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 $\boldsymbol{\theta}^*$ 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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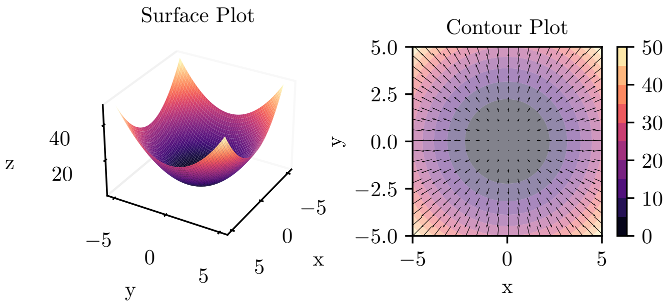
Key insight: Gradient points in direction of steepest ascent
So $-\nabla f$ points in direction of steepest descent!

Geometric Intuition with Level Sets



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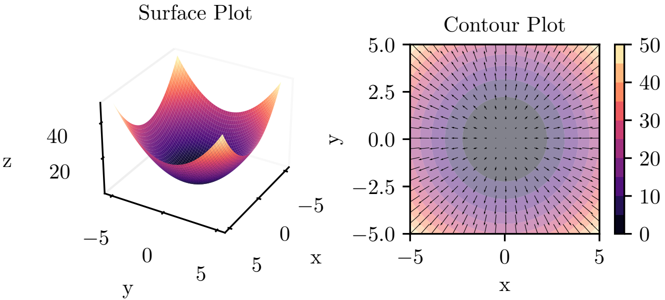

Mathematical definition: $\nabla f(x, y) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix}$

Taylor Series: The Mathematical Foundation

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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:

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

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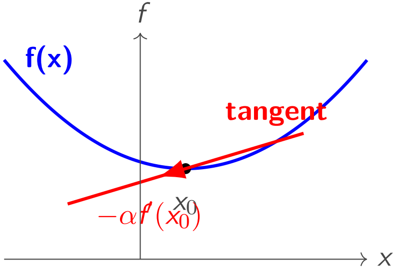
- **Second-order:** adds $\frac{1}{2}f''(x_0)(x - x_0)^2$ (quadratic)

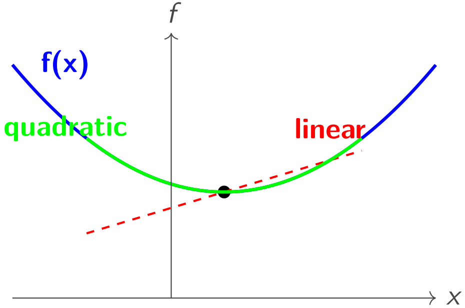
Visual: Tangent Line Approximation



Key Points:

Linear approximation gives us the direction to move!

Adding Quadratic Term



Key Points:

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

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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:

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

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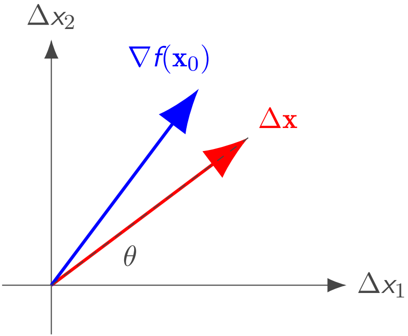
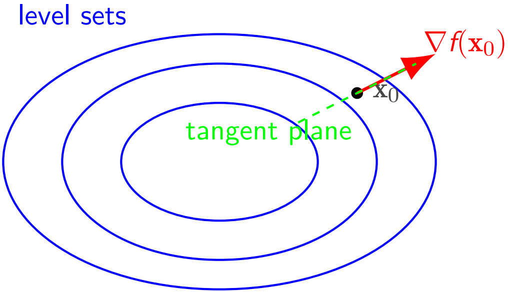
For 2D case: $\Delta\mathbf{x} = \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} = \begin{bmatrix} x_1 - x_{0,1} \\ x_2 - x_{0,2} \end{bmatrix}$



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

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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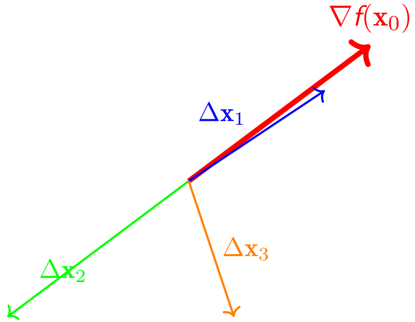
Important: Vector Geometry Reminder

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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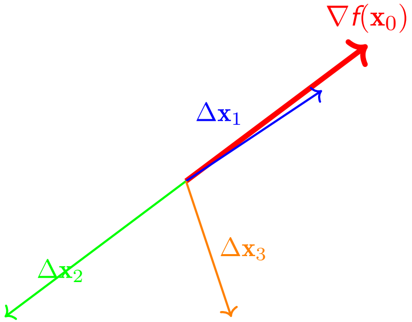

Dot products tell us the direction:

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

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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:

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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 $\boldsymbol{\theta}_0$

The Complete Algorithm

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Key hyperparameter: Learning rate α

Key Points:

Learning rate selection is crucial for success!

Learning Rate: The Step Size

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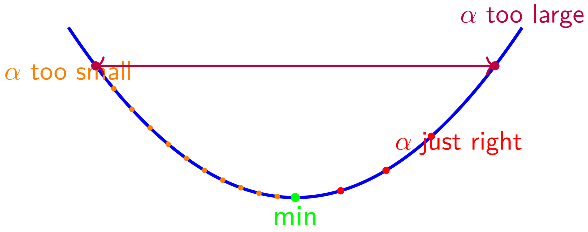
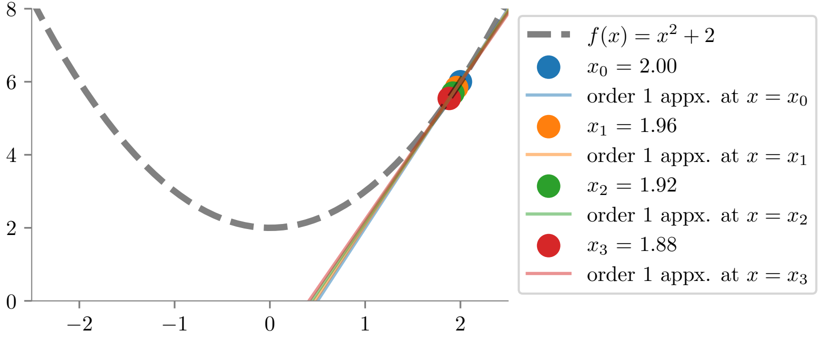


Learning Rate Visualization: Too Small

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

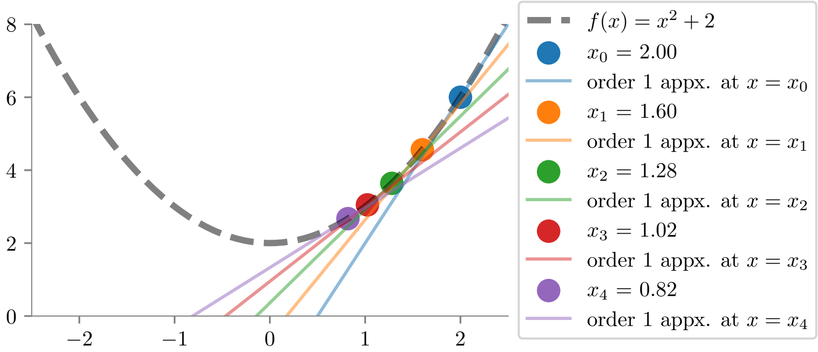


Important: Problem

Takes many iterations to reach the minimum. Computationally expensive!

Learning Rate: Just Right

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

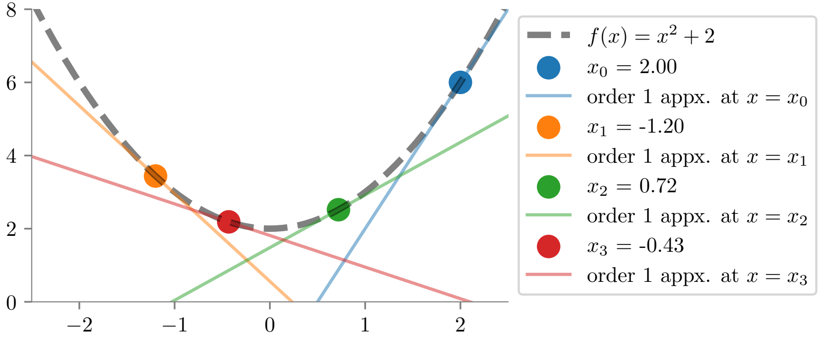


Key Points:

Perfect balance: Fast convergence + Stability

Learning Rate: Too Large

$\alpha = 0.8$: **Fast but may overshoot**

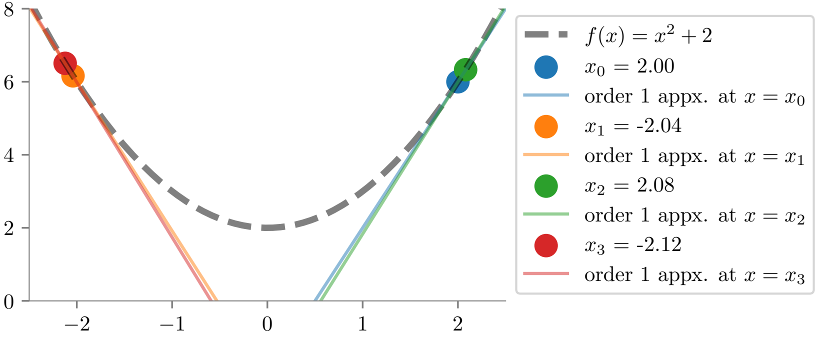


Important: Warning

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!

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):

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

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

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

Step-by-Step Example: Setup

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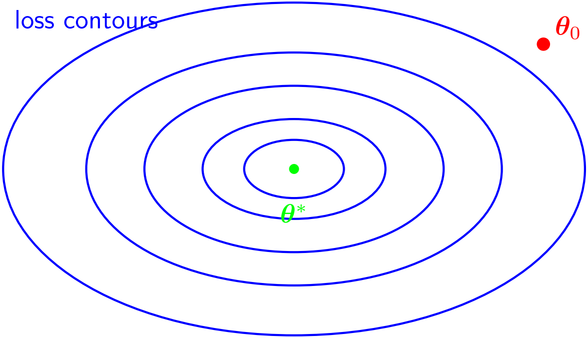
Key Points:

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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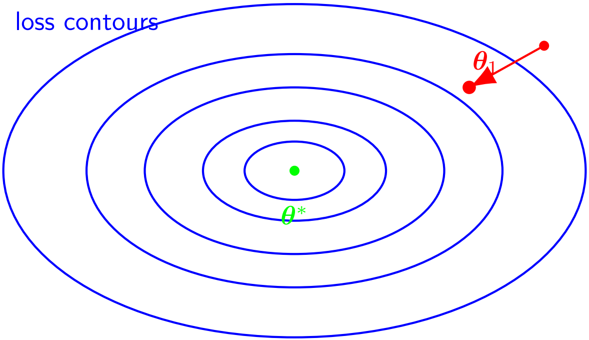

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Steps get smaller as we approach minimum (gradient magnitude decreases)!

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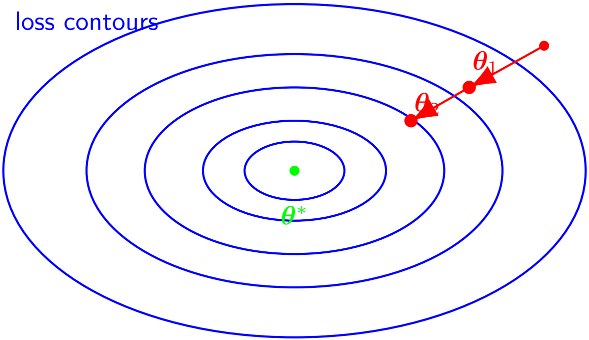

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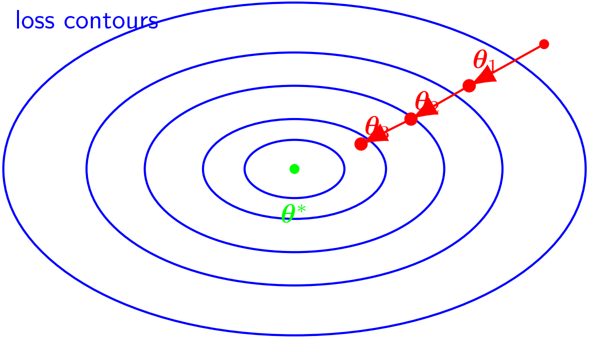

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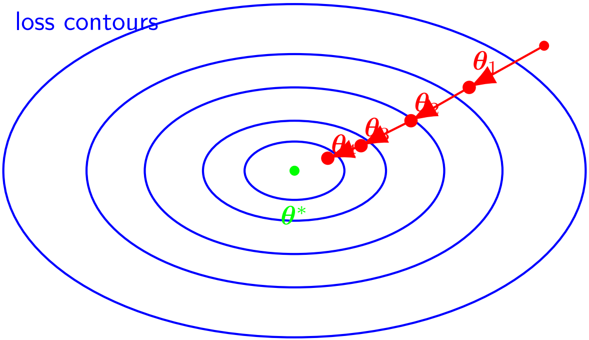

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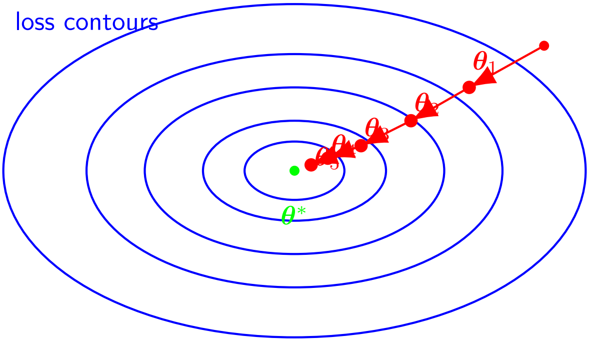

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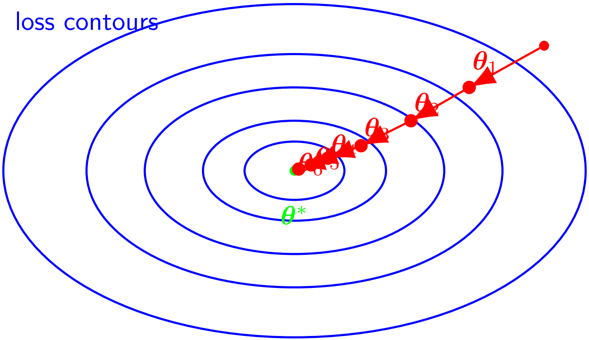

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Variants of Gradient Descent

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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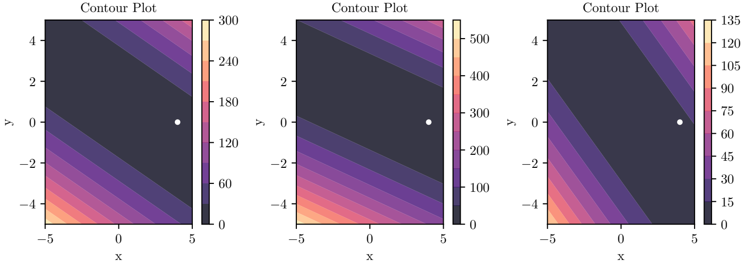
Key Points:

Modern ML Standard: Mini-batch GD with batch sizes 32-256

- Good balance of stability and efficiency
- Enables parallel computation (GPUs!)
- Better gradient estimates than pure SGD

SGD: The Noisy Path

SGD uses one sample at a time for updates



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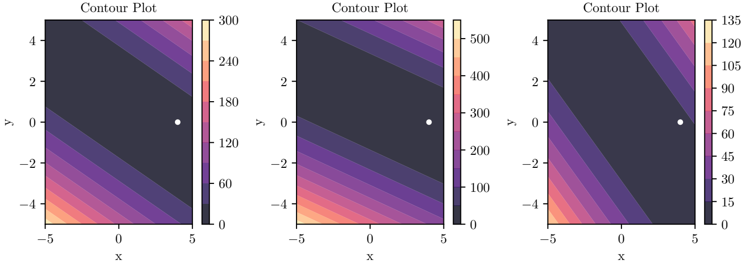

Trade-offs:

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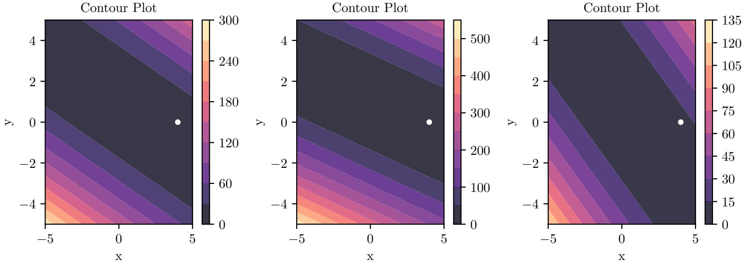

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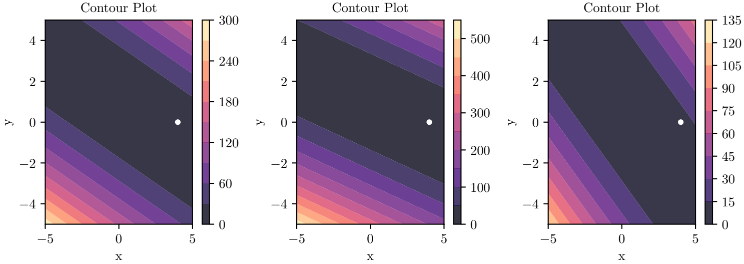

Trade-offs:

- **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

SGD as an Unbiased Estimator

True gradient (what we want):

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

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

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SGD gradient estimate (what we compute):

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

where $(\mathbf{x}_j, y_j)$ is sampled uniformly from $\{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$

The Unbiased Property: Mathematical Proof

Theorem: SGD Unbiased Estimator Property

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

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Detailed Proof:

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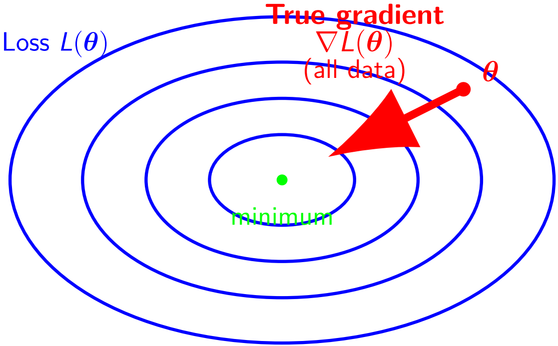
- Individual SGD steps may be "wrong"
- But they average to the correct direction over time
- Theoretical guarantee that justifies SGD's effectiveness
- The "noise" helps escape local minima in non-convex problems

Visual Intuition 1: Overall Loss Surface

True loss function using all data points:

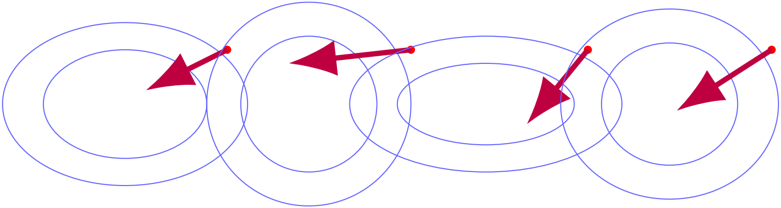


Key Points:

This is what we want: gradient computed using ALL data points

Visual Intuition 2: Individual Sample Loss Surfaces

Loss for individual data points (different shapes):



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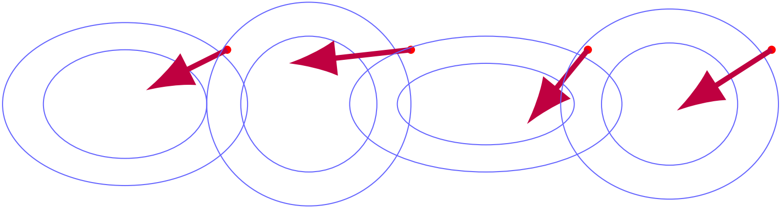

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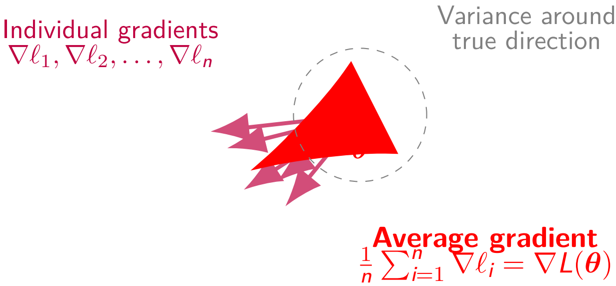
Important: Key Observation

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

Visual Intuition 3: Averaging Individual Gradients

The magic: Average of individual gradients = True gradient

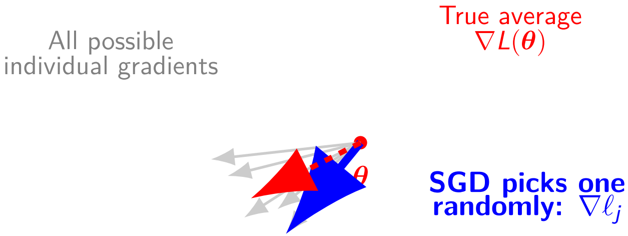


Theorem: Visual Proof of Unbiasedness

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

GD vs Normal Equation: Complexity

For linear regression:

Important: Normal Equation

$\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
Time: $\mathcal{O}(d^2 n + d^3)$
Space: $\mathcal{O}(d^2)$

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

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

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

Beyond Basic Gradient Descent

Modern optimizers improve upon vanilla GD:

- **Momentum:** $\mathbf{v}_{t+1} = \beta \mathbf{v}_t + (1 - \beta)\mathbf{g}_t$
- **AdaGrad:** Adaptive per-parameter learning rates

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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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- **Mixed precision:** 16-bit + 32-bit arithmetic

Practical Considerations

Learning Rate Selection Strategies

Common approaches:

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- 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 3: Poor Feature Scaling

Problem: Different scales cause poor convergence
Solution: Standardize features: $(x - \mu)/\sigma$

Summary and Key Takeaways

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- **Theoretical properties:** Unbiased estimator guarantees
- **Practical wisdom:** Learning rates, scaling, diagnostics

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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!