STAT 4830: Numerical optimization for data science and ML

Lecture 4: How to compute gradients in PyTorch

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Manual Gradient Computation

Consider computing this gradient by hand:

$$f(w) = \frac{1}{2}\|\tanh(W_2\mathrm{ReLU}(W_1x + b_1) + b_2) - y\|^2$$

annoying

Automatic Differentiation

PyTorch provides:

```
# Define complex function
def f(x, W1, b1, W2, b2):
    h = torch.relu(W1 @ x + b1)
    return 0.5 * torch.sum(
        (torch.tanh(W2 @ h + b2) - y)**2
    )

# Get gradient automatically
f.backward()
```

Key benefits:

1. Automatic gradient computation
2. Handles any differentiable function
3. Memory efficient implementation
4. Scales to large problems

Three Key Ideas

1. **Computational Graph**
2. **Reverse-Mode Differentiation**
3. **Memory-Efficient Implementation**

Outline

1. Computing Gradients

```
Function → Graph → Gradient
```

2. Gradient Descent

```
Gradient → Update → Repeat
```

3. Neural Networks

```
Features → Layers → Loss
```

A Simple Example: Polynomial Function

Let's start with a one-dimensional function:

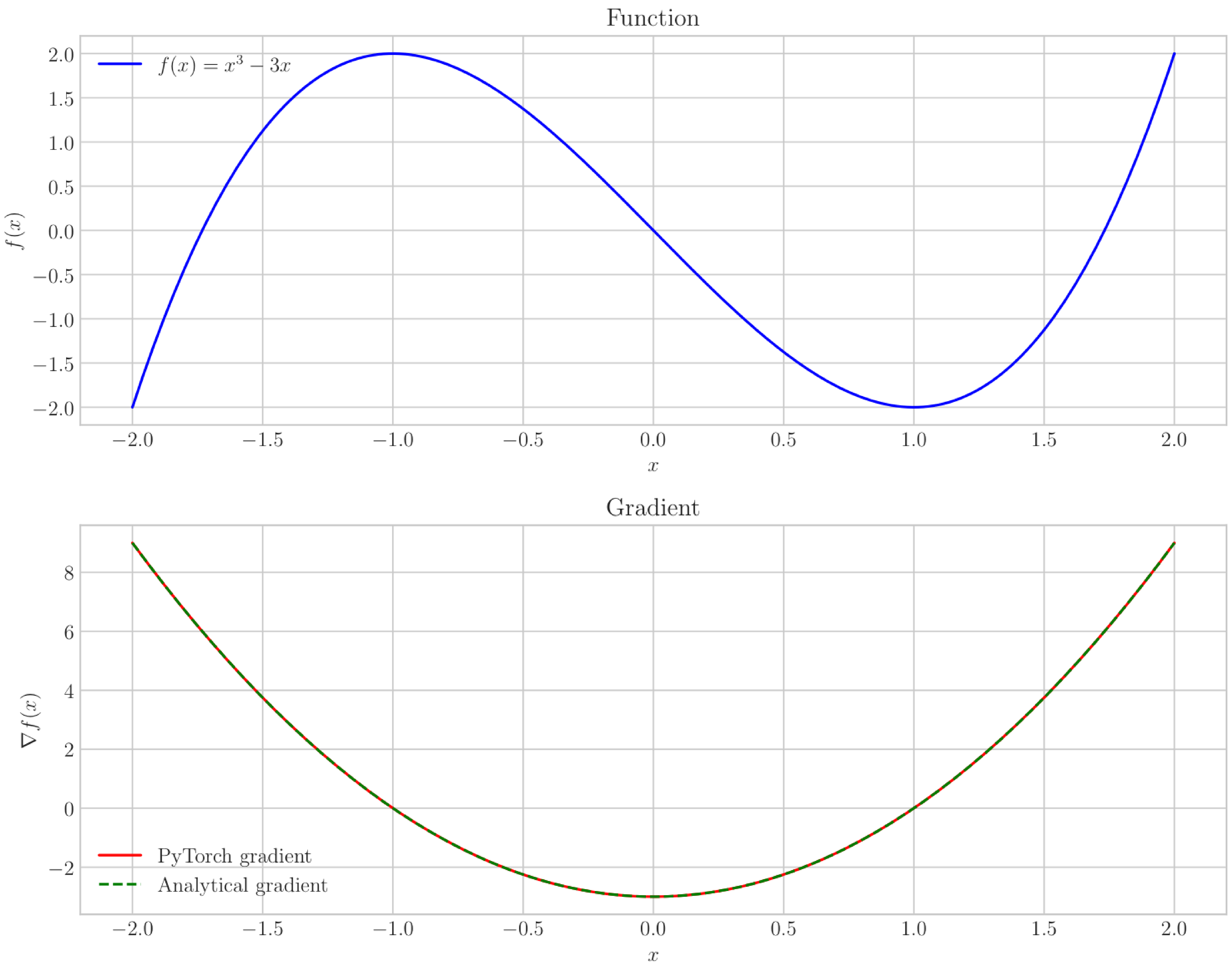
$$f(x) = x^3 - 3x$$

Manual gradient computation:

$$\frac{d}{dx} f(x) = 3x^2 - 3$$

PyTorch automates this:

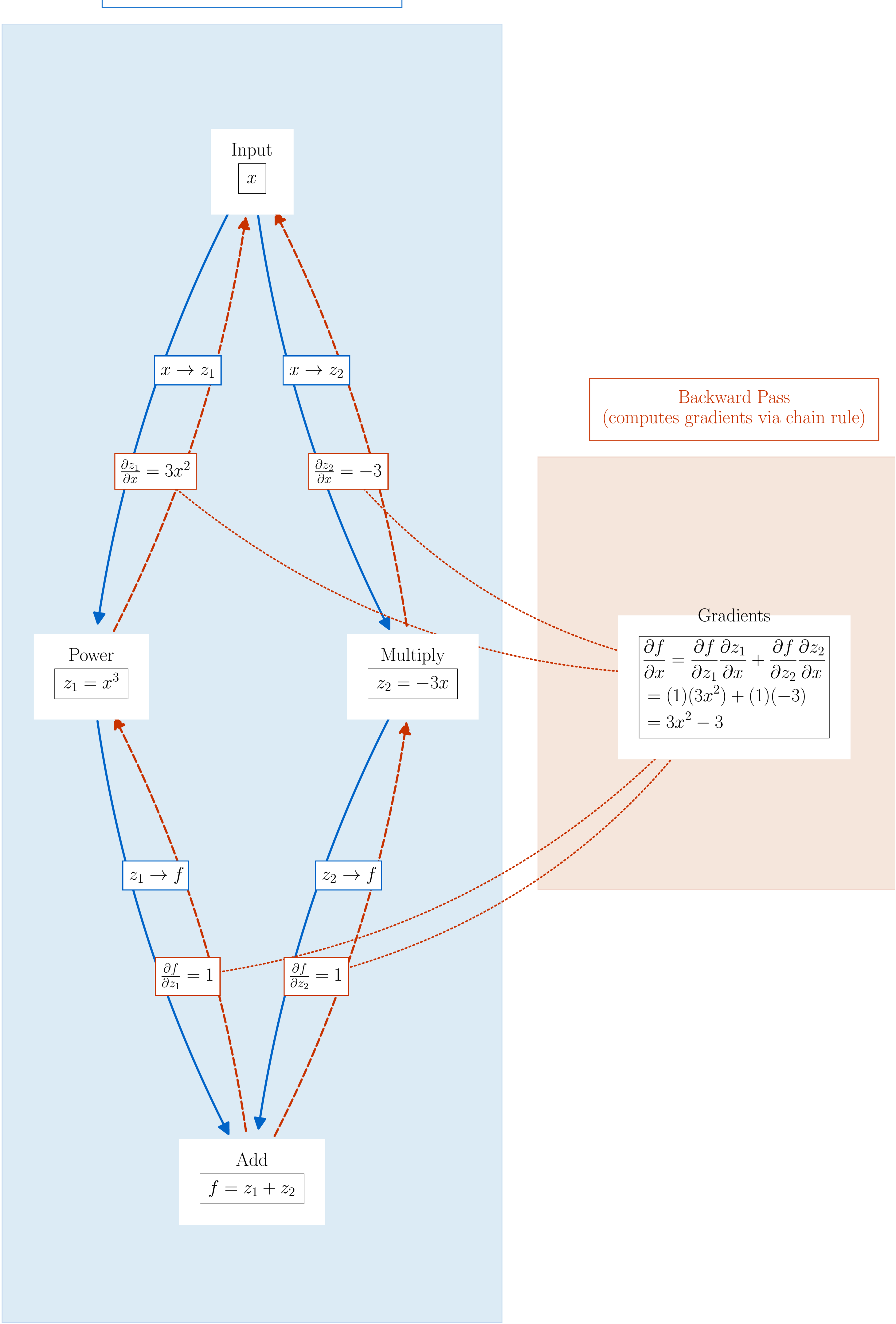
```
x = torch.tensor([1.0], requires_grad=True) # Gradient Tracking
y = x**3 - 3*x # Forward Pass
y.backward() # Backward Pass
print(f"f'(1) = {x.grad}") # Gradient Access
```


Function
$f(x) = x^3 - 3x$
$f(x)$
x
Gradient
PyTorch gradient
Analytical gradient
$\nabla f(x)$
x

How does PyTorch do this?

- **Forward pass:** When you evaluate a function, PyTorch computes a *computational graph* that records all operations like addition, multiplication, powers, etc.
- **Backward pass:** PyTorch traverses the graph in reverse order to compute the gradient, using what is essentially an efficient implementation of the chain rule.

The graph



Input
x
$x \to z_1$
$x \to z_2$
$\frac{\partial z_1}{\partial x} = 3x^2$
$\frac{\partial z_2}{\partial x} = -3$
Backward Pass
(computes gradients via chain rule)
Power
$z_1 = x^3$
Multiply
$z_2 = -3x$
Gradients
$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial z_1}\frac{\partial z_1}{\partial x} + \frac{\partial f}{\partial z_2}\frac{\partial z_2}{\partial x}$
$= (1)(3x^2) + (1)(-3)$
$= 3x^2 - 3$
$z_1 \to f$
$z_2 \to f$
$\frac{\partial f}{\partial z_1} = 1$
$\frac{\partial f}{\partial z_2} = 1$
Add
$f = z_1 + z_2$

Building the Computational Graph

Each node in the graph:

- Stores output value from forward pass
- Contains function for local gradients
- Maintains references to inputs

For $f(x) = x^3 - 3x$, we build:

1. Input node storing x
2. Power node computing $z_1 = x^3$
3. Multiply node computing $z_2 = -3x$
4. Add node forming $f = z_1 + z_2$

Computing Gradients: The Process

Starting State:

- Initialize $\frac{\partial f}{\partial f} = 1$ at output
- All other gradients start at 0

Algorithm:

1. Process nodes in reverse order
2. Compute local gradients
3. Multiply by incoming gradient
4. Add to input gradients

backward(): Step by Step

1. Output Node ($f = z_1 + z_2$):

- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial z_1} = 1$, $\frac{\partial f}{\partial z_2} = 1$
- Propagate to both input nodes

2. Power Node ($z_1 = x^3$):

- Incoming gradient: 1
- Local gradient: $\frac{\partial z_1}{\partial x} = 3x^2$
- Contribute: $\frac{\partial f}{\partial x} \mathrel{+}= (1)3x^2$

3. Multiply Node ($z_2 = -3x$):

- Incoming gradient: 1
- Local gradient: $\frac{\partial z_2}{\partial x} = -3$
- Contribute: $\frac{\partial f}{\partial x} \mathrel{+}= (1)(-3)$

4. Input Node (x):

- Accumulates from both paths
- (-3) from multiply node
- $(3x^2)$ from power node
- Final gradient: $\frac{\partial f}{\partial x} = 3x^2 - 3$

Two Implementation Approaches

1. Using `backward()`

```
# Create graph
x.requires_grad = True
z = g(x)
y = h(z)

# Compute gradients
y.backward()
grad = x.grad  # Stored in tensor
```

Best for:

- Training loops
- Multiple gradients
- Memory efficiency

2. Using `autograd.grad()`

```
# Create graph
x.requires_grad = True
z = g(x)
y = h(z)

# Direct computation
grad = torch.autograd.grad(y, x)[0]
```

Best for:

- One-off gradients
- Direct access
- Higher derivatives

Common Pitfall 1: In-place Operations

Problem:

- In-place operations can break gradient computation
- They modify values needed for backward pass

Example:

```python
x = torch.tensor([4.0], requires_grad=True)
y = torch.sqrt(x)  # y is 2.0
# Need y=2.0 to compute d/dx sqrt(x)=1/(2sqrt(x))

try:
    y.add_(1)  # In-place: y becomes 3.0
    # Original y=2.0 is lost! Can't compute
    # gradient of sqrt anymore
    z = 3 * y
    z.backward()  # Error: lost value needed
except RuntimeError as e:
    print("Error: sqrt needs original output")
```

Solution:

```python
x = torch.tensor([4.0], requires_grad=True)
y = torch.sqrt(x)  # y is 2.0
# Create new tensor, preserving y=2.0
y = y + 1  # y_new is 3.0, but y=2.0 exists
z = 3 * y
z.backward()  # Works: can compute
# d/dx sqrt(x) = 1/(2sqrt(x)) using y=2.0
print(x.grad)  # tensor([0.7500])
# = 3 * 1/(2sqrt(4)) = 3 * 1/4 = 0.75
```

Key point:

- In-place ops destroy values needed for gradient
- Create new tensors to preserve computation graph

Common Pitfall 2: Memory Management

Problem:

- Tracking gradients uses memory
- Not needed during evaluation

Memory inefficient:

```
# Create large tensors
X = torch.randn(1000, 1000,
                requires_grad=True)
y = torch.randn(1000)

# Tracks all computations
loss = ((X @ X.t() @ y - y)**2).sum()
```

Solution:

```
# Disable gradient tracking
with torch.no_grad():
    # No computational graph built
    loss = ((X @ X.t() @ y - y)**2).sum()
```

Key point:

- Use `torch.no_grad()` for evaluation
- Saves memory and computation

Common Pitfall 3: Gradient Accumulation

Problem:

- Gradients accumulate by default
- Multiple backward passes add up

Wrong:

```
x = torch.tensor([1.0], requires_grad=True)
for _ in range(2):
    y = x**2  # grad = 2x
    y.backward()  # Gradients add up!
    x -= 0.1 * x.grad  # Wrong gradient
    print(f"grad: {x.grad}")
# First iter:  2x = 2(1.0) = 2.0
# Second iter: 2x = 2(0.8) = 1.6
#              BUT adds to previous 2.0
#              giving 2.0 + 1.6 = 3.6!
```

Solution:

```
x = torch.tensor([1.0], requires_grad=True)
for _ in range(2):
    y = x**2  # grad = 2x
    y.backward()
    with torch.no_grad():
        x -= 0.1 * x.grad
        x.grad.zero_()  # Clear gradients
    print(f"grad: {x.grad}")
# First iter:  2x = 2(1.0) = 2.0
# Second iter: 2x = 2(0.8) = 1.6
#              Clean gradient!
```

Key point:

- Zero gradients between updates
- Use `zero_grad()` in training loops

Beyond 1d: Least Squares

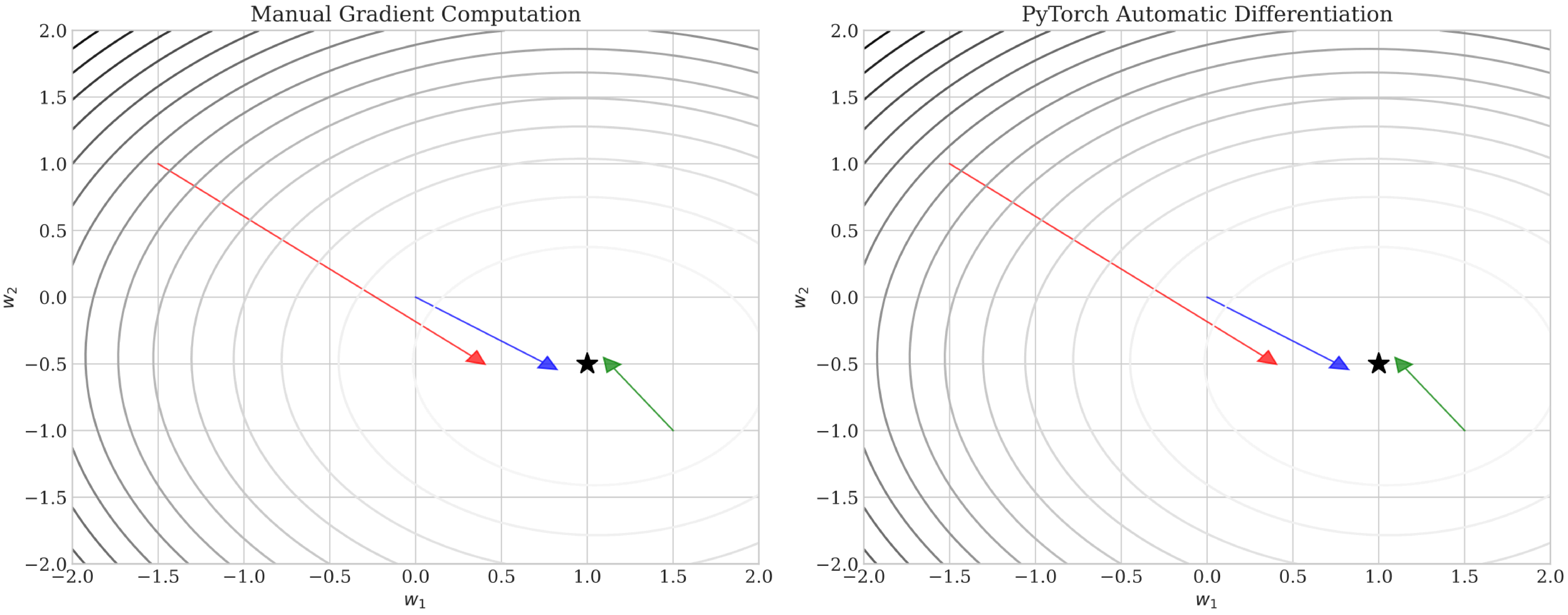
Manual gradient:

$$\nabla f = X^\top (Xw - y)$$

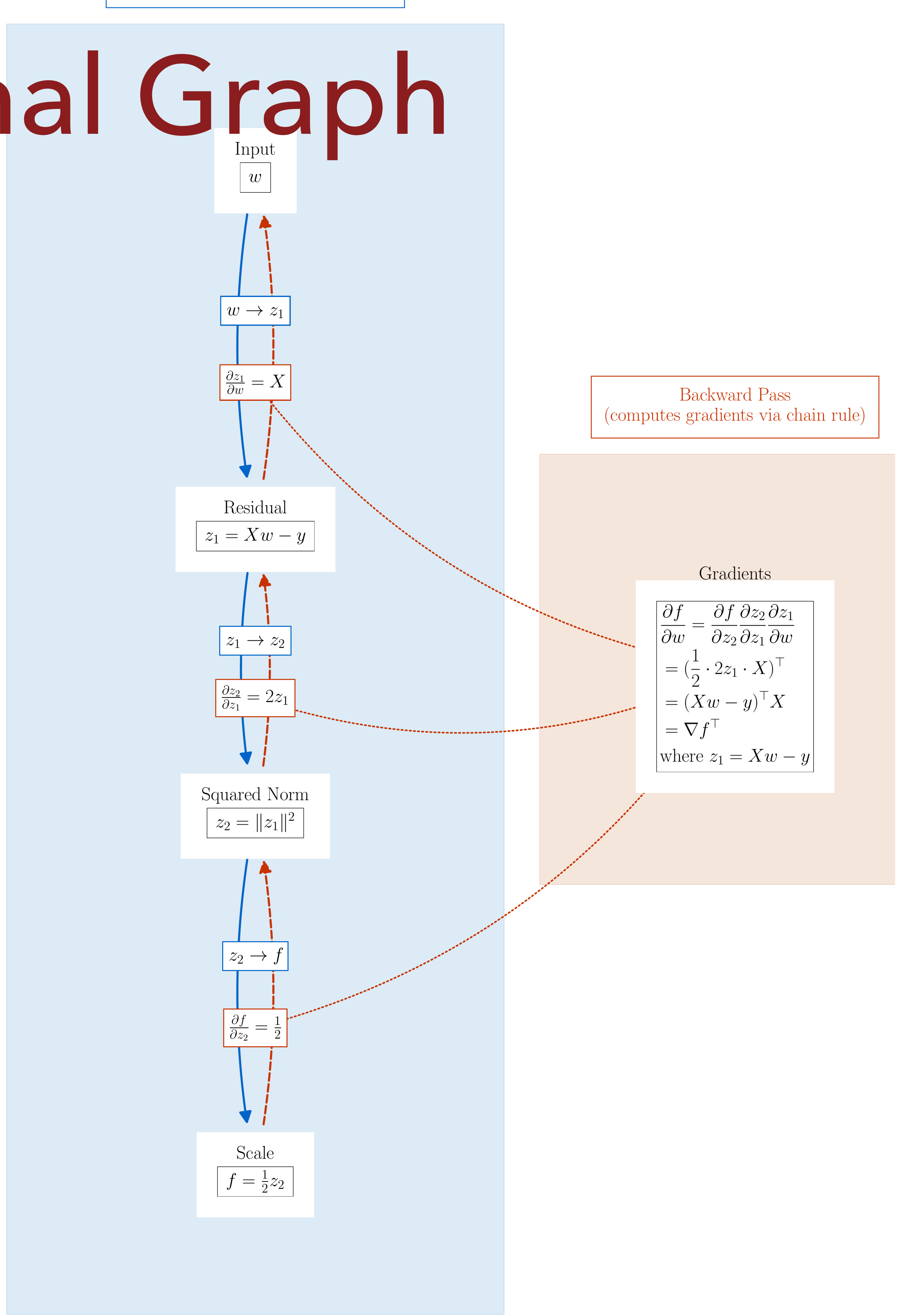
PyTorch gradient:

```
pred = X @ w
loss = 0.5*((pred - y)**2).sum()
loss.backward()
grad = w.grad
```

Agreement between manual and PyTorch



Computational Graph



Building the Least Squares Graph

For $f(w) = \frac{1}{2}\|Xw - y\|^2$, we build:

1. Input nodes storing $\mathbf{w}$
2. Residual node computing $\mathbf{z}_1 = \mathbf{X}\mathbf{w} - \mathbf{y}$
3. Square norm node computing $z_2 = \|\mathbf{z}_1\|^2$
4. Scale node forming $f = \frac{1}{2}z_2$

Computing Gradients: The Process

Subtlety: Total derivative vs gradient (more next time)

Starting State:

- Initialize $\frac{\partial f}{\partial f} = 1$ at output
- All other gradients start at 0

Algorithm:

1. Process nodes in reverse order
2. Compute local gradients
3. Multiply by incoming total derivative
4. Add to input total derivative

Least Squares: backward() Step 1

Output Node ($f = \frac{1}{2} z_2$):

- Incoming gradient: $\frac{\partial f}{\partial f} = 1$ (scalar)
- Total derivative: $\frac{\partial f}{\partial z_2} = \frac{1}{2}$ (scalar)
- Propagate to z_2 node: $\frac{\partial f}{\partial z_2} = \frac{1}{2}$ (1×1 matrix)

Least Squares: backward() Step 2

Square Norm Node ($z_2 = \|\mathbf{z}_1\|^2$):

- Incoming total derivative: $\frac{\partial f}{\partial z_2} = \frac{1}{2}$ (1×1 matrix)
- Local total derivative: $\frac{\partial z_2}{\partial \mathbf{z}_1} = \mathbf{2z}_1^\top$ (1×n matrix)
- Propagate to $\mathbf{z}_1$ node: $\frac{\partial f}{\partial \mathbf{z}_1} = \frac{\partial f}{\partial z_2} \frac{\partial z_2}{\partial \mathbf{z}_1} = \mathbf{z}_1^\top$ (1×n matrix)

Least Squares: backward() Step 3

Residual Node ($\mathbf{z}_1 = \mathbf{X}\mathbf{w} - \mathbf{y}$):

- Incoming total derivative: $\frac{\partial f}{\partial \mathbf{z}_1} = \mathbf{z}_1^\top$ (1×n matrix)
- Local total derivative: $\frac{\partial \mathbf{z}_1}{\partial \mathbf{w}} = \mathbf{X}$ (n×p matrix)
- Total derivative to $\mathbf{w}$ node: $\frac{\partial f}{\partial \mathbf{w}} = \mathbf{z}_1^\top \mathbf{X}$ (1×p matrix)

Least Squares: Final Step

Input Node ($\mathbf{w}$):

- Total derivative: $\frac{\partial f}{\partial \mathbf{w}} = \mathbf{z}_1^\top \mathbf{X}$ (1×p matrix)
- Convert to gradient: $\nabla f = (\frac{\partial f}{\partial \mathbf{w}})^\top = \mathbf{X}^\top \mathbf{z}_1$ (p×1 matrix)

Final computation:

$$\nabla f = \left(\frac{\partial z_1}{\partial w} \frac{\partial z_2}{\partial z_1} \frac{\partial f}{\partial z_2} \right)^\top = \mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

Applying Gradient Descent

Minimize least squares loss:

$$f(w) = \frac{1}{2}\|Xw - y\|^2$$

Manual implementation:

```
def manual_gradient(X, y, w):
    return X.T @ (X @ w - y)

w = torch.zeros(p)  # Initialize
for step in range(max_iters):
    grad = manual_gradient(X, y, w)
    w = w - alpha * grad
```

PyTorch Implementation

Same algorithm, automatic gradients:

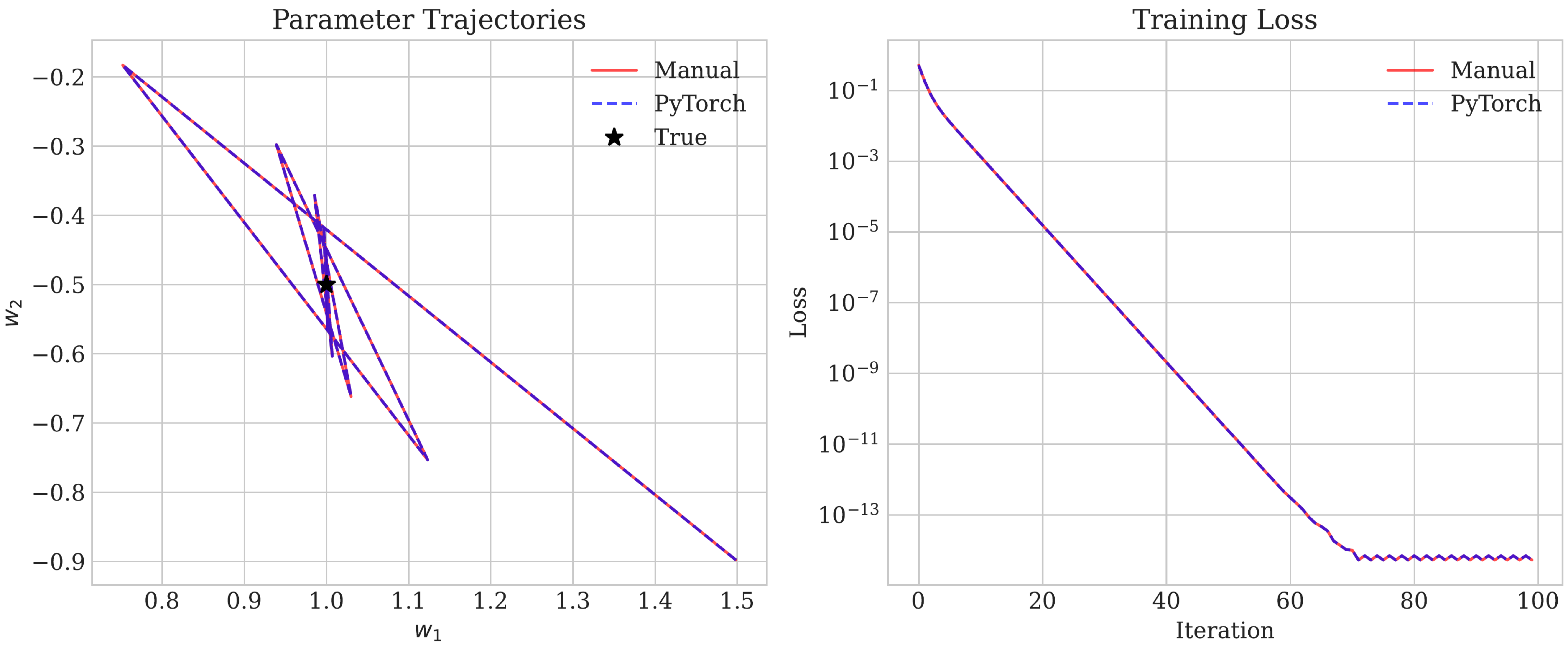
```
w = torch.zeros(p, requires_grad=True) # Initialize weights and require gradients

for step in range(max_iters):
    # Forward pass
    pred = X @ w
    loss = 0.5 * ((pred - y)**2).sum()

    # Backward pass
    loss.backward()

    # Update
    with torch.no_grad(): # Do not modify the computational graph
        w -= alpha * w.grad # update the weights
        w.grad.zero_() # reset the gradient to zero to avoid accumulation
```

Comparison of Approaches



From Linear to Neural Networks

Linear Model:

$$\mathbf{y} = \mathbf{X}\mathbf{w}$$

Neural Network:

$$\mathbf{h} = \tanh(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

$$P(y = 1 \mid x) = \sigma(\mathbf{w}_2^\top \mathbf{h} + b_2)$$

Key differences:

- Multiple transformations
- Nonlinear activations
- Learnable features

Neural Network Architecture

Layer composition:

```
Input → Linear₁ → Tanh → Linear₂ → Sigmoid
ℝᵈ      ℝʰˣᵈ      ℝʰ     ℝ¹ˣʰ      [0,1]
```

Dimensions:

- Input: $\mathbf{x} \in \mathbb{R}^d$
- Hidden: $\mathbf{h} \in \mathbb{R}^h$
- Output: $p \in [0, 1]$

Each layer adds:

- Linear transform
- Nonlinearity
- Learnable parameters

PyTorch Implementation

```
class BinaryClassifier(nn.Module):
    def __init__(self, d=784, h=32):
        super().__init__()
        # ℝᵈ → ℝʰ
        self.linear1 = nn.Linear(d, h)
        # ℝʰ → ℝ
        self.linear2 = nn.Linear(h, 1)

    def forward(self, x):
        # Hidden features
        h = torch.tanh(self.linear1(x))
        # Probability output
        return torch.sigmoid(
            self.linear2(h)
        )
```

Training Loop

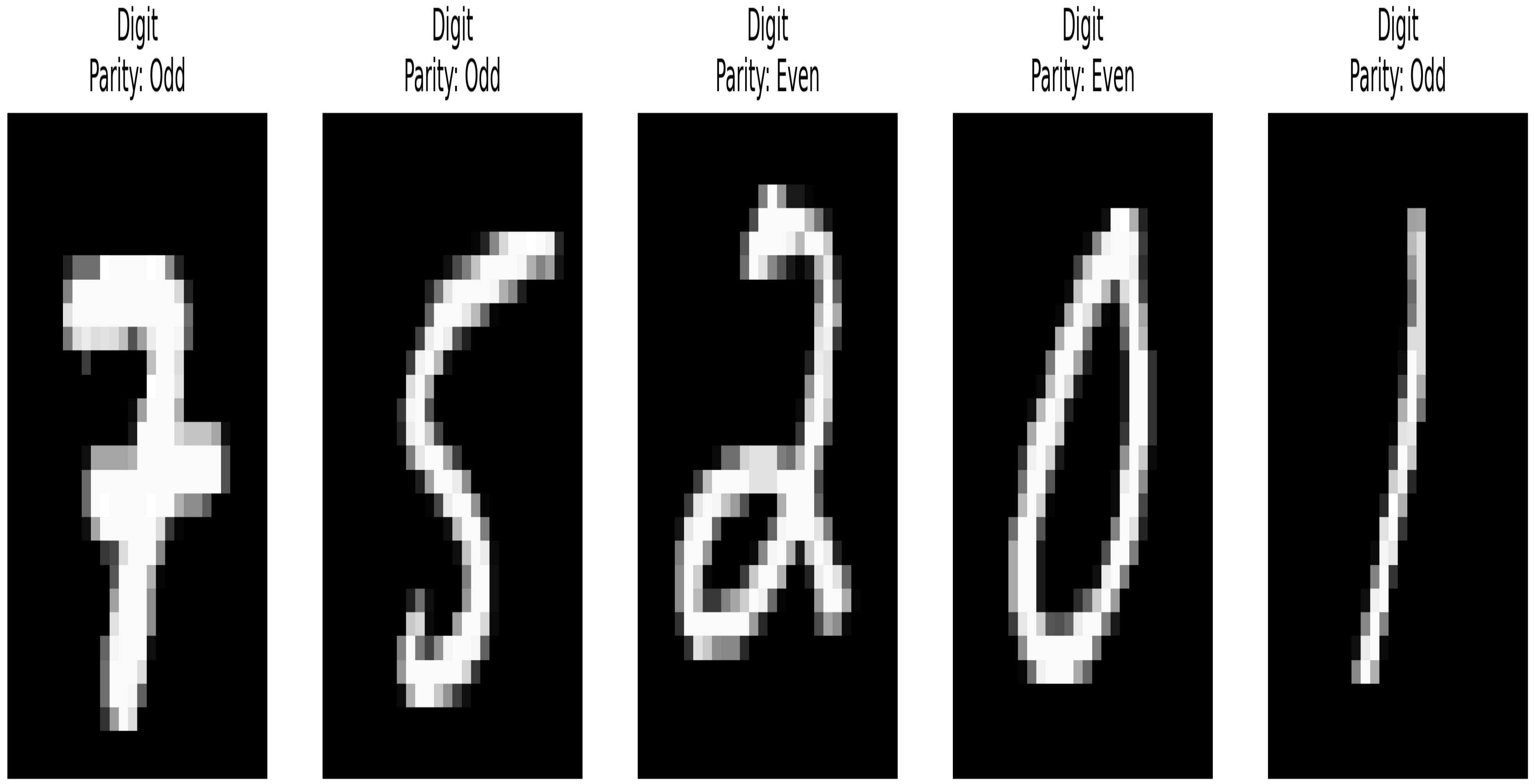
```python
def train_step(model, x, y, optimizer):
    # 1. Forward: compute prediction and loss
    pred = model(x)
    loss = criterion(y_pred.squeeze(), y_train)

    # 2. Backward: compute gradients
    optimizer.zero_grad()
    loss.backward()

    # 3. Update: apply gradients
    optimizer.step()

    return loss.item()
```

MNIST Classification: The Task



Dataset:

- 60,000 training images
- 10,000 test images
- 28×28 pixels each
- Binary labels (odd/even)

Preprocessing:

```
transform = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize(
        (0.1307,), (0.3081,)
    )
])

# Load data
train_dataset = datasets.MNIST(
    './data',
    train=True,
    transform=transform
)
```

Model Comparison: Architecture

Logistic Regression:

```
class Logistic(nn.Module):
    def __init__(self):
        super().__init__()
        self.linear = nn.Linear(784, 1)

    def forward(self, x):
        # Single linear layer
        return torch.sigmoid(
            self.linear(x.view(-1, 784))
        )
```

Neural Network:

```
class SimpleNN(nn.Module):
    def __init__(self):
        super().__init__()
        self.fc1 = nn.Linear(784, 32)
        self.fc2 = nn.Linear(32, 1)

    def forward(self, x):
        # Hidden layer with ReLU
        h = torch.relu(
            self.fc1(x.view(-1, 784))
        )
        # Output layer
        return torch.sigmoid(self.fc2(h))
```

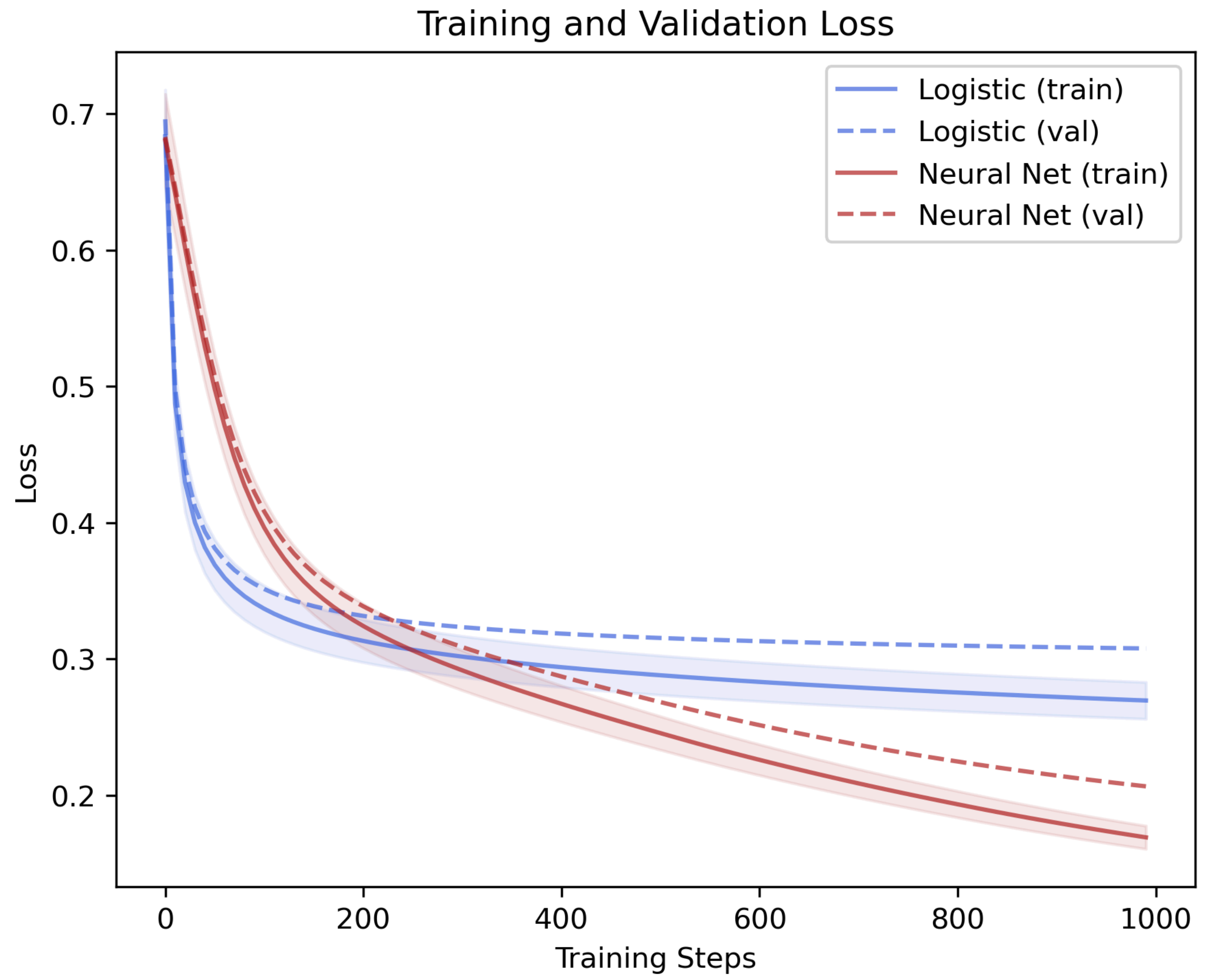
Training Process: Step by Step

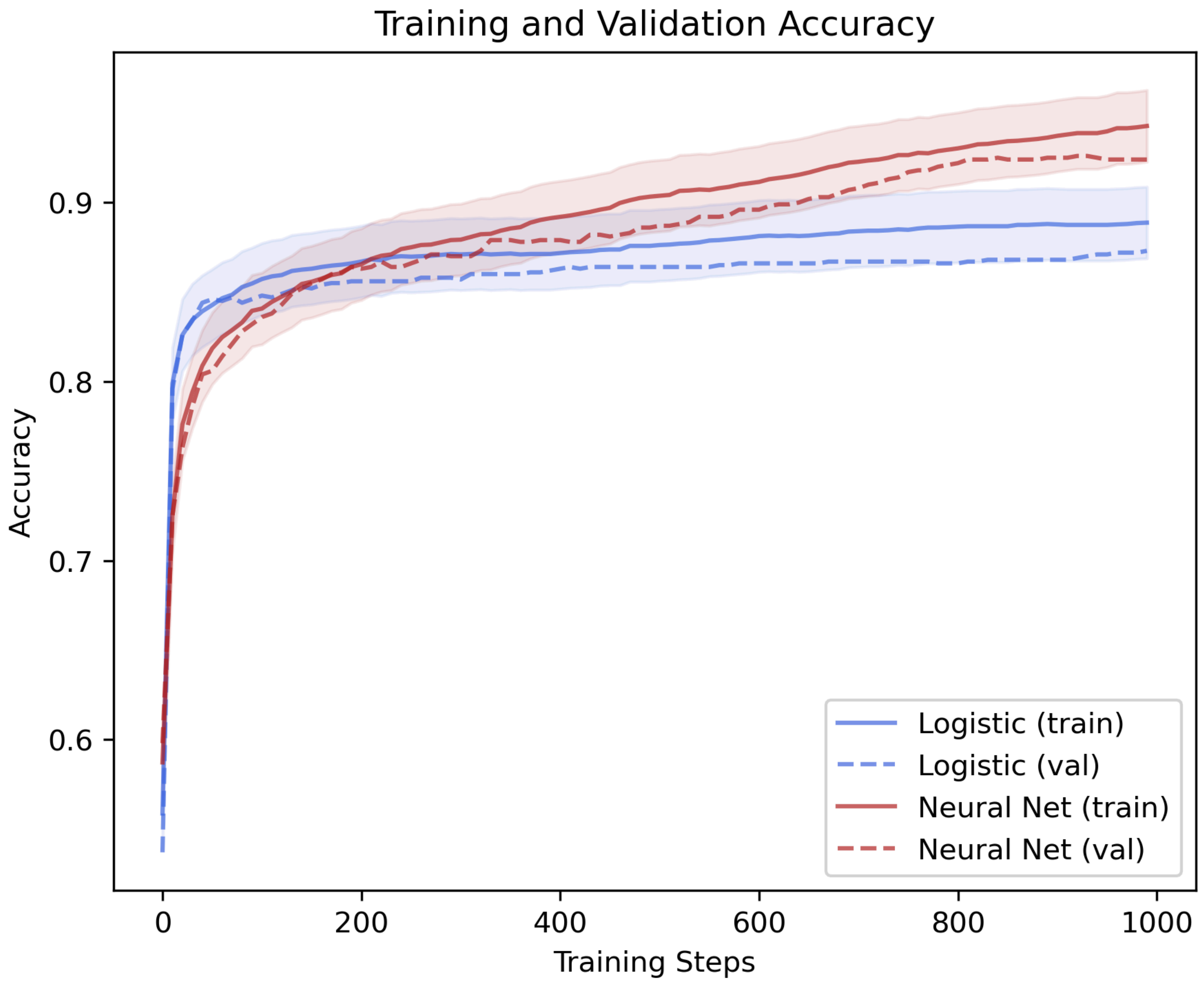
```
def train_model(model, X_train, y_train, X_val, y_val, alpha=0.01, n_steps=1000):
    for step in range(n_steps):
        # Forward pass
        y_pred = model(X_train)
        loss = criterion(y_pred.squeeze(), y_train)

        # Backward pass
        loss.backward()

        # Update parameters
        with torch.no_grad(): # Do not modify the computational graph
            for param in model.parameters():
                param -= alpha * param.grad # update the parameters
                param.grad.zero_() # reset the gradient to zero to avoid accumulation
```

Results Analysis





Final Results:

- Logistic: 87.30% accuracy
- Neural Net: 92.40% accuracy

Questions?

- Course website: https://damek.github.io/STAT-4830/
- Office hours: Listed on course website
- Email: damek@wharton.upenn.edu