Gradient Descent: The Foundation of Machine Learning Optimization

From Taylor Series to Modern Deep Learning

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Important: The Challenge

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

Gradient Intuition: Climbing Mountains

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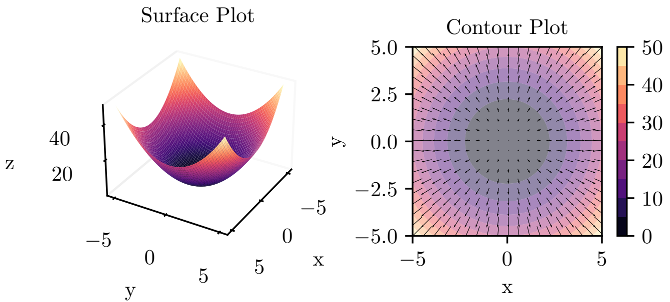
Key insight: Gradient points in direction of steepest ascent
So $-\nabla f$ points in direction of steepest descent!

Geometric Intuition with Level Sets



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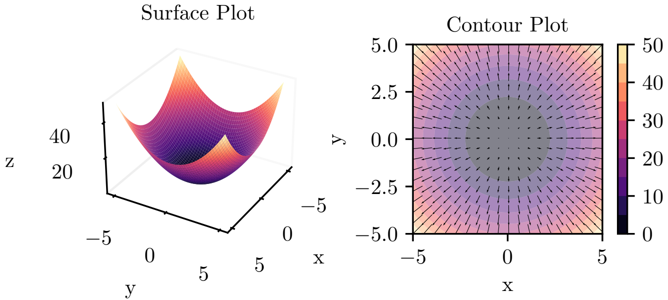

Mathematical definition: $\nabla f(x,y) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix}$

Taylor Series: The Mathematical Foundation

Why Taylor Series? The Key Insight

Example: The Core Idea

If we can't solve $\min f(\mathbf{x})$ exactly, let's approximate $f(\mathbf{x})$ locally!

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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:

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

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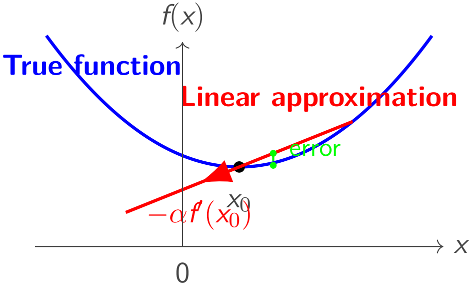
- **Second-order:** adds $\frac{1}{2}f''(x_0)(x - x_0)^2$ (quadratic)

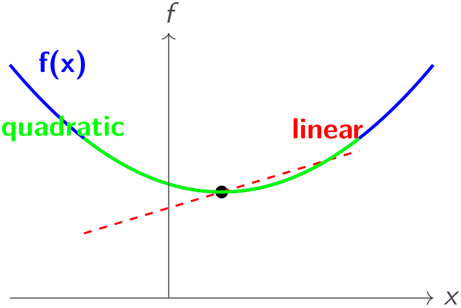
Visual: Tangent Line Approximation

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 $x_0 = 0$

Let's compute the derivatives:

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Taylor approximations:

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

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

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

Extension to Multiple Variables

For function $f(\mathrm{x})$ around point x_0:

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T(\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \nabla^2 f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) + \dots \quad (5)$$

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

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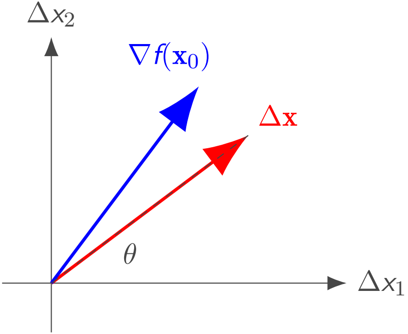
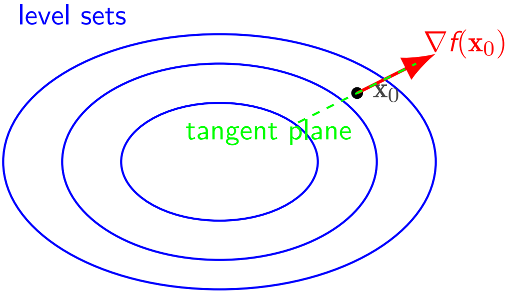
For 2D case: $\Delta\mathbf{x} = \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} = \begin{bmatrix} x_1 - x_{0,1} \\ x_2 - x_{0,2} \end{bmatrix}$



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

Why is Gradient Perpendicular to Level Sets?

Mathematical insight: Level set $= \{\mathbf{x} : f(\mathbf{x}) = c\}$ for constant c

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On level sets: Moving along the level curve keeps $f(\mathbf{x})$ constant

- If $\mathbf{x}(t)$ parameterizes level curve: $f(\mathbf{x}(t)) = c$ (constant)
- Taking derivative: $\frac{d}{dt} f(\mathbf{x}(t)) = \nabla f(\mathbf{x}) \cdot \mathbf{x}'(t) = 0$

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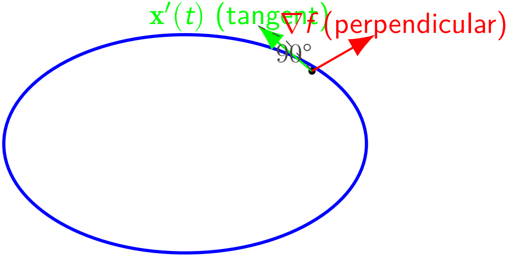

From Taylor Series to Gradient Descent

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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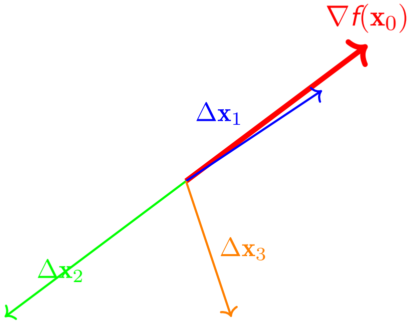
Important: Vector Geometry Reminder

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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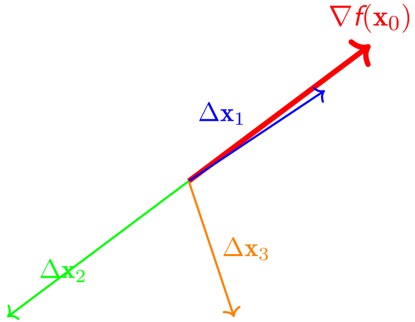

Dot products tell us the direction:

- $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}_1 > 0$ (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

This gives us the gradient descent update:

$$\mathbf{x}_{\mathsf{new}} = \mathbf{x}_{\mathsf{old}} - \alpha \nabla f(\mathbf{x}_{\mathsf{old}})$$

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- Uses only first derivatives (gradients)
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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 $\boldsymbol{\theta}_0$

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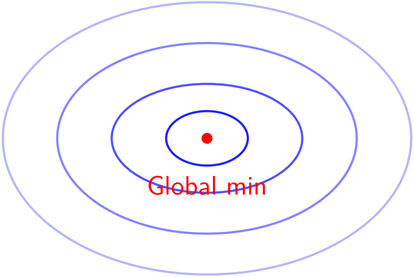
Key hyperparameter: Learning rate α

Key Points:

Learning rate selection is crucial for success!

Animated Gradient Descent in Action

Watch how gradient descent finds the minimum:



Loss surface $f(\boldsymbol{\theta})$

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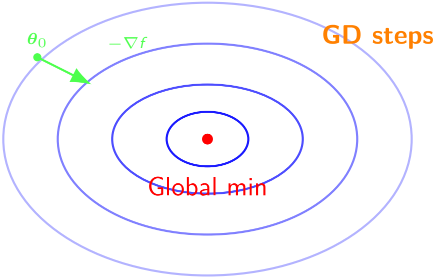

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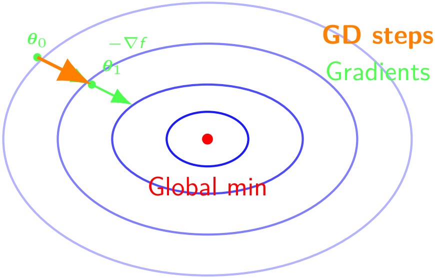

Loss surface $f(\boldsymbol{\theta})$

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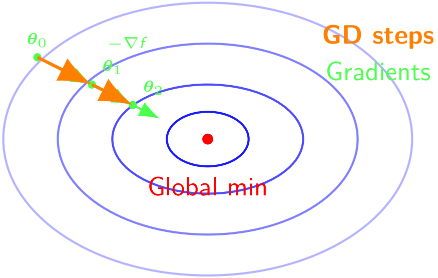

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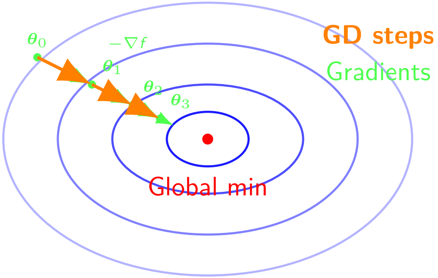

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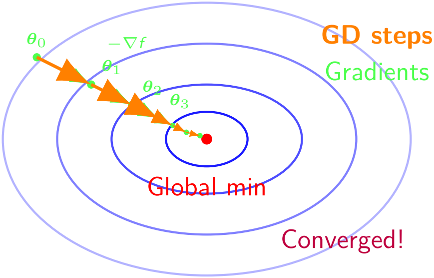

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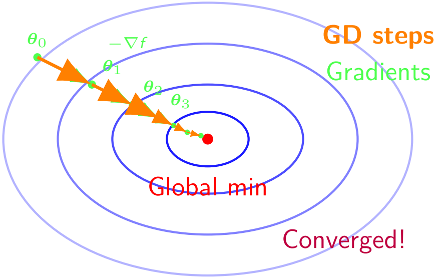

Loss surface $f(\boldsymbol{\theta})$

Theorem: Key Insight

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

Learning Rate: The Step Size

The learning rate α controls how big steps we take:

- **Too small α:** Slow convergence

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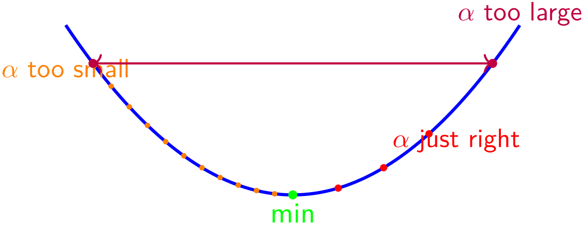
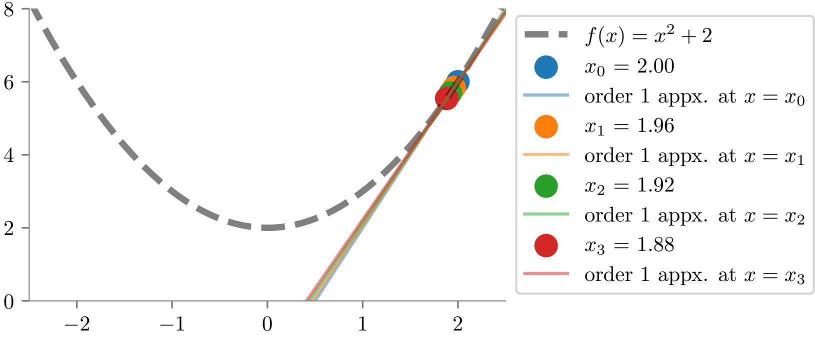


Learning Rate Visualization: Too Small

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

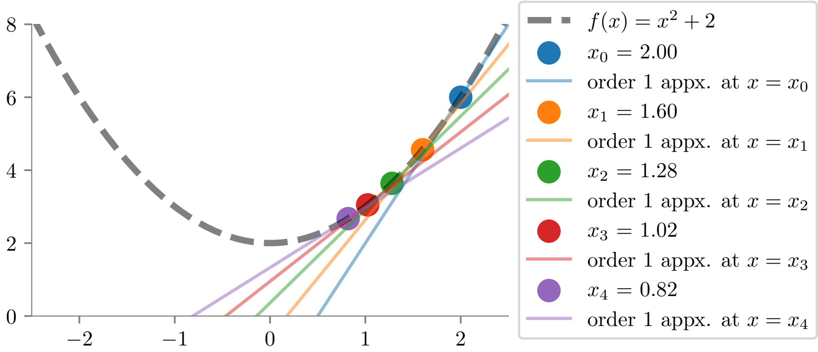


Important: Problem

Takes many iterations to reach the minimum. Computationally expensive!

Learning Rate: Just Right

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

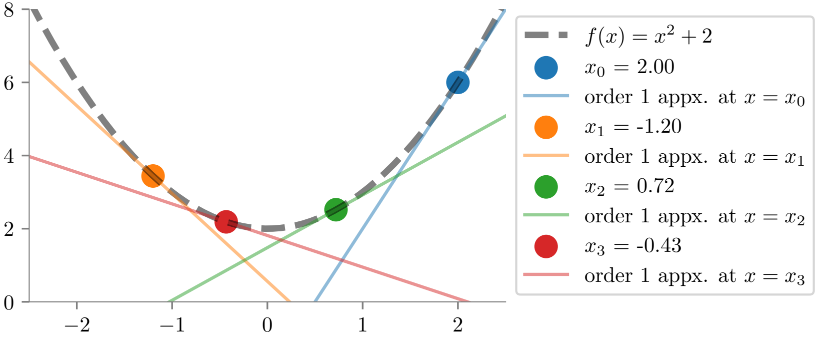


Key Points:

Perfect balance: Fast convergence + Stability

Learning Rate: Too Large

$\alpha = 0.8$: Fast but may overshoot

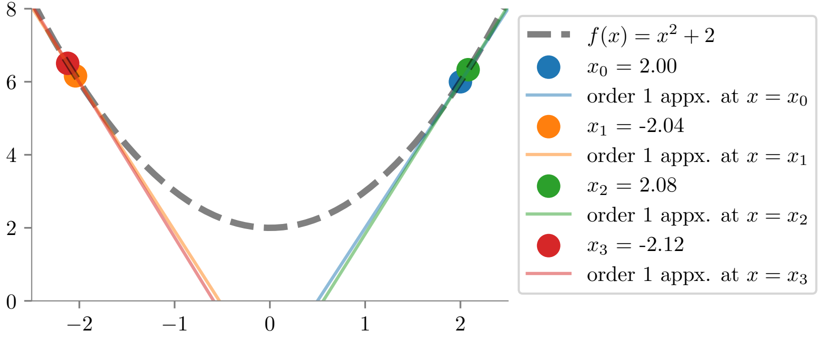


Important: Warning

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

Learning Rate: Disaster

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

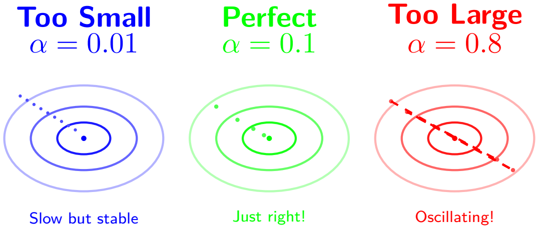


Important: Disaster Zone

The algorithm diverges. Always monitor your loss curves!

Learning Rate Showdown: All Together

Compare different learning rates side by side:



Theorem: Goldilocks Principle

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

Key Points:

Pro tip: Start with $\alpha \in [0.01, 0.1]$ and adjust based on loss curves

Gradient Descent for Linear Regression

Linear Regression: Our First Application

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

x	**y**
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2	2
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Cost Function (Mean Squared Error):

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

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

Computing Gradients for Linear Regression

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

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Let's compute each partial derivative:

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

$$= -\frac{2}{n} \sum_{i=1}^{n} \epsilon_i \tag{8}$$

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

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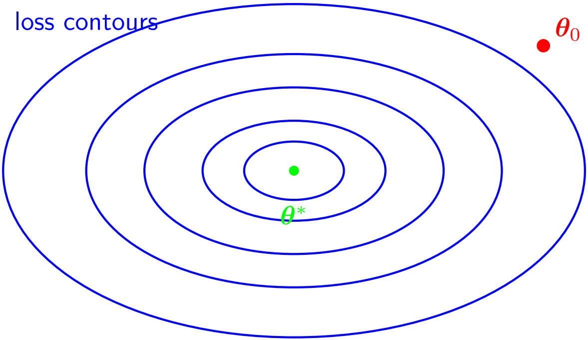
Key Points:

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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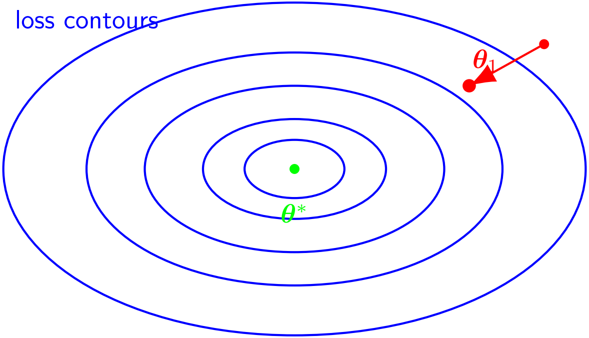

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Steps get smaller as we approach minimum (gradient magnitude decreases)!

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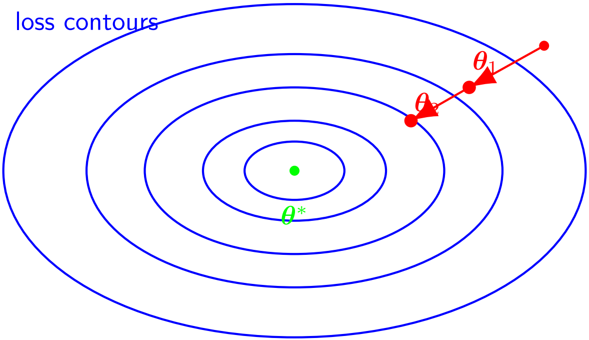

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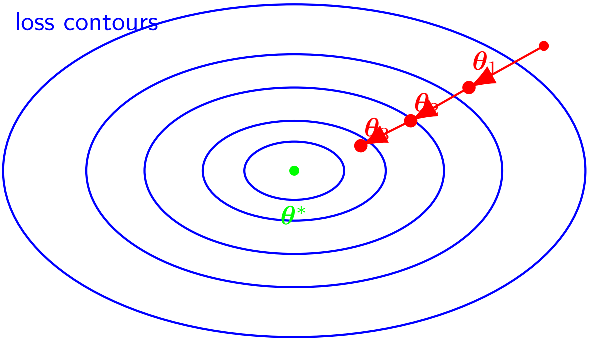

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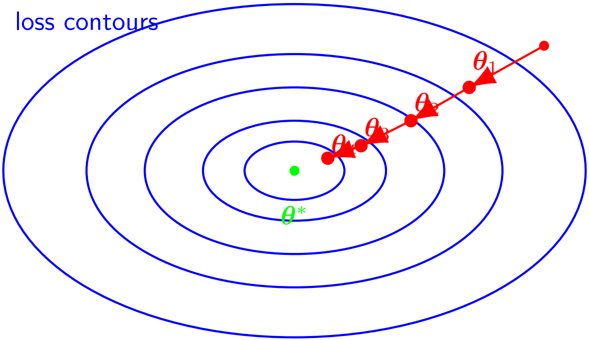

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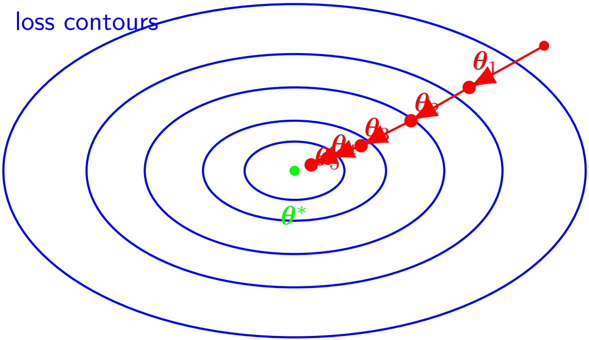

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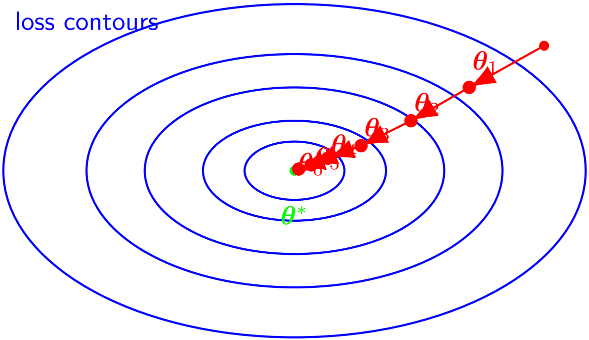

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Variants of Gradient Descent

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

SGD Step-by-Step Example: Setup

Same data, same initial values: $\theta_0 = 4, \theta_1 = 0$, $\alpha = 0.1$

x	**y**
1	1
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SGD: Use ONE sample per update

- **Iteration 1:** Pick sample $(\mathbf{x}_1, y_1) = (1, 1)$

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Compute gradients using ONLY sample 1:

- $\frac{\partial \ell_1}{\partial \theta_0} = -2\epsilon_1 = -2(-3) = 6$

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Key Points:

After sample 1: $(\theta_0, \theta_1) = (3.4, -0.6)$
Compare to batch GD: $(3.6, -0.67)$ - different path!

SGD Step-by-Step Example: Second Sample

Iteration 2: Pick sample $(\mathbf{x}_2, y_2) = (2, 2)$

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Gradients for sample 2:

- $\frac{\partial \ell_2}{\partial \theta_0} = -2(-0.2) = 0.4$

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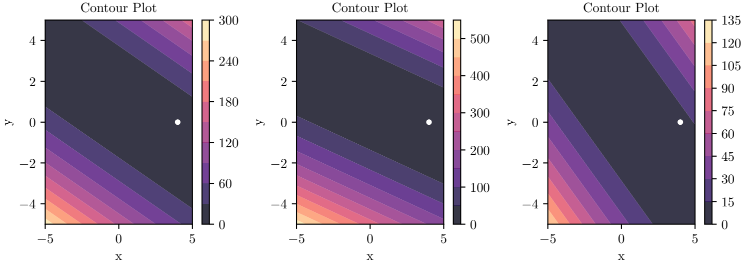
SGD: The Noisy Path

SGD uses one sample at a time for updates



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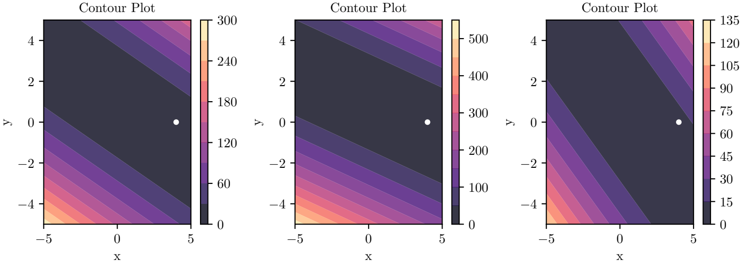

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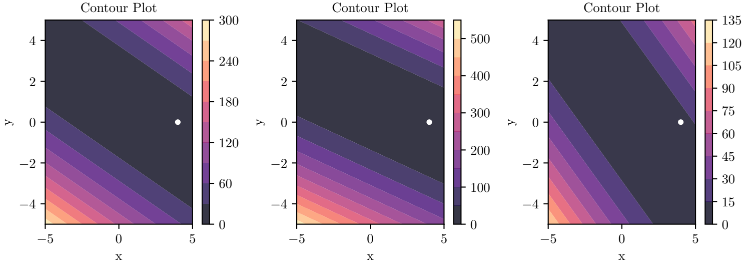

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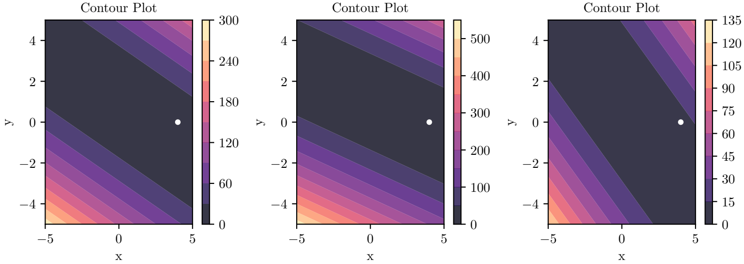

Trade-offs:

- **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:

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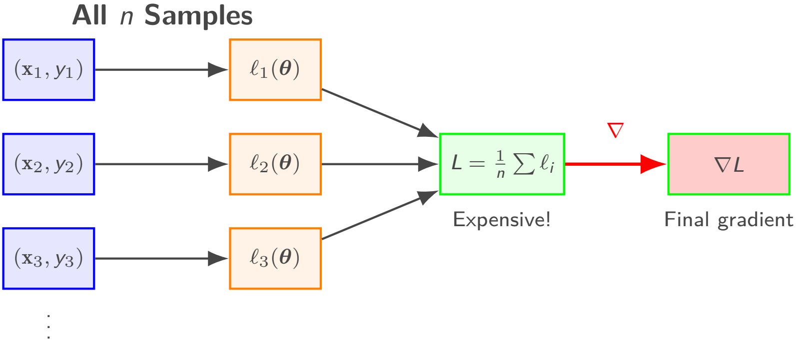
Important: The Problem

Computing $f(\mathbf{x}_i; \boldsymbol{\theta})$ for ALL n samples is too slow!
Need: Fast approximation that still gives good direction

Step 2: Computational Graph - Can We Break This?

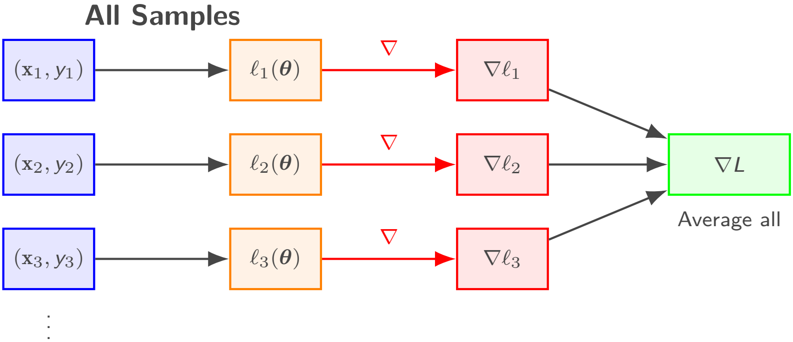
Current approach: Sum first, then take gradient



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:

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

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

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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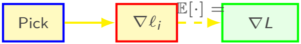

Important: Unbiased Property

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

The Unbiased Property: Mathematical Proof

Theorem: SGD Unbiased Estimator Property

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$$\begin{aligned}
\mathbb{E}[\nabla \tilde{L}(\boldsymbol{\theta})] &= \mathbb{E}\left[\nabla \ell(f(\mathbf{x}_j; \boldsymbol{\theta}), y_j)\right] && (13) \\
&= \sum_{i=1}^{n} P(\text{sample } i) \cdot \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) && (14) \\
&= \sum_{i=1}^{n} \frac{1}{n} \cdot \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) && (15) \\
&= \frac{1}{n} \sum_{i=1}^{n} \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) \qquad \text{(linearity of expectation)} && (16) \\
&= \nabla L(\boldsymbol{\theta}) \qquad \text{(from previous slide)} && (17)
\end{aligned}$$

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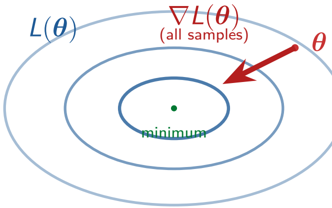
Practical implications:

- 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:

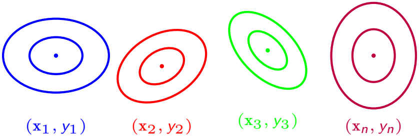


Key Points:

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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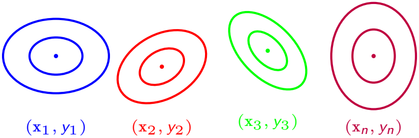
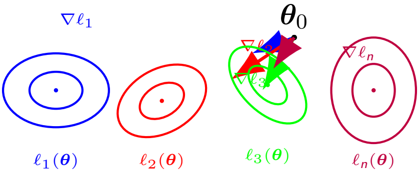


Important: Key Observation

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

Visual Intuition 3: Gradients from Same Starting Point

What happens when we evaluate gradients from the same point θ_0?



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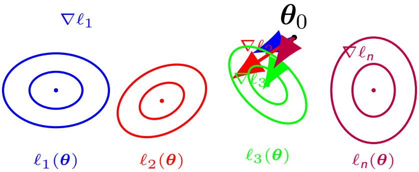
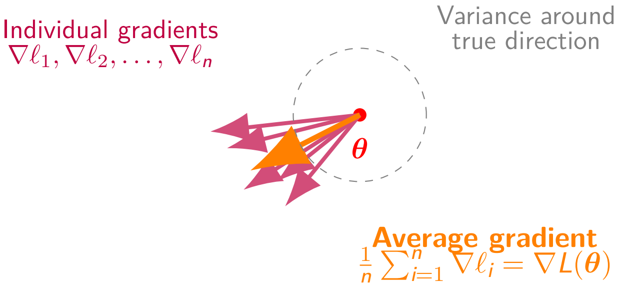


Theorem: Key Insight

From the **same point**, each loss surface gives a **different gradient direction**!

Visual Intuition 4: Averaging Individual Gradients

The magic: Average of individual gradients = True gradient

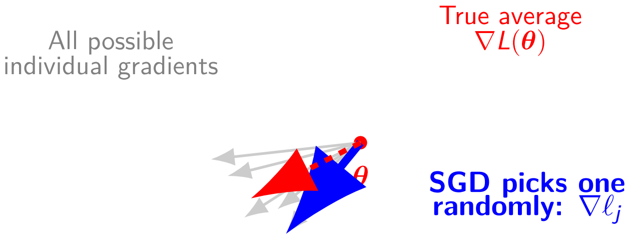


Theorem: Visual Proof of Unbiasedness

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:



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

Normal Equation: The Direct Approach

For linear regression, we can solve directly:

Definition: Normal Equation

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

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Key Points:

One computation gives the optimal $\hat{\boldsymbol{\theta}}$ - no learning rate needed!

Normal Equation: Step-by-Step Complexity

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Normal Equation: Matrix Inversion Cost

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Important: Memory Requirements

Space: Need to store $\mathbf{X}^T\mathbf{X}$ matrix
Size: $d \times d = d^2$ elements $\Rightarrow \mathcal{O}(d^2)$ space

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Key Points:

Total time: $\mathcal{O}(d^2 n + d^3)$ dominated by $\mathcal{O}(d^3)$ when d large

Gradient Descent: Iterative Approach

GD update rule for linear regression:

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Key Points:

Each iteration requires gradient computation - let's analyze the cost!

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Step 2: Compute $\mathbf{X}\boldsymbol{\theta} - \mathbf{y}$

- Element-wise subtraction of $n \times 1$ vectors

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- **Cost:** $\mathcal{O}(nd)$ operations

Step 2: Compute $\mathbf{X}\boldsymbol{\theta} - \mathbf{y}$

- Element-wise subtraction of $n \times 1$ vectors
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Key Points:

Per iteration: $\mathcal{O}(nd + n + nd + d) = \mathcal{O}(nd)$

GD vs Normal Equation: Final Complexity Comparison

Important: Normal Equation

$\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
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$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \alpha\mathbf{X}^T(\mathbf{X}\boldsymbol{\theta}_t - \mathbf{y})$
Time: $\mathcal{O}(T \cdot nd)$ for T iterations
Space: $\mathcal{O}(nd)$
Iterations: T (approximate solution)

GD vs Normal Equation: Final Complexity Comparison

Theorem: Trade-off

Normal equation: Fast but scales poorly with d
Gradient descent: Slower but scales better with d

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)
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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

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Key Points:

Every deep learning framework uses gradient descent variants!

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- **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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- Very slow progress $\rightarrow$ α too low
- Oscillating loss $\rightarrow$ Try momentum or smaller α

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Key Points:

Best practice: Use multiple criteria + validation performance

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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

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

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- 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!

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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!