Gradient Descent: The Foundation of Machine Learning

From Taylor Series to Modern Deep Learning

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The Core Machine Learning Challenge

Key Points:

Central Problem: Find the best parameters $\boldsymbol{\theta}^*$ for our model

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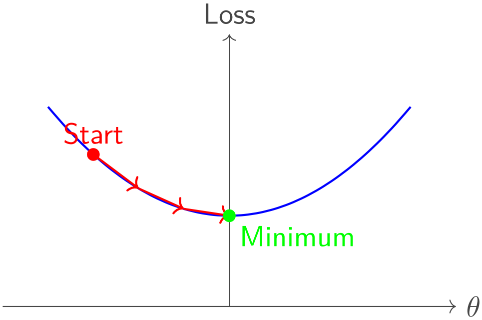
Important: The Challenge

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

Enter: Iterative Optimization

Since we can't solve directly, we use iterative methods:



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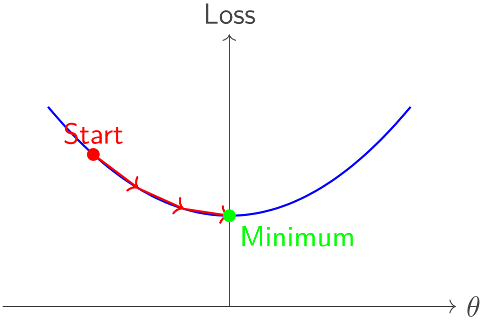

Definition: Gradient Descent

The workhorse algorithm that powers modern machine learning

Intuition: Following the Steepest Path

The Mountain Climbing Analogy

Imagine: You're lost in fog and want to reach the valley

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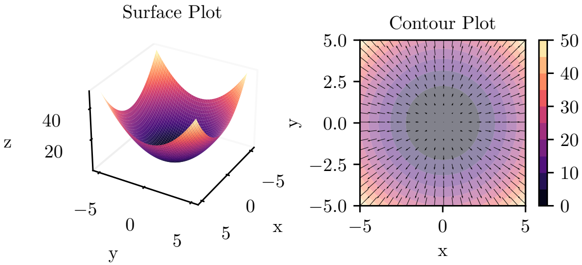
Mathematical Definition of Gradient



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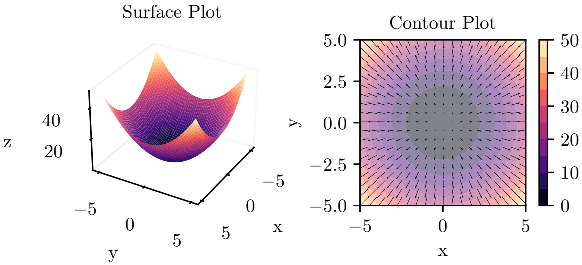

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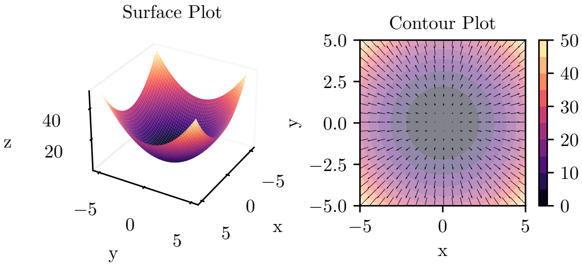

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Mathematical Foundation: Taylor Series

Why Taylor Series?

Example: The Core Idea

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Taylor series expansion around point x_0:

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

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- **1st order:** $f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T(\mathbf{x} - \mathbf{x}_0)$ (linear)
- **2nd order:** Includes curvature via Hessian

Taylor Series: Concrete Example

Let's approximate $f(x) = \cos(x)$ **around** $x_0 = 0$:

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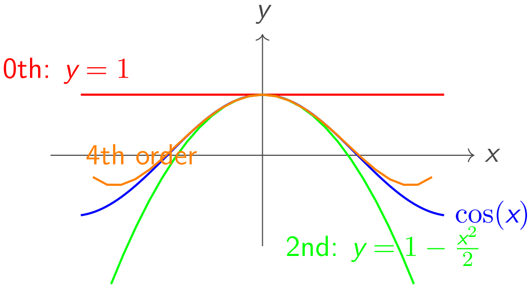
Taylor approximations:

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

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

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

Visual: Taylor Approximations



Key Points: H

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

Derivation: 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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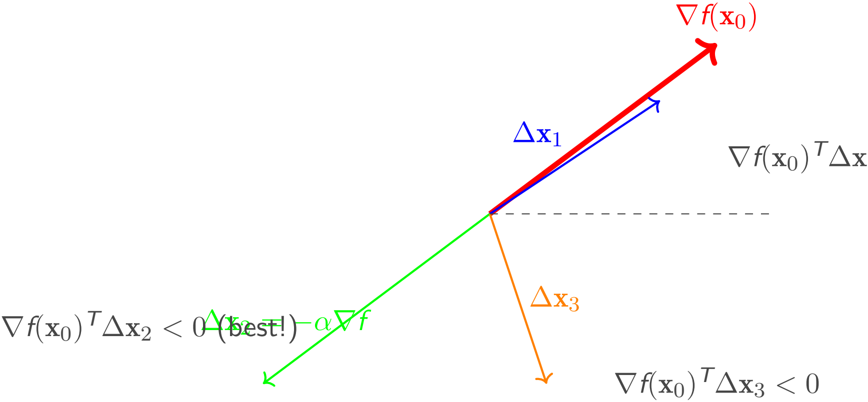
Important: Vector Geometry Reminder

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 with TikZ



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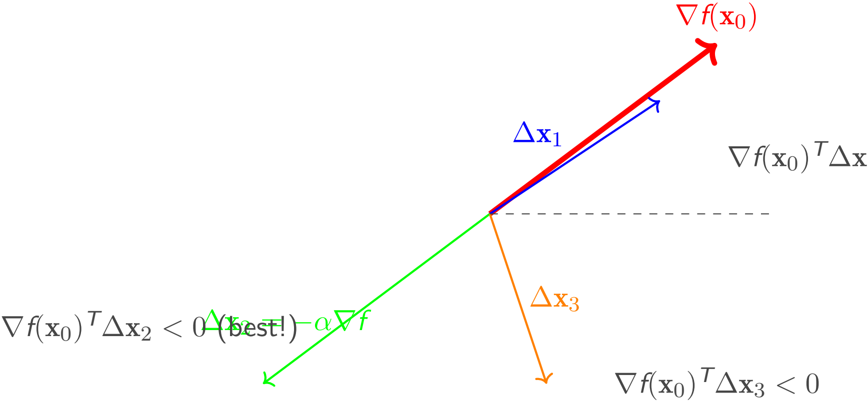

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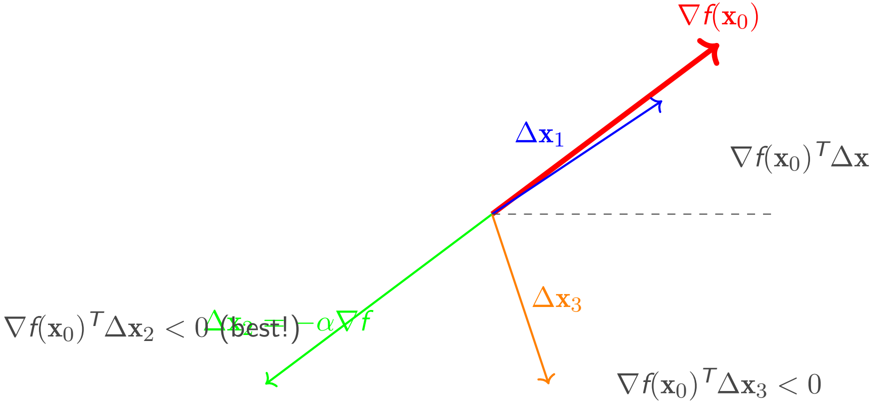

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Pop Quiz #1: Understanding the Derivation

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

Definition: Gradient Descent Algorithm

An iterative first-order optimization method for finding local minima

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Algorithm Steps:

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Key hyperparameter: Learning rate α

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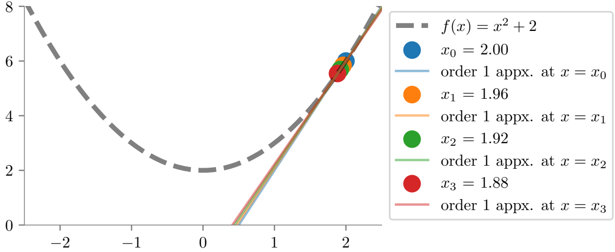
Key Points: L

earning rate selection is crucial for success!

Learning Rate Visualization: Too Small

$\alpha = 0.01$ - **Slow but steady**

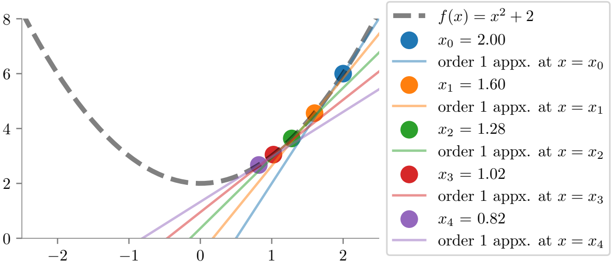


Important: Issue

Many iterations needed $\rightarrow$ Computationally expensive

Learning Rate Visualization: Just Right

$\alpha = 0.1$ - **The sweet spot**

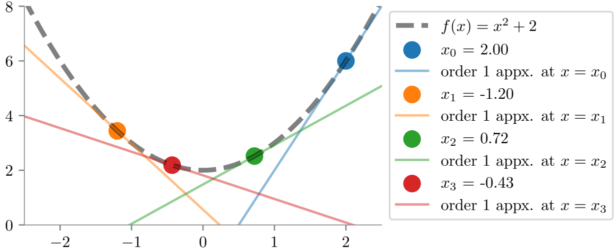


Key Points: P

erfect balance: Fast convergence + Stability

Learning Rate Visualization: Too Large

$\alpha = 0.8$ - **Getting risky**

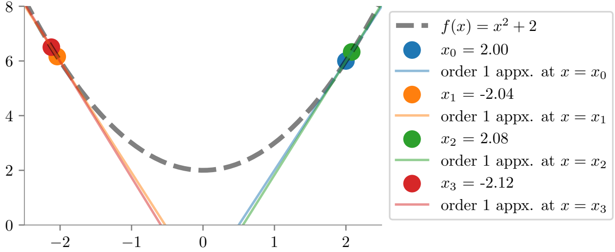


Important: Warning

Fast but oscillatory - watch for instability!

Learning Rate Visualization: Disaster

$\alpha = 1.01$ - **Complete failure**



Important: Disaster Zone

Function values explode! Always monitor your loss curves.

Application: Linear Regression

Our First Real Example

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):

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

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

Computing the Gradients

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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$$\frac{\partial \mathrm{MSE}}{\partial \theta_1} = \frac{2}{n} \sum_{i=1}^{n} (y_i - \theta_0 - \theta_1 x_i)(-x_i) \tag{8}$$

$$= -\frac{2}{n} \sum_{i=1}^{n} \epsilon_i x_i \tag{9}$$

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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- $\epsilon_3 = 3 - 4 = -1$

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Compute gradients:

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- $\theta_0^{(1)} = 4 - 0.1 \times 4 = 3.6$

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Parameter updates:

- $\theta_0^{(1)} = 4 - 0.1 \times 4 = 3.6$
- $\theta_1^{(1)} = 0 - 0.1 \times 6.67 = -0.67$

Step-by-Step Example: Updates

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- $\frac{\partial\,\mathrm{MSE}}{\partial\theta_0} = -\frac{2}{3}(-3-2-1) = 4$
- $\frac{\partial\,\mathrm{MSE}}{\partial\theta_1} = -\frac{2}{3}(-3\cdot 1-2\cdot 2-1\cdot 3) = 6.67$

Parameter updates:

- $\theta_0^{(1)} = 4 - 0.1 \times 4 = 3.6$
- $\theta_1^{(1)} = 0 - 0.1 \times 6.67 = -0.67$

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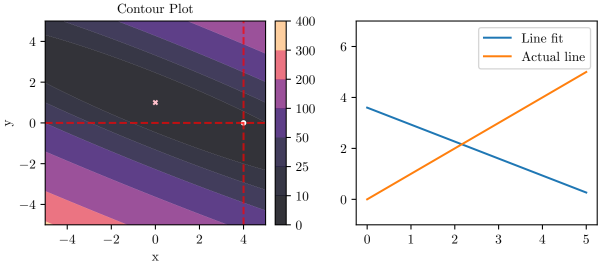
Key Points: N

ew parameters: $(\theta_0, \theta_1) = (3.6, -0.67)$
We moved closer to the true solution $(0, 1)$!

Visual Journey: GD in Action



Notice: Steps get smaller as we approach the minimum!

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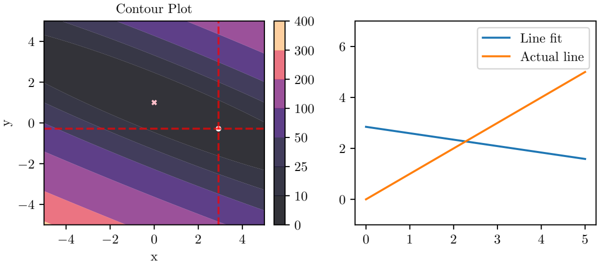

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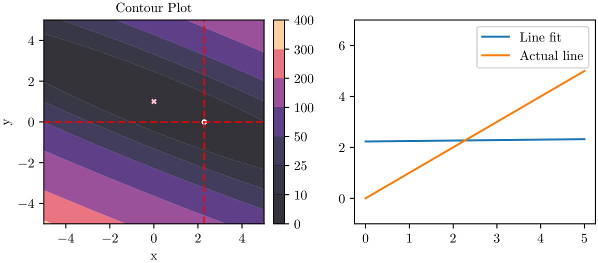

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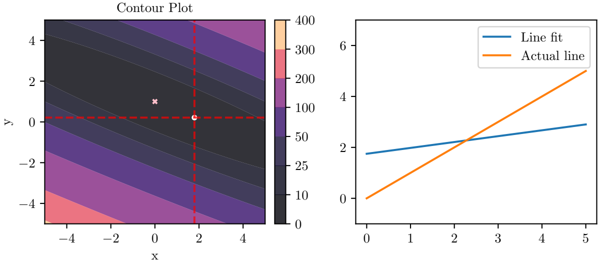

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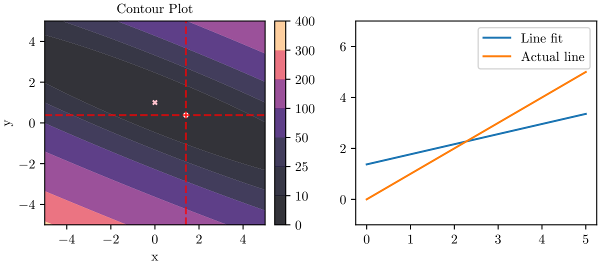

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Variants: Batch vs Stochastic vs Mini-batch

The Gradient Descent Family

Three variants based on data usage per update:

Definition: Batch Gradient Descent

Use ALL training data for each gradient computation

Definition: Stochastic Gradient Descent (SGD)

Use ONE sample for each gradient computation

Definition: Mini-batch Gradient Descent

Use a SMALL BATCH of samples for each gradient computation

Comparison: The Trade-offs

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

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Key Points:

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

- Good balance of stability and efficiency
- Enables GPU parallelization
- Better gradient estimates than pure SGD

Epochs vs Iterations

Definition: Iteration

One parameter update step

Definition: Epoch

One complete pass through the entire training dataset

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Important: Important

Always specify which metric when discussing convergence

Mathematical Properties

SGD as Unbiased Estimator

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

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Proof:

$$\begin{aligned}\mathbb{E}[\nabla \tilde{L}(\boldsymbol{\theta})] &= \mathbb{E}[\nabla \ell(f(\mathbf{x}; \boldsymbol{\theta}), y)] \\ &= \sum_{i=1}^{n} \frac{1}{n} \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i) = \nabla L(\boldsymbol{\theta})\end{aligned}$$

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Key Points:

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Example: Intuition

Like asking random people for directions:

- Each answer might be slightly off
- But with no systematic bias, the average is correct

Advanced SGD Theory

For detailed mathematical analysis, see:

Computational Complexity

GD vs Normal Equation: When to Use What?

For linear regression, we have two options:

Important: Normal Equation

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

Scenario	**Normal Eq.**	**Gradient Desc.**
Few features ($d < 1000$)	Yes	Yes
Many features ($d > 10000$)	No	Yes
Non-linear models	No	Yes
Large datasets	No	Yes
Need exact solution	Yes	No
Online learning	No	Yes

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Key Points:

Modern ML: Gradient descent dominates due to:

- High-dimensional problems (d very large)
- Non-linear models (neural networks)
- Large datasets (n very large)

Pop Quiz #2: Complexity Analysis

Answer this!

Dataset: $n = 10^6$ samples, $d = 10^3$ features
Questions:

1. Normal equation complexity?
2. GD complexity for 100 iterations?
3. Which would you choose?
4. What if $d = 10^6$?

Modern Extensions

Beyond Basic Gradient Descent

Modern optimizers address GD limitations:

- **Momentum:** Accelerates in consistent directions

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Example: Why These Improvements?

- Handle different parameter scales
- Accelerate convergence
- Reduce oscillations
- Better for non-convex landscapes

Gradient Descent in Deep Learning

Key Points: E

very deep learning framework uses gradient descent variants!

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- **Automatic differentiation:** PyTorch/TensorFlow magic
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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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Important: Warning Signs

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

Convergence Criteria

When to stop optimization:

- **Gradient norm:** $\|\nabla f(\boldsymbol{\theta})\| < \epsilon$

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Key Points:

Best practice: Use multiple criteria + validation performance

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Important: Pitfall 1: Poor Initialization

Problem: Starting at bad points
Solution: Xavier/He initialization

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Important: Pitfall 3: Poor Feature Scaling

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

Summary and Takeaways

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- **Practical aspects:** Learning rates, convergence

Looking Ahead

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

Final Pop Quiz #3

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 is always better than GD
5. GD can find global minima for any function

Thank You!

Questions?

Next lecture: Advanced Optimization Techniques
Practice: Implement GD for your favorite ML model!