



Gradient Descent

DS 4400 | Machine Learning and Data Mining I

Zohair Shafi

Spring 2026

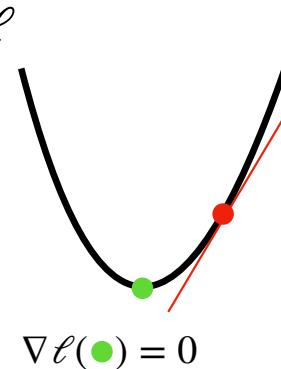
Wednesday | January 21, 2026

Optimizing Loss Functions

- For any loss function $\ell(\theta)$
 - To find minimum, set $\underbrace{\nabla \ell = 0}$ and solve for θ

$$\ell(\theta) := \frac{1}{m} \sum (y - \hat{y})^2$$

$\nabla \ell(\bullet)$ points in direction of steepest ascent



Optimizing Loss Functions

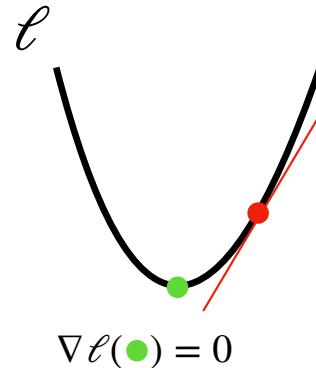
$x \in \mathbb{R}^{m \times n}$ - # features.
data

$$\theta = \underbrace{(x^T x)^{-1}}_{\text{matrix inverse}} \cdot x^T y$$

$$x^T x \rightarrow \boxed{n \times n}$$

- For any loss function $\ell(\theta)$
 - To find minimum, set $\nabla \ell = 0$ and solve for θ
 - This is called the **closed form solution**
 - But it's not always possible to find closed form solutions, especially when there are a large number of parameters
 - Inverting a matrix is a costly operation - most common methods have complexity $\underline{O(n^3)}$ $\rightarrow 100^3$

$\nabla \ell(\bullet)$ points in direction of steepest ascent

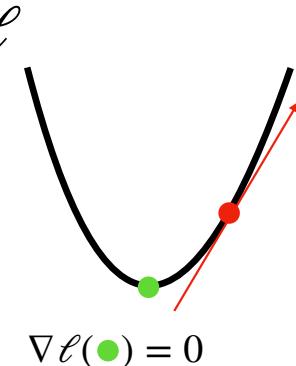


Optimizing Loss Functions

- This is where Gradient Descent comes in
 - Practical and efficient - has $O(mTn)$ where m is number of training points, T is number of epochs and n is number of features
 - Generally applicable to different loss functions
 - Convergence guarantees for certain types of loss functions (e.g., convex functions)

data
#feat

$\nabla \ell(\bullet)$ points in direction of steepest ascent

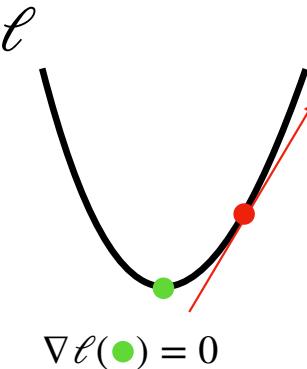


Optimizing Loss Functions

- What is gradient descent?



$\nabla \ell(\bullet)$ points in direction of steepest ascent

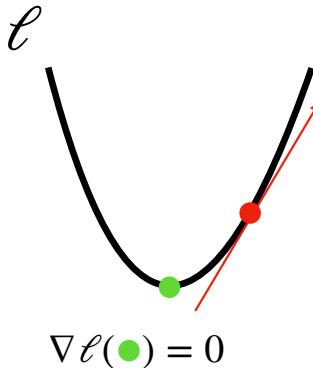


Optimizing Loss Functions

- What is gradient descent?



$\nabla \ell(\bullet)$ points in direction of steepest ascent

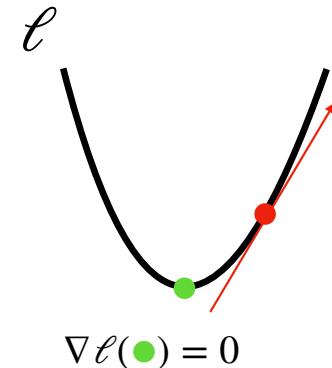


Optimizing Loss Functions

- What is gradient descent?

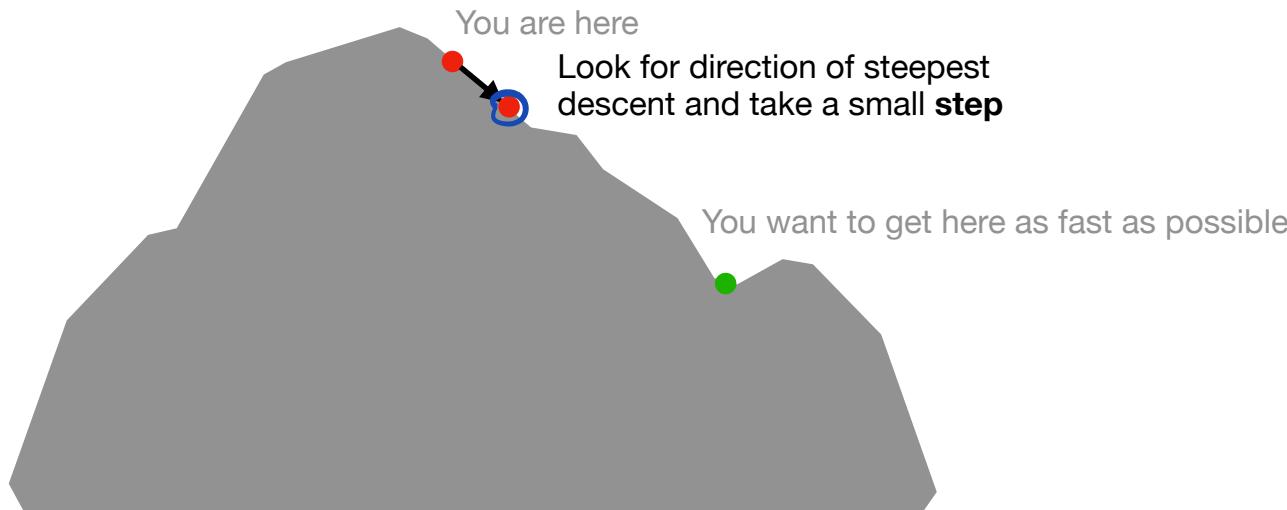


$\nabla \ell(\bullet)$ points in direction of steepest ascent

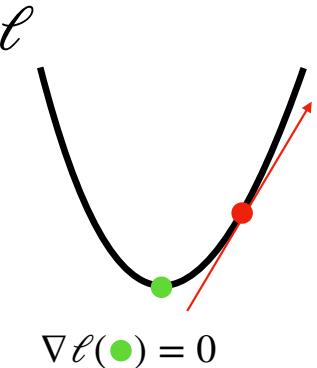


Optimizing Loss Functions

- What is gradient descent?



$\nabla \ell(\bullet)$ points in direction of steepest ascent

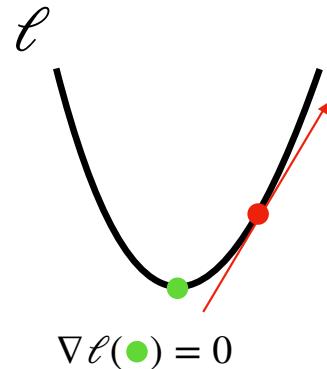


Optimizing Loss Functions

- What is gradient descent?

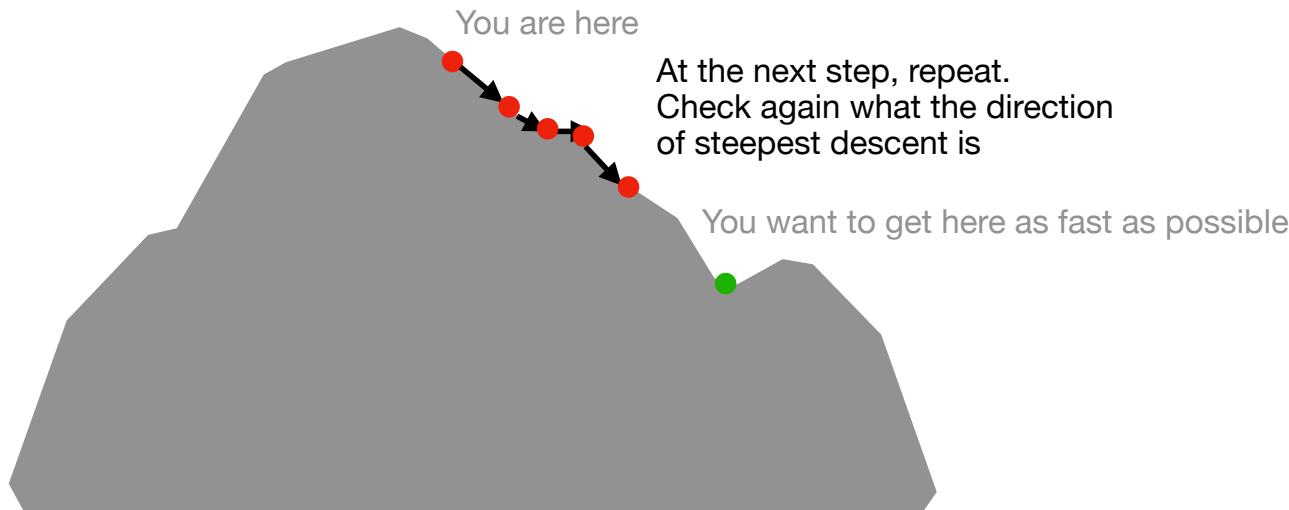


$\nabla \ell(\bullet)$ points in direction of steepest ascent

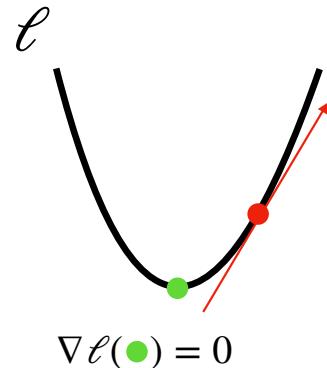


Optimizing Loss Functions

- What is gradient descent?

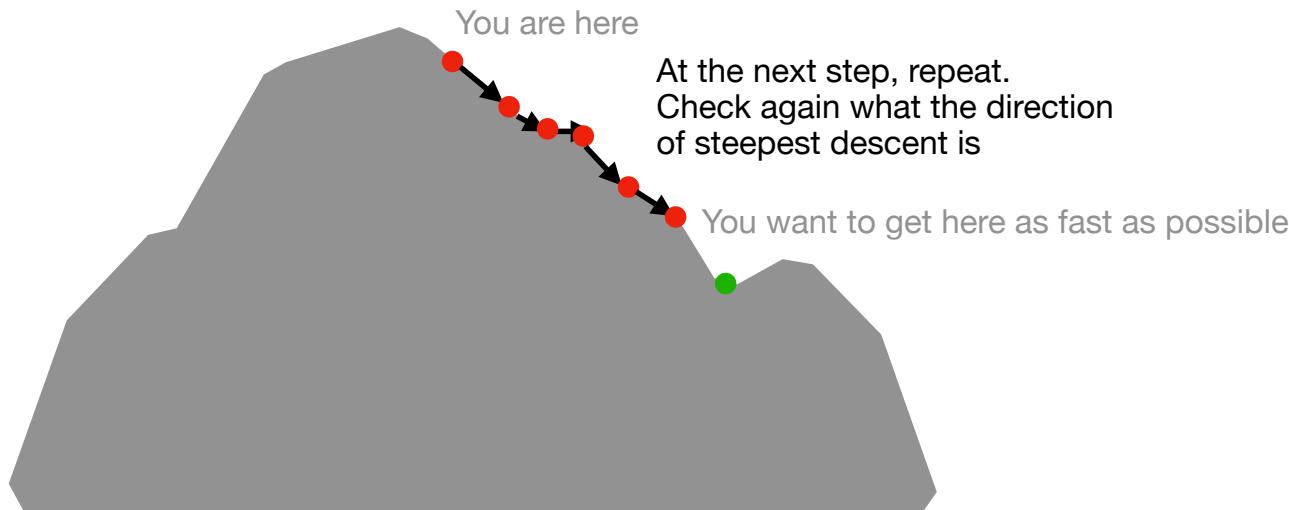


$\nabla \ell(\bullet)$ points in direction of steepest ascent

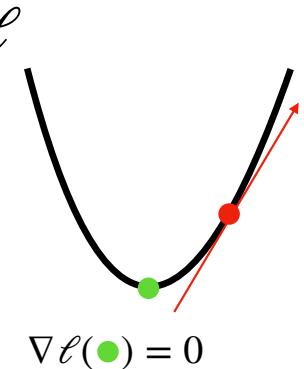


Optimizing Loss Functions

- What is gradient descent?

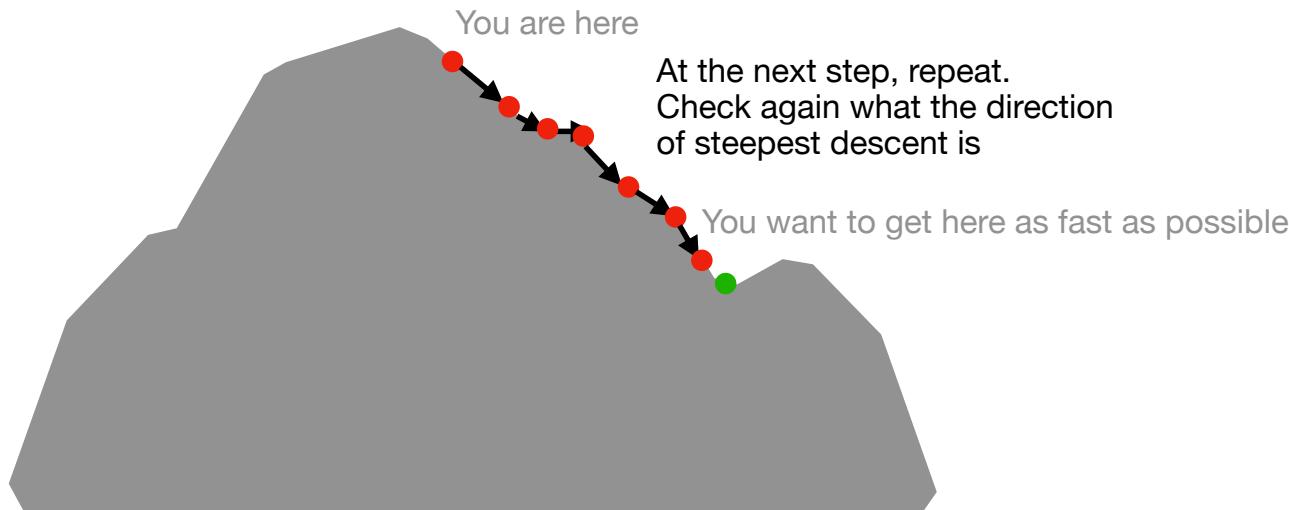


$\nabla \ell(\bullet)$ points in direction of steepest ascent

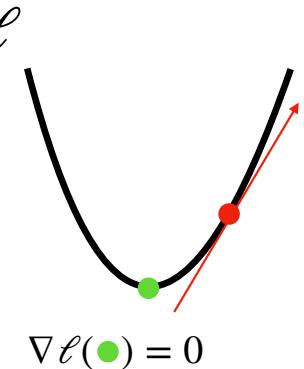


Optimizing Loss Functions

- What is gradient descent?

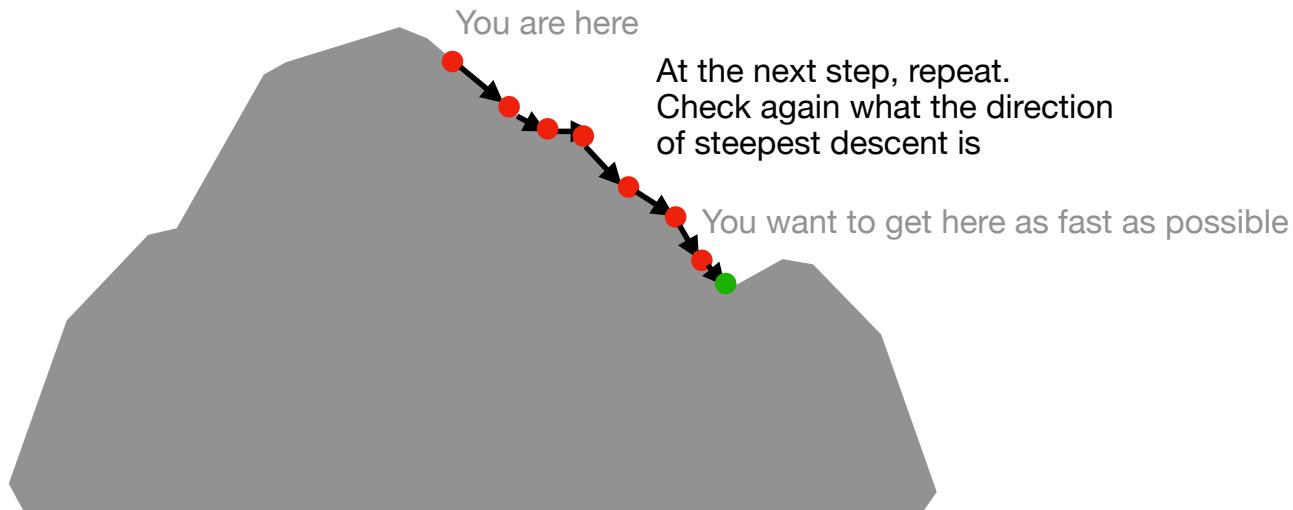


$\nabla \ell(\bullet)$ points in direction of steepest ascent

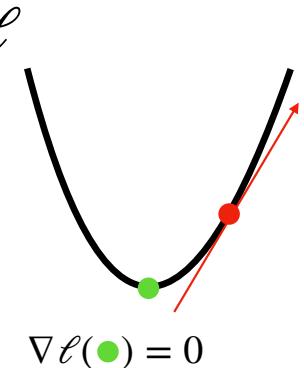


Optimizing Loss Functions

- What is gradient descent?

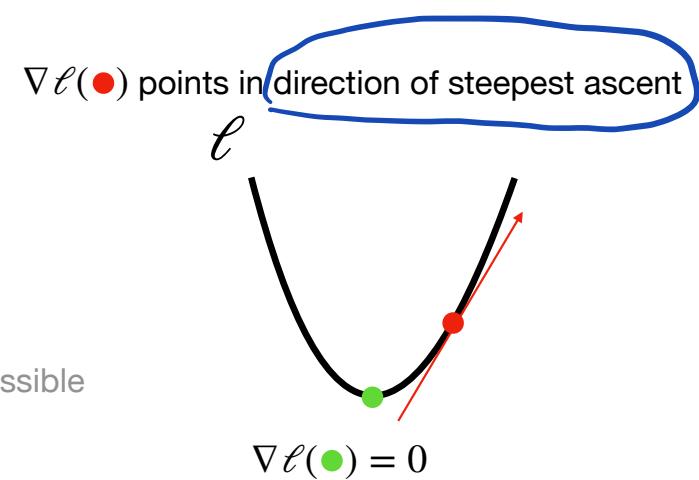
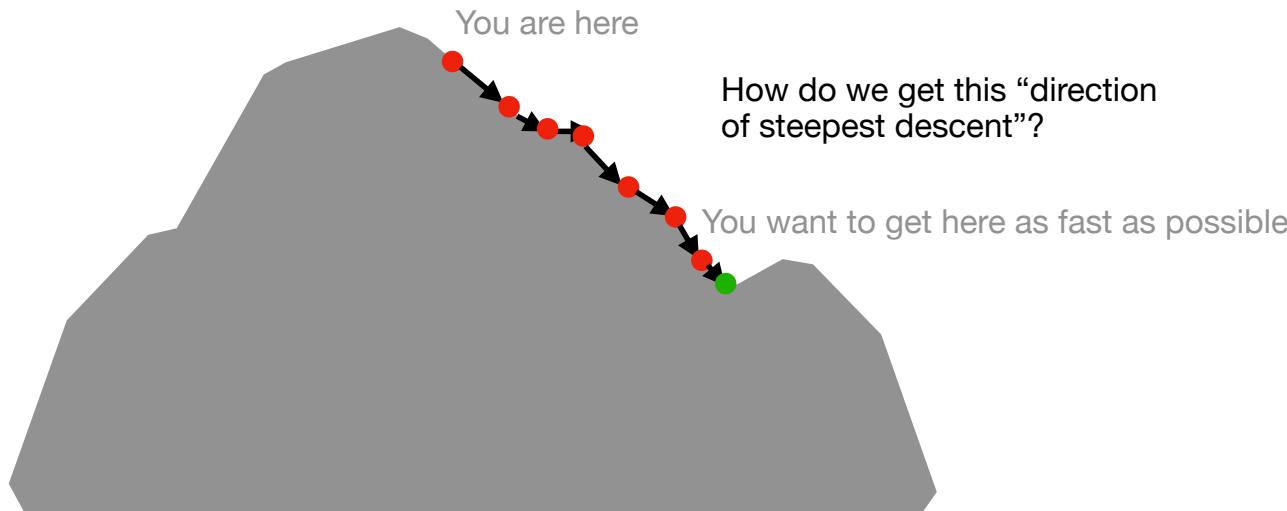


$\nabla \ell(\bullet)$ points in direction of steepest ascent



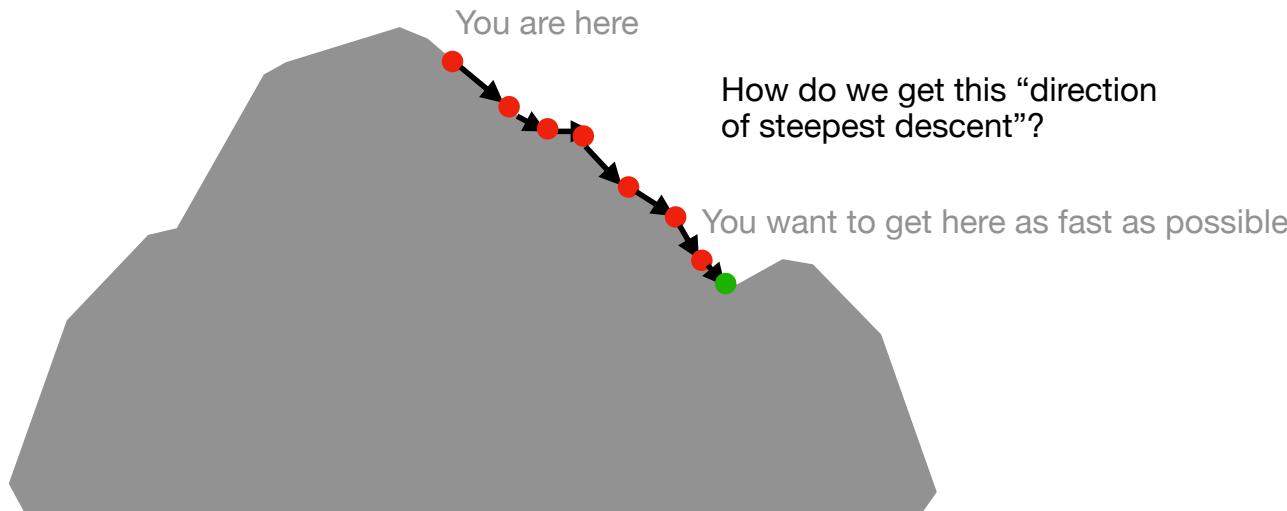
Optimizing Loss Functions

- What is gradient descent?

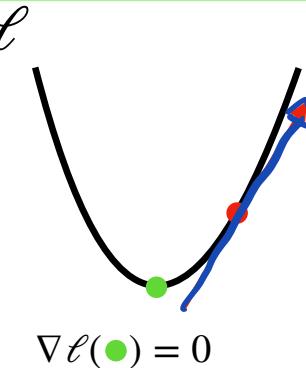


Optimizing Loss Functions

- What is gradient descent?

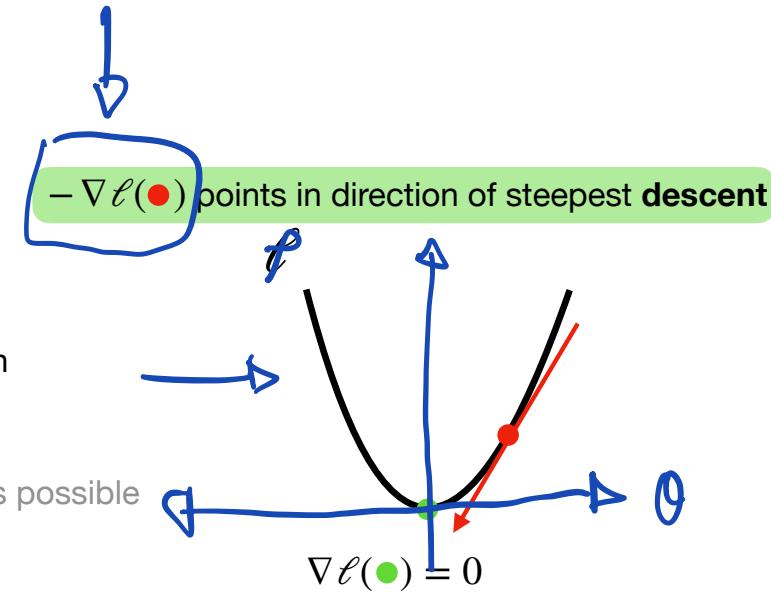
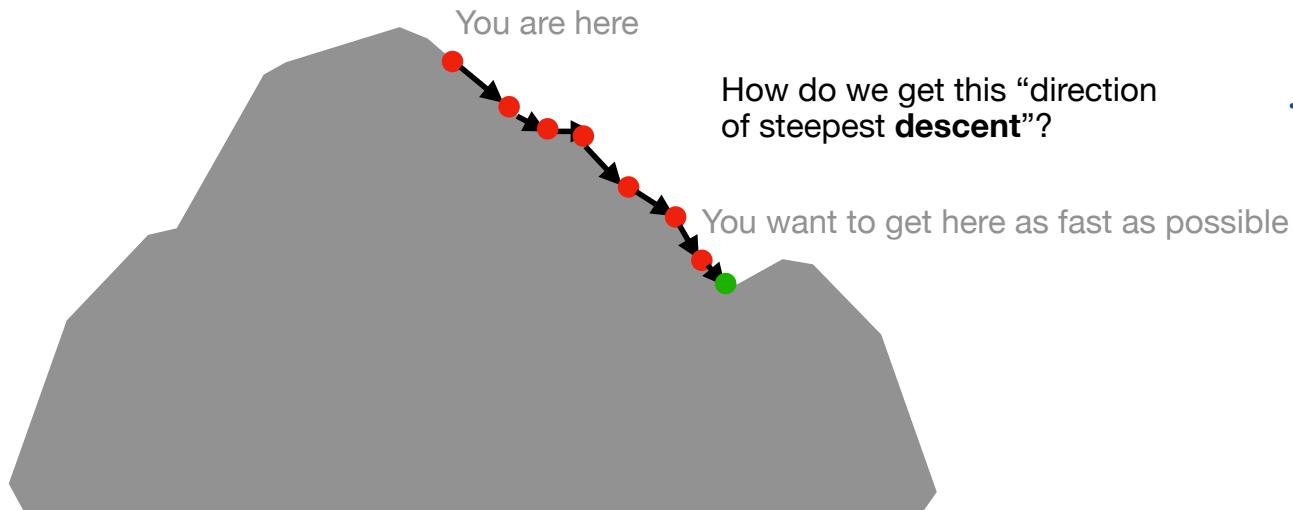


$\nabla \ell(\bullet)$ points in direction of steepest ascent



Optimizing Loss Functions

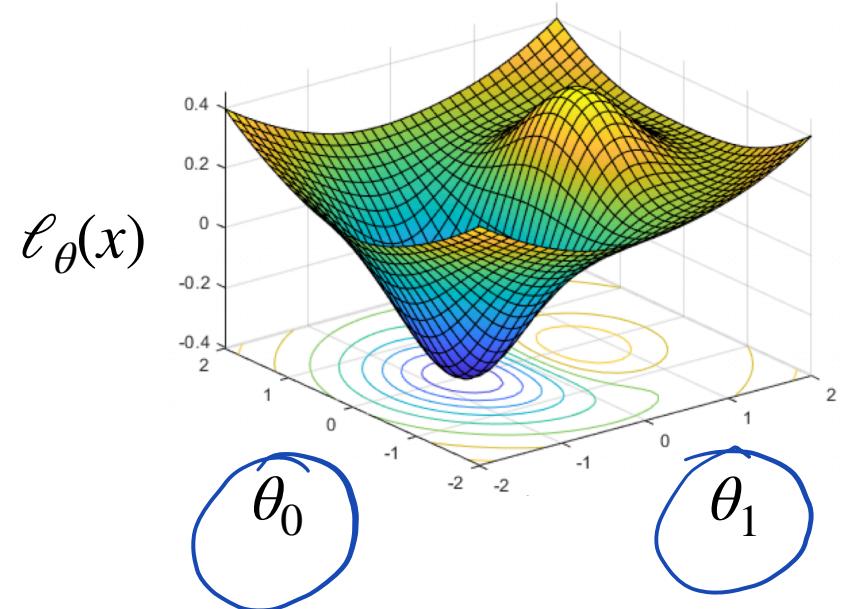
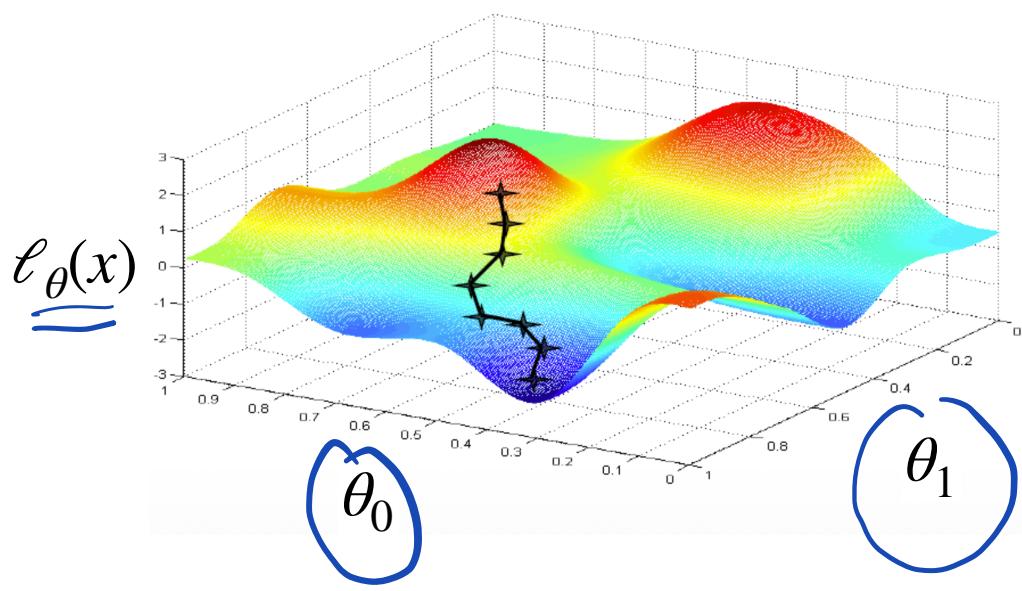
- What is gradient descent?



In the plot above, you have a **single** parameter θ

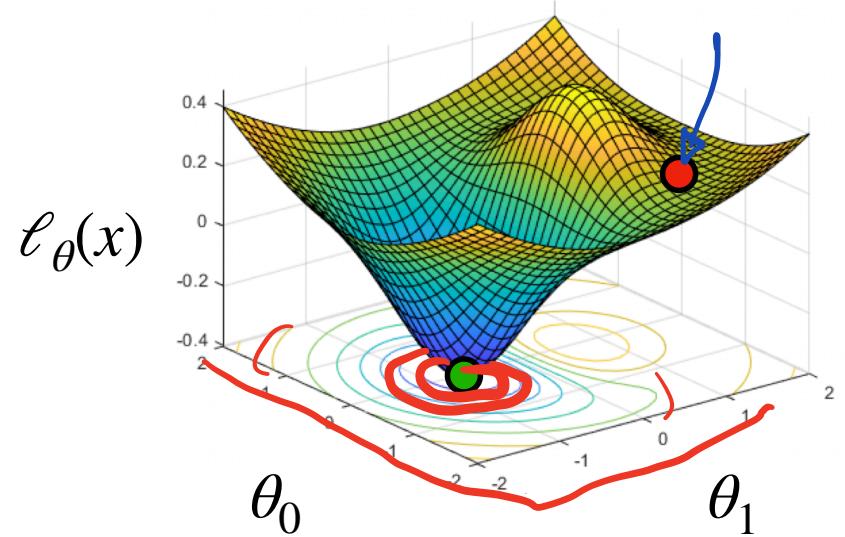
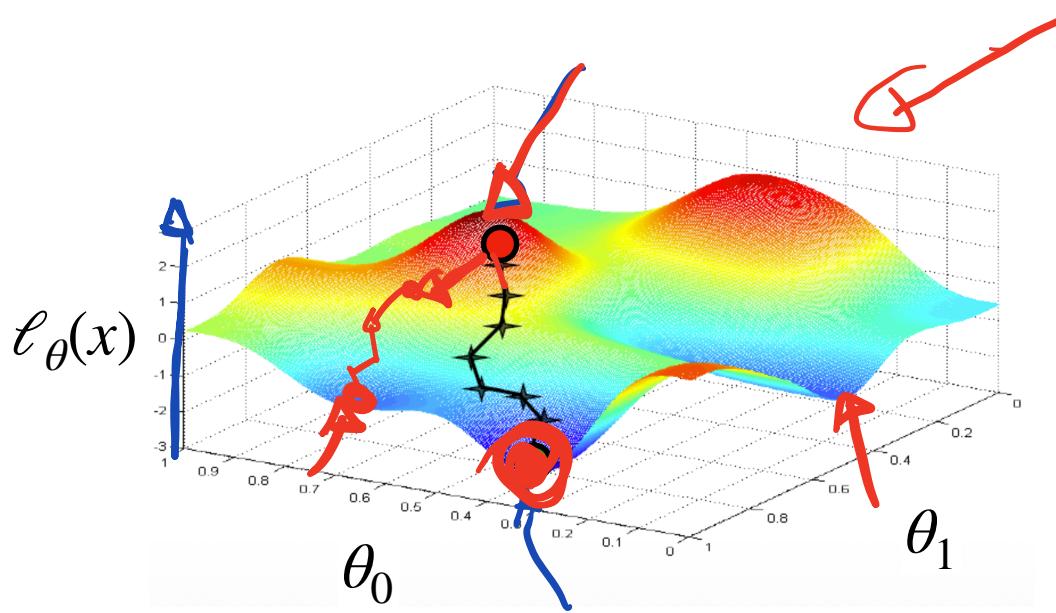
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



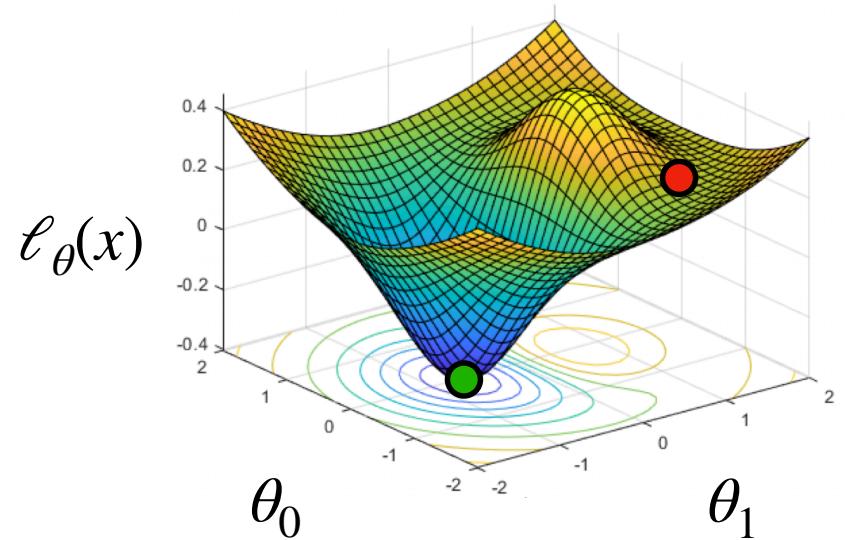
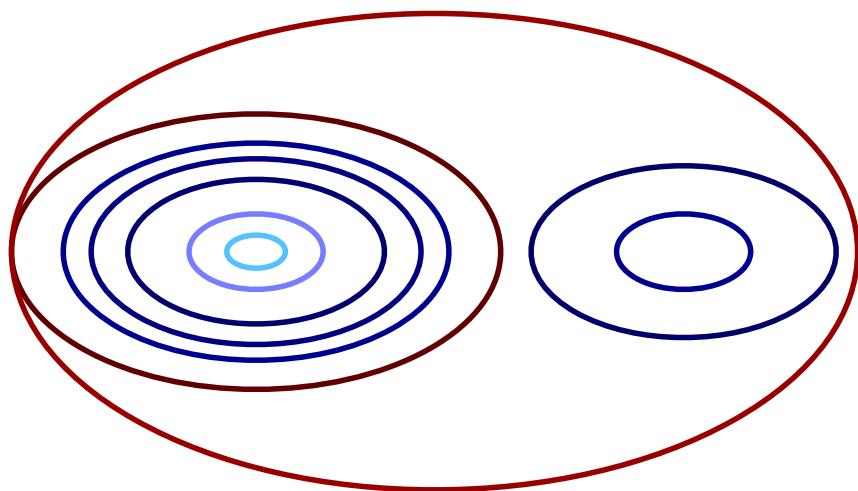
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



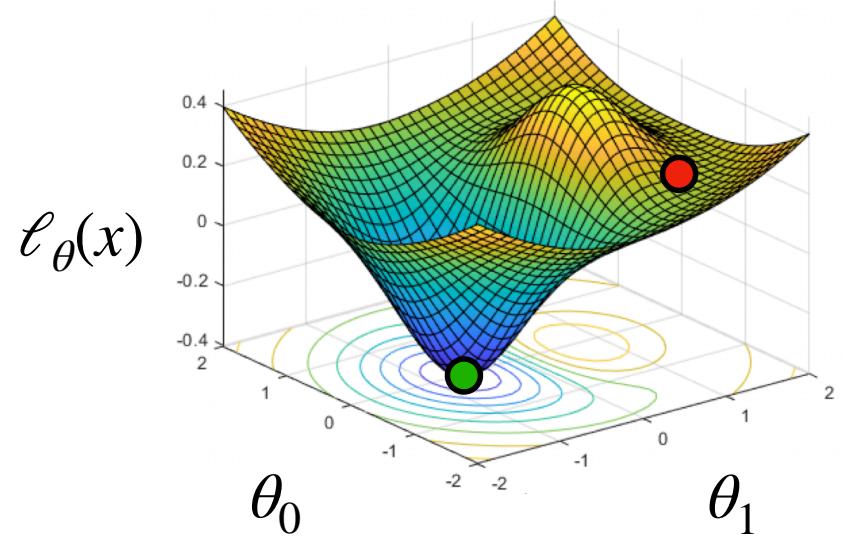
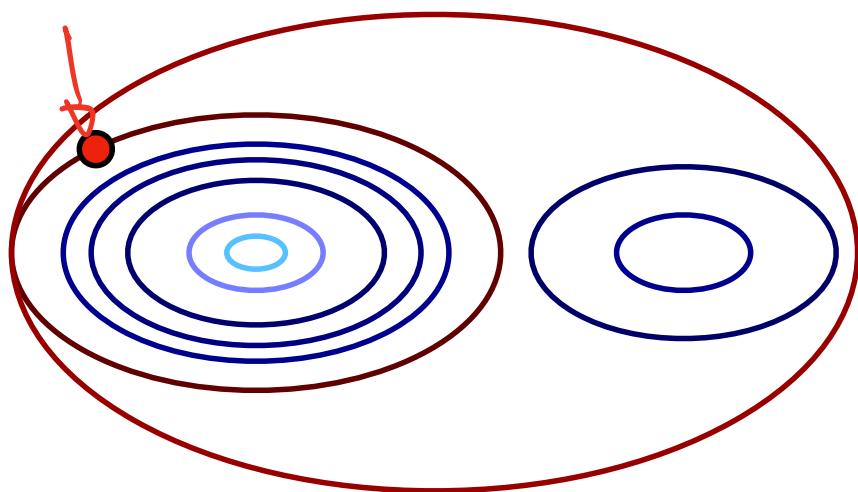
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



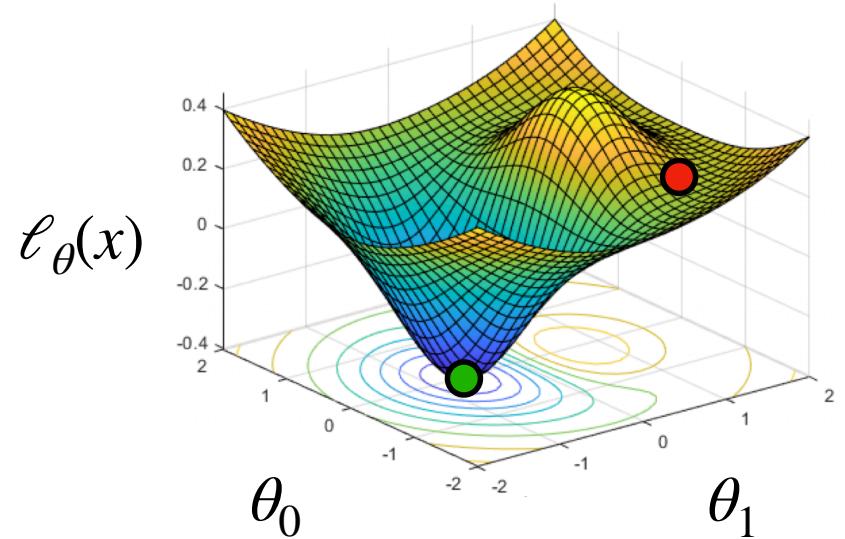
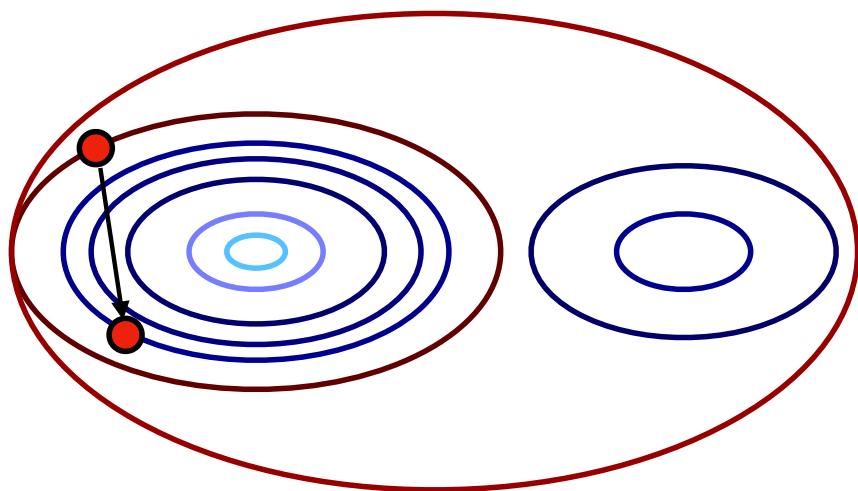
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



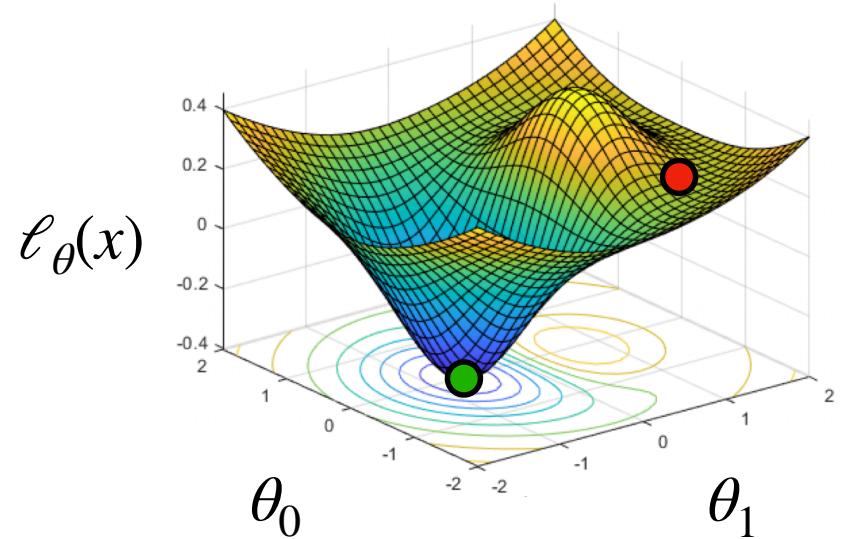
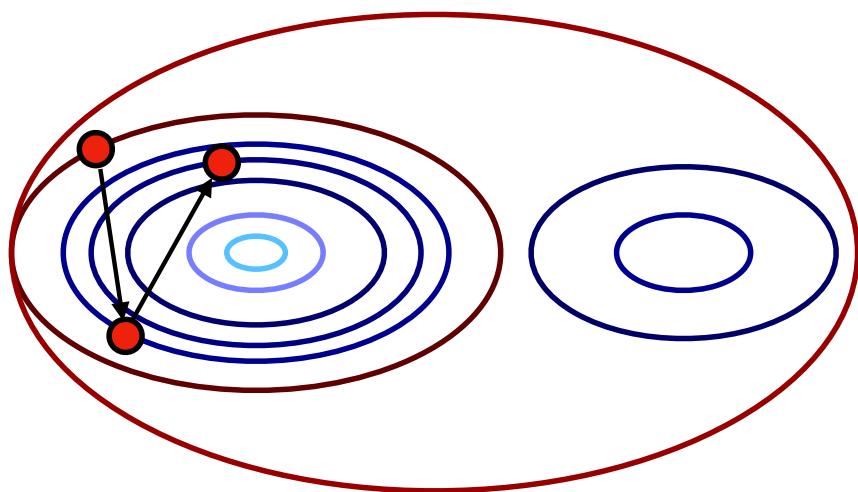
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



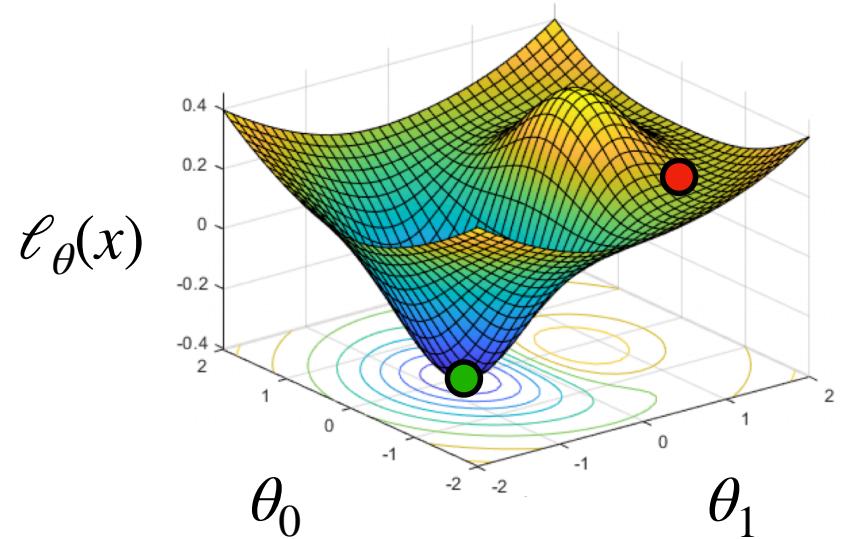
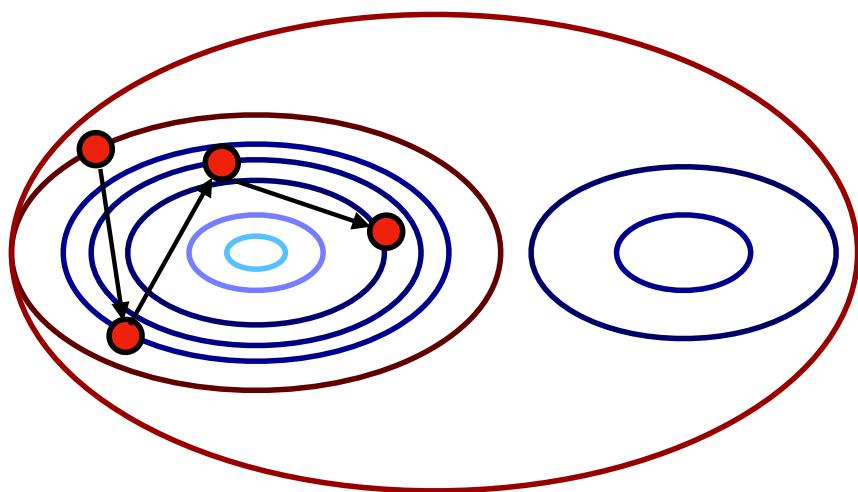
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



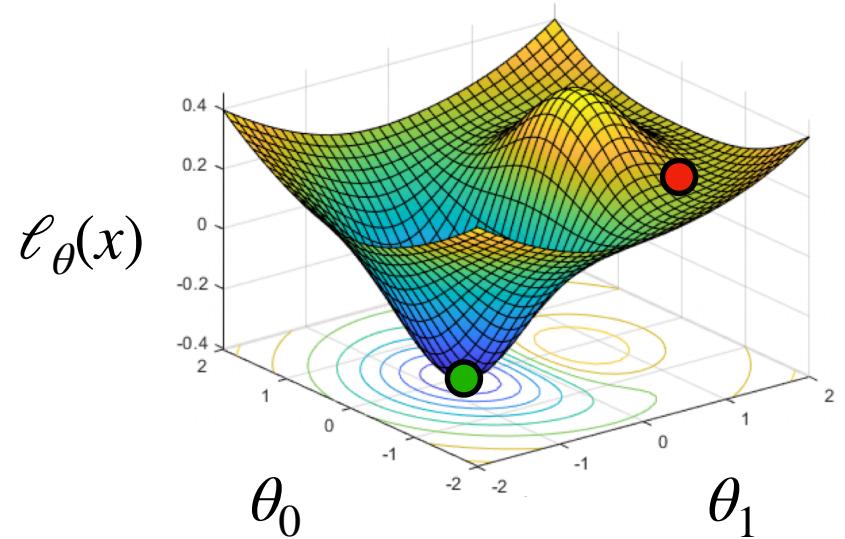
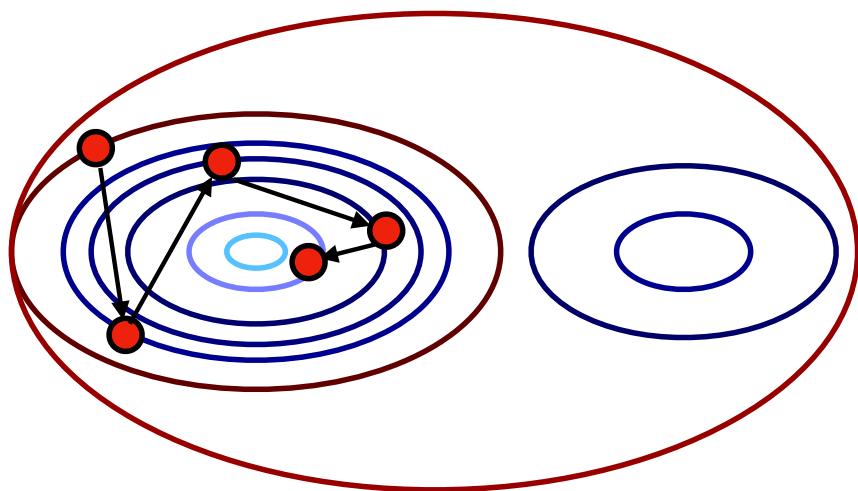
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



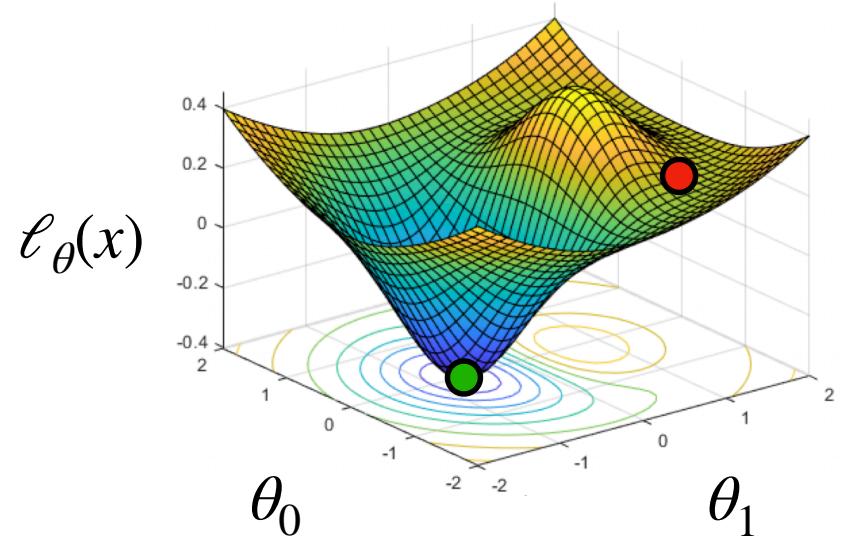
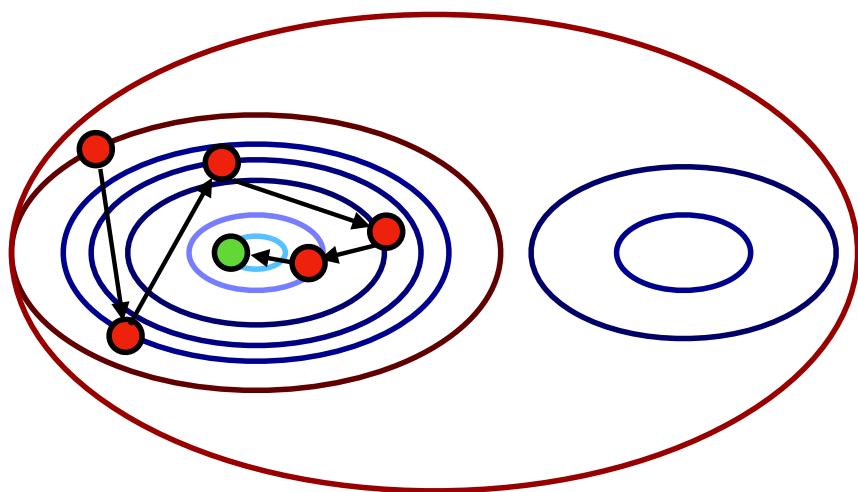
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



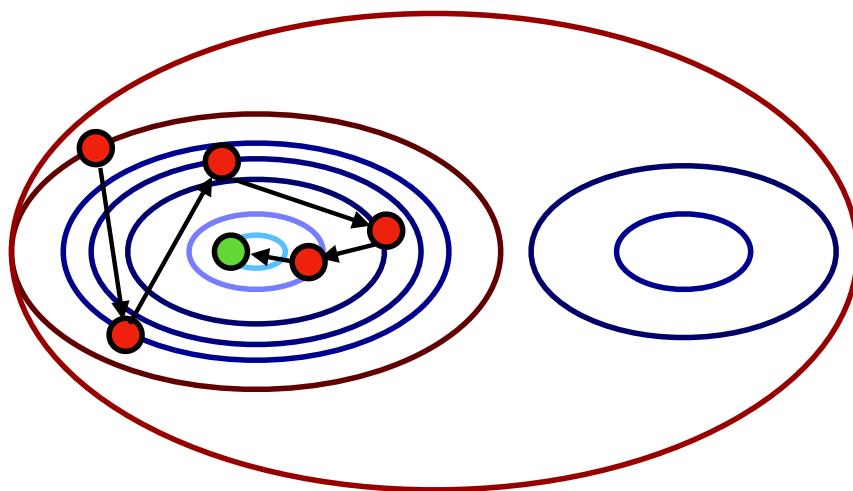
Optimizing Loss Functions

- What does the loss landscape look like with multiple learnable parameters?



Optimizing Loss Functions

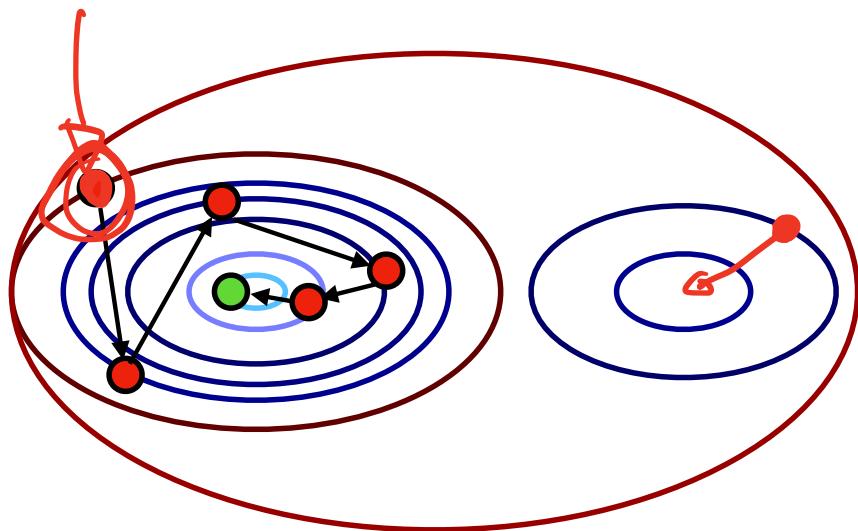
Gradient Descent - Formulation



$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \underbrace{\theta_0 - \theta_1 x_i}_{\hat{y}})^2$$

Optimizing Loss Functions

Gradient Descent - Formulation

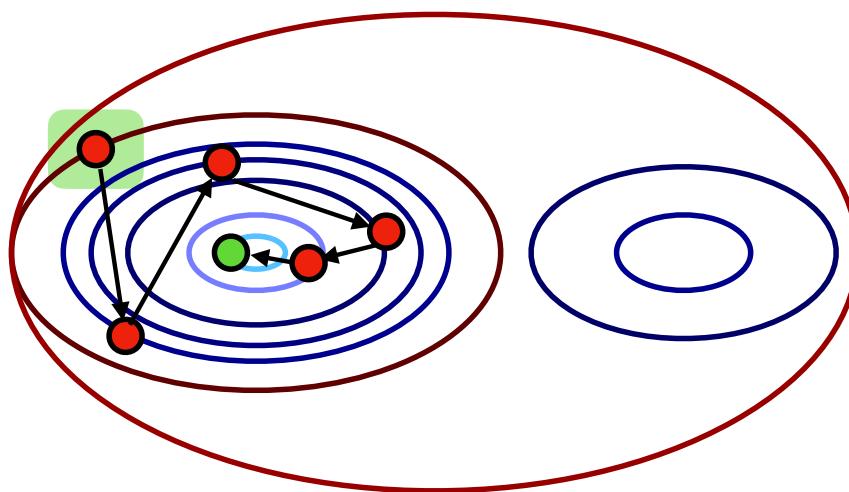


$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

Optimizing Loss Functions

Gradient Descent - Formulation



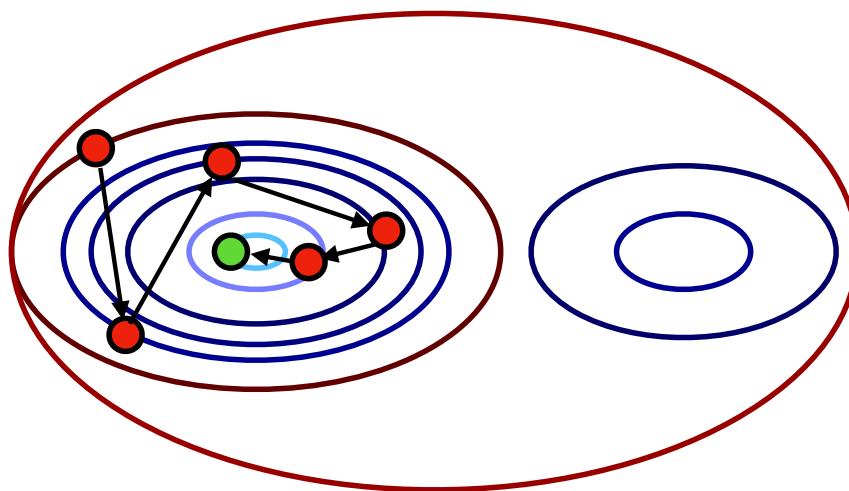
$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

This is going to be your “starting point” on the loss landscape

Optimizing Loss Functions

Gradient Descent - Formulation



$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

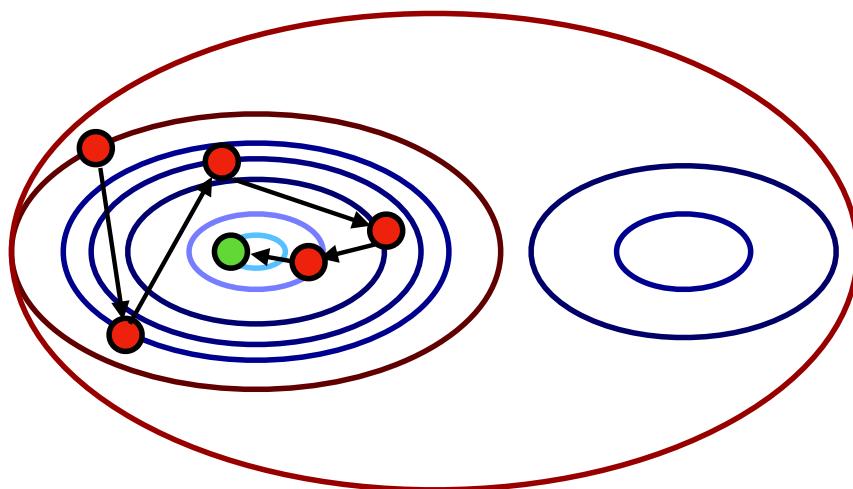
Step 1: Initialize θ_0, θ_1

Step 2: Repeat Until Convergence

$$\theta_j \leftarrow \theta_j - \alpha \cdot \frac{\partial \ell_{\theta}(x)}{\partial \theta_j}$$

Optimizing Loss Functions

Gradient Descent - Formulation



$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

Step 2: Repeat Until Convergence

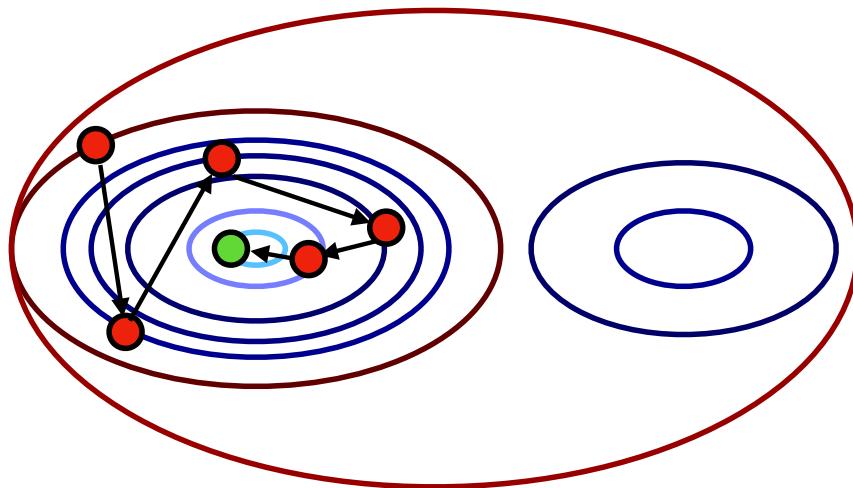
$$\theta_j \leftarrow \theta_j - \alpha \cdot \frac{\partial \ell_{\theta}(x)}{\partial \theta_j}$$

Negative of partial derivative points
in the direction of steepest descent

Optimizing Loss Functions

Gradient Descent - Formulation

2
lr



$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

Step 2: Repeat Until Convergence

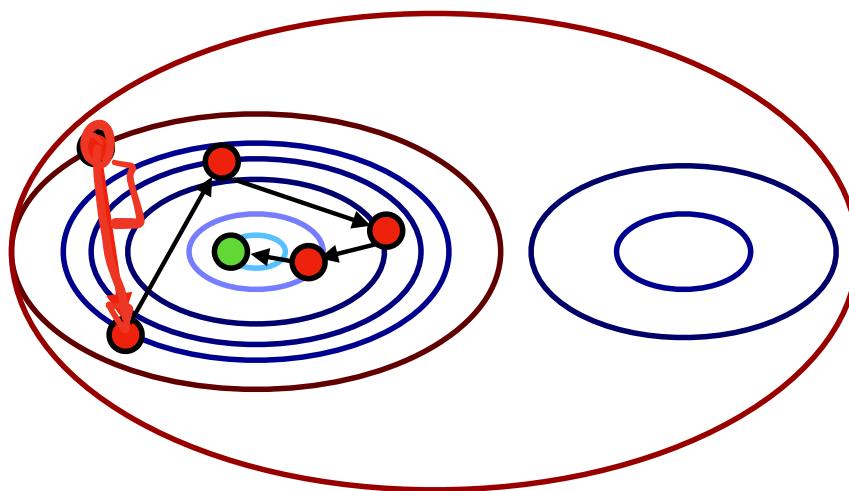
$$\theta_j \leftarrow \theta_j - \alpha \cdot \frac{\partial \ell_{\theta}(x)}{\partial \theta_j}$$

α : Learning Rate

Optimizing Loss Functions

Gradient Descent - Formulation

α controls how big a step to take



$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

Step 2: Repeat Until Convergence

$$\theta_j \leftarrow \theta_j - \alpha \cdot \boxed{\frac{\partial \ell_{\theta}(x)}{\partial \theta_j}}$$

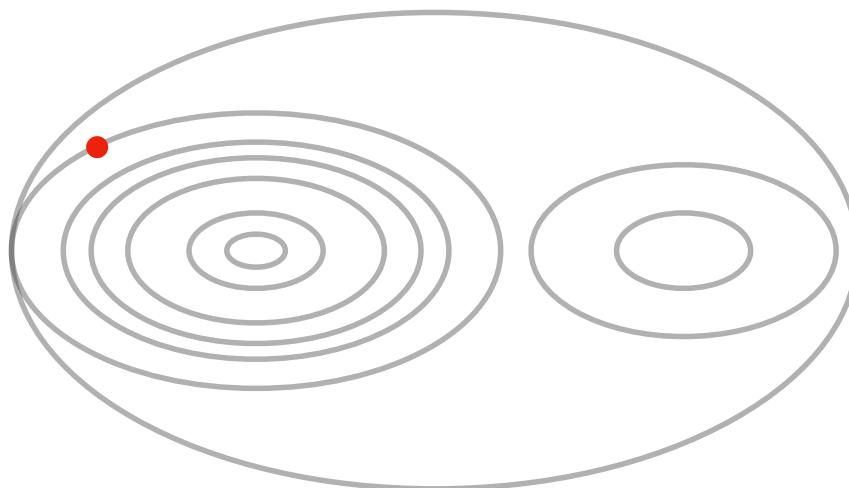
α : Learning Rate

Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$



10^{-3}

$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

Step 2: Repeat Until Convergence

$$\theta_j \leftarrow \theta_j - \alpha \cdot \frac{\partial \ell_{\theta}(x)}{\partial \theta_j}$$

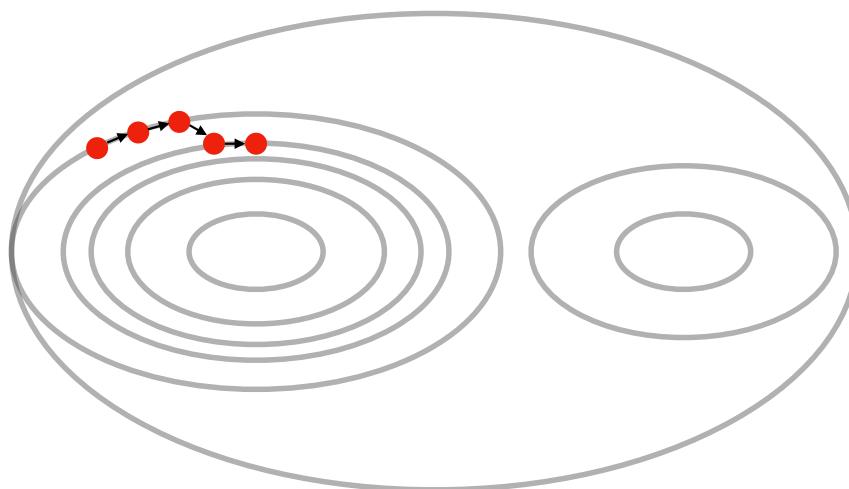
α : Learning Rate

Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$



$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

Step 2: Repeat Until Convergence

$$\theta_j \leftarrow \theta_j - \alpha \cdot \frac{\partial \ell_{\theta}(x)}{\partial \theta_j}$$

α : Learning Rate

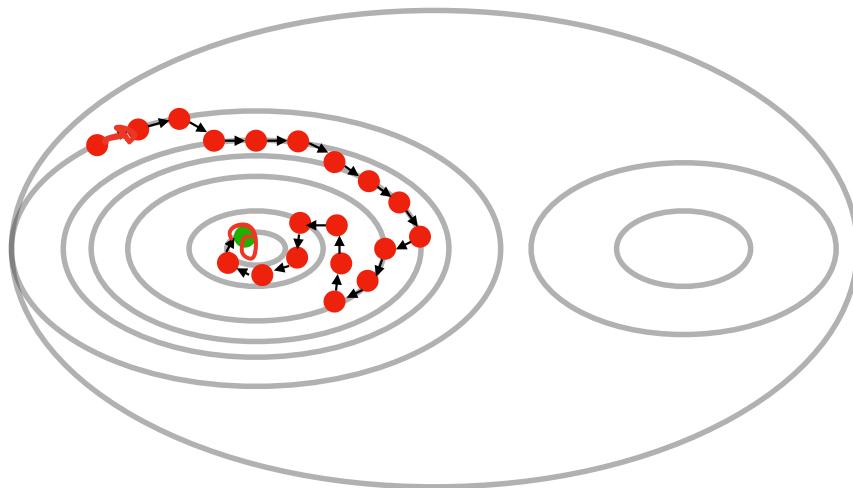
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

$$\begin{matrix} 10^{-2} \\ \downarrow \\ 10^{-8} \end{matrix}$$



$$\ell_{\theta}(x) = \frac{1}{m} \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$$

Step 1: Initialize θ_0, θ_1

Step 2: Repeat Until Convergence

$$\theta_j \leftarrow \theta_j - \alpha \cdot \frac{\partial \ell_{\theta}(x)}{\partial \theta_j}$$

α : Learning Rate

Optimizing Loss Functions

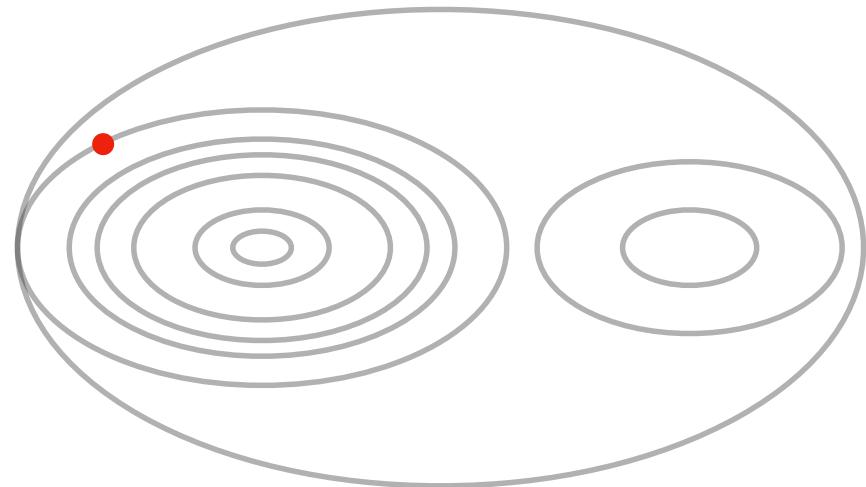
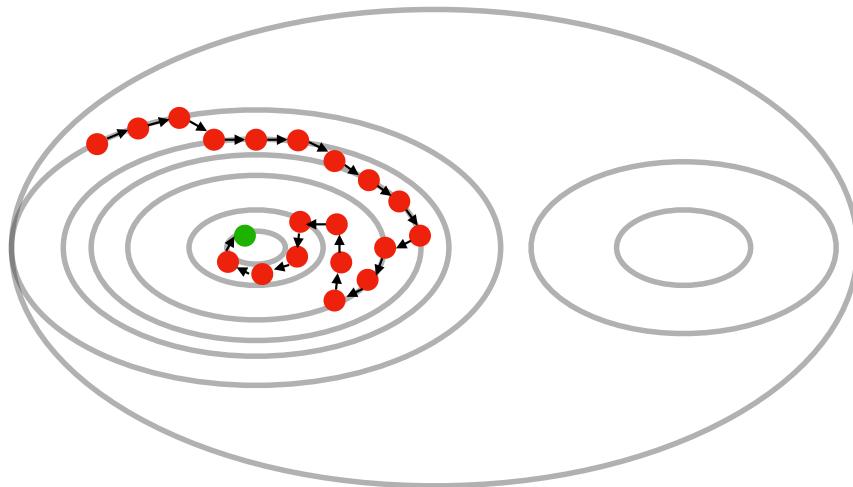
Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

What happens when α is too large?

Say $\alpha = 10$

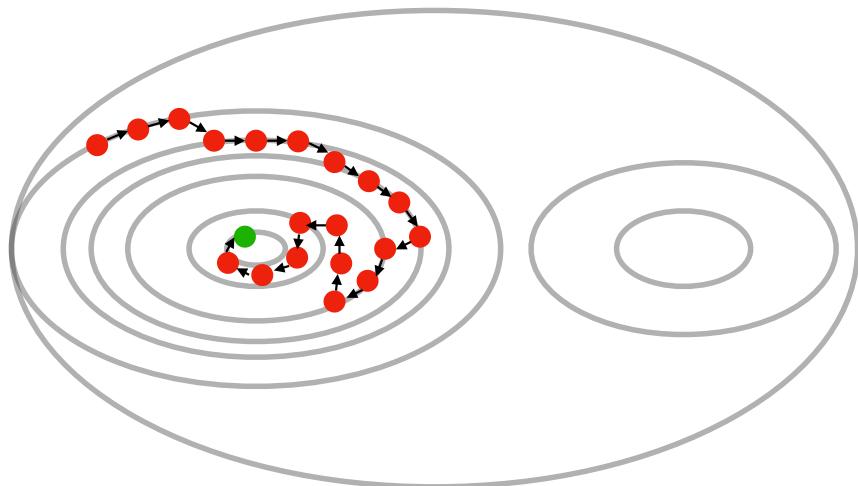


Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

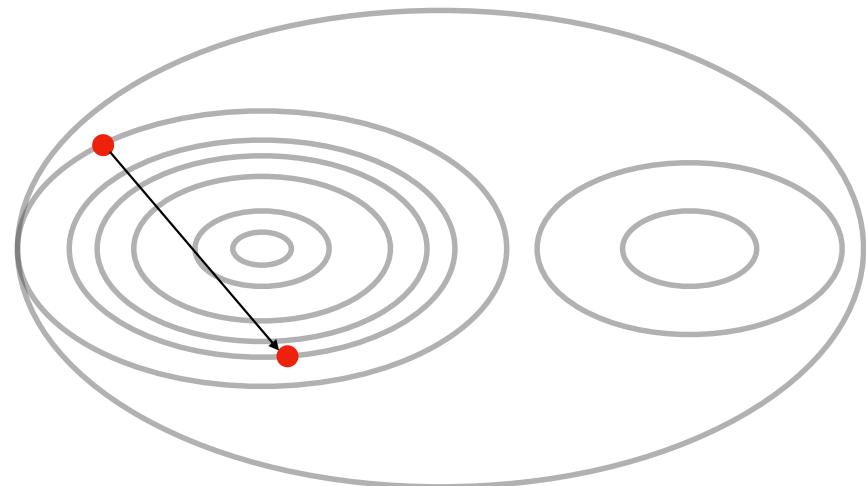
What happens when α is too small?

Say $\alpha = 10^{-5}$



What happens when α is too large?

Say $\alpha = 10$

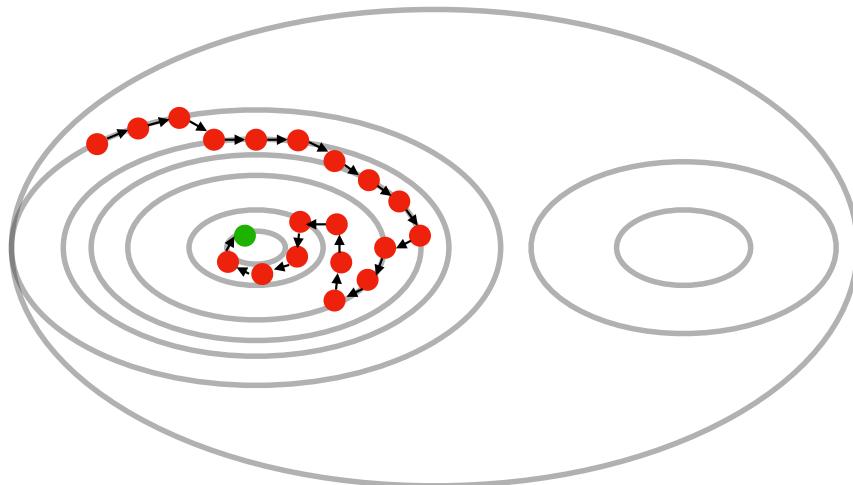


Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

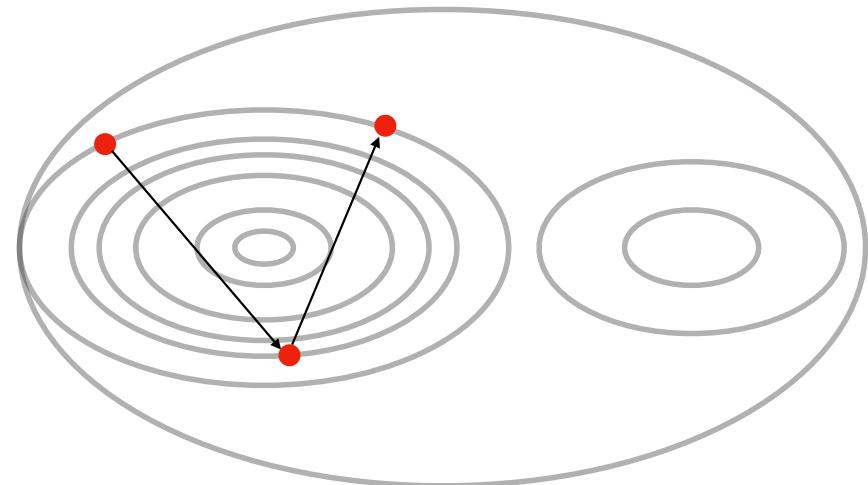
What happens when α is too small?

Say $\alpha = 10^{-5}$



What happens when α is too large?

Say $\alpha = 10$

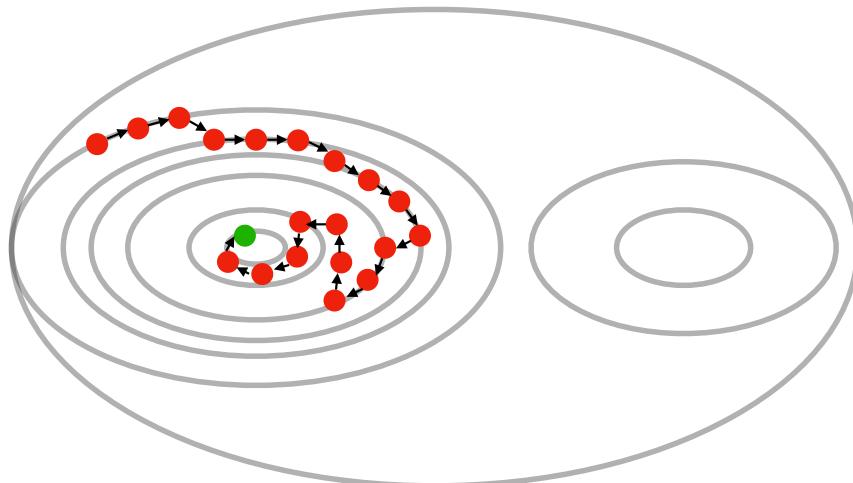


Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

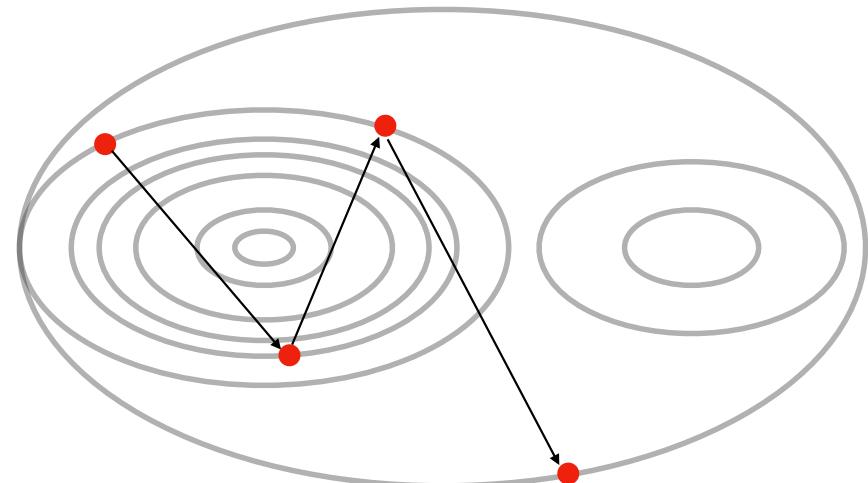
What happens when α is too small?

Say $\alpha = 10^{-5}$



What happens when α is too large?

Say $\alpha = 10$



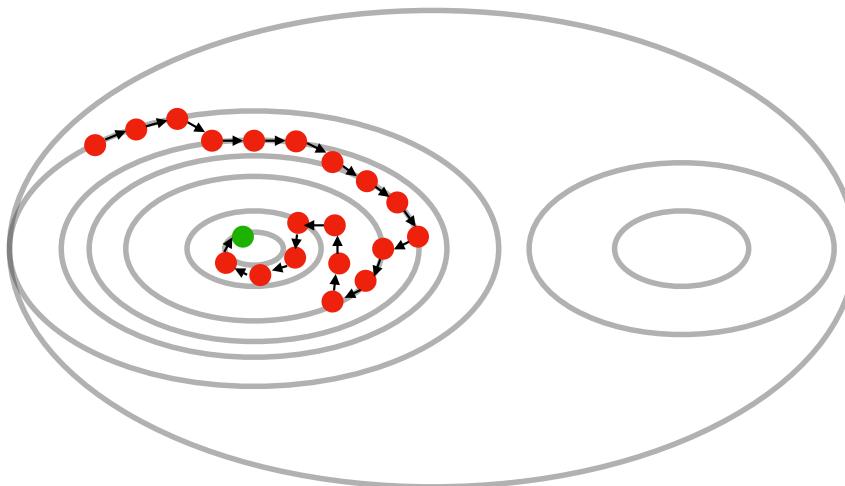
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

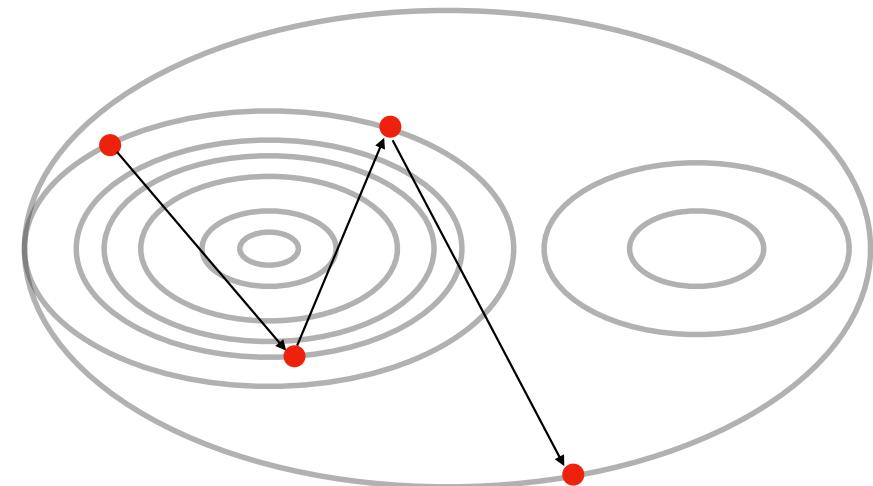
Say $\alpha = 10^{-5}$

With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$



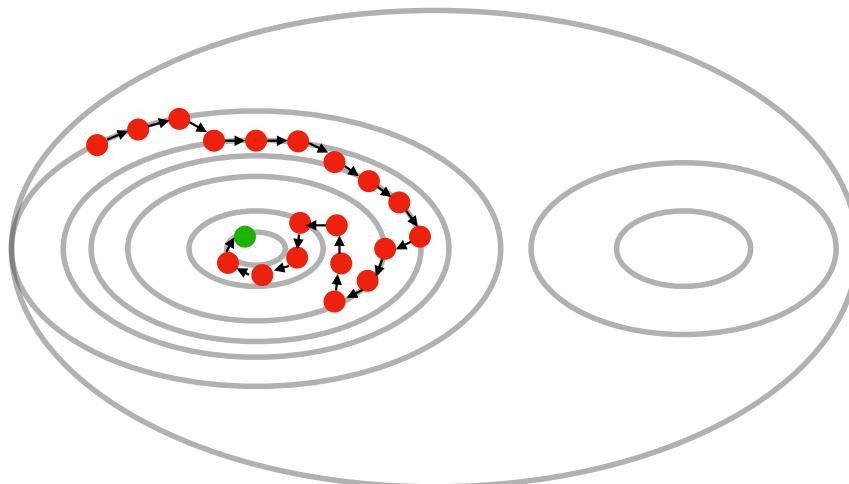
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

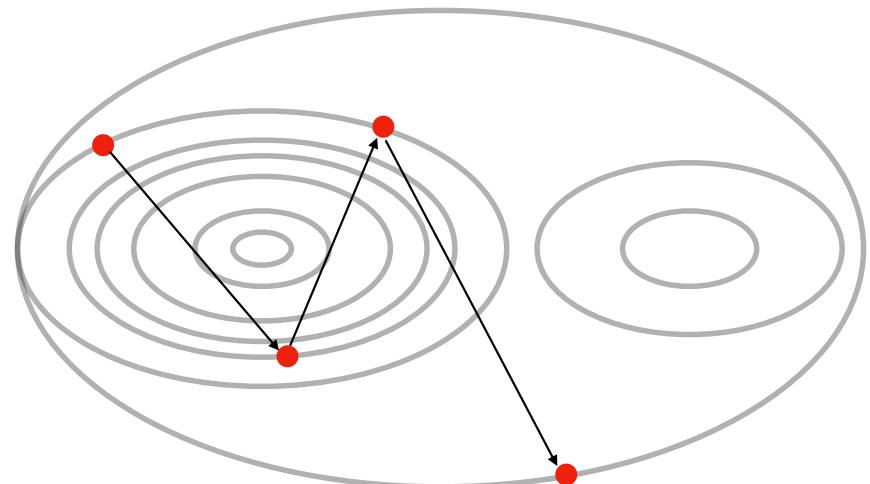
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



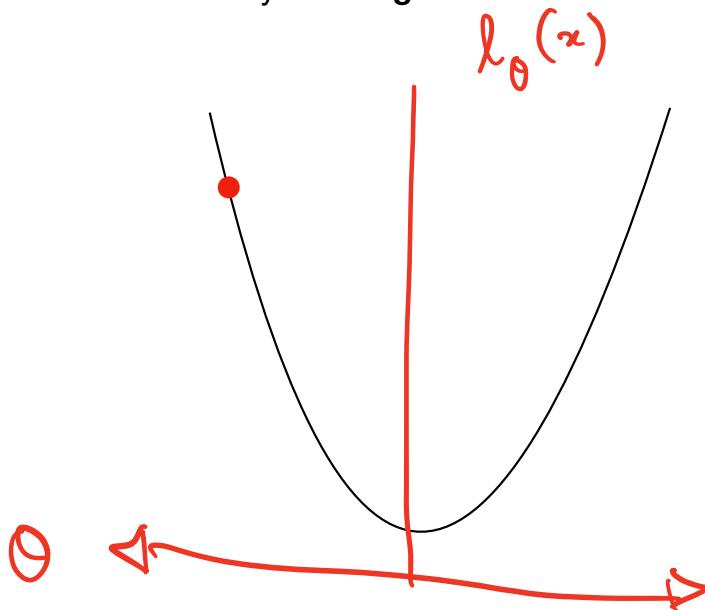
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

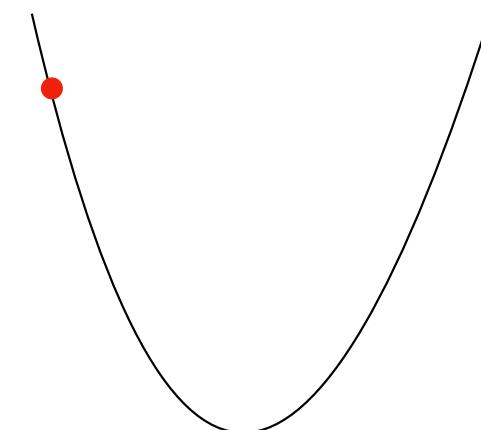
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



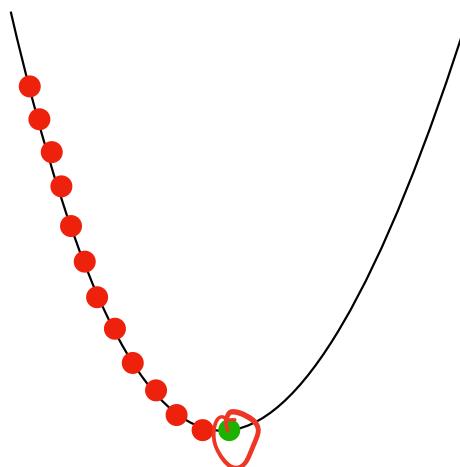
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

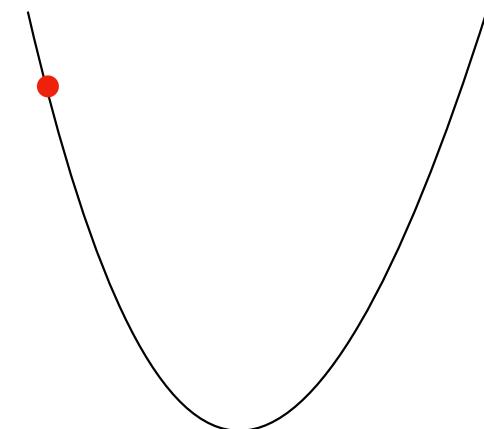
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



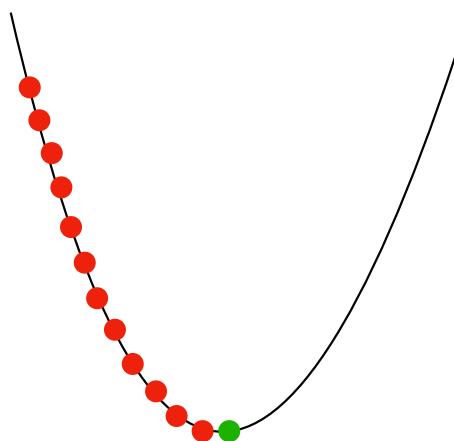
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

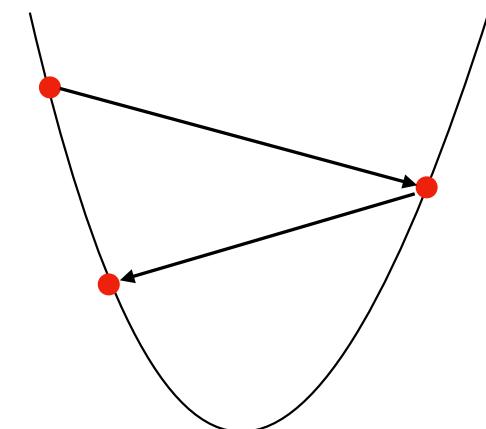
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



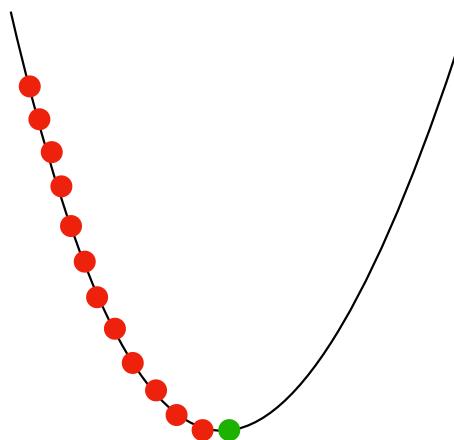
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

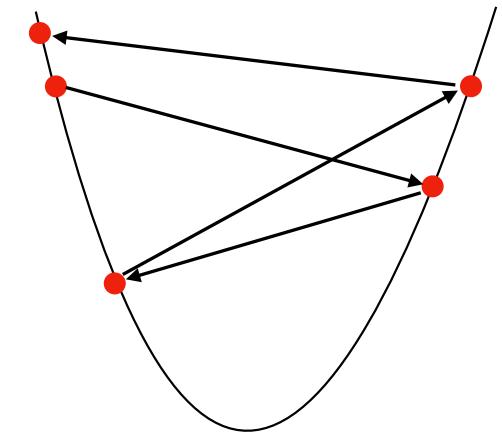
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



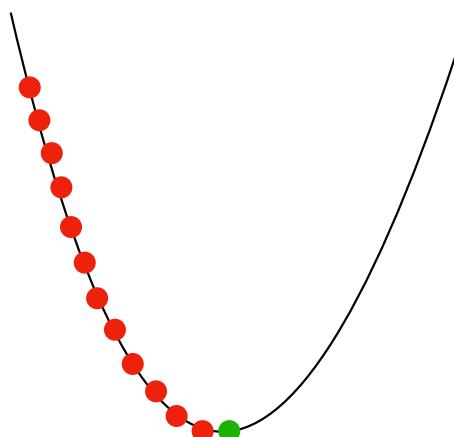
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

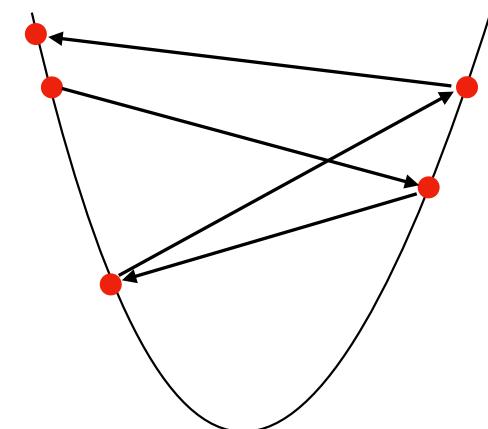
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



You might not always diverge, but converging might still not be possible

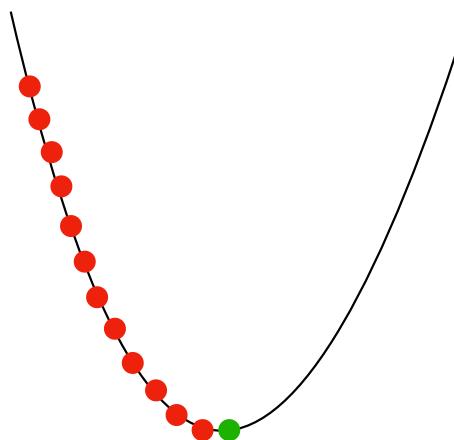
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

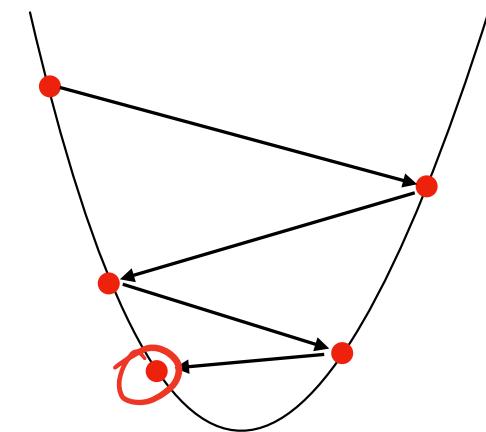
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



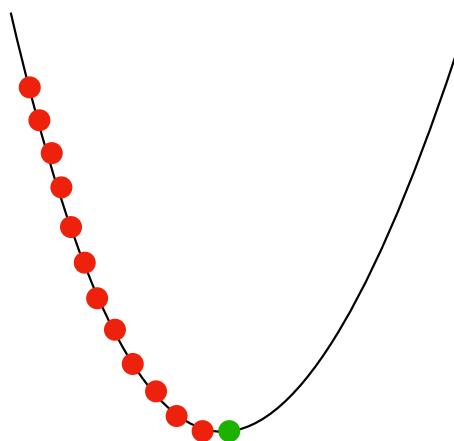
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

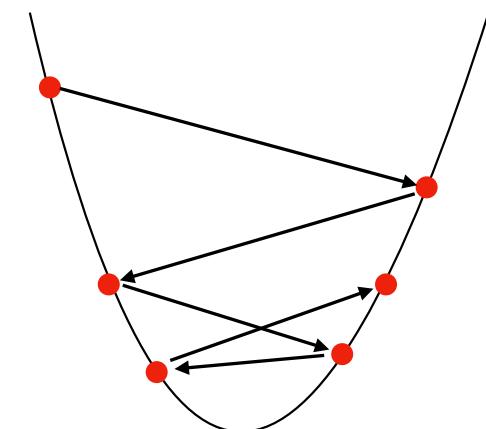
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



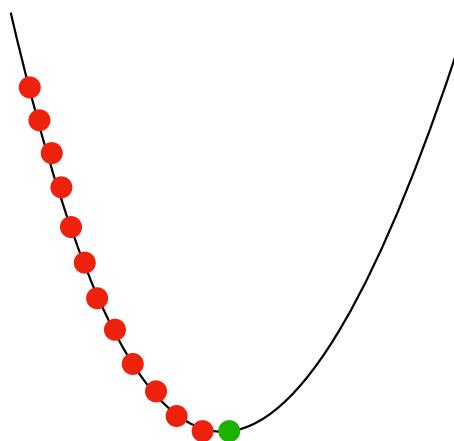
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

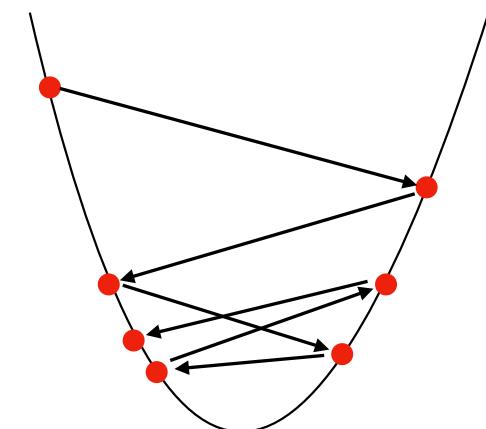
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



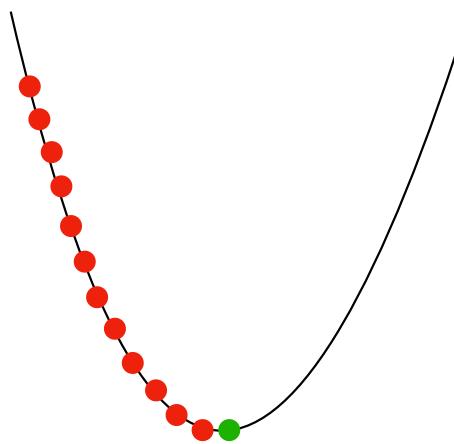
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

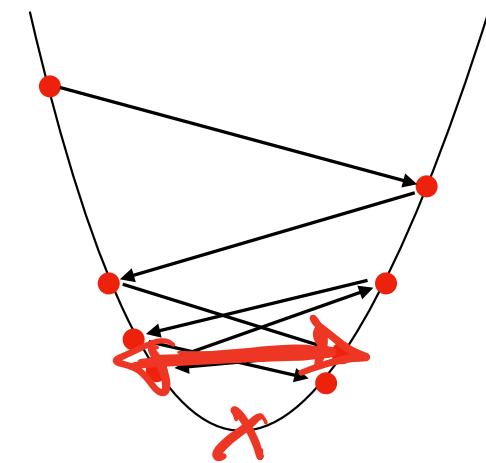
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



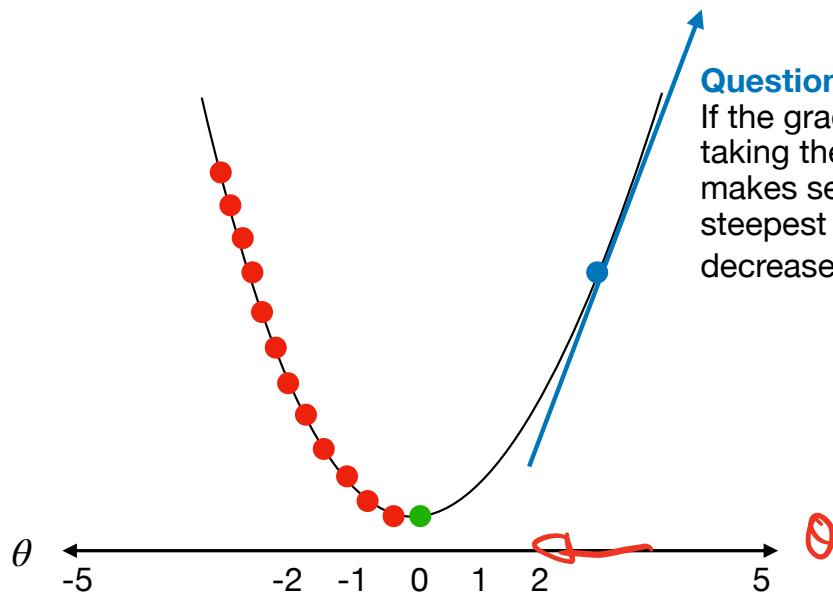
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

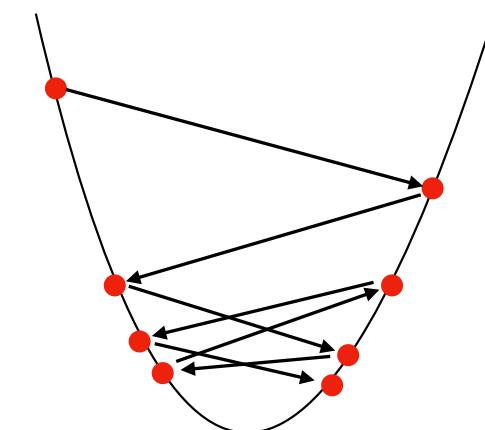
With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge



Question:
If the gradient here is positive, taking the negative of the gradient makes sense to get direction of steepest descent - i.e., we decrease the value of θ

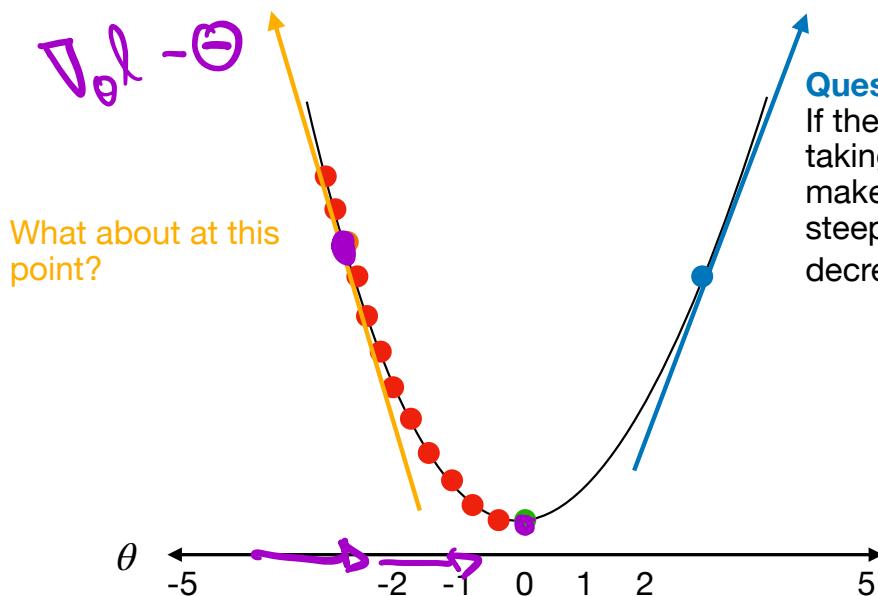
Optimizing Loss Functions

Gradient Descent - Effect of Learning Rate

What happens when α is too small?

Say $\alpha = 10^{-5}$

With a small learning rate α , if the loss function is convex, the optimization will eventually **converge**



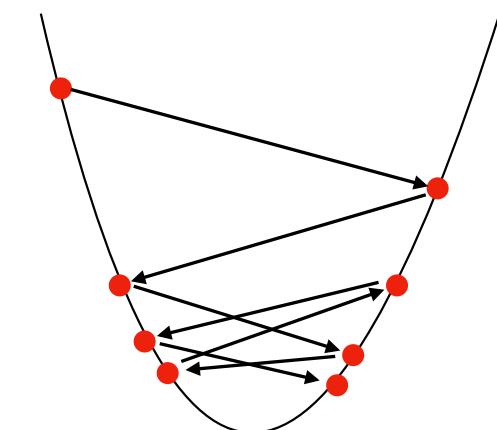
What about at this point?

What happens when α is too large?

Say $\alpha = 10$

With a large learning rate α , if the loss function is convex, the optimization could possibly start **diverging** and never converge

Question:
If the gradient here is positive, taking the negative of the gradient makes sense to get direction of steepest descent - i.e., we decrease the value of θ

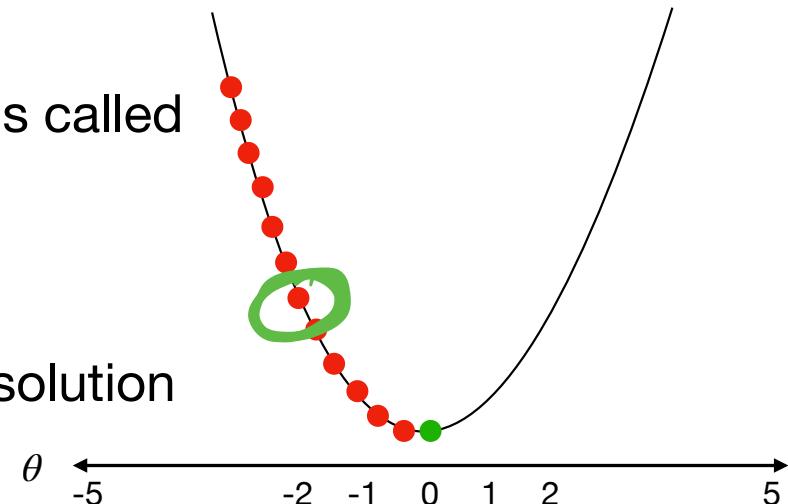


Optimizing Loss Functions

Gradient Descent - Stopping Criterion

$x \rightarrow 500$ []
3

- When do you stop your iterations?
 - Maximum Iteration →
 - Each iteration through the training dataset is called an “epoch” → 1000
 - Terminate after a fixed number of epochs
 - Simple, but provides no guarantees about solution quality



Optimizing Loss Functions

Gradient Descent - Stopping Criterion

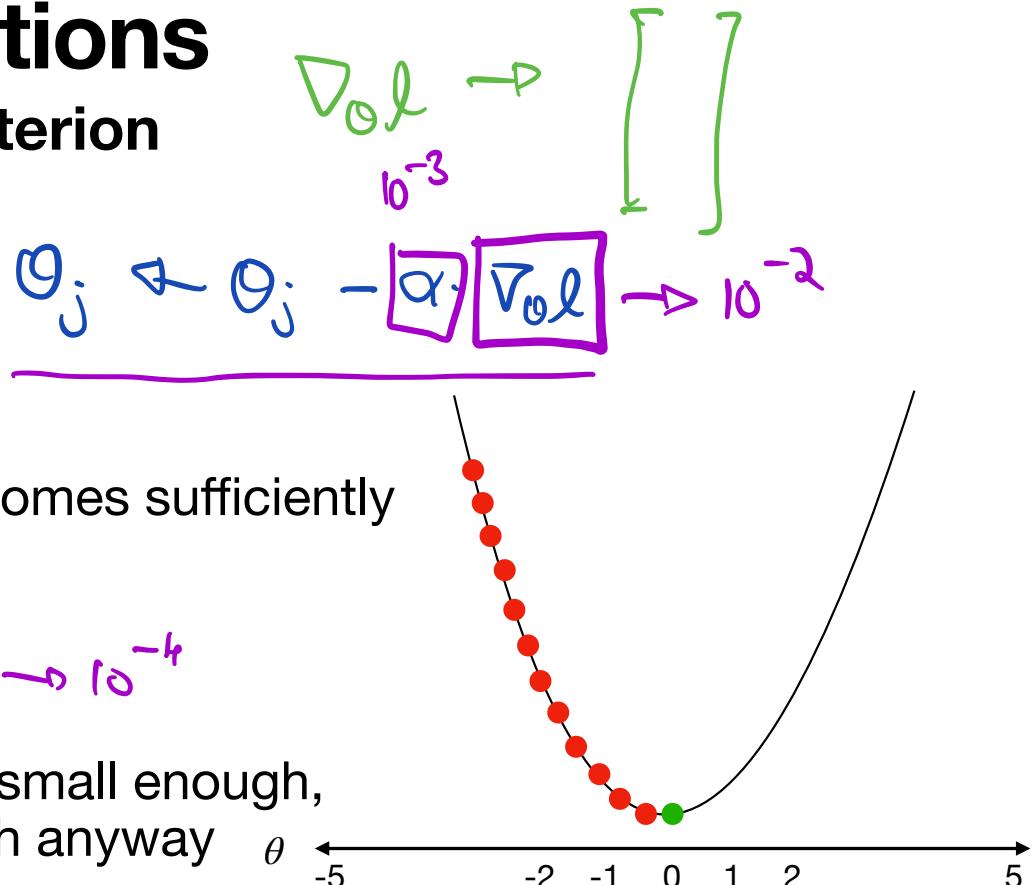
- When do you stop your iterations?

- Gradient Norm Threshold

- Terminate when the gradient becomes sufficiently small

$$\|\nabla \ell_\theta(x)\|_2 \leq \epsilon \rightarrow 10^{-4}$$

- At this point, if the gradients are small enough, the parameters won't move much anyway

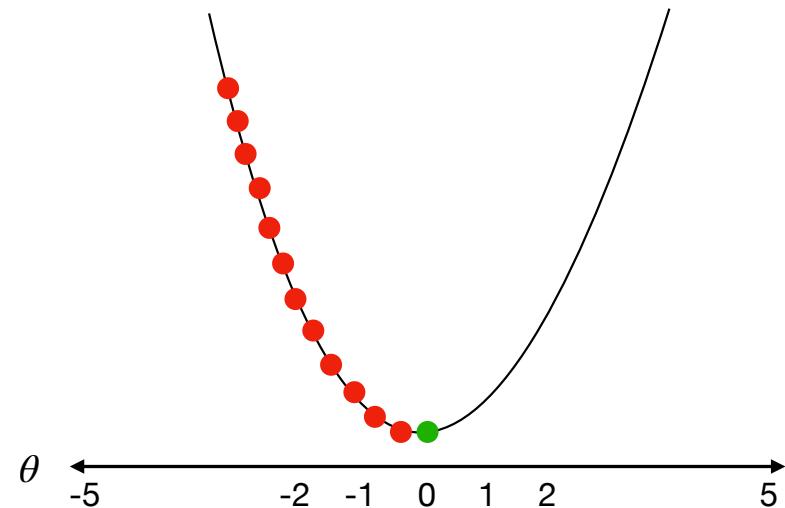
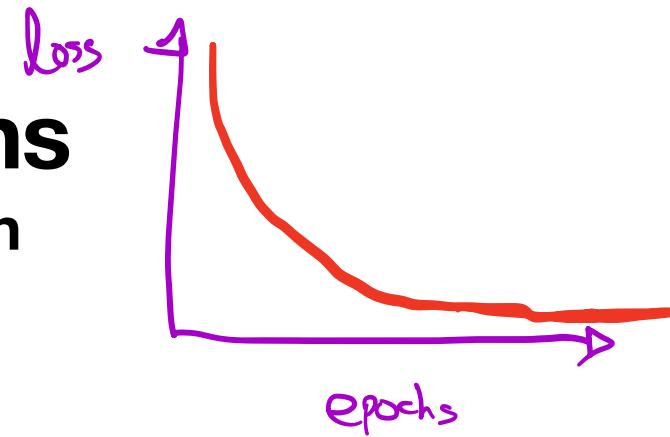


Optimizing Loss Functions

Gradient Descent - Stopping Criterion

- When do you stop your iterations?
 - Function Value Change
 - Terminate when the loss stops changing meaningfully

$$|\ell_{\theta_t}(x) - \ell_{\theta_{t-1}}(x)| \leq \epsilon$$



Optimizing Loss Functions

Gradient Descent - Stopping Criterion

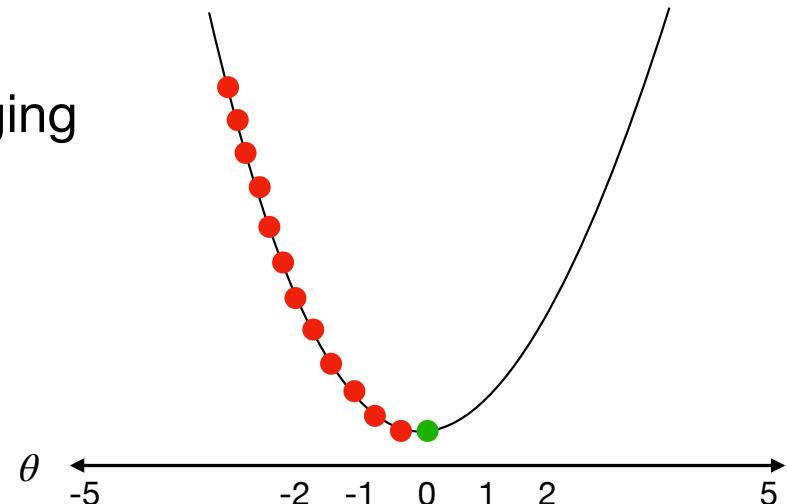
- When do you stop your iterations?
 - Parameter Value Change
 - Terminate when the parameters stop changing meaningfully

$$|\theta_t - \theta_{t-1}| \leq \epsilon$$



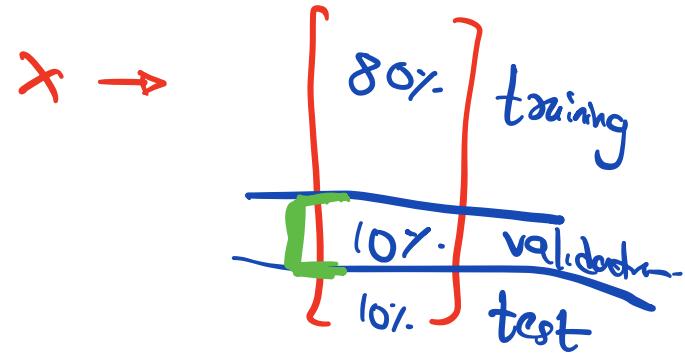
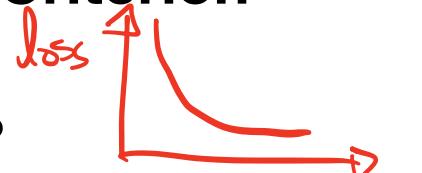
Prev
Slate

$$\rightarrow |l(\theta_t) - l(\theta_{t-1})|$$

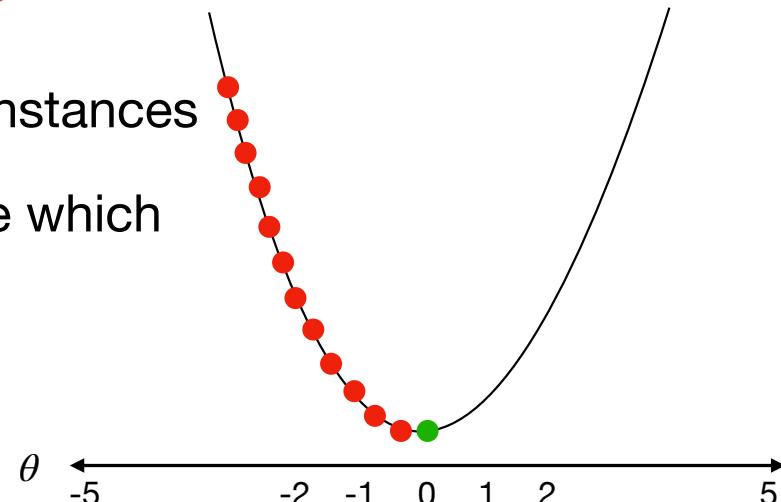
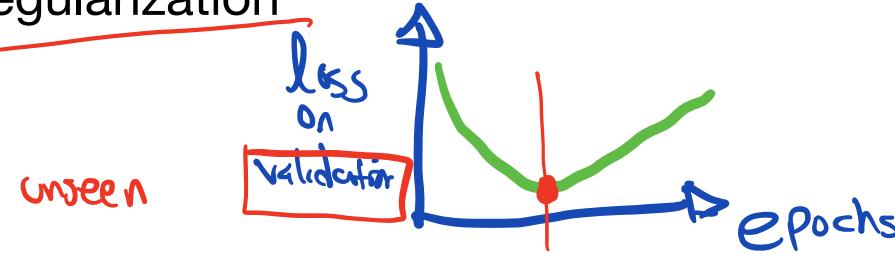


Optimizing Loss Functions

Gradient Descent - Stopping Criterion



- When do you stop your iterations?
 - Validation Based Stopping (Early Stopping)
 - Monitor performance on a validation set of instances
 - Stop when validation loss begins to increase which signals overfitting
 - Serves as both stopping criterion and regularization

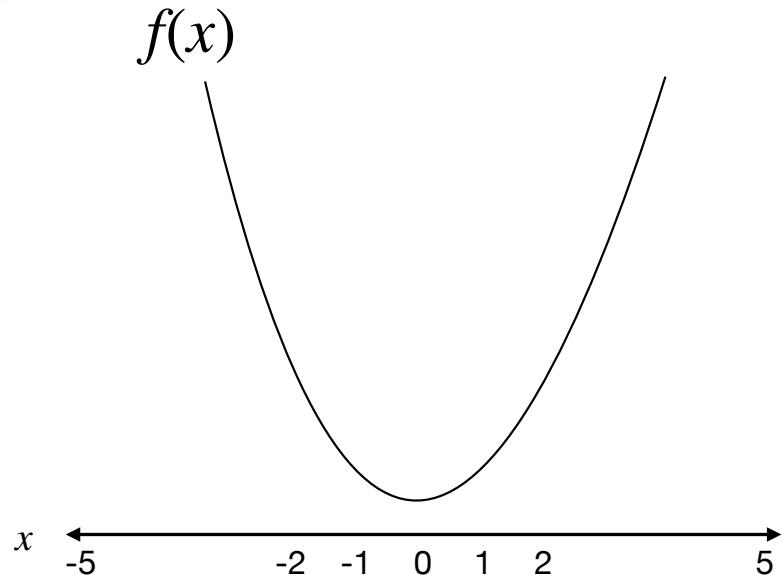


Optimizing Loss Functions

Gradient Descent - Convexity

- A function f is convex if for all points in its domain (input) and for all $\lambda \in [0,1]$

$$\rightarrow f(\underbrace{\lambda x + (1 - \lambda)y}_{\text{convex combination}}) \leq \underbrace{\lambda f(x)}_{\text{line segment}} + (1 - \lambda)f(y)$$

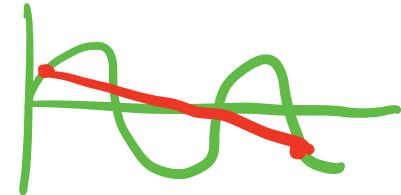
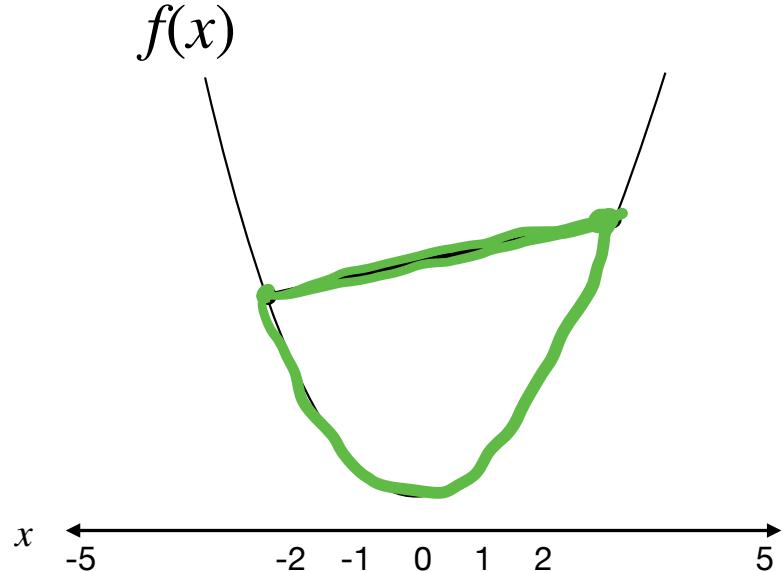
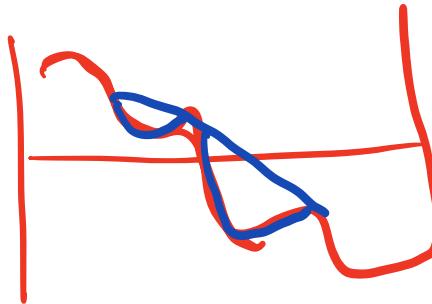
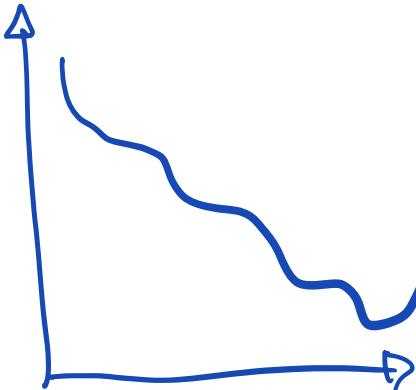


Optimizing Loss Functions

Gradient Descent - Convexity

- A function f is convex if for all points in its domain (input) and for all $\lambda \in [0,1]$

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y)$$



Optimizing Loss Functions

Gradient Descent - Convexity

- A function f is convex if for all points in its domain (input) and for all $\lambda \in [0,1]$

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y)$$

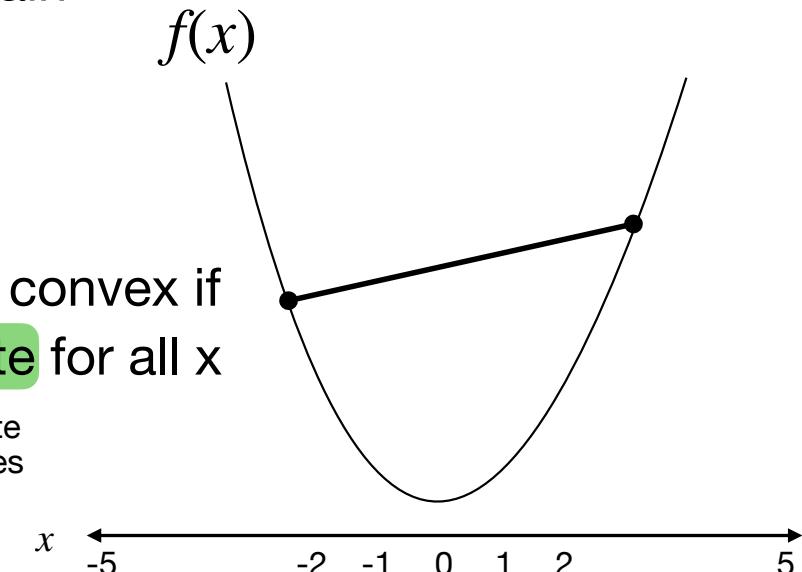
- For more complicated functions, a function f is convex if the Hessian matrix $H(x)$ is positive semi-definite for all x

Second order derivative or derivative of the Jacobian

A matrix is positive semi-definite if and only if all of its eigenvalues are strictly greater than 0

Symmetric

$$\nabla f_0 = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \dots \end{bmatrix}$$



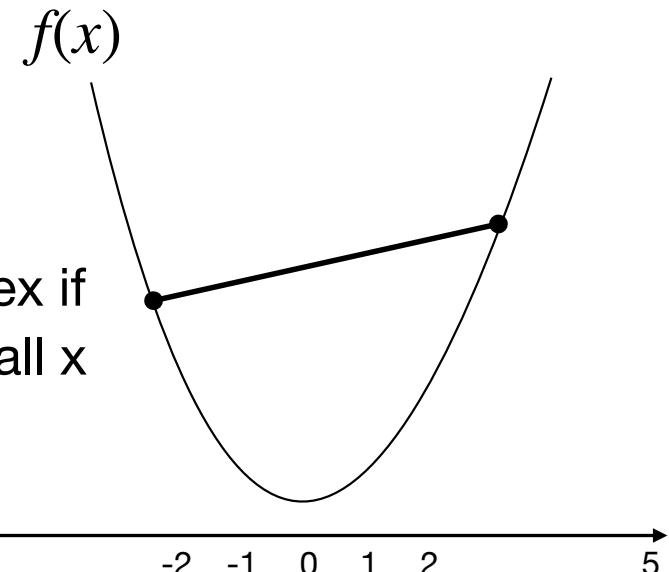
Optimizing Loss Functions

Gradient Descent - Convexity

- A function f is convex if for all points in its domain (input) and for all $\lambda \in [0,1]$

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y)$$

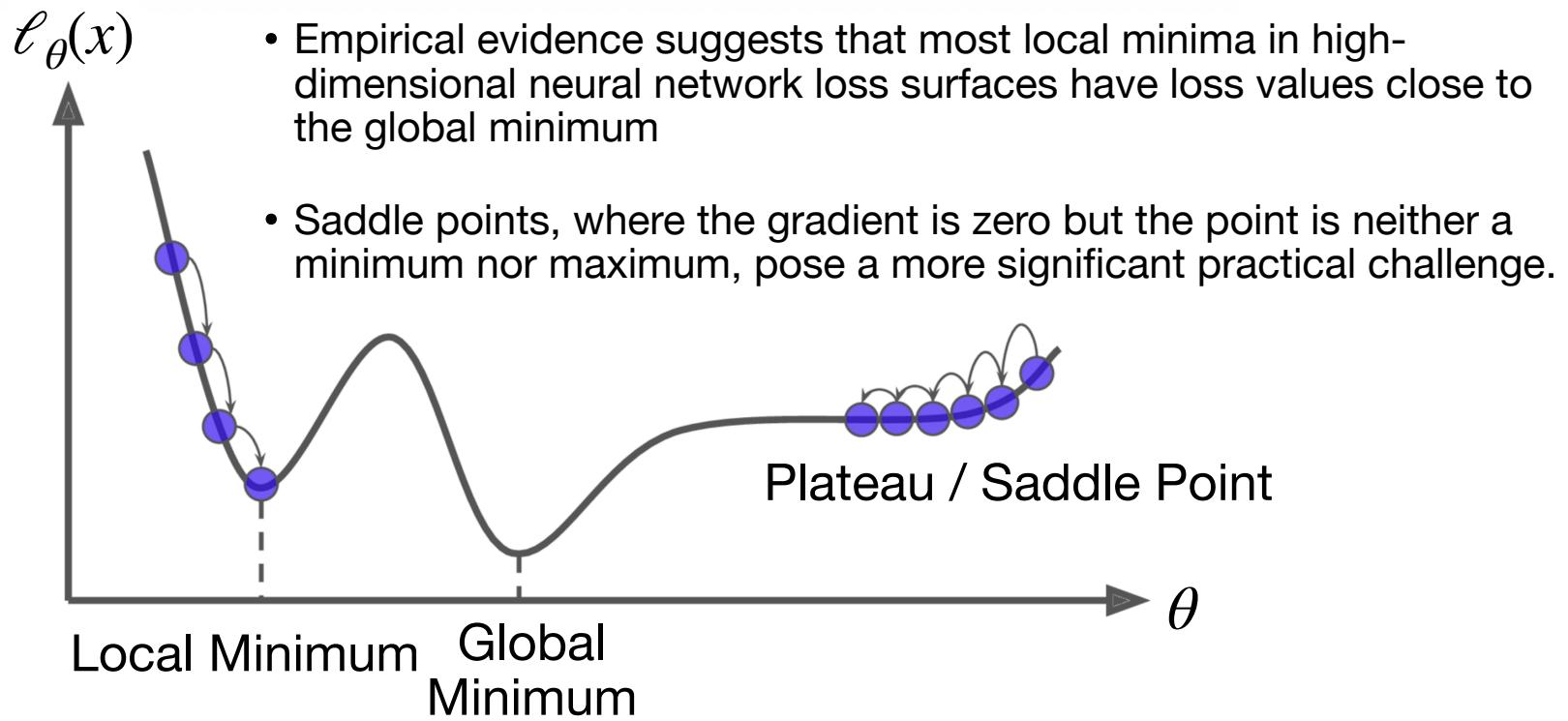
- For more complicated functions, a function f is convex if the Hessian matrix $H(x)$ is positive semi-definite for all x
- If a function is convex, gradient descent is guaranteed to converge given the right learning rate since every local minimum is a global minimum



Optimizing Loss Functions

Gradient Descent - More Complicated Functions

- Most deep learning models however have **highly non-convex** loss landscapes



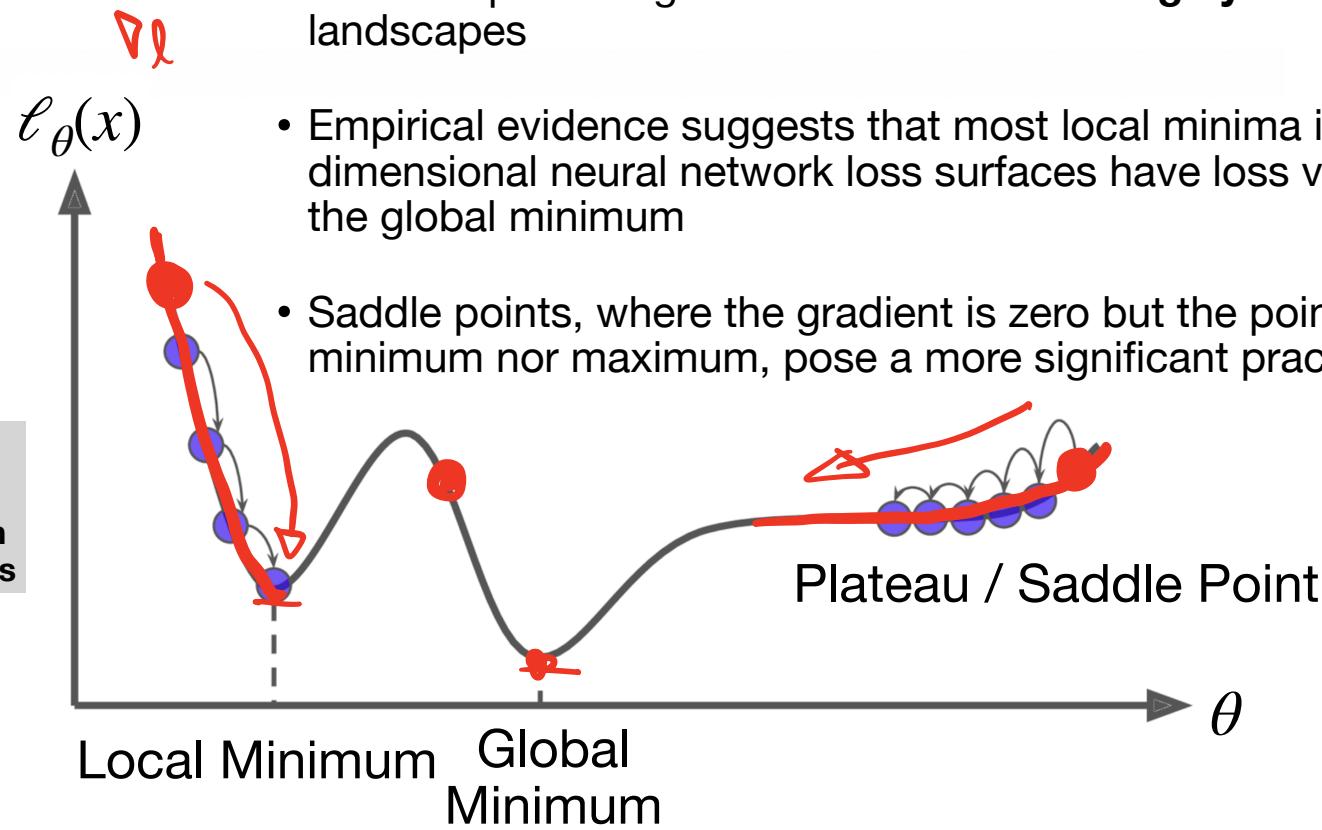
Optimizing Loss Functions

Gradient Descent - More Complicated Functions

- Most deep learning models however have **highly non-convex** loss landscapes
- Empirical evidence suggests that most local minima in high-dimensional neural network loss surfaces have loss values close to the global minimum
- Saddle points, where the gradient is zero but the point is neither a minimum nor maximum, pose a more significant practical challenge.

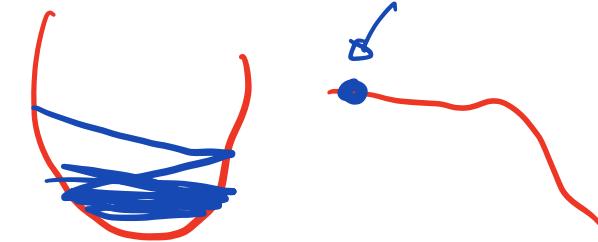
Initialization is an issue.

We will talk about it when
we get to neural networks



Optimizing Loss Functions

Gradient Descent - Convergence Issues



- **Oscillation:** When the learning rate is **too large** or the loss surface has regions of high curvature, the algorithm oscillates around the minimum rather than converging smoothly.
- **Slow convergence in flat regions:** When gradients are small, parameter updates become negligible, leading to extremely slow progress.
- **Divergence:** If the learning rate exceeds a certain value for convex functions, the algorithm can **diverge** entirely, with the loss increasing without bound.
- Saddle points: In high dimensions, saddle points are ubiquitous. The **gradient at a saddle point is zero**, causing standard gradient descent to stall.

Optimizing Loss Functions

Gradient Descent - Practical Fixes

$$x \leftarrow \frac{x - \mu}{\sigma}$$

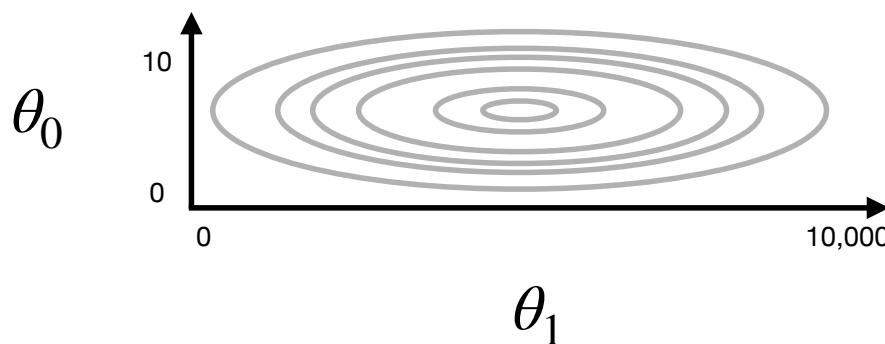
mean
↓
Covariance

- Feature Scaling
 - Remember we want all input features $x_1, x_2 \dots x_n$ to be in similar ranges
 - When features have different scales, the loss surface becomes elongated (ill-conditioned).

Optimizing Loss Functions

Gradient Descent - Practical Fixes

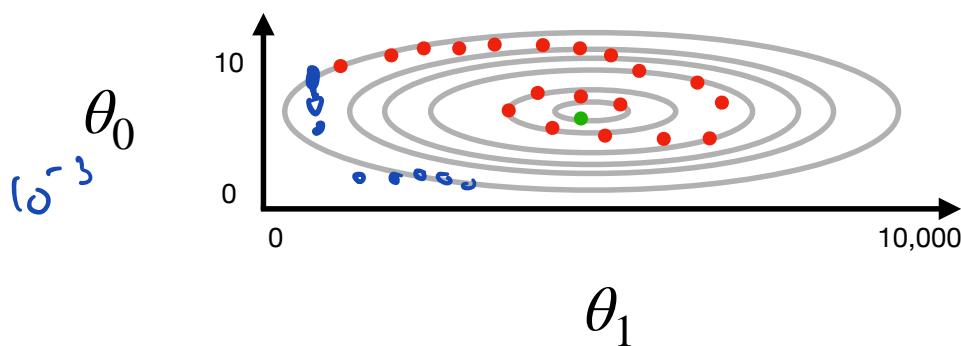
- Feature Scaling
 - Remember we want all input features $x_1, x_2 \dots x_n$ to be in similar ranges
 - When features have different scales, the loss surface becomes elongated (ill-conditioned).



Optimizing Loss Functions

Gradient Descent - Practical Fixes

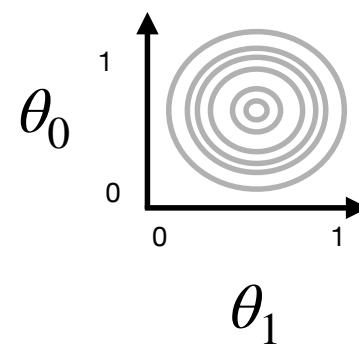
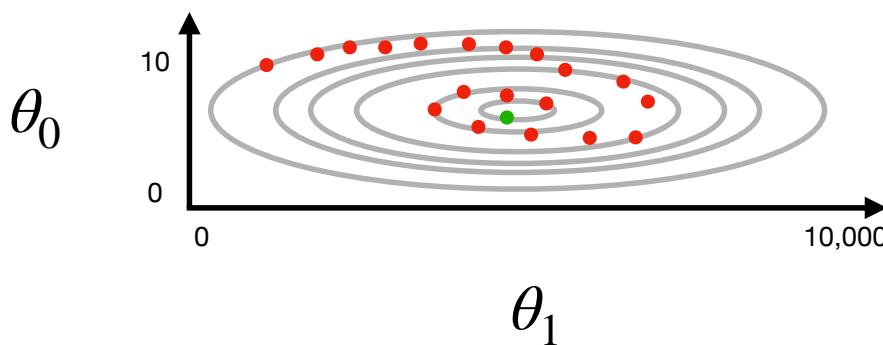
- Feature Scaling
 - Remember we want all input features $x_1, x_2 \dots x_n$ to be in similar ranges
 - When features have different scales, the loss surface becomes elongated (ill-conditioned).



Optimizing Loss Functions

Gradient Descent - Practical Fixes

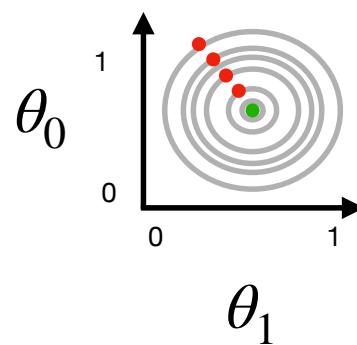
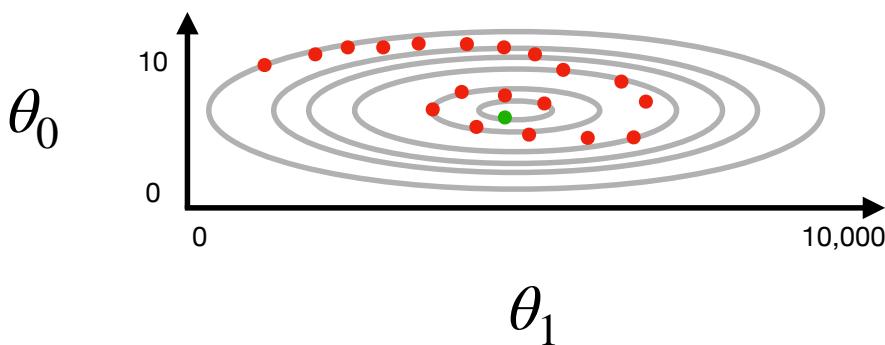
- Feature Scaling
 - Remember we want all input features $x_1, x_2 \dots x_n$ to be in similar ranges
 - When features have different scales, the loss surface becomes elongated (ill-conditioned).



Optimizing Loss Functions

Gradient Descent - Practical Fixes

- Feature Scaling
 - Remember we want all input features $x_1, x_2 \dots x_n$ to be in similar ranges
 - When features have different scales, the loss surface becomes elongated (ill-conditioned).



This dramatically accelerates the optimization process

This also allows having one single learning rate for all parameters

Optimizing Loss Functions

Gradient Descent - Practical Fixes

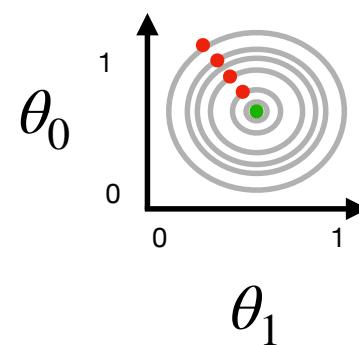
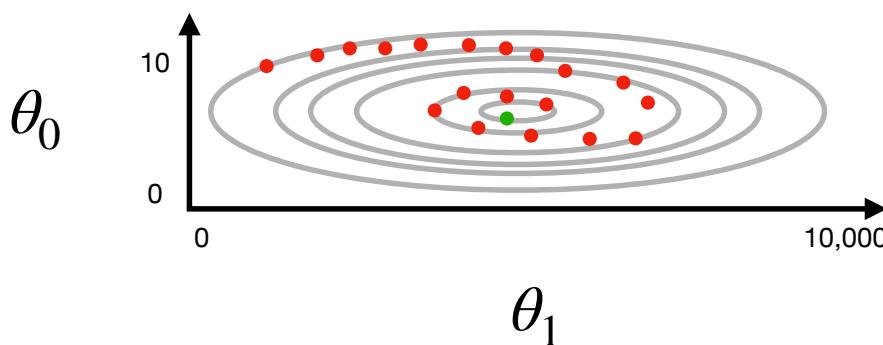
$$x_{\text{train}} \leftarrow \frac{x - \bar{x}_{\text{train}}}{s_{\text{train}}}$$

$$x_{\text{test}} \leftarrow \frac{x - \bar{x}_{\text{train}}}{s_{\text{train}}}$$

NOTE: Scaling parameters (mean, standard deviation, min, max) must be computed only on training data and then applied to validation and test data to prevent data leakage.

- Feature Scaling
 - Remember we want all input features $x_1, x_2 \dots x_n$ to be in similar ranges
 - When features have different scales, the loss surface becomes elongated (ill-conditioned).

$$\frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$



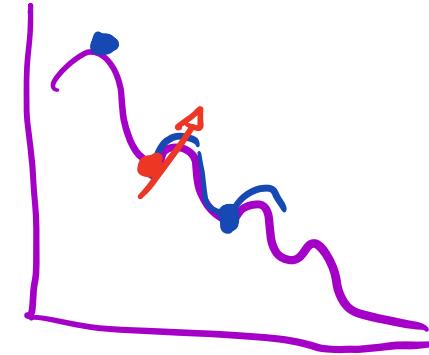
This dramatically accelerates the optimization process

This also allows having one single learning rate for all parameters

Optimizing Loss Functions

Gradient Descent - Momentum

- Standard gradient descent can oscillate in ravines
 - Areas where the surface curves **more steeply in one dimension** than another
 - Or they can get stuck in plateau / saddle points
- Momentum helps accelerate gradient descent by accumulating velocity in **directions of consistent gradient**



$$\theta_j \leftarrow \theta_j - \alpha \cdot \frac{\partial \ell_{\theta}(x)}{\partial \theta_j}$$
$$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}$$

Optimizing Loss Functions

Gradient Descent - Momentum

- Momentum helps accelerate gradient descent by accumulating velocity in **directions of consistent gradient**

With Momentum

$$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}$$
$$v_t = \beta v_{t-1} + \nabla \ell_{\theta_{t-1}}$$
$$\theta_t = \theta_{t-1} - \alpha \cdot v_t$$
$$v_t = \beta \cdot v_{t-1} + \nabla \ell_{\theta_{t-1}}$$

Optimizing Loss Functions

Gradient Descent - Momentum

$$V_{10} = \beta V_q + \nabla \ell_{\theta_q}$$

- Momentum helps accelerate gradient descent by accumulating velocity in **directions of consistent gradient**

$$V_q = \beta V_8 + \nabla \ell_{\theta_8}$$

$$V_1 = \beta V_0 + \nabla \ell_{\theta_0}$$

$$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}$$

$$V_2 = \beta V_1 + \nabla \ell_{\theta_1}$$

With Momentum

$$V_2 = \beta (\beta V_0 + \nabla \ell_{\theta_0}) + \nabla \ell_{\theta_1}$$

Velocity Vector

$$v_t = \underbrace{\beta \cdot v_{t-1}}_{\text{green}} + \underbrace{\nabla \ell_{\theta_{t-1}}}_{\text{red}}$$

$$\theta_t = \theta_{t-1} - \alpha \cdot v_t$$

$$V_3 :$$

$$V_{10} = \beta (V_9 + \nabla \ell \beta (V_8 + \dots \nabla \ell \beta (V_1 + \dots \nabla \ell)))$$

Optimizing Loss Functions

Gradient Descent - Momentum

- Momentum helps accelerate gradient descent by accumulating velocity in **directions of consistent gradient**

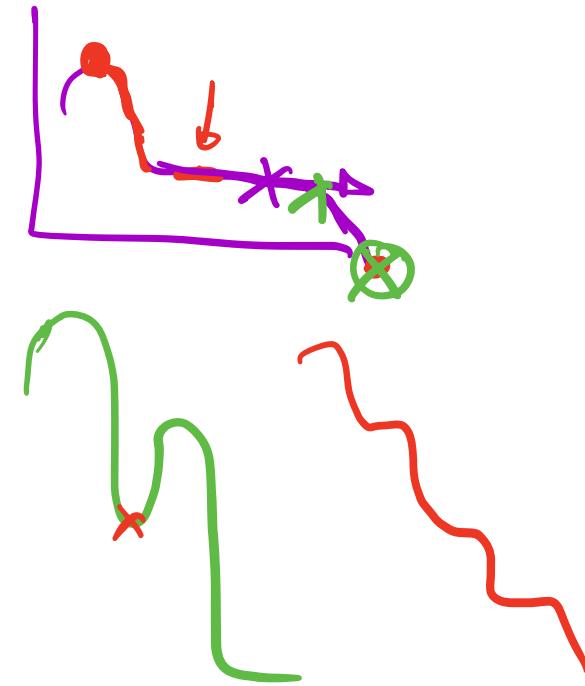
$$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}$$

With Momentum

β is the momentum coefficient, typically set to 0.9

$$v_t = \beta \cdot v_{t-1} + \nabla \ell_{\theta_{t-1}}$$

$$\theta_t = \theta_{t-1} - \alpha \cdot v_t$$



Optimizing Loss Functions

Gradient Descent - Momentum

- Momentum helps accelerate gradient descent by accumulating velocity in **directions of consistent gradient**

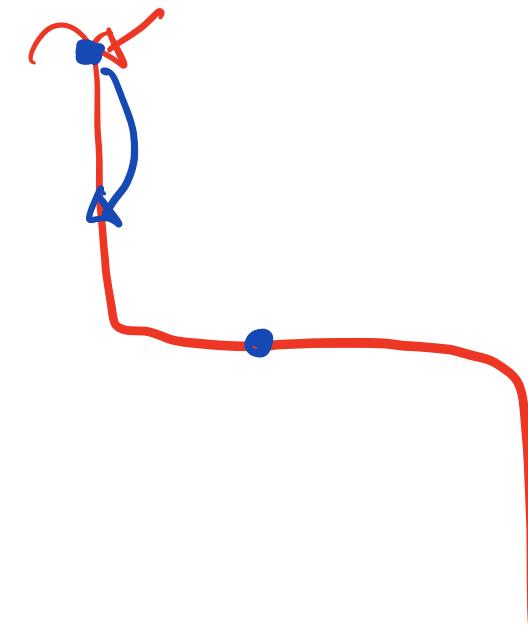
$$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}$$

With Momentum

If $\beta = 0$, you get back standard gradient descent

$$v_t = \beta \cdot v_{t-1} + \nabla \ell_{\theta_{t-1}}$$

$$\theta_t = \theta_{t-1} - \alpha \cdot v_t$$



Optimizing Loss Functions

Gradient Descent - Momentum

- Momentum helps accelerate gradient descent by accumulating velocity in **directions of consistent gradient**

$$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}$$

With Momentum

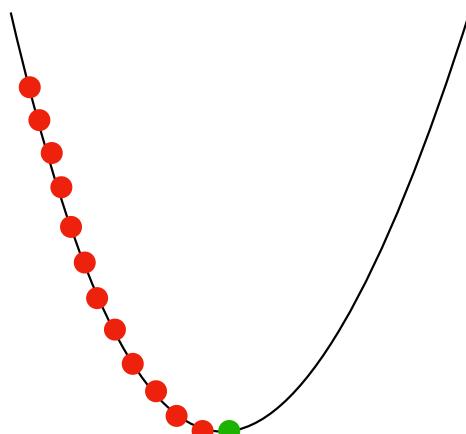
→ $v_t = \beta \cdot v_{t-1} + \nabla \ell_{\theta_{t-1}}$

$$\theta_t = \theta_{t-1} - \boxed{\alpha} \cdot v_t$$

Think of momentum as gravity pulling a ball down a hill, the momentum will carry the ball through any flat or even small uphill regions

Optimizing Loss Functions

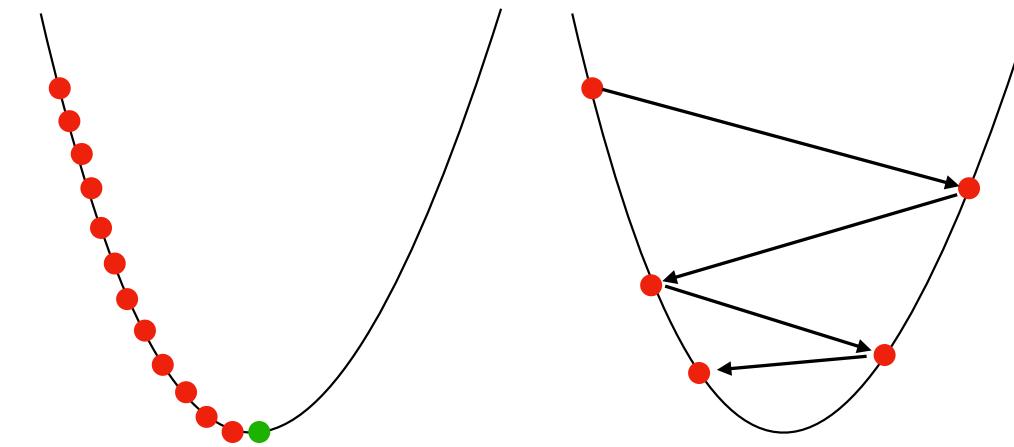
Gradient Descent - Adaptive Step Sizes



α is too small
Finds the optimal but too slow

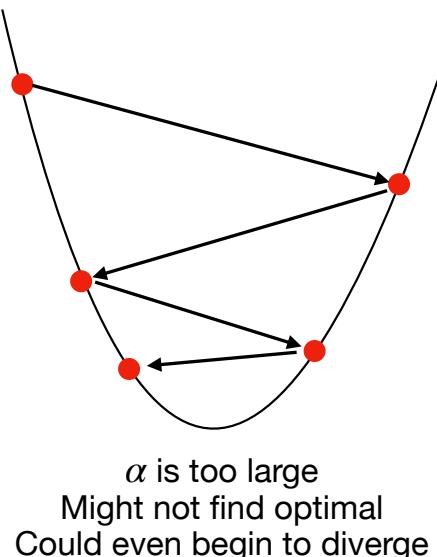
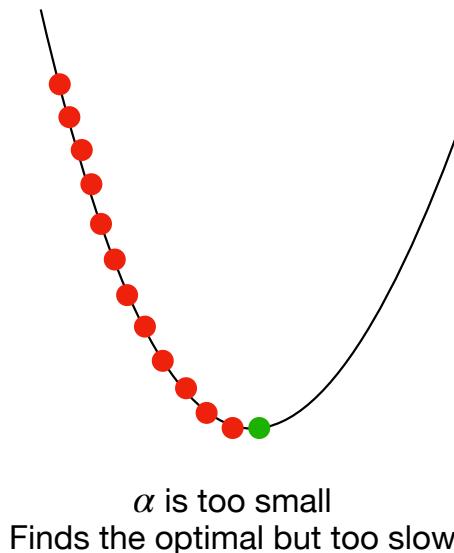
Optimizing Loss Functions

Gradient Descent - Adaptive Step Sizes



Optimizing Loss Functions

Gradient Descent - Adaptive Step Sizes

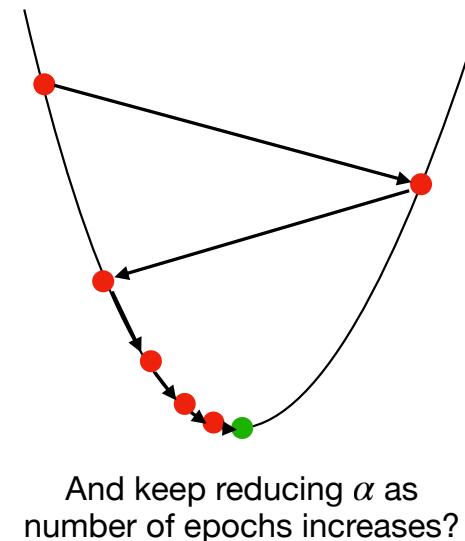
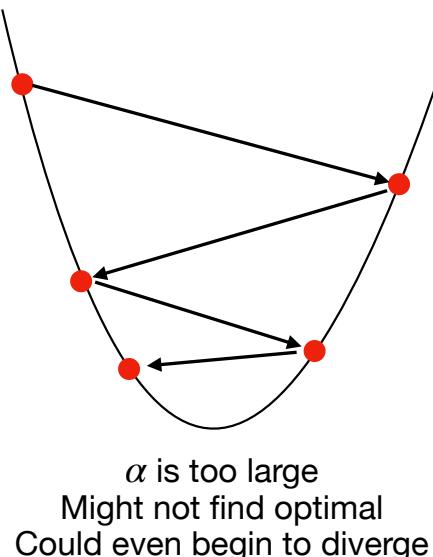
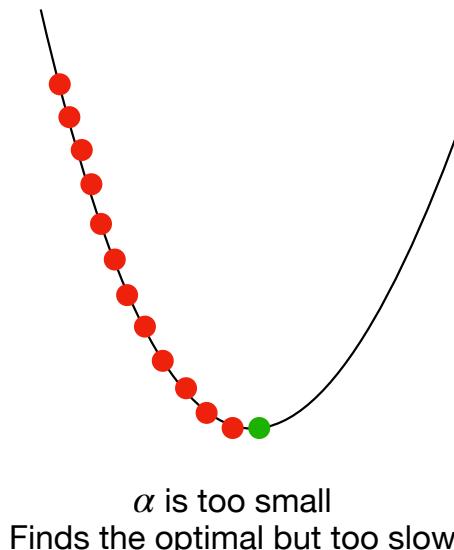


A graph of a convex loss function. The gradient descent path (red dots with arrows) starts with a very large step that overshoots the minimum. Subsequent steps are much smaller, converging quickly to the minimum. This illustrates the use of adaptive step sizes to handle different scales in the gradient.

What if you set α to be large initially?

Optimizing Loss Functions

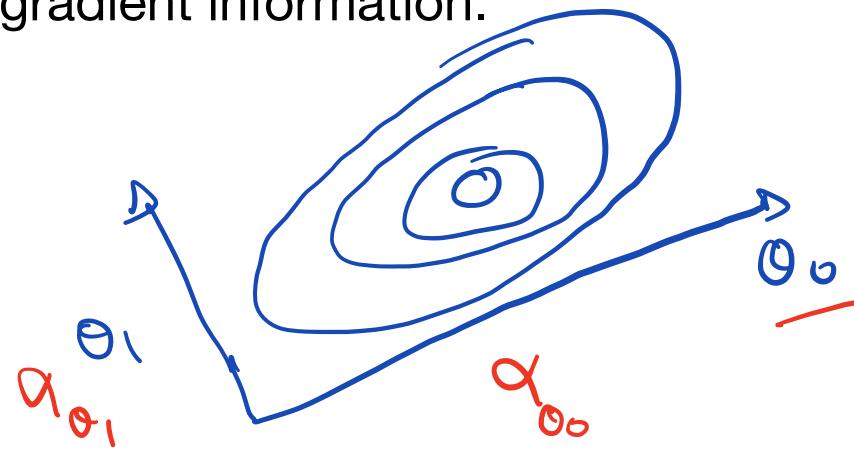
Gradient Descent - Adaptive Step Sizes



Optimizing Loss Functions

Gradient Descent - Per Parameter Adaptive Learning Rates

- A single global learning rate may be suboptimal
 - Some parameters might benefit from larger updates while others need smaller ones.
 - Adaptive methods adjust the learning rate for each parameter individually based on historical gradient information.



Optimizing Loss Functions

Gradient Descent - AdaGrad

- AdaGrad adapts the learning rate for **each parameter** based on the sum of squared historical gradients

$$\begin{aligned} G_t &= G_{t-1} + (\nabla \ell_{\theta_{t-1}})^2 \\ \theta_t &= \theta_{t-1} - \frac{\alpha}{\sqrt{G_t + \epsilon}} \cdot \nabla \ell_{\theta_{t-1}} \end{aligned}$$

Optimizing Loss Functions

Gradient Descent - AdaGrad

- AdaGrad adapts the learning rate for **each parameter** based on the sum of squared historical gradients

$$G_t \neq G_{t-1}$$

$$\rightarrow G_t = G_{t-1} + (\nabla \ell_{\theta_{t-1}})^2$$
$$\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{G_t} + \epsilon} \cdot \nabla \ell_{\theta_{t-1}}$$

$$G_t = \begin{bmatrix} G_{\theta_0} \\ G_{\theta_1} \\ G_{\theta_2} \end{bmatrix}$$
$$\nabla \ell = \begin{bmatrix} \nabla_{\theta_0} \\ \nabla_{\theta_1} \\ \nabla_{\theta_2} \end{bmatrix}$$

- Parameters with large historical gradients receive smaller updates
- Parameters with small historical gradients receive larger updates
- The limitation is that the accumulated sum G_t grows monotonically, eventually making the learning rate vanishingly small.

Optimizing Loss Functions

Gradient Descent - AdaGrad

- AdaGrad adapts the learning rate for **each parameter** based on the sum of squared historical gradients

$$G_t = G_{t-1} + (\nabla \ell_{\theta_{t-1}})^2$$
$$\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{G_t} + \epsilon} \cdot \nabla \ell_{\theta_{t-1}}$$

The diagram illustrates the AdaGrad update rule. It shows the formula $\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{G_t} + \epsilon} \cdot \nabla \ell_{\theta_{t-1}}$. A blue bracket encloses the term $\frac{\alpha}{\sqrt{G_t} + \epsilon}$, which represents the adaptive learning rate. The term $\sqrt{G_t} + \epsilon$ is highlighted with a blue box, indicating that it is the sum of the previous squared gradient and a small constant ϵ to prevent division by zero.

- Parameters with large historical gradients receive smaller updates
- Parameters with small historical gradients receive larger updates
- The limitation is that the accumulated sum G_t grows monotonically, eventually making the learning rate vanishingly small.

Optimizing Loss Functions

Gradient Descent - RMSProp

- RMSprop addresses AdaGrad's diminishing learning rate by using an exponentially decaying average of squared gradients

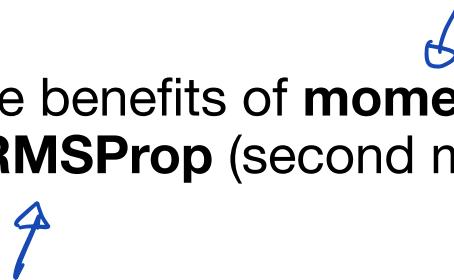
$$\rightarrow G_t = \rho \cdot G_{t-1} + (1 - \rho) \cdot (\nabla \ell_{\theta_{t-1}})^2$$
$$\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{G_t + \epsilon}} \cdot \nabla \ell_{\theta_{t-1}}$$

- The decay rate ρ is typically set to 0.9.
- This prevents the learning rate from decaying to zero while still adapting to the gradient scale.

Optimizing Loss Functions

Gradient Descent - ADAM

- Adam (**A**daptive **M**oment Estimation) combines the benefits of **momentum** (first moment) with the adaptive learning rates of **RMSProp** (second moment)



Optimizing Loss Functions

Gradient Descent - ADAM

- Adam (**A**daptive **M**oment **E**stimation) combines the benefits of **momentum** (first moment) with the adaptive learning rates of **RMSProp** (second moment)

Adam maintains **two** moving averages

$$\text{First Moment (mean): } m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla \ell_{\theta_{t-1}}$$

$$\text{Second Moment (variance): } v_t = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla \ell_{\theta_{t-1}})^2$$

Optimizing Loss Functions

Gradient Descent - ADAM

- Adam (**A**daptive **M**oment Estimation) combines the benefits of **momentum** (first moment) with the adaptive learning rates of **RMSProp** (second moment)

Adam maintains **two** moving averages

$$\text{First Moment (mean): } \boxed{m_t} = \beta_1 m_{t-1} + (1 - \beta_1) \boxed{\nabla \ell_{\theta_{t-1}}}$$

$$\text{Second Moment (variance): } \boxed{v_t} = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla \ell_{\theta_{t-1}})^2$$

$$\text{Update: } \theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{v_t} + \epsilon} \cdot \boxed{m_t}$$

Optimizing Loss Functions

Gradient Descent - ADAM

- Adam (**Adaptive Moment Estimation**) combines the benefits of **momentum** (first moment) with the adaptive learning rates of **RMSProp** (second moment)

Adam maintains **two** moving averages



Bias Correction:
Important for early iterations when estimates are biased towards 0

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$

$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

First Moment (mean): $m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla \ell_{\theta_{t-1}}$

Second Moment (variance): $v_t = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla \ell_{\theta_{t-1}})^2$

Update: $\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{\hat{v}_t} + \epsilon} \cdot \hat{m}_t$

Optimizing Loss Functions

Gradient Descent - ADAM

- Adam (**Adaptive Moment Estimation**) combines the benefits of **momentum** (first moment) with the adaptive learning rates of **RMSProp** (second moment)

Adam maintains **two** moving averages

$$\text{First Moment (mean): } m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla \ell_{\theta_{t-1}}$$

$$\text{Second Moment (variance): } v_t = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla \ell_{\theta_{t-1}})^2$$

$$\text{Update: } \theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{\hat{v}_t} + \epsilon} \cdot \hat{m}_t$$

Default Hyperparameters: $\beta_1 = 0.9, \beta_2 = 0.999, \alpha = 10^{-3}$

Bias Correction:
Important for early iterations when estimates are biased towards 0

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$

$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

- Batch Gradient Descent
 - Use **entire training set per epoch**
 - The whole training dataset is used to compute a single parameter update

$$x = \begin{bmatrix} & \\ 1000 & \end{bmatrix}$$

$$\theta_t = \theta_{t-1} - \alpha \frac{1}{m} \sum_{i=1}^m \nabla \ell_{\theta_{t-1}}(x_i, y_i)$$

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

- Batch Gradient Descent
 - Use **entire training set per epoch**
 - The whole training dataset is used to compute a single parameter update
 - One epoch leads to **one** parameter update

$$\theta_t = \theta_{t-1} - \alpha \frac{1}{m} \sum_{i=1}^m \nabla \ell_{\theta_{t-1}}(x_i, y_i)$$

Sum over the whole training dataset

$$w_t \leftarrow w_{t-1} + \alpha \cdot \nabla_{w_{t-1}}$$

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

- Stochastic Gradient Descent

$$x \in \mathbb{R}^{1000}$$

- Use **one** randomly selected training data point at each step
- Parameters are updated after looking at each data point
- One epoch leads to **m** parameter updates

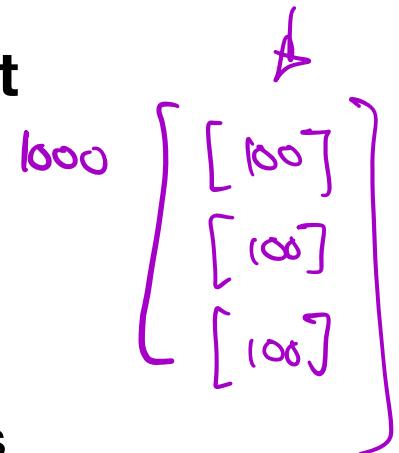
$M=3$

# bed	sq.ft.	$\theta_t = \theta_{t-1} - \alpha \nabla \ell_{\theta_{t-1}}(x_i, y_i)$
5	5000	\leftarrow
4	4000	\leftarrow
1	650	\leftarrow

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

- Mini-Batch Gradient Descent
 - A compromise between batch and stochastic variants
 - Use a small batch of randomly sampled training data points
 - Typical batch sizes are $B = 32, 64, 128, 256, 512, 1024$



$$\theta_t = \theta_{t-1} - \alpha \frac{1}{B} \sum_{i=1}^B \nabla \ell_{\theta_{t-1}}(x_i, y_i)$$

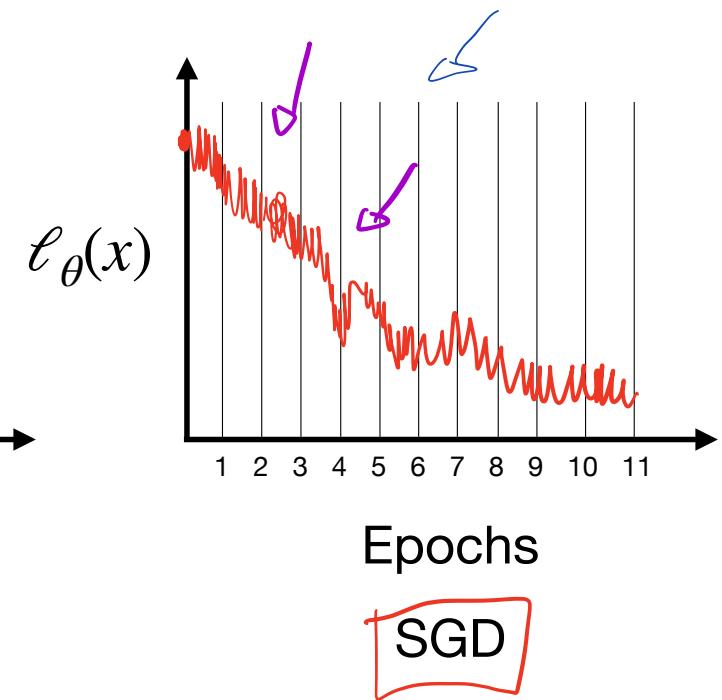
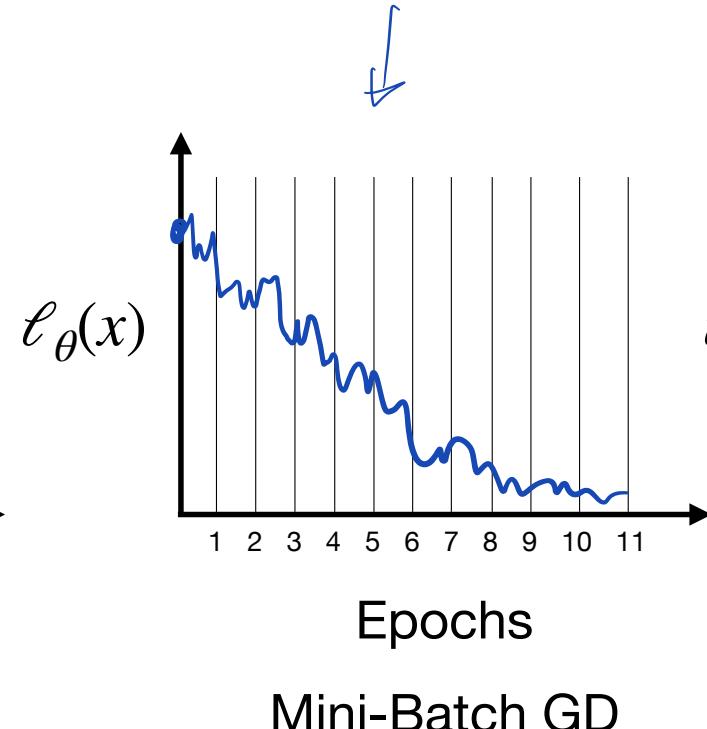
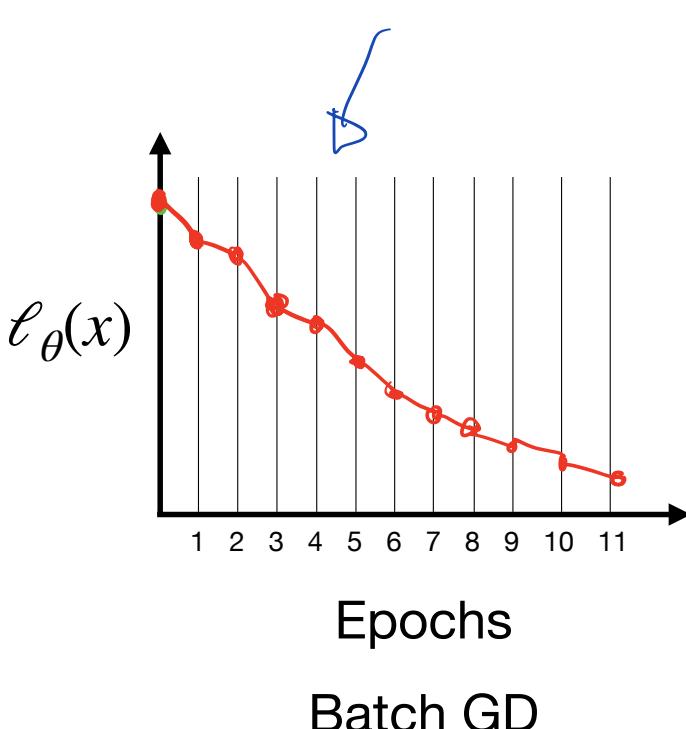
1 epoch → 10 updates

$$m/B$$

$$m = 1000$$
$$B = 100$$

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent



SGD

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

Batch Pros:

Stable Convergence: No noise in gradient estimates means smooth, predictable progress toward the minimum

Guaranteed Descent: Each update is guaranteed to reduce the loss (with appropriate learning rate)

Simple learning rate selection: The lack of noise means you can often use larger learning rates without instability

Parallelizable Gradient Computation The sum over all samples can be computed in parallel across multiple processors

Stochastic Pros:

Fast Updates: Each parameter update is computationally cheap, allowing rapid initial progress.

Memory Efficient: Only one sample needs to be in memory at a time.

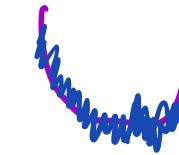
Escapes Local Minima: The inherent noise helps the algorithm escape shallow local minima and saddle points. The stochasticity acts as implicit regularization

Online Learning: Can naturally incorporate new data as it arrives - just perform an update on each new sample

Better Generalization: The noise can prevent overfitting to the training set.

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent



Batch Cons:

Computationally Expensive: For large datasets, computing the full gradient is very slow. A dataset with 10 million samples requires processing all 10 million before a single update.

Memory Intensive: The entire dataset must fit in memory.

Redundant Computation: Many datasets contain redundant or similar samples. BGD computes gradients for all of them even when a subset would provide nearly the same information.

Poor Escape From Local Minima: The deterministic nature means the algorithm follows the same path every time and can get permanently stuck in local minima or saddle points.

Slow for Online Learning: Cannot incorporate new data without reprocessing everything.

Stochastic Cons:

High Variance: Individual gradient estimates can be very noisy, causing erratic updates.

Unstable Convergence: The loss curve is noisy. The algorithm may step away from the minimum even when near it.

Requires Learning Rate Decay: To converge to a minimum (rather than oscillating around it), the **learning rate must decrease** over time, adding hyperparameters.

Poor Hardware Utilization: Modern GPUs are optimized for **parallel operations on batches**, not sequential single-sample operations. SGD fails to exploit this.

Sensitive to Sample Ordering: The order in which samples are presented can affect results, requiring careful shuffling.

Gradient Descent

Batch vs Mini-Batch vs Stochastic Gradient Descent

Mini-Batch

Variance Reduction: Averaging over B samples reduces gradient variance by a factor of B compared to pure SGD, while still maintaining some beneficial noise

- **Hardware Efficiency:** GPUs perform matrix operations in parallel. A batch size of 64 is nearly as fast as a batch size of 1 on modern hardware, giving essentially 64x speedup over SGD
- **Memory-Computation Tradeoff:** Batch size can be tuned to maximize GPU memory utilization without requiring the full dataset
- **Balances Exploration and Exploitation:** Enough noise to escape poor regions, enough signal to make consistent progress.

Gradient Descent

Gradient Descent vs Closed Form

Gradient Descent

- + Linear increase in m (# training data) and n (# features)
- + Generally applicable to multiple models
- + Guaranteed to reach global optimum for convex functions and appropriate learning rate
- Need to choose learning rate α and stopping conditions
- Need to choose optimization method (Adam, RMSProp etc..)
- Might get stuck in local optima / saddle point
- Needs feature scaling

$$m < n^3$$
$$m < n^2$$

Closed Form

$$\theta = (X^T X)^{-1} X^T Y$$

- + No parameter tuning
- + Gives global optimum
- Not generally applicable to any learning algorithm
- Slow computation - scales with n^3 where n is number of features

Summary and Next Class

- Summary
 - We saw how gradient descent works
 - We saw issues with gradient descent and how to address them
 - We saw multiple optimizers commonly used in gradient descent
 - We saw types of gradient descent (batch, mini-batch, stochastic)
- Next Class - Classification, cross-validation and logistic regression