Deep Learning Course

Lesson 3 -Backpropagation, and Gradient Descent

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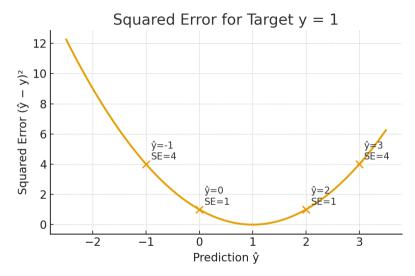
What does it mean to "improve" a model?

- In regression, we predict one or more numbers. We "improve" the model when predictions get closer to the true targets.
- The discrepancy is called the **loss**. A common choice is the **squared error**:

$$\mathsf{SE}(\hat{y},y) = (\hat{y} - y)^2.$$

- Key properties:
 - SE \geq 0: the error is never negative.
 - Larger deviations are penalized more strongly (quadratic growth).
- Example: if the target is y = 1
 - Predicting $\hat{y} = 0$ or 2 gives error 1
 - Predicting $\hat{y} = -1$ or 3 gives error 4





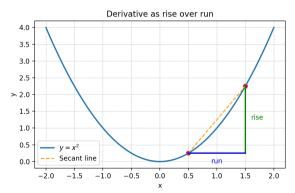
Example with target y = 1: predictions $\hat{y} = 0$ or 2 give error 1; predictions $\hat{y} = -1$ or 3 give error 4.

Our goal: reducing the error

- Once we can measure the error (loss), the next step is to minimize it.
- Intuitively, we want to **go downhill** in the loss landscape moving toward smaller and smaller values.
- The parameters of the network (weights and biases) determine where we are on this landscape.
- The question becomes: In which direction should we move the parameters to make the loss smaller?

How do we go downhill? Thanks to derivatives!

- The **derivative** tells us how a function changes when its input changes.
- Intuitively, it measures the **slope** or **tilt** of the curve at a given point.
- A positive derivative means the function is increasing; a negative derivative means it is decreasing.
- When we want to **minimize** a function, we move in the direction where the derivative is **negative** that is, downhill.



Formal definition of the derivative

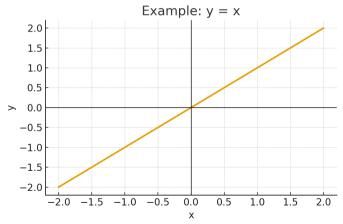
- The derivative of a function f(x) at a point x_0 measures the instantaneous rate of change of f at that point.
- Formally, it is defined as the limit of the average rate of change:

$$f'(x_0) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

- The smaller the Δx , the closer the secant line gets to the tangent line.
- Geometrically, the derivative corresponds to the slope of the tangent line to the curve y = f(x) at x_0 .
- If this limit exists, the function is said to be **differentiable** at x_0 .

Example: y = x

- Consider the simple function y = x.
- It is a straight line passing through the origin.
- Question: What is the value of the derivative?



Derivative of y = x

- Let f(x) = x.
- By definition, the derivative is

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

• Substituting f(x) = x:

$$f'(x) = \lim_{\Delta x \to 0} \frac{(x + \Delta x) - x}{\Delta x}.$$

• Simplifying the numerator:

$$f'(x) = \lim_{\Delta x \to 0} \frac{\Delta x}{\Delta x} = \lim_{\Delta x \to 0} 1 = 1.$$

Result

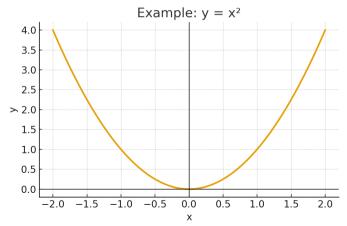
For all x, the derivative of y = x is f'(x) = 1.



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Example: $y = x^2$

- Consider the quadratic function $y = x^2$.
- Notice that it is a curved shape opening upward.
- Question: What is the value of the derivative of $y = x^2$?



Derivative of $y = x^2$

- Let $f(x) = x^2$.
- By definition of the derivative:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

• Substitute $f(x) = x^2$:

$$f'(x) = \lim_{h \to 0} \frac{(x+h)^2 - x^2}{h}.$$

• Expand the square:

$$f'(x) = \lim_{h \to 0} \frac{x^2 + 2xh + h^2 - x^2}{h}.$$

Simplify the numerator:

$$f'(x) = \lim_{h \to 0} \frac{2xh + h^2}{h} = \lim_{h \to 0} (2x + h).$$

• Taking the limit:

$$f'(x)=2x.$$

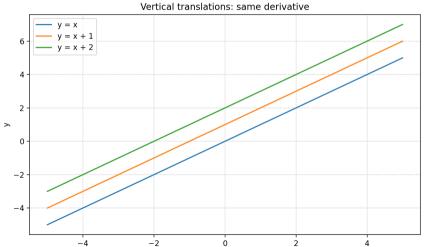
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Result

For all x, the derivative of $y = x^2$ is f'(x) = 2x.

Vertical translations do not change the derivative

- Functions y = x, y = x + 1, y = x + 2 share the same slope 1.
- Adding a constant shifts the graph but does *not* change the derivative.



Introduction to Partial Derivatives

- When a function depends on more than one variable, such as f(x, y), we can study how the function changes with respect to each variable separately.
- The **partial derivative** measures how the function changes when we vary one variable while keeping the others constant.
- In practice, when taking the derivative with respect to one variable, the other variables are treated as if they were **constants**.
- Formally:

$$\frac{\partial f}{\partial x} = \lim_{h \to 0} \frac{f(x+h,y) - f(x,y)}{h}, \quad \frac{\partial f}{\partial y} = \lim_{h \to 0} \frac{f(x,y+h) - f(x,y)}{h}.$$

• Example: if $f(x, y) = x^2 + 3y$,

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial f}{\partial y} = 3.$$

• Partial derivatives are fundamental in multivariable calculus and in machine learning, where loss functions often depend on many parameters.

What happens when x is a vector?

- When x is a vector $x = [x_1, x_2, \dots, x_n]$, the function f(x) depends on multiple variables at once.
- Taking the derivative of f with respect to x means computing the partial derivative with respect to each component.
- The result is a **vector** called the **gradient**:

$$abla_x f(x) = egin{bmatrix} rac{\partial f}{\partial x_1} \ rac{\partial f}{\partial x_2} \ dots \ rac{\partial f}{\partial x_n} \end{pmatrix}.$$

- Each component of the gradient tells us how much f(x) changes when we vary one coordinate, keeping the others constant.
- The gradient points in the direction of the **steepest increase** of the function.



When both input and output are vectors

Sometimes a function takes a vector as input and returns a vector as output:

$$f: \mathbb{R}^n \to \mathbb{R}^m$$
.

• Example:

$$f(x) = \begin{bmatrix} x_1 + 2x_2 \\ 3x_1 - x_2 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

- In this case, we cannot describe the derivative with a single vector.
- Instead, we use a matrix of partial derivatives, called the Jacobian matrix:

$$J_f(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}.$$

- Each row corresponds to the gradient of one output component with respect to all input components.
- The Jacobian generalizes the concept of the derivative to vector-valued functions.

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Computing the Jacobian from the previous example

Recall the function:

$$f(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \end{bmatrix} = \begin{bmatrix} x_1 + 2x_2 \\ 3x_1 - x_2 \end{bmatrix}.$$

• Compute the partial derivatives of each component:

$$\frac{\partial f_1}{\partial x_1} = 1, \quad \frac{\partial f_1}{\partial x_2} = 2,$$

$$\frac{\partial f_2}{\partial x_1} = 3, \quad \frac{\partial f_2}{\partial x_2} = -1.$$

• Therefore, the **Jacobian matrix** is:

$$J_f(x) = \begin{bmatrix} 1 & 2 \\ 3 & -1 \end{bmatrix}.$$

 \bullet Each row represents the gradient of one output component with respect to the input vector x.

When x is itself a function: the Chain Rule

- Sometimes the variable x is not a simple number or vector, but rather another function.
- Example: if y = f(u) and u = g(x), then y ultimately depends on x through g.
- To find how y changes with respect to x, we use the **Chain Rule**.
- The Chain Rule connects the rate of change of f with respect to u and the rate of change of u with respect to x:

$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx}.$$

- Intuitively, we are "chaining" together the effects of each transformation.
- This concept is fundamental in backpropagation, where each layer of a neural network applies the Chain Rule to propagate gradients backward.



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Returning to our main goal: reducing the error

- We now have all the tools we need to return to our original problem: reducing the loss.
- We know how to compute the error between the target value and the predicted value.
- However, what we truly want to know is: How should we change the weights so that the error decreases?
- The loss depends on the weights indirectly:

$$Loss = L(\hat{y}, y) = L(f(x; W), y).$$

ullet Thanks to derivatives and the Chain Rule, we can measure how small changes in the weights W affect the loss:

$$\frac{\partial L}{\partial W}$$

- This derivative tells us the direction in which to adjust the weights to reduce the error.
- The process of computing these derivatives layer by layer is called backpropagation.

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Using the Chain Rule to express $\frac{dL}{dW}$

• In a neural network, the loss L depends on the weights W through several intermediate variables:

$$x \rightarrow z = xW + b \rightarrow \hat{y} = f(z) \rightarrow L(\hat{y}, y)$$

• To compute how the loss changes with respect to the weights, we apply the **Chain Rule**:

$$\frac{dL}{dW} = \frac{dL}{d\hat{y}} \cdot \frac{d\hat{y}}{dz} \cdot \frac{dz}{dW}.$$

- Each term in this product captures a different part of the dependency:
 - $\frac{dL}{d\hat{v}}$: how the loss changes with the predicted output,
 - $\frac{d\hat{y}}{dz}$: how the activation output changes with the pre-activation, $\frac{dz}{dW}$: how the pre-activation changes with the weights.
- This decomposition allows us to compute gradients efficiently, step by step, moving backward through the network.

Forward pass with $\hat{y} = f(xW^T)$ - part 1

• Let the input vector be:

$$x = \begin{bmatrix} x_1 & x_2 \end{bmatrix}, \quad W = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix}.$$

• Since W has shape 3×2 , we compute:

$$z = xW^T$$
.

• Expanding element by element:

$$z_1 = x_1 w_{11} + x_2 w_{12},$$

 $z_2 = x_1 w_{21} + x_2 w_{22},$
 $z_3 = x_1 w_{31} + x_2 w_{32}.$

• The activation function *f* is applied elementwise:

$$\hat{y} = f(z) = [f(z_1), f(z_2), f(z_3)].$$

• At this stage, we have completed the **forward pass**, producing the predicted output \hat{y} .

Forward pass with $\hat{y} = f(xW^T)$ - part 2

• Suppose the true target is:

$$y = \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix}$$
.

• We define the loss using the **squared error**:

$$L = \frac{1}{2} \sum_{i=1}^{3} (\hat{y}_i - y_i)^2.$$

• The division by 2 is a mathematical convenience: when we later take the derivative, the exponent 2 and the factor $\frac{1}{2}$ cancel out neatly:

$$\frac{d}{d\hat{y}_i}\left(\frac{1}{2}(\hat{y}_i-y_i)^2\right)=(\hat{y}_i-y_i).$$

- This simplification makes the gradient expressions cleaner and easier to interpret.
- Therefore, the forward computation gives:

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$$x \xrightarrow{W^T} z \xrightarrow{f} \hat{y} \xrightarrow{L} \text{Loss.}$$

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Computing $\frac{dL}{d\hat{y}}$

Recall the loss function for our example:

$$L = \frac{1}{2} \sum_{i=1}^{3} (\hat{y}_i - y_i)^2.$$

• To find how the loss changes with respect to the predicted outputs \hat{y} , we take the derivative with respect to each component \hat{v}_i :

$$\frac{\partial L}{\partial \hat{y}_i} = \frac{\partial}{\partial \hat{y}_i} \left(\frac{1}{2} (\hat{y}_i - y_i)^2 \right).$$

Applying the derivative:

$$\frac{\partial L}{\partial \hat{y}_i} = (\hat{y}_i - y_i).$$

• In vector form:

$$\frac{dL}{d\hat{y}} = [\hat{y}_1 - y_1, \quad \hat{y}_2 - y_2, \quad \hat{y}_3 - y_3].$$



Computing $\frac{d\hat{y}}{dz}$: general case

Recall that:

$$z_1 = x_1 w_{11} + x_2 w_{12},$$

 $z_2 = x_1 w_{21} + x_2 w_{22},$
 $z_3 = x_1 w_{31} + x_2 w_{32}.$

• The activation function f transforms z into:

$$\hat{y} = f(z)$$

• Since both \hat{y} and z are vectors, the derivative of one with respect to the other is a **Jacobian matrix**:

$$\frac{d\hat{y}}{dz} = \begin{bmatrix} \frac{\partial \hat{y}_1}{\partial z_1} & \frac{\partial \hat{y}_1}{\partial z_2} & \frac{\partial \hat{y}_1}{\partial z_3} \\ \frac{\partial \hat{y}_2}{\partial z_1} & \frac{\partial \hat{y}_2}{\partial z_2} & \frac{\partial \hat{y}_2}{\partial z_3} \\ \frac{\partial \hat{y}_3}{\partial z_1} & \frac{\partial \hat{y}_3}{\partial z_2} & \frac{\partial \hat{y}_3}{\partial z_3} \end{bmatrix}.$$

- Each element represents how a small change in one component of z affects one component of \hat{y} .
- In general, this matrix may contain nonzero off-diagonal terms if the activation function couples multiple outputs.

Simplification for pointwise activation functions (e.g. ReLU)

• For most neural network activations, such as ReLU, sigmoid, or tanh, the function acts **independently** on each component of z:

$$\hat{y}_i = f(z_i).$$

- This means that changing z_i affects only \hat{y}_i , and not any other component.
- As a result, the Jacobian matrix becomes diagonal:

$$\frac{d\hat{y}}{dz} = \begin{bmatrix} f'(z_1) & 0 & 0 \\ 0 & f'(z_2) & 0 \\ 0 & 0 & f'(z_3) \end{bmatrix}.$$

For the ReLU activation:

$$f(z_i) = \max(0, z_i) \quad \Rightarrow \quad f'(z_i) = \begin{cases} 1 & \text{if } z_i > 0, \\ 0 & \text{if } z_i \leq 0. \end{cases}$$

• This diagonal structure is what makes backpropagation efficient, since each neuron's derivative depends only on its own activation.

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Understanding $\frac{dz}{dW}$: step by step

• Recall that:

$$z_1 = x_1 w_{11} + x_2 w_{12}, \quad z_2 = x_1 w_{21} + x_2 w_{22}.$$

• If we take the derivative of z_1 with respect to the weights in the first row $W_1 = [w_{11}, w_{12}]$:

$$\frac{\partial z_1}{\partial W_1} = \begin{bmatrix} \frac{\partial z_1}{\partial w_{11}} & \frac{\partial z_1}{\partial w_{12}} \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} = x.$$

ullet However, if we take the derivative of z_1 with respect to the second row of weights $W_2=[w_{21},w_{22}]$:

$$\frac{\partial z_1}{\partial W_2} = \begin{bmatrix} \frac{\partial z_1}{\partial w_{21}} & \frac{\partial z_1}{\partial w_{22}} \end{bmatrix} = \begin{bmatrix} 0 & 0 \end{bmatrix}.$$

- This shows that z_1 depends only on the first row of W, while z_2 depends only on the second row.
- Each neuron is connected only to its own set of weights.

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Building the full Jacobian $\frac{dz}{dW}$

• Extending the previous reasoning to all components z_1, z_2, z_3 :

$$z_i = x_1 w_{i1} + x_2 w_{i2}, \quad i = 1, 2, 3.$$

• Each z_i depends only on the weights in its own row $W_i = [w_{i1}, w_{i2}]$:

$$\frac{\partial z_i}{\partial W_j} = \begin{cases} x & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

• Therefore, the full Jacobian is a block matrix:

$$\frac{dz}{dW} = \begin{bmatrix} x & 0 & 0\\ 0 & x & 0\\ 0 & 0 & x \end{bmatrix},$$

where each block $x = [x_1, x_2]$ represents how one neuron's output changes with its own weights.

Recap: structure of the full derivative

We expressed the gradient of the loss with respect to the weights using the Chain Rule:

$$\frac{dL}{dW} = \frac{dL}{d\hat{y}} \cdot \frac{d\hat{y}}{dz} \cdot \frac{dz}{dW}.$$

- Each component describes a different relationship in the network:

 - $\frac{dL}{d\hat{y}} = \hat{y} y$ measures how the loss changes with the predicted output. $\frac{d\hat{y}}{dz} = \text{diag}(f'(z_1), f'(z_2), f'(z_3))$ describes how the activation function transforms the signal.
- These two parts together form the gradient that flows backward through the output laver.

Recap: how z depends on the weights

• The third term, $\frac{dz}{dW}$, shows how each pre-activation depends on its own weights:

$$z_i = x_1 w_{i1} + x_2 w_{i2} \quad \Rightarrow \quad \frac{\partial z_i}{\partial W_i} = x.$$

Cross-dependencies are zero:

$$\frac{\partial z_i}{\partial W_j} = \begin{cases} x & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

• Putting all terms together, the gradient for each neuron becomes:

$$\frac{dL}{dW_i} = (\hat{y}_i - y_i) f'(z_i) x.$$

- Each neuron's update depends on:
 - **1** The prediction error $(\hat{y}_i y_i)$,
 - 2 The local slope $f'(z_i)$,
 - The input vector *x*.



Introducing the concept of δ'

• To simplify notation, we group the terms that measure the local error for each neuron:

$$\delta_i = (\hat{y}_i - y_i) f'(z_i).$$

• The vector form is:

$$\boldsymbol{\delta} = \begin{bmatrix} \delta_1 & \delta_2 & \delta_3 \end{bmatrix} = (\hat{y} - y) \odot f'(z),$$

where \odot denotes elementwise multiplication.

- Intuitively:
 - $(\hat{y} y)$ tells us the prediction error,
 - f'(z) scales that error according to the local slope of the activation.
- ullet δ represents the **error signal** that will be propagated backward through the network.

Simplified gradient using δ

• Using the definition of δ_i , the gradient with respect to the weights becomes:

$$\frac{dL}{dW_i} = \delta_i x.$$

• In matrix form, stacking all neurons together:

$$\frac{dL}{dW} = \boldsymbol{\delta}^T x.$$

- This compact expression shows that:
 - ullet the gradient is the **outer product** between the input x and the error signal δ ,
 - each neuron's weight update is proportional to the input values that produced the error.
- This formulation is the foundation of backpropagation.



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From Jacobians to outer product: make the multiplication explicit

We start from the chain rule:

$$\frac{dL}{dW} = \underbrace{\frac{dL}{d\hat{y}}}_{1\times 3} \underbrace{\frac{d\hat{y}}{dz}}_{3\times 3} \underbrace{\frac{dz}{dW}}_{\text{block matrix}}.$$

For a pointwise activation, $\frac{d\hat{y}}{dz} = \operatorname{diag}(f'(z_1), f'(z_2), f'(z_3))$. Define $\delta := \frac{dL}{dz} = (\hat{y} - y) \odot f'(z)$ so that $\frac{dL}{d\hat{y}} \frac{d\hat{y}}{dz} = \delta$ (shape 1×3).

The last factor has block-diagonal structure because each z_i depends only on W_i :

$$\frac{dz}{dW} = \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix}, \text{ each block } x = [x_1 \ x_2] \text{ has shape } 1 \times 2.$$

Now multiply the vector $\delta = [\delta_1 \ \delta_2 \ \delta_3]$ by this block matrix:

$$\delta \cdot \frac{dz}{dW} = \left[\delta_1 x \mid \delta_2 x \mid \delta_3 x \right],$$

a 1×6 row obtained by concatenating the three 1×2 blocks.



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Where the outer product comes from

The row $\left[\delta_1 x \mid \delta_2 x \mid \delta_3 x\right]$ groups the contributions per neuron. If we reshape these two-wide blocks into rows, we obtain a 3×2 matrix:

$$\frac{dL}{dW} \equiv \begin{bmatrix} \delta_1 x \\ \delta_2 x \\ \delta_3 x \end{bmatrix} = \begin{bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \end{bmatrix} \begin{bmatrix} x_1 & x_2 \end{bmatrix} = \delta^T x.$$

Elementwise this means

$$\frac{\partial L}{\partial w_{ik}} = \delta_i\,x_k, \quad i \in \{1,2,3\}, \ k \in \{1,2\}.$$

Why it collapses to an outer product:

- **1** $\frac{d\hat{y}}{dz}$ is diagonal for pointwise activations, so cross terms vanish when forming δ .
- ② Each z_i depends only on the weights in row W_i , making $\frac{dz}{dW}$ block-diagonal with identical x blocks.

These two structural diagonals turn the general Jacobian product into the outer product $\delta^T x$.

What about the bias *b*?

• Until now we ignored the bias term b, but it is present in the full expression:

$$z = xW^T + b$$
.

• The bias affects each neuron additively, so the derivative of z_i with respect to b_i is simply:

$$\frac{\partial z_i}{\partial b_i} = 1.$$

• Therefore, using the Chain Rule:

$$\frac{dL}{db_i} = \frac{dL}{dz_i} \cdot \frac{dz_i}{db_i} = \delta_i.$$

• In vector form:

$$\frac{dL}{db} = \delta.$$

ullet Each bias term has the same gradient as its corresponding neuron's δ_i .

Embedding the bias inside the input vector

To simplify notation, we can include the bias in the weight matrix by augmenting the input:

$$\tilde{x} = \begin{bmatrix} x_1 & x_2 & 1 \end{bmatrix}, \quad \tilde{W} = \begin{bmatrix} w_{11} & w_{12} & b_1 \\ w_{21} & w_{22} & b_2 \\ w_{31} & w_{32} & b_3 \end{bmatrix}.$$

• The forward pass becomes:

$$z = \tilde{x} \, \tilde{W}^T$$
.

• The gradient keeps the same form:

$$\frac{dL}{d\tilde{W}} = \boldsymbol{\delta}^T \tilde{\mathbf{x}},$$

and the last column of $rac{dL}{d ilde{W}}$ corresponds exactly to $rac{dL}{db}=\delta.$

• This trick allows us to treat the bias as just another weight connected to a constant input 1.

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From backpropagation to gradient descent

• After computing all gradients through backpropagation, we know how the loss changes with respect to each parameter:

$$\frac{dL}{dW}$$
, $\frac{dL}{db}$.

- The next step is to actually update the parameters in order to reduce the loss.
- The idea of gradient descent is simple:

new parameter = old parameter - η · gradient,

where η is the **learning rate**.

Applied to our case:

$$W \leftarrow W - \eta \frac{dL}{dW}, \quad b \leftarrow b - \eta \frac{dL}{db}.$$

- The learning rate controls the size of each update:
 - ullet too large o overshoot the minimum,
 - ullet too small o very slow convergence.
- This iterative process gradually moves the network's parameters downhill in the loss landscape.

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Lab time (1/3) - Forward pass exercise

- Let's practice the full forward computation with a simple example.
- Given:

$$x = [1, 2], \quad W = \begin{bmatrix} 3 & 2 \\ 4 & 1 \\ 5 & 2 \end{bmatrix}, \quad y = [1, 4, 4].$$

Definitions:

$$z = xW^T$$
, $\hat{y} = \text{ReLU}(z)$, $L = \frac{1}{2}(\hat{y} - y)^2$.

- Tasks:
 - Compute the vector z.
 - ② Apply the ReLU activation to get \hat{y} .
 - Compute the loss L.
- Hint: Remember that ReLU is defined as $ReLU(z_i) = max(0, z_i)$.

Question: What are the values of z, \hat{y} , and L?



Lab time (1/3) - Solution

Given:

$$x = [1, 2], \quad W = \begin{bmatrix} 3 & 2 \\ 4 & 1 \\ 5 & 2 \end{bmatrix}, \quad y = [1, 4, 4].$$

• Compute $z = xW^T$:

$$z_1 = 1 \cdot 3 + 2 \cdot 2 = 7,$$

 $z_2 = 1 \cdot 4 + 2 \cdot 1 = 6,$
 $z_3 = 1 \cdot 5 + 2 \cdot 2 = 9.$

Apply ReLU activation:

$$\hat{y} = \text{ReLU}(z) = [7, 6, 9].$$

Compute the loss:

$$L = \frac{1}{2} \sum_{i} (\hat{y}_i - y_i)^2 = \frac{1}{2} \left[(7 - 1)^2 + (6 - 4)^2 + (9 - 4)^2 \right] = \frac{1}{2} (36 + 4 + 25) = \frac{65}{2} = 32.5.$$

• Result:

$$z = [7, 6, 9], \quad \hat{y} = [7, 6, 9], \quad L = 32.5.$$



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Lab time (2/3): compute the gradients (task)

Given the same setup:

$$x = [1, 2], \quad W = \begin{bmatrix} 3 & 2 \\ 4 & 1 \\ 5 & 2 \end{bmatrix}, \quad y = [1, 4, 4], \quad z = xW^T, \quad \hat{y} = \text{ReLU}(z), \quad L = \frac{1}{2} \sum_i (\hat{y}_i - y_i)^2.$$

Tasks

- ② Compute $\frac{d\hat{y}}{dz}$ for ReLU and then $\frac{dL}{dz}$.
- Combine the parts to obtain $\frac{dL}{dW}$.

Hints:

$$\operatorname{ReLU}(u) = \max(0, u), \quad \operatorname{ReLU}'(u) = \begin{cases} 1 & u > 0 \\ 0 & u \leq 0 \end{cases}$$

Lab time (2/3): compute the gradients (solution)

From the forward pass:

$$z = [7, 6, 9], \quad \hat{y} = [7, 6, 9].$$

1.
$$\frac{dL}{d\hat{y}} = \hat{y} - y = [6, 2, 5].$$

- **2.** For ReLU at these $z_i > 0$: $\frac{d\hat{y}}{dz} = \text{diag}(1,1,1)$. Hence $\frac{dL}{dz} = \frac{dL}{d\hat{y}} \frac{d\hat{y}}{dz} = [6,2,5]$. Define $\delta := \frac{dL}{dz} = [6,2,5]$.
- **3.** Since $z_i = x_1 w_{i1} + x_2 w_{i2}$, $\frac{\partial z_i}{\partial W_i} = x = [1, 2]$, $\frac{\partial z_i}{\partial W_i} = 0$ for $i \neq j$.
- 4. Row-wise gradient:

$$\frac{dL}{dW_i} = \delta_i \times \quad \Rightarrow \quad \frac{dL}{dW} = \begin{bmatrix} 6 \\ 2 \\ 5 \end{bmatrix} \begin{bmatrix} 1 & 2 \end{bmatrix} = \begin{bmatrix} 6 & 12 \\ 2 & 4 \\ 5 & 10 \end{bmatrix}.$$



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Lab time (3/3) - Applying gradient descent (question)

We now use the results from the previous exercise. Given:

$$x = [1, 2], \quad W = \begin{bmatrix} 3 & 2 \\ 4 & 1 \\ 5 & 2 \end{bmatrix}, \quad y = [1, 4, 4],$$

and we already computed:

$$\frac{dL}{dW} = \begin{bmatrix} 6 & 12\\ 2 & 4\\ 5 & 10 \end{bmatrix}.$$

We will now apply gradient descent to update the weights:

$$W_{\mathsf{new}} = W - \eta rac{dL}{dW}.$$

Tasks:

- Choose a learning rate $\eta = 0.1$.
- 2 Compute the updated weights W_{new} .
- ullet Interpret what happens to each row of W.

Question: What are the new values of W after one gradient descent step?

Lab time (3/3) - Applying gradient descent (solution)

Using $\eta = 0.1$:

$$W_{\text{new}} = W - \eta \frac{dL}{dW} = \begin{bmatrix} 3 & 2 \\ 4 & 1 \\ 5 & 2 \end{bmatrix} - 0.1 \times \begin{bmatrix} 6 & 12 \\ 2 & 4 \\ 5 & 10 \end{bmatrix}.$$

Compute the update:

$$0.1 \times \begin{bmatrix} 6 & 12 \\ 2 & 4 \\ 5 & 10 \end{bmatrix} = \begin{bmatrix} 0.6 & 1.2 \\ 0.2 & 0.4 \\ 0.5 & 1.0 \end{bmatrix}.$$

Subtract from W:

$$W_{\text{new}} = \begin{bmatrix} 3 - 0.6 & 2 - 1.2 \\ 4 - 0.2 & 1 - 0.4 \\ 5 - 0.5 & 2 - 1.0 \end{bmatrix} = \begin{bmatrix} 2.4 & 0.8 \\ 3.8 & 0.6 \\ 4.5 & 1.0 \end{bmatrix}.$$

Result:

$$W_{\text{new}} = \begin{bmatrix} 2.4 & 0.8 \\ 3.8 & 0.6 \\ 4.5 & 1.0 \end{bmatrix}.$$

Each weight has moved slightly **downhill** in the direction opposite to its gradient.

New loss after weight update

After applying the gradient descent step, the new weights are:

$$W_{\mathsf{new}} = egin{bmatrix} 2.4 & 0.8 \\ 3.8 & 0.6 \\ 4.5 & 1.0 \end{bmatrix}.$$

Now recompute the forward pass:

$$z_{\mathsf{new}} = x W_{\mathsf{new}}^T, \quad \hat{y}_{\mathsf{new}} = \mathsf{ReLU}(z_{\mathsf{new}}), \quad L_{\mathsf{new}} = \frac{1}{2} \sum_i (\hat{y}_{\mathsf{new},i} - y_i)^2.$$

Step 1: Compute z_{new}

$$z_{\text{new}} = [1, 2] \begin{bmatrix} 2.4 & 3.8 & 4.5 \\ 0.8 & 0.6 & 1.0 \end{bmatrix} = [4.0, 5.0, 6.5].$$

Step 2: Apply ReLU:

$$\hat{y}_{\text{new}} = [4.0, 5.0, 6.5].$$



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New loss after weight update

Step 3: Compute new loss:

$$L_{\text{new}} = \frac{1}{2}[(4-1)^2 + (5-4)^2 + (6.5-4)^2] = \frac{1}{2}(9+1+6.25) = 8.125.$$

Result: The new loss is

$$L_{\text{new}} = 8.125,$$

a significant reduction from the previous L = 32.5.

Two Layers Network, forward setup & assumptions (single sample)

Input:
$$x \in \mathbb{R}^{1 \times d}$$

$$z_1 = xW_1^\top + b_1 \quad (z_1 \in \mathbb{R}^{1 \times h}),$$

$$h = f_1(z_1) \quad \text{(pointwise)} \quad (h \in \mathbb{R}^{1 \times h}),$$

$$z_2 = hW_2^\top + b_2 \quad (z_2 \in \mathbb{R}^{1 \times k}),$$

$$\hat{y} = f_2(z_2) \quad \text{(pointwise)},$$
Squared Error (SE): $L(\hat{y}, y) = \frac{1}{2} ||\hat{y} - y||_2^2.$

Shapes: $W_1 \in \mathbb{R}^{h \times d}$, $b_1 \in \mathbb{R}^h$, $W_2 \in \mathbb{R}^{k \times h}$, $b_2 \in \mathbb{R}^k$.

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Full chain first (no shortcuts)

Goal: gradients w.r.t. parameters of both layers.

Second layer

$$\frac{\partial L}{\partial W_2} = \underbrace{\frac{\partial L}{\partial \hat{y}}}_{1 \times k} \underbrace{\frac{\partial \hat{y}}{\partial z_2}}_{k \times k} \underbrace{\frac{\partial z_2}{\partial W_2}}_{k \times (kh)}, \qquad \frac{\partial L}{\partial b_2} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_2} \frac{\partial z_2}{\partial b_2}.$$

First layer

$$\frac{\partial L}{\partial W_1} = \underbrace{\frac{\partial L}{\partial \hat{y}}}_{1 \times k} \underbrace{\frac{\partial \hat{y}}{\partial z_2}}_{k \times k} \underbrace{\frac{\partial z_2}{\partial h}}_{k \times h} \underbrace{\frac{\partial h}{\partial z_1}}_{h \times h} \underbrace{\frac{\partial z_1}{\partial W_1}}_{h \times (hd)}$$

(and analogously for $\partial L/\partial b_1$).



Compute the 5 Pieces (Pointwise Activations)

- 1) $\frac{\partial L}{\partial \hat{y}} = \hat{y} y \in \mathbb{R}^{1 \times k}$ (for MSE; replace accordingly for a generic loss).
- 2) $\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{z}_2} = \operatorname{diag}(f_2'(\mathbf{z}_2)) \in \mathbb{R}^{k \times k}$.
- 3) $\frac{\partial z_2}{\partial h} = W_2 \in \mathbb{R}^{k \times h} \text{ since } z_2 = h W_2^{\top}.$
- **4)** $\frac{\partial h}{\partial z_1} = \operatorname{diag}(f'_1(z_1)) \in \mathbb{R}^{h \times h}.$
- 5) $\frac{\partial z_1}{\partial W_i}$: as a Jacobian wrt $\text{vec}(W_1) \in \mathbb{R}^{hd}$ (row-major):



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Introduce Deltas (δ_2, δ_1)

Define the layer-2 and layer-1 pre-activation gradients:

$$\delta_2 := \frac{\partial L}{\partial z_2} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_2} = (\hat{y} - y) \odot f_2'(z_2) \in \mathbb{R}^{1 \times k}.$$

$$\delta_1 := \frac{\partial L}{\partial z_1} = (\delta_2 W_2) \odot f_1'(z_1) \in \mathbb{R}^{1 \times h}.$$

Assembling the chain for the first layer

Chain:

$$\frac{\partial L}{\partial \text{vec}(W_1)} = \underbrace{\delta_2}_{1 \times k} \underbrace{W_2}_{k \times h} \underbrace{\text{diag}(f'(z_1))}_{h \times h} \underbrace{(I_h \otimes x^\top)}_{h \times hd}.$$

Define the hidden-layer delta

$$\delta_1 := (\delta_2 W_2) \circ f'(z_1)$$
 $(1 \times h),$

then

$$\boxed{\frac{\partial L}{\partial W_1} = \delta_1^\top x} \quad (h \times d), \qquad \boxed{\frac{\partial L}{\partial b_1} = \delta_1} \quad (h).$$

Generalization: L Layers, Pointwise Activations

Forward for $I = 1, \ldots, L$:

$$z^{(l)} = h^{(l-1)} W^{(l)^{\top}}, \qquad h^{(l)} = f^{(l)} (z^{(l)}), \quad h^{(0)} = x.$$

Define pre-activation deltas:

$$\delta^{(L)} = \frac{\partial L}{\partial h^{(L)}} \odot f^{(L)'}(z^{(L)}), \qquad \delta^{(I)} = \left(\delta^{(I+1)}W^{(I+1)}\right) \odot f^{(I)'}(z^{(I)}), \quad I = L-1, \ldots, 1.$$

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Summary of all gradients for multilayer gradient descent

Quantity	Meaning	Formula
$\delta^{(L)}$	Error at output layer	$(\hat{y}-y)\odot f'(z^{(L)})$
$\delta^{(\prime)}$	Error at hidden layer I	$(\delta^{(l+1)}W^{(l+1)})\odot f'(z^{(l)})$
$rac{\partial L}{\partial W^{(I)}}$	Gradient w.r.t. weights	$\delta^{(\prime)^{ op}} h^{(\prime-1)}$
$rac{\partial m{L}}{\partial m{b}^{(I)}}$	Gradient w.r.t. biases	$\delta^{(I)}$
$rac{\partial L}{\partial h^{(I)}}$	Gradient passed to previous layer	$\delta^{(l+1)}W^{(l+1)}$

Update rule for each layer:

$$W^{(l)} \leftarrow W^{(l)} - \eta \frac{\partial L}{\partial W^{(l)}}, \qquad b^{(l)} \leftarrow b^{(l)} - \eta \frac{\partial L}{\partial b^{(l)}}.$$

Note: $h^{(0)} = x$ (the input), and the recursion for δ continues backward until the first layer.

Lab time: Implement backpropagation in a two-layer network

- Goal: implement a simple two-layer neural network from scratch in NumPy.
- The network should have:

```
Input: 2 \rightarrow Hidden: 3 \rightarrow Output: 3
```

- Use ReLU as activation for the hidden layer and a linear output for regression.
- Implement two main functions:
 - forward(x) computes \hat{y} and stores intermediate values for backward.
 - backward(y, cache) computes all gradients using the chain rule.
 - steps(grads, lr) update the weights using the calculated gradients.
- Perform the update step inside a simple loop to observe how the loss decreases over epochs.
- Suggested structure:
 - **1** Initialize W_1, b_1, W_2, b_2 with random values.
 - 2 Compute z_1, h, z_2, \hat{y} .
 - **3** Compute the loss $L = \frac{1}{2} ||\hat{y} y||^2$.
 - **1** Backpropagate and update parameters with learning rate η .
- Challenge: print the loss at each iteration and verify that it decreases.



```
import numpy as np
def relu(u):
    return np.maximum(0.0, u)
def relu grad(u):
    return (u > 0).astype(u.dtype)
class TwoLayerNet:
    def init (self, in dim=2, hidden dim=3, out dim=3, seed=0):
        np.random.seed(seed)
        self.W1 = np.random.randn(hidden_dim, in_dim)
        self.b1 = np.zeros(hidden_dim)
        self.W2 = np.random.randn(out dim. hidden dim)
        self.b2 = np.zeros(out dim)
    def forward(self. x):
        z1 = x @ self.W1.T + self.b1
        h = relu(z1)
        z^2 = h @ self.W2.T + self.b2
        y_hat = z2
        cache = {"x": x, "z1": z1, "h": h, "z2": z2, "y_hat": y_hat, "W2": self.W2.copy()}
        return v hat, cache
```

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```
def backward(self, y, cache):
    x, z1, h, z2, y_hat, W2 = (
        cache["x"], cache["z1"], cache["h"], cache["z2"], cache["y hat"], cache["W2"]
    diff = v hat - v
    loss = 0.5 * np.sum(diff**2)
    # Output layer
    delta2 = diff
    dW2 = np.outer(delta2, h)
    db2 = delta2
    # Hidden laver
    dh = delta2 @ W2
    delta1 = dh * relu_grad(z1)
    dW1 = np.outer(delta1, x)
    db1 = delta1
    grads = {"W1": dW1, "b1": db1, "W2": dW2, "b2": db2}
    return grads, loss
```

```
def step(self, grads, lr=0.01):
        self.W1 -= lr * grads["W1"]
        self.b1 -= lr * grads["b1"]
        self.W2 -= lr * grads["W2"]
        self.b2 -= lr * grads["b2"]
# ---- training loop ----
net = TwoLaverNet(seed=0)
x = np.array([1.0, 2.0])
y = np.array([1.0, 4.0, 4.0])
lr = 0.1
for epoch in range(20):
    v hat, cache = net.forward(x)
    grads, loss = net.backward(y, cache)
    net.step(grads, lr=lr)
    print(f"Epoch {epoch+1:02d} | Loss: {loss:.4f}")
```

From single sample to batch processing

• So far, we computed gradients for a single training example:

$$x \in \mathbb{R}^{d_{\text{in}}}, \qquad y \in \mathbb{R}^{d_{\text{out}}}.$$

• In practice, we process many samples at once using a batch:

$$X \in \mathbb{R}^{m \times d_{\text{in}}}, \qquad Y \in \mathbb{R}^{m \times d_{\text{out}}},$$

where m is the batch size.

• Forward pass (for the whole batch):

$$Z^{(1)} = XW^{(1)^{\top}} + b^{(1)}, \qquad H = f(Z^{(1)}),$$

$$Z^{(2)} = HW^{(2)^{\top}} + b^{(2)}, \qquad \hat{Y} = f(Z^{(2)}).$$

• Loss (mean squared error for the batch):

$$L = \frac{1}{2m} \|\hat{Y} - Y\|_F^2.$$



Backpropagation over batches

• Compute the gradients for all samples in the batch:

$$\delta^{(2)} = (\hat{Y} - Y) \odot f'(Z^{(2)}),$$

$$\frac{\partial L}{\partial W^{(2)}} = \frac{1}{m} \delta^{(2)^{\top}} H, \qquad \frac{\partial L}{\partial b^{(2)}} = \frac{1}{m} \sum_{i=1}^{m} \delta_{i}^{(2)},$$

$$\delta^{(1)} = (\delta^{(2)} W^{(2)}) \odot f'(Z^{(1)}), \qquad \frac{\partial L}{\partial W^{(1)}} = \frac{1}{m} \delta^{(1)^{\top}} X.$$

• The gradient descent update remains identical:

$$W^{(l)} \leftarrow W^{(l)} - \eta \frac{\partial L}{\partial W^{(l)}}, \qquad b^{(l)} \leftarrow b^{(l)} - \eta \frac{\partial L}{\partial b^{(l)}}.$$

• Each row of $\delta^{(l)}$ corresponds to one sample in the batch.



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Summary of all gradients for multilayer gradient descent (batch version)

Quantity	Meaning	Formula (batch size m)
$\Delta^{(L)}$	Error at output layer	$(\hat{Y} - Y) \odot f'(Z^{(L)})$
$\Delta^{(I)}$	Error at hidden layer I	$(\Delta^{(l+1)}W^{(l+1)})\odot f'(Z^{(l)})$
$rac{\partial L}{\partial W^{(I)}}$	Gradient w.r.t. weights	$\frac{1}{m}\Delta^{(\prime)^\top}H^{(l-1)}$
$rac{\partial L}{\partial b^{(I)}}$	Gradient w.r.t. biases	$\frac{1}{m}\sum_{i=1}^m \Delta_{i:}^{(I)}$
$rac{\partial L}{\partial H^{(I)}}$	Gradient passed to previous layer	$\Delta^{(l+1)} \mathcal{W}^{(l+1)}$

Update rule for each layer:

$$W^{(l)} \leftarrow W^{(l)} - \eta \frac{\partial L}{\partial W^{(l)}}, \qquad b^{(l)} \leftarrow b^{(l)} - \eta \frac{\partial L}{\partial b^{(l)}}.$$

Note:

- $X = H^{(0)}$ represents the batch input.
- Each row of $\Delta^{(l)}$ corresponds to one training sample.
- The factor $\frac{1}{m}$ ensures averaging over the batch.



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Lab time: extend the code to support batches

Goal: modify your two-layer (2-3-3) network to process a **batch** of m samples instead of a single input. **Tasks**

- Update forward() to accept a batch X and return \hat{Y} and the cached variables.
- ② Update backward() to use the batched derivatives and average over m.

class TwoLayerNet:

```
def init (self. in dim=2. hidden dim=3. out dim=3. seed=0):
    np.random.seed(seed)
    self.W1 = np.random.randn(hidden_dim, in_dim)
    self.b1 = np.zeros(hidden_dim)
    self.W2 = np.random.randn(out dim, hidden dim)
    self.b2 = np.zeros(out dim)
def forward(self, X):
   Z1 = X @ self.W1.T + self.b1
   H = relu(Z1)
   Z2 = H @ self.W2.T + self.b2
    Y hat = Z2
   cache = {
        "X": X, "Z1": Z1, "H": H, "Z2": Z2, "Y_hat": Y_hat,
        "W2": self.W2.copy()
   return Y_hat, cache
```

```
def backward(self, Y, cache):
    X, Z1, H, Z2, Y hat, W2 = (
        cache["X"], cache["Z1"], cache["H"], cache["Z2"], cache["Y hat"], cache["W2"]
   m = X.shape[0]
    Diff = Y hat - Y
                                                   # (m, out dim)
    loss = 0.5 / m * np.sum(Diff**2)
    # Output layer (linear): dY hat/dZ2 = 1
    Delta2 = Diff
                                                   # (m. out dim)
    dW2 = (Delta2.T @ H) / m
                                                   # (out dim. hidden dim)
    db2 = Delta2.mean(axis=0)
                                                   # (out dim.)
    # Hidden layer
    dH = Delta2 @ W2
                                                   # (m. hidden dim)
    Delta1 = dH * relu grad(Z1)
                                                   # (m. hidden dim)
    dW1 = (Delta1.T @ X) / m
                                                   # (hidden dim. in dim)
                                                   # (hidden dim.)
    db1 = Delta1.mean(axis=0)
    grads = {"W1": dW1, "b1": db1, "W2": dW2, "b2": db2}
    return grads, loss
```

```
if __name__ == "__main__":
    net = TwoLayerNet(seed=0, hidden dim=1000)
    n = 1000
    X = np.random.uniform(-10, 10, size=(n, 2))
    # Y: \[ \tau x 1 * * 2 \], \( x 2 * * 2 \], \( 2 * x 1 * x 2 \]
    Y = np.column_stack((
        X[:, 0]**2.
        X[:. 1]**2.
        2 * X[:, 0] * X[:, 1]
    ))
    for epoch in range(10000):
        Y hat, cache = net.forward(X/20)
        grads, loss = net.backward(Y, cache)
        net.step(grads, lr=0.01)
        print(f"Epoch {epoch+1:02d} | Loss: {loss:.4f}")
Y_{hat} = net.forward([[3/20,-1/20]]) #Extepcted [9, 1, -6]
print(Y_hat)
```

Lab time: train your TwoLayerNet on MNIST

Goal: use your simple TwoLayerNet class (with linear output and MSE loss on one-hot labels) to train a neural network on the MNIST dataset.

Instructions: Load the MNIST dataset:

- ullet Each image is 28 imes 28, flatten it into a vector of 784 values.
- Normalize pixel values to the range [0, 1].
- Convert integer labels (0–9) into one-hot vectors of length 10.

Create your model:

```
net = TwoLayerNet(in_dim=784, hidden_dim=128, out_dim=10)
```

Lab time: train your TwoLayerNet on MNIST

Train using the **entire dataset as a single batch**:

- Perform one forward pass on all samples.
- Compute gradients with backward.
- Apply the update step with step.
- Repeat for several epochs.

After each epoch:

- Print the average loss.
- Compute accuracy using np.argmax(y_hat, axis=1).

Note: if the dataset does not fit in memory, you can split it into smaller mini-batches and repeat the same steps for each batch.

Challenge: Observe how the network learns over time - monitor how the loss decreases and accuracy increases, even with this simple setup.

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```
#...
def normalize_fit(X):
    mean = X.mean(axis=0, keepdims=True).astype(np.float32)
    std = X.std(axis=0, keepdims=True).astype(np.float32)
    std[std < 1e-6] = 1e-6
    return mean, std

def normalize_apply(X, mean, std):
    return (X - mean) / std</pre>
```

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```
if name == " main ":
   Xtr = np.load("train images.npy").astype(np.float32)
   vtr = np.load("train labels.npv").astvpe(np.int64)
   Xte = np.load("test images.npy").astype(np.float32)
   vte = np.load("test labels.npy").astype(np.int64)
   Xtr /= 255.0: Xte /= 255.0
   mean. std = normalize fit(Xtr)
   Xtr = normalize_apply(Xtr, mean, std)
   Xte = normalize apply(Xte, mean, std)
   ytr = np.eye(10)[ytr]
   model = TwoLaverNet(in dim=784, hidden dim=32, out dim=10)
   for epoch in range(1000):
       Y hat, cache = model.forward(Xtr)
       grads, loss = model.backward(vtr, cache)
       model.step(grads, lr=0.0005)
       print(f"Epoch {epoch+1:02d} | Loss: {loss:.4f}")
   Y_pred,_ = model.forward(Xte)
   Y_pred = np.argmax(Y_pred,axis=1)
   accuracy = np.sum(Y pred==vte)/Y pred.shape[0]
   print(f"Accuracy: {accuracy: .4f}")
```

Thanks!

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