# Introduction to Optimization in Machine Learning

Course:
INFO-6154 Data Science and Machine Learning

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# What Is Optimization in ML?

Optimization is the mathematical process of adjusting model parameters to minimize a specific objective function, known as the **loss function**. In machine learning, this is how models *learn from data*.

### Gradient Descent Flow (from scratch)

```python
# Loss function: f(x) = (x - 3)^2
x = 0                          # Initial guess
lr = 0.1                       # Learning rate
for i in range(10):
    grad = 2 * (x - 3)         # Derivative of f(x)
    x -= lr * grad             # Update step
```

# What Is Optimization in ML?

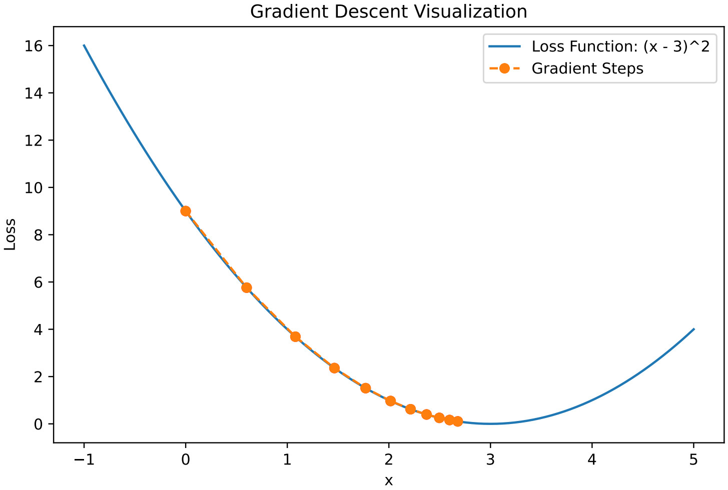
**Definition**

In the context of machine learning, **optimization** refers to the process of finding the best model parameters that minimize (or maximize) a predefined loss function on the training data.

**Why is it essential for model training?**

- Without optimization, models cannot adjust to learn from data.
- All training procedures – from linear regression to deep neural networks – rely on optimization algorithms to adjust weights.
- The quality of the optimization directly affects model performance.

# What Is Optimization in ML?



# What Is Optimization in ML?

**Insight**

Optimization is not a post-processing step – it *is* the core of the learning process itself.

**Optimization vs. Inference**

- **Optimization** happens during training: finding the best parameters.
- **Inference** happens during testing/deployment: using the learned parameters to make predictions.
- The optimization phase enables inference to work properly.

**Note**

Do not confuse model *training* (which involves optimization) with *using* the model (inference).

# Key Components of Optimization

1. **Loss Function**
   - Measures how far predictions are from the true values.
   - Defines the objective to minimize.
   - Common examples: Mean Squared Error (MSE), Cross-Entropy Loss.
2. **Model Parameters**
   - The internal values (like weights) that the model adjusts during training.
   - These are what optimization seeks to improve.
3. **Optimizer**
   - The algorithm that updates model parameters based on the loss.
   - Examples: Gradient Descent, Adam, RMSProp.
4. **Training Data**
   - The source of feedback for optimization.
   - Includes features $X$ and true labels $Y$.

# Key Components of Optimization

## All Key Components in One View

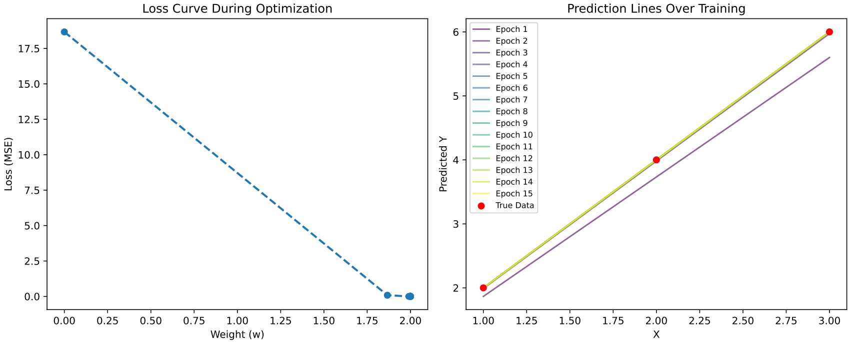
```
# 1. Training Data
X = [1, 2, 3]
Y = [2, 4, 6]  # True values

# 2. Parameters (initialize weight)
w = 0.0

# 3. Loss Function: MSE
def loss(w):
    return sum((w*x - y)**2 for x, y in zip(X, Y)) / len(X)

# 4. Optimizer: Gradient Descent
lr = 0.1
for _ in range(10):
    grad = sum(2 * x * (w*x - y) for x, y in zip(X, Y)) /
        len(X)
    w = w - lr * grad
```

# Key Components of Optimization



# Key Components of Optimization

## Real-World Example: AI for Medical Diagnosis

- **Loss Function** – Penalizes incorrect diagnosis (e.g., missing a cancer case).
- **Parameters** – Weights in the neural network that analyze CT scans.
- **Optimizer** – Algorithm adjusting weights to reduce false negatives.
- **Training Data** – Thousands of labeled scans (e.g., benign vs. malignant).

## Insight

Well-optimized AI models in healthcare reduce diagnostic errors and improve early detection rates.

# Types of Problems Optimization Solves in ML

Optimization in machine learning is not limited to one kind of task – it underpins a wide variety of problems by defining and minimizing suitable loss functions.

**1. Classification**

- Predicting discrete categories (e.g., spam vs. not spam, positive vs. negative).
- **Common Loss**: Cross-Entropy Loss.
- **Example**: Classifying skin lesions as benign or malignant from dermoscopic images.

**2. Regression**

- Predicting continuous values.
- **Common Loss**: Mean Squared Error (MSE).
- **Example**: Predicting house prices or ICU patient length-of-stay.

# Types of Problems Optimization Solves in ML

## Comparing Loss Types in Classification

```
# Predicted probabilities from sigmoid
preds = 1 / (1 + np.exp(-w * X))

# Mean Squared Error
mse = np.mean((preds - labels)**2)

# Cross-Entropy Loss
ce = -np.mean(labels * np.log(preds) +
              (1 - labels) * np.log(1 - preds))
```

## Warning

Applying the wrong loss type (e.g., using regression loss for a classification task) can cause the optimizer to converge on meaningless or harmful solutions.

# Practical Failures of Optimization

Even with well-designed models and datasets, optimization can fail in subtle or catastrophic ways. Understanding these pitfalls is crucial for diagnosing poor model performance.

**1. Non-Convergence**

- The optimizer fails to reduce the loss meaningfully.
- Can be caused by a poor learning rate, bad initialization, or vanishing/exploding gradients.
- **Example**: Deep CNN on X-ray images not improving due to poor learning rate scheduling.

**2. Stuck in Local Minima or Saddle Points**

- The model reaches a point where gradients are small but performance is poor.
- Especially problematic in non-convex functions like those in neural networks.

# Practical Failures of Optimization

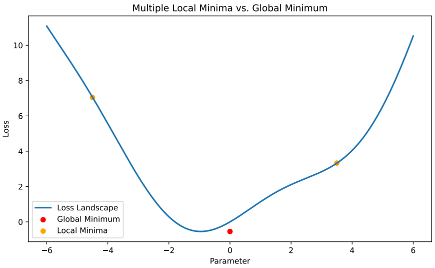



Figure 1: *

Local Minima vs Global Minimum

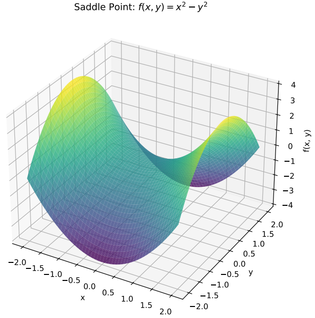


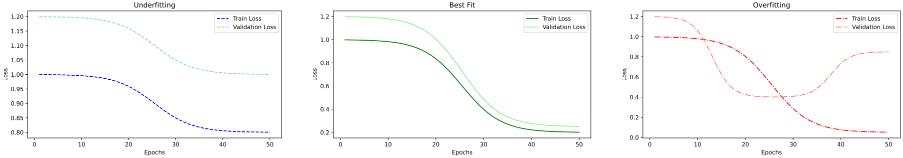

Figure 2: *

Saddle Point Landscape

# Practical Failures of Optimization

## 3. Overfitting

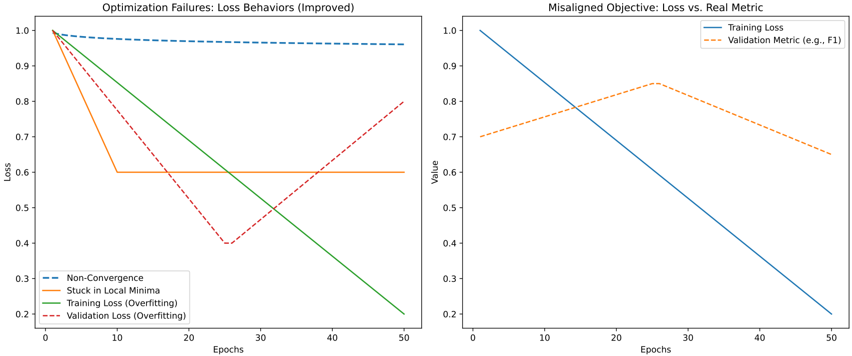
- The optimizer fits the training data too well, harming generalization.
- Caused by overtraining or lack of regularization.
- **Example**: A fraud detection model that performs perfectly on historical data but fails in deployment.



# Practical Failures of Optimization

**4. Misaligned Objectives**

- The loss being minimized doesn't match the real-world goal.
- **Example**: Optimizing for accuracy in a highly imbalanced cancer screening dataset.
- Real goal may be sensitivity or F1 score, not raw accuracy.



# Practical Failures of Optimization

## Key Pitfalls to Watch For

- Loss decreases, but validation performance is poor.
- Model performs well on paper but fails in production.
- Training behaves erratically with large gradients or exploding loss.

## Tip

Always monitor both training and validation metrics. Use visualizations like loss curves to catch optimization issues early.

# Real-World Problem Framing and Optimization

Many machine learning projects fail not because of poor models – but because the problem was *framed incorrectly* from the start.

**Why framing matters:**

- The way we define the prediction target, features, and loss function shapes the entire optimization process.
- A misaligned problem frame leads to optimizing the wrong thing.

**Common Mistakes in Problem Framing**

- Predicting a variable that cannot be reliably measured.
- Using poor proxies (e.g., clicks instead of satisfaction).
- Treating subjective or noisy data as ground truth.
- Ignoring domain-specific constraints (e.g., false positives in healthcare).

**Example: Predicting Hospital Readmissions**

- Goal: Reduce costly and preventable readmissions.
- Naive label: Any readmission within 30 days.

# Real-World Problem Framing and Optimization

- Problem: Some readmissions are medically necessary or unrelated.
- Result: Optimizer penalizes the model for clinically valid outcomes.

**Takeaway**

Bad framing leads to bad labels, bad loss functions, and ultimately – bad models.

**Role of Domain Expertise**

- Helps define meaningful prediction targets.
- Guides which features to include or exclude.
- Informs what types of errors are tolerable or critical.

**Best Practice**

Start every ML project with a clearly defined real-world objective and discuss how it will be reflected in your loss function and data structure.

# Examples and Mini Case Studies

Letâs explore how optimization decisions play out in real-world projects – especially when the loss function does not align well with actual goals.

**Case Study 1: Customer Churn Prediction**

- **Business Goal**: Retain high-value customers to reduce revenue loss.
- **Naive ML Goal**: Predict if a customer will churn (binary classification).
- **Common Pitfall**: Optimizing for log-loss or AUC, regardless of customer value.
- **Better Framing**: Weight the loss function by customer lifetime value (CLV).

# Examples and Mini Case Studies

**Optimization Adjustment**

Instead of treating all churns equally, the loss could penalize errors on high-value customers more heavily.

**Case Study 2: Fraud Detection**

- **Business Goal**: Catch fraudulent transactions while minimizing friction for real users.
- **Naive ML Goal**: Minimize classification error.
- **Challenge**: Fraud cases are rare and false positives harm user experience.
- **Better Framing**: Optimize for precision-recall balance or F1 score. Use cost-sensitive loss if available.

# Examples and Mini Case Studies

**Impact**

Aligning the optimization objective with business priorities significantly improves model utility and adoption.

**Tip**

Don’t rely solely on off-the-shelf loss functions. Customize your optimization objective to match the problemâs real-world context.

# Takeaways: Setting the Right Optimization Mindset

Understanding optimization is more than just knowing algorithms – itâs about having the right mindset when designing and training models.

**Key Conceptual Shifts**

- **Loss** is what the model optimizes – not necessarily what we care about.
- **Metric** is what we report – it may not guide training unless we make it part of the loss.
- **Optimization** is not interpretation – the most accurate model may be the least explainable.

**Warning**

A model learns what you tell it to optimize – not what you wish it would learn.

# Takeaways: Setting the Right Optimization Mindset

**Good Optimization Practice Starts With:**

- Framing the problem in real-world terms.
- Choosing a loss function that reflects your goal.
- Anticipating practical failures during training.

**Closing Thought**

Before you optimize a model, make sure you're solving the right problem – with the right signal.