Optimization Algorithms in Deep Learning

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Recap: Regression and Classification

Supervised Learning: General Framework

- **Goal:** Learn (estimate) a function $f(\mathbf{x}; \mathbf{w})$ that maps several input features $\mathbf{x}$ to an output variable y.

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- **Prediction:** Once $\hat{\mathbf{w}}$ is obtained, use

$$\hat{y} = f(\mathbf{x}; \hat{\mathbf{w}})$$

for new input $\mathbf{x}$.

Regression Models

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- **Ordinary Least Squares (OLS) solution:**

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

where

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- **Important Note**: For all regression types of problems, we might not get the closed-form expressions of $\hat{\mathbf{w}}$.

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- **Prediction:** Assign the class with the highest predicted probability

$$\hat{y}_i = \arg \max_{k \in \{1, \dots, K\}} P(Y = k \mid \mathbf{x}_i, \mathbf{w})$$

Role of Gradients and Hessians in Optimization

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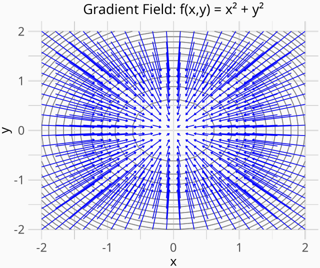

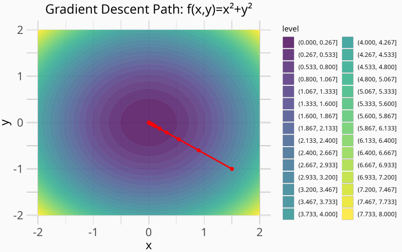

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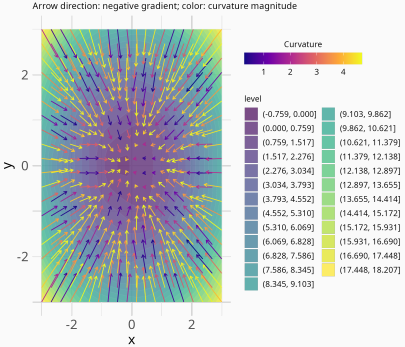

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Famous Optimization Algorithms Used in Deep Learning

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- **Scalability:** Mini-batch version enables training on massive datasets

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- $\boldsymbol{w}$: Model parameters (e.g., weights)
- $\mathcal{L}(\boldsymbol{w})$: Loss function (e.g., Mean Squared Error, Log Loss)
- η: Learning rate (step size)
- $\nabla_w \mathcal{L}(\boldsymbol{w})$: Gradient (direction of steepest ascent)

Gradient Descent: The Core Idea

- **Goal:** Minimize a loss function $L(w)$ to find the best model parameters w for regression/classification.
- **Intuition:** Find the lowest point in a valley by always walking downhill.

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Motivation: Fundamental algorithm for training models like Linear Regression and Logistic Regression.

Batch Gradient Descent: The Standard Version

Algorithm:

1. Initialize parameters $\boldsymbol{w}$ randomly.
2. **Compute Gradient** over the **entire dataset**:

$$\nabla_w \mathcal{L}(\boldsymbol{w}) = \frac{1}{n} \sum_{i=1}^{n} \nabla_w \text{Loss}(f_w(\boldsymbol{x}^{(i)}), y^{(i)})$$

3. **Update:** $\boldsymbol{w} = \boldsymbol{w} - \eta \nabla_w \mathcal{L}(\boldsymbol{w})$
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Characteristics:

- ✓ **Pros:** Stable convergence. Guaranteed for convex functions.
- × **Cons:** Very slow for large datasets. One update requires a full data pass.

Stochastic Gradient Descent (SGD)

Core Idea: Use a **single, random** training example $(\boldsymbol{x}^{(i)}, y^{(i)})$ to compute a noisy gradient.

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Algorithm per Epoch (one complete pass through data):

1. Shuffle the entire dataset.
2. For each example (input) i in the dataset:
   2.1 Compute gradient for one example: $\nabla_w \mathcal{L}(\boldsymbol{w}; \boldsymbol{x}^{(i)}, y^{(i)})$
   2.2 Update immediately: $\boldsymbol{w} = \boldsymbol{w} - \eta \nabla_w \mathcal{L}(\boldsymbol{w}; \boldsymbol{x}^{(i)}, y^{(i)})$

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Key Properties:

- ✓ **Pros:** Extremely fast per update. Can escape local minima due to noise.
- × **Cons:** Very noisy path. Loss may fluctuate heavily. Harder to converge precisely.

Mini-batch Gradient Descent

Core Idea: The best compromise. Use a small random subset (a **mini-batch**) of size b to compute the gradient.

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Key Properties:

- ✓ **Pros:** Efficient and leverages GPU parallelism. More stable than SGD.
- × **Cons:** Introduces the batch size b as a new hyperparameter to tune.

Comparison: GD, SGD, and Mini-batch GD

Criterion	Batch GD	Stochastic GD	Mini-batch GD
Gradient	Full dataset	Single example	Small batch (b)
Speed/Update	Slow	Very Fast	Fast
Stability	Smooth	Noisy	Moderate
Memory	High	Low	Medium
Parallelization	Difficult	No	Excellent
Use Case	Small datasets	Large datasets	Deep Learning

Conclusion: For most modern machine learning tasks, especially deep learning, Mini-batch Gradient Descent is the preferred algorithm.