Gradient Descent: The Foundation of ML Optimization

From Taylor Series to Modern Deep Learning

Nipun Batra and Teaching Staff

IIT Gandhinagar

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Outline

The Core ML Problem

$$\min_{\boldsymbol{\theta}} f(\boldsymbol{\theta})$$

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Examples everywhere:

- Linear regression: $\min(y - \mathbf{X}\theta)^2$
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Challenge: Most ML problems have no closed-form solution

Geometric Intuition: Climbing Mountains

Imagine hiking in fog to reach the valley:

- Feel slope beneath your feet
- **Strategy:** Step in steepest downhill direction
- **Gradient** = steepest uphill
- **Negative gradient** = steepest downhill

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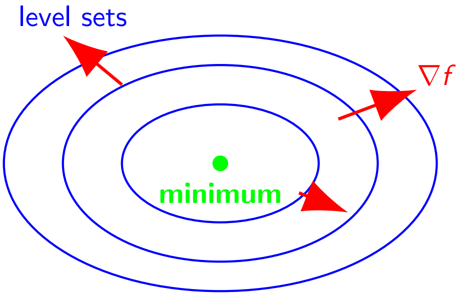

Think!

Why does following $-\nabla f$ lead us toward the minimum?

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(Solution in Appendix)

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Key insight: If we can't solve $\min f(\mathbf{x})$ exactly, approximate $f(\mathbf{x})$ locally!

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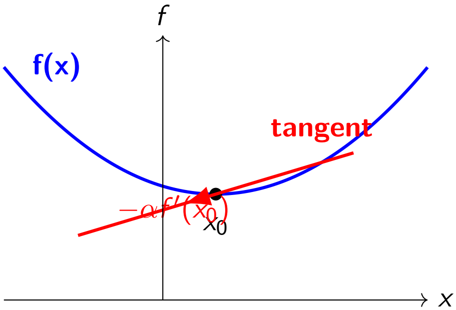
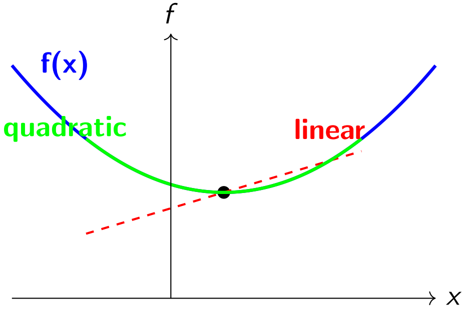
- **Zero-order:** $f(x) \approx f(x_0)$ (constant)
- **First-order:** adds linear term (tangent)
- **Second-order:** adds quadratic curvature

Visual: Tangent Line Approximation



Visual: Adding Quadratic Term



Key insight: Higher-order terms give better approximations!

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

$$
\begin{align}
f(0) &= \cos(0) = 1 \tag{1}\\
f'(0) &= -\sin(0) = 0 \tag{2}\\
f''(0) &= -\cos(0) = -1 \tag{3}\\
f'''(0) &= \sin(0) = 0 \tag{4}\\
f^{(4)}(0) &= \cos(0) = 1 \tag{5}
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Taylor approximations:

$$\text{0th order:} \quad f(x) \approx 1 \tag{6}$$
$$\text{2nd order:} \quad f(x) \approx 1 - \frac{x^2}{2} \tag{7}$$
$$\text{4th order:} \quad f(x) \approx 1 - \frac{x^2}{2} + \frac{x^4}{24} \tag{8}$$

Multivariate Taylor Series

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T \Delta \mathbf{x} + \frac{1}{2} \Delta \mathbf{x}^T \nabla^2 f(\mathbf{x}_0) \Delta \mathbf{x}$$

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where $\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}_0$

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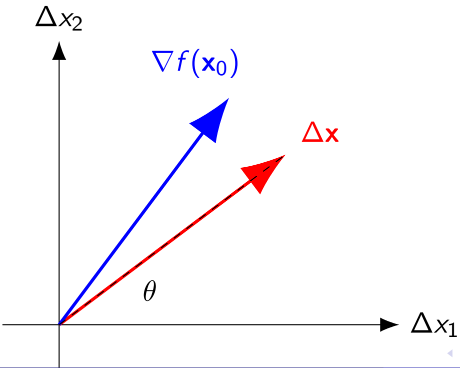
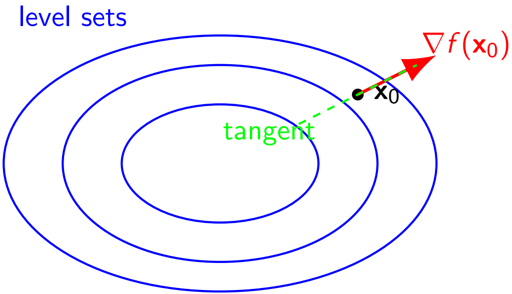


Visual: Multivariate Case with Level Sets



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

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

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

The Gradient Descent Algorithm

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Algorithm:

1. **Initialize:** θ_0 (random or educated guess)
2. **For** $t = 0, 1, 2, \ldots$ until convergence:
    - Compute gradient: $\mathbf{g}_t = \nabla f(\boldsymbol{\theta}_t)$
    - Update parameters: $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \alpha \mathbf{g}_t$
    - Check convergence: $|\mathbf{g}_t| < \epsilon$

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Key properties:

- First-order method (uses gradients, not Hessians)
- Greedy local search
- Guaranteed convergence for convex functions

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

x	y
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Cost Function (Mean Squared Error):

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

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

Computing Gradients for Linear Regression

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

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

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Matrix form: $\nabla \text{MSE}(\boldsymbol{\theta}) = \frac{2}{n}\mathbf{X}^T(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$

Step-by-Step Example

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

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- Errors: $\epsilon_1 = -3$, $\epsilon_2 = -2$, $\epsilon_3 = -1$
- $\frac{\partial \text{MSE}}{\partial \theta_0} = -\frac{2}{3}(-6) = 4$
- $\frac{\partial \text{MSE}}{\partial \theta_1} = -\frac{2}{3}(-10) = 6.67$
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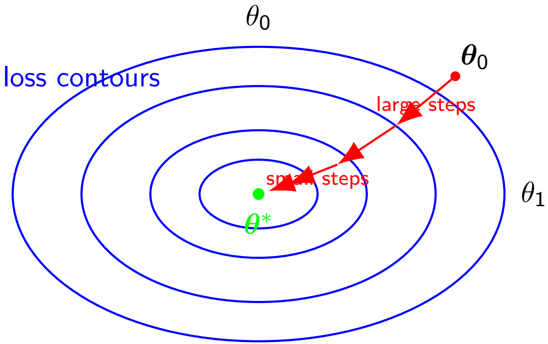
New parameters: $(\theta_0, \theta_1) = (3.6, -0.67)$

Visual: GD Path on Loss Surface



Notice: Algorithm takes larger steps when gradient is large!

The Gradient Descent Family

Three main variants based on data usage per update:

Method	**Data per update**	**Updates per epoch**	**Convergence**
Batch GD	n (all)	1	Smooth
SGD	1	n	Noisy
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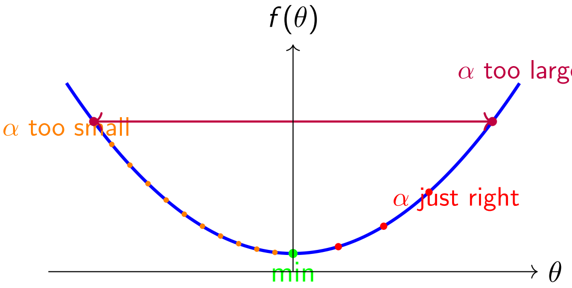
Modern ML: Mini-batch GD with batch sizes 32-256 is most common

- Good balance of stability and efficiency
- Enables parallel computation (GPUs love batches!)

Learning Rate Effects



Pop Quiz #1

For dataset with 1000 samples and batch size 50:

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2. If SGD takes 1000 epochs to converge, roughly how many epochs should mini-batch take?
3. Why might SGD be noisier than batch GD?

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(Solutions in Appendix)

Convergence Rates for Convex Functions

L-smooth convex: $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\|$
With step size $\alpha \in (0, 1/L]$:

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μ-strongly convex + L-smooth:

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \leq \left(1 - \frac{\mu}{L}\right)^t (f(\mathbf{x}_0) - f(\mathbf{x}^*))$$

Rate: Linear convergence! Condition number $\kappa = L/\mu$

SGD as Unbiased Estimator

True gradient: $\nabla L(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \nabla \ell(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i)$
SGD gradient estimate: $\nabla \tilde{L}(\boldsymbol{\theta}) = \nabla \ell(f(\mathbf{x}; \boldsymbol{\theta}), y)$, where $(\mathbf{x}, y)$ is sampled uniformly from $\{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$

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Proof sketch:

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

Implication: Individual SGD steps might be "wrong", but average in correct direction!

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Intuitive analogy: Asking random people for directions

- Individual answers might be slightly off
- But if no systematic bias, average direction is correct
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The noise can be beneficial:

- Helps escape local minima in non-convex problems
- Provides implicit regularization
- Enables online learning

GD vs Normal Equation

For linear regression:
Normal equation: $\hat{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

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When to use which?

- Few features ($d < 1000$): Normal equation
- Many features ($d > 10000$): Gradient descent
- Non-linear models: Only gradient descent works

Beyond Basic Gradient Descent

Momentum: $\mathbf{v}_{t+1} = \beta \mathbf{v}_t + (1-\beta)\mathbf{g}_t$, $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \alpha \mathbf{v}_{t+1}$
Adam: Combines momentum + adaptive learning rates

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \frac{\alpha}{\sqrt{\hat{\mathbf{v}}_t} + \epsilon}\hat{\mathbf{m}}_t$$

Defaults: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$

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Why these improvements?

- Handle different parameter scales automatically
- Accelerate convergence in relevant directions
- Reduce oscillations in narrow valleys

Second-Order Methods

Newton's method: $\theta_{t+1} = \theta_t - \alpha[\nabla^2 f(\theta_t)]^{-1} \nabla f(\theta_t)$
Gauss-Newton: For least squares problems
L-BFGS: Quasi-Newton method (approximates Hessian)

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Line search methods: Adaptive step size via Armijo condition

Gradient Descent in Deep Learning

Every modern deep learning framework uses GD variants!
Key extensions:

- **Backpropagation:** Efficient gradient computation
- **Automatic differentiation:** PyTorch/TensorFlow handle gradients
- **GPU acceleration:** Parallel mini-batch gradients
- **Mixed precision:** 16-bit + 32-bit arithmetic

Learning Rate Selection

Common strategies:

- Grid search: $\alpha \in \{0.001, 0.01, 0.1, 1.0\}$
- Learning rate schedules: Start high, decay over time
- Adaptive methods: Let algorithm adjust automatically
- Learning rate finder: Gradually increase and watch loss

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Warning signs:

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

Other Practical Considerations

Feature scaling: Standardize features: $(x - \mu)/\sigma$

Convergence criteria:

- Gradient magnitude: $\|\nabla f(\boldsymbol{\theta})\| < \epsilon$
- Function change: $|f(\boldsymbol{\theta}_{t+1}) - f(\boldsymbol{\theta}_t)| < \epsilon$
- Maximum iterations: Simple upper bound

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Common pitfalls:

- Poor initialization (use Xavier/He for neural networks)
- Poor feature scaling (different parameter scales)
- Not monitoring validation performance

Think!

For L-smooth function, why might $\alpha > 2/L$ cause divergence on a quadratic?

Think!

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(Solution in Appendix)

What We've Learned

Core journey:

- **Mathematical foundation:** Taylor series approximation
- **Key insight:** Follow $-\nabla f$ for steepest descent
- **Algorithm:** $\theta_{t+1} = \theta_t - \alpha \nabla f(\theta_t)$
- **Variants:** Batch, SGD, mini-batch (use mini-batch!)
- **Theory:** Convergence rates depend on function properties

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From theory to practice:

- Tune learning rates carefully
- Scale features properly
- Monitor diagnostics
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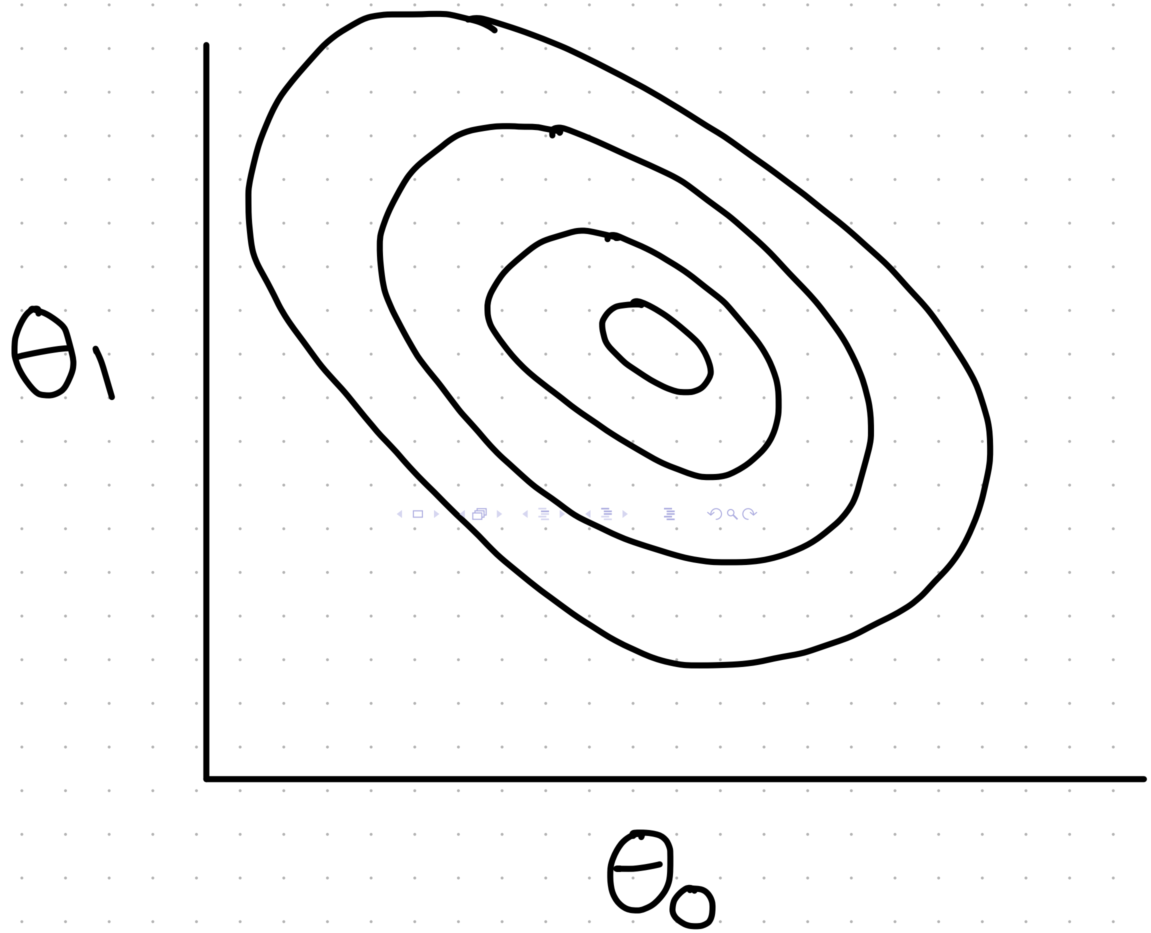
Gradient descent powers modern machine learning!

Deep Dive: Stochastic Gradient Descent Theory

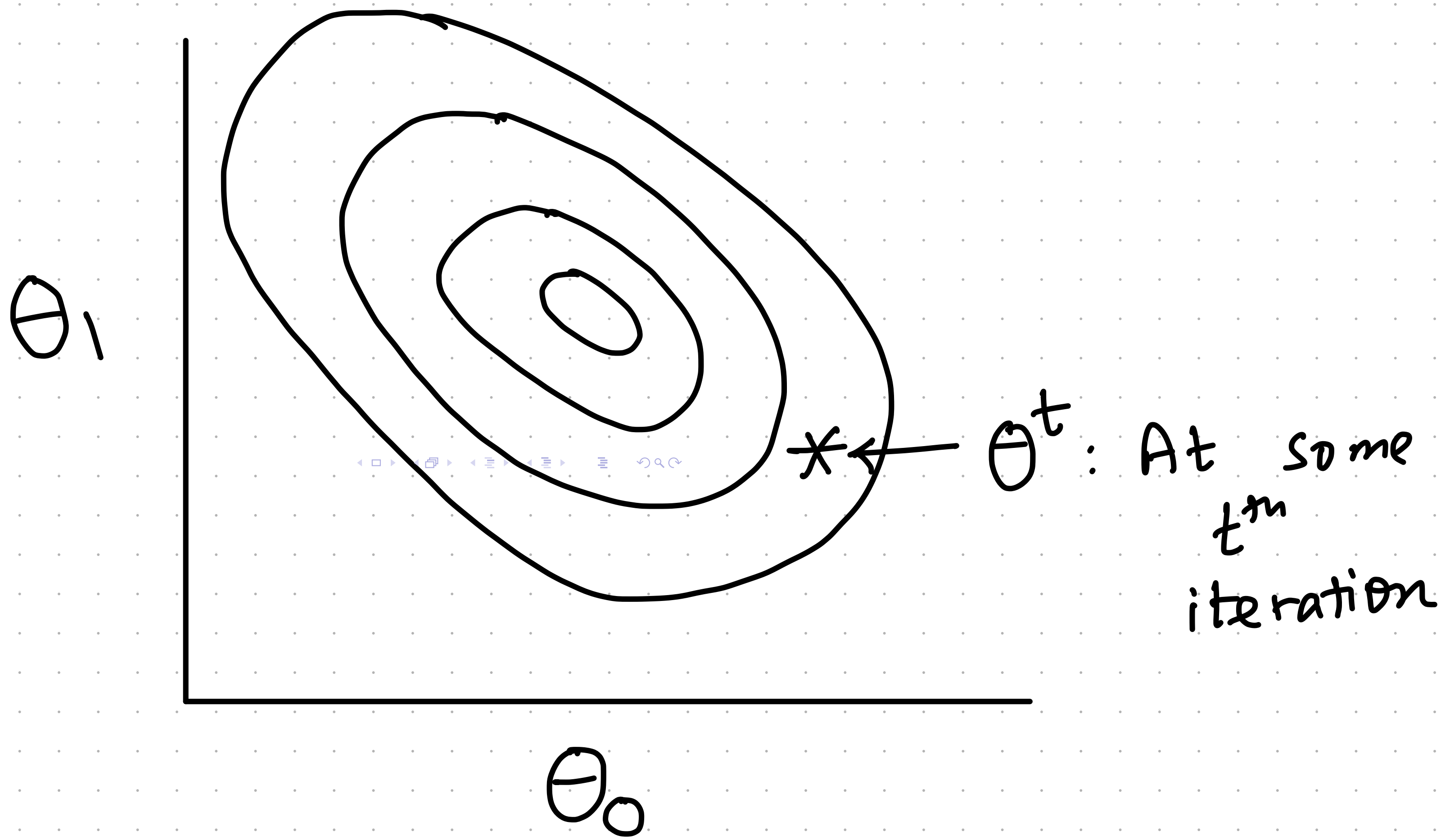
For comprehensive mathematical analysis:

X	y
$— \; x_1^T \; —$	y_1
$\vdots$	
$— \; x_N^T \; —$	y_N

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



LOSS SURFACE OVER 'N' EXAMPLES



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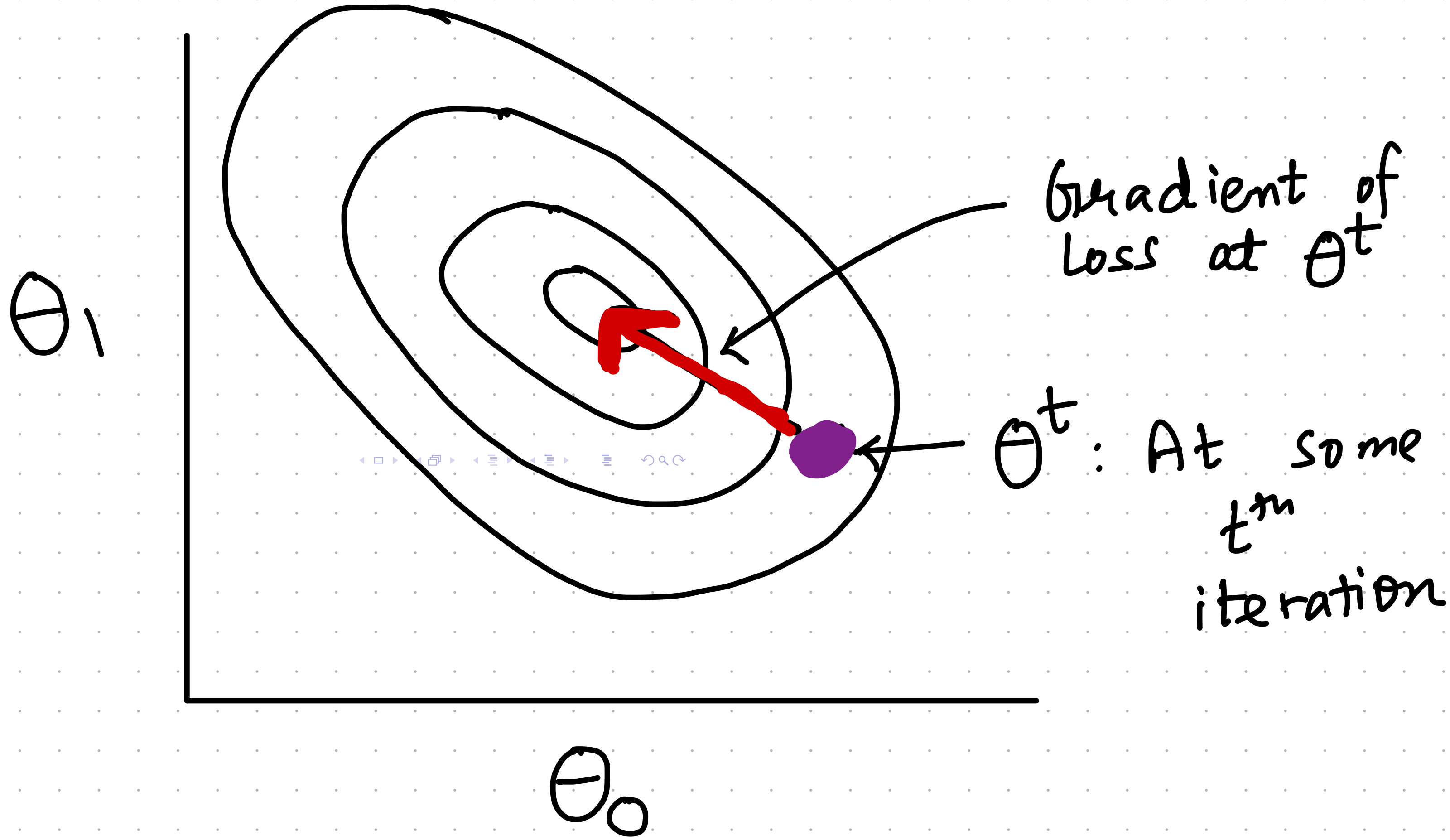

LOSS SURFACE OVER "N" EXAMPLES

Think! Solutions

Think! 1: Why does $-\nabla f$ lead toward minimum?
The gradient $\nabla f(\mathbf{x})$ points in direction of steepest *ascent*. To *descend* (minimize), we go in the opposite direction: $-\nabla f(\mathbf{x})$.

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Think! 2: Why might $\alpha > 2/L$ cause divergence?
For quadratic $f(x) = \frac{L}{2}x^2$, we have $f'(x) = Lx$. The update becomes:
$x_{t+1} = x_t - \alpha L x_t = (1 - \alpha L)x_t$.
If $\alpha L > 2$, then $|1 - \alpha L| > 1$, causing the sequence to diverge.

Pop Quiz Solutions

Pop Quiz #1: For 1000 samples, batch size 50:

1. Mini-batch iterations per epoch: $1000/50 = 20$
2. If SGD takes 1000 epochs, mini-batch might take ≈ 50 epochs (rough estimate)
3. SGD is noisier because it uses only 1 sample per update vs. all samples for batch GD

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Additional insight: The noise in SGD can actually help escape local minima in non-convex optimization problems!

References & Further Reading

Essential references:

- Boyd & Vandenberghe: *Convex Optimization*
- Nocedal & Wright: *Numerical Optimization*
- Goodfellow et al.: *Deep Learning*, Chapters 4 & 8

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Interactive resources:

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