Automatic Differentiation

Outline

- Recap neural networks and backpropagation
- Simple minimization examples
- Example with partial derivatives and a compute graph
- Partial derivatives and compute graphs for a one-layer network
- Partial derivatives and compute graphs for a two-layer network
- Automatic differentiation in code

Recap: Neural Networks and Backpropagation

- Take five minutes to draw
  - Whatever will help you remember (no correct or incorrect drawings)
  - You'll keep a running drawing log the rest of the semester

Automatic Differentiation (AD)

- Distinct from
  - Symbolic differentiation (exact, slow, must have symbolic representation)
  - Numerical differentiation (approximation/imprecise, fast, flexible)

- Forms of AD
  - Forward mode AD (exact, fast, flexible)
  - Reverse mode AD (exact, faster, flexible) (used by PyTorch as the default[1])

- Some terms
  - Differentiation: Process of finding a derivative
  - Derivative: The rate of change of a function (sometimes at a specific point)
  - Partial derivative: Derivative of a function with respect to one of several variables
  - Gradient: All partial derivatives

$$f(a) = 4(a-2)^2 - 3$$

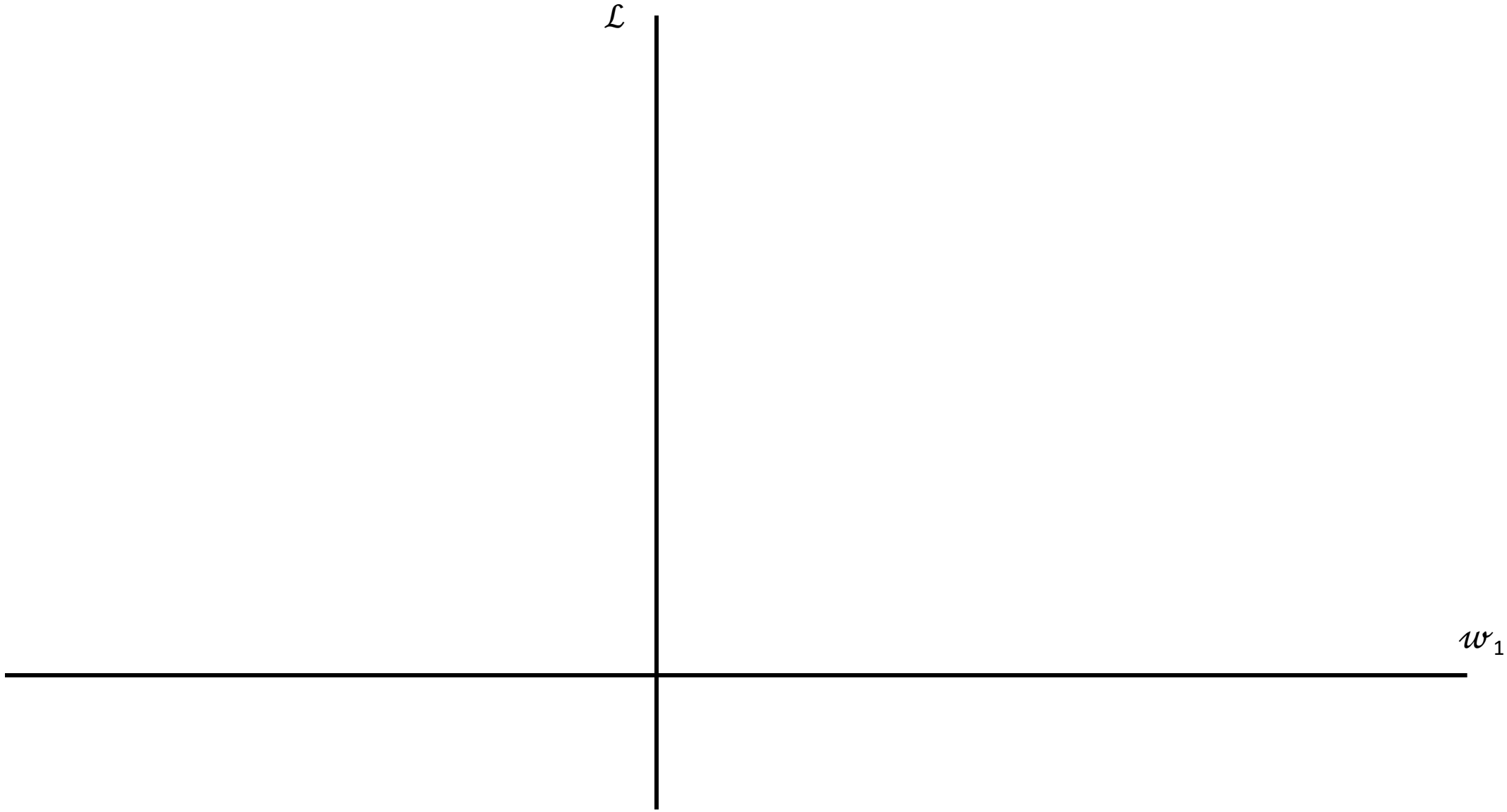
Plot

Closed-form solution

https://www.desmos.com/calculator/utlqlqutld

$f(a) = 4a^2 - 3$, where $a = 1.8$ and $a = 2.2$

Plot and Gradient Descent


$\mathcal{L}$
w_1

$$f(a, b, c, d) = b(a - c)^2 - d$$

$$f(a,b) = a^3 b^2$$

Minimize with respect to a

One-Layer Network (MSE and Sigmoid) Compute Graph

- $Z = XW^T + b$
- $A = \sigma(Z)$
- $\mathcal{L} = \frac{1}{2}(A - Y)^2$

Two-Layer Network (MSE and Sigmoid)

- $Z^{[1]} = A^{[0]}W^{[1]T} + b^{[1]T}$
- $A^{[1]} = \sigma\left(Z^{[1]}\right)$
- $Z^{[2]} = A^{[1]}W^{[2]T} + b^{[2]T}$
- $A^{[2]} = \sigma(Z^{[2]})$
- $\mathcal{L} = \frac{1}{2}\left(A^{[2]} - Y\right)^2$

Manual Differentiation

- How does the derivation change if we add hidden layers?
- How does the derivation change if we change the activation function?
- How does the derivation change if we change the loss function?

Automatic Differentiation (Autodiff, Autograd)

```
# Forward propagation A0 = X, Yhat = A2
Z1 = linear(A0, W1, b1)
A1 = sigmoid(Z1)
Z2 = linear(A1, W2, b2)
A2 = sigmoid(Z2)

# Compute loss as the mean-square-error
bce_loss = torch.mean(Y * torch.log(A2) + (1 - Y) * torch.log(1 - Yhat))

learning_rate = 0.01 # aka alpha or α
```

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```
# Compute gradients for W^[2] and b^[2]
dL_dY = (Y / Yhat - (1 - Y) / (1 - Yhat)) / 2
dY_dZ2 = Yhat * (1 - Yhat)
dZ2 = dL_dY * dY_dZ2
dW2 = (1 / N) * dZ2.T @ A1
db2 = dZ2.mean(dim=0)

# Compute gradients for W^[1] and b^[1]
dZ1 = dZ2 @ W2 * ((A1 * (1 - A1)))
dW1 = (1 / N) * dZ1.T @ X
db1 = dZ1.mean(dim=0)

W1 -= learning_rate * dW1
b1 -= learning_rate * db2
W2 -= learning_rate * dW2
b2 -= learning_rate * db2
```

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W1 -= learning_rate * dW1
b1 -= learning_rate * db2
W2 -= learning_rate * dW2
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```

```
bce_loss.backward()

W1 -= learning_rate * W1.grad
b1 -= learning_rate * b1.grad
W2 -= learning_rate * W2.grad
b2 -= learning_rate * b2.grad
```

Creating the Compute Graph

```python
# Sigmoid compute node from matrix.py
def sigmoid(self) -> Matrix:
    """Element-wise sigmoid."""
    result = Matrix(self.data.sigmoid(), children=(self,))

    def _gradient() -> None:
        self.grad += result.data * (1 - result.data) * result.grad

    result._gradient = _gradient
    return result
```

matrix.py

```python
# Sigmoid math from list2d.py
def sigmoid(self) -> List2D:
    vals = [
        [sigmoid(self.vals[i][j]) for j in range(self.ncol)]
        for i in range(self.nrow)
    ]
    return List2D(*self.shape, vals)
```

list2d.py

Creating the Compute Graph

```python
def sigmoid(self) -> Matrix:
    """Element-wise sigmoid."""
    result = Matrix(self.data.sigmoid(), children=(self,))

    def _gradient() -> None:
        self.grad += result.data * (1 - result.data) * result.grad

    result._gradient = _gradient
    return result
```

```python
def __matmul__(self, rhs: Matrix) -> Matrix:
    """Matrix multiplication: self @ rhs."""
    result = Matrix(self.data @ rhs.data, children=(self, rhs))

    def _gradient() -> None:
        self.grad += result.grad @ rhs.data.T
        rhs.grad += self.data.T @ result.grad

    result._gradient = _gradient
    return result
```

```python
def __add__(self, rhs: float | int | Matrix) -> Matrix:
    """Element-wise addition."""
    rhs_vals = rhs.data if isinstance(rhs, Matrix) else rhs
    children = (self, rhs) if isinstance(rhs, Matrix) else (self,)
    result = Matrix(self.data + rhs_vals, children=children)

    def _gradient() -> None:
        self.grad += result.grad.unbroadcast(*self.shape)
        if isinstance(rhs, Matrix):
            rhs.grad += result.grad.unbroadcast(*rhs.shape)

    result._gradient = _gradient
    return result
```

Backpropagation (.backward)

```
def backward(self) -> None:
    """Compute all gradients using backpropagation."""

    sorted_nodes: list[Matrix] = []
    visited: set[Matrix] = set()

    # Sort all elements in the compute graph using a topological ordering (DFS)
    # (Creating a closure here for convenience; capturing sorted_nodes and visited)
    def topological_sort(node: Matrix) -> None:
        if node not in visited:
            visited.add(node)
            for child in node._children:
                topological_sort(child)
            sorted_nodes.append(node)

    # Perform the topological sort
    topological_sort(self)

    # Initialize all gradients with ones
    self.grad.ones_()

    # Update gradients from output to input (backwards)
    for node in reversed(sorted_nodes):
        node._gradient()
```