

CSC 561: Neural Networks and Deep Learning

Gradient Descent

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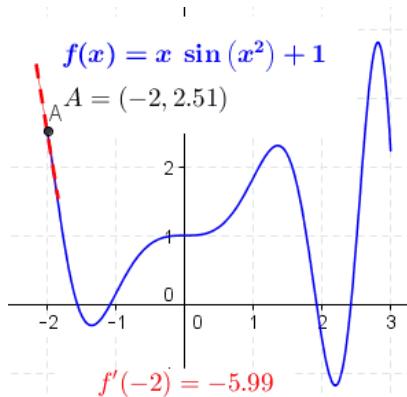


The gradient

From calculus ...

- Given a function $f(x)$, its derivative $f'(x)$ tells us how much a very small increment to the argument will change the value of the function
 - steepness of the function at x
 - rate of change at x
- Positive slope
 - very small increase in x **increases** $f(x)$
- Negative slope
 - very small increase in x **decreases** $f(x)$

Scalar function of scalar argument



For a function $y = f(x)$ the derivative is given by $f'(x) = \alpha$, such that $\Delta y = \alpha \Delta x$

Scalar function of vector argument

- Input is now a column vector \mathbf{x} $y = f(\mathbf{x})$
- note that $\Delta\mathbf{x}$ is also a vector $\Delta\mathbf{y} = \alpha\Delta\mathbf{x}$
- Derivative** is a row vector $\alpha = [\alpha_1, \alpha_2, \dots, \alpha_d]$
- partial derivative α_i indicates how y changes when x_i is incremented, also represented as $\frac{\partial y}{\partial x_i}$

$$\Delta y = \frac{\partial y}{\partial x_1} \Delta x_1 + \frac{\partial y}{\partial x_2} \Delta x_2 + \dots + \frac{\partial y}{\partial x_d} \Delta x_d$$

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Examples

- What is the derivative of:

$$f(\mathbf{x}) = x_1^3 + 2x_2 + 5x_3^4?$$

$$f(x, y, z) = x^3 + 2y + 5z^4?$$

$$f(x, y, z) = x^3y^2 + 2xy + 5yz^4?$$

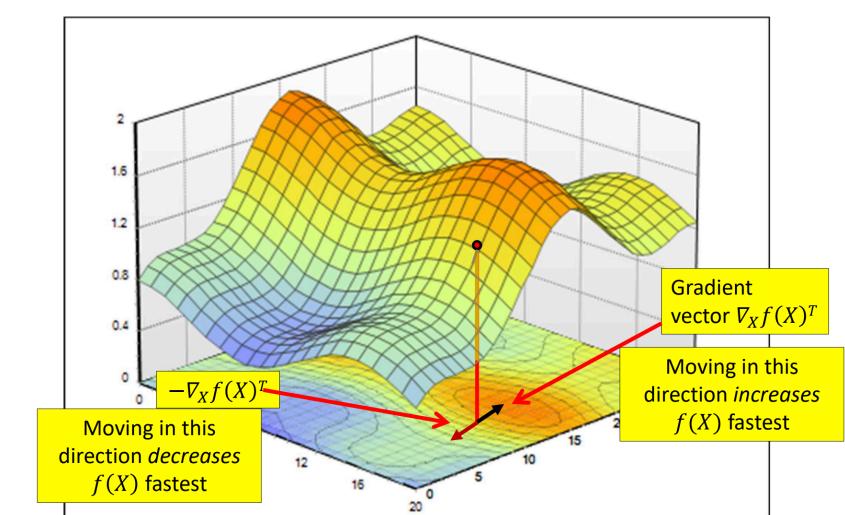
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Gradient

- A **gradient** is the transpose of the **derivative**
- a column vector of partial derivatives

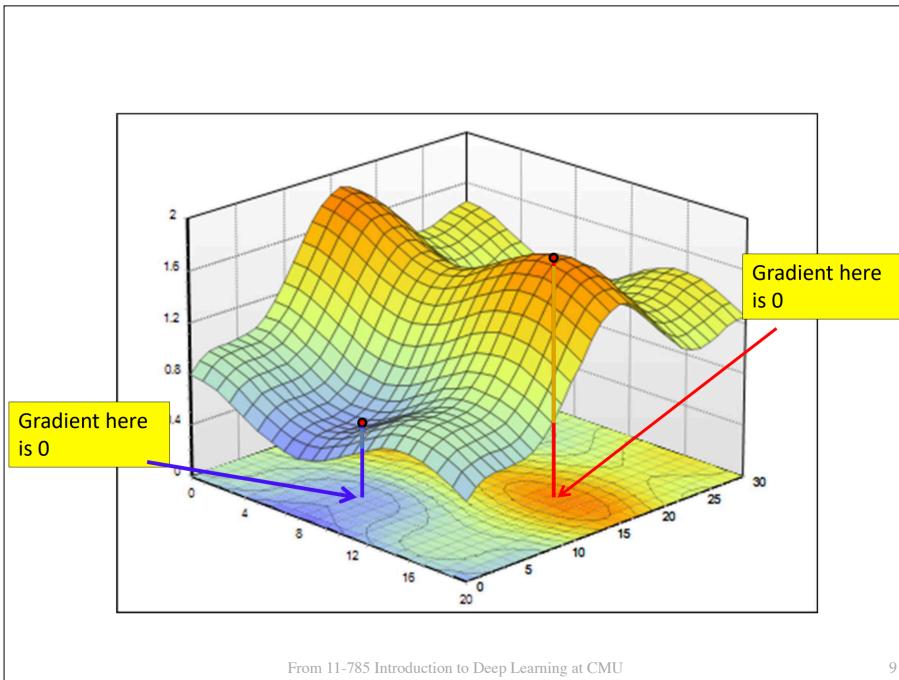
$$\nabla_{\mathbf{x}} f(\mathbf{x})^T = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_d} \end{bmatrix}$$

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From 11-785 Introduction to Deep Learning at CMU

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The Hessian

- Square matrix containing all second-order partial derivatives

$$\nabla_{\mathbf{x}}^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_d \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_d \partial x_d} \end{bmatrix}$$

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Unconstrained optimization

- Given a multivariate function $f(\mathbf{x})$
 - ✓ calculate the derivative $\nabla_{\mathbf{x}} f(\mathbf{x})$ and solve for \mathbf{x} where the derivative is zero
 - ✓ compute the Hessian at solution \mathbf{x}^*
 - if positive definite (positive eigenvalues) then it is a **local minima**
 - if negative definite (negative eigenvalues) then it is a **local maxima**
- Example
 - ✓ $f(x, y, z) = x^3 + 3x^2y - yz^3 + z^2$

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Gradient descent

Alternative solution

- Iterative methods

- apply an update rule iteratively until finding the solution (or approximating it)

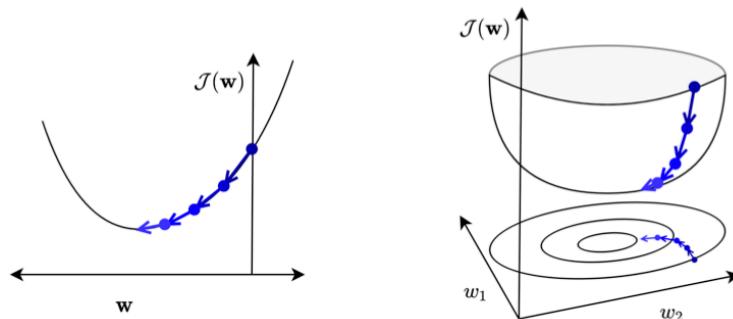
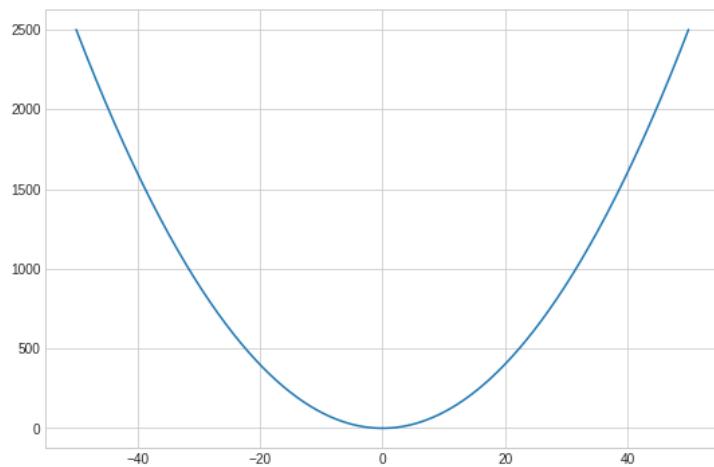


Figure from https://www.cs.toronto.edu/~rgrosse/courses/csc311_f21/lectures/lec03.pdf

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Example: $f(x) = x^2$



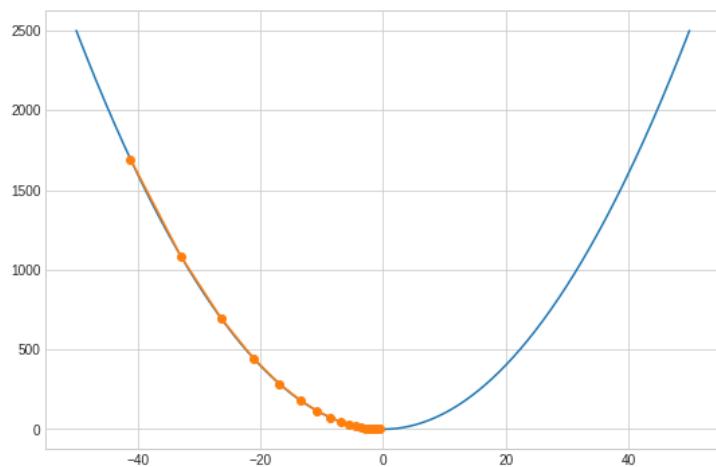
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Gradient descent

- Optimization technique used to find the value of x where $f(x)$ is **minimum**
 - guess a starting point
 - walk iteratively (taking steps) in the **opposite direction** of the function's gradient
- Alternatively, to find the **maximum**, walk in the **direction** of the gradient (gradient ascent)
- Step size (a.k.a. **learning rate**) is critical
 - hyperparameter

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Example: $f(x) = x^2$



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Show me the code

```
# define a function and its derivative
f = lambda x: x ** 2
df = lambda x: 2 * x

# apply gradient descent
n_steps, l_rate = 10, 2

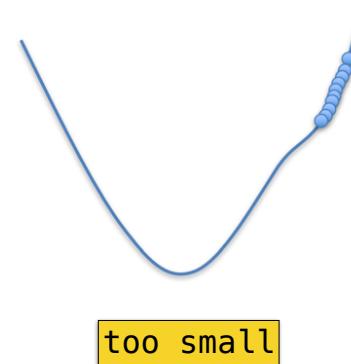
solution = np.random.randint(-50, 50)

for i in range(n_steps):
    solution = solution - (l_rate * df(solution))
    print(f'{solution:.4f}')
```

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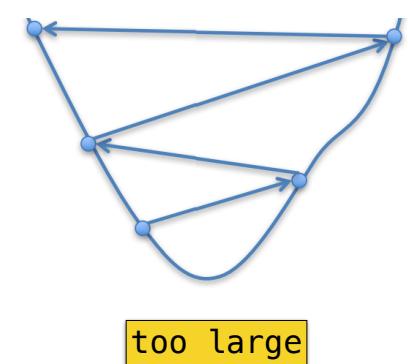
The learning rate

slow convergence



too small

overshoots, may not converge



too large

https://www.cc.gatech.edu/~bboots3/CS4641-Fall2018/Lecture3/03_LinearRegression.pdf

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Playground

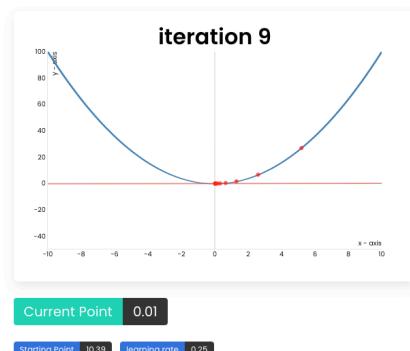


Hey there!
Let's play with
gradient descent.

This mini-app acts as an
interactive supplement to Teach
LA's curriculum on linear
regression and gradient descent.

[Lesson \(do this first!\)](#)

[Playground](#)



<https://uclaacm.github.io/gradient-descent-visualiser/>

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Gradient descent and machine learning

Learning (minimizing the loss)

- Want to minimize the **empirical risk**

$$\mathbf{w}^* = \arg \min_{\mathbf{w}} J(\mathbf{w})$$

$$\mathbf{w}^* = \arg \min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^n l(h_{\mathbf{w}}, x_i, y_i)$$

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Learning (minimizing the loss)

- Can use gradient descent

- iteratively update the desired **parameters (weights)** until convergence or a maximum number of iterations

$$\mathbf{w}^* = \arg \min_{\mathbf{w}} J(\mathbf{w})$$

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla_{\mathbf{w}} J(\mathbf{w}^{(t)})$$

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Updating the parameters

- Full** gradient descent

- a.k.a. batch gradient descent

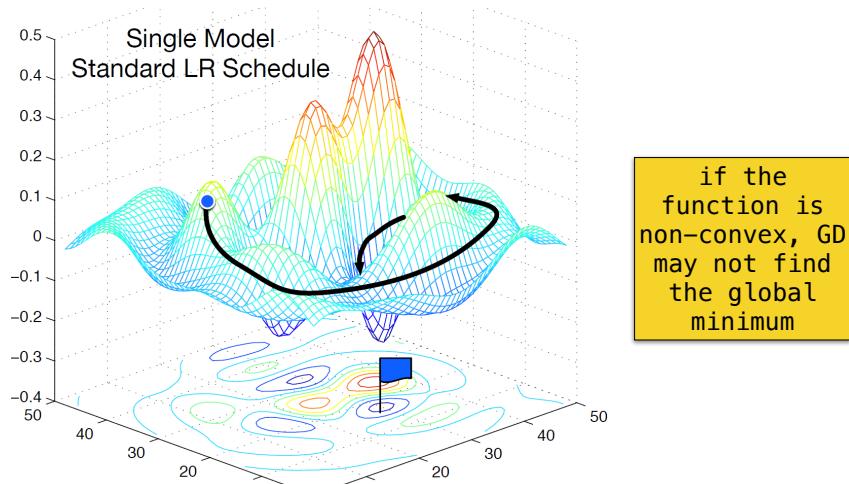
- update parameters after calculating the gradient using the entire training data

- Mini-batch** gradient descent

- update parameters after calculating the gradient using subsets of the training data (mini-batches)

- Stochastic** gradient descent

- update parameters after calculating the gradient using a single datapoint



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$$\mathbf{w}^{(t)} \rightarrow \mathbf{w}^{(t+1)} \rightarrow \mathbf{w}^{(t+2)} \rightarrow \dots$$

can be slow
on large
datasets

full gradient
descent

requires a full
pass over the
training data

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$$\mathbf{w}^{(t)} \rightarrow \mathbf{w}^{(t+1)} \rightarrow \mathbf{w}^{(t+2)} \rightarrow \dots$$

mini-batch
gradient descent

use a subset
(mini-batch) at
each iteration

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$$\mathbf{w}^{(t)} \rightarrow \mathbf{w}^{(t+1)} \rightarrow \mathbf{w}^{(t+2)} \rightarrow \dots$$

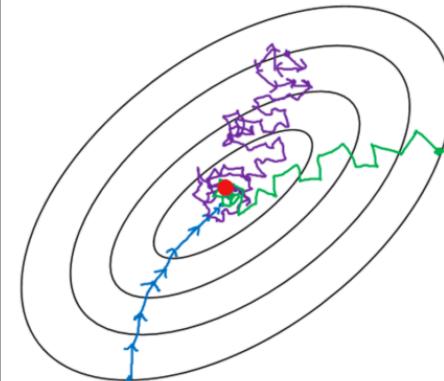
scalable but
with high
variance
(loss
increasing
at some
iterations)

stochastic
gradient descent

use a single
datapoint at
each iteration

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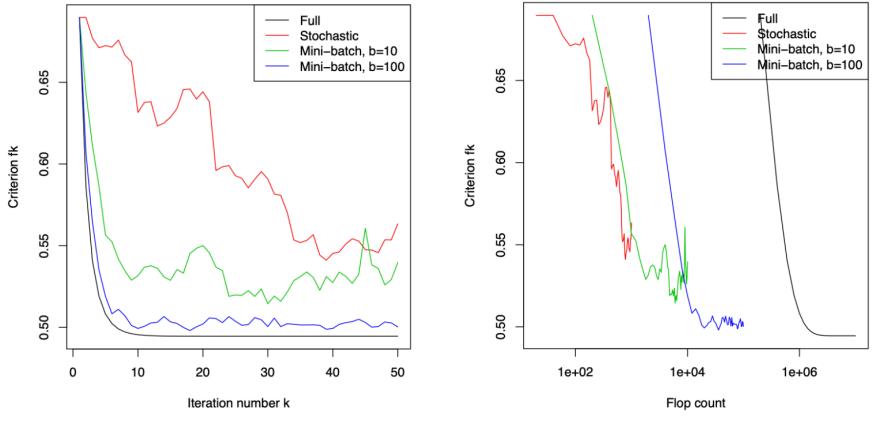
Convergence



- Batch gradient descent
- Mini-batch gradient Descent
- Stochastic gradient descent

Efficiency

Consider logistic regression with 10000 training samples and $\mathbf{x}_i \in \mathbb{R}^{20}$



Credit: Ryan Tibshirani, Convex Optimization 10-725

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Remarks on mini-batch and stochastic GD

- Both are **unbiased** estimators of the full gradient
- Both can march toward a solution before even seeing all the data
- Constant** computational cost of each weight update
 - regardless the length of the training data
- SGD with a fixed learning rate cannot guarantee convergence
 - it does not minimize the gradient of the full data directly
 - must shrink** learning rate during training

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