Deep Learning Lab Course 2018

Labs:
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(Robotics) Wolfram Burgard,
(Machine Learning) Frank Hutter,
(Neurorobotics) Joschka Boedecker

University of Freiburg

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Technical Issues

- **Location:** Tuesday, 14:00 - 16:00, building 082, room 00 006 (Kinohoersaal)
- **Remark:** We will be there for questions every week from 14:00 - 16:00.
  - *We expect you to work on your own.* Your attendance is required during lectures/presentations
  - *We expect you have basic knowledge in ML (e.g. heard the Machine Learning lecture).*
- **Contact information (tutors):**

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- **Homepage:** http://dl-lab.informatik.uni-freiburg.de/

Schedule and outline

- **Phase 1**
  - **Today:** introduction deep learning (lecture).
  - **16.10 - 30.10** Assignment 1
  - **23.10:** Q/A session
  - **30.10:** introduction convolutional neural networks (lecture), hand in Assignment 1
  - **30.10 - 13.11:** Assignment 2
  - **06.11:** Q/A session

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- **Phase 2 (split into different tracks)**
  - **13.11 - 18.12:** lectures and exercises of the different tracks

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- **Phase 2 (split into different tracks)**
  - **13.11 - 18.12:** lectures and exercises of the different tracks
- **Phase 3:**
  - **08.01:** start of the final projects
  - **15.01:** Q/A session
  - **22.01:** Q/A session
  - **29.01:** Q/A session
  - **05.02:** poster session

Tracks (tentative topics)

- **Track 1 Reinforcement Learning / Robotics**
  - Robot navigation
  - Deep reinforcement learning

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- **Track 1 Reinforcement Learning / Robotics**
  - Robot navigation
  - Deep reinforcement learning
- **Track 2 AutoML / Computer Vision**
  - Image segmentation
  - Autoencoders
  - Generative adversarial networks
  - Architecture search and hyperparameter optimization

Evaluation of Exercises

for each exercise:

- solve coding exercise alone
- hand-in **short** 1-2 page report explaining your results, typically accompanied by 1-2 figures (e.g. learning curves / table with comparisons)
- hand in your code

Final Project

- We will provide a list of different projects but feel free to propose own ideas
- You will split up into small groups of 3 - 4 persons for the final project
- At the end we will organize a poster session where you have to present your results
- **You need to register for the exams**

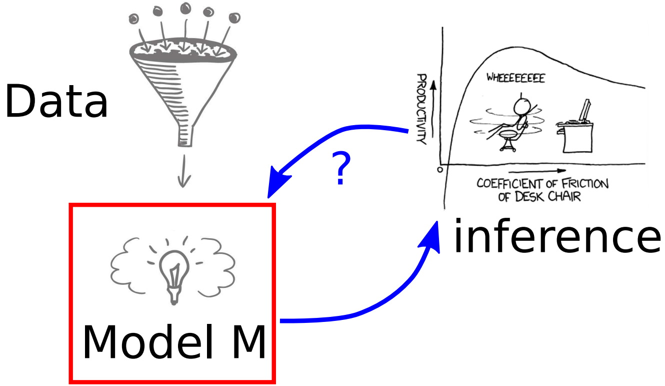
Today...

- **Lecture:** Short recap on how MLPs (feed-forward neural networks) work and how to train them
- **First assignment:** implement a simple MLP in numpy and train it on MNIST dataset (more on this at the end)

What you need to do after today's class

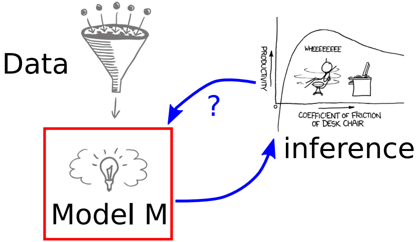
- decide whether you want to take the course and which track you want to join
- if you are enrolled in HISinONE for different tracks, unregister from all tracks except the one you want to take
- start working on exercise 1

(Deep) Machine Learning Overview



1. Learn Model **M** from the data
2. Let the model **M** infer unknown quantities from data

(Deep) Machine Learning Overview



Data	Sensory Information	Query
Labeled Images	An image	Is a cat in the image?
Transcribed Speech	A speech segment	What is this person saying?
Paraphrases	A pair of sentences	Is this sentence a paraphrase?
Movie Ratings	Ratings of Y and by X	Will a user X like a movie Y?
Parallel Corpora	A Finnish sentence	What is "moi" in English?

(Examples by Kyunghyun Cho)

Machine Learning Overview

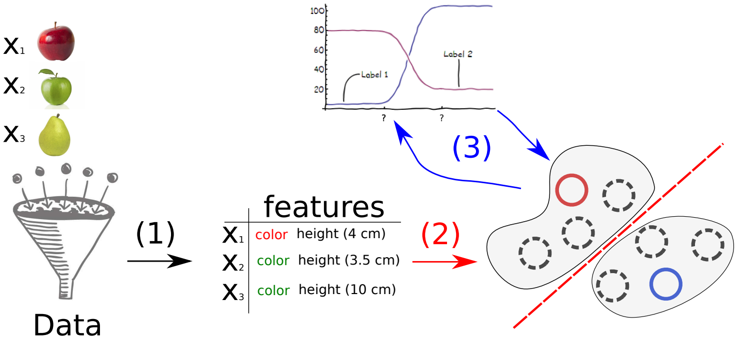
What is the difference between deep learning and a standard machine learning pipeline ?

Standard Machine Learning Pipeline

(1) Engineer good features (**not learned**)

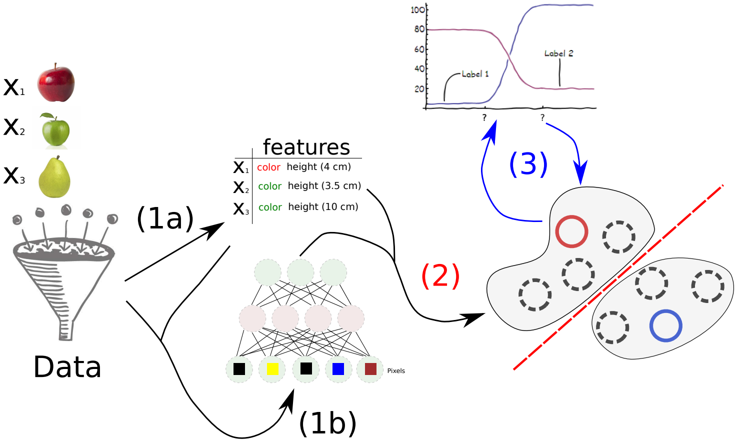
(2) Learn Model

(3) Inference e.g. classes of unseen data



Unsupervised Feature Learning Pipeline

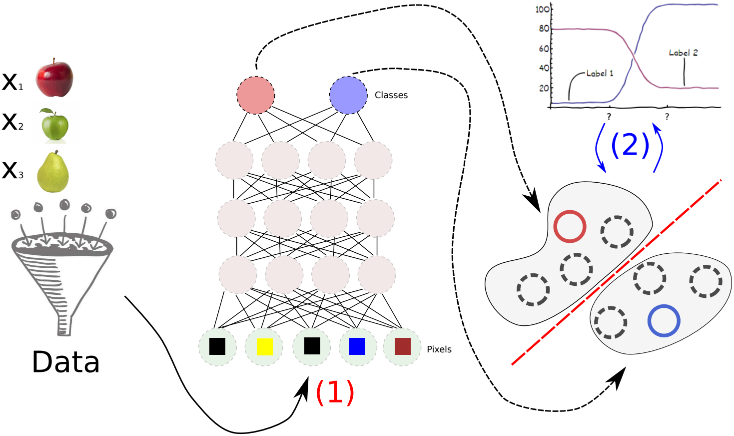
(1a) Maybe engineer good features (**not learned**)
(1b) Learn (deep) representation unsupervisedly
(2) Learn Model
(3) Inference e.g. classes of unseen data



Supervised Deep Learning Pipeline

(1) Jointly Learn everything with a deep architecture

(2) Inference e.g. classes of unseen data



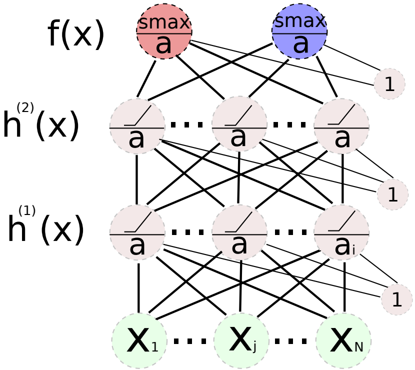
Training supervised feed-forward neural networks

- Let's formalize!
- **We are given:**
  - Dataset $D = \{(\mathbf{x}^1, \mathbf{y}^1), \ldots, (\mathbf{x}^N, \mathbf{y}^N)\}$
  - A neural network with parameters θ which implements a function $f_\theta(\mathbf{x})$
- **We want to learn:**
  - The parameters θ such that $\forall i \in [1, N] : f_\theta(\mathbf{x}^i) = \mathbf{y}^i$

Training supervised feed-forward neural networks

- A neural network with parameters θ which implements a function $f_\theta(\mathbf{x})$

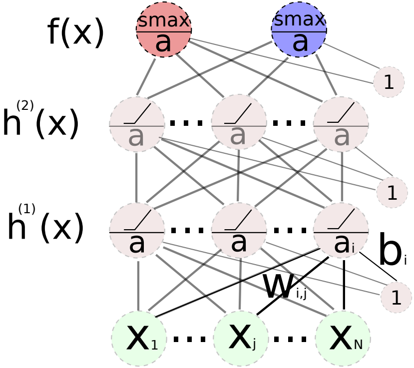
$\rightarrow$ θ is given by the network weights w and bias terms b



Neural network forward-pass

- Computing $f_\theta(\mathbf{x})$ for a neural network is a forward-pass

- unit i **activation**:
  $$a_i = \sum_{j=i}^{N} w_{i,j} x_j + b_i$$
- unit i **output**:
  $h_i^{(1)}(\mathbf{x}) = t(a_i)$ where $t(\cdot)$ is an activation or transfer function

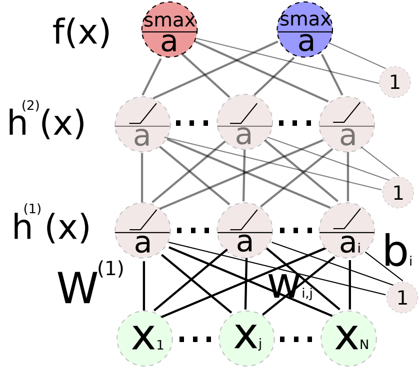


Neural network forward-pass

- Computing $f_\theta(\mathbf{x})$ for a neural network is a forward-pass

alternatively (and much faster) use vector notation:

- layer **activation**: $\mathbf{a}^{(1)} = \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}$
- layer **output**: $h^{(1)}(\mathbf{x}) = t(\mathbf{a}^{(1)})$ where $t(\cdot)$ is applied element wise

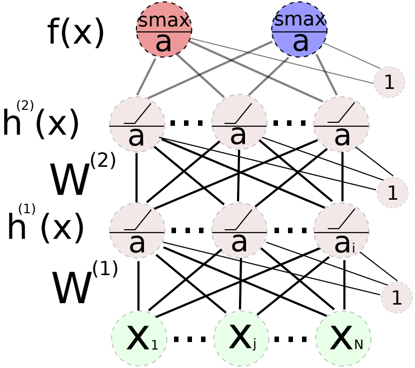


Neural network forward-pass

- Computing $f_\theta(\mathbf{x})$ for a neural network is a forward-pass

Second layer

- layer 2 **activation**: $\mathbf{a}^{(2)} = \mathbf{W}^{(2)} h^{(1)}(\mathbf{x}) + \mathbf{b}^{(2)}$
- layer 2 **output**: $h^{(1)}(\mathbf{x}) = t(\mathbf{a}^{(2)})$ where $t(\cdot)$ is applied element wise

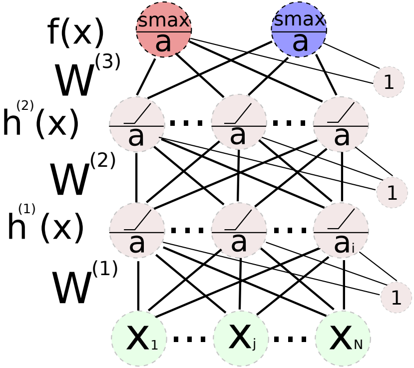


Neural network forward-pass

- Computing $f_\theta(\mathbf{x})$ for a neural network is a forward-pass

Output layer

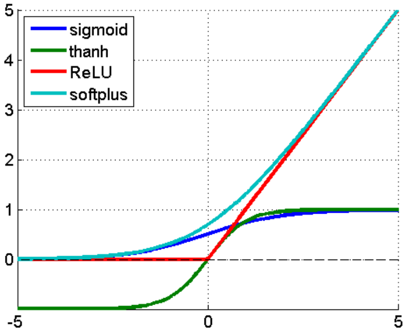
- output layer **activation**: $\mathbf{a}^{(3)} = \mathbf{W}^{(3)} h^{(2)}(\mathbf{x}) + \mathbf{b}^{(3)}$
- network **output**: $f(\mathbf{x}) = o(\mathbf{a}^{(3)})$ where $o(\cdot)$ is the output nonlinearity
- for **classification** use softmax: $o_i(z) = \frac{e^{z_i}}{\sum_{j=1}^{|z|} e^{z_j}}$



Training supervised feed-forward neural networks

- Neural network activation functions
- Typical nonlinearities for hidden layers are: $tanh(a_i)$, sigmoid $\sigma(a_i) = \dfrac{1}{1+e^{-a_i}}$, ReLU $relu(a_i) = max(a_i, 0)$
- tanh and sigmoid are both **squashing** non-linearities
- ReLU just **thresholds** at 0

→ Why not linear ?



Training supervised feed-forward neural networks

- Train parameters θ such that $\forall i \in [1, N] : f_\theta(\mathbf{x}^i) = \mathbf{y}^i$

Training supervised feed-forward neural networks

- Train parameters θ such that $\forall i \in [1, N] : f_\theta(\mathbf{x}^i) = \mathbf{y}^i$
- We can do this via minimizing the empirical risk on our dataset D

$$\min_\theta L(f_\theta, D) = \min_\theta \frac{1}{N} \sum_{i=1}^{N} l(f_\theta(\mathbf{x}^i), \mathbf{y}^i), \tag{1}$$

where $l(\cdot, \cdot)$ is a per example loss

Training supervised feed-forward neural networks

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- For regression often use the squared loss:

$$l(f_\theta(\mathbf{x}), \mathbf{y}) = \frac{1}{2} \sum_{j=1}^{M} (f_{j,\theta}(\mathbf{x}) - y_j)^2$$

- For M-class classification use the negative log likelihood:

$$l(f_\theta(\mathbf{x}), \mathbf{y}) = \sum_{j}^{M} -log(f_{j,\theta}(\mathbf{x})) \cdot y_j$$

Gradient descent

- The simplest approach to minimizing $\min_{\theta} L(f_\theta, D)$ is gradient descent

Gradient descent:
$\theta^0 \leftarrow$ init randomly
do

- $\theta^{t+1} = \theta^t - \gamma \dfrac{\partial L(f_\theta, D)}{\partial \theta}$

while $\left(L(f_{\theta^{t+1}}, V) - L(f_{\theta^t}, V)\right)^2 > \epsilon$

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- Where V is a validation dataset (why not use D ?)
- Remember in our case: $L(f_\theta, D) = \dfrac{1}{N} \sum_{i=1}^{N} l(f_\theta(\mathbf{x}^i), \mathbf{y}^i)$
- We will get to computing the derivatives shortly

Gradient descent

- Gradient descent example: $D = \{(x^1, y^1), \ldots, (x^{100}, y^{100})\}$ with

$$x \sim \mathcal{U}[0, 1]$$
$$y = 3 \cdot x + \epsilon \text{ where } \epsilon \sim \mathcal{N}(0, 0.1)$$

Gradient descent

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- **Learn** parameters θ of function $f_\theta(x) = \theta x$ using loss

$$l(f_\theta(x), y) = \frac{1}{2}\|f_\theta(\mathbf{x}) - \mathbf{y}\|_2^2 = \frac{1}{2}(f_\theta(x) - y)^2$$

$$\frac{\partial L(f_\theta, D)}{\partial \theta} = \frac{1}{N}\sum_{i=1}^{N} \frac{\partial l(f_\theta, D)}{\partial \theta} = \frac{1}{N}\sum_{i=1}^{N}(\theta x - y)x$$

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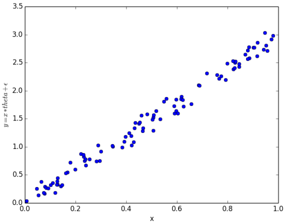

Gradient descent

- Gradient descent example $\gamma = 2$.

gradient descent

Stochastic Gradient descent (SGD)

- There are two problems with gradient descent:
  1. We have to find a good γ
  2. Computing the gradient is expensive if the training dataset is large!
- Problem 2 can be attacked with online optimization (we will have a look at this)
- Problem 1 remains but can be tackled via second order methods or other advanced optimization algorithms (rprop/rmsprop, adagrad)

Gradient descent

1. We have to find a good γ ($\gamma = 2.$, $\gamma = 5.$)

gradient descent 2

Stochastic Gradient descent (SGD)

2 Computing the gradient is expensive if the training dataset is large!
- What if we would only evaluate f on parts of the data ?

Stochastic Gradient Descent:
$\theta^0 \leftarrow$ init randomly
do

- $(\mathbf{x}', \mathbf{y}') \sim D$
  sample example from dataset D
- $\theta^{t+1} = \theta^t - \gamma^t \frac{\partial l(f_\theta(\mathbf{x}'), \mathbf{y}')}{\partial \theta}$

while $(L(f_{\theta^{t+1}}, V) - L(f_{\theta^t}, V))^2 > \epsilon$
where $\sum_{t=1}^{\infty} \gamma^t \rightarrow \infty$ and $\sum_{t=1}^{\infty} (\gamma^t)^2 < \infty$
(γ should go to zero but not too fast)

Stochastic Gradient descent (SGD)

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while $(L(f_{\theta^{t+1}}, V) - L(f_{\theta^t}, V))^2 > \epsilon$

where $\sum_{t=1}^{\infty} \gamma^t \rightarrow \infty$ and $\sum_{t=1}^{\infty} (\gamma^t)^2 < \infty$

(γ should go to zero but not too fast)

$\rightarrow$ SGD can speed up optimization for large datasets

$\rightarrow$ but can yield very noisy updates

$\rightarrow$ in practice mini-batches are used
(compute $l(\cdot, \cdot)$ for several samples and average)

$\rightarrow$ we still have to find a learning rate shedule γ^t

Stochastic Gradient descent (SGD)

→ Same data, assuming that gradient evaluation on all data takes 4 times as much time as evaluating a single datapoint

(gradient descent ($\gamma = 2$), stochastic gradient descent ($\gamma^t = 0.01\frac{1}{t}$))

sgd

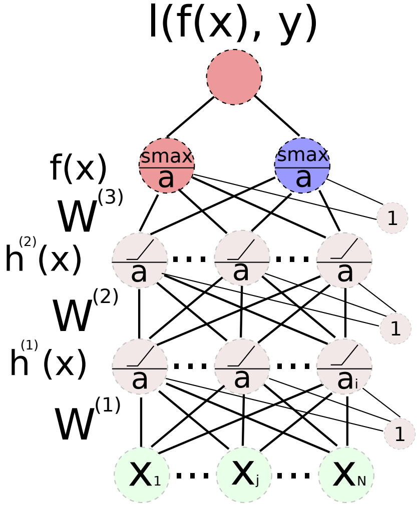
Neural Network backward pass

$\rightarrow$ Now how do we compute the gradient for a network ?

- Use the chain rule:

$$\frac{\partial f(g(x))}{\partial x} = \frac{\partial f(g(x))}{\partial g(x)} \frac{\partial g(x)}{\partial x}$$

- first compute loss on output layer
- then backpropagate to get $\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{W}^{(3)}}$ and $\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{a}^{(3)}}$

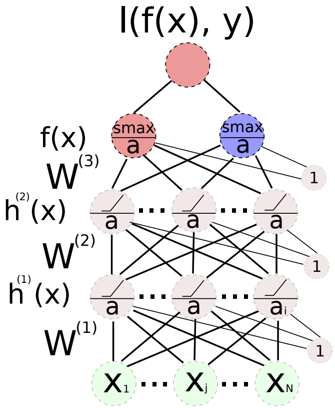


Neural Network backward pass

machine learning lab

→ Now how do we compute the gradient for a network ?

- gradient wrt. layer 3 **weights**:
  $$\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{W}^{(3)}} = \frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{a}^{(3)}} \frac{\partial \mathbf{a}^{(3)}}{\mathbf{W}^{(3)}}$$
- assuming l is NLL and softmax outputs, gradient wrt. layer 3 activation is:
  $$\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{a}^{(3)}} = -(\mathbf{y} - f(x))$$
  $\mathbf{y}$ is one-hot encoded
- gradient of $\mathbf{a}$ wrt. $\mathbf{W}^{(3)}$:
  $$\frac{\partial \mathbf{a}^{(3)}}{\partial \mathbf{W}^{(3)}} = h^{(2)}(\mathbf{x})^T$$



→ recall
$\mathbf{a}^{(3)} = \mathbf{W}^{(3)} h^{(2)}(\mathbf{x}) + \mathbf{b}^{(3)}$

Neural Network backward pass

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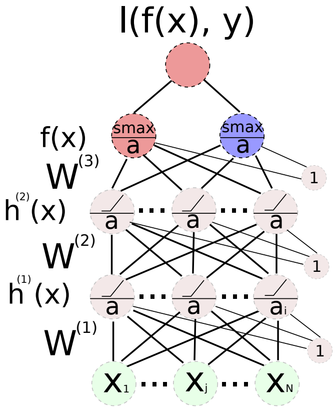
- gradient of **a** wrt. $\mathbf{W}^{(3)}$:
  $$\frac{\partial \mathbf{a}^{(3)}}{\partial \mathbf{W}^{(3)}} = h^{(2)}(\mathbf{x})^T$$
- combined:
  $$\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{W}^{(3)}} = -(\mathbf{y} - f(x))(h^{(2)}(\mathbf{x}))^T$$



$\rightarrow$ recall
$\mathbf{a}^{(3)} = \mathbf{W}^{(3)} h^{(2)}(\mathbf{x}) + \mathbf{b}^{(3)}$

Neural Network backward pass

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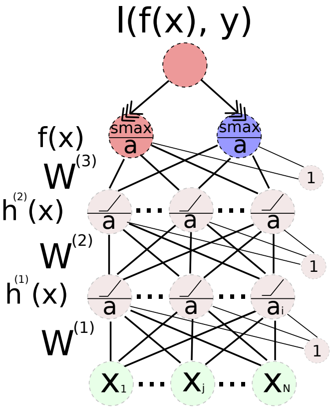
- assuming l is NLL and softmax outputs, gradient wrt. layer 3 activation is:
  $$\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{a}^{(3)}} = -(\mathbf{y} - f(x))$$
- gradient of **a** wrt. $\mathbf{W}^{(3)}$:
  $$\frac{\partial \mathbf{a}^{(3)}}{\partial \mathbf{W}^{(3)}} = (h^{(2)}(\mathbf{x}))^T$$
- gradient wrt. **previous layer**:

$$\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial h^{(2)}(\mathbf{x})} = \frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{a}^{(3)}} \frac{\partial \mathbf{a}^{(3)}}{\partial h^{(2)}(\mathbf{x})}$$
$$= \left(\mathbf{W}^{(3)}\right)^T \frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{a}^{(3)}}$$

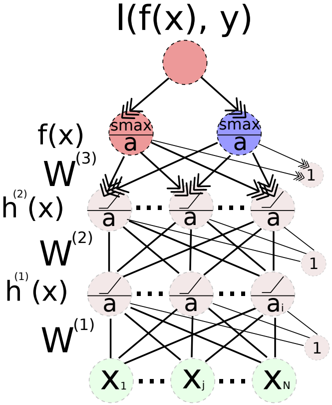


$\rightarrow$ recall
$\mathbf{a}^{(3)} = \mathbf{W}^{(3)} h^{(2)}(\mathbf{x}) + \mathbf{b}^{(3)}$

Neural Network backward pass

$\rightarrow$ Now how do we compute the gradient for a network ?

- gradient wrt. layer 2 **weights**:
$$\frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial \mathbf{W}^{(2)}} = \frac{\partial l(f(\mathbf{x}), \mathbf{y})}{\partial h^{(2)}(\mathbf{x})} \frac{\partial h^{(2)}(\mathbf{x})}{\partial \mathbf{a}^{(2)}} \frac{\partial \mathbf{a}^{(2)}}{\mathbf{W}^{(2)}}$$
- same schema as before just have to consider computing derivative of activation function $\frac{\partial h^{(2)}(\mathbf{x})}{\partial \mathbf{a}^{(2)}}$, e.g. for sigmoid $\sigma(\cdot)$
$$\frac{\partial h^{(2)}(\mathbf{x})}{\partial \mathbf{a}^{(2)}} = \sigma(a_i)(1 - a_i)$$
- and backprop even further



$\rightarrow$ recall
$$\mathbf{a}^{(3)} = \mathbf{W}^{(3)} h^{(2)}(\mathbf{x}) + \mathbf{b}^{(3)}$$

Gradient Checking

- $\rightarrow$ Backward-pass is just repeated application of the **chain rule**
- $\rightarrow$ However, there is a huge potential for bugs ...
- $\rightarrow$ Gradient checking to the rescue (simply check code via finite-differences):

Gradient Checking:

$\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \dots)$ init randomly

$\mathbf{x} \leftarrow$ init randomly ; $\mathbf{y} \leftarrow$ init randomly

$g_{\text{analytic}} \leftarrow$ compute gradient $\dfrac{\partial l(f_\theta(\mathbf{x}), \mathbf{y})}{\partial \theta}$ via backprop

for i in $\#\theta$

- $\hat{\theta} = \theta$
- $\hat{\theta}_i = \hat{\theta}_i + \epsilon$
- $g_{\text{numeric}} = \dfrac{l(f_{\hat{\theta}}(x), \mathbf{y}) - l(f_\theta(x), \mathbf{y})}{\epsilon}$
- assert($\|g_{\text{numeric}} - g_{\text{analytic}}\| < \epsilon$)

- can also be used to test partial implementations (i.e. layers, activation functions)
  - $\rightarrow$ simply remove loss computation and backprop **ones**

Overfitting

- If you train the parameters of a large network $\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \dots)$ you will see overfitting!
  $\rightarrow L(f_\theta(x), D) \ll L(f_\theta(x), V)$
- This can be at least partly conquered with regularization

Overfitting

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  $\rightarrow L(f_\theta(x), D) \ll L(f_\theta(x), V)$
- This can be at least partly conquered with regularization
  - **weight decay:** change cost (and gradient)

$$L(f_\theta, D) = \frac{1}{N} \min_\theta \sum_{i=1}^{N} l(f_\theta(\mathbf{x}^i), \mathbf{y}^i) + \frac{1}{\#\theta} \sum_{i}^{\#\theta} \|\theta_i\|^2$$

$\rightarrow$ enforces small weights (occams razor)

Overfitting

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  $\rightarrow L(f_\theta(x), D) \ll L(f_\theta(x), V)$
- This can be at least partly conquered with regularization
  - **weight decay:** change cost (and gradient)

$$L(f_\theta, D) = \frac{1}{N} \min_\theta \sum_{i=1}^{N} l(f_\theta(\mathbf{x}^i), \mathbf{y}^i) + \frac{1}{\#\theta} \sum_{i}^{\#\theta} \|\theta_i\|^2$$

    $\rightarrow$ enforces small weights (occams razor)
  - **dropout:** kill $\approx 50\%$ of the activations in each hidden layer **during training** forward pass. Multiply hidden activations by $\frac{1}{2}$ **during testing**
    $\rightarrow$ prevents co-adaptation / enforces robustness to noise

Overfitting

- If you train the parameters of a large network $\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \dots)$ you will see overfitting!
  $\rightarrow L(f_\theta(x), D) \ll L(f_\theta(x), V)$
- This can be at least partly conquered with regularization
  - **weight decay:** change cost (and gradient)

$$L(f_\theta, D) = \frac{1}{N} \min_\theta \sum_{i=1}^{N} l(f_\theta(\mathbf{x}^i), \mathbf{y}^i) + \frac{1}{\#\theta} \sum_{i}^{\#\theta} \|\theta_i\|^2$$

    $\rightarrow$ enforces small weights (occams razor)
  - **dropout:** kill $\approx 50\%$ of the activations in each hidden layer **during training** forward pass. Multiply hidden activations by $\frac{1}{2}$ **during testing**
    $\rightarrow$ prevents co-adaptation / enforces robustness to noise
  - Many, many more !

Assignment

- **Implementation:** Implement a simple feed-forward neural network by completing the provided *stub* this includes:
  - possibility to use 2-4 layers
  - sigmoid/tanh and ReLU for the hidden layer
  - softmax output layer
  - optimization via gradient descent (gd)
  - optimization via stochastic gradient descent (sgd)
  - weight initialization with random noise **(!!!)** (use normal distribution with changing std. deviation for now)
- Bonus points for testing some advanced ideas:
  - implement dropout, weight decay
  - implement a different optimizer (rprop, rmsprop, adagrad)
- **Code stub:** `https://github.com/aisrobots/dl-lab-2018`
- **Evaluation:**
  - Find good parameters (learning rate, number of iterations etc.) using a validation set (usually take the last 10k examples from the training set)
  - After optimizing parameters run on the full dataset and test once on the test-set (you should be able to reach $\approx 1.6 - 1.8\%$ error)
- **Submission:** Clone our github repo and send us the link to your github/bitbucket repo including your solution code and the report as a pdf-file. Email to kleinaa@cs.uni-freiburg.de with subject: **dl-lab-course 18**

Slide Information

- **Thanks to Tobias Springenberg who generated most of these slides for the DL Lab Course WS 2016/2017.**