Gradient Descent: The Foundation of Machine Learning Optimization

From Taylor Series to Modern Deep Learning

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Mathematical Foundations

Key Points:

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

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Examples everywhere:

• Linear regression: Minimize $(y - X\theta)^2$

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Important: The Challenge

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

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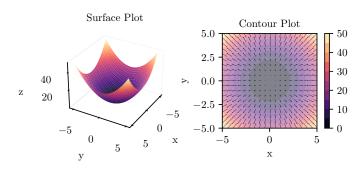
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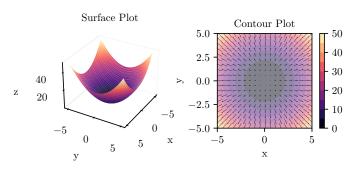
Key Points:

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

Example: The Core Idea

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Important: Taylor Series Power

Any smooth function can be approximated by polynomials!

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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Different orders of approximation:

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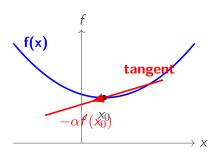
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- **Second-order:** adds $\frac{1}{2}f'(x_0)(x-x_0)^2$ (quadratic)

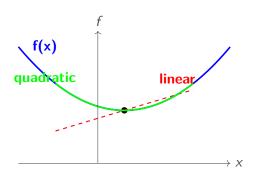
Visual: Tangent Line Approximation



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

Let's compute the derivatives:

•
$$f(0) = \cos(0) = 1$$

•
$$f(0) = -\sin(0) = 0$$

•
$$f''(0) = -\cos(0) = -1$$

•
$$f''(0) = \sin(0) = 0$$

•
$$f^{(4)}(0) = \cos(0) = 1$$

Taylor approximations:

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

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

For function f(x) around point x_0 :

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

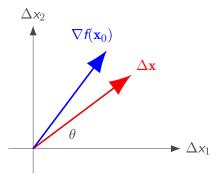
Understanding the Linear Term

The first-order term: $\nabla \mathit{f}(x_0)^T \Delta x$ where $\Delta x = x - x_0$

Understanding the Linear Term

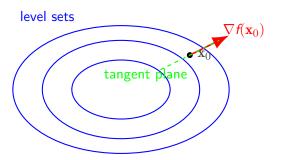
The first-order term: $\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}$ where $\Delta \mathbf{x} = \mathbf{x} - \mathbf{x}_0$

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

Goal: Find Δx such that $\mathit{f}(x_0 + \Delta x) < \mathit{f}(x_0)$

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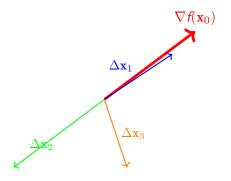
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Important: Vector Geometry Reminder

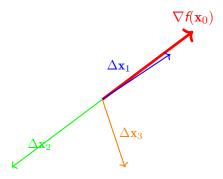
For vectors $\mathbf{a}, \mathbf{b} \colon \mathbf{a}^T \mathbf{b} = |\mathbf{a}| |\mathbf{b}| \cos(\theta)$

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)

Definition: Optimal Choice

$$\Delta \mathbf{x} = -\alpha \nabla \mathbf{f}(\mathbf{x}_0), \quad \alpha > 0$$

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Key Points:

This gives us the fundamental gradient descent step!

This gives us the gradient descent update:

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Key properties:

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- Greedy local search
- 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

Algorithm Steps:

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The Complete Algorithm

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Key hyperparameter: Learning rate α

Key Points:

Learning rate selection is crucial for success!

The learning rate α controls how big steps we take:

• Too small α : Slow convergence

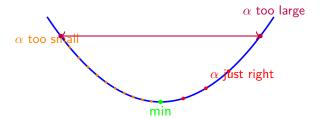
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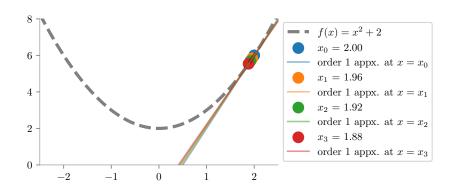
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Learning Rate Visualization: Too Small

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

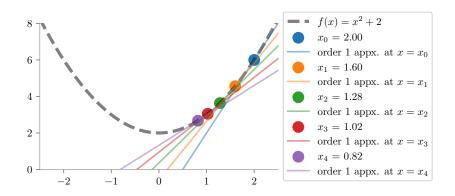


Important: Problem

Takes many iterations to reach the minimum. Computationally expensive!

Learning Rate: Just Right

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

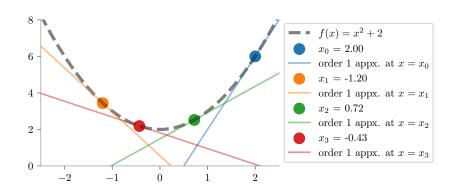


Key Points:

Perfect balance: Fast convergence + Stability

Learning Rate: Too Large

 $\alpha = 0.8$: Fast but may overshoot

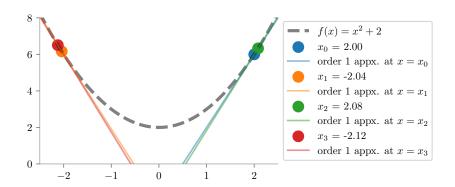


Important: Warning

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!

Gradient Descent for Linear Regression

Linear Regression: Our First Application

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

X	у
1	1
2	2
3	3

Linear Regression: Our First Application

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Cost Function (Mean Squared Error):

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

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

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Let's compute each partial derivative:

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

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

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

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

•
$$\hat{y}_1 = \theta_0 + \theta_1 \cdot 1 = 4 + 0 \cdot 1 = 4$$

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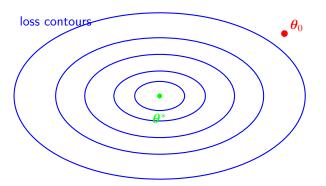
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Key Points:

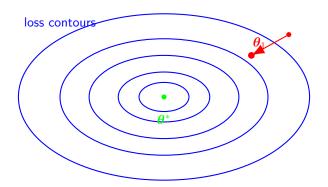
New parameters: $(\theta_0, \theta_1) = (3.6, -0.67)$

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

Visual Journey: Gradient Descent in Action



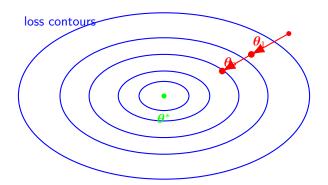
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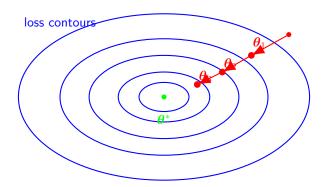
Steps get smaller as we approach minimum (gradient magnitude decreases)!

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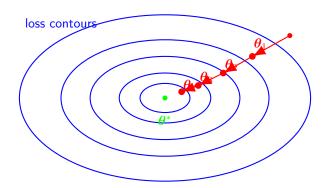


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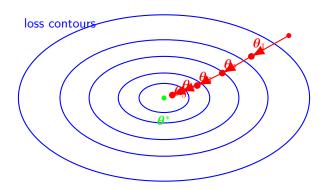
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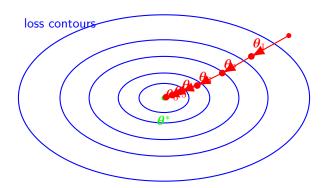
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Variants of Gradient Descent

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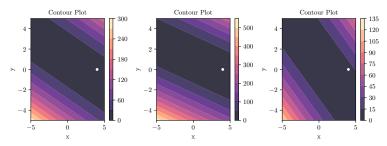
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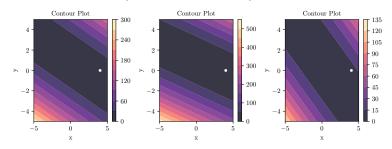
Modern ML Standard: Mini-batch GD with batch sizes 32-256

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

SGD uses one sample at a time for updates



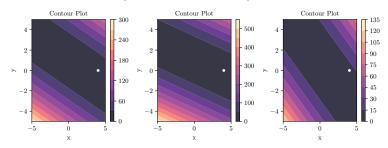
SGD uses one sample at a time for updates



Trade-offs:

Pro: Fast updates, can escape local minima

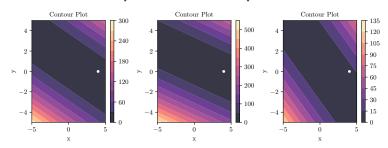
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Trade-offs:

- 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):

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

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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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$$= \sum_{i=1}^{n} P(\text{sample } i) \cdot \nabla \ell(f(\mathbf{x}_{i}; \boldsymbol{\theta}), y_{i})$$
 (12)

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Example: Intuitive Analogy

Like asking random people for directions:

• Each person's answer might be slightly off

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

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

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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: O(nd)

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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- Accelerate convergence in relevant directions
- Reduce oscillations in narrow valleys

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- Automatic differentiation: PyTorch/TensorFlow magic
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- **Mixed precision:** 16-bit + 32-bit arithmetic

Practical Considerations

Common approaches:

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

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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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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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Gradient descent is the backbone of modern machine learning!

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Journey recap:

Mathematical foundation: Taylor series derivation

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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

Next steps for mastery:

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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 $x = 2 0.1 \times 4 = 1.6$
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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!