Machine Intelligence 1

1.3 Multi-layer Perceptrons

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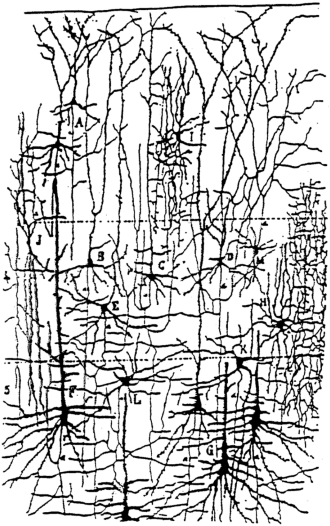
1.3.1 Classes of Neural Networks

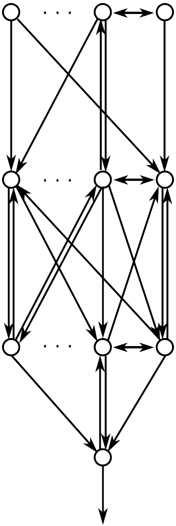
Graphs representing neural networks

Design principles inspired by biology

- architecture:
  - simple elements
  - massively parallel systems
  - low precision and robustness
  - distributed representation of information
  - no separation between data and program
- inductive learning:
  - data driven, adaptive systems
  - learning and self-organization vs. deduction and programming
  - often seen as a plus: biologically inspired learning rules

Graphs representing neural networks





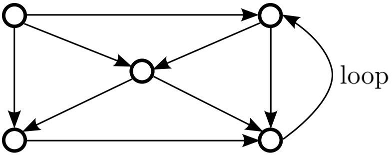
neural network
$\downarrow$
directed graph

(connectionist) neuron
$\downarrow$
node of the graph

neural connection
$\downarrow$
weighted edge

Recurrent Neural Networks (RNNs)

Recurrent networks $\hat{=}$ directed graphs containing cycles



- dynamical systems
- spatio-temporal pattern analysis
- sequence processing
- associative memory and pattern completion

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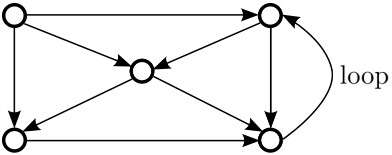


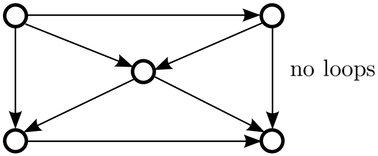
- dynamical systems
- spatio-temporal pattern analysis
- sequence processing
- associative memory and pattern completion

Examples:

Hopfield networks (Hopfield, 1982)
Boltzmann machines (Ackley, Hinton & Sejnowski, 1985)
Infinite **I**mpulse **R**esponse (IIR) networks (Crochiere & Oppenheim, 1975)
Long **S**hort-**T**erm **M**emory networks (LSTM, Hochreiter & Schmidhuber, 1997)
Deep Recurrent Neural Networks (Pascanu, Gulcehre, Cyho & Bengio, 2014)

Feedforward Neural Networks (FFN)

Feedforward Networks $\widehat{=}$ directed acyclic graphs (DAGs)



- association between variables
- prediction of attributes

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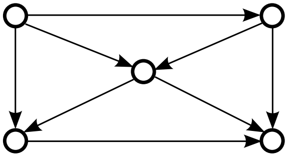

- association between variables
- prediction of attributes

Examples:

Multi**l**ayer-**P**erceptron (MLP, Rumelhart, Hinton & Williams, 1986
Radial **B**asis **F**unction network (RBF, Broomhead & Lowe, 1988)
Support **V**ector **M**achines (SVM, Cortes & Vapnik, 1995)
Deep **B**elief **N**etworks (DBN, Hinton, Osidero & Teh, 2006; Mnih et al., 2016)

Prediction of attributes

real-valued attributes: regression problems

$f: \mathbb{R}^N \rightarrow \mathbb{R}$	(or subsets)	one target value
$f: \mathbb{R}^N \rightarrow \mathbb{R}^M$	(or subsets)	multivariate attributes

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ordinal attributes: classification problems

$f : \mathbb{R}^N \to \mathcal{S}$	where $\mathcal{S}$ is a set of attributes $\{a_1, a_2, \dots, a_M\}$
$f : \mathbb{R}^N \to \{-1, +1\}$	special case: two class problems

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predicting probabilities

$f_k : \mathbb{R}^N \to [0, 1] \subset \mathbb{R}$ probability of attribute a_k from $\mathcal{S}$

s.t. $\sum_{k=1}^{M} f_k(\cdot) = 1$ constrains all $f_k(\cdot)$ to be probabilities

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structured input / structured output

$f : \mathcal{X} \to \mathcal{Y}$ where $\mathcal{X}$ and $\mathcal{Y}$ are sets of structures, e.g. graphs or sentences

see Baklr, Hofmann, Schölkopf, Smola, Taskar and Vishwanathan (Eds.): Predicting structured data, 2007

1.3.2 The Multi-layer-Perceptron for Regression

Overview inductive learning

data representation

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model class

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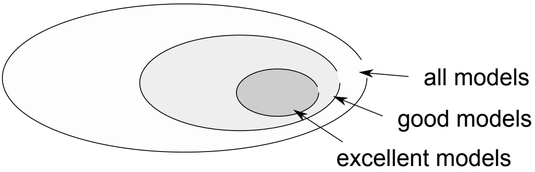
performance measure

↓

optimization

↓

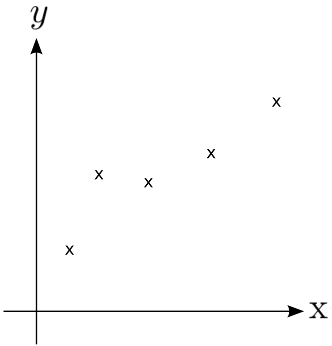
validation



data representation

Our example: regression with one real-valued attirbute

- input feature vectors: $\underline{\mathbf{x}} \in \mathbb{R}^N$
- output attributes: $y_T \in \mathbb{R}$
- training set: $\{\underline{\mathbf{x}}^{(\alpha)}, y_T^{(\alpha)}\}_{\alpha=1}^{p}$



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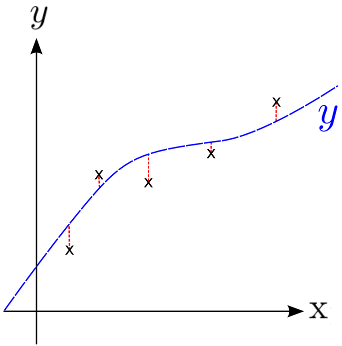
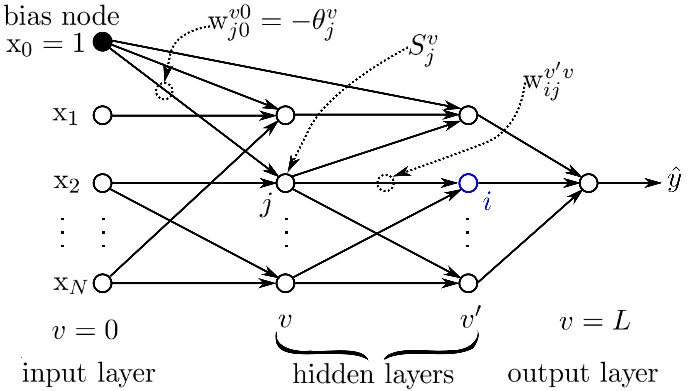
- output attributes: $y_T \in \mathbb{R}$
- training set: $\{\underline{\mathbf{x}}^{(\alpha)}, y_T^{(\alpha)}\}_{\alpha=1}^p$
- label function: $y_T = y(\underline{\mathbf{x}}) + \text{noise}$



model class

Multi-layer perceptrons (MLPs)

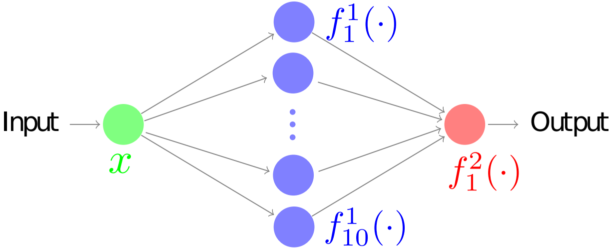
- layered FFN $\hat{y}(\cdot;\underline{\mathbf{w}})$ models label function $y(\cdot)$



- $S_i^{v'} = f_i^{v'}(h_i^{v'}) \overset{\text{e.g.}}{=} \tanh(h_i^{v'})\,, \quad h_i^{v'} = \sum_{j=0}^{N} w_{ij}^{v'v} S_j^v$

Model class: one example

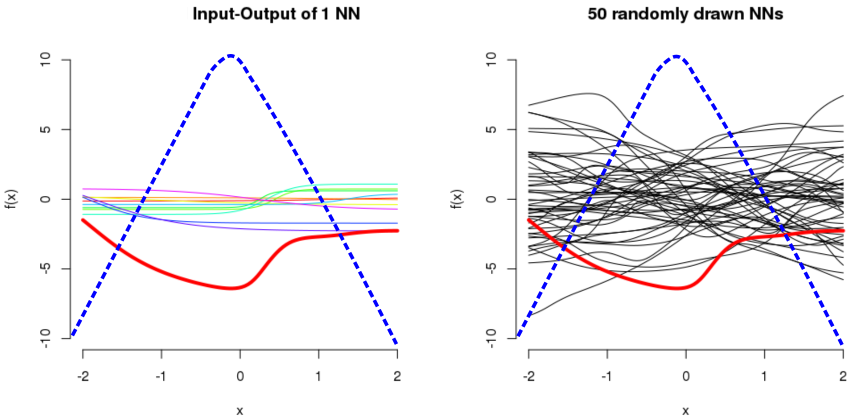
1 input, 1 output, 1 hidden layer with 10 units



$$\hat{y}(x) \quad = \quad f_1^2\Big(\sum_{i=1}^{10} w_{1i}^{21}\, f_i^1(w_{i1}^{10}\, x - w_{i0}^{10})\Big)$$

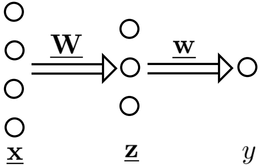
$$f_i^1(a) = \tanh(a) \text{ \& } f_1^2(a) = a$$

Model class: one example



(parameters drawn from Gaussian distribution)

Linear transfer functions



$$
\begin{aligned}
y &= \underline{\mathbf{w}}^{\top}\underline{\mathbf{z}} \quad = \quad \underline{\mathbf{w}}^{\top}\underline{\mathbf{W}}\,\underline{\mathbf{x}} \\
&= (\underline{\mathbf{W}}^{\top}\underline{\mathbf{w}})^{\top}\underline{\mathbf{x}} \quad = \quad \underline{\hat{\mathbf{w}}}^{\top}\underline{\mathbf{x}} \\
&\widehat{=} \quad \text{connectionist neuron}
\end{aligned}
$$

MLPs are universal approximators

Funahashi (1989)

Let $y^*_{(\underline{\mathbf{x}})}$ be a continuous, real valued function over a compact interval K and

$$\hat{y}_{(\underline{\mathbf{x}})} = \sum_{i=1}^{M} \mathrm{w}_i^{21} f\Big(\sum_{j=1}^{N} \mathrm{w}_{ij}^{10} \mathrm{x}_j - \theta_i\Big)$$

be a three-layered MLP with a non-constant, bounded, monotonously increasing and continuous function $f : \mathbb{R} \to \mathbb{R}$.

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be a three-layered MLP with a non-constant, bounded, monotonously increasing and continuous function $f : \mathbb{R} \to \mathbb{R}$.

Then there exists a set of parameters $M, N \in \mathbb{N}$ and $\mathrm{w}_i^{21}, \mathrm{w}_{ij}^{10}, \theta_i \in \mathbb{R}$ such that for every $\varepsilon > 0$:

$$\max_{\underline{\mathbf{x}} \in K} \Big| \hat{y}_{(\underline{\mathbf{x}})} - y^*_{(\underline{\mathbf{x}})} \Big| \leq \varepsilon$$

Funahashi (1989) On the approximate realization of continuous mappings by neural networks. Neur Netw, 2:183–192
Hornik et al. (1989) Multilayer Feedforward Networks are Universal Approximators. Neur Netw, 2:359–366.

1.3.3 Performance Measures and Model Selection

Cost functions

$$\underbrace{\underline{\mathbf{x}} \in \mathbb{R}^N}_{\text{feature vector}} \longrightarrow \underbrace{y \in \mathbb{R}}_{\text{attribute}}$$

y_T: true value of attribute
$y(\underline{\mathbf{x}})$: predicted value of attribute (e.g. by MLP)

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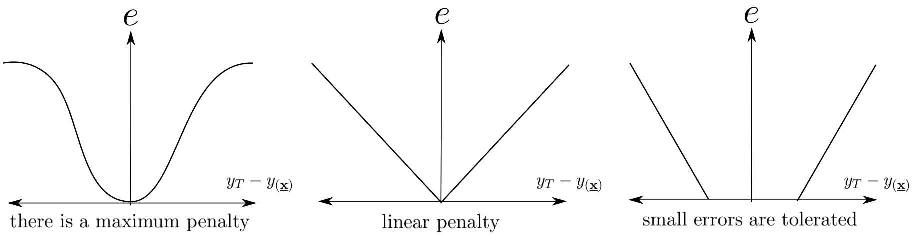
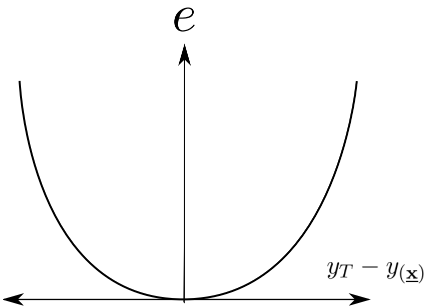
individual cost $e(y_T, \underline{\mathbf{x}})$



several choices ⇒ predictor will depend on error measure!

Lecture example: quadratic error



$$e(y_T, \underline{\mathbf{x}}) \quad = \quad \frac{1}{2}\Big(y(\underline{\mathbf{x}}) - y_T\Big)^2$$

- Gaussian noise on attributes
- sensitive against “outliers”

Performance measure

Generalization error

$$E^G \quad := \quad < e >_{y_T, \underline{\mathbf{x}}} \quad = \quad \iint d\underline{\mathbf{x}}\, dy_T \; P_{(y_T, \underline{\mathbf{x}})} \, e_{(y_T, \underline{\mathbf{x}})}$$

$P_{(y_T, \underline{\mathbf{x}})}$: joint Probability Density Function (PDF) of observations

Performance measure

Generalization error

$$E^G \quad := \quad < e >_{y_T, \underline{\mathbf{x}}} \quad = \quad \iint d\underline{\mathbf{x}}\, dy_T\; P_{(y_T, \underline{\mathbf{x}})}\, e_{(y_T, \underline{\mathbf{x}})}$$

$P_{(y_T, \underline{\mathbf{x}})}$: joint Probability Density Function (PDF) of observations

"good" predictor: low value of E^G
"bad" predictor: high value of E^G

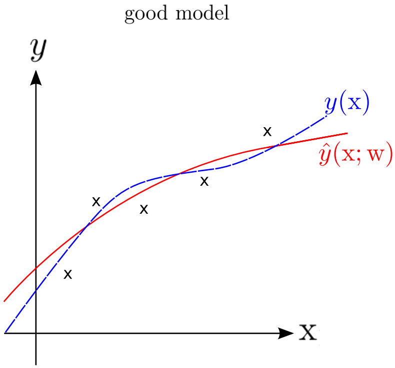
$$E^G \overset{!}{=} \min$$

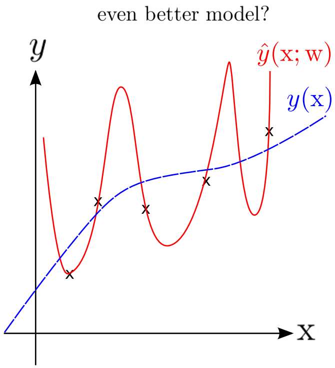
but: $P(y_T|\underline{\mathbf{x}})$ **is not known**

Principle of Empirical Risk Minimization (ERM)

math. expectation (E^G)	$\rightarrow$	empirical average (E^T)
$E^G := \int d\underline{\mathbf{x}} dy_T \ P(y_T, \underline{\mathbf{x}}) e(y_T, \underline{\mathbf{x}})$	$\rightarrow$	$E^T := \frac{1}{p} \sum_{\alpha=1}^{p} e^{(\alpha)}$
generalization error	$\rightarrow$	training error
$E^G \overset{!}{=} \min$	$\rightarrow$	$E^T \overset{!}{=} \min$

Consequences?

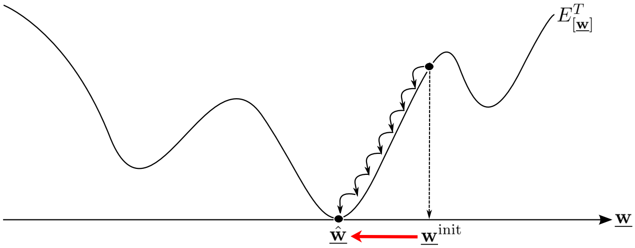




1.3.4 Optimization of Model Parameters: Gradient Descent

Gradient descent

training error E^T for the given training set: $E^T_{[\underline{\mathbf{w}}]} = \frac{1}{p} \sum\limits_{\alpha=1}^{p} e^{(\alpha)}_{[\underline{\mathbf{w}}]}$



$$w_{ij}^{v'v}(t+1) \quad = \quad w_{ij}^{v'v}(t) \quad - \quad \underbrace{\hat{\eta}}_{\text{learning step}} \quad \underbrace{\frac{\partial E^T_{[\underline{\mathbf{w}}]}}{\partial \mathrm{w}_{ij}^{v'v}}}_{\text{gradient vector}}$$

Calculation of the gradient

$$\frac{\partial E^T_{[\underline{\mathbf{w}}]}}{\partial \mathrm{w}^{v'v}_{ij}} = \frac{1}{p}\sum_{\alpha=1}^{p} \underbrace{\frac{\partial e^{(\alpha)}_{[\underline{\mathbf{w}}]}}{\partial \mathrm{w}^{v'v}_{ij}}}_{\substack{\text{individual} \\ \text{cost}}} = \frac{1}{p}\sum_{\alpha=1}^{p} \underbrace{\frac{\partial e^{(\alpha)}_{[\underline{\mathbf{w}}]}}{\partial y(\underline{\mathbf{x}}^{(\alpha)}, \underline{\mathbf{w}})}}_{\substack{\text{factor depending} \\ \text{on cost function}}} \cdot \underbrace{\frac{\partial y(\underline{\mathbf{x}}^{(\alpha)}, \underline{\mathbf{w}})}{\partial \mathrm{w}^{v'v}_{ij}}}_{\substack{\text{factor depending on} \\ \text{model class (e.g. MLP)}}}$$

Calculation of the error term

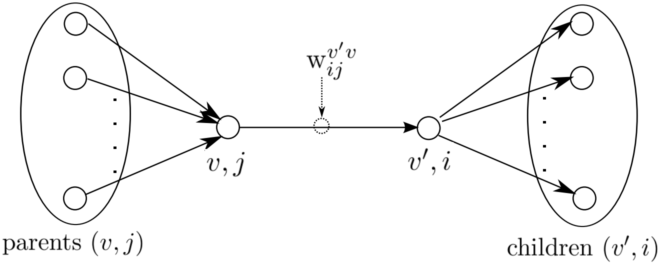
Quadratic Error

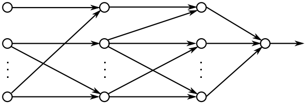
$$e(y_T, \underline{\mathbf{x}}) = \frac{1}{2}\big(y_T - y(\underline{\mathbf{x}})\big)^2 \qquad \Rightarrow \qquad \frac{\partial e^{(\alpha)}_{[\underline{\mathbf{w}}]}}{\partial y_{(\underline{\mathbf{x}}^{(\alpha)}, \underline{\mathbf{w}})}} = y_{(\underline{\mathbf{x}}^{(\alpha)}, \underline{\mathbf{w}})} - y_T$$

1.3.5 The Backpropagation Method

Gradients in neural networks

$$\frac{\partial y(\underline{\mathbf{x}}^{(\alpha)}, \underline{\mathbf{w}})}{\partial \mathrm{w}_{ij}^{v'v}}$$





see blackboard for derivation

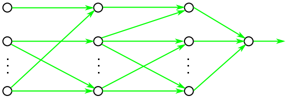
Summary of the backpropagation method

initialization of weights and thresholds
while *stopping criterion not met* **do**

$\text{gradient}_{ij}^{v'v} := 0\,, \quad \forall w_{ij}^{v'v}$

for $\alpha \in \{1, \ldots, p\}$ **do**

$h_i^0 := x_i^\alpha\,, \quad \forall i$ // forward propagation

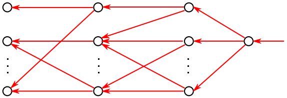


for $v' \in \{1, \ldots, L\}$ **do**

$$h_i^{v'} := \sum_{(v',i)\in C(v,j)} w_{ij}^{v'v} f_j^v(h_j^v)\,, \quad \forall i$$

end

$\delta_i^L := f'(h_i^L)\,, \quad \forall i$ // backward propagation



for $v' \in \{L-1, \ldots, 1\}$ **do**

$$\delta_i^{v'} := {f'}_i^{v'}(h_i^{v'}) \sum_{(\beta,k)\in C(v',i)} \delta_k^\beta\, w_{ki}^{\beta v'}\,, \quad \forall i$$

end

$\text{gradient}_{ij}^{v'v} := \text{gradient}_{ij}^{v'v} + \frac{\partial e^{(\alpha)}}{\partial y}\, \delta_i^{v'}\, f_j^v(h_j^v)\,, \quad \forall w_{ij}^{v'v}$ // average

end

$w_{ij}^{v'v} := w_{ij}^{v'v} - \frac{\hat{\eta}}{p}\,\text{gradient}_{ij}^{v'v}\,, \quad \forall w_{ij}^{v'v}$ // gradient descend step

end

Summary of the backpropagation method

initialization of weights and thresholds
while *stopping criterion not met* **do**

  gradient$_{ij}^{v'v} := 0\,, \quad \forall w_{ij}^{v'v}$
  for $\alpha \in \{1, \dots, p\}$ **do**
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    for $v' \in \{1, \dots, L\}$ **do**
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  end
  $w_{ij}^{v'v} := w_{ij}^{v'v} - \frac{\hat{\eta}}{p}$ gradient$_{ij}^{v'v}\,, \quad \forall w_{ij}^{v'v}$ // gradient descend step
end

computational and memory complexity

$\mathcal{O}(n)$,

n: number of weights

Initialization and stopping criteria

Initialization: random numbers, such that h_i^v approx. $\mathcal{O}(1)$

$\rightarrow$ too **large**?

$\rightarrow$ too **small**?

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$\rightarrow$ too **large**: transfer function saturates and gradients become too small

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Initialization and stopping criteria

Initialization: random numbers, such that h_i^v approx. $\mathcal{O}(1)$

$\rightarrow$ too **large**: transfer function saturates and gradients become too small

$\rightarrow$ too **small**: neurons operate in the linear regime of f

Stopping criteria:

$\rightsquigarrow$ fixed number of iterations

$\rightsquigarrow$ fixed CPU-time

$\rightsquigarrow$ E^T falls below a predefined value

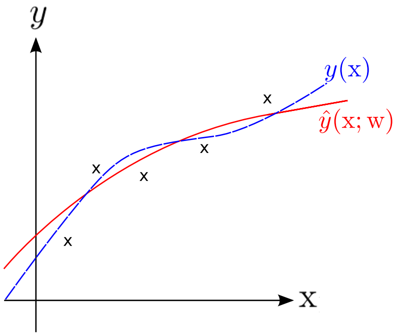
$\rightsquigarrow$ $\frac{\Delta E^T}{E^T}$ falls below a predefined value

$\rightsquigarrow$ validation criterion fulfilled

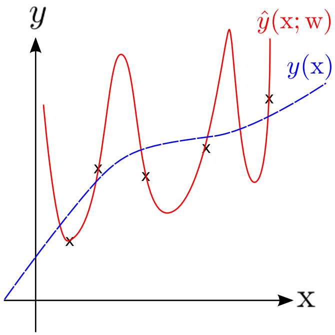
1.3.6 Validation of Model Selection

Overfitting

good model



even better model?



Assessment of prediction quality

Test set method

observations $\begin{cases} \text{training data } \left\{\left(\underline{\mathbf{x}}^{(\alpha)}, y_T^{(\alpha)}\right)\right\}, \alpha \in \{1, \ldots, p\} \\ \rightarrow E^T \text{ selects model parameters} \\ \\ \end{cases}$

$$\hat{E}^T \quad = \quad \frac{1}{p} \sum_{\alpha=1}^{q} e^{(\alpha)}$$

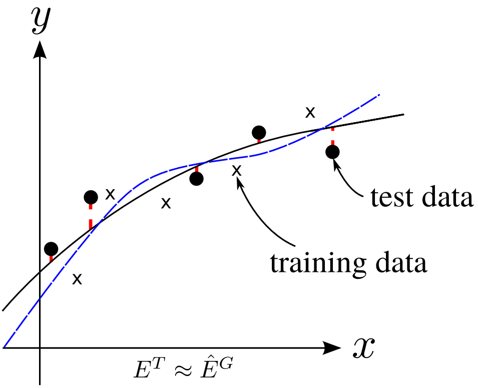
Assessment of prediction quality

Test set method

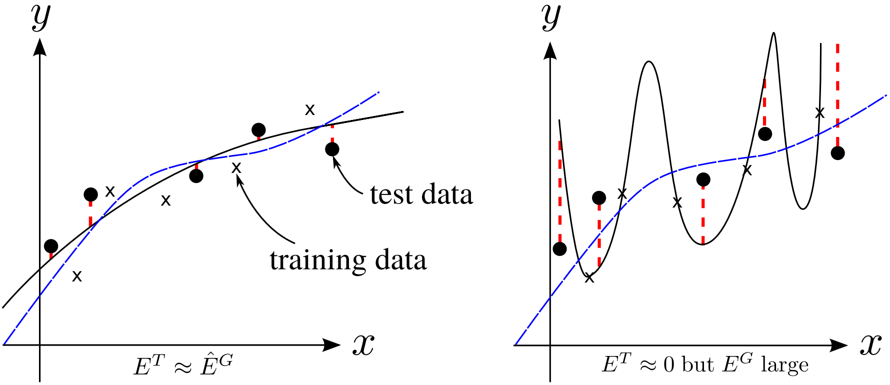
$$\text{observations} \begin{cases} \text{training data } \left\{\left(\underline{\mathbf{x}}^{(\alpha)}, y_T^{(\alpha)}\right)\right\}, \alpha \in \{1, \ldots, p\} \\ \rightarrow E^T \text{ selects model parameters} \\ \text{test data } \left\{\left(\underline{\mathbf{x}}^{(\beta)}, y_T^{(\beta)}\right)\right\}, \beta \in \{1, \ldots, q\} \\ \rightarrow \hat{E}^G \text{ estimates generalization error} \end{cases}$$

$$\hat{E}^G \quad = \quad \frac{1}{q} \sum_{\beta=1}^{q} e^{(\beta)}$$

Test set method

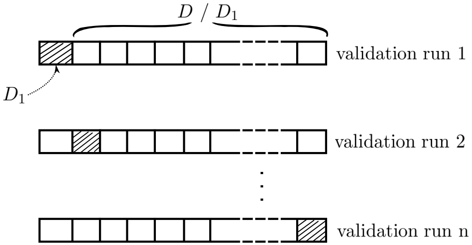


Test set method



Resampling methods: n-fold cross-validation

Observations $D \to n$ disjunct sets D_j, $\bigcup_{j=1}^{n} D_j = D$



Training of n networks on the training datasets D / D_j
Estimation of E^G:

$$\widehat{E}^G = \frac{1}{p} \sum_j \sum_{\alpha \in D_j} e^{(\alpha)}$$

Typical choice: $n \in \{5, \ldots, 10\}$ $n = p$: leave-one-out cross-validation

Variance of the cross-validation estimator

Remarks

- n-fold cross-validation is only used for estimating E^G
- each of the n folds results in a different solution (set of parameters)
- All data are used for selecting the model parameters

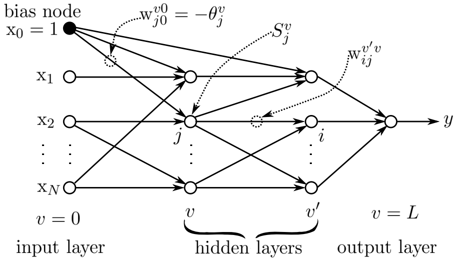
$$\mathrm{var}\left(\widehat{E}^G\right) = \frac{n-1}{n} \sum_{j=1}^{n} \Big(\underbrace{\widehat{E}_j^G}_{\substack{\text{test error} \\ \text{on } D_j}} - \widehat{E}^G \Big)^2$$

End of Section 1.3

the following slides contain

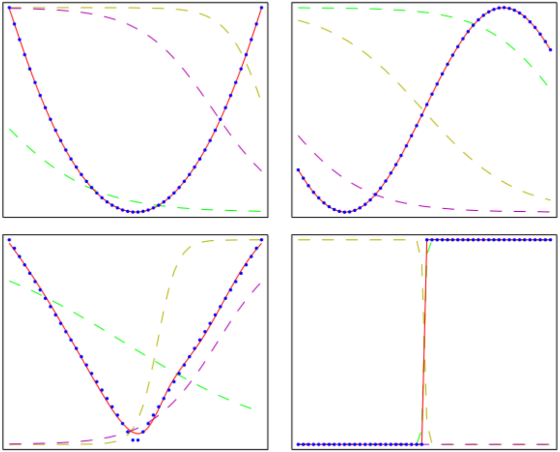
OPTIONAL MATERIAL

Multi-layer perceptrons: nomenclature



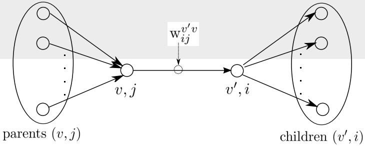
S_j^v	activity of neuron (v, j)	(layer,unit)
$S_0^v = x_0 = 1$	activity of bias neuron	
$S_i^0 = x_i$	input to MLP, i^{th} component	
$S_i^L = y$	output of MLP	
$w_{ij}^{v'v}$	connection weight between neurons (v, j) and (v', i)	
$w_{j0}^{v0} = \theta_j^v$	connection weight between bias node and neuron (v, j)	
$h_i^{v'}$	$= \sum_j w_{ij}^{vv-1} S_j^{v-1} \quad = \quad$ total input of neuron (v', i)	
$f_i^{v'}$	transfer function of neuron (v', i)	

Illustration: ERM with MLPs (Bishop 2009)



fitted MLPs with 1 hidden layer of 3 neurons

The Credit Assignment Problem



How do the weights $w_{ij}^{v'v}$ of hidden units $S_i^{v'}$ contribute to the error?

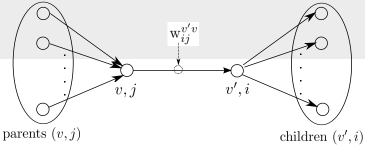
Solution: smart application of the chain rule

$$\frac{\partial y}{\partial \mathrm{w}_{ij}^{v'v}} = \underbrace{\frac{\partial y}{\partial h_i^{v'}}}_{\substack{:=\delta_i^{v'} \\ \text{"local error"} \\ \text{at neuron} \\ (v',i)}} \cdot \underbrace{\frac{\partial h_i^{v'}}{\partial \mathrm{w}_{ij}^{v'v}}}_{\substack{=S_j^v \\ \text{activity} \\ \text{of neuron} \\ (v,j)}}$$

Forward propagation: calculation of activities (parents $\rightarrow$ children)

$$S_j^0 = \mathrm{x}_j^{(\alpha)} \quad \rightarrow \quad S_i^{v'} = f\Big(\sum_{(v',i) \in C(v,j)} \mathrm{w}_{ij}^{v'v} S_j^v \Big)$$

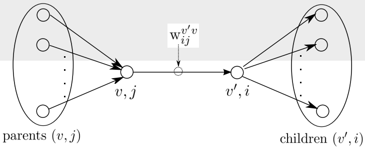
Backpropagation



Backpropagation: calculation of "local errors" (children $\rightarrow$ parents)

$$\delta_i^L = \underbrace{f'(h_i^{v'})}_{=1 \text{ for identity}} \quad \text{and} \quad \delta_i^{v'} = \sum_{(v'',k) \in C(v',i)} \frac{\partial y}{\partial h_k^{v''}} \cdot \frac{\partial h_k^{v''}}{\partial h_i^{v'}}, \quad \forall v' \neq L$$

Backpropagation



Backpropagation: calculation of "local errors" (children → parents)

$$\delta_i^L = \underbrace{f'(h_i^{v'})}_{=1 \text{ for identity}} \quad \text{and} \quad \delta_i^{v'} = \sum_{(v'',k) \in C(v',i)} \frac{\partial y}{\partial h_k^{v''}} \cdot \frac{\partial h_k^{v''}}{\partial h_i^{v'}}, \quad \forall v' \neq L$$

rewrite using $\frac{\partial y}{\partial h_k^{v''}} = \delta_k^{v''}$

$$\delta_i^{v'} = \sum_{(v'',k) \in C(v',i)} \delta_k^{v''} \cdot w_{ki}^{v''v'} f'(h_i^{v'}) = f'(h_i^{v'}) \sum_{(v'',k) \in C(v',i)} \delta_k^{v''} w_{ki}^{v''v'}$$

Computational complexity: $O(n)$, n: number of weights & thresholds