Neural Networks

Volker Tresp

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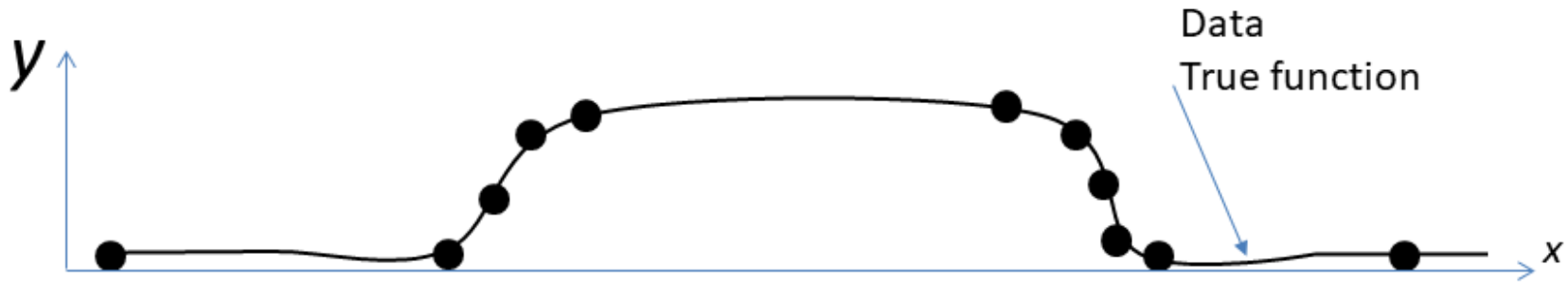
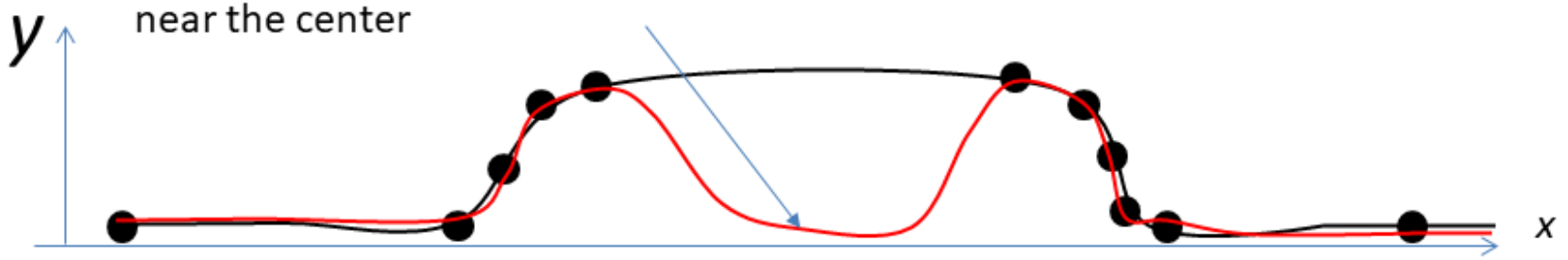
Introduction

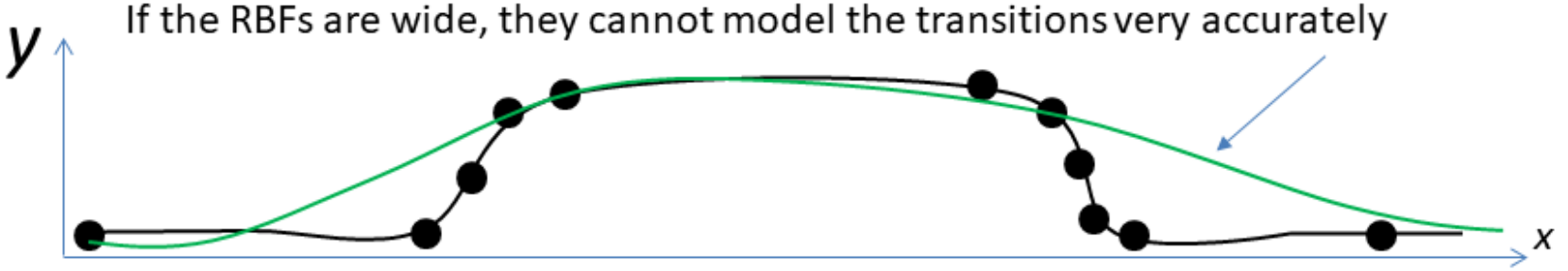
- In many applications, data might be uniformly distributed in input space, but complexity in y-space might be nonuniform
- In the next slide the function has two areas of high complexity; RBF approaches, with a notion of uniform complexity, have problems



If the RBFs are narrow, I might need a lot of them and the prediction is bad near the center



If the RBFs are wide, they cannot model the transitions very accurately



Sigmoidal Basis Functions

- A sigmoidal basis function has the form

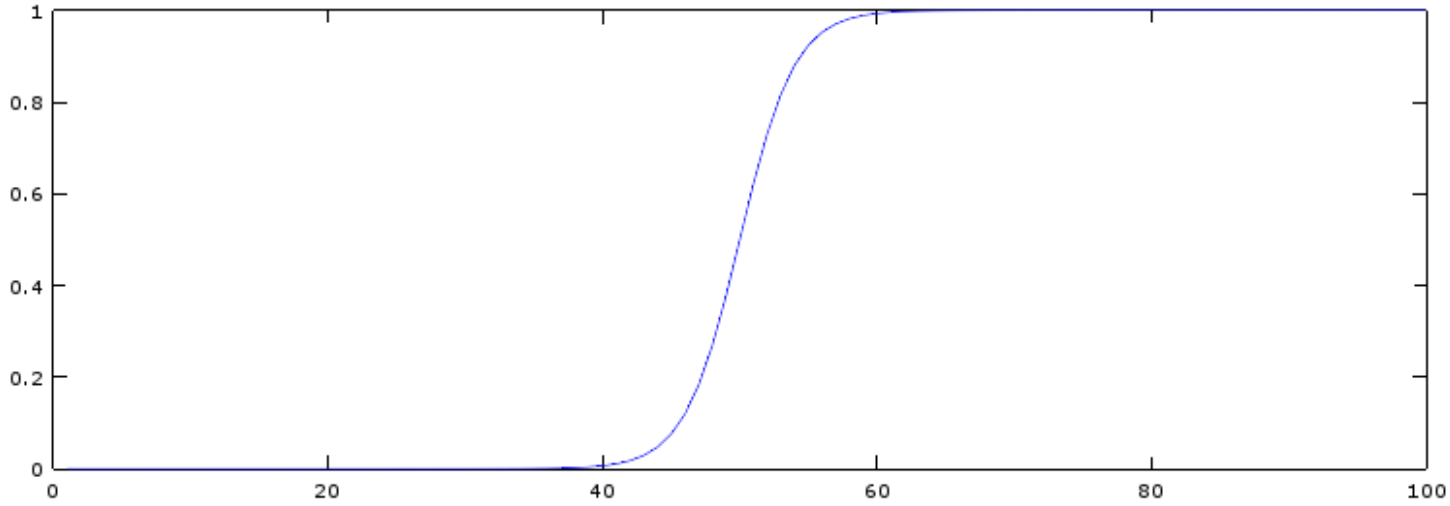
$$\text{sig}(vx + v_0)$$

where

$$\text{sig}(arg) = \frac{1}{1 + \exp(-arg)}$$

- The function is only complex near its center where $arg \approx 0$
- Important: **To get the location and the slope at the center, we need to adapt the inner parameters** v_0, v. There is no closed-form solution for the estimate of those parameters: we need to use gradient-based approaches like SGD

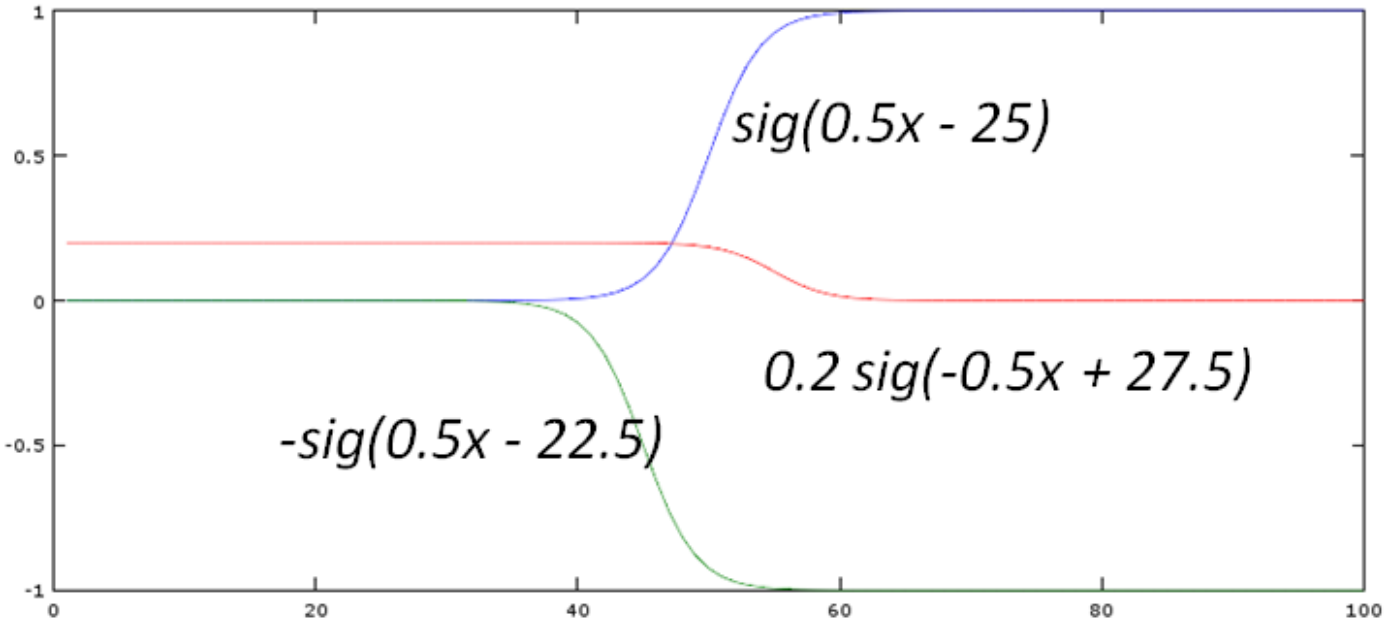
sig(0.5x - 25)

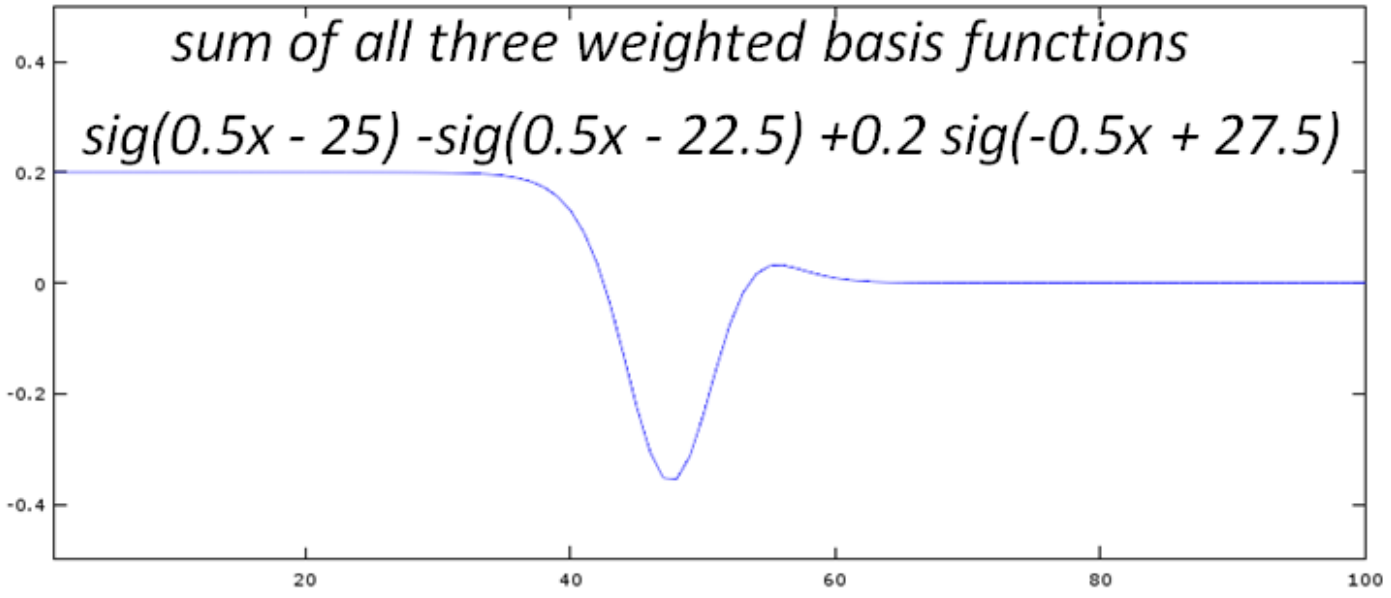


Several Sigmoidal Basis Functions

- With several weighted sigmoidal basis functions, we are able to model a variety of functions with local complexity

$$f(x) = w_0 + \sum_{h=1}^{H} w_h \, \mathsf{sig}(v_h x + v_{h,0})$$


sig(0.5x - 25)
0.2 sig(-0.5x + 27.5)
-sig(0.5x - 22.5)
1
0.5
0
-0.5
-1
0
20
40
60
80
100


sum of all three weighted basis functions
sig(0.5x - 25) -sig(0.5x - 22.5) +0.2 sig(-0.5x + 27.5)
0.4
0.2
0
-0.2
-0.4
20
40
60
80
100

Overcomplete Basis

- Another approch would be to select a sparse subset in an overcomplete basis
- This is the approach used in Wavelets, Sparse coding, ...

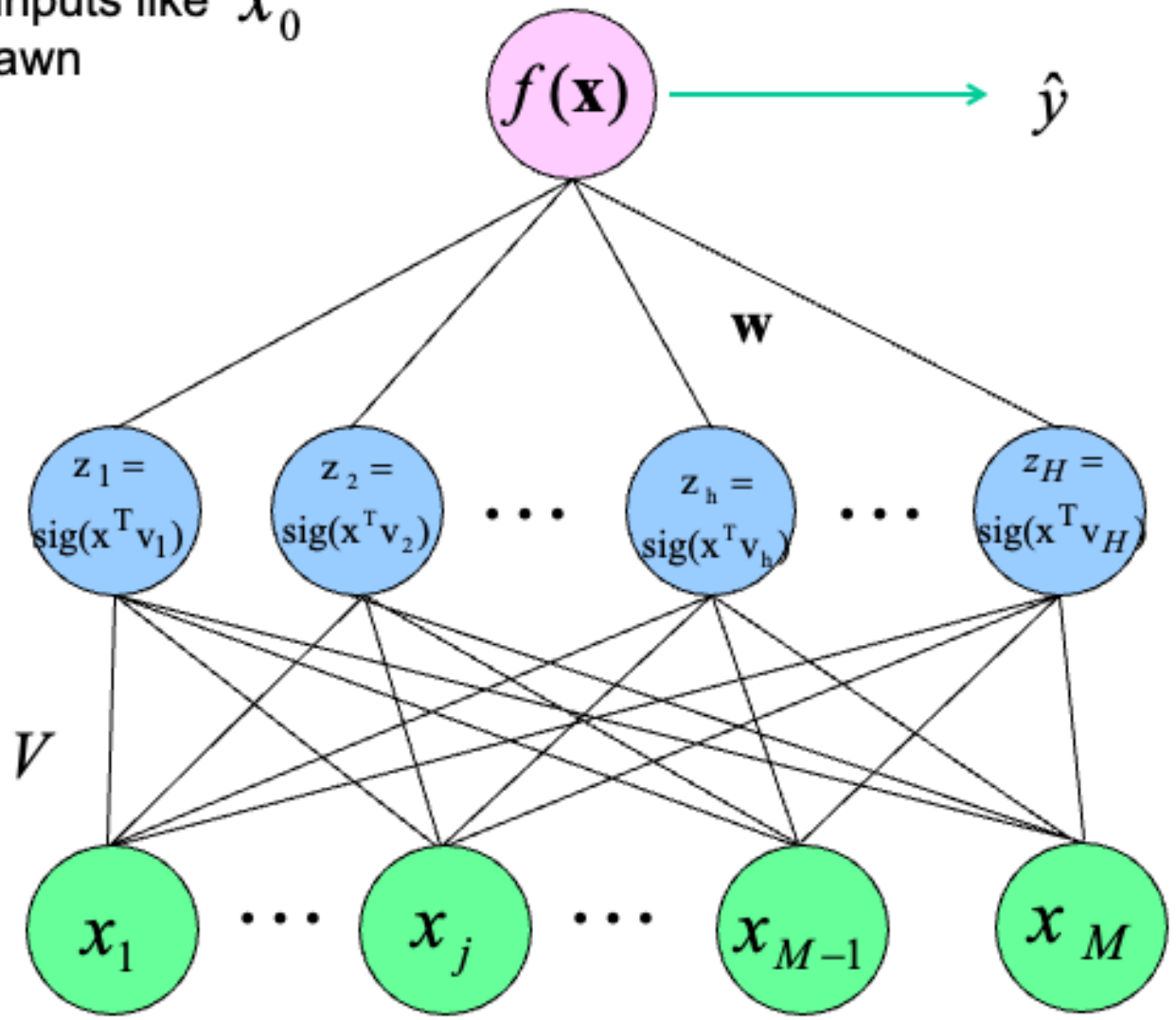
Multidimensional Input Space

- With several sigmoidal basis functions, we are able to model a variety of functions with local complexity *in a high dimensional input space*

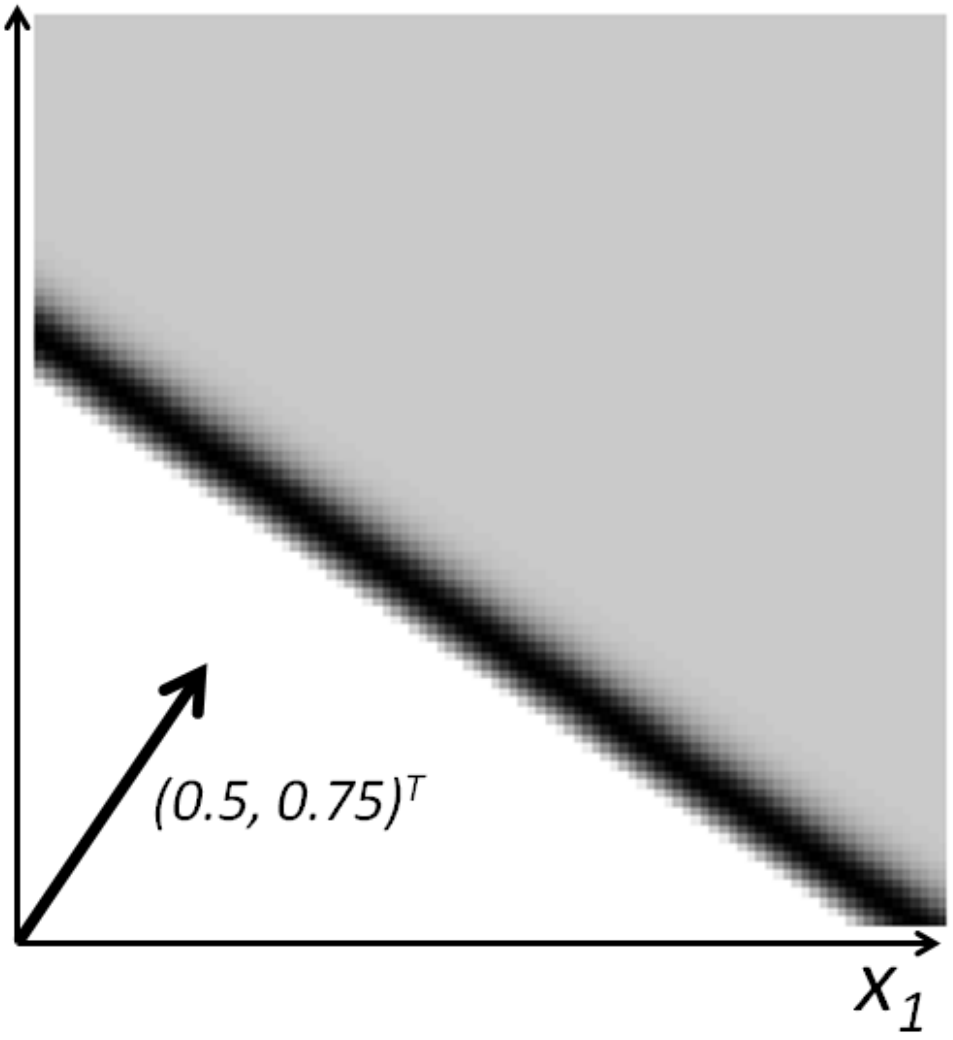
$$f(\mathbf{x}) = w_0 + \sum_{h=1}^{H} w_h \,\mathrm{sig}\left(v_{h,0} + \sum_{j=1}^{M} v_{h,j} x_j\right)$$

- This equation describes neural network, more specifically, a Multilayer Perceptron with one hidden layer

Constant inputs like x_0 are not drawn



$sig(0.5x_1+0.75x_2 - 25)$
$-sig(0.5x_1 +0.75x_2 - 22.5)$
$+0.2\ sig(-0.5x_1 -0.75x_2 + 27.5)$



Dimensionality Reduction

- Note that the neural network can also performs dimensionality reduction: in the figure, any components orthogonal to $(0.5, 0.75)^T$ are ignored
- So neural networks are well suited for large M, small smoothness m and noisy features, if the function has high complexity only in the projection on some low-dimensional subspaces

Neural Networks: Essential Advantages

- Neural Networks are universal approximators: any continuous function can be approximated arbitrarily well (with a sufficient number of neural basis functions)
- Naturally, they can solve the XOR problem and at the time (mid 1980's) were considered the response to the criticism by Minsky and Papert with respect to the limited power of the single Perceptron
- Important advantage of Neural Networks: a good function fit can often (for a large class of important function classes) be achieved with a **small number of** neural basis functions
- Neural Networks scale well with input dimensions

Flexible Models: Neural Networks

- For regression, the output of a neural network is the weighted sum of basis functions

$$\widehat{y} = f(\mathbf{x}) = w_0 + \sum_{h=1}^{H} w_h \text{sig}(\mathbf{x}^T \mathbf{v}_h)$$

- Note, that in addition to the output weights $\mathbf{w}$, the neural network also has inner weights $\mathbf{v}_h$

Notation

- $\mathbf{x} = 1, x_1, \ldots, x_j, \ldots, x_M$: inputs (with constant)
- $\mathbf{z} = 1, z_1, z_2, \ldots, z_h, \ldots, z_H$: Outputs of the H hidden units (with constant)
- $v_{h,j}$: weight from input j to hidden unit h
- y: single neural network output; $H(M+1) + (H+1)$ adjustable parameters
- w_h: weight from hidden unit h to output y
- $y_1, \ldots, y_k, \ldots, y_K$: K neural network outputs; $H(M+1) + K(H+1)$ adjustable parameters
- $w_{k,h}$: weight from hidden unit h to output k

Neural Basis Functions

- Special form of the basis functions

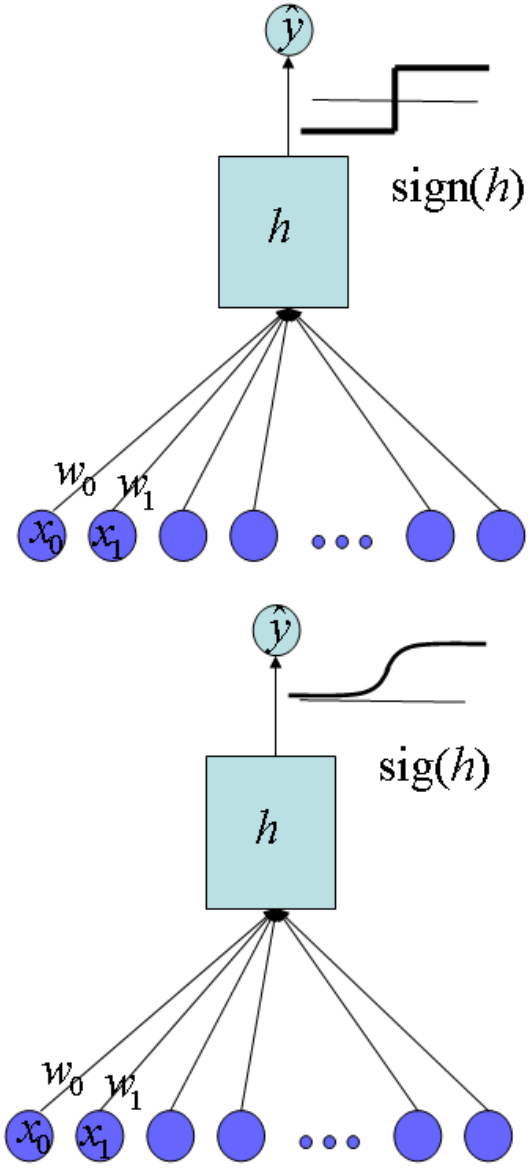
$$z_h = \text{sig}(\mathbf{x}^T \mathbf{v}_h) = \text{sig}\left(v_{h,0} + \sum_{j=1}^{M} v_{h,j} x_j \right)$$

  using the *logistic function*

$$\text{sig}(arg) = \frac{1}{1 + \exp(-arg)}$$

- Adaption of the inner parameters $v_{h,j}$ of the basis functions!

Hard and Soft (sigmoid) Transfer Functions



- First, the activation function of the neurons in the hidden layer are calculated as the weighted sum of the inputs as

$$h(\mathbf{x}) = \sum_{j=0}^{M} w_j x_j$$

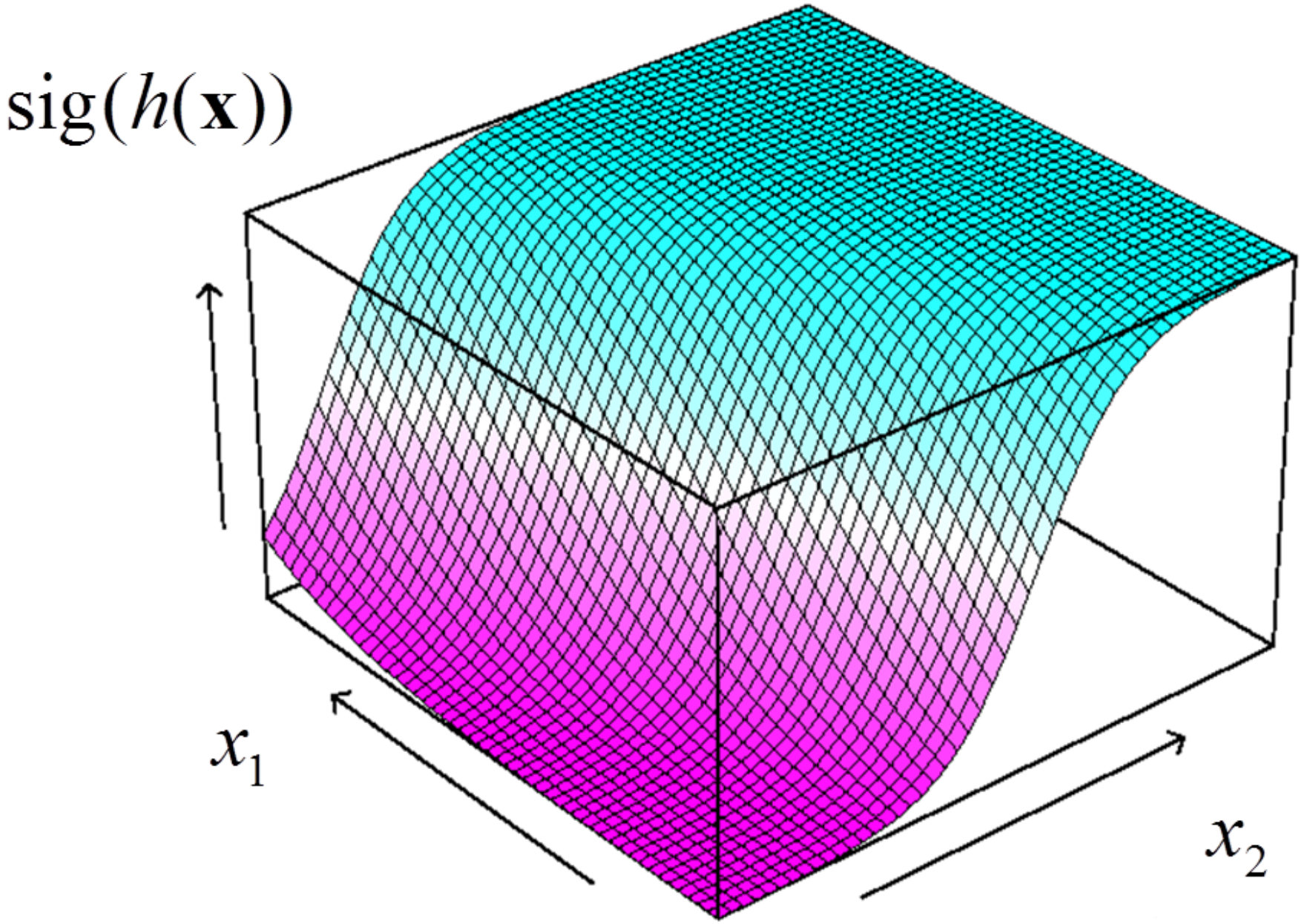
(note: $x_0 = 1$ is a constant input, so that w_0 corresponds to the bias)

- The sigmoid neuron has a soft (sigmoid) transfer function

$$\textbf{Perceptron}: \quad \hat{y} = \text{sign}(h(\mathbf{x}))$$

Sigmoidal neuron: $\quad \hat{y} = \text{sig}(h(\mathbf{x}))$

Transfer Function


sig(h(x))
x1
x2

Separating Hyperplane

- Definition of the hyperplane

$$\text{sig}\left(\sum_{j=0}^{M} v_{h,j} x_j\right) = 0.5$$

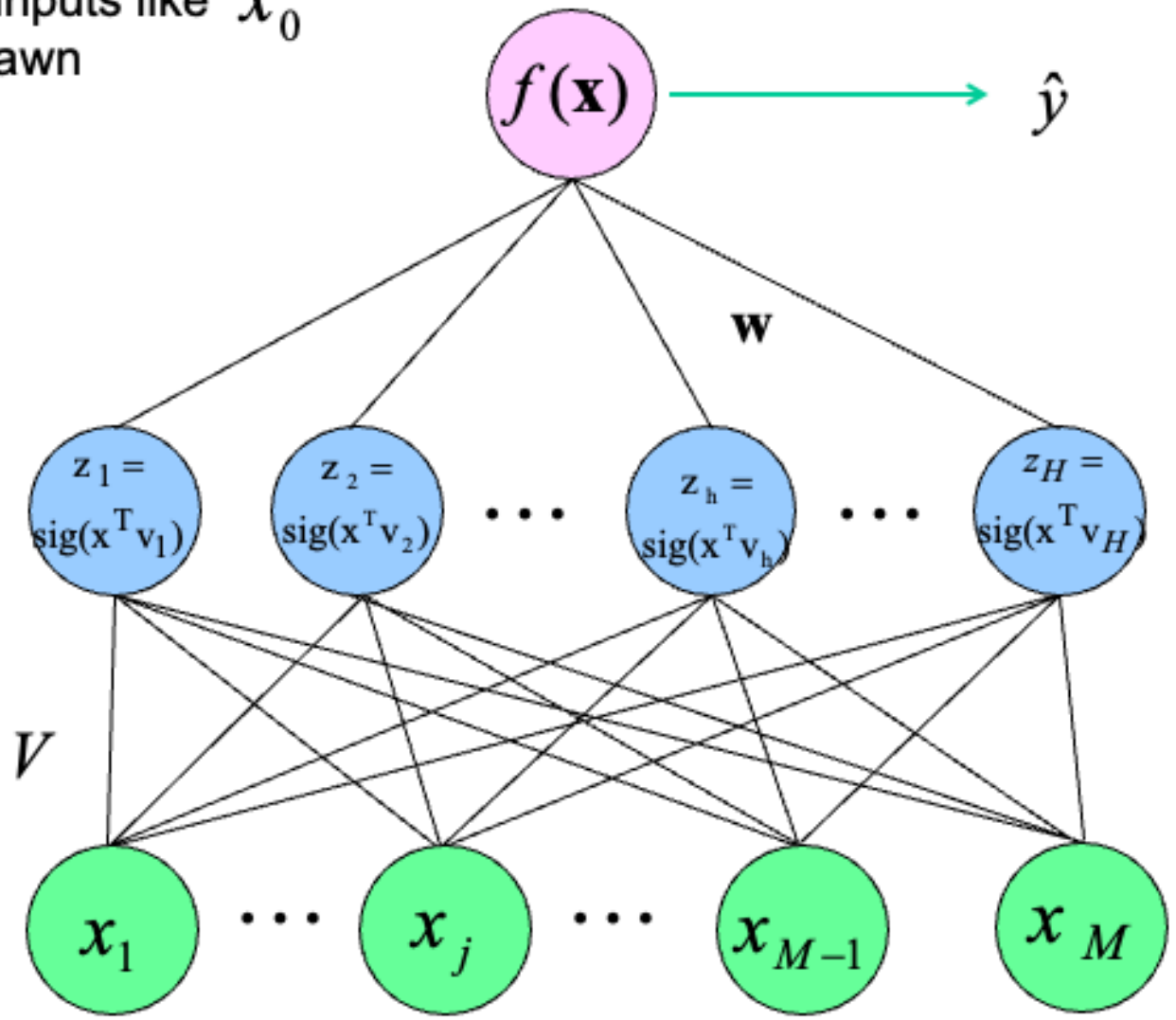
  which means that:

$$\sum_{j=0}^{M} v_{h,j} x_j = 0$$

- "carpet over a step"

Architecture of a Neural Network

Constant inputs like x_0 are not drawn



Variants

- For a **2-class neural network classifier** apply the sigmoid transfer function to the output neuron, and calculate

$$\widehat{y} = \text{sig}(f(\mathbf{x})) = \text{sig}(\mathbf{z}^T\mathbf{w})$$

- For **multi-class tasks** (e.g., recognizing digits $0, 1, \ldots, 9$), one uses several output neurons. For example, to classify K digits

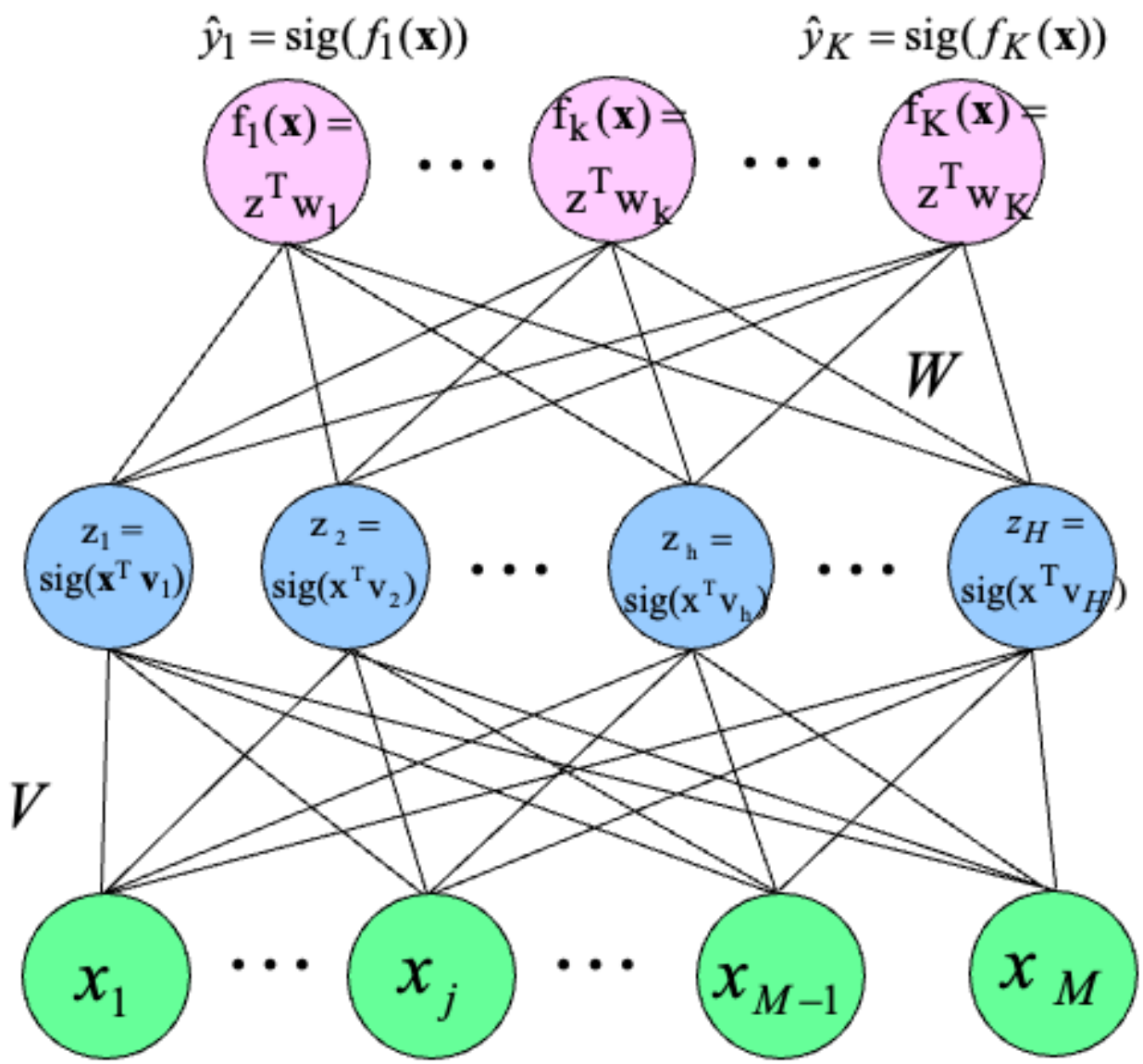
$$\widehat{y}_k = \text{sig}(f_k(\mathbf{x})) = \text{sig}(\mathbf{z}^T\mathbf{w}_k) \quad k = 1, 2, \ldots, K$$

  and one decides for class l, with $l = \arg\max_k(\widehat{y}_k)$

- (Nowadays on typically uses the softmax cost function (discussed further down)

- A Neural Network with at least one hidden layer is called a Multilayer Perceptron (MLP)

Architecture of a Neural Network for Several Classes


$\hat{y}_1 = \text{sig}(f_1(\mathbf{x}))$
$\hat{y}_K = \text{sig}(f_K(\mathbf{x}))$
$f_1(\mathbf{x}) = z^T w_1$
$f_k(\mathbf{x}) = z^T w_k$
$f_K(\mathbf{x}) = z^T w_K$
W
$z_1 = \text{sig}(\mathbf{x}^T \mathbf{v}_1)$
$z_2 = \text{sig}(x^T v_2)$
$z_h = \text{sig}(x^T v_h)$
$z_H = \text{sig}(x^T v_H)$
V
x_1
x_j
x_{M-1}
x_M

Learning Multiple-Class Classifiers

- The goal again is the minimization of the squared error calculated over all training patterns and all outputs

$$\text{cost} = \sum_{i=1}^{N} \text{cost}_i$$

  with $\text{cost}_i = \sum_{k=1}^{K} (y_{i,k} - \widehat{y}_{i,k})^2$

- The least squares solution for V cannot be calculated in closed-form
- Typically both W and V are trained via (stochastic) gradient descent

Adaption of the Output Weights

- The gradient of the cost function for an output weight for pattern i becomes

$$\frac{\partial \text{cost}_i}{\partial w_{k,h}} = -2\delta_{i,k} z_{i,h}$$

where

$$\delta_{i,k} = \text{sig}'(\mathbf{z}_i^T \mathbf{w}_k)[y_{i,k} - \hat{y}_{i,k}]$$

is the back propagated error signal (error back propagation). Note, that $\delta_{i,k}$ is attached to an output node k.

Adaption of the Output Weights (cont'd)

- The pattern based gradient descent learning becomes (pattern: i, output: k, hidden: h):

$$w_{k,h} \leftarrow w_{k,h} + \eta \delta_{i,k} z_{i,h}$$

- Another example of a **delta-rule**

The Derivative of the Sigmoid Transfer Function with Respect to the Argument

... can be written elegantly as

$$\mathrm{sig}'(in) = \frac{\exp(-in)}{(1+\exp(-in))^2} = \mathrm{sig}(in)(1-\mathrm{sig}(in))$$

Thus

$$\delta_{i,k} = \widehat{y}_{i,k}(1-\widehat{y}_{i,k})\ (y_{i,k}-\widehat{y}_{i,k})$$

Adaptation of the Input Weights

- The gradient of an input weight with respect to the cost function for pattern i becomes

$$\frac{\partial \text{cost}_i}{\partial v_{h,j}} = -2\delta_{i,h}x_{i,j}$$

  with the back propagated error

$$\delta_{i,h} = \text{sig}'(\mathbf{x}_i^T \mathbf{v}_h) \sum_{k=1}^{K} w_{k,h}\delta_{i,k} = z_{i,h}(1 - z_{i,h}) \sum_{k=1}^{K} w_{k,h}\delta_{i,k}$$

- Note, that $\delta_{i,h}$ is attached to hidden node h.

Adaptation of the Input Weights (cont'd)

- For the pattern based gradient descent, we get (pattern: *i*, hidden: *h*, input: *j*):

$$v_{h,j} \leftarrow v_{h,j} + \eta \delta_{i,h} x_{i,j}$$

Pattern-based Learning

- Iterate over all training patterns
- Let $\mathbf{x}_i$ be the training data point at iteration t
  - Apply $\mathbf{x}_i$ and calculate $\mathbf{z}_i, \hat{\mathbf{y}}_i$ (*forward propagation*)
  - Via *error backpropagation* calculate the $\delta_{i,h}, \delta_{i,k}$
  - Adapt

$$w_{k,h} \leftarrow w_{k,h} + \eta \delta_{i,k} z_{i,h}$$

$$v_{h,j} \leftarrow v_{h,j} + \eta \delta_{i,h} x_{i,j}$$

- All operations are "local": biologically plausible

Complexity Analysis

- Neural networks work well in all situations covered in the discussion on basis function, except for Case I. (curse of dimensionality)
- In particular, they offer an excellent solution for Case Ia (sparse basis).

Neural Networks and Overfitting

- In comparison to conventional statistical models, a Neural Network has a huge number of free parameters, which might easily lead to over fitting
- The two most common ways to fight over fitting are regularization and stopped-training
- Let's first discuss regularization

Neural Networks: Regularization

- We introduce regularization terms and get

$$\text{cost}^{pen} = \sum_{i=1}^{N} \text{cost}_i + \lambda_1 \sum_{k=1}^{K} \sum_{h=0}^{H} w_{k,h}^2 + \lambda_2 \sum_{h=0}^{H} \sum_{j=0}^{M} v_{h,j}^2$$

- The learning rules change to (with *weight decay term*, the constant bias is typically not regularized)

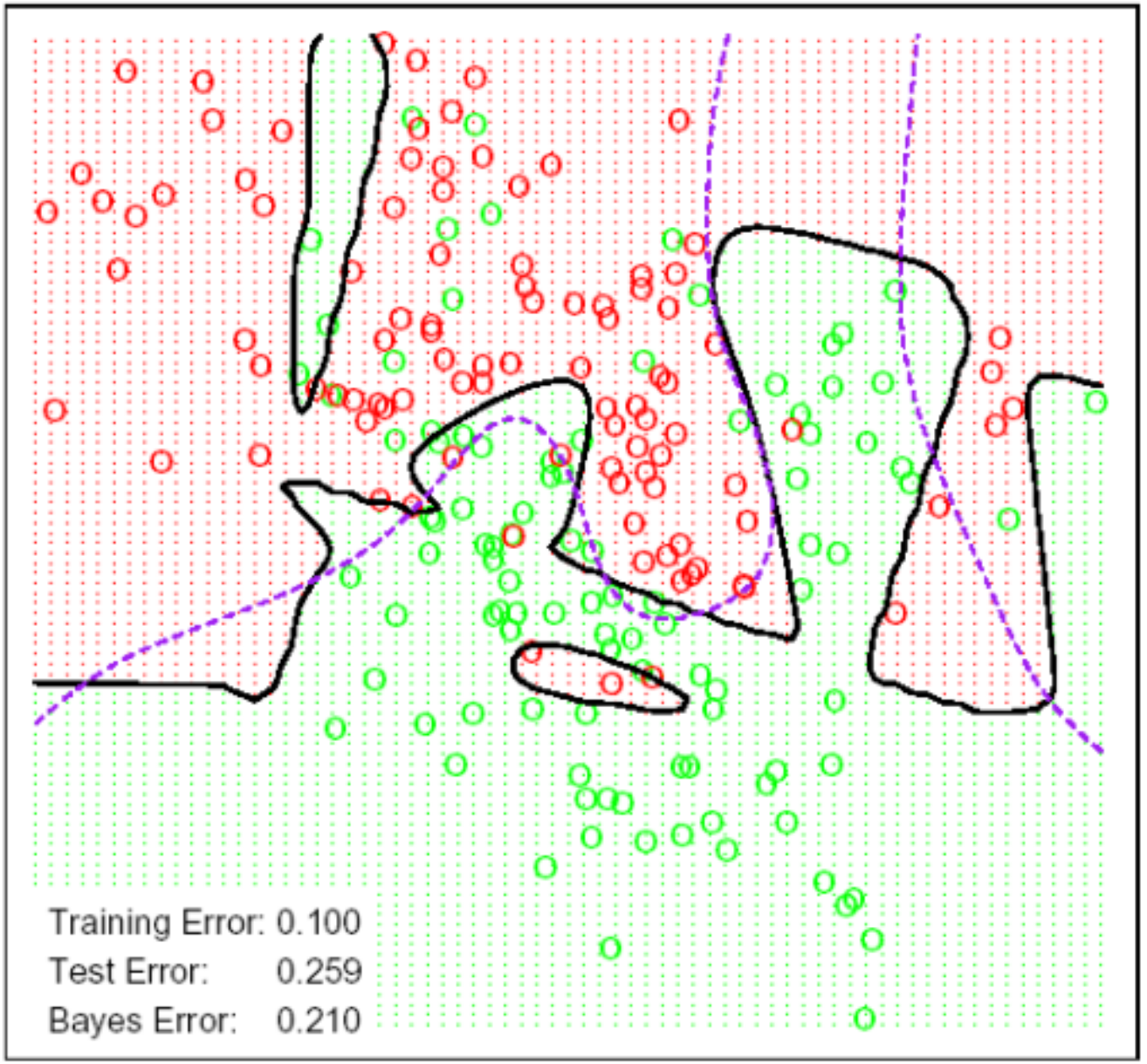
$$w_{k,h} \leftarrow w_{k,h} + \eta \left(\delta_{i,k} z_{i,h} - \frac{\lambda_1}{N} w_{k,h} \right)$$

$$v_{h,j} \leftarrow v_{h,j} + \eta \left(\delta_{i,h} x_{i,j} - \frac{\lambda_2}{N} v_{h,j} \right)$$

Artificial Example

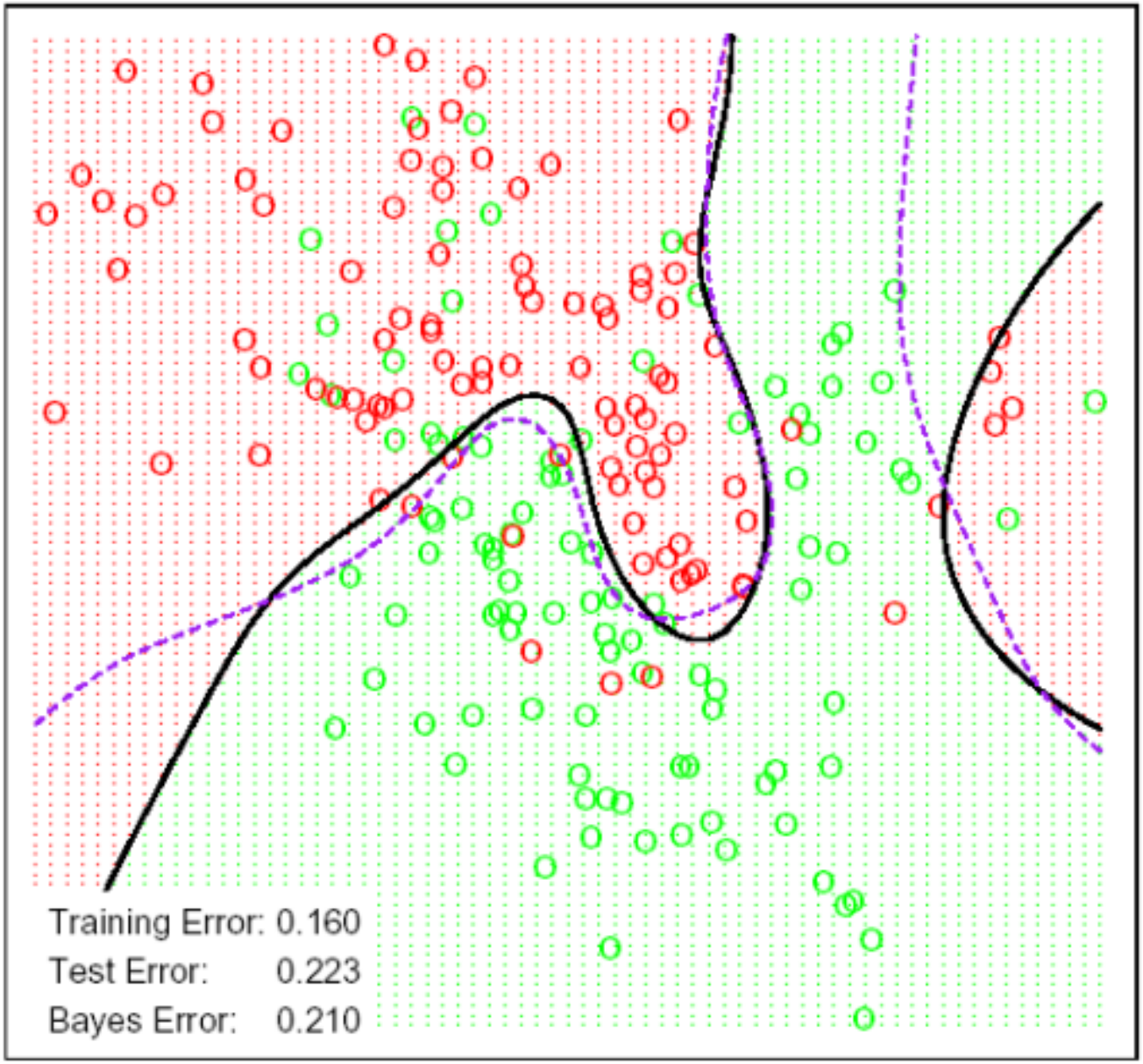
- Data for two classes (red/green circles) are generated
- Classes overlap
- The optimal separating boundary is shown dashed
- A neural network without regularization shows over fitting (continuous line)

Neural Network - 10 Units, No Weight Decay



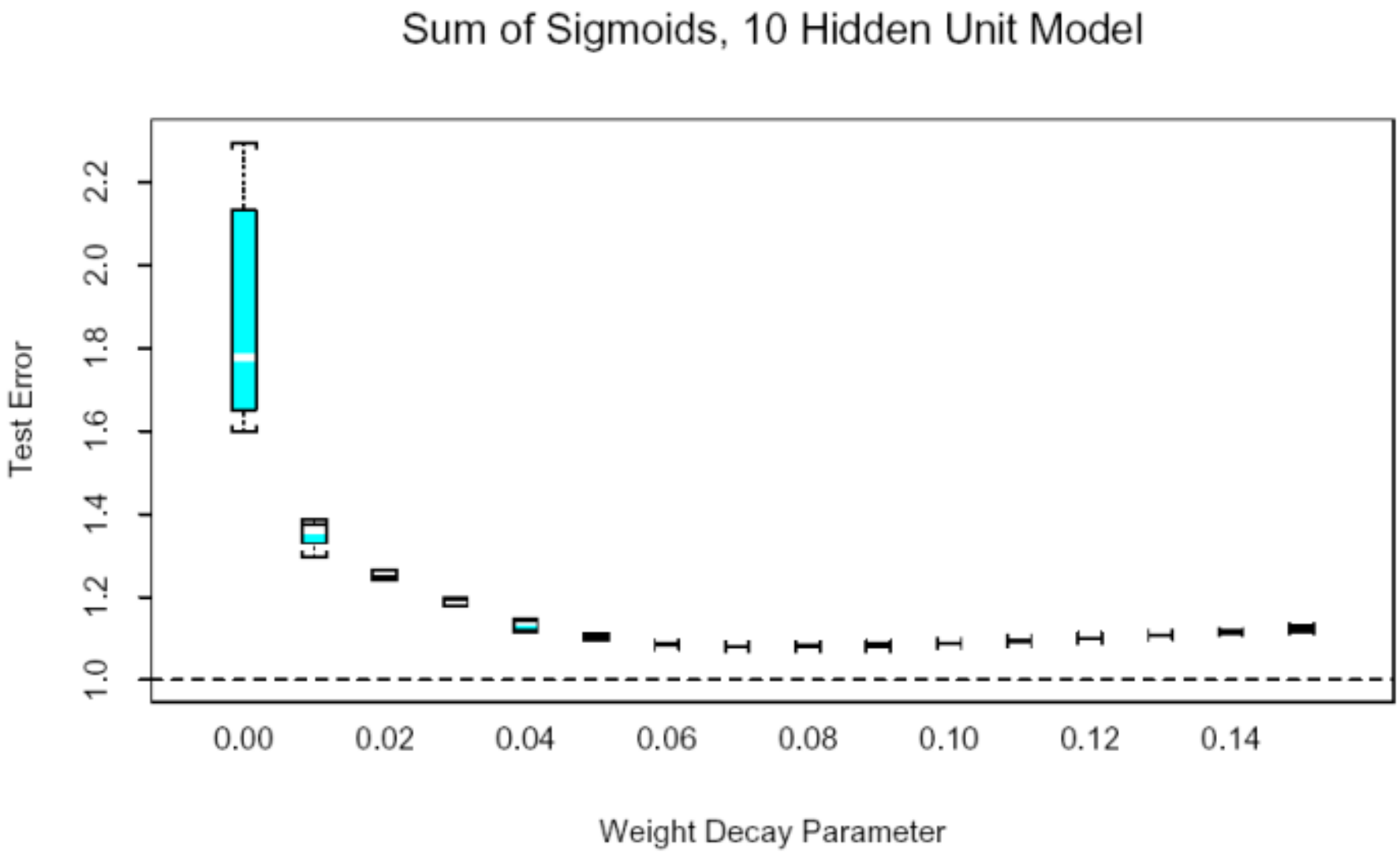
Same Example with Regularization

- With regularization ($\lambda_1 = \lambda_2 = 0.02$) the separating plane is closer to the true class boundaries
- The training error is smaller with the unregularized network, the test error is smaller with the regularized network


Neural Network - 10 Units, Weight Decay=0.02
Training Error: 0.160
Test Error: 0.223
Bayes Error: 0.210

Optimized Regularization Parameters

- The regularization parameter is varied between 0 and 0.15
- The vertical axis shows the test error for many independent experiments
- The best test error is achieved with regularization parameter 0.07
- The test error varies a lot with no regularization


Sum of Sigmoids, 10 Hidden Unit Model
Test Error
1.0
1.2
1.4
1.6
1.8
2.0
2.2
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Weight Decay Parameter

Variations

- Use more than one hidden layer (see deep learning)
- Use $\tanh(arg) \in (-1, 1)$ instead of $\text{sig}(arg) \in (0, 1)$
- For the $\tanh(arg)$, use targets $y \in \{-1, 1\}$, instead of $y \in \{0, 1\}$
- Often: Use $\tanh(arg)$ in the hidden layer and $\text{sig}(arg)$ in the output layer (for binary classes) and $\text{softmax}(arg)$ for multiple classes

Cross-entropy Cost Function for Binary Classification

- We use $\widehat{y} = \mathsf{sig}(\eta)$ with $\eta = \mathbf{z}^T\mathbf{w}$
- The likelihood for pattern i is $L_i = \widehat{y}_i^{y_i}(1-\widehat{y}_i)^{1-y_i}$ (to be maximized)
- With $y_i \in \{0, 1\}$, the cross-entropy loss for pattern i is the logarithm of the negative log-likelihood, as

$$\begin{aligned}\mathsf{cost}_i^{CE} &= -y_i \log \widehat{y}_i - (1-y_i)\log(1-\widehat{y}_i) \\ &= -y_i\eta + \log(1+\exp(\eta))\end{aligned}$$

  and the gradient becomes

$$\frac{\partial \mathsf{cost}_i^{CE}}{\partial w_h} = -(y_i - \widehat{y}_i)z_{i,h}$$

- (homework!) Nowadays, the cross-entropy cost function is typically being used

Delta Rules

- Thus, for the cross-entropy cost function, we get for the **delta-rule**:

$$\delta_i = (y_i - \widehat{y}_i).$$

  with $\widehat{y}_i \in (0, 1)$

- This is identical to the delta-rule for the Perceptron, only there, $\widehat{y}_i \in \{0, 1\}$
- Recall that for the (old-style) neural network for binary classification,

$$\delta_i = \text{sig}'(\mathbf{z}_i^T \mathbf{w})(y_i - \widehat{y}_i)$$

Cross-entropy Cost Function for Multiple Classes

- Often the outputs are mutual exclusive: a handwritten digit is exactly one out of 10 digit
- As activation, one uses the softmax function with $f_{i,k} = \sum_{h=0}^{H} w_{k,h} z_{i,h}$

$$\widehat{y}_{i,k} = \frac{\exp f_{i,k}}{\sum_{k'=1}^{K} \exp f_{i,k'}}$$

- The likelihood for pattern i is $L_i = \prod_k \widehat{y}_{i,k}^{y_{i,k}}$ (to be maximized)
- The cost term (one hot encoding with $y_{i,k} \in \{0, 1\}$) is the logarithm of the negative log-likelihood, as

$$\text{cost}_i^{CE} = \left(-\sum_k y_{i,k} \exp f_{i,k} \right) + \left(\log \sum_{k'=1}^{K} \exp f_{i,k'} \right)$$

Cross-entropy Cost Function for Multiple Classes (cont'd)

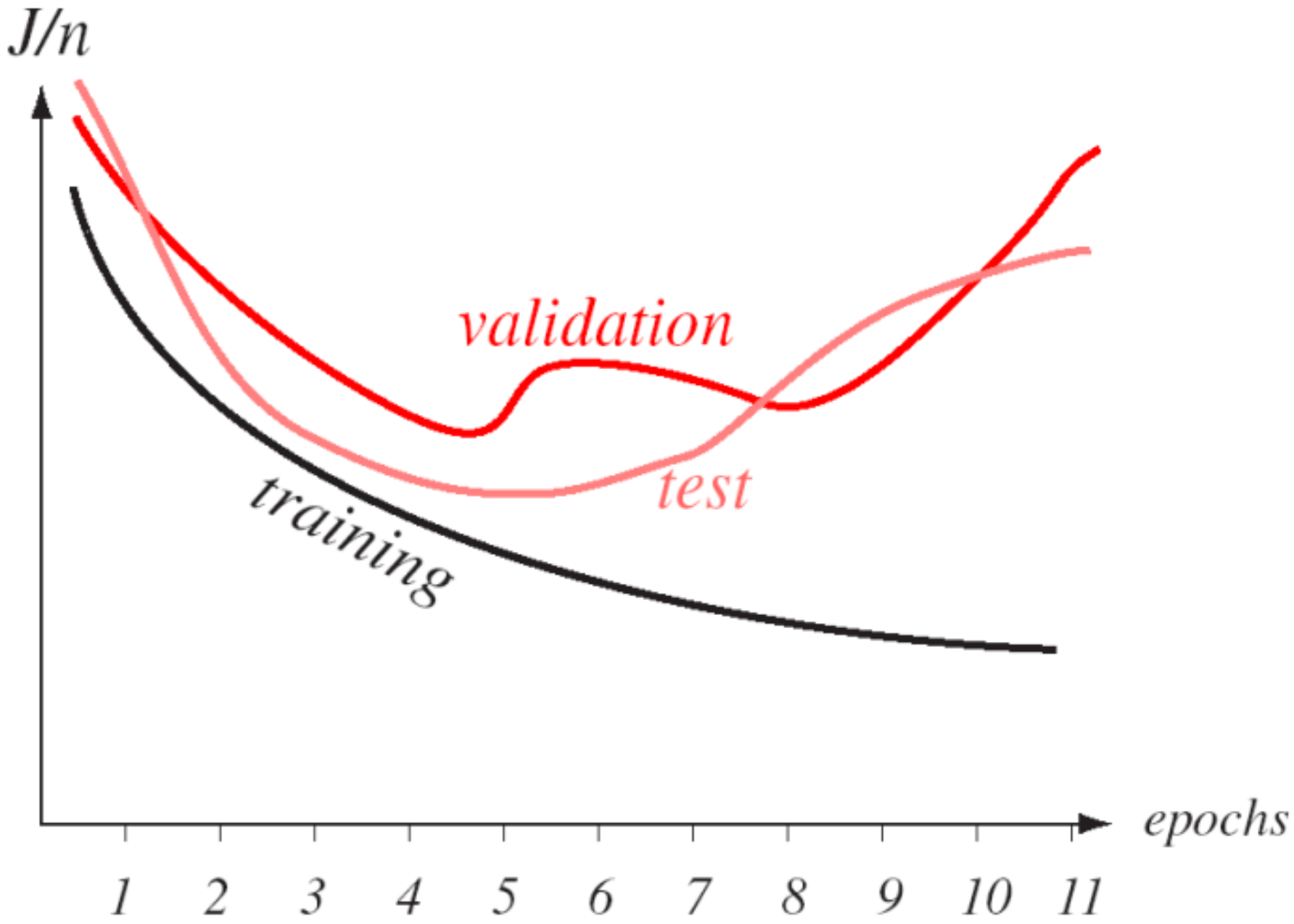
- The partial derivative,

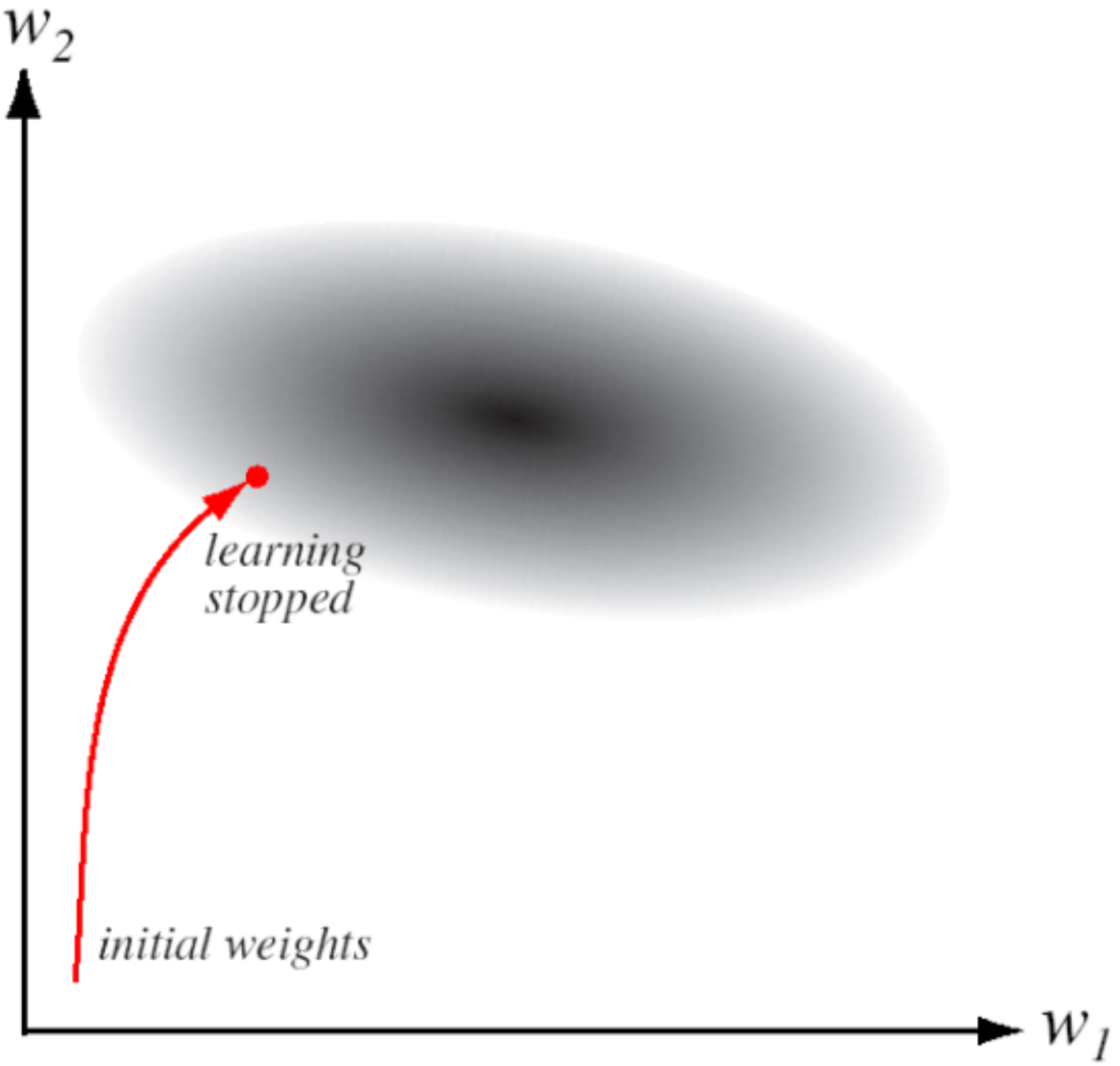
$$\frac{\partial \text{cost}_i^{CE}}{\partial w_{k,h}} = -(y_{i,k} - \hat{y}_{i,k}) z_{i,h}$$

- (homework!) Nowadays, the cross-entropy cost function is being used

Regularization with Stopped-Training

- In the next picture you can see a typical behaviour of training error and test error as a function of training time (an epoch is one pass through all data during learning)
- As expected the training error steadily decreases with epochs
- As expected, the test error first decreases as well; maybe surprisingly there is a minimum, after which the test error increases
- Explanation: During training, the degrees of freedom in the neural network slowly increase; with too many degrees of freedom, overfitting occurs
- It is possible to regularize a neural network by simply stopping the adaptation at the right moment (regularization by stopped-training)


J/n
validation
test
training
epochs
1
2
3
4
5
6
7
8
9
10
11


w_2
learning
stopped
initial weights
w_1

Optimizing the Learning Rate η

- Convergence can be influenced by the learning rate η
- Next figure: if the learning rate is too small, convergence can be very slow, if too large the iterations can oscillate and even diverge
- The learning rate can be adapted to the learning process ("Adaptive Learning Rate Control"); a popular variant is called Adaptive Moment Estimation (Adam) (see deep learning lecture)

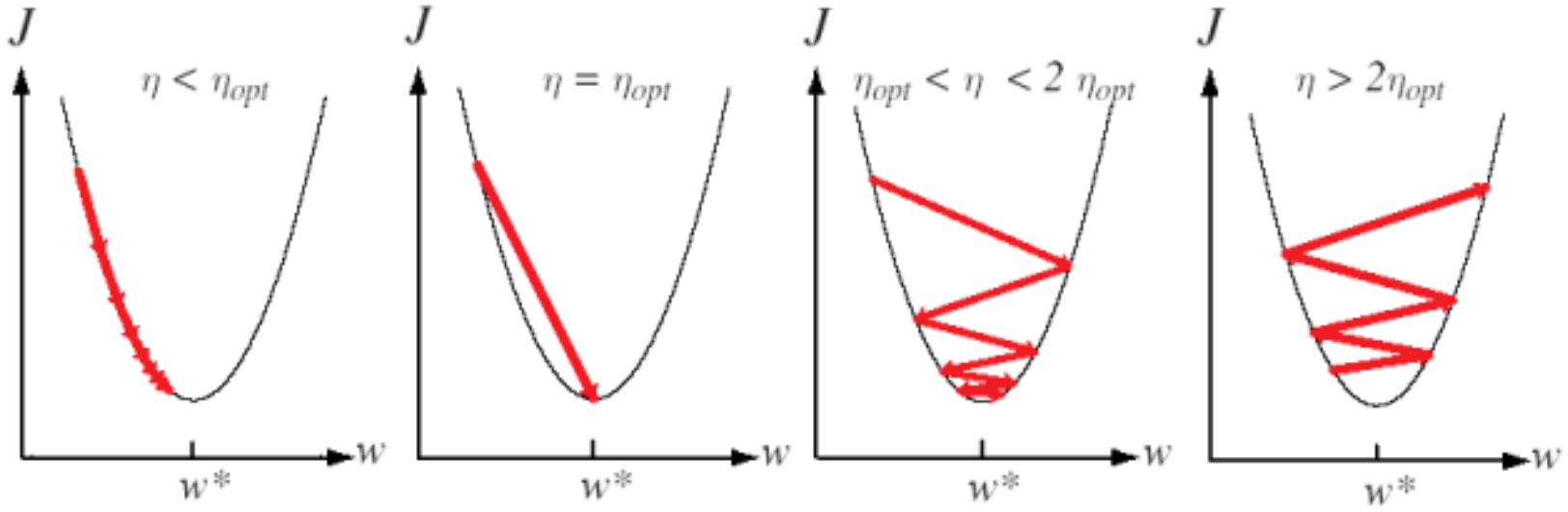
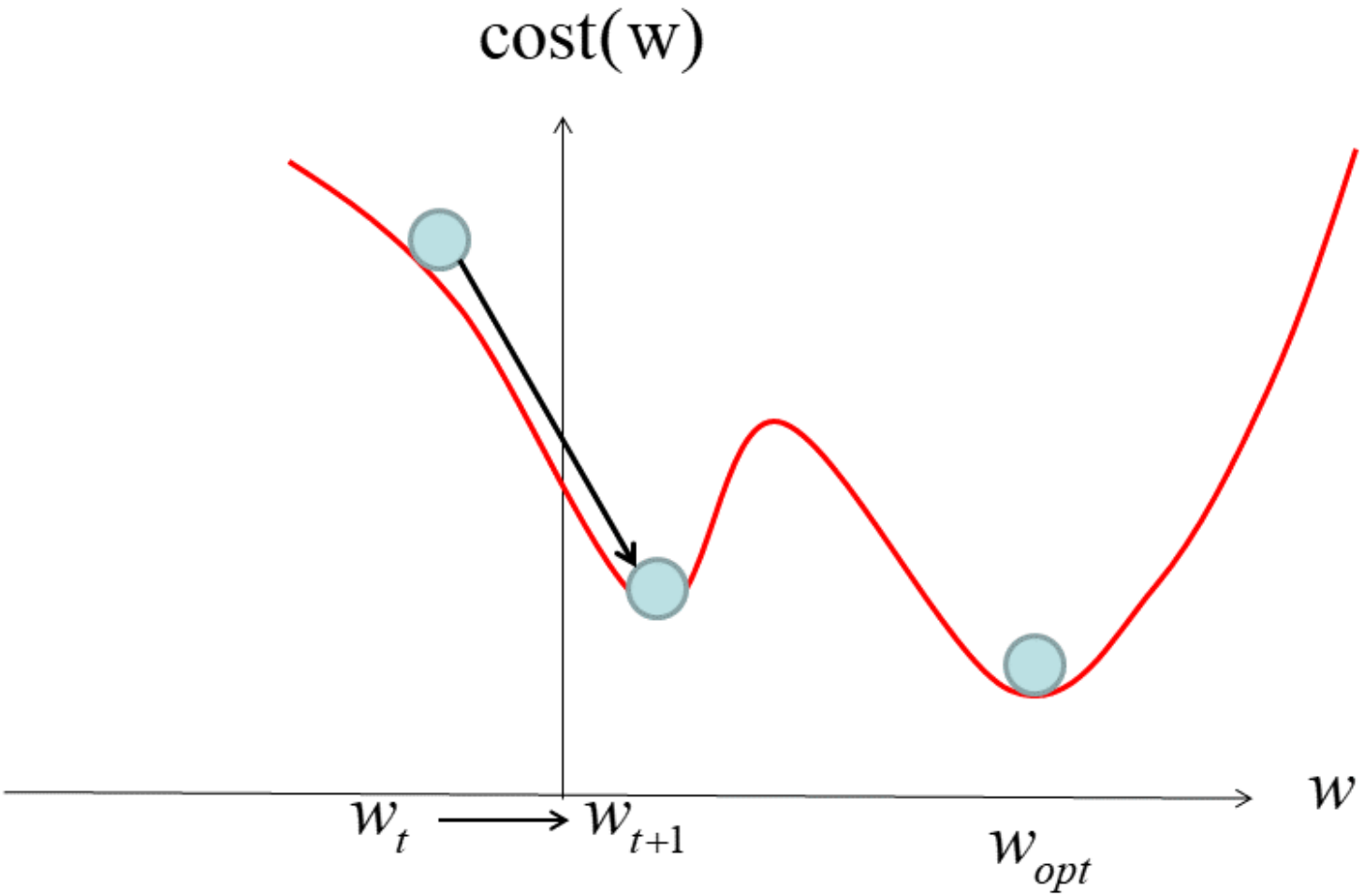
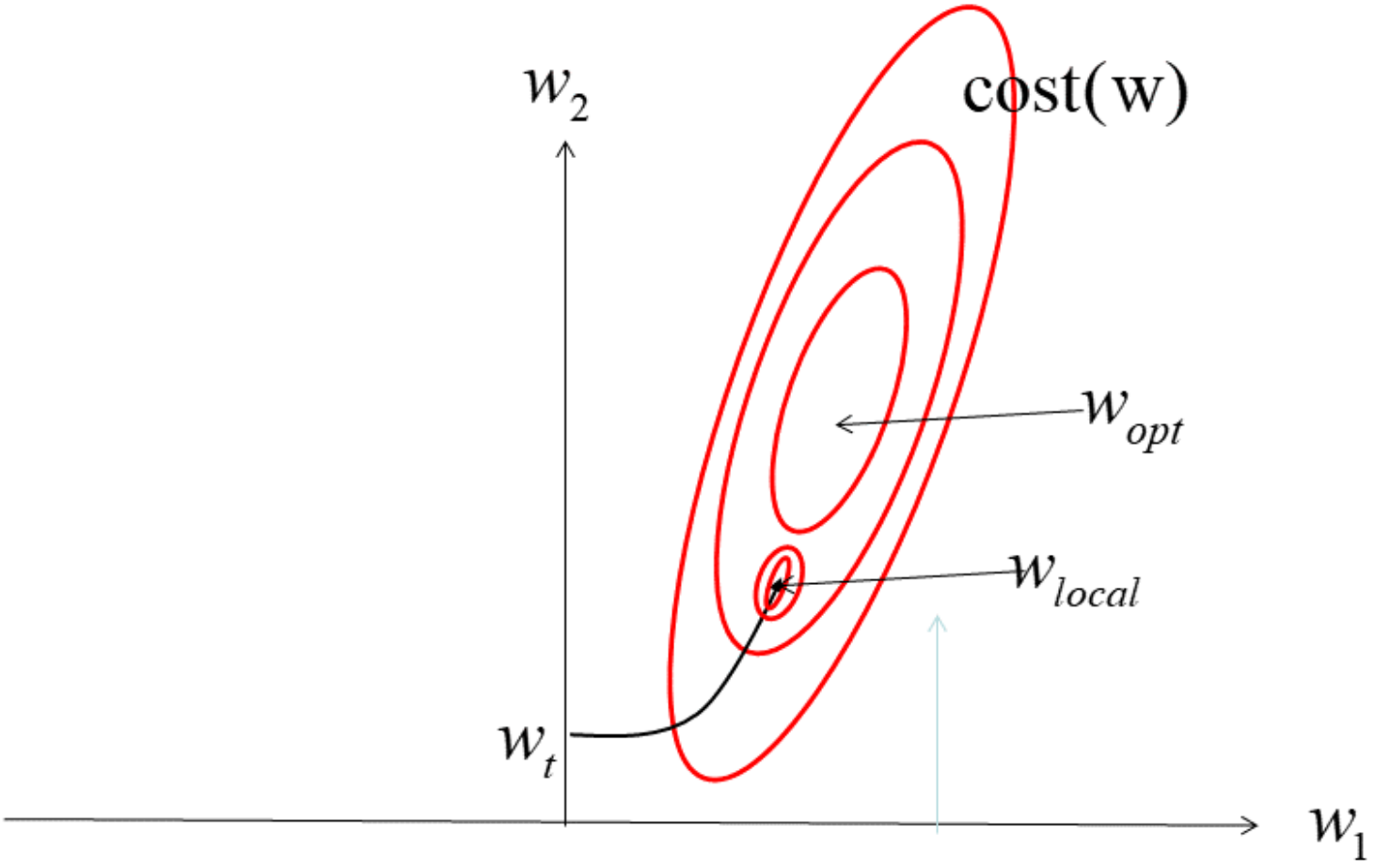


FIGURE 6.16. Gradient descent in a one-dimensional quadratic criterion with different learning rates. If $\eta < \eta_{opt}$, convergence is assured, but training can be needlessly slow. If $\eta = \eta_{opt}$, a single learning step suffices to find the error minimum. If $\eta_{opt} < \eta < 2\eta_{opt}$, the system will oscillate but nevertheless converge, but training is needlessly slow. If $\eta > 2\eta_{opt}$, the system diverges. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

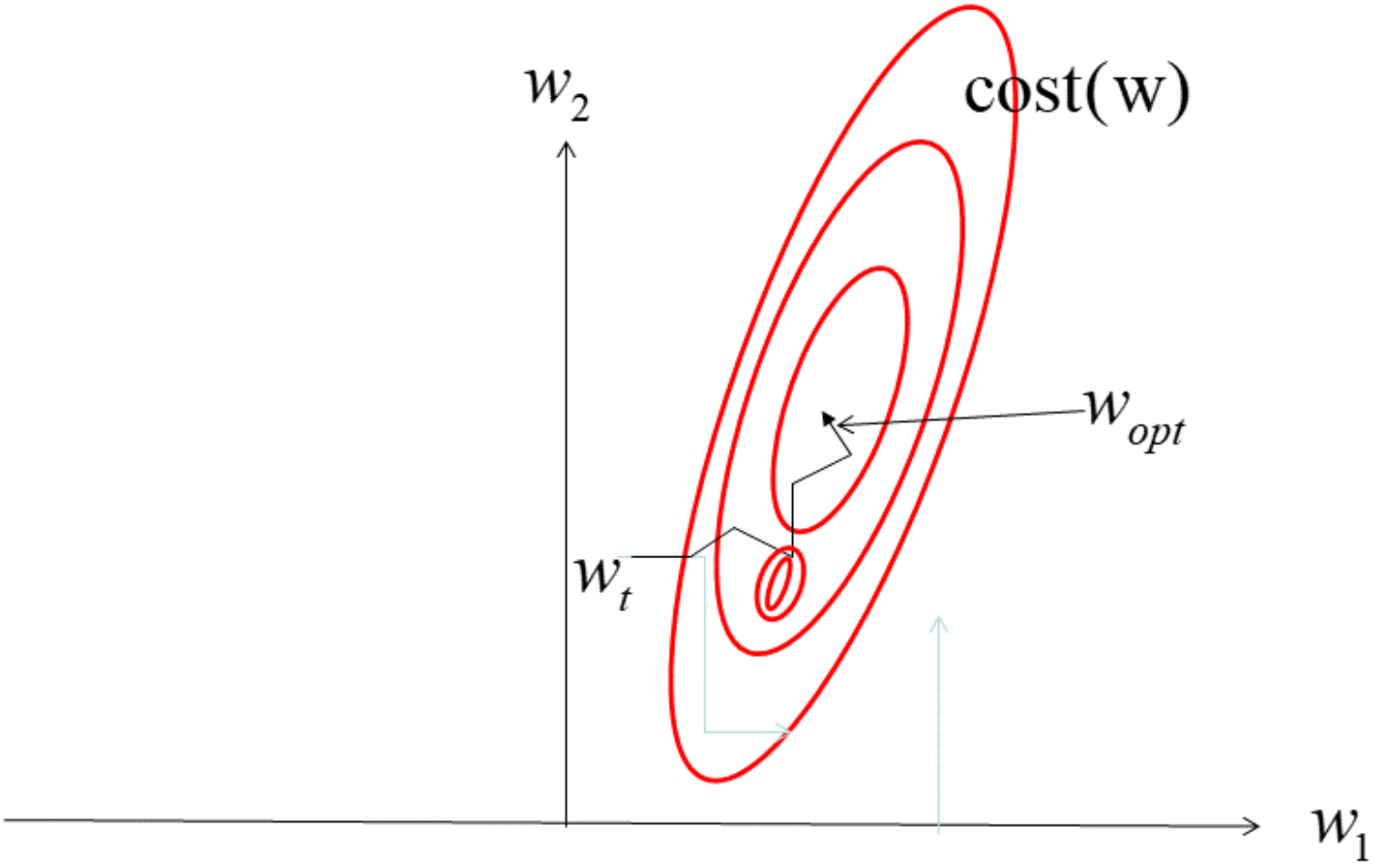
Local Solutions


cost(w)
w_t
w_{t+1}
w_{opt}
w

Local Solutions


w_2
cost(w)
w_{opt}
w_{local}
w_t
w_1

SGD has Fewer Problems with Local Optima

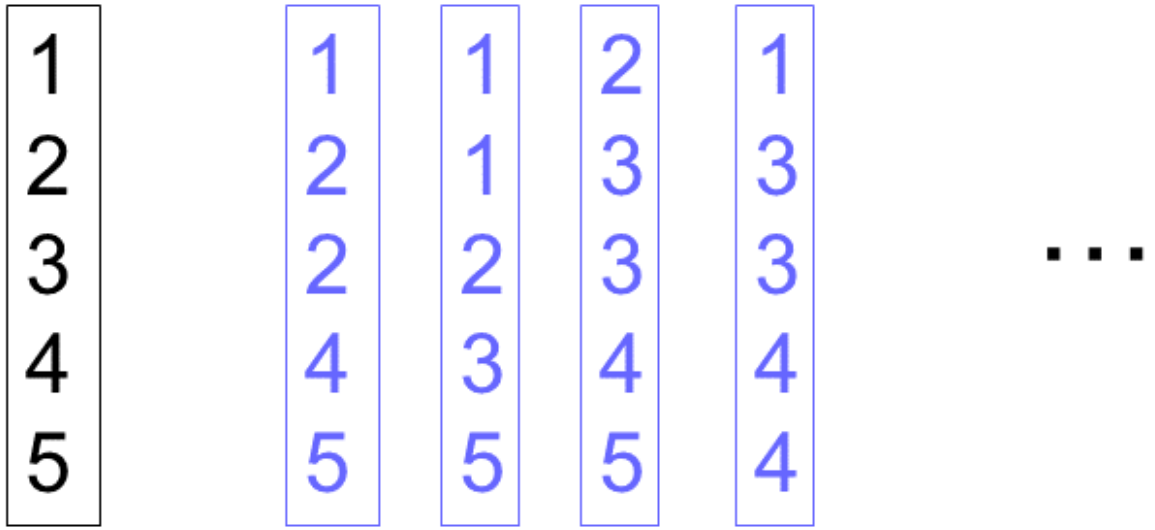

w_2
cost(w)
w_{opt}
w_t
w_1

Dealing with Local Optima

- Restart: Simply repeat training with different initial values and take the best one
- Committee: Repeat training with different initial values and take all of them: for regression, simply average the responses, for classification, take a majority vote

Bagging

- Bagging: Bootstrap AGGregatING
- Committee as before, but each neural network is trained on a different bootstrap sample of the training data
- Bootstrap sample: From N training data, randomly select N data points *with replacement*. This means one generates a new training data set with again N data points but where some data points of the original set occur more than once and some not at all
- If you apply this committee idea to decision trees you get Random Forests (used to win many Kaggle competitions; now often beaten by deep neural networks)


1
2
3
4
5
1 2 2 4 5
1 1 2 3 5
2 3 3 4 5
1 3 3 4 4
...
Original data
Bootstrap sample

Conclusion

- Neural Networks are very powerful and show excellent performance
- Training can be complex and slow, but one might say with some justification, that a neural network really learns something: the optimal representation of the data in the hidden layer
- Predictions are fast!
- Neural Networks are universal approximators and have excellent approximation properties
- Key: Basis functions are not predifined by some more or less smart procedure (as in fixed basis function approaches) but the learning algorithm attempts to find the "optimal", problem specific basis functions
- Disadvantage: training a neural network is something of an art; a number of hyper parameters have to be tuned (number of hidden neurons, learning rate, regularization parameters, ...)

Conclusion (cont'd)

- Not all problems can be formulated as a neural network learning problem (but surprisingly many real world problems)
- Disadvantage: A trained neural network finds a local optimum. The solution is not unique, e.g. depends on the initialization of the parameters. Solutions: multiple runs, committee machines
- Note added in 2016; Computing libraries like Theano, TensorFlow, Keras, and PyTorch use symbolic differentiation; you never have to program backprop: calculating the gradient manually is error prone and tedious for complex structured models

APPENDIX: Approximation Accuracy of Neural Networks

Complexity Measure

- How many hidden neurons are required for a certain approximation accuracy?
- Define the complexity measure C_f as

$$\int |\omega||\tilde{f}(\omega)|\, d\omega = C_f,$$

  where $\tilde{f}(\omega)$ is the Fourier transform of $f(\mathbf{x})$. ω is the frequency vector in M dimensions. C_f penalizes (assigns a high value to) rough functions containing high frequency components!
- So, *roughness* $\approx C_f$
- The target function class $\mathcal{F}$ now consists of all functions with a complexity measure smaller or equal to C_f
- We consider again

$$\|\mathbf{f} - \mathbf{g}\|_B^2 = \frac{1}{V_B} \int_B (f(\mathbf{x}) - g(\mathbf{x}))^2 d\mathbf{x}$$

Here V_B is the volume of the unit ball B in M dimensions

Main Result

- Our model class $\mathcal{M}$ consists of neural networks with one hidden layer
- Barron showed that for each target $f(\mathbf{x})$, with a finite C_f, there is a neural network with one hidden layer, with

$$\|\mathbf{f} - \mathbf{f}_{\mathbf{w}}\|_B^2 \leq \frac{4C_f^2}{H} \tag{1}$$

- We can then estimate the number of neurons in the hidden layer as

$$H = \mathcal{O}\left(\textit{accuracy} \times C_f^2\right)$$

  The number of parameters is dominated by the number of parameters in the layer between input and hidden; thus,

$$M_P = \mathcal{O}\left(M \times \textit{accuracy} \times C_f^2\right)$$

- Recall that before we got for fixed basis functions

$$M_\phi = M_P = \mathcal{O}\left(\textit{accuracy}^{M \times \textit{roughness}}\right)$$

Main Result (cont'd)

- For important function classes it could be shown that C_f only increases weakly (e.g., proportional) with M
- Examples where C_f only increases weakly (e.g., proportional) with M: The functions become very smooth in high dimensions (Case III (smooth)), or in Case Ia (sparse basis); neural networks also do well in Ib (manifold), and, of course, II (blessing) and IV (smooth)
- Quellen: V. Tresp. Die besonderen Eigenschaften Neuraler Netze bei der Approximation von Funktionen. *Kuenstliche Intelligenz,* Nr. 4., 1995.

  A. Barron. Universal Approximation Bounds for Superpositions of a Sigmoidal Function. *IEEE Trans. Information Theory,* Vol. 39, Nr. 3, 1993.