Deep Learning & Applied AI

Stochastic gradient descent

Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

2nd semester a.y. 2019/2020 · March 23, 2020

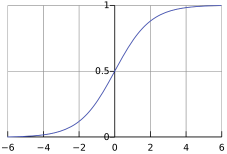
Logistic regression

We got to the following convex loss:

$$\ell_\Theta(\{x_i, y_i\}) = -\sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b))$$

Here, σ is the nonlinear logistic sigmoid:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



σ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_{\Theta} \ell_{\Theta} = 0$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$\nabla_\Theta \left(y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) \right)$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$\nabla_\Theta y_i \ln(\sigma(ax_i + b)) + \nabla_\Theta (1 - y_i) \ln(1 - \sigma(ax_i + b))$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \ln(\sigma(ax_i + b)) + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial h}{\partial a}$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial}{\partial a} a x_i + b$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i)\ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i)\nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial \sigma(ax_i + b)}{\partial(ax_i + b)} \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial}{\partial (ax_i + b)} \frac{1}{1 + e^{-(ax_i + b)}} \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i)\ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i)\nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{e^{-(ax_i + b)}}{(1 + e^{-(ax_i + b)})^2} \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i+b)}} \frac{e^{-(ax_i+b)}}{1 + e^{-(ax_i+b)}} \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i + b)}} \frac{(1 + e^{-(ax_i + b)}) - 1}{1 + e^{-(ax_i + b)}} \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i + b)}} (1 - \frac{1}{1 + e^{-(ax_i + b)}}) \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i)\nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial \ln(\sigma(ax_i + b))}{\partial \sigma(ax_i + b)} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{1}{\sigma(ax_i + b)} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{1}{\sigma(ax_i + b)} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b)) x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b)) x_i$$

And similarly for the second term and for all parameters.

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system to solve for the parameters.

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(a x_i + b)) = (1 - \sigma(a x_i + b)) x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system to solve for the parameters.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(a x_i + b)) = (1 - \sigma(a x_i + b)) x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system to solve for the parameters.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	loss	solution
linear regression		
linear regression + Tikhonov		
logistic regression		

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(a x_i + b)) = (1 - \sigma(a x_i + b)) x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system to solve for the parameters.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	**loss**	**solution**
linear regression	convex	
linear regression + Tikhonov	convex	
logistic regression	convex	

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(a x_i + b)) = (1 - \sigma(a x_i + b)) x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system to solve for the parameters.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	
logistic regression	convex	

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system to solve for the parameters.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system to solve for the parameters.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	nonlinear optimization

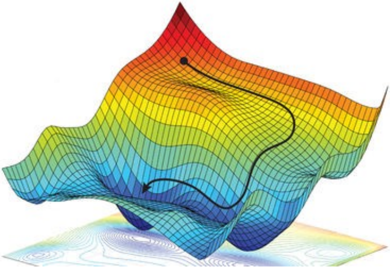
Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

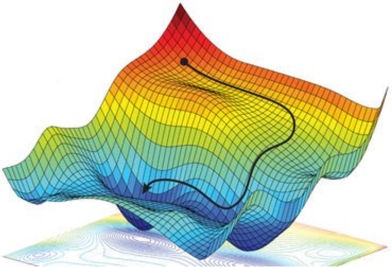
Example of a loss function $\ell_{\boldsymbol{\Theta}} : \mathbb{R}^2 \to \mathbb{R}$:



Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

Example of a loss function $\ell_{\boldsymbol{\Theta}} : \mathbb{R}^2 \to \mathbb{R}$:



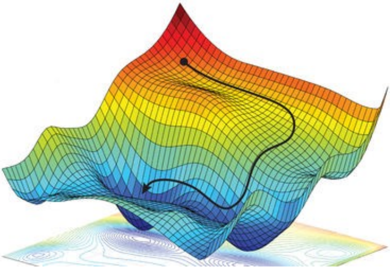
Overall idea: Move where the function decreases the most.

1. Start from some point $\boldsymbol{\Theta}^{(0)} \in \mathbb{R}^2$.

Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

Example of a loss function $\ell_{\boldsymbol{\Theta}} : \mathbb{R}^2 \to \mathbb{R}$:



Overall idea: Move where the function decreases the most.

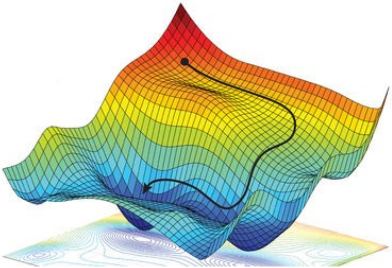
1. Start from some point $\boldsymbol{\Theta}^{(0)} \in \mathbb{R}^2$.
2. Iteratively compute:

$$\boldsymbol{\Theta}^{(t+1)} = \boldsymbol{\Theta}^{(t)} - \alpha \nabla \ell_{\boldsymbol{\Theta}^{(t)}}$$

Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

Example of a loss function $\ell_{\boldsymbol{\Theta}} : \mathbb{R}^2 \to \mathbb{R}$:



Overall idea: Move where the function decreases the most.

1. Start from some point $\boldsymbol{\Theta}^{(0)} \in \mathbb{R}^2$.
2. Iteratively compute:

$$\boldsymbol{\Theta}^{(t+1)} = \boldsymbol{\Theta}^{(t)} - \alpha \nabla \ell_{\boldsymbol{\Theta}^{(t)}}$$

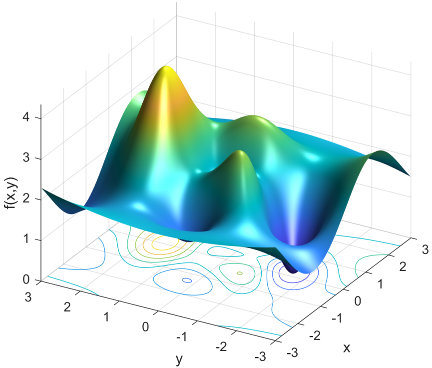
3. Stop when a minimum is reached.

Gradient descent

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

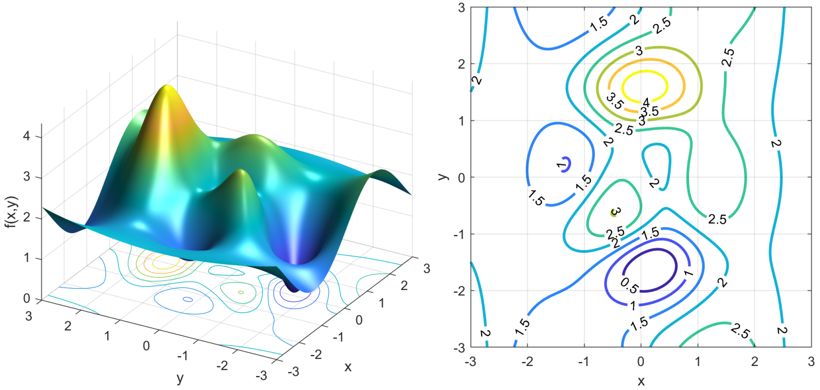
Gradient descent

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$



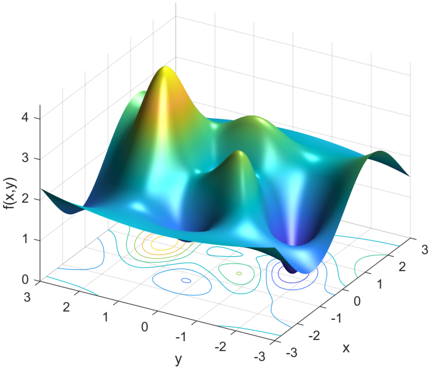
Gradient descent

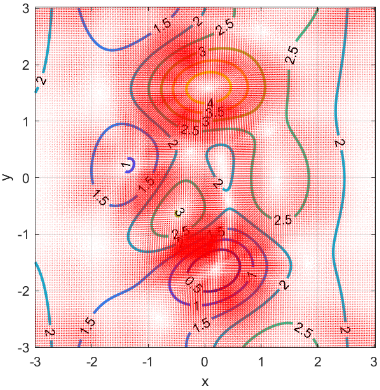
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$



Gradient descent

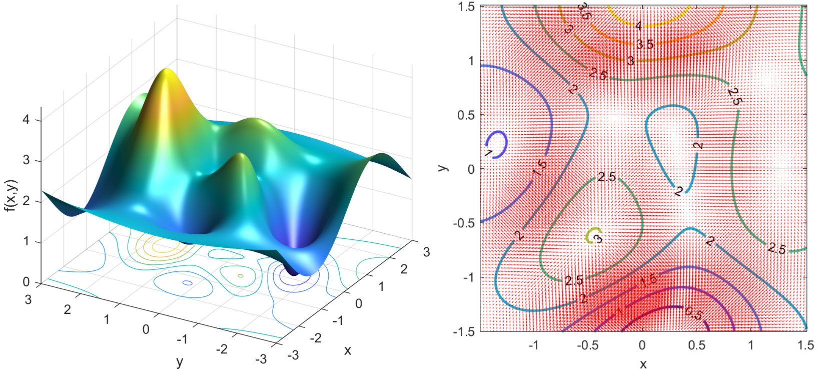
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$





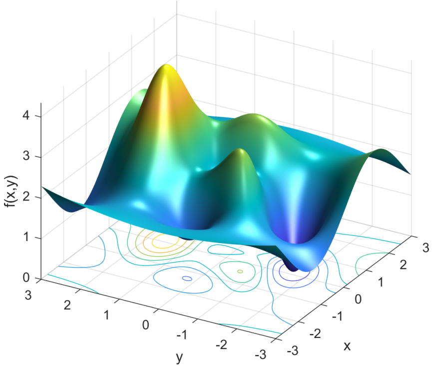
Gradient descent

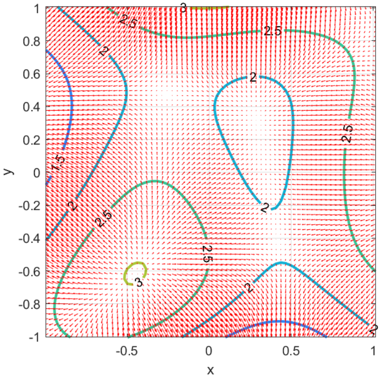
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$



Gradient descent

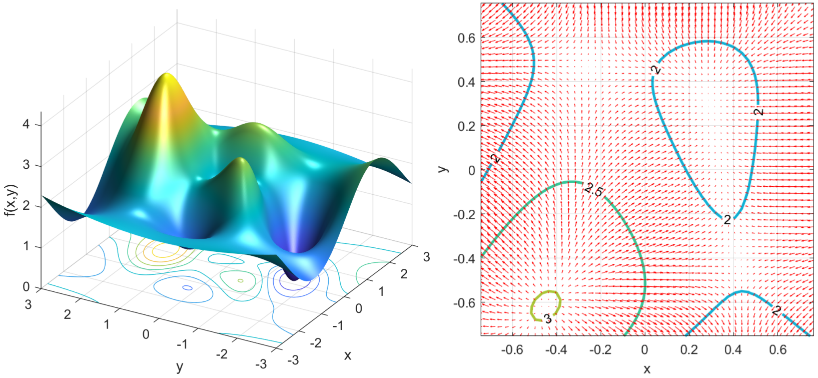
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$





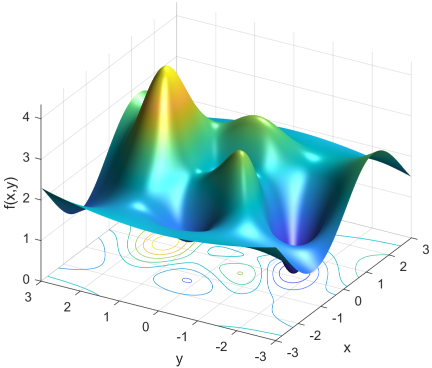
Gradient descent

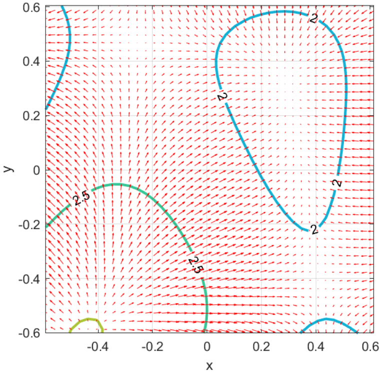
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$



Gradient descent

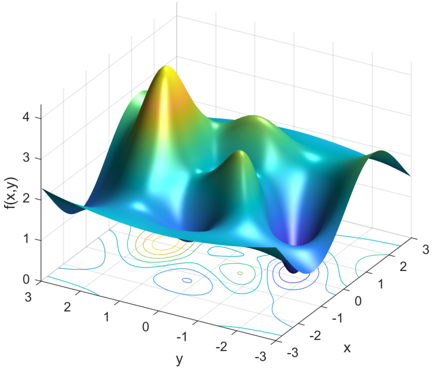
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

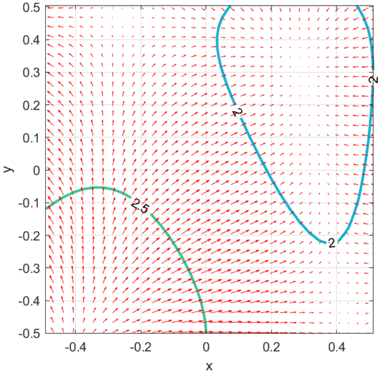




Gradient descent

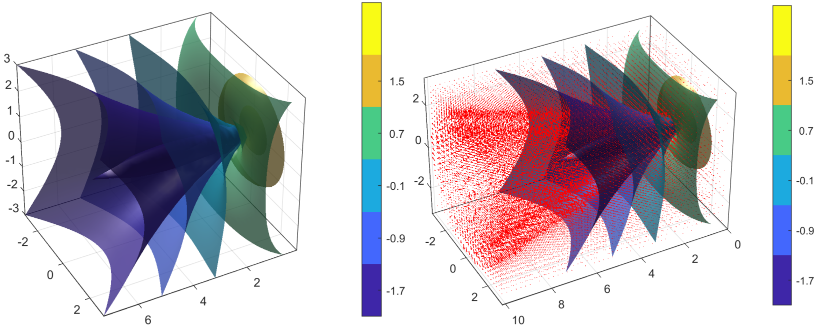
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$





Gradient descent: High dimensions

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

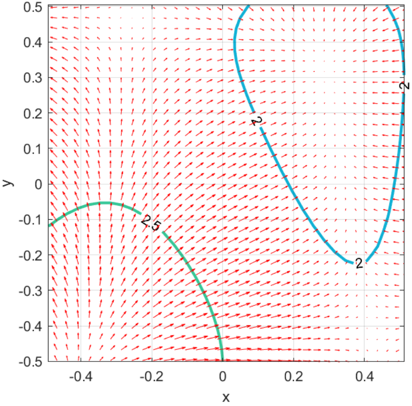


All we say is also valid in $\gg 2$ dimensions.

Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

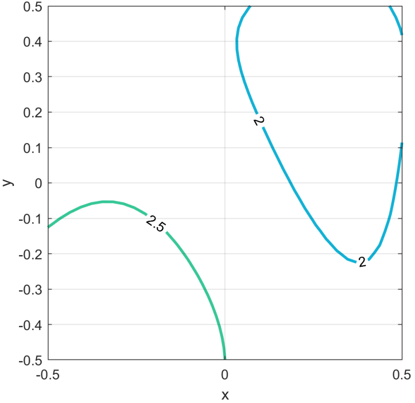
The gradient is orthogonal to level curves / level surfaces.



Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

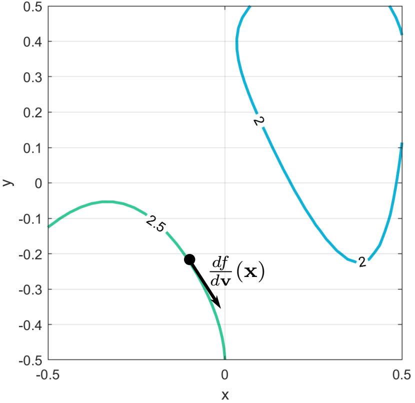
The gradient is orthogonal to level curves / level surfaces.



Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

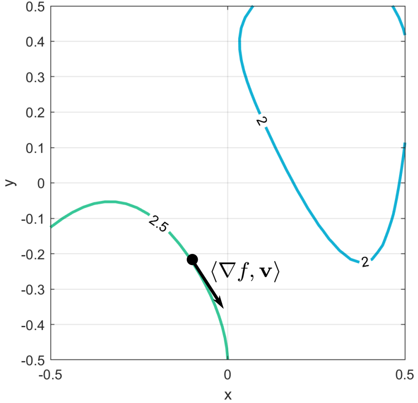
The gradient is orthogonal to level curves / level surfaces.



Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

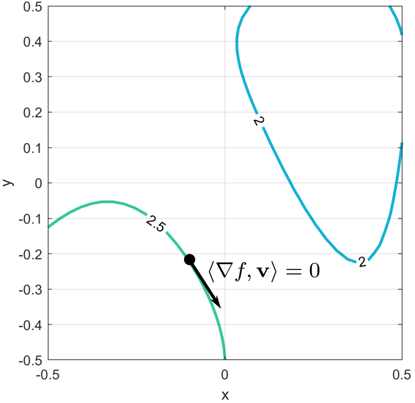
The gradient is orthogonal to level curves / level surfaces.



Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The gradient is orthogonal to level curves / level surfaces.

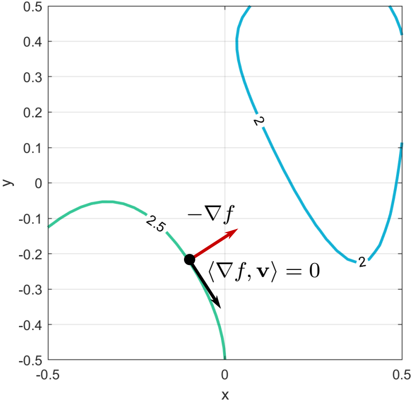


The directional derivative is zero along isocurves.

Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The gradient is orthogonal to level curves / level surfaces.



The directional derivative is zero along isocurves.

Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

Recall:

f has partial (or even directional) derivatives $\not\Rightarrow$ f is differentiable

Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

Recall:

$$f \text{ has partial (or even directional) derivatives} \not\Rightarrow f \text{ is differentiable}$$

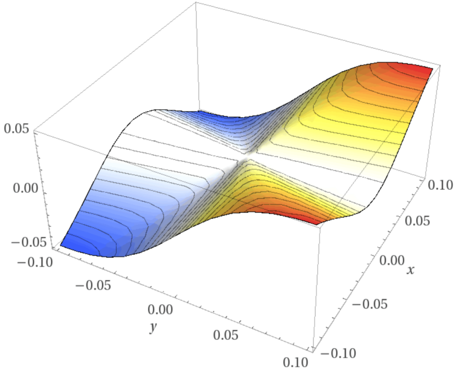
$$f \text{ has continuous gradient} \Rightarrow f \text{ is differentiable}$$

Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

Example in $\mathbb{R}^2$: $f(x, y) = \begin{cases} 0 & \text{at } (0,0) \\ \frac{x^2 y}{x^2+y^2} & \text{elsewhere} \end{cases}$



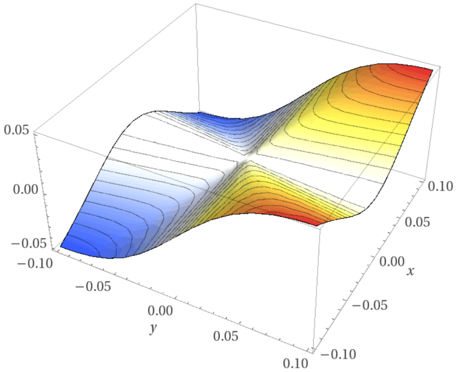
Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

Example in $\mathbb{R}^2$: $f(x, y) = \begin{cases} 0 & \text{at } (0,0) \\ \frac{x^2 y}{x^2+y^2} & \text{elsewhere} \end{cases}$

$\frac{\partial}{\partial y} f(x, 0) = 1$ for $x \neq 0$



Gradient descent: Differentiability

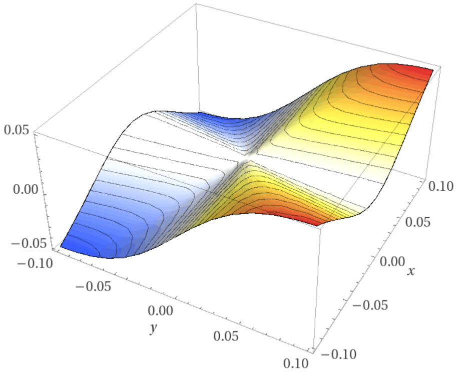
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

Example in $\mathbb{R}^2$: $f(x,y) = \begin{cases} 0 & \text{at } (0,0) \\ \frac{x^2 y}{x^2+y^2} & \text{elsewhere} \end{cases}$

$\frac{\partial}{\partial y} f(x,0) = 1$ for $x \neq 0$

$\frac{\partial}{\partial y} f(0,y) = 0$ for $y \neq 0$



Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

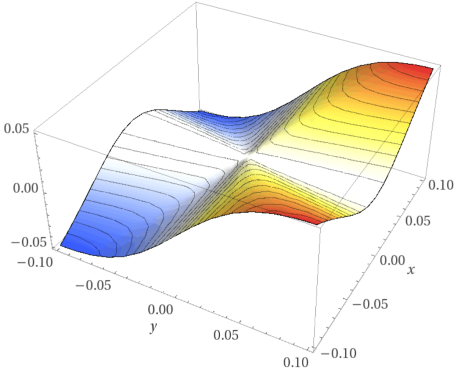
Gradient descent requires f to be differentiable at all points.

Example in $\mathbb{R}^2$: $f(x,y) = \begin{cases} 0 & \text{at } (0,0) \\ \frac{x^2 y}{x^2+y^2} & \text{elsewhere} \end{cases}$

$\frac{\partial}{\partial y} f(x,0) = 1$ for $x \neq 0$

$\frac{\partial}{\partial y} f(0,y) = 0$ for $y \neq 0$

$\Rightarrow \frac{\partial}{\partial y} f(x,y)$ discontinuous at $(0,0)$



Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

Example in $\mathbb{R}^2$: $f(x, y) = \begin{cases} 0 & \text{at } (0,0) \\ \frac{x^2 y}{x^2+y^2} & \text{elsewhere} \end{cases}$

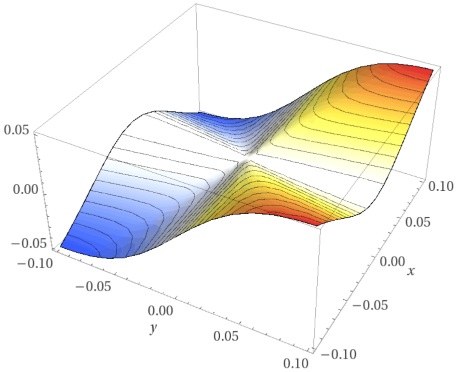
$\frac{\partial}{\partial y} f(x, 0) = 1$ for $x \neq 0$

$\frac{\partial}{\partial y} f(0, y) = 0$ for $y \neq 0$

$\Rightarrow \frac{\partial}{\partial y} f(x, y)$ discontinuous at $(0, 0)$

the partial derivatives of f are defined everywhere, but are discontinuous at the origin

$\Rightarrow f$ is not differentiable



Gradient descent: Stationary points

A stationary point is such that:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \cancelto{0}{\alpha \nabla f(\mathbf{x}^{(t)})}$$

Gradient descent "gets stuck" at stationary points.

Gradient descent: Stationary points

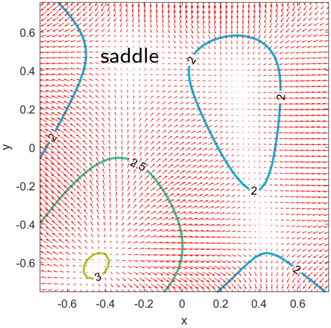
A stationary point is such that:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \cancel{\nabla f(\mathbf{x}^{(t)})}^{\,0}$$

Gradient descent "gets stuck" at stationary points.

However:

- Stationary point $\not\Rightarrow$ local minimum



Gradient descent: Stationary points

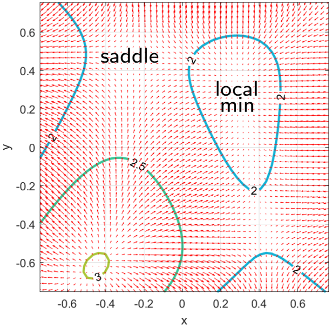
A stationary point is such that:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \cancelto{0}{\nabla f(\mathbf{x}^{(t)})}$$

Gradient descent "gets stuck" at stationary points.

However:

- Stationary point $\not\Rightarrow$ local minimum $\not\Rightarrow$ global minimum.



Gradient descent: Stationary points

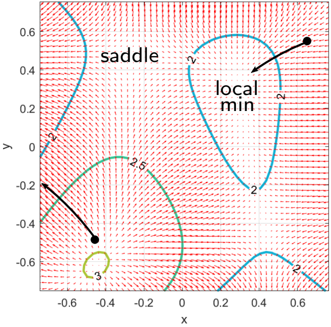
A stationary point is such that:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \cancelto{0}{\nabla f(\mathbf{x}^{(t)})}$$

Gradient descent "gets stuck" at stationary points.

However:

- Stationary point $\not\Rightarrow$ local minimum $\not\Rightarrow$ global minimum.
- Which stationary point depends on the initialization.



Gradient descent: Learning rate

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The parameter $\alpha > 0$ is also called learning rate in ML.

Gradient descent: Learning rate

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The parameter $\alpha > 0$ is also called learning rate in ML.

Remark: The length of a step is not simply α, but $\alpha \|\nabla f\|$.

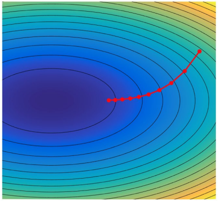
Gradient descent: Learning rate

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The parameter $\alpha > 0$ is also called learning rate in ML.

Remark: The length of a step is not simply α, but $\alpha\|\nabla f\|$.

- Too small: slow convergence speed



small α

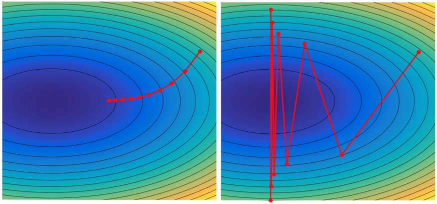
Gradient descent: Learning rate

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The parameter $\alpha > 0$ is also called learning rate in ML.

Remark: The length of a step is not simply α, but $\alpha \|\nabla f\|$.

- Too small: slow convergence speed
- Too big: risk of overshooting



small α large α

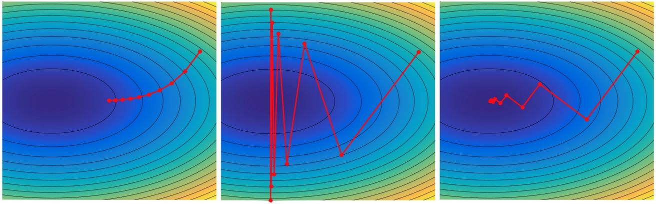
Gradient descent: Learning rate

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The parameter $\alpha > 0$ is also called learning rate in ML.

Remark: The length of a step is not simply α, but $\alpha \|\nabla f\|$.

- Too small: slow convergence speed
- Too big: risk of overshooting
- Optimal values can be found via line search algorithms



small α | large α | optimal α

$\arg\min_\alpha f(\mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)}))$

Decay and momentum

The learning rate can be adaptive or follow a schedule.

Decay and momentum

The learning rate can be adaptive or follow a schedule.

- Decrease α according to a decay parameter ρ:
  Examples:

$$\alpha^{(t+1)} = (1-\frac{t}{\rho})\alpha^{(0)}+\frac{t}{\rho}\alpha^{(\rho)}\,, \quad \alpha^{(t+1)} = \frac{\alpha^{(t)}}{1+\rho t}\,, \quad \alpha^{(t+1)} = \alpha^{(0)}e^{-\rho t}$$

Decay and momentum

The learning rate can be adaptive or follow a schedule.

- Decrease α according to a decay parameter ρ:

  Examples:

$$\alpha^{(t+1)} = (1-\frac{t}{\rho})\alpha^{(0)}+\frac{t}{\rho}\alpha^{(\rho)}\,, \quad \alpha^{(t+1)} = \frac{\alpha^{(t)}}{1+\rho t}\,, \quad \alpha^{(t+1)} = \alpha^{(0)}e^{-\rho t}$$

- Accumulate past gradients and keep moving in their direction:

$$\begin{aligned} \mathbf{v}^{(t+1)} &= \lambda \mathbf{v}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)}) \quad \text{momentum} \\ \mathbf{x}^{(t+1)} &= \mathbf{x}^{(t)} + \mathbf{v}^{(t+1)} \end{aligned}$$

Decay and momentum

The learning rate can be adaptive or follow a schedule.

- Decrease α according to a decay parameter ρ:

  Examples:

  $$\alpha^{(t+1)} = (1-\frac{t}{\rho})\alpha^{(0)}+\frac{t}{\rho}\alpha^{(\rho)}\,, \quad \alpha^{(t+1)} = \frac{\alpha^{(t)}}{1+\rho t}\,, \quad \alpha^{(t+1)} = \alpha^{(0)}e^{-\rho t}$$

- Accumulate past gradients and keep moving in their direction:

  $$\begin{aligned} \mathbf{v}^{(t+1)} &= \lambda \mathbf{v}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)}) \quad \text{momentum} \\ \mathbf{x}^{(t+1)} &= \mathbf{x}^{(t)} + \mathbf{v}^{(t+1)} \end{aligned}$$

  Step length $\propto$ how aligned is the sequence of gradients.

  $$\frac{1}{1-\lambda}\alpha\|\nabla f\|$$

Decay and momentum

The learning rate can be adaptive or follow a schedule.

- Decrease α according to a decay parameter ρ:

  Examples:

$$\alpha^{(t+1)} = (1-\frac{t}{\rho})\alpha^{(0)}+\frac{t}{\rho}\alpha^{(\rho)}\,, \quad \alpha^{(t+1)} = \frac{\alpha^{(t)}}{1+\rho t}\,, \quad \alpha^{(t+1)} = \alpha^{(0)}e^{-\rho t}$$

- Accumulate past gradients and keep moving in their direction:

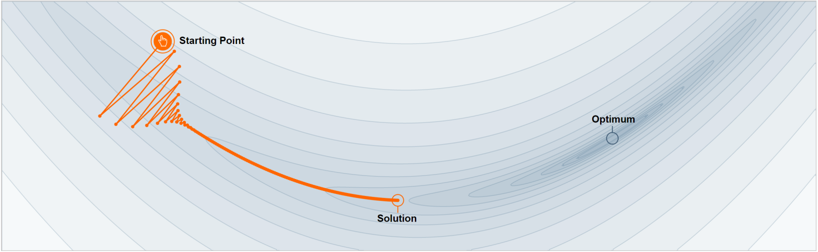
$$\mathbf{v}^{(t+1)} = \lambda\mathbf{v}^{(t)} - \alpha\nabla f(\mathbf{x}^{(t)}) \quad \text{momentum}$$
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} + \mathbf{v}^{(t+1)}$$

  Step length $\propto$ how aligned is the sequence of gradients.

$$\frac{1}{1-\lambda}\alpha\|\nabla f\|$$

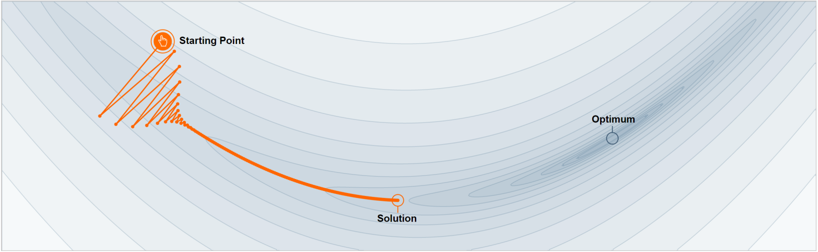
  Acceleration effect for big λ + escape from local minima.

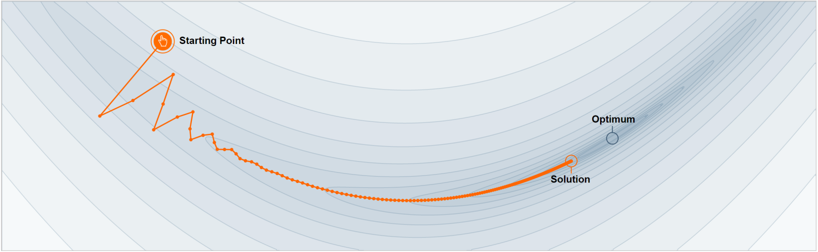
Momentum



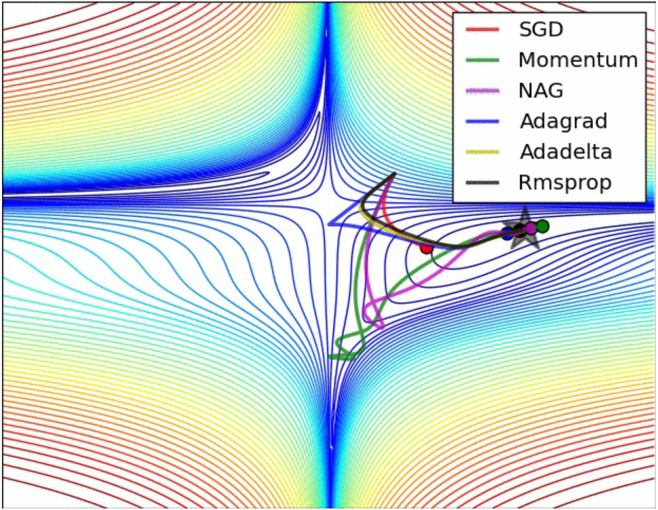
Goh, "Why momentum really works", Distill 2017

Momentum





Goh, “Why momentum really works”, Distill 2017


SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)})$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)})$$
$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} - \alpha \nabla f(\mathbf{x}^{(1)})$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\begin{aligned}
\mathbf{x}^{(1)} &= \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)}) \\
\mathbf{x}^{(2)} &= \mathbf{x}^{(1)} - \alpha \nabla f(\mathbf{x}^{(1)}) \\
&= \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)}) - \alpha \nabla f(\mathbf{x}^{(1)})
\end{aligned}$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$
\begin{aligned}
\mathbf{x}^{(1)} &= \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)}) \\
\mathbf{x}^{(2)} &= \mathbf{x}^{(1)} - \alpha \nabla f(\mathbf{x}^{(1)}) \\
&= \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)}) - \alpha \nabla f(\mathbf{x}^{(1)}) \\
&\vdots \\
\mathbf{x}^{(t+1)} &= \mathbf{x}^{(0)} - \alpha \sum_{i=1}^{t} \nabla f(\mathbf{x}^{(t)})
\end{aligned}
$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} - \alpha \sum_{i=1}^{t} \nabla f(\mathbf{x}^{(t)})$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} - \alpha \sum_{i=1}^{t} \nabla f(\mathbf{x}^{(t)})$$

With momentum:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=1}^{t} \frac{1 - \lambda^{t+1-i}}{1 - \lambda} \nabla f(\mathbf{x}^{(t)})$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} - \alpha \sum_{i=1}^{t} \nabla f(\mathbf{x}^{(t)})$$

With momentum:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=1}^{t} \frac{1-\lambda^{t+1-i}}{1-\lambda} \nabla f(\mathbf{x}^{(t)})$$

The more general form:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=1}^{t} \gamma_i^t \nabla f(\mathbf{x}^{(t)}) \quad \text{for some } \gamma_i$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} - \alpha \sum_{i=1}^{t} \nabla f(\mathbf{x}^{(t)})$$

With momentum:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=1}^{t} \frac{1 - \lambda^{t+1-i}}{1 - \lambda} \nabla f(\mathbf{x}^{(t)})$$

The more general form:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=1}^{t} \Gamma_i^t \nabla f(\mathbf{x}^{(t)}) \quad \text{for some diag. matrix } \Gamma_i$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} - \alpha \sum_{i=1}^{t} \nabla f(\mathbf{x}^{(t)})$$

With momentum:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=1}^{t} \frac{1 - \lambda^{t+1-i}}{1 - \lambda} \nabla f(\mathbf{x}^{(t)})$$

The more general form:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=1}^{t} \Gamma_i^t \nabla f(\mathbf{x}^{(t)}) \quad \text{for some diag. matrix } \Gamma_i$$

generalizes optimization algorithms like ADAM, AdaGrad, etc.

Gradient descent for deep learning

Gradient descent can be applied to nonconvex problems, without optimality guarantees.

Gradient descent for deep learning

Gradient descent can be applied to nonconvex problems, without optimality guarantees.

In order to gain generalization, the following consideration is crucial:

We are rarely interested in the global optimum.

Gradient descent for deep learning

Gradient descent can be applied to nonconvex problems, without optimality guarantees.

In order to gain generalization, the following consideration is crucial:

We are rarely interested in the global optimum.

Even for convex problems like:

- Linear regression
- Logistic regression

We get more efficient and numerically stable solutions.

Gradient descent for deep learning

Gradient descent can be applied to nonconvex problems, without optimality guarantees.

In order to gain generalization, the following consideration is crucial:

We are rarely interested in the global optimum.

Even for convex problems like:

- Linear regression ($\mathbf{X}$ can be huge and must be inverted/factorized)
- Logistic regression

We get more efficient and numerically stable solutions.

Gradient descent for deep learning

Gradient descent can be applied to nonconvex problems, without optimality guarantees.

In order to gain generalization, the following consideration is crucial:

We are rarely interested in the global optimum.

Even for convex problems like:

- Linear regression ($\mathbf{X}$ can be huge and must be inverted/factorized)
- Logistic regression (no closed form solution)

We get more efficient and numerically stable solutions.

Gradient descent for deep learning

In the general DL setting:

Each parameter gets updated so as to decrease the loss:

$$\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \alpha \frac{\partial \ell}{\partial \boldsymbol{\theta}_i}$$

The gradient tells us how to modify the parameters.

Gradient descent for deep learning

In the general DL setting:

Each parameter gets updated so as to decrease the loss:

$$\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \alpha \frac{\partial \ell}{\partial \boldsymbol{\theta}_i}$$

The gradient tells us how to modify the parameters.

- $\boldsymbol{\theta}$ stores the neural network parameters, possibly millions

Gradient descent for deep learning

In the general DL setting:

Each parameter gets updated so as to decrease the loss:

$$\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \alpha \frac{\partial \ell}{\partial \boldsymbol{\theta}_i}$$

The gradient tells us how to modify the parameters.

- $\boldsymbol{\theta}$ stores the neural network parameters, possibly millions
- The loss can be non-convex and non-differentiable
  Cannot even apply gradient descent!

Gradient descent for deep learning

In the general DL setting:

Each parameter gets updated so as to decrease the loss:

$$\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \alpha \frac{\partial \ell}{\partial \boldsymbol{\theta}_i}$$

The gradient tells us how to modify the parameters.

- $\boldsymbol{\theta}$ stores the neural network parameters, possibly millions
- The loss can be non-convex and non-differentiable
  Cannot even apply gradient descent!
- Must address computational complexity and numerical stability

Gradient descent for deep learning

In the general DL setting:

Each parameter gets updated so as to decrease the loss:

$$\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \alpha \frac{\partial \ell}{\partial \boldsymbol{\theta}_i}$$

The gradient tells us how to modify the parameters.

- $\boldsymbol{\theta}$ stores the neural network parameters, possibly millions
- The loss can be non-convex and non-differentiable
  Cannot even apply gradient descent!
- Must address computational complexity and numerical stability

Very often in DL we confront problems that have well defined solutions in mathematical terms, but require extra care and tweaking in practice.

Stochastic gradient descent

Recall that the loss is usually defined over n training examples:

$$\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f_\Theta(x_i))^2$$

Stochastic gradient descent

Recall that the loss is usually defined over n training examples:

$$\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n} \sum_{i=1}^{n} \hat{\ell}_\Theta(\{x_i, y_i\})$$

Stochastic gradient descent

Recall that the loss is usually defined over n training examples:

$$\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n} \sum_{i=1}^{n} \hat{\ell}_\Theta(\{x_i, y_i\})$$

which requires computing the gradient for each term in the summation:

$$\nabla \ell_\Theta(\{x_i, y_i\}) = \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\{x_i, y_i\})$$

Stochastic gradient descent

Recall that the loss is usually defined over n training examples:

$$\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n}\sum_{i=1}^{n} \hat{\ell}_\Theta(\{x_i, y_i\})$$

which requires computing the gradient for each term in the summation:

$$\nabla\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n}\sum_{i=1}^{n} \nabla\hat{\ell}_\Theta(\{x_i, y_i\})$$

Two bottlenecks make gradient descent impractical:

- Number of examples
- Number of parameters

Wilson and Martinez, "The general inefficiency of batch training for gradient descent learning", Neural Networks 2003

Stochastic gradient descent

$$\nabla \ell_\Theta(\{x_i, y_i\}) = \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\{x_i, y_i\})$$

Stochastic gradient descent

$$\nabla \ell_\Theta(\mathcal{T}) = \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

Stochastic gradient descent

$$\nabla \ell_\Theta(\mathcal{T}) = \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

Compute $\nabla \ell_\Theta$ for a small representative subset of $m \ll n$ examples:

$$\frac{1}{m} \sum_{i=1}^{m} \nabla \hat{\ell}_\Theta(\mathcal{B}) \approx \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

The mini-batch $\mathcal{B} \subset \mathcal{T}$ is drawn uniformly.

Stochastic gradient descent

$$\nabla \ell_\Theta(\mathcal{T}) = \frac{1}{n}\sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

Compute $\nabla \ell_\Theta$ for a small representative subset of $m \ll n$ examples:

$$\frac{1}{m}\sum_{i=1}^{m} \nabla \hat{\ell}_\Theta(\mathcal{B}) \approx \frac{1}{n}\sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

The mini-batch $\mathcal{B} \subset \mathcal{T}$ is drawn uniformly.

The true gradient $\nabla \ell_\Theta$ is approximated, but with a significant speed-up.

Example: MNIST dataset

$$n = 60,000\,,\ m = 10 \quad \Rightarrow \quad 6,000 \times \ \text{speedup}$$

Stochastic gradient descent

The algorithm is as follows:

1. Initialize $\boldsymbol{\theta}$.

Stochastic gradient descent

The algorithm is as follows:

1. Initialize $\boldsymbol{\theta}$.
2. Pick a mini-batch $\mathcal{B}$.

Stochastic gradient descent

The algorithm is as follows:

1. Initialize $\boldsymbol{\theta}$.
2. Pick a mini-batch $\mathcal{B}$.
3. Update with the downhill step (use momentum if desired):

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla \ell_{\boldsymbol{\theta}}(\mathcal{B})$$

Stochastic gradient descent

The algorithm is as follows:

1. Initialize $\boldsymbol{\theta}$.
2. Pick a mini-batch $\mathcal{B}$.
3. Update with the downhill step (use momentum if desired):

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla \ell_{\boldsymbol{\theta}}(\mathcal{B})$$

4. Go back to step (2).

Stochastic gradient descent

The algorithm is as follows:

1. Initialize $\boldsymbol{\theta}$.
2. Pick a mini-batch $\mathcal{B}$.
3. Update with the downhill step (use momentum if desired):

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla \ell_{\boldsymbol{\theta}}(\mathcal{B})$$

4. Go back to step (2).

When steps (2)-(4) cover the entire training set $\mathcal{T}$ we have an epoch.

Like gradient descent, the algorithm proceeds for many epochs.

Stochastic gradient descent

The algorithm is as follows:

1. Initialize $\boldsymbol{\theta}$.
2. Pick a mini-batch $\mathcal{B}$.
3. Update with the downhill step (use momentum if desired):

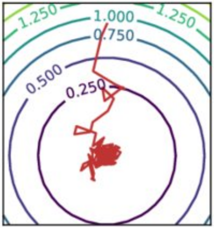
$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla \ell_{\boldsymbol{\theta}}(\mathcal{B})$$

4. Go back to step (2).

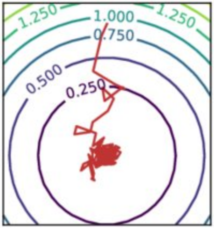
When steps (2)-(4) cover the entire training set $\mathcal{T}$ we have an epoch.
Like gradient descent, the algorithm proceeds for many epochs.

Remark: The update cost is constant regardless of the size of $\mathcal{T}$.

Stochastic gradient descent



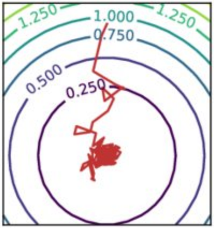
Stochastic gradient descent

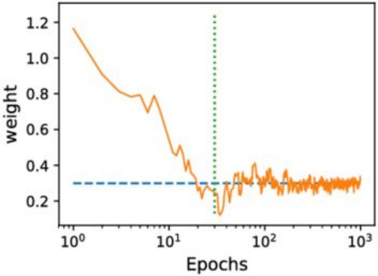


SGD does not stop at the minimum.

Oscillations are due to the noise induced by the random sampling.

Stochastic gradient descent





SGD does not stop at the minimum.

Oscillations are due to the noise induced by the random sampling.

Asymptotic upper bounds

$$\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f_\Theta(x_i))^2$$

Asymptotic upper bounds

$$\ell(\{f_\Theta(x_i), y_i\}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f_\Theta(x_i))^2$$

Asymptotic upper bounds

$$\ell(\{f_\Theta(x_i), y_i\}) = \frac{1}{n}\sum_{i=1}^{n}\hat{\ell}(\{f_\Theta(x_i), y_i\})$$

Asymptotic upper bounds

$$\ell(f_\Theta) = \frac{1}{n}\sum_{i=1}^{n}\hat{\ell}(f_\Theta)$$

Asymptotic upper bounds

For a convex problem, there is a true minimizer:

$$f^* = \arg\min_f \ell(f)$$

Asymptotic upper bounds

For a convex problem, consider the inequality:

$$|\ell(f_\Theta) - \ell(f^*)| < \rho$$

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

Asymptotic upper bounds

For a convex problem, consider the inequality:

$$|\underbrace{\ell(f_\Theta)}_{\text{GD/SGD}} - \underbrace{\ell(f^*)}_{\text{true}}| < \underbrace{\rho}_{\text{accuracy}}$$

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

Asymptotic upper bounds

For a convex problem, consider the inequality:

$$|\underbrace{\ell(f_\Theta)}_{\text{GD/SGD}} - \underbrace{\ell(f^*)}_{\text{true}}| < \underbrace{\rho}_{\text{accuracy}}$$

n training examples
d parameters
κ, ν are constants related to the conditioning of the problem

	cost per iteration	**iterations to reach ρ**
GD	$O(nd)$	$O(\kappa \log \frac{1}{\rho})$
SGD	$O(d)$	$\frac{\nu\kappa^2}{\rho} + o(\frac{1}{\rho})$

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

Asymptotic upper bounds

For a convex problem, consider the inequality:

$$|\underbrace{\ell(f_\Theta)}_{\text{GD/SGD}} - \underbrace{\ell(f^*)}_{\text{true}}| < \underbrace{\rho}_{\text{accuracy}}$$

n training examples
d parameters
κ, ν are constants related to the conditioning of the problem

	cost per iteration	**iterations to reach ρ**
GD	$O(nd)$	$O(\kappa \log \frac{1}{\rho})$
SGD	$O(d)$	$\frac{\nu\kappa^2}{\rho} + o(\frac{1}{\rho})$

SGD does not depend on the number of examples, implying better generalization

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

Stochastic gradient descent

Some practical considerations:

- Needs the training data to be shuffled to avoid data bias.

Stochastic gradient descent

Some practical considerations:

- Needs the training data to be shuffled to avoid data bias.

$$\frac{1}{m}\sum_{i=1}^{m}\nabla\hat{\ell}_{\Theta}(\mathcal{B}) \not\approx \frac{1}{n}\sum_{i=1}^{n}\nabla\hat{\ell}_{\Theta}(\mathcal{T})$$

Stochastic gradient descent

Some practical considerations:

- Needs the training data to be shuffled to avoid data bias.
- Each mini-batch can be processed in parallel.
  Batch size is limited by hardware.

Stochastic gradient descent

Some practical considerations:

- Needs the training data to be shuffled to avoid data bias.
- Each mini-batch can be processed in parallel.
  Batch size is limited by hardware.
- Large datasets: more steps to reach convergence.
  Remarkably rapid initial progress and slow asymptotic convergence.

Stochastic gradient descent

Some practical considerations:

- Needs the training data to be shuffled to avoid data bias.
- Each mini-batch can be processed in parallel.
  Batch size is limited by hardware.
- Large datasets: more steps to reach convergence.
  Remarkably rapid initial progress and slow asymptotic convergence.
- Small mini-batches can offer a regularizing effect.
  Very small batches $\rightarrow$ high variance in the estimation of the gradient
  $\rightarrow$ use a small learning rate to maintain stability.

Stochastic gradient descent

Some practical considerations:

- Needs the training data to be shuffled to avoid data bias.
- Each mini-batch can be processed in parallel.
  Batch size is limited by hardware.
- Large datasets: more steps to reach convergence.
  Remarkably rapid initial progress and slow asymptotic convergence.
- Small mini-batches can offer a regularizing effect.
  Very small batches $\rightarrow$ high variance in the estimation of the gradient
  $\rightarrow$ use a small learning rate to maintain stability.

SGD can find a low value of the loss quickly enough to be useful, even if it's not a minimum.

Suggested reading

Approachable explanation of differentiability in higher dimensions:
https://mathinsight.org/differentiability_multivariable_subtleties

Distill article on why momentum really works:
https://distill.pub/2017/momentum/

Seminal paper on using mini-batches for training:
http://axon.cs.byu.edu/papers/Wilson.nn03.batch.pdf

Seminal paper on GD vs. SGD performance:
https://papers.nips.cc/paper/3323-the-tradeoffs-of-large-scale-learning.pdf