Statistics for Hackers

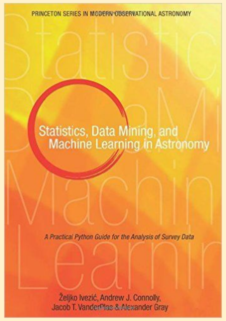
Jake VanderPlas @jakevdp

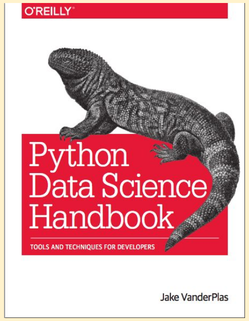
Sept 17, 2015

About Me

Jake VanderPlas *(Twitter/Github: jakevdp)*

- Astronomer by training
- Data Scientist at UW eScience Institute
- Active in Python science & open source
- Blog at *Pythonic Perambulations*
- Author of two books:





Statistics is **Hard**.

Statistics is Hard.

Using programming skills,
it can be easy.

Sometimes the questions are complicated and the answers are simple.

– Dr. Seuss (attr)

My thesis today:

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

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*.

Assuming a fair coin, compute probability of seeing 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)

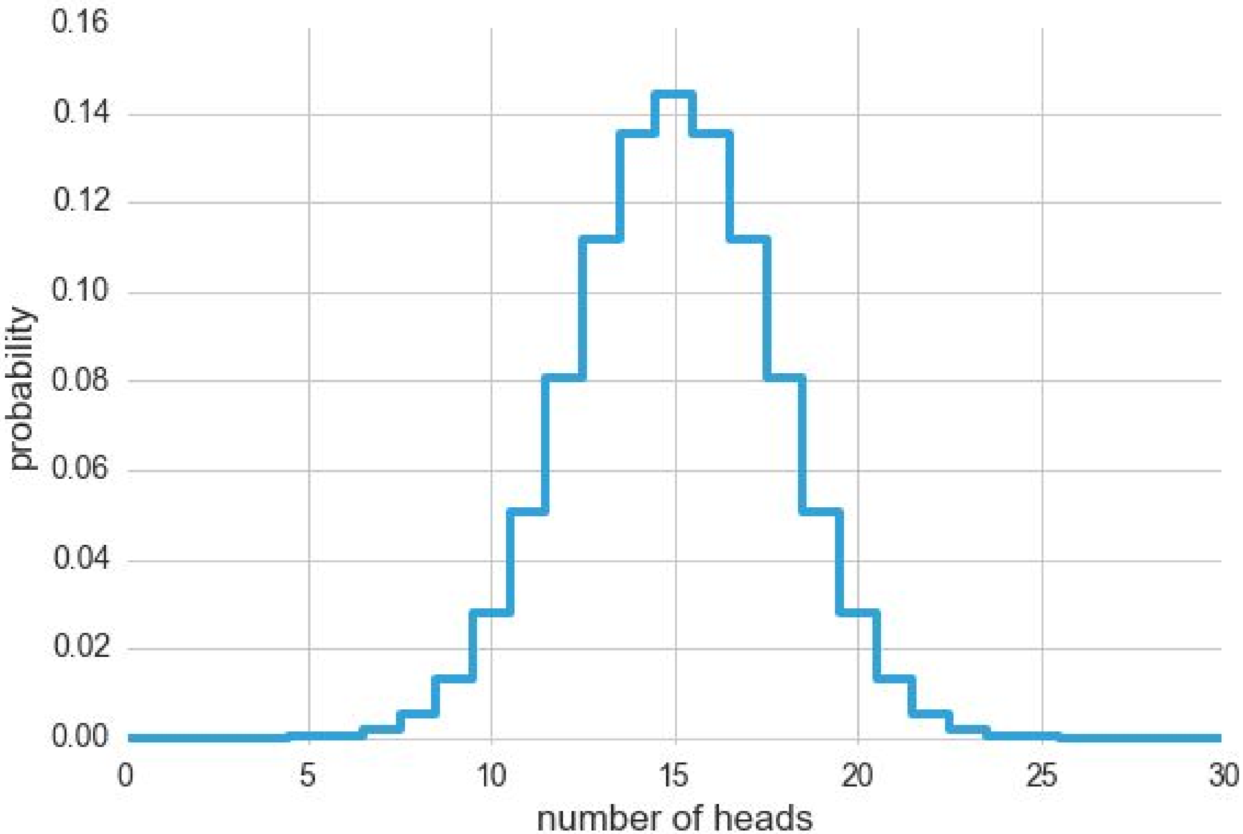
Probability of N_H heads

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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Classic Method:

$N_H = 22, \; N_T = 8$

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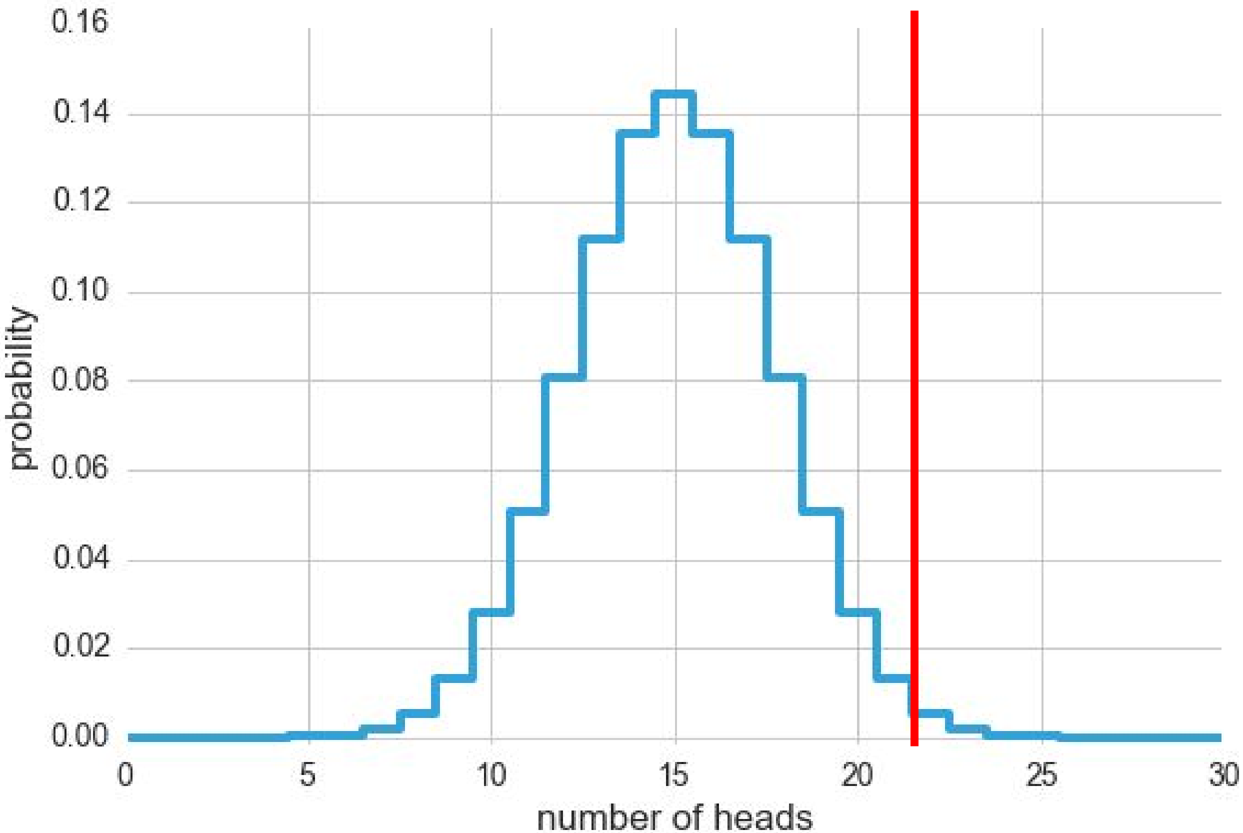

Classic Method:

$N_H = 22,\ N_T = 8$

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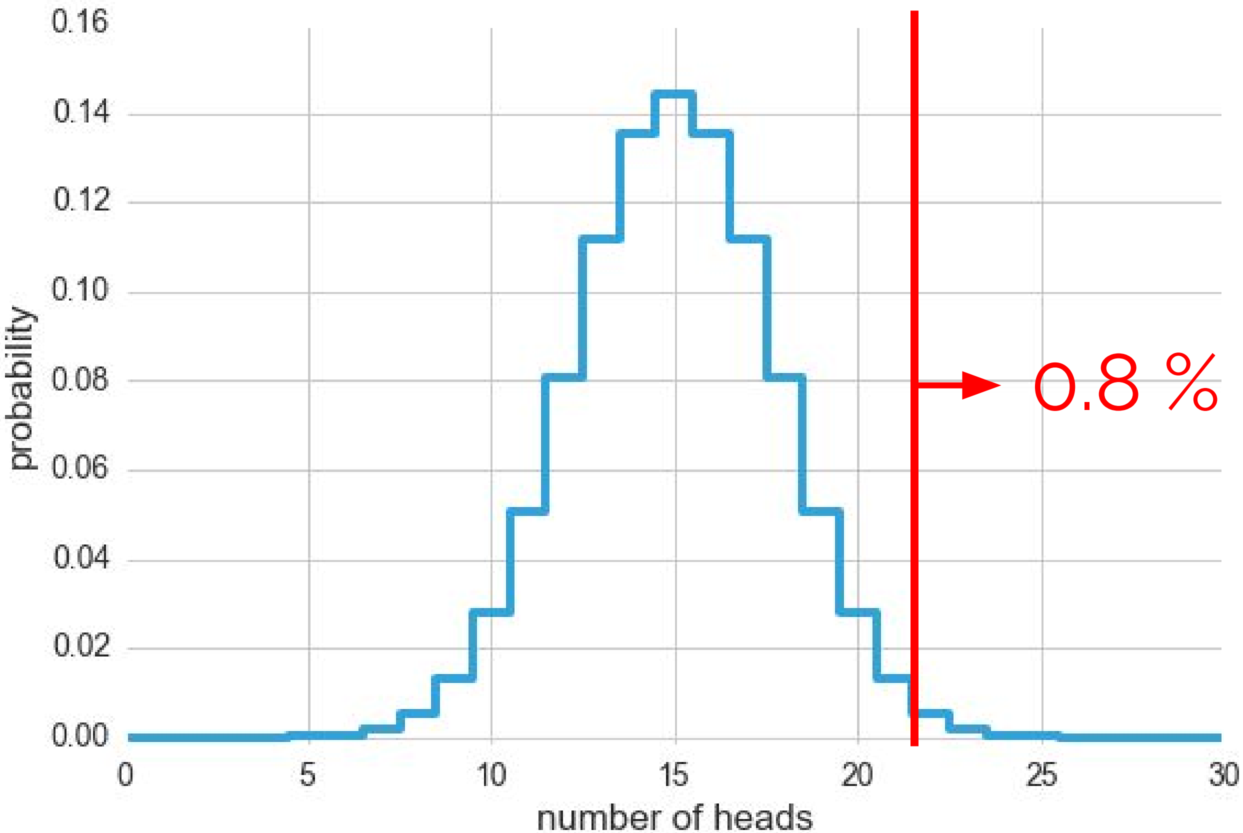
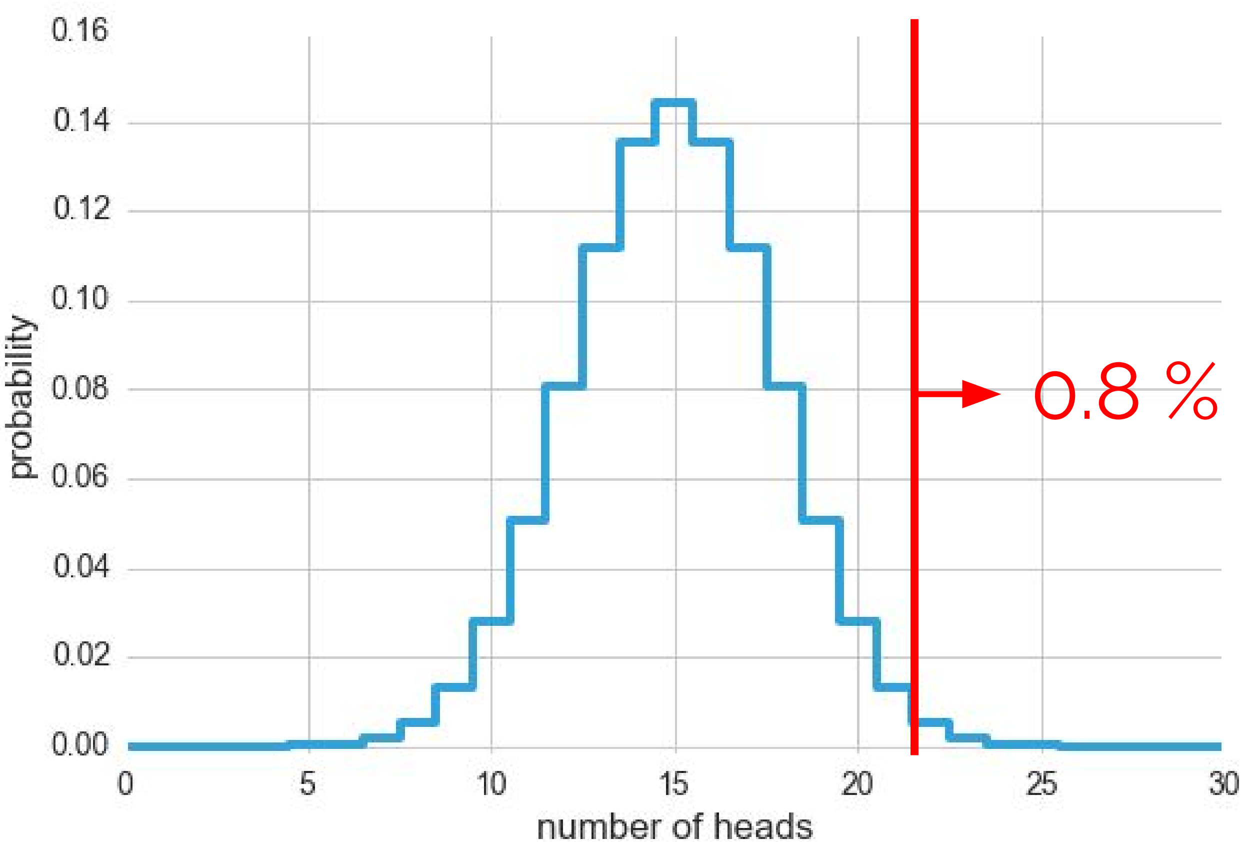


Classic Method:

$N_H = 22,\ N_T = 8$

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!

```python
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.

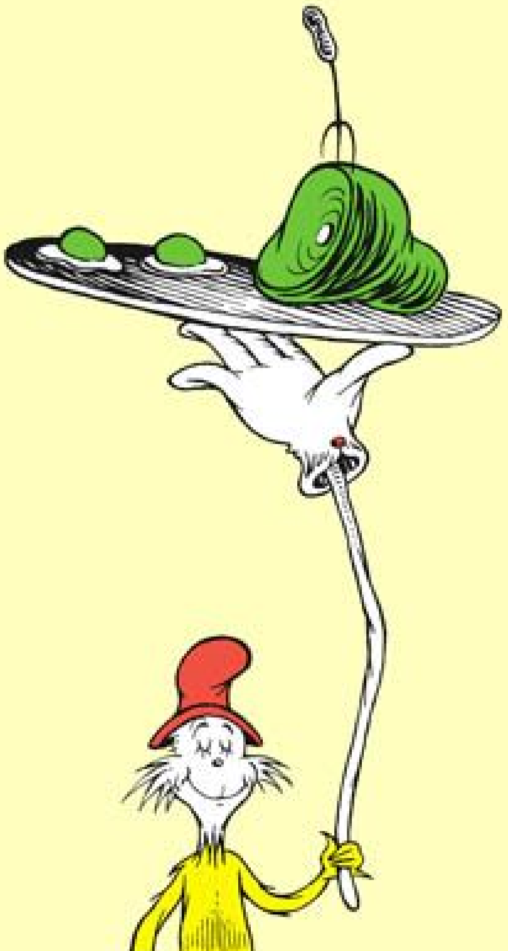
In general . . .

Computing the Sampling Distribution is Hard.

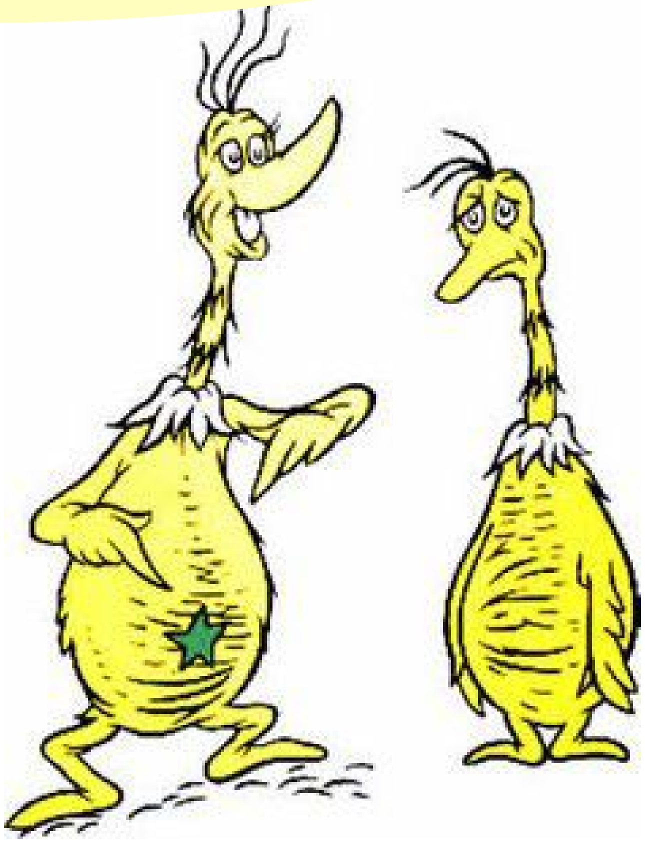
Simulating the Sampling Distribution is Easy.

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 . . .

*adapted from John Rauser's
Statistics Without All The Agonizing Pain

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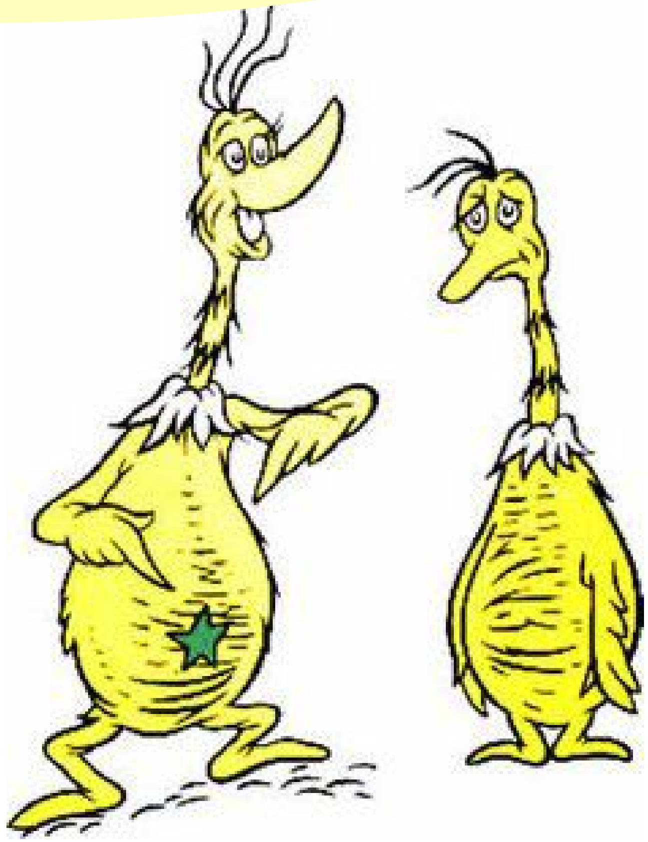
Sneeches:
Stars and Intelligence



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

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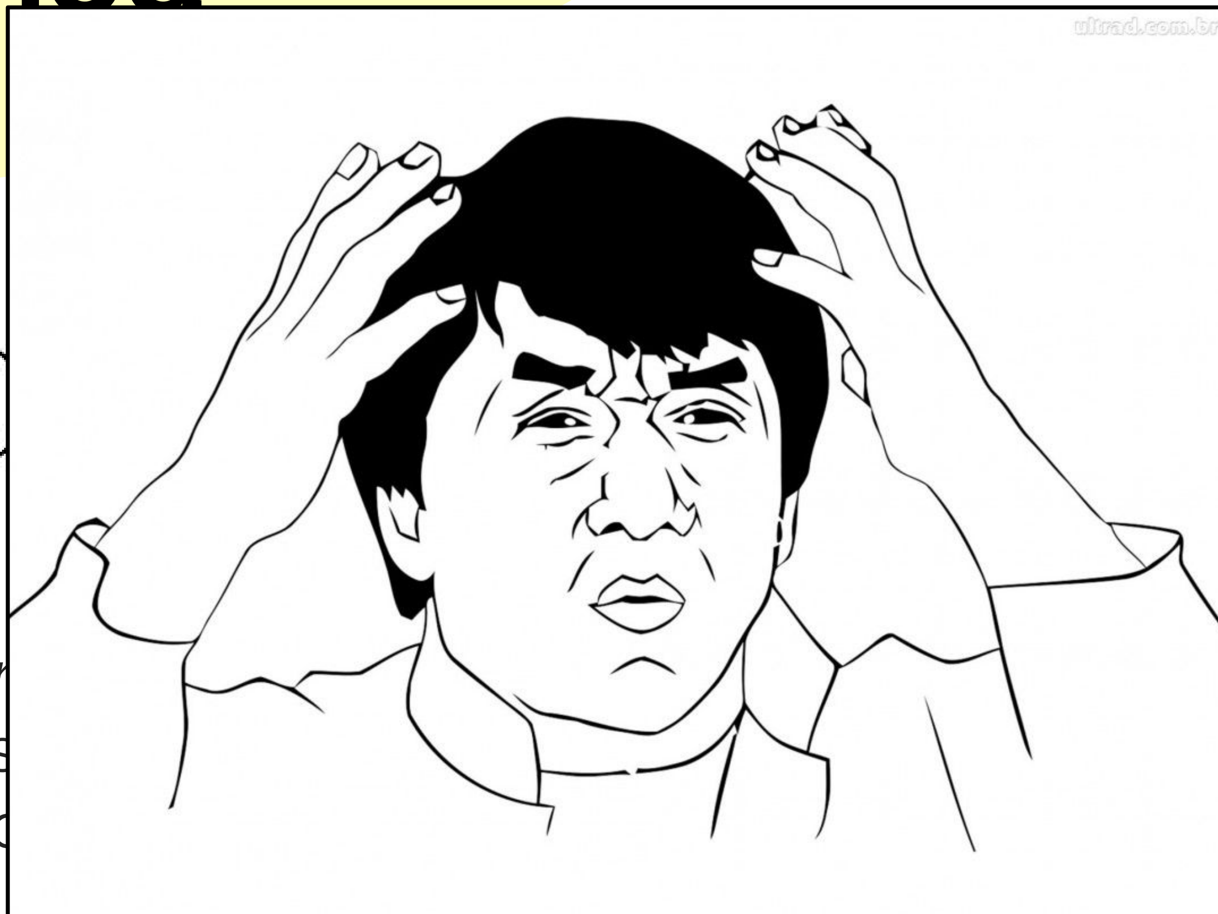
$$p(t;\nu) \quad \Big) ^{-\frac{\nu+1}{2}}$$



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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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1.7959

Classic Method

$$t > t_{crit}$$

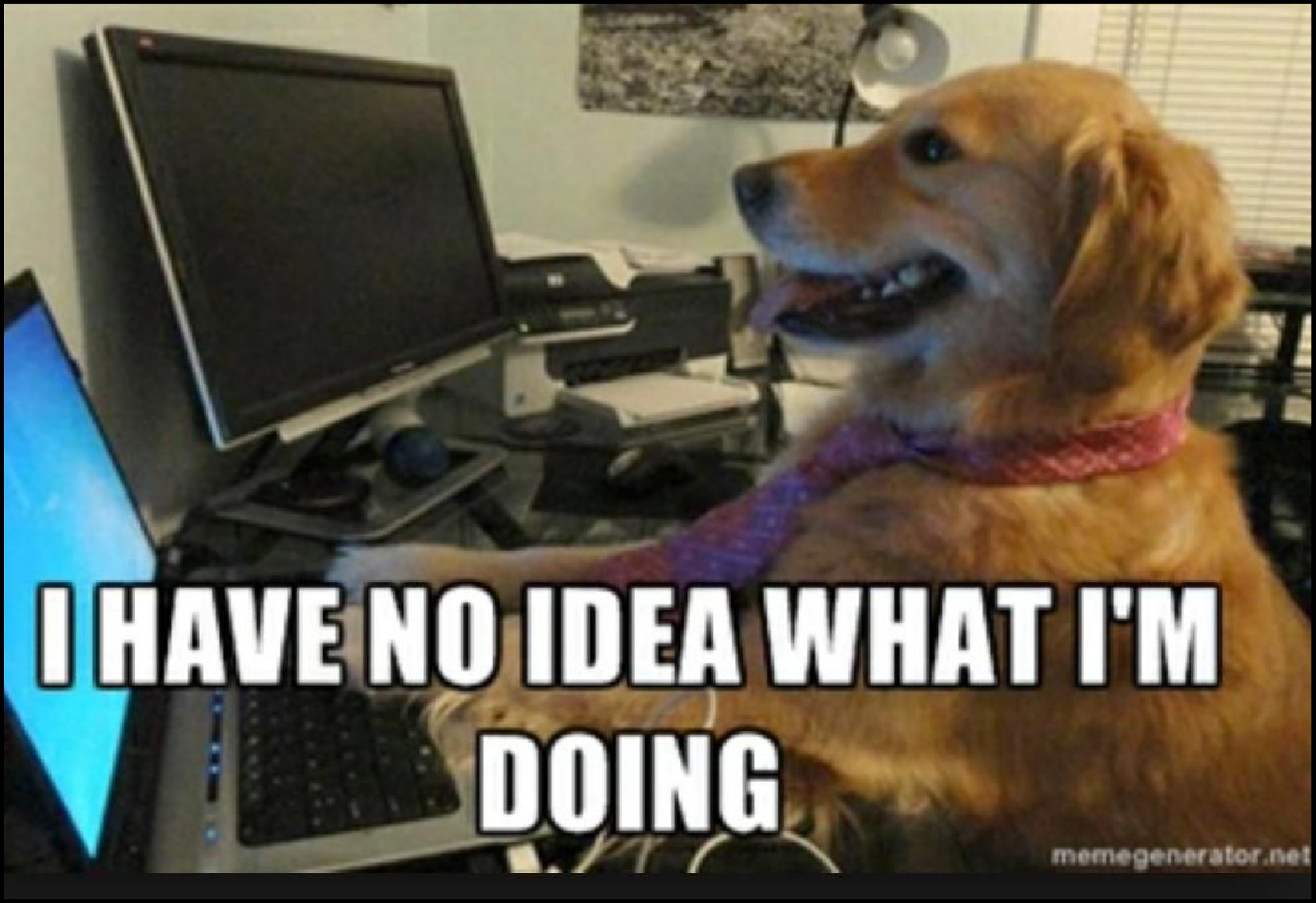
Classic Method

$$0.932 > 1.796$$

Classic Method

$$\cancel{0.932 > 1.796}$$

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

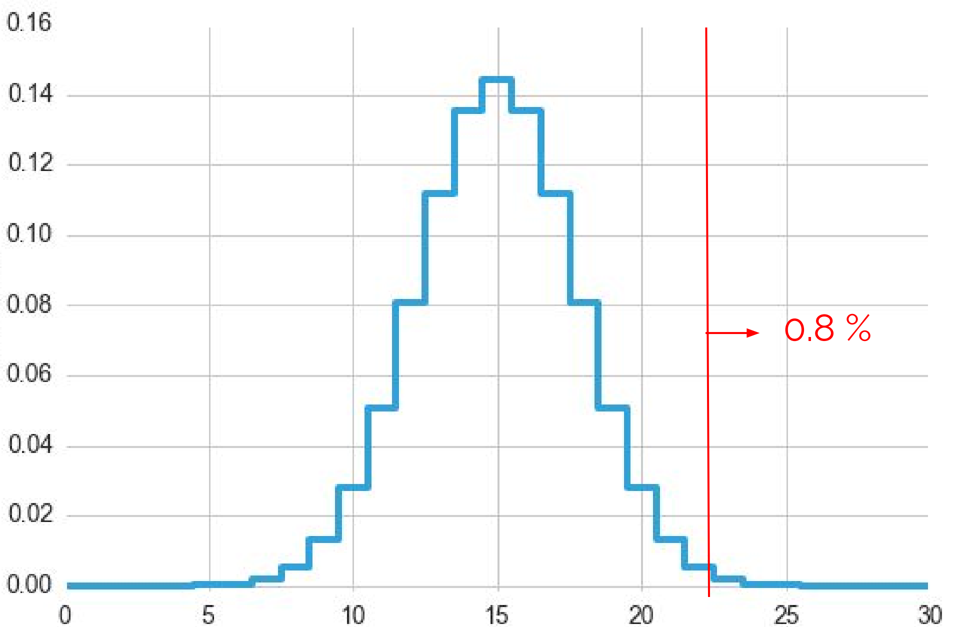

I HAVE NO IDEA WHAT I'M DOING
memegenerator.net

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

Problem:
Unlike coin flipping, we *don't* have a probabilistic model . . .

Problem:
Unlike coin flipping, we *don't* have a probabilistic 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
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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

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1. Shuffle Labels
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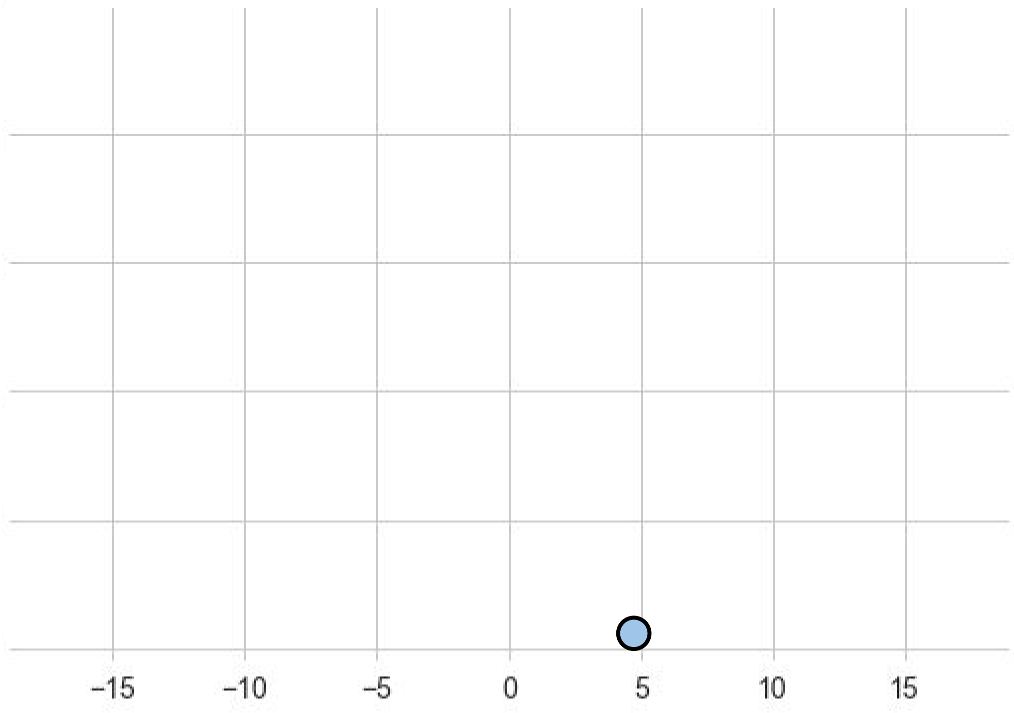

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1. **Shuffle Labels**
2. Rearrange
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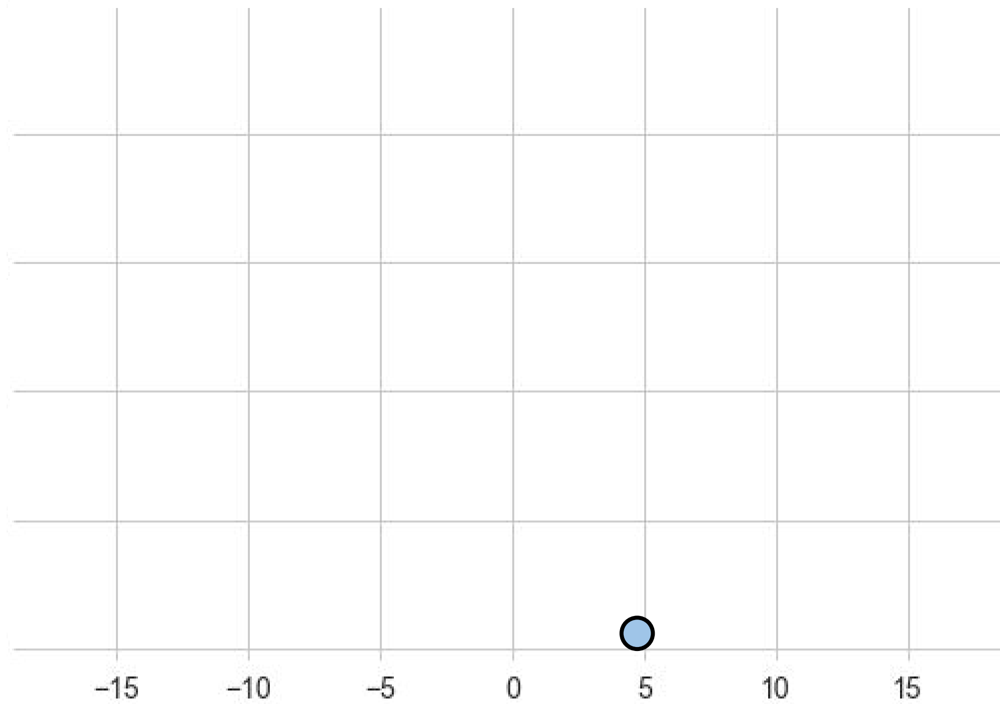

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84	56	72	69
61	63	74	57
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		76	91
		99	69

1. Shuffle Labels
2. Rearrange
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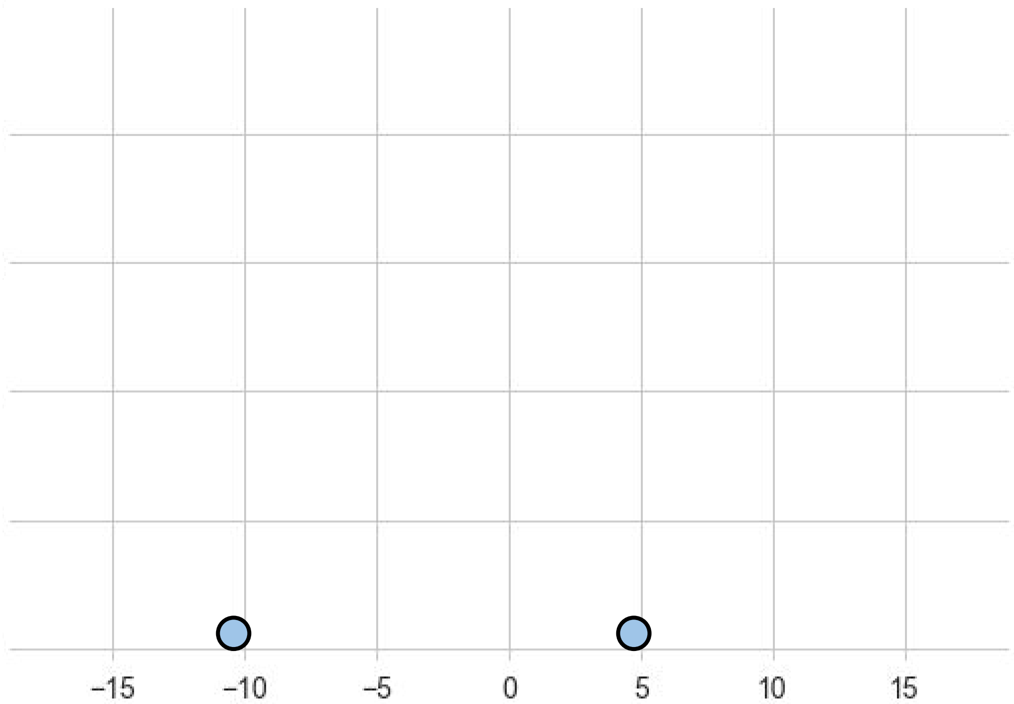

★ mean: 62.6

× mean: 74.1

difference: -11.6

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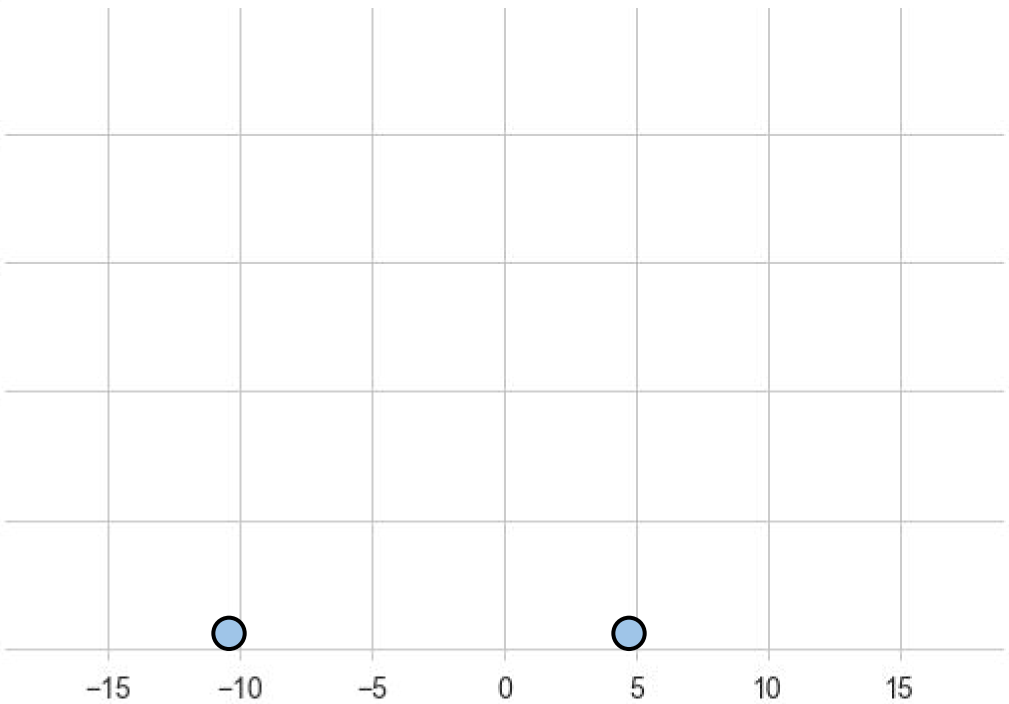
★		×	
84	56	72	69
61	63	74	57
65	66	81	87
62	44	46	69
		76	91
		99	69

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



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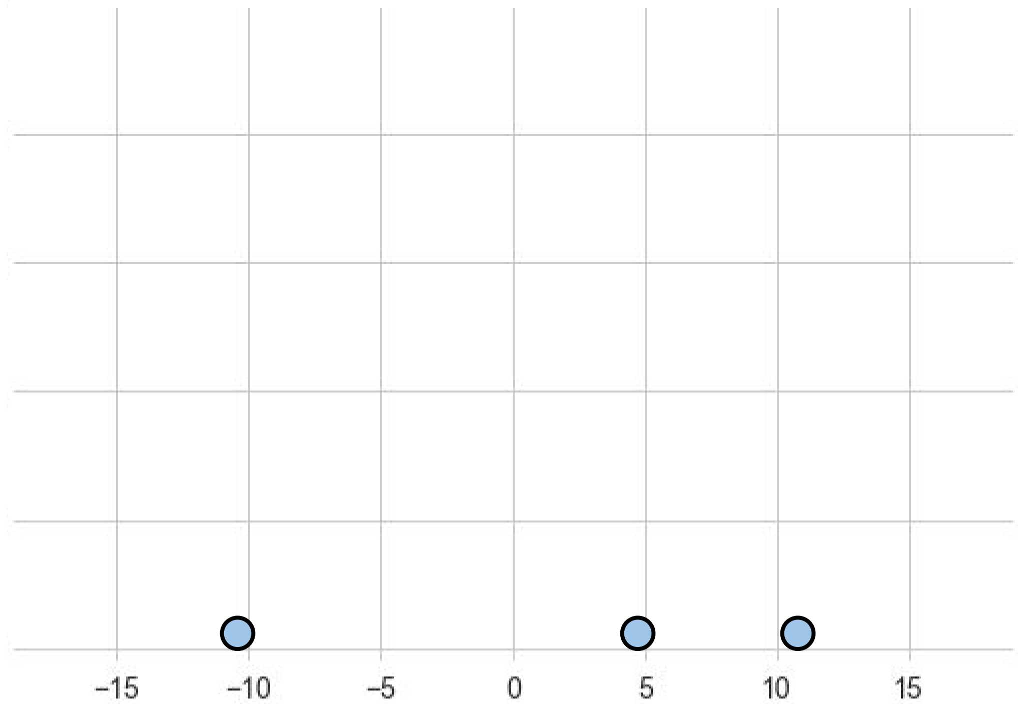
★		×	
74	56	72	69
61	63	84	57
87	76	81	65
91	99	46	69
		66	62
		44	69

★ mean: 75.9

× mean: 65.3

difference: 10.6

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



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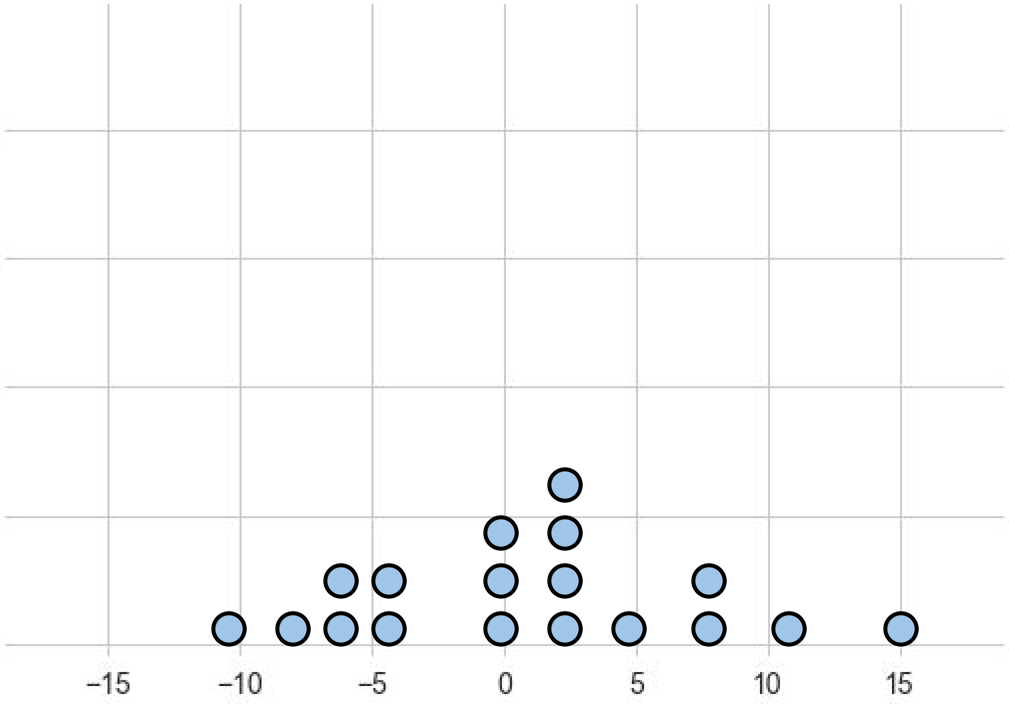

★		×	
84	81	69	69
61	69	87	74
65	76	56	57
99	44	46	63
		66	91
		62	72

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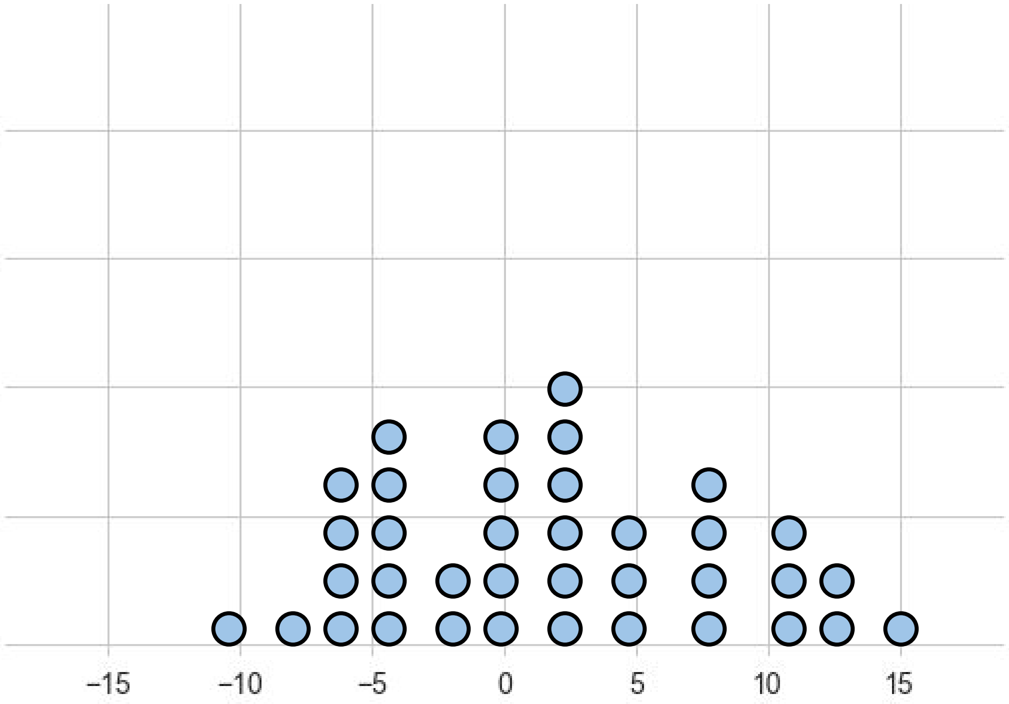
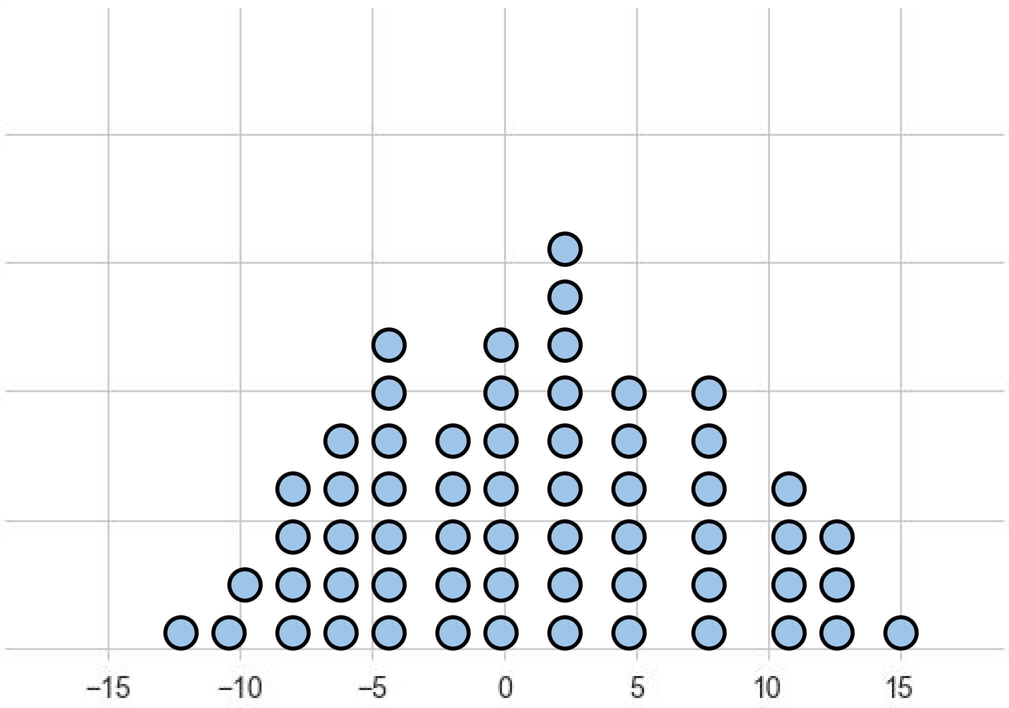


★		×	
74	62	72	57
61	63	84	69
87	81	76	65
91	99	46	69
		66	56
		44	69

1. Shuffle Labels
2. Rearrange
3. Compute means



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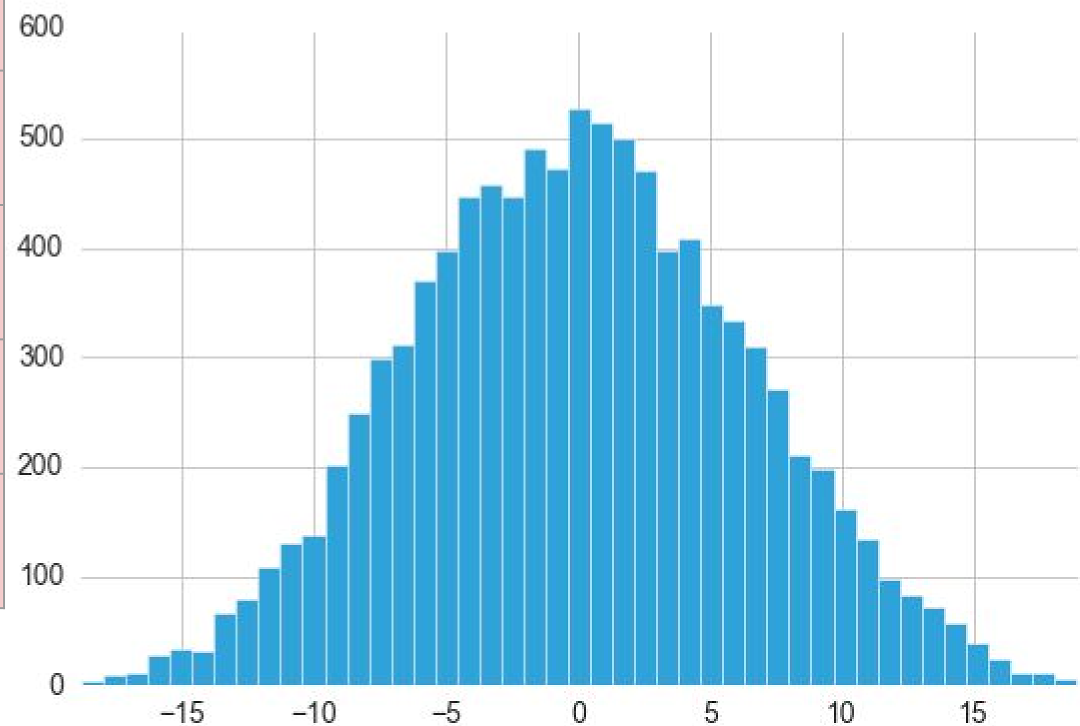
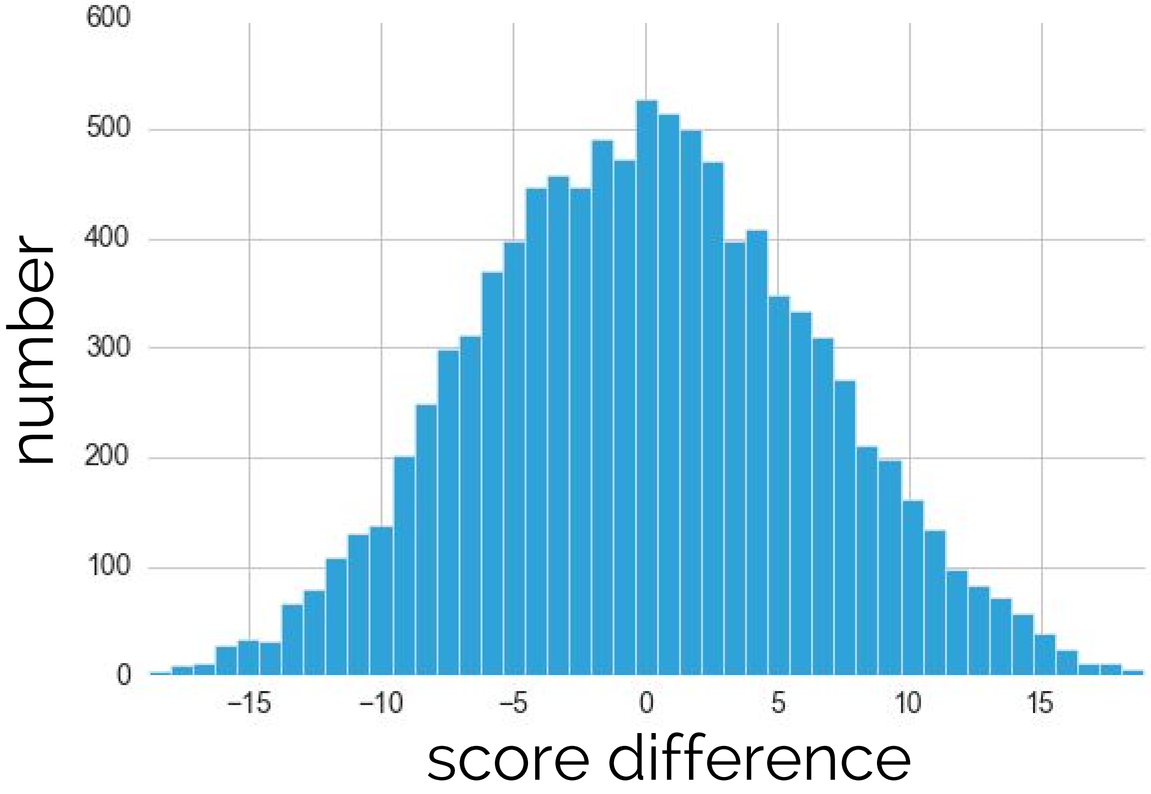
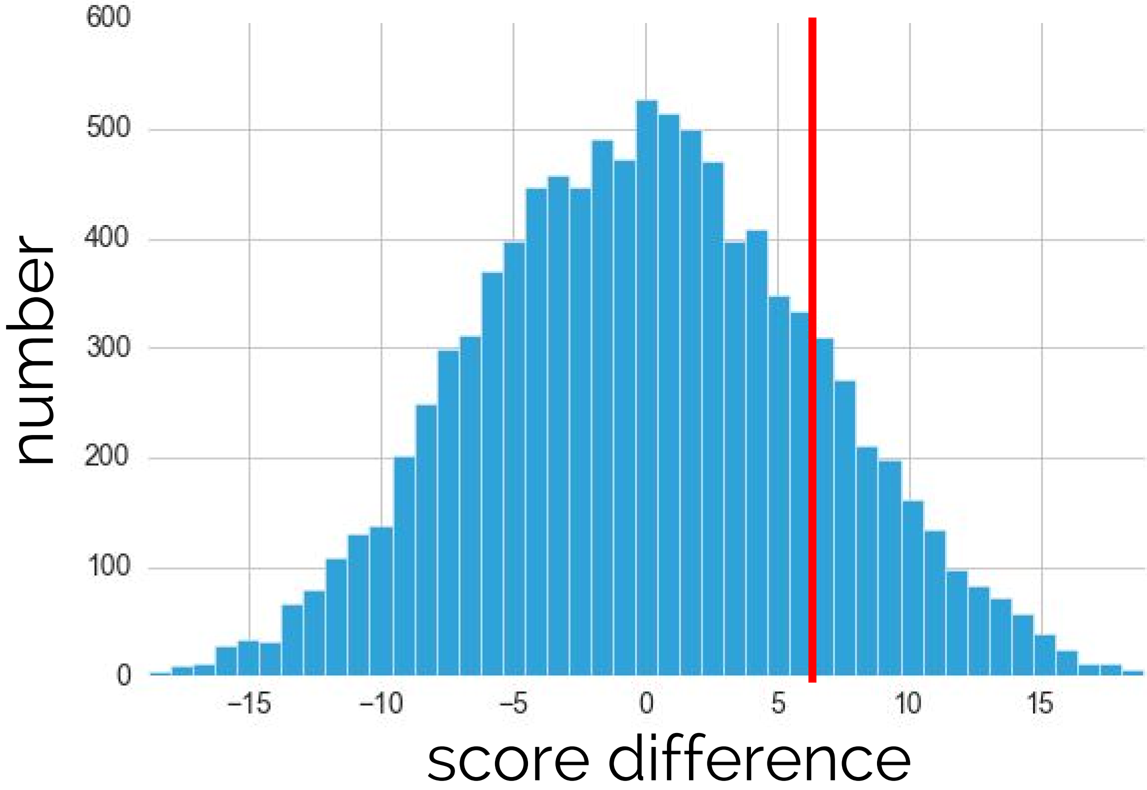
2. Rearrange
3. Compute means




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


600
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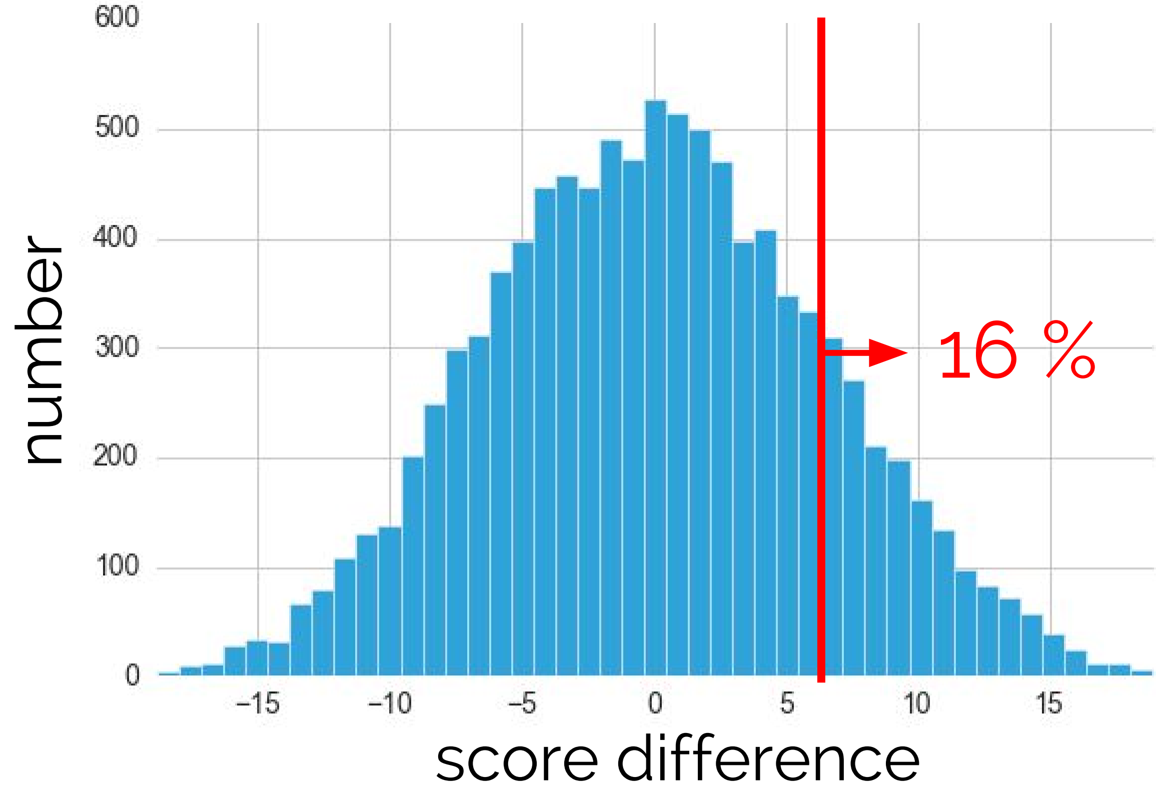

$$\frac{N_{>6.6}}{N_{tot}} = \frac{1608}{10000} = 0.16$$

“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.

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Notes on Shuffling:

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

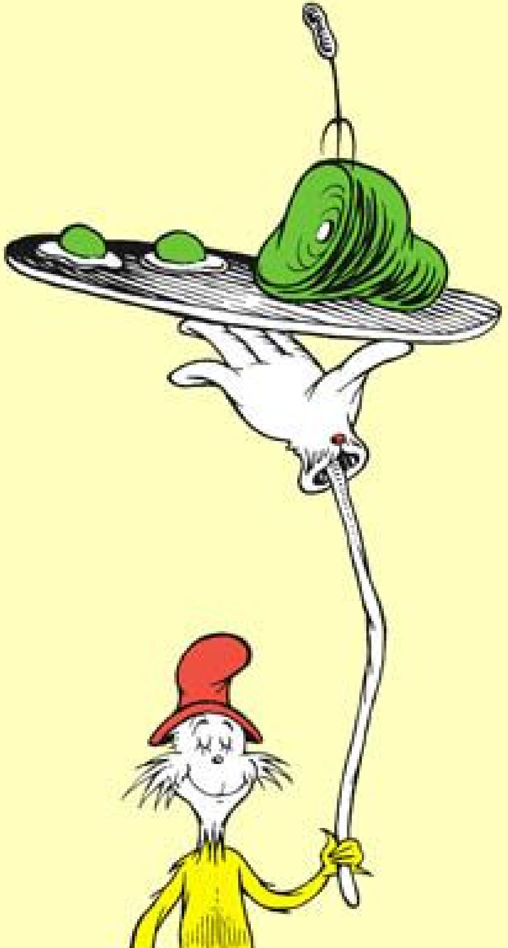
- Like all methods, it will only work if your samples are representative – always be careful about selection biases!

- Needs care for correlated data

- For more discussion & references, see *Statistics is Easy* by Shasha & Wilson

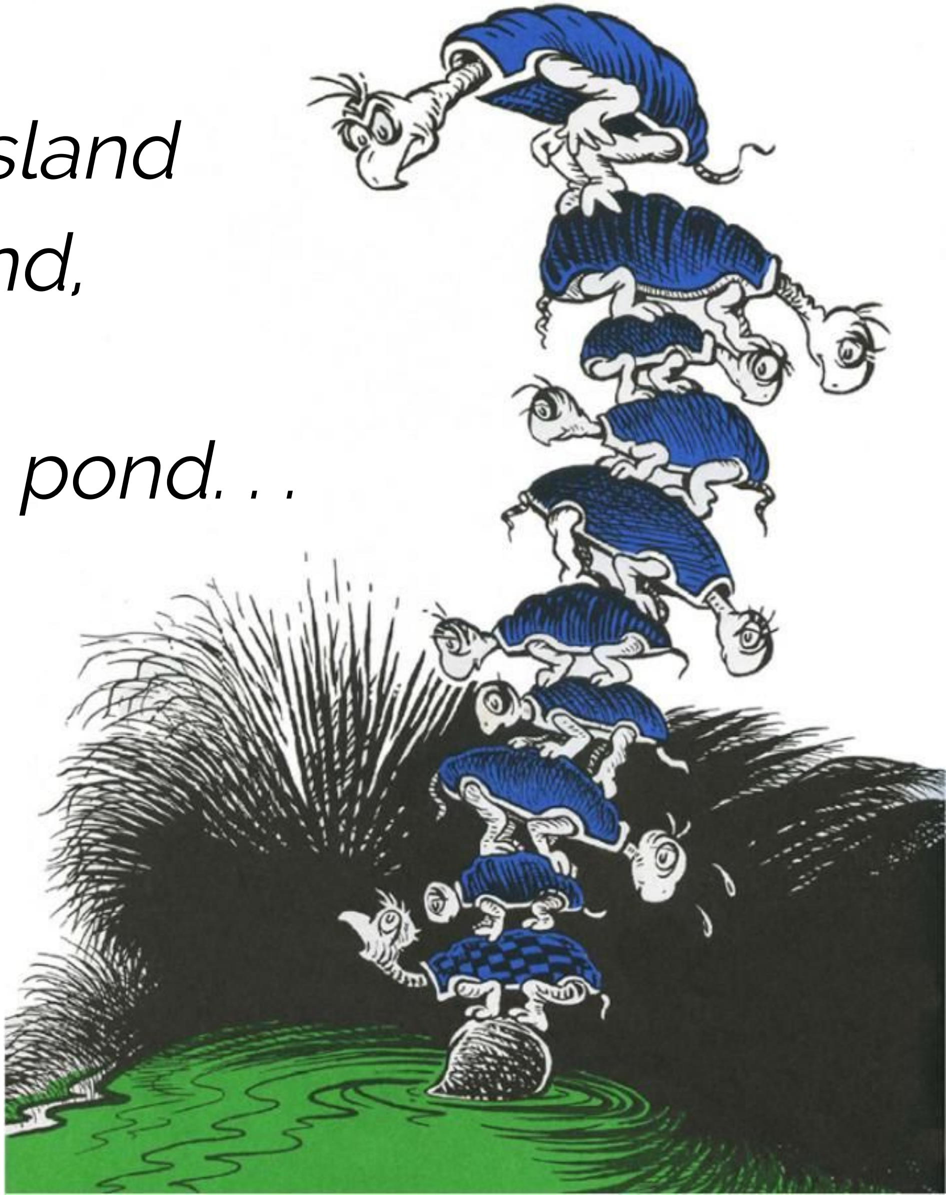
Four Recipes for Hacking Statistics:

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:
We need a way to simulate samples, but we don't have a generating model . . .

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We need a way to simulate samples, but 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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21									

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21	19								

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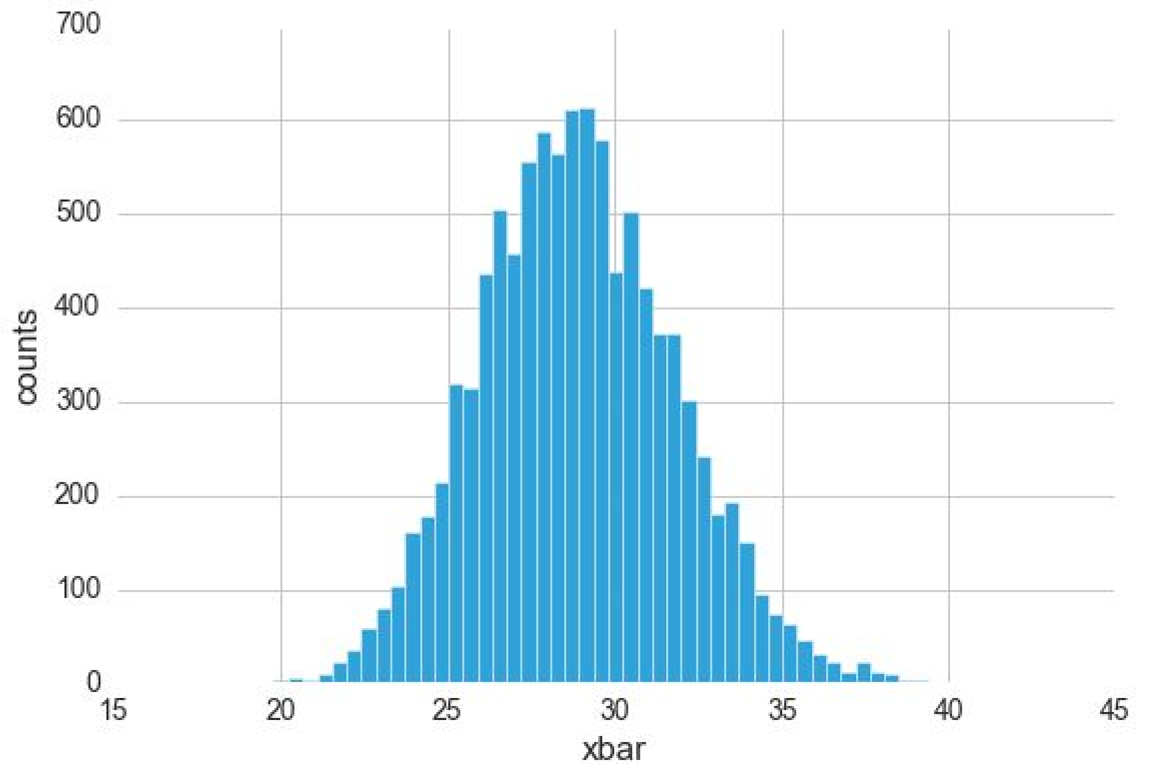
→ 31.05

**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)
```

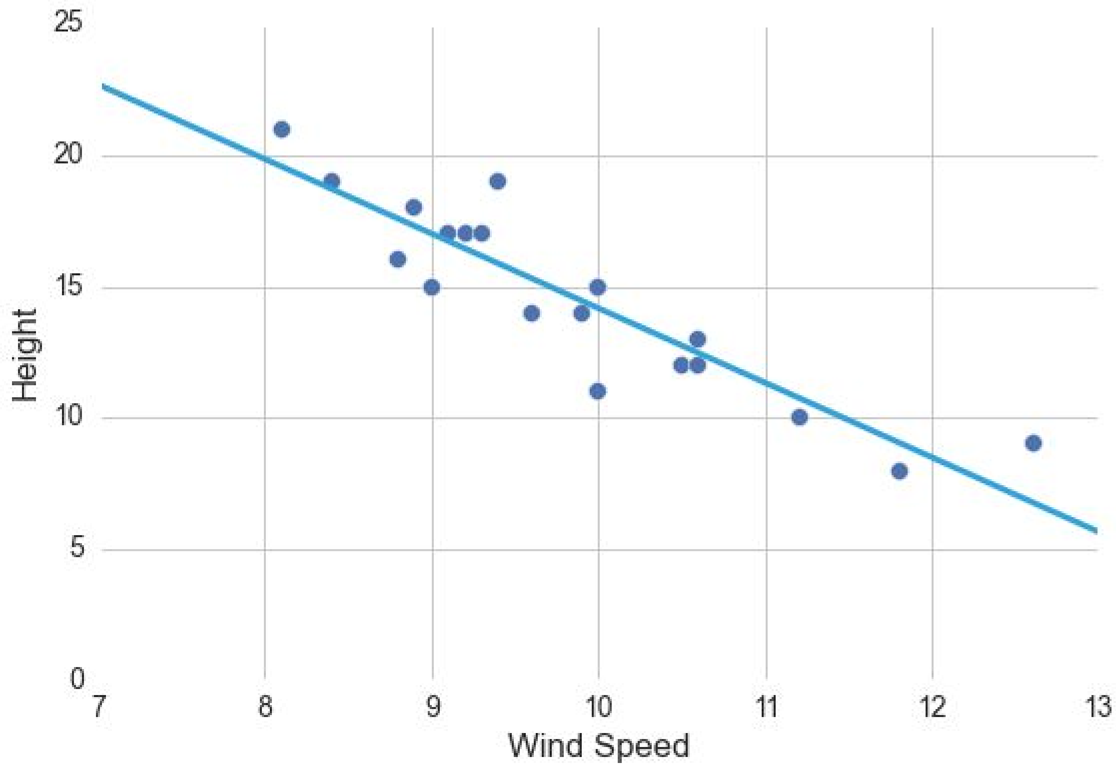
Height = 29 ± 3 turtles



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?



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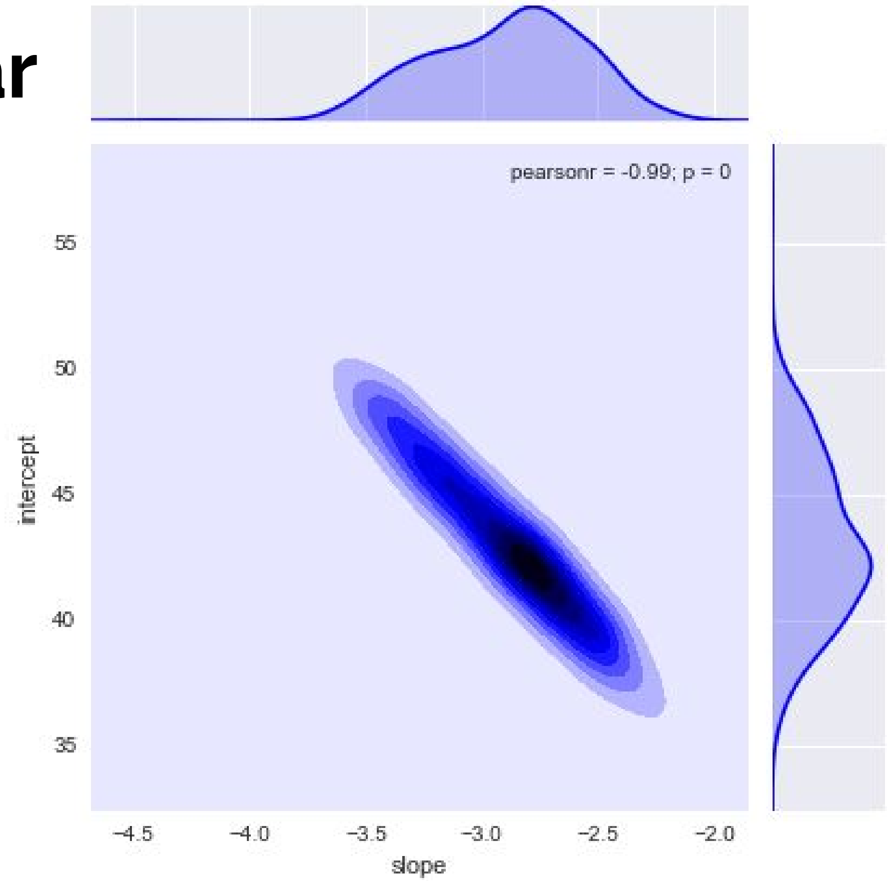



```
for i in range(10000):
    i = randint(20, size=20)
    slope, intercept = fit(x[i], y[i])
    results[i] = (slope, intercept)
```

Notes on Bootstrapping:

- Bootstrap resampling rests on sound theoretical grounds.

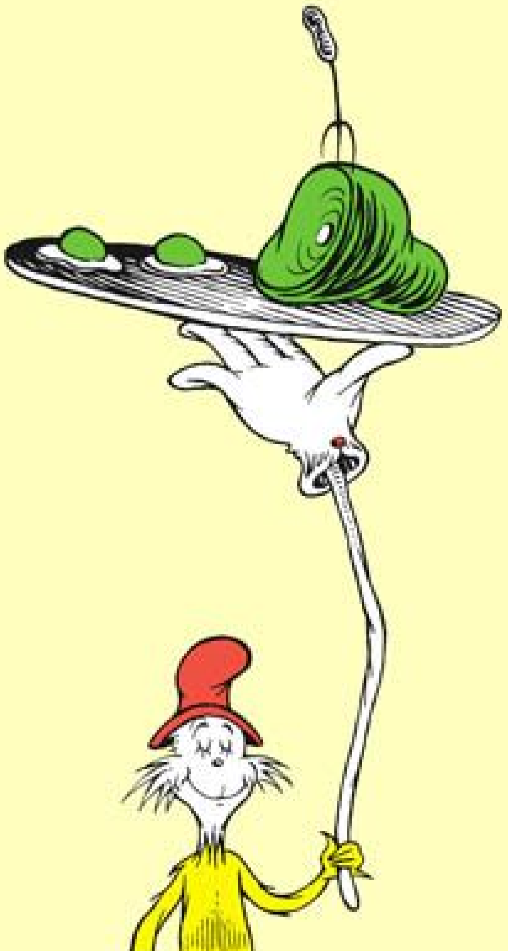
- Bootstrapping doesn't work well for rank-based statistics (e.g. maximum value)

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

- Always be careful about selection biases & correlated data!

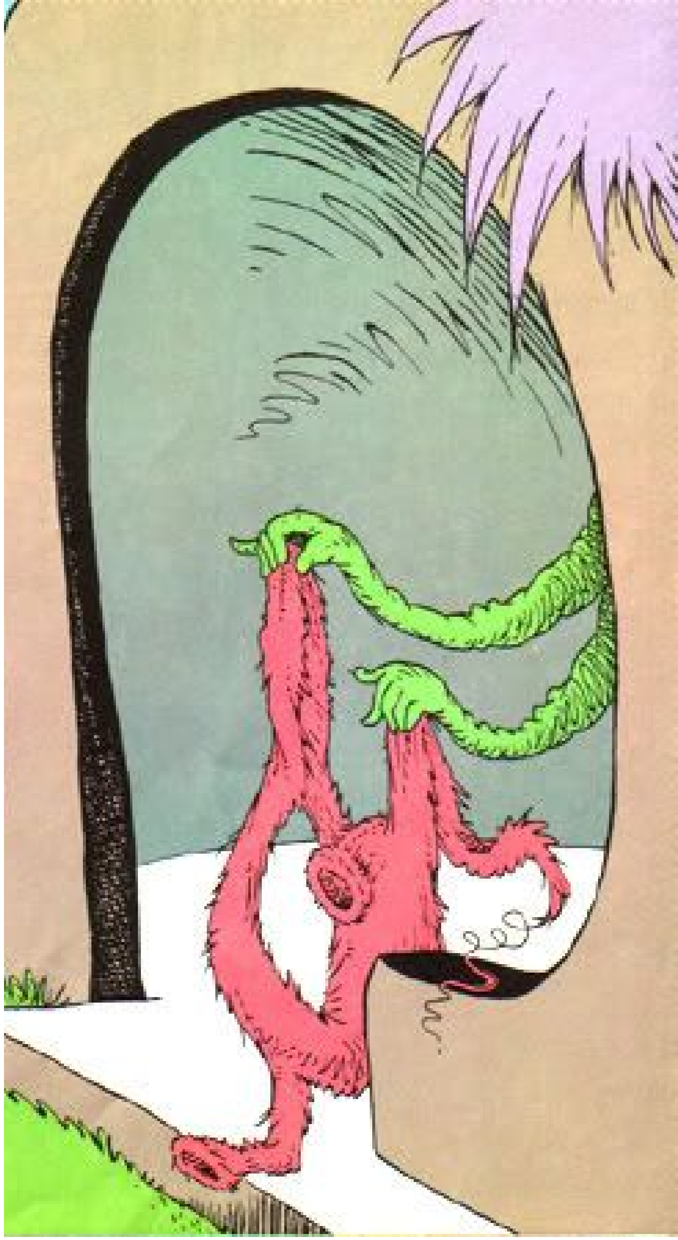
Four Recipes for Hacking Statistics:

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!



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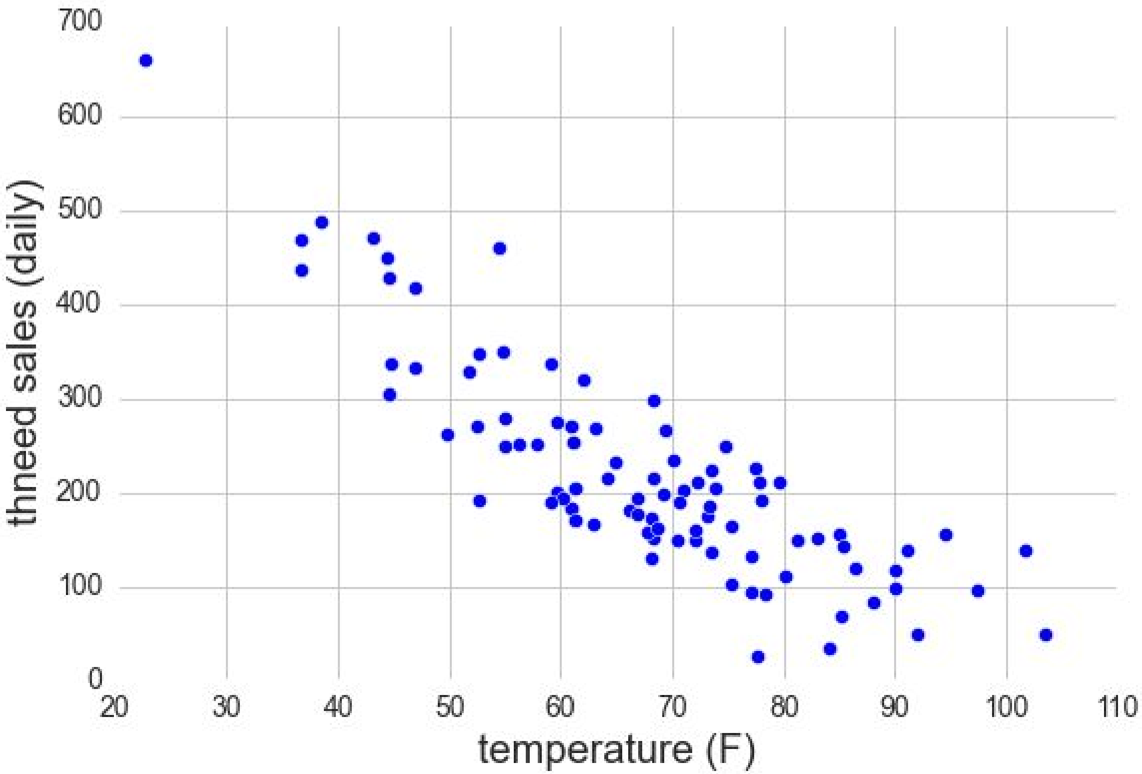
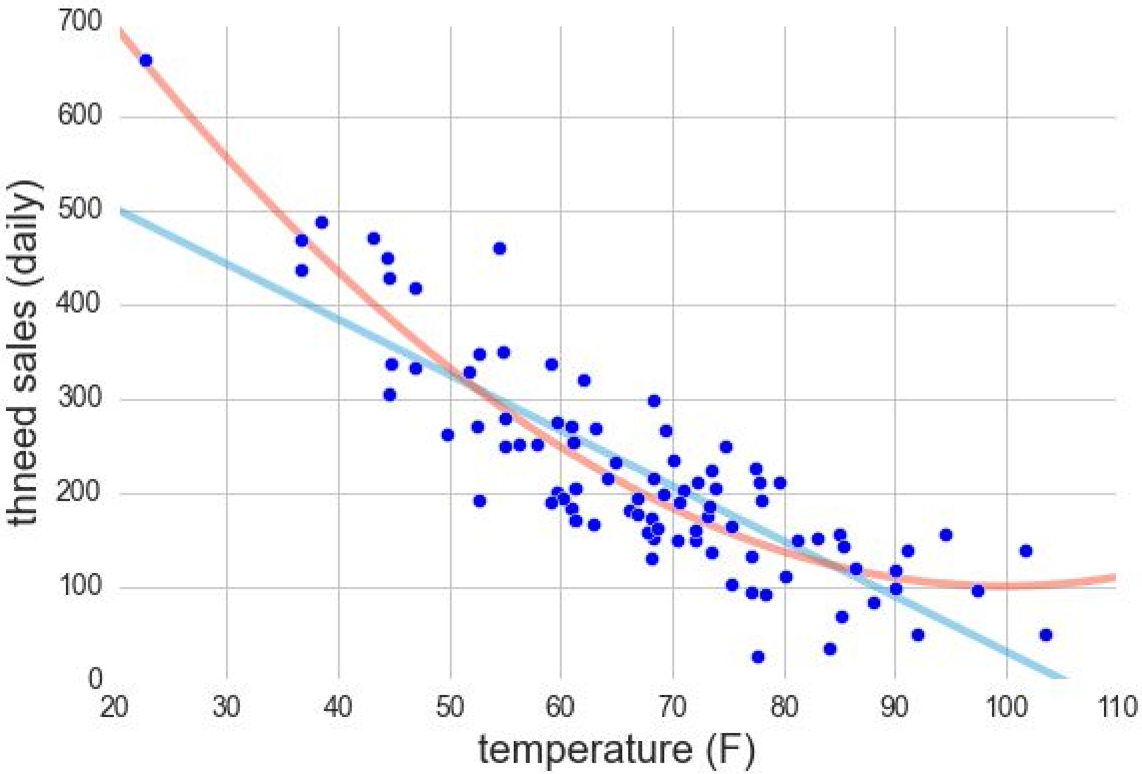
Thneed sales seem to show a trend with temperature . . .



Jake VanderPlas

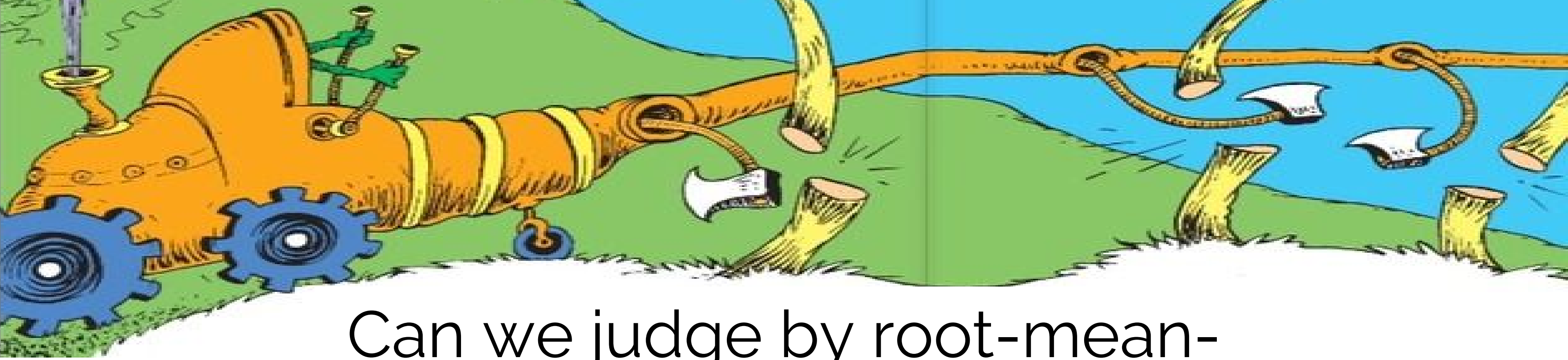
But which model is a better fit?



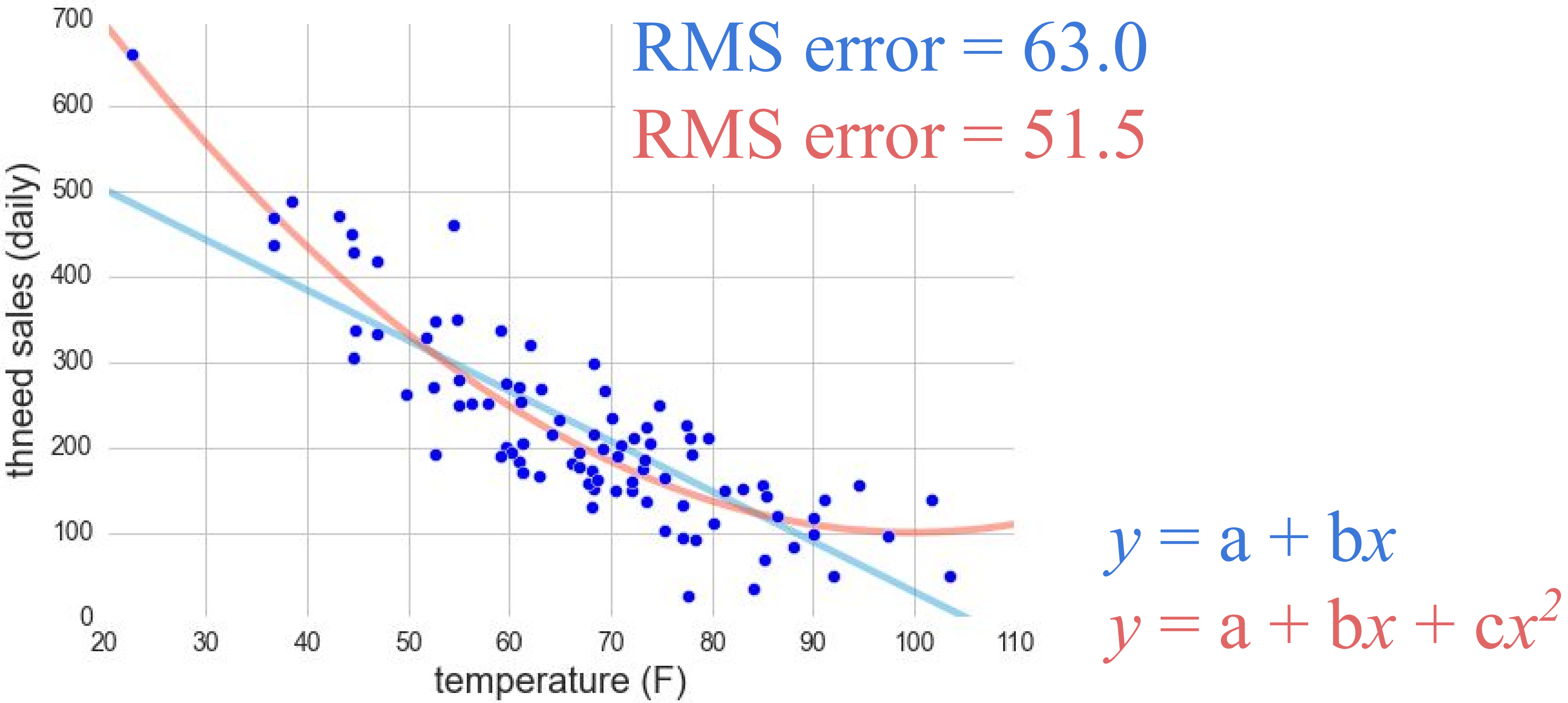
$$y = a + bx$$

$$y = a + bx + cx^2$$

Jake VanderPlas

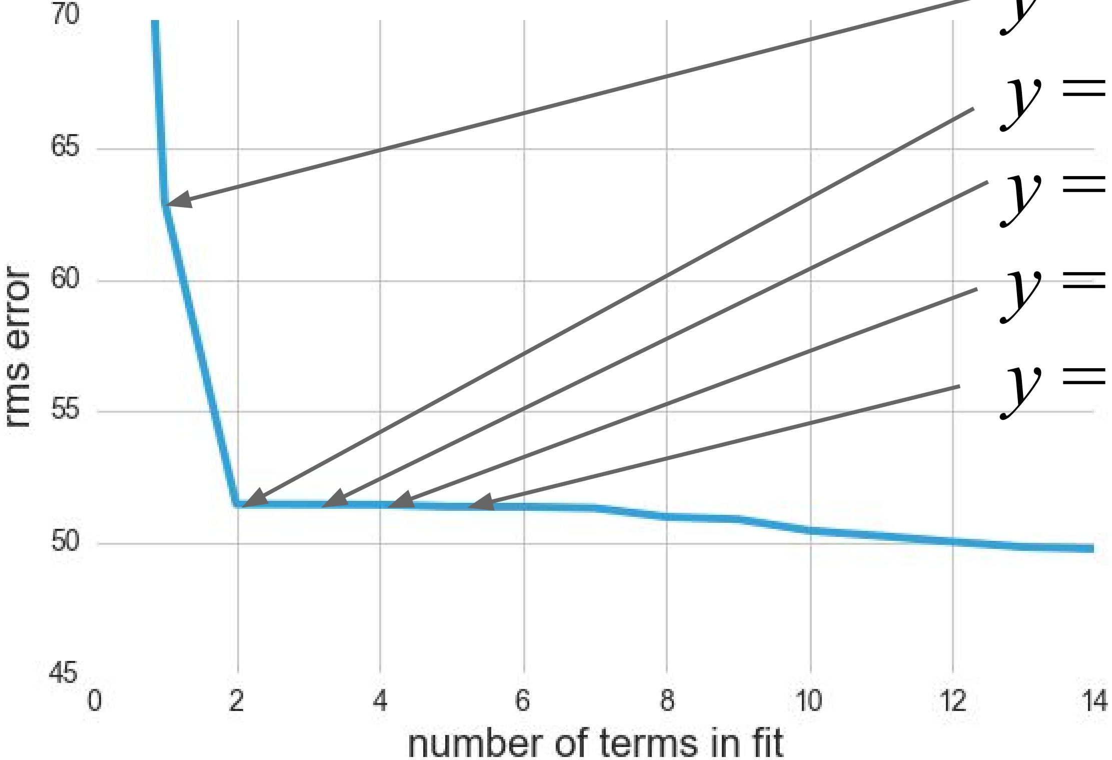


Can we judge by root-mean-square error?



Jake VanderPlas

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



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

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

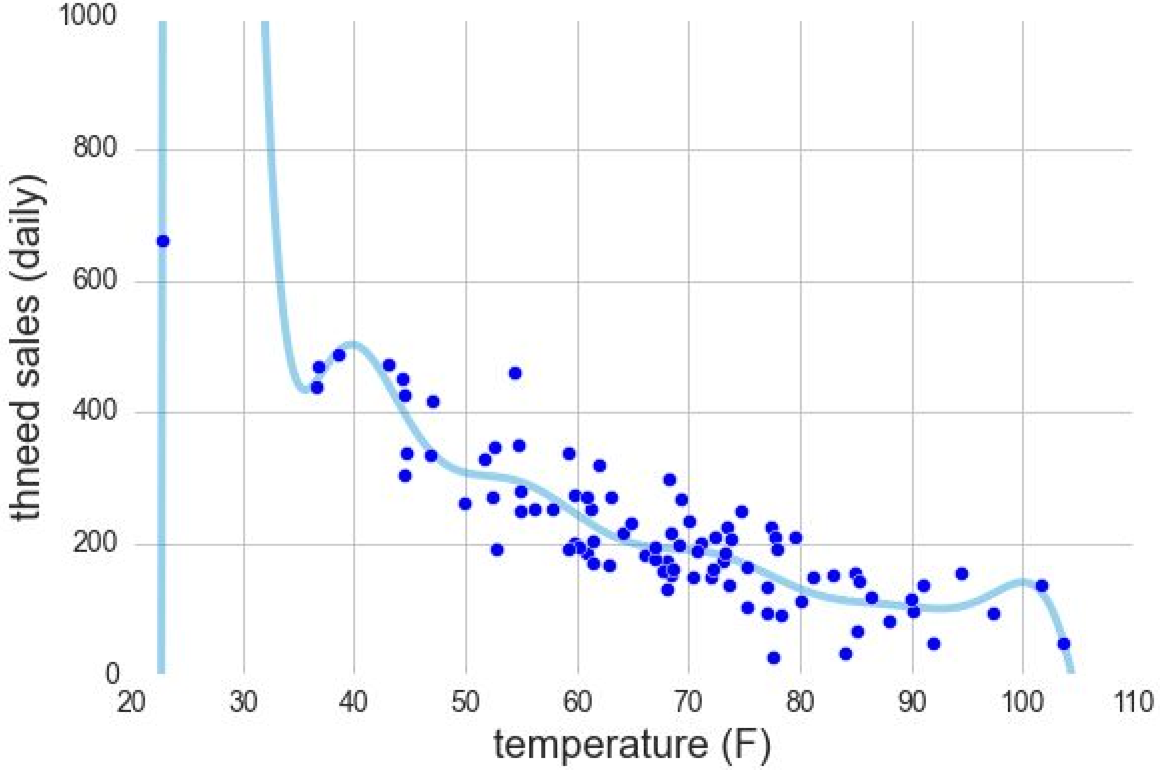
$$y = \mathrm{a} + \mathrm{b}x + \mathrm{c}x^2 + \mathrm{d}x^3$$

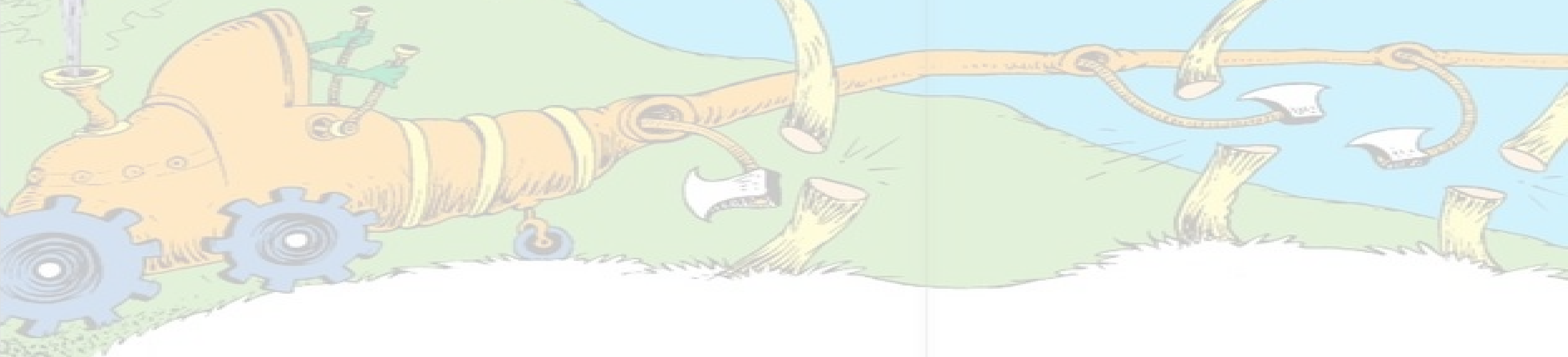
$$y = \mathrm{a} + \mathrm{b}x + \mathrm{c}x^2 + \mathrm{d}x^3 + \mathrm{e}x^4$$

$$y = \mathrm{a} + \cdots$$

RMS error does not tell the whole story.

$$y = a + bx + cx^2 + dx^3 + ex^4 + fx^5 + \cdots + nx^{14}$$





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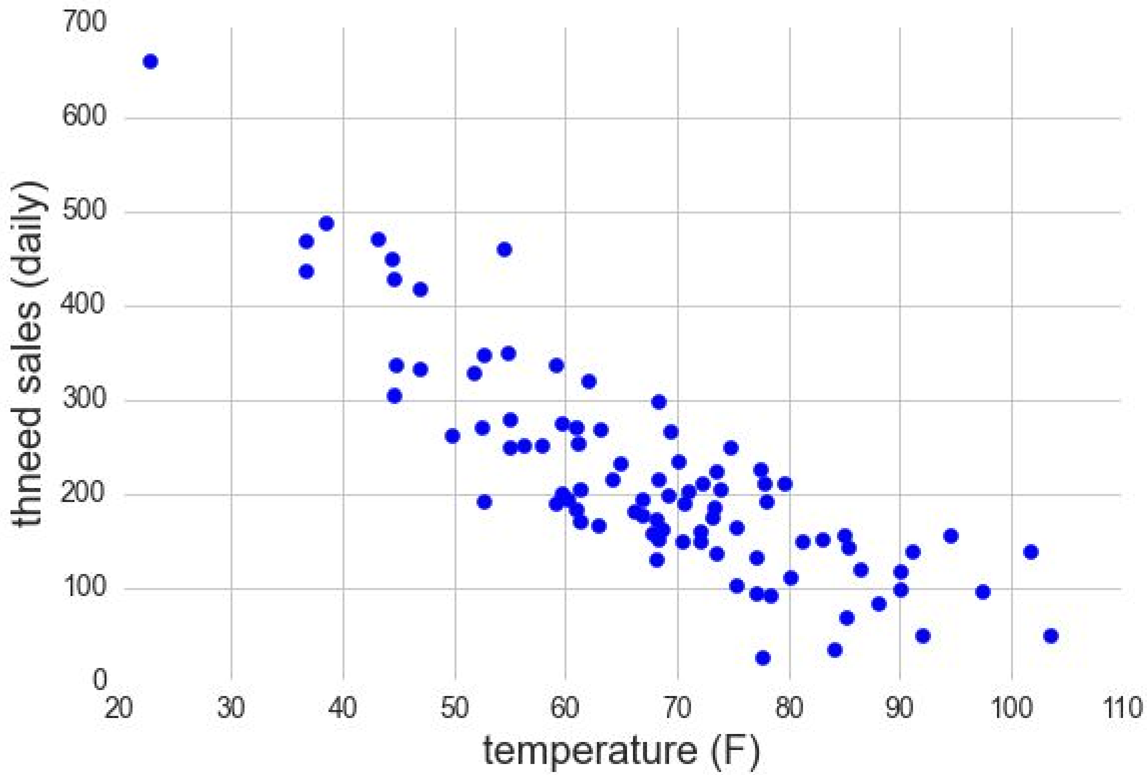
Can estimate degrees of freedom easily because the models are *nested* . . .

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

Now plug in all our numbers and . . .

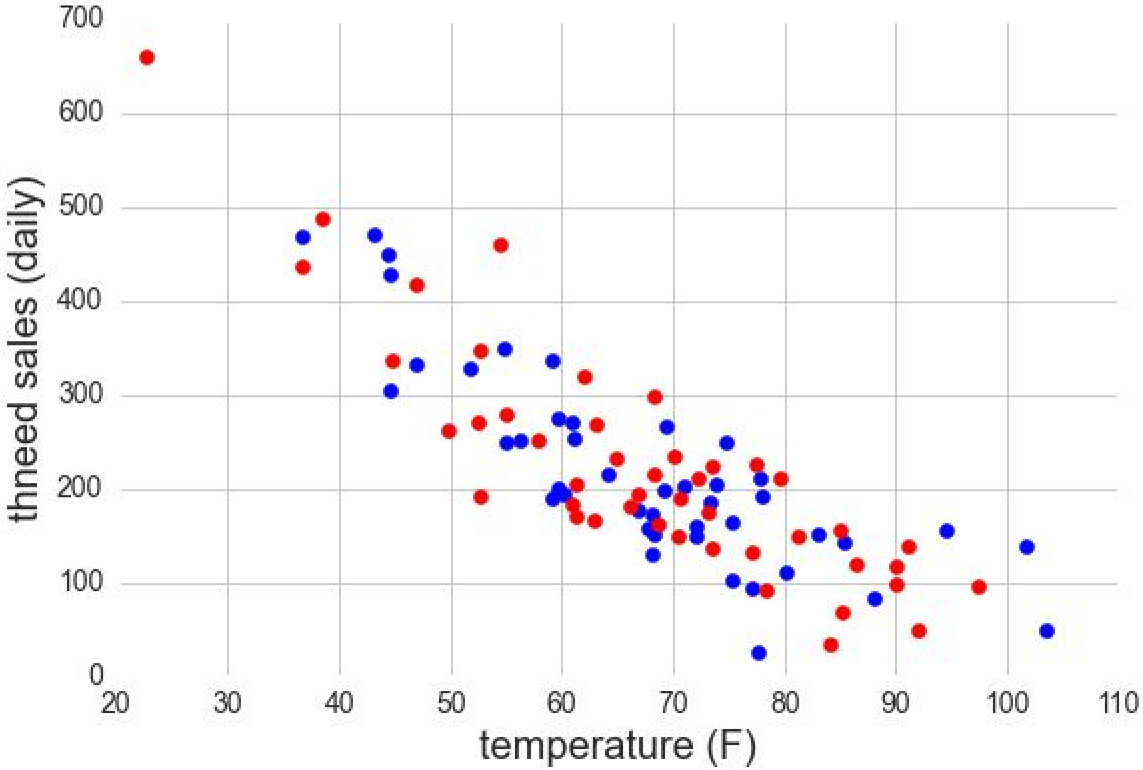
Easier Way:
Cross Validation

Cross-Validation



Cross-Validation

1. Randomly Split data



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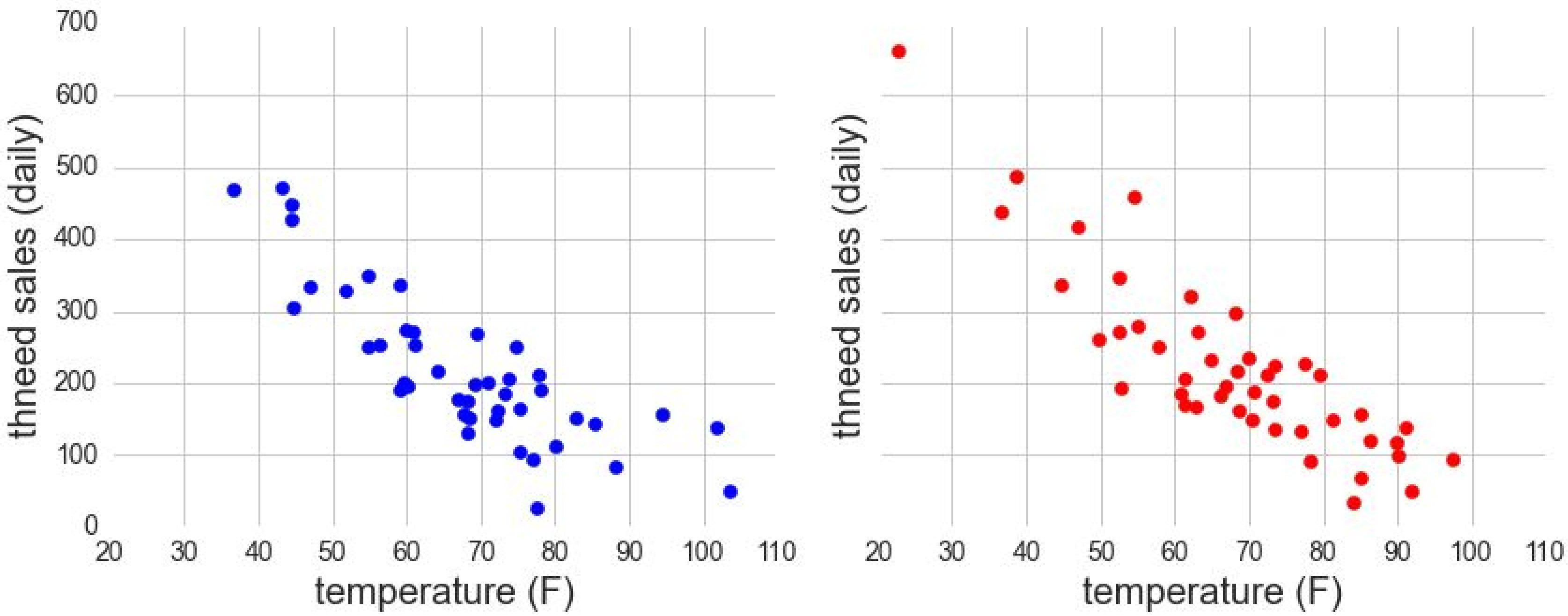
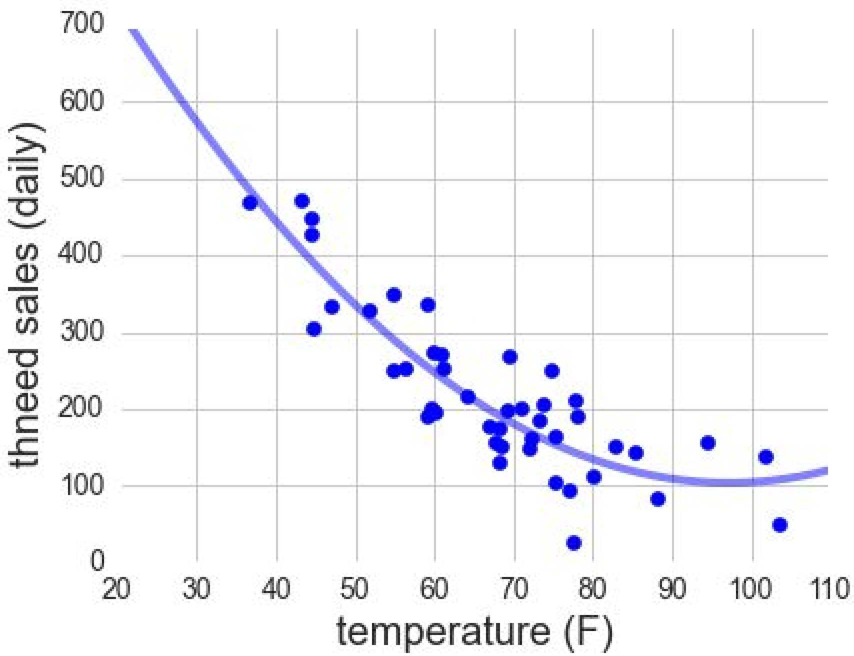
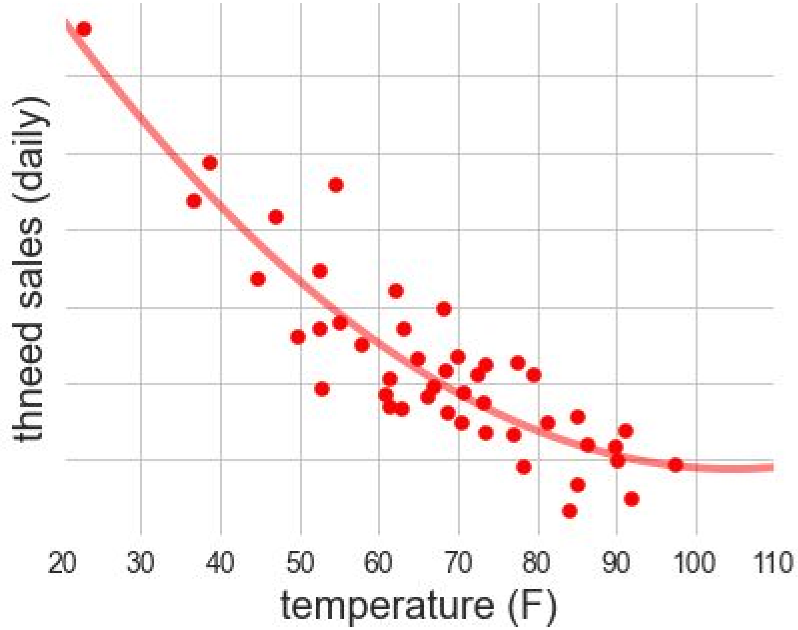


Jake VanderPlas

Cross-Validation

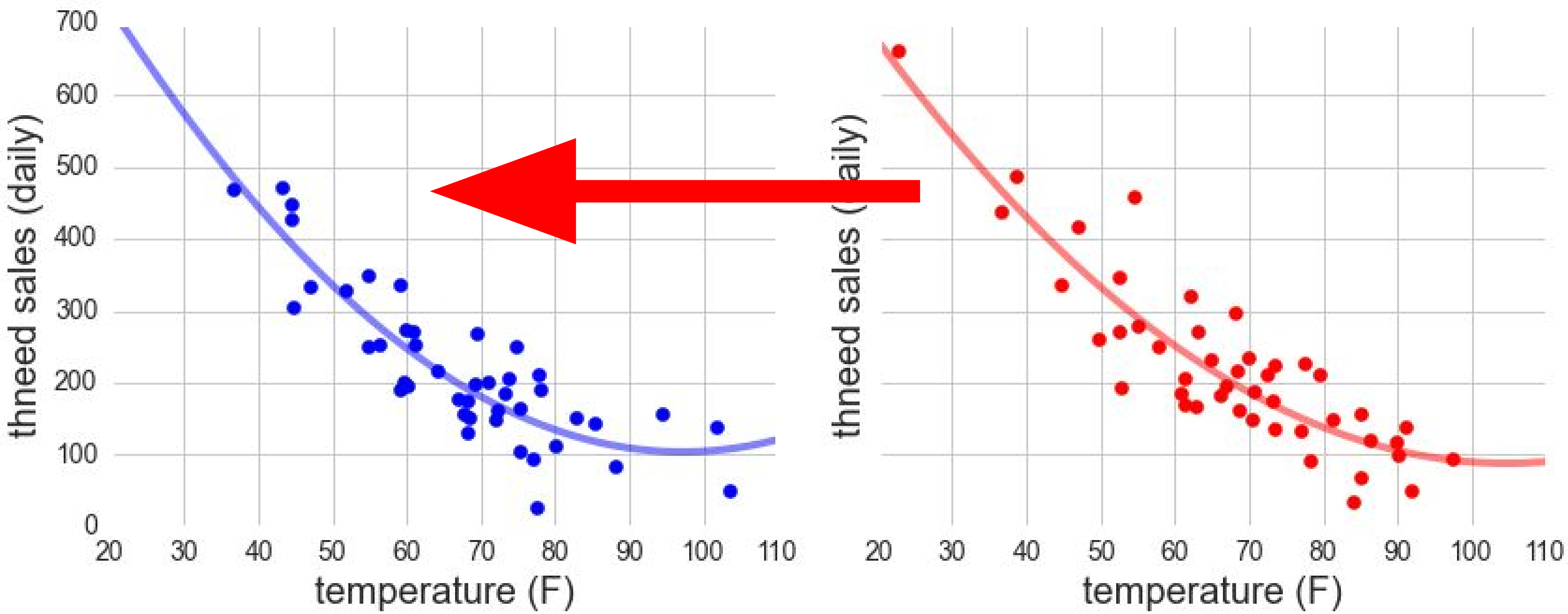
2. Find the best model for each subset





Cross-Validation

3. Compare models across subsets



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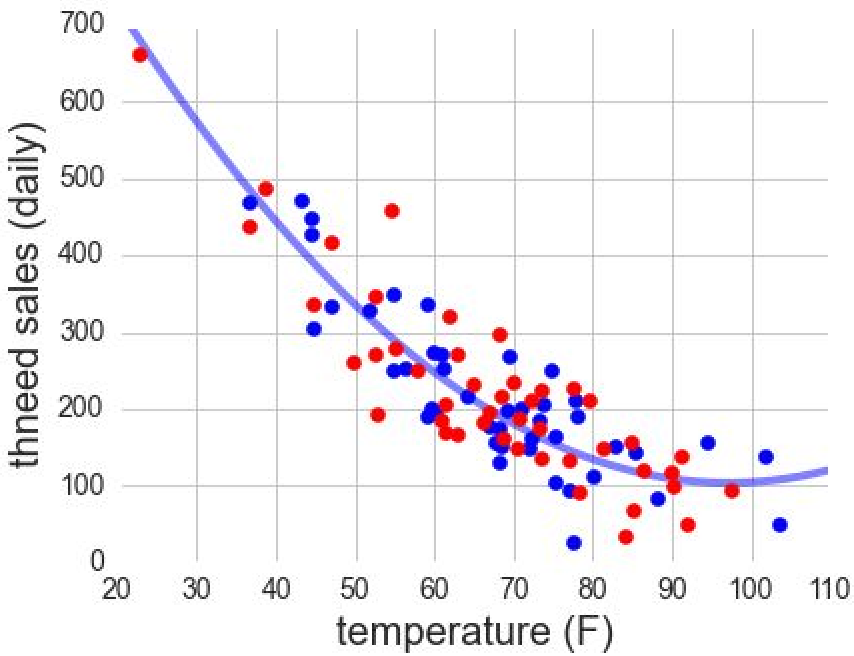

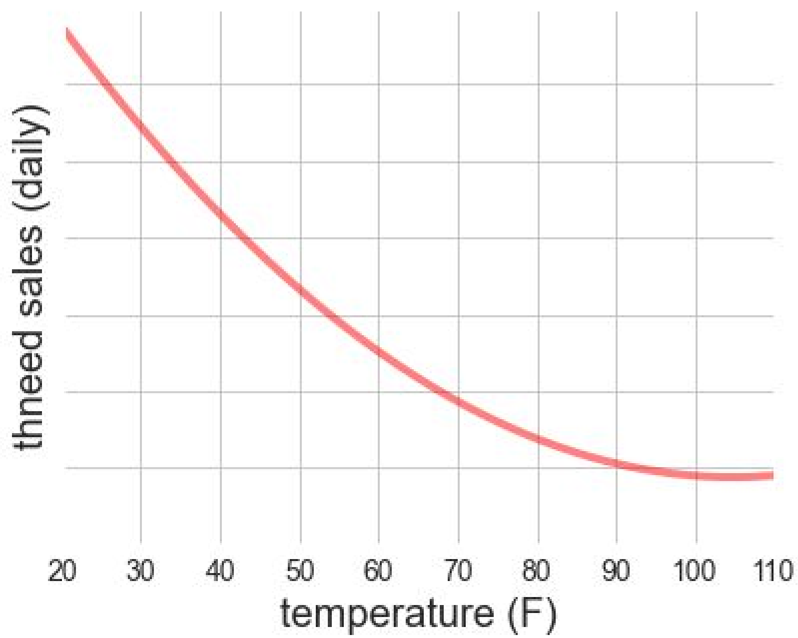

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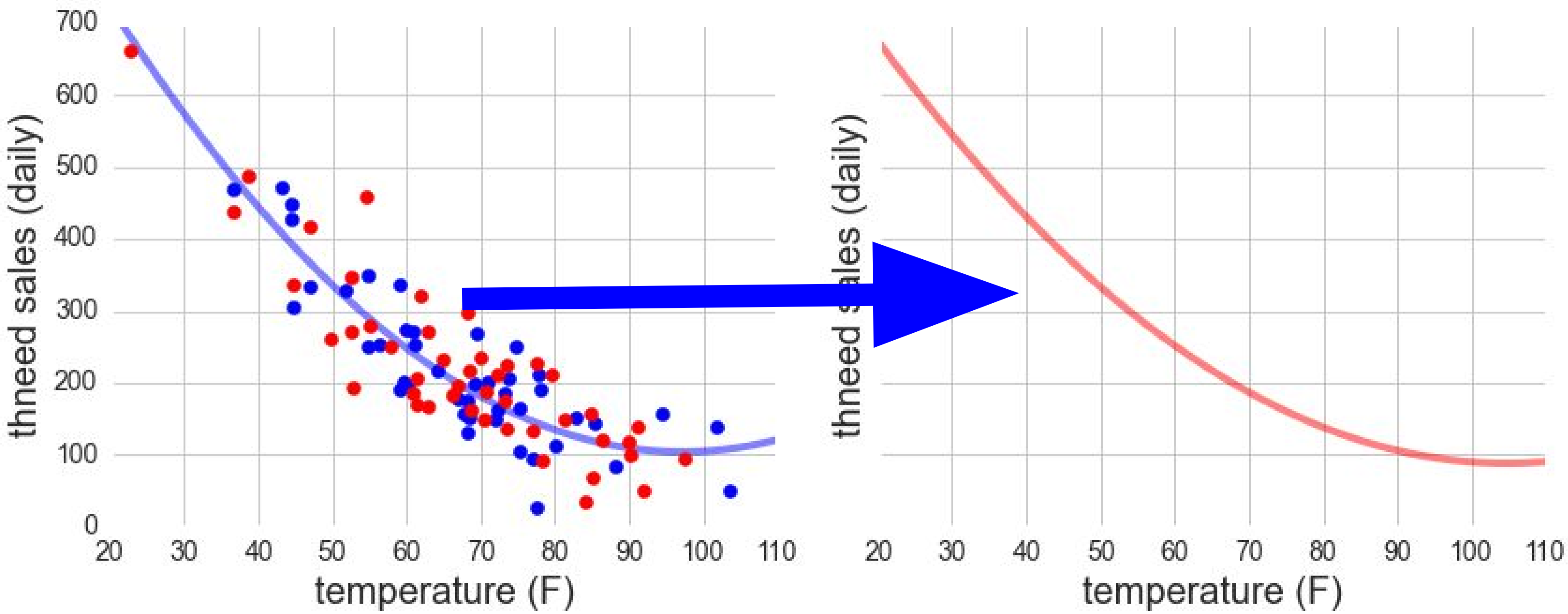

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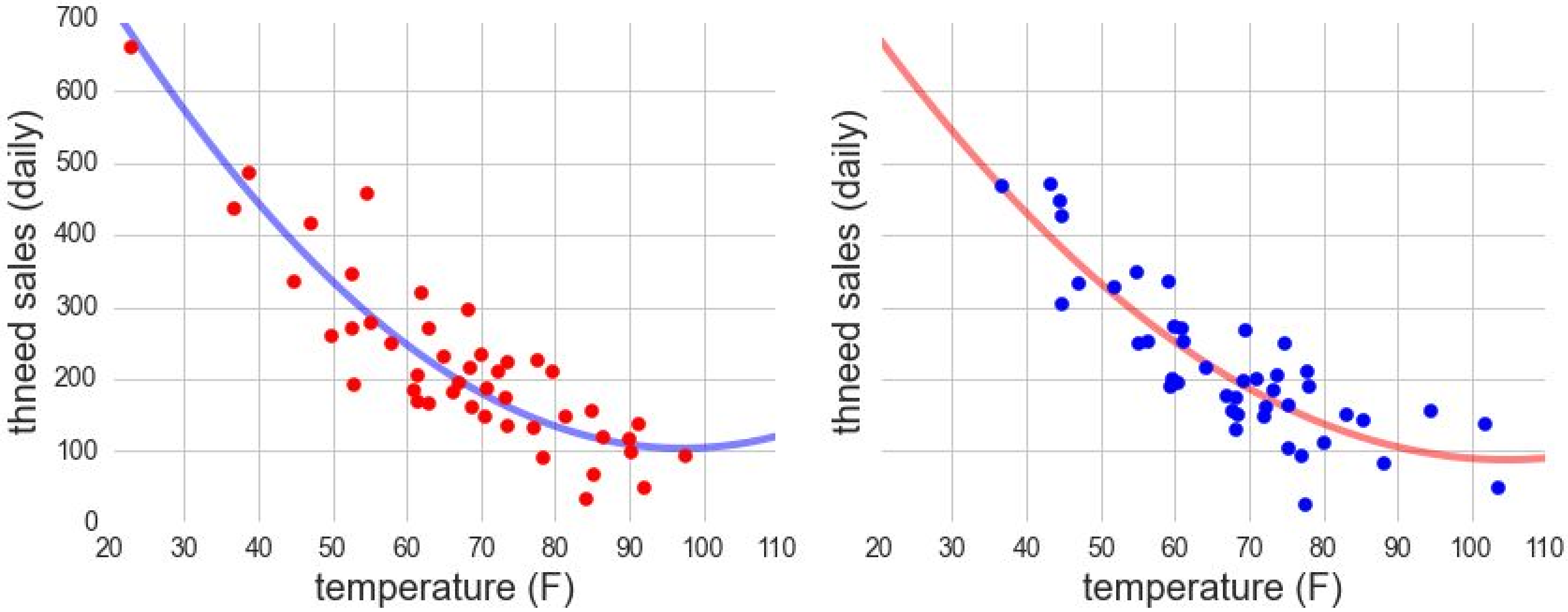
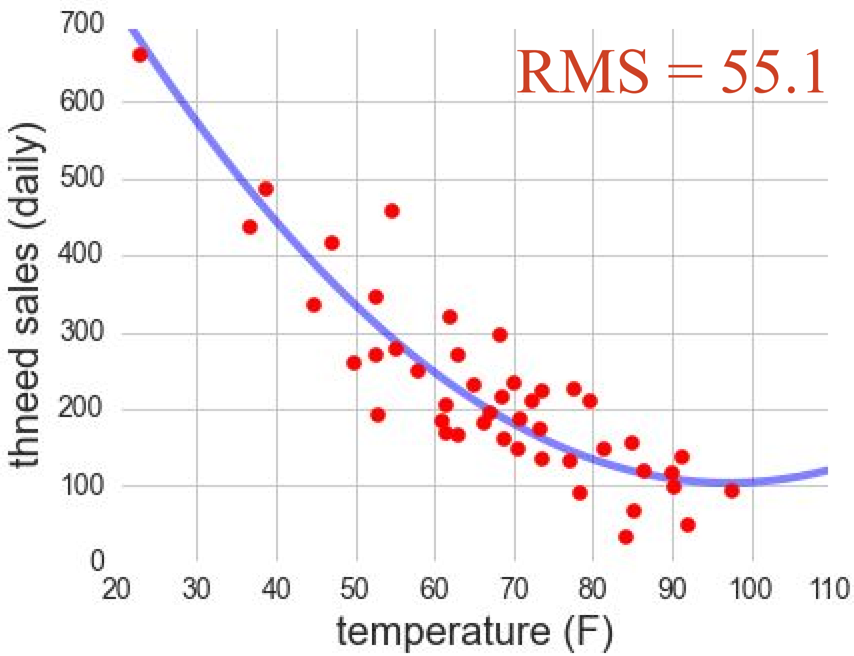
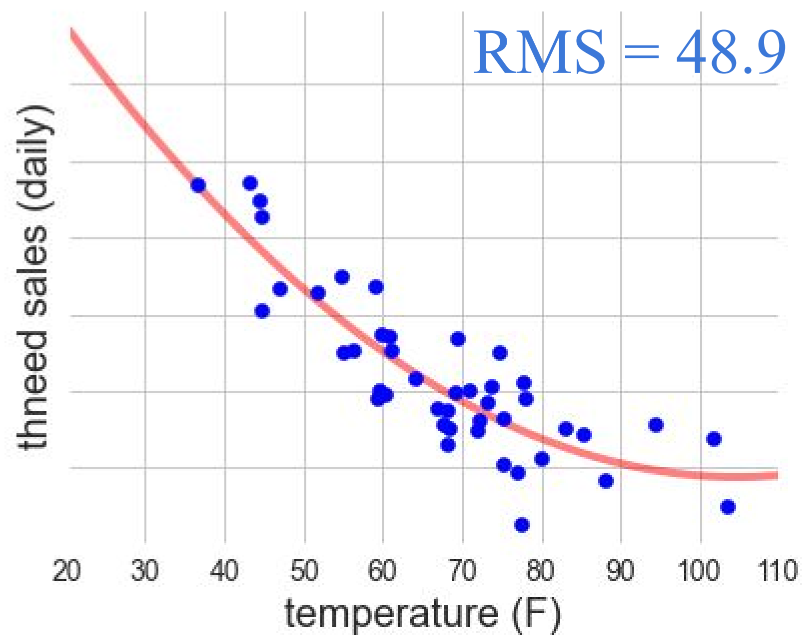


Cross-Validation

4. Compute RMS error for each

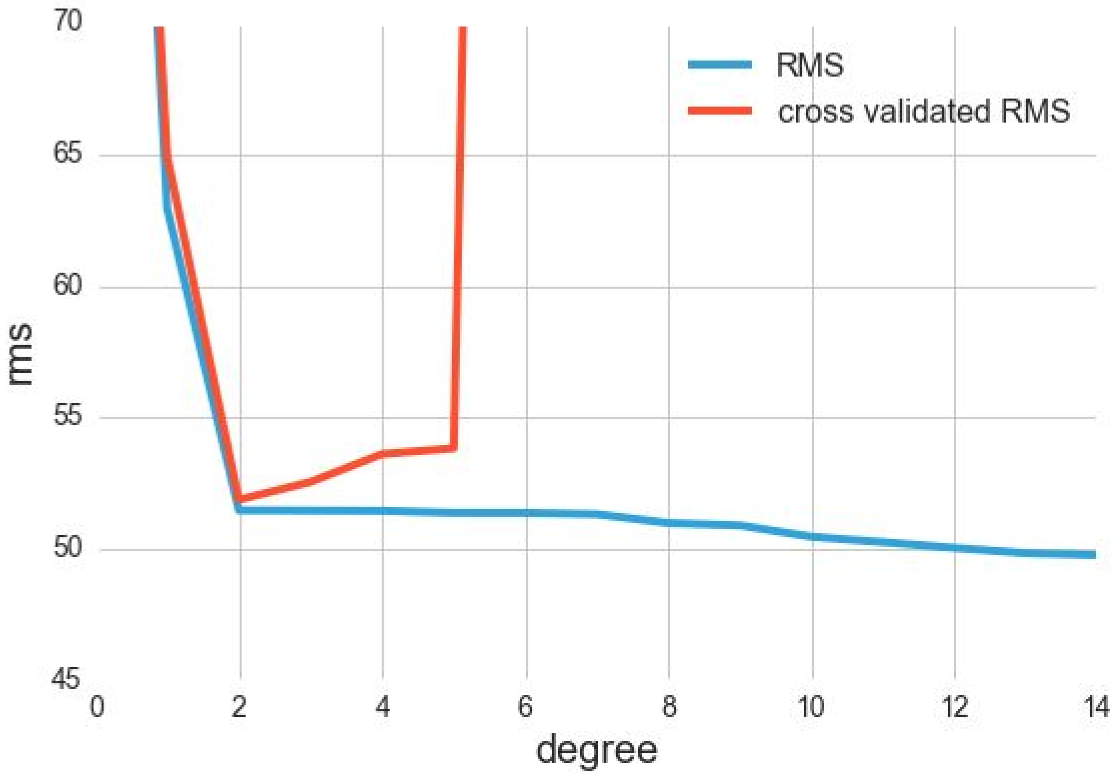




RMS estimate = 52.1

Cross-Validation

5. Compare cross-validated RMS for models:



Cross-Validation

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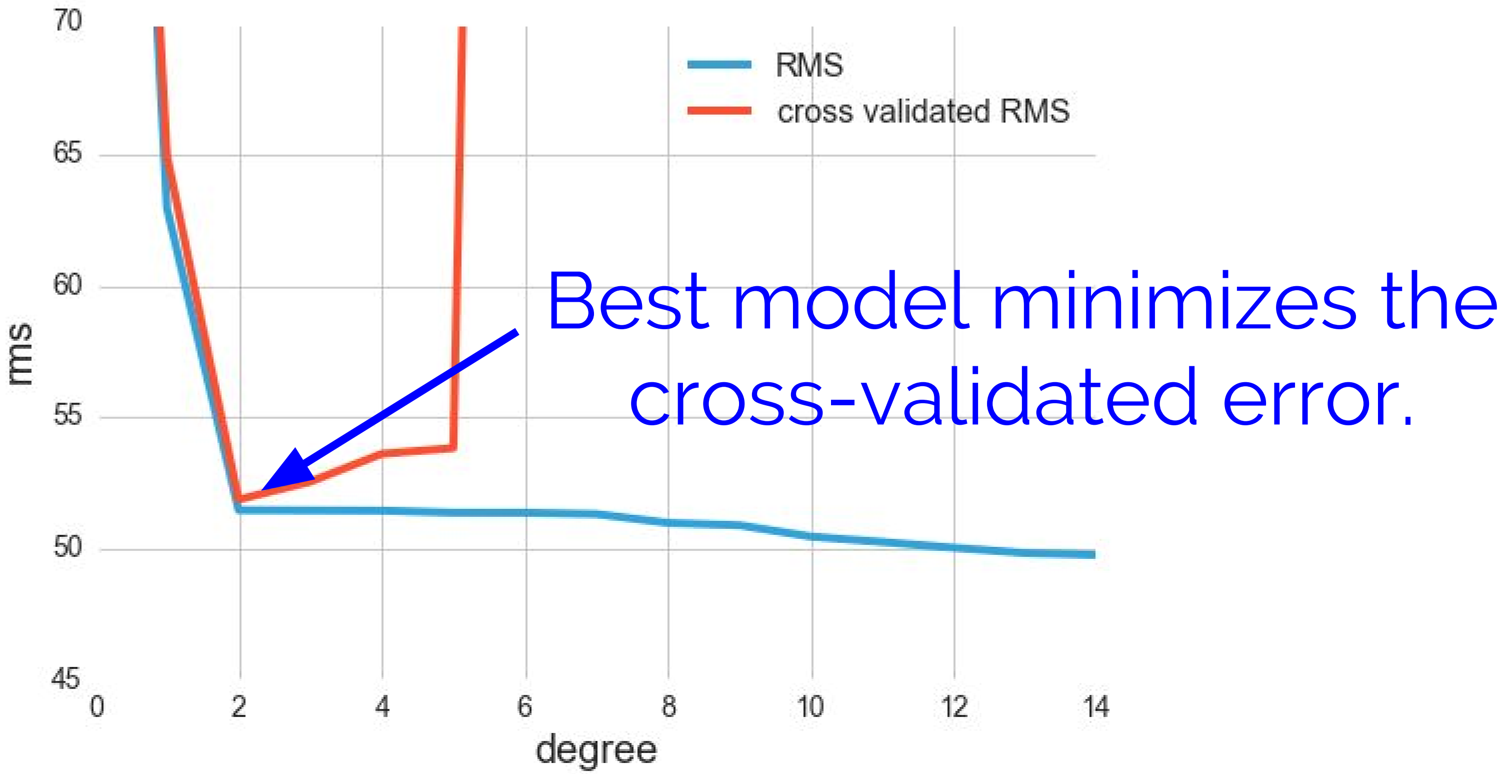
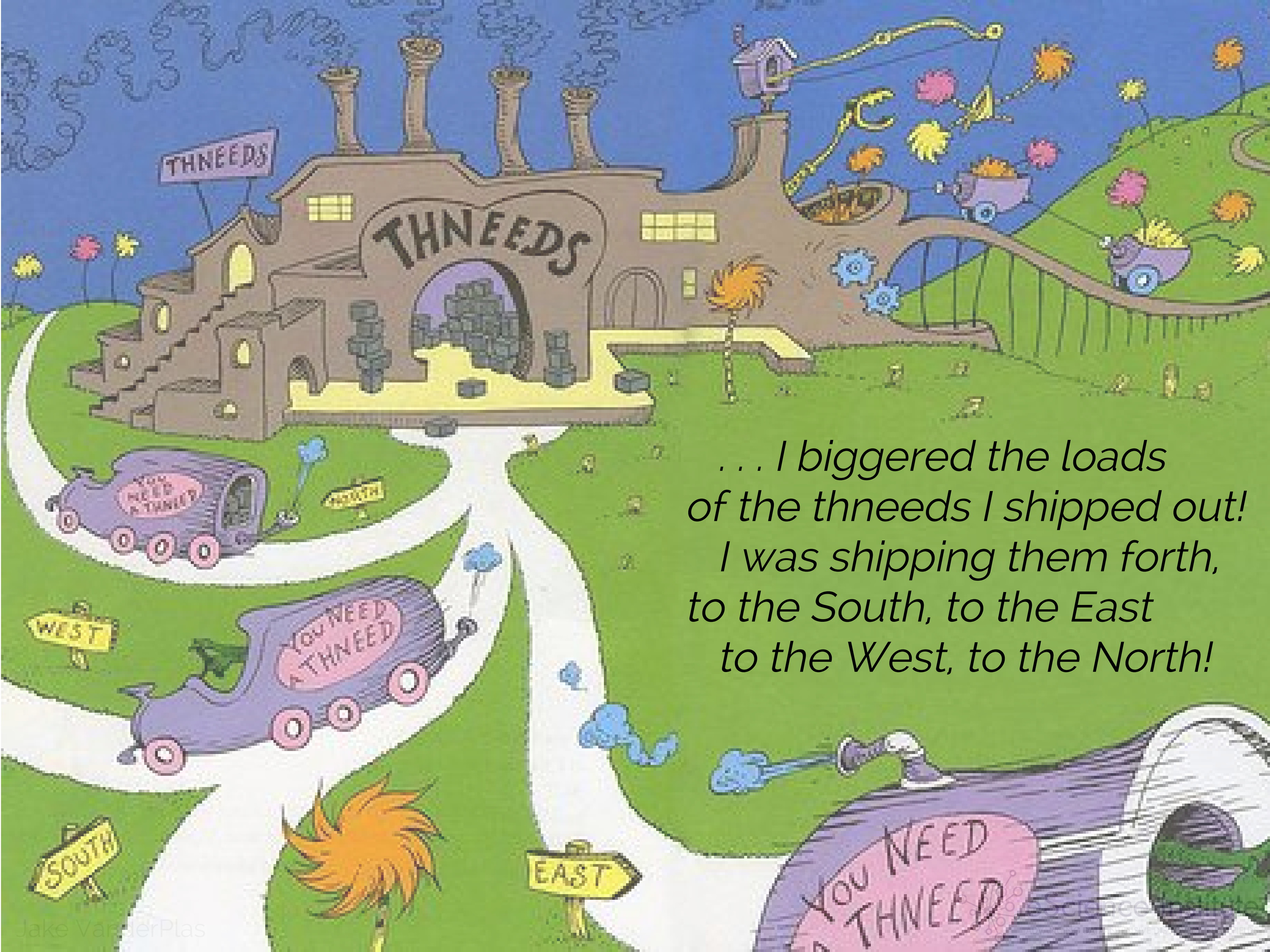




. . . I biggered the loads
of the thneeds I shipped out!
I was shipping them forth,
to the South, to the East
to the West, to the North!

Notes on Cross-Validation:

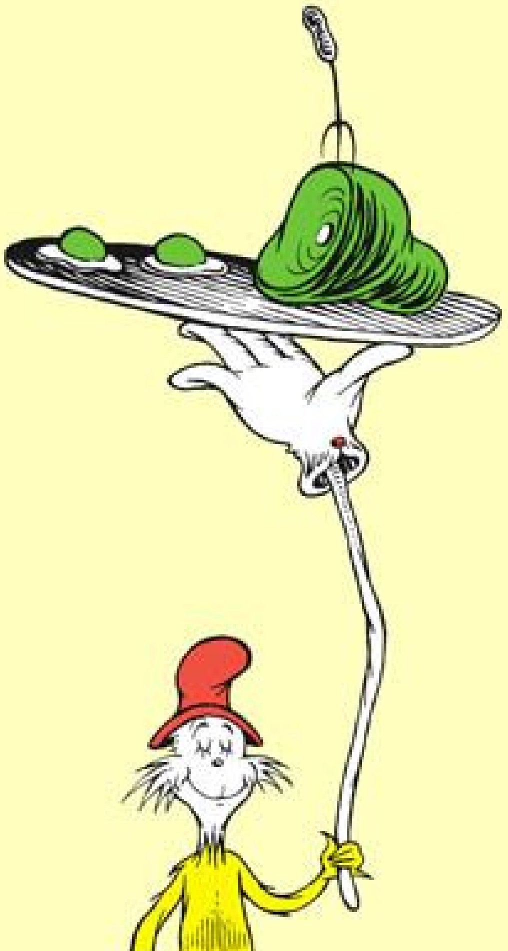
- This was **"2-fold" cross-validation**; other CV schemes exist & may perform better for your data (see e.g. scikit-learn docs)

- 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 correlations 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 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-Pillon)

- **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)

Sometimes the questions are complicated and the answers are simple.

– Dr. Seuss (attr)

~ Thank You! ~

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