ELEC2870 - Machine learning: regression and dimensionality reduction

Nonlinear regression with Multi-Layer Perceptrons

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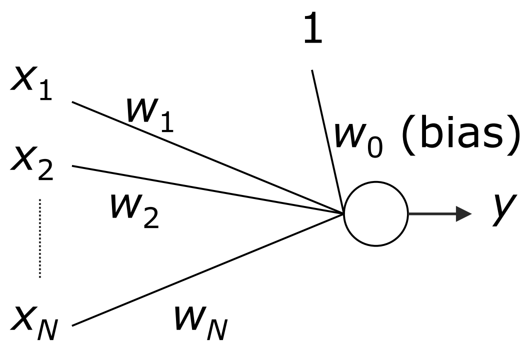
Outline

- Motivation
- Single-layer nonlinear regression
- Multi-layer perceptron
  - Model
  - MLP with threshold units
  - Number of layers
  - Learning
    - Error back-propagation
    - Weight adjustment
- Applications

Nonlinear regression: motivation

- Remember the linear model

$$y = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$



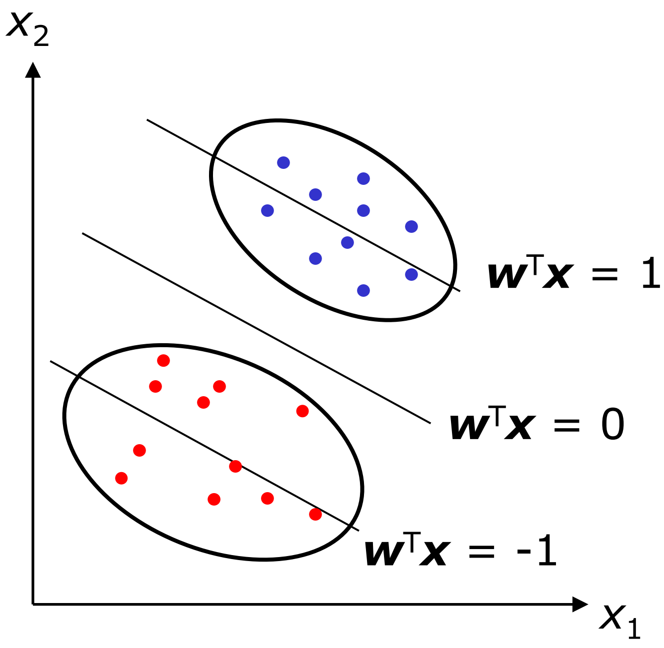
- and the sum-of-squares criterion

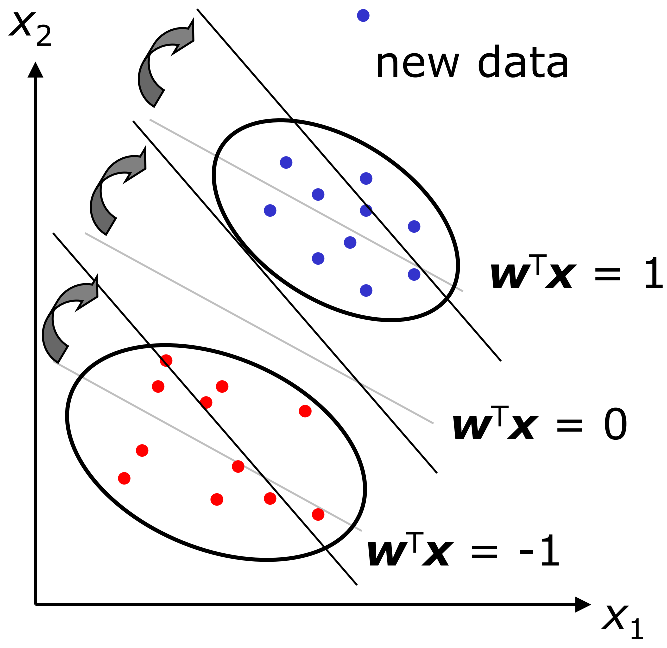
$$E = \frac{1}{P}\sum_{p=1}^{P}\left(t^p - y^p\right)^2 = \frac{1}{P}\sum_{p=1}^{P}\left(t^p - \mathbf{w}^{\mathrm{T}}\mathbf{x}^p\right)^2$$

- The influence of a *large* single error on this criterion is *very large* (because the error is squared)

Nonlinear regression: motivation

- When the dataset is quite small, a single outlier may have a dramatic influence:

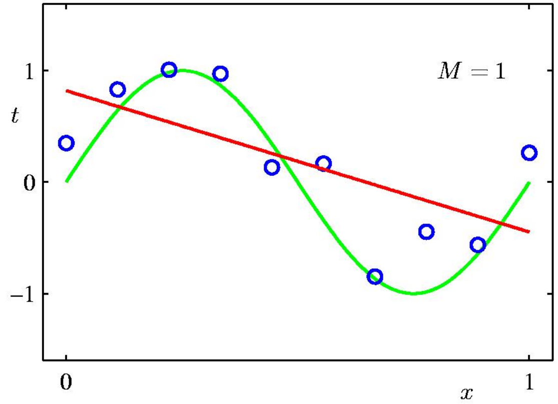




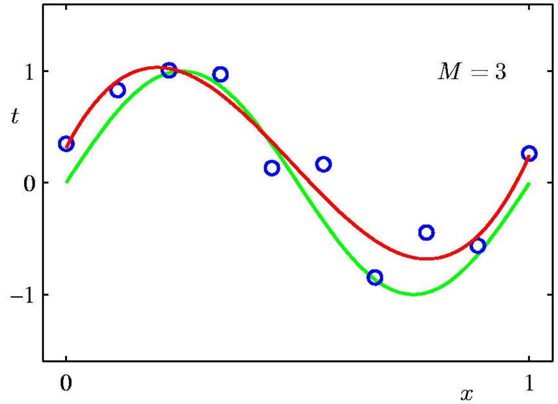
- This is true both in classification and regression!

Nonlinear regression: motivation

- Remember also that a linear model simply does not the expected job…
  - Linear model



  - Nonlinear model



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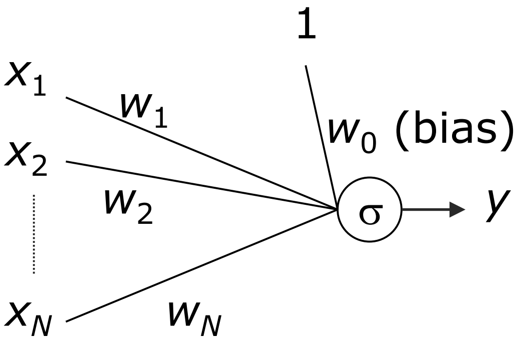
Single-layer nonlinear regression

- Model identical to linear regression, but with *nonlinear activation function*

$$y = \sigma\left(\mathbf{w}^{\mathsf{T}}\mathbf{x}\right)$$



- The error function becomes

$$E = \frac{1}{P}\sum_{k=1}^{P}\left(t^k - \sigma\left(\mathbf{w}^{\mathsf{T}}\mathbf{x}^k\right)\right)^2$$

- And the stochastic gradient descent rule

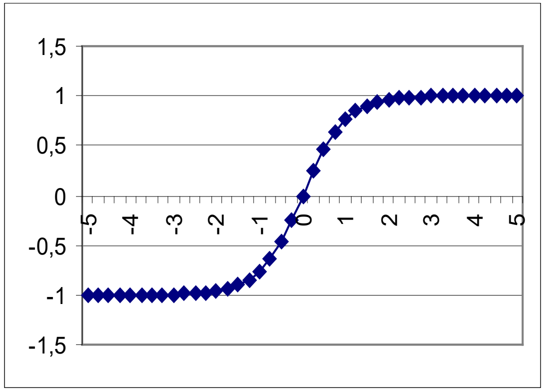
$$\boxed{\boldsymbol{w}(t+1) = \boldsymbol{w}(t) + \frac{2}{P}\alpha\left(t^k - \sigma\left(\boldsymbol{w}(t)^{\mathsf{T}}\boldsymbol{x}^k\right)\right)\boldsymbol{x}^k \left.\frac{\partial\sigma}{\partial p}\right|_{p=\boldsymbol{w}(t)^{\mathsf{T}}\boldsymbol{x}^k}}$$

(sometimes called the *generalized delta rule*)

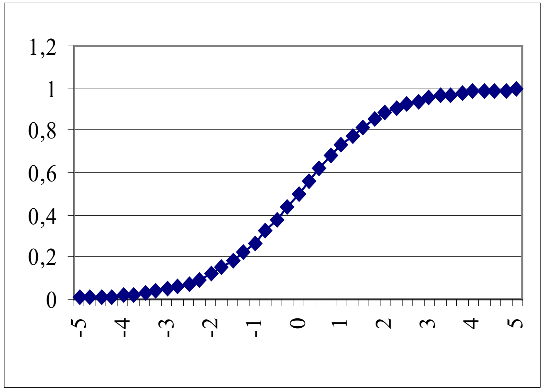
Nonlinear activation functions

- Commonly used non-linear activation function

hyperbolic tangent

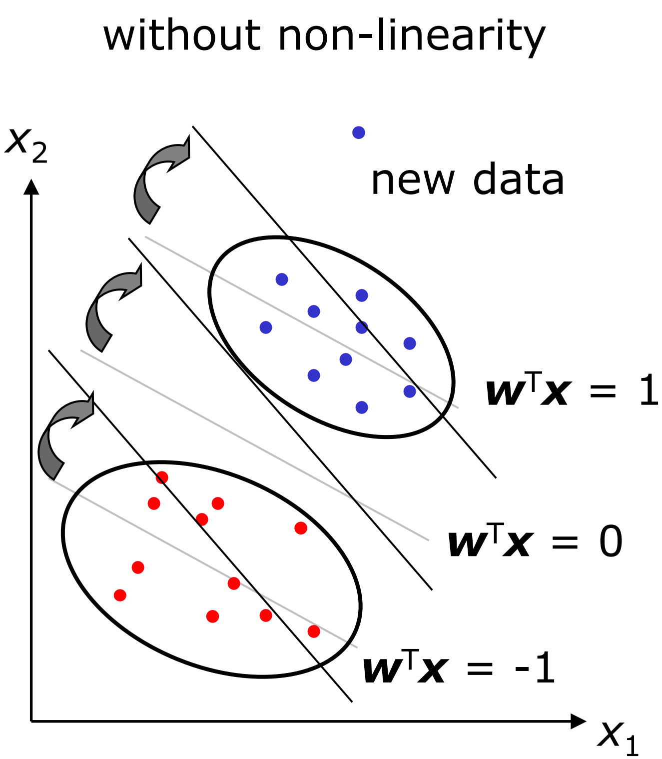


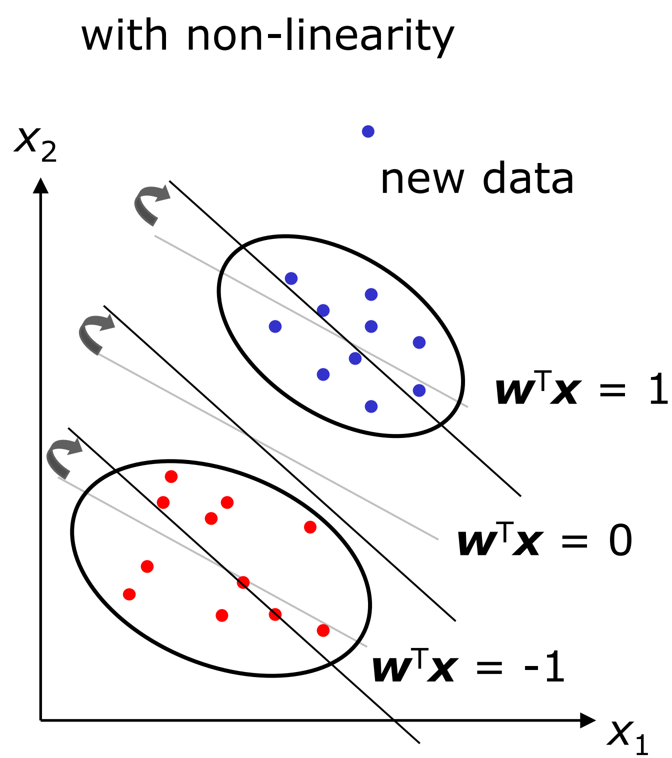
logistic function



- any slope
- slope can be a parameter
- logistic function: used to estimate posterior probabilities

Nonlinear effect on outliers





- Why? Because $\left|\sigma\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}^k\right)\right|$ never exceedes one, therefore $t^k - \sigma\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}^k\right)$ is almost 0 for well-classified points
- Not so simple in regression

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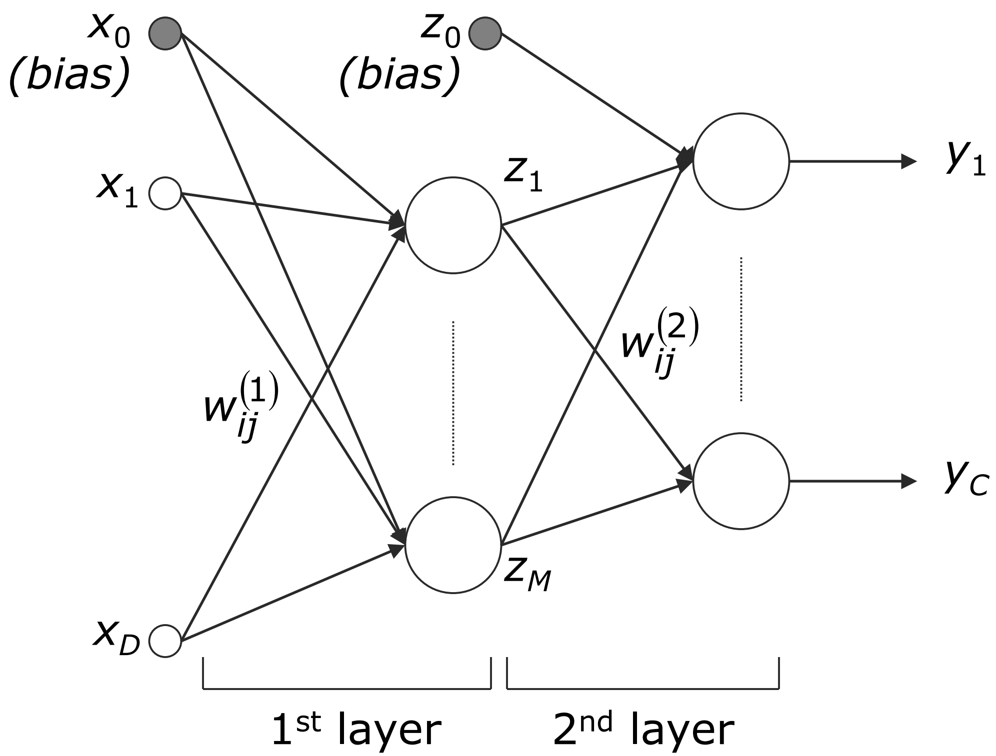
Multi-Layer Perceptron (MLP)

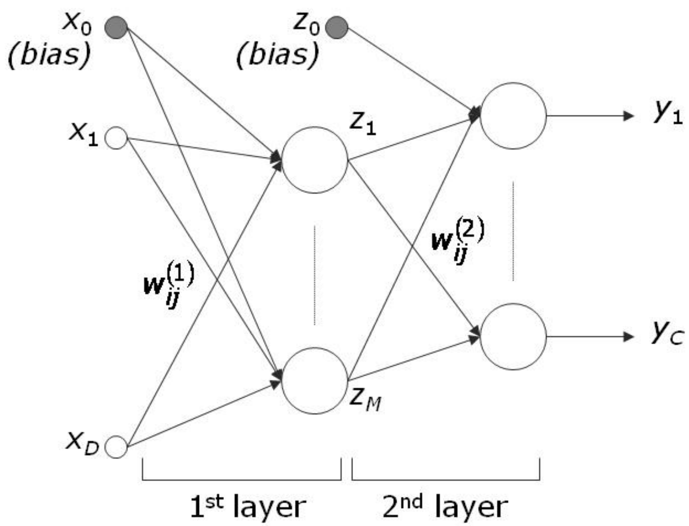
- several layers of weights and activation units



Multi-Layer Perceptron

$$y_k(\mathbf{x}) = h\left(\sum_{i=0}^{M} w_{ki}^{(2)} g\left(\sum_{j=0}^{D} w_{ij}^{(1)} x_j\right)\right)$$

$$\mathbf{y}(\mathbf{x}) = \mathbf{h}\left(\mathbf{w}^{(2)}\mathbf{g}\left(\mathbf{w}^{(1)}\mathbf{x}\right)\right)$$



- Convention: 2 layers of weights (in literature: sometimes 3 layers of *units* or *neurons*)
- *g* and *h* can be threshold (sign) units or continuous ones
- *h* can be linear but not *g* (otherwise only one layer)

Multi-Layer Perceptron

- How many layers
  - can we use ?
  - should we use ?

- In theory:
  - Any number of layers (see back-propagation algorithm)

- In practice:
  - More layers means more $w_{ij}^{(l)}$ parameters
  - Is it really needed?
  - How many layers do we need to approximate any function?

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MLP with threshold units

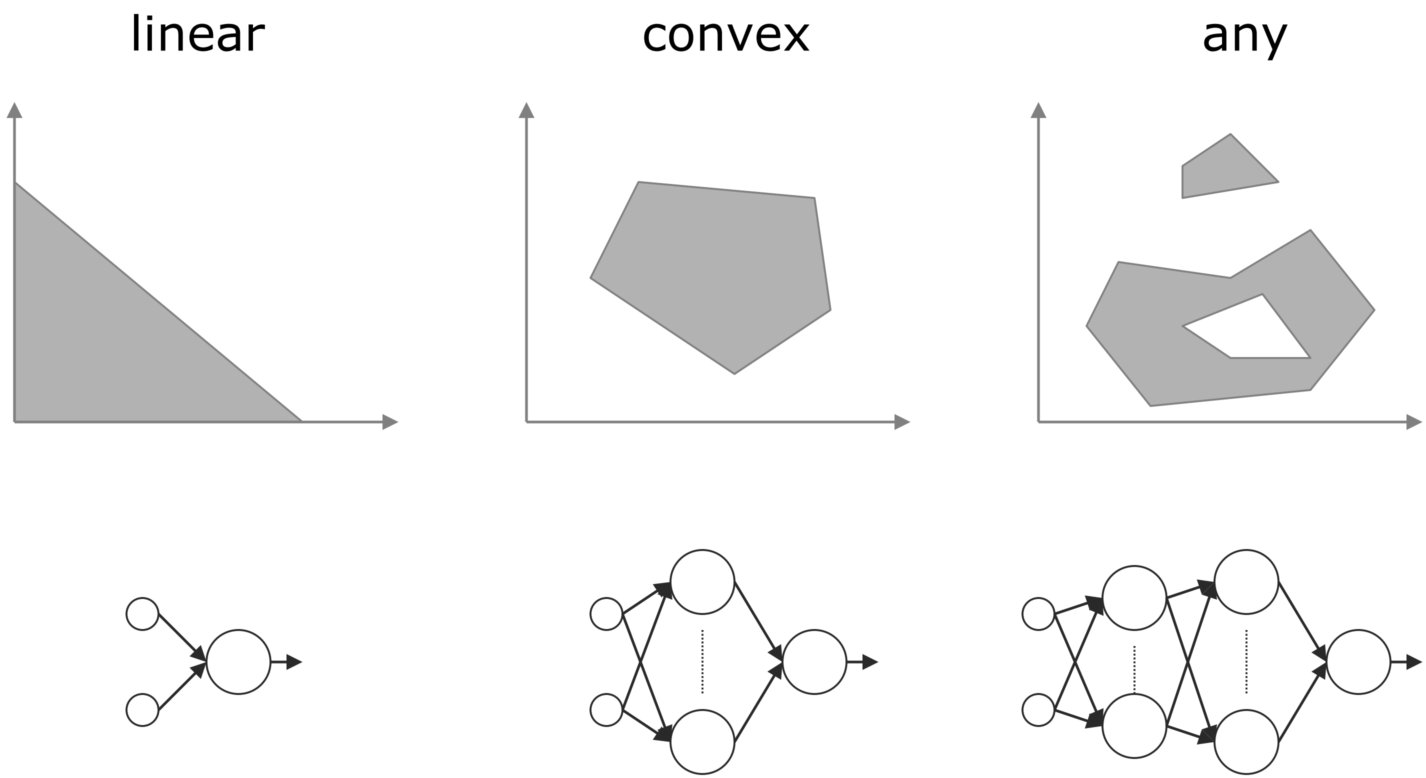
Warning: this is NOT the traditional MLP !

- We discusss the *MLP with thresold units* first to get an intuition about the number of layers
- But then we forget it immediately!
- *Why? Because threshold units means discontinuities, so no algorithm…*

- Outputs:
  - threshold units (all layers) → binary outputs
- Inputs:
  - binary inputs: Boolean function network
    - 2 layers (max.) for any function
    - look-up table without generalisation
  - continuous inputs (classification)
    - data become binary after 1^{st} layer
    - shape of decision boundaries depend on # layers

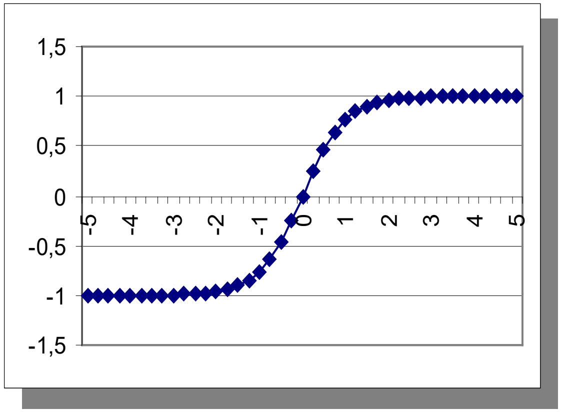
MLP with threshold units

Warning: this is NOT the traditional MLP !



Multi-Layer Perceptron

- General case (no more threshold units!)
- non-linear activation function: sigmoid or hyperbolic tangent
  - at least for “hidden” layers
  - output layer can be linear (otherwise limited output range)



- used for
  - approximation of functions
  - classification

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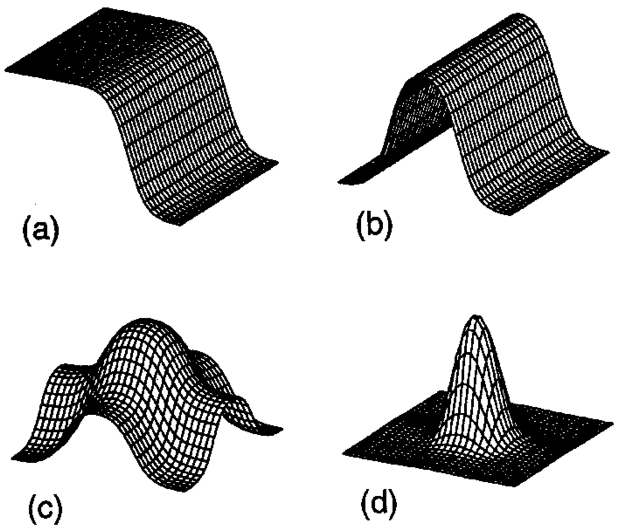
Number of layers

- A 3-layers network can approximate
  - any function
  - with any precision
- Indeed:
  - A 2-layers network can approximate a local function



2 layers:
(a) sigmoid
(b) sum of 2 sigmoids
(c) sum of 4 sigmoids
(d) sigmoid of sum
(bell-shaped local function)

  - A 3-layers network can thus approximate any sum of local functions

Number of layers

- That was intuition…
- Mathematically, it can be proven that

> A **2**-layer MLP can approximate arbitrarily well any (functional) continuous mapping, provided the number M of hidden units is sufficiently large

- This is called the *universal approximation property*
- It is theory: in practice, if M is too high, overfitting!
- It also valid for decision boundaries (classification)

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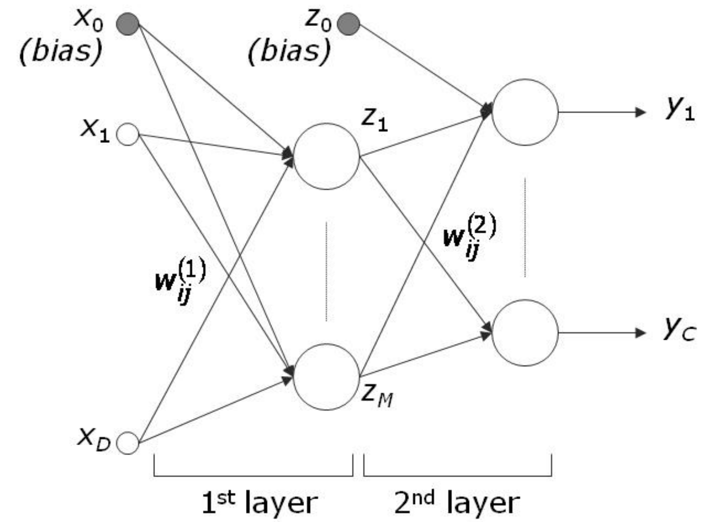
Learning in MLP

- Learning =
  - definition of an error criterion E
  - evaluation of derivatives of E w.r.t. parameters w
  - adjustments of parameters w according to derivatives



$$y_k(\mathbf{x}) = h\left(\sum_{i=0}^{M} w_{ki}^{(2)} g\left(\sum_{j=0}^{D} w_{ij}^{(1)} x_j\right)\right)$$

- Error criterion $$E = \frac{1}{P}\sum_{p=1}^{P} E^p(y_1,\ldots,y_C)$$

- Batch / stochastic learning
  - Batch learning (all samples together): E
  - on-line, stochastic (one sample at each iteration): E^p
- In the following, we omit p (stochastic learning)

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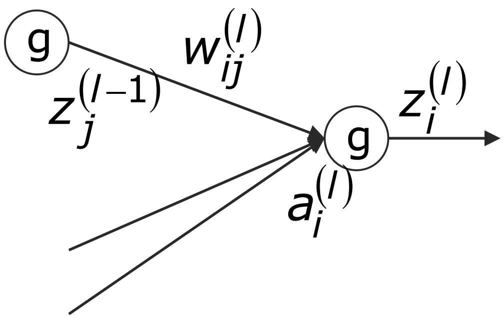
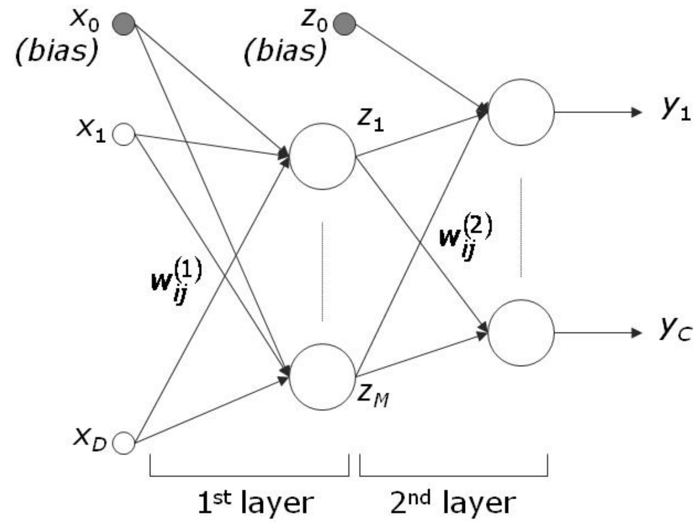
Error back-propagation

- Some notations

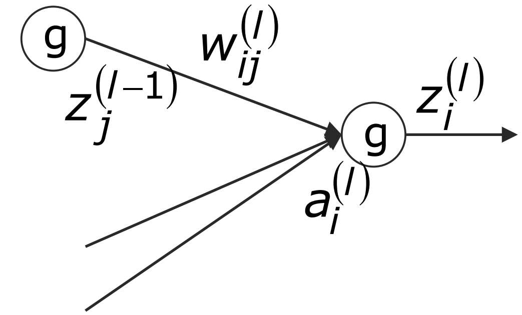


$$a_i^{(l)} = \sum_j w_{ij}^{(l)} z_j^{(l-1)}$$



Error back-propagation

$$a_i^{(l)} = \sum_j w_{ij}^{(l)} z_j^{(l-1)}$$



- Gradient descent: evaluation of $\dfrac{\partial E}{\partial w_{ij}^{(l)}}$

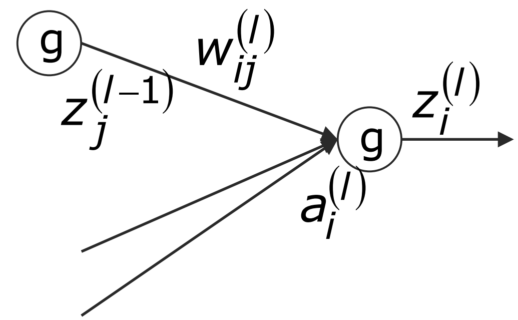
$$\frac{\partial E}{\partial w_{ij}^{(l)}} = \frac{\partial E}{\partial a_i^{(l)}} \frac{\partial a_i^{(l)}}{\partial w_{ij}^{(l)}}$$

$$= \delta_i^{(l)} z_j^{(l-1)} \longleftarrow$$

$\delta_i^{(l)} \equiv \dfrac{\partial E}{\partial a_i^{(l)}}$ to evaluate

Error back-propagation

$$\delta_i^{(l)} \equiv \frac{\partial E}{\partial a_i^{(l)}} \quad \text{to evaluate}$$



- For output units

$$\delta_i^{(l)} = \frac{\partial E}{\partial a_i^{(l)}} = \frac{\partial E}{\partial y_i^{(l)}} \frac{\partial y_i^{(l)}}{\partial a_i^{(l)}}$$

$$= \frac{\partial E}{\partial y_i^{(l)}} g'\left(a_i^{(l)}\right)$$

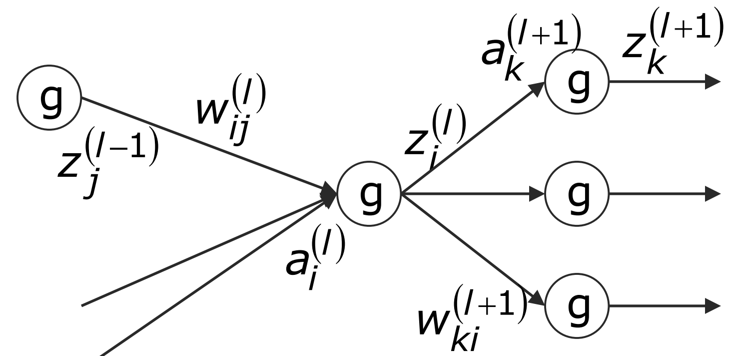
known

derivative of error criterion (known): $E = (t_i - y_i)^2$

$$\Rightarrow \frac{\partial E}{\partial y_i} = -2(t_i - y_i)$$

Error back-propagation

$$\delta_i^{(l)} \equiv \frac{\partial E}{\partial a_i^{(l)}} \quad \text{to evaluate}$$



- For hidden units

$$\delta_i^{(l)} = \frac{\partial E}{\partial a_i^{(l)}} = \sum_k \frac{\partial E}{\partial a_k^{(l+1)}} \frac{\partial a_k^{(l+1)}}{\partial a_i^{(l)}}$$

$$= \sum_k \left(\delta_k^{(l+1)} \frac{\partial \left(\sum_{j \in (l)} w_{kj}^{(l+1)} z_j^{(l)} \right)}{\partial a_i^{(l)}} \right)$$

$$= \sum_k \left(\delta_k^{(l+1)} w_{ki}^{(l+1)} g'\left(a_i^{(l)}\right) \right) = g'\left(a_i^{(l)}\right) \sum_k \left(\delta_k^{(l+1)} w_{ki}^{(l+1)} \right)$$

The error term (δ) is expressed as a combination of errors in the next layer

Error back-propagation

- Algorithm:
  - Apply an input vector $\boldsymbol{x}^k$ and propagate it through the network to evaluate all activations $z_i^{(l)}$ and neuron outputs $a_i^{(l)}$
  - Evaluate error terms $\delta_i^{(o)}$ in output layer
  - Back-propagate error terms $\delta_i^{(l)}$ to find error terms $\delta_i^{(l-1)}$
  - Evaluate all derivatives $\dfrac{\partial E}{\partial w_{ij}^{(l)}} = \delta_i^{(l)} z_j^{(l-1)}$
  - Adjust weights according to derivatives and a gradient descent scheme

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Weight adjustment

- Gradient descent is nice, but…
  - it can be very slow (when there are many parameters)
  - it is easily stuck in local minima
  - it is quite easy to do better…

- Now we have the derivatives $\dfrac{\partial E}{\partial w_{ij}^{(l)}}$, how to adjust weights?
- Notations:
  - weight update $\partial \mathbf{w} \equiv \mathbf{w}(t+1) - \mathbf{w}(t)$
  - gradient $\left(\dfrac{\partial E}{\partial \mathbf{w}}\right)^T \equiv \left(\dfrac{\partial E}{\partial w_1} \dfrac{\partial E}{\partial w_2} \cdots \dfrac{\partial E}{\partial w_D}\right)$
  - Hessian

$$H \equiv \left(\frac{\partial^2 E}{\partial \mathbf{w}^2}\right) \equiv \begin{pmatrix} \dfrac{\partial^2 E}{\partial {w_1}^2} & \dfrac{\partial^2 E}{\partial w_1 \partial w_2} & \cdots & \dfrac{\partial^2 E}{\partial w_1 \partial w_D} \\ \vdots & \vdots & & \vdots \\ \dfrac{\partial^2 E}{\partial w_D \partial w_1} & \dfrac{\partial^2 E}{\partial w_D \partial w_2} & \cdots & \dfrac{\partial^2 E}{\partial {w_D}^2} \end{pmatrix}$$

Indices are changed for simplicity of notations:

$$w_{ij}^{(l)},\ \forall i, j, l$$

$$\Downarrow$$

$$w_i, 1 \le i \le D$$

Weight adjustment

- First-order methods :

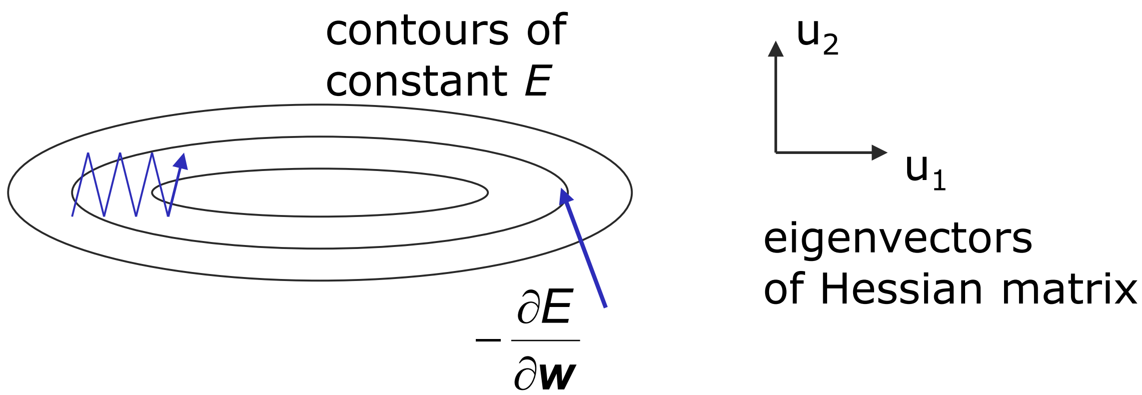
$$E(\mathbf{w}(t+1)) = E(\mathbf{w}(t)) + \left(\left.\frac{\partial E}{\partial \mathbf{w}}\right|_{\mathbf{w}(t)} \right)^T (\mathbf{w}(t+1) - \mathbf{w}(t))$$

$$= E(\mathbf{w}(t)) + \left(\left.\frac{\partial E}{\partial \mathbf{w}}\right|_{\mathbf{w}(t)} \right)^T \delta\mathbf{w}$$

  - For a $\delta\boldsymbol{w}$ of a given magnitude, largest $|\delta E|$ is found when gradient and weight update vectors are parallel
  - Adaptation rule: $\boxed{\mathbf{w}(t+1) = \mathbf{w}(t) - \alpha \left.\frac{\partial E}{\partial \mathbf{w}}\right|_{\mathbf{w}(t)}}$
  - This is gradient descent; nice, isn't it?

Weight adjustment

- First-order methods
  - Note that $-\dfrac{\partial E}{\partial \mathbf{w}}$ does not point towards the minimum of E !



Weight adjustment

- First-order methods: improvements
  - Momentum : to avoid sharp changes in gradient direction (stochastic scheme, outliers, etc.)

$$\mathbf{w}(t+1) = \mathbf{w}(t) - \alpha \left.\frac{\partial E}{\partial \mathbf{w}}\right|_{\mathbf{w}(t)} + \beta\left(\mathbf{w}(t) - \mathbf{w}(t-1)\right)$$

β =~0.9

Weight adjustment

- First-order methods: improvements
  - adaptive learning rate α

$$w_{ij}(t+1) = w_{ij}(t) - \alpha_{ij}(t) \left.\frac{\partial E}{\partial w_{ij}}\right|_{\mathbf{w}(t)}$$

$$\delta w_{ij}(t-1)\delta w_{ij}(t) > 0 \;\Rightarrow\; \alpha_{ij}(t+1) = \alpha_{ij}(t) + \kappa$$
$$\delta w_{ij}(t-1)\delta w_{ij}(t) < 0 \;\Rightarrow\; \alpha_{ij}(t+1) = \alpha_{ij}(t) - \kappa$$

    - Need for maximum safe step size
    - This is more or less the « delta-bar-delta » rule

Weight adjustment

- Second-order methods (Newton's method)

$$E(\mathbf{w}(t+1)) = E(\mathbf{w}(t)) + \left(\left. \frac{\partial E}{\partial \mathbf{w}} \right|_{\mathbf{w}(t)} \right)^T \delta\mathbf{w} + \frac{1}{2} \delta\mathbf{w}^T \left. \frac{\partial^2 E}{\partial \mathbf{w}^2} \right|_{\mathbf{w}(t)} \delta\mathbf{w}$$

- Stationary point (zero derivative) of this quadratic form:

$$\delta\mathbf{w} = -\left(\left. \frac{\partial^2 E}{\partial \mathbf{w}^2} \right|_{\mathbf{w}(t)} \right)^{-1} \left. \frac{\partial E}{\partial \mathbf{w}} \right|_{\mathbf{w}(t)}$$

- Adaptation rule:
  - minimum: move in this direction
  - maximum or saddle point: move in conjugate direction
  - Many "conjugate gradient" rules (some are line searches)

Weight adjustment

- Second-order methods (Newton's method)

$$\delta \mathbf{w} = -\left(\left. \frac{\partial^2 E}{\partial \mathbf{w}^2} \right|_{\mathbf{w}(t)} \right)^{-1} \left. \frac{\partial E}{\partial \mathbf{w}} \right|_{\mathbf{w}(t)}$$

- Hessian matrix difficult to compute → various approximations
  - Successive estimations
  - Diagonal terms only (quasi-Newton)
- Levenberg–Marquardt is another efficient algorithm

Weight adjustment

- What about the size of the step?

- Stochatic way: small α
  - but if too small: slow
  - and if too large: jumps over the minimum

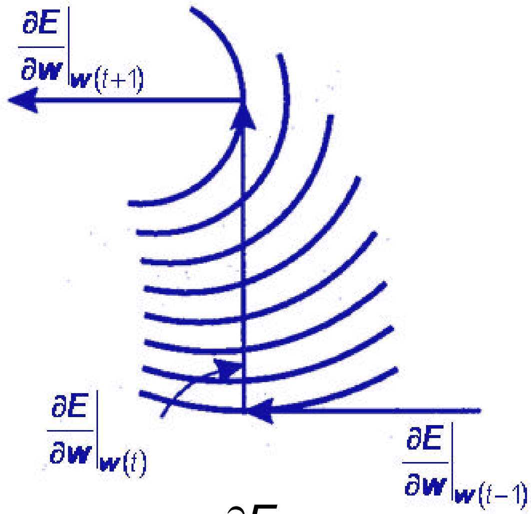
- Other solution: line search $\mathbf{w}(t+1) = \mathbf{w}(t) + \lambda(t)\mathbf{d}(t)$
  - go as far as possible in the chosen direction $\mathbf{d}(t)$
  - Implicit use of the Hessian matrix
  - If *d(t)* is the gradient at each time step: $\mathbf{d}(t) = \left.\frac{\partial E}{\partial \mathbf{w}}\right|_{\mathbf{w}(t)}$

$$\frac{\partial}{\partial \lambda} E(\mathbf{w}(t) + \lambda \mathbf{d}(t)) = 0 \quad \text{thus} \quad \left.\frac{\partial E}{\partial \mathbf{w}}\right|_{\mathbf{w}(t+1)} \mathbf{d}(t) = 0$$

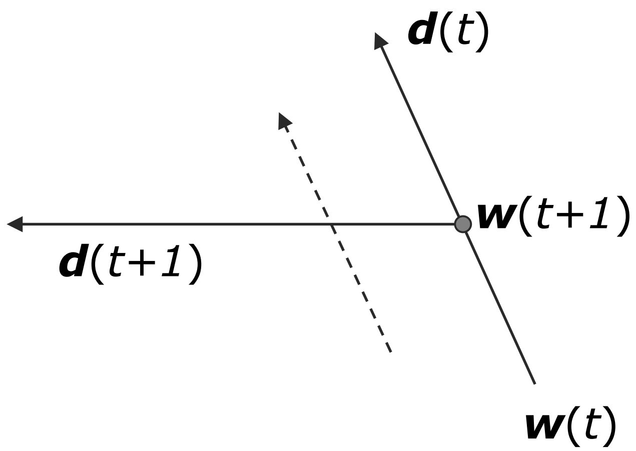
  - So successive directions are always orthogonal!

Weight adjustment

- Successive directions are orthogonal (line search)
  - Not good for speed of convergence



  - Use *conjugate* gradients:
    New direction is chosen so that the component of the gradient $\frac{\partial E}{\partial \mathbf{w}}$ parallel to the previous direction remains 0
    - Conjugate gradients make implicit use of the Hessian matrix



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Applications

- Some (old…) applications of MLP

- In fact some applications of nonlinear regression with machine learning! (not specific to MLP)

  1. A standard nonlinear model
  2. Several ways to use similar models for the same goal
  3. The interpolation-extrapolation question

Application: function approximation

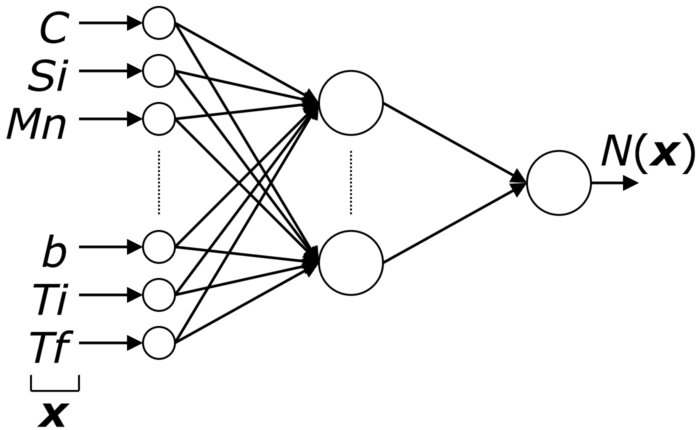
- Standard multivariate regression (function approximation)
- Application to process optimisation (estimation of physical properties, based on chemical composition and process parameters)

$$\alpha = f\left(C, Si, Mn, P, S, Al, N, Cu, Cr, Ni, Sn, V, Mo, Ti, Nb, B, d, b, Ti, Tf\right)$$

- "relative yield stress" α of different steel qualities
- inputs:
  - 16 chemical additives
  - plate's thickness d and width b
  - temperatures before (Ti) and after (Tf) rolling

From "Estimating material properties for process optimization", T. Poppe & T. Martinetz (Siemans AG), in ICANN'93 (Amsterdam, The Netherlands) proceedings, S. Gielen & B. Kappen eds., Sringer-Verlag, 1993

Application: function approximation



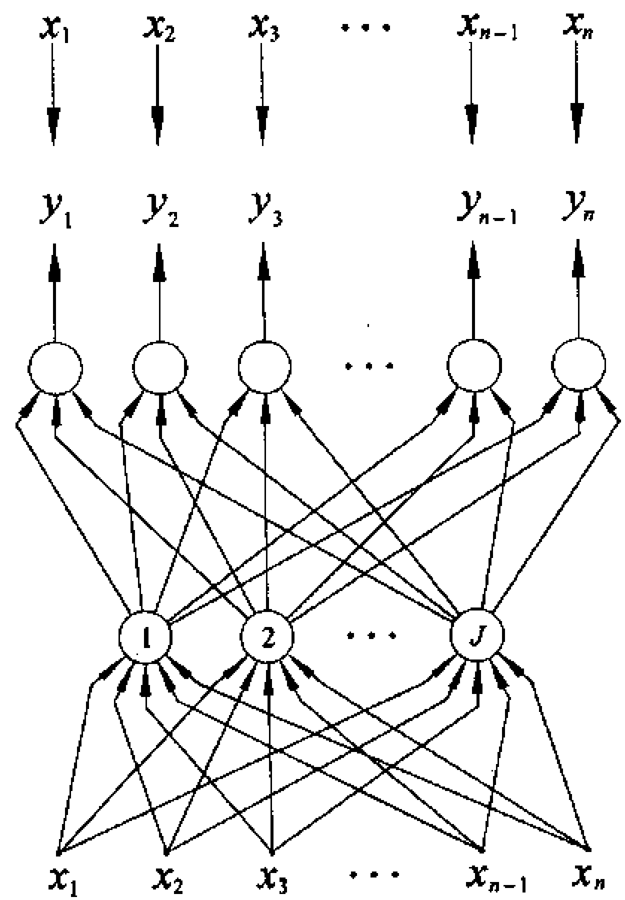
$$E = \sum_{p=1}^{P} E^p(\mathbf{x}) = \sum_{p=1}^{P} \left(\alpha^p - N\left(\mathbf{x}^p\right)\right)^2$$

- 1 hidden layer
- 10 hidden units
- training set: 9000 pairs
- test set: 3000 pairs
- on-line training

- Results:
  - Physical characterisation: RMS = 53.6 %
  - MLP learning: RMS = 34.9 %

Application: image compression 1

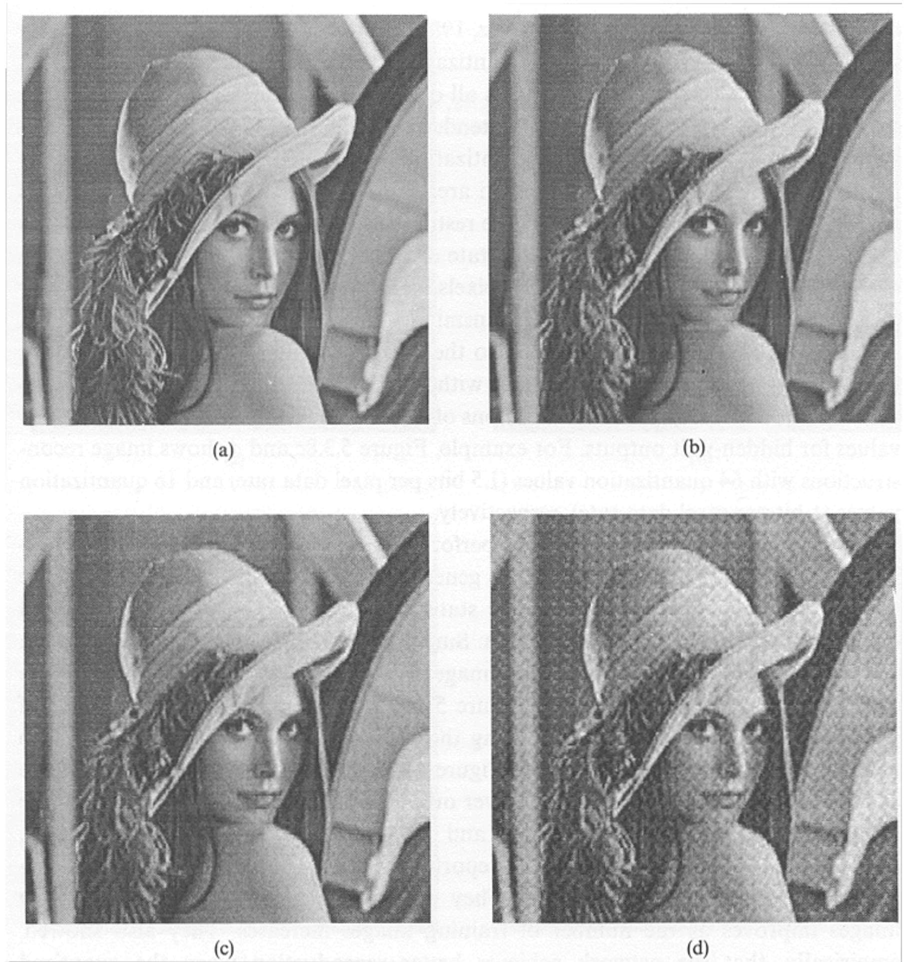
- lossy compression scheme (example)
- original image split into 8x8 pixel regions
- each 64-features vector sent in auto-associative MLP
- hidden layer: 16 neurons
- compression ration: 16/64



From: M. Hassoun, Fundamentals of artificial neural networks, MIT Press, 1995

Application: image compression 1

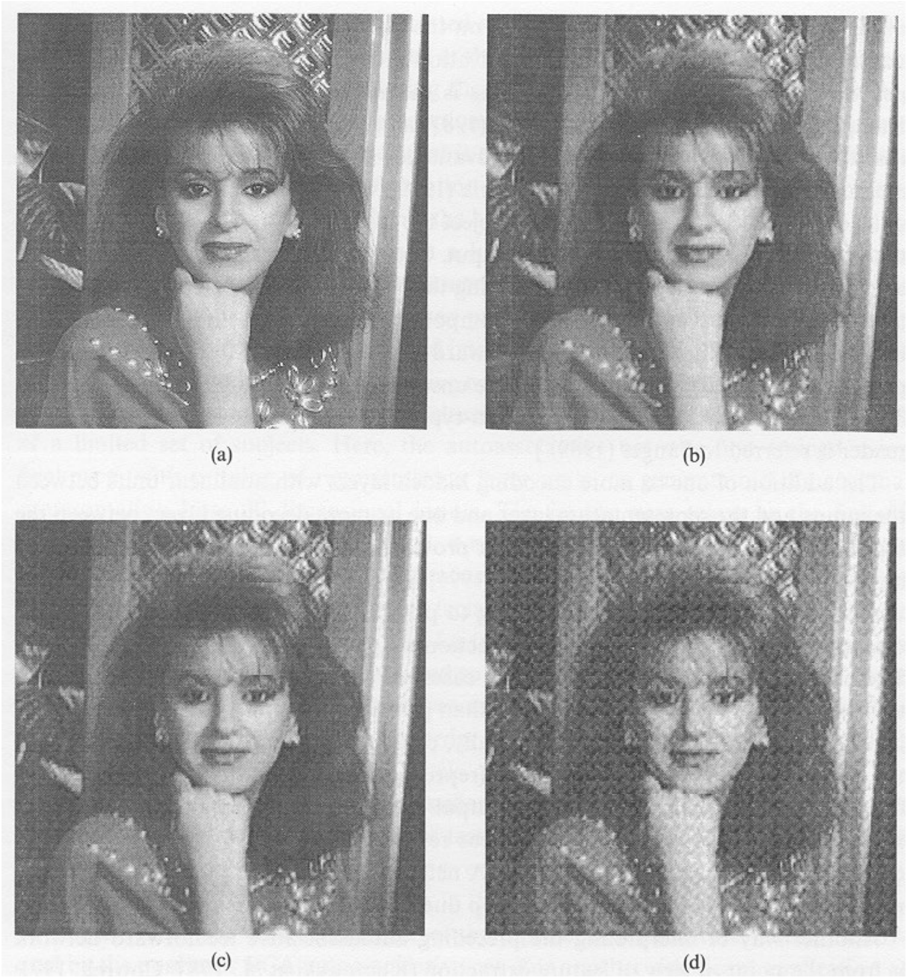
- result on training image
  - (a) original
  - (b) compressed
  - (c) compressed + quantized (1.5 bit/pixel)
  - (d) compressed + quantized (1 bit/pixel)



From: M. Hassoun, Fundamentals of artificial neural networks, MIT Press, 1995

Application: image compression 1

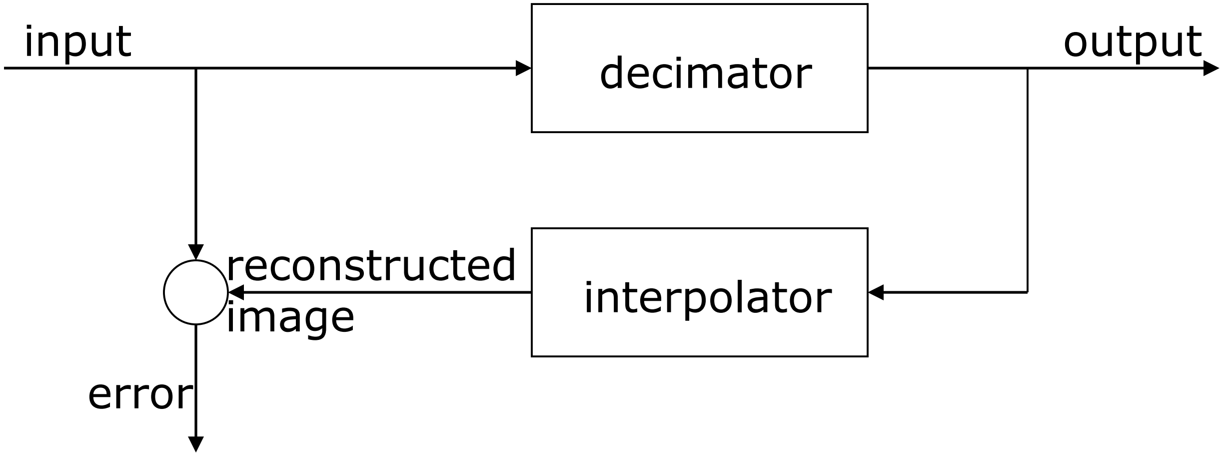
- result on testimage
  - (a) original
  - (b) compressed
  - (c) compressed + quantized (1.5 bit/pixel)
  - (d) compressed + quantized (1 bit/pixel)



From: M. Hassoun, Fundamentals of artificial neural networks, MIT Press, 1995

Application: image compression 2

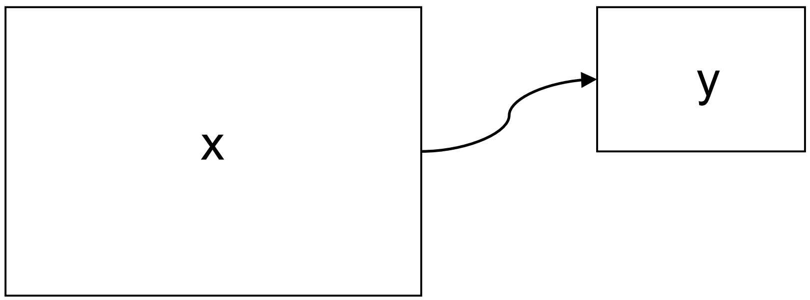
- lossless compression scheme (example)
- *Laplacian pyramids*



- If output and error are transmitted: lossless compression ! (interpolator function also needed of course)

Application: image compression 2

- Decimator: (half-band filter) + downsampler ← anti-aliasing



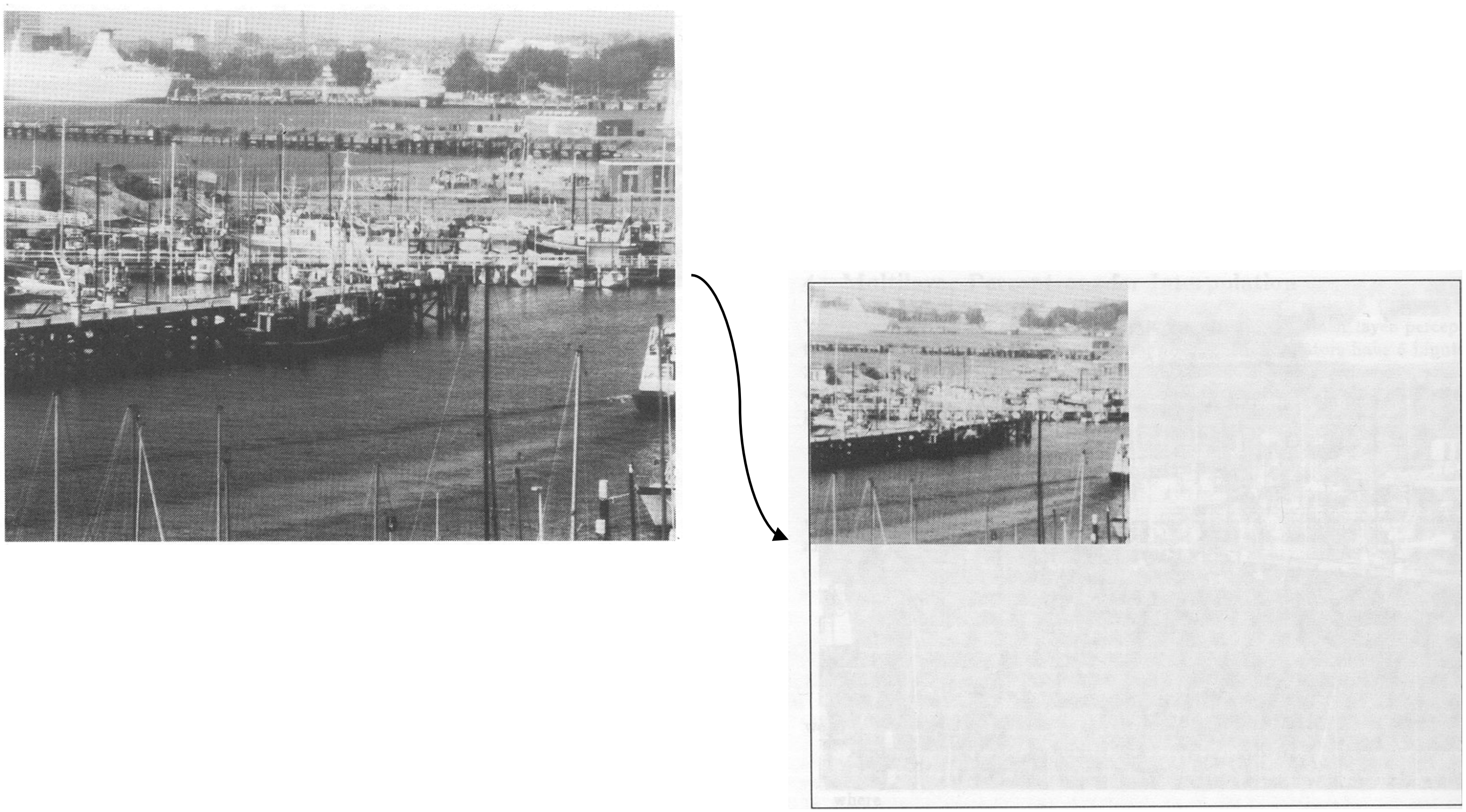
- Interpolator: upsampler + (half-band filter) ← smoothing

Application: image compression 2

- Traditional Laplace pyramids: decimator and interpolator are linear
- MLP: interpolator is non-linear
  - → better reconstruction
  - → smaller error
  - → better compression ratio for error with entropic coder

- entropic coder: better ratio if more zeroes

Application: image compression 2



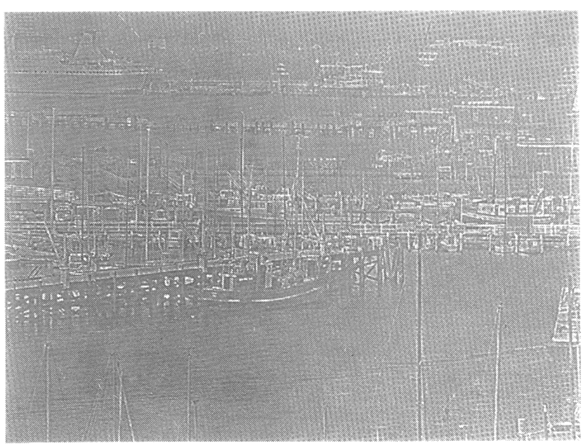
From “Laplacian pyramid with multilayer perceptrons interpolators”, B. Simon, B. Macq, M. Verleysen, in ESANN’93 (Bruges, Belgium) proceedings,D-Facto publications, 1993

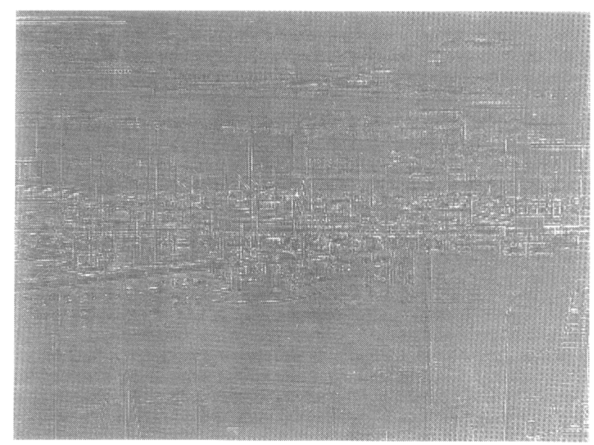
Application: image compression 2

linear

MLP

reconstructed images



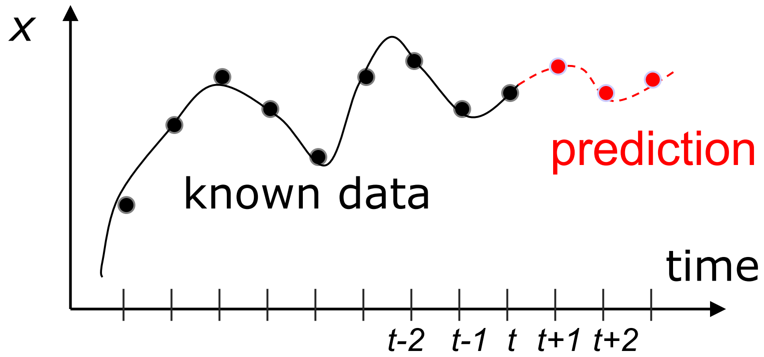


differences

From “Laplacian pyramid with multilayer perceptrons interpolators”, B. Simon, B. Macq, M. Verleysen, in ESANN’93 (Bruges, Belgium) proceedings,D-Facto publications, 1993

Application: time series forecasting

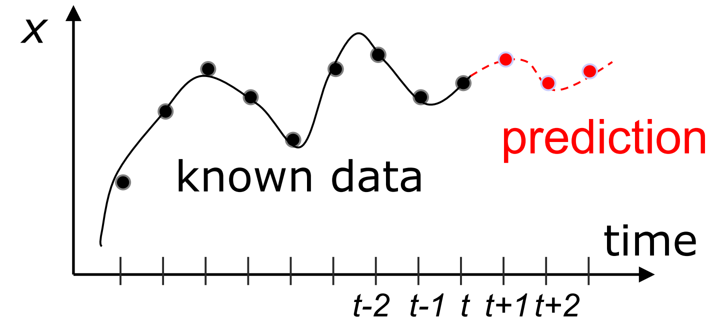
- Time series:



- Applications:
  - finance (stock market index, exchange rates, etc.)
  - electricity / gas consumption
  - etc.

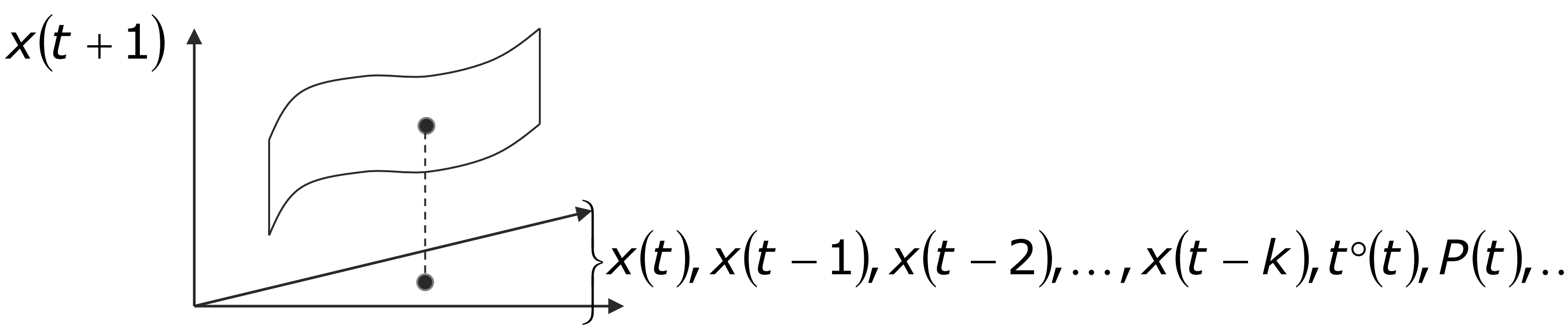
Application: time series forecasting

- Time series forecasting = function approximation



$$x(t+1) = f\big(\underbrace{x(t), x(t-1), x(t-2), \dots, x(t-k)}_{\text{past values}}, \underbrace{t^{\circ}(t), P(t), \dots}_{\text{inputs (exogenous variables)}}\big)$$

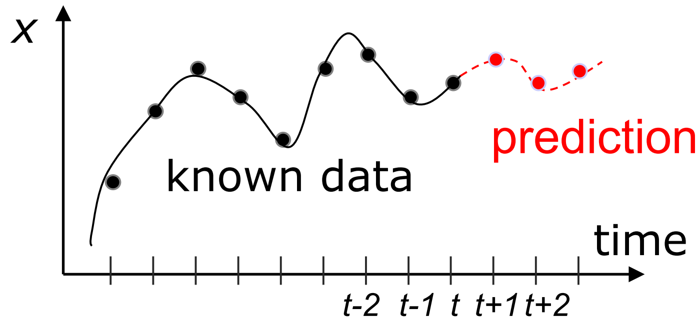
- New point in *inside* the surface



- So it is really interpolation, not extrapolation!

Application: time series forecasting

- Long-term forecasting



- To predict $x(t+2)$ we can use
  - the true value
  - the estimated value

  of $x(t+1)$