Neural Networks.

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Introduction and Rehearsal

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

Notation

In *supervised learning*, we work with

- an observation described by a vector $\boldsymbol{x} = (x_1, \ldots, x_D)$,
- the corresponding true value of the dependent variable y, and
- the prediction of a model $\widehat{y} = f_{\boldsymbol{w}}(\boldsymbol{x})$, where the model parameters are in vector $\boldsymbol{w}$.

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

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- the prediction of a model $\widehat{y} = f_{\boldsymbol{w}}(\boldsymbol{x})$, where the model parameters are in vector $\boldsymbol{w}$.
- Very often, we use *homogeneous coordinates* and matrix notation, and represent the whole training data set as $T = (\boldsymbol{X}, \boldsymbol{y})$, where

$$\boldsymbol{X} = \begin{pmatrix} 1 & \boldsymbol{x}^{(1)} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(|T|)} \end{pmatrix}, \qquad \text{and} \qquad \boldsymbol{y} = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(|T|)} \end{pmatrix}.$$

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

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Learning then amounts to finding such model parameters $\boldsymbol{w}^*$ which minimize certain loss (or energy) function:

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} J(\boldsymbol{w}, T)$$

Multiple linear regression

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

Multiple linear regression model:

$$\widehat{y} = f_w(\boldsymbol{x}) = w_1 x_1 + w_2 x_2 + \ldots + w_D x_D = \boldsymbol{x}\boldsymbol{w}^T$$

The minimum of

$$J_{MSE}(\boldsymbol{w}) = \frac{1}{|T|} \sum_{i=1}^{|T|} \left(y^{(i)} - \widehat{y}^{(i)} \right)^2,$$

is given by

$$\boldsymbol{w}^* = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y},$$

or found by numerical optimization.

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Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

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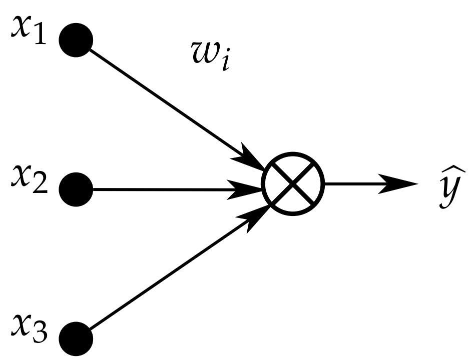
or found by numerical optimization.

Multiple regression as a **linear neuron**:



Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

Logistic regression

Logistic regression model:

$$\hat{y} = f(\boldsymbol{w}, \boldsymbol{x}) = g(\boldsymbol{x}\boldsymbol{w}^T),$$

where

$$g(z) = \frac{1}{1 + e^{-z}}$$

is the **sigmoid** (a.k.a **logistic**) function.

- No explicit equation for the optimal weights.
- The only option is to find the optimum numerically, usually by some form of gradient descent.

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

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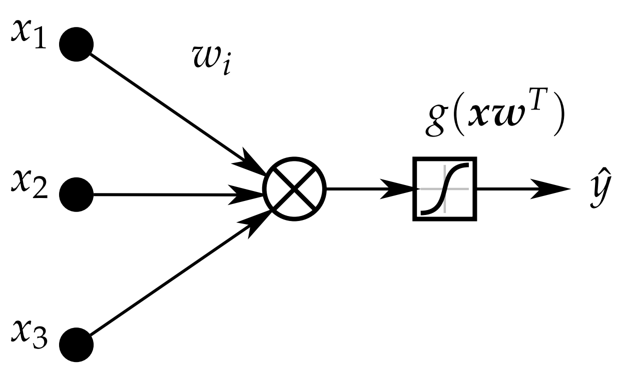
Logistic regression as a **non-linear neuron**:



Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

Gradient descent algorithm

- Given a function $J(\boldsymbol{w})$ that should be minimized,
- start with a guess of $\boldsymbol{w}$, and change it so that $J(\boldsymbol{w})$ decreases, i.e.
- update our current guess of $\boldsymbol{w}$ by taking a step in the direction opposite to the gradient:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \alpha \nabla J(\boldsymbol{w}), \text{ i.e.}$$

$$w_d \leftarrow w_d - \alpha \frac{\partial}{\partial w_d} J(\boldsymbol{w}),$$

where all w_ds are updated simultaneously and α is a **learning rate** (step size).

- For cost functions given as the sum across the training examples

$$J(\boldsymbol{w}) = \sum_{i=1}^{|T|} E(\boldsymbol{w}, \boldsymbol{x}^{(i)}, y^{(i)}),$$

we can concentrate on a single training example because

$$\frac{\partial}{\partial w_d} J(\boldsymbol{w}) = \sum_{i=1}^{|T|} \frac{\partial}{\partial w_d} E(\boldsymbol{w}, \boldsymbol{x}^{(i)}, y^{(i)}),$$

and we can drop the indices over training data set:

$$E = E(\boldsymbol{w}, \boldsymbol{x}, y).$$

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

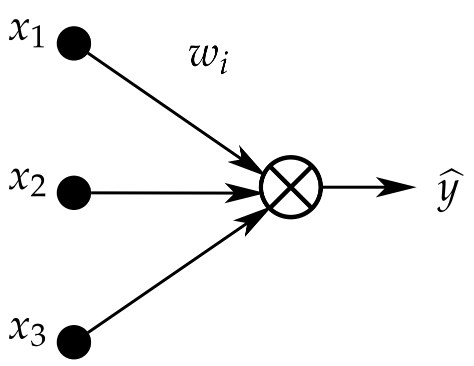
Gradient Descent

Regularization

RBF Networks

Summary

Example: Gradient for multiple regression and squared loss



Assuming the squared error loss

$$E(\boldsymbol{w}, \boldsymbol{x}, y) = \frac{1}{2}(y - \widehat{y})^2 = \frac{1}{2}(y - \boldsymbol{x}\boldsymbol{w}^T)^2,$$

we can compute the derivatives using the chain rule as

$$\begin{aligned}
\frac{\partial E}{\partial w_d} &= \frac{\partial E}{\partial \widehat{y}} \frac{\partial \widehat{y}}{\partial w_d}, \text{ where} \\
\frac{\partial E}{\partial \widehat{y}} &= \frac{\partial}{\partial \widehat{y}} \frac{1}{2}(y - \widehat{y})^2 = -(y - \widehat{y}), \text{ and} \\
\frac{\partial \widehat{y}}{\partial w_d} &= \frac{\partial}{\partial w_d} \boldsymbol{x}\boldsymbol{w}^T = x_d,
\end{aligned}$$

and thus

$$\frac{\partial E}{\partial w_d} = \frac{\partial E}{\partial \widehat{y}} \frac{\partial \widehat{y}}{\partial w_d} = -(y - \widehat{y})x_d.$$

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

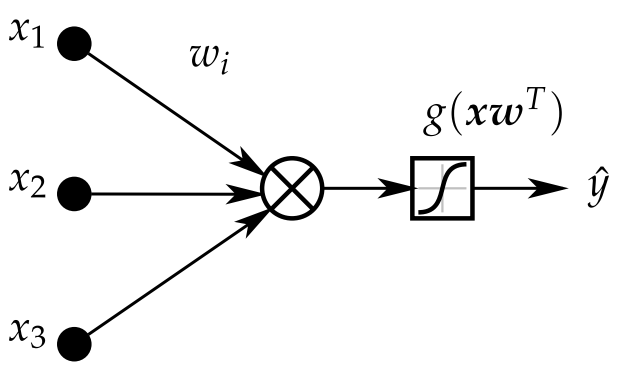
Gradient Descent

Regularization

RBF Networks

Summary

Example: Gradient for logistic regression and crossentropy loss



Nonlinear *activation* function:

$$g(a) = \frac{1}{1+e^{-a}}$$

Note that

$$g'(a) = g(a)\left(1 - g(a)\right).$$

Example: Gradient for logistic regression and crossentropy loss

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

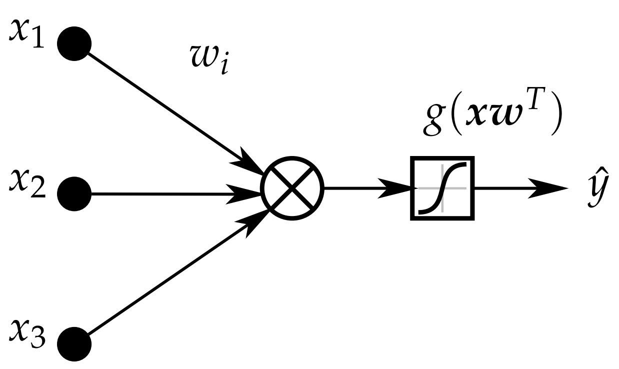
Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary



Nonlinear *activation* function:

$$g(a) = \frac{1}{1+e^{-a}}$$

Note that

$$g'(a) = g(a)\,(1 - g(a))\,.$$

Assuming the crossentropy loss

$$E(\boldsymbol{w}, \boldsymbol{x}, y) = -y \log \widehat{y} - (1-y)\log(1-\widehat{y}),$$

we can compute the derivatives using the chain rule as

$$\frac{\partial E}{\partial w_d} = \frac{\partial E}{\partial \widehat{y}} \frac{\partial \widehat{y}}{\partial a} \frac{\partial a}{\partial w_d}, \text{ where}$$

$$\frac{\partial E}{\partial \widehat{y}} = -\frac{y}{\widehat{y}} + \frac{1-y}{1-\widehat{y}} = -\frac{y-\widehat{y}}{\widehat{y}(1-\widehat{y})},$$

$$\frac{\partial \widehat{y}}{\partial a} = \widehat{y}(1-\widehat{y}), \text{ and } \frac{\partial a}{\partial w_d} = \frac{\partial}{\partial w_d}\boldsymbol{x}\boldsymbol{w}^T = x_d,$$

and thus

$$\frac{\partial E}{\partial w_d} = \frac{\partial E}{\partial \widehat{y}} \frac{\partial \widehat{y}}{\partial a} \frac{\partial a}{\partial w_d} = -(y-\widehat{y})x_d.$$

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

Relations to neural networks

- Above, we derived training algorithms (based on gradient descent) for linear regression model and linear classification model.
- Note the similarity with the *perceptron algorithm* ("just add certain part of a misclassified training example to the weight vector").
- Units like those above are used as **building blocks** for more complex/flexible models!

Intro
- Notation
- Multiple regression
- Logistic regression
- Gradient descent
- Ex: Grad. for MR
- Ex: Grad. for LR
- Relations to NN

Multilayer FFN

Gradient Descent

Regularization

RBF Networks

Summary

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- Units like those above are used as **building blocks** for more complex/flexible models!

A more complex/flexible model:

$$\widehat{y} = g^{OUT}\left(\sum_{k=1}^{K} w_k^{HID} g_k^{HID}\left(\sum_{d=1}^{D} w_{kd}^{IN} x_d\right)\right),$$

which is

- a nonlinear function of
  - a linear combination of
    - nonlinear functions of
      - linear combinations of inputs.

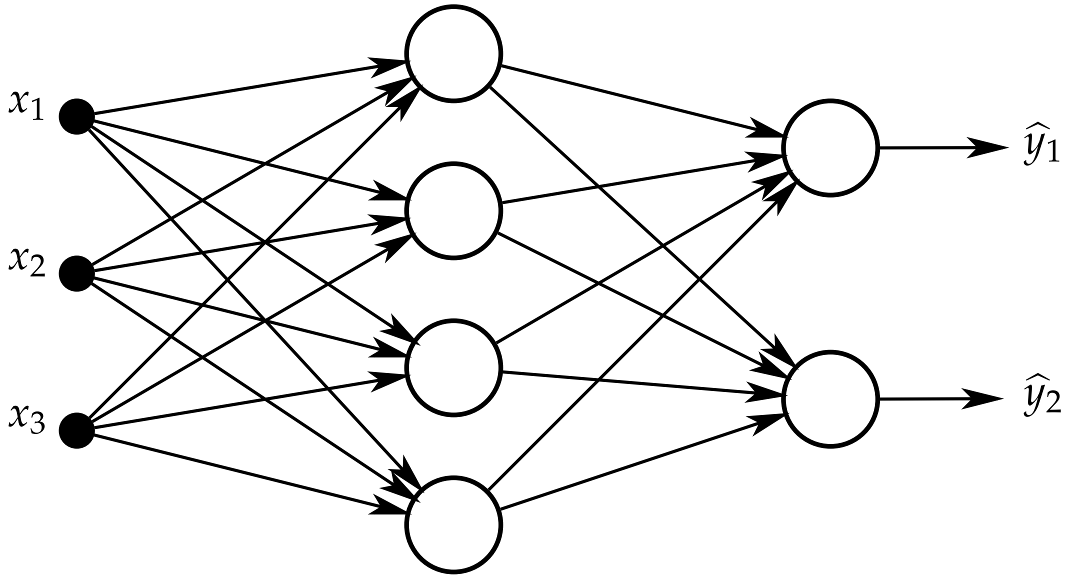
Multilayer Feedforward Networks

Intro
Multilayer FFN
• MLP
• MLP: A look inside
• Activation functions
• MLP: Learning
• BP
• BP algorithm
• BP: Example
• BP Efficiency
• Loss functions
Gradient Descent
Regularization
RBF Networks
Summary

MLP

Multilayer perceptron (MLP)

- Multilayer feedforward network:
  - the „signal“ is propagated from inputs towards outputs; no feedback connections exist.
- It realizes mapping from $\mathcal{R}^D \longrightarrow \mathcal{R}^C$, where D is the number of object features, and C is the number of output variables.
  - For binary classification and regression, a single output is sufficient.
  - For classification into multiple classes, 1-of-N encoding is usually used.
- **Universal approximation theorem:** A MLP with a single hidden layer with sufficient (but finite) number of neurons can approximate any continuous function arbitrarily well (under mild assumptions on the activation functions).



Intro

Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

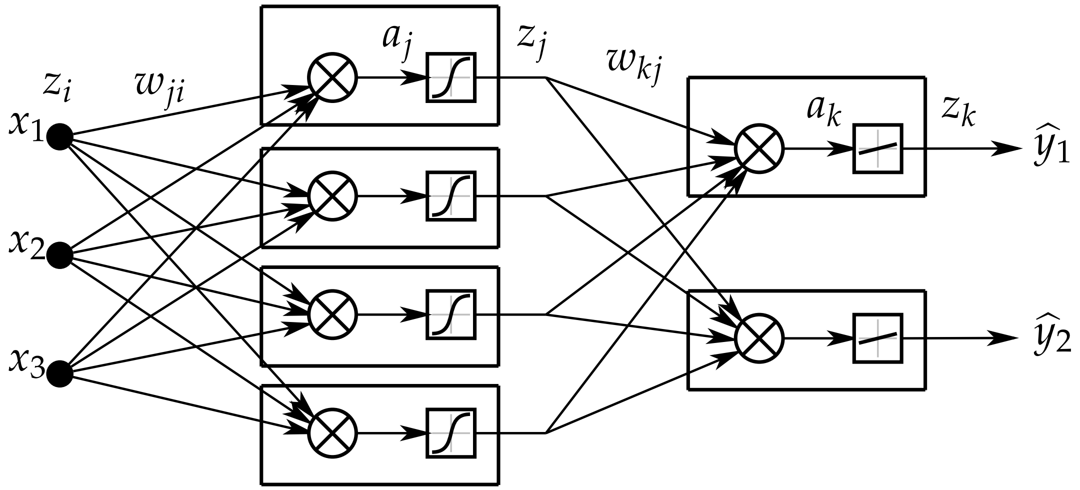
Gradient Descent

Regularization

RBF Networks

Summary

MLP: A look inside



Forward propagation:

- Given all the weights $\boldsymbol{w}$ and activation functions g, we can for a single input vector $\boldsymbol{x}$ easilly compute the estimate of the output vector $\widehat{\boldsymbol{y}}$ by iteratively evaluating in individual layers:

$$a_j = \sum_{i \in Src(j)} w_{ji} z_i \tag{1}$$

$$z_j = g(a_j) \tag{2}$$

- Note that
  - z_i in (1) may be the *outputs of hidden layers neurons* or the *inputs* x_i, and
  - z_j in (2) may be the the *outputs of hidden layers neurons* or the *outputs* $\widehat{y}_k$.

Activation functions

Intro

Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

Gradient Descent

Regularization

RBF Networks

Summary

- Identity: $g(a) = a$
- Binary step: $g(a) = \begin{cases} 0 & \text{for} \quad a < 0, \\ 1 & \text{for} \quad a \geq 0 \end{cases}$
- Logistic (sigmoid): $g(a) = \sigma(a) = \frac{1}{1+e^{-a}}$
- Hyperbolic tangent: $g(a) = \tanh(a) = 2\sigma(a) - 1$
- Rectified Linear unit (ReLU): $g(a) = \max(0, a) = \begin{cases} 0 & \text{for} \quad a < 0, \\ a & \text{for} \quad a \geq 0 \end{cases}$
- Leaky ReLU: $g(a) = \begin{cases} 0.01a & \text{for} \quad a < 0, \\ a & \text{for} \quad a \geq 0 \end{cases}$
- . . .

MLP: Learning

How to train a NN (i.e. find suitable $\boldsymbol{w}$) given the training data set $(\boldsymbol{X}, \boldsymbol{y})$?

Intro
Multilayer FFN
● MLP
● MLP: A look inside
● Activation functions
● MLP: Learning
● BP
● BP algorithm
● BP: Example
● BP Efficiency
● Loss functions
Gradient Descent
Regularization
RBF Networks
Summary

Intro
Multilayer FFN
• MLP
• MLP: A look inside
• Activation functions
• MLP: Learning
• BP
• BP algorithm
• BP: Example
• BP Efficiency
• Loss functions
Gradient Descent
Regularization
RBF Networks
Summary

MLP: Learning

How to train a NN (i.e. find suitable $\boldsymbol{w}$) given the training data set $(\boldsymbol{X}, \boldsymbol{y})$?

In principle, MLP can be trained in the same way as a single-layer NN using a gradient descent algorithm:

- Define the loss function to be minimized, e.g. squared error loss:

$$J(\boldsymbol{w}) = \sum_{i=1}^{|T|} E(\boldsymbol{w}, \boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)}) = \frac{1}{2} \sum_{i=1}^{|T|} \sum_{k=1}^{C} (y_{ik} - \widehat{y}_{ik})^2, \quad \text{where}$$

$$E(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2} \sum_{k=1}^{C} (y_k - \widehat{y}_k)^2.$$

  $|T|$ is the size of the training set, and C is the number of outputs of NN.

- Compute the gradient of the loss function w.r.t. individual weights:

$$\nabla E(\boldsymbol{w}) = \left(\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \ldots, \frac{\partial E}{\partial w_W} \right).$$

- Make a step in the direction opposite to the gradient to update the weights:

$$w_d \longleftarrow w_d - \eta \frac{\partial E}{\partial w_d} \quad \text{for } d = 1, \ldots, W.$$

How to compute the individual derivatives?

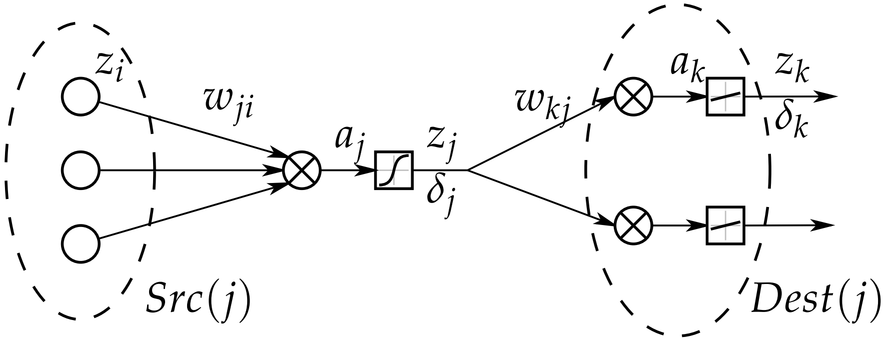
Error backpropagation

Error backpropagation (BP) is the algorithm for computing $\frac{\partial E}{\partial w_d}$.

Error backpropagation

Error backpropagation (BP) is the algorithm for computing $\frac{\partial E}{\partial w_d}$.

Consider only $\frac{\partial E}{\partial w_d}$ because
$\frac{\partial J}{\partial w_d} = \sum_n \frac{\partial}{\partial w_d} E(\boldsymbol{w}, \boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)})$.



E depends on w_{ji} only via a_j:

$$\frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial a_j}\frac{\partial a_j}{\partial w_{ji}} \tag{3}$$

Let's introduce the so called *error* δ_j:

$$\delta_j = \frac{\partial E}{\partial a_j} \tag{4}$$

From (1) we can derive:

$$\frac{\partial a_j}{\partial w_{ji}} = z_i \tag{5}$$

Substituting (4) and (5) into (3):

$$\frac{\partial E}{\partial w_{ji}} = \delta_j z_i, \tag{6}$$

where

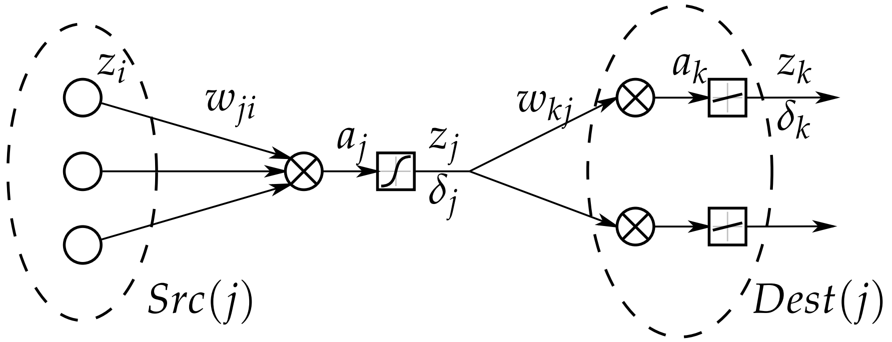
δ_j	is the error of the neuron on the output of the
z_i	is the input of the edge $i \rightarrow j$.

"The more we excite edge $i \rightarrow j$ (big z_i) and the larger is the error of the neuron on its output (large δ_j), the more sensitive is the loss function E to the change of w_{ji}."

- All values z_i are known from forward pass,
- to compute the gradient, we need to compute all δ_j.

Error backpropagation (cont.)

We need to compute the *errors* δ_j.



For the output layer:

$$\delta_k = \frac{\partial E}{\partial a_k}$$

E depends on a_k only via $\widehat{y}_k = g(a_k)$:

$$\delta_k = \frac{\partial E}{\partial a_k} = \frac{\partial E}{\partial \widehat{y}_k}\frac{\partial \widehat{y}_k}{\partial a_k} = g'(a_k)\frac{\partial E}{\partial \widehat{y}_k} \qquad (7)$$

For the hidden layers:

$$\delta_j = \frac{\partial E}{\partial a_j}$$

E depends on a_j via all a_k, $k \in Dest(j)$:

$$\begin{aligned}\delta_j = \frac{\partial E}{\partial a_j} &= \sum_{k\in Dest(j)} \frac{\partial E}{\partial a_k}\frac{\partial a_k}{\partial a_j} = \\ &= \sum_{k\in Dest(j)} \delta_k \frac{\partial a_k}{\partial a_j} = \\ &= g'(a_j)\sum_{k\in Dest(j)} w_{kj}\delta_k, \qquad (8)\end{aligned}$$

because

$$a_k = \sum_{j\in Src(k)} w_{kj}z_j = \sum_{j\in Src(k)} w_{kj}g(a_j),$$

and thus $\frac{\partial a_k}{\partial a_j} = w_{kj}g'(a_j)$

"The error δ_k is distributed to δ_j in the lower layer according to the weight w_{kj} (which is the speed of growth of the linear combination a_k) and according to the size of $g'(a_j)$ (which is the speed of growth of the activation function)."

Intro
Multilayer FFN
• MLP
• MLP: A look inside
• Activation functions
• MLP: Learning
• BP
• BP algorithm
• BP: Example
• BP Efficiency
• Loss functions
Gradient Descent
Regularization
RBF Networks
Summary

Error backpropagation algorithm

Algorithm 1: Error Backpropagation: the computation of derivatives $\frac{\partial E}{\partial w_d}$.

```
1 begin
2     Perform a forward pass for observation $\boldsymbol{x}$. This will result in values of all $a_j$ and $z_j$
        for the vector $\boldsymbol{x}$.
3     Evaluate the error $\delta_k$ for the output layer (using Eq. 7):
          $$\delta_k = g'(a_k)\frac{\partial E}{\partial \hat{y}_k}$$
4     Using Eq. 8, propagate the errors $\delta_k$ back to get all the remaining $\delta_j$:
          $$\delta_j = g'(a_j)\sum_{k\in Dest(j)} w_{kj}\delta_k$$
5     Using Eq. 6, evaluate all the derivatives to get the whole gradient:
          $$\frac{\partial E}{\partial w_{ji}} = \delta_j z_i$$
```

Error backpropagation: Example

Intro

Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

Gradient Descent

Regularization

RBF Networks

Summary

NN with a single hidden layer:

- Squared error loss: $E = \frac{1}{2}\sum_{k=1}^{C}(y_k - \widehat{y}_k)^2$
- Activation func. in the output layer: identity $g_k(a_k) = a_k, \quad g'_k(a_k) = 1$
- Activation func. in the hidden layer: sigmoidal $g_j(a_j) = \frac{1}{1+e^{-a_j}}, \quad g'_j(a_j) = z_j(1 - z_j)$

Intro
Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

Gradient Descent
Regularization
RBF Networks
Summary

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Computing the errors δ:

- Output layer: $\delta_k = g_k'(a_k)\frac{\partial E}{\partial \widehat{y}_k} = -(y_k - \widehat{y}_k)$

Intro
Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

Gradient Descent
Regularization
RBF Networks
Summary

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Computing the errors δ:

- Output layer: $\delta_k = g'_k(a_k)\frac{\partial E}{\partial \widehat{y}_k} = -(y_k - \widehat{y}_k)$
- Hidden layer: $\delta_j = g'_j(a_j)\sum_{k\in Dest(j)} w_{kj}\delta_k = z_j(1-z_j)\sum_{k\in Dest(j)} w_{kj}\delta_k$

Intro

Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

Gradient Descent

Regularization

RBF Networks

Summary

Error backpropagation: Example

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- Activation func. in the hidden layer: sigmoidal $g_j(a_j) = \frac{1}{1+e^{-a_j}}, \quad g_j'(a_j) = z_j(1 - z_j)$

Computing the errors δ:

- Output layer: $\delta_k = g_k'(a_k)\frac{\partial E}{\partial \widehat{y}_k} = -(y_k - \widehat{y}_k)$
- Hidden layer: $\delta_j = g_j'(a_j) \sum_{k \in Dest(j)} w_{kj}\delta_k = z_j(1 - z_j) \sum_{k \in Dest(j)} w_{kj}\delta_k$

Computation of all the partial derivatives:

$$\frac{\partial E}{\partial w_{ji}} = \delta_j x_i \qquad\qquad \frac{\partial E}{\partial w_{kj}} = \delta_k z_j$$

Error backpropagation: Example

Intro

Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

Gradient Descent

Regularization

RBF Networks

Summary

NN with a single hidden layer:

- Squared error loss: $E = \frac{1}{2} \sum_{k=1}^{C} (y_k - \widehat{y}_k)^2$
- Activation func. in the output layer: identity $g_k(a_k) = a_k, \quad g'_k(a_k) = 1$
- Activation func. in the hidden layer: sigmoidal $g_j(a_j) = \frac{1}{1+e^{-a_j}}, \quad g'_j(a_j) = z_j(1 - z_j)$

Computing the errors δ:

- Output layer: $\delta_k = g'_k(a_k) \frac{\partial E}{\partial \widehat{y}_k} = -(y_k - \widehat{y}_k)$
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Computation of all the partial derivatives:

$$\frac{\partial E}{\partial w_{ji}} = \delta_j x_i \qquad \frac{\partial E}{\partial w_{kj}} = \delta_k z_j$$

Online learning:

$$w_{ji} \longleftarrow w_{ji} - \eta \delta_j x_i$$
$$w_{kj} \longleftarrow w_{kj} - \eta \delta_k z_j$$

Batch learning:

$$w_{ji} \longleftarrow w_{ji} - \eta \sum_{n=1}^{|T|} \delta_j^{(n)} x_i^{(n)}$$
$$w_{kj} \longleftarrow w_{kj} - \eta \sum_{n=1}^{|T|} \delta_k^{(n)} z_j^{(n)}$$

Intro
Multilayer FFN
- MLP
- MLP: A look inside
- Activation functions
- MLP: Learning
- BP
- BP algorithm
- BP: Example
- BP Efficiency
- Loss functions

Gradient Descent
Regularization
RBF Networks
Summary

Error backpropagation efficiency

Let W be the number of weights in the network (the number of parameters being optimized).

- The evaluation of E for a single observation requires $\mathcal{O}(W)$ operations (evaluation of $w_{ji}z_i$ dominates, evaluation of $g(a_j)$ is neglected).

We need to compute W derivatives for each observation:

- Classical approach:
  - Find explicit equations for $\frac{\partial E}{\partial w_{ji}}$.
  - To compute each of them $\mathcal{O}(W)$ steps are required.
  - In total, $\mathcal{O}(W^2)$ steps for a single training example.
- Backpropagation:
  - Requires only $\mathcal{O}(W)$ steps for a single training example.

Loss functions

Task	Suggested loss function
Binary classification	Cross-entropy: $J = -\sum_{i=1}^{\lvert T \rvert} \left[y^{(i)} \log \widehat{y}^{(i)} + (1 - y^{(i)}) \log(1 - \widehat{y}^{(i)}) \right]$
Multinomial classification	Multinomial cross-entropy: $J = -\sum_{i=1}^{\lvert T \rvert} \sum_{k=1}^{C} I(y^{(i)} = k) \log \widehat{y}_k^{(i)}$
Regression	Squared error: $J = \sum_{i=1}^{\lvert T \rvert} (y^{(i)} - \widehat{y}^{(i)})^2$
Multi-output regression	Squared error: $J = \sum_{i=1}^{\lvert T \rvert} \sum_{k=1}^{C} (y_k^{(i)} - \widehat{y}_k^{(i)})^2$

Note: often, mean errors are used.

- Computed as the average w.r.t. the number of training examples $\lvert T \rvert$.
- The optimum is in the same point, of course.

Gradient Descent

Learning rate annealing

Intro
Multilayer FFN
Gradient Descent
- Learning rate
- Weights update
- Momentum
- GD improvements
Regularization
RBF Networks
Summary

Task: find such parameters $\boldsymbol{w}^*$ which minimize the model cost over the training set, i.e.

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y})$$

Intro
Multilayer FFN
Gradient Descent
- Learning rate
- Weights update
- Momentum
- GD improvements
Regularization
RBF Networks
Summary

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Gradient descent: $\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta^{(t)} \nabla J(\boldsymbol{w}^{(t)})$,
where $\eta^{(t)} > 0$ is the **learning rate** or **step size** at iteration t.

Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

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Learning rate decay:

- Decrease the learning rate in time.
- **Step decay:** reduce the learning rate every few iterations by certain factor, e.g. $\frac{1}{2}$.
- **Exponential decay:** $\eta^{(t)} = \eta_0 e^{-kt}$
- **Hyperbolic decay:** $\eta^{(t)} = \frac{\eta_0}{1+kt}$

Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

Weights update

When should we update the weights?

- **Batch learning:**
  - Compute the gradient w.r.t. all the training examples (epoch).
  - Several epochs are required to train the network.
  - Inefficient for redundant datasets.
- **Online learning:**
  - Compute the gradient w.r.t. a single training example only.
  - **Stochastic Gradient Descent (SGD)**
  - Converges almost surely to local minimum when $\eta^{(t)}$ decreases appropriately in time.
- **Mini-batch learning:**
  - Compute the gradient w.r.t. a small subset of the training examples.
  - A compromise between the above 2 extremes.

Momentum

Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

Momentum

- Perform the update in an analogy to physical systems: a particle with certain mass and velocity gets acceleration from the gradient ("force") of the loss function:

$$\boldsymbol{v}^{(t+1)} = \mu\boldsymbol{v}^{(t)} + \eta^{(t)}\nabla J(\boldsymbol{w}^{(t)})$$
$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \boldsymbol{v}^{(t+1)}$$

- SGD with momentum tends to keep traveling in the same direction, preventing oscillations.
- It builds the velocity in directions with consistent (but possibly small) gradient.

Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

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- SGD with momentum tends to keep traveling in the same direction, preventing oscillations.
- It builds the velocity in directions with consistent (but possibly small) gradient.

Nesterov's Momentum

- Slightly different update equations:

$$\begin{aligned} \boldsymbol{v}^{(t+1)} &= \mu \boldsymbol{v}^{(t)} + \eta^{(t)} \nabla J(\boldsymbol{w}^{(t)} + \mu \boldsymbol{v}^{(t)}) \\ \boldsymbol{w}^{(t+1)} &= \boldsymbol{w}^{(t)} + \boldsymbol{v}^{(t+1)} \end{aligned}$$

- Classic momentum corrects the velocity using gradient at $\boldsymbol{w}^{(t)}$; Nesterov uses gradient at $\boldsymbol{w}^{(t)} + \mu \boldsymbol{v}^{(t)}$ which is more similar to $\boldsymbol{w}^{(t+1)}$.
- Stronger theoretical convergence guarantees; slightly better in practice.

Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

Further gradient descent improvements

Resilient Propagation (Rprop)

- $\frac{\partial J}{\partial w_d}$ may differ a lot for different parameters w_d.
- Rprop does not use the value, only its *sign* to adapt the step size for each weight separately.
- Often, an order of magnitude faster than basic GD.
- Does not work well for mini-batches.

Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

Further gradient descent improvements

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Adaptive Gradient (Adagrad)

- Idea: Reduce learning rates for parameters having high values of gradient.

Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

Further gradient descent improvements

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- Similar to AdaGrad, but employs a moving average of the gradient values.
- Can be seen as a generalization of Rprop, can work also with mini-batches.

Intro
Multilayer FFN
Gradient Descent
- Learning rate
- Weights update
- Momentum
- GD improvements
Regularization
RBF Networks
Summary

Further gradient descent improvements

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Intro
Multilayer FFN
Gradient Descent
• Learning rate
• Weights update
• Momentum
• GD improvements
Regularization
RBF Networks
Summary

Further gradient descent improvements

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See also:

- `http://sebastianruder.com/optimizing-gradient-descent/`
- `http://cs231n.github.io/neural-networks-3/`
- `http://cs231n.github.io/assets/nn3/opt2.gif`, `http://cs231n.github.io/assets/nn3/opt1.gif`

Regularization

Overfitting and regularization

Intro
Multilayer FFN
Gradient Descent
Regularization
- Ridge
- Dropout
RBF Networks
Summary

Overfitting in NN is often characterized by weight values that are very large in magnitude. How to deal with it?

- Get more data.
- Use a simpler model (less hidden layers, less neurons, different activation functions).
- Use *regularization* (penalize the model complexity).

Intro
Multilayer FFN
Gradient Descent
Regularization
• Ridge
• Dropout
RBF Networks
Summary

Overfitting and regularization

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Ridge regularization:

- Modified loss function, e.g. for squared error:

$$J'(\boldsymbol{w}) = J(\boldsymbol{w}) + \text{penalty} = \frac{1}{2m}\sum_{i=1}^{m}\left(y^{(i)} - \boldsymbol{x}^{(i)}\boldsymbol{w}^T\right)^2 + \frac{\alpha}{m}\sum_{d=1}^{D} w_d^2.$$

- Modified weight update in GD:

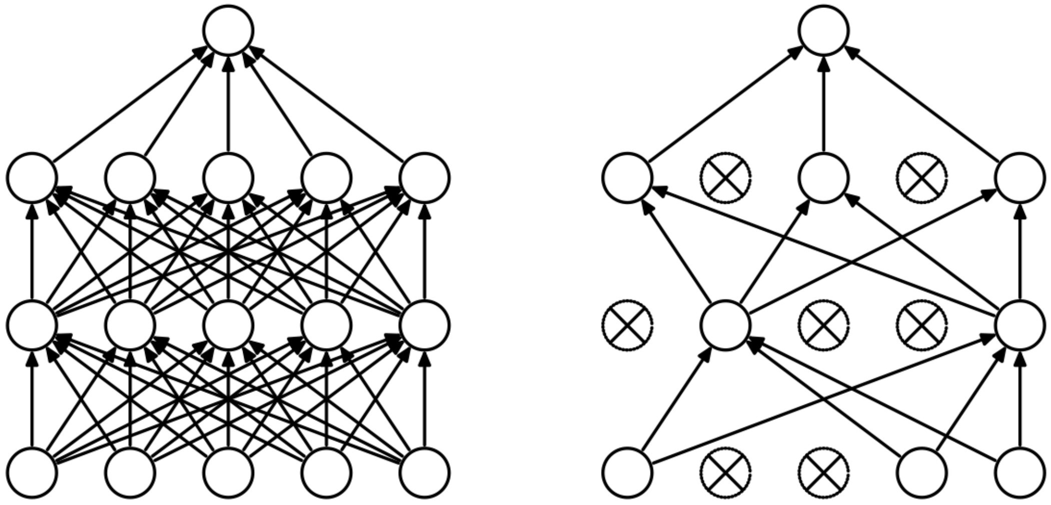
$$w_d \leftarrow w_d - \eta\frac{\partial J'}{\partial w_d} = \underbrace{\left(1 - \frac{\eta\alpha}{m}\right)}_{\text{weight decay}} w_d - \eta\frac{\partial J}{\partial w_d},$$

  where η is the learning rate, α is the regularization strength, m is the number of examples in the batch.
- The biases (weights connected to constant 1) should not be regularized!

Intro
Multilayer FFN
Gradient Descent
Regularization
• Ridge
• Dropout
RBF Networks
Summary

Dropout

- Idea: Average many NNs, share weights to make it computationally feasible.
- For each training example, omit each neuron with certain probability (often $p = 0.5$).
- This is like sampling from 2^N networks where N is the number of units.
- Only a small part of the 2^N networks is actually sampled.
- Prevents coadaptation of feature vectors.

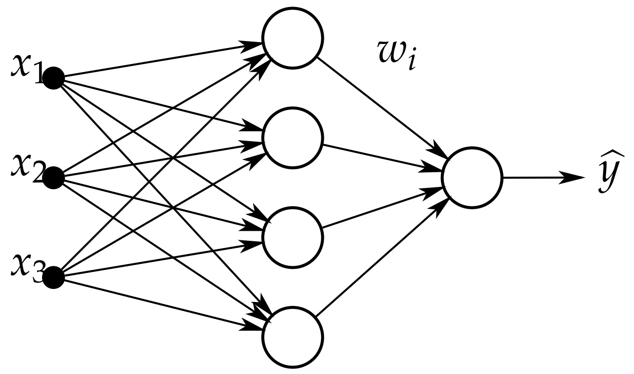

(a) Standard Neural Net (b) After applying dropout.

Srivastava et al.: A Simple Way to Prevent Neural Networks from Overfitting, 2014

Radial Basis Function Networks

RBF networks

A simple RBF network:



RBF networks

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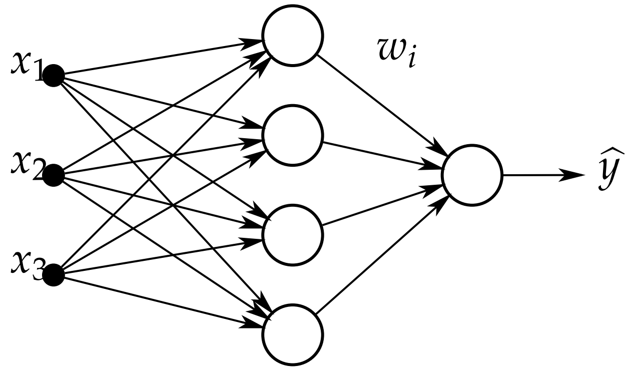


RBF network realizes function

$$\widehat{y} = \sum_{i=1}^{N} w_i \rho\left(|\boldsymbol{x} - \boldsymbol{c_i}|\right)$$

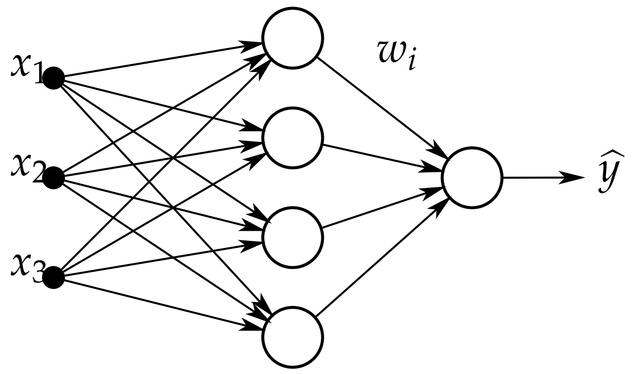
where

- N is the number of RBF neurons in the hidden layer,
- $\boldsymbol{c}_i$ is a centroid of the ith neuron, and
- w_i are the weights of the output linear combination.
- RBF function ρ is usually Gaussian

$$\rho\left(|\boldsymbol{x} - \boldsymbol{c_i}|\right) = \exp\left(-\frac{|\boldsymbol{x} - \boldsymbol{c}_i|^2}{\sigma^2}\right)$$

RBF networks

A simple RBF network:



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RBF functions are local:

- changing the parameters of one neuron has only a small effect on network predictions for points far away from the neuron centroid.

RBF networks are universal approximators:

- With sufficient number of neurons they are able to approximate any continuous function with arbitrary precision.

To train the network we must learn

- the weights w_i,
- the centroids $\boldsymbol{c}_i$, and
- the “sizes” of RBF functions σ^2.

Learning is usually done in 2 phases:

1. learn the centroids $\boldsymbol{c}_i$ (e.g. using k-means),
2. learn weights w_i.

RBF network extensions

Normalized architecture

The network function is

$$\widehat{y} = \sum_{i=1}^{N} w_i u\left(|\boldsymbol{x} - \boldsymbol{c_i}|\right)$$

where u is a *normalized RBF*:

$$u\left(|\boldsymbol{x} - \boldsymbol{c_i}|\right) = \frac{\rho\left(|\boldsymbol{x} - \boldsymbol{c_i}|\right)}{\sum_{j=1}^{N} \rho\left(|\boldsymbol{x} - \boldsymbol{c_j}|\right)}$$

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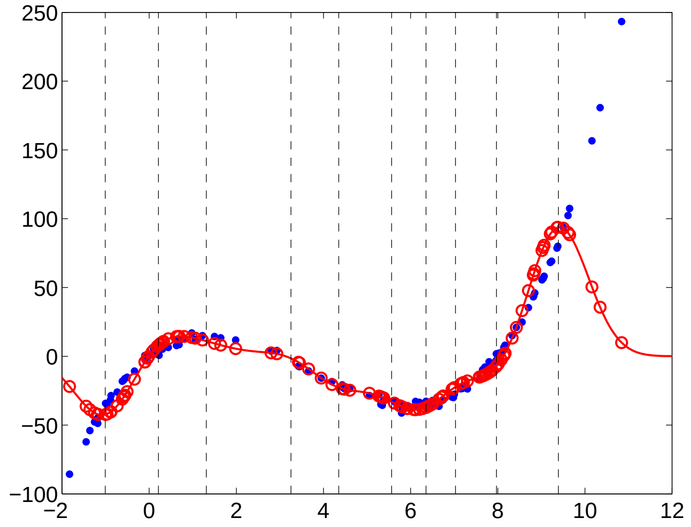
Unnormalized architecture:



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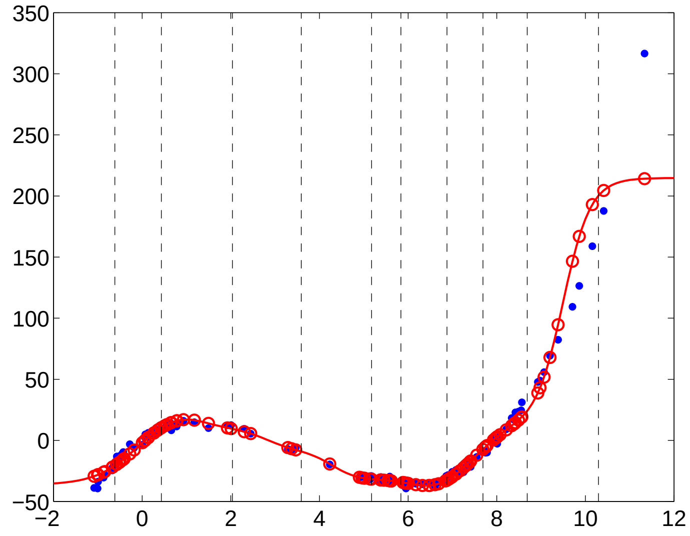

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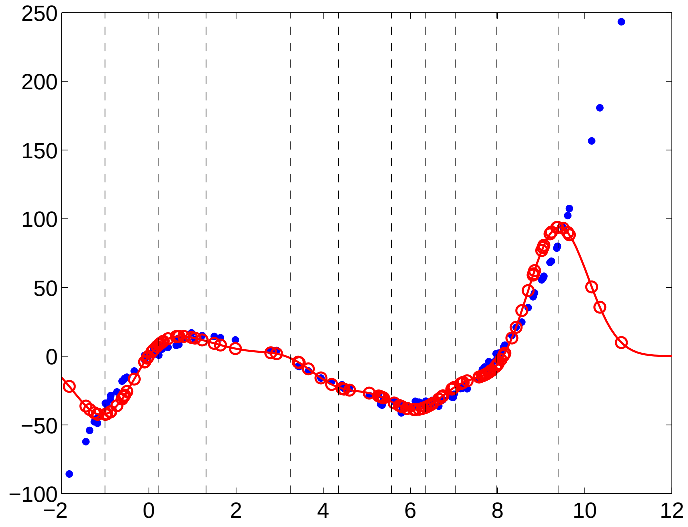

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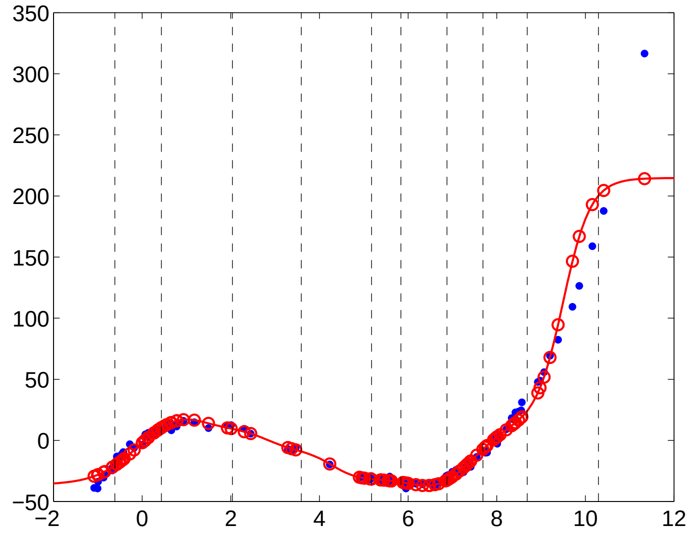

Mixture of locally linear models

For unnormalized architecture:

$$\hat{y} = \sum_{i=1}^{N} \left(a_i + \boldsymbol{b}_i\left(\boldsymbol{x} - \boldsymbol{c_i}\right)\right) \rho\left(|\boldsymbol{x} - \boldsymbol{c_i}|\right) \text{ nebo}$$

For normalized architecture:

$$\hat{y} = \sum_{i=1}^{N} \left(a_i + \boldsymbol{b}_i\left(\boldsymbol{x} - \boldsymbol{c_i}\right)\right) u\left(|\boldsymbol{x} - \boldsymbol{c_i}|\right)$$

Summary

Competencies

After this lecture, a student shall be able to . . .

- describe the model of a simple neuron, and explain its relation to multivariate regression and logistic regrassion;
- explain how to find weights of a single neuron using gradient descent (GD) algorithm;
- derive the update equations used in GD to optimize the weights of a single neuron for various loss functions and various activation functions;
- describe a multilayer feedforward network and discuss its usage and characteristics;
- compare the use of GD in case of a single neuron and in case of NN, discuss similarities and differences;
- explain the error backpropagation (BP) algorithm — its purpose and principle;
- implement BP algorithm for a simple NN, and suggest how the implementation should be modified to allow application for complex networks;
- discuss the purpose of various modifications of GD algorithm (learning rate decay, weight update schedule, momentum, . . .);
- discuss the regularization options for NN (weight decay, dropout);
- describe RBF networks and explain their main differences to MLP.