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. 26.10.	(1)	0. Introduction
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Fri. 9.11.	(3)	A.2 Linear Classification
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Fri. 30.11.	(6)	B.1 Nearest-Neighbor Models
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Fri. 11.1.	(10)	B.5 A First Look at Bayesian and Markov Networks
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Outline

1. Network Topologies

2. Stochastic Gradient Descent (Backpropagation)

3. Regularization

Outline

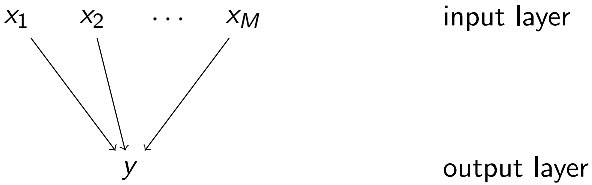
Logistic Regression

logistic regression:

$$\hat{y}(x) := \hat{p}(y = 1 \mid x) = \text{logistic}(\beta^T x), \quad x \in \mathbb{R}^M$$

Note: $\text{logistic}(x) := 1/(1 + e^{-x})$.

Logistic Regression (0 hidden layers)

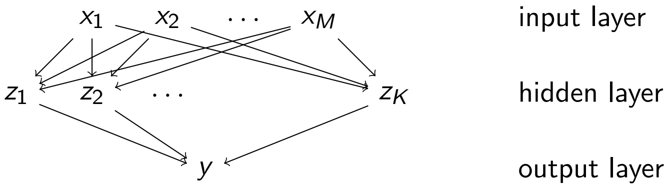


logistic regression:

$$\hat{y}(x) := \hat{p}(y = 1 \mid x) = \text{logistic}(\beta^T x), \quad x \in \mathbb{R}^M$$

Note: $\text{logistic}(x) := 1/(1 + e^{-x})$.

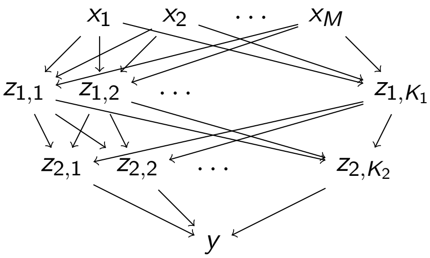
Feedforward Neural Network (1 hidden layer)



feedforward neural network (1 hidden layer):

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

Feedforward Neural Network (2 hidden layers)



input layer

1st hidden layer

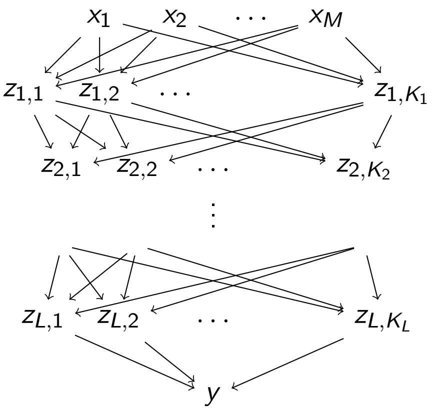
2nd hidden layer

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)



input layer

1st hidden layer

2nd hidden layer

$\vdots$

Lth hidden layer

output layer

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

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

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

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

$$\text{softmax}: \ \mathbb{R}^T \rightarrow \mathbb{R}^T$$

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

$$= \begin{pmatrix} \frac{e^{u_1}}{\sum_{s=1}^{T} e^{u_s}} \\ \frac{e^{u_2}}{\sum_{s=1}^{T} e^{u_s}} \\ \vdots \\ \frac{e^{u_T}}{\sum_{s=1}^{T} e^{u_s}} \end{pmatrix}$$

Softmax

binary classification:

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

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 / 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

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

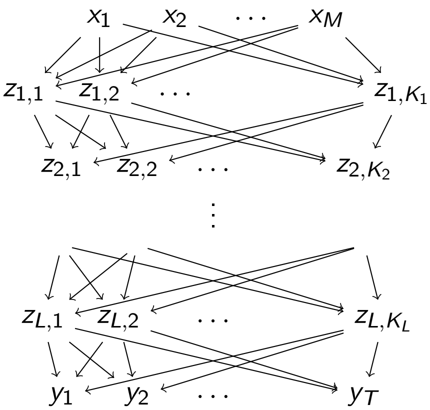
- softmax is a generalization of the logistic function from 2 to T classes.
- softmax is continuous and differentiable.
- softmax components sum to one:

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

- 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)



input layer

1st hidden layer

2nd hidden layer

⋮

Lth hidden layer

output layer

$$
\begin{aligned}
z_{1,k}(x) &:= s(\beta_{1,k}^T\, x), & k &= 1,\ldots,K_1, \quad x \in \mathbb{R}^M \\
z_{\ell,k}(x) &:= s(\beta_{\ell,k}^T\, z_{\ell-1}(x)), & \ell &= 2,\ldots,L, \quad k = 1,\ldots,K_\ell \\
\hat{y}_k(x) &:= s(\beta_{L+1,k}^T\, z_L(x)), & k &= 1,\ldots,T
\end{aligned}
$$

Feedforward Neural Network (L hidden layers, T outputs)

make it simple 1: each layer a vector

$$
\begin{array}{cl}
x & \text{input layer} \\
\downarrow & \\
z_1 & \text{1st hidden layer} \\
\downarrow & \\
z_2 & \text{2nd hidden layer} \\
\vdots & \vdots \\
\downarrow & \\
z_L & L\text{th hidden layer} \\
\downarrow & \\
y & \text{output layer}
\end{array}
$$

$$
\begin{aligned}
z_1(x) &:= s^\circ(\beta_1 x) & & \beta_1 \in \mathbb{R}^{K_1 \times M} \\
z_\ell(x) &:= s^\circ(\beta_\ell z_{\ell-1}(x)), \quad \ell = 2, \ldots, L, & & \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}} \\
\hat{y}(x) &:= s^\circ(\beta_{L+1} z_L(x)) & & \beta_{L+1} \in \mathbb{R}^{T \times K_L}
\end{aligned}
$$

Feedforward Neural Network (L hidden layers, T outputs)

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

$$
\begin{array}{ll}
z_0 & \text{input layer} \\
\downarrow & \\
z_1 & \text{1st hidden layer} \\
\downarrow & \\
z_2 & \text{2nd hidden layer} \\
\vdots & \vdots \\
\downarrow & \\
z_L & L\text{th hidden layer} \\
\downarrow & \\
z_{L+1} & \text{output layer}
\end{array}
$$

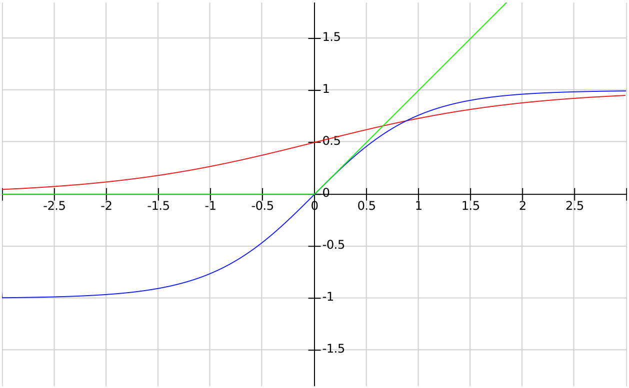
$$z_\ell(x) := s^\circ(\beta_\ell \, z_{\ell-1}(x)), \quad \ell = 1, \ldots, L+1 \qquad \beta_\ell \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$$

with $z_0 := x, \quad \hat{y}(x) := z_{L+1}(x), \quad K_1 := M, \quad K_{L+1} := T$

Activation Functions

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

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



red: logistic, blue: tanh, green: rect

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:

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

gradient (vector):

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

function/map with N inputs, M outputs:

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

Jacobian (matrix):

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

Vector Calculus Refresh – Chain Rule

function composition:

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

chain rule:

$$\nabla(g \circ f)(x) = Df(x)^T (\nabla g)(f(x))$$

Vector Calculus Refresh – Elementwise Function Application

function with single input, single output:

$$f : \mathbb{R} \rightarrow \mathbb{R}$$
$$x \mapsto f(x)$$

elementwise function application:

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

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:

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

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:

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

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:

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

with $z_0 := x, \quad \hat{y}(x) := z_{L+1}(x), \quad K_1 := M, \quad K_{L+1} := T$

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:

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

with $z_0 := x, \quad \hat{y}(x) := z_{L+1}(x), \quad K_1 := M, \quad K_{L+1} := T$

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:

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

with $z_0 := x, \quad \hat{y}(x) := (z_{L+1} \circ u_{L+1} \circ z_L \circ u_L \circ \cdots \circ z_1 \circ u_1)(x), \quad K_1 := M, \quad K_{L+1} := T$

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:

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

$$z_\ell(u_\ell) := s^\circ(u_\ell)$$

with $z_0 := x, \quad \hat{y}(x) := (z_{L+1} \circ u_{L+1} \circ z_L \circ u_L \circ \cdots \circ z_1 \circ u_1)(x), \quad K_1 := M, \quad K_{L+1} := T$

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

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

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:

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

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:

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

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**$(\ldots)$:
      return β
  raise exception "not converged in I iterations"

where

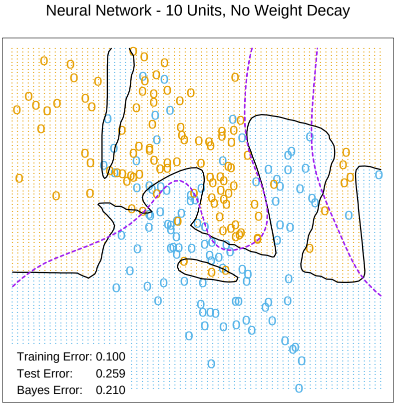
- L number of layers
- K layer sizes
- s activation function
- $\nabla\mathcal{L}$ loss gradient
- λ regularization weight
- η step length schedule
- I number of iterations

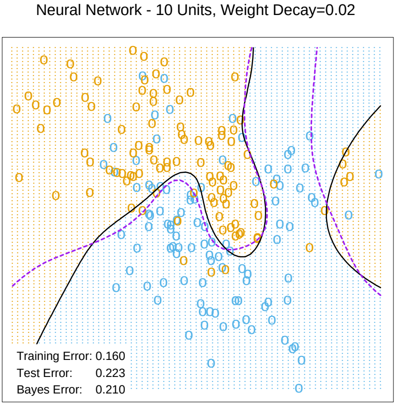
Outline

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]

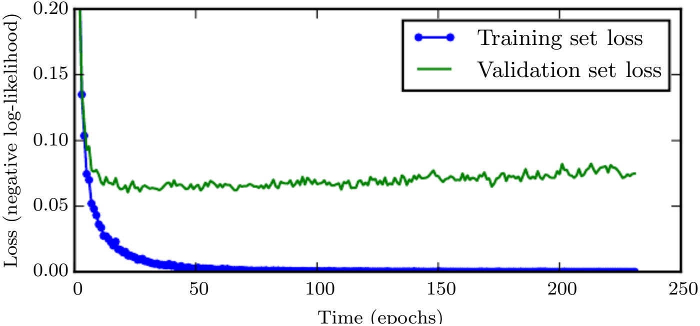
L2 regularization / Example





[Hastie et al., 2005, p. 39

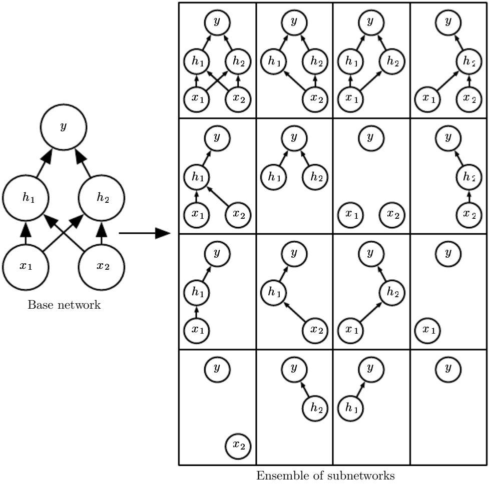
Early Stopping



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

Early stopping works with any iterative learning algorithm.

Dropout



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

Summary (1/3)

- (Feedforward) Neural networks are supervised parametric models
  - 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**)
  - usually using **minibatches** for a few ten or hundred instances.

Summary (2/3)

- 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 (3/3)

- 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
    - 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.

References

Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. The Mit Press, Cambridge, Massachusetts, November 2016. ISBN 978-0-262-03561-3.

Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin. *The Elements of Statistical Learning: Data Mining, Inference and Prediction*, volume 27. Springer, 2005.

Sergey Ioffe and Christian Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. In *International Conference on Machine Learning*, pages 448–456, 2015.

Günter Klambauer, Thomas Unterthiner, Andreas Mayr, and Sepp Hochreiter. Self-Normalizing Neural Networks. *arXiv preprint arXiv:1706.02515*, 2017.

Kevin P. Murphy. *Machine Learning: A Probabilistic Perspective*. The MIT Press, 2012.

Nitish Srivastava, Geoffrey E. Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: A simple way to prevent neural networks from overfitting. *Journal of machine learning research*, 15(1):1929–1958, 2014.