DeepLearning on FPGAs

Artificial Neural Networks: Backpropagation and more

Sebastian Buschjäger

Technische Universität Dortmund - Fakultät Informatik - Lehrstuhl 8

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Recap: Homework

Question: So whats your accuracy?
Question: What about speed?

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Some remark about notation: In the previous slides I used θ twice with different meaning

1) As "bias" parameter for the perceptron
2) As vector-to-be-optimized by gradient descent

$\Rightarrow$ This is now changed. θ will always be used in a general fashion as the vector-to-be-optimized.

Any questions / remarks / whatsoever?

Recap: Data Mining (1)

Important concepts:

- **Feature Engineering** is key to solve Data Mining tasks
- **Deep Learning** combines learning and Feature Engineering
- **Data Mining approach:**
  - Specify model family ($\rightarrow$ perceptron)
  - Specify optimization procedure ($\rightarrow$ gradient descent)
  - Specify a cost / loss function ($\rightarrow$ RMSE or cross-entropy)

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Perceptron: A linear classifier $f\colon \mathbb{R}^d \rightarrow \{0, 1\}$ with

$$\widehat{f}(\vec{x}) = \begin{cases} +1 & \text{if } \sum_{i=1}^{d} w_i \cdot x_i \geq b \\ 0 & \text{else} \end{cases}$$

Recap: Data Mining (2)

Optimization procedure: Gradient descent

$$\widehat{\theta}^{new} = \widehat{\theta}^{old} - \alpha \cdot \nabla_{\theta} \ell(\mathcal{D}, \widehat{\theta}^{old})$$

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Loss function: RMSE or cross-entropy

$$\ell(\mathcal{D}, \widehat{\theta}) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(y_i - f_{\widehat{\theta}}(\vec{x}_i)\right)^2}$$

$$\ell(\mathcal{D}, \widehat{\theta}) = -\frac{1}{N} \sum_{i=1}^{N} \left(y_i \ln\left(f_{\widehat{\theta}}(\vec{x}_i)\right) + (1 - y_i) \ln\left(1 - f_{\widehat{\theta}}(\vec{x}_i)\right)\right)$$

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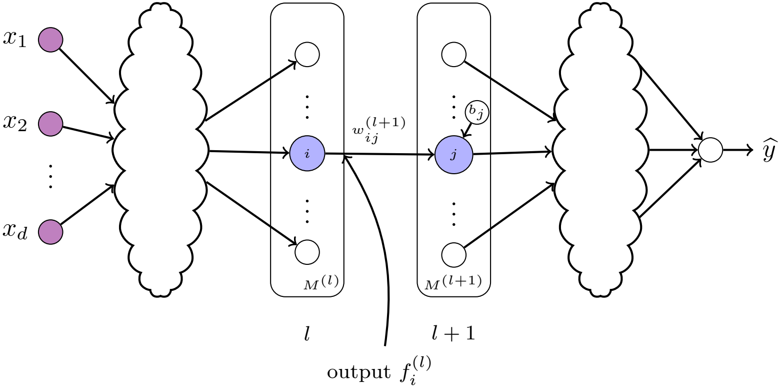
So far: Training of single perceptron
Now: Training of multi-layer perceptron (MLP)

MLP: Some Notation (1)



$\mathbf{w_{i,j}^{(l+1)}} \widehat{=}$ Weight from neuron i in layer l to neuron j in layer $l+1$

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Gradient descent:

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Loss function:

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Observation 1: Square-Root is monotone
Observation 2: Loss function depends on entire training data set!

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Note: For $\alpha \to 0$ it "almost surely" converges

MLP: Learning (3)

New loss function:

$$
\begin{aligned}
\ell(\mathcal{D}, \widehat{w}) &= \frac{1}{2}\left(y_i - \widehat{f}(\vec{x}_i)\right)^2 \\
\nabla_{\widehat{w}}\ell(\mathcal{D}, \widehat{w}) &= \frac{1}{2}2(y_i - \widehat{f}(\vec{x}_i))\frac{\partial \widehat{f}(\vec{x}_i)}{\partial \widehat{w}}
\end{aligned}
$$

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Observation: f is not continuous in 0 (it makes a step)
Thus: Impossible to derive $\nabla_{\widehat{w}}\ell(\mathcal{D}, w)$ in 0, because f is not differentiable in 0!

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Solution: We need to make f continuous

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Bonus: This seems to be a little closer to real neurons

Bonus 2: We have non-linearity inside the network (more later)

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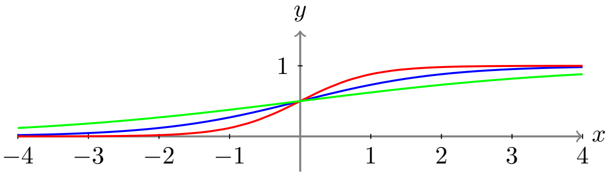
Idea: Use sigmoid **activation** function



$$\sigma(z) = \frac{1}{1+e^{-\beta \cdot z}}, \beta \in \mathbb{R}_{>0}$$

Note: β controls slope around 0

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&= \beta(1-\sigma(z))\sigma(z)
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Thus: Given L layer in total

- **Internally:** We use $f_j^{(l+1)} = \sigma\left(\sum_{i=0}^{M^{(l)}} w_{i,j}^{(l+1)} f_i^{(l)} + b_j^{(l+1)}\right)$
- **Prediction:** Is mapped to 0 or 1:

$$\widehat{f}(\vec{x}) = \begin{cases} +1 & \text{if } \sigma\left(\sum_{i=0}^{M^{(L-1)}} w_i^{(L)} f_i^{(L-1)} + b^{(L)}\right) \geq 0 \\ 0 & \text{else} \end{cases}$$

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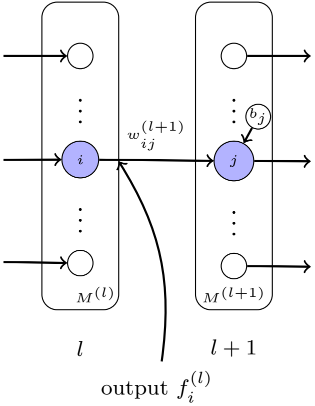
Learning with gradient descent:

$$w_{i,j}^{(l)} = w_{i,j}^{(l)} - \alpha \cdot \frac{\partial \ell}{\partial w_{i,j}^{(l)}}$$

$$b_j^{(l)} = b_j^{(l)} - \alpha \cdot \frac{\partial \ell}{\partial b_j^{(l)}}$$

MLP: Notation Recap

Note: Too many l and ℓ's: Use $E = \ell$ (loss) for easier reading



$$\textbf{find} : \frac{\partial E}{\partial w_{i,j}^{(l)}}, \frac{\partial E}{\partial b_j^{(l)}}$$

$$M^{(l)} \;\hat{=}\; \#\text{Neurons in layer } l$$

$$y_j^{(l+1)} = \sum_{i=0}^{M^{(l)}} w_{i,j}^{(l+1)} f_i^{(l)} + b_j^{(l+1)}$$

$$f_j^{(l+1)} = \sigma\left(y_j^{(l+1)}\right)$$

$$\sigma(z) = \frac{1}{1+e^{-\beta \cdot z}}, \beta = 1$$

. . .

. . .

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Backpropagation for sigmoid activation / RMSE loss

Gradient step:

$$
\begin{aligned}
w_{i,j}^{(l)} &= w_{i,j}^{(l)} - \alpha \cdot \delta_j^{(l)} f_i^{(l-1)} \\
b_j^{(l)} &= b_j^{(l)} - \alpha \cdot \delta_j^{(l)}
\end{aligned}
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Recursion:

$$
\begin{aligned}
\delta_j^{(l-1)} &= f_j^{(l-1)} \left(1 - f_j^{(l-1)}\right) \sum_{k=1}^{M^{(l)}} \delta_k^{(l)} w_{j,k}^{(l)} \\
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derivative of loss function

Backpropagation for activation h / loss ℓ

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\delta_j^{(l-1)} &= \frac{\partial h(y_i^{(l-1)})}{\partial y_i^{(l-1)}} \sum_{k=1}^{M^{(l)}} \delta_k^{(l)} w_{j,k}^{(l)} \\
\delta_j^{(L)} &= \frac{\partial \ell(y_i^{(L)})}{\partial y_i^{(L)}} \cdot \frac{\partial h(y_i^{(L)})}{\partial y_i^{(L)}}
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Backpropagation: Different notation

Notation: We used scalar notation so far

Fact: Same results can be derived using matrix-vector notation

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$$\delta^{(l-1)} = \left(W^{(l)}\right)^T \delta^{(l)} \odot \frac{\partial h(y^{(l-1)})}{\partial y^{(l-1)}}$$

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vectorial derivative!

Hadamard-product / Schur-product: piecewise multiplication

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- Each layer implements delta computation
- Output-layer implements delta computation with loss function
- Layers are either connected to each other and recursively call backprop. or some "control" function performs backprop.

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Thus: Arbitrary network architectures can be realised without changing learning algorithm

Network architectures

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Some general ideas:

- **Non-linear activation:** A network should contain at least one layer with non-linear activation function for better learning
- **Sparse activation:** To prevent over-fitting, only a few neurons of the network should be active at the same time
- **Fast convergence:** The loss function / activation function should allow a fast convergence in the first few epochs
- **Feature extraction:** Combining multiple layers in deeper networks usually allows (higher) level feature extraction

Backpropagation: Vanishing gradients

Observation 1: $\sigma(z) = \frac{1}{1+e^{-\beta \cdot z}} \in [0, 1]$

Observation 2: $\frac{\partial \sigma(z)}{\partial z} = \sigma(z) \cdot (1 - \sigma(z)) \in [0, 1]$

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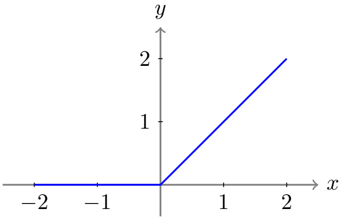
So far: No fundamental solution found, but a few suggestions

- Change activation function
- Exploit different optimization methods
- Use more data / carefully adjust stepsizes
- Reduce number of parameters / depth of network

New activation function: ReLu

Rectified Linear (ReLu):



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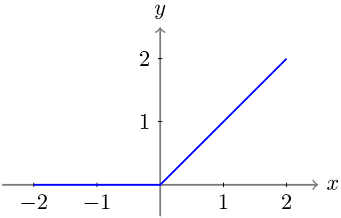

$$h(z) = \begin{cases} z & \text{if } z \geq 0 \\ 0 & \text{else} \end{cases} = max(0, z)$$

$$\frac{\partial h(z)}{\partial z} = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{else} \end{cases}$$

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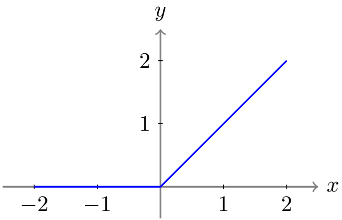

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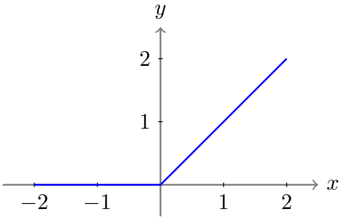

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Note: ReLu is not differentiable in $z = 0$!

But: Usually that is not a problem

- **Practical:** $z = 0$ is pretty rare, just use 0 there. It works well
- **Mathematical:** There exists a subgradient of $h(z)$ at 0

ReLu(2)

Subgradients: A gradient shows the direct of the steepest descent
$\Rightarrow$ If a function is not differentiable, it has no steepest descent
$\Rightarrow$ There might be multiple (equally) "steepest descents"

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For ReLu: We can choose $\frac{\partial h(z)}{\partial z}\Big|_{z=0}$ from $[0, 1]$
Big Note: Using a subgradient does not guarantee that our loss function decreases! We might change weights to the worse!

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$\Rightarrow$ There might be multiple (equally) "steepest descents"

For ReLu: We can choose $\frac{\partial h(z)}{\partial z}\Big|_{z=0}$ from $[0,1]$
Big Note: Using a subgradient does not guarantee that our loss function decreases! We might change weights to the worse!

Nice properties of ReLu:

- Super-easy forward, backward and derivative computation
- Either activates or deactivates a neuron (sparsity)
- Less problems with gradient vanishing, since error is multiplied by 1 or 0
- Still gives network non-linear activation

Improve convergence for GD: Simple improvements

Gradient descent:

$$\widehat{\theta}^{new} = \widehat{\theta}^{old} - \alpha \cdot \nabla_\theta \ell(\mathcal{D}, \widehat{\theta}^{old})$$

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(Mini-)Batch: Compute derivatives for multiple examples and average direction (allows parallel computation of gradient)

$$\widehat{\theta}^{new} = \widehat{\theta}^{old} - \alpha \cdot \frac{1}{K} \sum_{i=0}^{K} \nabla_\theta \ell(\vec{x}_i, \widehat{\theta}^{old})$$

Note: For Mini-Batch approaches the convergence is not guranteed theoretically

Improve convergence: Stepsize

What about the stepsize?

- If its to small, you will learn slow ($\rightarrow$ more data required)
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Practical suggestion: Simple heuristic

- Try out different stepsizes on small subsample of data
- Pick that one that most reduces the loss
- Use it for on the full dataset

Sidenote: Changing the stepsize while training also possible

Improve convergence: Loss functions

Recap: $\delta_j^{(L)}$ should be relatively large for faster learning:

$$\delta_j^{(L)} = \frac{\partial \ell(y_i^{(L)})}{\partial y_i^{(L)}} \cdot \frac{\partial h(y_i^{(L)})}{\partial y_i^{(L)}} = \frac{\partial \ell(\widehat{y})}{\partial \widehat{y}} \cdot \frac{\partial h(\widehat{y}))}{\partial \widehat{y}}$$

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$\rightarrow \delta_j^{(L)} = \frac{\widehat{y}-y}{(1-\widehat{y})\widehat{y}} \cdot \frac{\partial h(\widehat{y}))}{\partial \widehat{y}} = \widehat{y} - y$ cancels small sigmoid values

Improve Convergence: Start solution

Where do we start?

In SGD: Start with some θ. SGD will walk us the right direction

Important: For NN (specifically for MSE + sigmoid activation) we need "sane" initialization:

$$\begin{aligned} \delta_j^{(L)} &= -\left(y_i - f_j^{(L)}\right) f_j^{(L)} \left(1 - f_j^{(L)}\right) \\ \Rightarrow \delta_j^{(L)} &= 0, \text{ if } f_j^{(L)} = 0 \text{ or } f_j^{(L)} = 1 \end{aligned}$$

Therefore: Init weights randomly with gaussian distribution

$$w_{ij}^{(l)} \sim \mathcal{N}(0, \varepsilon) \text{ with } \varepsilon = 0.001 - 0.1$$

Bonus: Negative weights are also present

Summary

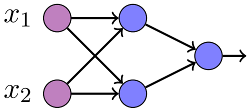
Important concepts:

- **For parameter optimization** we define a loss function
- **For parameter optimization** we use gradient descent
- **Neurons** have activation functions to ensure non-linearity and differentiability
- **Backpropagation** is an algorithm to compute the gradient
- **Non-linear and sparse** networks are usually better
- **Various techniques** can be used to improve convergence speed

Homework

Homework until next meeting

- Implement the following network to solve the XOR problem



- Implement backpropagation for this network
  - Try a simple solution first: Hardcode one activation / one loss function with fixed access to data structures
- If you feel comfortable, add new activation / loss functions

Tip 1: Verify that the proposed network uses 9 parameters
Tip 2: Start with $\alpha = 1.0$ and 10000 training examples
Note: We will later use `C`, so please use `C` or a `C`-like language
Question: Can you reduce the number of examples necessary?