Machine Learning

B. Supervised Learning: Nonlinear Models
B.2. Neural Networks

Lars Schmidt-Thieme

Information Systems and Machine Learning Lab (ISMLL)
Institute for Computer Science
University of Hildesheim, Germany

Syllabus

Fri. 25.10.	(1)	0. Introduction
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Fri. 1.11.	(2)	A.1 Linear Regression
Fri. 8.11.	(3)	A.2 Linear Classification
Fri. 15.11.	(4)	A.3 Regularization
Fri. 22.11.	(5)	A.4 High-dimensional Data
		B. Supervised Learning: Nonlinear Models
Fri. 29.11.	(6)	B.1 Nearest-Neighbor Models
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Fri. 13.12.	(8)	B.3 Decision Trees
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Fri. 10.1.	(10)	B.5 A First Look at Bayesian and Markov Networks
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Outline

Outline

Logistic Regression

logistic regression:

$$\begin{aligned}\hat{y}(x) := \hat{p}(y = 1 \mid x) &= \text{logistic}(\beta^T x) \\ &= 1/(1 + e^{-\beta^T x}) = 1/(1 + e^{-\sum_{m=1}^{M} \beta_m x_m}), \quad x \in \mathbb{R}^M\end{aligned}$$

Logistic Regression (0 hidden layers)

$$\begin{tikzcd} x_1 \arrow[dr] & x_2 \arrow[d] & \cdots & x_M \arrow[dll] & \text{input layer} \\ & y & & & \text{output layer} \end{tikzcd}$$

logistic regression:

$$\begin{aligned} \hat{y}(x) &:= \hat{p}(y = 1 \mid x) = \text{logistic}(\beta^T x) \\ &= 1/(1 + e^{-\beta^T x}) = 1/(1 + e^{-\sum_{m=1}^{M} \beta_m x_m}), \quad x \in \mathbb{R}^M \end{aligned}$$

Feedforward Neural Network (1 hidden layer)

$$\begin{tikzcd}
 & x_1 \arrow[dl] \arrow[d] \arrow[drrr] & x_2 \arrow[dll] \arrow[dl] \arrow[drr] & \cdots & x_M \arrow[dllll] \arrow[dlll] \arrow[d] & \text{input layer} \\
z_1 \arrow[drr] & z_2 \arrow[dr] & \cdots & & z_K \arrow[dll] & \text{hidden layer} \\
 & & y & & & \text{output layer}
\end{tikzcd}$$

feedforward neural network (1 hidden layer):

$$
\begin{aligned}
z_k(x) :=& \operatorname{logistic}(\beta_{1,k}^T x), \quad k = 1, \ldots, K, x \in \mathbb{R}^M \\
\hat{y}(x) :=& \operatorname{logistic}(\beta_2^T z(x))
\end{aligned}
$$

Feedforward Neural Network (2 hidden layers)

$$\begin{tikzcd}
 & x_1 \arrow[dl] \arrow[d] \arrow[drrrr] & x_2 \arrow[dll] \arrow[dl] \arrow[drrr] & \cdots & x_M \arrow[dllll] \arrow[dlll] \arrow[dr] & \\
z_{1,1} \arrow[d] \arrow[dr] \arrow[drrrr] & z_{1,2} \arrow[dl] \arrow[d] \arrow[drrr] & \cdots & & & z_{1,K_1} \arrow[dlllll] \arrow[dllll] \arrow[dl] \\
z_{2,1} \arrow[drr] & z_{2,2} \arrow[dr] & \cdots & & z_{2,K_2} \arrow[dll] & \\
 & & y & & &
\end{tikzcd}$$

input layer

1st hidden layer

2nd hidden layer

output layer

feedforward neural network (2 hidden layers):

$$\begin{aligned}
z_{1,k}(x) :=& \text{logistic}(\beta_{1,k}^T x), & k = 1, \ldots, K_1, \quad x \in \mathbb{R}^M \\
z_{2,k}(x) :=& \text{logistic}(\beta_{2,k}^T z_1(x)), & k = 1, \ldots, K_2 \\
\hat{y}(x) :=& \text{logistic}(\beta_3^T z_2(x))
\end{aligned}$$

Feedforward Neural Network (L hidden layers)

$$\begin{tikzcd}
 & x_1 \arrow[dl] \arrow[d] \arrow[drrr] & x_2 \arrow[dll] \arrow[dl] \arrow[drr] & \cdots & x_M \arrow[dllll] \arrow[dlll] \arrow[d] & \text{input layer} \\
z_{1,1} \arrow[d] \arrow[dr] \arrow[drrrr] & z_{1,2} \arrow[dl] \arrow[d] \arrow[drrr] & \cdots & & z_{1,K_1} \arrow[dllll] \arrow[dlll] \arrow[d] & \text{1st hidden layer} \\
z_{2,1} & z_{2,2} & \cdots & & z_{2,K_2} & \text{2nd hidden layer} \\
 & & \vdots & & & \vdots \\
z_{L,1} \arrow[drr] & z_{L,2} \arrow[dr] & \cdots & & z_{L,K_L} \arrow[dll] & L\text{th hidden layer} \\
 & & y & & & \text{output layer}
\end{tikzcd}$$

$$z_{1,k}(x) := \text{logistic}(\beta_{1,k}^T\, x), \qquad k = 1, \ldots, K_1, x \in \mathbb{R}^M$$

$$z_{\ell,k}(x) := \text{logistic}(\beta_{\ell,k}^T\, z_{\ell-1}(x)), \qquad \ell = 2, \ldots, L, k = 1, \ldots, K_\ell$$

$$\hat{y}(x) := \text{logistic}(\beta_{L+1}^T\, z_L(x))$$

Different Targets y

Binary classification:

$$\hat{y}(x) := \hat{p}(y = 1 \mid x) = \text{logistic}(\beta_{L+1}^T z_L(x)), \qquad \beta_{L+1} \in \mathbb{R}^{K_L}$$

Regression:

$$\hat{y}(x) := \beta_{L+1}^T z_L(x), \qquad \beta_{L+1} \in \mathbb{R}^{K_L}$$

Regression with multiple outputs:

$$\hat{y}(x) := \beta_{L+1} z_L(x), \qquad \beta_{L+1} \in \mathbb{R}^{T \times K_L} \text{ a matrix!}$$

Multi-class classification:

$$\hat{y}(x) := \hat{p}(y \mid x) = \text{softmax}(\beta_{L+1} z_L(x)), \qquad \beta_{L+1} \in \mathbb{R}^{T \times K_L}$$

Notes:

- L hidden layers
- at hidden nodes always are logistic/sigmoid functions (**activation function**, **transfer function**).

Softmax

$$
\begin{aligned}
\text{softmax} : \ & \mathbb{R}^T \rightarrow \mathbb{R}^T \\
\text{softmax}(u) := & \left(\frac{e^{u_t}}{\sum_{s=1}^T e^{u_s}} \right)_{t=1:T}, \quad u \in \mathbb{R}^T \\
= & \begin{pmatrix} \frac{e^{u_1}}{\sum_{s=1}^T e^{u_s}} \\ \frac{e^{u_2}}{\sum_{s=1}^T e^{u_s}} \\ \vdots \\ \frac{e^{u_T}}{\sum_{s=1}^T e^{u_s}} \end{pmatrix}
\end{aligned}
$$

Softmax

binary classification:

$$\begin{aligned}\hat{y}(x) &:= \hat{p}(y=1 \mid x) = \text{logistic}(\beta_{L+1}^T z_L(x)) \\ &= \text{logistic}(u_{L+1}(x)), \quad u_{L+1}(x) := \beta_{L+1}^T z_L(x), \beta_{L+1} \in \mathbb{R}^{K_L}\end{aligned}$$

$$\text{logistic}(u) := \frac{1}{1+e^{-u}}$$

multi-class classification:

$$\begin{aligned}\hat{y}(x) &:= \hat{p}(y \mid x) = (\hat{p}(y=t \mid x))_{t=1:T} = \text{softmax}(\beta_{L+1} z_L(x)) \\ &= \text{softmax}(u_{L+1}(x)), \quad u_{L+1}(x) := \beta_{L+1} z_L(x), \beta_{L+1} \in \mathbb{R}^{T\times}\end{aligned}$$

$$\text{softmax}(u) := \left(\frac{e^{u_t}}{\sum_{s=1}^T e^{u_s}}\right)_{t=1:T}, \quad u \in \mathbb{R}^T$$

Softmax / Generalization of the Logistic

binary classification:

$$\hat{y}(x) := \hat{p}(y = 1 \mid x) = \text{logistic}(\beta_{L+1}^T z_L(x))$$
$$= \text{logistic}(u_{L+1}(x)), \quad u_{L+1}(x) := \beta_{L+1}^T z_L(x), \beta_{L+1} \in \mathbb{R}^{K_L}$$

$$\text{logistic}(u) := \frac{1}{1+e^{-u}} = \frac{e^u}{1+e^u} = \begin{pmatrix} \frac{e^0}{e^0+e^u} \\ \frac{e^u}{e^0+e^u} \end{pmatrix}_2 = (\text{softmax}(\begin{pmatrix} 0 \\ u \end{pmatrix}))_2$$

$$\begin{pmatrix} \hat{p}(y=0 \mid x) \\ \hat{p}(y=1 \mid x) \end{pmatrix} = \text{softmax}(\begin{pmatrix} 0 \\ u_{L+1}(x) \end{pmatrix})$$

multi-class classification:

$$\hat{y}(x) := \hat{p}(y \mid x) = (\hat{p}(y = t \mid x))_{t=1:T} = \text{softmax}(\beta_{L+1} z_L(x))$$
$$= \text{softmax}(u_{L+1}(x)), \quad u_{L+1}(x) := \beta_{L+1} z_L(x), \beta_{L+1} \in \mathbb{R}^{T\times}$$

$$\text{softmax}(u) := \left(\frac{e^{u_t}}{\sum_{s=1}^T e^{u_s}}\right)_{t=1:T}, \quad u \in \mathbb{R}^T$$

Softmax Properties

$$\text{softmax}(u) := \left(\frac{e^{u_t}}{\sum_{s=1}^{T} e^{u_s}} \right)_{t=1:T}, \quad u \in \mathbb{R}^T$$

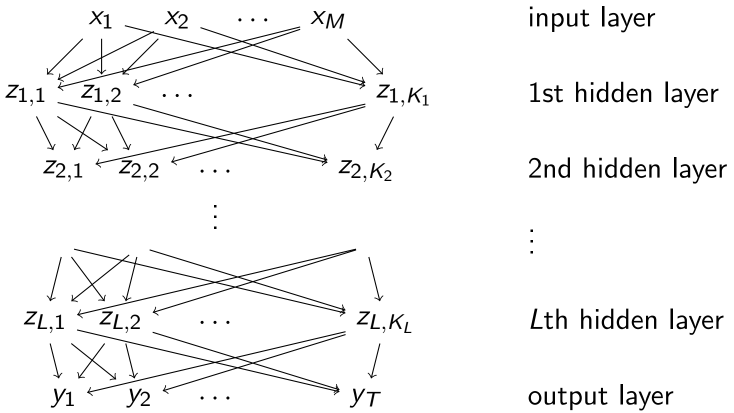
- softmax is a generalization of the logistic function from 2 to T classes.
- softmax is continuous and differentiable.
- softmax components sum to one:

$$\sum_{t=1}^{T} (\text{softmax}(u))_t = 1$$

- softmax in the limit approaches the maximum indicator:

$$\lim_{a \to \infty} \text{softmax}(a \cdot u) = (\mathbb{I}(u_t = u_{\max}))_{t=1:T}, \quad u_{\max} := \max_{s \in 1:T} u(s)$$

Feedforward Neural Network (L hidden layers, T outputs)


x_1 x_2 $\cdots$ x_M
input layer
$z_{1,1}$ $z_{1,2}$ $\cdots$ z_{1,K_1}
1st hidden layer
$z_{2,1}$ $z_{2,2}$ $\cdots$ z_{2,K_2}
2nd hidden layer
$\vdots$
$z_{L,1}$ $z_{L,2}$ $\cdots$ z_{L,K_L}
Lth hidden layer
y_1 y_2 $\cdots$ y_T
output layer

$$z_{1,k}(x) := s_1(\beta_{1,k}^T x), \qquad k = 1, \ldots, K_1, \quad x \in \mathbb{R}^M$$

$$z_{\ell,k}(x) := s_\ell(\beta_{\ell,k}^T z_{\ell-1}(x)), \quad \ell = 2, \ldots, L, \quad k = 1, \ldots, K_\ell$$

$$\hat{y}_k(x) := s_{L+1,k}(\beta_{L+1,.}^T z_L(x)), \quad k = 1, \ldots, T$$

Beware: for softmax s_{L+1} is **not** elementwise!

Feedforward Neural Network (L hidden layers, T outputs)

make it simple 1: each layer a vector

$$\begin{tikzcd}
x \arrow[d] & \text{input layer} \\
z_1 \arrow[d] & \text{1st hidden layer} \\
z_2 & \text{2nd hidden layer} \\
\vdots \arrow[d] & \vdots \\
z_L \arrow[d] & L\text{th hidden layer} \\
y & \text{output layer}
\end{tikzcd}$$

$$z_1(x) := s_1^\circ(\beta_1 x) \qquad \beta_1 \in \mathbb{R}^{K_1 \times M}$$

$$z_\ell(x) := s_\ell^\circ(\beta_\ell z_{\ell-1}(x)), \quad \ell = 2, \ldots, L, \qquad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$$

$$\hat{y}(x) := s_{L+1}(\beta_{L+1} z_L(x)) \qquad \beta_{L+1} \in \mathbb{R}^{T \times K_L}$$

Beware: for softmax s_{L+1} is **not** elementwise!

Feedforward Neural Network (L hidden layers, T outputs)

make it simple 2: rename x and $\hat{y}$ to z_0 and z_{L+1}

$$\begin{tikzcd}
z_0 \arrow[d] & \text{input layer} \\
z_1 \arrow[d] & \text{1st hidden layer} \\
z_2 & \text{2nd hidden layer} \\
\vdots \arrow[d] & \vdots \\
z_L \arrow[d] & L\text{th hidden layer} \\
z_{L+1} & \text{output layer}
\end{tikzcd}$$

$$z_\ell(x) := s_\ell(\beta_\ell \, z_{\ell-1}(x)), \quad \ell = 1, \ldots, L+1, \qquad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$$

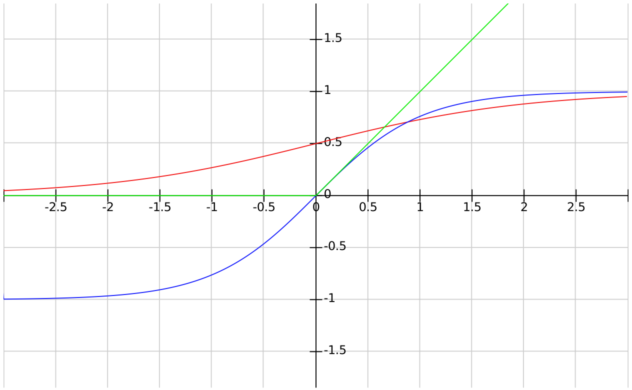
with $z_0 := x$, $\hat{y}(x) := z_{L+1}(x)$, $K_0 := M$, $K_{L+1} := T$, $s_\ell = s_\ell^\circ$ for $\ell \neq L+1$

Beware: for softmax s_{L+1} is **not** elementwise!

Activation Functions

Nowadays, usually the **rectifier** is used as activation function s (such nodes are called **ReLU**: **rectified linear unit**):

$$\text{rect}(x) := \max(0, x)$$



red: logistic, blue: tanh, green: rect

Parameters & Structure

- model:

$$z_\ell(x) := s_\ell(\beta_\ell \, z_{\ell-1}(x)), \quad \ell = 1, \ldots, L+1 \qquad \beta_\ell \in$$

with $z_0 := x$, $\hat{y}(x) := z_{L+1}(x)$, $K_0 := M$, $K_{L+1} := T$, $s_\ell = s^\circ_\ell$ for $\ell \neq L+1$

- parameters:

$$\beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}, \quad \ell = 1, \ldots, L+1$$

- structure:
  - $L \in \mathbb{N}_0$: number of hidden layers.
  - $K_\ell \in \mathbb{N}, \quad \ell = 1, \ldots, L$: size of hidden layer ℓ.
  - $s_\ell = s^\circ, \quad \ell = 1, \ldots, L$: activation function of hidden layer ℓ.
    (applied elementwise and usually not dependent on the layer ℓ)
  - s_{L+1}: output function.

Predicting with a Neural Network

```
**predict-nn**$(x, \beta, s)$ :
    $z_0 := x$
    for $\ell := 1, \ldots, L+1$ :
        $z_\ell := s_\ell^\circ(\beta_\ell \, z_{\ell-1})$
    return $z_{L+1}$
```

Network Topologies

- **feedforward neural network** (aka **multilayer perceptron**, MLP)
    - often just a single hidden layer is used
        - NN with single hidden layer is already a **universal approximator**
    - **skip arcs** can be used to connect layers skipping a hidden layer
    - usually layers are connected completely (**fully connected layer**), but sometimes **sparse connections** are used.
    - nodes & connections always form a DAG
- **recurrent neural network**
    - neural networks with backward connections / not a DAG.
    - used in language modeling
    - no simple probabilistic interpretation
    - nowadays usually rolled out to a feedforward net with tied weights
- **Hopfield networks** / **associative memory**:
    - symmetric connections between hidden units

Outline

Vector Calculus Refresh – Gradients & Jacobians

function with N inputs, single output:

$$\begin{aligned} f : \mathbb{R}^N &\to \mathbb{R} \\ x &\mapsto f(x_1, \ldots, x_N) \end{aligned}$$

gradient (vector):

$$\nabla f(x) := \left(\frac{\partial f}{\partial x_n}(x)\right)_{n=1:N}$$

function/map with N inputs, M outputs:

$$\begin{aligned} f : \mathbb{R}^N &\to \mathbb{R}^M \\ x &\mapsto (f_m(x_1, \ldots, x_N))_{m=1:M} \end{aligned}$$

Jacobian (matrix) / **total derivative**:

$$Df(x) := \left(\frac{\partial f_m}{\partial x_n}(x)\right)_{m=1:M,n=1:N}$$

Vector Calculus Refresh – Gradients & Jacobians

function with N inputs, single output:

$$\begin{aligned} f : \mathbb{R}^N &\to \mathbb{R} \\ x &\mapsto f(x_1, \ldots, x_N) \end{aligned}$$

gradient (vector):

$$\nabla f(x) := \left(\frac{\partial f}{\partial x_n}(x) \right)_{n=1:N} = (Df(x))^T$$

function/map with N inputs, M outputs:

$$\begin{aligned} f : \mathbb{R}^N &\to \mathbb{R}^M \\ x &\mapsto (f_m(x_1, \ldots, x_N))_{m=1:M} \end{aligned}$$

Jacobian (matrix) / **total derivative**:

$$Df(x) := \left(\frac{\partial f_m}{\partial x_n}(x) \right)_{m=1:M, n=1:N} = \begin{pmatrix} \nabla f_1(x)^T \\ \nabla f_2(x)^T \\ \vdots \\ \nabla f_M(x)^T \end{pmatrix}$$

Vector Calculus Refresh – Chain Rule

function composition:

$$\begin{array}{rccc} & X := \mathbb{R}^N & \xrightarrow{f} & Y := \mathbb{R}^M \\ f: & x & \mapsto & f(x) \end{array}$$

Vector Calculus Refresh – Chain Rule

function composition:

$$\begin{array}{llllll} & X := \mathbb{R}^N & \xrightarrow{f} & Y := \mathbb{R}^M & \xrightarrow{g} & Z := \mathbb{R} \\ f : & x & \mapsto & f(x) & & \\ g : & & & y & \mapsto & g(y) \end{array}$$

Vector Calculus Refresh – Chain Rule

function composition:

$$\begin{array}{rcccccc} & X := \mathbb{R}^N & \xrightarrow{f} & Y := \mathbb{R}^M & \xrightarrow{g} & Z := \mathbb{R} & \\ f: & x & \mapsto & f(x) & & & \\ g: & & & y & \mapsto & g(y) & \\ g \circ f: & x & & & \mapsto & (g \circ f)(x) & := g(f(x)) \end{array}$$

chain rule:

$$\begin{aligned} D(g \circ f)(x) &= Dg(f(x))\, Df(x) \\ \nabla(g \circ f)(x) &= Df(x)^T (\nabla g)(f(x)) \end{aligned}$$

Vector Calculus Refresh – Elementwise Function Application

function with single input, single output:

$$\begin{aligned} f : \mathbb{R} &\rightarrow \mathbb{R} \\ x &\mapsto f(x) \end{aligned}$$

elementwise function application:

$$\begin{aligned} f^\circ : \mathbb{R}^N &\rightarrow \mathbb{R}^N \\ x &\mapsto (f(x_n))_{n=1:N} = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_N) \end{pmatrix} \end{aligned}$$

its Jacobian:

$$Df^\circ(x) = \begin{pmatrix} f'(x_1) & & & \\ & f'(x_2) & & \\ & & \ddots & \\ & & & f'(x_N) \end{pmatrix} = \operatorname{diag}(f'^\circ(x))$$

Vector Calculus Refresh – Partial Gradients & Jacobians

function with N inputs, single output:

$$\begin{aligned} f : \mathbb{R}^N &\rightarrow \mathbb{R} \\ x &\mapsto f(x_1, \ldots, x_N) \end{aligned}$$

partial gradient (vector):

$$\nabla_I f(x) := \left(\frac{\partial f}{\partial x_n}(x) \right)_{n \in I}, \quad I \subseteq \{1, \ldots, N\}$$

function/map with N inputs, M outputs:

$$\begin{aligned} f : \mathbb{R}^N &\rightarrow \mathbb{R}^M \\ x &\mapsto (f_m(x_1, \ldots, x_N))_{m=1:M} \end{aligned}$$

partial Jacobian (matrix):

$$D_I f(x) := \left(\frac{\partial f_m}{\partial x_n}(x) \right)_{m=1:M, n \in I} \qquad I \subseteq \{1, \ldots, N\}$$

Objective Function

feedforward neural network, L hidden layers with $K_1, \ldots, K_L$ nodes each:

$$z_\ell(x) := s_\ell(\beta_\ell \, z_{\ell-1}(x)), \quad \ell = 1, \ldots, L+1, \qquad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$$

with $z_0 := x, \quad \hat{y}(x) := z_{L+1}(x), \quad K_0 := M, \quad K_{L+1} := T, \quad s_\ell = s^\circ_\ell$ for $\ell \neq L+1$

objective function:

$$f(\beta) := \frac{1}{N} \sum_{n=1}^{N} \mathcal{L}(y_n, \hat{y}(x_n)) + \frac{\lambda}{2} ||\beta||^2 = \frac{1}{N} \sum_{n=1}^{N} \mathcal{L}(\beta; x_n, y_n) + \frac{\lambda}{2} ||\beta||^2$$

loss for single sample:

$$\mathcal{L}(\beta; x, y) := \mathcal{L}(y, z_{L+1}(x))$$

Objective Function

feedforward neural network, L hidden layers with $K_1, \ldots, K_L$ nodes each:

$$\begin{aligned} u_\ell(x) &:= \beta_\ell \, z_{\ell-1}(x), \quad \ell = 1, \ldots, L+1, \quad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}} \\ z_\ell(x) &:= s_\ell^\circ(u_\ell(x)), \quad \ell = 1, \ldots, L \\ z_{L+1}(x) &:= s_{L+1}(u_\ell(x)) \end{aligned}$$

with $z_0 := x, \quad \hat{y}(x) := z_{L+1}(x), \quad K_0 := M, \quad K_{L+1} := T$

loss for single sample:

$\mathcal{L}(\beta; x, y) := \mathcal{L}(y, z_{L+1}(x))$

Objective Function

feedforward neural network, L hidden layers with $K_1, \ldots, K_L$ nodes each:

$$u_\ell(z_{\ell-1}) := \beta_\ell \, z_{\ell-1}, \quad \ell = 1, \ldots, L+1, \quad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$$

$$z_\ell(u_\ell) := s^\circ(u_\ell), \qquad z_{L+1}(u_{L+1}) := s_{L+1}(u_{L+1})$$

with $z_0 := x, \quad \hat{y}(x) := (z_{L+1} \circ u_{L+1} \circ z_L \circ u_L \circ \cdots \circ z_1 \circ u_1)(x), \quad K_0 := M, \quad K_{L+1} := T$

loss for single sample:

$$\mathcal{L}(\beta; x, y) := \mathcal{L}(y, z_{L+1}(x)) = (\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_\ell \circ u_\ell \circ \cdots z_1 \circ u_1)(x)$$

with pair loss $\mathcal{L}_y(z_{L+1}) := \text{loss}(y, z_{L+1})$

Objective Function

feedforward neural network, L hidden layers with $K_1, \ldots, K_L$ nodes each:

$$u_\ell(z_{\ell-1}) := \beta_\ell \, z_{\ell-1}, \quad \ell = 1, \ldots, L+1, \quad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$$

$$z_\ell(u_\ell) := s^\circ(u_\ell), \qquad z_{L+1}(u_{L+1}) := s_{L+1}(u_{L+1})$$

with $z_0 := x, \quad \hat{y}(x) := (z_{L+1} \circ u_{L+1} \circ z_L \circ u_L \circ \cdots \circ z_1 \circ u_1)(x), \quad K_0 := M, \quad K_{L+1} := T$

loss for single sample:

$$\mathcal{L}(\beta; x, y) := \mathcal{L}(y, z_{L+1}(x)) = (\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_\ell \circ u_\ell \circ \cdots z_1 \circ u_1)(x)$$

with pair loss $\mathcal{L}_y(z_{L+1}) := \text{loss}(y, z_{L+1})$

its gradients:

$$\nabla_{\beta_{\ell,k}} \mathcal{L}(\beta) = D_{\beta_{\ell,k}} u_\ell(z_{\ell-1})^T \nabla(\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_{\ell+1} \circ u_{\ell+1} \circ z_\ell)(u_\ell)$$

$$\nabla(\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_{\ell+1} \circ u_{\ell+1} \circ z_\ell)(u_\ell)$$

$$= D z_\ell^T D u_{\ell+1}^T \nabla(\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_{\ell+2} \circ u_{\ell+2} \circ z_{\ell+1})(u_{\ell+1})$$

Gradients / Recursion Scheme

single sample loss gradients:

$$\nabla_{\beta_{\ell,k}}\mathcal{L}(\beta) = D_{\beta_{\ell,k}} u_\ell(z_{\ell-1})^T \nabla(\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_{\ell+1} \circ u_{\ell+1} \circ z_\ell)(u_\ell)$$

$$\nabla(\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_{\ell+1} \circ u_{\ell+1} \circ z_\ell)(u_\ell)$$
$$= Dz_\ell^T Du_{\ell+1}^T \nabla(\mathcal{L}_y \circ z_{L+1} \circ u_{L+1} \circ \cdots z_{\ell+2} \circ u_{\ell+2} \circ z_{\ell+1})(u_{\ell+1})$$

establishes a recursive computation scheme:

$$\begin{aligned}\nabla_{\beta_{\ell,k}}\mathcal{L}(\beta) &= D_{\beta_{\ell,k}} u_\ell(z_{\ell-1})^T g_\ell(u_\ell)\\ g_\ell(u_\ell) &:= Dz_\ell^T Du_{\ell+1}^T\, g_{\ell+1}(u_{\ell+1})\\ g_{L+1}(u_{L+1}) &:= Dz_{L+1}^T \nabla \mathcal{L}_y(z_{L+1})\end{aligned}$$

Gradients / Components

$$u_\ell(z_{\ell-1}) := \beta_\ell\, z_{\ell-1}, \quad \ell = 1, \ldots, L+1, \quad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$$
$$z_\ell(u_\ell) := s^\circ(u_\ell), \qquad z_{L+1}(u_{L+1}) := s_{L+1}(u_{L+1})$$

single sample loss gradients:

$$\nabla_{\beta_{\ell,k}} \mathcal{L}(\beta) = D_{\beta_{\ell,k}} u_\ell(z_{\ell-1})^T g_\ell(u_\ell)$$
$$g_\ell(u_\ell) := Dz_\ell^T\, Du_{\ell+1}^T\, g_{\ell+1}(u_{\ell+1})$$
$$g_{L+1}(u_{L+1}) := Dz_{L+1}^T \nabla \mathcal{L}_y(z_{L+1})$$

components:

$$Du_\ell = \beta_\ell$$
$$Dz_\ell = \operatorname{diag}(s'^\circ(u_\ell))$$
$$D_{\beta_{\ell,k}} u_\ell = e_k\, z_{\ell-1}^T \qquad \rightsquigarrow \qquad \begin{aligned} \nabla_{\beta_{\ell,k}} \mathcal{L}(\beta) &= z_{\ell-1}\, e_k^T\, g_\ell(u_\ell) \\ \nabla_{\beta_\ell} \mathcal{L}(\beta) &= g_\ell(u_\ell)\, z_{\ell-1}^T \end{aligned}$$

Note: e_k denotes the k-th unit vector: $(e_k)_j := \mathbb{I}(k = j)$.
β_ℓ is a parameter matrix, thus $\nabla_{\beta_\ell} \mathcal{L}(\beta)$ is a matrix-shaped gradient!

Gradients / Sticking Everything Together

parameters:

$$\beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}, \quad \ell = 1 : L+1$$

feed forward:

$$\begin{aligned} z_0 &:= x \\ u_\ell &:= \beta_\ell \, z_{\ell-1}, \quad \ell = 1 : L+1 \\ z_\ell &:= s^\circ(u_\ell) \end{aligned}$$

back propagation:

$$\begin{aligned} g_{L+1}(u_{L+1}) &:= Ds_{L+1}(u_{L+1}) \, \nabla \mathcal{L}_y(z_{L+1}) \\ g_\ell(u_\ell) &:= \text{diag}(s'^\circ(u_\ell)) \, \beta_{\ell+1}^T \, g_{\ell+1}(u_{\ell+1}) \\ \nabla_{\beta_\ell} \mathcal{L}(\beta) &= g_\ell(u_\ell) \, z_{\ell-1}^T, \quad \ell = L+1 : 1 \text{ backwards} \\ \beta_\ell^{\text{next}} &:= \beta_\ell - \eta(\nabla_{\beta_\ell} \mathcal{L}(\beta) + \lambda \beta_\ell) \end{aligned}$$

SGD / Backpropagation

```
learn-nn-sgd($\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, L, K, s, \nabla\mathcal{L}, \lambda, \eta, I$):
  randomly initialize $\beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$, $\ell = 1 : L+1$
  for $i := 1, \ldots, I$:
    for $(x_n, y_n) \in \mathcal{D}^{\text{train}}$ in random order:
      $z_0 := x_n$                                                [feed forward]
      for $\ell := 1 : L+1$:
        $u_\ell := \beta_\ell \, z_{\ell-1}$
        $z_\ell := s^\circ(u_\ell)$
      $g_{L+1} := \text{diag}(s'^\circ(u_{L+1}))\nabla\mathcal{L}_{y_n}(z_{L+1})$      [back propagation]
      for $\ell := L+1 : 2$ backwards:
        $g_{\ell-1} := \text{diag}(s'^\circ(u_{\ell-1}))\, \beta_\ell^T \, g_\ell$
        $\beta_\ell := \beta_\ell - \eta_i(g_\ell \, z_{\ell-1}^T + \lambda\beta_\ell)$
      $\beta_1 := \beta_1 - \eta_i(g_1 \, z_0^T + \lambda\beta_1)$
    if converged(...):
      return $\beta$
  raise exception "not converged in $I$ iterations"
```

where

- L number of layers
- K layer sizes
- s activation function
- $\nabla\mathcal{L}$ loss gradient
- λ regularization weight
- η step length schedule
- I number of iterations

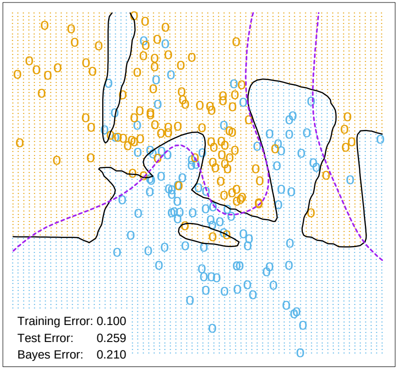
Outline

Regularization of Neural Networks

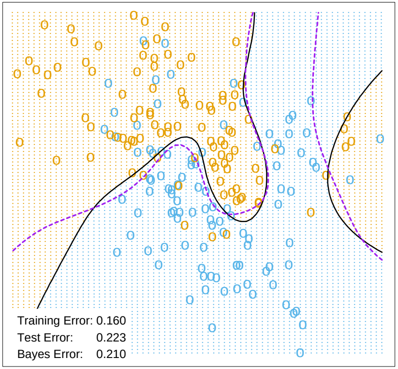
- generic, working with any model:
  - L2 regularization
    - aka **weight decay**
    - most frequently used method
  - L1 regularization
  - number of iterations as hyperparameter (**early stopping**)
- specific for neural networks:
  - **structural regularization**:
    - sufficiently small number of layers and sizes of layers
    - compare number of parameters with sample size!
  - **dropout** [Srivastava et al., 2014]
    - use random sample of input nodes and hidden nodes for each instance during training
  - **Batch normalization** [Ioffe and Szegedy, 2015]
    - standardize the values $z_{\ell,k}$ for each layer (for a minibatch).
  - **self-normalizing neural networks** [Klambauer et al., 2017]

L2 regularization / Example

Neural Network - 10 Units, No Weight Decay

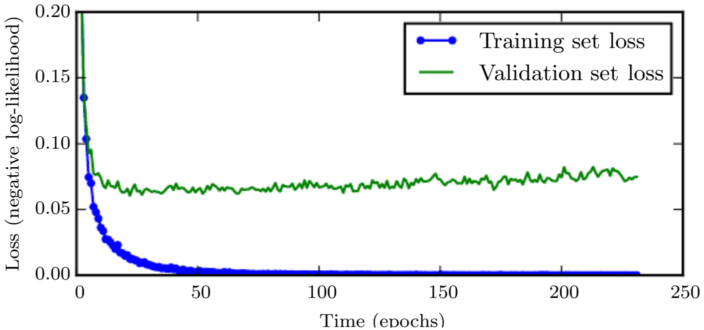


Neural Network - 10 Units, Weight Decay=0.02



[Hastie et al., 2005, p. 39

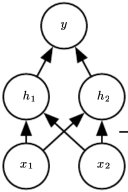
Early Stopping



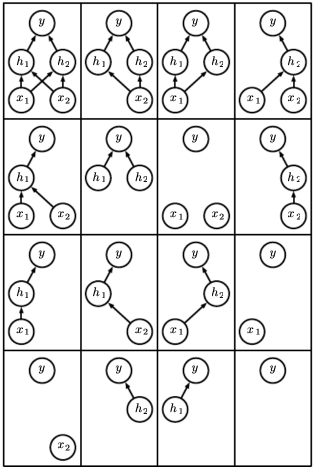
[source: Goodfellow et al. 2016, p. 239]

Early stopping works with any iterative learning algorithm.

Dropout



Base network



Ensemble of subnetworks

[source: Goodfellow et al. 2016, p. 252]

Summary (1/4)

- (Feedforward) Neural networks are parametrized models for supervised learning problems
  - arranged in several layers,
    - with the first layer being the inputs,
    - the last layer being the outputs,
    - intermediate/**hidden layers** representing subexpressions of the prediction function
      (not to be confused with latent variables!)
  - each layer composed of a **linear combination of the previous one**, with weights being parameters of the model,
  - and a **nonlinear activation function**,
    - usually the linear rectifier $\max(0, x)$
    - or a sigmoid function (logistic, tanh)
- Neural networks are learnt through Stochastic Gradient Descent
  - computation of the gradients in reverse order of computations of predictions (**backpropagation**)
  - [illegible]

Summary (2/4)

- The loss function of a neural network is **non-convex**.
- Neural networks can be learnt via Stochastic Gradient Descent
  - computation of the gradients in reverse order of computations of predictions (**backpropagation**)
  - usually using **minibatches** for a few ten or hundred instances.
  - starting from a **random initialization**.

Summary (3/4)

- As any other model, neural networks have to be regularized.
    - **structural regularization**:
        - number of nodes/layer and number of layers.
    - early stopping
    - L2 regularization (**weight decay**)
    - **dropout**: use a random sample of input and hidden nodes per example
- Neural networks can be extended in a rather straightforward way to work with sequential/time series, image data and any other kind of array data.
    - **convolutional neural networks**
    - **recurrent neural networks** (including LSTM, GRU)
    - these models belong to the most powerful models currently used in ML

Summary (4/4)

- A neural network with a single hidden layer can already approximate any function arbitrarily well.
  - **universal approximator**
  - if one adds arbitrarily many hidden nodes in that layer as necessary
  - but deeper networks with more than one hidden layer have shown to generalize better
    - esp. for structured data
    - make better use of a given number of parameters
    - **deep learning**

Further Readings

- See Murphy 2012, chapter 16.5 and Hastie et al. 2005, chapter 11.
- More detailed introduction in Goodfellow et al. 2016, chapter 6 and 7.

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