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Neural Networks

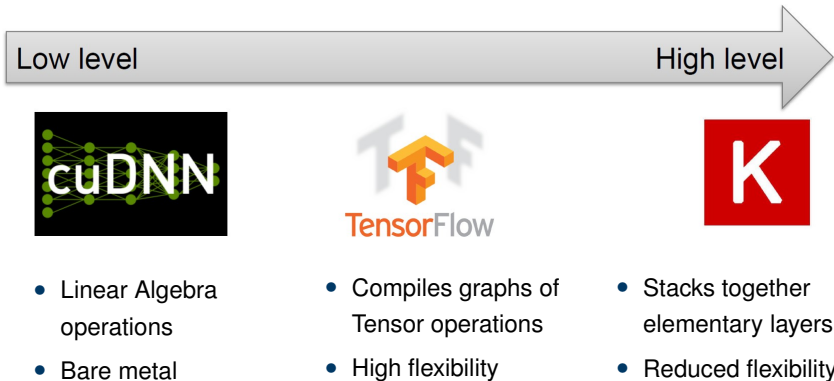
K. Breininger, V. Christlein, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle, M. Zinnen,
K. Packhäuser

Pattern Recognition Lab, Friedrich-Alexander University of Erlangen-Nürnberg

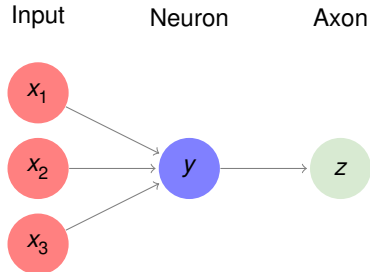
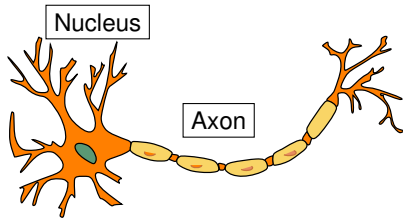
October 17, 2022



Flexibility vs. Abstraction



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
 - and only one data source
 - and one loss function

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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

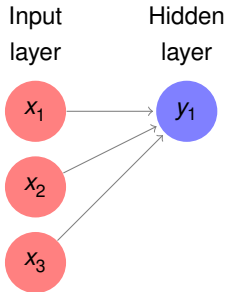


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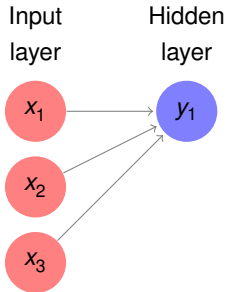
Fully Connected Layer



Forward



Forward

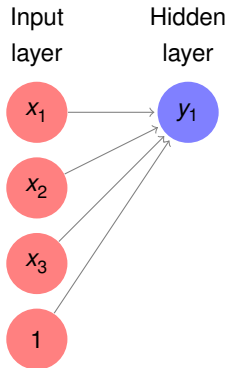


$$(w_1 \quad \dots \quad w_n) \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + w_{n+1} = \hat{y}$$

$$\mathbf{w}\mathbf{x} + \underbrace{w_{n+1}}_{\text{bias}} = \hat{y}$$

- Including the bias into the weight matrix results in a single matrix multiplication

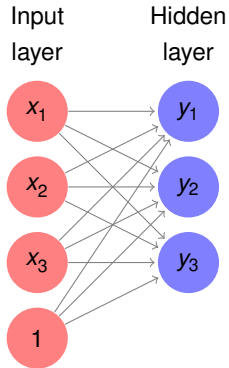
Forward



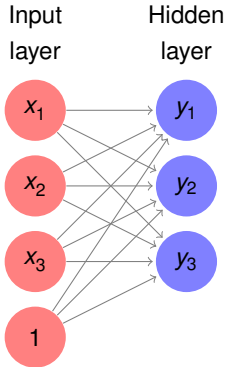
$$(w_1 \quad \dots \quad w_n \quad w_{n+1}) \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix} = \hat{y}$$

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

Forward



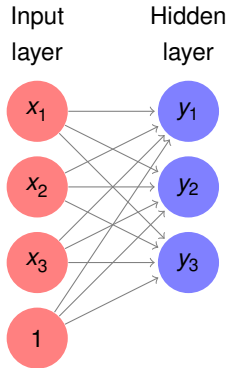
Forward



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

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

Forward



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

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

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} :

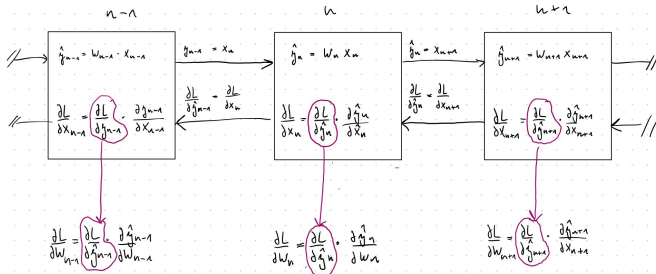
$$\mathbf{W}^{t+1} = \mathbf{W}^t - \eta \cdot \mathbf{E}_n \mathbf{X}^T \quad (3)$$

Note: Dynamic programming part of Backpropagation

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

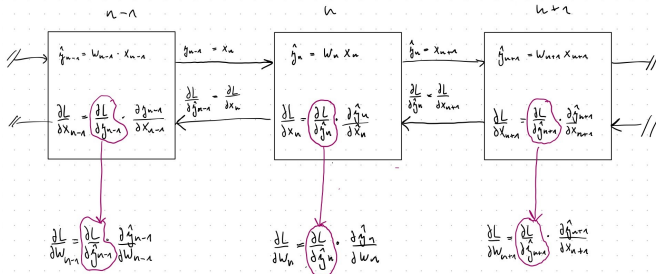
But what is E_n ?

- L denotes the loss and



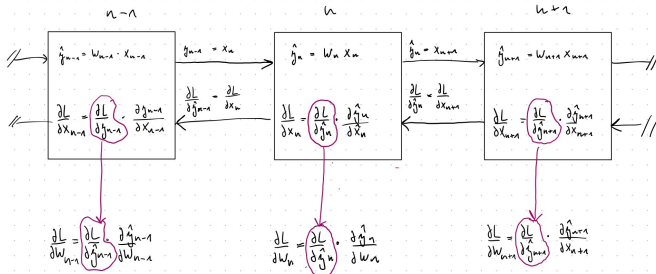
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- E_n is $\frac{\partial L}{\partial \hat{y}_n}$ of a layer n (center box down below in purple).



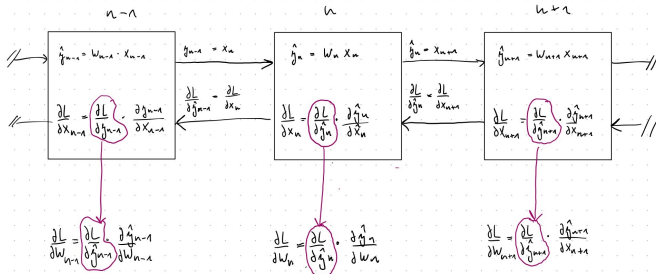
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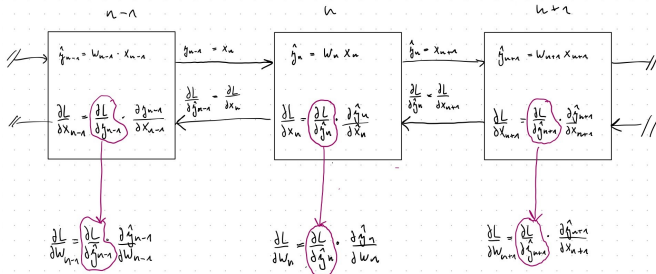
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- which is $E_{n-1} = \frac{\partial L}{\partial \hat{y}_{n-1}}$ of the next upper layer $n - 1$



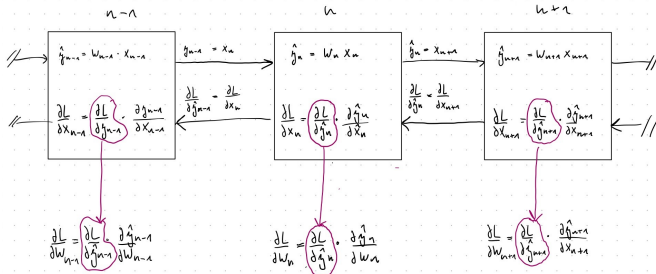
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- which is $E_{n-1} = \frac{\partial L}{\partial \hat{y}_{n-1}}$ of the next upper layer $n - 1$
- because the output of the layer $n - 1$ is the input of layer n : $\hat{y}_{n-1} = x_n$.



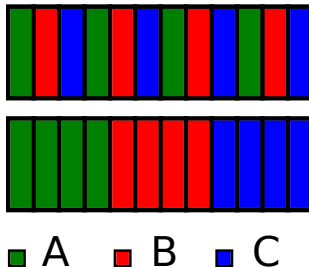
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- because the output of the layer $n - 1$ is the input of layer n : $\hat{y}_{n-1} = x_n$.
- Thus $\frac{\partial L}{\partial \hat{y}_{n-1}} = \frac{\partial L}{\partial x_n}$. This is **Backpropagation**!

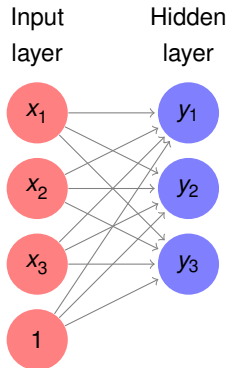


Memory Layout

- We don't want to have $X[:, 0]$ but $X[0]$ to access the batch
- We want the batch size to be the outermost loop
→ We have to adjust our formulas for the implementation
- We achieve it by transposition!



Forward - Our Memory Layout



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

$$(WX)^T = \hat{Y}^T \quad (4)$$

$$X^T W^T = \hat{Y}^T \quad (5)$$

Forward - Our Memory Layout

We transposed our equations

$$(\mathbf{W}\mathbf{X})^T = \hat{\mathbf{Y}}^T \quad (6)$$

$$\mathbf{X}^T \mathbf{W}^T = \hat{\mathbf{Y}}^T \quad (7)$$

but to benefit in our code from this new layout, we need to store our variables also in the transposed version. To differentiate the new and the old layout, the transposed versions of \mathbf{X} , \mathbf{W} , \mathbf{E} and $\hat{\mathbf{Y}}$ are now denoted with primes:

$$\mathbf{X}' = \mathbf{X}^T, \mathbf{W}' = \mathbf{W}^T, \mathbf{E}' = \mathbf{E}^T, \hat{\mathbf{Y}}' = \hat{\mathbf{Y}}^T \quad (8)$$

E.g. your python variable for the weights is now \mathbf{W}' , so we store our variables already in the transposed layout and compute everything in the new layout, like the forward pass:

$$\mathbf{X}' \mathbf{W}' = \hat{\mathbf{Y}}' \quad (9)$$

Backward - Our Memory Layout

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

$$\mathbf{E}'_{n-1} = \mathbf{E}'_n \mathbf{W}'^T \quad (10)$$

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

$$\mathbf{W}'^{t+1} = \mathbf{W}'^t - \eta \cdot \mathbf{X}'^T \mathbf{E}'_n \quad (11)$$

Note: Dynamic programming part of Backpropagation

- \mathbf{E}'_n : **error_tensor** passed downward
- \mathbf{E}'_n has always the same shape as \mathbf{Y}
- \mathbf{E}'_{n-1} has always the same shape as \mathbf{X}
- η : learning rate



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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.

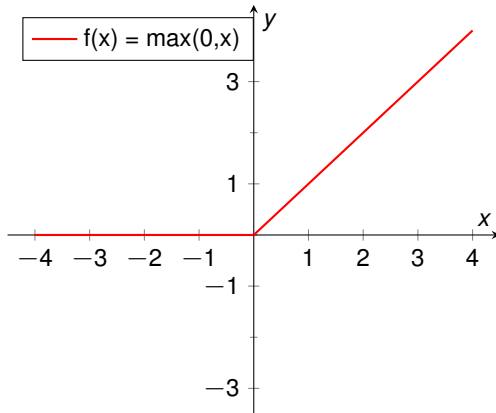


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ReLU Activation Function



Forward



Backward

ReLU is not continuously differentiable!

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ReLU is not continuously differentiable!

$$e_{n-1} = \begin{cases} 0 & \text{if } x \leq 0 \\ e_n & \text{else} \end{cases} \quad (12)$$

Note: DP part of Backpropagation yet again

Backward

ReLU is not continuously differentiable!

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- The scalar e is because activation functions operate elementwise on **E**

Backward

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Note: DP part of Backpropagation yet again

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

- 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 :

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^N \exp(x_j)} \quad (13)$$

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:

$$\mathbf{E}_{n-1} = \mathbf{y} \left(\mathbf{E}_n - \sum_{j=1}^N \mathbf{E}_{n,j} \hat{y}_j \right) \quad (14)$$

Backward

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- All operations are element-wise

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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

$$loss = \sum_{b=1}^B -\ln(\hat{y}_k + \epsilon) \text{ where } y_k = 1 \quad (15)$$

- 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

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- 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

$$\mathbf{E}_n = -\frac{y}{\hat{y} + \epsilon} \quad (16)$$

- The gradient prohibits predictions of 0 as well.

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$$\mathbf{E}_n = -\frac{y}{\hat{y} + \epsilon} \quad (16)$$

- 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?