

Gradient Descent: The Foundation of Machine Learning Optimization

From Taylor Series to Modern Deep Learning

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Mathematical Foundations

The Big Picture: Why Optimization Matters

Key Points:

Core ML Problem: Find best parameters θ^* for our model

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Important: The Challenge

Most ML problems have **no closed-form solution!**

Gradient Intuition: Climbing Mountains

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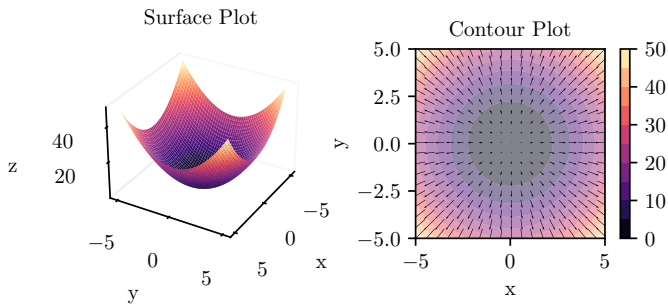
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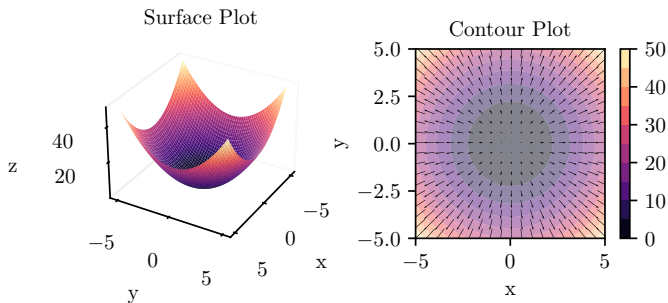
Key Points:

Key insight: Gradient points in direction of steepest **ascent**
So $-\nabla f$ points in direction of steepest **descent**!

Geometric Intuition with Level Sets



Geometric Intuition with Level Sets



Mathematical definition: $\nabla f(x, y) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix}$

Taylor Series: The Mathematical Foundation

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Example: The Core Idea

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Important: Taylor Series Power

Any smooth function can be approximated by polynomials!

Taylor Series: Starting with 1D

Taylor series expansion around point x_0 :

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 + \frac{1}{6}f'''(x_0)(x - x_0)^3 + \dots$$

(1)

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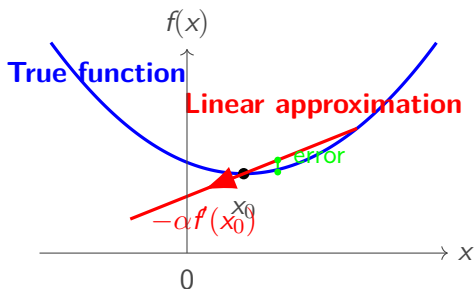
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- **Second-order:** adds $\frac{1}{2}f''(x_0)(x - x_0)^2$ (quadratic)

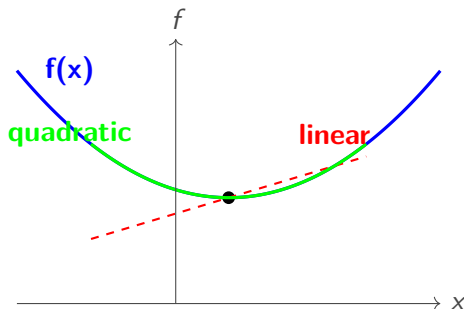
Visual: Tangent Line Approximation

Linear approximation: Use tangent line to approximate function locally



Key insight: Tangent gives best local linear approximation!

Adding Quadratic Term



Key Points:

Higher-order = better approximation, but 1st-order is often sufficient!

Concrete Example: $f(x) = \cos(x)$ at $x_0 = 0$

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Taylor approximations:

$$\text{0th order: } f(x) \approx 1 \quad (2)$$

$$\text{2nd order: } f(x) \approx 1 - \frac{x^2}{2} \quad (3)$$

$$\text{4th order: } f(x) \approx 1 - \frac{x^2}{2} + \frac{x^4}{24} \quad (4)$$

Extension to Multiple Variables

For function $f(\mathbf{x})$ around point \mathbf{x}_0 :

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T (\mathbf{x} - \mathbf{x}_0) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_0)^T \nabla^2 f(\mathbf{x}_0) (\mathbf{x} - \mathbf{x}_0) + \dots$$

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- $(\mathbf{x} - \mathbf{x}_0) = \Delta \mathbf{x}$ is the step vector

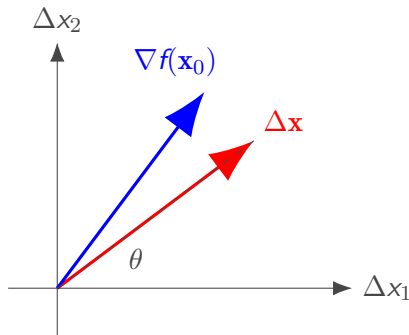
Understanding the Linear Term

The first-order term: $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}$ where $\Delta \mathbf{x} = \mathbf{x} - \mathbf{x}_0$

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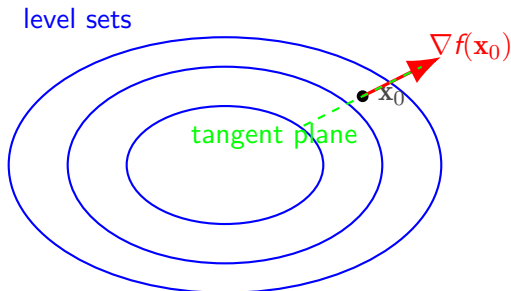
The first-order term: $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}$ where $\Delta \mathbf{x} = \mathbf{x} - \mathbf{x}_0$

For 2D case: $\Delta \mathbf{x} = \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} = \begin{bmatrix} x_1 - x_{0,1} \\ x_2 - x_{0,2} \end{bmatrix}$



Geometric interpretation: $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x} = |\nabla f| |\Delta \mathbf{x}| \cos \theta$

Visual: Multivariate Case with Level Sets



Key Points:

Gradient \perp level sets, tangent plane \perp gradient

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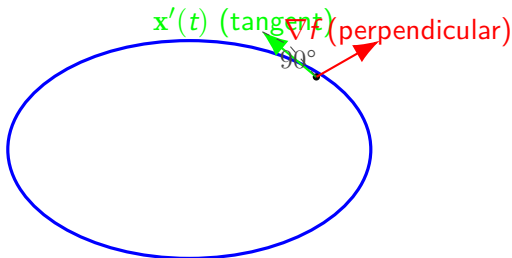
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From Taylor Series to Gradient Descent

The Key Question

Goal: Find $\Delta \mathbf{x}$ such that $f(\mathbf{x}_0 + \Delta \mathbf{x}) < f(\mathbf{x}_0)$

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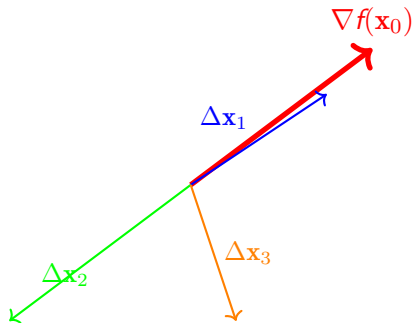
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Important: Vector Geometry Reminder

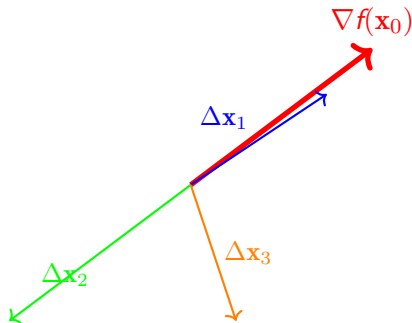
For vectors \mathbf{a}, \mathbf{b} : $\mathbf{a}^T \mathbf{b} = |\mathbf{a}| |\mathbf{b}| \cos(\theta)$

Most negative when: $\cos(\theta) = -1$ (opposite directions!)

Visual Derivation: Finding the Best Direction



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Dot products tell us the direction:

- $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}_1 > 0$ (increases function)
- $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}_2 < 0$ (decreases function - good!)
- $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}_3 < 0$ (decreases function)

The Optimal Choice: Direction of Steepest Descent

Definition: Optimal Choice

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Key Points:

This gives us the fundamental gradient descent step!

The Gradient Descent Update Rule

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- Guaranteed convergence for convex functions
- Foundation of modern machine learning

Pop Quiz #1: Understanding the Derivation

Answer this!

Consider $f(x) = x^2 + 2$ at point $x_0 = 2$.

Questions:

1. What is $f(x_0)$ and $f'(x_0)$?
2. Write the 1st-order Taylor approximation
3. If we take step $\Delta x = -0.1 \cdot f'(x_0)$, what is our new x ?
4. Will the function value decrease?

The Gradient Descent Algorithm

The Complete Algorithm

Algorithm Steps:

1. **Initialize:** Choose starting point θ_0

The Complete Algorithm

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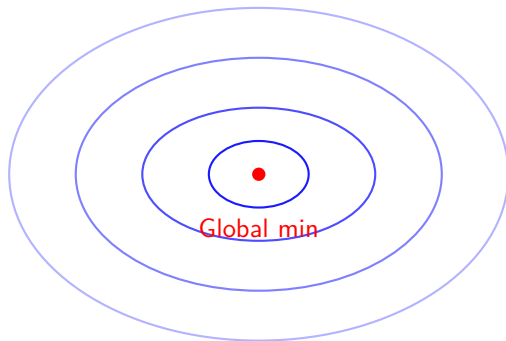
Key hyperparameter: Learning rate α

Key Points:

Learning rate selection is crucial for success!

Animated Gradient Descent in Action

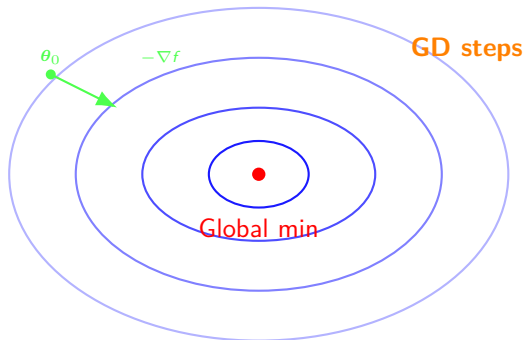
Watch how gradient descent finds the minimum:



Loss surface $f(\theta)$

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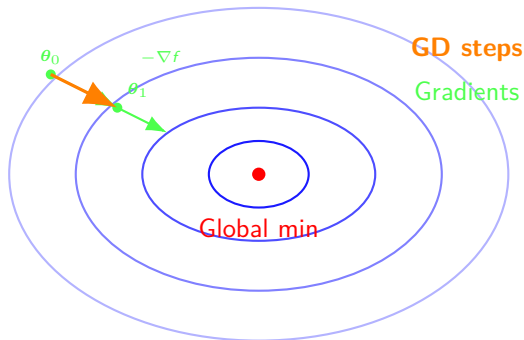
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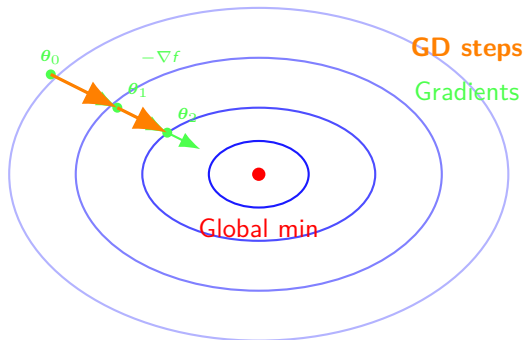
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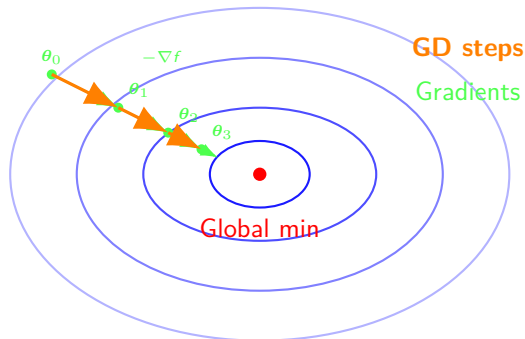
Watch how gradient descent finds the minimum:



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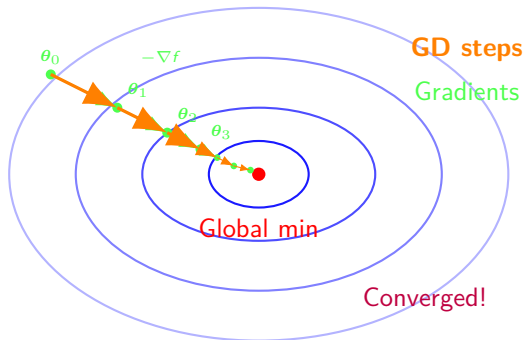
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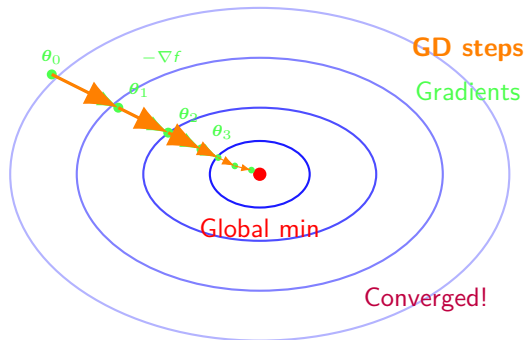
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Loss surface $f(\theta)$

Theorem: Key Insight

Steps get **smaller** as we approach the minimum because $|\nabla f| \rightarrow 0$!

Learning Rate: The Step Size

The learning rate α controls how big steps we take:

- **Too small α :** Slow convergence

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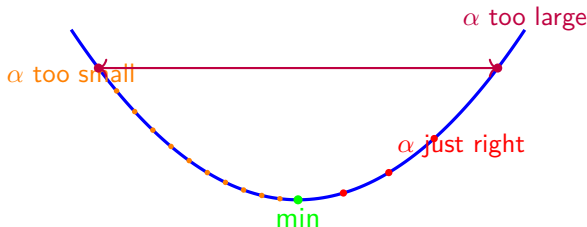
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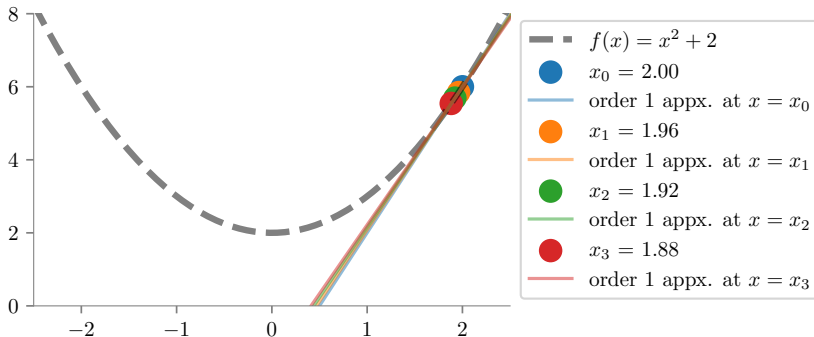
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Learning Rate Visualization: Too Small

$\alpha = 0.01$: **Convergence is slow but stable**

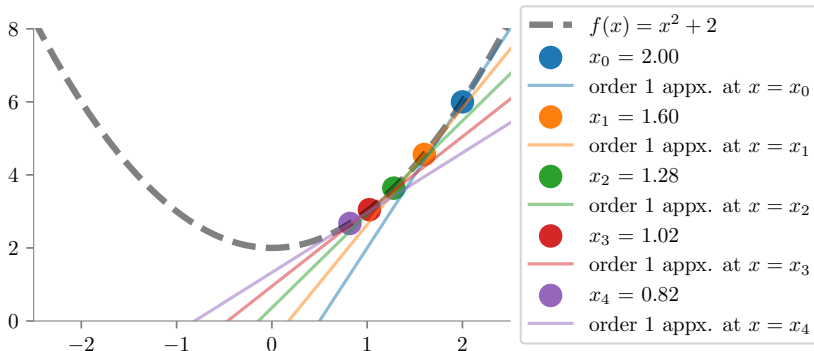


Important: Problem

Takes many iterations to reach the minimum. Computationally expensive!

Learning Rate: Just Right

$\alpha = 0.1$: **Good balance: Fast and stable convergence**

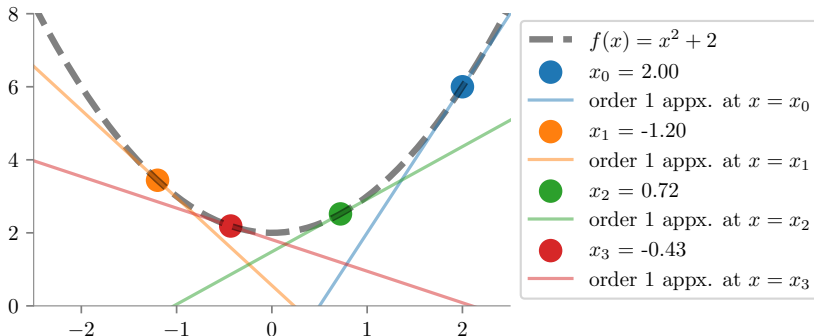


Key Points:

Perfect balance: Fast convergence + Stability

Learning Rate: Too Large

$\alpha = 0.8$: Fast but may overshoot

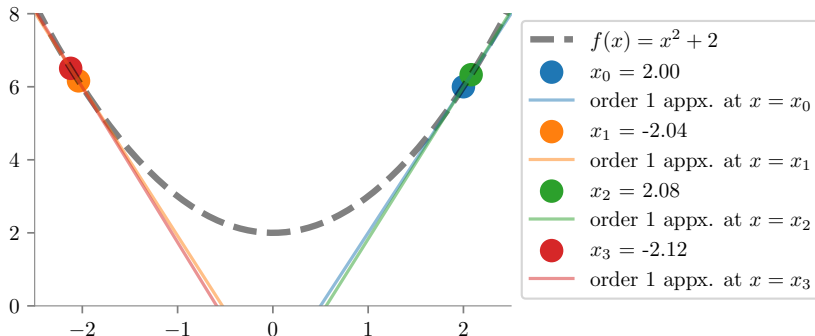


Important: Warning

Quick convergence but risk of instability. Watch out for oscillations!

Learning Rate: Disaster

$\alpha = 1.01$: **Divergence! Function values explode**



Important: Disaster Zone

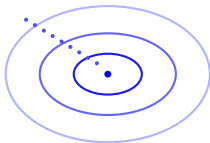
The algorithm diverges. Always monitor your loss curves!

Learning Rate Showdown: All Together

Compare different learning rates side by side:

Too Small

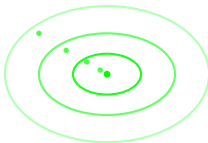
$$\alpha = 0.01$$



Slow but stable

Perfect

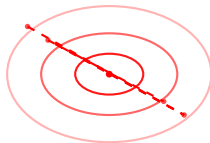
$$\alpha = 0.1$$



Just right!

Too Large

$$\alpha = 0.8$$



Oscillating!

Theorem: Goldilocks Principle

Not too small, not too large - learning rate must be **just right**!

Key Points:

Gradient Descent for Linear Regression

Linear Regression: Our First Application

Problem: Learn $y = \theta_0 + \theta_1 x$ from data

x	y
1	1
2	2
3	3

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Cost Function (Mean Squared Error):

$$\text{MSE}(\theta_0, \theta_1) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)^2$$

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Goal: $(\theta_0^*, \theta_1^*) = \arg \min_{\theta_0, \theta_1} \text{MSE}(\theta_0, \theta_1)$

Computing Gradients for Linear Regression

We need: $\nabla \text{MSE} = \begin{bmatrix} \frac{\partial \text{MSE}}{\partial \theta_0} \\ \frac{\partial \text{MSE}}{\partial \theta_1} \end{bmatrix}$

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Let's compute each partial derivative:

$$\frac{\partial \text{MSE}}{\partial \theta_0} = \frac{2}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)(-1) \quad (7)$$

$$= -\frac{2}{n} \sum_{i=1}^n \epsilon_i \quad (8)$$

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$$\frac{\partial \text{MSE}}{\partial \theta_1} = \frac{2}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)(-x_i) \quad (9)$$

$$= -\frac{2}{n} \sum_{i=1}^n \epsilon_i x_i \quad (10)$$

where $\epsilon_i = y_i - \hat{y}_i$ is the residual.

Step-by-Step Example: Setup

Initial values: $\theta_0 = 4, \theta_1 = 0$, **Learning rate:** $\alpha = 0.1$

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Parameter updates:

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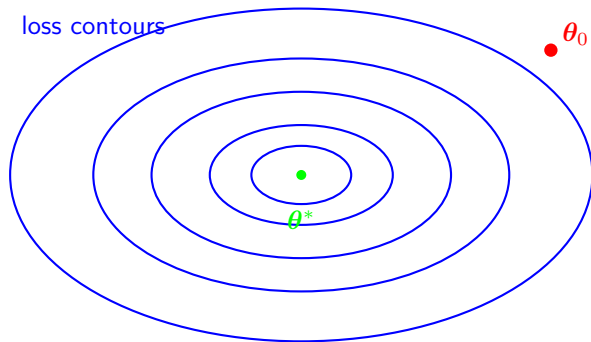
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Key Points:

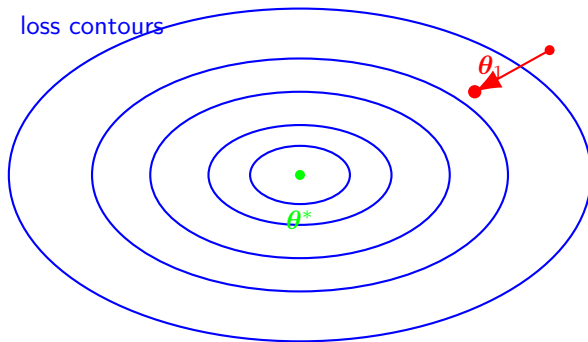
New parameters: $(\theta_0, \theta_1) = (3.6, -0.67)$

We moved closer to the true solution $(0, 1)$!

Visual Journey: Gradient Descent in Action



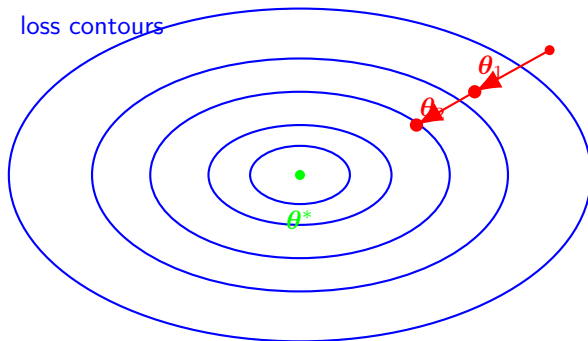
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Key Points:

Steps get smaller as we approach minimum (gradient magnitude decreases)!

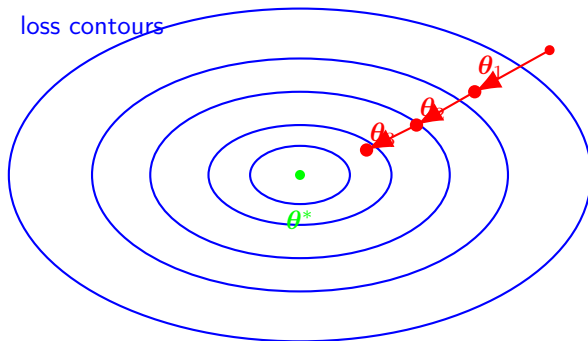
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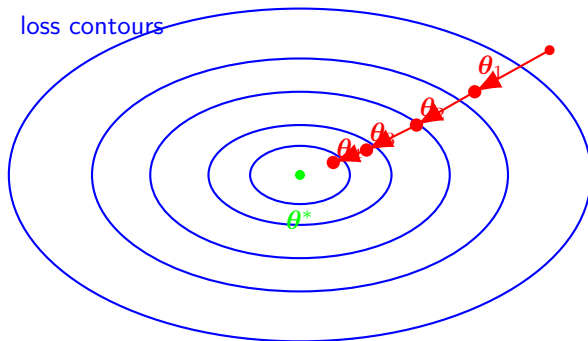
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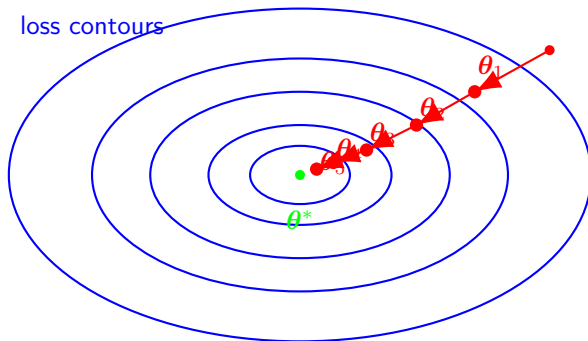
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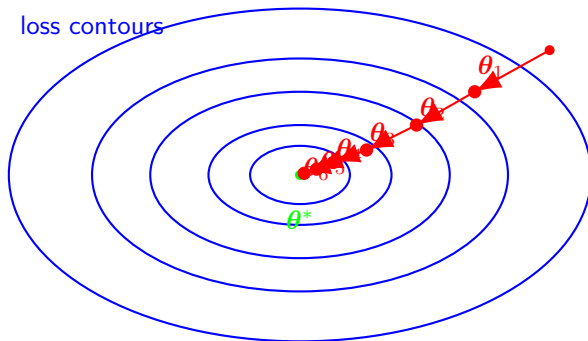
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Variants of Gradient Descent

The Gradient Descent Family

Three main variants based on data usage:

Definition: Batch Gradient Descent

Use **all** training data to compute each gradient

Definition: Stochastic Gradient Descent (SGD)

Use **one** sample to compute each gradient

Definition: Mini-batch Gradient Descent

Use a **small batch** of samples to compute each gradient

Comparison: Batch vs SGD vs Mini-batch

Method	Data/update	Updates/epoch	Convergence
Batch GD	n (all)	1	Smooth
SGD	1	n	Noisy
Mini-batch	b	n/b	Balanced

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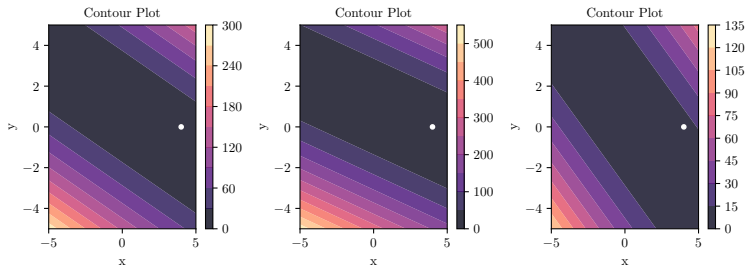
Key Points:

Standard: Mini-batch GD (batches 32-256)

- Balance of stability and efficiency
- Parallel computation on GPUs
- Better estimates than pure SGD

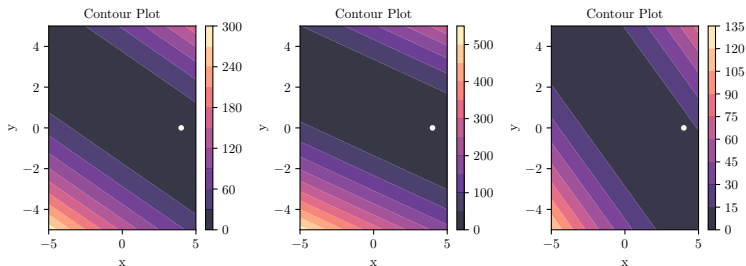
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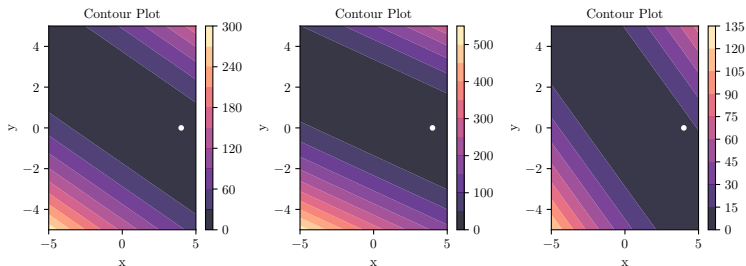


Trade-offs:

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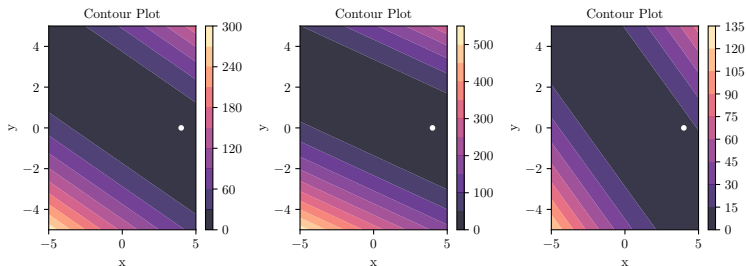


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Trade-offs:

- **Pro:** Fast updates, can escape local minima
- **Con:** Noisy convergence, may not reach exact minimum
- **Key insight:** Noise can be beneficial for non-convex problems!

Mathematical Properties

Step 1: The Modern ML Computational Challenge

Real-world machine learning problems:

- **Massive datasets:** $n = 1,000,000+$ examples (ImageNet, web data)

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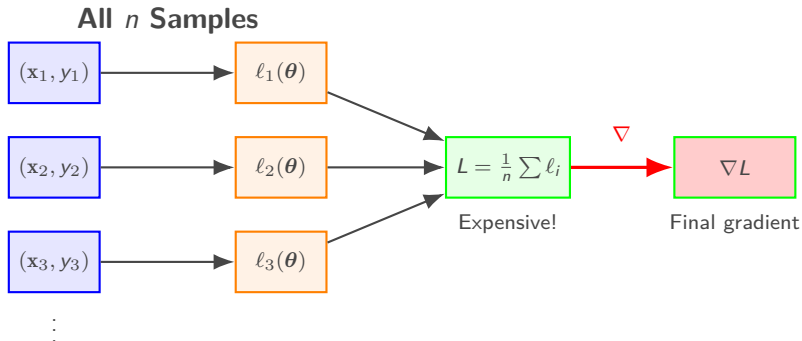
Important: The Problem

Computing $f(\mathbf{x}_i; \theta)$ for ALL n samples is too slow!

Need: Fast approximation that still gives good direction

Step 2: Computational Graph - Can We Break This?

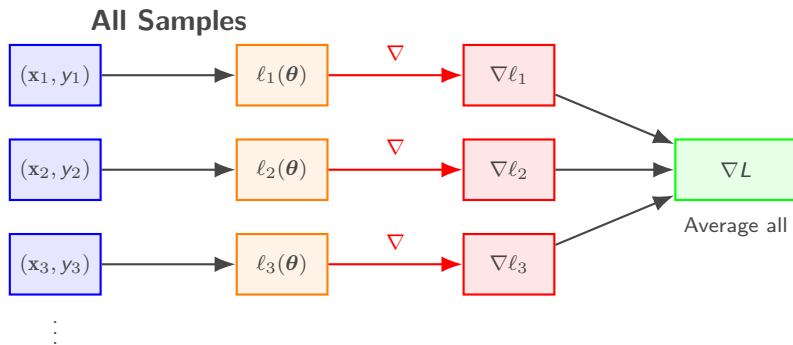
Current approach: Sum first, then take gradient



Key Points:

Problem: Computing losses for all n samples is expensive!

Step 3: The Linearity Insight - What If We Flip the Order?



Theorem: Linearity of Gradient

$$\nabla L = \frac{1}{n} \sum_{i=1}^n \nabla \ell_i$$

Step 4: The Mathematical Equivalence - Linearity of Gradient

Mathematical equivalence:

$$\nabla L(\boldsymbol{\theta}) = \nabla \left(\frac{1}{n} \sum_{i=1}^n \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) \right) \quad (11)$$

$$= \frac{1}{n} \sum_{i=1}^n \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) \quad (12)$$

Key Points:

This linearity property is the foundation for all gradient-based optimization!

Step 5: SGD as Unbiased Estimator - The Solution

SGD solution: Sample one gradient instead of all n !

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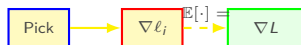
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Estimate: $\nabla \tilde{L}(\boldsymbol{\theta}) = \nabla \ell(f(\mathbf{x}_j; \boldsymbol{\theta}), y_j)$ for random j

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SGD solution: Sample one gradient instead of all n !

Estimate: $\nabla \tilde{L}(\theta) = \nabla \ell(f(\mathbf{x}_j; \theta), y_j)$ for random j



Important: Unbiased Property

$\mathbb{E}[\nabla \tilde{L}(\theta)] = \nabla L(\theta)$ - correct direction on average!

The Unbiased Property: Mathematical Proof

Theorem: SGD Unbiased Estimator Property

$$\mathbb{E}[\nabla \tilde{L}(\boldsymbol{\theta})] = \nabla L(\boldsymbol{\theta})$$

The Unbiased Property: Mathematical Proof

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$$\mathbb{E}[\nabla \tilde{L}(\boldsymbol{\theta})] = \mathbb{E}[\nabla \ell(f(\mathbf{x}_j; \boldsymbol{\theta}), y_j)] \quad (13)$$

$$= \sum_{i=1}^n P(\text{sample } i) \cdot \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) \quad (14)$$

$$= \sum_{i=1}^n \frac{1}{n} \cdot \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) \quad (15)$$

$$= \frac{1}{n} \sum_{i=1}^n \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) \quad (\text{linearity of expectation}) \quad (16)$$

$$= \nabla L(\boldsymbol{\theta}) \quad (\text{from previous slide}) \quad (17)$$

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Key Points:

Key insight: On average, SGD points in the correct direction!

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- Individual SGD steps may be “wrong”
- But they average to the correct direction over time
- Theoretical guarantee that justifies SGD’s effectiveness

Why Unbiasedness Matters

Key Points:

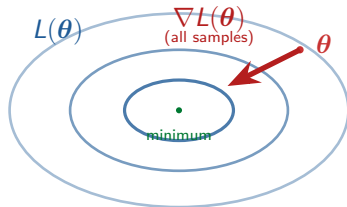
Key insight: On average, SGD points in the correct direction!

Practical implications:

- Individual SGD steps may be “wrong”
- But they average to the correct direction over time
- Theoretical guarantee that justifies SGD’s effectiveness
- The “noise” helps escape local minima in non-convex problems

Visual Intuition 1: Overall Loss Surface

True loss function using all data points:

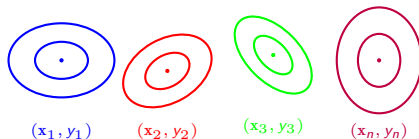


Key Points:

Gradient uses ALL data points for true direction

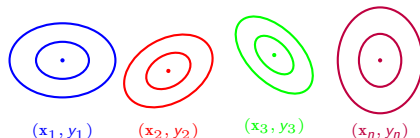
Visual Intuition 2: Individual Sample Loss Surfaces

Loss for individual data points (different shapes):



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Important: Key Observation

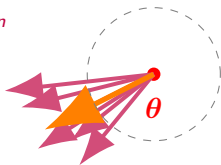
Each individual gradient points in a **different direction** - some variation!

Visual Intuition 3: Averaging Individual Gradients

The magic: Average of individual gradients = True gradient

Individual gradients
 $\nabla \ell_1, \nabla \ell_2, \dots, \nabla \ell_n$

Variance around
true direction



Average gradient
$$\frac{1}{n} \sum_{i=1}^n \nabla \ell_i = \nabla L(\theta)$$

Theorem: Visual Proof of Unbiasedness

Even though individual gradients vary, their average equals the true gradient!

Visual Intuition 4: SGD Sampling Process

SGD randomly picks one gradient at a time:

All possible
individual gradients

True average
 $\nabla L(\theta)$



SGD picks one
randomly: $\nabla \ell_j$

Key Points:

Key insight: Sometimes SGD goes "wrong" direction, but on average it's correct!

Why Unbiasedness Matters in Practice

Why Unbiasedness Matters in Practice

Example: Intuitive Analogy

Like asking random people for directions:

- Each person's answer might be slightly off
- But if there's no systematic bias, the average is correct
- SGD does the same with gradient estimates!

Computational Complexity

GD vs Normal Equation: Complexity

For linear regression:

Important: Normal Equation

$$\hat{\theta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Time: $\mathcal{O}(d^2 n + d^3)$

Space: $\mathcal{O}(d^2)$

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Key Points: Gradient Descent

$$\theta_{t+1} = \theta_t - \alpha \mathbf{X}^T (\mathbf{X} \theta_t - \mathbf{y})$$

Time: $\mathcal{O}(T \cdot nd)$ for T iterations

Space: $\mathcal{O}(nd)$

When to Use Which Method

Key Points:

Modern ML: Gradient descent dominates due to:

- High-dimensional data (d very large)
- Non-linear models (no normal equation exists)
- Large datasets (n very large)

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- **Online learning:** Only gradient descent works

Advanced Topics and Extensions

Beyond Basic Gradient Descent

Modern optimizers improve upon vanilla GD:

- **Momentum:** $\mathbf{v}_{t+1} = \beta \mathbf{v}_t + (1 - \beta) \mathbf{g}_t$

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- Reduce oscillations in narrow valleys

Gradient Descent in Deep Learning

Key Points:

Every deep learning framework uses gradient descent variants!

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- **GPU acceleration:** Parallel mini-batch processing
- **Mixed precision:** 16-bit + 32-bit arithmetic

Practical Considerations

Learning Rate Selection Strategies

Common approaches:

- **Grid search:** Try $\{0.001, 0.01, 0.1, 1.0\}$

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- Oscillating loss \rightarrow Try momentum or smaller α

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When to stop training?

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Key Points:

Best practice: Use multiple criteria + validation performance

Common Pitfalls

Important: Pitfall 1: Poor Initialization

Problem: Bad starting points

Solution: Xavier/He initialization

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Problem: Bad starting points

Solution: Xavier/He initialization

Important: Pitfall 2: Wrong Learning Rate

Problem: Divergence or slow convergence

Solution: Learning rate schedules, adaptive optimizers

Important: Pitfall 3: Poor Feature Scaling

Problem: Different scales cause poor convergence

Solution: Standardize features: $(x - \mu)/\sigma$

Summary and Key Takeaways

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- **Geometric intuition:** Steepest descent direction
- **Algorithm variants:** Batch, SGD, mini-batch
- **Theoretical properties:** Unbiased estimator guarantees
- **Practical wisdom:** Learning rates, scaling, diagnostics

From Theory to Practice

Next steps for mastery:

- Implement gradient descent from scratch

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Key Points:

Master gradient descent first - it's the foundation for everything else!

Final Pop Quiz #2

Answer this!

True or False?

1. SGD always converges faster than batch GD
2. Learning rates should decrease during training
3. SGD gradient estimates are unbiased
4. Normal equation always beats gradient descent
5. GD guarantees global minimum for any function

Deep Dive: Advanced Theory

For comprehensive mathematical analysis:

Important: Reference Materials

- SGD.pdf: Detailed convergence proofs
- Florian's estimators:
<https://florian.github.io/estimators/>
- Interactive notebooks for hands-on practice

Pop Quiz Solutions

Quiz #1 Solutions:

1. $f(2) = 6, f'(2) = 4$
2. $f(x) \approx 6 + 4(x - 2)$
3. New $x = 2 - 0.1 \times 4 = 1.6$
4. Yes, function decreases!

Pop Quiz Solutions

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4. Yes, function decreases!

Quiz #2 Solutions:

1. False - SGD faster per epoch, may need more epochs
2. True - schedules often improve convergence
3. True - key theoretical property
4. False - only for linear problems, small d
5. False - only local minima; global for convex only

Thank You!

Questions?

Next: Advanced Optimization Techniques

Practice: Implement GD for your favorite ML model!