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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The Big Picture: Why Optimization Matters

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Key Points: G

radient descent is the workhorse of modern machine learning!

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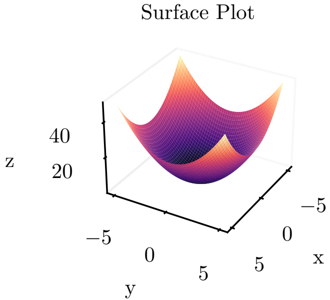

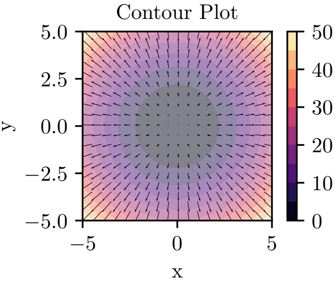

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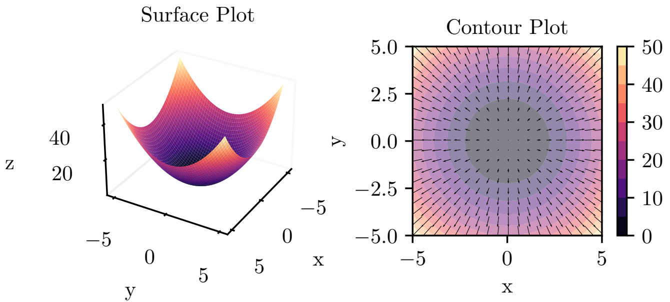
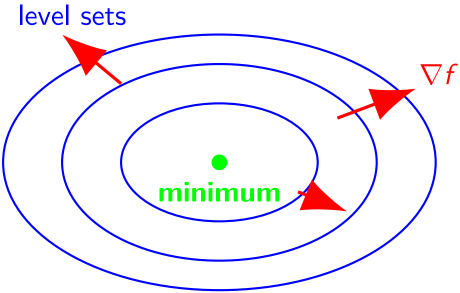


Geometric Intuition with Level Sets



Key Points: K

ey insight: Gradient $\perp$ level sets, points toward steepest ascent

Taylor Series: The Mathematical Foundation

Why Taylor Series? The Key Insight

Definition: The Core Idea

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

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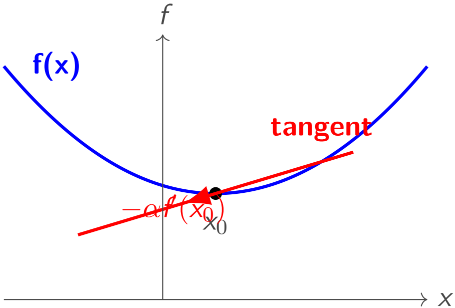
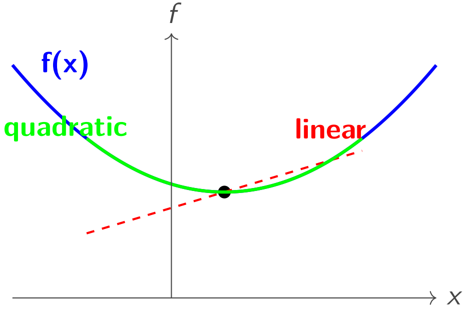
- **Second-order:** Includes curvature via Hessian $\nabla^2 f(\mathbf{x}_0)$

Univariate Taylor: Visual Understanding



Adding Quadratic Term



Important: Key Insight

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

Taylor Series: Concrete Example

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

- $f(0) = \cos(0) = 1$

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Taylor approximations:

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

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

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

Multivariate Taylor Series

Extension to multiple variables:

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

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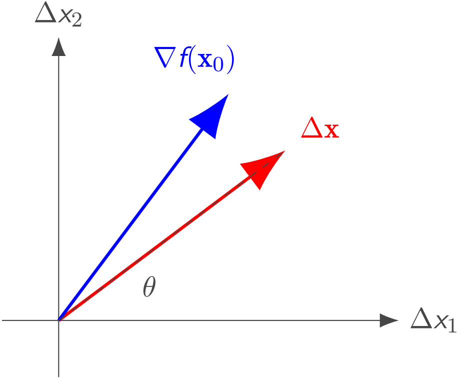
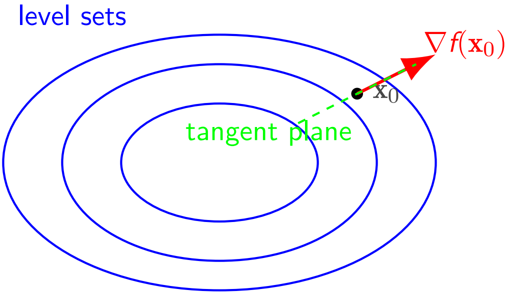


Linear term: $\nabla f(\mathbf{x}_0)^T \Delta\mathbf{x} = |\nabla f||\Delta\mathbf{x}| \cos\theta$

Visual: Multivariate Case with Level Sets



Key: Gradient $\perp$ level sets, tangent plane $\perp$ gradient

From Taylor Series to Gradient Descent

The Derivation: From Theory to Algorithm

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

For vectors $\mathbf{a}$ and $\mathbf{b}$: $\mathbf{a}^T\mathbf{b} = |\mathbf{a}||\mathbf{b}|\cos(\theta)$
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?

Pop Quiz #1: Solutions

Example: Solutions

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

1. $f(2) = 4 + 2 = 6$
2. $f'(x) = 2x$, so $f'(2) = 4$
3. $f(x) \approx 6 + 4(x - 2) = 4x - 2$
4. $\Delta x = -0.1 \times 4 = -0.4$, so $x_{new} = 2 - 0.4 = 1.6$

Gradient Descent Algorithm

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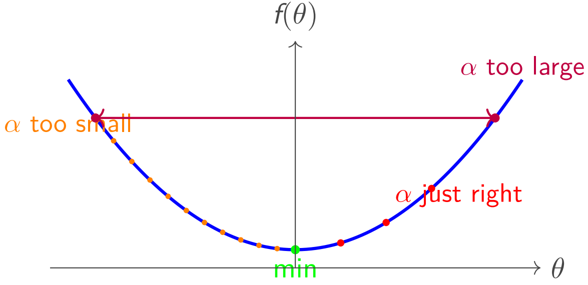
Key Points:

Key Properties:

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

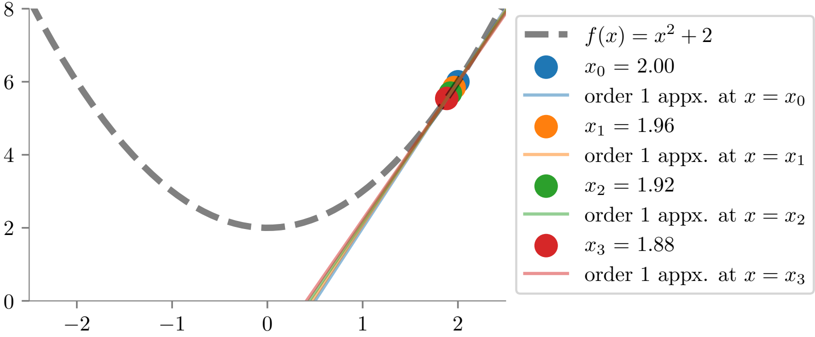
The Learning Rate: Your Step Size

The learning rate α controls how big steps we take



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

Convergence is slow but stable

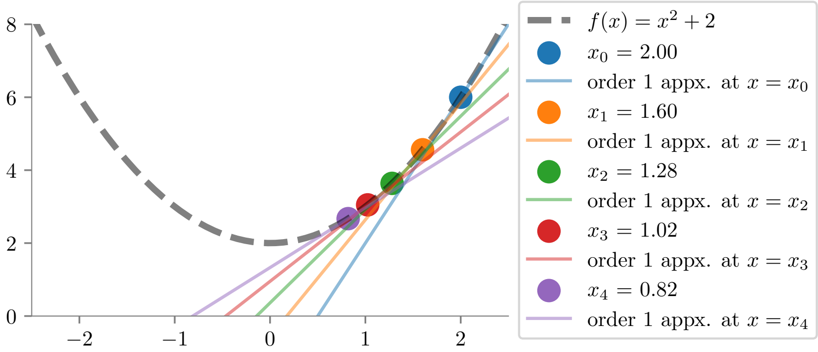


Important: Problem

Takes many iterations to reach the minimum. Computationally expensive!

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

Good balance: Fast and stable convergence

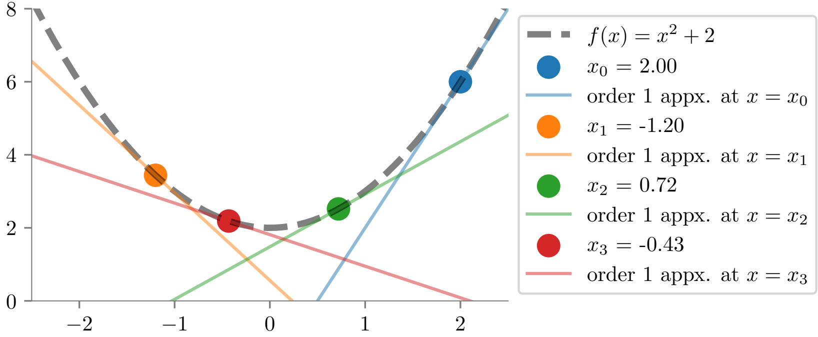


Key Points: T

his is often the sweet spot for many problems!

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

Fast but may overshoot

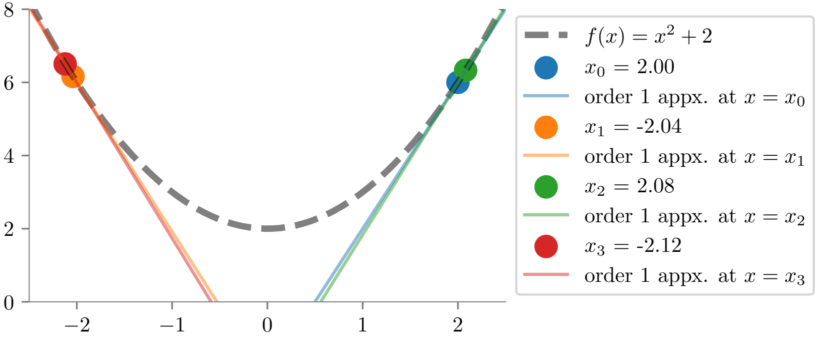


Important: Warning

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

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

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

Gradient Descent: Step-by-Step Example

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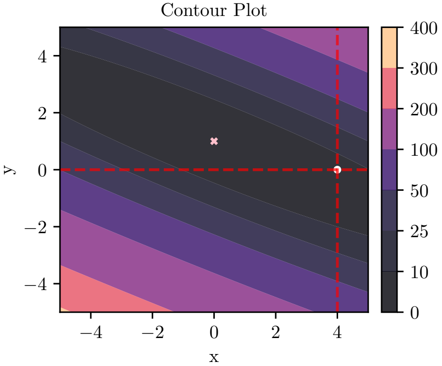
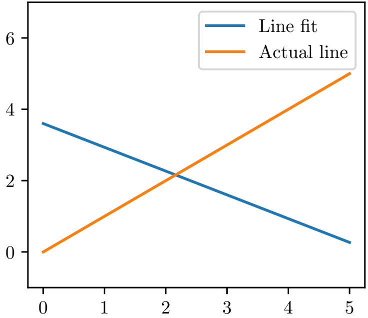
New parameters: $(\theta_0, \theta_1) = (3.6, -0.67)$

Visual Journey: Gradient Descent in Action

Let's watch gradient descent navigate the loss landscape:





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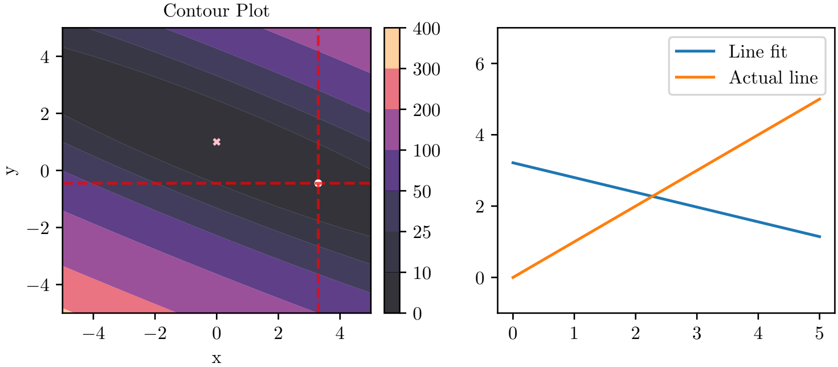

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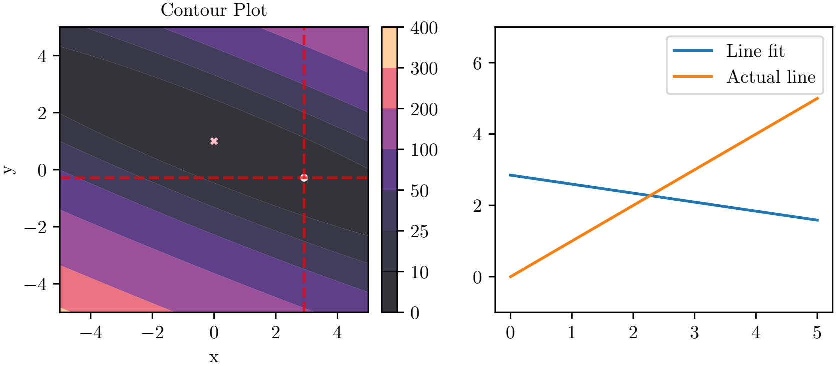

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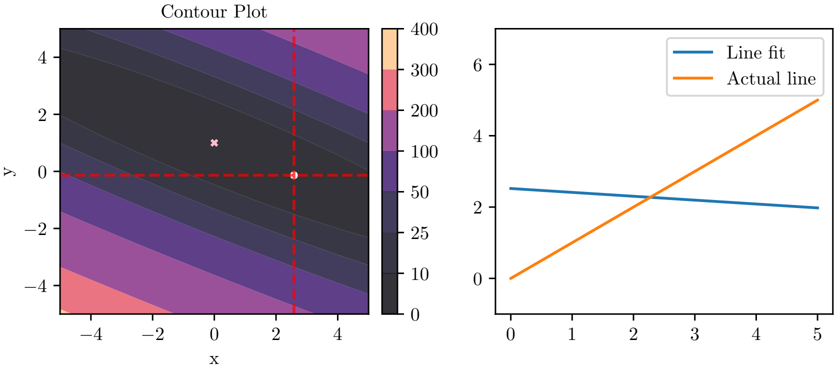

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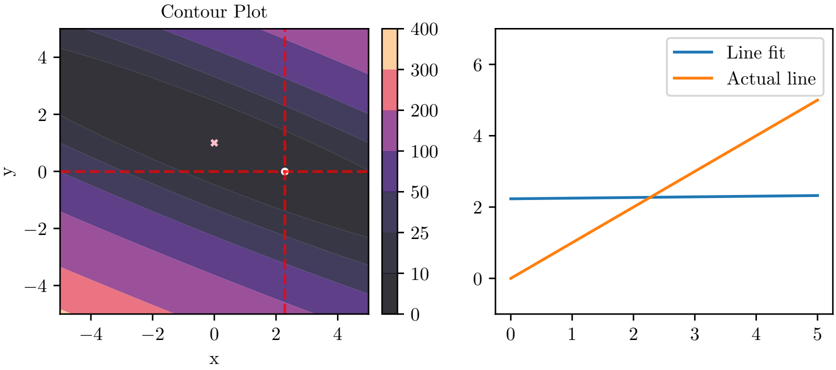

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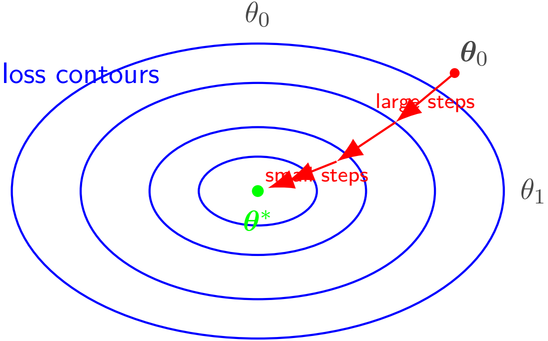
Visual: GD Path on Loss Surface (TikZ Version)



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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

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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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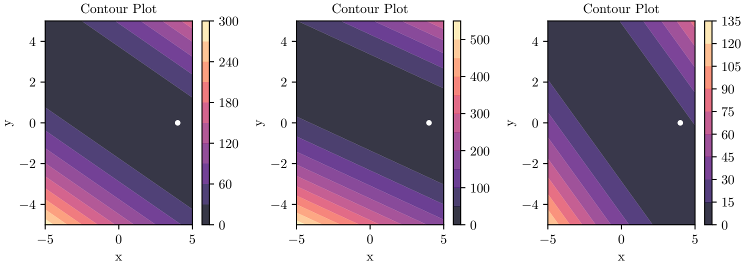
Key Points:

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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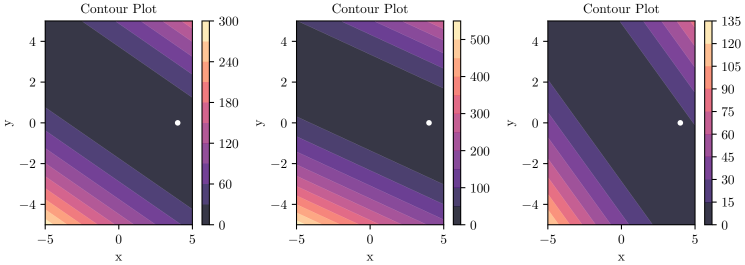

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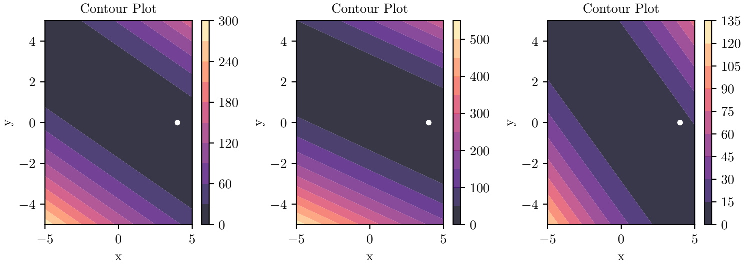

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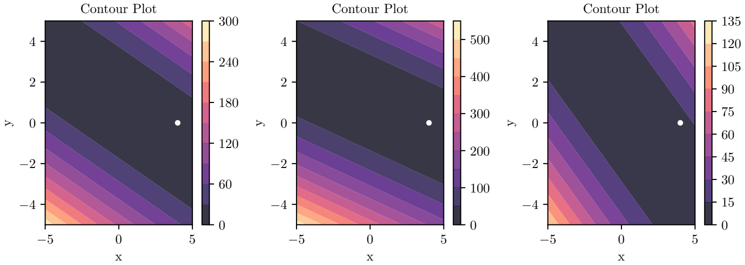

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- **Key insight:** The noise can be beneficial for non-convex problems!

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

Key Points: Gradient Descent

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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?

Pop Quiz #2: Solutions

Example: Solutions

For $n = 10^6$, $d = 10^3$:

1. Normal equation:
   $O(d^2 n + d^3) = O(10^{12} + 10^9) = O(10^{12})$
2. 100 GD iterations: $O(100 \cdot dn) = O(10^{11})$
3. Choose GD ($10\times$ faster)
4. If $d = 10^6$: Normal equation becomes $O(10^{18})$, GD becomes $O(10^{14})$ – definitely choose GD!

Advanced Topics and Extensions

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Modern deep learning uses advanced optimizers:

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- **AdaGrad:** Adaptive learning rates per parameter
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- **RMSprop:** Exponential moving average of squared gradients

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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- **GPU acceleration:** Parallel computation of mini-batch gradients
- **Mixed precision:** Use both 16-bit and 32-bit arithmetic

Practical Considerations

Choosing Learning Rates: Practical Tips

Key Points: L

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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

Convergence Criteria: When to Stop?

Common stopping criteria:

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

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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

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Important: Pitfall 1: Poor Initialization

Problem: Starting at bad points (e.g., all zeros)
Solution: Use Xavier/He initialization for neural networks

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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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From Theory to Practice: Next Steps

Practice opportunities:

- Implement gradient descent from scratch

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

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

Pop Quiz #3: Solutions

Example: Solutions

1. **False** - SGD converges faster per epoch but may need more epochs
2. **True** - Learning rate schedules often improve convergence
3. **True** - This is the key theoretical property of SGD
4. **False** - Normal equation only works for linear problems and small d
5. **False** - GD finds local minima; global minima only guaranteed for convex functions

Looking Ahead: Advanced Optimization

What's next in optimization?

- **Second-order methods:** Newton's method, L-BFGS

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- **Distributed optimization:** Federated learning, parameter servers
- **Meta-learning:** Learning to optimize

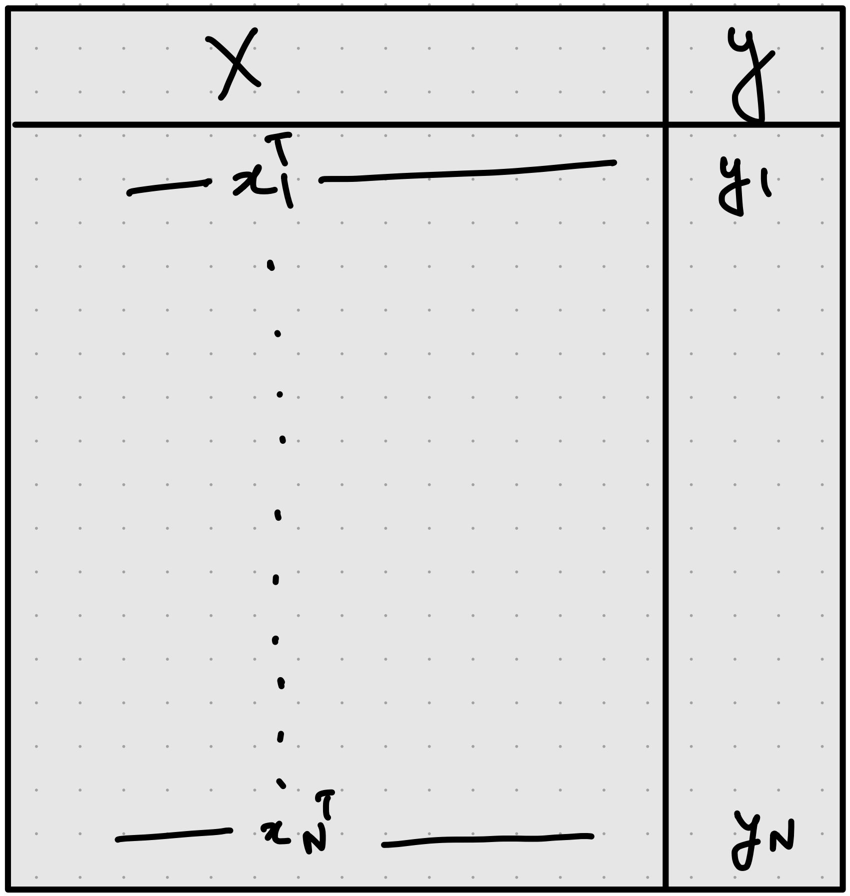
Additional Resources: SGD Deep Dive

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


X
y
x_1^T
y_1
x_N^T
y_N

X	y	$\hat{y} = f(x, \theta)$
— x_1^T —	y_1	$\hat{y}_1$
$\vdots$		$\vdots$
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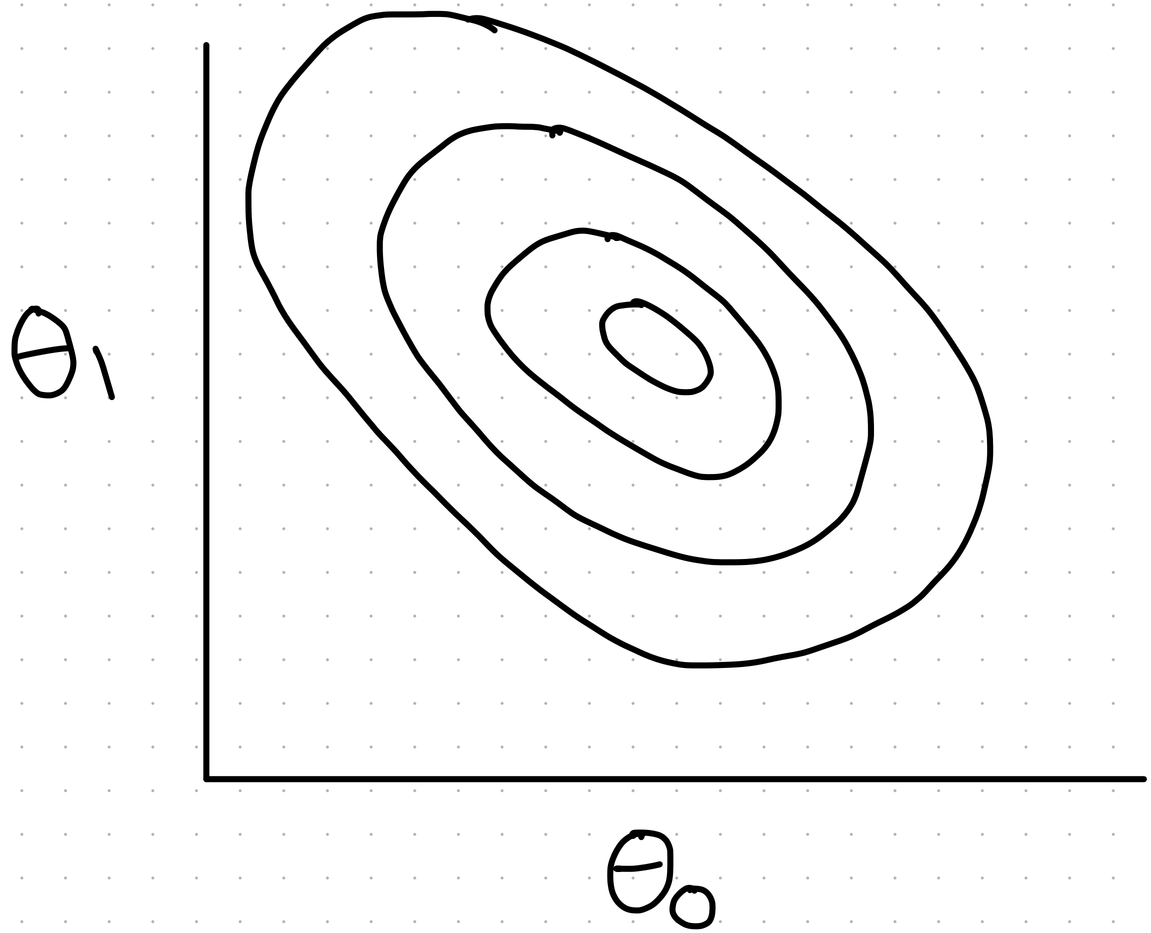

LOSS SURFACE OVER
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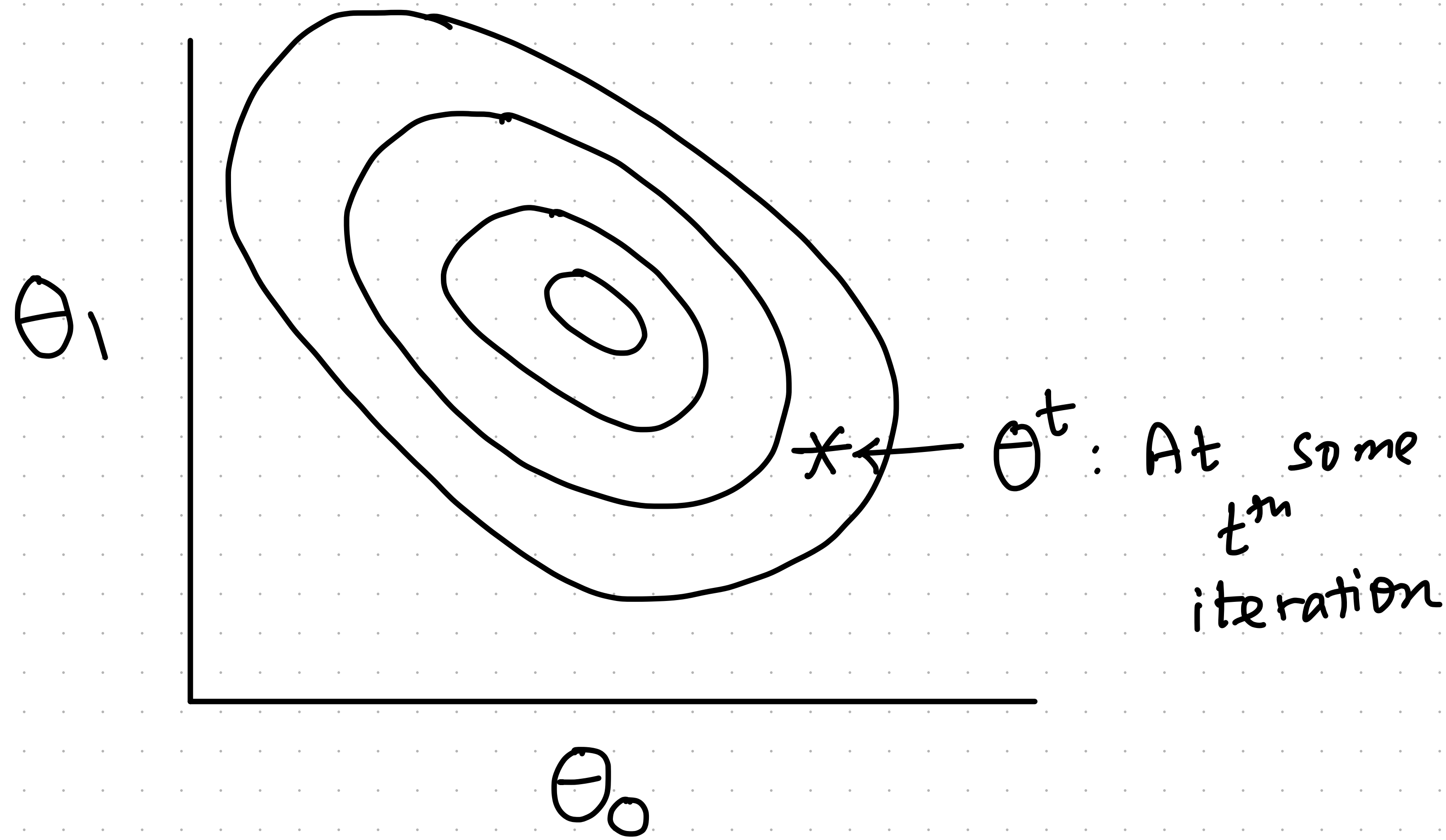

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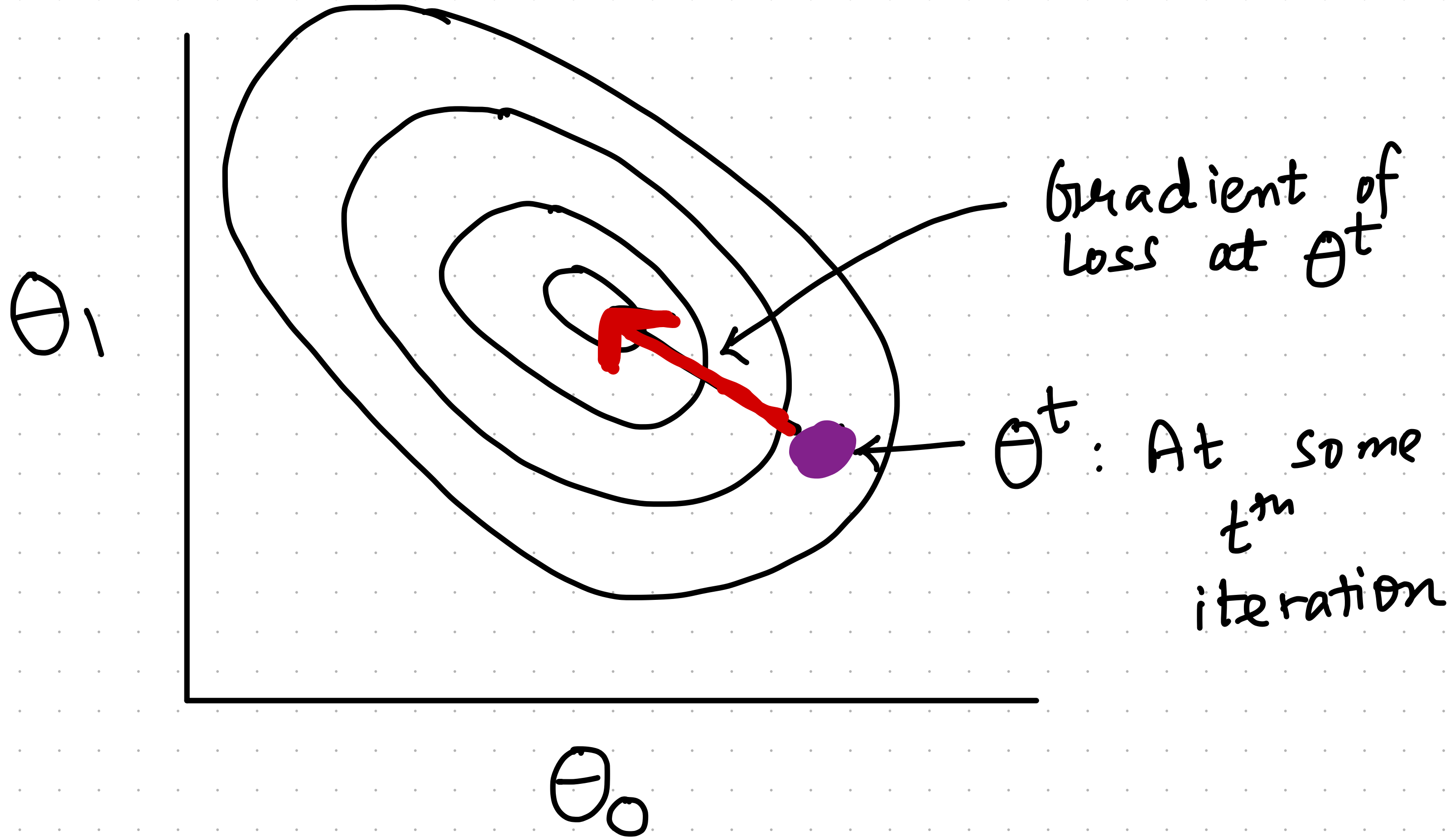

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Thank You!

Questions?

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