr(X = 1 \mid \theta) = \theta$
  - In the COVID example, if $\theta = 0.08$, we think 8% of the population has COVID
- Require that $0 \leq \theta \leq 1$ for a valid probability distribution



Digression: "inference" in statistics vs. ML

bonus!

- In machine learning, the usual terminology is:
  - "Learning" is the task of going from data $\mathbf{X}$ to parameters θ
  - "Inference" is the task of using the parameters θ to infer/predict something
- Statisticians sometimes use a "reverse" terminology:
  - Given data, you can "infer" parameters θ
  - Given parameters θ, you can predict something
- This is partly influenced by the history of the two communities:
  - Statisticians often assume there's a "true" parameter we can infer things about
  - ML hackers often focus on making predictions
- Some people use "inference" in both ways!
- We'll use the ML terminology

Inference task: computing probabilities

- An inference task: given θ, compute $\Pr(X = 0 \mid \theta)$
- We'll also sometimes write this as $p(0 \mid \theta)$
  - Be careful you know what we're abbreviating! "Explicit is better than implicit"

- Recall that probabilities add up to 1: since $X \in \{0, 1\}$,

$$\Pr(X = 0 \mid \theta) + \Pr(X = 1 \mid \theta) = 1$$

- Since $\Pr(X = 1 \mid \theta) = \theta$ by definition, this gives us

$$\Pr(X = 0 \mid \theta) + \theta = 1$$

- and so if $X \sim \mathrm{Bern}(\theta)$, we know $\Pr(X = 0 \mid \theta) = 1 - \theta$
- First inference task down!

Bernoulli distribution notation

- It's sometimes helpful to combine the Bernoulli distribution into one expression:

$$p(x \mid \theta) = \theta^x (1-\theta)^{1-x} = \theta^{\mathbb{1}(x=1)} (1-\theta)^{\mathbb{1}(x=0)}$$

- $\mathbb{1}$ is an "indicator function": $\mathbb{1}(E)$ is 1 if the condition E is true, and 0 if it's not

Aside: p for probability masses

bonus!

- If you're like me, you might be bothered by using a lowercase p in $p(0 \mid \theta)$
  - It's a probability mass, not a density!
- This is really really common among ML people, but when I first taught this class I started trying to change them all to P – or even to change everything to $\Pr$
- ...it got really really messy (why this is really really common among ML people)

- If you're like me, this might be reassuring:
  - p actually **is** a probability density for the Bernoulli distribution
  - It's just the Radon-Nikodym derivative wrt $\mu(A) = \mathbb{1}(0 \in A) + \mathbb{1}(1 \in A)$
- If you haven't seen measure-theoretic probability, don't worry – it's not actually relevant to this course

Outline

1. Bernoulli distributions
2. Bernoulli inference tasks

Inference task: computing dataset probabilities

- Inference task: given θ and an iid sample, compute $p(x^{(1)}, x^{(2)}, \ldots, x^{(n)} \mid \theta)$
- Also called the "likelihood": $\Pr\left(X^{(1)} = x^{(1)}, X^{(2)} = x^{(2)}, \ldots, X^{(n)} = x^{(n)} \mid \theta\right)$
  - Many ways to estimate/learn θ need this, e.g. maximum likelihood estimation
  - Also helpful in comparing models on validation/test data

- Assuming the $X^{(i)}$ are independent given θ, we have

$$p\left(x^{(1)}, x^{(2)}, \ldots, x^{(n)} \mid \theta\right) = \prod_{i=1}^{n} p\left(x^{(i)} \mid \theta\right)$$

  - We'll talk much more about conditional independence later in the course

Inference task: computing dataset probabilities

- Using the independence property, for example, $p(1, 0, 1, 1 \mid \theta)$ is

$$
\begin{aligned}
p\left(x^{(1)}, \ldots, x^{(4)} \mid \theta\right) &= \prod_{i=1}^{4} p\left(x^{(i)} \mid \theta\right) \\
&= p\left(x^{(1)} \mid \theta\right) \quad p\left(x^{(2)} \mid \theta\right) \quad p\left(x^{(3)} \mid \theta\right) \quad p\left(x^{(4)} \mid \theta\right) \\
&= \theta \quad (1-\theta) \quad \theta \quad \theta \\
&= \theta^{3}(1-\theta)
\end{aligned}
$$

- More generally, we can write

$$
\begin{aligned}
p(\mathbf{X} \mid \theta) &= \theta^{\sum_{i=1}^{n} x_i}(1-\theta)^{\sum_{i=1}^{n}(1-x_i)} \\
&= \theta^{\sum_{i=1}^{n} \mathbb{1}(x_i=1)}(1-\theta)^{\sum_{i=1}^{n} \mathbb{1}(x_i=0)} \\
&= \theta^{n_1}(1-\theta)^{n_0}
\end{aligned}
$$

Inference task: computing dataset probabilities

```python
n_1 = 0
n_0 = 0
for i in range(n):
    if X[i] == 1:
        n_1 += 1
    else:  # binary data
        n_0 += 1
p = theta ** n_1 * (1 - theta) ** n_0
```

Better version:

```python
n_1 = X.sum()
n_0 = X.shape[0] - n_1
log_p = n_1 * np.log(theta) \
      + n_0 * np.log1p(-theta)
```

- Computational complexity (of either): $\mathcal{O}(n)$
  - Look at each element once, doing a singe addition each time, then a constant number of operations for final value
- Operating in "log space" is very practically helpful:
  - If n is huge and/or θ is very close to 0 or 1, the probability is tiny
  - Calculation might underflow and return zero / be very inaccurate
  - Logarithms give you much bigger range of effective floating point computation
  - `np.log1p(t)` is $\log(1+t)$, but floats are much more accurate near 0 than 1!

Inference task: finding the mode ("decoding")

- Inference task: given θ, find the x that maximizes $p(x \mid \theta)$
  - "What's most likely to happen?"

- For Bernoulli models:
- If $\theta < 0.5$, the mode is $x = 0$
  - If $\theta = 0.03$, it's more likely that a random person **does not** have COVID-19.
- If $\theta > 0.5$, the mode is $x = 1$
  - If $\theta = 0.6$, it's more likely that a random person **does** have COVID-19 (uh-oh)
- If $\theta = 0.5$, both $x = 0$ and $x = 1$ are valid modes

- This process isn't very exciting for Bernoulli models.
  - For more complex models, it can be pretty hard (and important)
  - We'll see later than classification can be viewed as finding a (conditional) mode

Inference task: finding the most likely dataset

- Inference task: given θ, find the $\mathbf{X}$ that maximizes $p(\mathbf{X} \mid \theta)$
  - "What set of training example are we most likely to observe?"

- Recall for Bernoullis, $p(\mathbf{X} \mid \theta) = \theta^{n_1}(1-\theta)^{n_0}$

- If $\theta < 0.5$, the most likely dataset is $\mathbf{X} = (0, 0, 0, 0, \dots)$
  - $p(\mathbf{X} \mid \theta)$ is maximized if n_0 is as big as possible, and n_1 small
  - If $\theta = 0.3$, the "most likely" sample has zero positives!

- The modal dataset almost never represents "typical" behaviour.
  - If $\theta = 0.3$, we expect about 30% of samples to be 1, not 0%!
  - The modal $\mathbf{X}$ has the highest probability, but that probability might be really low
    - There are many datasets with some 1s in them
    - *Each one* is lower-probability than the all-zero dataset
    - As a whole they're overwhelmingly more likely

Inference task: sampling

- Inference task: given θ, generate X according to $p(X \mid \theta)$
  - Called sampling from the distribution

- Sampling is the "opposite" of density estimation:

$$\Pr(X = 1) = 0.4 \quad \xrightarrow{\text{sampling}} \quad \mathbf{X} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

- Given the model, your job is to generate IID examples
- Often write code to generate one sample, and call it many times

Why sample?

bonus!

- Sampling isn't especially interesting for Bernoulli distributions
  - Knowing θ tells you everything about the distribution

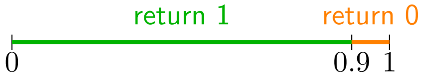
- But sampling will let us do neat things in more-complicated density models:
  - `thispersondoesnotexist.com`, DALL-E, ChatGPT, ...

- Sampling often helps us check whether the model is reasonable
  - If samples look nothing like the data, the model isn't very good

Inference task: sampling

- Basic ingredient of typical sampling methods:
- We assume we can sample uniformly on $[0, 1]$
- In practice, we use a "pseudo-random" number generator
  - `rng = np.random.default_rng(); t = rng.random()`
  - We won't talk about how this works; see CPSC 436R / Nick's book

- Consider sampling from $\mathrm{Bern}(0.9)$
  - 90% of the time, we should produce a 1
  - 10% of the time, we should produce a 0
- How can we do that with a sample from $U \sim \mathrm{Unif}([0, 1])$?
  - If $U \leq 0.9$, return 1; otherwise, return 0.



Inference task: sampling

- Sampling from $\mathrm{Bern}(\theta)$:
  - Generate $U \sim \mathrm{Unif}([0,1])$. If $U \leq \theta$, return 1; otherwise, return 0
- ```
  u = rng.random()
  if u <= theta:
      x = 1
  else:
      x = 0
  ```
  or `x = 1 if rng.random() <= theta else 0`
  or `x = (rng.random(t) <= theta).astype(int)`
- Assuming the uniform RNG costs $\mathcal{O}(1)$, generates a single sample in $\mathcal{O}(1)$ time
- To generate t samples, nothing smarter to do than just call it t times; $\mathcal{O}(t)$ cost
  ```

Summary

- Binary density estimation: models $\Pr(X = 1)$ given iid samples $x^{(1)}, \ldots, x^{(n)}$
- Bernoulli distribution over binary variables
  - Parameterized by $\theta \in [0, 1]$ with $\Pr(X = 1 \mid \theta) = \theta$
- Inference: computing things from models, like finding modes and sampling

- Next time: the exciting world of priors