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Neural Networks

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Pattern Recognition Lab, Friedrich-Alexander University of Erlangen-Nürnberg
November 8, 2020



Flexibility vs. Abstraction

Low level

High level



- Linear Algebra operations
- Bare metal

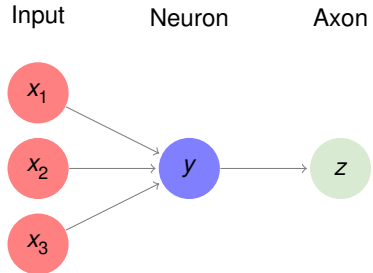
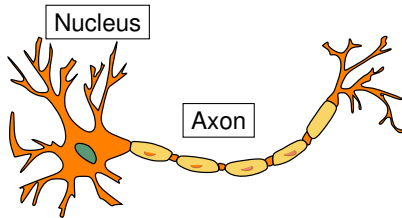


- Compiles graphs of Tensor operations
- High flexibility



- Stacks together elementary layers
- Reduced flexibility

Artificial Neural Networks



$$y = f\left(\sum_i^N w_i x_i\right)$$



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 - we allow only extremely simple graphs
 - with a list of layers
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- **recursively calls backward** on its layers passing the error
- in our case stores the loss over iterations, while in other frameworks this is commonly separated into an optimizer class

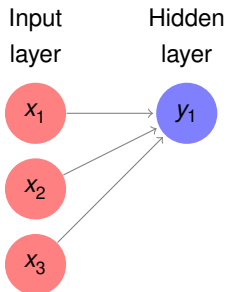


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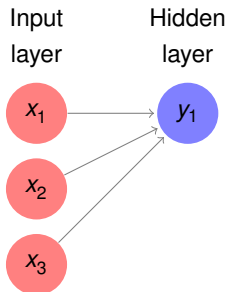
Fully Connected Layer



Forward



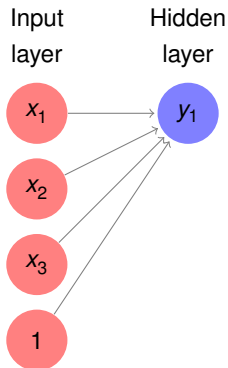
Forward



$$\begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}^T \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + w_{n+1} = \hat{y}$$

$$\mathbf{w}^T \mathbf{x} = \hat{y}$$

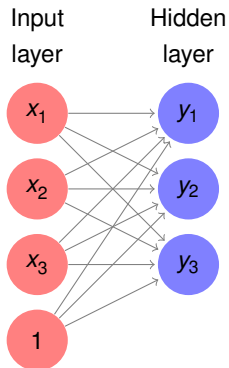
Forward



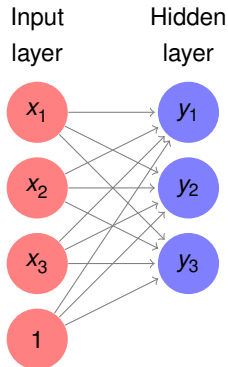
$$\begin{pmatrix} w_1 \\ \vdots \\ w_n \\ w_{n+1} \end{pmatrix}^T \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix} = \hat{y}$$

$$\mathbf{w}^T \mathbf{x} = \hat{y}$$

Forward



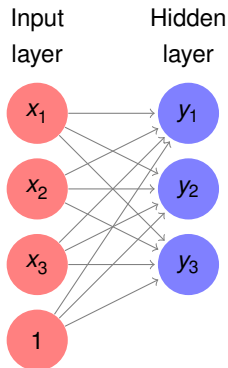
Forward



$$\begin{pmatrix} w_{1,1} & \dots & w_{1,m} \\ \vdots & \ddots & \vdots \\ w_{n,1} & \dots & w_{n,m} \\ w_{n+1,1} & \dots & w_{n+1,m} \end{pmatrix}^T \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix} = \begin{pmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_m \end{pmatrix}$$

$$\mathbf{W}\mathbf{x} = \hat{\mathbf{y}}$$

Forward



$$\begin{pmatrix} w_{1,1} & \dots & w_{1,m} \\ \vdots & \ddots & \vdots \\ w_{n,1} & \dots & w_{n,m} \\ w_{n+1,1} & \dots & w_{n+1,m} \end{pmatrix}^T \begin{pmatrix} x_{1,1} & \dots & x_{1,b} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \dots & x_{n,b} \\ 1 & \dots & 1 \end{pmatrix}$$

$$\mathbf{WX} = \hat{\mathbf{Y}} \quad (1)$$

Backward

- Return gradient with respect to **X**:

Backward

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$$\mathbf{E}_{n-1} = \mathbf{W}^T \mathbf{E}_n \quad (2)$$

- **E_n**: **error_tensor** passed downward

Backward

- Return gradient with respect to **X**:

$$\mathbf{E}_{n-1} = \mathbf{W}^T \mathbf{E}_n \quad (2)$$

- Update **W** using gradient with respect to **W**:

- **E_n**: **error_tensor** passed downward

Backward

- Return gradient with respect to \mathbf{X} :

$$\mathbf{E}_{n-1} = \mathbf{W}^T \mathbf{E}_n \quad (2)$$

- Update \mathbf{W} using gradient with respect to \mathbf{W} :

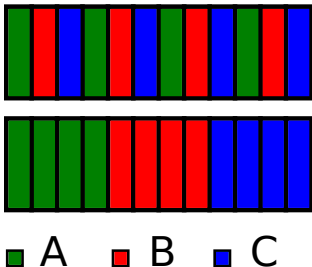
$$\mathbf{W}^{t+1} = \mathbf{W}^t - \eta \cdot \mathbf{E}_n \mathbf{X}^T \quad (3)$$

Note: Dynamic programming part of Backpropagation

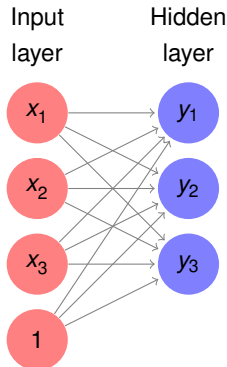
- \mathbf{E}_n : **error_tensor** passed downward
- η : learning rate

Memory Layout

- Numpy uses C ordering by default
- Wrong ordering will cause strided data access
- We want the batch size to be the outermost loop
→ We have to adjust our formulas for the implementation



Forward - Our Memory Layout



$$\begin{pmatrix} x_{1,1} & \dots & x_{1,b} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \dots & x_{n,b} \\ 1 & \dots & 1 \end{pmatrix}^T \begin{pmatrix} w_{1,1} & \dots & w_{1,m} \\ \vdots & \ddots & \vdots \\ w_{n,1} & \dots & w_{n,m} \\ w_{n+1,1} & \dots & w_{n+1,m} \end{pmatrix}$$

$$\mathbf{x}'\mathbf{w}' = \hat{\mathbf{y}}' \quad (4)$$

with

$$\mathbf{x}' = \mathbf{x}^T, \mathbf{w}' = \mathbf{w}^T, \hat{\mathbf{y}}' = \hat{\mathbf{y}}^T \quad (5)$$

$$\hat{\mathbf{y}}^T = (\mathbf{w}\mathbf{x})^T = \mathbf{x}^T\mathbf{w}^T \quad (6)$$

Backward - Our Memory Layout

- Return gradient with respect to \mathbf{X} :

$$\mathbf{E}'_{n-1} = \mathbf{E}'_n \mathbf{W}'^T \quad (7)$$

- Update \mathbf{W}' using gradient with respect to \mathbf{W}' :

$$\mathbf{W}'^{t+1} = \mathbf{W}'^t - \eta \cdot \mathbf{X}'^T \mathbf{E}'_n \quad (8)$$

Note: Dynamic programming part of Backpropagation

- \mathbf{E}'_n : **error_tensor** passed downward
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Basic Optimization



SGD

- In order to perform the aforementioned weight update we make use of a dedicated optimizer.
- In the first exercise we implement the Stochastic Gradient Descent Algorithm

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \underbrace{\nabla L(\mathbf{w}^{(k)})}_{\text{Gradient}}$$

where η denotes the learning rate.

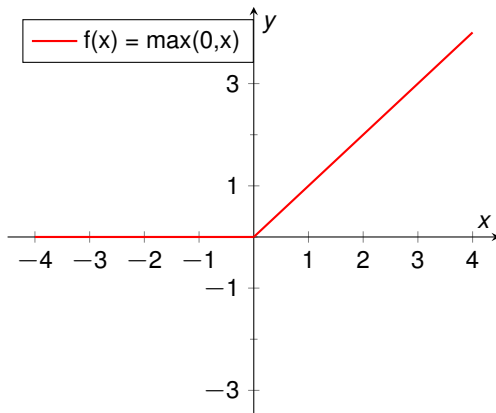


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ReLU Activation Function



Forward



Backward

ReLU is not continuously differentiable!

Backward

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$$e_{n-1} = \begin{cases} 0 & \text{if } x \leq 0 \\ e_n & \text{else} \end{cases} \quad (9)$$

Note: DP part of Backpropagation yet again

Backward

ReLU is not continuously differentiable!

$$e_{n-1} = \begin{cases} 0 & \text{if } x \leq 0 \\ e_n & \text{else} \end{cases} \quad (9)$$

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- The scalar e is because activation functions operate elementwise on \mathbf{E}

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ReLU is not continuously differentiable!

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- If you wonder about e_n instead of 1 consider that this is $\underbrace{\frac{\partial L}{\partial \hat{\mathbf{y}}}}_{\mathbf{E}} \cdot \underbrace{\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{x}}}_{\text{ReLU}}$



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SoftMax Activation Function



Forward

Labels as N -dimensional **one hot** vector \mathbf{y} :

$$\begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix}$$

Forward

Labels as N -dimensional **one hot** vector \mathbf{y} :

$$\begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix}$$

- Activation(Prediction) $\hat{\mathbf{y}}$ for every element of the batch of size B :

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^N \exp(x_j)} \quad (10)$$

Numeric

- If $x_k > 0 \rightarrow e^{x_k}$ might become very large
- To increase numerical stability x_k can be shifted
- $\tilde{x}_k = x_k - \max(\mathbf{x})$
- This leaves the scores unchanged!

Backward

- Compute for every element of the batch:

$$\mathbf{E}_{n-1} = \hat{y} \left(\mathbf{E}_n - \sum_{j=1}^N \mathbf{E}_{n,j} \hat{y}_j \right) \quad (11)$$

Backward

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- All operations are element-wise

Backward

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- All operations are element-wise
- Notice the similarity to the sigmoid gradient $\hat{y}(1 - \hat{y})$



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Cross Entropy Loss



Forward

$$loss = \sum_{b=1}^B -\ln(\hat{y}_k + \epsilon) \text{ where } y_k = 1 \quad (12)$$

- ϵ represents the smallest representable number. Take a look into *np.finfo.eps*
- ϵ increases stability for very wrong predictions to prevent values close to $\log(0)$

Forward

$$loss = \sum_{b=1}^B -\ln(\hat{y}_k + \epsilon) \text{ where } y_k = 1 \quad (12)$$

- ϵ represents the smallest representable number. Take a look into *np.finfo.eps*
- ϵ increases stability for very wrong predictions to prevent values close to $\log(0)$
- Notice: the Cross Entropy Loss requires predictions to be greater than 0,
- thus the Cross Entropy Loss works most stable with SoftMax predictions.

Backward

$$\mathbf{E}_n = -\frac{y}{\hat{y}} \quad (13)$$

- ϵ cancels out due to derivation. An additional ϵ would distort the gradient dramatically!
- The gradient prohibits predictions of 0 as well.

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- ϵ cancels out due to derivation. An additional ϵ would distort the gradient dramatically!
- The gradient prohibits predictions of 0 as well.
- Notice that this does **not** depend on an error \mathbf{E} .
→ it's the starting point of the recursive computation of gradients.



Thanks for listening.
Any questions?