DSC 140A

Probabilistic Modeling & Machine Learning

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**:

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

- 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 $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$ is too expensive.
  - ...

Today

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

DSC 140A

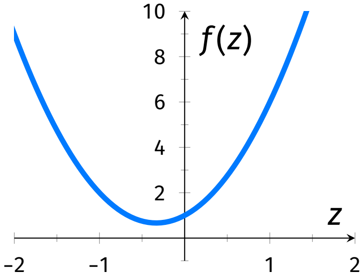
Probabilistic Modeling & Machine Learning

Lecture 3 | Part 2

What is the gradient?

What is the derivative?

- Consider $f(z) = 3z^2 + 2z + 1$.
  - What is the **slope** of the curve at $z = 1$?



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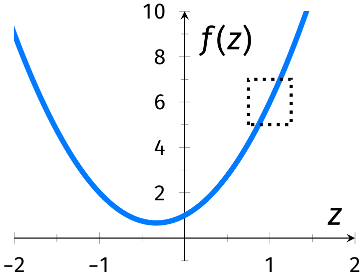

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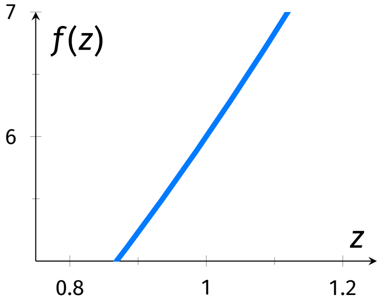


What is the derivative?

- The **derivative** gives the slope anywhere:

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

$$\frac{df}{dz}(z) =$$

The slope of the curve at $z = 1$:

$$\frac{df}{dz}(1) =$$

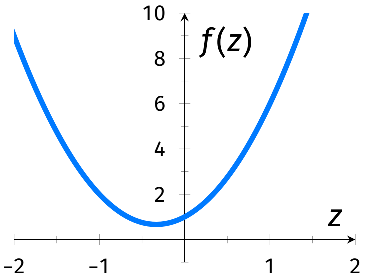
What type of object?

- 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: $\frac{df}{dz}(1) = 8$.

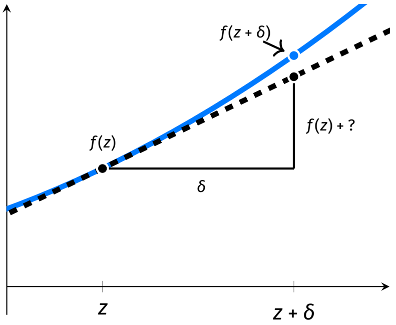
Sign of the Derivative

- If the derivative at a point is:
  - Positive: the function is **increasing**.
  - Negative: the function is **decreasing**.
  - Zero: the function is **flat**.



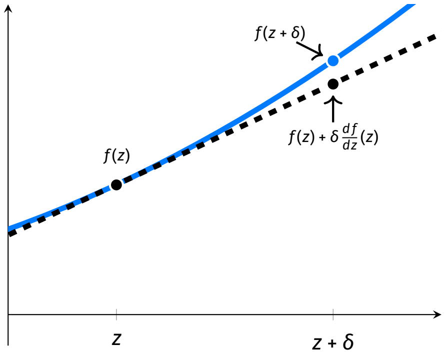
Exercise

What is the height of the dashed line at $z + \delta$?



Derivatives and Change

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

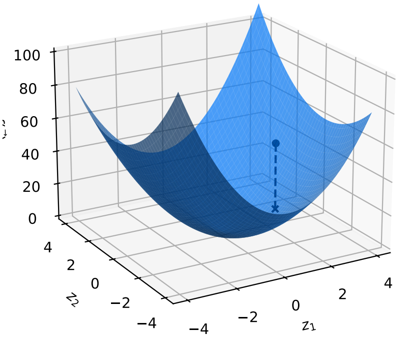


Increases and Decreases

- 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

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



Multivariate Functions

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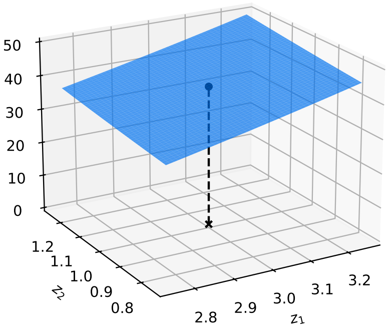


Partial Derivatives

- When f is a function of a vector $\vec{z} = (z_1, z_2)^T$, there are **two** slopes to talk about:

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

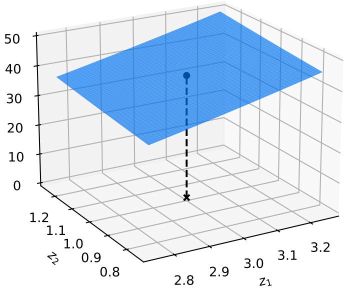
- $\frac{\partial f}{\partial z_2}$: slope in the z_2 direction.

Example

What is the slope of f at $(z_1, z_2) = (3, 1)$ in:

- The z_1 direction?
- The z_2 direction?

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



- $\frac{\partial f}{\partial z_1}(z_1, z_2) =$
- $\frac{\partial f}{\partial z_1}(3, 1) =$
- $\frac{\partial f}{\partial z_2}(z_1, z_2) =$
- $\frac{\partial f}{\partial z_2}(3, 1) =$

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?

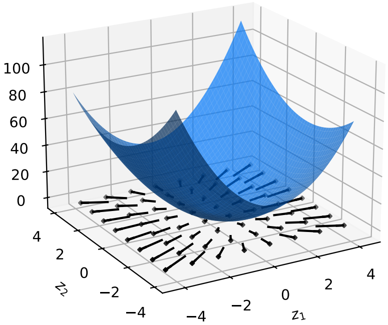
- The gradient of a function $f : \mathbb{R}^d \to \mathbb{R}$ is a **function**[1]:
  - Input: vector in $\mathbb{R}^d$.
  - Output: vector in $\mathbb{R}^d$.
  - Example: $\frac{df}{d\vec{z}}(\vec{z}) = (8z_1 + 2z_2, 2 + 2z_1)^T$.

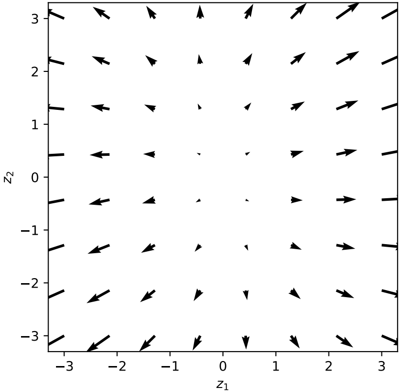
- The gradient of $f : \mathbb{R}^d \to \mathbb{R}$ **evaluated at a point** is a **vector** in $\mathbb{R}^d$:
  - Example: $\frac{df}{d\vec{z}}(3, 1) = (26, 8)^T$.

[1] Sometimes it is referred to as a **vector field**.

Gradient Fields

- The gradient can be viewed as a **vector field**:



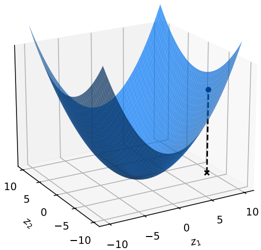


Meaning of Gradient Vector

- 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 ith component is the **slope** of f at $\vec{z}$ in the ith direction.

Exercise



Which of these could possibly be the gradient at the point $(9, -4)$?

- A) $(0, 0)$
- B) $(4, -1)$
- C) $(-4, -1)$
- D) $(-4, 1)$

Gradients and Change

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

- In multiple dimensions:

$$f(\vec{z}+\vec{\delta}) \approx f(\vec{z}) + \left(\delta_1 \times \frac{\partial f}{\partial z_1}(\vec{z})\right) + \left(\delta_2 \times \frac{\partial f}{\partial z_2}(\vec{z})\right) + \ldots$$

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

Exercise

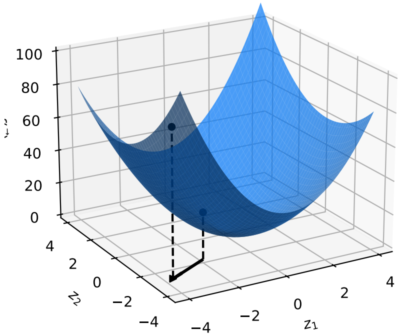
At a point $\vec{z} = (2,3)^T$, $f(\vec{z})$ is 7 and the gradient $\frac{df}{d\vec{z}}(\vec{z}) = (4,-2)^T$.

What is the approximate[a] value of $f(2.1, 3.1)$?

[a] Quality of approximation depends on second derivative.

Steepest Ascent

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

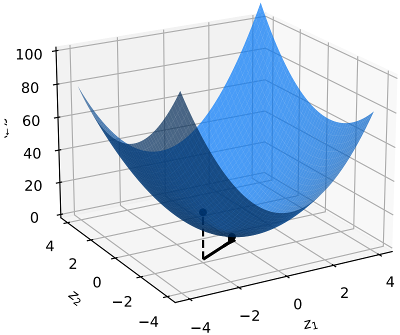


Proof

- 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

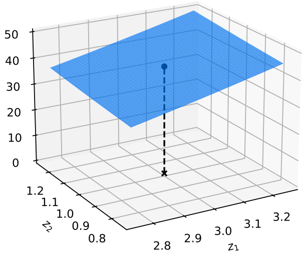
- The **negative** gradient points in the direction of **steepest descent**.



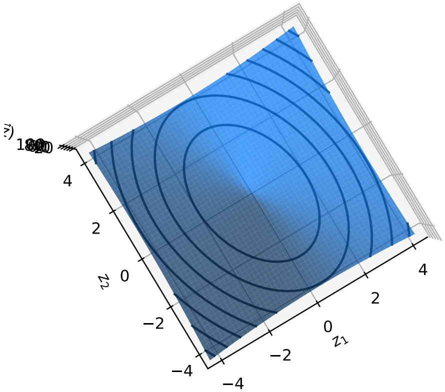
Why?

- The direction of steepest ascent is the **opposite** of the direction of steepest descent.

- Because, zoomed in, the function looks linear.

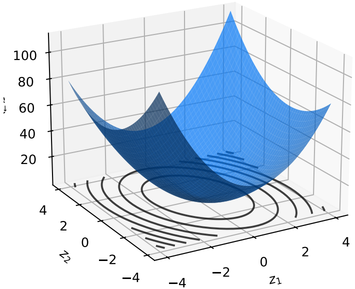


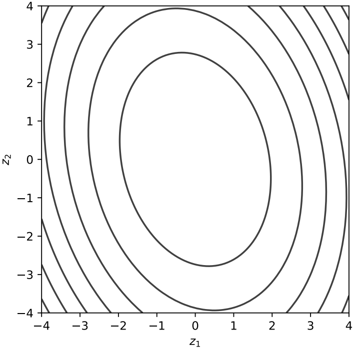
Contours



Contours

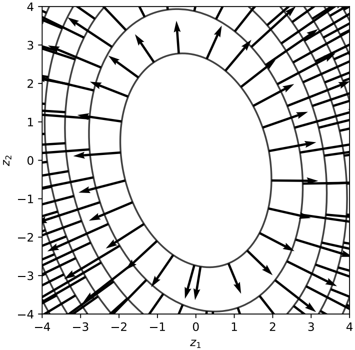
- The contours are the **level sets** of the function.





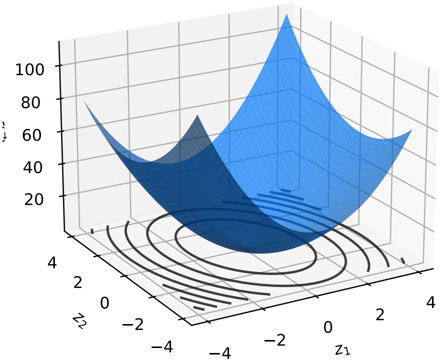
Contours and Gradients

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



Optimization

- To find a **minimum** (or **maximum**), look for where the gradient is $\vec{0}$.



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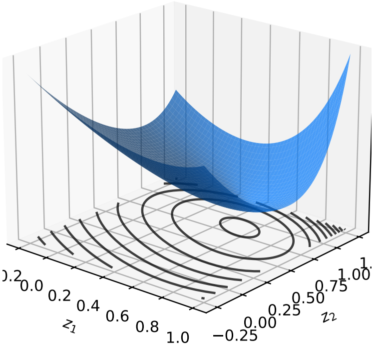
Probabilistic Modeling & Machine Learning

Lecture 3 | Part 3

Gradient Descent

Example

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



Example

- 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? **Not in closed form.**

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

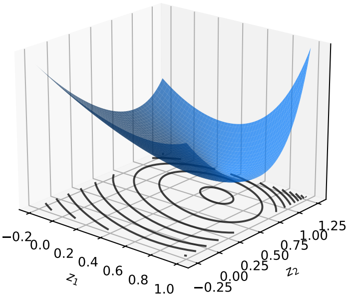
A Problem

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

[2]The 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 $(2, 1)^T$.

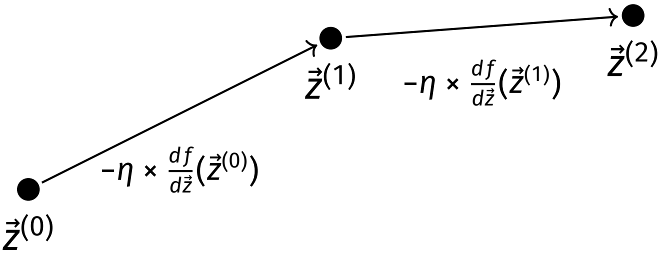
If you're trying to minimize $f(\vec{z})$, which place should you go to next?

- A) $(1, 1)$
- B) $(.8, .9)$
- C) $(1.2, 1.1)$

Direction of Steepest Descent

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

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

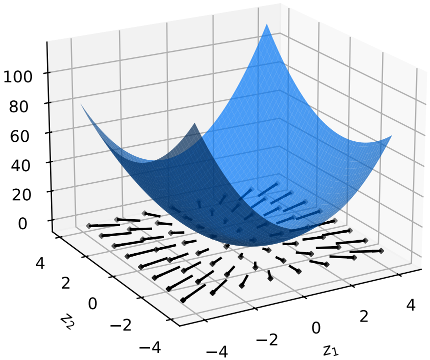


Gradient Descent

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



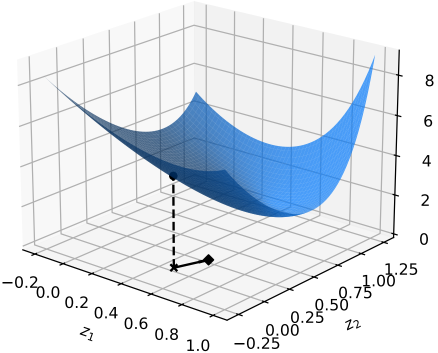
- Close to a minimum, gradient is small.
- **Idea:** stop when $\left\| \frac{df}{d\vec{z}}(\vec{z}^{(t)}) \right\|$ is small.
- **Alternative:** stop when $\|\vec{z}^{(t+1)} - \vec{z}^{(t)}\|$ is small.

```python
def gradient_descent(
    gradient, z_0, learning_rate, stop_threshold
):
    z = z_0
    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**.

Example



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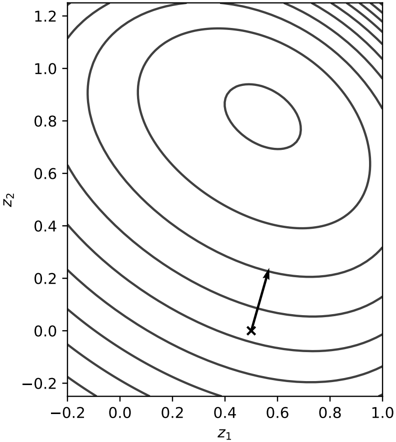

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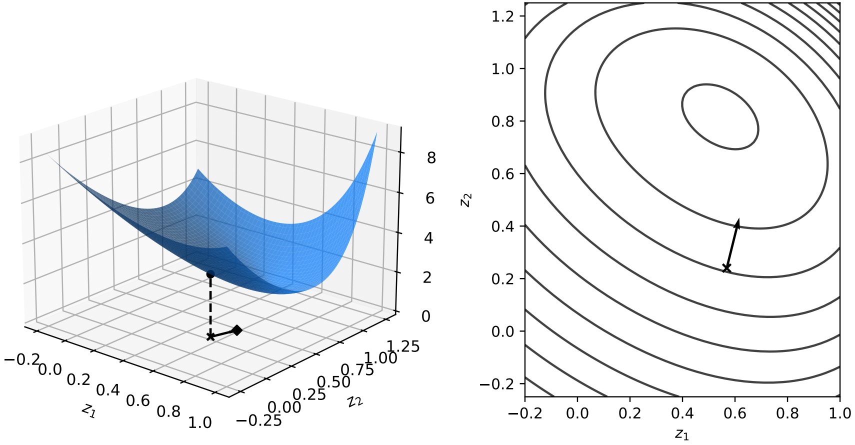
Example



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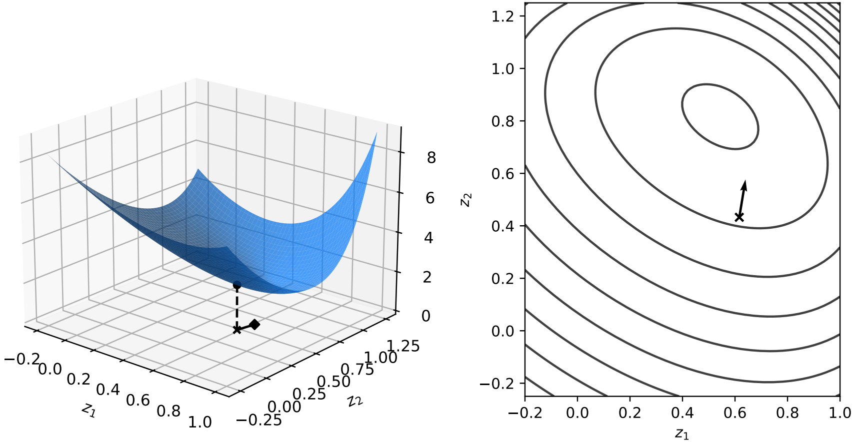
Example



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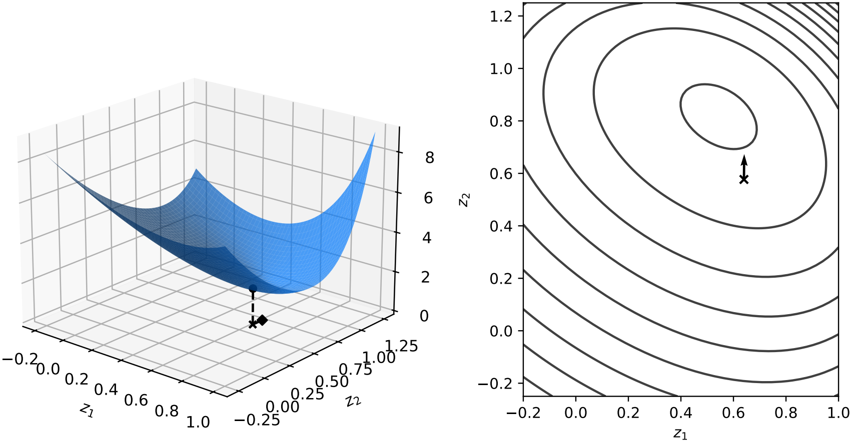
Example



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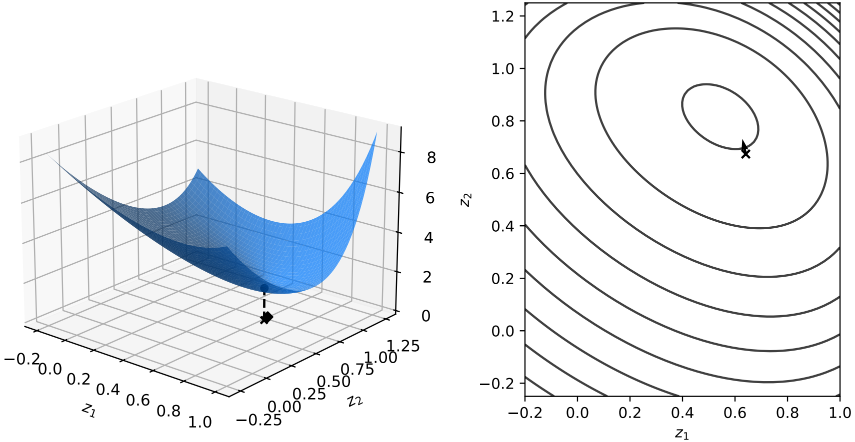

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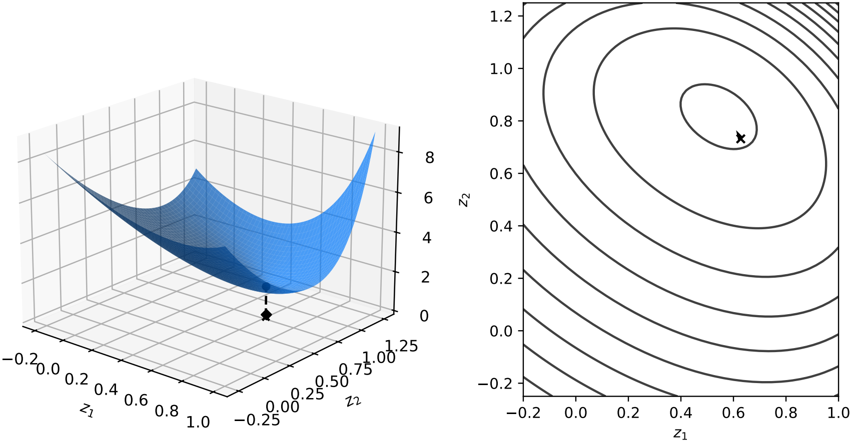
Example



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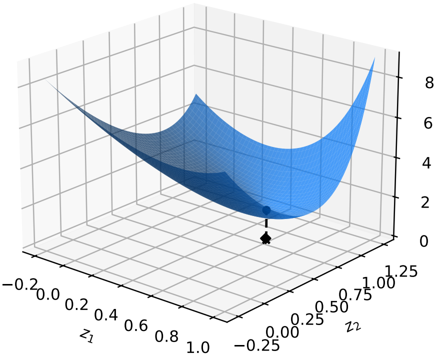
Example



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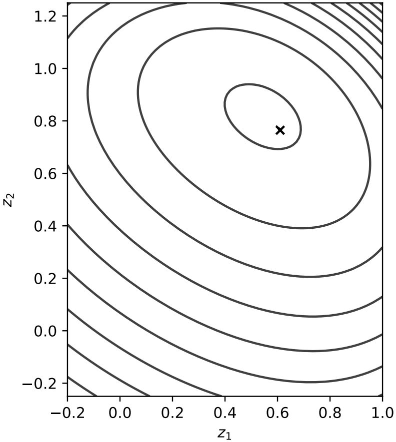

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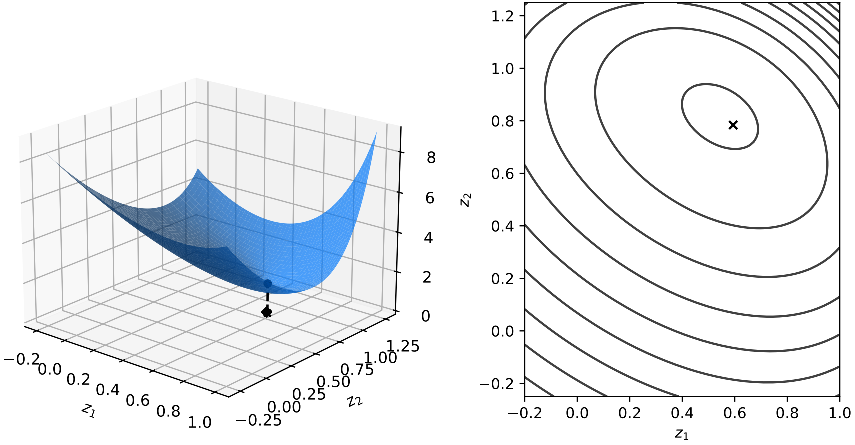
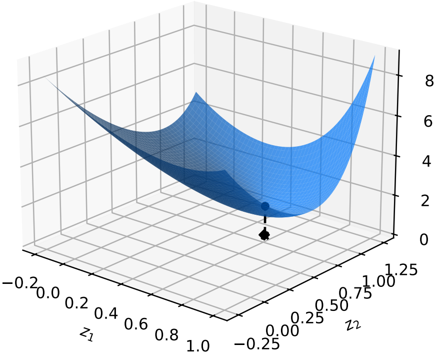
z_1

Example

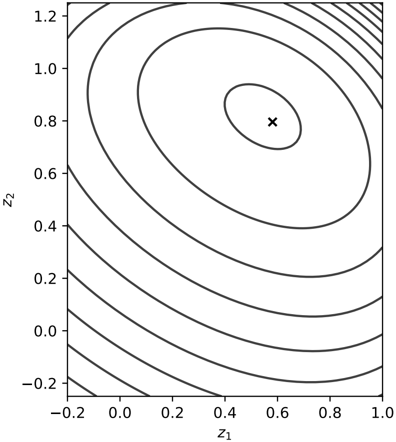


8
6
4
2
0
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
z_1
−0.25
0.00
0.25
0.50
0.75
1.00
1.25
z_2
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
z_2
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
z_1

Example

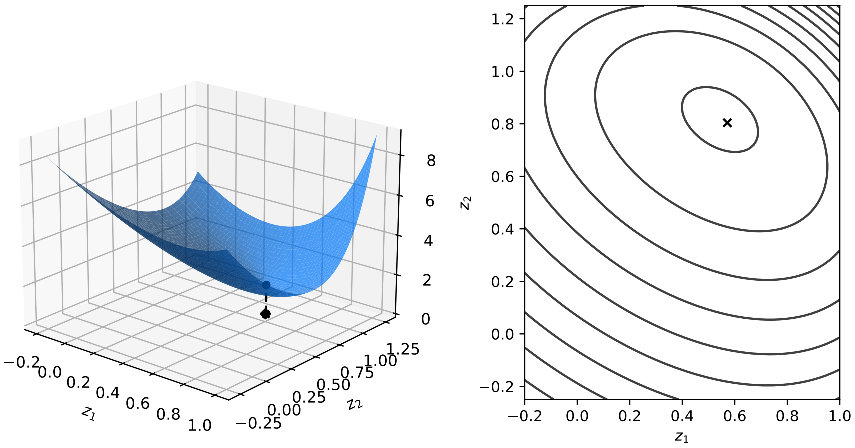


8
6
4
2
0
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
z_1
−0.25
0.00
0.25
0.50
0.75
1.00
1.25
z_2



1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
z_2
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
z_1

Example



8
6
4
2
0
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
z_1
−0.25
0.00
0.25
0.50
0.75
1.00
1.25
z_2
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
z_2
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
z_1

Exercise

Let $f(z_1, z_2) = z_1^4 + 3z_2^2 + z_1 z_2$.

Starting at $\vec{z}^{(0)} = (1, 1)$, what is the next point after one step of gradient descent with learning rate $\eta = 0.1$?

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Probabilistic Modeling & Machine Learning

Lecture 3 | Part 4

Gradient Descent for ERM

Gradient Descent for ERM

- In ERM, our goal is to minimize **empirical risk**:[3]

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

- Often, we can minimize using **gradient descent**.

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

The Gradient of the Risk

- The gradient of the empirical risk is:

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

- 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:

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

Exercise

Recall that the square loss for a linear predictor is: $(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2$.

What is the gradient of the square loss with respect to $\vec{w}$?

The Gradient of the MSE

- The gradient of the mean squared error is:[4]

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

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

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

Exercise

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

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

Gradient Descent for Least Squares

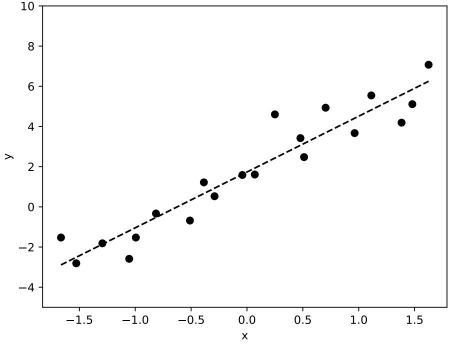
- We can perform least squares regression by solving the normal equations: $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$.

- 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

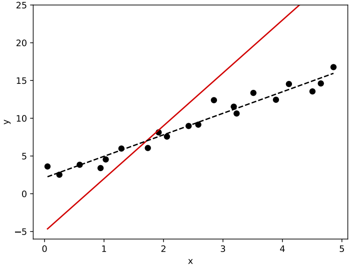
- We will run gradient descent to train a least squares regression model on the following data:



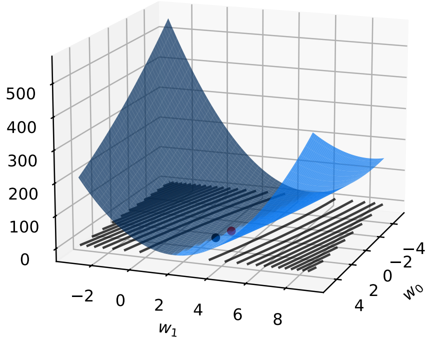
Exercise

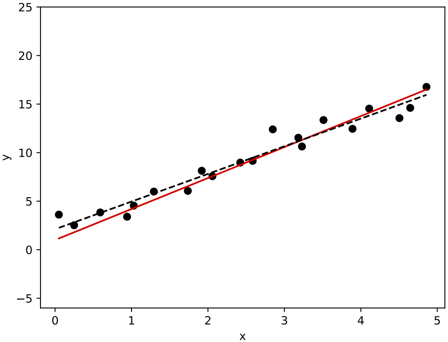
The plot below shows a linear prediction function using weight vector $\vec{w}^{(0)}$.

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

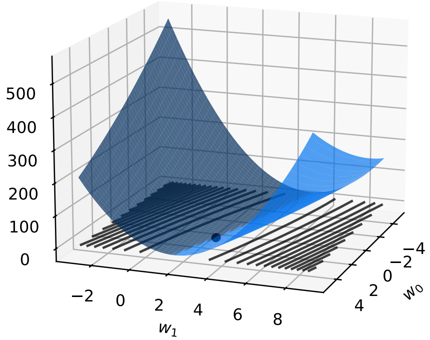


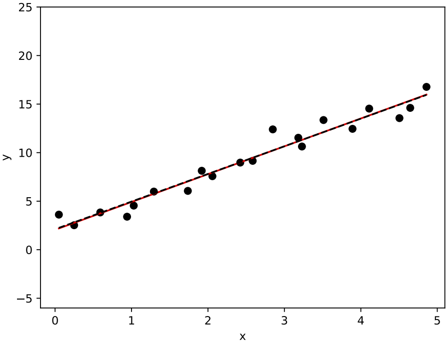
Iteration #40





Iteration #100





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Probabilistic Modeling & Machine Learning

Lecture 3 | Part 5

Appendix: From Theory to Practice

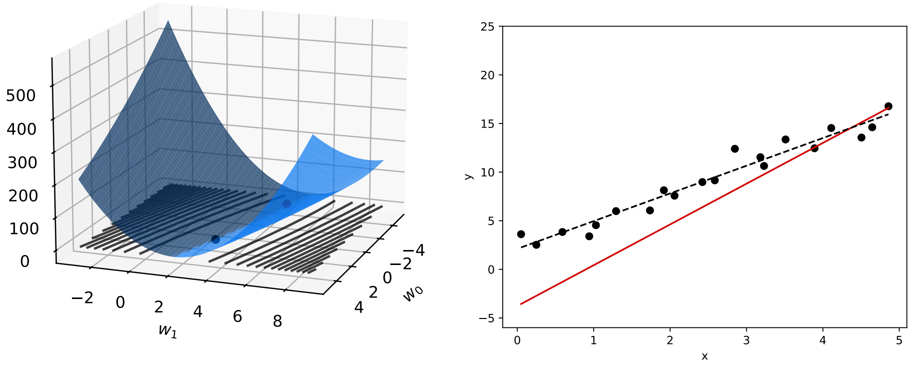
In Practice

- (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

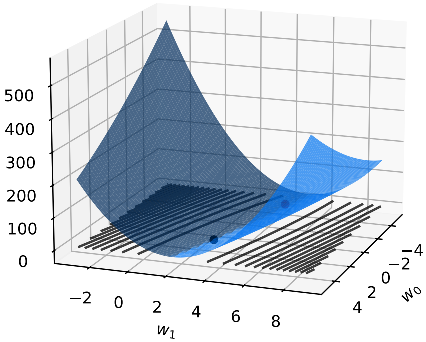

500
400
300
200
100
0
−2
0
2
4
6
8
w_1
−4
−2
0
2
4
w_0
25
20
15
10
5
0
−5
y
0
1
2
3
4
5
x

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

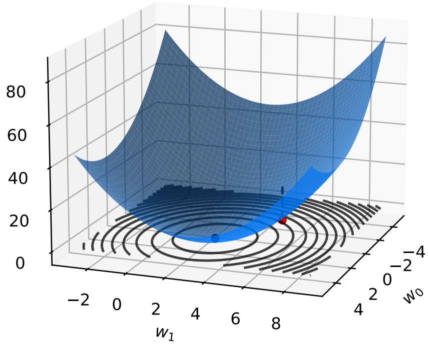
- When the contours are "long and skinny," you will be forced to pick a very small learning rate.

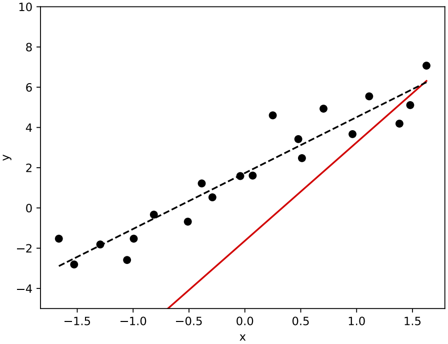


A Fix

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

Scaling





Next Time

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