

APSTA-GE 2352

Statistical Computing: Lecture 7

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NYU Grey Art Gallery

RIVER CENTER

WASHINGTON PL



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Announcements

- PS3 is now late
- PS4 is posted, due in two weeks
 - This is all numerical optimization
 - The PCA activity, while cool, got punted to PS5
 - Happened because the optimization activities are plenty long on their own

Check-In

- PollEv.com/klintkanopka

Motivating Problem

Numerical Optimization

- We have a function, $f(\mathbf{X}, \theta)$, where \mathbf{X} is data and θ are parameters
- Numerical optimization answers the question:

$$\operatorname{argmin}_{\theta} f(\mathbf{X}, \theta)$$

- From last week, remember argmin (or argmax) says: what value of θ minimizes (or maximizes) the output of $f(\mathbf{X}, \theta)$?
- Note that now \mathbf{X} is a matrix argument (that also contains our outcome, y) and θ is (often) a vector argument
- If we are using argmin, $f(\mathbf{X}, \theta)$ is often referred to as a *loss function*
 - Our goal is to write problems such that when we minimize the loss function, we've found the answer!

Just thinking about argmin

- How could we use a computer to minimize this?

$$\operatorname{argmin}_x x^2 - 2x - 3$$

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- Take the derivative with respect to x , set $\frac{df}{dx} = 0$, and solve

Just thinking about argmin

- How could we use a computer to minimize this?

$$\operatorname{argmin}_x x^2 - 2x - 3$$

- Take the derivative with respect to x , set $\frac{df}{dx} = 0$, and solve
- Make a list of possible x values, plug them in, and check which one gives the lowest value

Just thinking about argmin

- How could we use a computer to minimize this?

$$\operatorname{argmin}_x x^2 - 2x - 3$$

- Take the derivative with respect to x , set $\frac{df}{dx} = 0$, and solve
- Make a list of possible x values, plug them in, and check which one gives the lowest value
- Plot it and eyeball it

Just thinking about argmin

- How could we use a computer to minimize this?

$$\operatorname{argmin}_x x^2 - 2x - 3$$

- Take the derivative with respect to x , set $\frac{df}{dx} = 0$, and solve
- Make a list of possible x values, plug them in, and check which one gives the lowest value
- Plot it and eyeball it
- Some secret fourth thing???

How do we optimize?

- Remember that analytic solutions can be hard/impossible and grid search can be inefficient/slow/imprecise
- Numerical optimization leverages an algorithm to find a solution faster, more efficiently, and more precisely than grid search
- There are LOTS of algorithms with different tradeoffs
- We will develop my favorite one today
 - It might actually be my all-time favorite algorithm?

Tools

Single Precision Floating Point Numbers

- In computers, numbers are typically stored using 32 bits of memory
 - Each bit can have a value of either 0 or 1
 - This means that there are only 4,294,967,296 possible values
 - This has to cover every possible positive number, negative number, decimal, or super huge value
- The way computers handle this is using floating point numbers
 - Think of this as scientific notation
 - $2,395,423 \rightarrow 2.395423 \times 10^6$
- How is this stored?
 - One bit stores the sign (+/-)
 - Eight bits store the exponent (256 values, ranging from -126 to 127 with all 0s or 1s held back)
 - 23 bits stores the mantissa (this is about 6-8 decimal places of precision)
 - Importantly, the more extreme the value of the exponent, the less precise the entire number
 - This means nearly all computations contain some amount of rounding error

Monotonic Functions and Transformations

- A function is monotonic if it preserves order
- For a monotonic function, f :
 - $a > b \implies f(a) > f(b)$
- We will use the *log transformation* all the time in numerical optimization
- Because $\log(x)$ is a monotonic function:

$$\operatorname{argmin}_x f(x) = \operatorname{argmin}_x \log f(x)$$

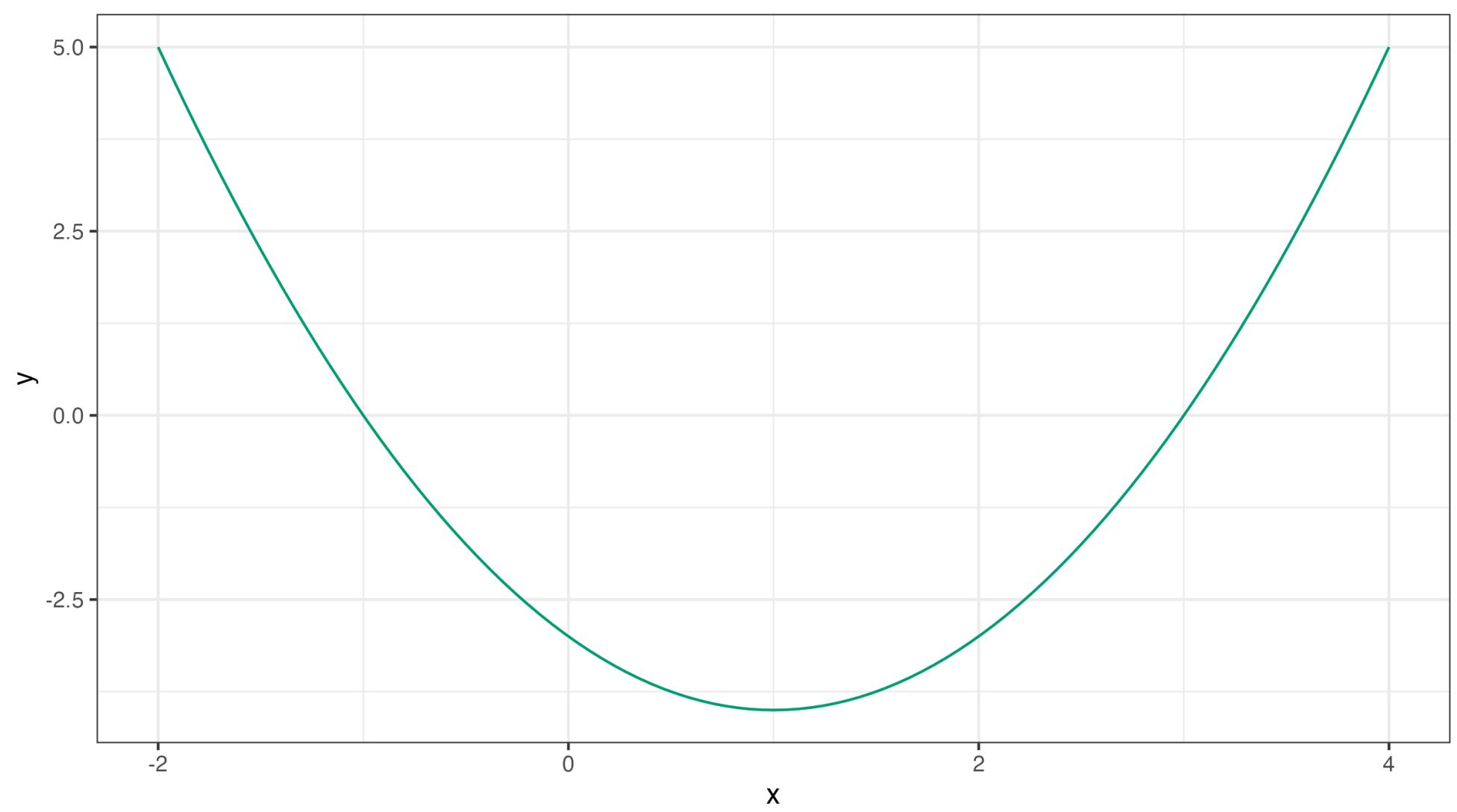
- You can turn multiplication into addition, leading to less extreme exponent values
 - $\log(ab) = \log(a) + \log(b)$
- The log transform maps positive numbers with negative exponents to negative numbers (with smaller exponents) and positive numbers with positive exponents into positive numbers (with smaller exponents)

Derivatives and Gradients

- Recall the derivative of a function with respect to a variable x is the slope of a line tangent to the function at a specific value of x
- The gradient is the multivariate (read: vector) generalization of the derivative
 - The gradient constructs a column vector of partial derivatives
 - If you think of a multivariate function as a surface, the gradient is a vector that points "uphill"
 - We write the derivative of f with respect to x as: $\frac{df}{dx}$
 - If f takes a vector argument, \mathbf{x} , of dimension k , we write the gradient of f as: ∇f

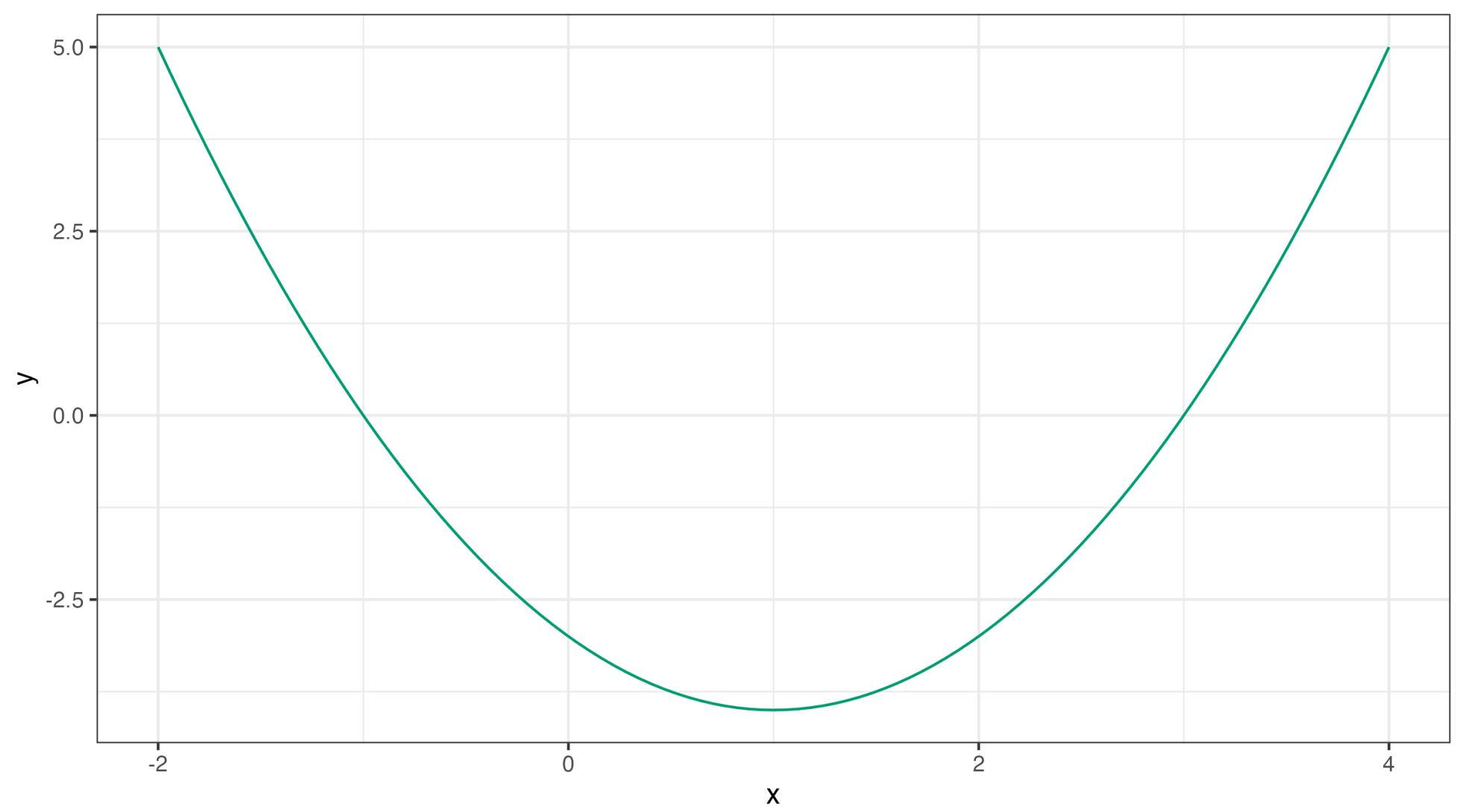
$$\nabla f = \frac{\partial f}{\partial \mathbf{x}} = \left[\frac{\partial f}{\partial x_1} \frac{\partial f}{\partial x_2} \cdots \frac{\partial f}{\partial x_k} \right]^\top$$

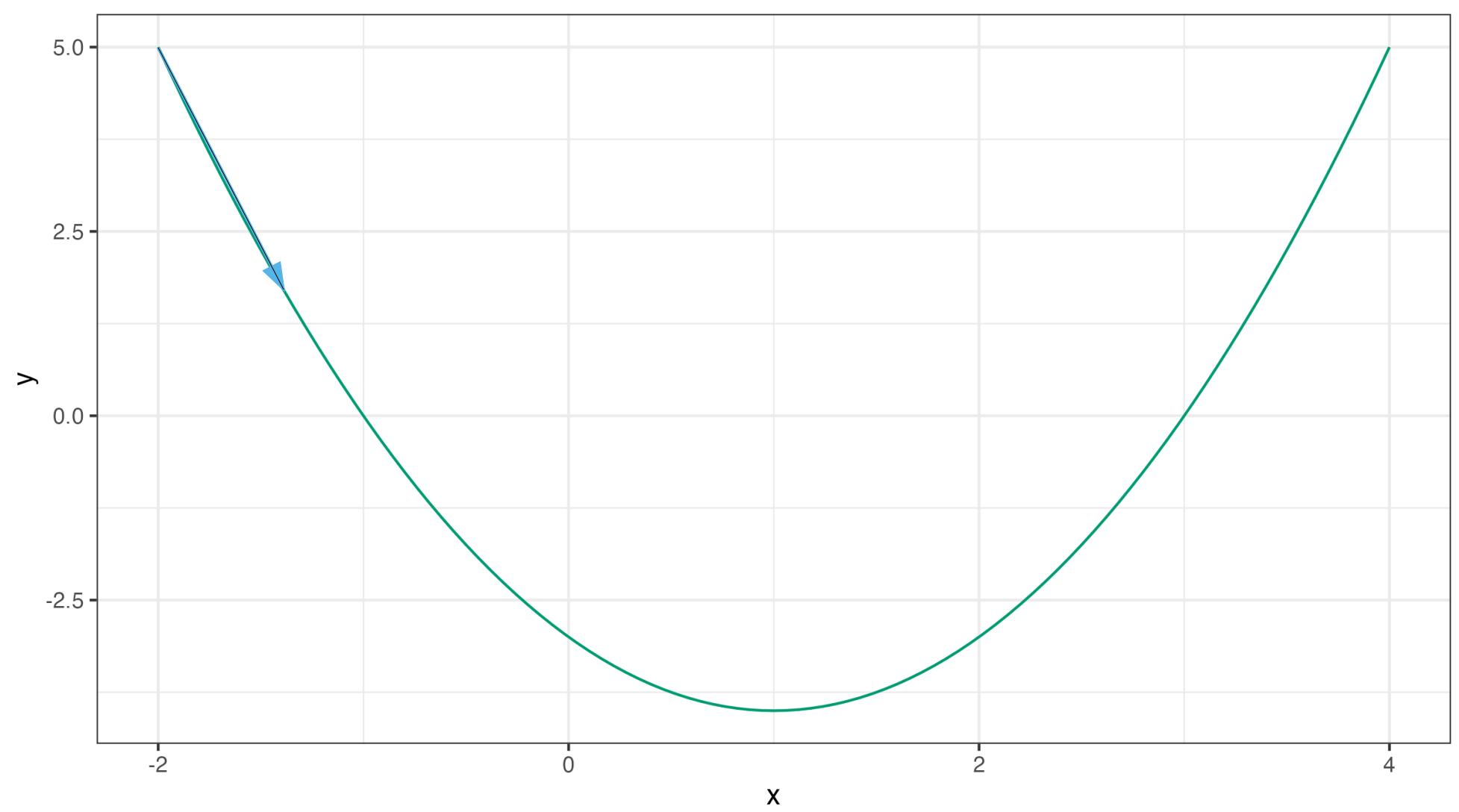
Algorithm: Gradient Descent

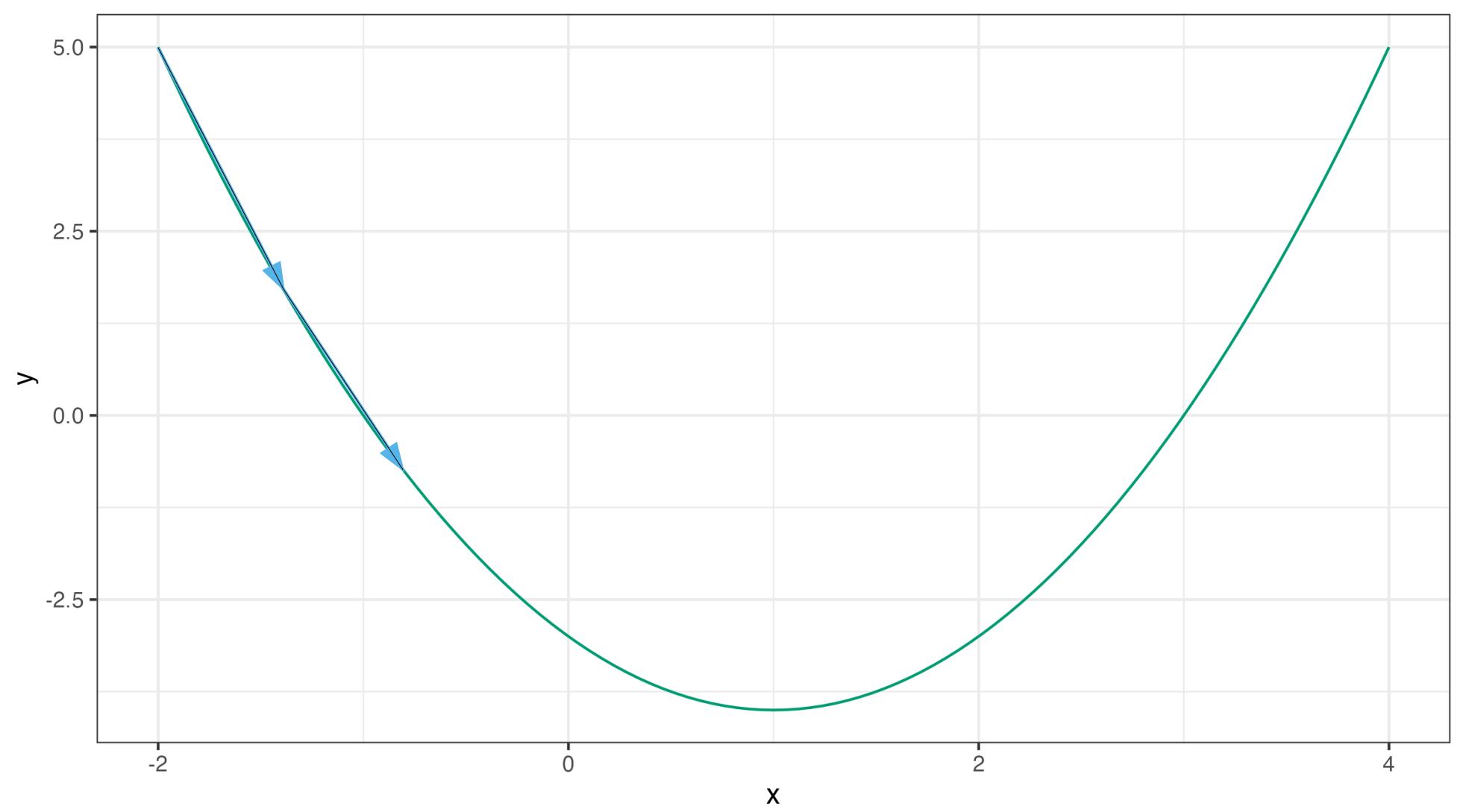


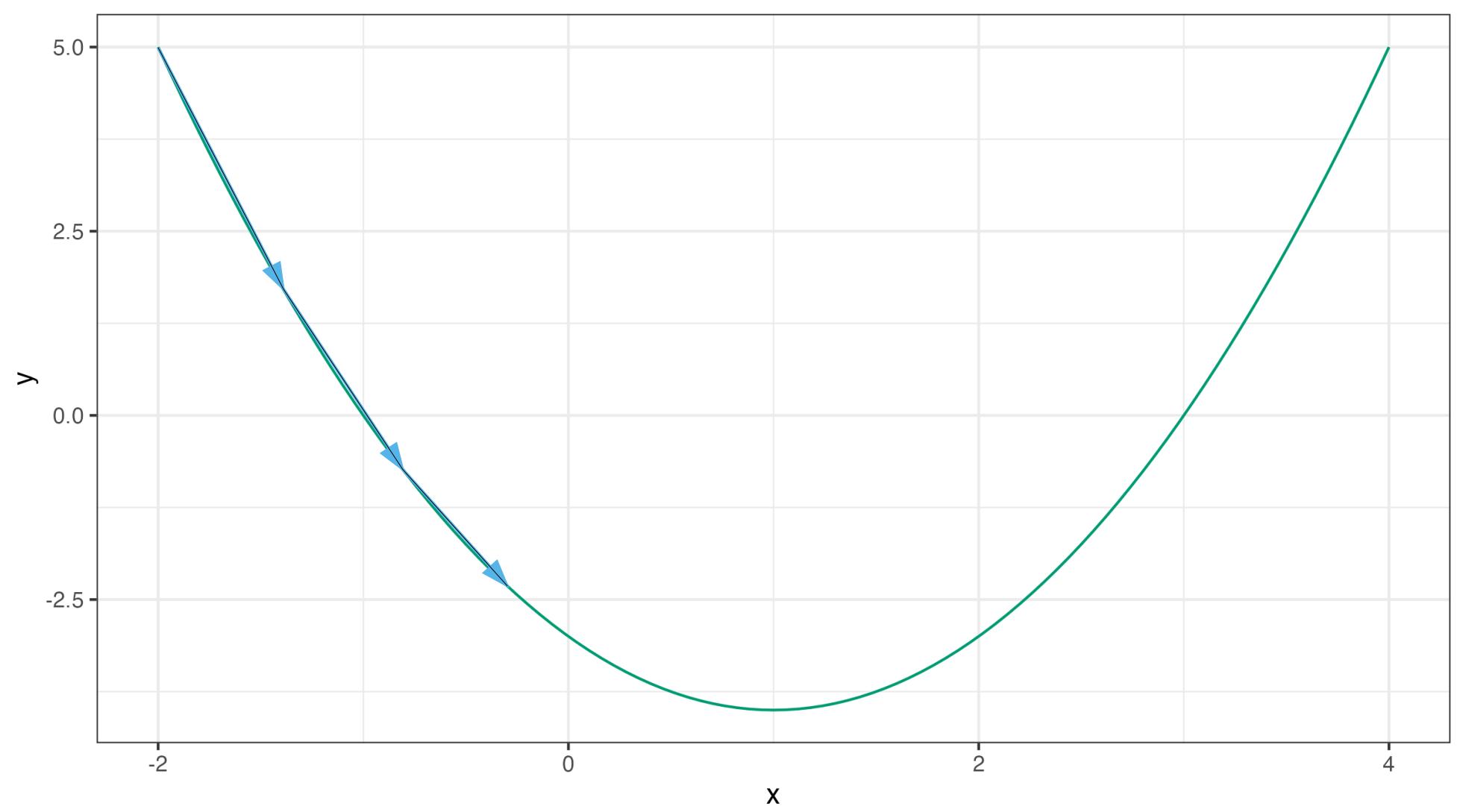
Gradient Descent

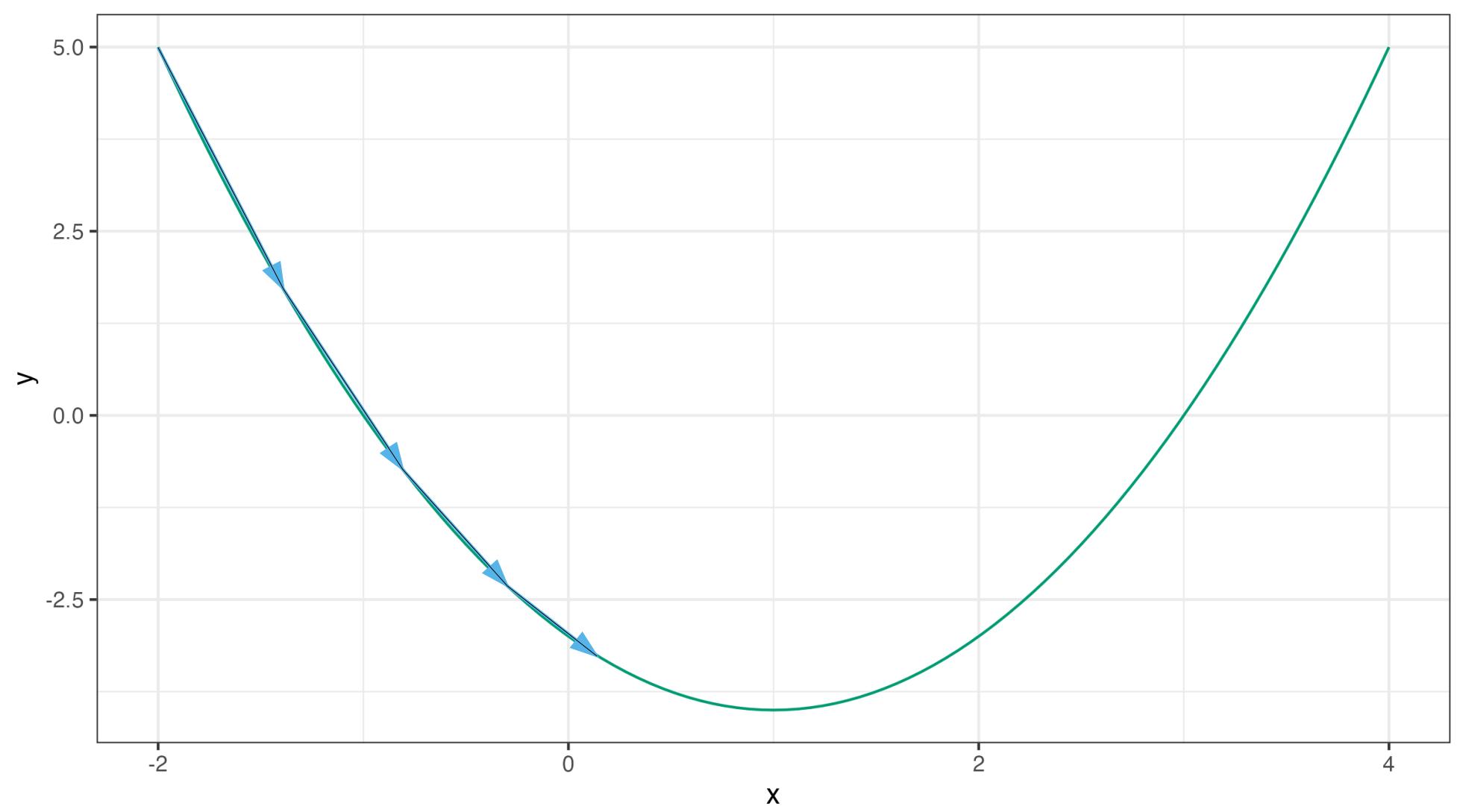
- Big idea: To find the minimum value of a function, we move downhill until we get to the bottom
- Algorithm: To find the argmin of a function f given parameter values θ_n at iteration n , and step size λ :
 1. Compute the gradient of f with respect to θ_n
 2. Find the next parameter values, θ_{n+1} , according to the update rule:
 - $\theta_{n+1} \leftarrow \theta_n - \lambda \nabla f$
 3. Repeat 1&2 until convergence
- What actually happens: Starting at some guess, use the gradient to repeatedly take steps “downhill” until you hit the bottom

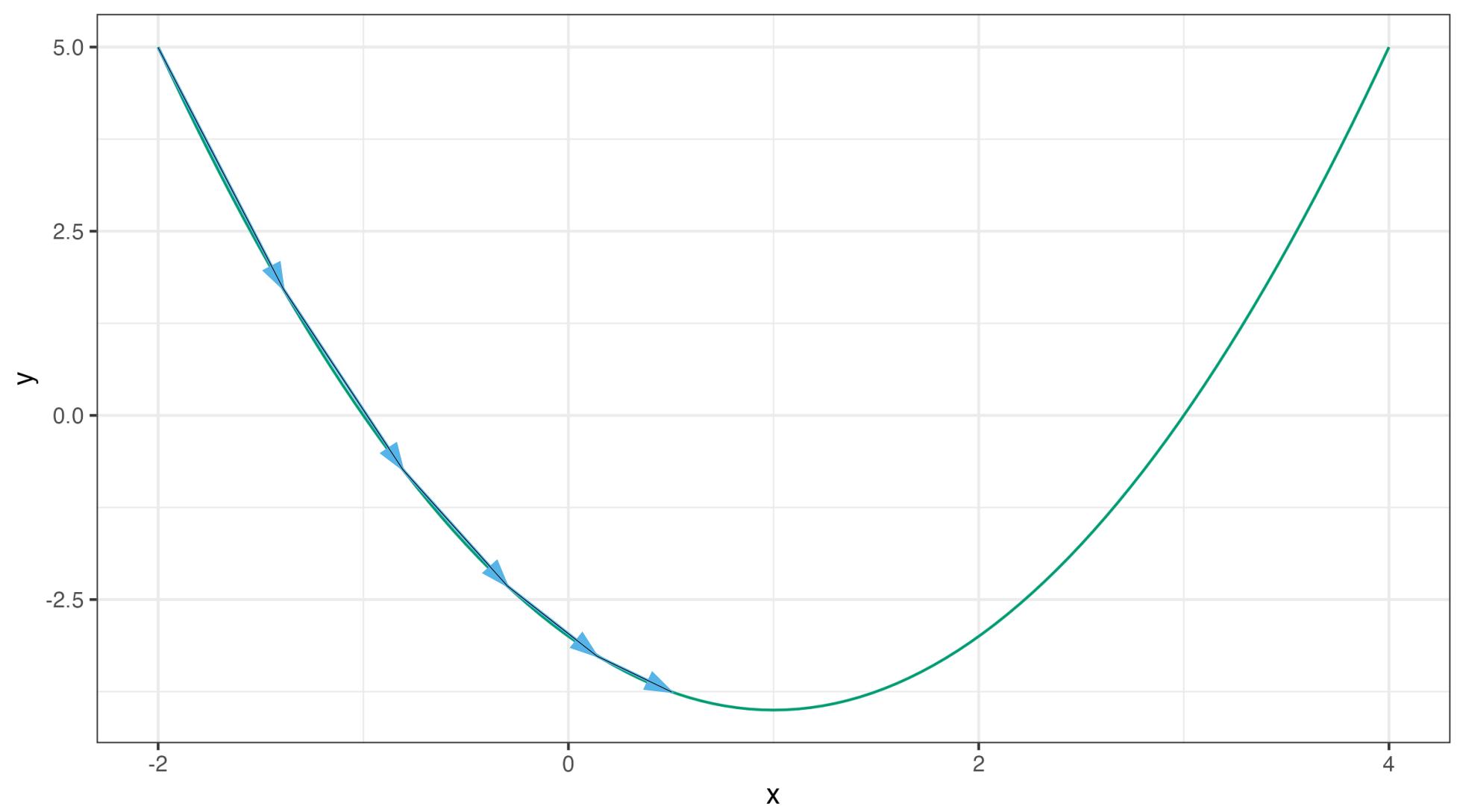


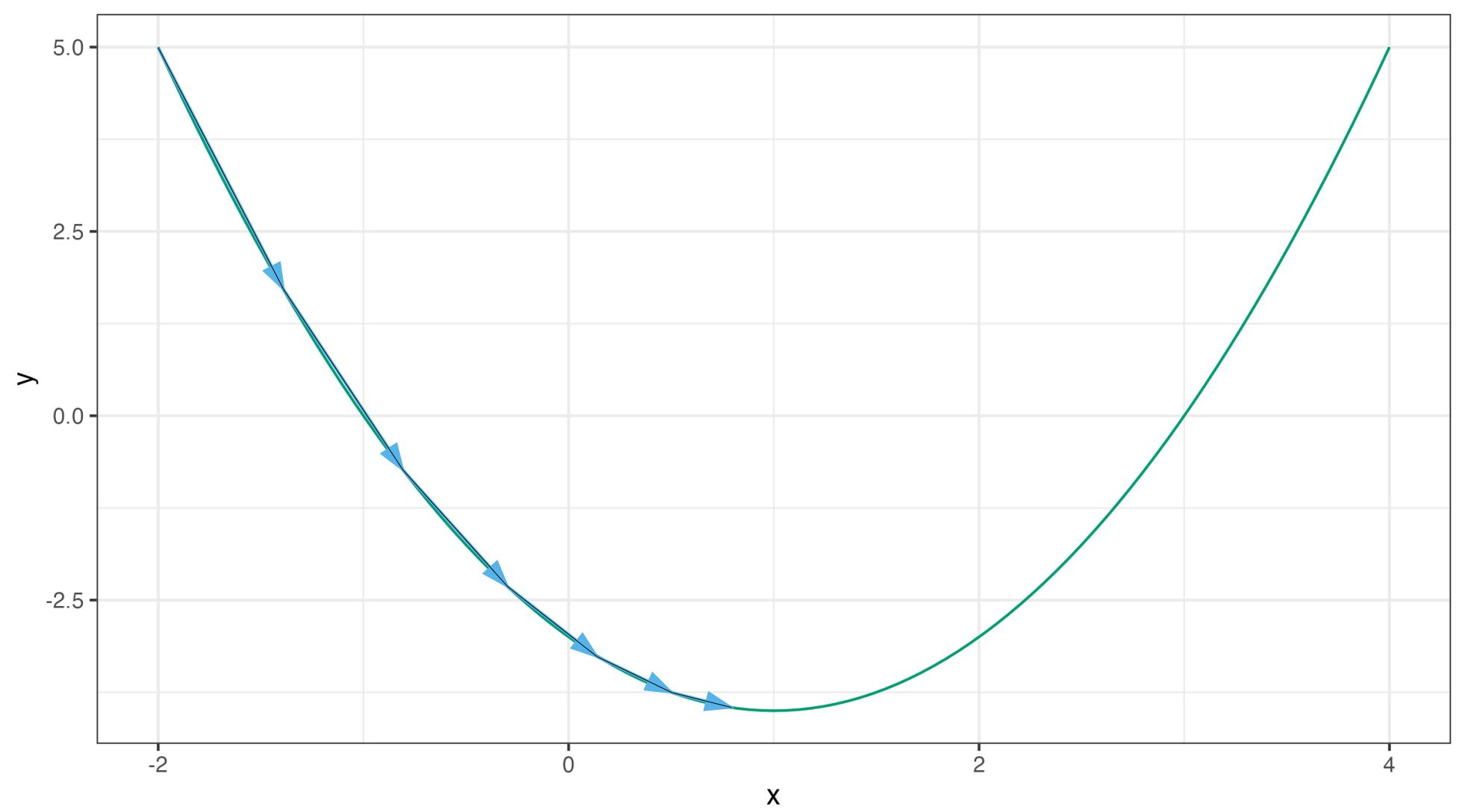


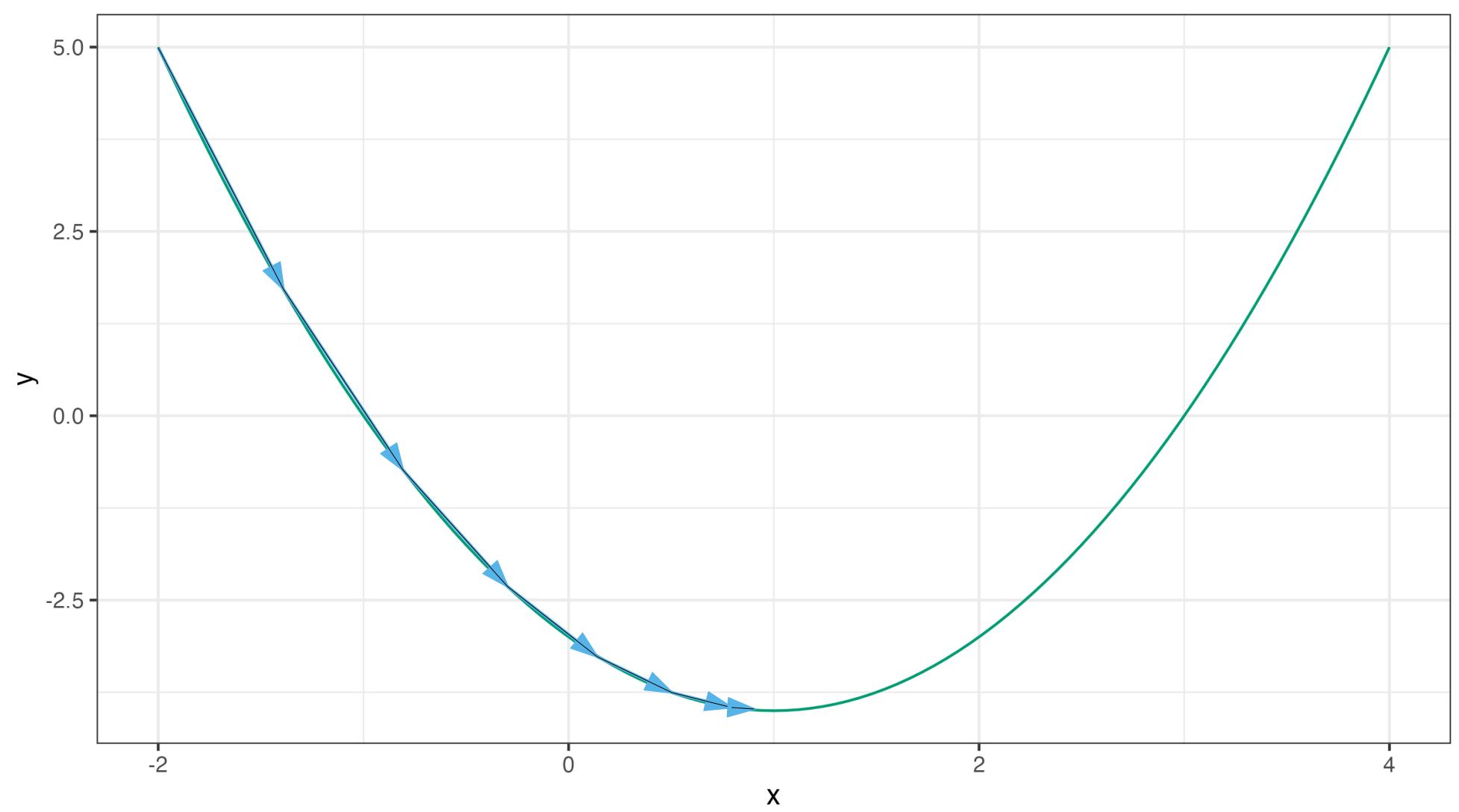


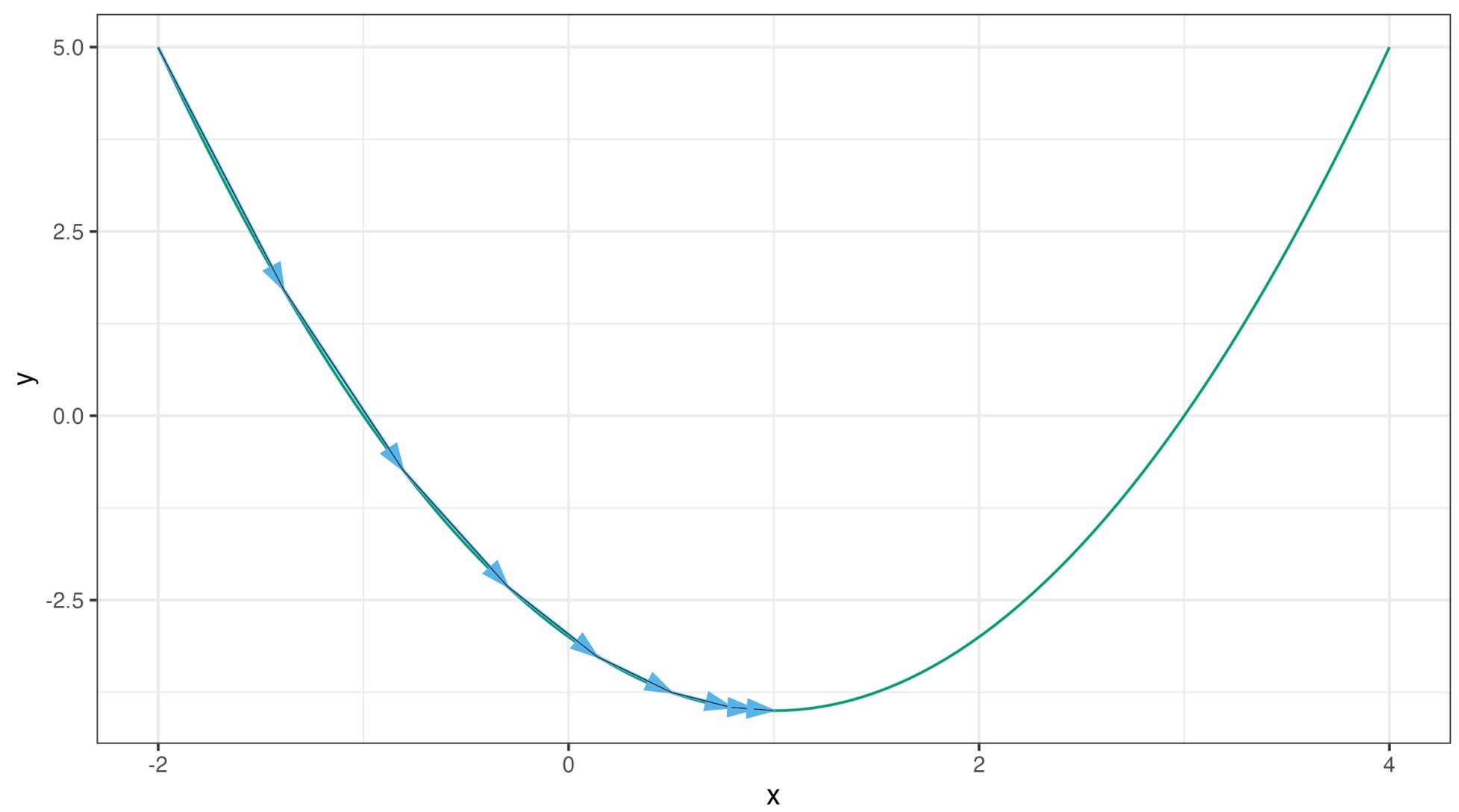












The OLS Loss Function

- So how do we write a loss function?
- Frame your solution as a minimization problem
 - Note that if you want to maximize something, it's the same as minimizing the negative of that thing
- Recall that OLS attempts to minimize the sum of squared residuals
 - For OLS with a single covariate x , outcome y , and coefficients, β_0, β_1 , write down the sum of squared residuals
 - Then how do we express that we want to minimize? What do we minimize with respect to?
 - What does this give us?

The OLS Loss Function

Set up the problem:

$$\underbrace{\sum_{x_i, y_i \in \mathbf{X}} (y_i - (\beta_0 + \beta_1 x_i))^2}_{\text{The sum of squared residuals}}$$

The OLS Loss Function

Set up the problem:

$$\underbrace{\operatorname{argmin}_{\beta}}_{\text{Find } \beta \text{ that minimizes}} \underbrace{\sum_{x_i, y_i \in \mathbf{X}} (y_i - (\beta_0 + \beta_1 x_i))^2}_{\text{The sum of squared residuals}}$$

The OLS Loss Function

Set up the problem:

$$\underbrace{\hat{\beta}}_{\text{Estimated coefficients}} = \underbrace{\operatorname{argmin}_{\beta}}_{\text{Find } \beta \text{ that minimizes}} \underbrace{\sum_{x_i, y_i \in \mathbf{X}} (y_i - (\beta_0 + \beta_1 x_i))^2}_{\text{The sum of squared residuals}}$$

Gradient Descent with OLS

- We start with our loss function:

$$\ell(\mathbf{X}, \beta) = \sum_{x_i, y_i \in \mathbf{X}} (y_i - (\beta_0 + \beta_1 x_i))^2$$

Gradient Descent with OLS

- We start with our loss function:

$$\ell(\mathbf{X}, \beta) = \sum_{x_i, y_i \in \mathbf{X}} (y_i - (\beta_0 + \beta_1 x_i))^2$$

- Now we need to take the gradient wrt the parameters we optimize over:

$$\nabla \ell(\mathbf{X}, \beta) = \begin{bmatrix} \frac{\partial \ell}{\partial \beta_0} \\ \frac{\partial \ell}{\partial \beta_1} \end{bmatrix}$$

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$$\nabla \ell(\mathbf{X}, \beta) = \begin{bmatrix} \frac{\partial \ell}{\partial \beta_0} \\ \frac{\partial \ell}{\partial \beta_1} \end{bmatrix}$$

- The gradient:

$$\nabla \ell(\mathbf{X}, \beta) = \begin{bmatrix} \frac{\partial \ell}{\partial \beta_0} \\ \frac{\partial \ell}{\partial \beta_1} \end{bmatrix} = \begin{bmatrix} \sum_{x_i, y_i \in \mathbf{X}} -2(y_i - (\beta_0 + \beta_1 x_i)) \\ \sum_{x_i, y_i \in \mathbf{X}} -2x_i(y_i - (\beta_0 + \beta_1 x_i)) \end{bmatrix}$$

Gradient Descent with OLS

Gradient Descent with OLS

- Next we pick a step size, λ
 - Smaller values of λ result in a more precise solution, but slower convergence time
 - Larger values of λ are less precise but converge faster
 - If you make λ too large, the optimization may become unstable and never converge!

Gradient Descent with OLS

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 - Larger values of λ are less precise but converge faster
 - If you make λ too large, the optimization may become unstable and never converge!
- Initialize starting values for your parameters
 - Lots of choices! Start at zero? Pick randomly?
- Update your parameters:
 - Recall $\theta_{n+1} \leftarrow \theta_n - \lambda \nabla f$
 - $\hat{\beta}_{0,n+1} \leftarrow \hat{\beta}_{0,n} + 2\lambda \sum_{x_i, y_i \in \mathbf{X}} (y_i - (\hat{\beta}_{0,n} + \hat{\beta}_{1,n} x_i))$
 - $\hat{\beta}_{1,n+1} \leftarrow \hat{\beta}_{1,n} + 2\lambda \sum_{x_i, y_i \in \mathbf{X}} x_i (y_i - (\hat{\beta}_{0,n} + \hat{\beta}_{1,n} x_i))$

Simulating some OLS data

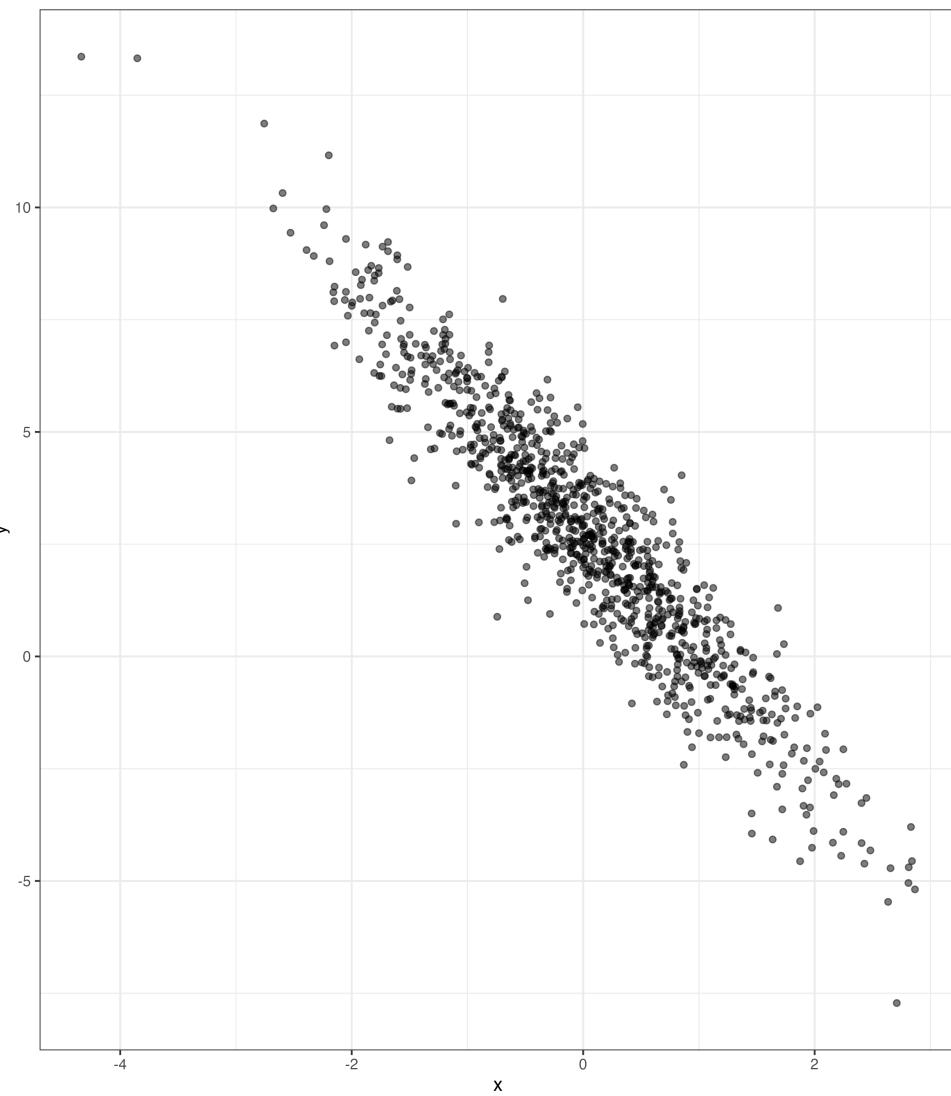
```
1 set.seed(242424)
2
3 N <- 1e3
4 true_beta <- c(2.718, -2.718)
5
6 d <- data.frame(x = rnorm(N))
7 d$y <- true_beta[1] + true_beta[2] * d$x + rnorm(N)
8
9 ols <- lm(y ~ x, d)
10 ols_beta <- coef(ols)
11 ols_beta
```

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9 ols <- lm(y ~ x, d)
10 ols_beta <- coef(ols)
11 ols_beta
12
13 # (Intercept)           x
14 #     2.783908    -2.686621
```

Simulating some OLS data

```
1 ggplot(d, aes(x = x, y = y)) +  
2   geom_point(alpha = 0.5) +  
3   theme_bw()
```



Implementing the Gradient Descent Update

```
1 lr <- 1e-4  
2 beta <- c(0, 0)
```

Implementing the Gradient Descent Update

```
1 lr <- 1e-4
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4 beta[1] <- beta[1] + 2 * lr * sum(d$y - (beta[1] + beta[2] * d$x))
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6
7 beta
8
9 # [1] 0.5407162 -0.5354659
```

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10
11 beta[1] <- beta[1] + 2 * lr * sum(d$y - (beta[1] + beta[2] * d$x))
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11 beta[1] <- beta[1] + 2 * lr * sum(d$y - (beta[1] + beta[2] * d$x))
12 beta[2] <- beta[2] + 2 * lr * sum(d$x * (d$y - (beta[1] + beta[2] * d$x)))
13
14 beta
15
16 # [1] 0.9764911 -0.9641414
```

How long until convergence? $\lambda = 10^{-4}$

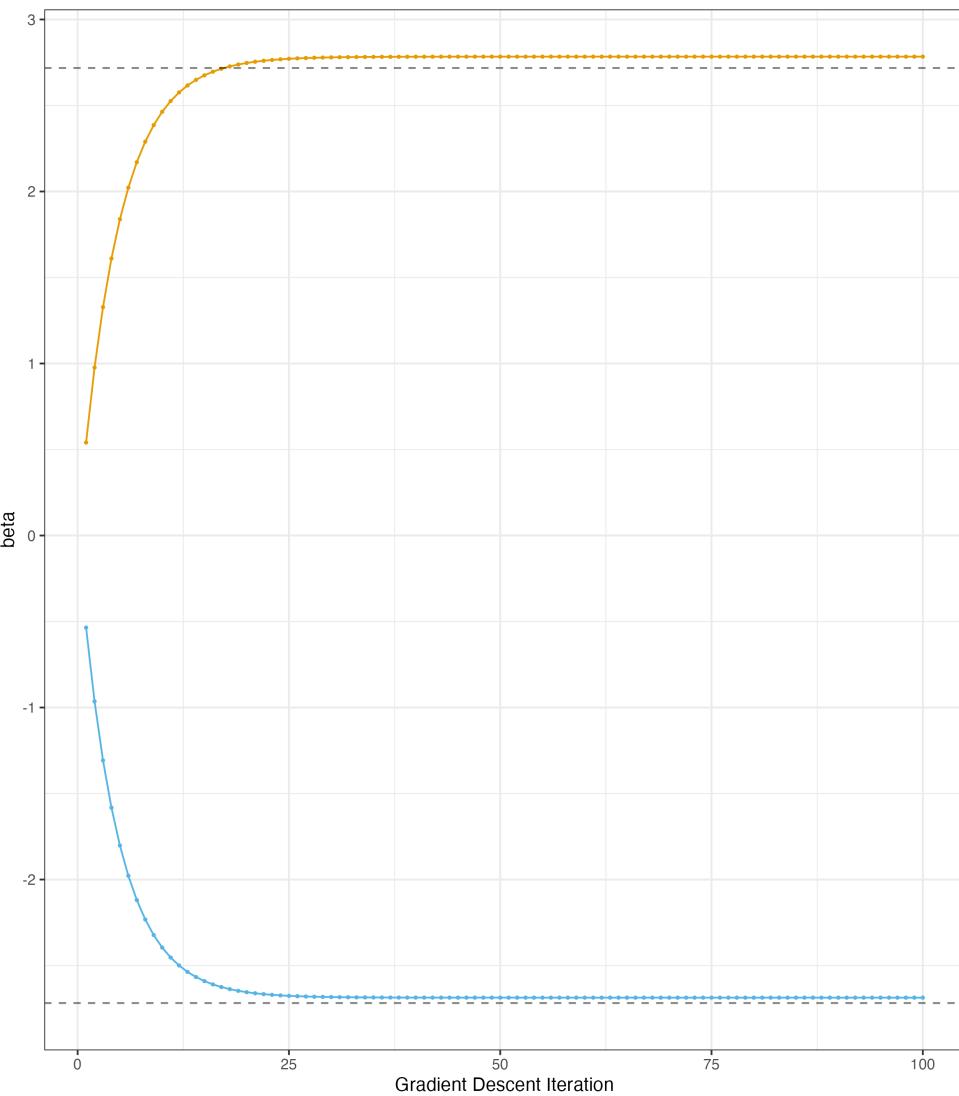
```
1 M <- 1e2
2 lr <- 1e-4
3 beta <- c(0, 0)
4 betas <- data.frame(i = 1:M, beta_0 = numeric(M), beta_1 = numeric(M))
5
6 for (i in 1:M) {
7   beta[1] <- beta[1] + 2 * lr * sum(d$y - (beta[1] + beta[2] * d$x))
8   beta[2] <- beta[2] + 2 * lr * sum(d$x * (d$y - (beta[1] + beta[2] * d$x)))
9
10  betas$beta_0[i] <- beta[1]
11  betas$beta_1[i] <- beta[2]
12 }
13
14 beta
15
16 # [1] 2.783908 -2.686621
```

$$\lambda = 10^{-4}$$

```

1  ggplot(betas, aes(x = i)) +
2    geom_line(aes(y = beta_0),
3               color = okabeito_colors(1)) +
4    geom_line(aes(y = beta_1),
5               color = okabeito_colors(2)) +
6    geom_point(aes(y = beta_0),
7               size = 0.5,
8               color = okabeito_colors(1)) +
9    geom_point(aes(y = beta_1),
10              size = 0.5,
11              color = okabeito_colors(2)) +
12    geom_hline(aes(yintercept = true_beta[1]),
13               lty = 2,
14               alpha = 0.5) +
15    geom_hline(aes(yintercept = true_beta[2]),
16               lty = 2,
17               alpha = 0.5) +
18    labs(x='Gradient Descent Iteration',
19          y = 'beta') +
20    theme_bw()

```



What about a faster learning rate? $\lambda = 10^{-3}$

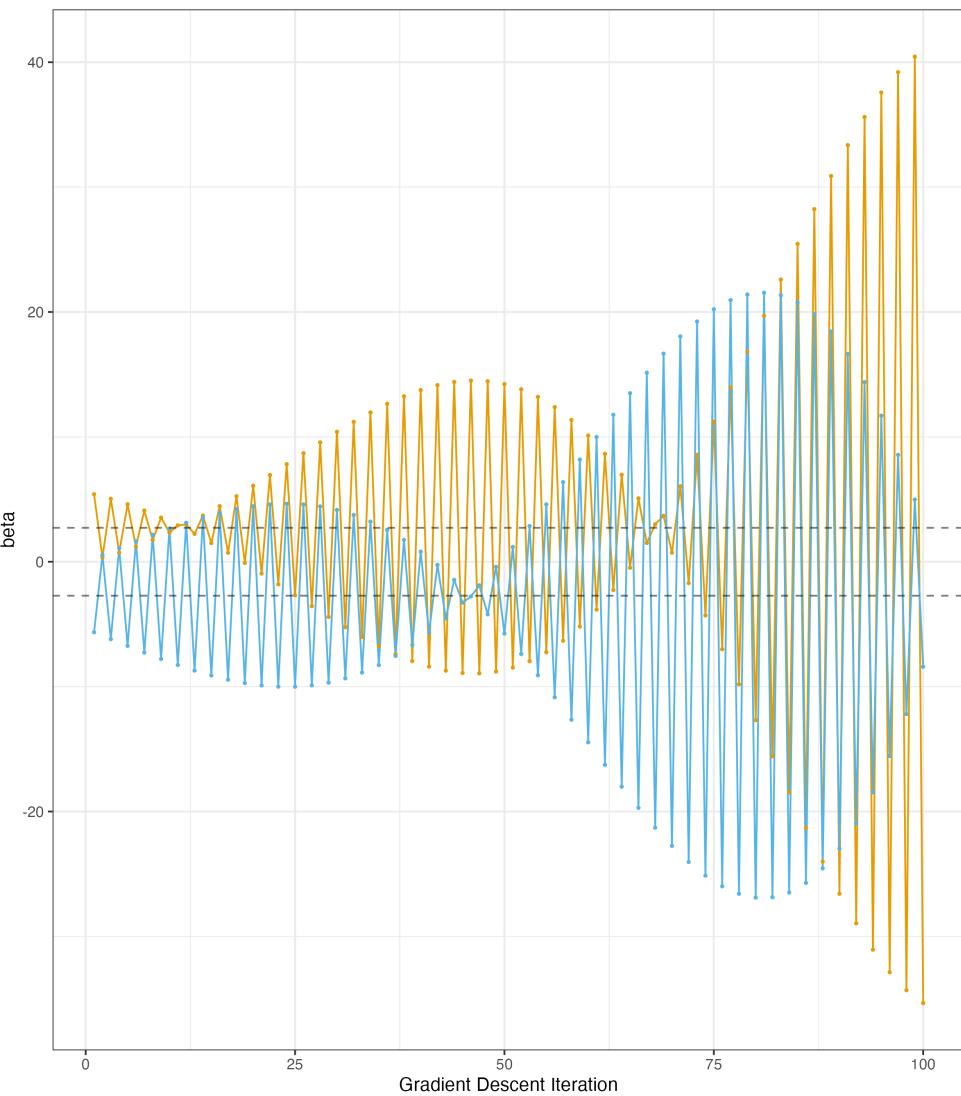
```
1 M <- 1e2
2 lr <- 1e-3
3 beta <- c(0, 0)
4 betas <- data.frame(i = 1:M, beta_0 = numeric(M), beta_1 = numeric(M))
5
6 for (i in 1:M) {
7   beta[1] <- beta[1] + 2 * lr * sum(d$y - (beta[1] + beta[2] * d$x))
8   beta[2] <- beta[2] + 2 * lr * sum(d$x * (d$y - (beta[1] + beta[2] * d$x)))
9
10  betas$beta_0[i] <- beta[1]
11  betas$beta_1[i] <- beta[2]
12 }
13
14 beta
15
16 # [1] -35.335523 -8.404527
```

$$\lambda = 10^{-3}$$

```

1  ggplot(betas, aes(x = i)) +
2    geom_line(aes(y = beta_0),
3               color = okabeito_colors(1)) +
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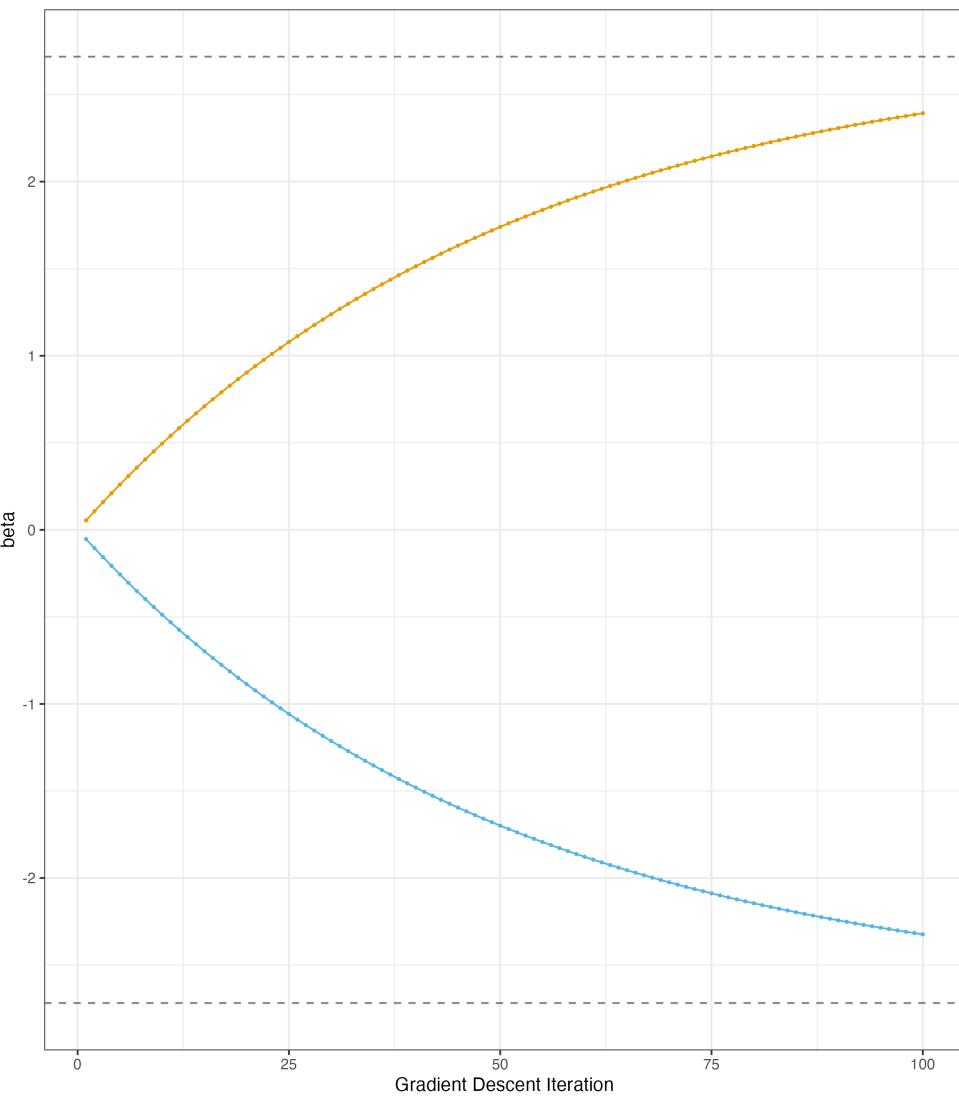


What about a slower learning rate? $\lambda = 10^{-5}$

```
1 M <- 1e2
2 lr <- 1e-5
3 beta <- c(0, 0)
4 betas <- data.frame(i = 1:M, beta_0 = numeric(M), beta_1 = numeric(M))
5
6 for (i in 1:M) {
7   beta[1] <- beta[1] + 2 * lr * sum(d$y - (beta[1] + beta[2] * d$x))
8   beta[2] <- beta[2] + 2 * lr * sum(d$x * (d$y - (beta[1] + beta[2] * d$x)))
9
10  betas$beta_0[i] <- beta[1]
11  betas$beta_1[i] <- beta[2]
12 }
13
14 beta
15
16 # [1] 2.392762 -2.323370
```

$$\lambda = 10^{-5}$$

```
1 ggplot(betas, aes(x = i)) +
2   geom_line(aes(y = beta_0),
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9   geom_point(aes(y = beta_1),
10            size = 0.5,
11            color = okabeito_colors(2)) +
12   geom_hline(aes(yintercept = true_beta[1]),
13              lty = 2,
14              alpha = 0.5) +
15   geom_hline(aes(yintercept = true_beta[2]),
16              lty = 2,
17              alpha = 0.5) +
18   labs(x='Gradient Descent Iteration',
19        y = 'beta') +
20   theme_bw()
```



When do you stop?

- The *easiest* way to do it is just pick a number of iterations and then stop
 - You may not reach the solution
 - You may take too many iterations that you didn't need to
- Typically we stop when the solution *converges*
 - Often this looks like picking a threshold value, ϵ
 - After every iteration, check to see how much the estimate has changed by
 - Stop when the change in parameter estimates is smaller than the threshold
 - Lets you set the level of precision you want in your answer
 - If your threshold is too small relative to the step size, the optimization routine may never converge

More Tools

Maximum Likelihood Estimation

Maximum Likelihood Estimation

- A linear regression assumes normally distributed error with constant error variance, or:

$$y_i \sim \mathcal{N}(\beta_0 + \beta_1 x_i, \sigma^2)$$

Maximum Likelihood Estimation

- A linear regression assumes normally distributed error with constant error variance, or:

$$y_i \sim \mathcal{N}(\beta_0 + \beta_1 x_i, \sigma^2)$$

- We can write down the *likelihood* (think Bayes' theorem) of observing a set of parameters conditioned on our observed data by multiplying together the normal density functions for each observation:

$$L(\beta | \mathbf{X}) = \prod_{y_i, x_i \in \mathbf{X}} \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2}$$

Log Transformin'

- We can make our lives way easier with a log transform! Why?

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- Multiplying lots of probabilities results in numerical instability by ending up with tiny numbers!

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- The log transform can turn these products into a sum!

$$\log \prod_{y_i, x_i \in \mathbf{X}} \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2} = \sum_{y_i, x_i \in \mathbf{X}} \log \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2}$$

Log Transformin'

- We can make our lives way easier with a log transform! Why?
- Multiplying lots of probabilities results in numerical instability by ending up with tiny numbers!
- The log transform can turn these products into a sum!

$$\begin{aligned} \log \prod_{y_i, x_i \in \mathbf{X}} \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2} &= \sum_{y_i, x_i \in \mathbf{X}} \log \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2} \\ &= \sum_{y_i, x_i \in \mathbf{X}} \log \frac{1}{\sigma \sqrt{2\pi}} + \log e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2} \end{aligned}$$

Log Transformin'

- We can make our lives way easier with a log transform! Why?
- Multiplying lots of probabilities results in numerical instability by ending up with tiny numbers!
- The log transform can turn these products into a sum!

$$\begin{aligned} \log \prod_{y_i, x_i \in \mathbf{X}} \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2} &= \sum_{y_i, x_i \in \mathbf{X}} \log \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2} \\ &= \sum_{y_i, x_i \in \mathbf{X}} \log \frac{1}{\sigma \sqrt{2\pi}} + \log e^{-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2} \\ &= \sum_{y_i, x_i \in \mathbf{X}} \log \frac{1}{\sigma \sqrt{2\pi}} - \frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2 \end{aligned}$$

Maximum (Log) Likelihood Estimation

- Maximum Likelihood Estimation (MLE) is just finding the values of your parameters that maximize the likelihood
- Because the log transform is monotonic, we can just maximize the log likelihood instead

$$\ell(\theta|\mathbf{X}) = \log L(\theta|\mathbf{X})$$

$$\hat{\theta} = \operatorname{argmax}_{\theta} L(\theta|\mathbf{X}) = \operatorname{argmax}_{\theta} \ell(\theta|\mathbf{X})$$

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- We have a few options on how this works:
 1. Take the gradient of the log likelihood and set it equal to zero to find the estimates $\hat{\theta}$ analytically
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 3. Some secret third thing that we haven't really discussed yet

MLE for OLS

$$\hat{\beta} = \operatorname{argmax}_{\beta} \left[\sum_{y_i, x_i \in \mathbf{X}} \log \frac{1}{\sigma \sqrt{2\pi}} - \frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma} \right)^2 \right]$$

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- Does this last line look familiar?

MLE for OLS

$$\hat{\beta} = \operatorname{argmin}_{\beta} \sum_{y_i, x_i \in \mathbf{X}} (y_i - (\beta_0 + \beta_1 x_i))^2$$

- The MLE for OLS is identical to minimizing the sum of squared residuals
- This is not always the case for other estimators, though!
- Now we have to actually minimize it—for this, we'll use `optim()`

optim()

All hail the greatest built-in function in base R, `optim()`

- `optim()` is a general purpose optimization function in R
- It has a bunch of different optimization methods and is used by just about every single modeling function under the hood
- `optim()` specifically does **argmin**
 - You write a function that takes parameters as inputs
 - You give `optim()` starting values for those parameters (as a vector) and the function to be argmin'd
 - `optim()` returns the values of the parameters that minimize the function
- **If you can write something as a maximization or minimization problem, `optim()` can solve it for you**
 - Caveats about convexity and identifiability and some other stuff

MLE with optim() for OLS

```
1 SumSquaredResid <- function(beta, d){  
2   # TODO: Compute sum of squared residual  
3   return(ssr)  
4 }
```

MLE with optim() for OLS

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11 # [1] 15666.95
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```

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21 mle_beta  
22  
23 # [1] 2.784030 -2.686716
```

Checking results

```
1 true_beta  
2 ols_beta  
3 gd_beta  
4 mle_beta
```

Checking results

```
1 true_beta  
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3 # [1] 2.718 -2.718  
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5 ols_beta  
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Checking results

```
1 true_beta  
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3 # [1] 2.718 -2.718  
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5 ols_beta  
6  
7 # (Intercept)          x  
8 #     2.783908    -2.686621  
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```

Some notes on optim()

- The function you minimize needs to output only a single scalar value
- The first argument of the function you minimize needs to be all the parameters you want to optimize, passed as a vector
- There are a whole bunch of options you can fiddle with in order to change convergence conditions, speed, or optimization algorithm
- If you make a function that also returns the gradient, you can gain a lot of speed and precision!
- Works best with *convex* problems
 - Otherwise you can get stuck in local minima!
 - If you can't be convex, just start from a bunch of random spots and take the best solution
 - If your problem involves finding where a function is equal to zero, squaring it and finding the minimum will do the job!

Wrap Up

Recap

- Numerical optimization is the most useful skill we learn in this course
- If you can frame something as an optimization problem, `optim()` can generally solve it
- Working in log space has tons of advantages, especially when you're dealing with probabilities

Final Thoughts

- PollEv.com/klintkanopka