Gradient Descent: The Foundation of Machine Learning Optimization

From Taylor Series to Modern Deep Learning

Nipun Batra and the teaching staff

IIT Gandhinagar

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

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Key Points: G

radient descent is the workhorse of modern machine learning!

Gradient Intuition: Climbing Mountains

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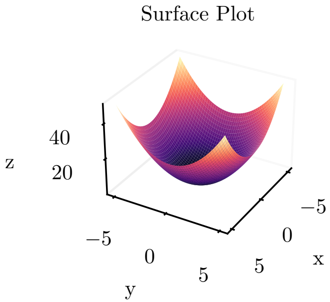

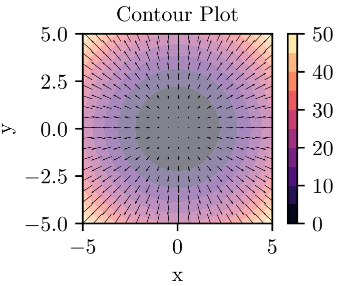

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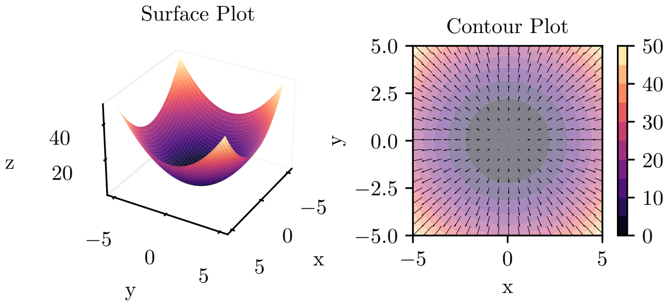

Taylor Series: The Mathematical Foundation

Why Taylor Series? The Local Approximation

Definition: The Key Insight

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Taylor series expansion around point $\mathbf{x}_0$:

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

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- **Second-order:** Includes curvature via Hessian $\nabla^2 f(\mathbf{x}_0)$

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Taylor approximations:

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

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

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Important: Key Insight

Higher-order terms give better approximations, but first-order is often sufficient for optimization!

From Taylor Series to Gradient Descent

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

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Example: Vector Geometry Insight

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

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Definition: Gradient Descent Update Rule

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

Pop Quiz #1: Taylor Series Understanding

Answer this!

Given $f(x) = x^2 + 2$ and expansion point $x_0 = 2$:
Questions:

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

Gradient Descent Algorithm

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Definition: Gradient Descent

An iterative first-order optimization algorithm for finding local minima of differentiable functions

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Key Points:

Key Properties:

- First-order method (uses gradients, not Hessians)

The Learning Rate: Your Step Size

The learning rate α controls how big steps we take

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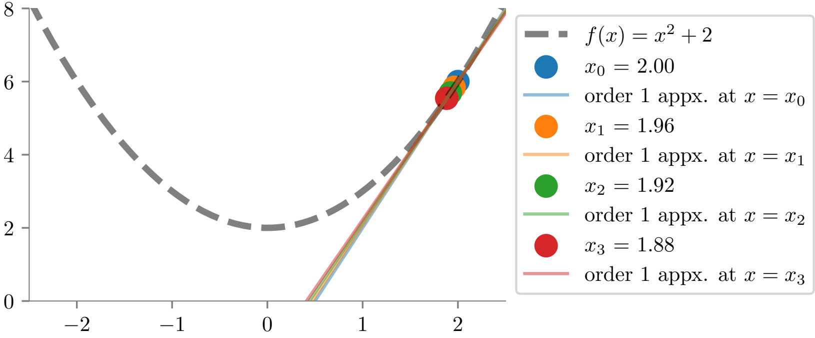
Let's see this visually...

Learning Rate: Too Small ($\alpha = 0.01$)

Convergence is slow but stable

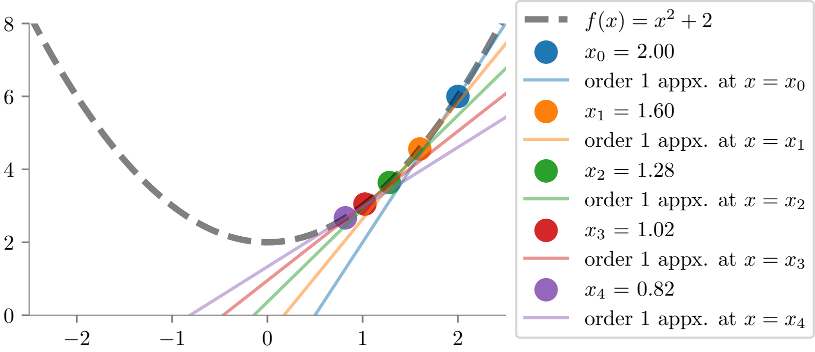


Important: Problem

Takes many iterations to reach the minimum. Computationally expensive!

Learning Rate: Just Right ($\alpha = 0.1$)

Good balance: Fast and stable convergence

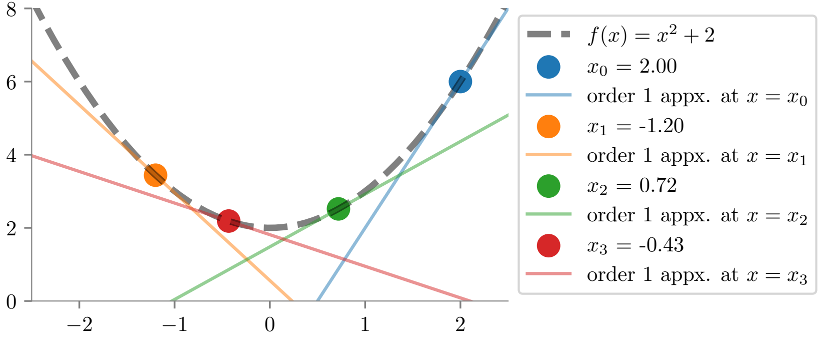


Key Points: T

his is often the sweet spot for many problems!

Learning Rate: Too Large ($\alpha = 0.8$)

Fast but may overshoot

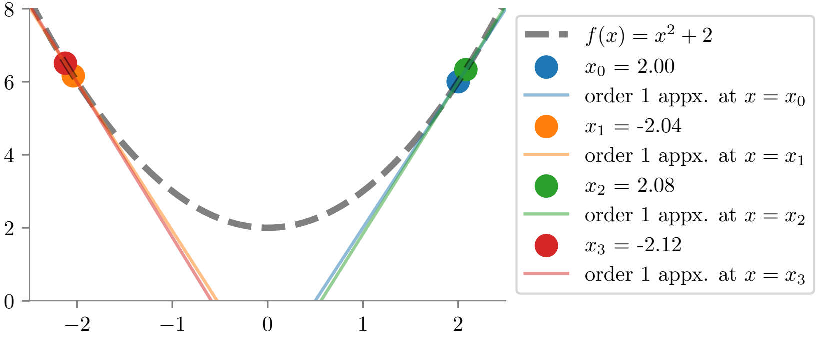


Important: Warning

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 Real 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):

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

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

Computing Gradients for Linear Regression

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

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Let's compute each partial derivative:

$$\frac{\partial \text{MSE}}{\partial \theta_0} = \frac{2}{n} \sum_{i=1}^{n} (y_i - \theta_0 - \theta_1 x_i)(-1) \tag{6}$$

$$= -\frac{2}{n} \sum_{i=1}^{n} \epsilon_i \tag{7}$$

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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.

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

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

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- $\frac{\partial \, \mathrm{MSE}}{\partial \theta_0} = -\frac{2}{3}(-3 - 2 - 1) = 4$
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- $\theta_0 = 4 - 0.1 \times 4 = 3.6$

Gradient Descent: Step-by-Step Example

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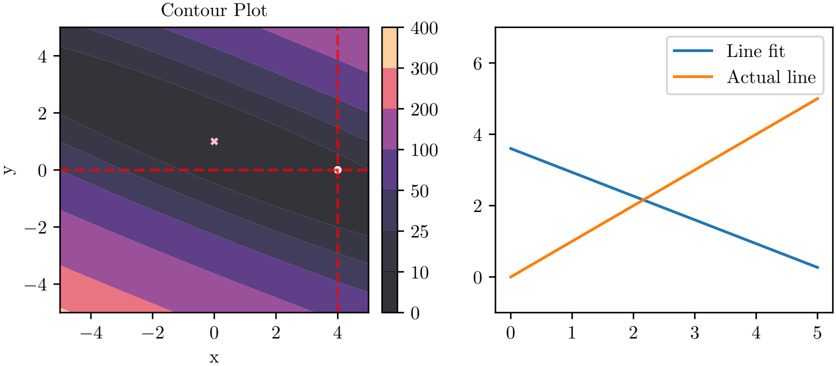
New parameters: $(\theta_0, \theta_1) = (3.6, -0.67)$

Visual Journey: Gradient Descent in Action

Let's watch gradient descent navigate the loss landscape:



Notice: The algorithm takes larger steps when gradient is large, smaller steps as it approaches the minimum!

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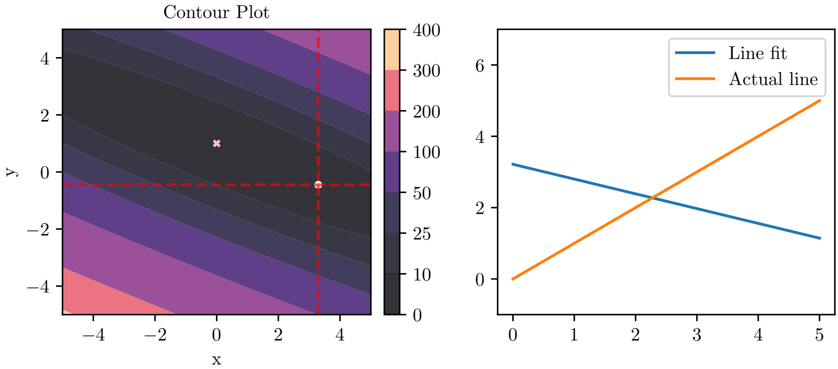

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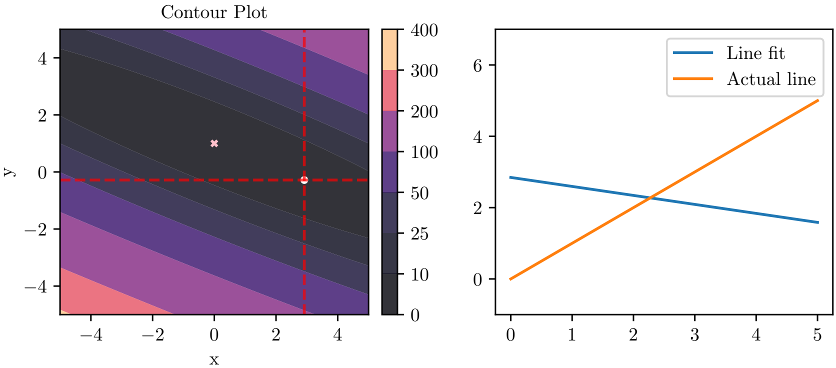

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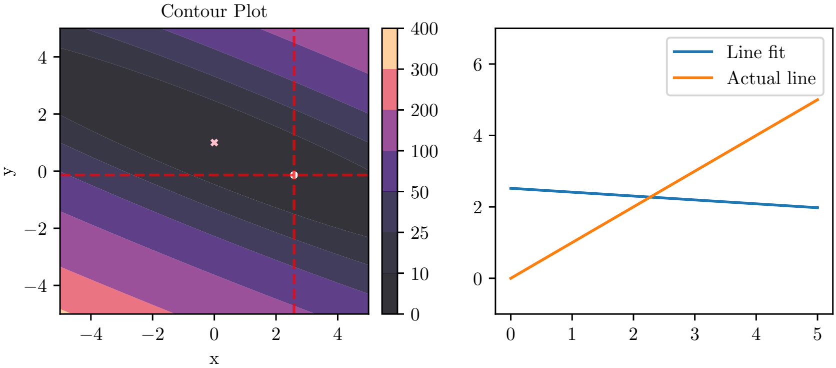

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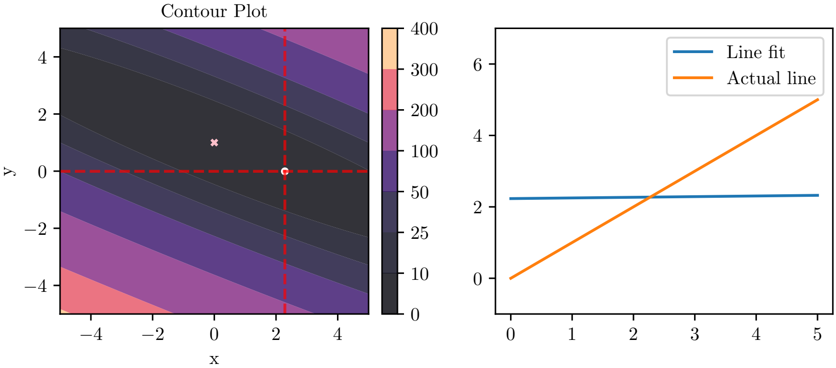

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Loss vs. Iterations: Convergence Curves

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Important: Debug Tip

If your loss curve is noisy, jagged, or increasing, check your learning rate!

Variants of Gradient Descent

The Gradient Descent Family

Three main variants based on how much data we use per update:

Definition: Batch Gradient Descent (GD)

Use all training data to compute each gradient

Definition: Stochastic Gradient Descent (SGD)

Use one sample to compute each gradient

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Trade-offs: Computational cost vs. convergence stability vs. memory usage

Batch vs Stochastic vs Mini-batch

Method	**Data per update**	**Updates per epoch**	**Converg**
Batch GD	n (all)	1	Smoo
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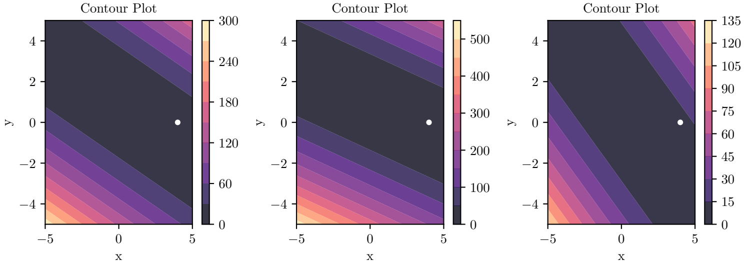
Key Points:

Modern ML: Mini-batch GD with batch sizes 32-256 is most common

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

Stochastic Gradient Descent: The Noisy Path

SGD uses one sample at a time for updates



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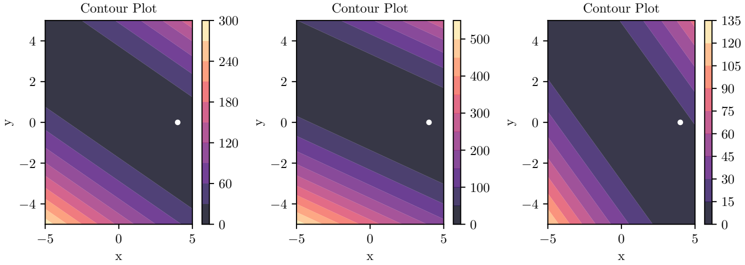

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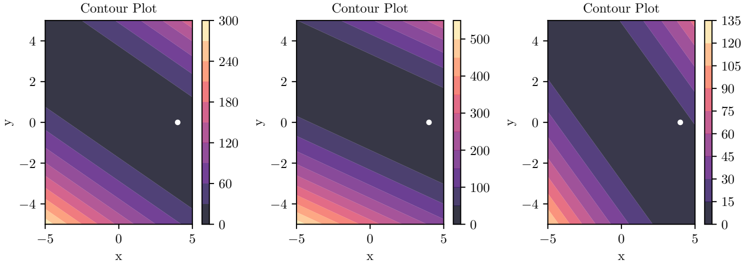

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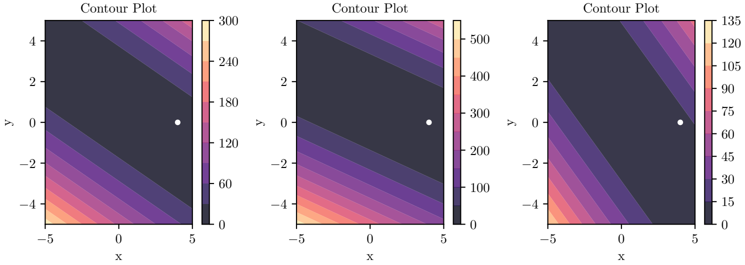

- **Pro:** Fast updates, can escape local minima due to noise
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- **Key insight:** The noise can be beneficial for non-convex problems!

Epochs vs Iterations: Important Distinction

Definition: Iteration

One parameter update step (one gradient computation and update)

Definition: Epoch

One complete pass through the entire training dataset

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Mathematical Properties

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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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Example: Intuitive Analogy

Imagine asking random people for directions to a destination:

- Individual answers might be slightly off

Computational Complexity

Computational Complexity: GD vs Normal Equation

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

Key Points: Gradient Descent

$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \alpha\mathbf{X}^T(\mathbf{X}\boldsymbol{\theta}_t - \mathbf{y})$
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- **Non-linear models:** Only gradient descent works

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

Pop Quiz #2: Complexity Comparison

Answer this!

You have a dataset with $n = 10^6$ samples and $d = 10^3$ features.

Questions:

1. What's the complexity of normal equation?
2. What's the complexity of 100 GD iterations?
3. Which method would you choose and why?
4. What if $d = 10^6$ instead?

Advanced Topics and Extensions

Beyond Basic Gradient Descent

Modern deep learning uses advanced optimizers:

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Example: Why These Improvements?

- Handle different parameter scales automatically
- Accelerate convergence in relevant directions
- Reduce oscillations in narrow valleys
- Better performance on non-convex landscapes

Gradient Descent in Deep Learning

Key Points: E

very modern deep learning framework uses gradient descent variants!

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- **Backpropagation:** Efficient gradient computation for neural networks

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Practical Considerations

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Important: Warning Signs

- Loss exploding $\rightarrow$ Learning rate too high
- Very slow convergence $\rightarrow$ Learning rate too low
- Oscillating loss $\rightarrow$ Try smaller learning rate or

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Common stopping criteria:

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Example: Practical Advice

- Always set a maximum iteration limit
- Monitor multiple criteria simultaneously
- Use validation set performance in practice
- Early stopping prevents overfitting

Common Pitfalls and How to Avoid Them

Important: Pitfall 1: Poor Initialization

Problem: Starting at bad points (e.g., all zeros)
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Important: Pitfall 3: Poor Feature Scaling

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

Summary and Key Takeaways

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Key Points: G

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- Compare batch vs SGD vs mini-batch
- Visualize convergence paths

Pop Quiz #3: Comprehensive Review

Answer this!

True or False?

1. SGD always converges faster than batch gradient descent
2. The learning rate should decrease as training progresses
3. SGD gradient estimates are unbiased
4. Normal equation is always better than gradient descent
5. Gradient descent can only find global minima

Looking Ahead: Advanced Optimization

What's next in optimization?

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

Additional Resources: SGD Deep Dive

For detailed mathematical analysis and proofs:

Important: Reference Material

See "SGD.pdf" in the assets folder for:

- Formal convergence proofs
- Variance analysis of SGD
- Advanced theoretical properties
- Comparison with other optimization methods

Thank You!

Questions?

Next: Advanced Optimization Techniques
Practice: Implement gradient descent for your favorite ML model!