

# STAT 4830: Numerical optimization for data science and ML

Lecture 0: Introduction

Professor Damek Davis

# Course overview

- **Focus:** Numerical optimization for data science and ML
- **Tools:** PyTorch, Python, occasional use of other libraries
- **Format:** Lecture-based
- **Final Project:** Incrementally developed throughout semester

# Prerequisites

- Basic calculus and linear algebra (Math 2400)
- Basic probability (Stat 4300)
- Python programming experience
- No advanced optimization/ML background needed

# Why PyTorch?

- Modern auto-differentiation frameworks drive deep learning success
- Enables rapid experimentation with:
  - New model architectures and
  - Novel optimization algorithms
- More flexible than traditional solver-based tools

# Preview: spam classification

Let's start with a practical example:

- How do we automatically filter spam emails?
- Demonstrates core optimization concepts
- Shows PyTorch in action

# How computers read email

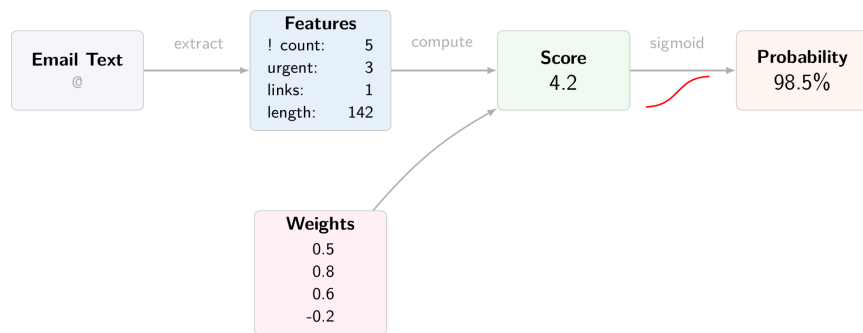
```
email1 = ""  
Subject: URGENT! You've won $1,000,000!!!  
Dear Friend! Act NOW to claim your PRIZE money!!!  
""  
  
email2 = ""  
Subject: Team meeting tomorrow  
Hi everyone, Just a reminder about our 2pm sync.  
""
```

# Feature extraction

Convert text to numbers:

```
def extract_features(email):
    features = {
        'exclamation_count': email.count('!'),
        'urgent_words': len(['urgent', 'act now', 'prize']
                            & set(email.lower().split())),
        'suspicious_links': len([link for link in email.split()
                                if 'www' in link]),
        'time_sent': email.timestamp.hour,
        'length': len(email)
    }
    return features
```

# Classification process



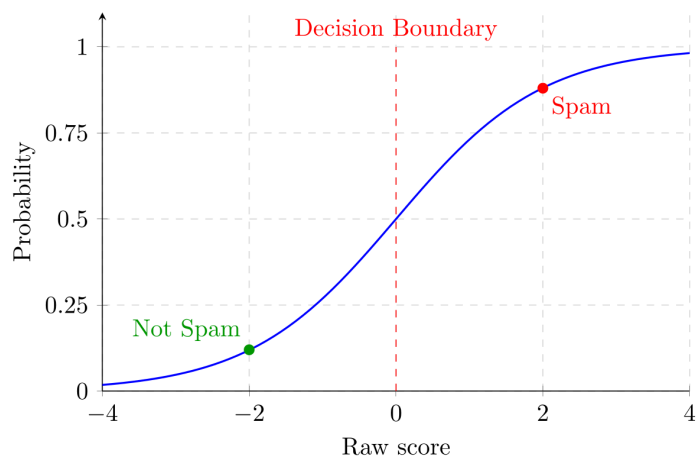
1. Extract numeric features
2. Multiply by weights
3. Sum weighted features
4. Convert to probability



# The sigmoid function

Converts any number into a probability (0-1):

```
def sigmoid(x):  
    return 1 / (1 + torch.exp(-x))
```



# Mathematical formulation

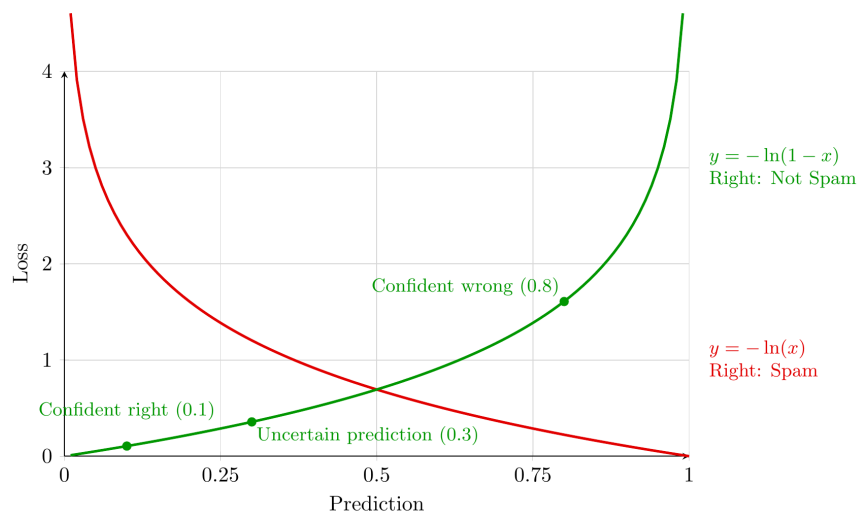
Our optimization problem:

$$\min_w \frac{1}{n} \sum_{i=1}^n [-y_i \log(\sigma(x_i^\top w)) - (1 - y_i) \log(1 - \sigma(x_i^\top w))]$$

Where:

- $w$  = weights vector
- $x_i$  = feature vector
- $y_i$  = true label (0/1)
- $\sigma$  = sigmoid function

# Cross-entropy loss

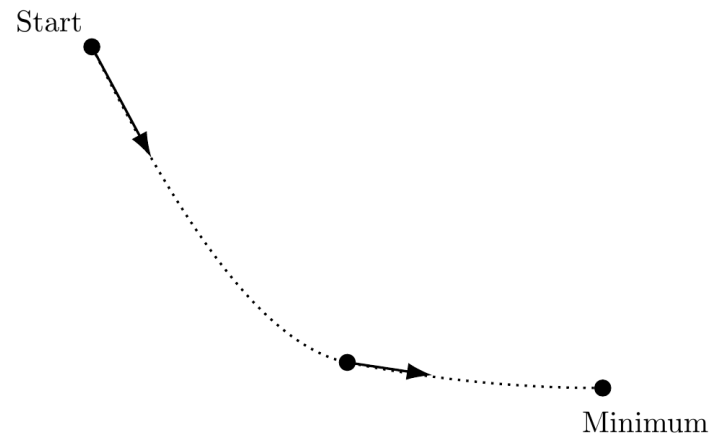


- Penalizes wrong predictions
- Rewards confident correct predictions
- Creates balanced learning

# How Gradient Descent Works

The optimization process works like hiking:

1. Look around you (measure gradient)
2. Take a step downhill
3. Repeat until you reach the bottom



# The optimization loop

Each iteration:

1. **Measure** how well current weights classify emails
2. **Calculate** gradient (direction of steepest error reduction)
3. **Update** weights by stepping in this direction
4. **Repeat** until convergence

The learning rate controls step size:

- Too small → slow progress
- Too large → overshooting

# PyTorch: What, how, and why

**What:** Modern framework for optimization and deep learning

**How:**

- Tracks operations in a computational graph
- Automatically computes gradients
- Enables parallel computation (CPU/GPU)

**Why:**

- Automates the hardest part (gradients)
- Makes experimentation fast
- Scales from simple to complex models

# Inside PyTorch: Tensors and autograd

```
# Tensors: The building blocks
x = torch.tensor([1.0, 2.0], requires_grad=True)
y = x * 2
z = y.sum()

# Automatic differentiation
z.backward() # Computes gradients
print(x.grad) # Shows  $\partial z / \partial x$ 
```

PyTorch builds a graph of operations, enabling automatic gradient computation.

# Implementation in PyTorch

```
# Initialize
weights = torch.randn(5, requires_grad=True)
learning_rate = 0.01

for _ in range(1000):
    # Forward pass
    predictions = spam_score(features, weights)
    loss = cross_entropy_loss(predictions, true_labels)

    # Backward pass
    loss.backward()

    # Update weights
    with torch.no_grad():
        weights -= learning_rate * weights.grad
        weights.grad.zero_()
```

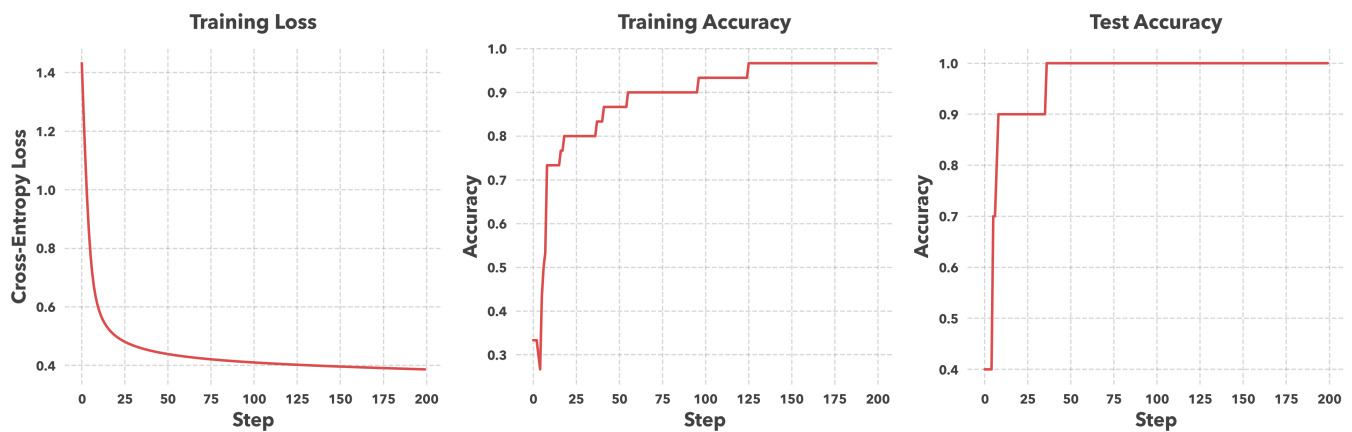


# Try it yourself!

 [Open in Colab](#)

- Complete implementation in the notebook
- Experiment with different learning rates
- See how the loss changes during training
- Test the model on new emails

# Training results



Three key metrics:

- **Loss** and **Training accuracy**: Performance on known data.
- **Test accuracy**: Performance on new emails

# Course structure

1. Linear algebra & direct methods
2. Problem formulations & classical software
3. Calculus for optimization
4. Automatic differentiation & PyTorch
5. First-order methods
6. Second-order methods
7. Advanced topics
8. Modern deep learning practice

# Learning outcomes

By course end, you'll be able to:

1. Model real problems as optimization problems
2. Select appropriate algorithms
3. Implement solutions in PyTorch
4. Apply optimization to practical problems
5. Conduct optimization research

# Getting started

- Review the syllabus
- Set up Python environment
- Try the [Colab notebook](#)
- Start thinking about project ideas

# Questions?

- Course website: <https://damek.github.io/STAT-4830/>
- Office hours: Listed on the course website
- Email: [damek@wharton.upenn.edu](mailto:damek@wharton.upenn.edu)
- Discord: Check email for invite.