Neural Networks

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Flexibility vs. Abstraction

Low level High level

- Linear Algebra operations
- Bare metal

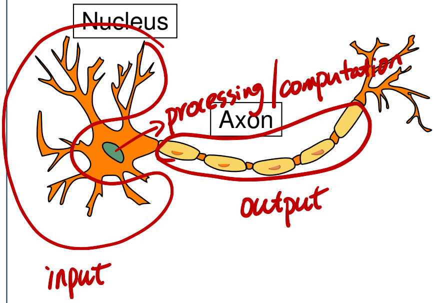
- Compiles graphs of Tensor operations
- High flexibility

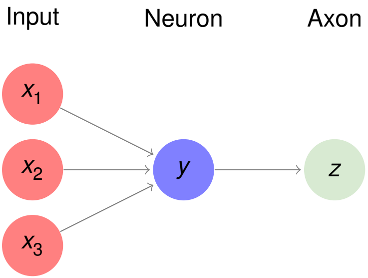
- Stacks together elementary layers
- Reduced flexibility

Artifical Neural Networks

Terminology:

- error tensor E / E_{n-1} : $\frac{\partial L}{\partial y}$
- "Layer" : activation function becomes a layer





$$\mathbf{y} = f\Big(\sum_{i}^{N} w_i x_i\Big)$$

non-linear function

Neural Network

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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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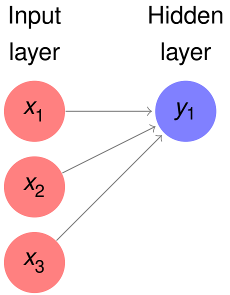
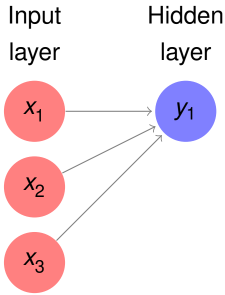
- **recursively calls forward** on its layers passing the input-data feed forward data
- **recursively calls backward** on its layers passing the error backpropagation/optimization parameters
- in our case stores the loss over iterations, while in other frameworks this is commonly separated into an optimizer class

Fully Connected Layer

Forward



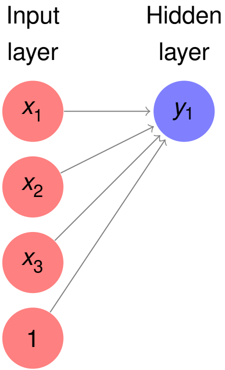
Forward



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

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

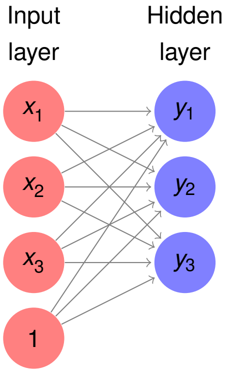
Forward



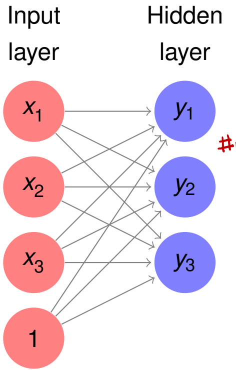
$$\begin{pmatrix} w_1 \\ \vdots \\ w_n \\ w_{n+1} \end{pmatrix}^T \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix} = \hat{y}$$

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

Forward



Forward



#output m

#input n

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

$m \times n$ $\quad$ $n \times 1$ $\quad$ $m \times 1$

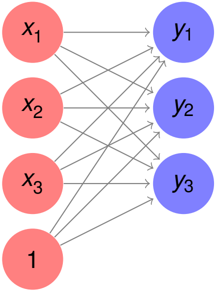
$$\mathbf{W}\mathbf{x} = \hat{\mathbf{y}}$$

$(\ )^T$

Forward

Input layer

Hidden layer



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

batch dimension

$$\mathbf{W}\mathbf{X} = \hat{\mathbf{Y}} \tag{1}$$

Backward $\begin{cases} \nabla x \\ \nabla w \end{cases}$

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

Backward

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

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

- $\mathbf{E_n}$: **error_tensor** passed downward

Backward

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

- $\mathbf{E_n}$: **error_tensor** passed downward

Backward

$E: \frac{\partial}{\partial \text{input}}$

- 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**:

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

$\frac{\partial L}{\partial w}$

Note: Dynamic programming part of Backpropagation

- $\mathbf{E_n}$: **error_tensor** passed downward
- η: learning rate

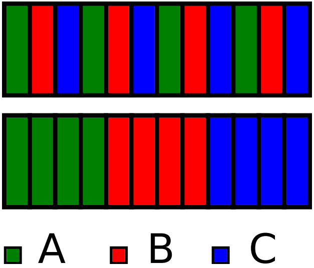
Memory Layout

C: a[0][0], a[0][1], a[0][2], a[1][0], a[1][1]... 从左到右

F: a[0][0], a[1][0], a[2][0], a[0][1], a[1][1]... 从上到下

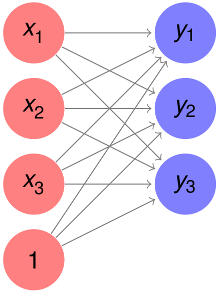
Contiguous 连续存储

- Numpy uses C ordering by default
- Wrong ordering will cause 大跨距 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

Input layer   Hidden layer



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

$$\mathbf{X}'\mathbf{W}' = \hat{\mathbf{Y}}' \tag{4}$$

with

$$\mathbf{X}' = \mathbf{X}^\mathsf{T},\ \mathbf{W}' = \mathbf{W}^\mathsf{T},\ \hat{\mathbf{Y}}' = \hat{\mathbf{Y}}^\mathsf{T} \tag{5}$$

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

Backward - Our Memory Layout

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

$$\mathbf{E}'_{\mathbf{n-1}} = \mathbf{E}'_{\mathbf{n}}\mathbf{W}'^{\mathbf{T}} \tag{7}$$

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

W updates for fully connected layer

$$\boxed{\mathbf{W}'^{t+1} = \mathbf{W}'^{t} - \eta \cdot \mathbf{X}'^{\mathbf{T}}\mathbf{E}'_{\mathbf{n}}} \tag{8}$$

Note: Dynamic programming part of Backpropagation

- $\mathbf{E}'_{\mathbf{n}}$: **error_tensor** passed downward
- η: learning rate

Basic Optimization

SGD

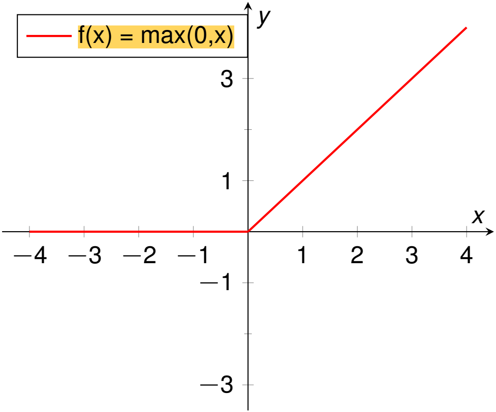
- In order to perform the aforementioned weight update we make use of a dedicated optimizer.
- In the first exercise we implement the Stochastic Gradient Descent Algorithm

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

where η denotes the learning rate.

ReLU Activation Function

Forward



Backward

ReLU is not continuously differentiable!

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

Note: DP part of Backpropagation yet again

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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 $\underbrace{\frac{\partial L}{\partial \hat{\mathbf{y}}}}_{\mathbf{E}} \cdot \underbrace{\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{x}}}_{\text{ReLU}}$

?

SoftMax Activation Function

Forward

Labels as N-dimensional **one hot vector y**: $\begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix}$

Forward

Labels as N-dimensional **one hot vector y**: $\begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix}$

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

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

?

Numeric

- If $x_k > 0 \to e^{x_k}$ 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:

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

$j = 1 \rightsquigarrow batch\_size.$

Backward

- Compute for every element of the batch:

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- All operations are element-wise

Backward

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

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

Cross Entropy Loss

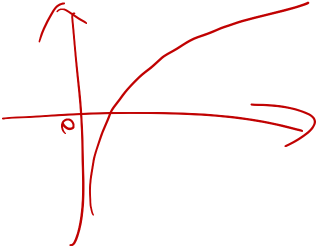
Compute Loss for Classification / Distribution

Forward

B↑, Loss↑

$$loss = \sum_{b=1}^{B} -\ln\left(\hat{y}_k + \epsilon\right) \;\; \textbf{where} \; y_k = 1 \qquad (12)$$

- 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 $log(0)$



exploding gradient

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 CrossEntropy Loss requires predictions to be greater than 0,
- thus the CrossEntropyLoss works most stable with softmax predictions.

Backward

$$\mathbf{E}_n = -\frac{y}{\hat{y}} \tag{13}$$

- 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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- The gradient prohibits predictions of 0 as well.
- Notice that this does **not** depend on an error **E**.
  $\rightarrow$ it's the starting point of the recursive computation of gradients.

Thanks for listening.

Any questions?