Statistics for Hackers

Jake VanderPlas
PyCon 2016

< About Me >

- Astronomer by training
- Statistician by accident
- Active in Python science & open source
- Data Scientist at UW eScience Institute
- @**jakevdp** on Twitter & Github

Statistics for Hackers

Statistics for Hackers

Hacker *(n.)*

1. A person who is trying to steal your grandma's bank password.

Hacker *(n.)*

1. ~~A person who is trying to steal your grandma's bank password.~~
2. A person whose natural approach to problem-solving involves writing *code*.

Statistics is Hard.

Statistics is Hard.

Using programming skills,
it can be easy.

My thesis today:

If you can write a for-loop, you can do statistics

Statistics is fundamentally about

Asking the Right Question.

Sometimes the questions are complicated and the answers are simple.

– *Dr. Seuss (attr)*

Warm-up

Warm-up:

Coin Toss

You toss a coin **30** times and see **22** heads. Is it a fair coin?


A fair coin should show 15 heads in 30 tosses. This coin is biased.
Even a fair coin could show 22 heads in 30 tosses. It might be just chance.

Classic Method:

Assume the Skeptic is correct: test the *Null Hypothesis.*

What is the probability of a fair coin showing 22 heads simply by chance?

Classic Method:

$N_H = 22,\ N_T = 8$

Start computing probabilities . . .

$$P(H) = \frac{1}{2}$$

$$P(HH) = \left(\frac{1}{2}\right)^2$$

Classic Method:

$N_H = 22, \; N_T = 8$

$$P(HHT) = \left(\frac{1}{2}\right)^3$$

$$\begin{aligned} P(2H,\ 1T) = \quad & P(HHT) \\ & +P(HTH) \\ & +P(THH) \\ = \ & \frac{3}{8} \end{aligned}$$

Classic Method:

$N_H = 22,\ N_T = 8$

$$P(N_H, N_T) = \binom{N}{N_H}\left(\frac{1}{2}\right)^{N_H}\left(1 - \frac{1}{2}\right)^{N_T}$$

Number of arrangements (binomial coefficient)

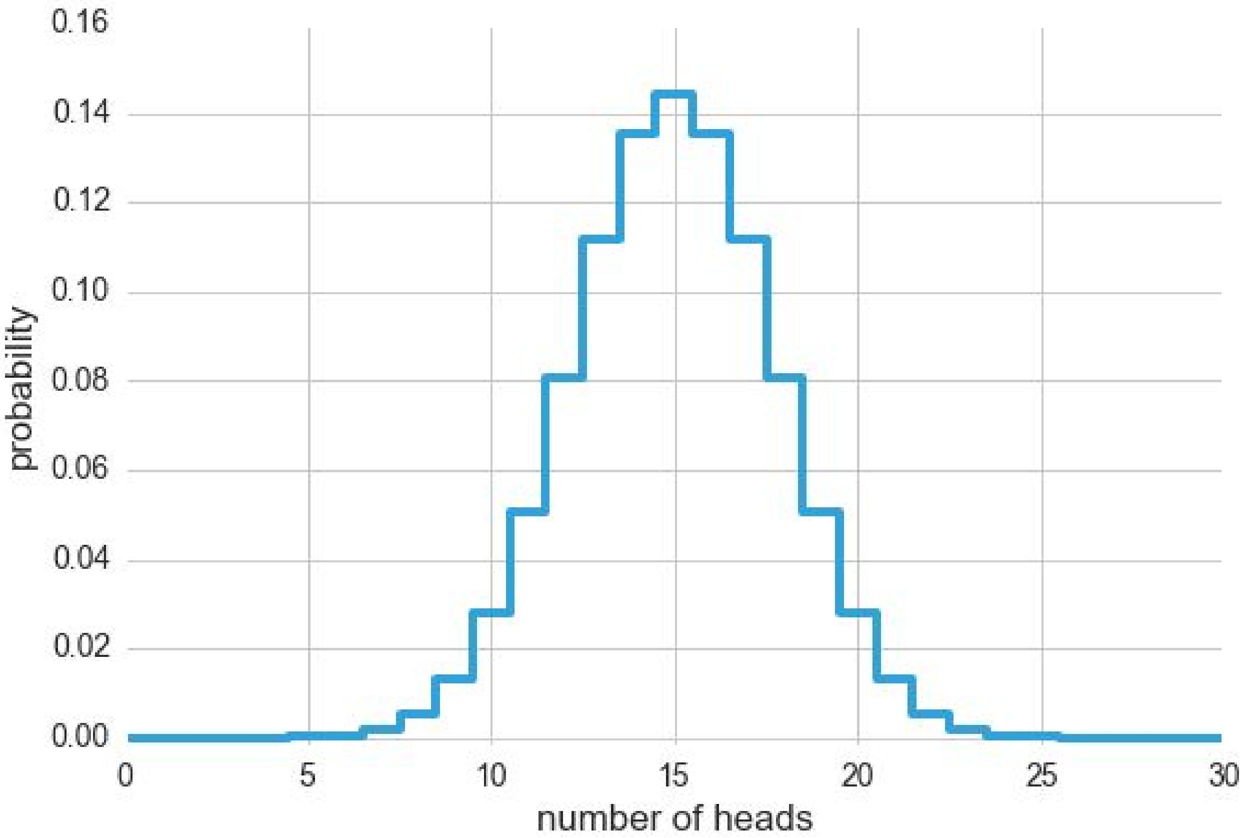
Probability of N_H heads

Probability of N_T tails

Classic Method:

$N_H = 22,\ N_T = 8$

$$P(N_H, N_T) = \binom{N}{N_H}\left(\frac{1}{2}\right)^{N_H}\left(1 - \frac{1}{2}\right)^{N_T}$$



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$$N_H = 22, \; N_T = 8$$

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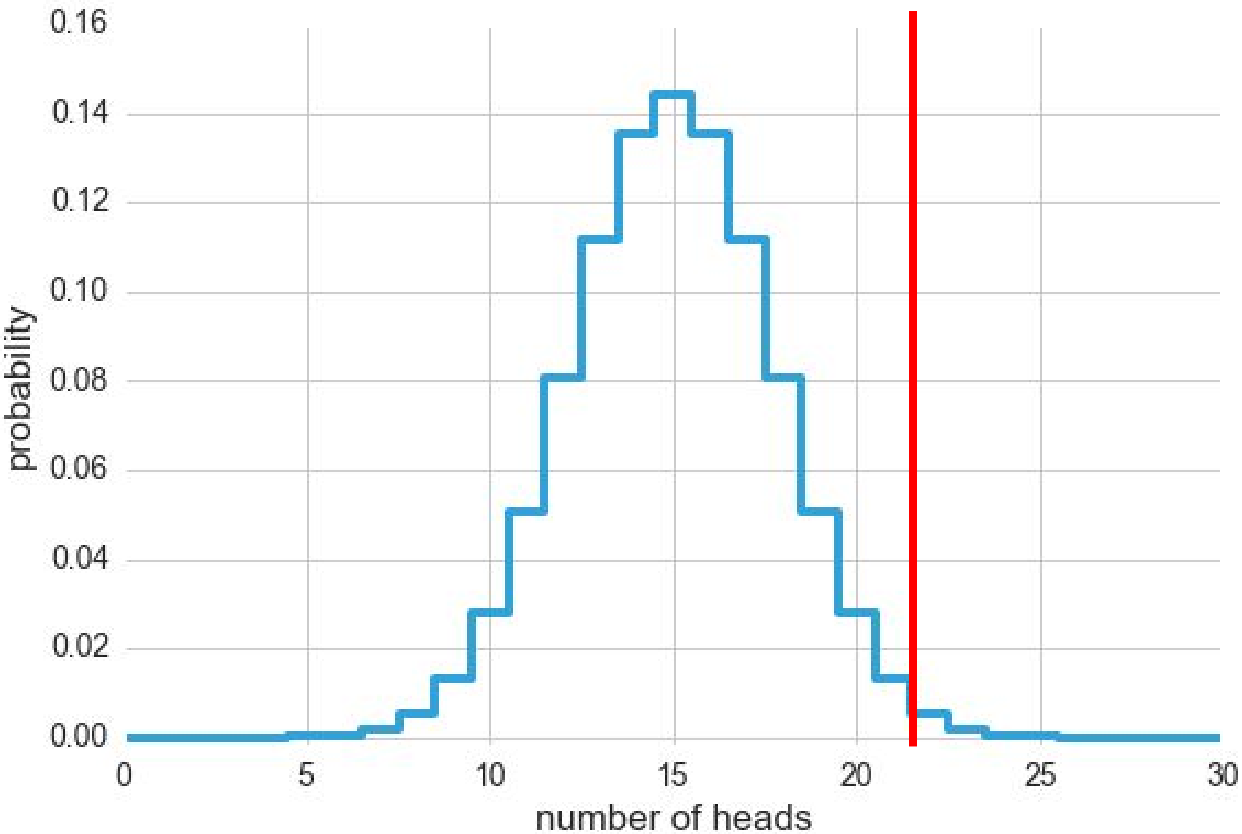

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$$N_H = 22, \; N_T = 8$$

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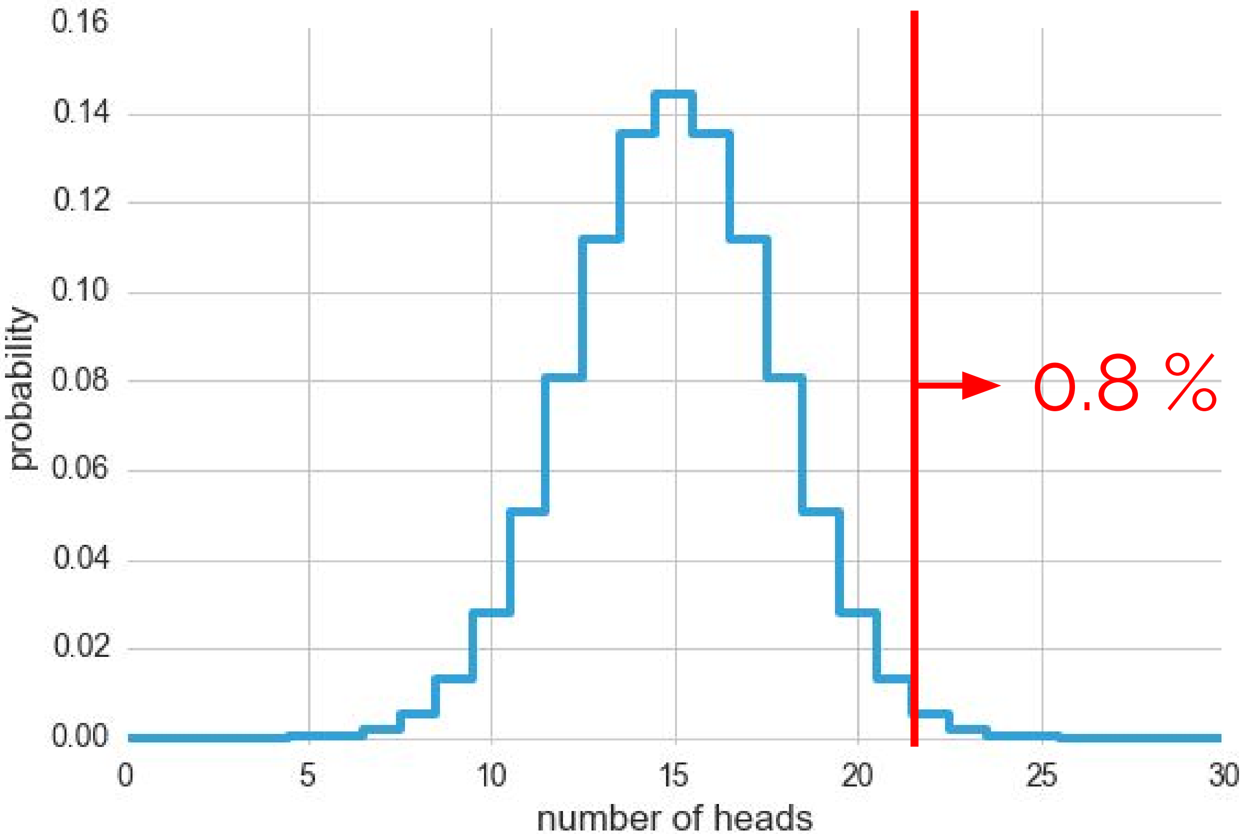
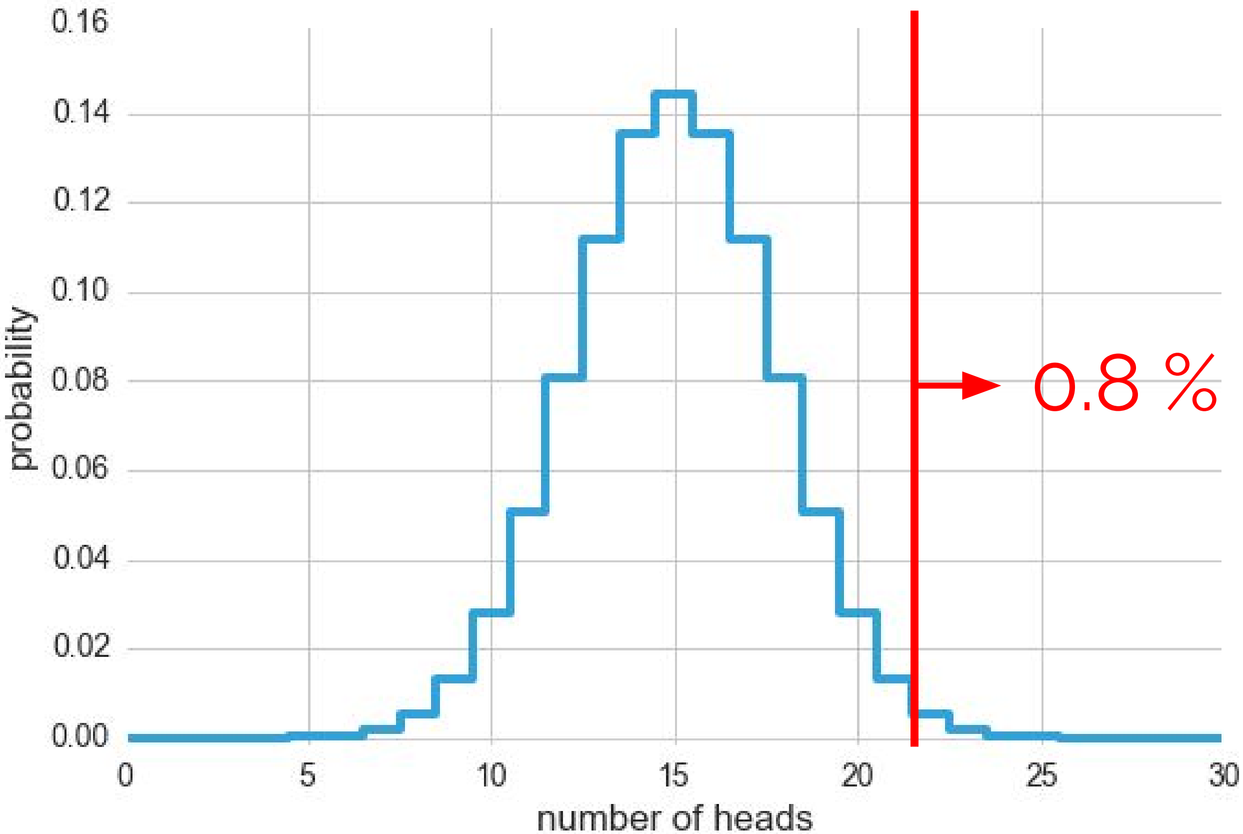


Classic Method:

$N_H = 22,\ N_T = 8$

Probability of 0.8% (i.e. p = 0.008) of observations given a fair coin.

→ **reject fair coin hypothesis at $p < 0.05$**



Could there be an easier way?

Easier Method:

Just simulate it!

```
M = 0
for i in range(10000):
    trials = randint(2, size=30)
    if (trials.sum() >= 22):
        M += 1
p = M / 10000 # 0.008149
```

→ reject fair coin at $p = 0.008$

In general . . .

Computing the Sampling Distribution is Hard.

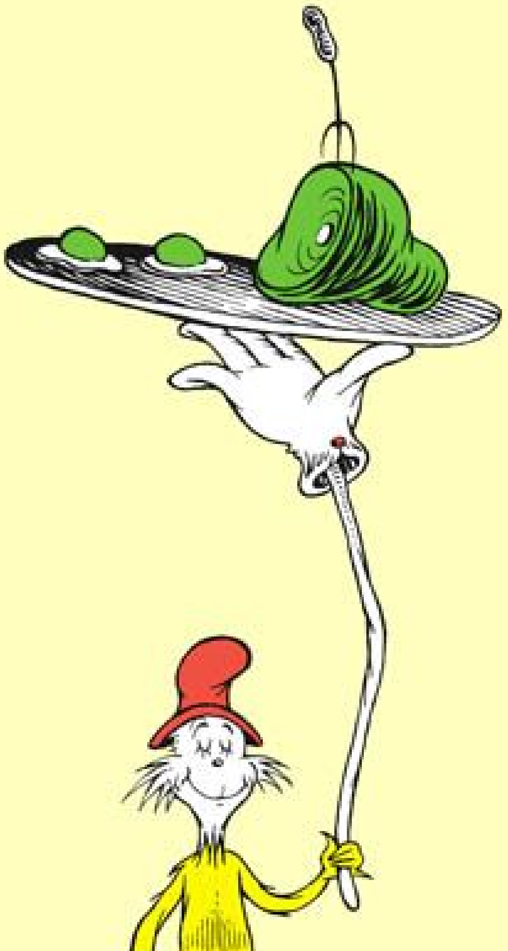
In general . . .

Computing the Sampling Distribution is Hard.

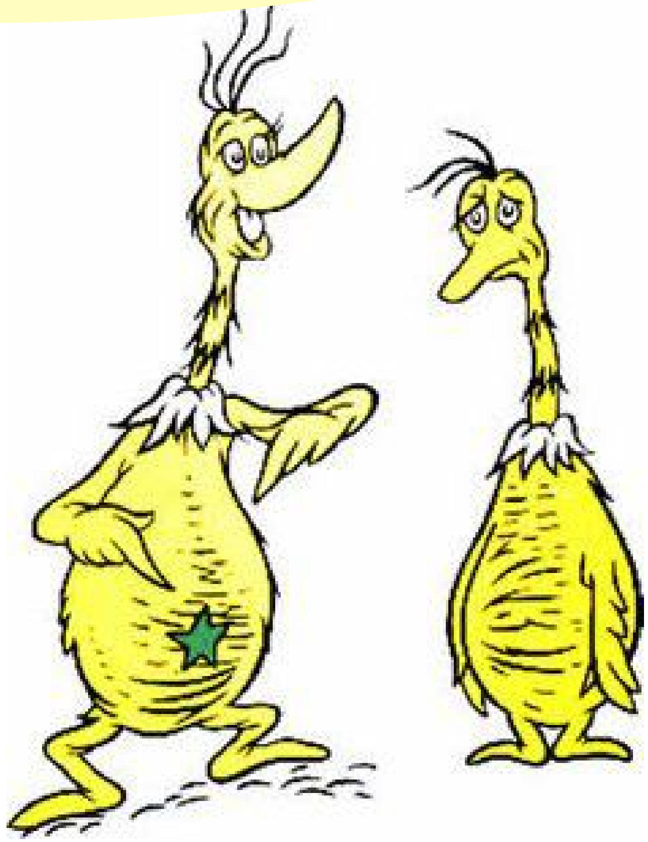
Simulating the Sampling Distribution is Easy.

Four Recipes for Hacking Statistics:

1. Direct Simulation ✓
2. Shuffling
3. Bootstrapping
4. Cross Validation



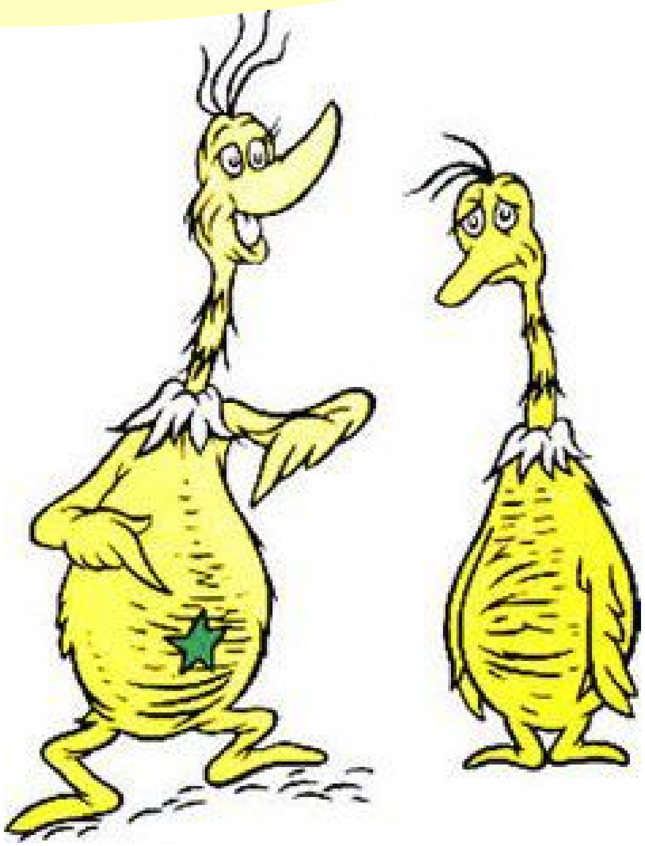
Sneeches:
Stars and Intelligence



Now, the Star-Belly Sneetches
had bellies with stars.
The Plain-Belly Sneetches
had none upon thars . . .

*inspired by John Rauser's
Statistics Without All The Agonizing Pain

Sneeches:
Stars and Intelligence



Test Scores

★		×	
84	72	81	69
57	46	74	61
63	76	56	87
99	91	69	65
		66	44
		62	69

★ mean: 73.5
× mean: 66.9
difference: 6.6

Is this difference of 6.6 statistically significant?

★ mean: 73.5
× mean: 66.9
difference: 6.6

Classic Method

(Welch's t-test)

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

Classic Method

(Welch's t-test)

$$t = \frac{73.5 - 66.9}{\sqrt{\frac{316.3}{8} + \frac{124.8}{12}}} = 0.932$$

Classic Method

(Student's t distribution)

$$p(t;\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi}\,\Gamma\left(\frac{\nu}{2}\right)}\left(1+\frac{t^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

Classic Method

(Student's t distribution)

$$p(t;\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi}\,\Gamma\left(\frac{\nu}{2}\right)}\left(1+\frac{t^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

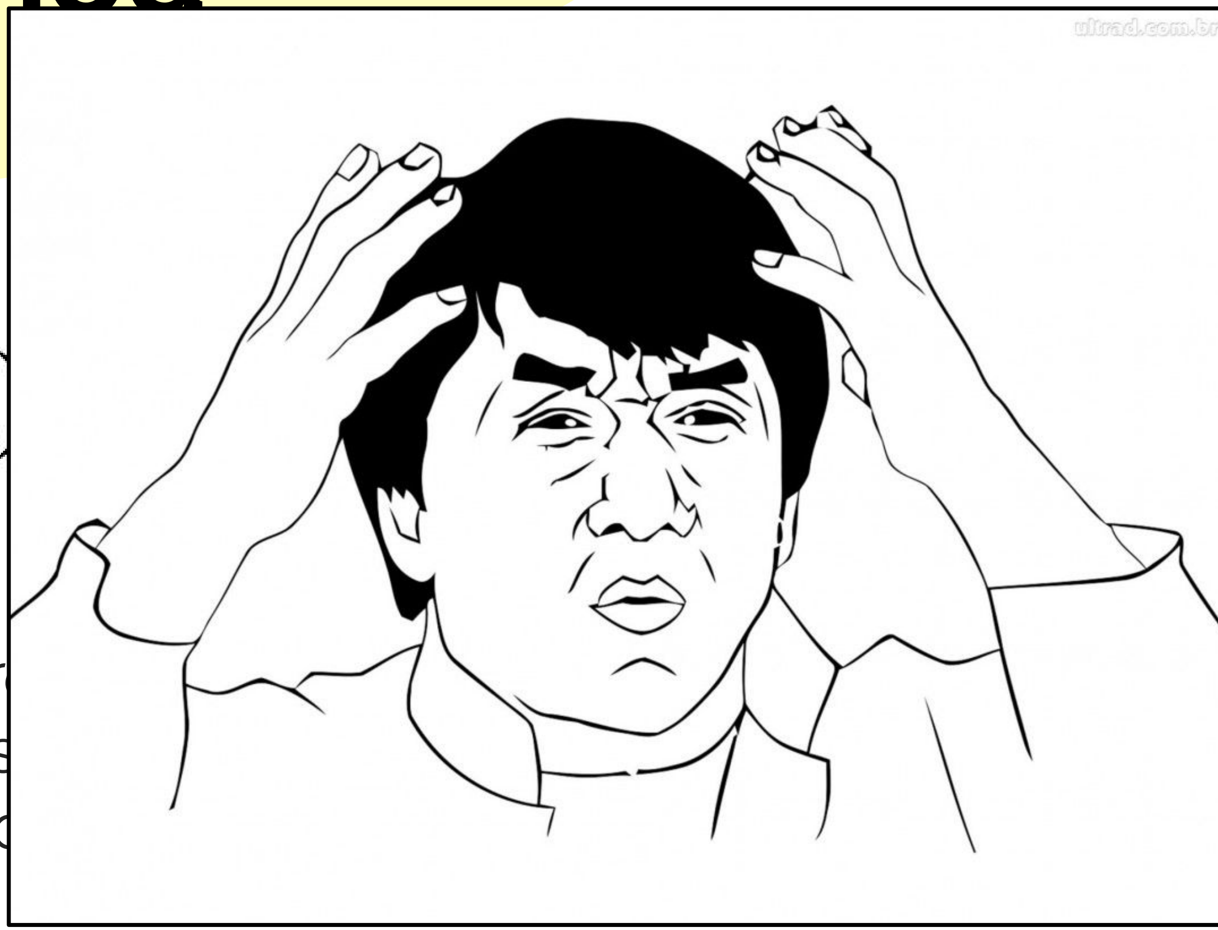
Degree of Freedom: "The number of independent ways by which a dynamic system can move, without violating any constraint imposed on it."

-Wikipedia

Classic Method

(Student's t distribution)

$$p(t;\nu) \quad \ldots \quad \Big)^{-\frac{\nu+1}{2}}$$



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Classic Method

(Welch–Satterthwaite equation)

$$\nu \approx \frac{\left(\frac{s_1^2}{N_1} + \frac{s_2^2}{N_2}\right)^2}{\frac{s_1^4}{N_1^2(N_1-1)} + \frac{s_2^4}{N_2^2(N_2-1)}}$$

Classic Method

(Welch–Satterthwaite equation)

$$\nu \approx \frac{\left(\frac{316.3}{8} + \frac{124.8}{12}\right)^2}{\frac{316.3^2}{8^2(8-1)} + \frac{124.8^2}{12^2(12-1)}} = 10.7$$

Classic
Methoc

α (1 tail)	0.05	0.025	0.01	0.005	0.0025	0.001	0.0005
α (2 tail)	0.1	0.05	0.02	0.01	0.005	0.002	0.001
df							
1	6.3138	12.7065	31.8193	63.6551	127.3447	318.4930	636.0450
2	2.9200	4.3026	6.9646	9.9247	14.0887	22.3276	31.5989
3	2.3534	3.1824	4.5407	5.8408	7.4534	10.2145	12.9242
4	2.1319	2.7764	3.7470	4.6041	5.5976	7.1732	8.6103
5	2.0150	2.5706	3.3650	4.0322	4.7734	5.8934	6.8688
6	1.9432	2.4469	3.1426	3.7074	4.3168	5.2076	5.9589
7	1.8946	2.3646	2.9980	3.4995	4.0294	4.7852	5.4079
8	1.8595	2.3060	2.8965	3.3554	3.8325	4.5008	5.0414
9	1.8331	2.2621	2.8214	3.2498	3.6896	4.2969	4.7809
10	1.8124	2.2282	2.7638	3.1693	3.5814	4.1437	4.5869
11	1.7959	2.2010	2.7181	3.1058	3.4966	4.0247	4.4369
12	1.7823	2.1788	2.6810	3.0545	3.4284	3.9296	4.3178
13	1.7709	2.1604	2.6503	3.0123	3.3725	3.8520	4.2208
14	1.7613	2.1448	2.6245	2.9768	3.3257	3.7874	4.1404
15	1.7530	2.1314	2.6025	2.9467	3.2860	3.7328	4.0728
16	1.7459	2.1199	2.5835	2.9208	3.2520	3.6861	4.0150
17	1.7396	2.1098	2.5669	2.8983	3.2224	3.6458	3.9651
18	1.7341	2.1009	2.5524	2.8784	3.1966	3.6105	3.9216
19	1.7291	2.0930	2.5395	2.8609	3.1737	3.5794	3.8834
20	1.7247	2.0860	2.5280	2.8454	3.1534	3.5518	3.8495

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9	1.8331	2.2621	2.8214	3.2498	3.6896	4.2969	4.7809
10	[illegible]	[illegible]	2.7638	3.1693	3.5814	4.1437	4.5869
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Classic Method

$$t > t_{crit}$$

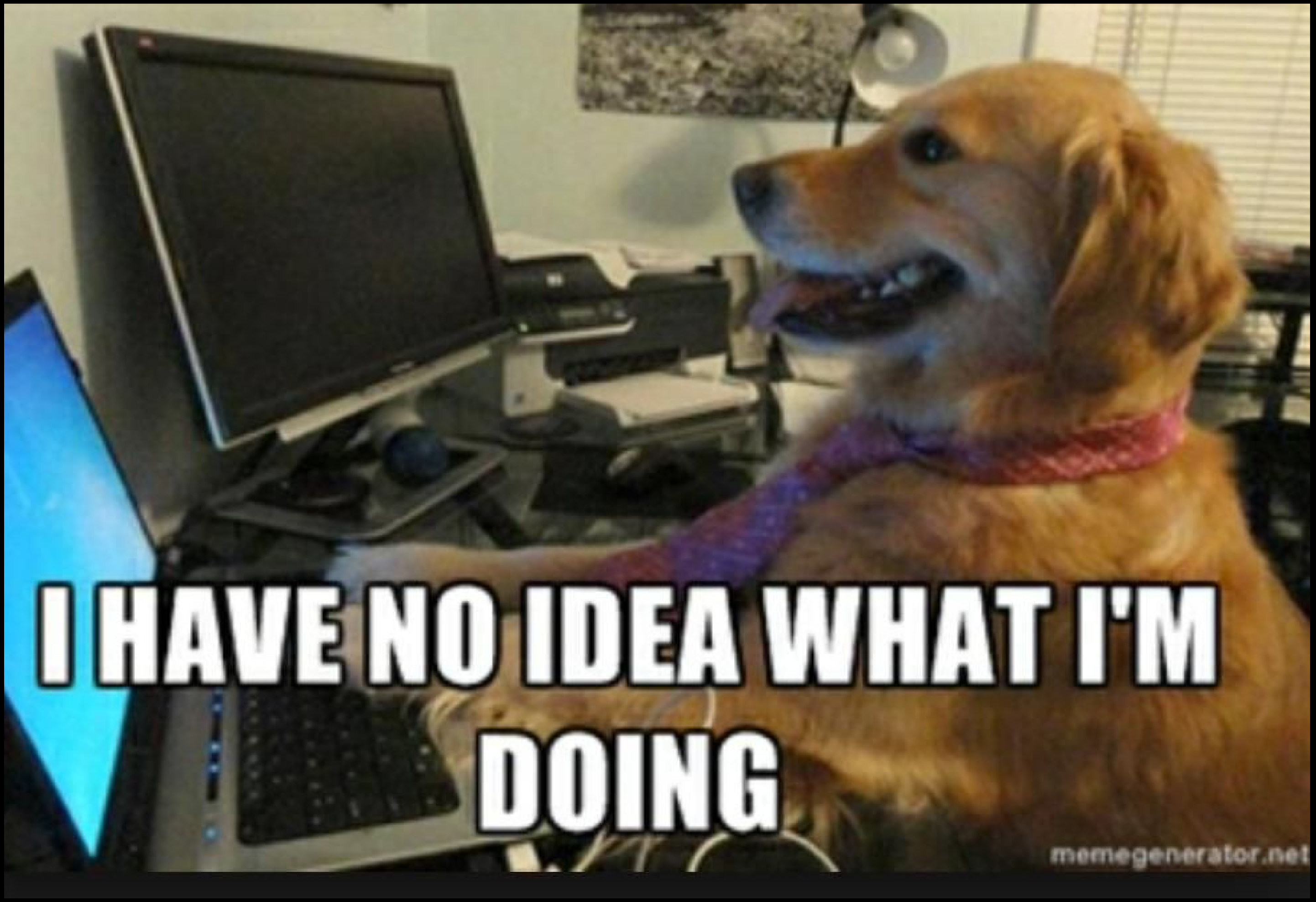
Classic Method

$$0.932 > 1.796$$

Classic Method

$$\cancel{0.932 > 1.796}$$

“The difference of 6.6 is not significant at the p=0.05 level”


I HAVE NO IDEA WHAT I'M DOING
memegenerator.net

The biggest problem:

We've entirely lost-track of what question we're answering!

< One popular alternative . . . >

“Why don’t you just . . .”

```
from statsmodels.stats.weightstats import ttest_ind
t, p, dof = ttest_ind(group1, group2,
                      alternative='larger',
                      usevar='unequal')
print(p)  # 0.186
```

< One popular alternative . . . >

"Why don't you just . . ."

```
from statsmodels.stats.weightstats import ttest_ind
t, p, dof = ttest_ind(group1, group2,
                      alternative='larger',
                      usevar='unequal')
print(p)  # 0.186
```

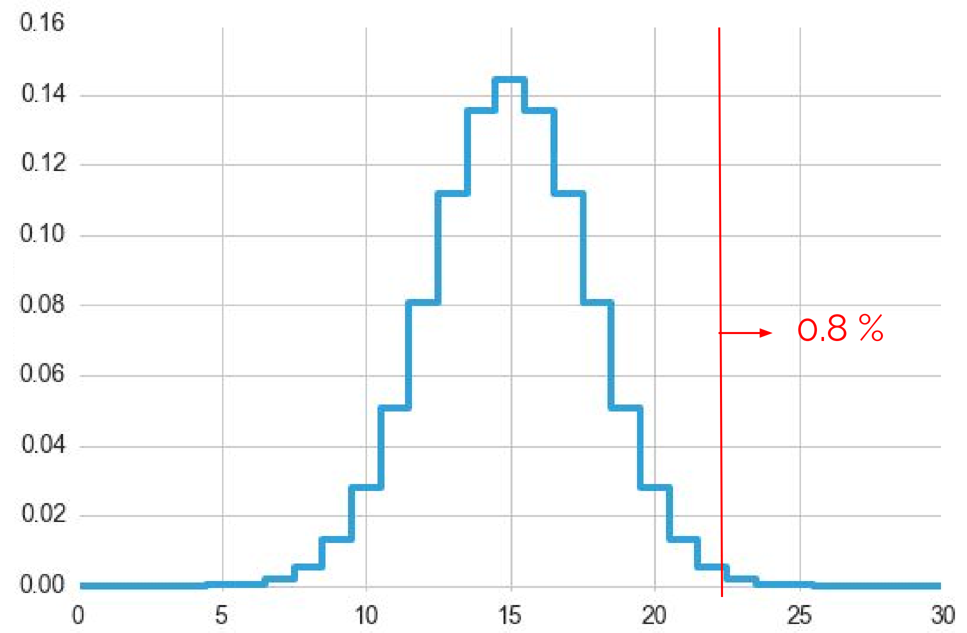
. . . But what question is this answering?

Stepping Back...

The deep meaning lies in the *sampling distribution:*

$$p(t;\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi}\,\Gamma\left(\frac{\nu}{2}\right)}\left(1+\frac{t^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

Same principle as the coin example:



Let’s use a sampling method instead

The Problem:

Unlike coin flipping, we *don't* have a generative model . . .

The Problem:

Unlike coin flipping, we *don't* have a generative model . . .

Solution:

Shuffling

★		×	
84	72	81	69
57	46	74	61
63	76	56	87
99	91	69	65
		66	44
		62	69

Idea:
Simulate the distribution by *shuffling* the labels repeatedly and computing the desired statistic.

Motivation:
if the labels really don't matter, then switching them shouldn't change the result!

★		×	
84	72	81	69
57	46	74	61
63	76	56	87
99	91	69	65
		66	44
		62	69

1. Shuffle Labels
2. Rearrange
3. Compute means

★		×	
84	72	81	69
57	46	74	61
63	76	56	87
99	91	69	65
		66	44
		62	69

1. **Shuffle Labels**
2. Rearrange
3. Compute means

★		×	
84	81	72	69
61	69	74	57
65	76	56	87
99	44	46	63
		66	91
		62	69

1. Shuffle Labels
2. **Rearrange**
3. Compute means

★		×	
84	81	72	69
61	69	74	57
65	76	56	87
99	44	46	63
		66	91
		62	69

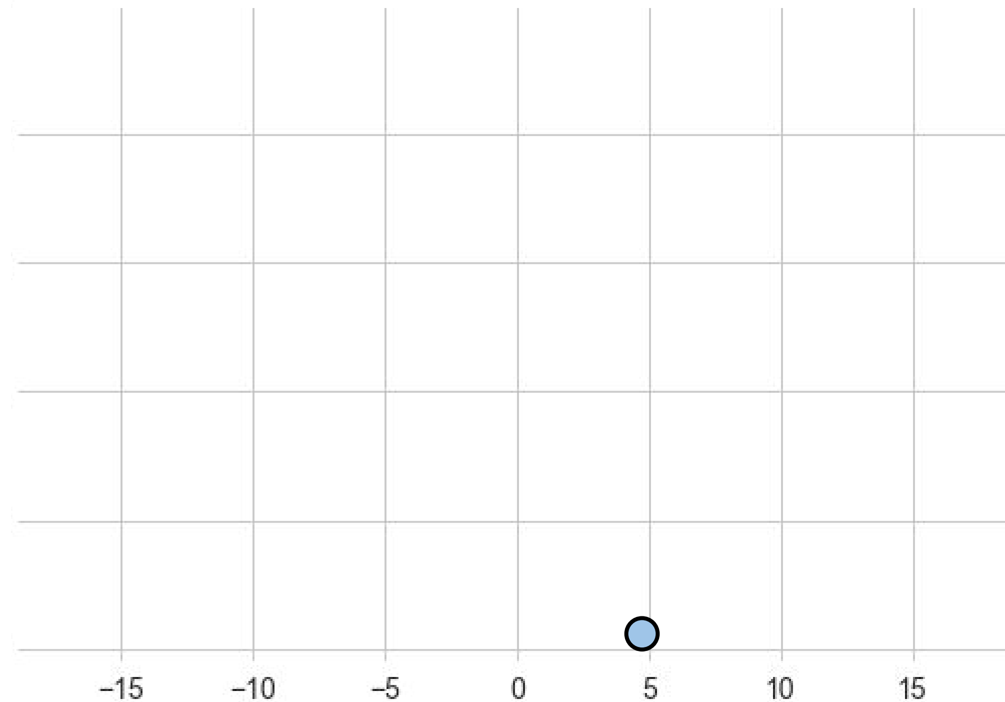
1. Shuffle Labels
2. Rearrange
3. **Compute means**

★ mean: 72.4
× mean: 67.6
difference: 4.8

★		×	
84	81	72	69
61	69	74	57
65	76	56	87
99	44	46	63
		66	91
		62	69

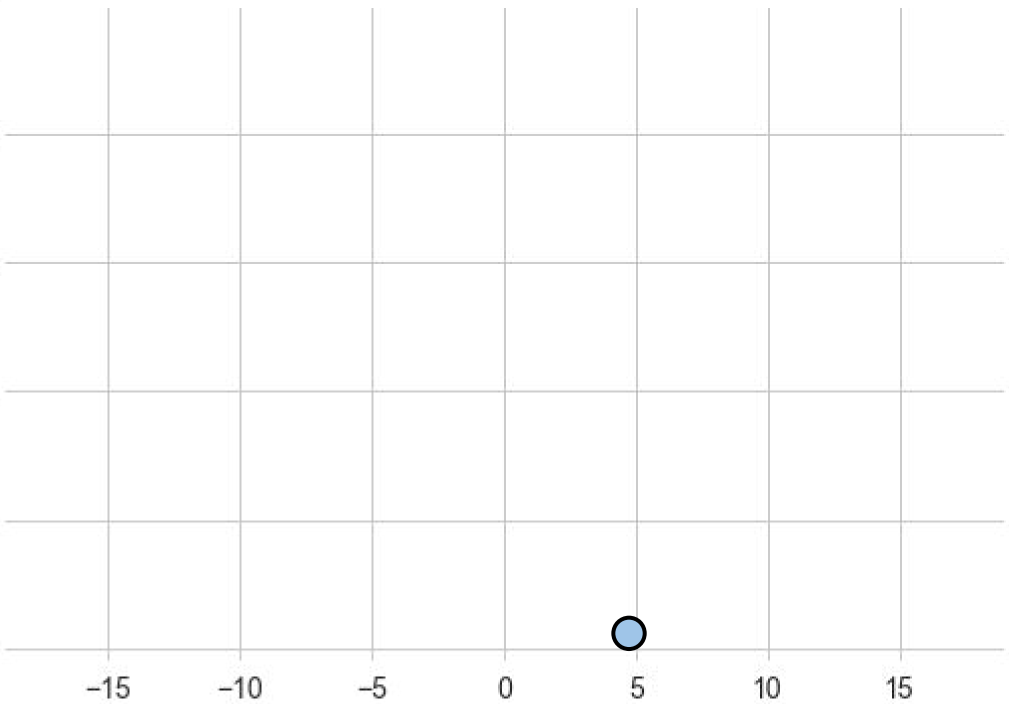
★ mean: 72.4
× mean: 67.6
difference: 4.8

1. Shuffle Labels
2. Rearrange
3. **Compute means**



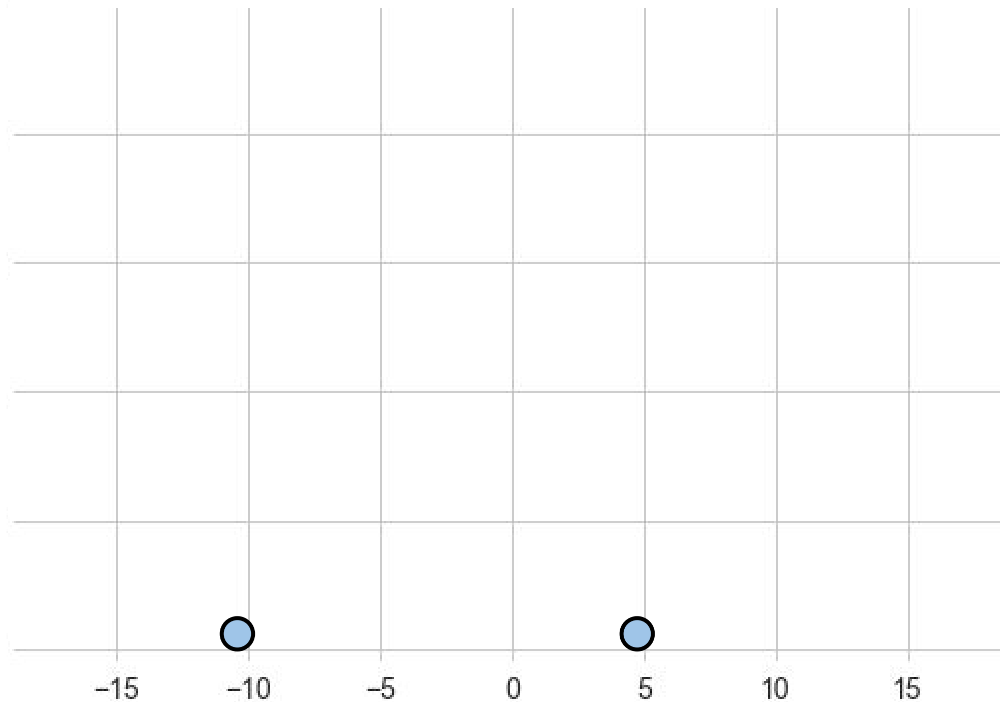
★		×	
84	81	72	69
61	69	74	57
65	76	56	87
99	44	46	63
		66	91
		62	69

1. **Shuffle Labels**
2. Rearrange
3. Compute means



★		×	
84	56	72	69
61	63	74	57
65	66	81	87
62	44	46	69
		76	91
		99	69

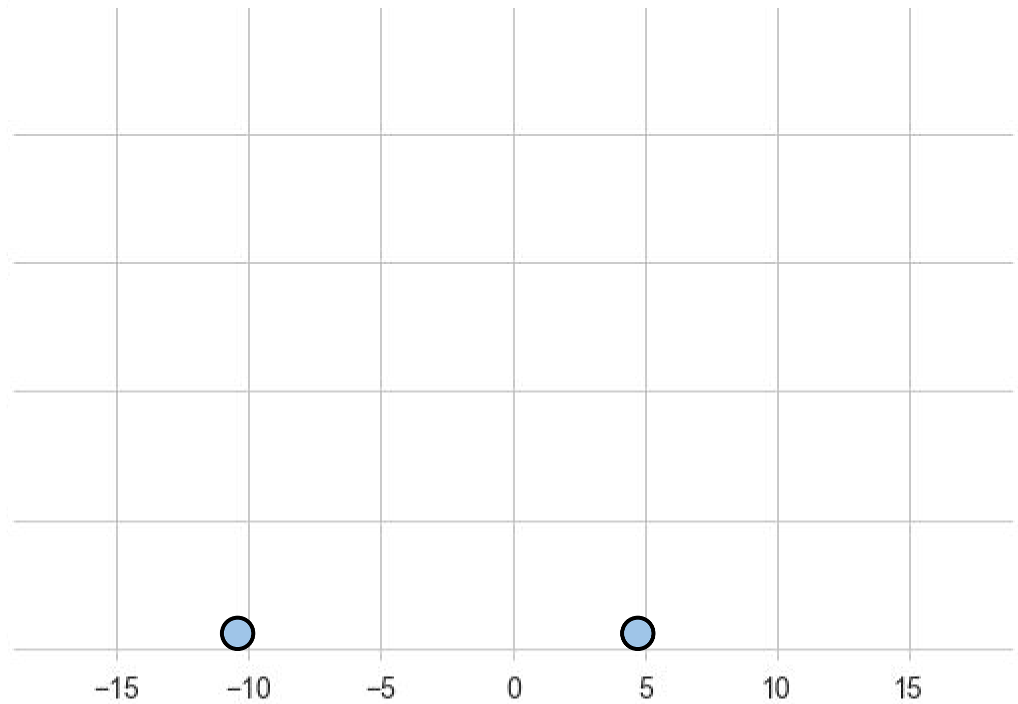
1. Shuffle Labels
2. Rearrange
3. **Compute means**



★ mean: 62.6
× mean: 74.1
difference: -11.6

★		×	
84	56	72	69
61	63	74	57
65	66	81	87
62	44	46	69
		76	91
		99	69

1. **Shuffle Labels**
2. Rearrange
3. Compute means



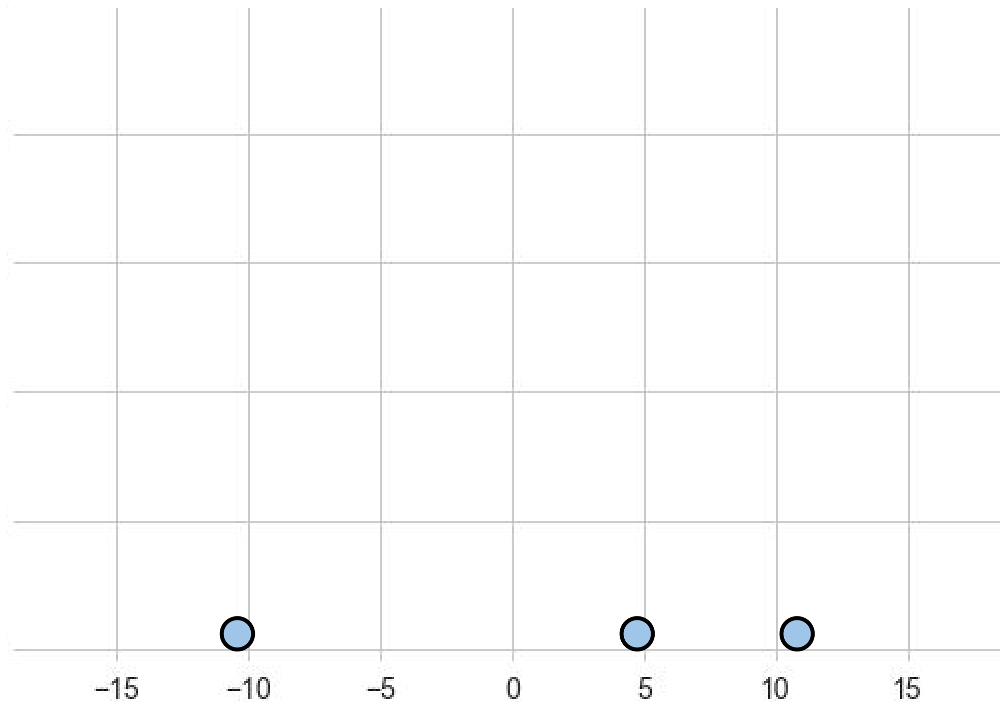
★		×	
74	56	72	69
61	63	84	57
87	76	81	65
91	99	46	69
		66	62
		44	69

★ mean: 75.9

× mean: 65.3

difference: 10.6

1. Shuffle Labels
2. Rearrange
3. **Compute means**



★		×	
84	56	72	69
61	63	74	57
65	66	81	87
62	44	46	69
		76	91
		99	69

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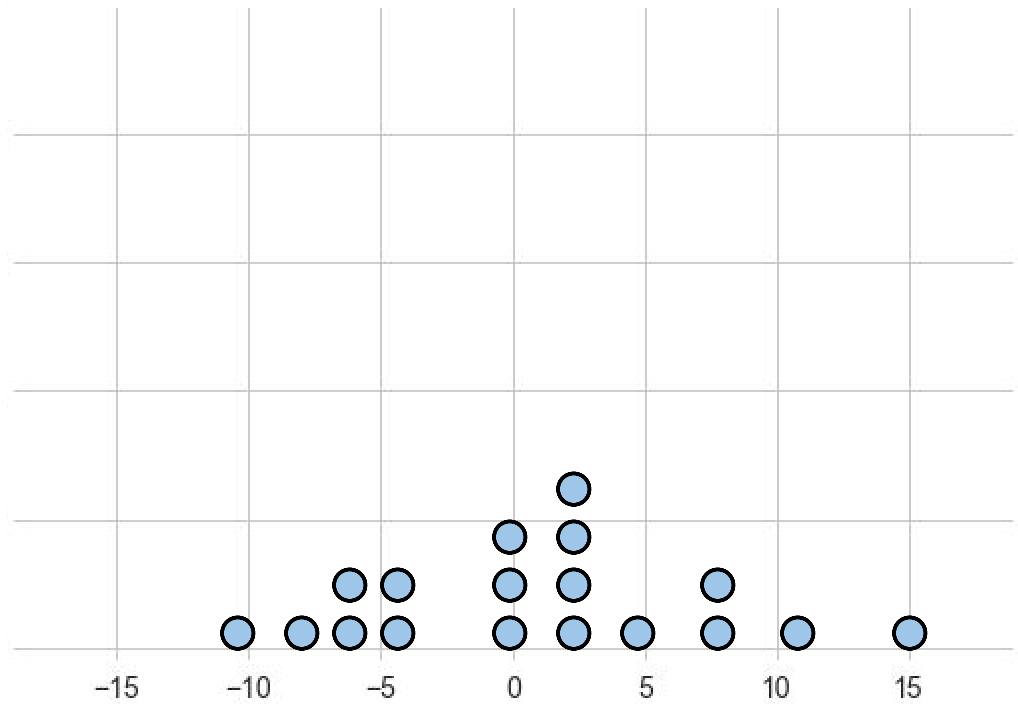
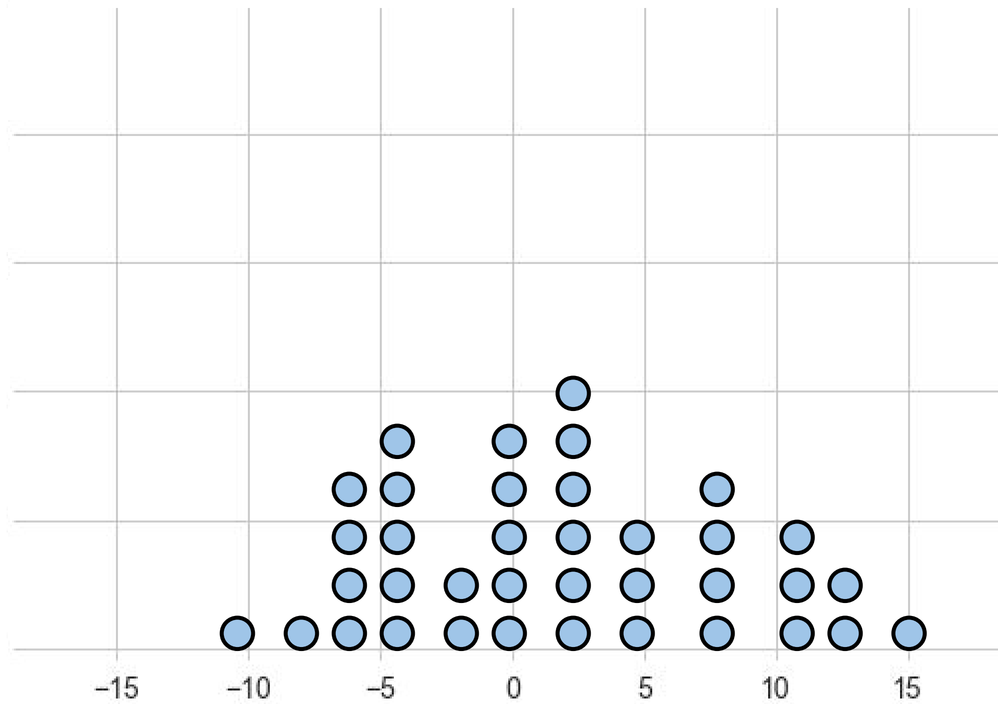


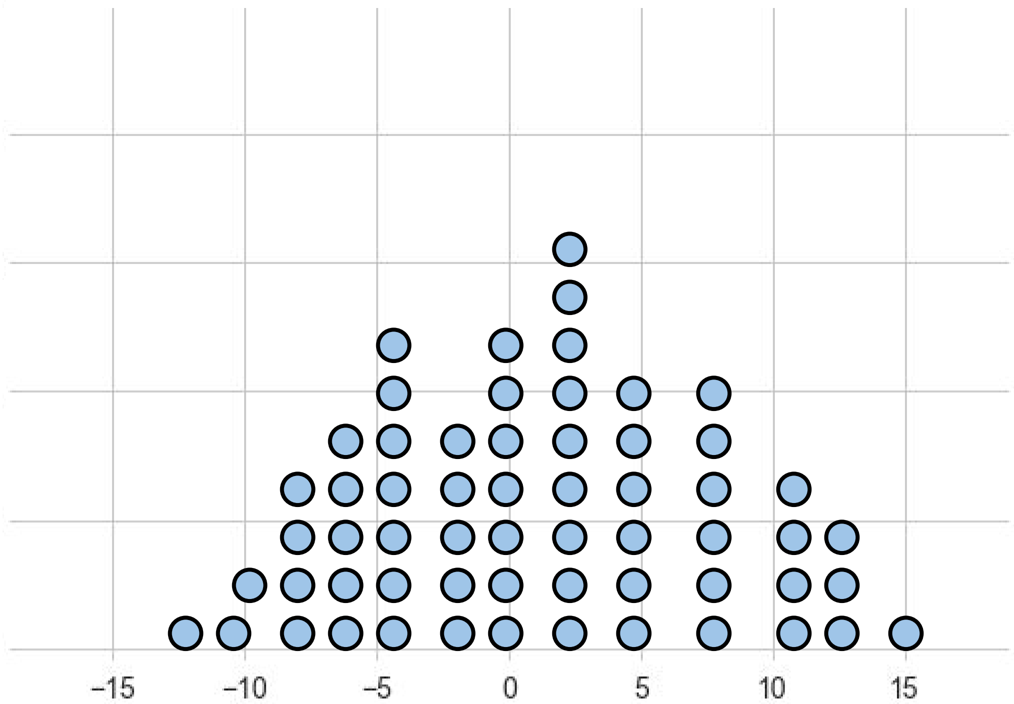
★		×	
84	81	69	69
61	69	87	74
65	76	56	57
99	44	46	63
		66	91
		62	72

1. Shuffle Labels
2. Rearrange
3. Compute means



★		×	
74	62	72	57
61	63	84	69
87	81	76	65
91	99	46	69
		66	56
		44	69

1. Shuffle Labels
2. Rearrange
3. Compute means



★		×	
84	81	72	69
61	69	74	57
65	76	56	87
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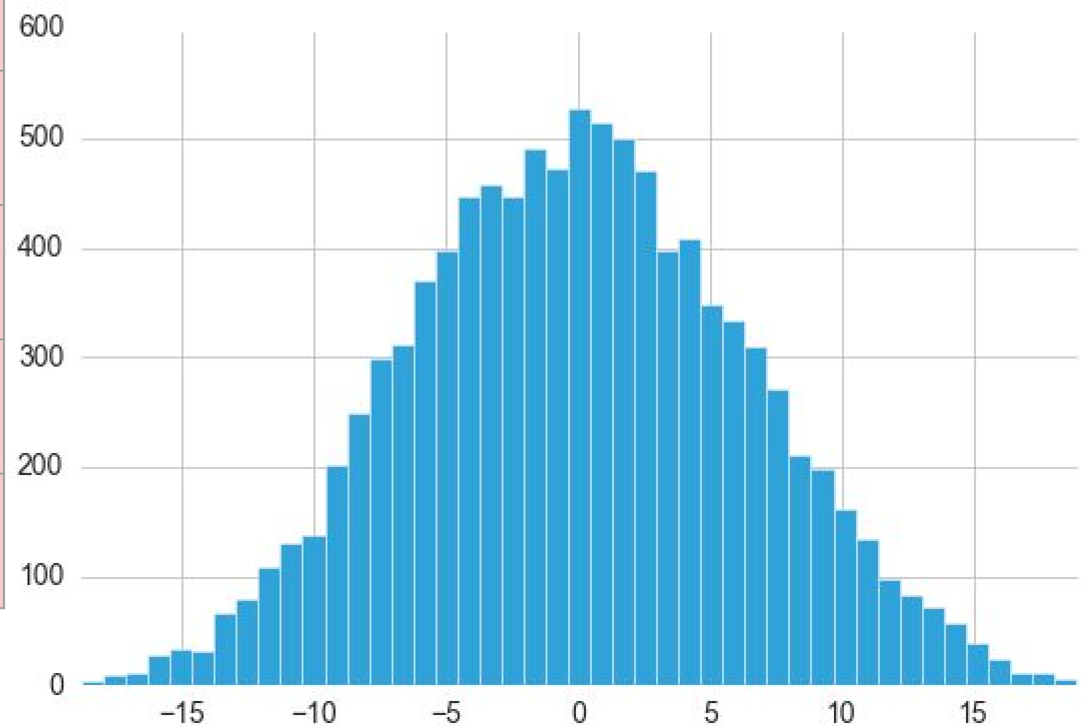
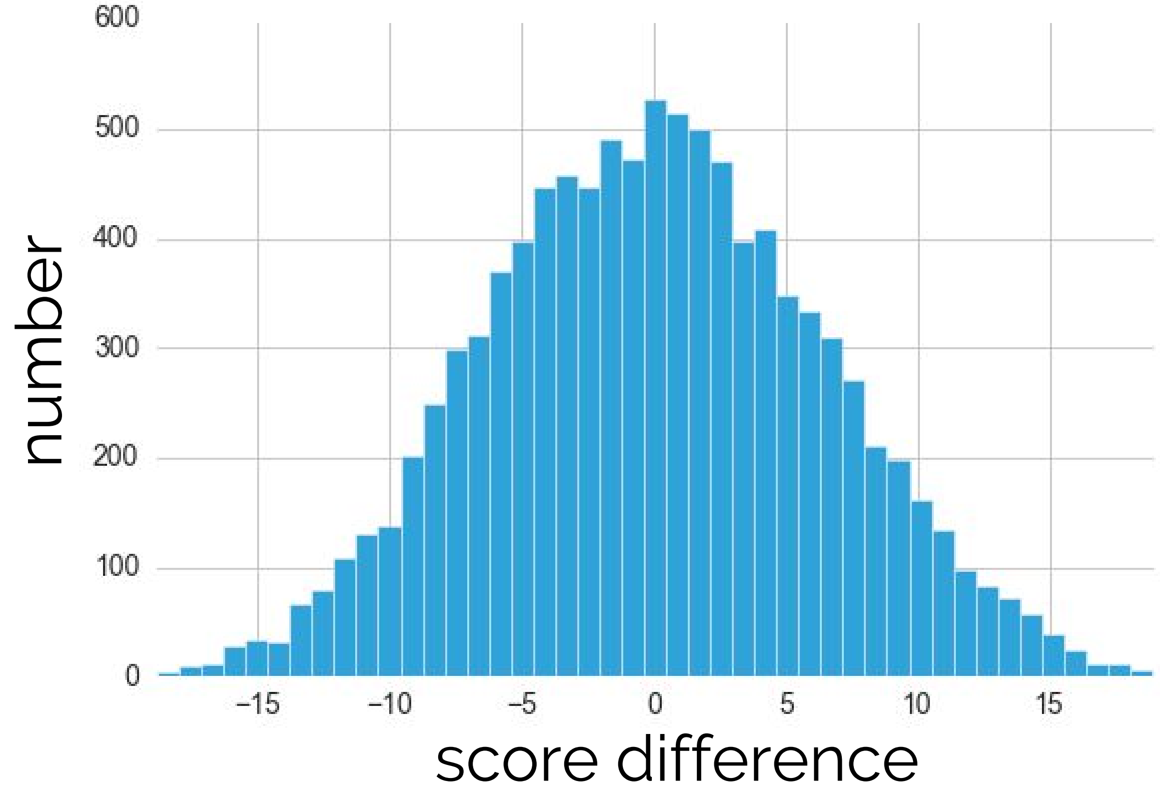
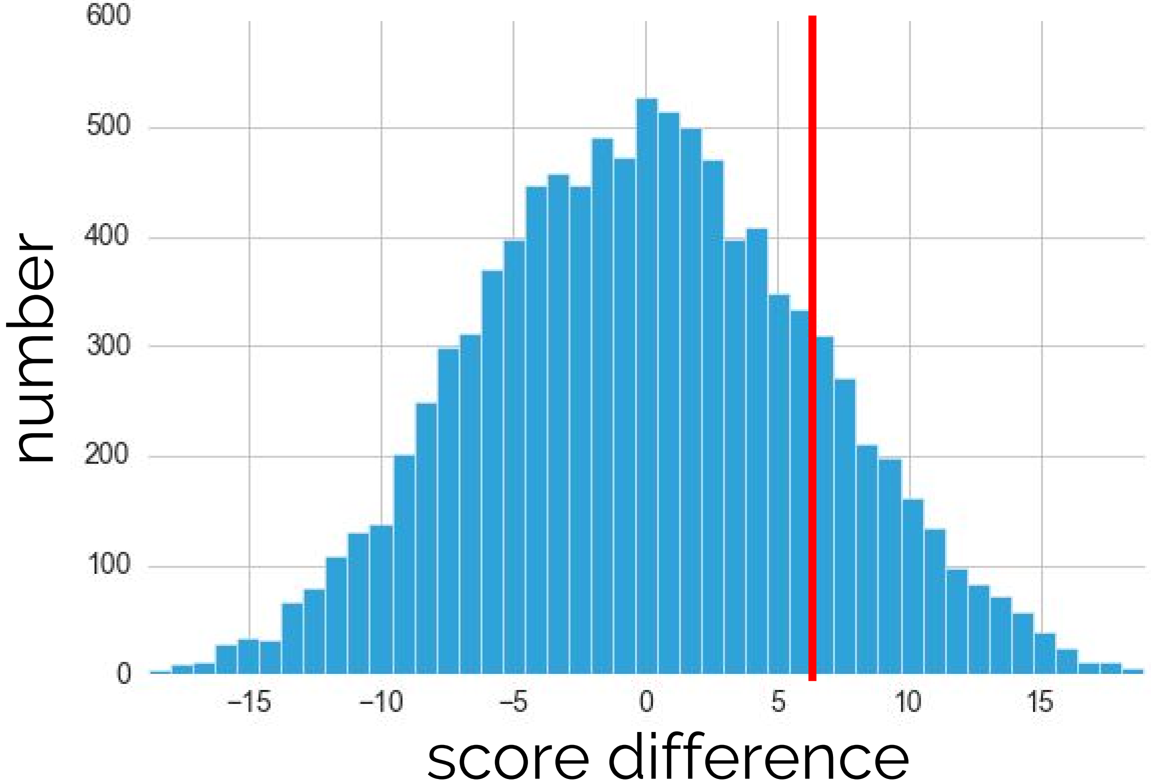
3. Compute means





600
500
400
300
200
100
0
number
−15
−10
−5
0
5
10
15
score difference


600
500
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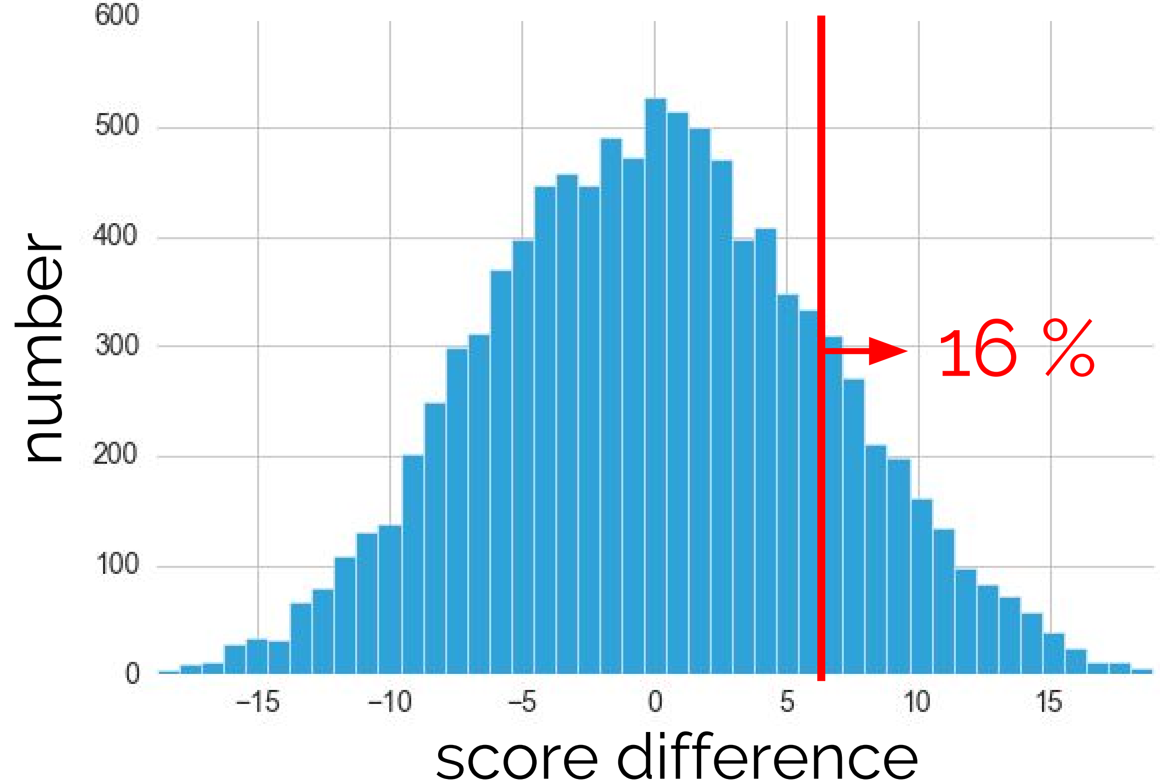


$$\frac{N_{>6.6}}{N_{tot}} = \frac{1608}{10000} = 0.16$$

“A difference of 6.6 is not significant at p = 0.05.”

That day, all the Sneetches
forgot about stars
And whether they had one,
or not, upon thars.

Notes on Shuffling:

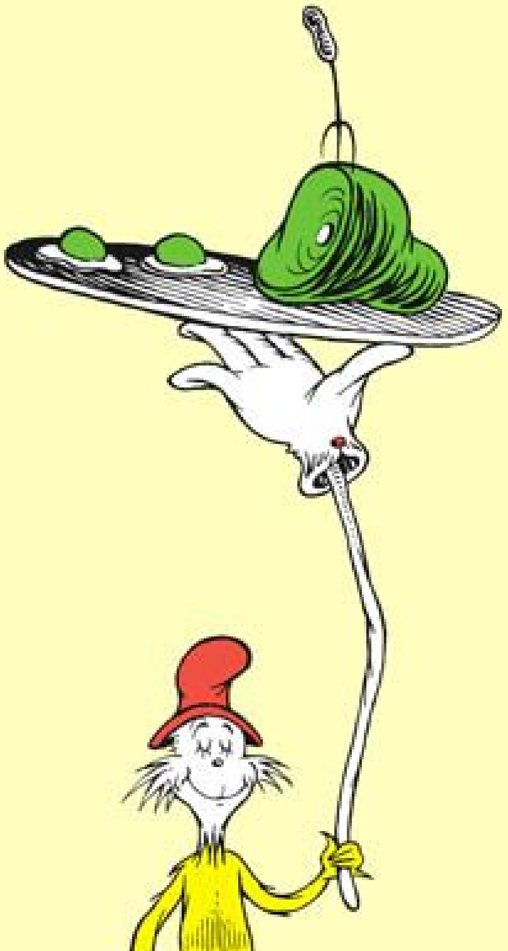
- Works when the *Null Hypothesis* assumes two groups are equivalent

- Like all methods, it will only work if your samples are representative – always be careful about selection biases!

- Needs care for non-independent trials. Good discussion in Simon's *Resampling: The New Statistics*

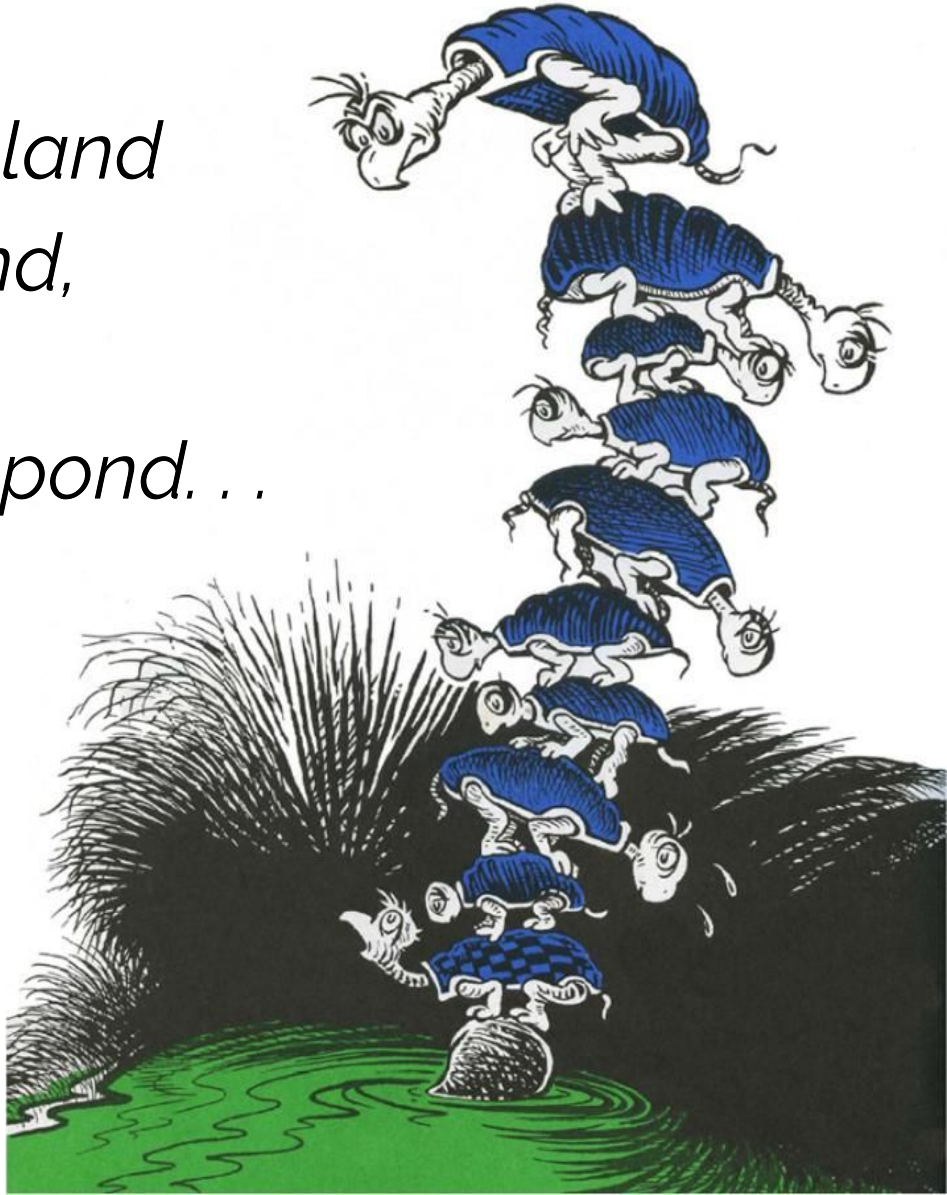
Four Recipes for Hacking Statistics:

1. Direct Simulation ✓
2. Shuffling ✓
3. Bootstrapping
4. Cross Validation



Yertle's Turtle Tower

On the far-away island
of Sala-ma-Sond,
Yertle the Turtle
was king of the pond. . .



How High can Yertle stack his turtles?

Observe 20 of Yertle's turtle towers . . .

# of turtles									
48	24	32	61	51	12	32	18	19	24
21	41	29	21	25	23	42	18	23	13

- What is the mean of the number of turtles in Yertle's stack?
- What is the uncertainty on this estimate?

Classic Method:

Sample Mean:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i = 28.9$$

Standard Error of the Mean:

$$\sigma_{\bar{x}} = \frac{1}{\sqrt{N}} \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2} = 3.0$$

What assumptions go into these formulae?

Can we use sampling instead?

Problem:
As before, we don't have a generating model . . .

Problem:
As before, we don't have a generating model . . .

Solution:
Bootstrap Resampling

Bootstrap Resampling:

48	24	51	12
21	41	25	23
32	61	19	24
29	21	23	13
32	18	42	18

Idea:
Simulate the distribution by *drawing samples with replacement.*

Motivation:
The data estimates its own distribution – we draw random samples from this distribution.

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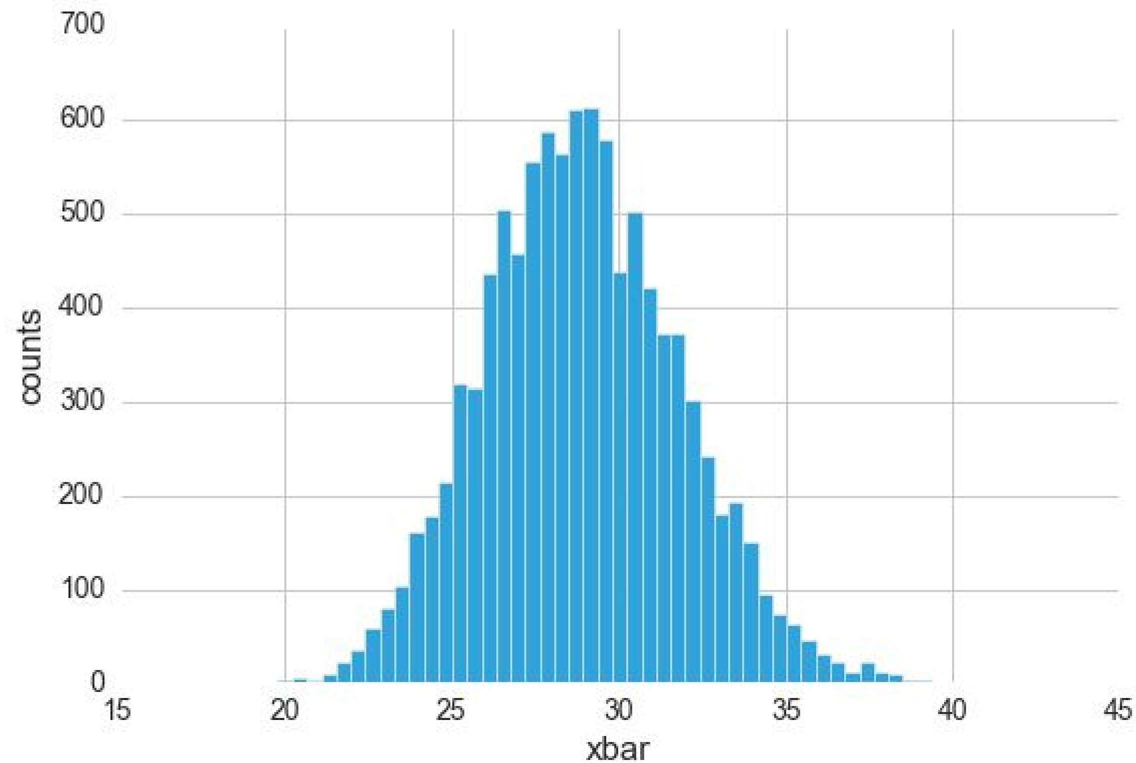
→ 31.05

Repeat this several thousand times . . .

Recovers The Analytic Estimate!

```
for i in range(10000):
    sample = N[randint(20, size=20)]
    xbar[i] = mean(sample)
mean(xbar), std(xbar)
# (28.9, 2.9)
```

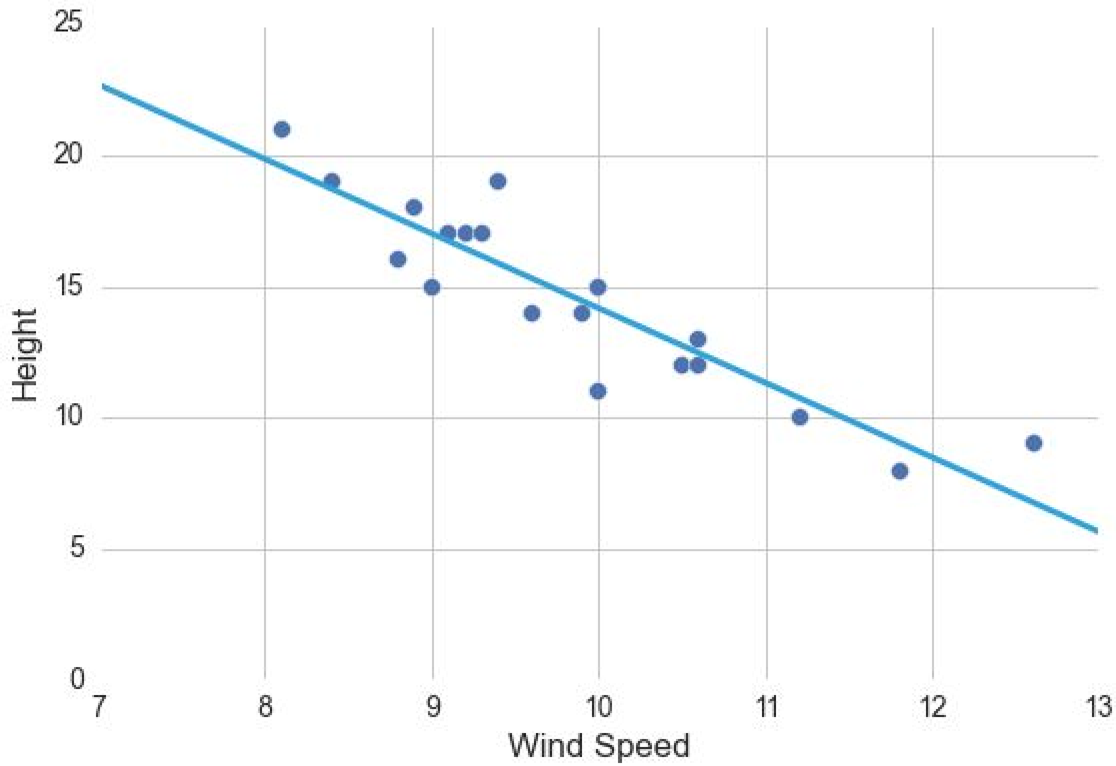
Height = 29 ± 3 turtles



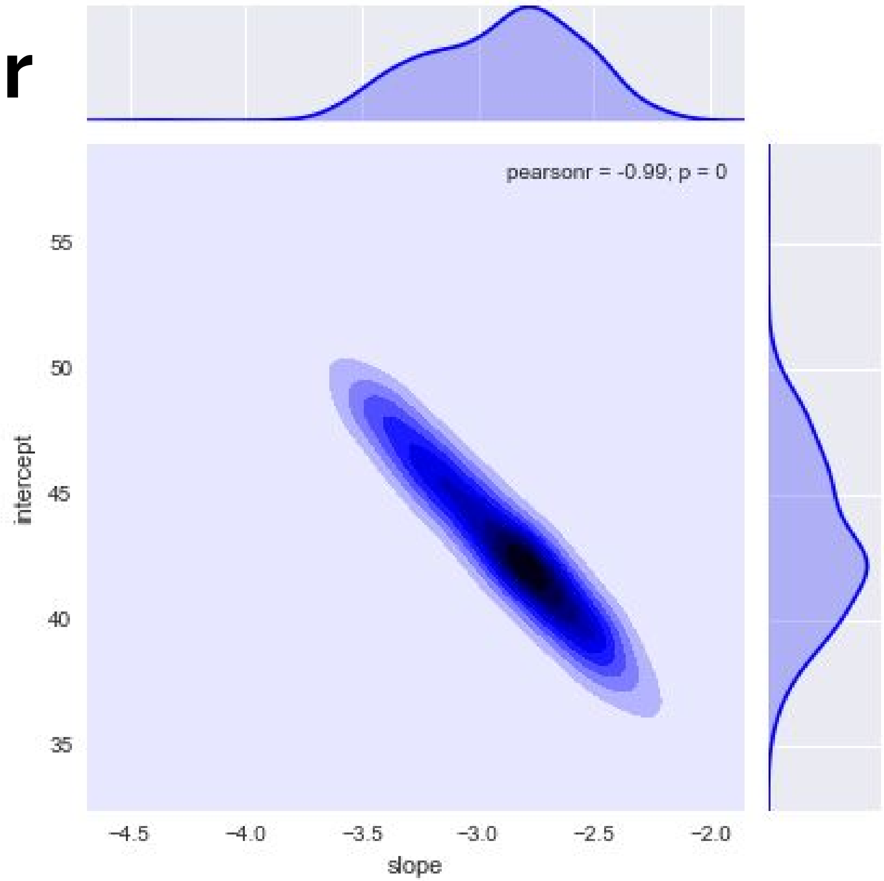
Bootstrap sampling can be applied even to more involved statistics

Bootstrap on Linear Regression:

What is the relationship between speed of wind and the height of the Yertle's turtle tower?



Bootstrap on Linear Regression:




```
for i in range(10000):
    i = randint(20, size=20)
    slope, intercept = fit(x[i], y[i])
    results[i] = (slope, intercept)
```

Notes on Bootstrapping:

- Bootstrap resampling is well-studied and rests on solid theoretical grounds.

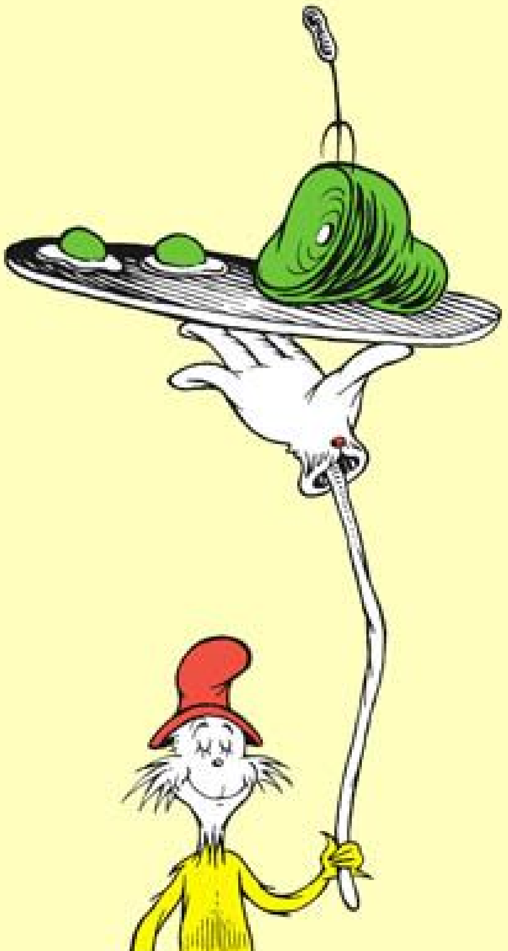
- Bootstrapping often doesn't work well for rank-based statistics (e.g. maximum value)

- Works poorly with very few samples (N > 20 is a good rule of thumb)

- As always, be careful about selection biases & non-independent data!

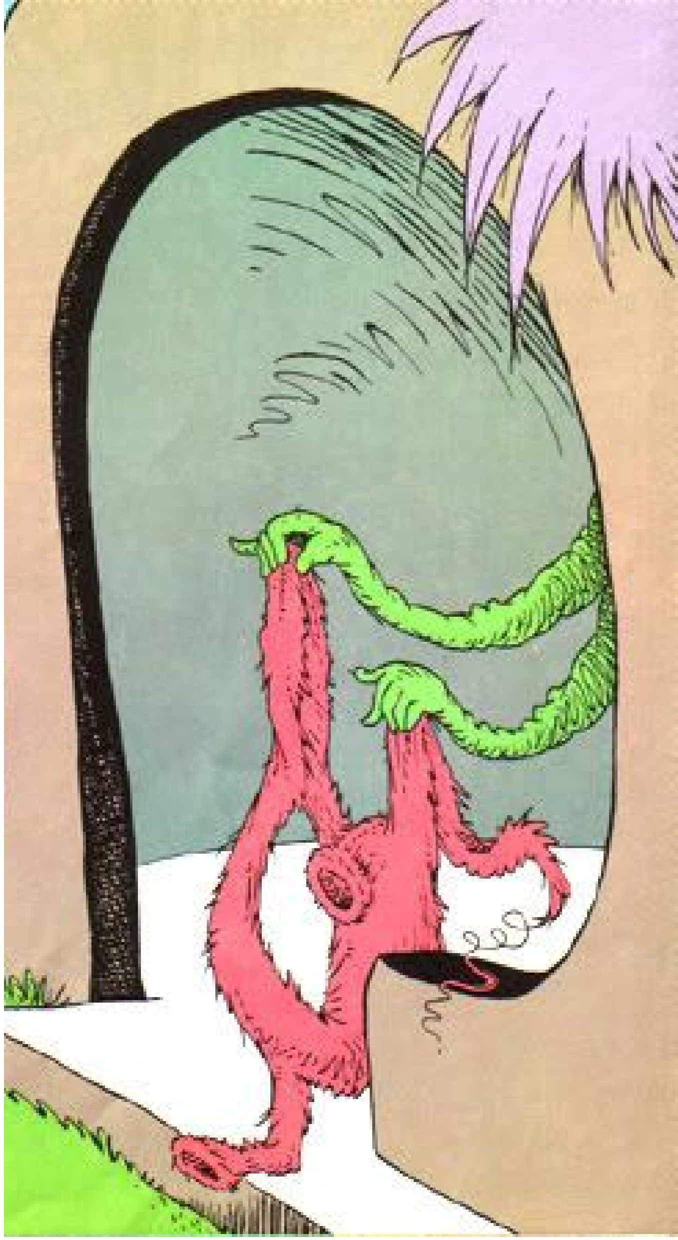
Four Recipes for Hacking Statistics:

1. Direct Simulation ✓
2. Shuffling ✓
3. Bootstrapping ✓
4. Cross Validation

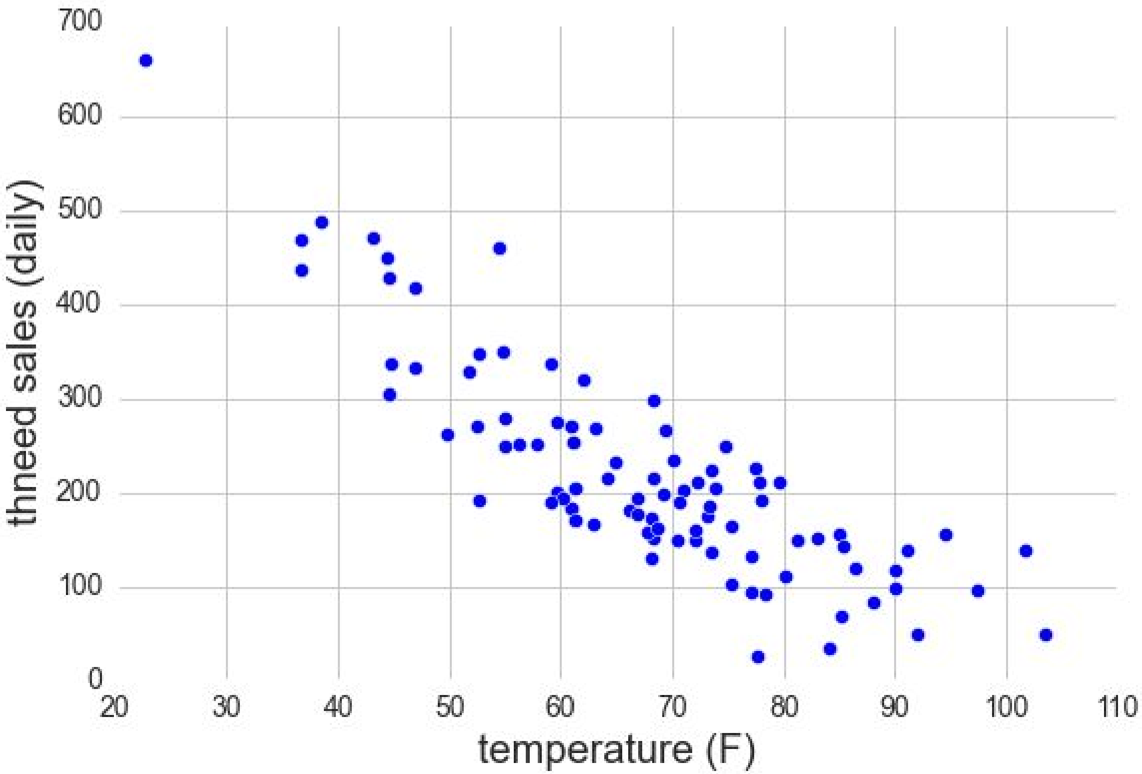


Onceler Industries:
Sales of Thneeds

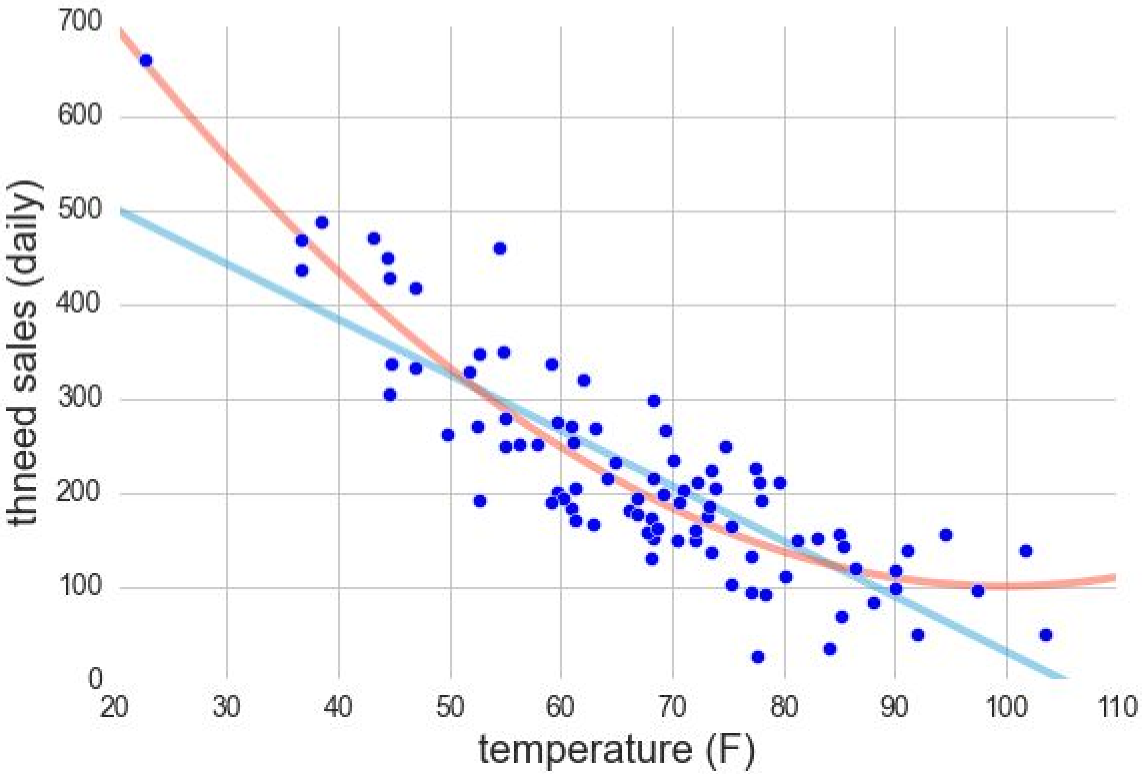
I'm being quite useful!
This thing is a Thneed.
A Thneed's a Fine-Something-
That-All-People-Need!



Thneed sales seem to show a trend with temperature . . .

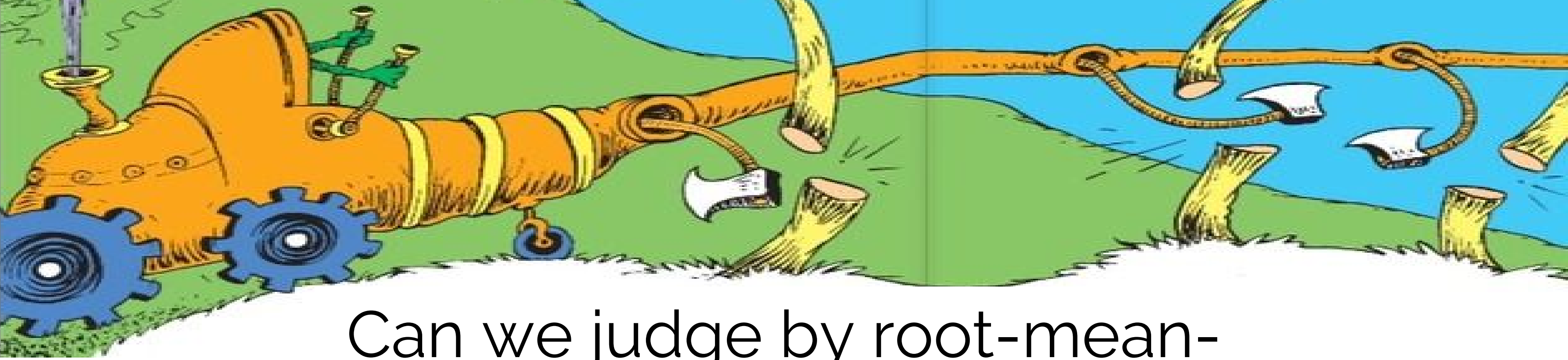


But which model is a better fit?

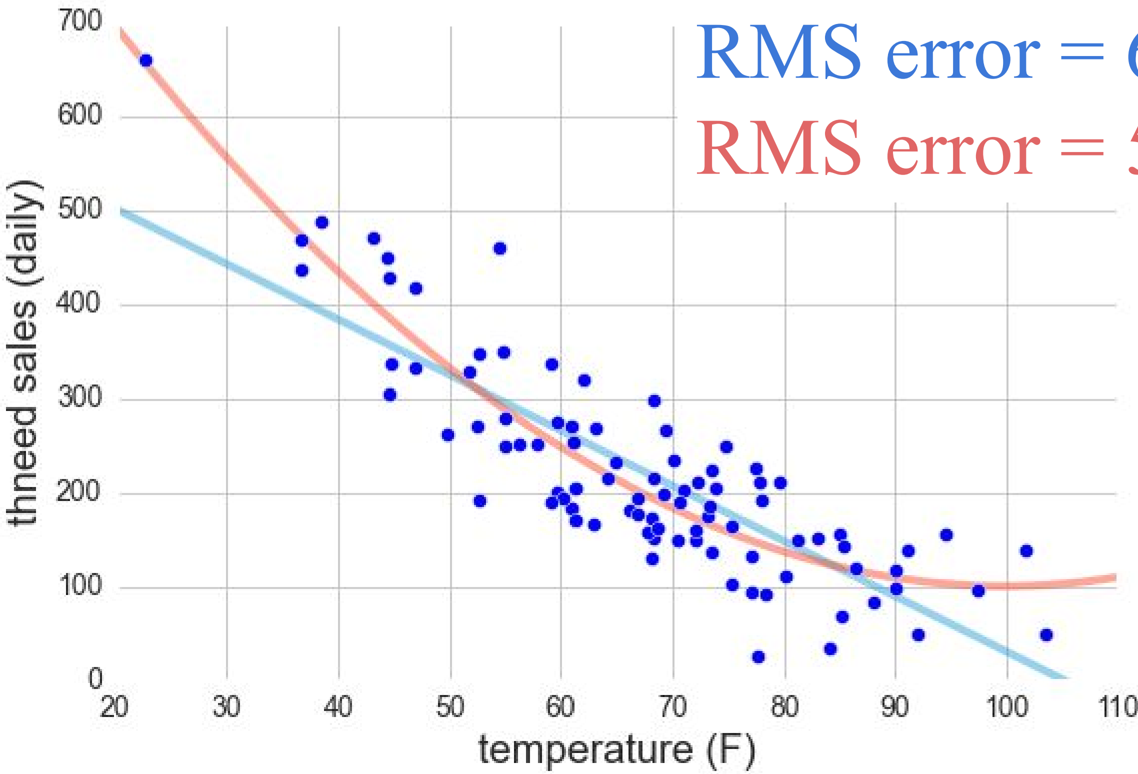


$$y = \mathrm{a} + \mathrm{b}x$$

$$y = \mathrm{a} + \mathrm{b}x + \mathrm{c}x^2$$



Can we judge by root-mean-square error?



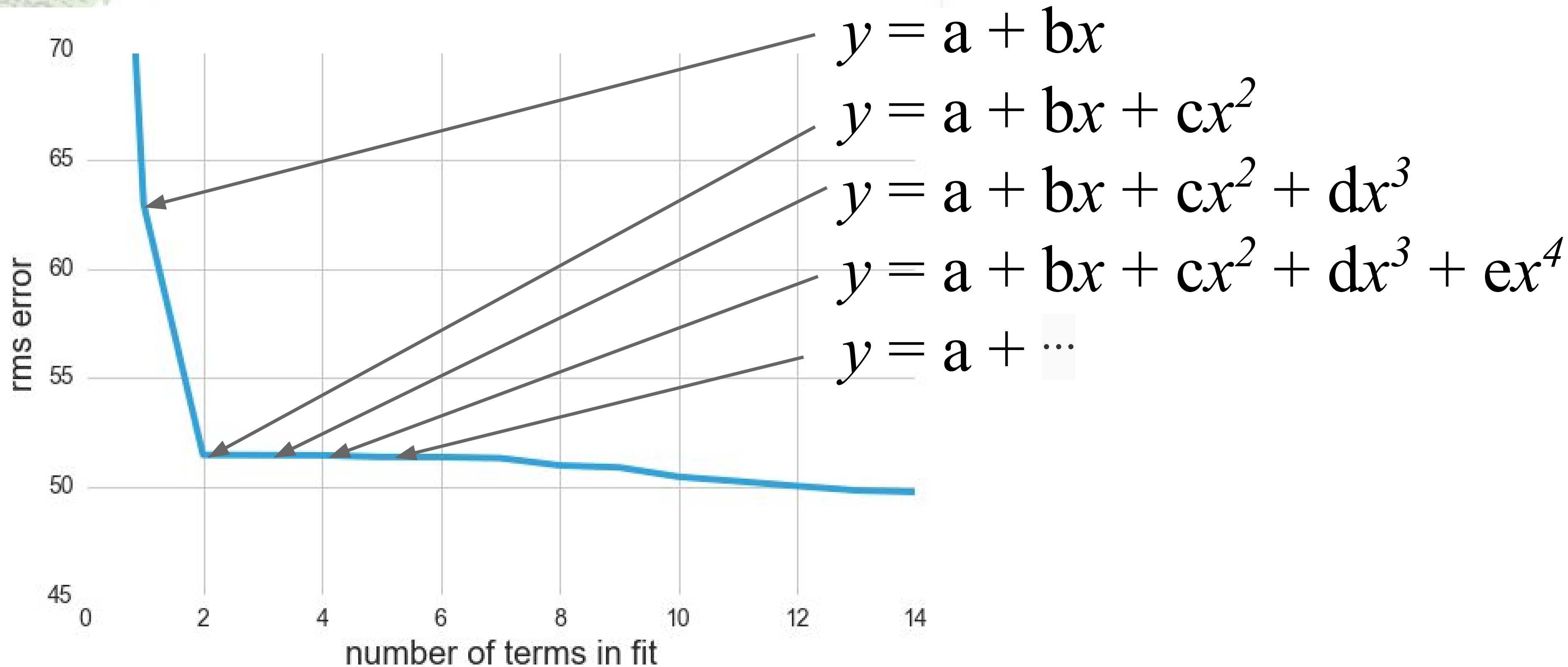
RMS error = 63.0

RMS error = 51.5

$y = \mathrm{a} + \mathrm{b}x$

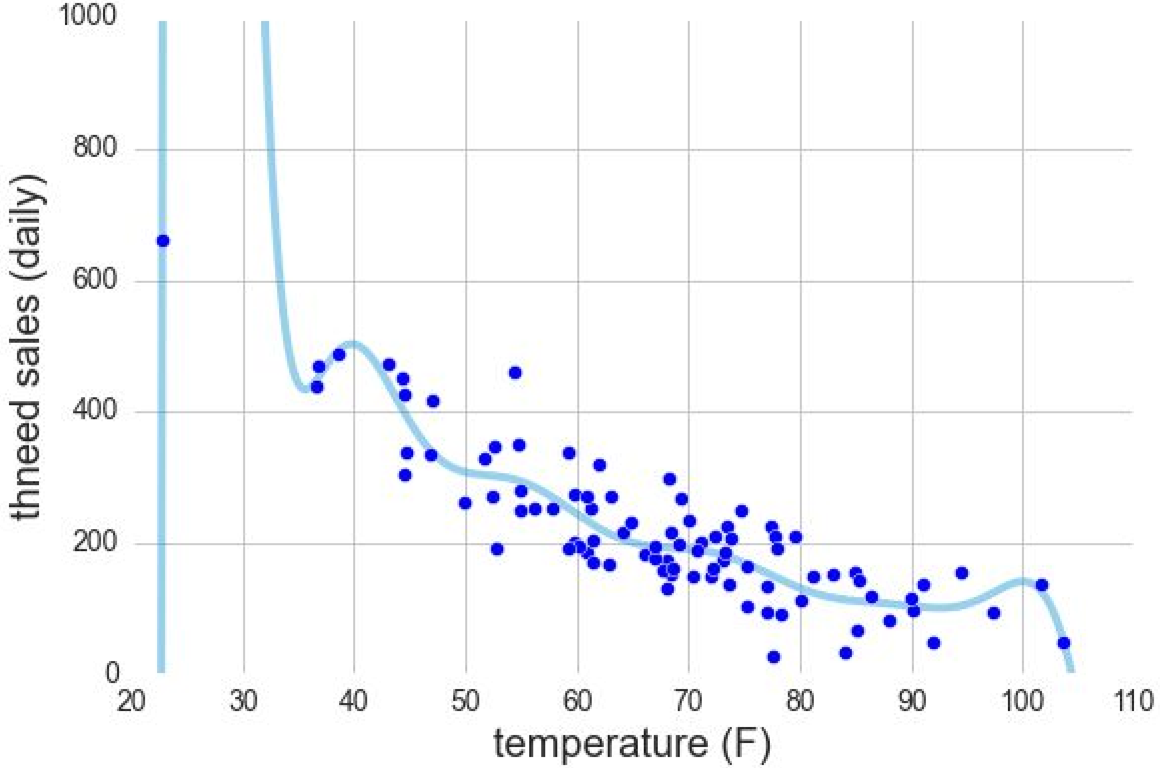
$y = \mathrm{a} + \mathrm{b}x + \mathrm{c}x^2$

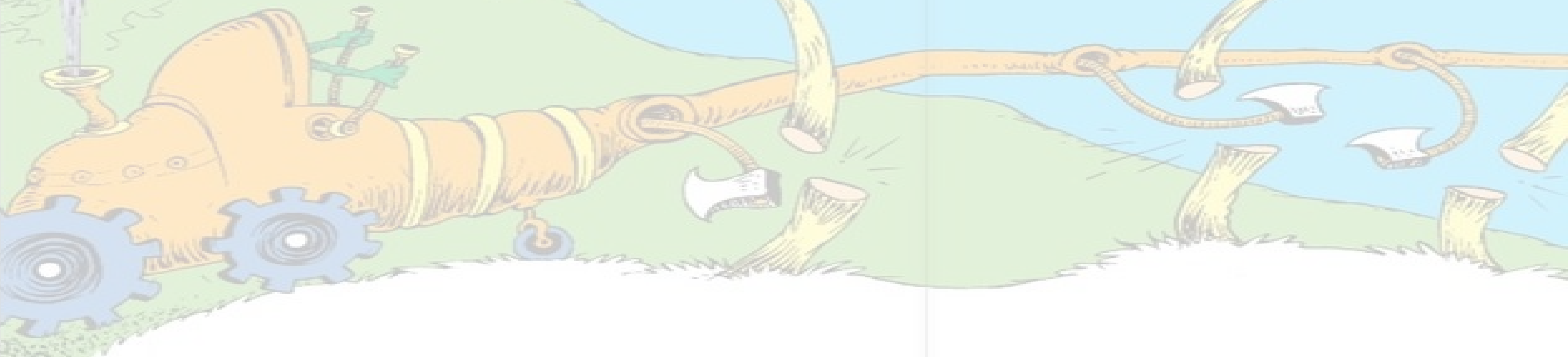
In general, more flexible models will *always* have a lower RMS error.



RMS error does not tell the whole story.

$$y = \mathrm{a} + \mathrm{b}x + \mathrm{c}x^2 + \mathrm{d}x^3 + \mathrm{e}x^4 + \mathrm{f}x^5 + \cdots + \mathrm{n}x^{14}$$





Not to worry:
Statistics has figured this out.

Classic Method

Difference in Mean Squared Error follows chi-square distribution:

$$p(x;\nu) = \frac{1}{2^{\nu/2}\Gamma\left(\frac{\nu}{2}\right)} x^{\frac{\nu}{2}-1} e^{-\frac{x}{2}}$$

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Can estimate degrees of freedom easily because the models are *nested* . . .

$$\nu \approx \nu_2 - \nu_1$$
$$\nu_2 \approx (N - d_2)$$
$$\nu_1 \approx (N - d_1)$$

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$$\nu \approx \nu_2 - \nu_1$$

$$\nu_2 \approx (N - d_2)$$

$$\nu_1 \approx (N - d_1)$$

Plug in our numbers . . .

Classic Method

Wait… what question were we trying to answer again?

Difference in Mean Squared Error follows chi-square distribution

$$p(x;\nu) = \frac{1}{2^{\nu/2}\Gamma\left(\frac{\nu}{2}\right)} x^{\frac{\nu}{2}-1} e^{-\frac{x}{2}}$$

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$$\nu \approx \nu_2 - \nu_1$$

$$\nu_2 \approx (N - d_2)$$

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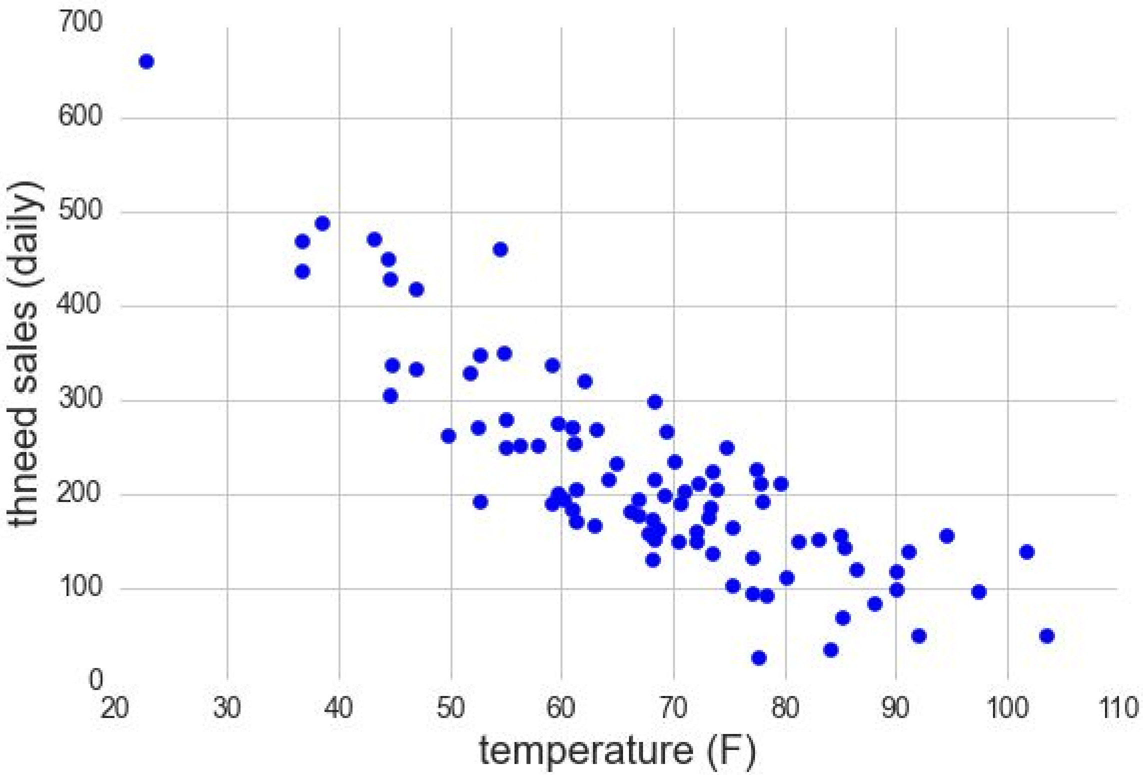
Plug in our numbers . . .

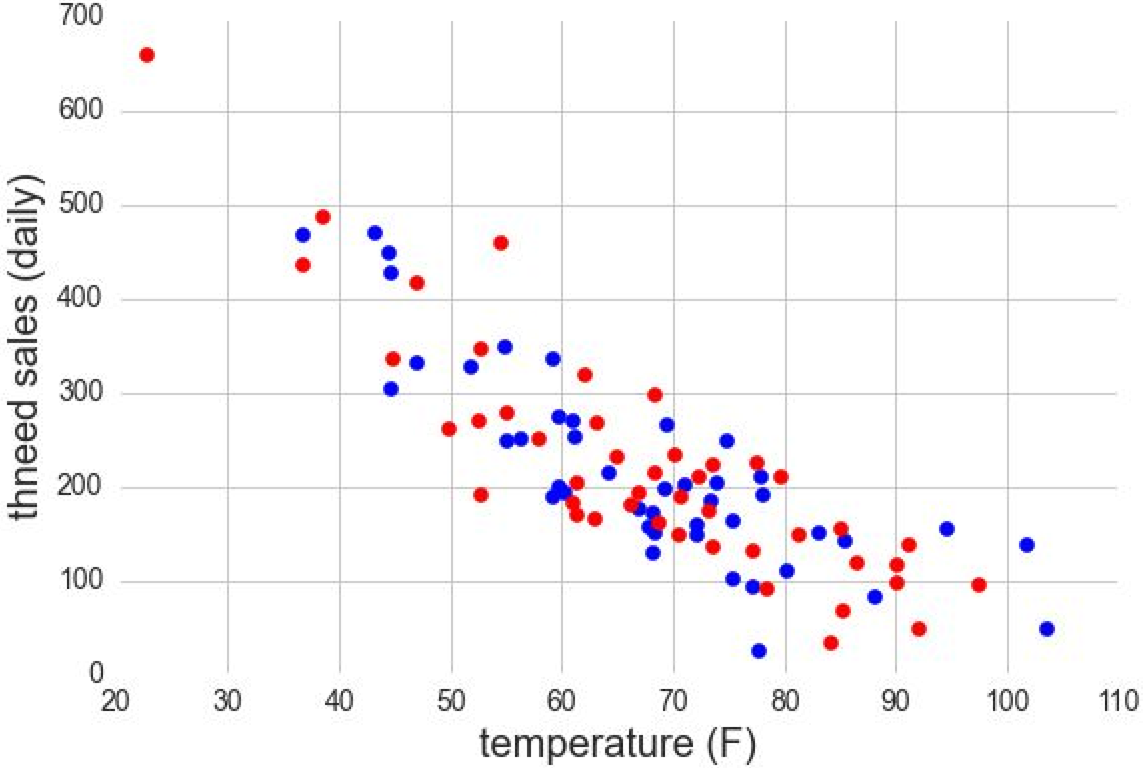
Another Approach: Cross Validation

Cross-Validation



Cross-Validation

1. Randomly Split data



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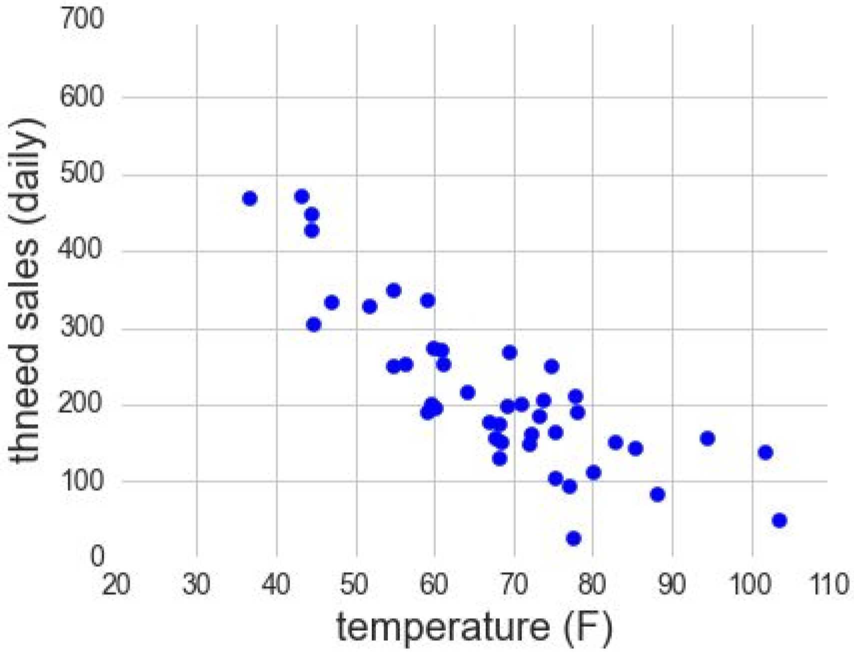
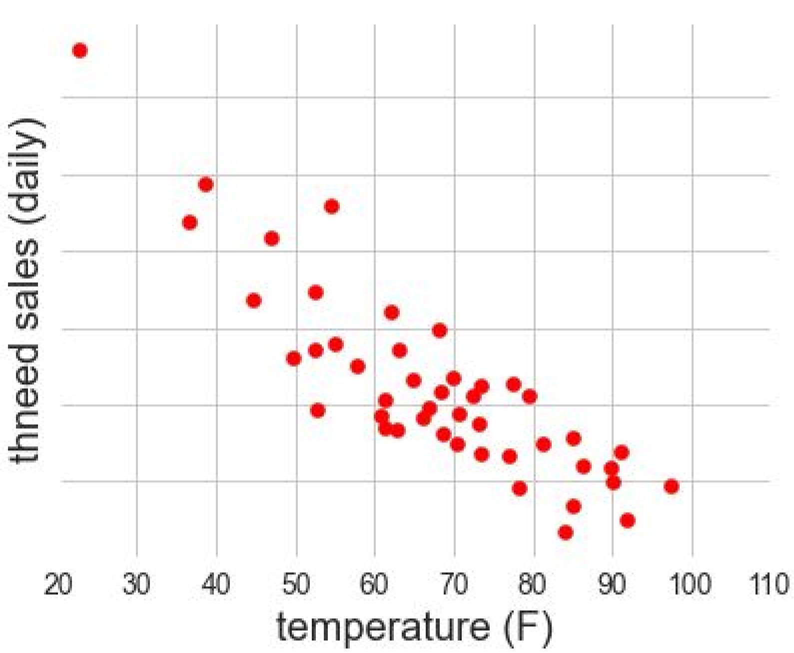
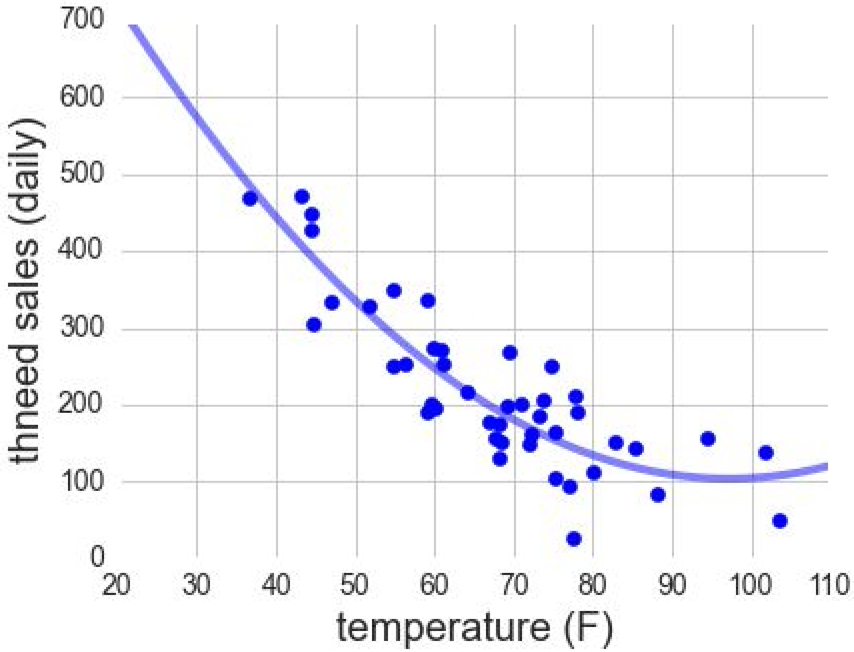
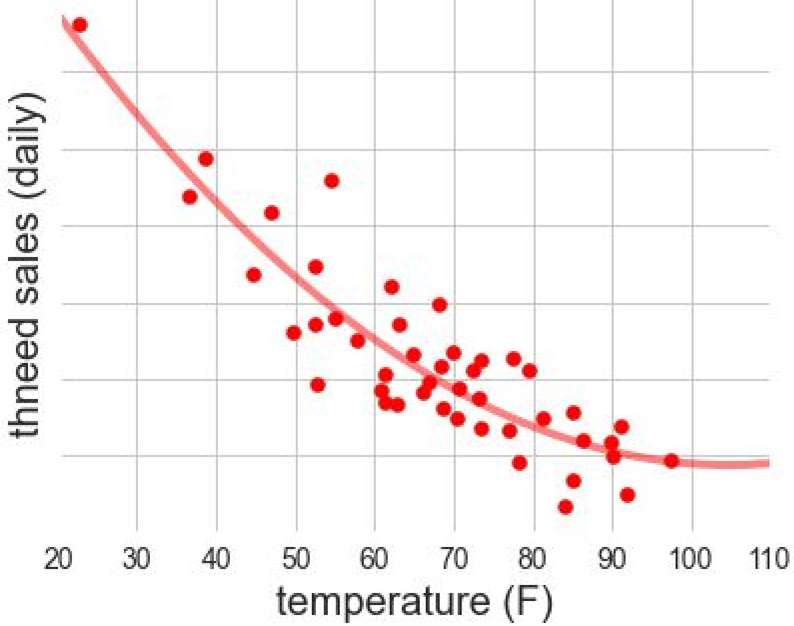




Cross-Validation

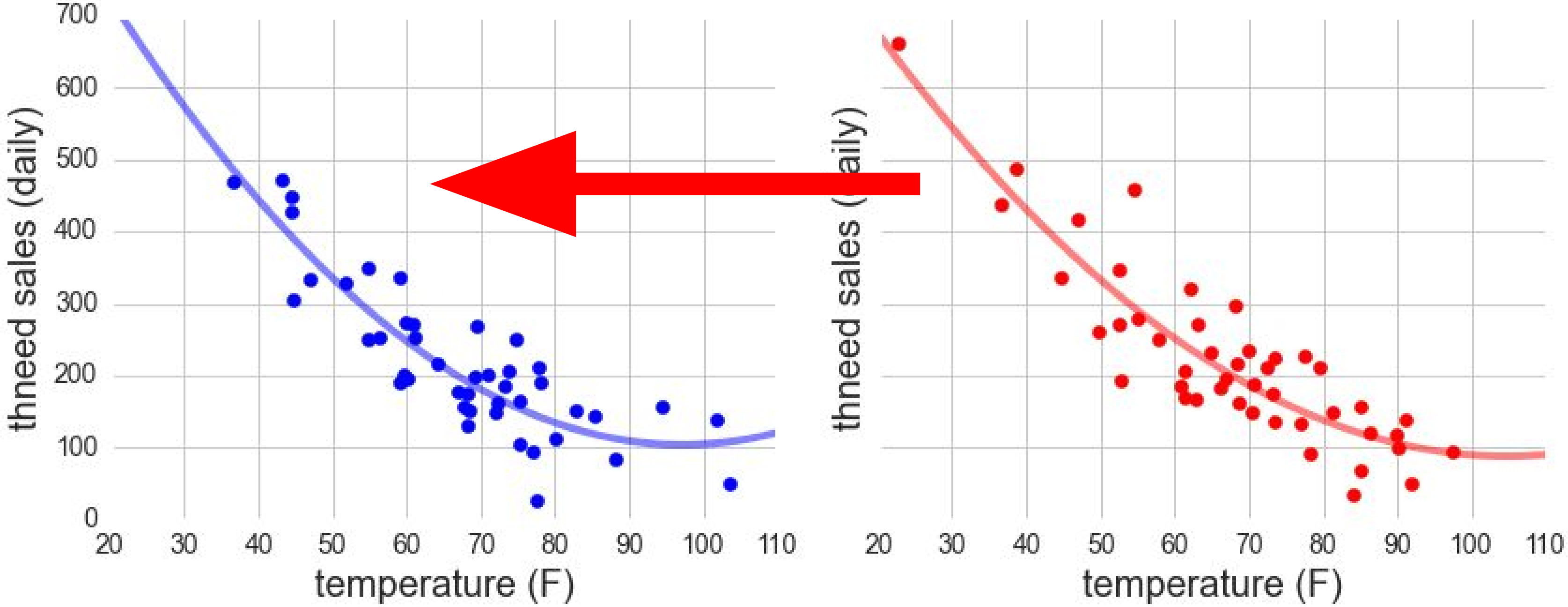
2. Find the best model for each subset





Cross-Validation

3. Compare models across subsets



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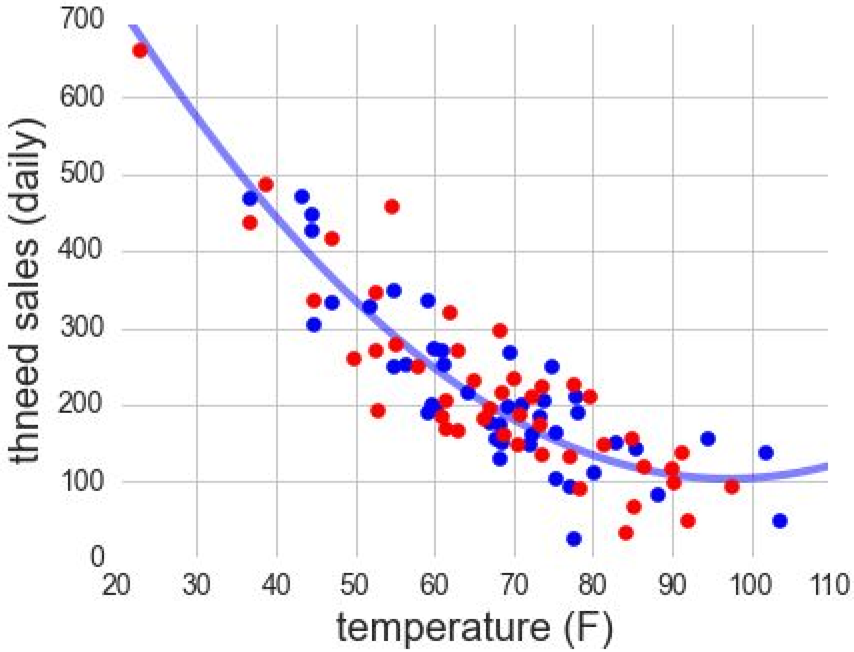

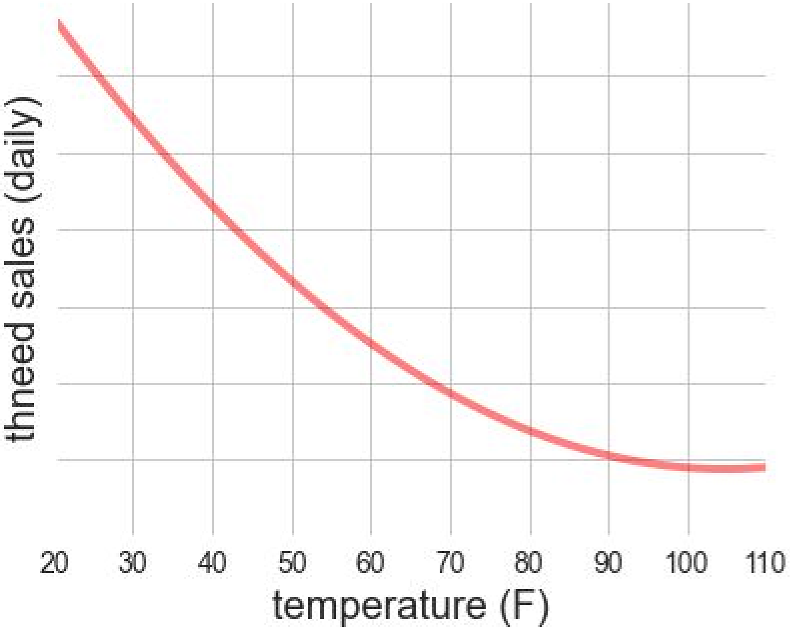

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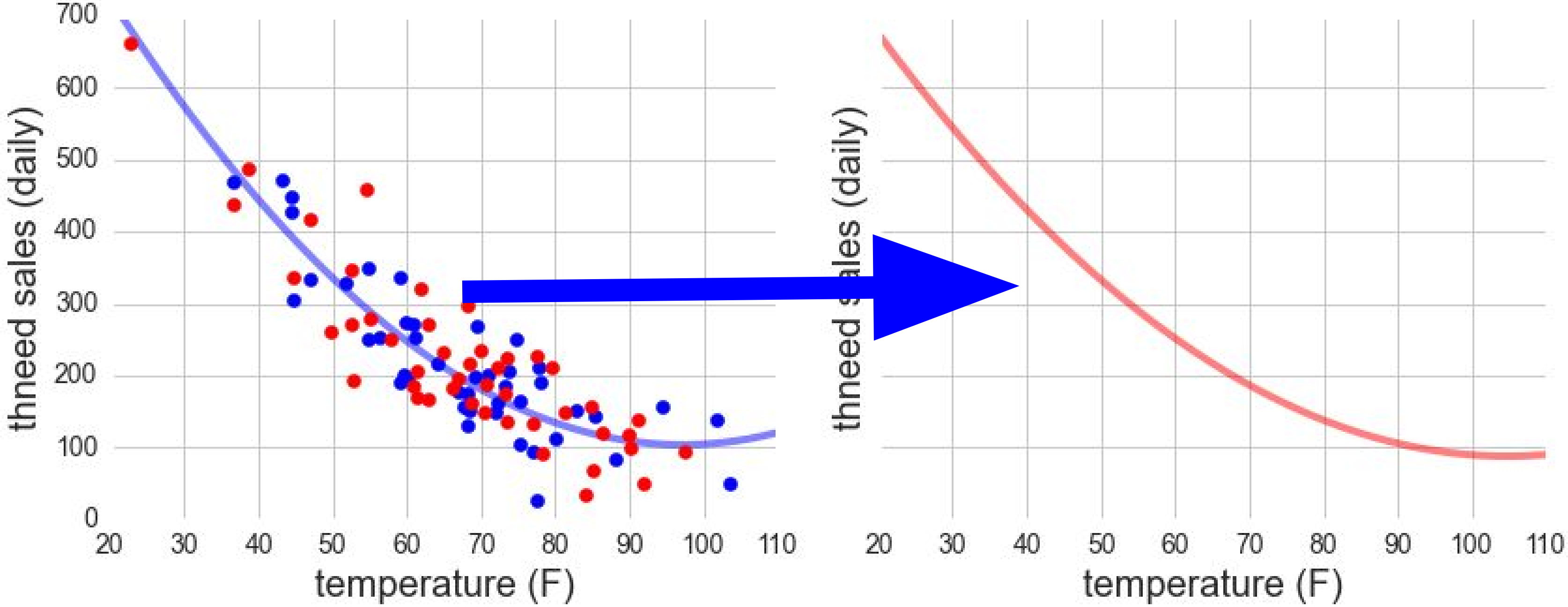

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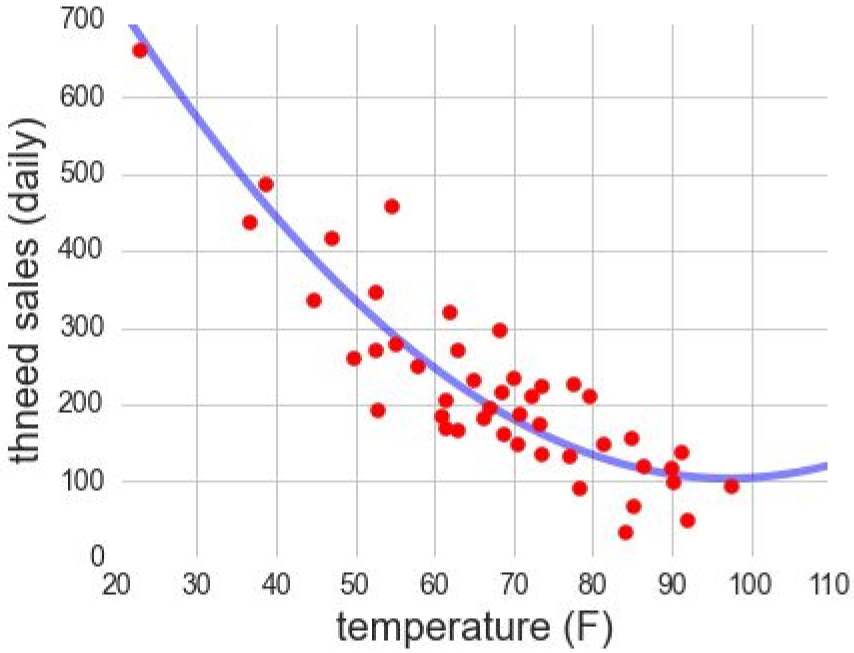
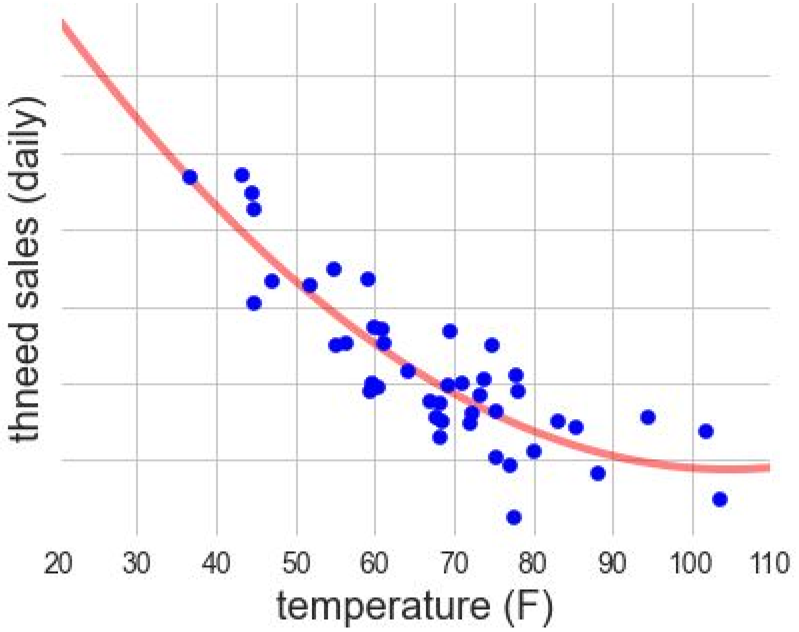
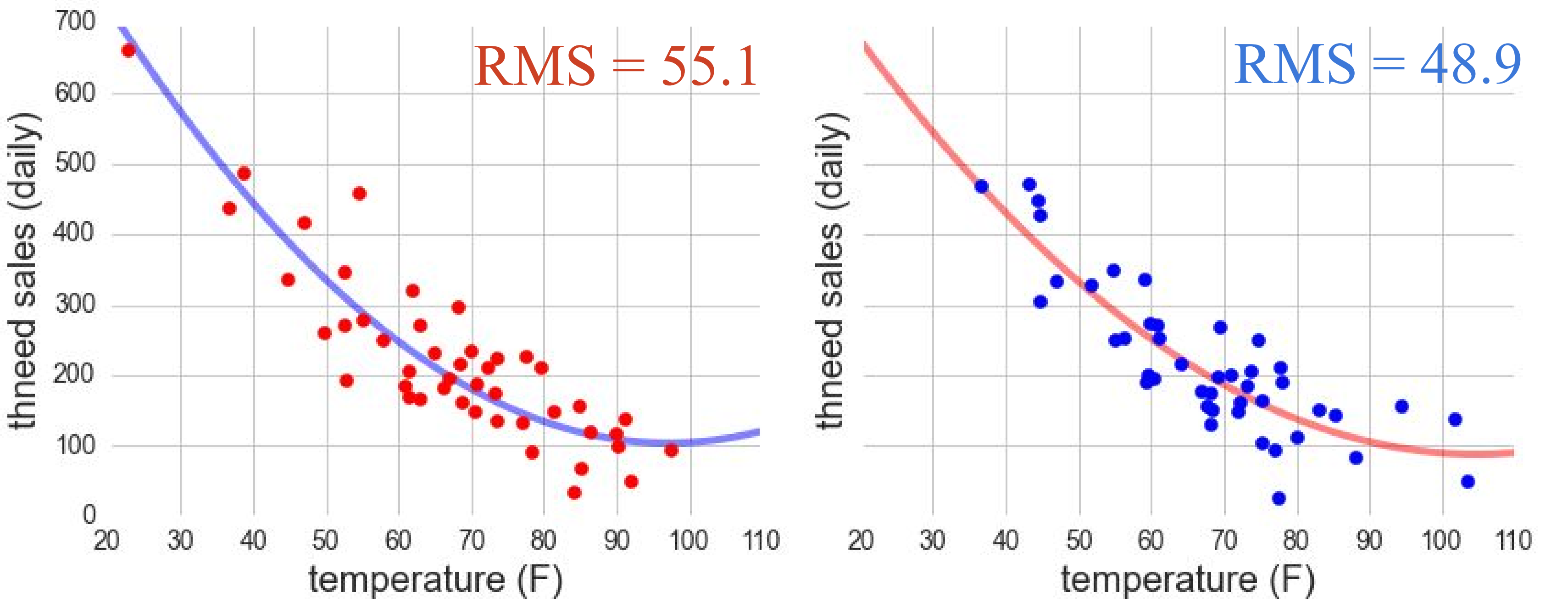




Cross-Validation

4. Compute RMS error for each



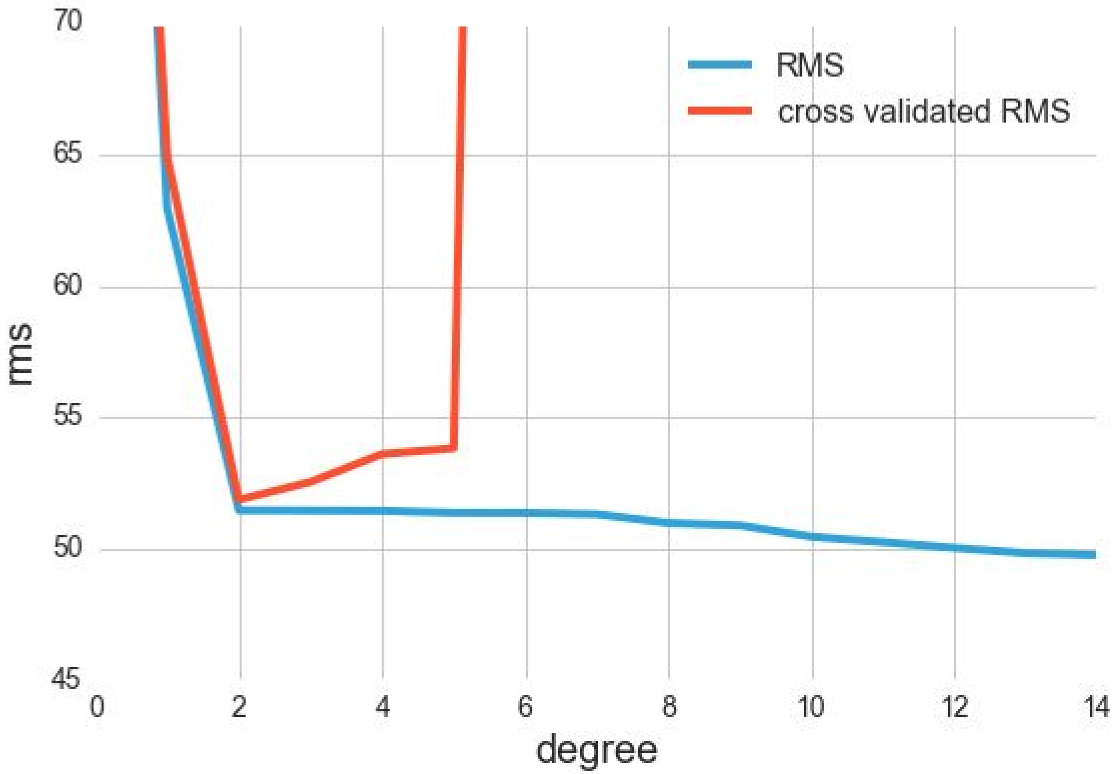
RMS estimate = 52.1

Cross-Validation

Repeat for as long as you have patience . . .

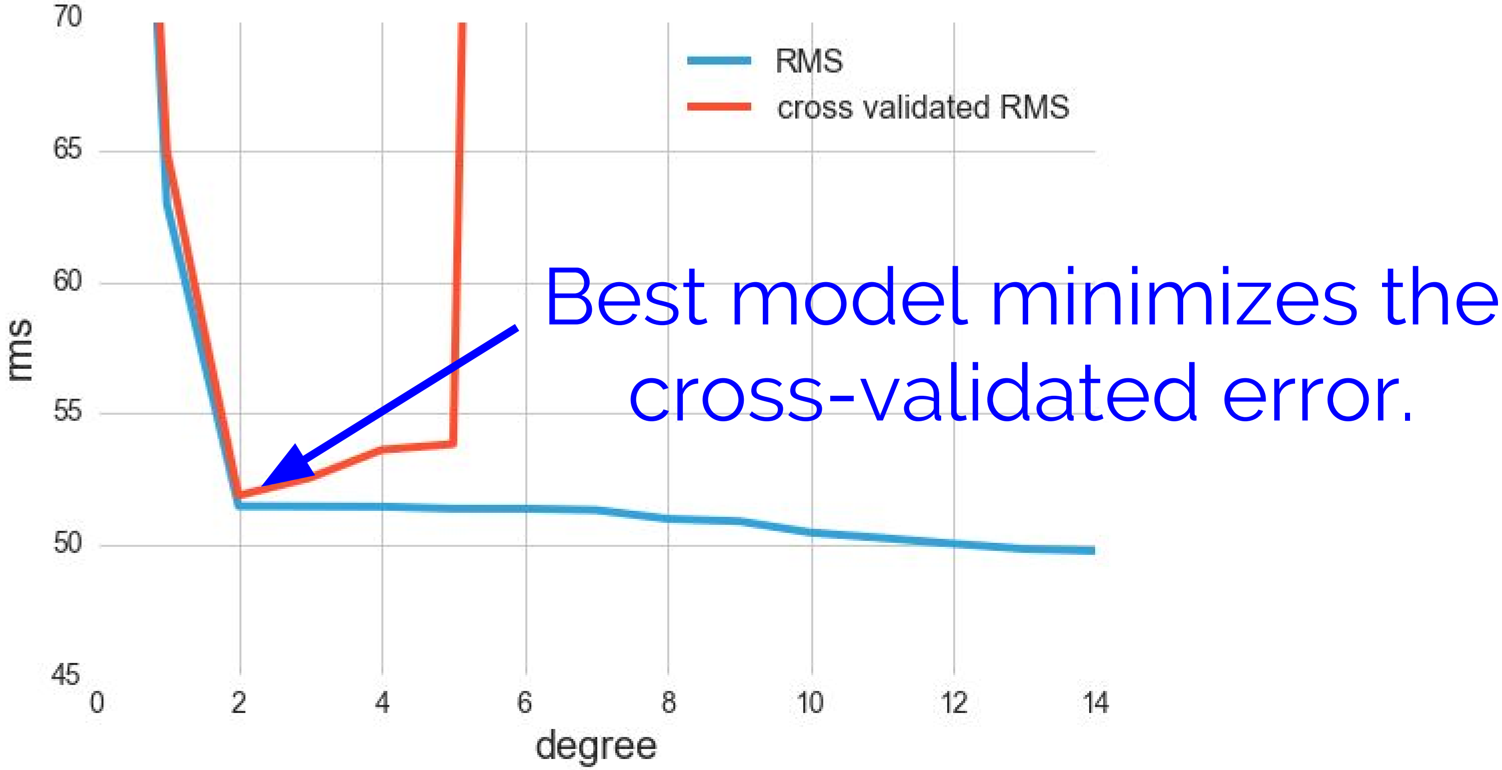
Cross-Validation

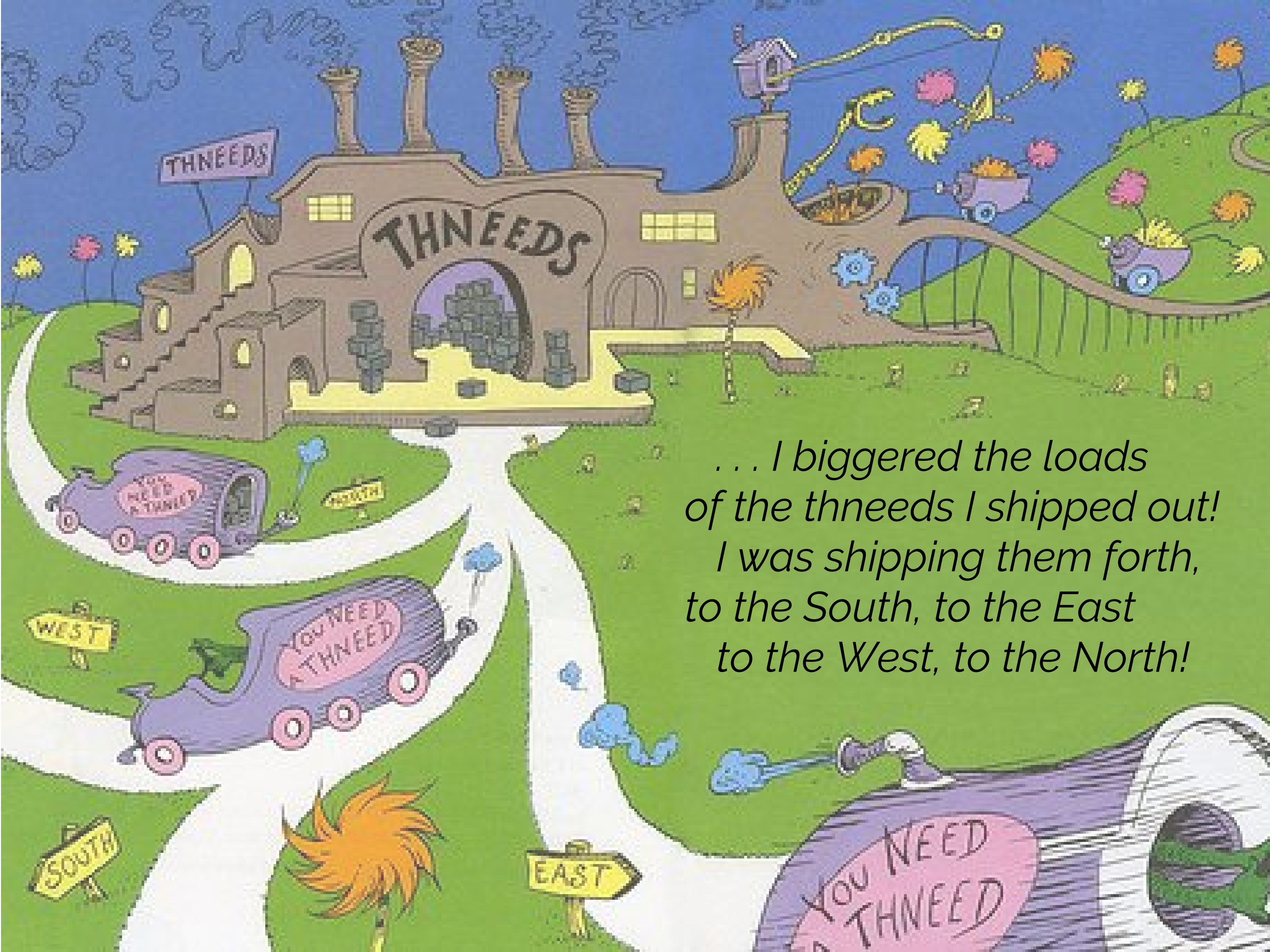
5. Compare cross-validated RMS for models:



Cross-Validation

5. Compare cross-validated RMS for models:





. . . I biggered the loads
of the thneeds I shipped out!
I was shipping them forth,
to the South, to the East
to the West, to the North!

Notes on Cross-Validation:

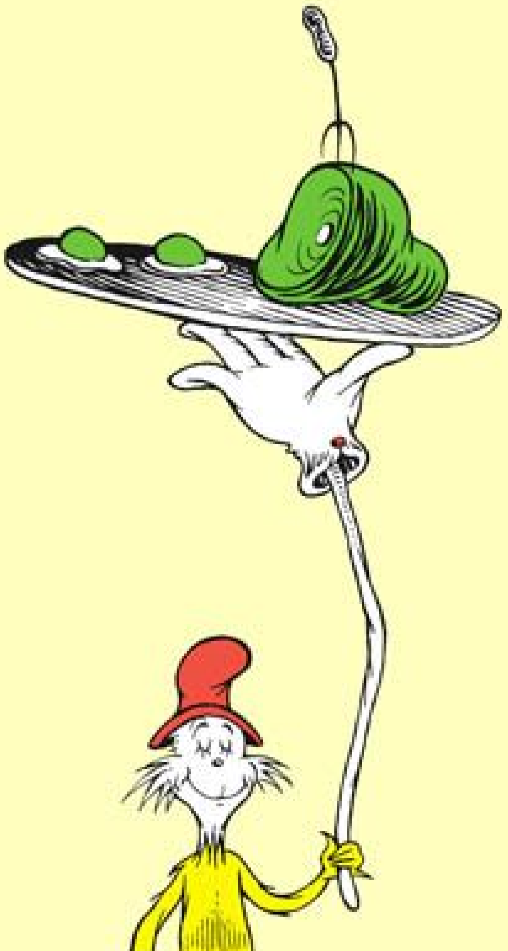
- This was **“2-fold” cross-validation**; other CV schemes exist & may perform better for your data (see e.g. scikit-learn docs)

- Cross-validation is the go-to method for model evaluation in **machine learning**, as statistics of the models are often not known in the classical sense.

- Again: caveats about selection bias and independence in data.

Four Recipes for Hacking Statistics:

1. Direct Simulation ✓
2. Shuffling ✓
3. Bootstrapping ✓
4. Cross Validation ✓



Sampling Methods
allow you to use intuitive **computational**
approaches in place of often
non-intuitive statistical rules.

If you can write a for-loop
you can do statistical analysis.

Things I didn't have time for:

- **Bayesian Methods:** very intuitive & powerful approaches to more sophisticated modeling.
(see e.g. *Bayesian Methods for Hackers* by Cam Davidson-Pilon)

- **Selection Bias:** if you get data selection wrong, you'll have a bad time.
(See Chris Fonnesbeck's Scipy 2015 talk, *Statistical Thinking for Data Science*)

- **Detailed considerations** on use of sampling, shuffling, and bootstrapping.
(I recommend *Statistics Is Easy* by Shasha & Wilson
And *Resampling: The New Statistics* by Julian Simon)

Sometimes the questions are complicated and the answers are simple.

– Dr. Seuss (attr)

~ Thank You! ~

Email: jakevdp@uw.edu

Twitter: @jakevdp

Github: jakevdp

Web: http://vanderplas.com/

Blog: http://jakevdp.github.io/

Slides available at
http://speakerdeck.com/jakevdp/statistics-for-hackers/