Train artificial neural networks

ANDREAS LANGER, LUND UNIVERSITY

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- a directed graph (V, E)

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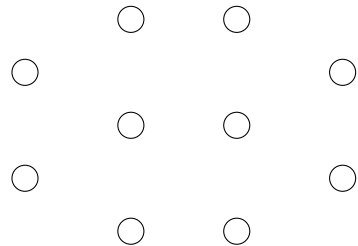

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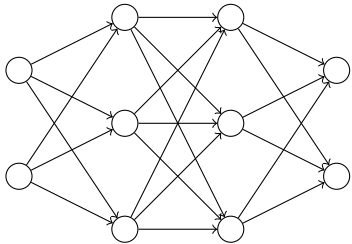

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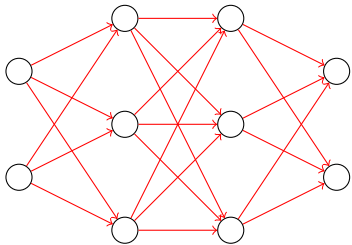

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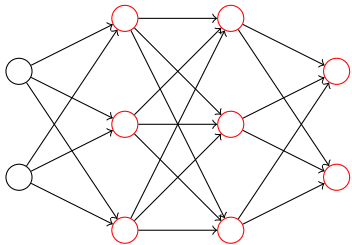

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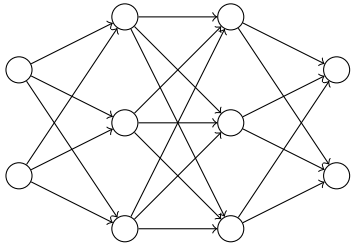
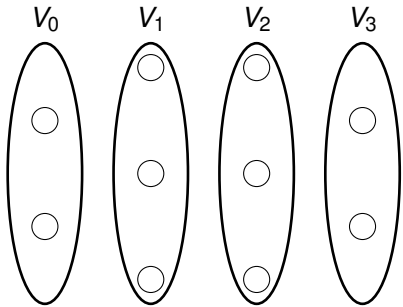


$\Rightarrow$ Neural networks are characterized by the tuple (V, E, σ, w).

Requirements to the network

(i) The net is layered: Set of nodes V has decomposition into $T+1$, $T \in \mathbb{N}$, (non-empty) disjoint subsets $V_i \subset V$, $i = 0, \ldots, T$, i.e. $V = \bigcup_{i=0}^{T} V_i$.



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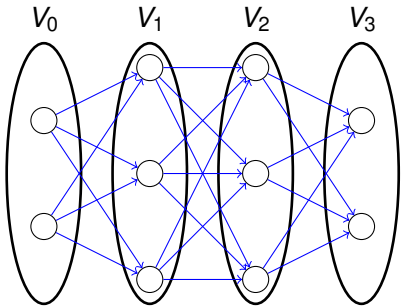

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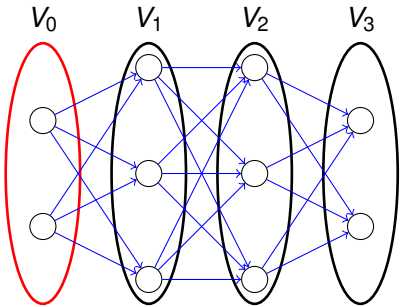

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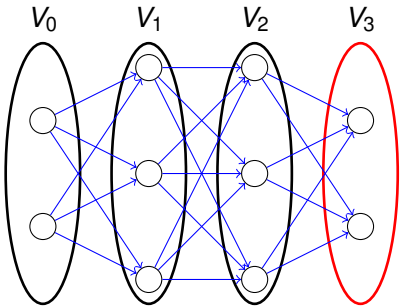

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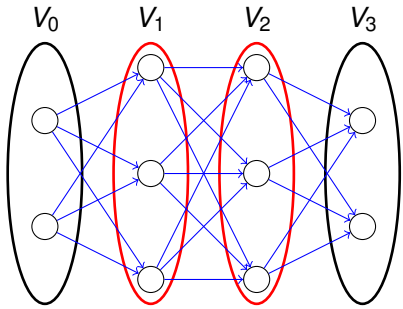

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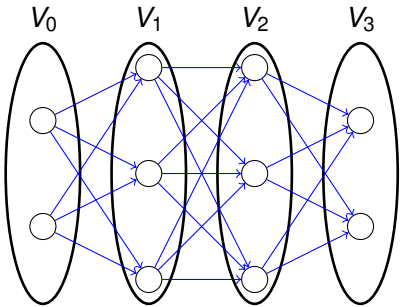

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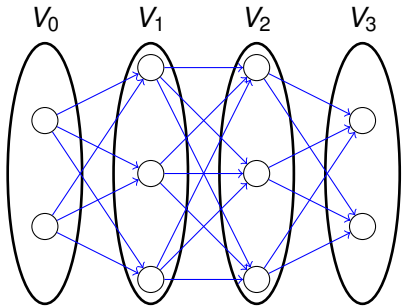
- $\max_{t=0,\dots,T} |V_t|$ .... width of the network



Input – Output

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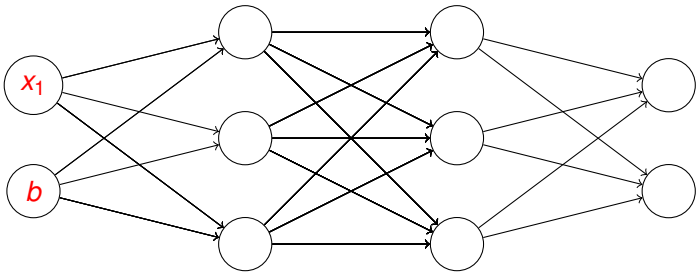

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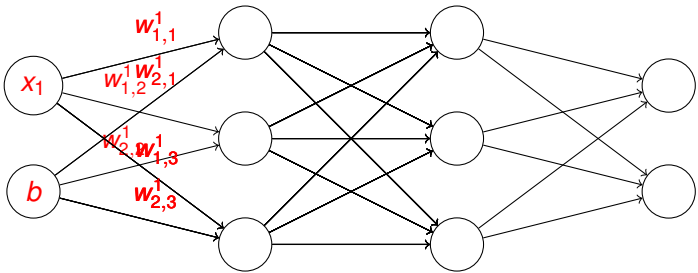

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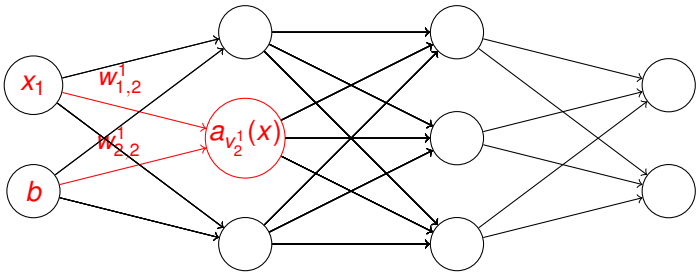

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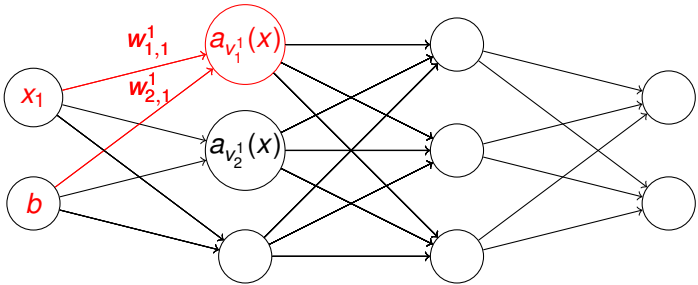

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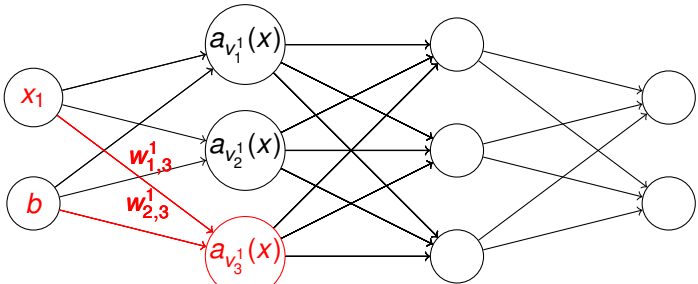

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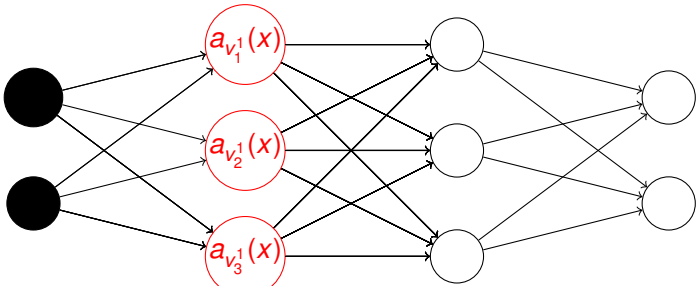

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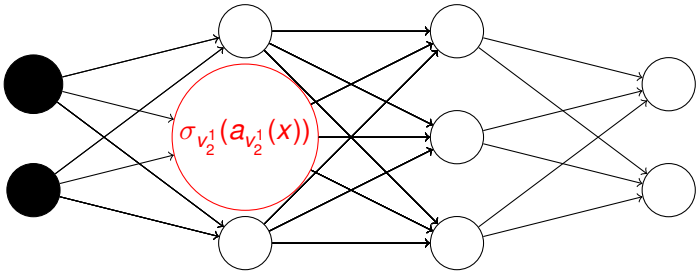

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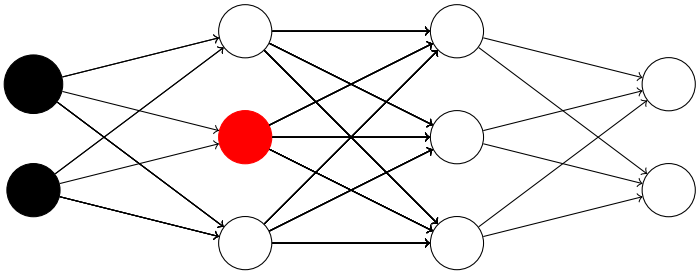

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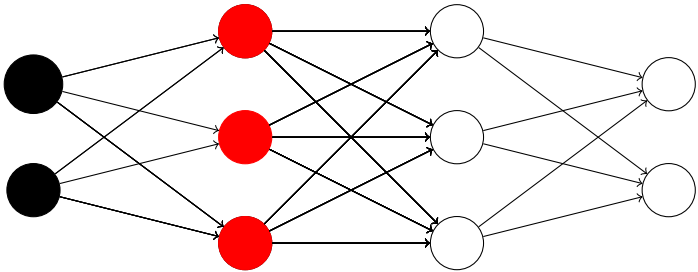

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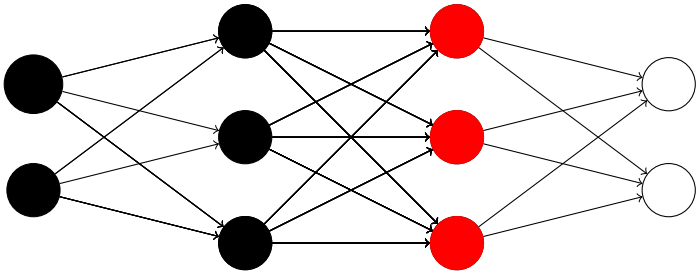

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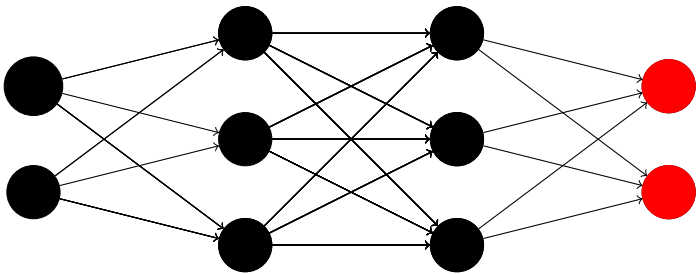
   Output of the net: $h(x) := (o_{v_i^T}(x))_{i=1}^{|V_T|} \in \mathbb{R}^{|V_T|}$



Examples of activation functions

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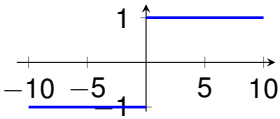

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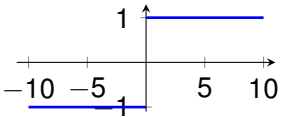
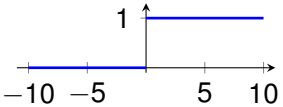


- Unit step function: $\sigma_{\text{step}}(x) := \begin{cases} +1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$



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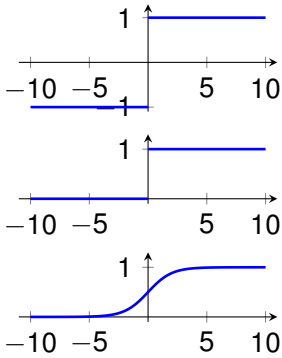

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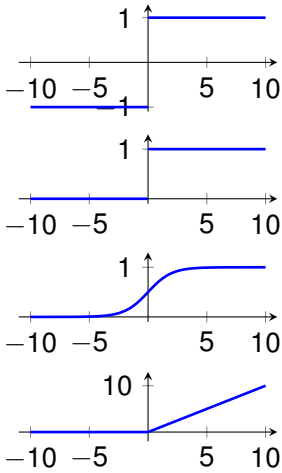
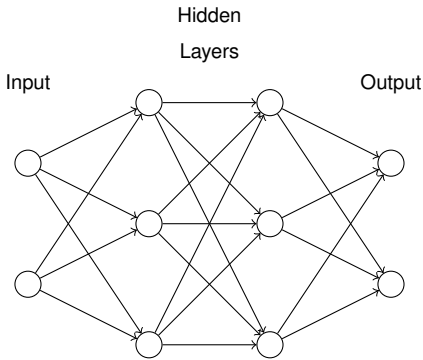
- Rectified linear unit (ReLU): $\sigma_{\text{ReLU}}(x) := \max\{0, x\}$

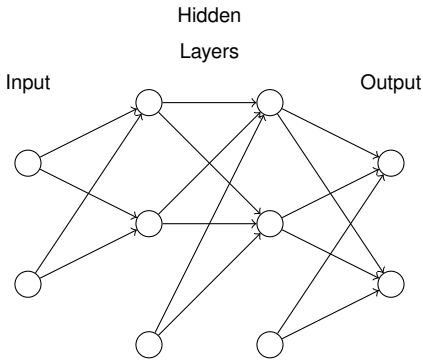


Neural Nets



Feedforward
neural network (FNN)

Neural Nets



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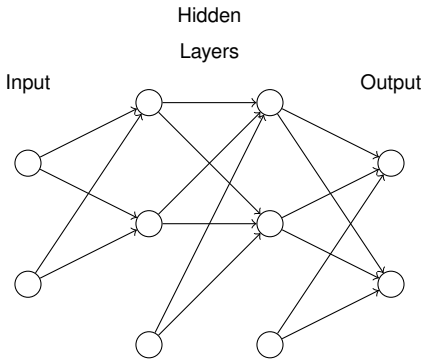

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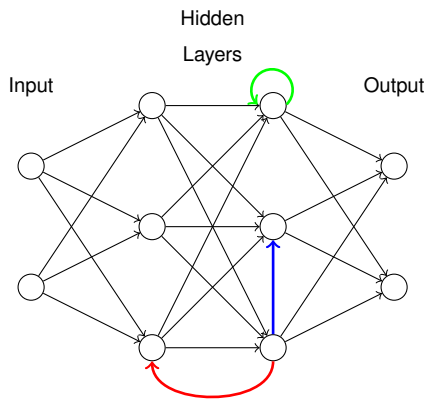

Recurrent neural network (RNN)

What are artificial neural networks used for?

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- Adaptivity: Machine learning tools adapt to the input data. Example:
  - Decoding of handwriting, where the program can adapt to handwriting of different users.
  - Spam filter: automatic adaptation to the change of spam e-mails.

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Learning

Supervised/unsupervised learning

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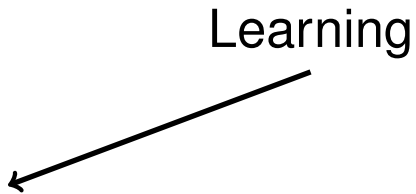
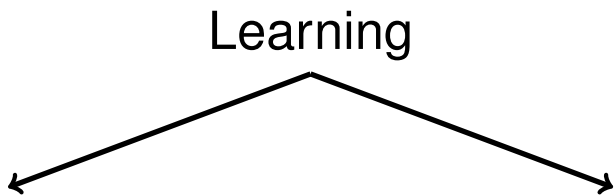


Supervised learning: Learning based on training data $\Rightarrow$ Mapping rule that can predict classification of unknown data.
Example: Emails classified as spam or not spam $\rightarrow$ Spam-Filter.

Supervised/unsupervised learning



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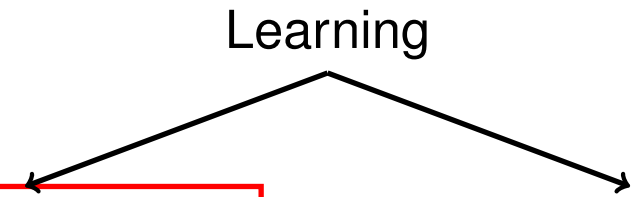

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- Learning algorithm $A : \bigcup_{m \in \mathbb{N}} (X \times Y)^m \to H$, $S \mapsto h_S$: The task of the learning algorithm is to link a data point $x \in X$ with a correct label.

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Risk

- Loss function $\ell : Y \times Y \to [0, \infty)$:
  Example:
  1. 0-1 loss: $\ell_{0-1}(y, h(x)) := \begin{cases} 0 & \text{falls } h(x) = y \\ 1 & \text{falls } h(x) \neq y \end{cases}$
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Attention: The probability distribution P is not known!

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Types of learning problems

Regression:

- Output space Y is continuous; e.g. $Y = \mathbb{R}$
- Loss function measures continuous distance between points; e.g. $\ell = \ell_2$
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Classification:

- Output space Y is discrete; e.g. $Y = \{0, 1\}$ (binary classification)
- Usual loss function is $\ell = \ell_{0-1}$
  $\Rightarrow \mathcal{R}_P(h) = \mathop{\mathbb{E}}_{(x,y)\sim P}(\ell(y, h(x))) = \mathop{\mathbb{P}}_{(x,y)\sim P}[h(x) \neq y]$

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FNN - learning problem

How does the FNN fit into the statistical learning problem?

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- FNN maps an element $x \in X = \mathbb{R}^{|V_0|-1}$ into the output space $Y = \mathbb{R}^{|V_T|}$. I.e. let (V, E, σ, w) fixed, then

$$h_{V,E,\sigma,w} : X \to Y.$$

FNN forms a hypothesis class

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- We assume: Architecture (V, E, σ) given

$$\Rightarrow \ H_{V,E,\sigma} := \{h_{V,E,\sigma,w} : X \to Y \mid \ w : E \to \mathbb{R}\}.$$

- Learning means, choose $h_{V,E,\sigma,w} \in H_{V,E,\sigma}$ by fitting the weights w to the training data S.

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Empirical risk

How can a learning algorithm try to minimize the risk via the hypothesis class without knowing the probability distribution?

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Remedy:

- Training data: We can compute the empirical risk

$$\mathcal{R}_S(h) := \frac{1}{m} \sum_{i=1}^{m} \ell(y_i, h(x_i)).$$

$\Rightarrow$ empirical risk minimization (ERM)

$$\inf_{h \in H} \mathcal{R}_S(h)$$

If $|H| < \infty \Rightarrow$ existence of a minimum is guaranteed.

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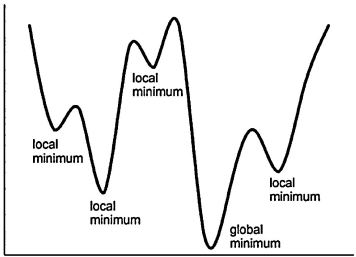
Characterization of a Solution

For a function $f : H \to \mathbb{R}$ a candidate $w^* \in H$ is called

- global minimizer of f in H, if

$$f(w^*) \leq f(w) \quad \text{for all } w \in H$$



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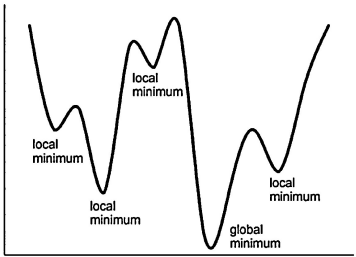

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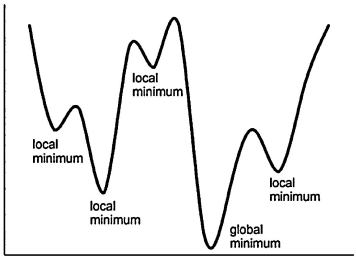

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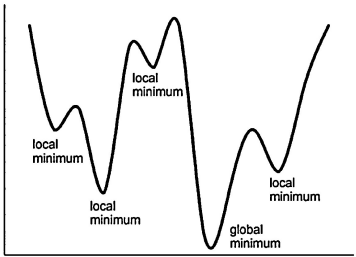

Existence of minimizer

Under which conditions has

$$\min_{w \in H} f(w)$$

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Under which conditions has

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a solution?

- If $|H| < \infty$.
- If there exists an $w_0 \in H$ such that the level set

$$\mathcal{L}_f(w_0) := \{w \in H \mid f(w) \leq f(w_0)\}$$

is compact and f lower semi-continuous (Theorem of Weierstraß).

Definition

A set H is compact, if every sequence in H has a convergent subsequence whose limit belongs to H.

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Training

- Find hypotheses in $H_{V,E,\sigma}$ which has minimal risk $\rightarrow$ adjust edge weights w.
- Risk $\mathcal{R}_P(w) := \int_{X \times Y} \ell(y, h_w) \, \mathrm{d}P(x, y)$ cannot be directly minimized.
- ERM: $\min_{w \in \mathbb{R}^{|E|}} \{\mathcal{R}_S(w) := \frac{1}{m} \sum_{i=1}^{m} \ell(y_i, h_w(x_i))\}$

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- Gradient descent method:

Algorithmus Gradient descent method

Initialize: $w^0 \in \mathbb{R}^{|E|}$
for $j = 0, 1, 2, \ldots$ **do**
  Choose step size s^j
  $w^{j+1} = w^j - s^j \nabla_w \mathcal{R}_S(w^j)$
end for

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Stochastic gradient method

- For a lot of training data S, the calculation of the gradient is computationally very intensive, since a gradient has to be calculated for each data item $(x, y) \in S$.

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- For a lot of training data S, the calculation of the gradient is computationally very intensive, since a gradient has to be calculated for each data item $(x, y) \in S$.
- Remedy: Stochastic gradient method (SGD)

Idea of SGD:

- Random (uniformly distributed) selection of $\tilde{m} \ll m$ training data from S
- $w^{j+1} = w^j - s^j \frac{1}{\tilde{m}} \sum_{i=1}^{\tilde{m}} \nabla_w \ell(y_{j_i}, h_{w^j}(x_{j_i}))$ $\tilde{m}$ is called mini-batch size
- Often $\tilde{m} = 1$

Stochastic gradient method (cont.)

Algorithmus Stochastic gradient method

Initialize: $w^0 \in \mathbb{R}^{|E|}$
for $j = 0, 1, 2, \ldots$ **do**
  Choose randomly $(x, y) \in S$
  Set $d^j = -\nabla_w \ell(y, h_{w^j}(x))$
  Choose step-size s^j (e.g. $s^j = \frac{1}{c(j+1)}$, $c > 0$)
  $w^{j+1} = w^j + s^j d^j$
end for

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Note: Let $w = w^j$ and (x_i, y_i) be randomly chosen from S

$$\mathop{\mathbb{E}}_{(x_i,y_i)\sim U}[\nabla_w \ell(y_i, h_w(x_i))] = \sum_{i=1}^{m} \nabla_w \ell(y_i, h_w(x_i)) \cdot \mathbb{P}[Z = (x_i, y_i)] = \frac{1}{m} \sum_{i=1}^{m} \nabla_w \ell(y_i, h_w(x_i))$$
$$= \nabla_w \mathcal{R}_S(w)$$

Descent method

Consider $\min_{w \in \mathbb{R}^n} f(w)$ with $f : \mathbb{R}^n \to \mathbb{R}$ continuously differentiable.

Algorithmus Descent method

Initialize: $w^0 \in R^n$
for $j = 0, 1, 2, \ldots$ **do**
  Compute a descent direction d^j
  Compute a step-size s^j,such that $f(w^j + s^j d^j) < f(w^j)$
  Set $w^{j+1} = w^j + s^j d^j$
end for

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Descent direction - Criterion

Definition (Descent direction)

A direction $d \in \mathbb{R}^n \setminus \{0\}$ is called descent direction of the function f in $x \in \mathbb{R}^n$, if there exists an $\bar{s} > 0$ with

$$f(x + sd) < f(x) \qquad \forall s \in (0, \bar{s}).$$

Lemma

Let $f : \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable in $x \in \mathbb{R}^n$. If $d \in \mathbb{R}^n$ fulfills the inequality

$$\nabla f(x)^T d < 0,$$

then d is a descent direction of f in x.

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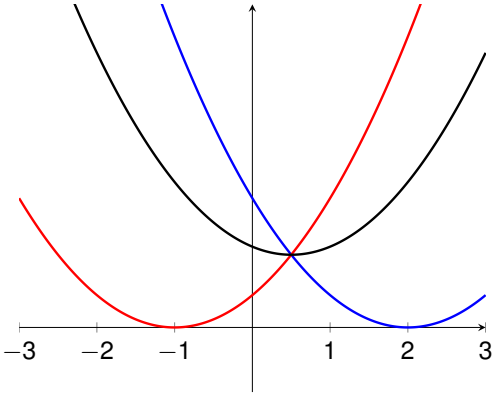
SGD is not a descent method

Example:

- $f(x) = \frac{1}{2}(f_1(x) + f_2(x))$ with $f_1(x) = \frac{1}{2}(x-2)^2$ and $f_2(x) = \frac{1}{2}(x+1)^2$.



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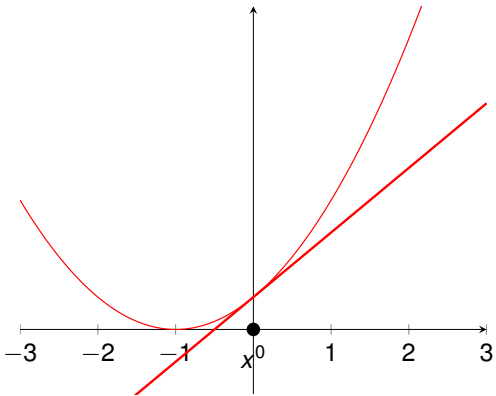
- Set $x^0 = 0$ and randomly choose $i = 2 \Rightarrow d^0 = -\nabla f_2(x^0) = -1$.



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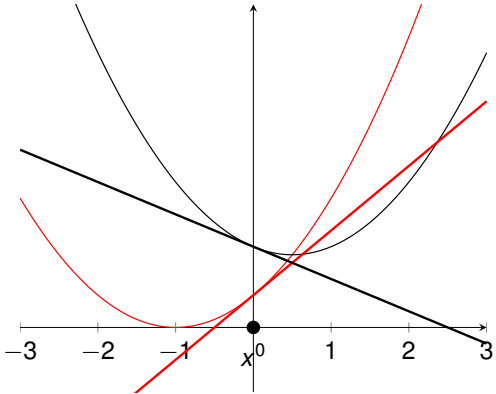

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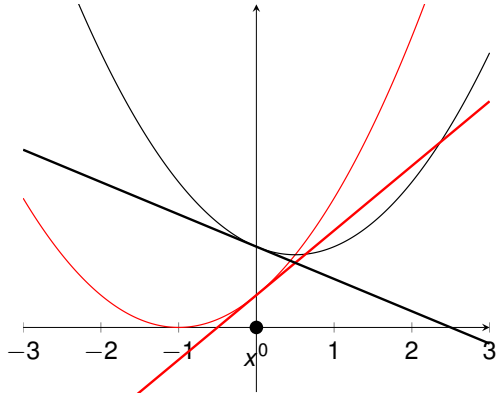

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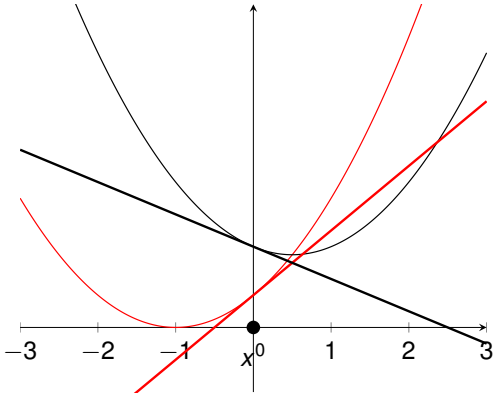

$\Rightarrow$ stochastic gradient method is not a descent method in general.

SGD for FNN

Algorithmus stochastic gradient method for FNN

Parameter: Stopping criteria
step-sizes $(s^1, s^2, \ldots)$
Input: Layered FNN-architecture (V, E)
Differentiable activation function $\sigma : \mathbb{R} \to \mathbb{R}$
Initialize: Choose $w^0 \in \mathbb{R}^{|E|}$ randomly
for $j = 0, 1, 2, \ldots$ **do**
Choose randomly $(x, y) \in S$
Compute the gradient $g^j = \nabla_w \ell(y, h_{w^j}(x))$ (using backpropagation)
Set $w^{j+1} = w^j - s^j g^j$
end for

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Backpropagation for FNN

Notation:

- Loss function $\ell(y_i, h_w(x_i)) =: \ell^i(w) = \frac{1}{2}\sum_{a=1}^{|V_T|}(h_a - y^a)^2$
- For simplicity let $\ell(w) = \ell^i(w)$
- $h_j = o_{T,j}$, $j = 1, \ldots, |V_T|$
- $o_{t,j} = \sigma(a_{t,j})$, $j = 1, \ldots, |V_t|$, $t = 1, \ldots, T$
- $a_{t,j} = \sum_{r=1}^{|V_{t-1}|} w_{rj}^t o_{t-1,r}$, $j = 1, \ldots, |V_t|$, $t = 1, \ldots, T$
- w_{rj}^t is the weight from V_{t-1} to V_t

Derivative of ℓ w.r.t. w_{rj}^t:

$$\frac{\partial \ell}{\partial w_{rj}^t} = \frac{\partial \ell}{\partial a_{t,j}} \frac{\partial a_{t,j}}{\partial w_{rj}^t} = \underbrace{\frac{\partial \ell}{\partial o_{t,j}}}_{=:\delta_{t,j}} \sigma'(a_{t,j}) o_{t-1,r} = \delta_{t,j} \sigma'(a_{t,j}) o_{t-1,r}$$

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Computation of $\delta_{t,j}$

- Case 1: $t = T$

$$\frac{\partial \ell}{\partial w_{rj}^T} = \underbrace{\frac{\partial \ell}{\partial o_{T,j}}}_{=\delta_{T,j}} \sigma'(a_{T,j}) o_{T-1,r} = (h_j - y^j)\sigma'(a_{T,j}) o_{T-1,r} = \delta_{T,j}\sigma'(a_{T,j}) o_{T-1,r}$$

- Case 2: $t = T - 1$

$$\frac{\partial \ell}{\partial w_{rj}^{T-1}} = \frac{\partial \ell}{\partial o_{T-1,j}} \frac{\partial o_{T-1,j}}{\partial w_{rj}^{T-1}} = \sum_{i=1}^{|V_T|} \frac{\partial \ell}{\partial a_{T,i}} \frac{\partial a_{T,i}}{\partial o_{T-1,j}} \frac{\partial o_{T-1,j}}{\partial w_{rj}^{T-1}}$$

$$= \underbrace{\sum_{i=1}^{|V_T|} \delta_{T,i}\sigma'(a_{T,i}) w_{ji}^T}_{\delta_{T-1,j}} \sigma'(a_{T-1,j}) o_{T-2,r}$$

$$\Rightarrow \delta_{t,j} = \begin{cases} h_j - y^j & \text{if } t = T \\ \sum_{i=1}^{|V_{t+1}|} \delta_{t+1,i}\sigma'(a_{t+1,i}) w_{ji}^{t+1} & \text{else} \end{cases}$$

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Backpropagation as algorithm

1. **Input:** Input of x, determine the output of the input layer.
2. **Feedforward:** Compute a_{t_j} and $o_{t,j}$ for all t, j.
3. **Output Error:** Compute $\delta_{T,j}$
4. **Backpropagate the Error:** Determine recursively $\delta_{t,j}$ for $t = T-1, \ldots, 1$
5. **Output:** $\frac{\partial \ell}{\partial w_{rj}^t} = \delta_{t,j}\sigma'(a_{t,j})o_{t-1,r}$ for all r, j, t.

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Formulation of an attack

Given:

- Neural network (V, E, σ, w) and hence $h_w : X(= \mathbb{R}^n) \to Y(= \mathbb{R}^{|V_T|})$
- Loss function $\ell : Y \times Y \to \mathbb{R}$
- $x \in X = \mathbb{R}^n$ (can also be from $S_{|x}$) with $h_w(x) = y \in Y$
- Target classification $\tilde{y} \in Y$ (not always used)

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Formulation of the attack problem: Solve

$$\inf_{\tilde{x} \in X} \|x - \tilde{x}\| \qquad \text{subject to} \quad h_w(\tilde{x}) = \tilde{y}$$

- This approach minimizes the change (disturbance) while the constraint requires the classification $\tilde{y}$.
- If $h_w(x) = \tilde{y}$, then the minimization problem is trivial, as the solution is $\tilde{x}^* = x$.

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(A) The probably first attack

For simplicity let $\mathfrak{L}(x, y) := \ell(y, h_w(x))$.

Approach of [Szegedy, Zaremba, Sutskever, Bruna, Erhan, Goodfellow, Fergus 2014]

- Formulate the following unrestricted optimization problem

$$\min_{\tilde{x} \in X} \alpha \|x - \tilde{x}\|_2 + \mathfrak{L}(\tilde{x}, \tilde{y})$$

  with $\alpha > 0$.
- Solution method: L-BFGS

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(B) Gradient methods

- Approach of [Goodfellow, Shlens, Szegedy 2015]
  - Linearization: $\mathfrak{L}(x+\delta, y) \approx \mathfrak{L}(x, y) + \delta^T \nabla_x \mathfrak{L}(x, y)$
  - We want to choose $\delta \in \mathbb{R}^n$ such that $\delta^T \nabla_x \mathfrak{L}(x, y)$ is maximal, where $\|\delta\|_\infty \leq \epsilon$ is sufficiently small.
  - Choose $\delta = \epsilon \operatorname{sign}(\nabla_x \mathfrak{L}(x, y)) \Rightarrow \delta^T \nabla_x \mathfrak{L}(x, y) = \epsilon \operatorname{sign}(\nabla_x \mathfrak{L}(x, y))^T \nabla_x \mathfrak{L}(x, y) \geq 0$
  - $\epsilon > 0$ specifies the size of the change (step size)
  - $\tilde{x} = x + \epsilon \operatorname{sign}(\nabla_x \mathfrak{L}(x, y))$
  - δ is not a descent direction. BUT $-\delta$ is a descent direction!

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(iv) Use target classification $\tilde{y}$ [Kurakin, Goodfellow, Bengio 2017]

$$\tilde{x} = x - \epsilon \operatorname{sign}(\nabla_x \mathfrak{L}(x, \tilde{y}))$$

Can also be extended iteratively.

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(C) DeepFool [Moosavi-Dezfooli, Fawzi, Froosard 2016]

Assumptions:

- Consider binary classification, i.e. $Y = \{-1, +1\}$.
- $h_w(x) = \sigma_{\text{sign}}(f(x))$
- $f : \mathbb{R}^n \to \mathbb{R}$ an affine classifier $f(x) = \langle w, x \rangle + b$, $w \in \mathbb{R}^n$, $b \in \mathbb{R}$
- $F := \{x \in \mathbb{R}^n \mid f(x) = 0\}$ is the separating affine hyperplane.

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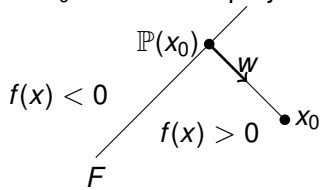
- Let $x_0 \in \mathbb{R}^n$. Then project x_0 onto F:



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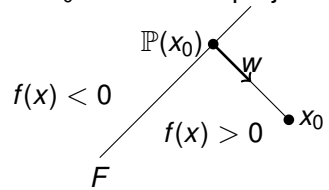

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- Extension to nonlinear functions f and multiclass problems

Questions