ECE 20875

Python for Data Science

David Inouye and Qiang Qiu

(Adapted from material developed by Profs. Milind Kulkarni, Stanley Chan, Chris Brinton, David Inouye, Qiang Qiu)

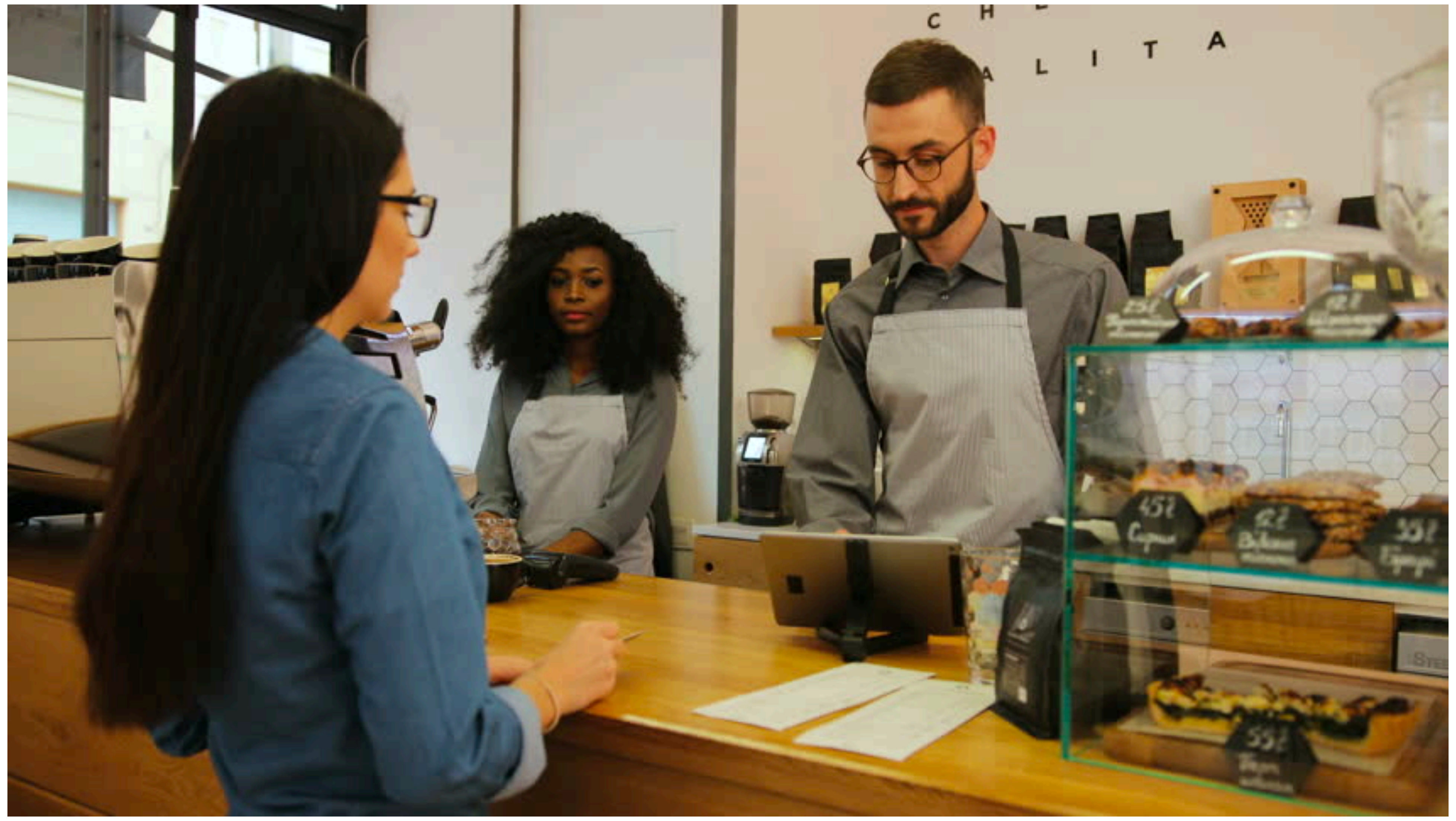
Histograms

a problem

- You're managing a coffee shop
- Assuming you want to maximize profit, how much coffee should you buy for each day?
    - Too much → Surplus, waste money :(
    - Too little → Unsatisfied demand, under-caffeinated customers :(
- What should you do?

collect data

- Count how many people get coffee in a day
  - Day 1: 37 people
  - Likely different each day of the week, and the type of coffee (cold brew, late, etc.) also has an impact
  - Assume such factors do not matter (problem is still interesting!)
- Should we just get enough coffee for 37 people?



(keep) collect(ing) data

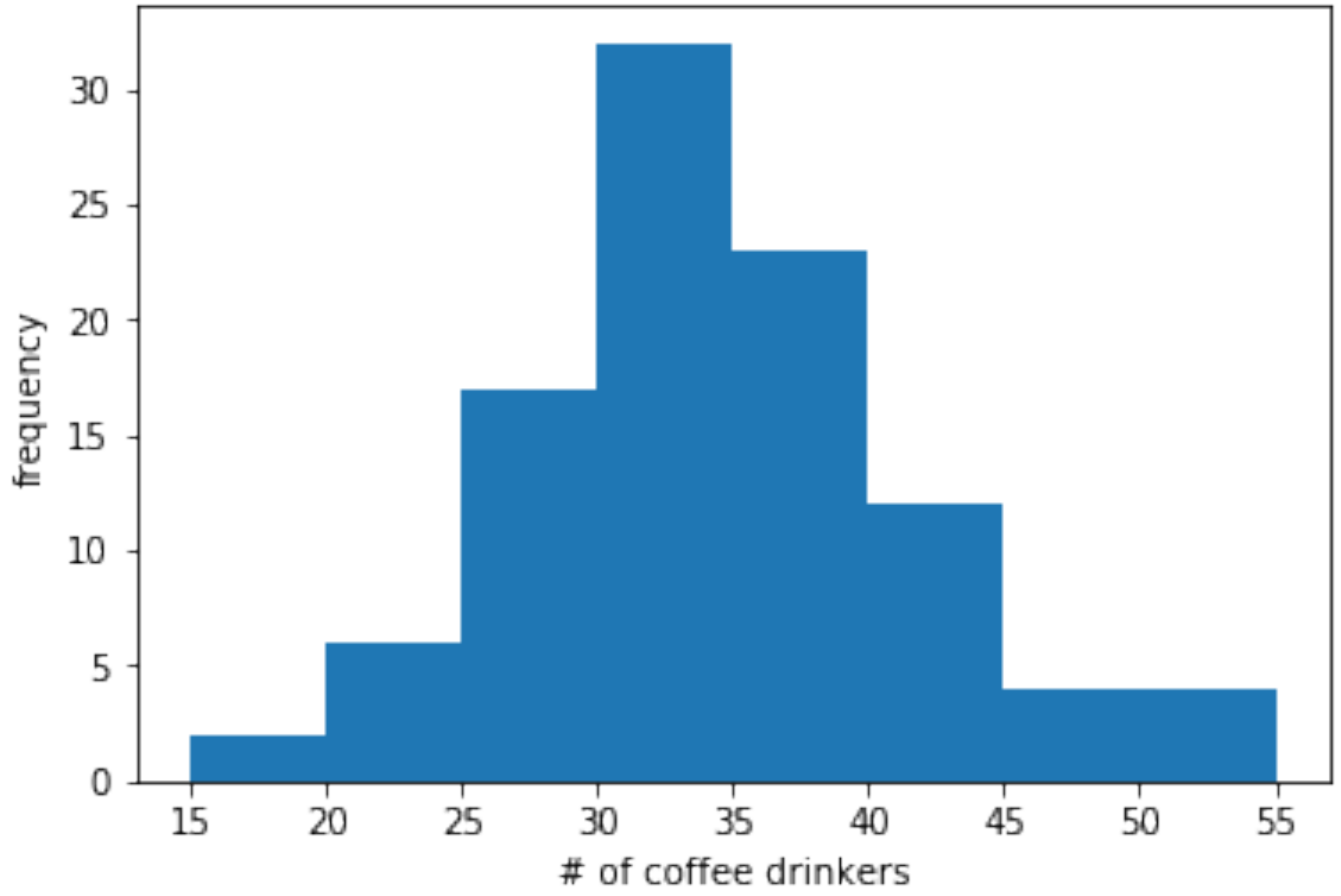
- Day 2: 43
- Day 3: 48
- Day 4: 41
- Day 5: 46
- Day 6: 19 (!)
- Day 7: 38
- …

100 days later ...

```
[37, 43, 48, 41, 46, 19, 28, 35, 34, 38,
31, 32, 32, 23, 23, 33, 35, 39, 34, 28,
39, 28, 29, 38, 28, 30, 25, 35, 39, 35,
31, 28, 25, 26, 15, 31, 28, 32, 40, 21,
34, 38, 30, 47, 34, 31, 51, 30, 41, 36,
33, 51, 22, 25, 29, 50, 32, 39, 25, 37,
54, 33, 36, 25, 30, 22, 41, 35, 31, 40,
30, 33, 27, 36, 27, 34, 24, 41, 37, 29,
48, 40, 31, 32, 33, 32, 40, 31, 32, 40,
31, 33, 32, 38, 37, 41, 37, 39, 38, 42]
```

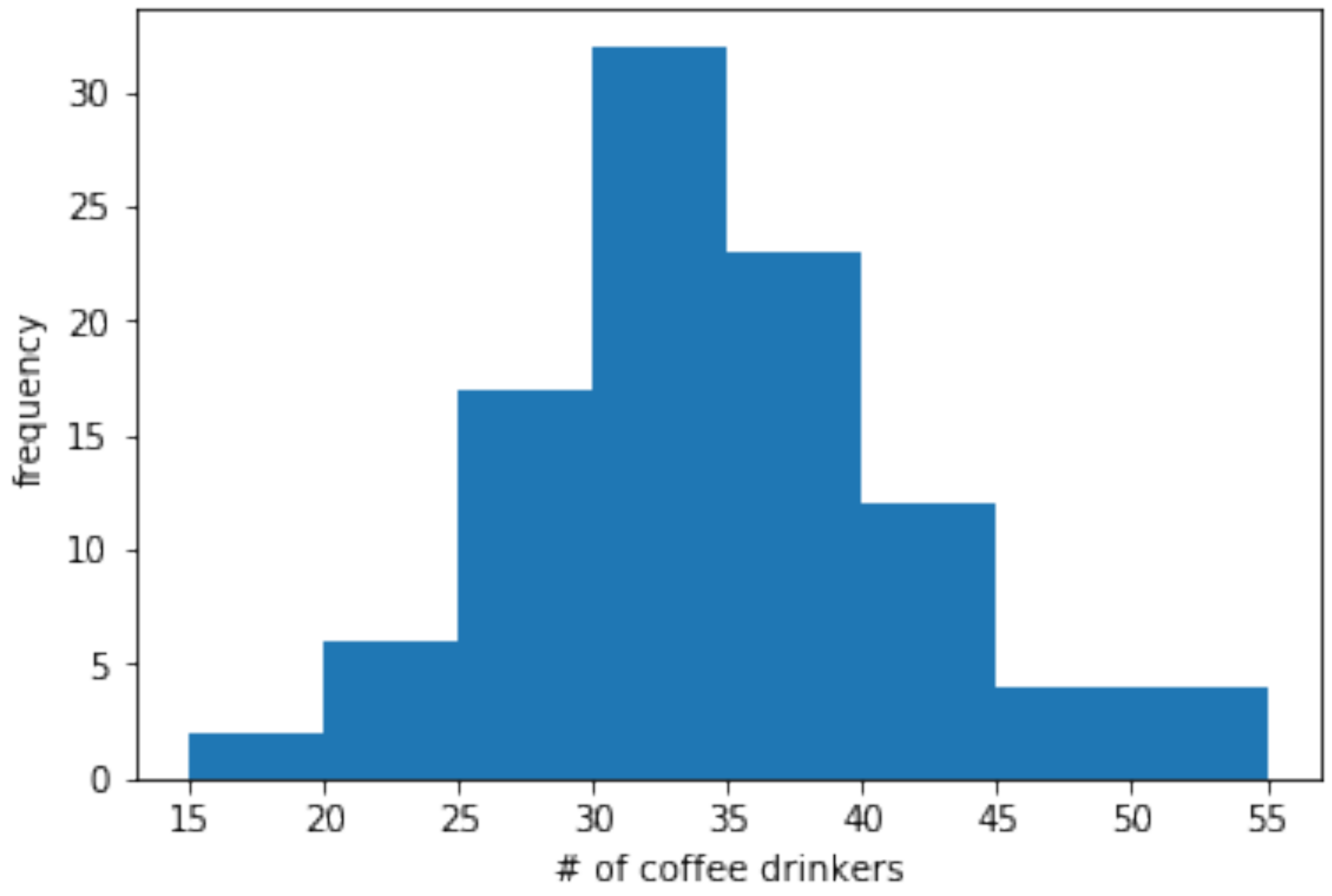
visualize the data

- Staring at a list of numbers is not very illuminating
- Visualizing the data in a useful way can help reveal patterns
  - **Data visualization** is an important subset of data science
- Since the data consists of a single, numeric variable, we can try a **histogram**



building a histogram

- A histogram visualizes observations of a random variable d
- Each bar in a histogram is a **bin**
  $x_1, x_2, \ldots$
- Each observation is placed into one bin
  $x_1 : 15 \leq d < 20,\ x_2 : 20 \leq d < 25, \ldots$
- The **count** (size/height) of each bin is the number of observations in that bin
  $x_1 : 2,\ x_2 : 6, \ldots$




```
import matplotlib.pyplot as plt
_ = plt.hist(data, bins=8, range=(15,55))
plt.xlabel('# of coffee drinkers')
plt.ylabel('frequency')
plt.show()
```

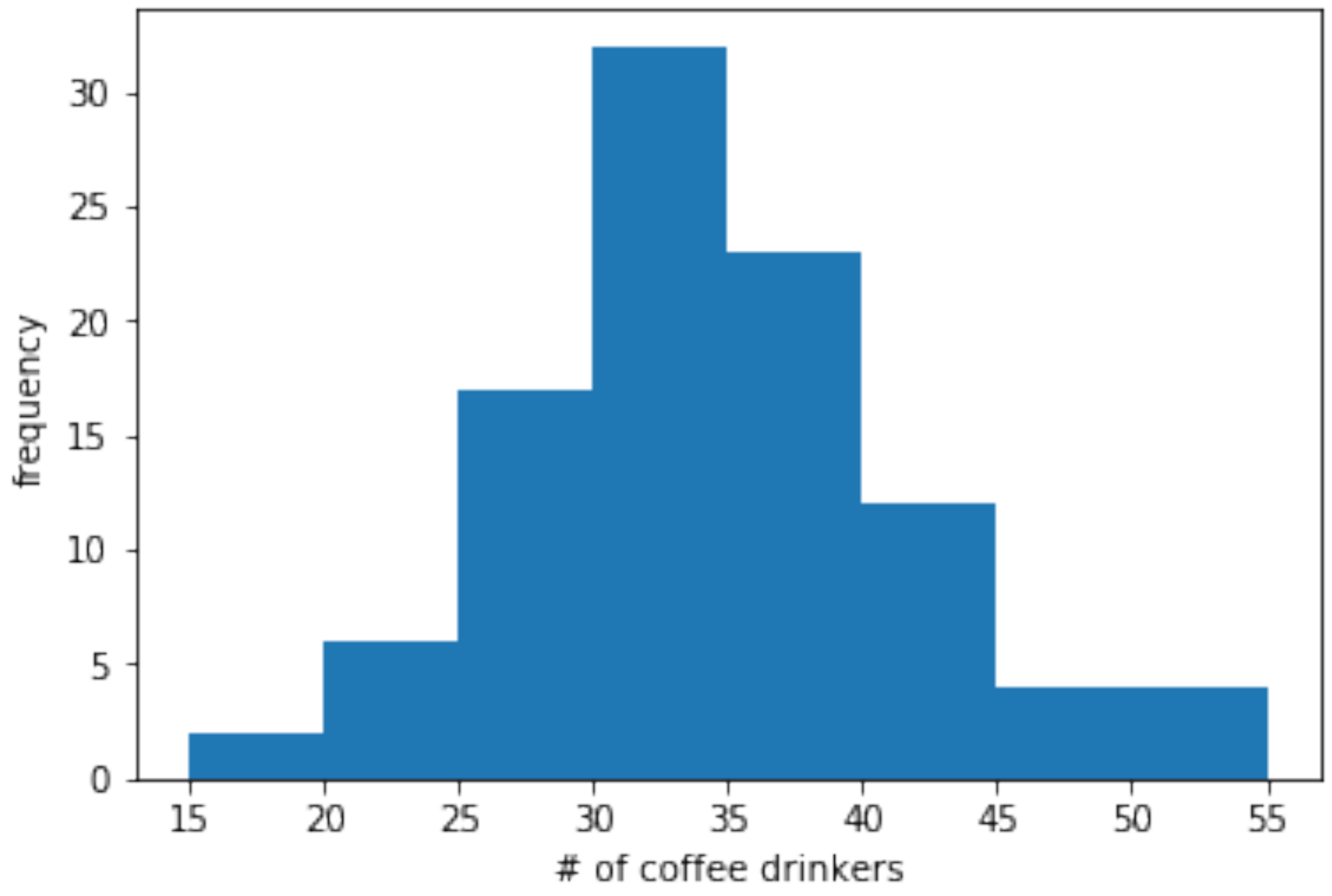
building a histogram

- The empirical (measured) **frequency** of each bin is the fraction of data in that bin

$$\hat{p}_1 = x_1 / \sum_k x_k = 0.02, \;\; \hat{p}_2 = x_2 / \sum_k x_k = 0.06, \ldots$$

Note that $\sum_k \hat{p}_k = 1$

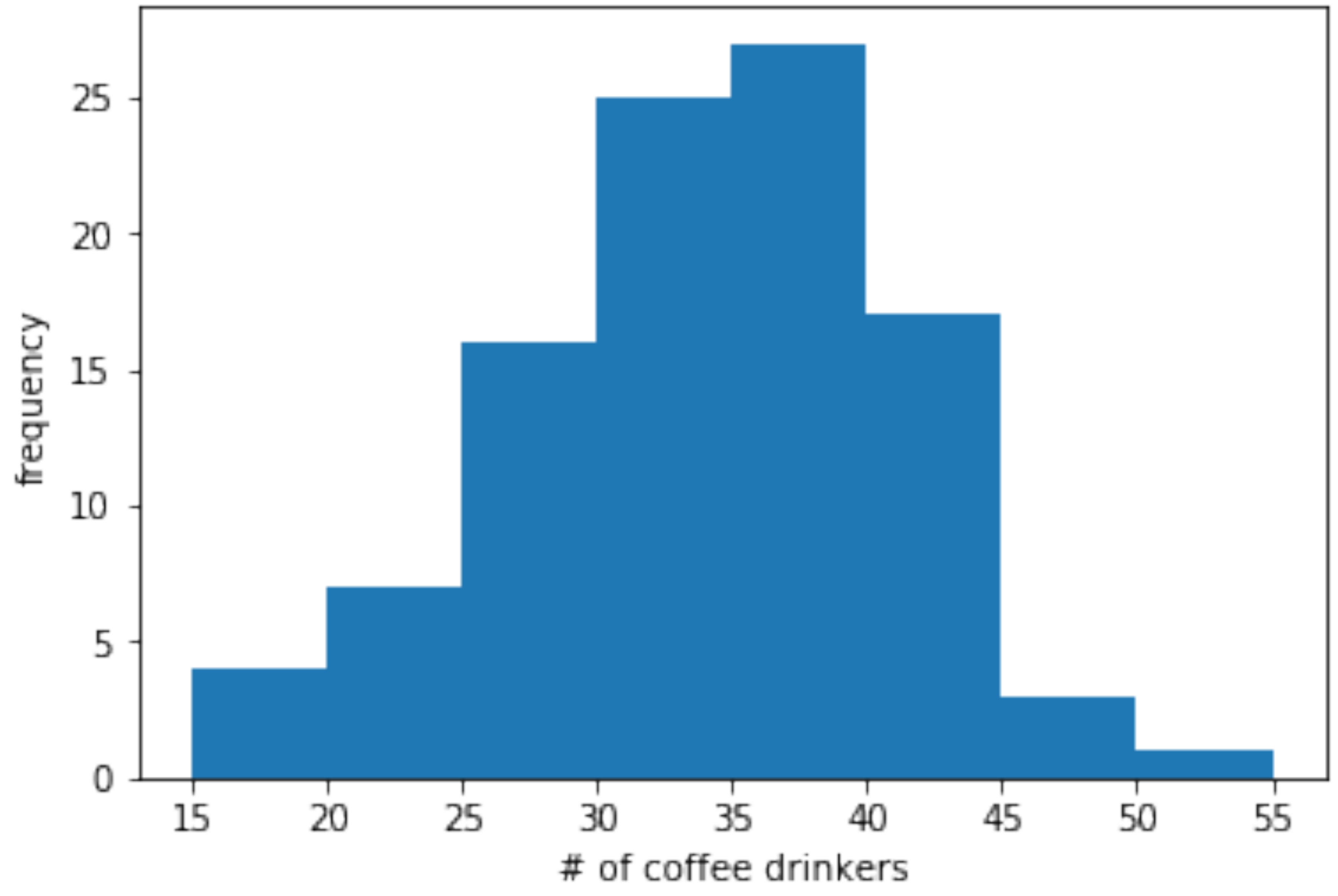
- Often, count is also referred to as frequency
  - The y-axis numbers telling us what exactly is plotted
  - (More details on later slides)




```
_ = plt.hist(data, bins=8, range=(15,55))
plt.xlabel('# of coffee drinkers')
plt.ylabel('frequency')
```

repeating the experiment

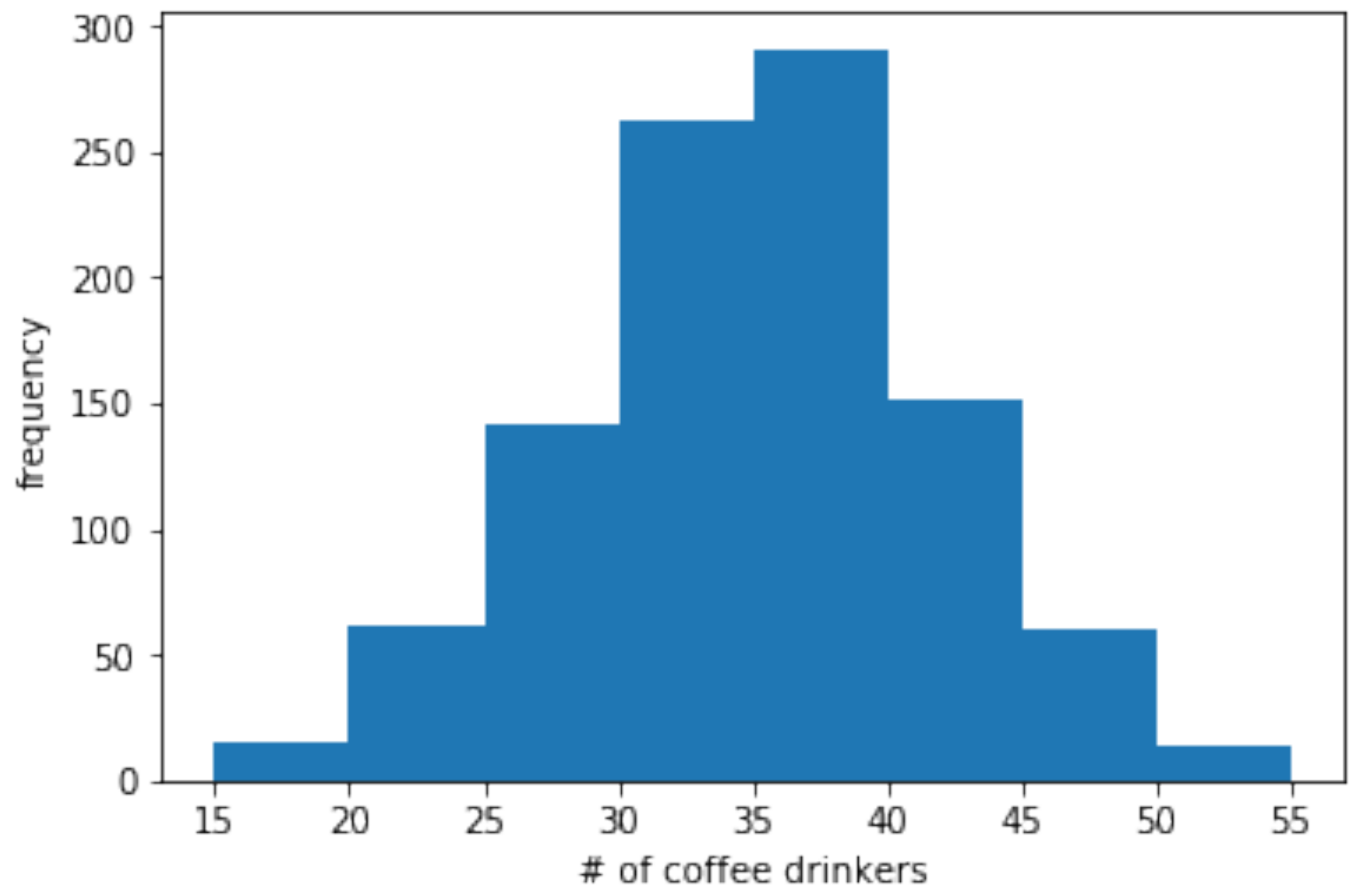
- Remember: This histogram comes from observed data
- If we repeat the experiment, we might not get the same histogram!
    - In fact, there will almost surely be some difference at this sample size
- This is because what we have is a **sample** of the true distribution




```
_ = plt.hist(data, bins=8, range=(15,55))
plt.xlabel('# of coffee drinkers')
plt.ylabel('frequency')
```

collecting a larger sample

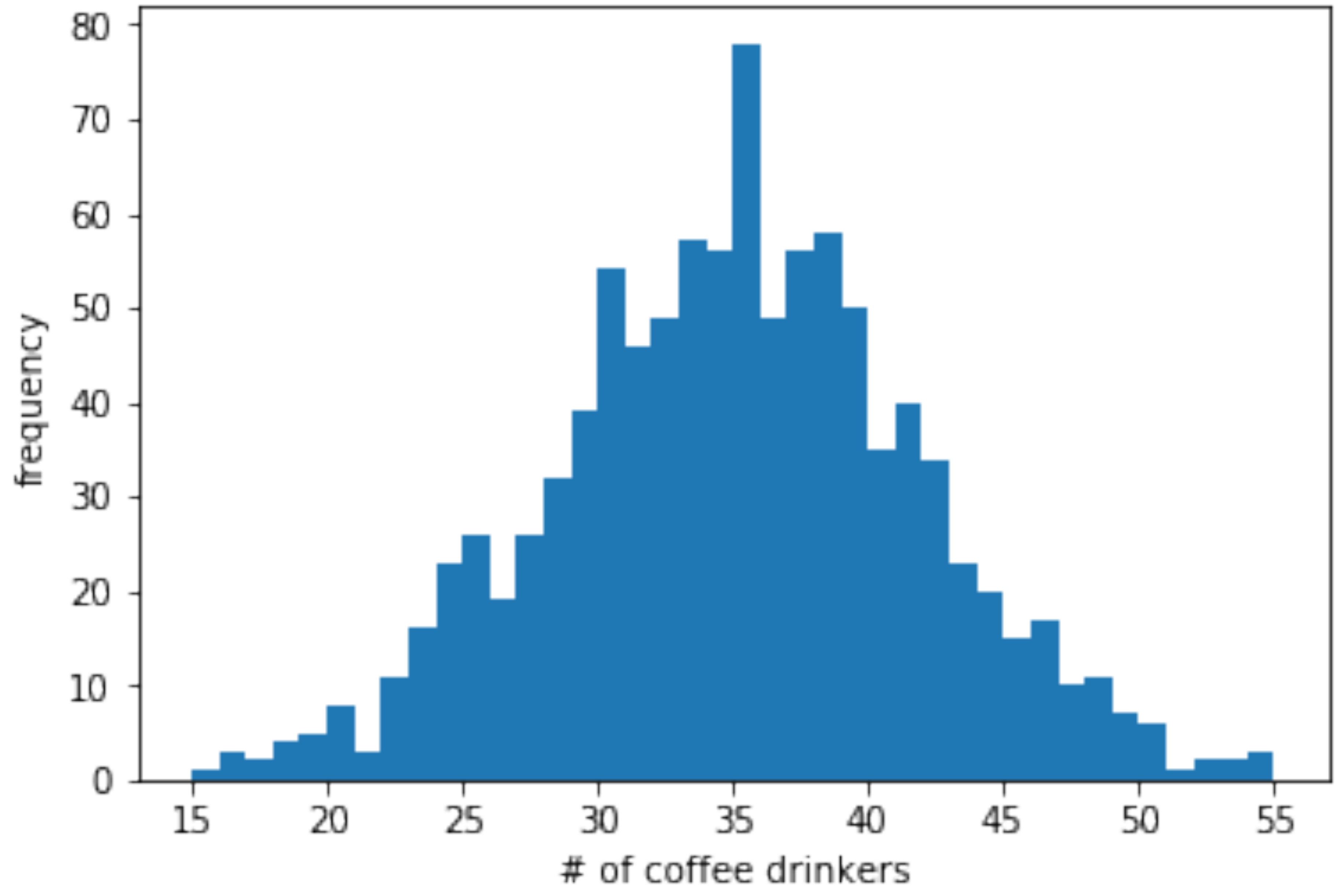
- Suppose we collect 1000 observations instead of 100
- The result on the right looks basically the same!
- Using the same number of bins
  - Each bin has more observations in it
  - But the relative frequencies are not changing much
- But now that we have a larger sample, we can add more bins to see a *finer granularity* of the distribution




```
_ = plt.hist(data, bins=8, range=(15,55))
plt.xlabel('# of coffee drinkers')
plt.ylabel('frequency')
```

adding more bins

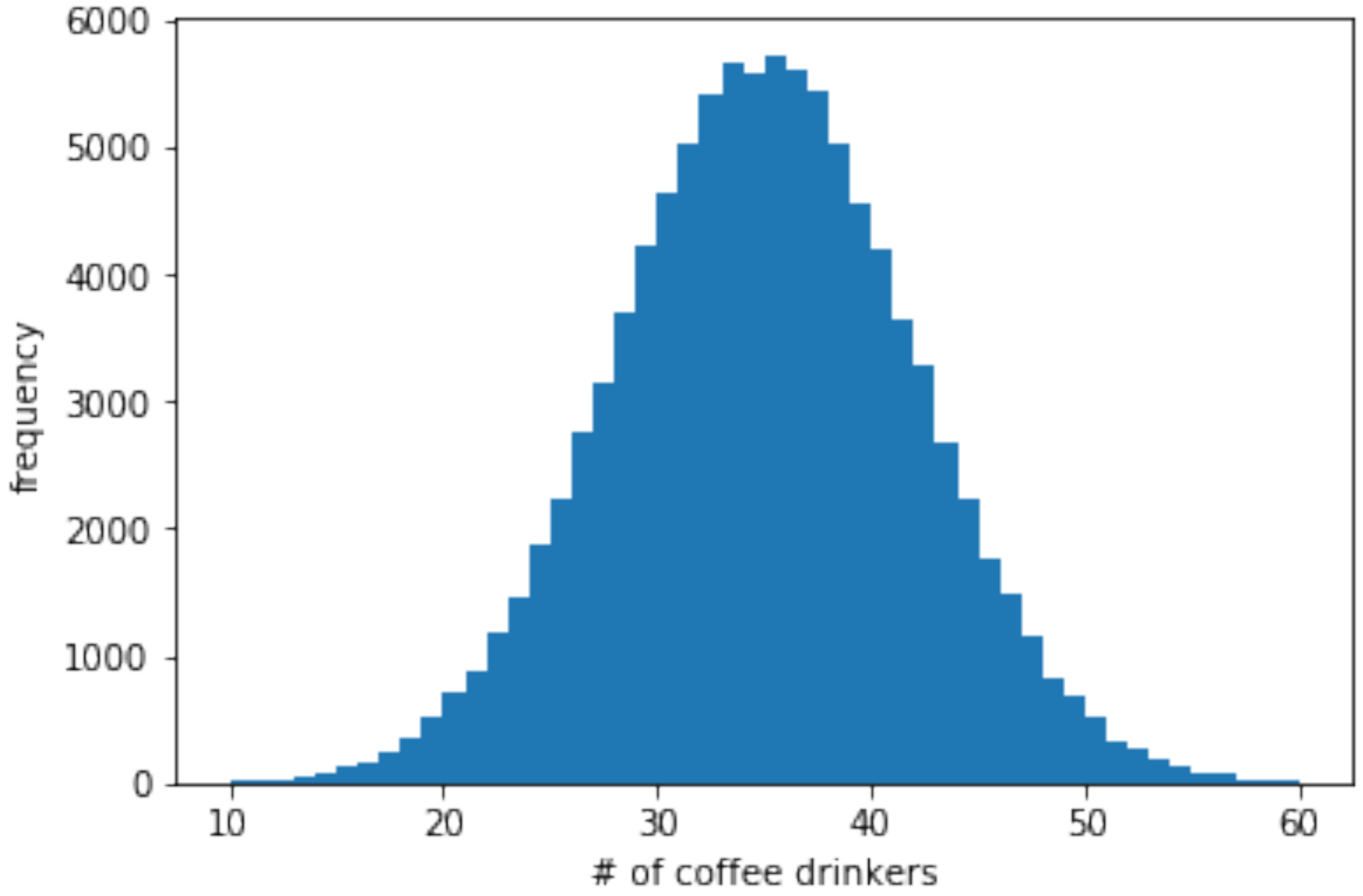
- This looks better!
- Gives us a good sense of what the data looks like, and what the underlying distribution is
- What would happen if we used more than 40 bins here?




```
_ = plt.hist(data, bins=40, range=(15,55))
plt.xlabel('# of coffee drinkers')
plt.ylabel('frequency')
```

adding even more data

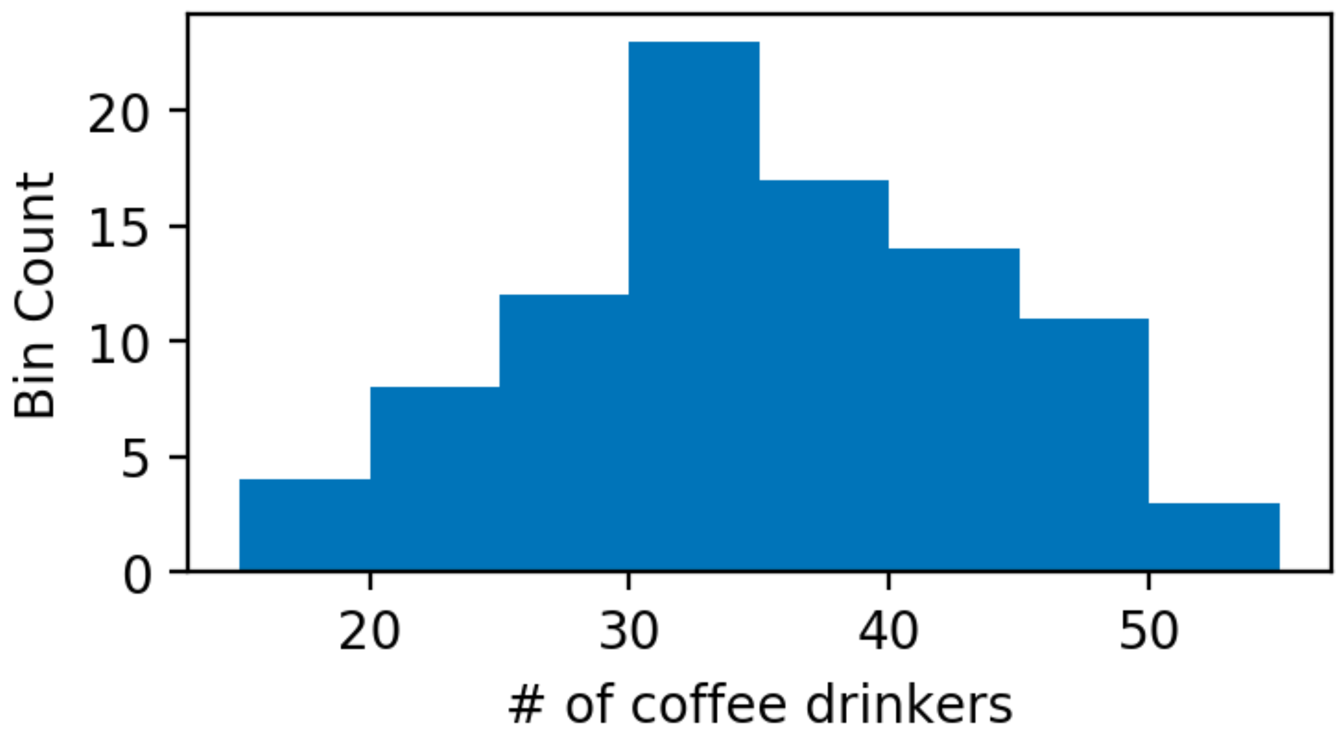
- This looks even better!
- As we add more data points, our histogram looks more and more like the “true” shape of the underlying distribution
  - We’ll get in to what this means when we talk about distributions and sampling

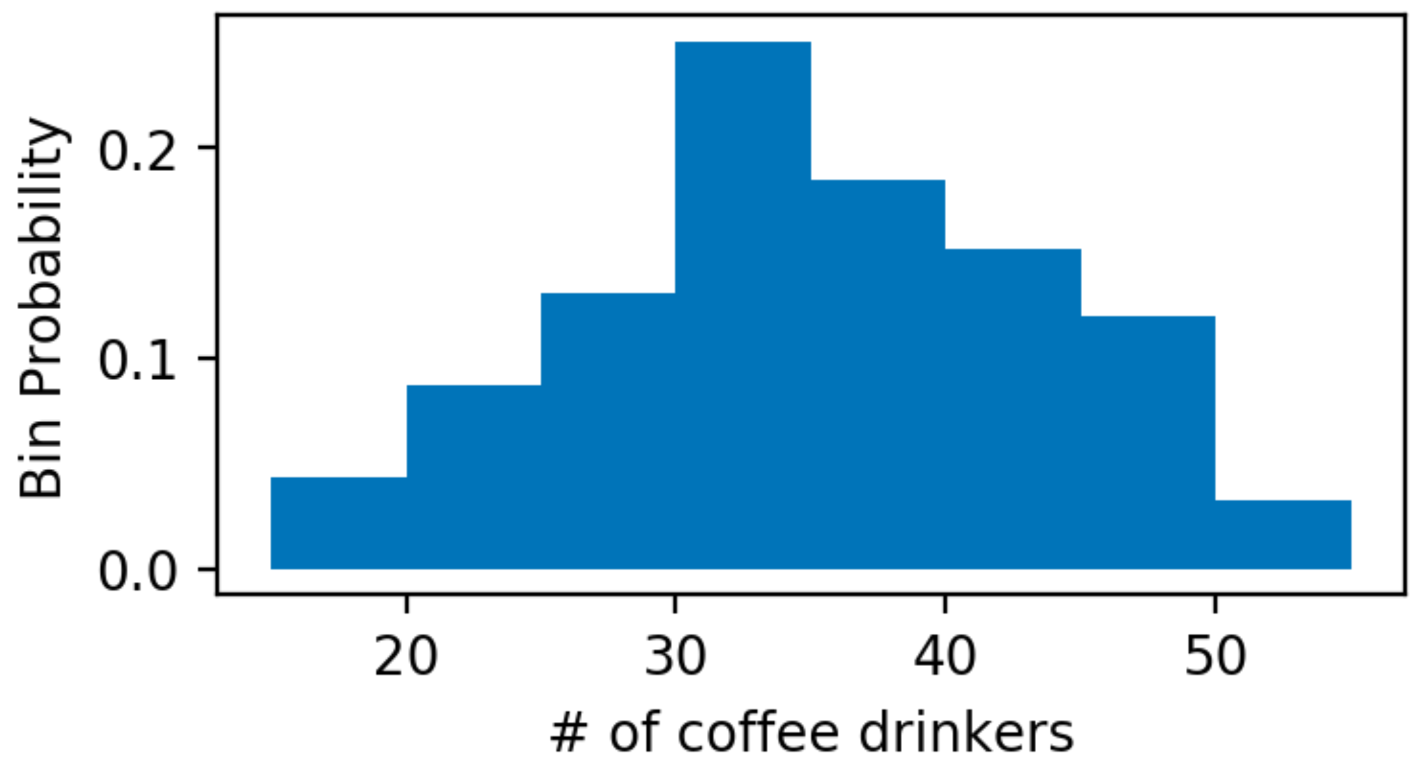


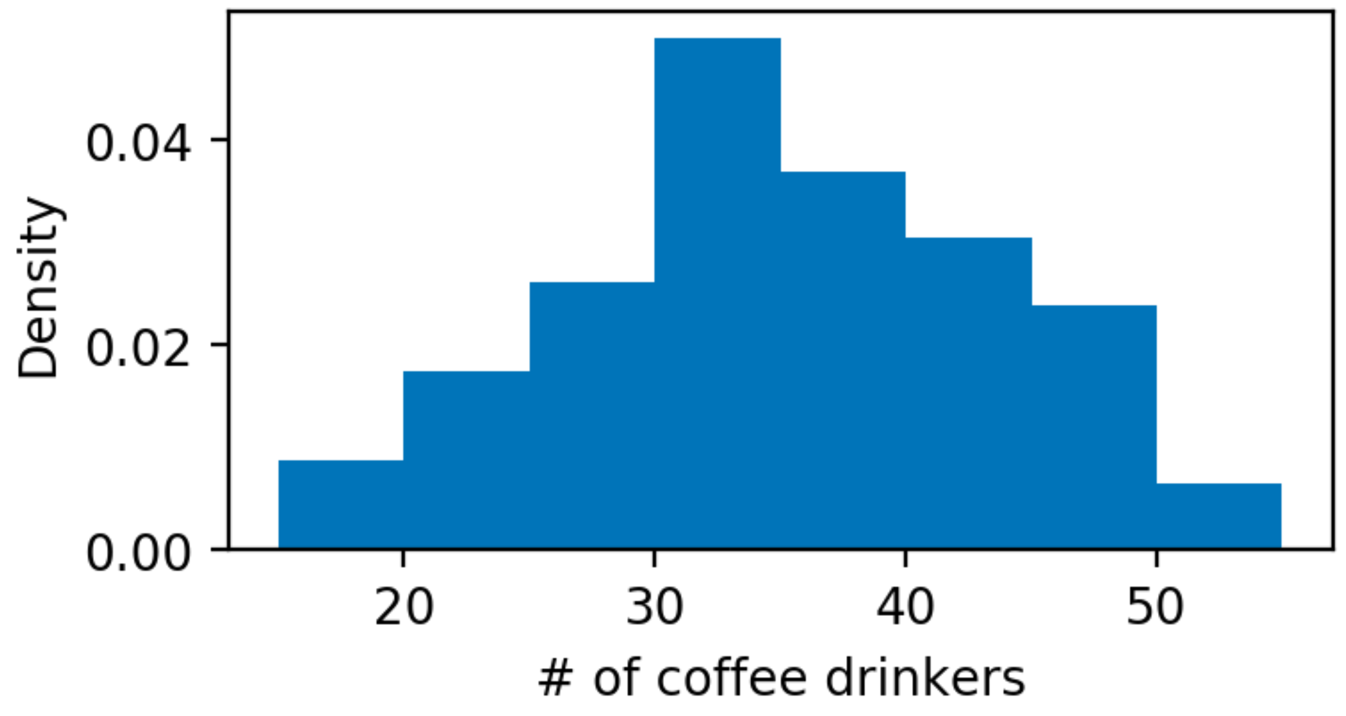

```
_ = plt.hist(data, bins=40, range=(15,55))
plt.xlabel('# of coffee drinkers')
plt.ylabel('frequency')
```

histogram bin normalization

- **<u>Count</u>** - y-axis is the count in each bin, denoted x_k
  - $\sum_{k=1}^{n} x_k = m$, sum of all bins is total number of samples m
- **<u>Probability</u>** - y-axis is probability for each bin, denoted $\hat{p}_k = \frac{x_k}{\sum_l x_l}$
  - $\sum_k \hat{p}_k = 1$, sum of all bin probabilities is 1
- **<u>Density</u>** - y-axis is normalized by both probability and **bin width**, $\hat{d}_k = \frac{\hat{p}_k}{w}$
  - So $\sum_k w\hat{d}_k = 1$, i.e., the **area under the curve** is 1
- “Frequency” can be used for both “count” and “probability” above



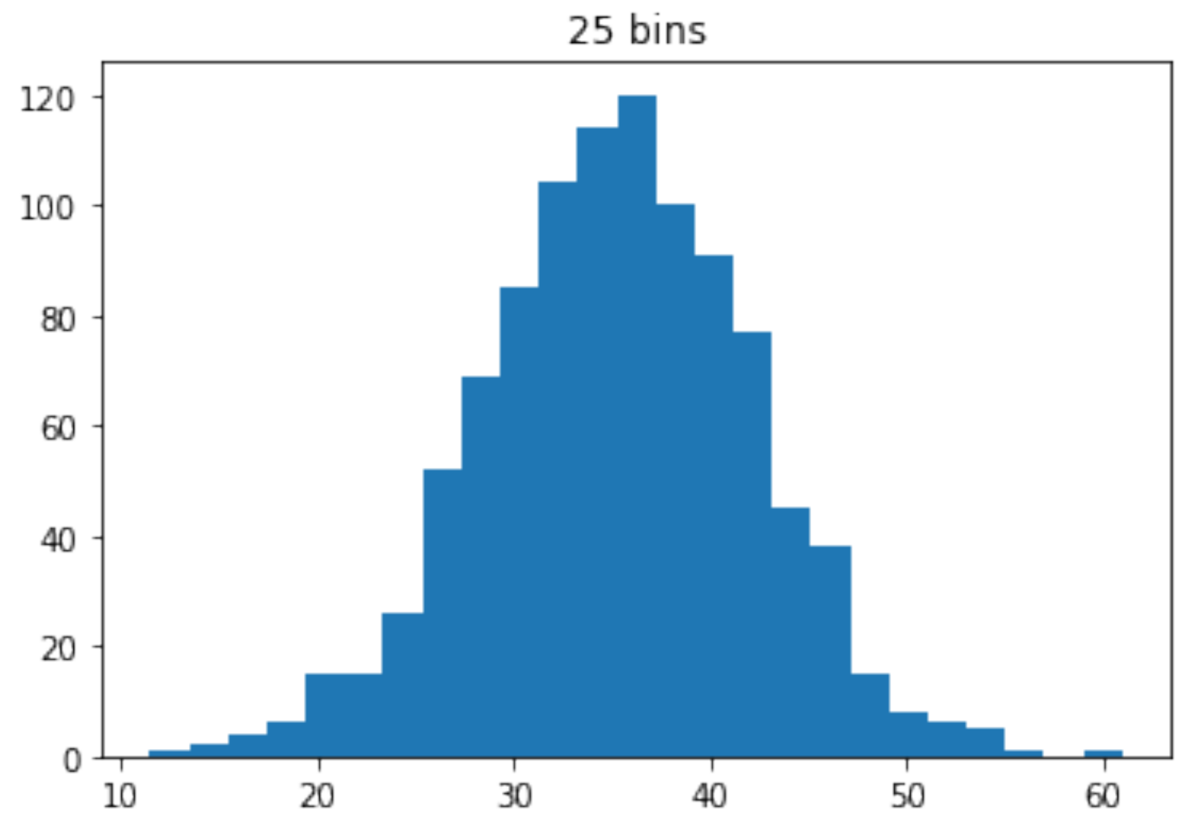


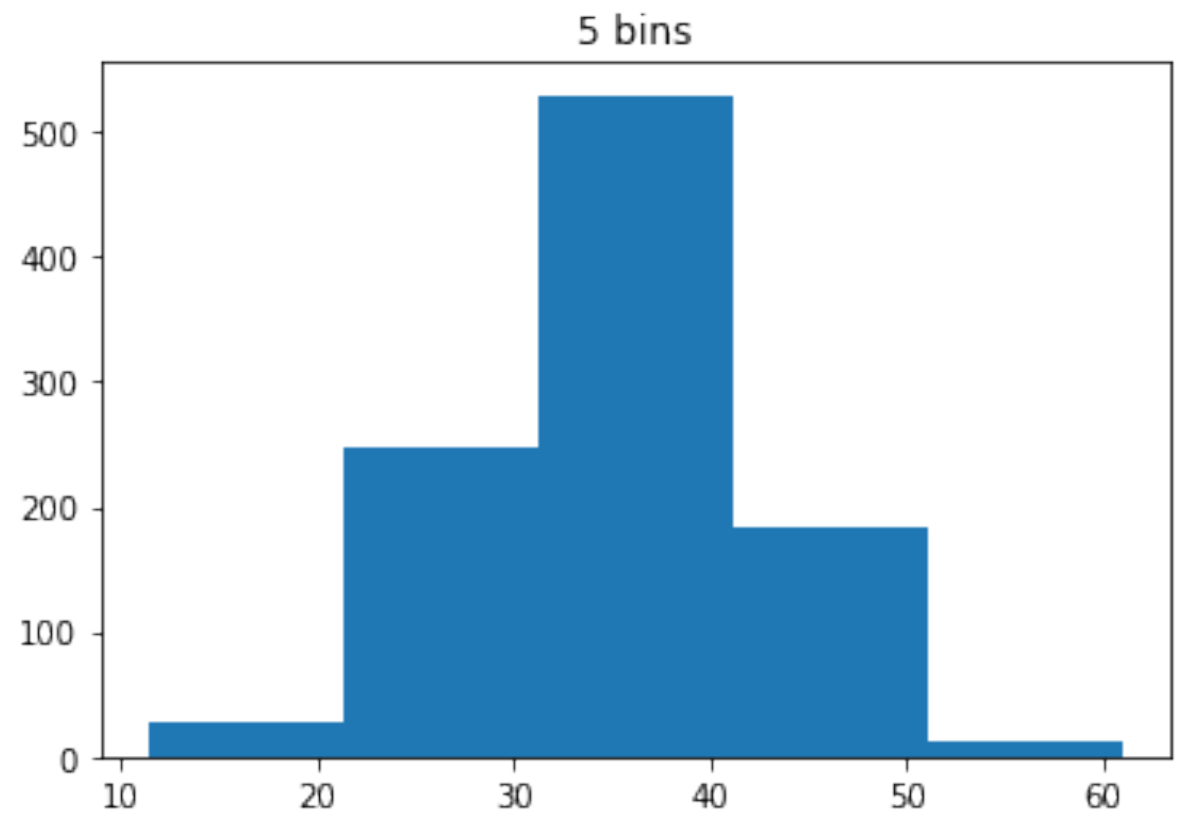


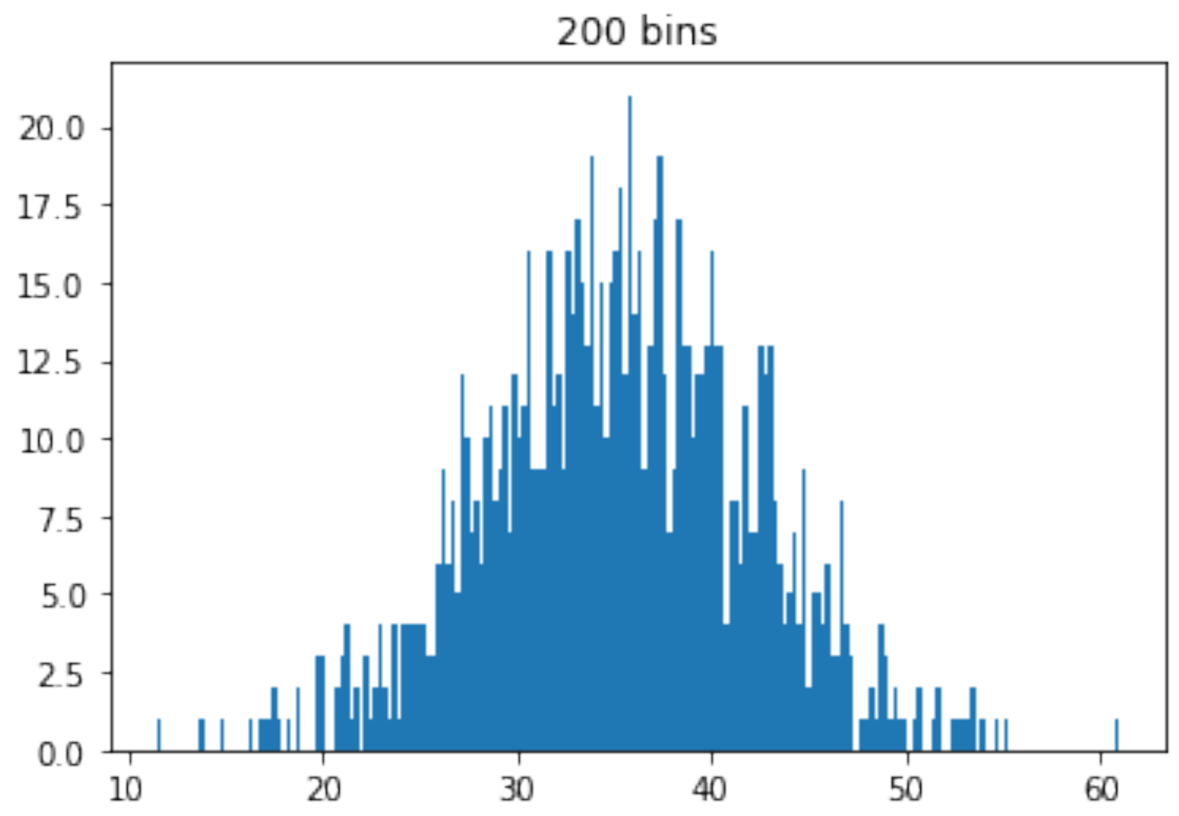

```
_ = plt.hist(data, bins=8,
range=(15,55), density='True')
```

choice of bins

- The histogram has a few parameters
  - Number of bins n, width of bins w, and even number of samples m can be viewed as one
  - Bins don't even have to be homogeneous
- Several formulas have been proposed for choosing n and w based on the sample
  - Square root: $n = \lceil \sqrt{m} \rceil$
  - Sturges' formula: $n = \lceil \log_2 m \rceil + 1$
  - Rice rule: $n = \lceil 2m^{1/3} \rceil$
  - Scott's normal reference rule: $w = 3.5\hat{\sigma}/m^{1/3}$
- How do we reason about the "optimal" choice?

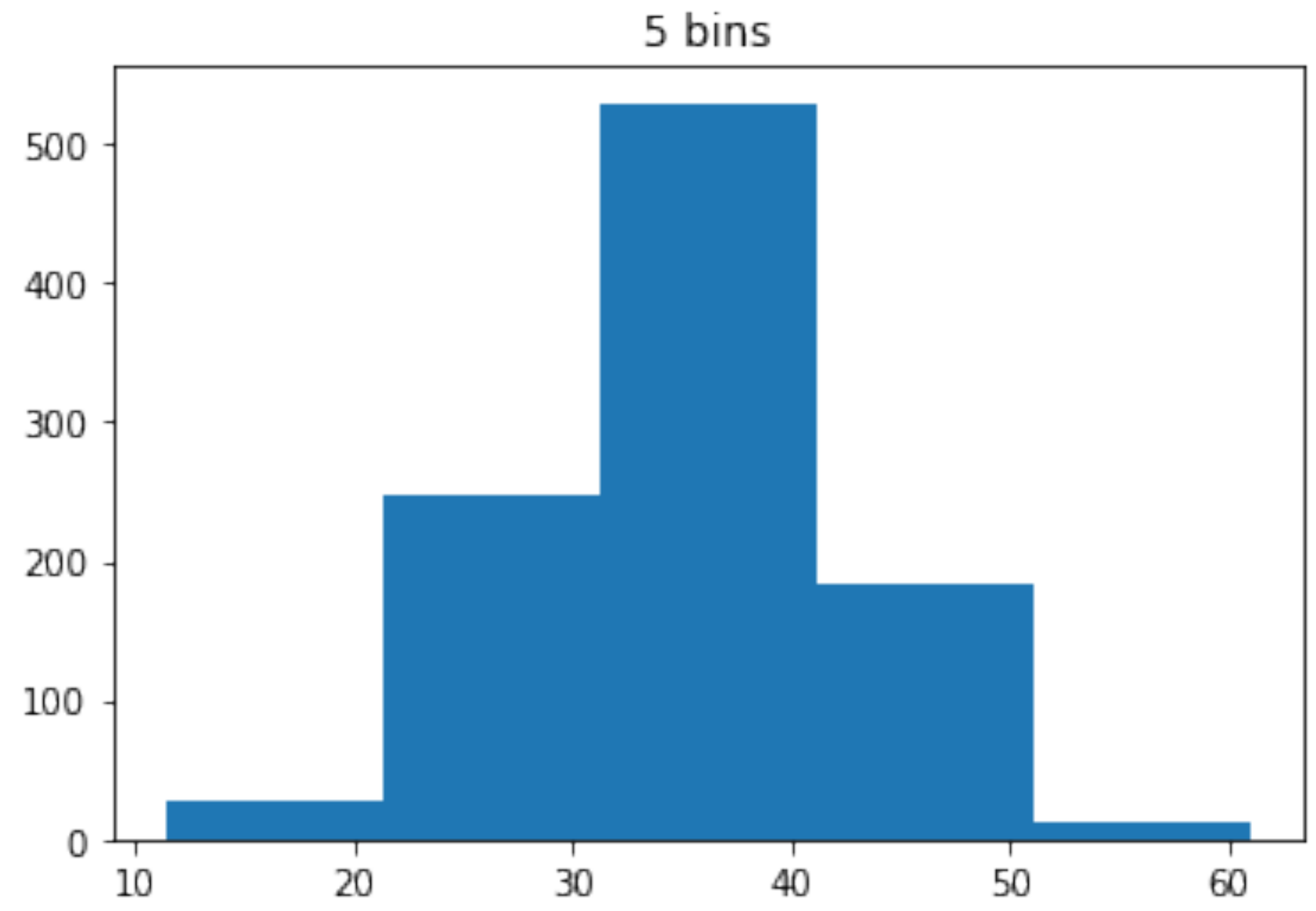


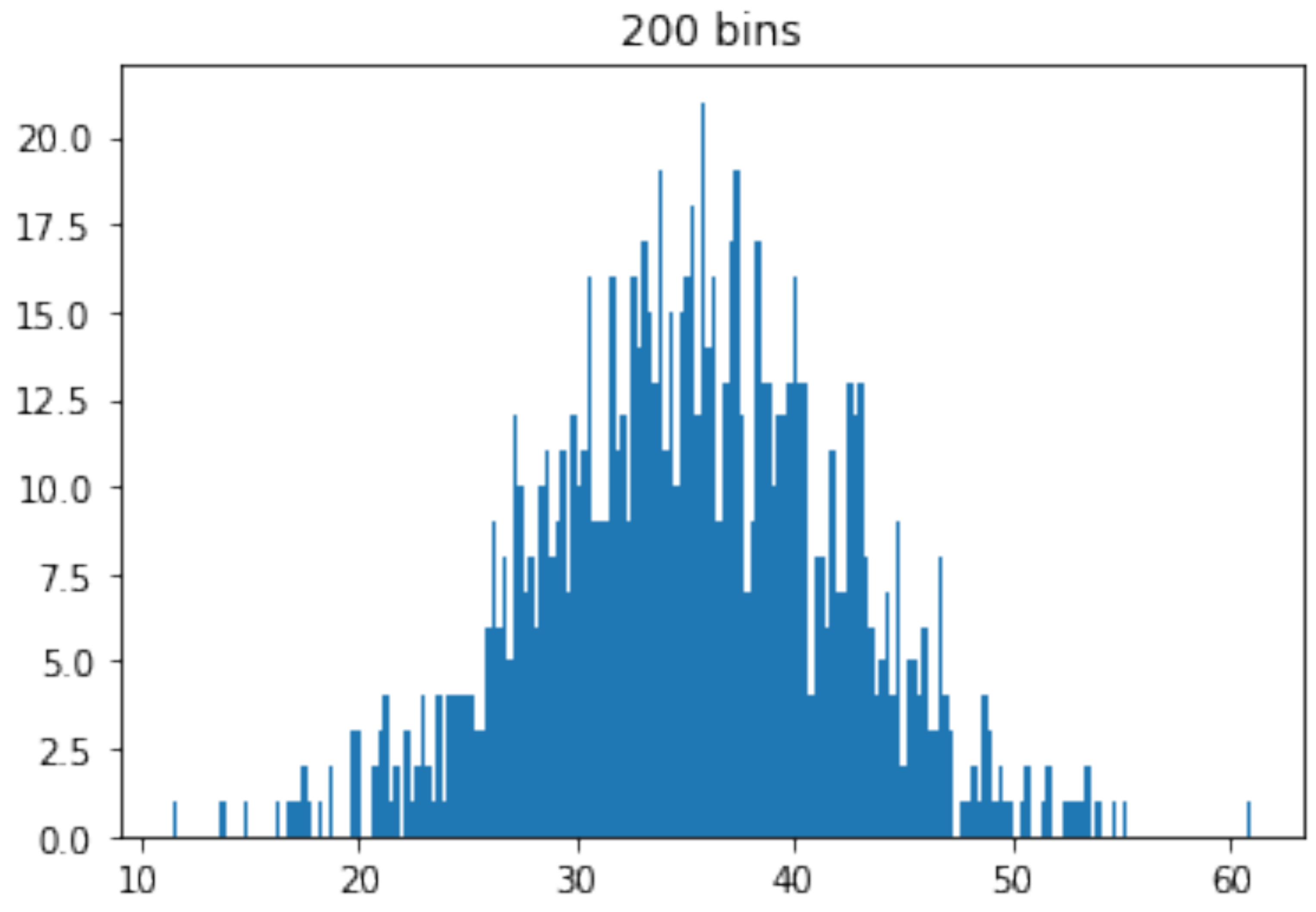




bin width intuition

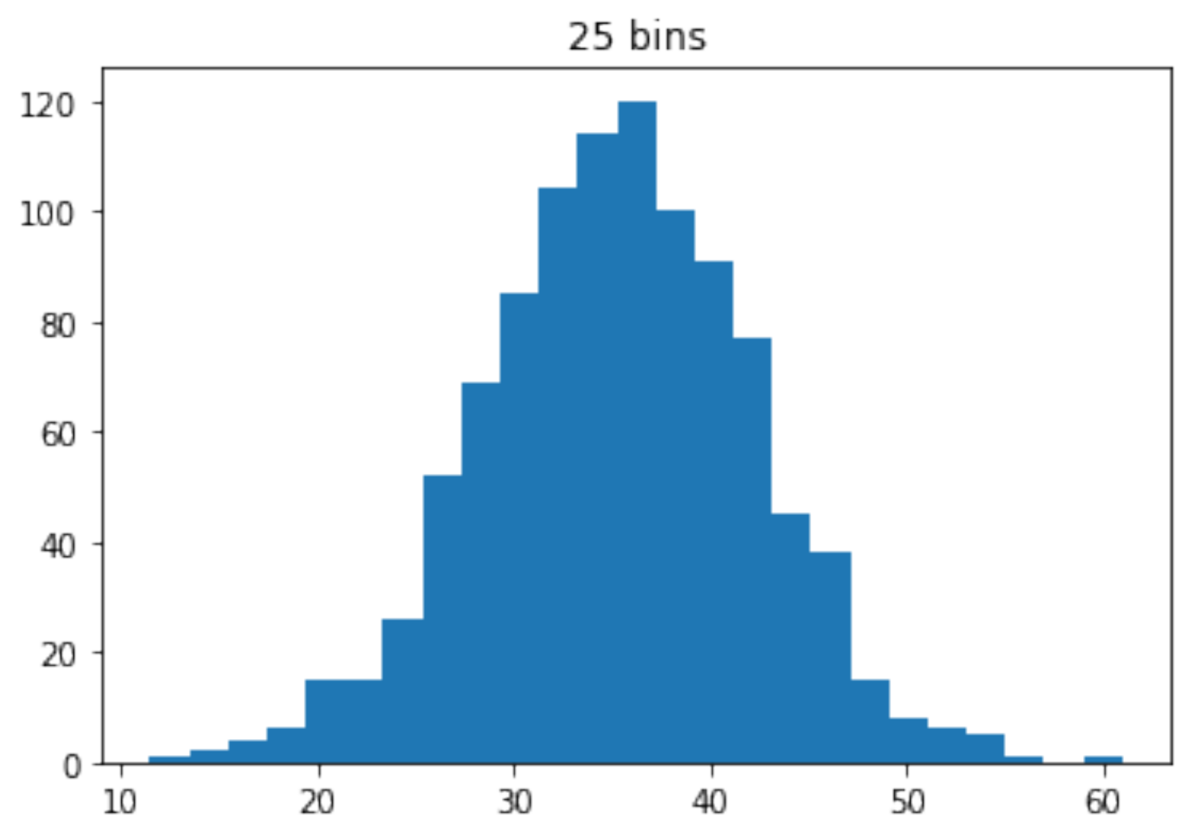
- Choosing large bin size w
  - Broad range of points (some rare, some common) put into the same bin and given the same estimate
- Choosing small bin size w
  - Each bin is based on fewer samples, so harder to estimate how likely the bin is
  - In the limit: Buckets of size 0 (is it practical?)
- So how do we choose the bin size in general?

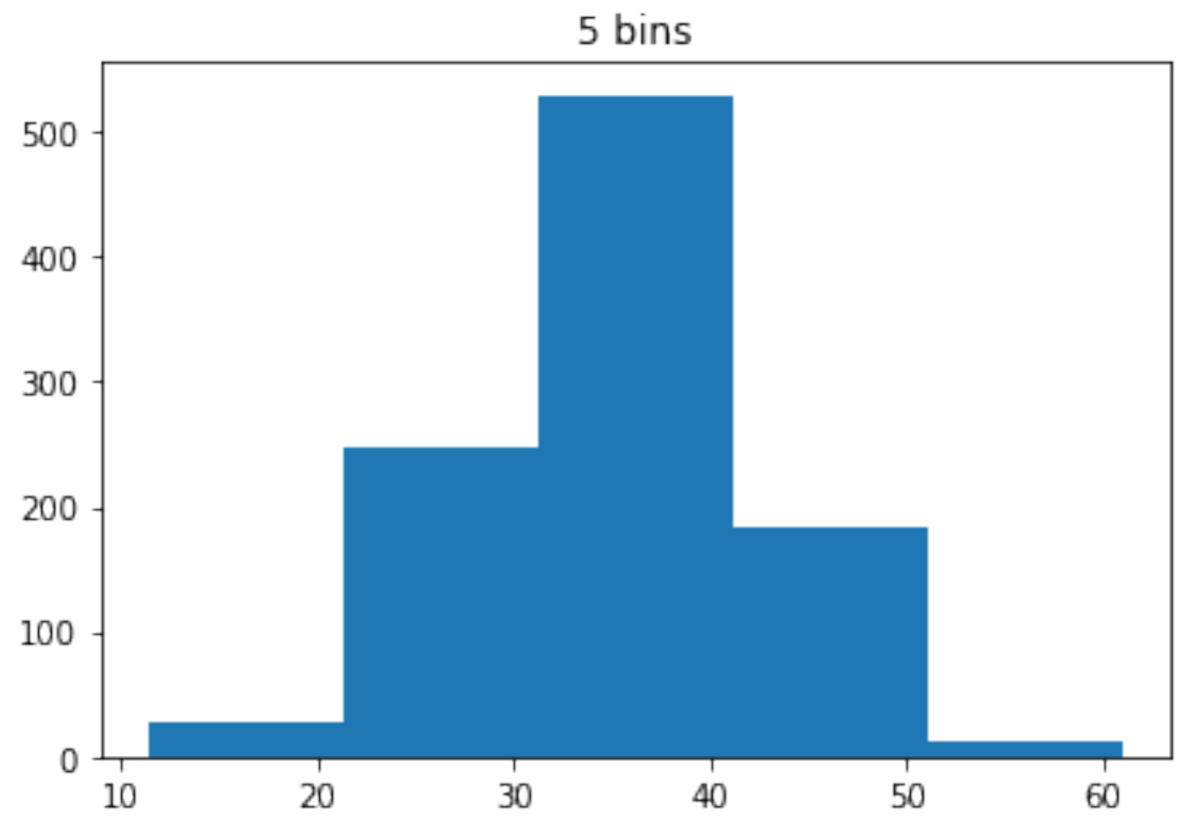


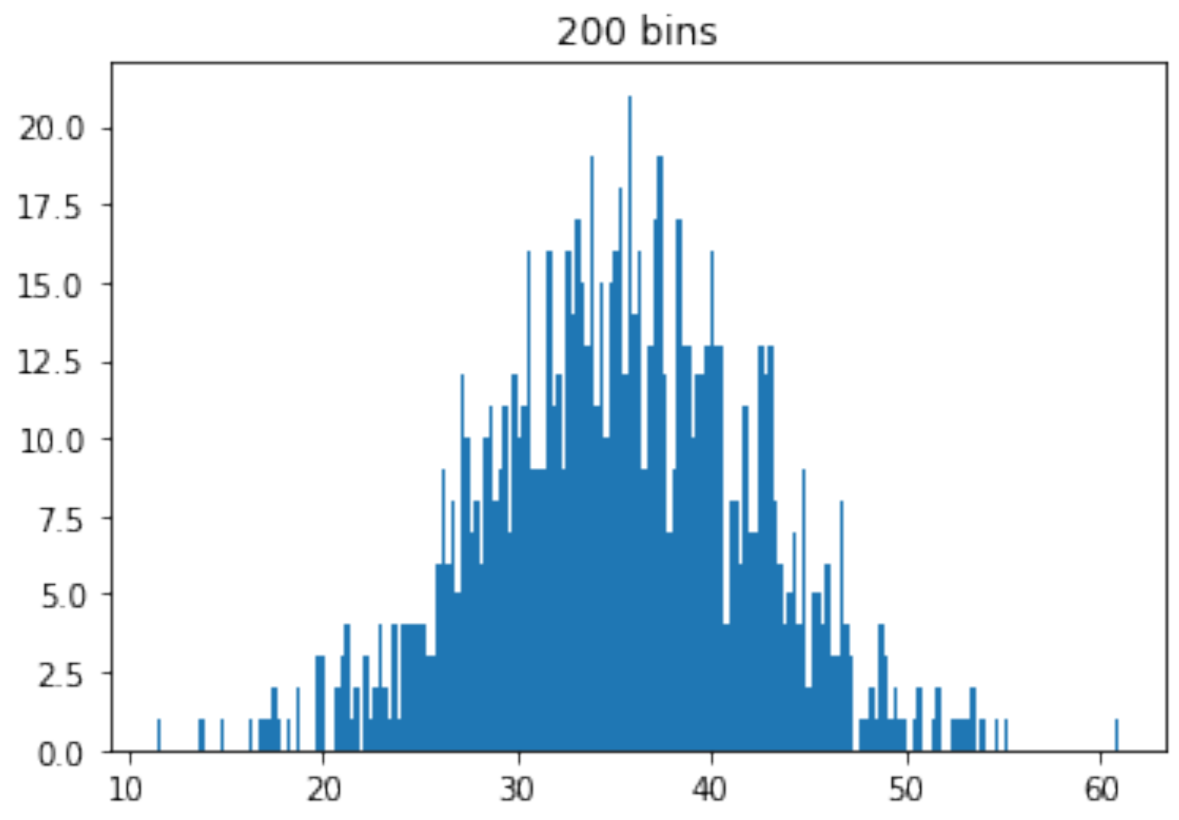


evaluation of histograms

- We can choose many different bin widths w (or equivalently the number of bins n)
- How do we **evaluate** which bin width w is better?
  - *Visual appeal* - Which is most visually appealing to humans?
  - *Usefulness* - Which helps the owner know how much coffee to make?
  - *Mathematical metrics* - Which satisfies some mathematical notion of goodness? (Ideally this is tied to *usefulness*)
- We will focus on **mathematical metrics**

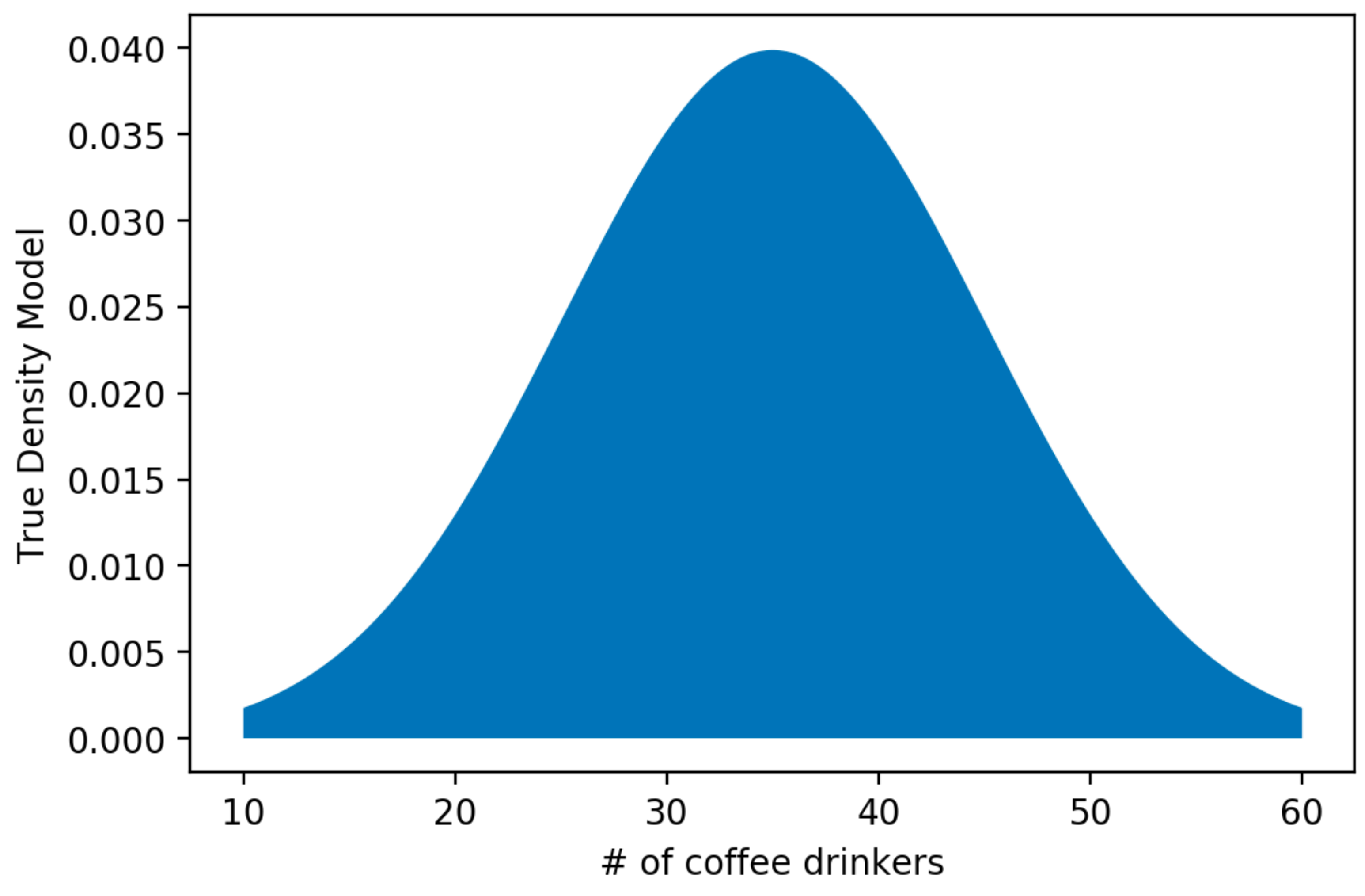


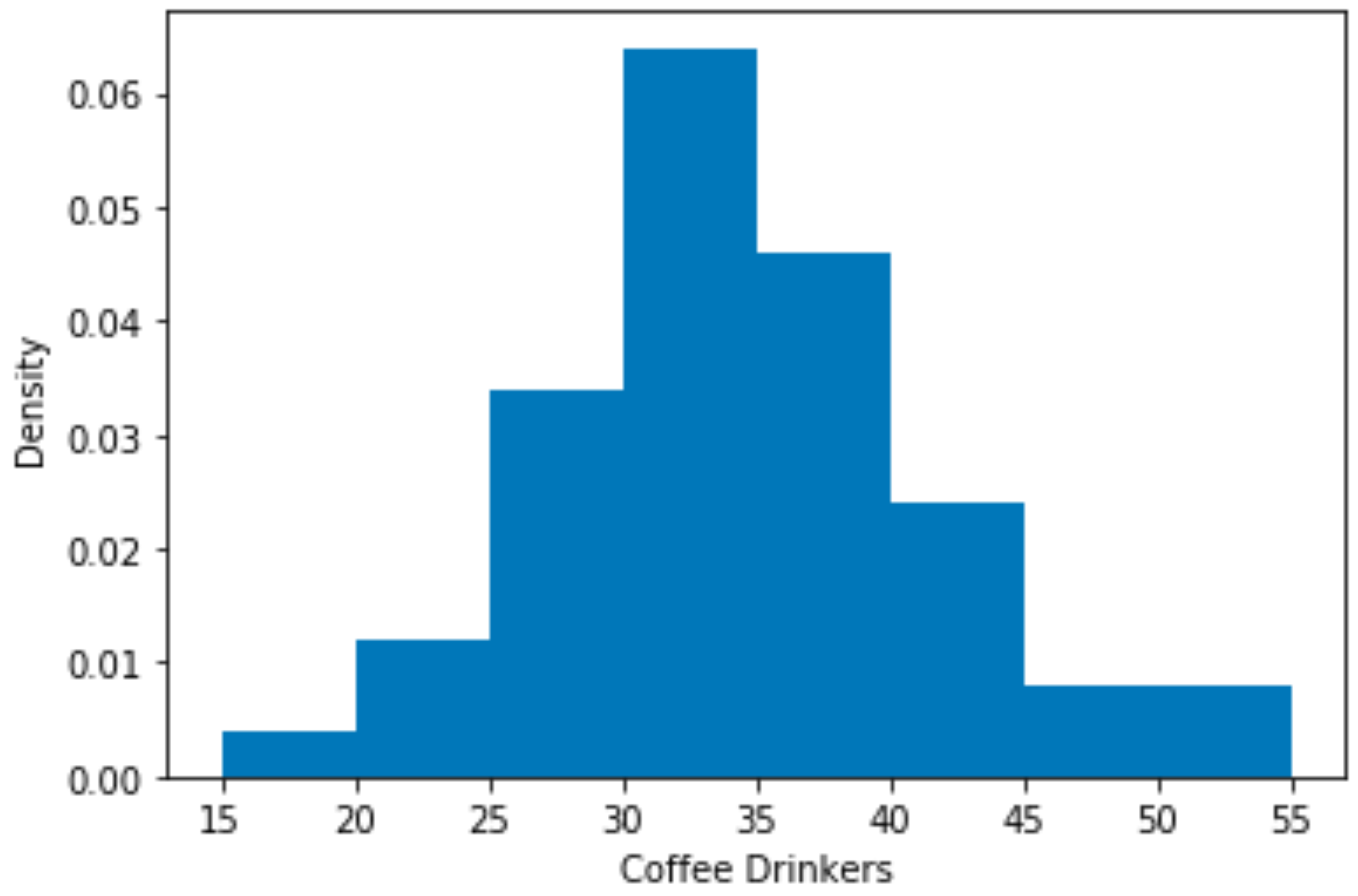




estimated vs. “true” model

- First, we *assume* there is some **“true” underlying model** (often denoted by $f(x)$) for the phenomena of interest
  - Importantly, this “true” model is **unknown** (or **hidden**)
  - For example, we don’t know before collecting data the distribution of coffee purchases.
  - Even after collecting data, we can only **estimate** the distribution.
- Histograms are an **estimate** (or **approximation**, often denoted by $\hat{f}(x)$) of the true distribution.



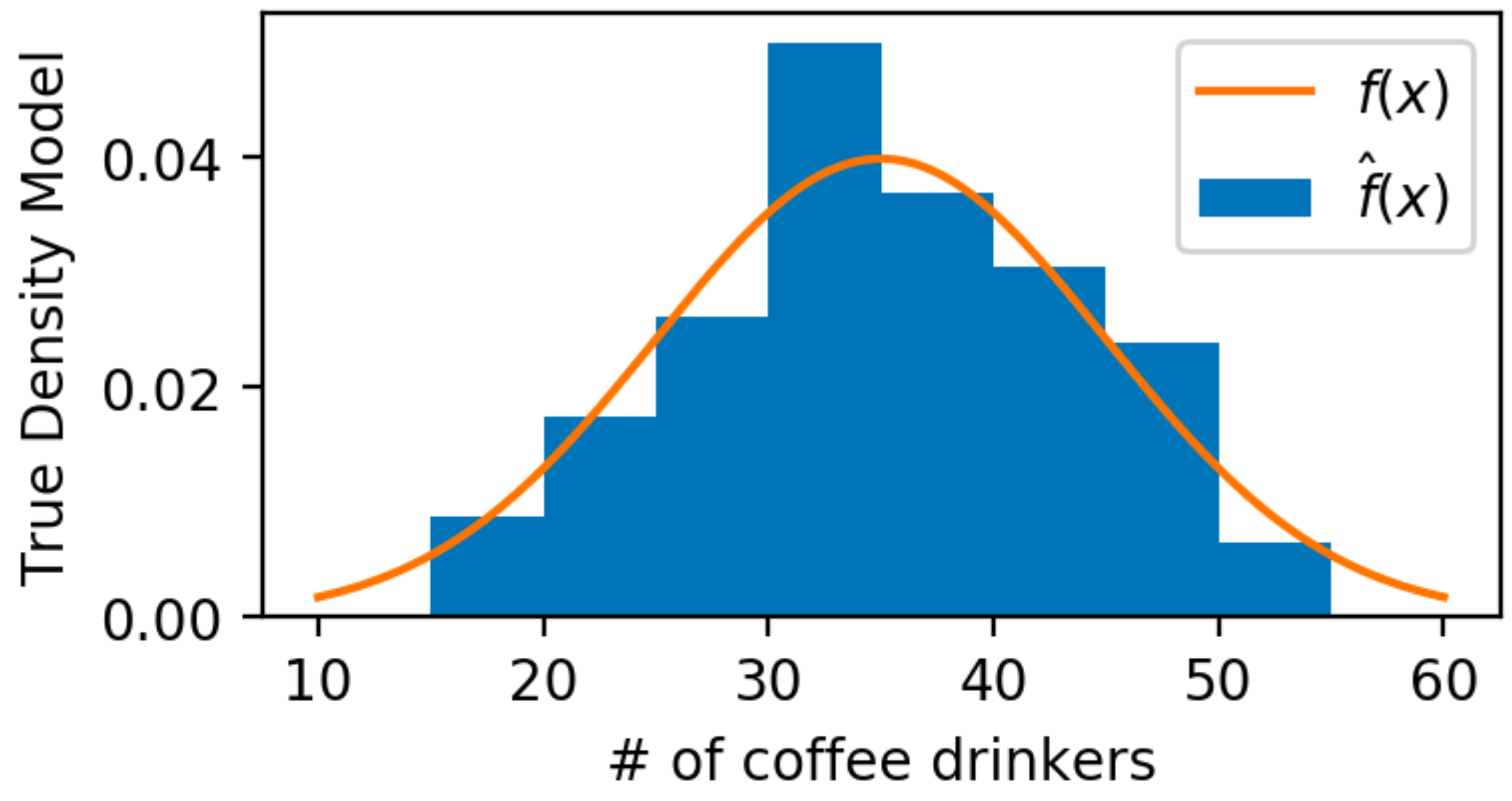


minimizing the estimation error

- We can pick the bin size w that minimizes the error of estimating a point
- The **Integrated Square Error (ISE)** of a histogram can be written as a function of the bin width (i.e., the smoothing parameter

$$L(w) = \int \left(\hat{f}_m(x) - f(x) \right)^2 dx$$

  - Here, $\hat{f}_m(x)$ is the density estimate of the histogram with m samples
  - However, $f(x)$ is the "true" but *unknown* model, so how do we compute $L(w)$?



estimating the error with samples

- The Integrated Square Error (ISE):

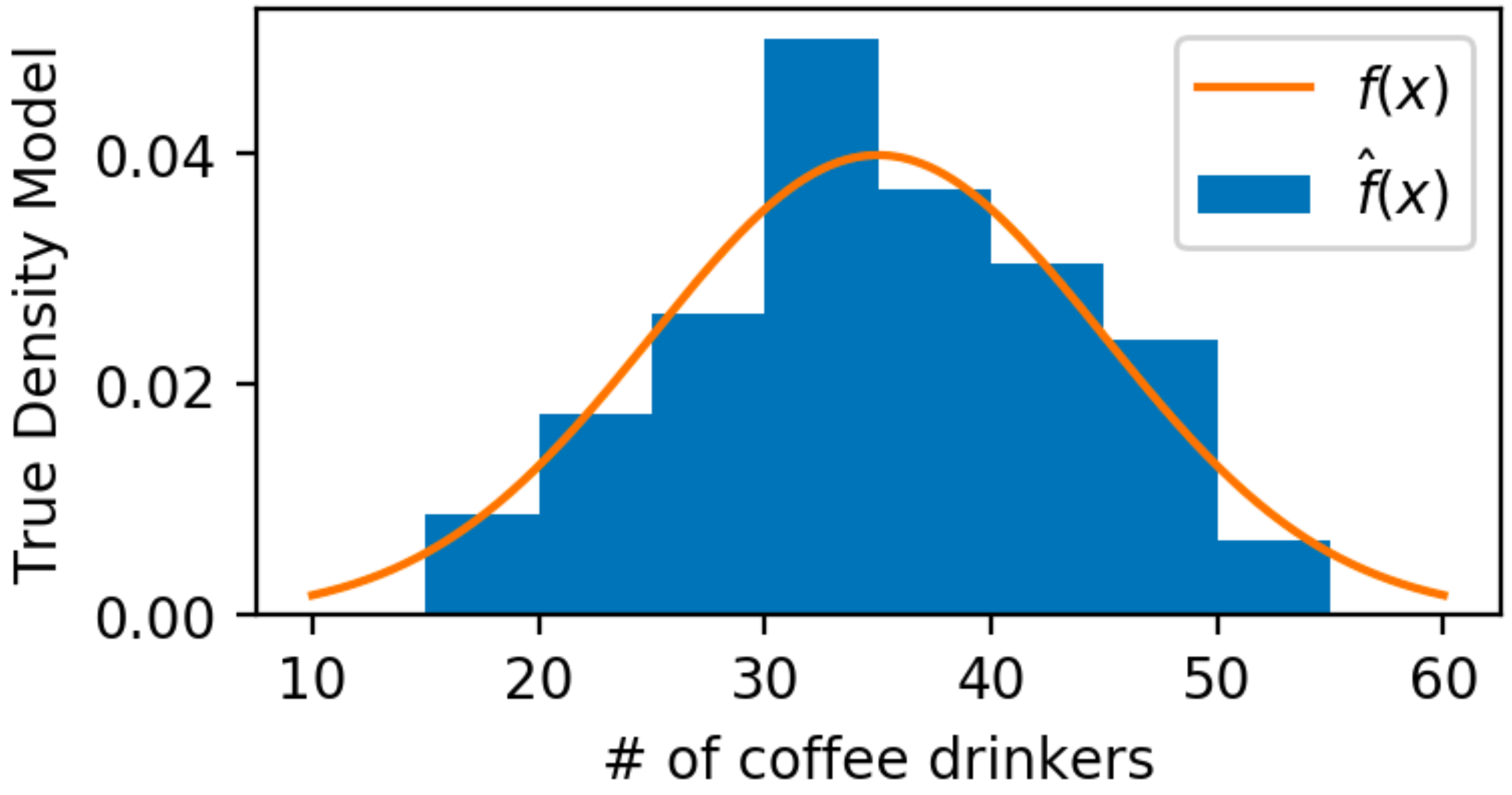
$$L(w) = \int \left(\hat{f}_m(x) - f(x) \right)^2 dx$$

- We can approximate with data samples by $L(w) \approx J(w) + constant$, where

$$J(w) = \frac{2}{(m-1)w} - \frac{m+1}{(m-1)w}(\hat{p}_1^2 + \hat{p}_2^2 + \cdots + \hat{p}_n^2)$$

  - w is bin width, m is the number of samples and $\hat{p}_k$, $k = 1,\ldots,n$ are the bin probabilities

- We can choose the "optimal" bin width by minimizing $J(w)$, which approximates $L(w)$!



minimizing $J(w)$

- The brute-force way is to try as many values of w as possible and choose the best
- Better to work with n here in this case, since there is a finite number of possibilities
- For each $n = 1, \ldots, m$:
  - calculate w
  - use this to calculate J

  Plot the results, choose the best one
- To narrow down the number of values we need to try, **grid search** procedures are also possible

Testing all numbers of bins