732A99/TDDE01 Machine Learning

Lecture 3c Block 1: Neural Networks

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Contents

Literature

- Main source
  - Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Sections 5.1-5.3.3 and 5.5.2.
- Additional source
  - Hastie, T., Tibshirani, R. and Friedman, J. *The Elements of Statistical Learning*. Springer, 2009. Chapter 11.

Neural Networks

- Consider binary classification with input space $\mathbb{R}^D$. Consider a training set $\{(\boldsymbol{x}_n, t_n)\}$ where $t_n \in \{-1, +1\}$.

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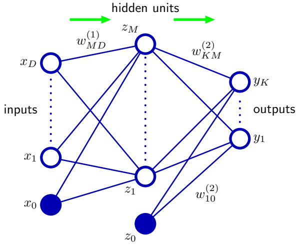
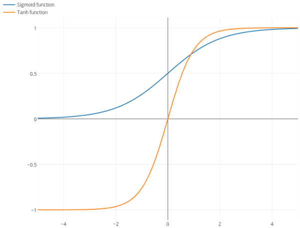
- NNs imply a user-defined number of data-selected basis functions.

Neural Networks





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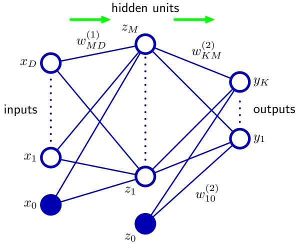

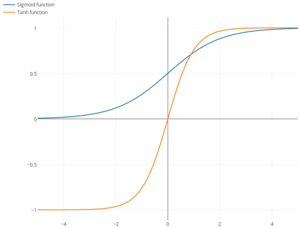

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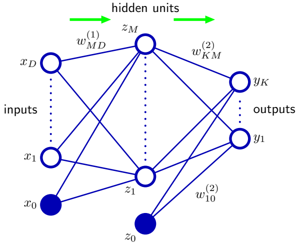

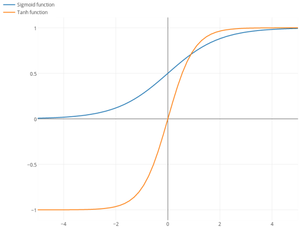

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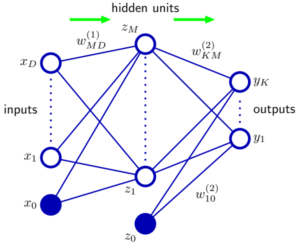
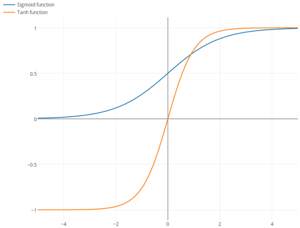
Neural Networks





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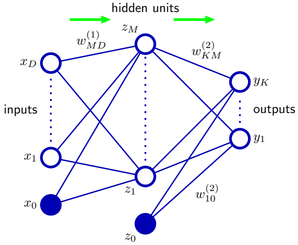

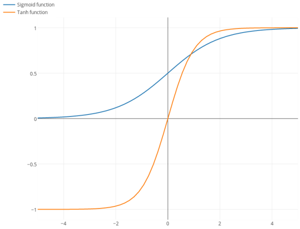

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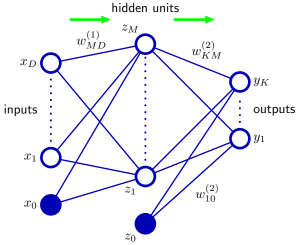

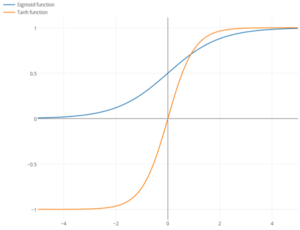

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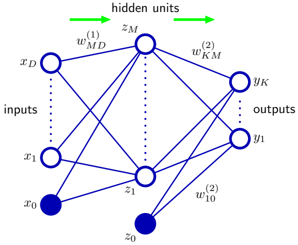

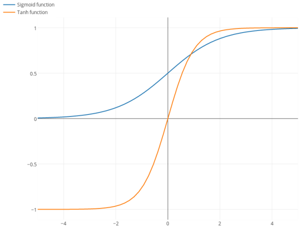

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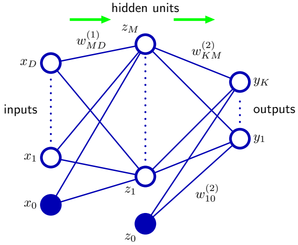

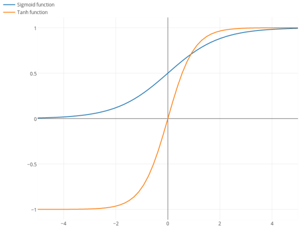

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- Two-layer NN:

$$y_k(\boldsymbol{x}) = \sigma\Big(\sum_j w_{kj}^{(2)} h\Big(\sum_i w_{ji}^{(1)} x_i + w_{j0}^{(1)}\Big) + w_{k0}^{(2)}\Big)$$

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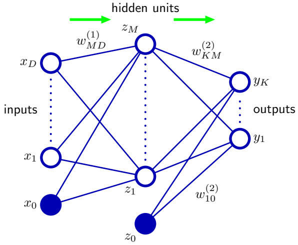

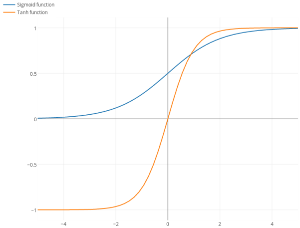

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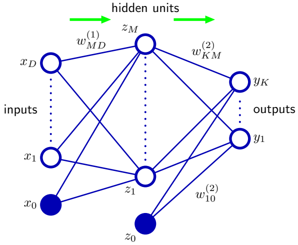
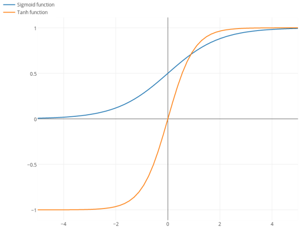
Neural Networks





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- All the previous is, of course, generalizable to more layers.

Neural Networks

- For a large variety of activation functions, the two-layer NN can uniformly approximate any continuous function to arbitrary accuracy provided enough hidden units. Easy to fit the parameters ? Overfitting ?!

Figure 5.3 Illustration of the capability of a multilayer perceptron to approximate four different functions comprising (a) $f(x) = x^2$, (b) $f(x) = \sin(x)$, (c), $f(x) = |x|$, and (d) $f(x) = H(x)$ where $H(x)$ is the Heaviside step function. In each case, $N = 50$ data points, shown as blue dots, have been sampled uniformly in x over the interval $(-1, 1)$ and the corresponding values of $f(x)$ evaluated. These data points are then used to train a two-layer network having 3 hidden units with 'tanh' activation functions and linear output units. The resulting network functions are shown by the red curves, and the outputs of the three hidden units are shown by the three dashed curves.

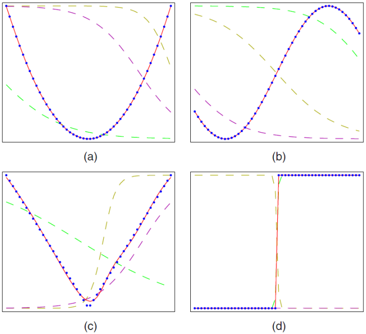
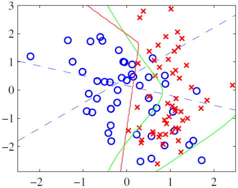
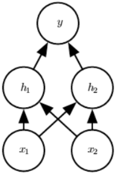


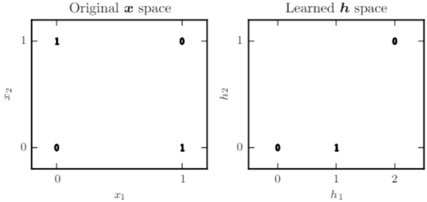
Figure 5.4 Example of the solution of a simple two-class classification problem involving synthetic data using a neural network having two inputs, two hidden units with 'tanh' activation functions, and a single output having a logistic sigmoid activation function. The dashed blue lines show the $z = 0.5$ contours for each of the hidden units, and the red line shows the $y = 0.5$ decision surface for the network. For comparison, the green line denotes the optimal decision boundary computed from the distributions used to generate the data.



Neural Networks

- Solving the XOR problem with NNs.
- No line shatters the points in the original space.
- The NN represents a mapping of the input space to an alternative space where a line can shatter the points. Note that the points (0,1) and (1,0) are mapped both to the point (1,0).
- **It resembles SVMs**.





$$w_{11}^{(1)} = w_{12}^{(1)} = w_{21}^{(1)} = w_{22}^{(1)} = 1$$
$$w_{10}^{(1)} = 0,\ w_{20}^{(1)} = -1$$
$$h_j = z_j = h(a_j) = \max\{0, a_j\}$$
$$w_{11}^{(2)} = 1,\ w_{12}^{(2)} = -2$$
$$w_{10}^{(2)} = 0$$
$$y = y_k = a_k$$

Backpropagation Algorithm

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Backprojection Algorithm

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- This error function can be justified from a maximum likelihood approach to learning $\boldsymbol{w}$. To see it, **assume** that

$$p(t_k|\boldsymbol{x}, \boldsymbol{w}, \sigma) = \mathcal{N}(t_k|y_k(\boldsymbol{x}), \sigma)$$

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  which is equivalent to the sum-of-squares error function for a given σ.
- If σ is not given, then we can find the ML estimates of $\boldsymbol{w}$, plug them into the log likelihood function, and maximize it with respect to σ.

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  where $\eta_t > 0$ is the learning rate ($\sum_t \eta_t = \infty$ and $\sum_t \eta_t^2 < \infty$ to ensure convergence, e.g. $\eta_t = 1/t$).

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- Sequential, stochastic or online gradient descent

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta_t \nabla E_n(\boldsymbol{w}^{t})$$

  where n is chosen randomly or sequentially.

Backpropagation Algorithm

- The weight space is highly multimodal and, thus, we have to resort to approximate iterative methods to minimize the previous expression.
- Batch gradient descent

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta_t \nabla E(\boldsymbol{w}^{t})$$

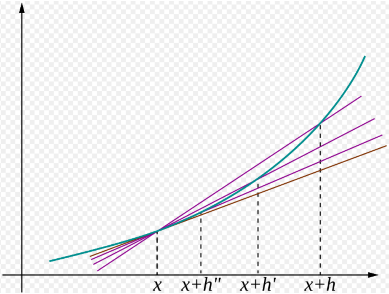
  where $\eta_t > 0$ is the learning rate ($\sum_t \eta_t = \infty$ and $\sum_t \eta_t^2 < \infty$ to ensure convergence, e.g. $\eta_t = 1/t$).
- Sequential, stochastic or online gradient descent

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta_t \nabla E_n(\boldsymbol{w}^{t})$$

  where n is chosen randomly or sequentially.
- Sequential gradient descent is less affected by the multimodality problem, as a local minimum of the whole data will not be generally a local minimum of each individual point.

Backpropagation Algorithm

- Recall that $f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$



- Recall that $\nabla E_n(\boldsymbol{w}^t)$ is a vector whose components are the partial derivatives of $E_n(\boldsymbol{w}^t)$.

Backpropagation Algorithm

- Since E_n depends on w_{ji} only via a_j, and $a_j = \sum_i w_{ji} x_i$, then

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j} x_i = \delta_j x_i$$

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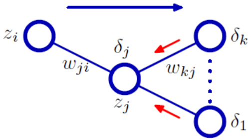

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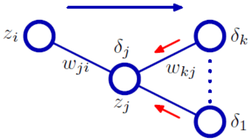

- For classification, we minimize the negative log likelihood function, a.k.a. cross-entropy error function:

$$E_n(\boldsymbol{w}) = -\sum_k \left[t_{nk} \ln y_k(\boldsymbol{x}_n) + (1 - t_{nk}) \ln(1 - y_k(\boldsymbol{x}_n)) \right]$$

with $t_{nk} \in \{0, 1\}$ and $y_k(\boldsymbol{x}_n) = \sigma(a_k)$. Then, again

$$\frac{\partial E_n}{\partial w_{kj}} = \delta_k z_j \text{ and } \delta_k = \frac{\partial E_n}{\partial a_k} = y_k - t_k$$

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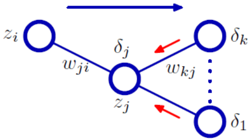

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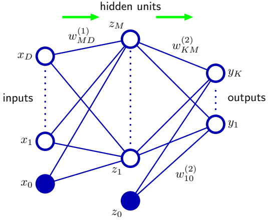
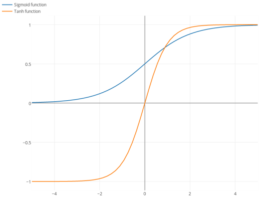
- This is an example of embarrassingly parallel algorithm.

Backpropagation Algorithm





- Example: $y_k = a_k$, and $z_j = h(a_j) = \tanh(a_j)$ where $\tanh(a) = \frac{\exp(a)-\exp(-a)}{\exp(a)+\exp(-a)}$.

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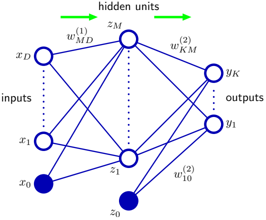

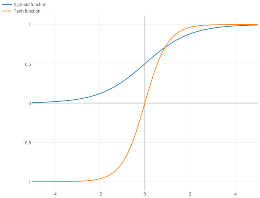

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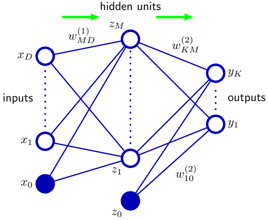

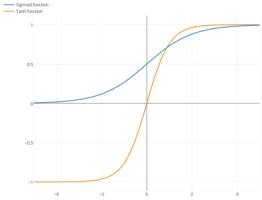

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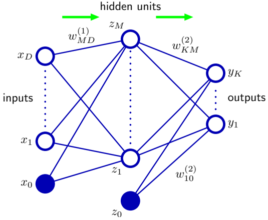

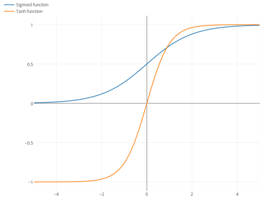

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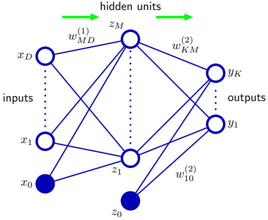

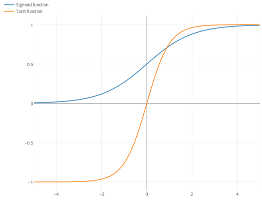

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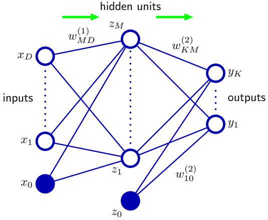

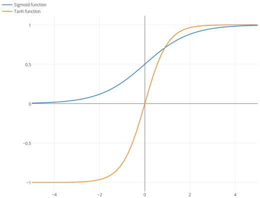

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  - Initialize the weights to almost-zero values so that the initial model is almost-linear, i.e. the sigmoid function is almost-linear around the zero. Let the algorithm to introduce non-linearities where needed.
    - Note however that this initialization makes the sigmoid function take a value around half its saturation level. That is why the hyperbolic tangent function is sometimes preferred in practice.

Regularization

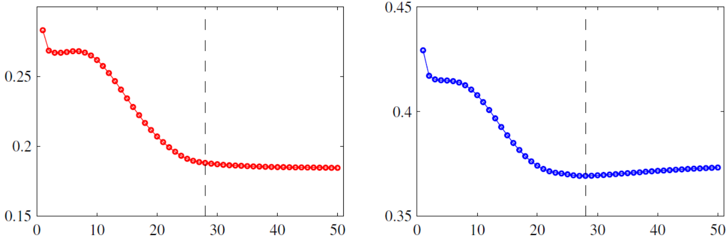

Figure 5.12 An illustration of the behaviour of training set error (left) and validation set error (right) during a typical training session, as a function of the iteration step, for the sinusoidal data set. The goal of achieving the best generalization performance suggests that training should be stopped at the point shown by the vertical dashed lines, corresponding to the minimum of the validation set error.

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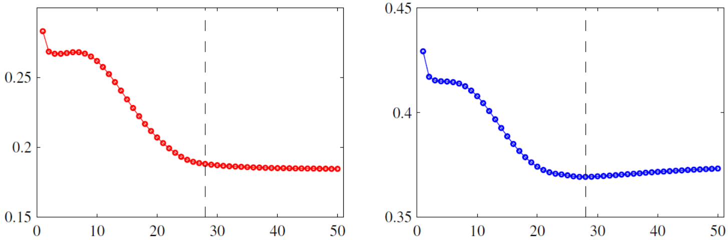

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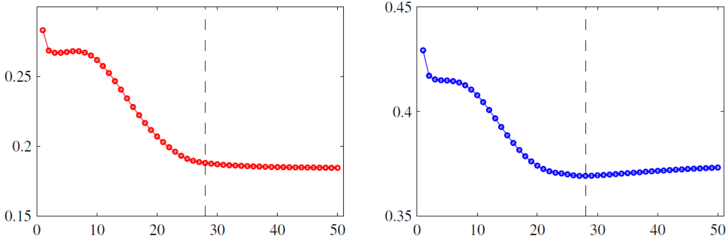

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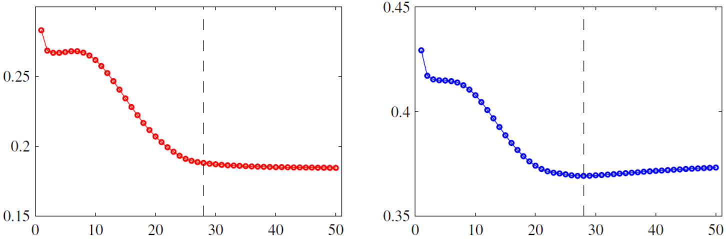

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- Regularization when learning the structure:
  - Cross-validation.
  - Penalizing complexity according to

$$E(\boldsymbol{w}) + \frac{\lambda}{2}||\boldsymbol{w}||^2 \text{ or } E(\boldsymbol{w}) + \frac{\lambda_1}{2}||\boldsymbol{w}^{(1)}||^2 + \frac{\lambda_2}{2}||\boldsymbol{w}^{(2)}||^2$$

    and choose λ, or λ_1 and λ_2 by cross-validation. Note that the effect of the penalty is simply to add λw_{ji} and λw_{kj}, or $\lambda_1 w_{ji}$ and $\lambda_2 w_{kj}$ to the appropriate derivatives.

Summary

- NNs: Nonlinear mapping from input to output.
- Extremely expressive.
- Training: Backpropagation algorithm, and regularization.