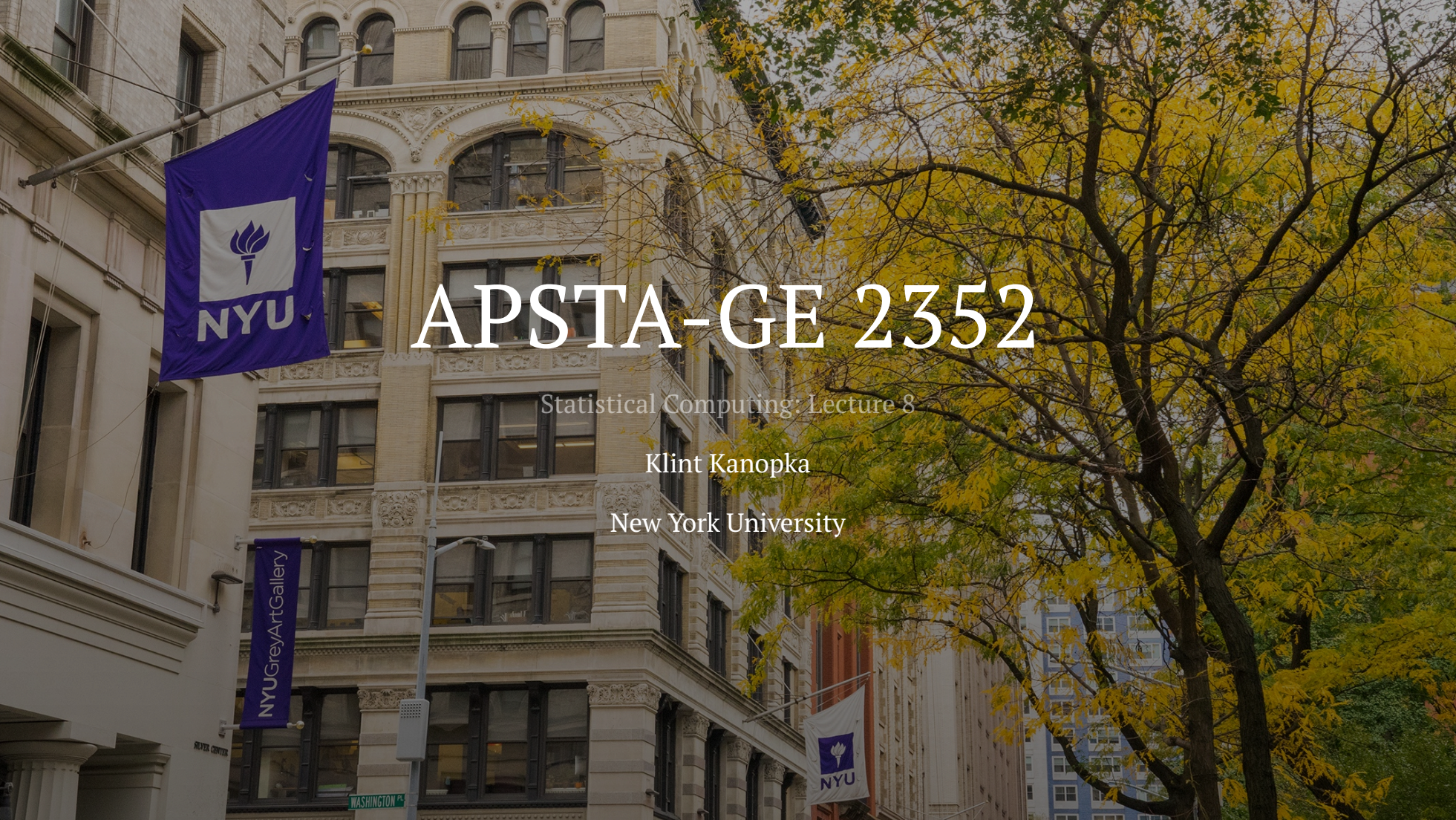

APSTA-GE 2352

Statistical Computing: Lecture 8

Klint Kanopka

New York University

Table of Contents

1. Statistical Computing - Week 8
    1. Table of Contents
    2. Announcements
    3. Vector Norms
2. Motivating Problem
    1. Overfitting
3. Dealing with Overfitting
    1. Regularization
    2. Ridge Regression
    3. LASSO Regression
4. More Resampling Methods
    1. The Central Limit Theorem
    2. The Jackknife
    3. The Bootstrap
5. Wrap Up
    1. Recap

Announcements

- PS4 due the day before Halloween
  - Very spooky
  - How's it going?
- If you haven't already, please do the mid-semester survey
  - https://forms.gle/Ljh25bvYeoAL5dEU8

Check-In

- PollEv.com/klintkanopka

Vector Norms

- We often want to talk about the *length* of a vector, but how do we measure length?
- Conceptually, think of the length of a vector as the distance it spans from the origin
- We'll talk about two types of norms today

The Euclidean Norm

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- The Euclidean distance a vector extends in space from the origin

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$$||\vec{x}||_2 = \sqrt{\sum_{k=1}^{K} x_k^2}$$

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$$||\vec{x}||_2 = \sqrt{x_1^2 + \cdots + x_k^2}$$

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$$||\vec{x}||_1 = \sum_{k=1}^{K} |x_k|$$

$$||\vec{x}||_1 = |x_1| + \cdots + |x_k|$$

Motivating Problem

Overfitting

```r
d <- data.frame(x = rnorm(50))
d$y <- -1.5 + 3*d$x + rnorm(50, sd=0.5)

m <- lm(y~x, d)
coef(m)
```

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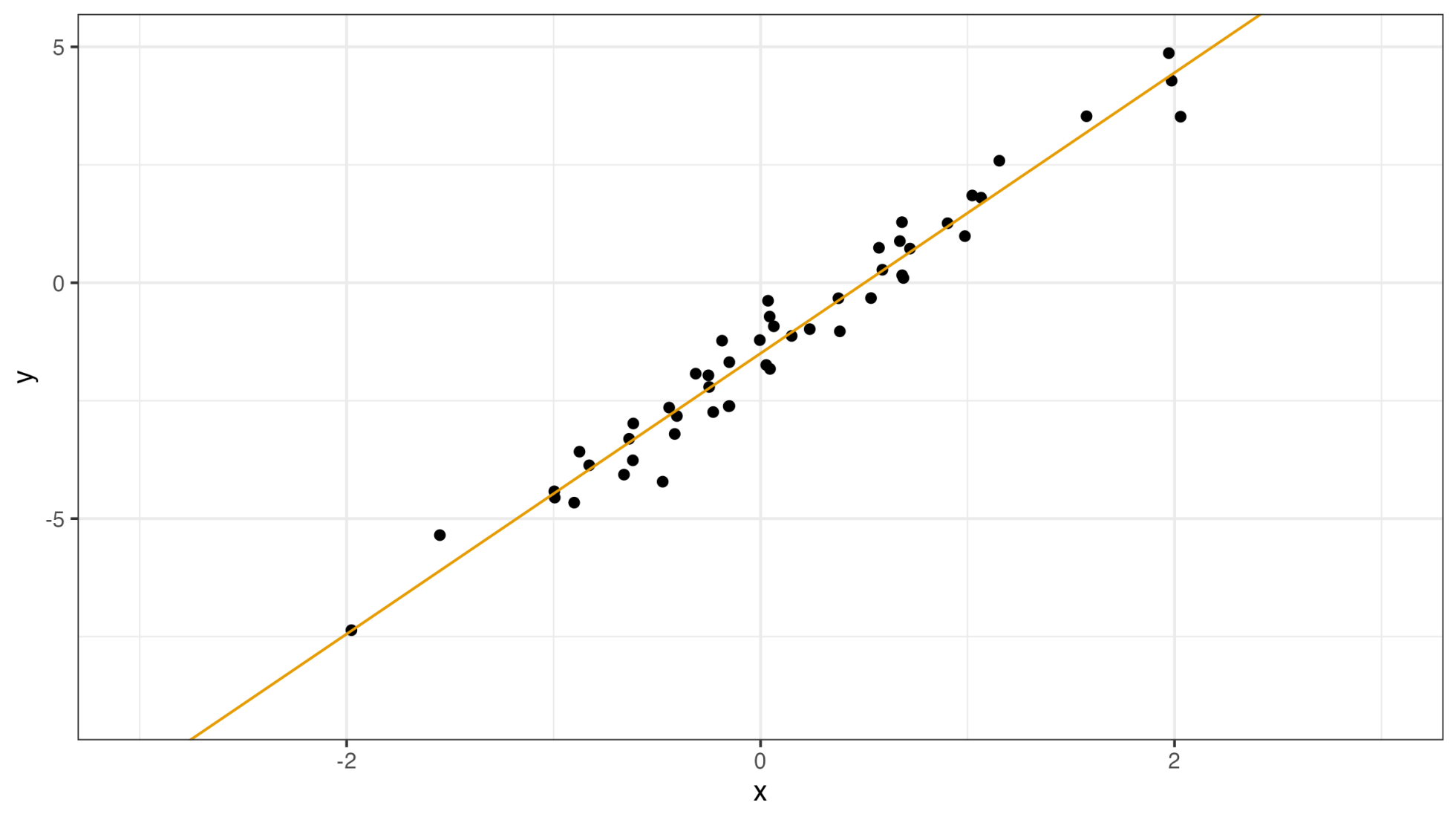
d <- data.frame(x = rnorm(50))
d$y <- -1.5 + 3*d$x + rnorm(50, sd=0.5)

m <- lm(y~x, d)
coef(m)

# (Intercept)           x
#  -1.425421    2.883035
```


5
0
-5
y
-2
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2
x

Overfitting

```
d2 <- rbind(d, data.frame(x=2, y=-8))

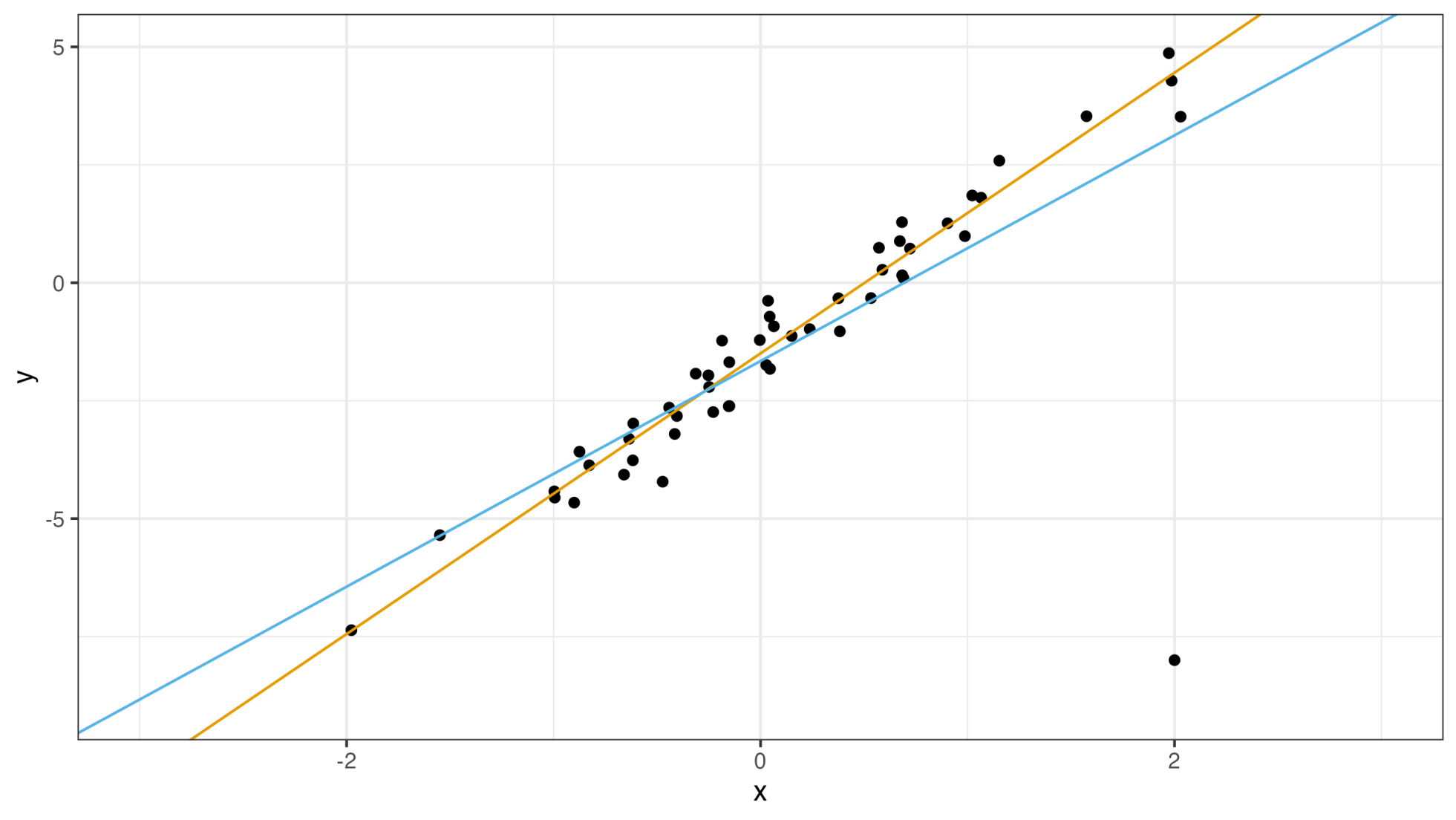
m2 <- lm(y~x, d2)
coef(m2)
```

Overfitting

```r
d2 <- rbind(d, data.frame(x=2, y=-8))

m2 <- lm(y~x, d2)
coef(m2)

# (Intercept)           x
#   -1.659093    2.391916
```


5
0
-5
y
-2
0
2
x

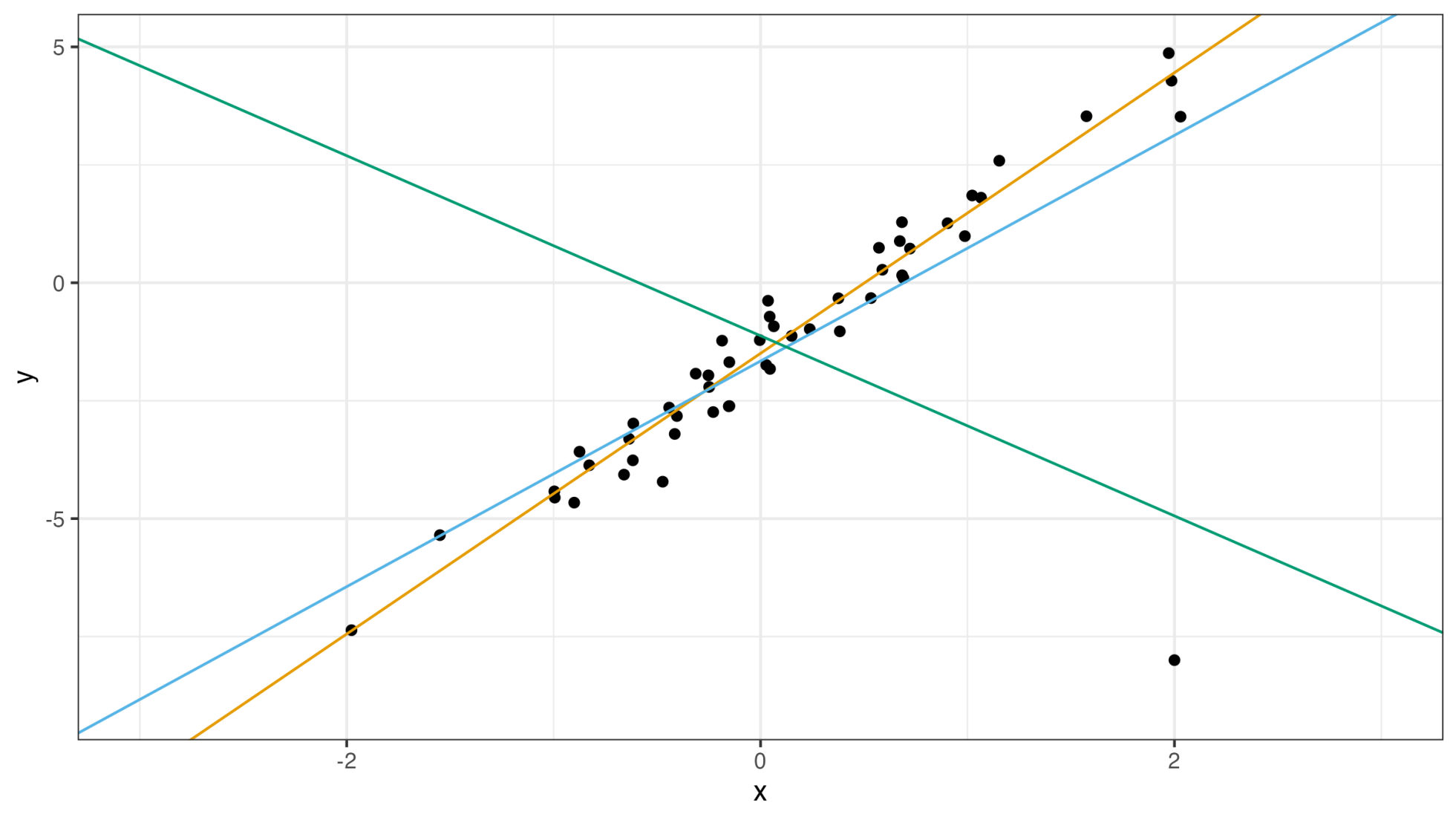
Overfitting

```
d3 <- rbind(d2, data.frame(x=50, y=-100))
m3 <- lm(y~x, d3)
coef(m3)
```

Overfitting

```r
d3 <- rbind(d2, data.frame(x=50, y=-100))
m3 <- lm(y~x, d3)
coef(m3)

# (Intercept)           x
#   -1.124650   -1.908941
```


5
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y
-2
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x

Overfitting

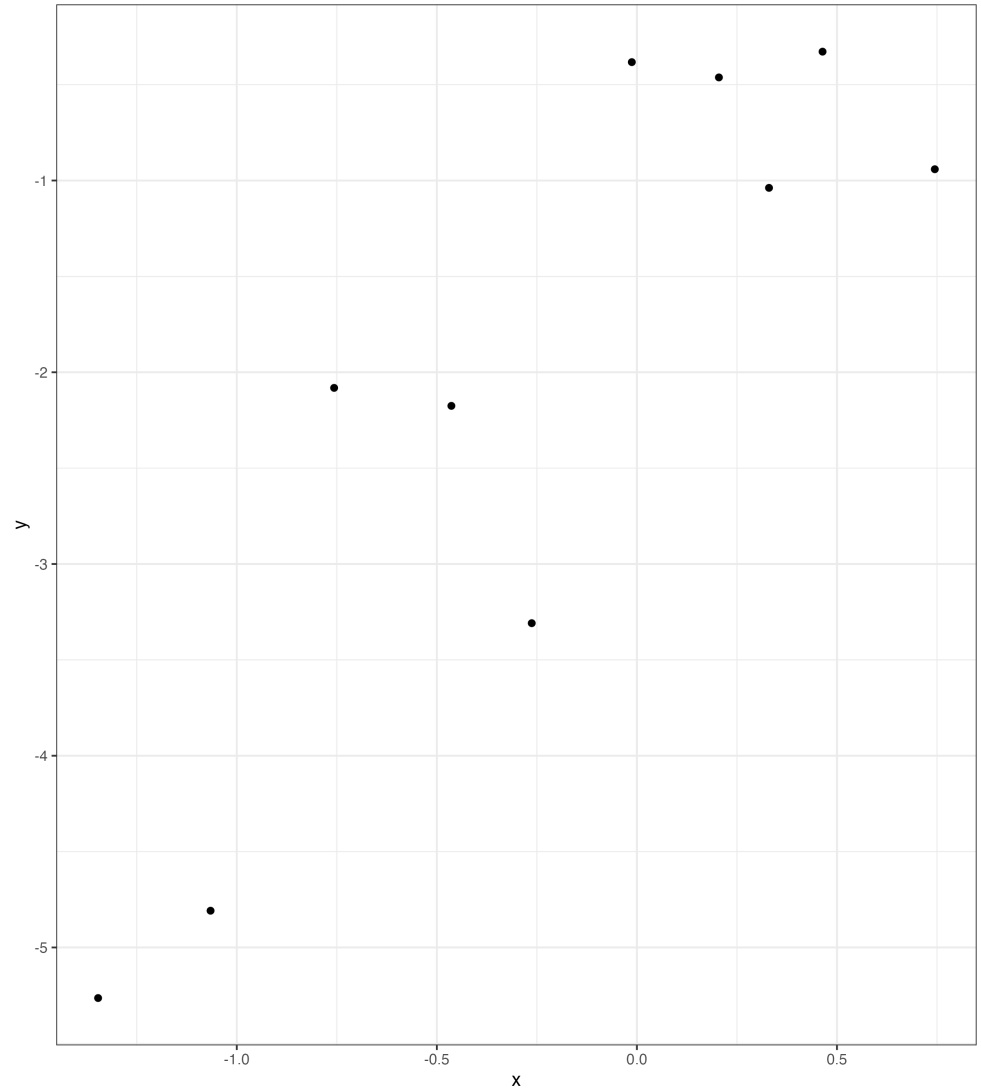
- *Overfitting* occurs when the model you are estimating has too much flexibility and can make large adjustments for small variations in the data it is fit to (or *trained on*)
- Overfitting hurts the ability of your model to *generalize*, or make reasonable predictions with data it hasn't seen yet (we call these predictions *out of sample*, or OOS)
- Overfitting often occurs under one of two conditions:
  1. The individual parameter estimates grow too large
  2. Your model has a large number of estimable parameters relative to the amount of data

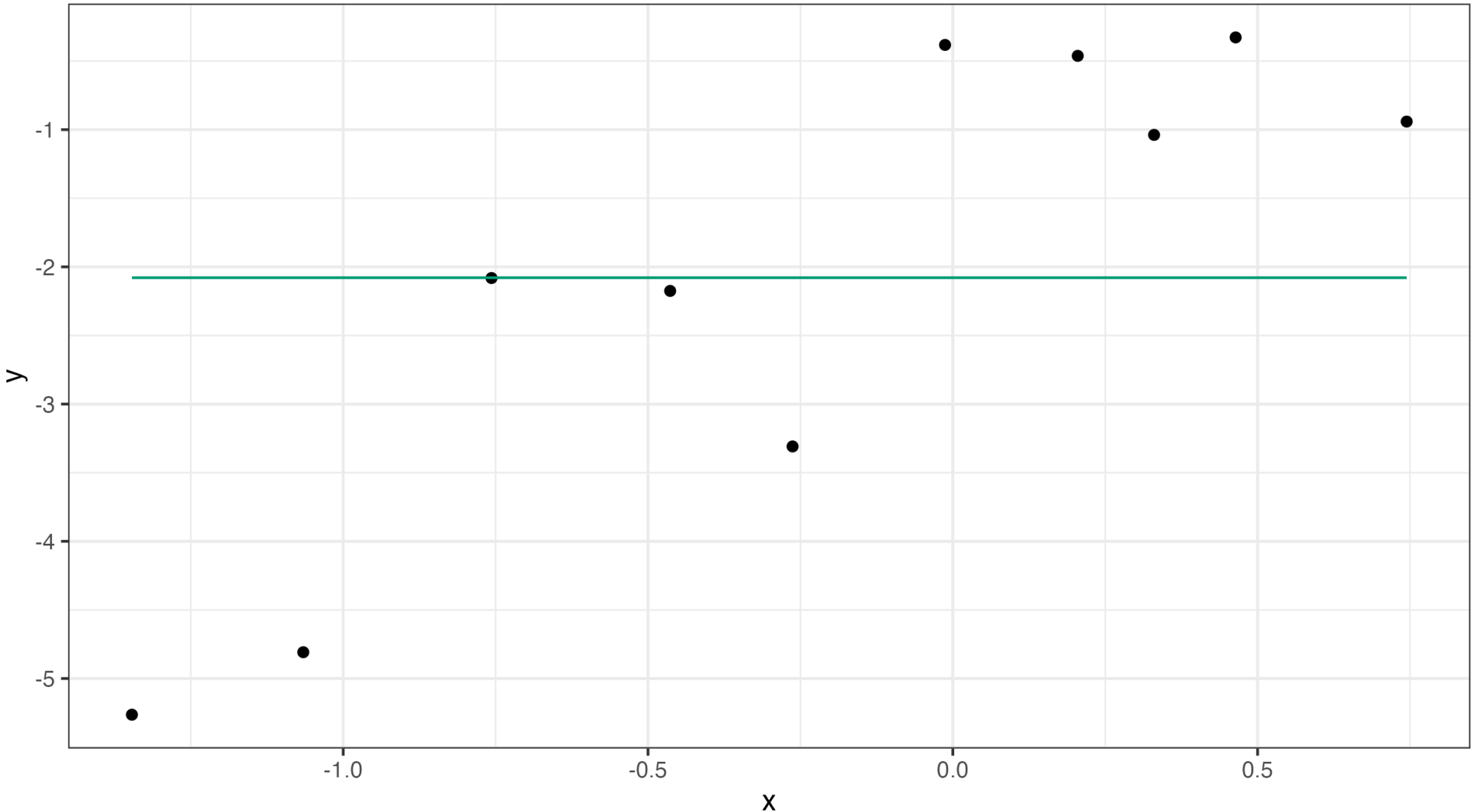
Overfitting

- What happens when functions become too flexible?
- We'll plot ten data points and then a polynomial function of best fit

```
d <- data.frame(x = rnorm(10))
d$y <- -1.5 + 3*d$x + rnorm(10)

ggplot(d, aes(x=x, y=y)) +
  geom_point() +
  theme_minimal()
```




-1
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-4
-5
y
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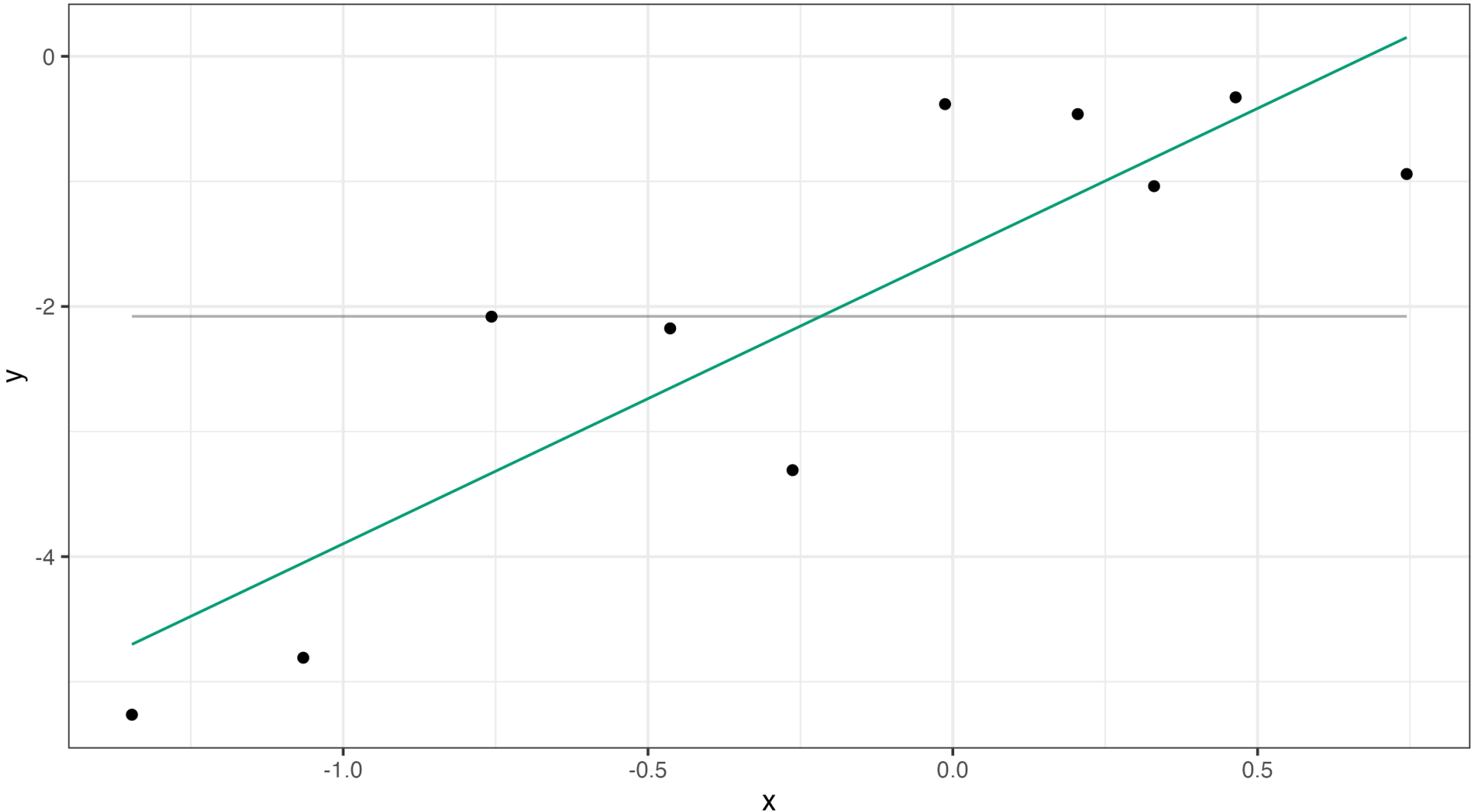
0.0
0.5
x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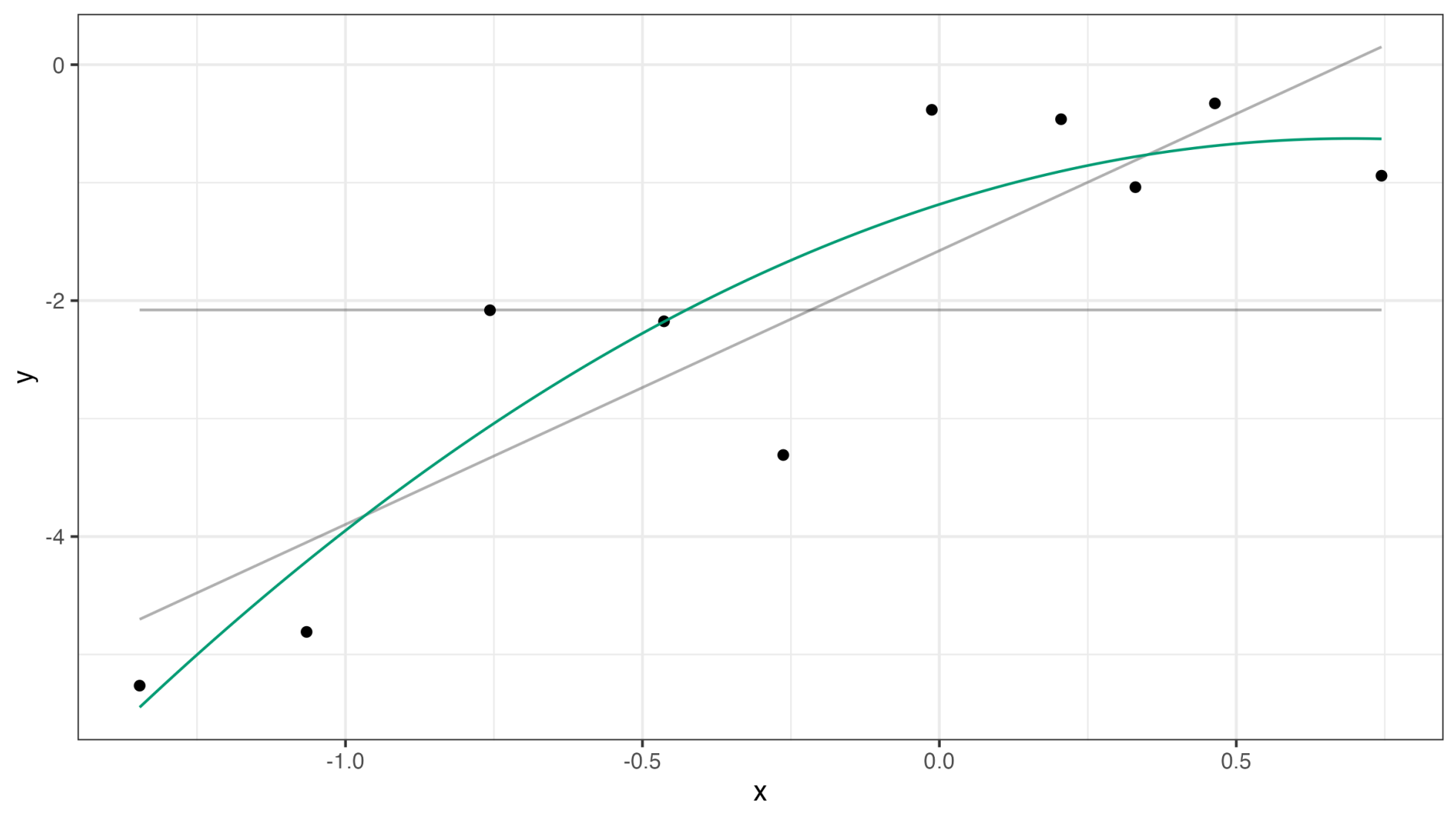
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y
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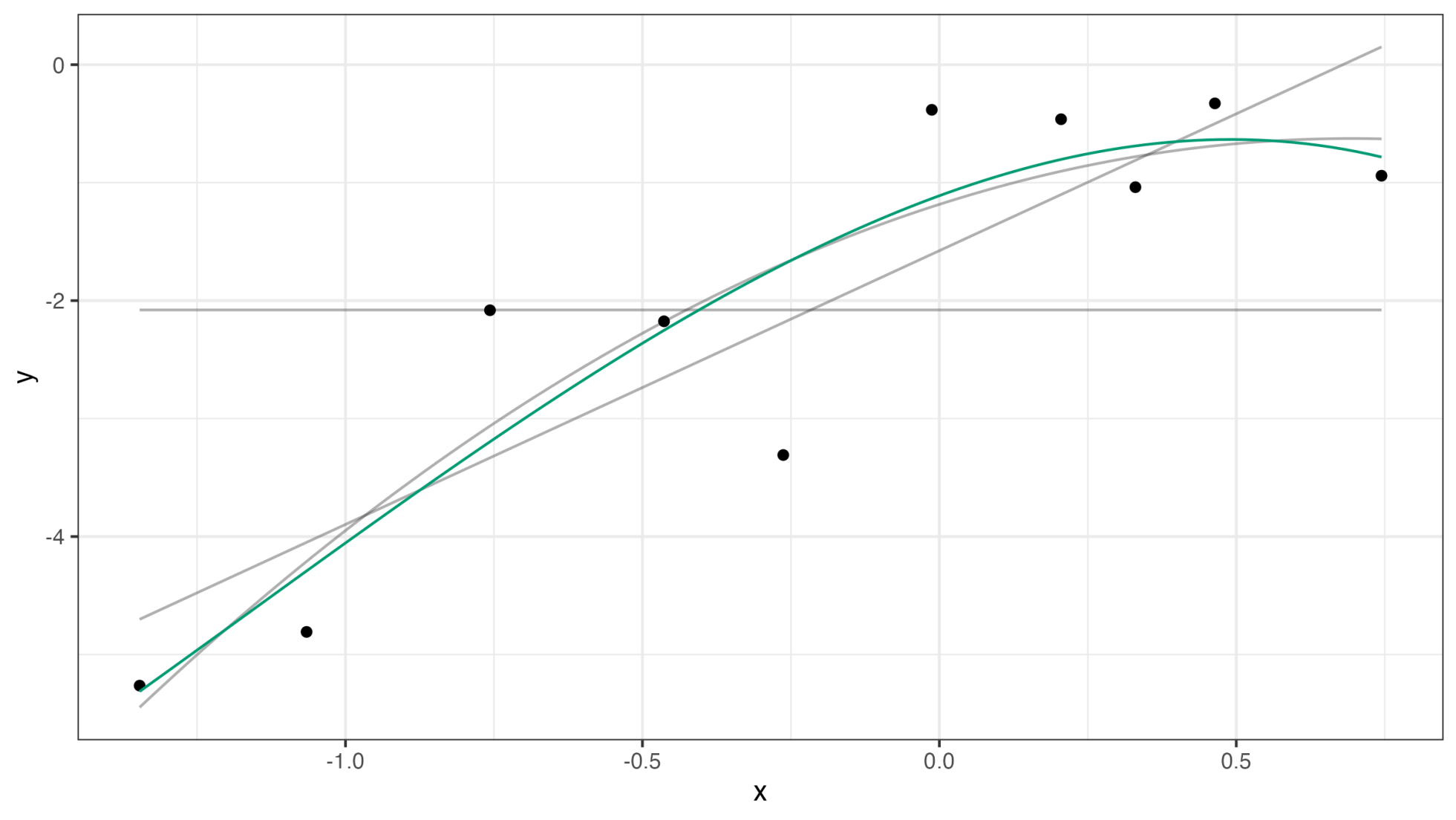
0.0
0.5
x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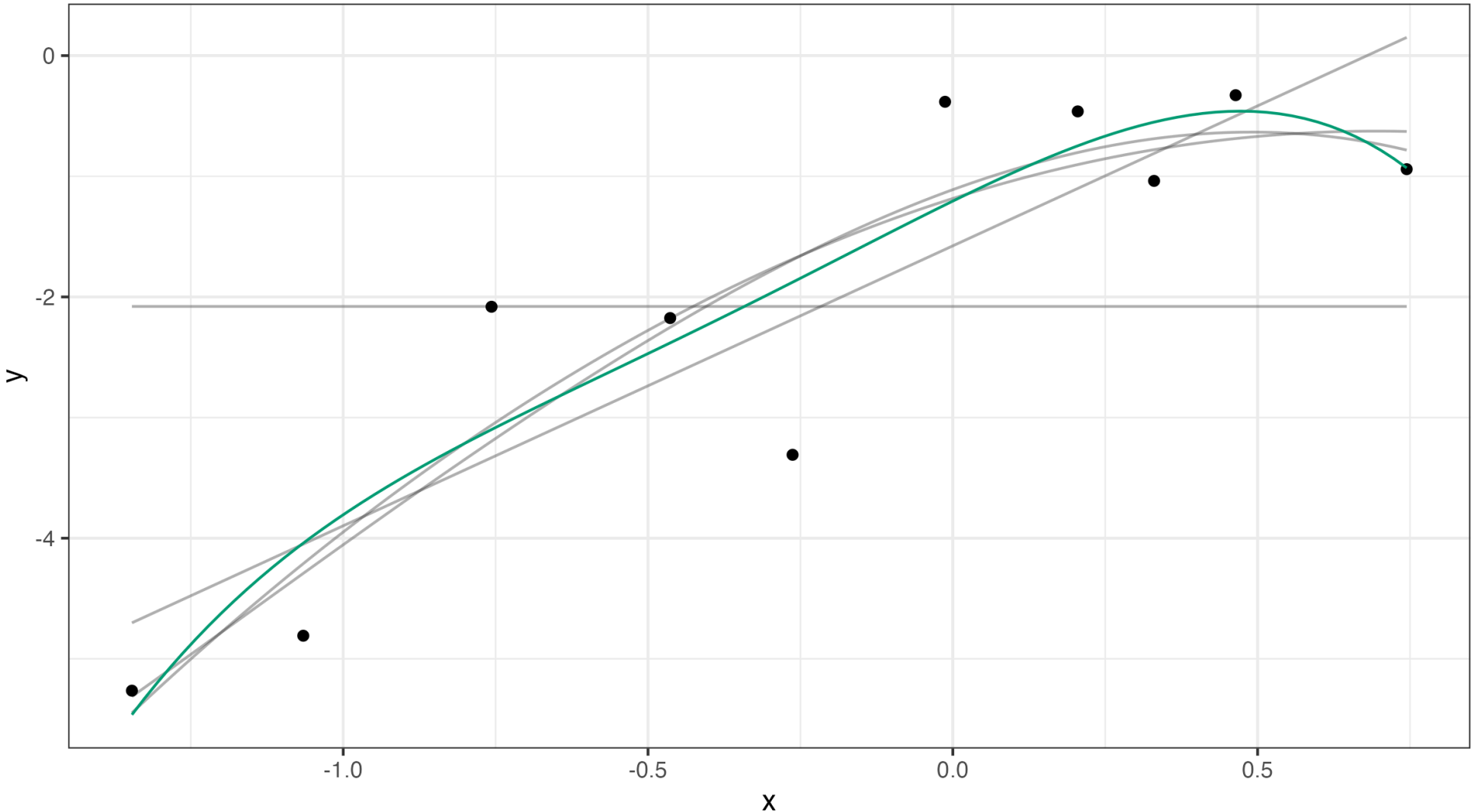
x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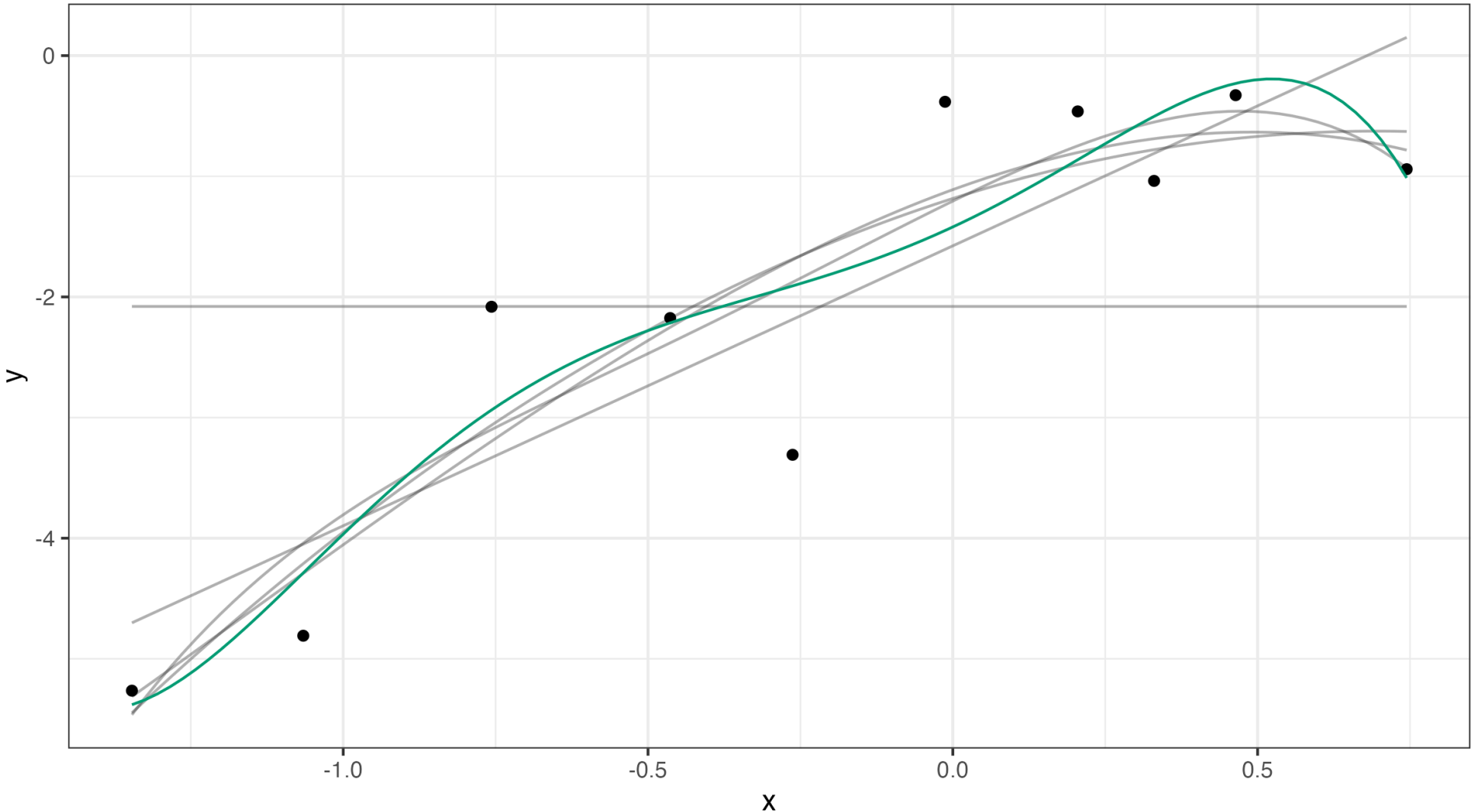
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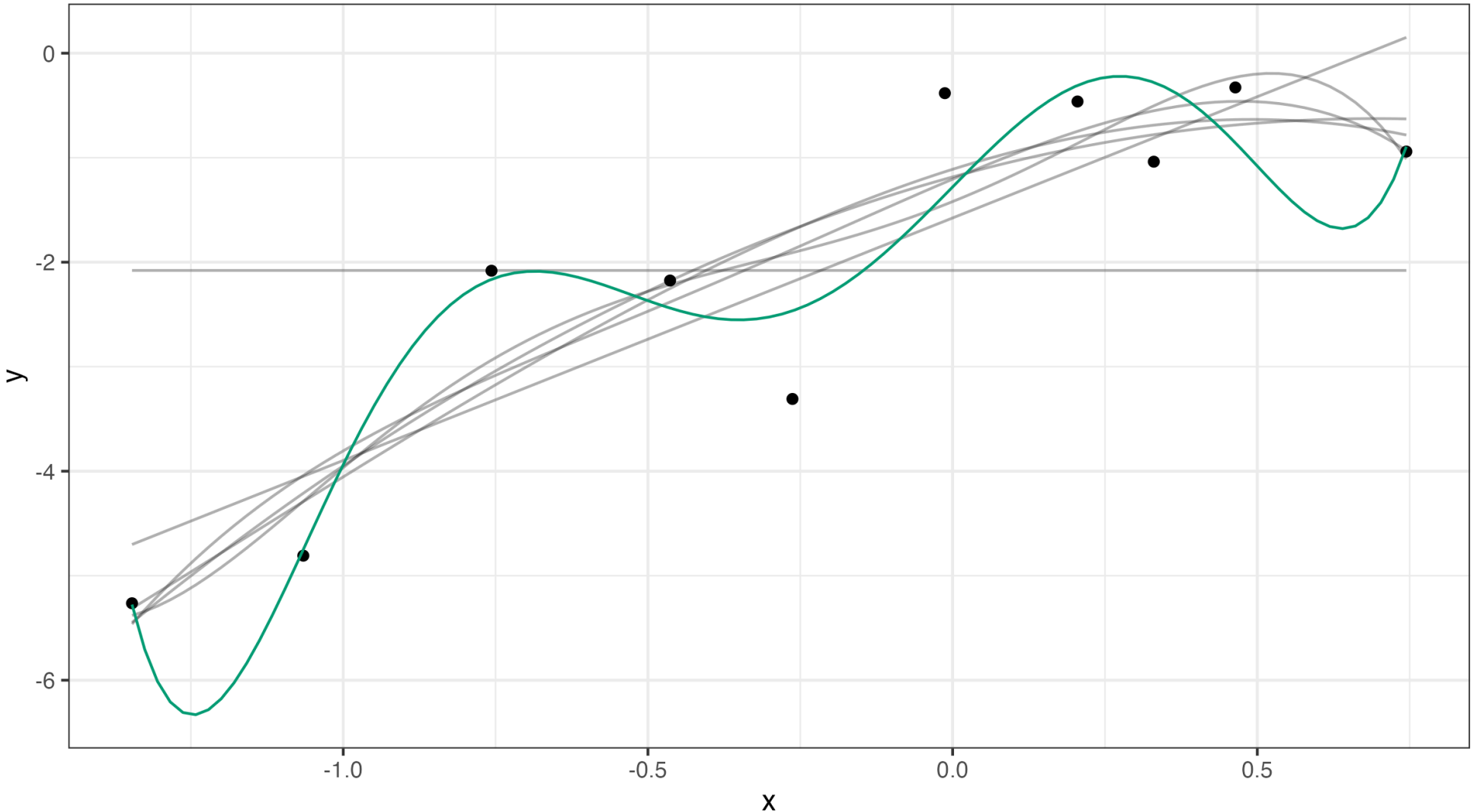
-0.5
0.0
0.5
x


0
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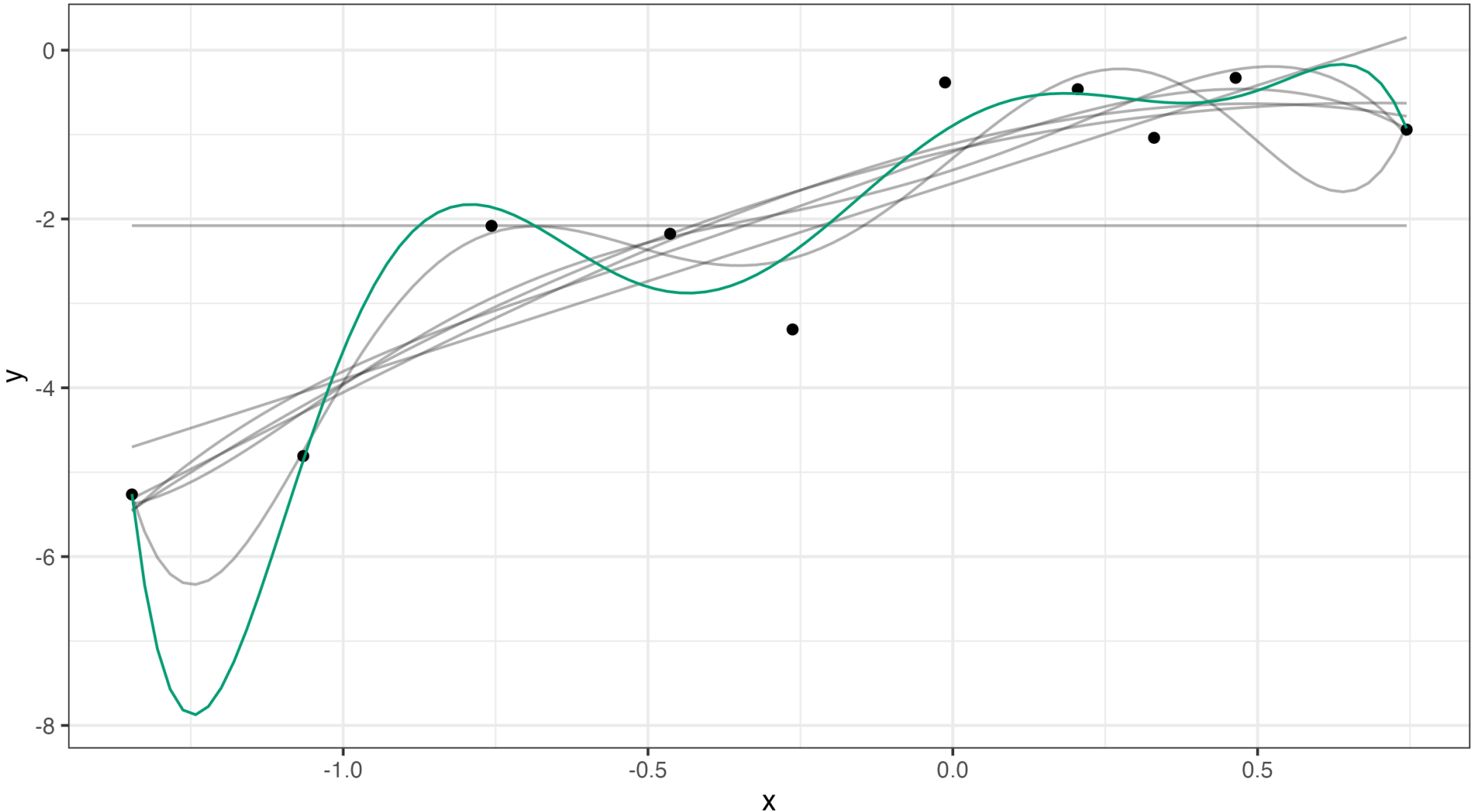
-4
-6
y
-1.0
-0.5
0.0
0.5
x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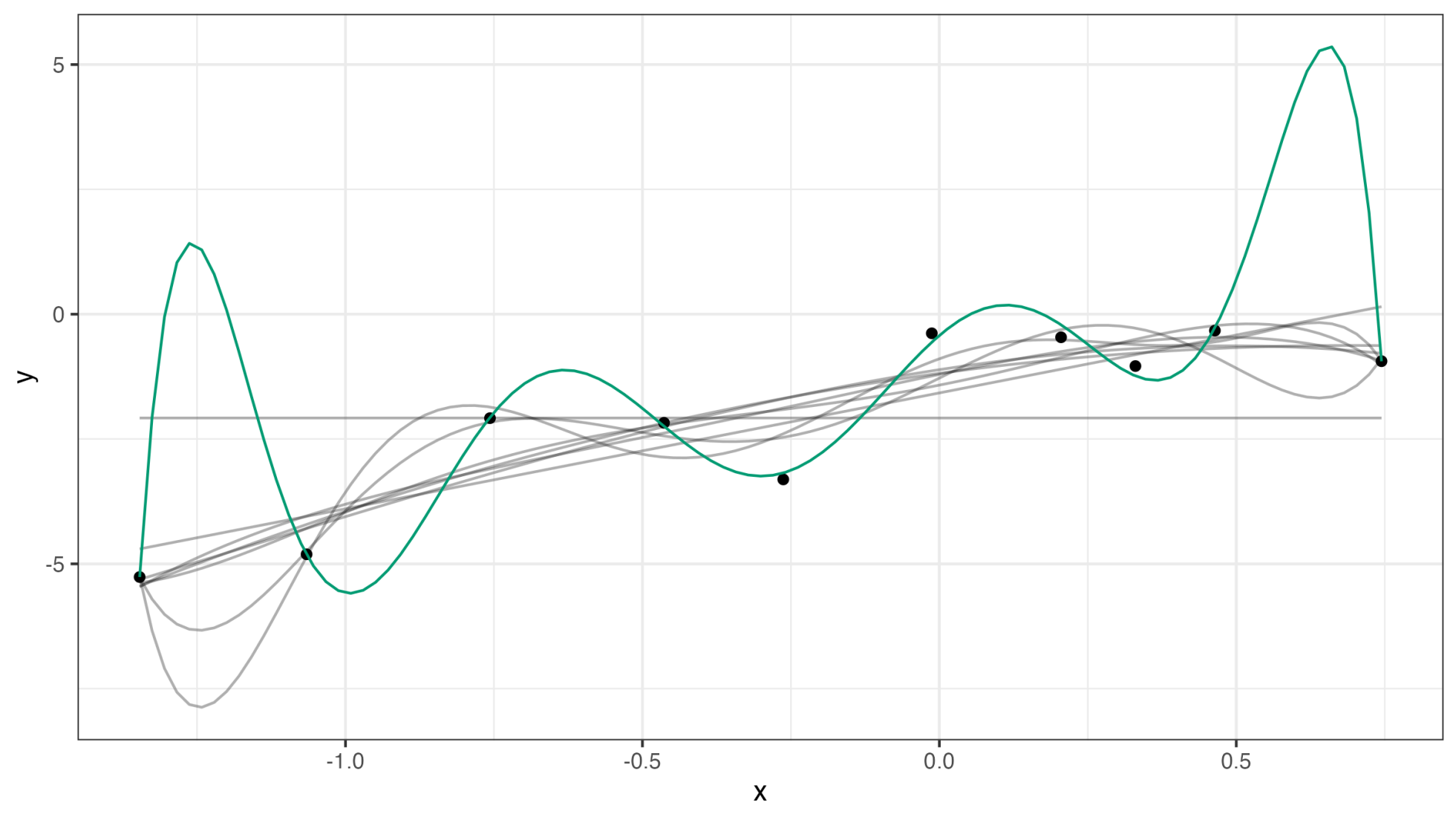
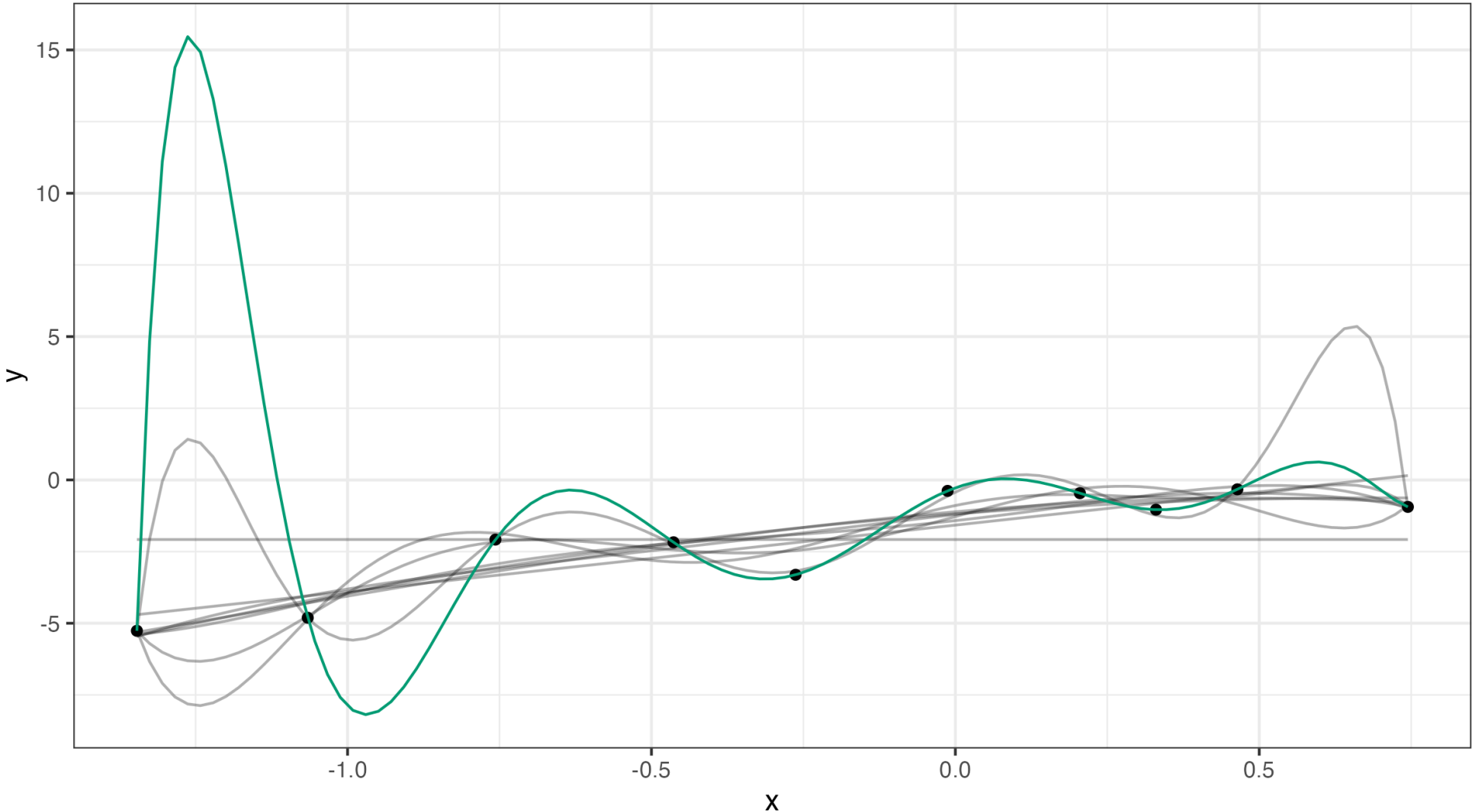
0.0
0.5
x


5
0
-5
y
-1.0
-0.5
0.0
0.5
x


15
10
5
0
-5
y
-1.0
-0.5
0.0
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x

Dealing with Overfitting

Regularization

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- Downside: Induces some bias in your parameter estimates
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  - You can control how much bias you introduce, however!

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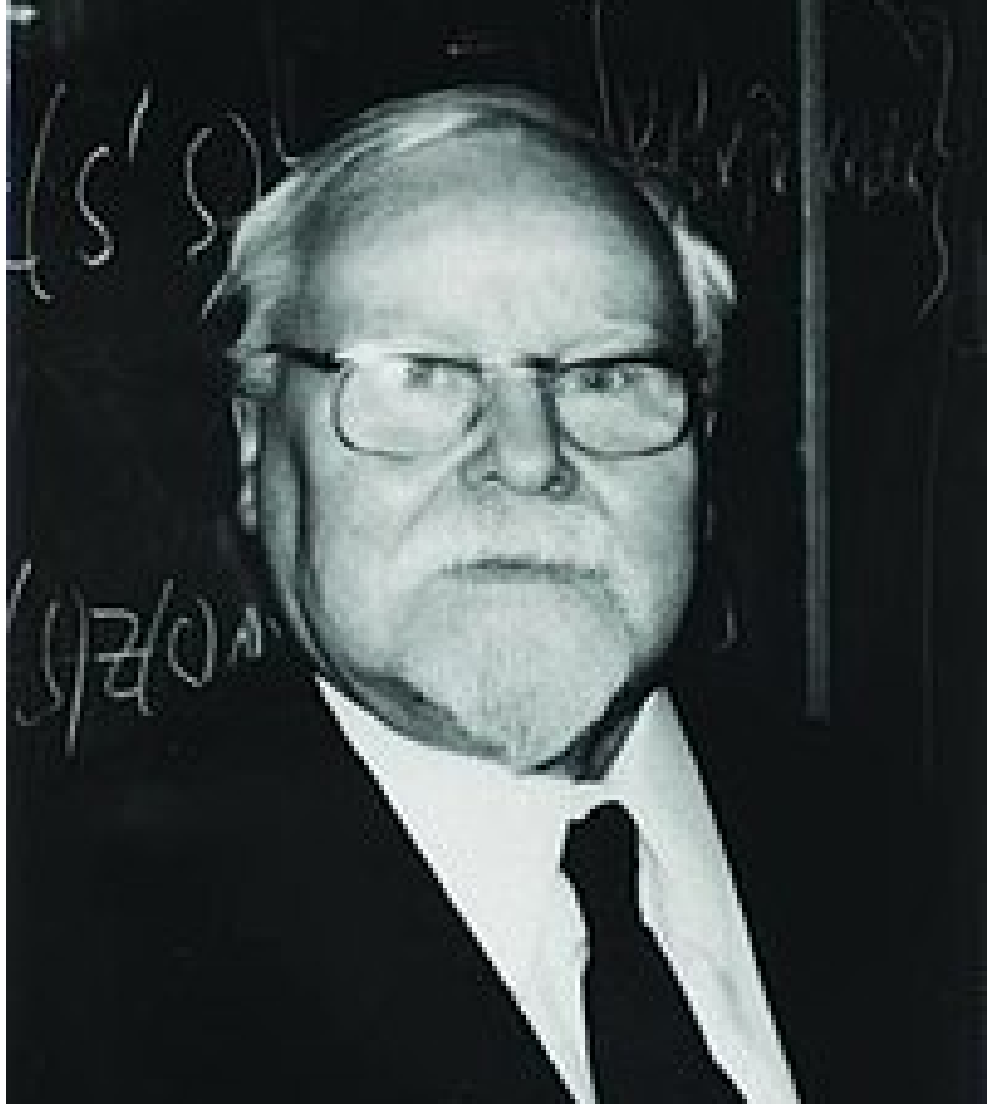
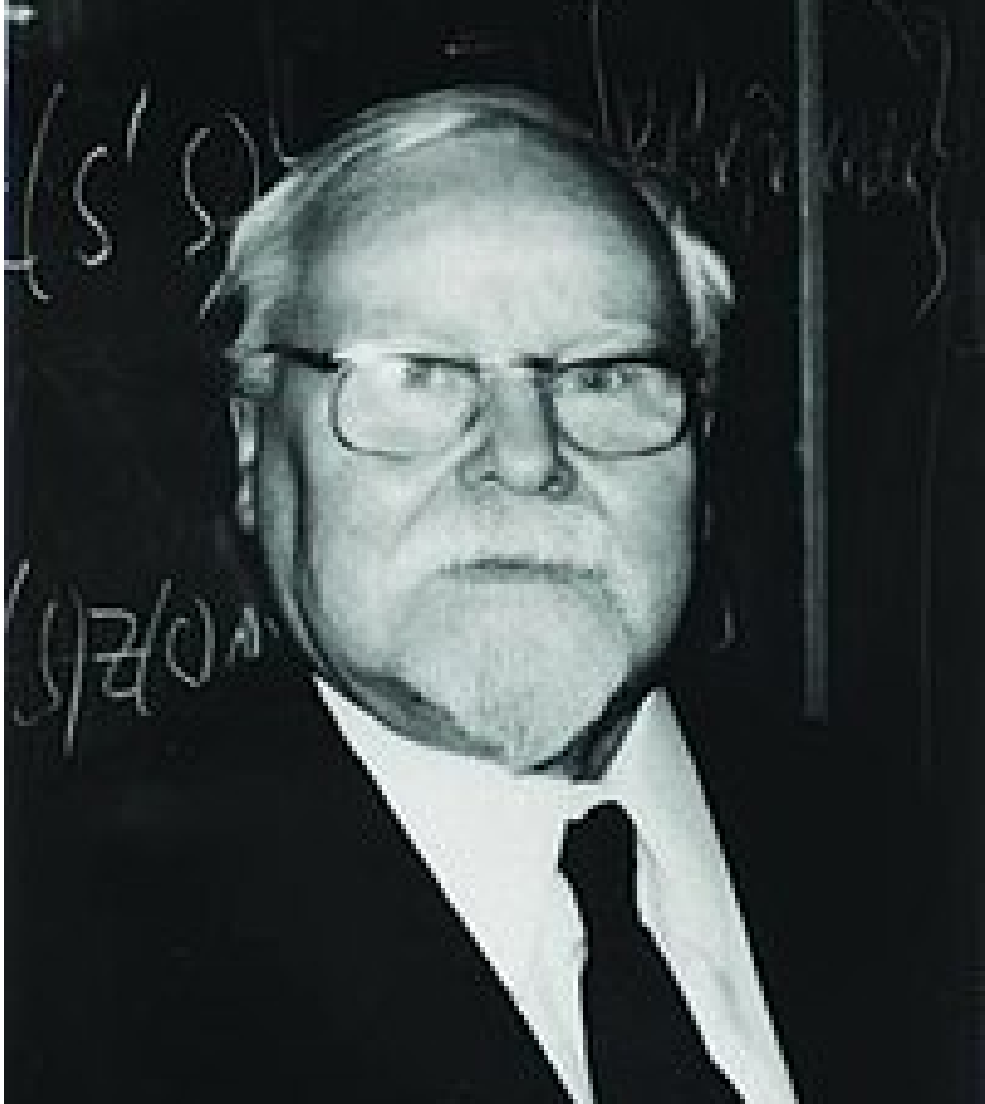
- Downside: Induces some bias in your parameter estimates
  - This means you technically get "the wrong answer" when you go to interpret coefficients
  - You can control how much bias you introduce, however!
- Upsides: Lots!
  - Helps models generalize to OOS data
  - Useful when you have multicollinearity
  - Can allow you to estimate models that would be otherwise unidentified
  - Easy to implement
  - Works with (almost) any type of model

Andrey Tikhonov (1906-1993)



Andrey Tikhonov (1906-1993)

- Soviet mathematician



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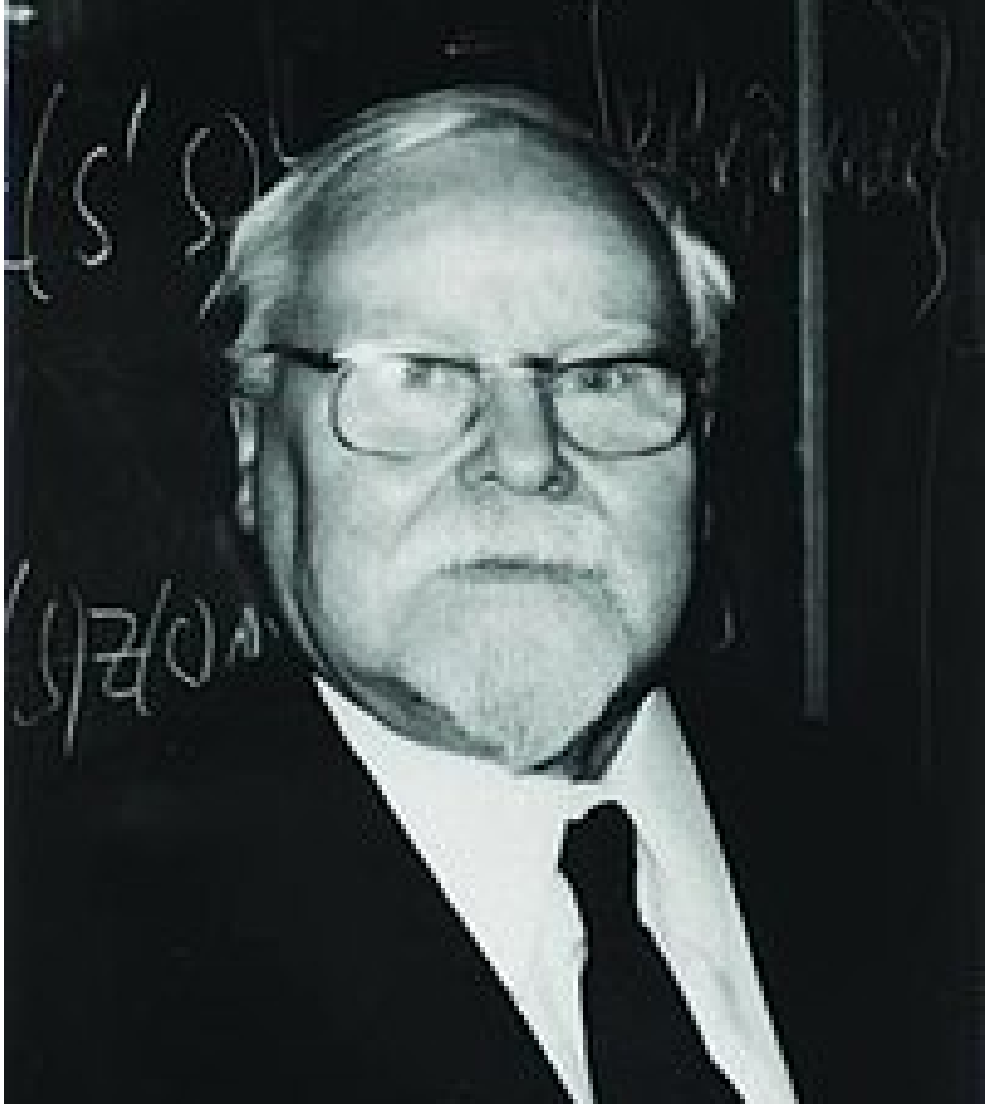

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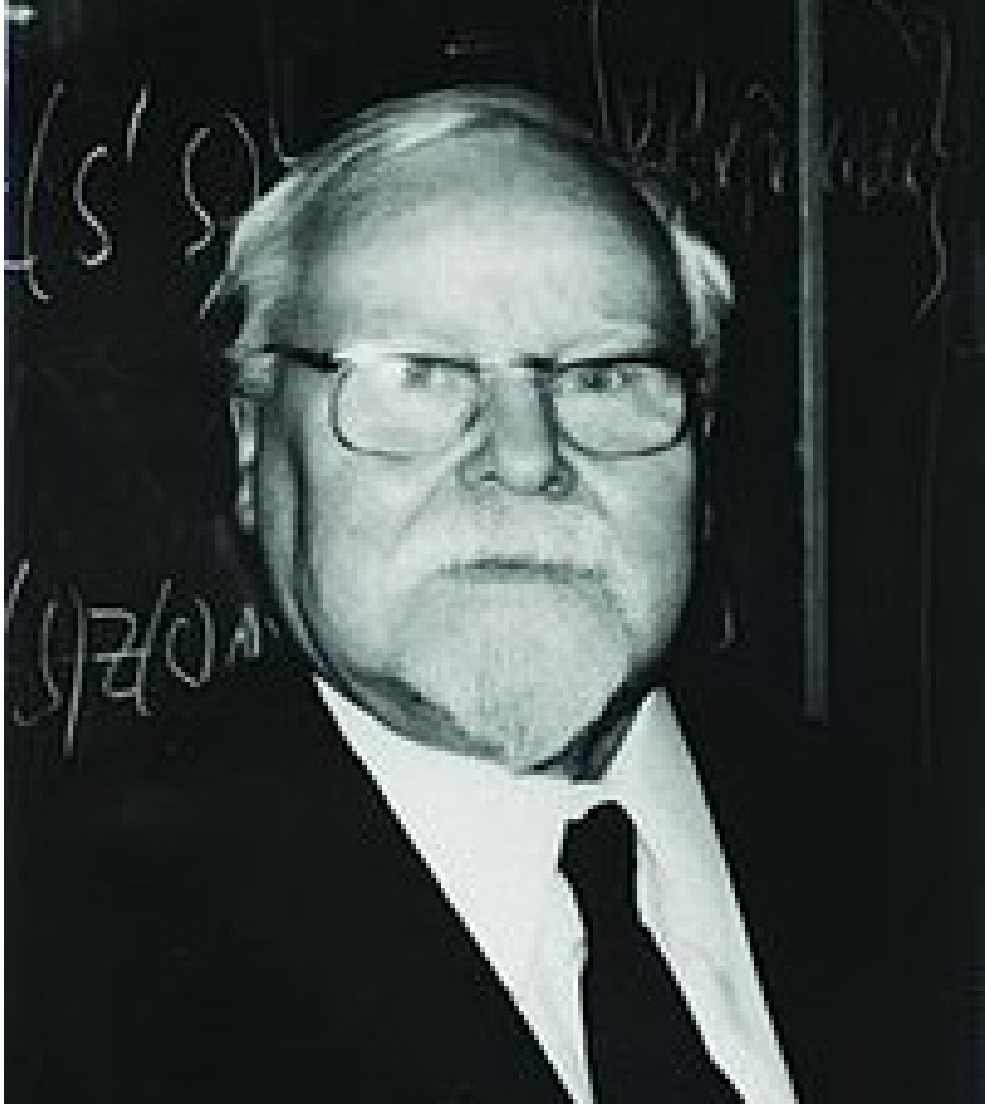

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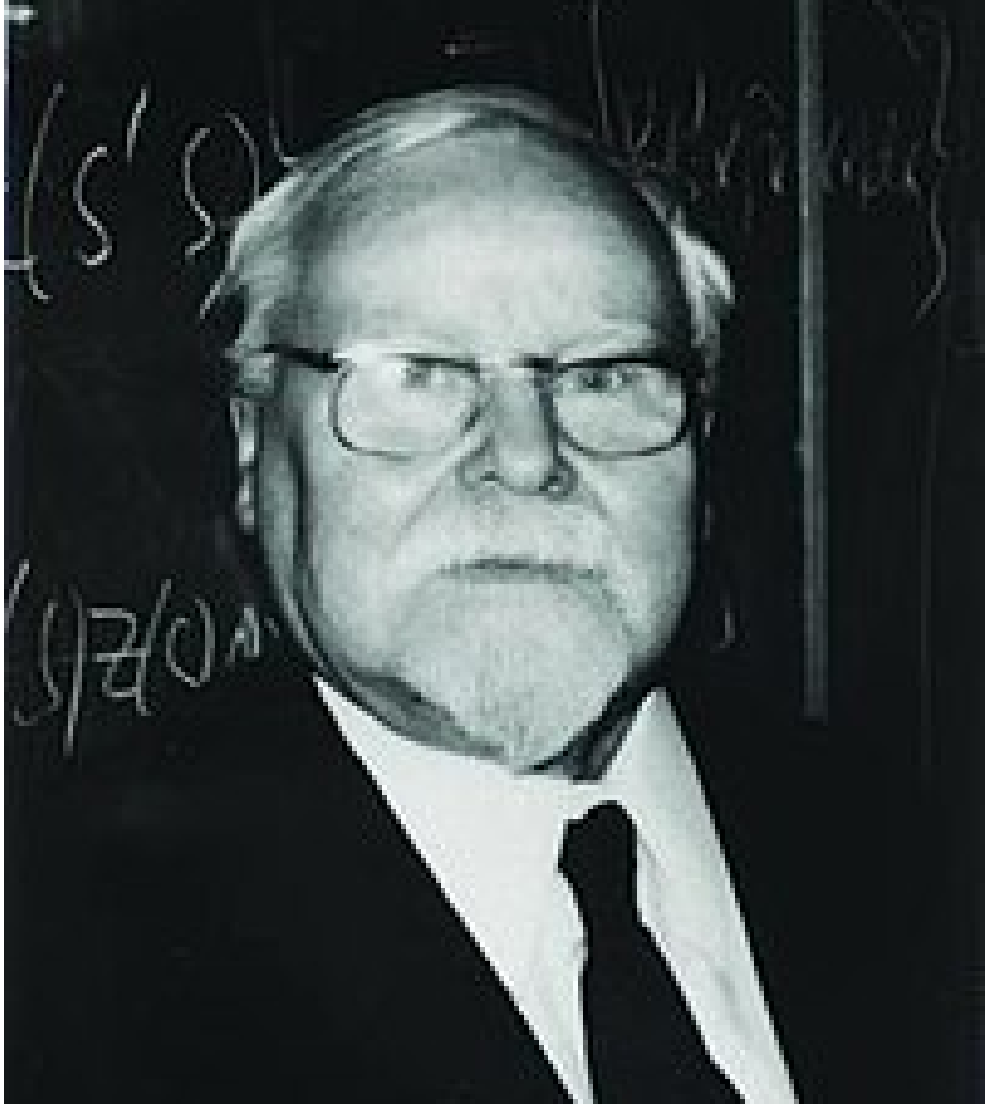
- Active in topology and mathematical physics (among other things)
- Recipient of the Lenin Prize (1966)
- Twice named Hero of Socialist Labor (1954, 1986)



Ridge Regression

- **Core Idea:** We will conduct a linear regression, but add a penalty proportional to the L^2 norm of the vector of coefficients, β
- This type of penalty is called the Ridge Penalty, Ridge Regularization, or L^2 Regularization
- Not just useful for linear regressions!
- Recall the OLS loss function that minimizes the squared error:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{\mathbf{x}_i, y_i \in \mathbf{X}} \left(y_i - \mathbf{x}_i \beta \right)^2$$

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- Now we add the Ridge penalty:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{\mathbf{x}_i, y_i \in \mathbf{X}} \left(y_i - \mathbf{x}_i \beta\right)^2 \underbrace{+\lambda ||\beta||_2^2}_{\text{Ridge Penalty}}$$

- Note that minimizing the SSE is the same as minimizing the MSE!

Ridge Regression

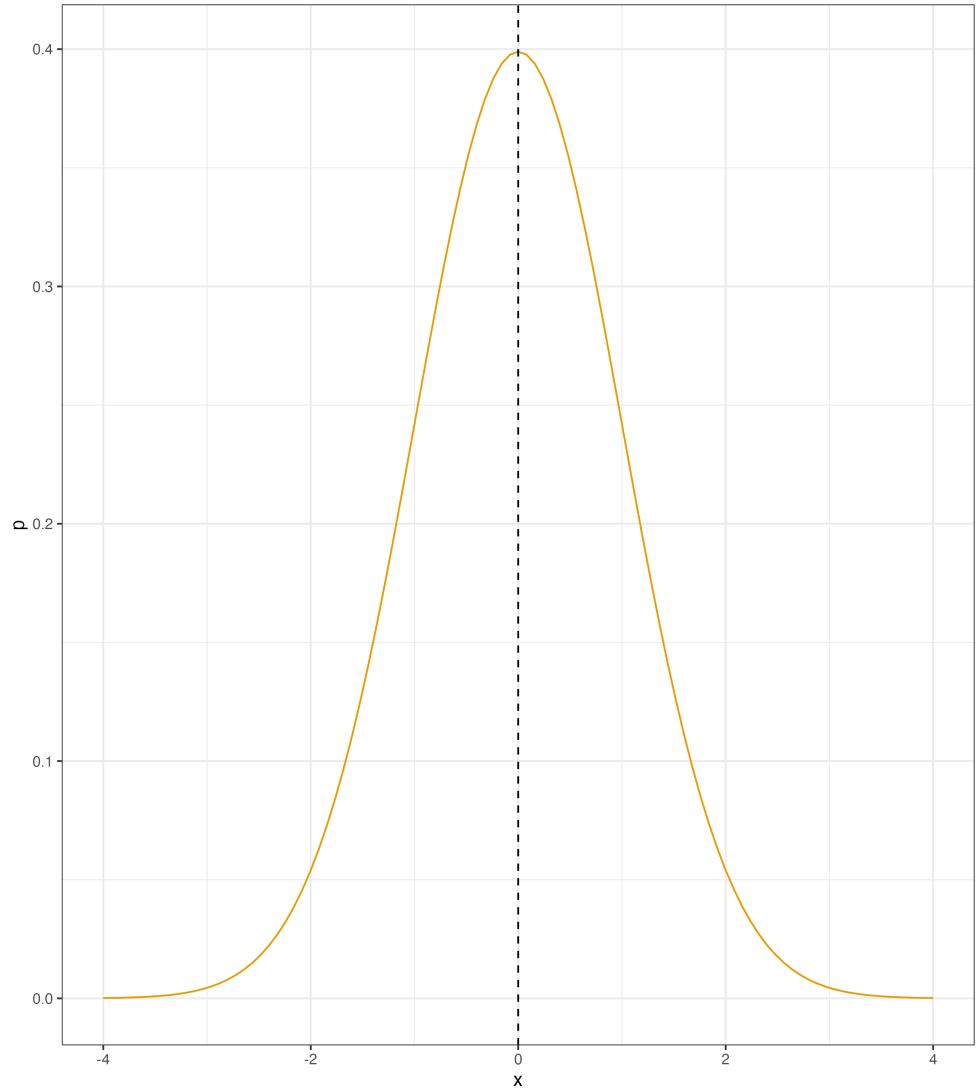
- Recall the loss function:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{\mathbf{x}_i, y_i \in \mathbf{X}} \left(y_i - \mathbf{x}_i \beta\right)^2 \underbrace{+\lambda ||\beta||_2^2}_{\text{Ridge Penalty}}$$

- So what happens here?
  - The left part of the argmin tries to minimize the MSE
  - The right part tries to minimize the length of the vector β
- So who wins?
  - It depends on λ, often called the *regularization parameter*
  - If $\lambda = 0$, there is no regularization, and we recover OLS exactly
  - For $\lambda > 0$, the optimization problem has to consider the size of β
  - As $\lambda \to \infty$, the only thing that matters is reducing the size of β until $||\beta||_2 = 0$
  - The larger λ is, the more β is shrunk toward zero
  - This is how you control how much regularization (and how much bias) you induce

The Ridge Penalty Puts a Normal Prior on β

- We think that the elements of β should be normally distributed
- They are *most likely* to be *nearly* zero
- The value of λ controls how much shrinkage toward zero is experienced
- Another way to think about λ is that it controls the *variance* of the normal prior
- When you get to multilevel models, think of random effects as similar to regularization!
- Typically, we pick λ to maximize OOS predictive performance, either by holding out a *test set* or through cross-validation



One Quick Note on Maximizing a Penalized Likelihood

- This is how we minimize squared error:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_i \left(y_i - \mathbf{x}_i\beta\right)^2 + \lambda||\beta||_2^2$$

- This is how we maximize the log likelihood:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmax}} \; -\sum_i \left(y_i - \mathbf{x}_i\beta\right)^2 - \lambda||\beta||_2^2$$

What about other types of regularization?

- Remember that we said overfitting occurs if your parameters are too big or if you have too many
- Ridge only solves the first problem. What about the second?
- Turns out, we can do this using Least Absolute Shrinkage and Selection Operator (LASSO)
- This is implemented through another penalized loss function

Robert Tibshirani (born 1956)

- Professor of Statistics at Stanford University
- Student of Bradley Efron
- Invented Generalized Additive Models (GAMs)
- Wrote *The Elements of Statistical Learning*
- Wrote *An Introduction to Statistical Learning*

LASSO Regression

- **Core Idea:** We will conduct a linear regression, but add a penalty proportional to the L^1 norm of the vector of coefficients, β
- This type of penalty is called the LASSO Penalty, LASSO Regularization, or L^1 Regularization
- Still not just useful for linear regressions!
- Recall the OLS loss function that minimizes the squared error:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{\mathbf{x}_i, y_i \in \mathbf{X}} \left(y_i - \mathbf{x}_i \beta\right)^2$$

- Now we add the LASSO penalty:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{\mathbf{x}_i, y_i \in \mathbf{X}} \left(y_i - \mathbf{x}_i \beta\right)^2 \underbrace{+\lambda ||\beta||_1}_{\text{LASSO Penalty}}$$

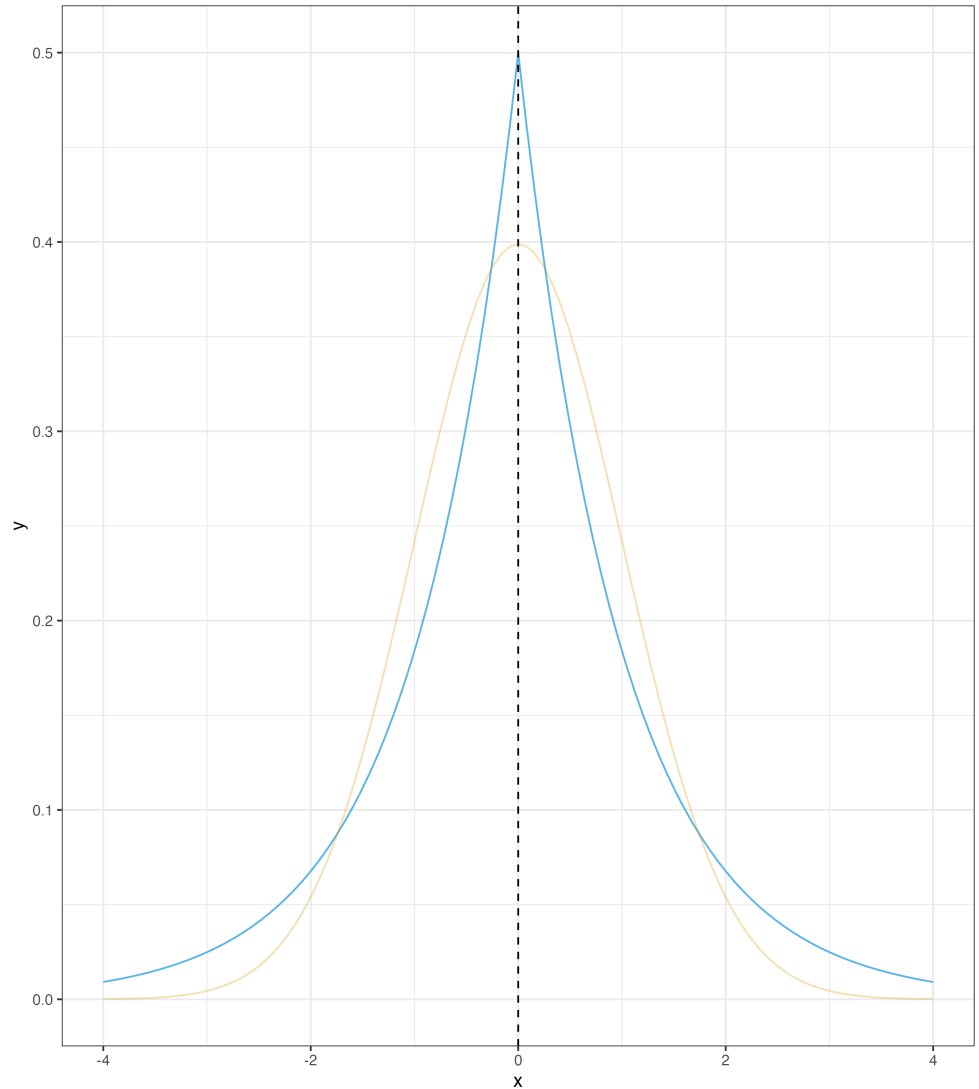
LASSO Regression

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{\mathbf{x}_i, y_i \in \mathbf{X}} \left(y_i - \mathbf{x}_i \beta\right)^2 \underbrace{+\lambda ||\beta||_1}_{\text{LASSO Penalty}}$$

- So what happens here?
  - The left part of the argmin tries to minimize the MSE
  - The right part tries to minimize the length of the vector β, but in kind of a different way from the Ridge penalty!
- So what changes?
  - Note that as $\beta, \epsilon \to 0, |\beta + \epsilon| - |\beta| > (\beta + \epsilon)^2 - \beta^2$
  - This gives a loss function with a LASSO penalty extra incentive to force some coefficients to be zero!
  - The Ridge penalty will uniformly shrink coefficients toward zero, while the LASSO penalty will force some number of coefficients to be *precisely* zero
  - This effectively drops variables with less predictive value from your model (which is the "selection" part of LASSO)
  - Higher values of λ will drop more variables

LASSO Penalty Puts a Laplace Prior on β

- This means we think that the elements of β should be Laplace distributed
- This means they are *most likely* to be *exactly* zero, but with enough evidence they can take on any value
- The value of λ controls how aggressively coefficients are forced to be zero
- Again, we pick the λ value to maximize OOS predictive performance, either by holding out a *test set* of some data or through cross-validation



More Resampling Methods

The Central Limit Theorem

- Core to statistics, because it says "normal distributions are worth understanding" even though most data is not actually normally distributed!
- $\{X_1, X_2, \ldots, X_n\}$ are i.i.d. random variables with:
  - $\mathrm{E}[X_i] = \mu$
  - $\mathrm{Var}[X_i] = \sigma^2$
- We define the *sample mean*: $\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$

The Central Limit Theorem

- As n grows large, the *distribution of sample means* converges to:

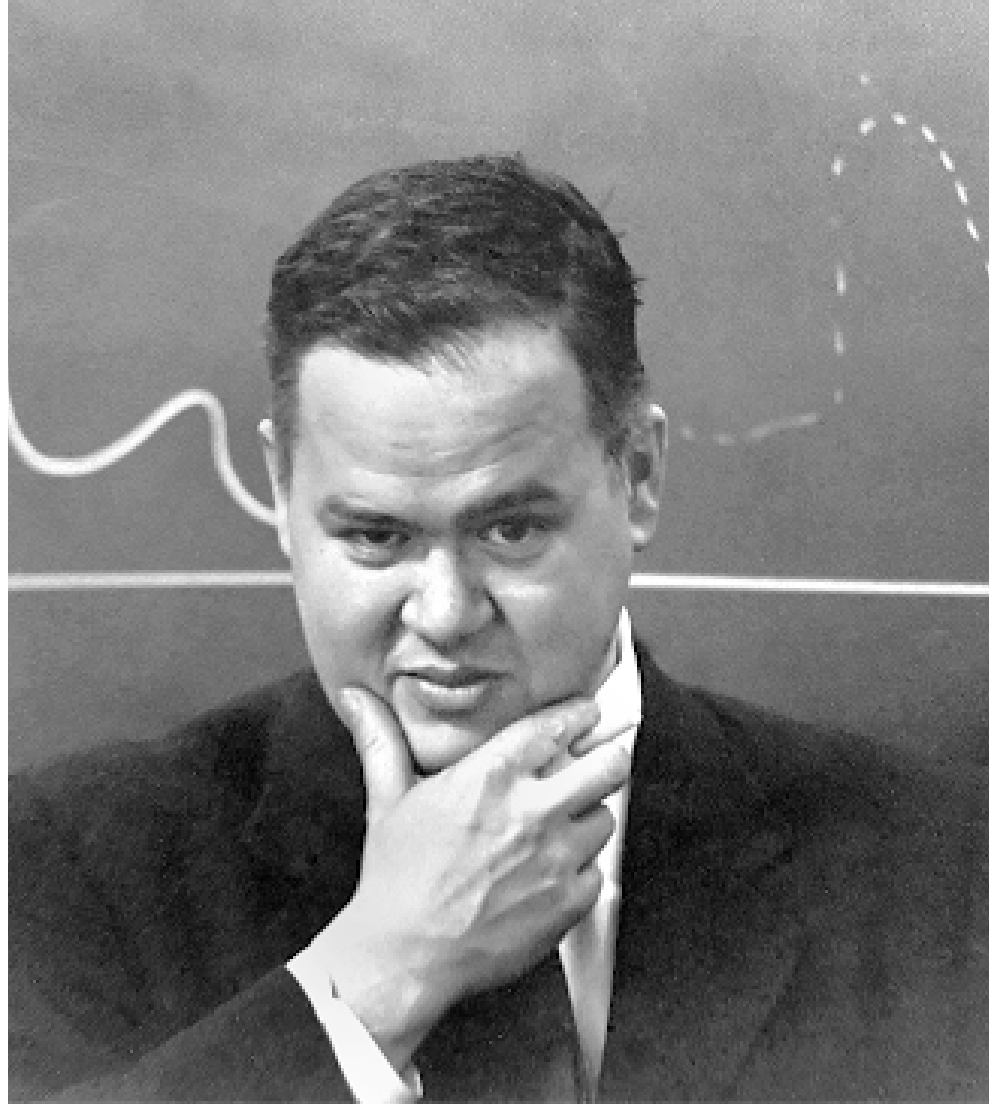
$$\bar{X}_i \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right)$$

- This holds even if X_i is not normally distributed!
- This only applies to sample means!

Resampling Methods

- We want to reason about populations from samples
- The CLT helps a lot, but it doesn't do everything!
- **Core idea:** The distribution of the data you have is your best guess at the distribution of the population
- But what do we do with this?

John Tukey (1915-2000)



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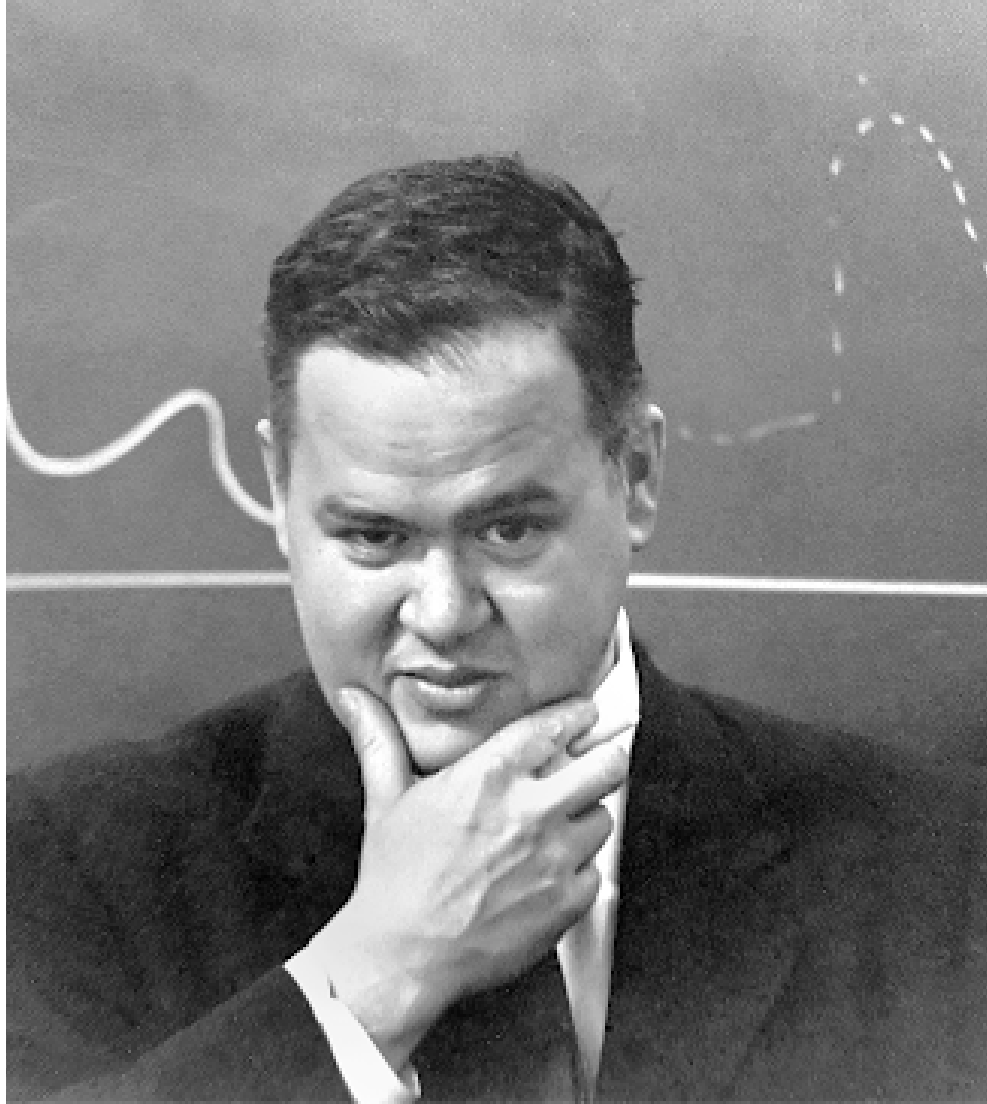

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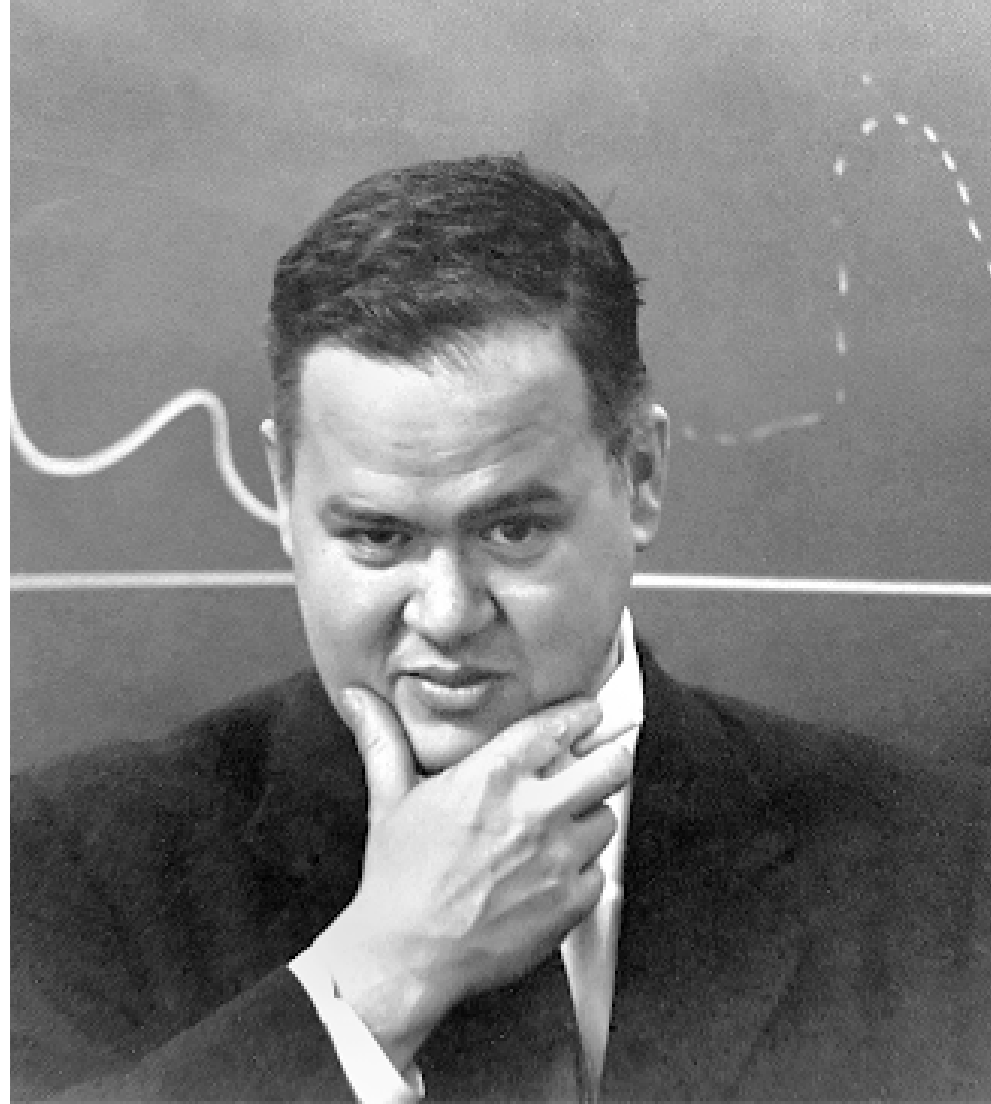

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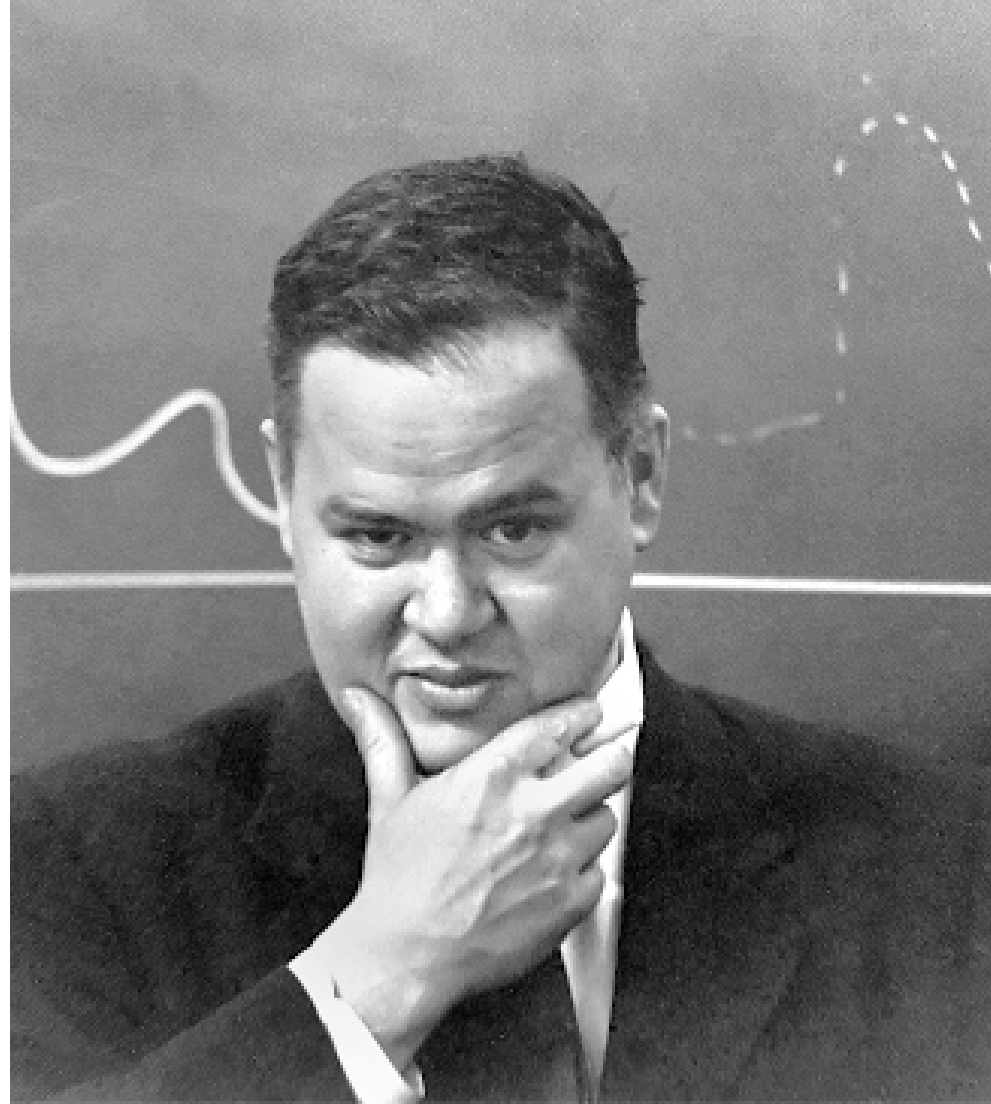

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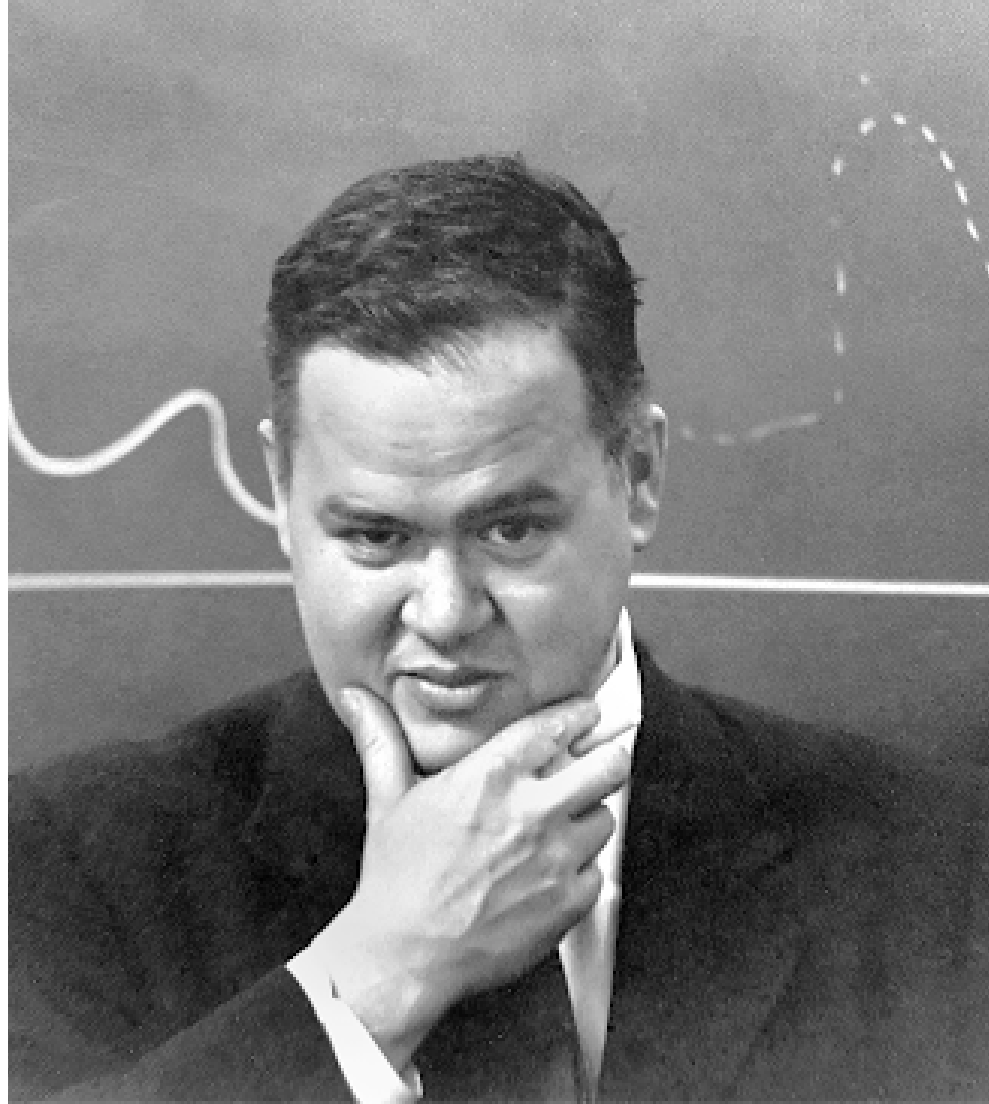

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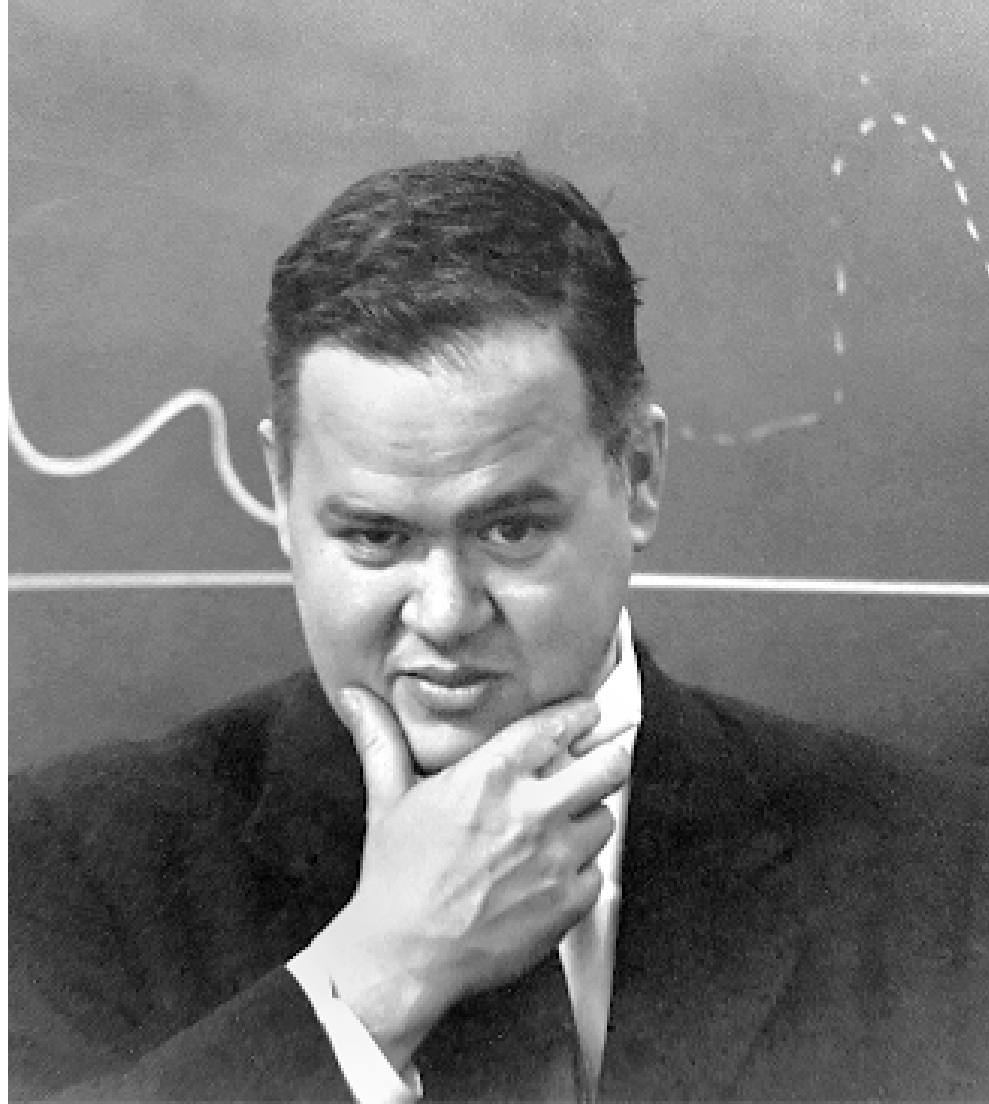

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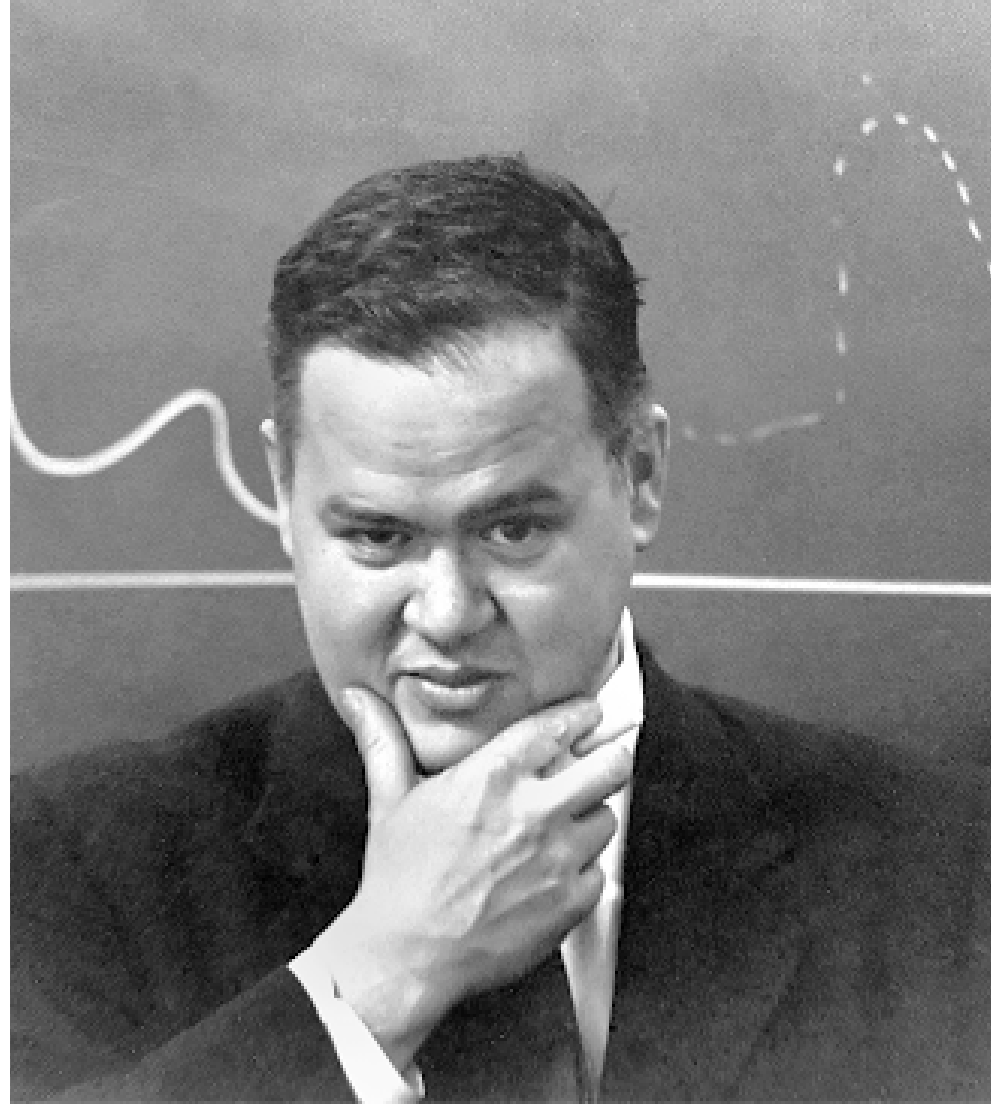
- Certified badass



What did Tukey give us today?

The Jackknife

- Thanks Tukey!
- "Rough and ready" tool to solve statistical problems when the exact solution might be hard or unknown
- **Core idea:** We take our data, make new datasets by dropping single observations, compute our statistic of interest, and then look at the distribution

The Jackknife

- We have $\{X_1, X_2, \ldots, X_n\}$, which are i.i.d. samples from some population
- We care about some estimator or statistic in the population, $f(X_i)$ We often think that: $\mathrm{E}[f(X_i)] = f\left(\{X_1, X_2, \ldots, X_n\}\right)$
- But this tells us nothing about the bias or variance of that estimator!

The Jackknife

- From your dataset of length n, create n new resampled datasets of length $n - 1$, each missing one observation
- Compute your estimator or statistic on each resampled dataset
- Aggregate these statistics to get your jackknife estimate
  - The mean of the estimator in jackknife samples can be used to understand bias
  - The variance of the estimator in jackknife samples can be used to quantify uncertainty
  - Does not require the CLT to apply to the estimator!

The Bootstrap

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- **Resampling's Core Idea:** The distribution of the data you have is your best guess at the distribution of the population

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The Bootstrap

- **Resampling's Core Idea:** The distribution of the data you have is your best guess at the distribution of the population
- **Jackknife's Core Idea:** We take our data, make new datasets by dropping single observations, compute our statistic of interest, and then look at the distribution
- **Bootstrap's Core Idea:** We take our data and make new datasets by resampling *with replacement* from our original dataset to approximate the population. Then we compute our statistic of interest on each resampled dataset and look at the distribution

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  - MacArthur Prize Fellowship
  - Membership in the National Academy of Sciences and the American Academy of Arts and Sciences
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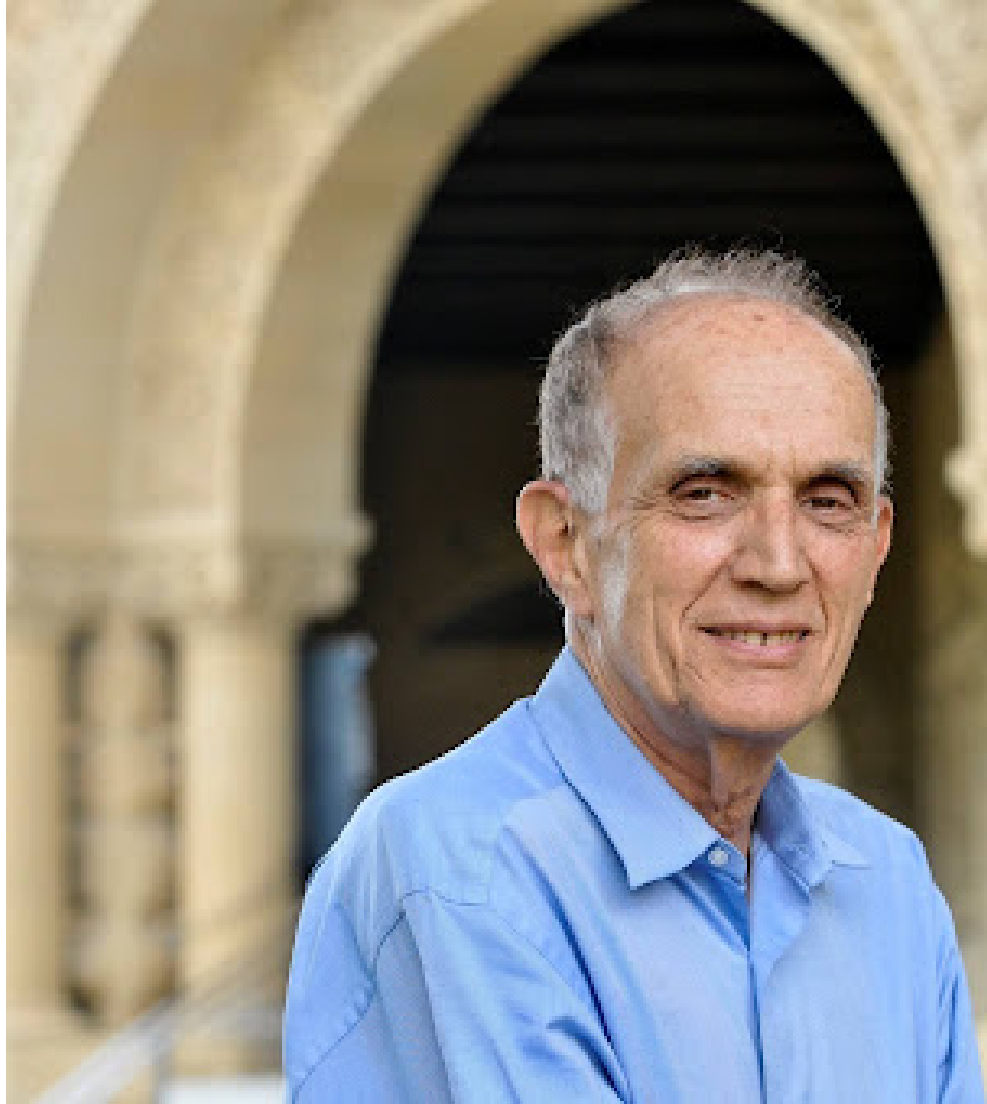

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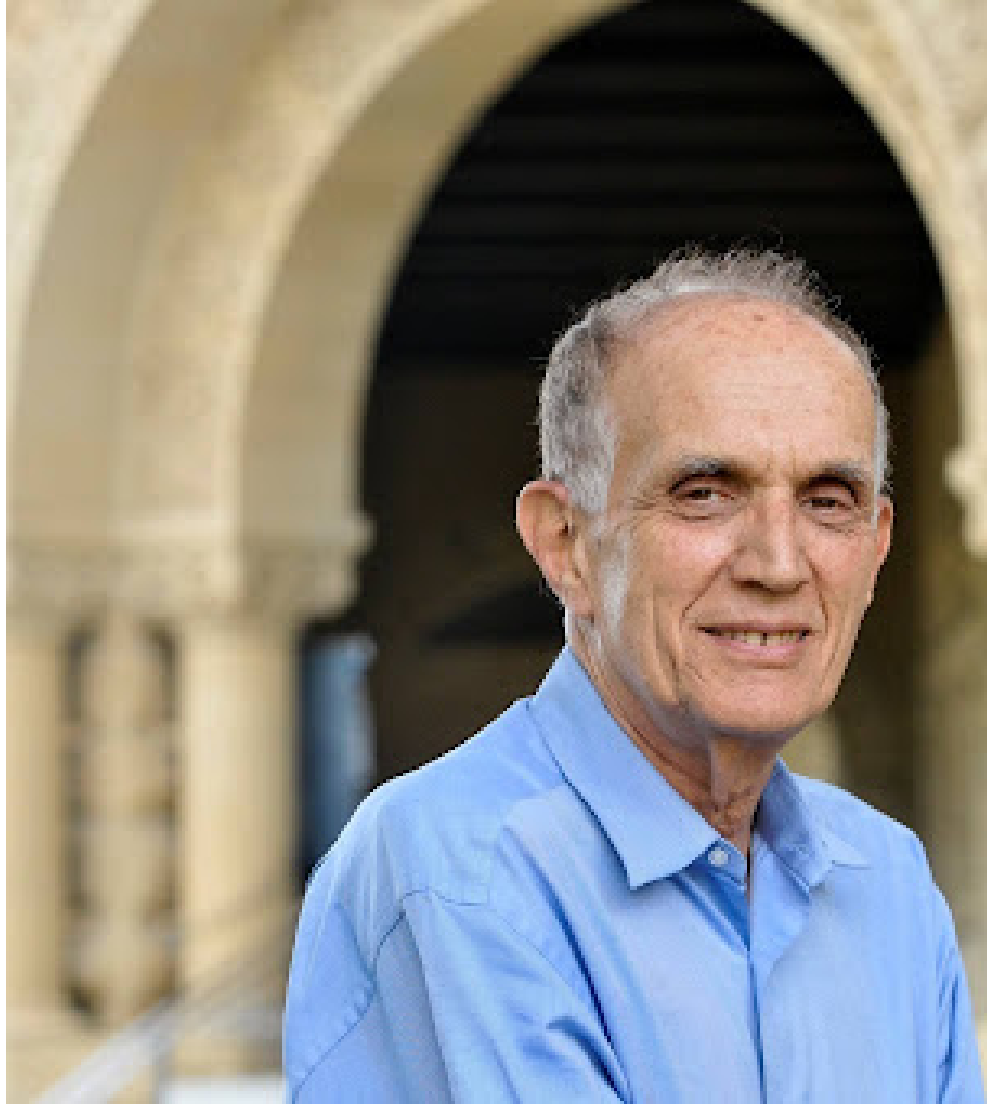

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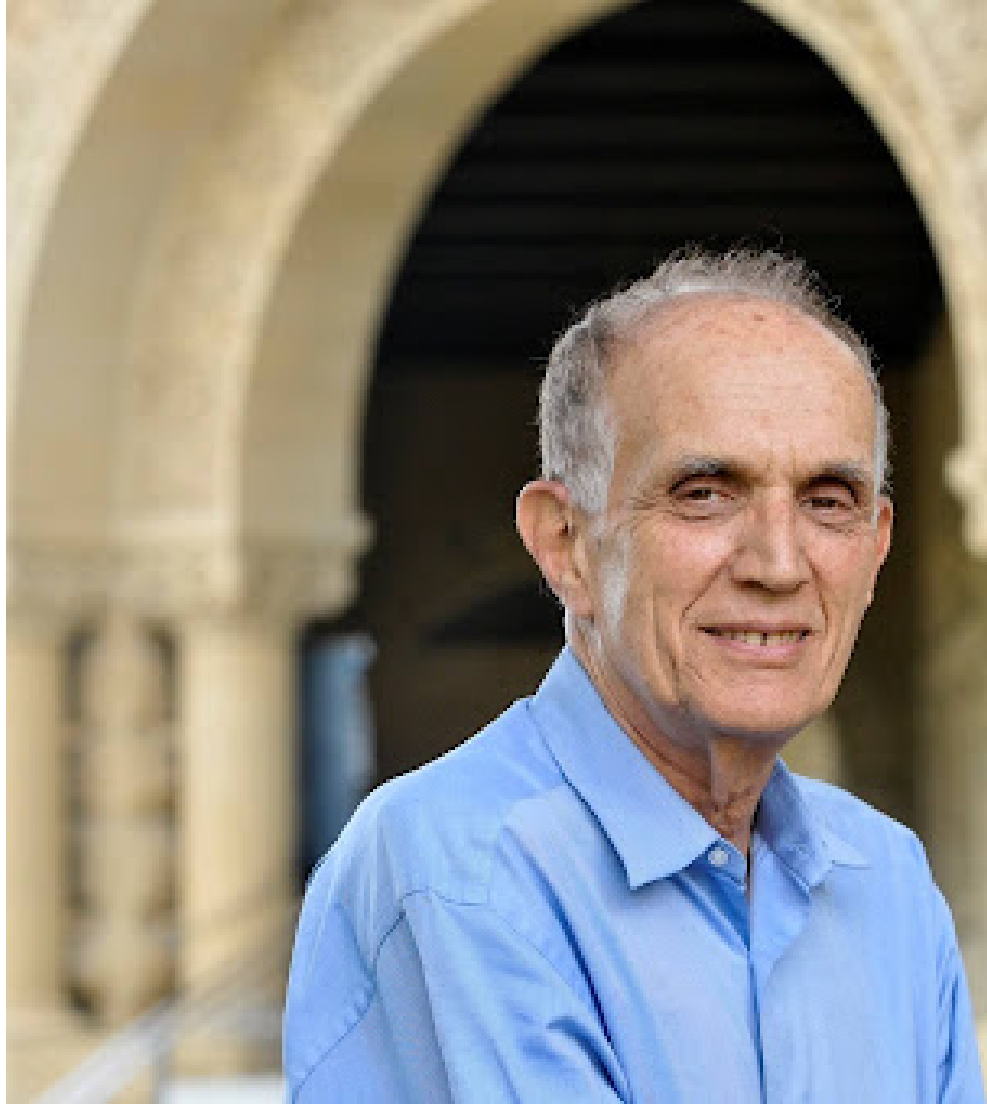

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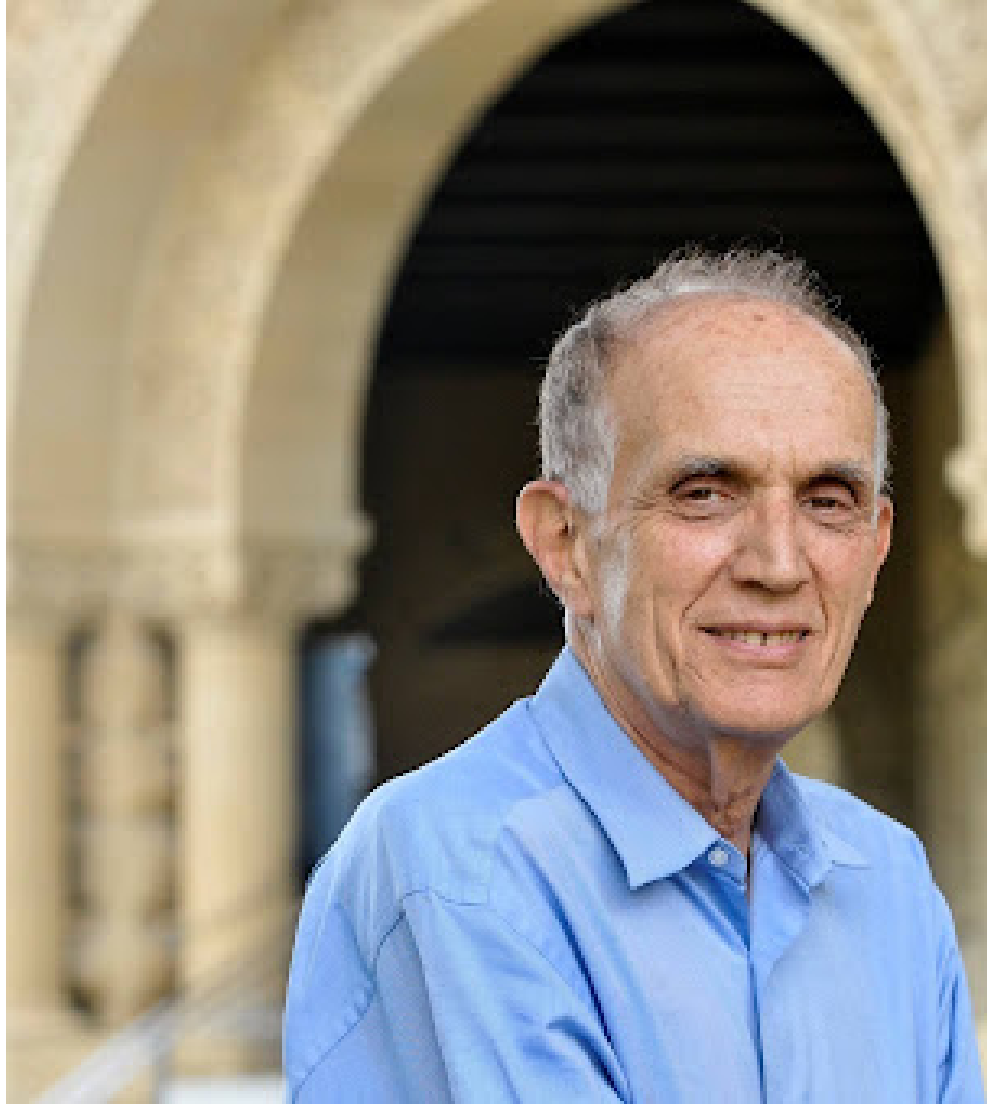

The Bootstrap

- It works for basically anything!
- Your data describes an *empirical distribution function* - this is an approximation of the cumulative distribution function (CDF)
- The empirical distribution function (eCDF) converges to the CDF
- The bootstrap uses resampling with replacement to build new eCDFs
- Because we resample with replacement, we can have many more eCDFs *with the same sample size as the original data* than the jackknife
- Data are guaranteed to be drawn from the population of interest!
- Often used for bias, variance, and constructing confidence intervals
- Does not require the CLT to apply to your estimator!

How to Bootstrap

1. Compute your estimate in the full sample with N observations
2. Draw M bootstrap samples, each of length N, from the original dataset *with replacement*
3. Compute your estimate on each bootstrap sample
4. Use the distribution of bootstrap estimates to:

- Check the original estimate for bias (using the mean value)
- Find the variance of a standard error of the estimate (using the variance or sd)
- Construct a confidence interval (by looking at the end points of the middle 95% of the distribution of bootstrap estimates)

Applied Bootstrapping

```r
d <- data.frame(x = rnorm(1e2))
d$y <- -1.5 + 3*d$x + rnorm(1e2)

m <- lm(y~x, d)


summary(m)$coefficients
```

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#              Estimate Std. Error   t value     Pr(>|t|)
# (Intercept) -1.486122 0.09547956 -15.56482 3.078629e-28
# x            3.101451 0.09144205  33.91712 5.913505e-56
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#        x
# 3.101451
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1. Write a function that extracts the coefficient we care about
2. Then we add resampling
3. Run it a bunch of times

```
Beta1Boot <- function(d){

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replicate(5, Beta1Boot(d))
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```

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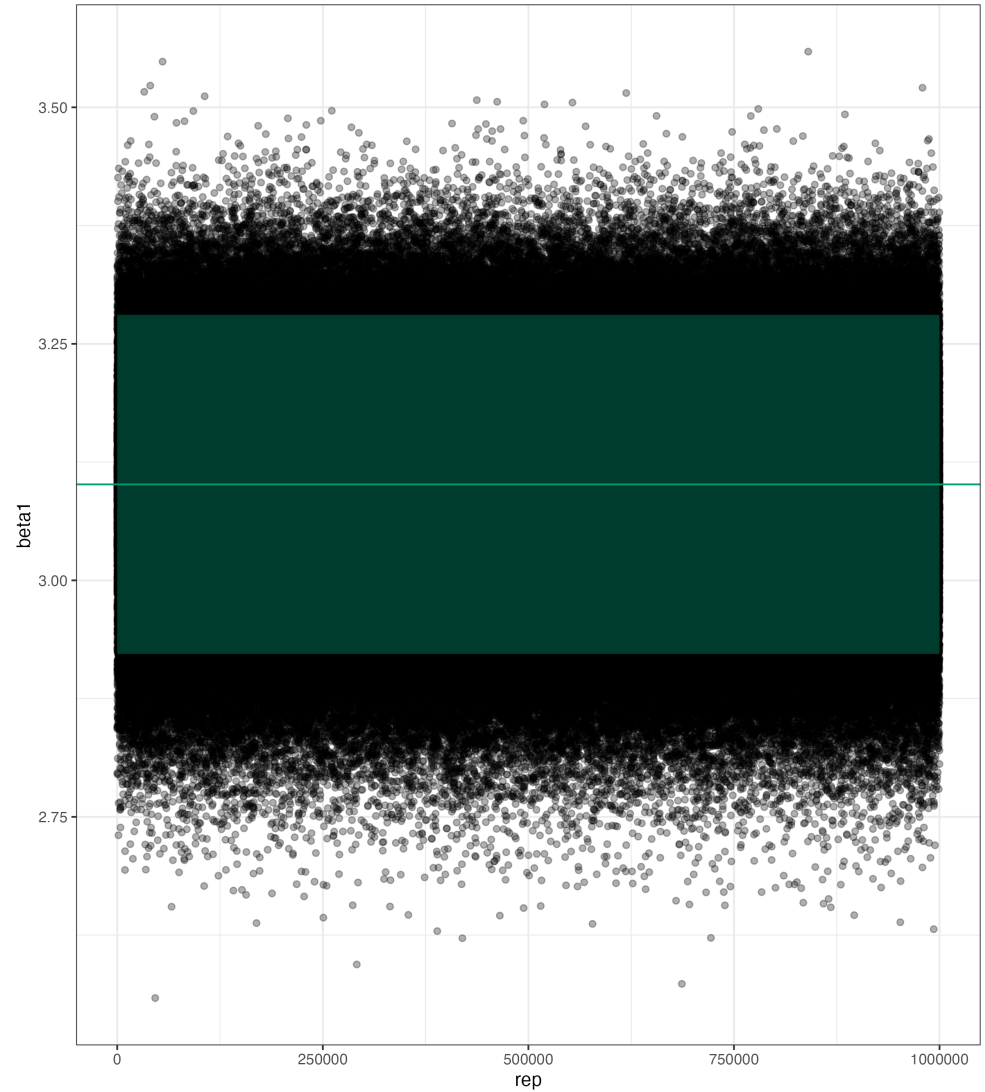
N_boot <- 1e6
boot <- data.frame(rep = 1:N_boot,
                   beta1 = replicate(N_boot, Beta1Boot(d)))
```

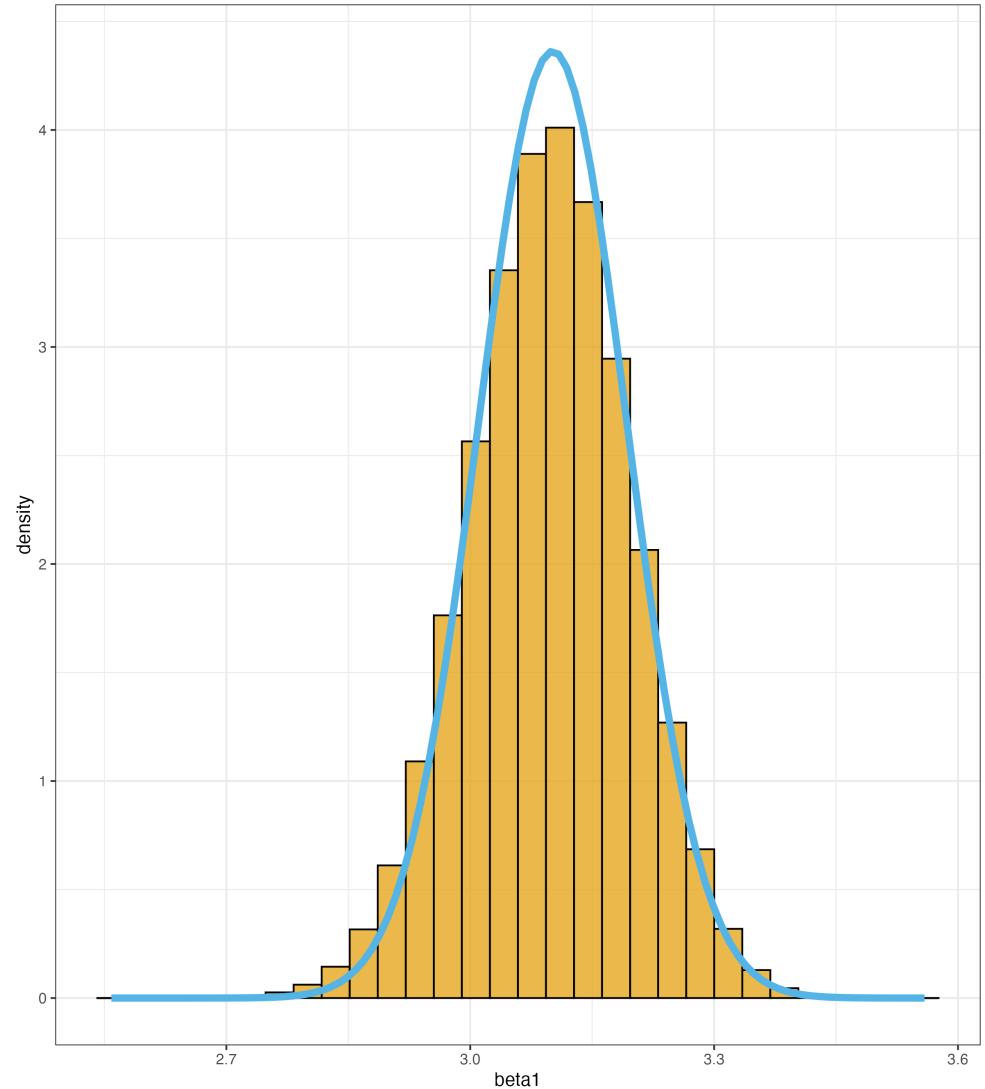
Applied Bootstrapping

```
ggplot(boot, aes(x = rep, y = beta1)) +
  geom_point(alpha = 0.3) +
  geom_hline(
    aes(
      yintercept =
        summary(m)$coefficients[2, 1]),
      color = okabeito_colors(3)
  ) +
  geom_ribbon(
    aes(
      ymin =
        summary(m)$coefficients[2, 1] -
        1.96*summary(m)$coefficients[2, 2],
      ymax =
        summary(m)$coefficients[2, 1] +
        1.96*summary(m)$coefficients[2, 2]
    ),
    fill = okabeito_colors(3),
    alpha = 0.4
  ) +
  theme_bw()
```



Applied Bootstrapping

```
ggplot(boot, aes(x = beta1)) +
  geom_histogram(
    aes(y = after_stat(density)),
    bins = 30,
    color = 'black',
    fill = okabeito_colors(1),
    alpha = 0.7
  ) +
  geom_function(
    fun = dnorm,
    size = 2,
    color = okabeito_colors(2),
    args = list(
      mean = summary(m)$coefficients[2, 1],
      sd = summary(m)$coefficients[2, 2]
    )
  ) +
  theme_bw()
```



Applied Boostrapping

- `lm()` estimate, SE, and 95% CI:

```
summary(m)$coefficients[2,1:2]
c(summary(m)$coefficients[2,1] - 1.96*summary(m)$coefficients[2,2],
  summary(m)$coefficients[2,1] + 1.96*summary(m)$coefficients[2,2])
```

- Bootstrapped estimate, SE, and 95% CI:

```
c(mean(boot$beta1), sd(boot$beta1))
quantile(boot$beta1, c(0.025, 0.975))
```

Applied Boostrapping

- `lm()` estimate, SE, and 95% CI:

```r
summary(m)$coefficients[2,1:2]

#   Estimate Std. Error
# 3.10145067 0.09144205

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# [1] 2.922224 3.280677
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- Bootstrapped estimate, SE, and 95% CI:

```r
c(mean(boot$beta1), sd(boot$beta1))

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#     2.5%    97.5%
# 2.897704 3.286801
```

Wrap Up

Recap

- Regularization puts a penalty on the likelihood proportional to the length of the parameter vector
  - This shrinks parameters toward zero
  - Ridge regression shrinks them slightly
  - LASSO regression tends to force parameters to be zero
- Resampling is a way to estimate things that are difficult to know analytically
  - The jackknife drops single observations to create new datasets of approximately the same size
  - The bootstrap resamples *with replacement* to create new datasets the same size as your old data
- Regularization and the bootstrap are probably the two most generalizable applied techniques you'll learn here!

Final Thoughts

- PollEv.com/klintkanopka