

Lecture 3 | Part 1

Recap

Empirical Risk

Last time, we framed the problem of learning as minimizing the empirical risk.

$$R(H) = \frac{1}{n} \sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}), y_i)$$

▶ In the case where *H* is linear::

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), y_i)$$

Minimizing Empirical Risk

- Picking different loss functions changes the optimization problem.
- If we use square loss:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} (\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i)^2$$

We can minimize by setting the gradient to zero.

• We get:
$$\vec{w} = (X^T X)^{-1} X^T \vec{y}$$
.

Minimizing Empirical Risk

▶ But sometimes we can't use this approach.
 ▶ If R is not differentiable (absolute loss).
 ▶ If computing w* = (X^TX)⁻¹X^Tv is too expensive.

Today

- A general, very popular approach to optimization: gradient descent.
- Instead of solving for w^{*} "all at once", we'll iterate towards it.



Lecture 3 | Part 2 What is the gradient?

Consider f(z) = 3z² + 2z + 1.
 What is the slope of the curve at z = 1?



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 What is the slope of the curve at z = 1?







The derivative gives the slope anywhere:

$$f(z) = 3z^2 + 2z + 1$$

$$\frac{df}{dz}(z) = \frac{6z+2}{2}$$

The slope of the curve at z = 1:

$$\frac{df}{dz}(1) = 6 + 2 = 8$$

What type of object?

- The derivative of $f : \mathbb{R} \to \mathbb{R}$ is a **function**:
 - Input: scalar.
 - Output: scalar.
 - Example: $\frac{df}{dz}(z) = 6z + 2$.
- The derivative evaluated at a point is a scalar:
 Example: df/dz(1) = 8.

Sign of the Derivative

If the derivative at a point is:

- Positive: the function is increasing.
- Negative: the function is decreasing.
- Zero: the function is **flat**.





Derivatives and Change

The derivative tells us **how much** the function changes with an infinitesimal increase in z.



Increases and Decreases

- The sign of the derivative tells us if the function is increasing or decreasing.
 - Positive: f is increasing at z.
 - Negative: f is decreasing at z.

Multivariate Functions



Multivariate Functions

Now consider
$$f(\vec{z}) = f(z_1, z_2) = 4z_1^2 + 2z_2 + 2z_1z_2$$
.
What is the **slope** of the surface at $(z_1, z_2) = (3, 1)$?



Partial Derivatives

When f is a function of a vector z = (z₁, z₂)^T, there are two slopes to talk about:

•
$$\frac{\partial f}{\partial z_1}$$
: slope in the z_1 direction.

$$\frac{\partial f}{\partial z_2}$$
: slope in the z_2 direction.

Example

What is the slope of f at (z₁, z₂) = (3, 1) in:
 The z₁ direction?
 The z₂ direction?

$$f(\vec{z}) = 4z_1^2 + 2z_2 + 2z_1z_2$$



$$\frac{\partial f}{\partial z_1}(z_1, z_2) = 8z_1 + 2z_2$$

$$\frac{\partial f}{\partial z_1}(3, 1) = 8 \cdot 3 + 2 \cdot 1 = 26$$

$$\frac{\partial f}{\partial z_2}(z_1, z_2) = 2 + 2 \cdot 2 \cdot 1$$

$$\frac{\partial f}{\partial z_2}(3, 1) = 2 + 2 \cdot 3 = 8$$

What is the gradient?

We can package the partial derivatives into a single object: the gradient.

$$\frac{df}{d\vec{z}}(\vec{z}) = \begin{pmatrix} \frac{\partial f}{\partial z_1}(\vec{z}) \\ \frac{\partial f}{\partial z_2}(\vec{z}) \end{pmatrix}$$

What is the gradient?

▶ In general, if $f : \mathbb{R}^d \to \mathbb{R}$, then the gradient is:

$$\frac{df}{d\vec{z}}(\vec{z}) = \begin{pmatrix} \frac{\partial f}{\partial z_1}(\vec{z}) \\ \frac{\partial f}{\partial z_2}(\vec{z}) \\ \vdots \\ \frac{\partial f}{\partial z_d}(\vec{z}) \end{pmatrix}$$

What type of object?

- The gradient of a function $f : \mathbb{R}^d \to \mathbb{R}$ is a **function**¹:
 - ▶ Input: vector in \mathbb{R}^d .
 - Output: vector in \mathbb{R}^d .
 - Example: $\frac{df}{d\vec{z}}(\vec{z}) = (8z_1 + 2z_2, 2 + 2z_1)^T$.
- ► The gradient of $f : \mathbb{R}^d \to \mathbb{R}$ evaluated at a point is a vector in \mathbb{R}^d : Example: $\frac{df}{dt^2}(3,1) = (26,8)^T$.

¹Sometimes it is referred to as a vector field.

Gradient Fields

The gradient can be viewed as a vector field:



Meaning of Gradient Vector

- The gradient of a function $f : \mathbb{R}^d \to \mathbb{R}$ at a point \vec{z} is a vector in \mathbb{R}^d .
- The *i*th component is the **slope** of *f* at *z* in the *i*th direction.



Gradients and Change

• Recall:
$$f(z + \delta) \approx f(z) + \delta \times \frac{df}{dz}(z)$$
.

In multiple dimensions:

$$\begin{split} f(\vec{z} + \vec{\delta}) &\approx f(\vec{z}) + \left(\delta_1 \times \frac{\partial f}{\partial z_1}(\vec{z})\right) + \left(\delta_2 \times \frac{\partial f}{\partial z_2}(\vec{z})\right) + \dots \\ &\approx f(\vec{z}) + \vec{\delta} \cdot \frac{df}{d\vec{z}}(\vec{z}) \end{split}$$

$$f(2.1,3.1) \approx f(2,3) + (2.1-2) \cdot \frac{\partial f}{\partial z_1}(2.3) + (3.1-3) \cdot \frac{\partial f}{\partial z_2}(2.3)$$

$$\mp + 0.1 \times 4 + 0.1 \times (-2) = \pm 4.4 - .2$$

Exercise

At a point $\vec{z} = (2,3)^T$, $f(\vec{z})$ is 7 and the gradient $\frac{df}{d\vec{z}}(\vec{z}) = (4,-2)^T$.

What is the approximate^a value of f(2.1, 3.1)?

^aQuality of approximation depends on second derivative.

Steepest Ascent

Key property: the gradient vector points in the direction of steepest ascent.



Proof

► Remember:
$$f(\vec{z} + \vec{\delta}) \approx f(\vec{z}) + \vec{\delta} \cdot \frac{df}{d\vec{z}}(\vec{z})$$
.

So the total change is
$$\vec{\delta} \cdot \frac{df}{d\vec{z}}(\vec{z})$$
.

Also remember:
$$\vec{\delta} \cdot \frac{df}{d\vec{z}}(\vec{z}) = \|\vec{\delta}\| \left\| \frac{df}{d\vec{z}}(\vec{z}) \right\| \cos \theta$$
.

So the increase in *f* is maximized when $\theta = 0$. That is, when $\vec{\delta}$ points in the direction of $\frac{df}{d\vec{z}}(\vec{z})$.

Steepest Descent

The negative gradient points in the direction of steepest descent.



Why?

- The direction of steepest ascent is the **opposite** of the direction of steepest descent.
- Because, zoomed in, the function looks linear.


















The contours are the level sets of the function.



Contours and Gradients

► The gradient is **orthogonal** to the contours.



Optimization

► To find a **minimum** (or **maximum**), look for where the gradient is 0.





Lecture 3 | Part 3

Gradient Descent

► **Goal:** minimize
$$f(\vec{z}) = e^{z_1^2 + z_2^2} + (z_1 - 2)^2 + (z_2 - 3)^2$$
.



Try solving
$$\frac{df}{d\vec{z}}(\vec{z}) = 0$$
.

► The gradient is:

$$\frac{df}{d\vec{z}}(\vec{z}) = \begin{pmatrix} 2z_1 e^{z_1^2 + z_2^2} + 2(z_1 - 2) \\ 2z_2 e^{z_1^2 + z_2^2} + 2(z_2 - 3) \end{pmatrix}$$

Can we solve the system?

$$2z_1e^{z_1^2+z_2^2} + 2(z_1 - 2) = 0$$

$$2z_2e^{z_1^2+z_2^2} + 2(z_2 - 3) = 0$$

Try solving
$$\frac{df}{d\vec{z}}(\vec{z}) = 0$$
.

► The gradient is:

$$\frac{df}{d\vec{z}}(\vec{z}) = \begin{pmatrix} 2z_1e^{z_1^2+z_2^2}+2(z_1-2)\\ 2z_2e^{z_1^2+z_2^2}+2(z_2-3) \end{pmatrix}$$

Can we solve the system? Not in closed form.

$$2z_1e^{z_1^2+z_2^2} + 2(z_1 - 2) = 0$$

$$2z_2e^{z_1^2+z_2^2} + 2(z_2 - 3) = 0$$

A Problem

- ► The function **is differentiable**².
- But we can't set gradient to zero and solve.
- **How do we find the minimum**?

²The gradient exists everywhere.

A Solution

- Idea: iterate towards a minimum, step by step.
- Start at an arbitrary location.
- At every step, move in direction of steepest descent.
 - ▶ i.e., the negative gradient.



Exercise

The gradient of a function $f(\vec{z})$ at (1, 1) is $(2, 1)^T$. If you're trying to minimize $f(\vec{z})$, which place should you go to next?



• If η is the **learning rate**, then the next step is:

$$\vec{z}^{(t+1)}=\vec{z}^{(t)}-\eta\times\frac{df}{d\vec{z}}(\vec{z}^{(t)})$$



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Gradient Descent

To minimize $f(\vec{z})$:

- Pick arbitrary starting point $\vec{z}^{(0)}$, learning rate $\eta > 0$
- Until convergence, repeat:
 - **Compute gradient:** $\frac{df}{d\vec{z}}(\vec{z}^{(t)})$ at $\vec{z}^{(t)}$.
 - **Update:** $\vec{z}^{(t+1)} = \vec{z}^{(t)} \eta \times \frac{df}{d\vec{z}}(\vec{z}^{(t)}).$
- When converged, return $\vec{z}^{(t)}$.
 - It is (approximately) a local minimum.

Stopping Criterion



- Close to a minimum, gradient is small.
- Idea: stop when $\left\| \frac{df}{d\vec{z}}(\vec{z}^{(t)}) \right\|$ is small.
 - Alternative: stop when $\|\vec{z}^{(t+1)} \vec{z}^{(t)}\|$ is small.

```
def gradient descent(
    gradient, z o, learning rate, stop threshold
):
    Z = Z \Theta
    while True:
        z new = z - learning rate * gradient(z)
        if np.linalg.norm(z new - z) < stop threshold:
            break
        z = z new
    return z new
```

Picking Parameters

- The learning rate and stopping threshold are parameters.
- They need to be chosen carefully for each problem.
- If not, the algorithm may not converge.

























Lecture 3 | Part 4

Gradient Descent for ERM

Gradient Descent for ERM

In ERM, our goal is to minimize empirical risk:³

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, y_i)$$

Often, we can minimize using gradient descent.

³We've assumed H is a linear prediction function.

 $\frac{d}{dx} \left[f(x) + g(x) \right]$ The Gradient of the Risk $\frac{d}{dx} \left[f(x) + g(x) \right]$ The gradient of the empirical risk is:

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{d}{d\vec{w}} \left(\frac{1}{n} \sum_{i=1}^{n} \ell(\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, y_i) \right)$$
$$= \frac{1}{n} \sum_{i=1}^{n} \frac{d\ell}{d\vec{w}} (\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, y_i)$$

Gradient of risk is average gradient of loss.

As far as we can go without knowing the loss.
The Gradient of the MSE

Recall: the mean squared error is the empirical risk with respect to the square loss:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} (\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2$$

► The gradient is:

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{d}{d\vec{w}} (\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2$$

$$\frac{d}{dw} (xw - y)^{2} = 2(xw - y) \cdot \frac{d}{dw} (xw - y) = 2(xw - y) \times \frac{d}{dw} (xw) = x$$

$$\frac{d}{dw} (xw) = x$$
Exercise
$$\frac{d}{dw} (xw) = \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} = 2 \left[Aug(x^{(i)}) \cdot \vec{w} - y_{i} \right]^{2} = \frac{1}{2} \times \frac{1}{2} \times$$

The Gradient of the MSE

The gradient of the mean squared error is:⁴

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n} \sum_{i=1}^{n} (\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i) \operatorname{Aug}(\vec{x}^{(i)})$$

• Each training point $\vec{x}^{(i)}$ contributes to the gradient.

⁴We saw before that $\frac{dR}{dw}(\vec{w}) = 2X^T X \vec{w} - 2X^T \vec{y}$. These two are actually equal.

Exercise

What will be the gradient if every prediction is exactly correct?

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n} \sum_{i=1}^{n} (\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i) \operatorname{Aug}(\vec{x}^{(i)})$$
Zero

Gradient Descent for Least Squares

- ► We can perform least squares regression by solving the normal equations: $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$.
- But we can find the same solution using gradient descent:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta \times \frac{2}{n} \sum_{i=1}^{n} (\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w}^{(t)} - y_i) \operatorname{Aug}(\vec{x}^{(i)})$$

Example

We will run gradient descent to train a least squares regression model on the following data:



Exercise

The plot below shows a linear prediction function using weight vector $\vec{w}^{(0)}$.

What is the sign of the **second** entry of $\frac{dR}{d\vec{w}}(\vec{w}^{(0)})$?















































Lecture 3 | Part 5

Appendix: From Theory to Practice

In Practice

- ► (S)GD is **heavily used** in machine learning.
- Can be used to solve many optimization problems.
- But it can be tricky to get working.

Learning Rate

The learning rate has to be chosen carefully.

- If too large, the algorithm may diverge.
- If too small, the algorithm may converge slowly.










Diverging

- ► To diagnose, print $R(\vec{w})$ at each iteration.
- If it is increasing consistently, the algorithm is diverging.
- Fix: decrease the learning rate.
 But not by too much! Then it may converge too slowly.

Problem

When the contours are "long and skinny," you will be forced to pick a very small learning rate.



A Fix

- Scaling (standardizing) the features can help.
- This makes the contours more circular.
- Doesn't change the prediction!















Next Time

- How do we minimize the risk with respect to absolute loss?
- When is gradient descent guaranteed to converge?