Introduction to Statistical Machine Learning

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Outlines

Part IX

Neural Networks 1

Basis Functions

- The basis functions play a crucial role in the algorithms explored so far.
- Number and parameters of basis functions fixed before learning starts (e.g. Linear Regression and Linear Classification).
- Number of basis functions fixed, parameters of the basis functions are adaptive (e.g. Neural Networks).
- Center basis function on the data, select a subset of basis functions in the training phase (e.g. Support Vector Machines, Relevance Vector Machines).

Outline

- The functional form of the network model (including special parametrisation of the basis functions).
- How to determine the network parameters within the maximum likelihood framework? (Solution of a nonlinear optimisation problem.)
- Error backpropagation : efficiently evaluate the derivatives of the log likelihood function with respect to the network parameters.
- Various approaches to regularise neural networks.

Feed-forward Network Functions

- Same goal as before: Decompose the target t

$$t(\mathbf{x}) = y(\mathbf{x}, \mathbf{w}) + \epsilon(\mathbf{x})$$

  where $\epsilon(\mathbf{x})$ is the residual error.

- (Generalised) Linear Model

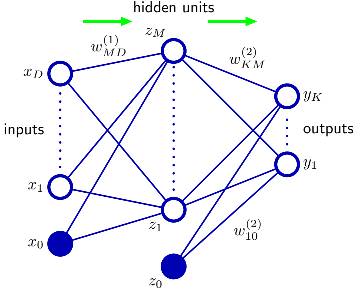
$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=0}^{M} w_j \phi_j(\mathbf{x})\right)$$

  where $\boldsymbol{\phi} = (\phi_0, \dots, \phi_M)^T$ is the fixed model basis and $\mathbf{w} = (w_0, \dots, w_M)^T$ are the model parameter.

- For regression: $f(\cdot)$ is the identity function.
- For classification: $f(\cdot)$ is a nonlinear activation function.
- Goal : Let $\phi_j(\mathbf{x})$ depend on parameters, and then adjust these parameters together with $\mathbf{w}$.

Feed-forward Network Functions

- Goal : Let $\phi_j(\mathbf{x})$ depend on parameters, and then adjust these parameters together with $\mathbf{w}$.
- Many ways to do this.
- Neural networks use basis functions which follow the same form as the (generalised) linear model.
- EACH basis function is itself a nonlinear function of an adaptive linear combination of the inputs.



Functional Transformations

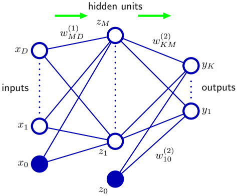
- Construct M linear combinations of the input variables $x_1, \dots, x_D$ in the form

$$\underbrace{a_j}_{\text{activations}} = \sum_{i=1}^{D} \underbrace{w_{ji}^{(1)}}_{\text{weights}} x_i + \underbrace{w_{j0}^{(1)}}_{\text{bias}} \qquad j = 1, \dots, M$$

- Apply a differentiable, nonlinear activation function $h(\cdot)$ to get the output of the hidden units

$$z_j = h(a_j)$$

- $h(\cdot)$ is typically sigmoidal or $\tanh$.



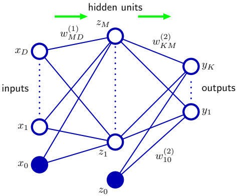
Functional Transformations

- The outputs of the hidden units are again linearly combined

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)} \qquad k = 1, \dots, K$$

- Apply again a differentiable, nonlinear activation function $g(\cdot)$ to get the network outputs y_k

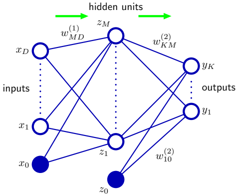
$$y_k = g(a_k)$$



Functional Transformations

- The activation function $g(\cdot)$ is determined by the nature of the data and the distribution of the target variables.
- For standard regression: $g(\cdot)$ is the identity function so that $y_k = a_k$.
- For multiple binary classification, $g(\cdot)$ is a logistic sigmoid function

$$y_k = \sigma(a_k) = \frac{1}{1 + \exp(-a_k)}$$

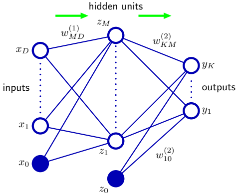


Functional Transformations

- Combine all transformations into one formula

$$y_k(\mathbf{x}, \mathbf{w}) = g\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}\right) + w_{k0}^{(2)}\right)$$

where $\mathbf{w}$ contains all weight and bias parameters.

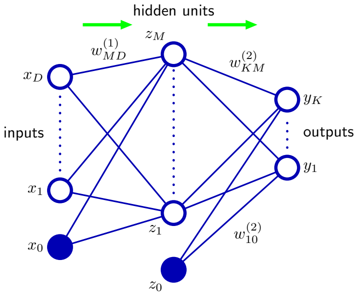


Functional Transformations

- As before, the biases can be absorbed into the weights by introducing an extra input $x_0 = 1$ and a hidden unit $z_0 = 1$.

$$y_k(\mathbf{x}, \mathbf{w}) = g\left(\sum_{j=0}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right)$$

where $\mathbf{w}$ now contains all weight and bias parameters.

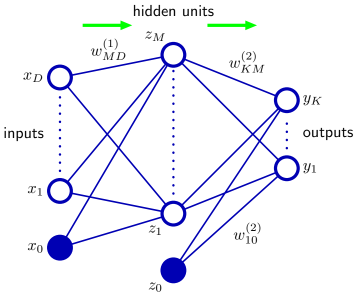


Comparison to Perceptron

- A neural network looks like a multilayer perceptron.
- But perceptron's nonlinear activation function was a step function. Not smooth. Not differentiable.

$$f(a) = \begin{cases} +1, & a \geq 0 \\ -1, & a < 0 \end{cases}$$

- The activation functions $h(\cdot)$ and $g(\cdot)$ of a neural network are smooth and differentiable.



Linear Activation Functions

- If all activation functions are linear functions then there exists an equivalent network without hidden units. (Composition of linear functions is a linear function.)
- But if the number of hidden units in this case is smaller than the number of input or output units, the resulting linear function are not the most general.
- Dimensionality reduction.
- Principal Component Analysis (comes later in the lecture).
- Generally, most neural networks use nonlinear activation functions as the goal is to approximate a nonlinear mapping from the input space to the outputs.

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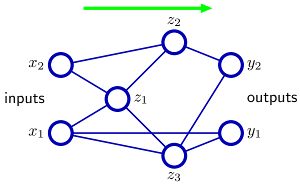
Extensions of the Neural Network Architecture

- Add more hidden layers.
- Some units may be not fully connected to the next layer.
- Some links may skip over one or several subsequent layer(s).
- Still in the framework of feed-forward networks.
- Note: If information is allowed to flow also backwards, we get a graph with cycles. This is called a recurrent neural network which can exhibit a very different dynamical behaviour (e.g. may have state, may exhibit chaos). Not further considered here.



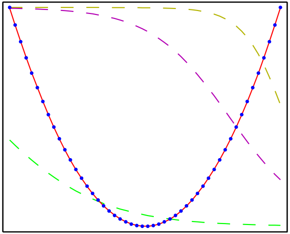
Neural Networks as Universal Function Approximators

- Feed-forward neural networks are universal approximators.
- Example: A two-layer neural network with linear outputs can uniformly approximate any continuous function on a compact input domain to arbitrary accuracy if it has enough hidden units.
- Holds for a wide range of hidden unit activation functions, but NOT for polynomials.
- Remaining big question : Where do we get the appropriate settings for the weights from? With other words, how do we learn the weights from training examples?

Aproximation Capabilities of Neural Networks

- Neural network approximating

$$f(x) = x^2$$

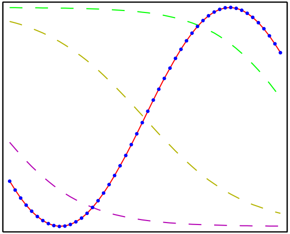


Two-layer network with 3 hidden units ($\tanh$ activation functions) and linear outputs trained on 50 data points sampled from the interval $(-1, 1)$. Red: resulting output. Dashed: Output of the hidden units.

Aproximation Capabilities of Neural Networks

- Neural network approximating

$$f(x) = \sin(x)$$



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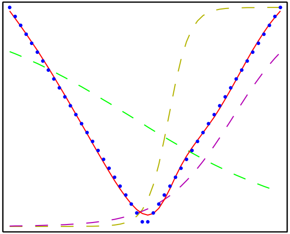
Aproximation Capabilities of Neural Networks

- Neural network approximating

$$f(x) = |x|$$

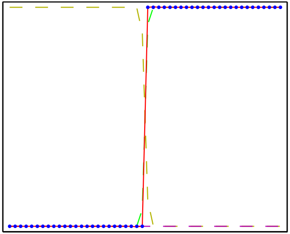


Two-layer network with 3 hidden units ($\tanh$ activation functions) and linear outputs trained on 50 data points sampled from the interval $(-1, 1)$. Red: resulting output. Dashed: Output of the hidden units.

Aproximation Capabilities of Neural Networks

- Neural network approximating Heaviside function

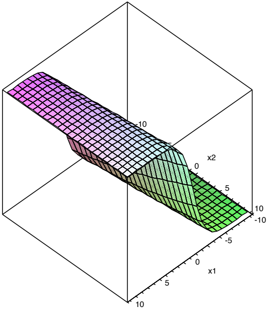
$$f(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$



Two-layer network with 3 hidden units ($\tanh$ activation functions) and linear outputs trained on 50 data points sampled from the interval $(-1, 1)$. Red: resulting output. Dashed: Output of the hidden units.

Variable Basis Functions in a Neural Networks

- Hidden layer nodes represent parametrised basis functions



$z = \sigma(w_0 + w_1 x_1 + w_2 x_2)$ for $(w_0, w_1, w_2) = (0.0, 1.0, 0.1)$

Variable Basis Functions in a Neural Networks

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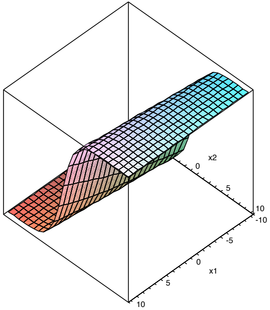

$z = \sigma(w_0 + w_1 x_1 + w_2 x_2)$ for $(w_0, w_1, w_2) = (0.0, 0.1, 1.0)$

Variable Basis Functions in a Neural Networks

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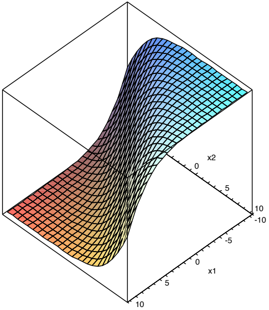
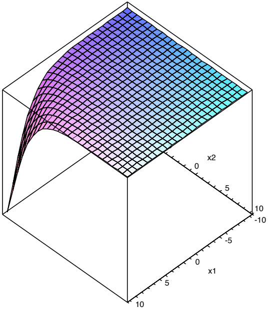


$z = \sigma(w_0 + w_1 x_1 + w_2 x_2)$ for $(w_0, w_1, w_2) = (0.0, -0.5, 0.5)$

Variable Basis Functions in a Neural Networks

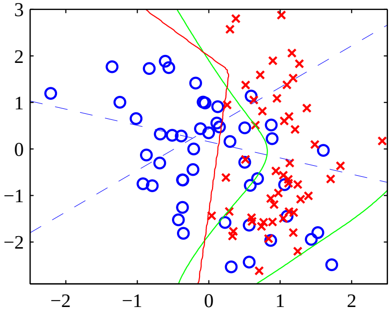
- Hidden layer nodes represent parametrised basis functions



$$z = \sigma(w_0 + w_1 x_1 + w_2 x_2) \text{ for } (w_0, w_1, w_2) = (10.0, -0.5, 0.5)$$

Aproximation Capabilities of Neural Networks

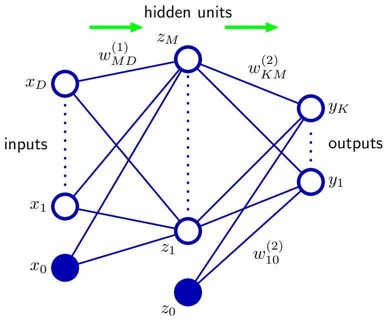
- Neural network for two-class classification.
- 2 inputs, 2 hidden units with $\tanh$ activation function, 1 output with logistic sigmoid activation function.



Red: $y = 0.5$ decision boundary. Dashed blue: $z = 0.5$ hidden unit contours. Green: Optimal decision boundary from the known data distribution.

Weight-space Symmetries

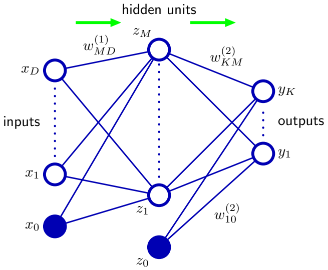
- Given a set of weights $\mathbf{w}$. This fixes a mapping from the input space to the output space.
- Does there exist another set of weights realising the same mapping?
- Assume $\tanh$ activation function for the hidden units. As $\tanh$ is an odd function: $\tanh(-a) = -\tanh(a)$.
- Change the sign of all inputs to a hidden unit and outputs of this hidden unit: Mapping stays the same.



Weight-space Symmetries

- M hidden units, therefore 2^M equivalent weight vectors.
- Furthermore, exchange all of the weights going into and out of a hidden unit with the corresponding weights of another hidden unit. Mapping stays the same. $M!$ symmetries.
- Overall weight space symmetry : $M!\,2^M$

M	1	2	3	4	5	6	7
$M!\,2^M$	2	8	48	384	3840	46080	645120



Parameter Optimisation

- Assume the error $E(\mathbf{w})$ is a smooth function of the weights.
- Smallest value will occur at a critical point for which

$$\nabla E(\mathbf{w}) = 0.$$

- This could be a minimum, maxium, or saddle point.
- Furthermore, because of symmetry in weight space, there are at least $M!\,2^M$ other critical points with the same value for the error.

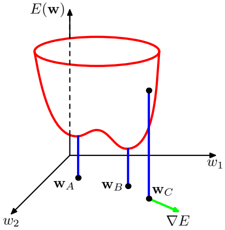
Parameter Optimisation

Definition (Global Minimum)

A point $\mathbf{w}^*$ for which the error $E(\mathbf{w}^*)$ is smaller than any other error $E(\mathbf{w})$.

Definition (Local Minimum)

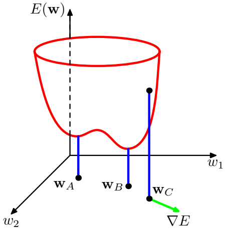
A point $\mathbf{w}^*$ for which the error $E(\mathbf{w}^*)$ is smaller than any other error $E(\mathbf{w})$ in some neighbourhood of $\mathbf{w}^*$.



Parameter Optimisation

- Finding the global minimum is difficult in general (would have to check everywhere) unless the error function comes from a special class (e.g. smooth convex functions have only one minimum).
- Error functions for neural networks are not convex (symmetries!).
- But finding a local minimum might be sufficient.
- Use iterative methods with weight vector update $\Delta \mathbf{w}^{(\tau)}$ to find a local minimum.

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \Delta \mathbf{w}^{(\tau)}$$



Local Quadratic Approximation

- Around a minimum $\mathbf{w}^*$ we can approximate

$$E(\mathbf{w}) \simeq E(\mathbf{w}^*) + \frac{1}{2}(\mathbf{w} - \mathbf{w}^*)^T \mathbf{H}(\mathbf{w} - \mathbf{w}^*),$$

  where the Hessian $\mathbf{H}$ is evaluated at $\mathbf{w}^*$.
- Using a set $\{\mathbf{u}_i\}$ of orthonormal eigenvectors of $\mathbf{H}$,

$$\mathbf{H}\mathbf{u}_i = \lambda_i \mathbf{u}_i,$$

  to expand

$$\mathbf{w} - \mathbf{w}^* = \sum_i \alpha_i \mathbf{u}_i.$$

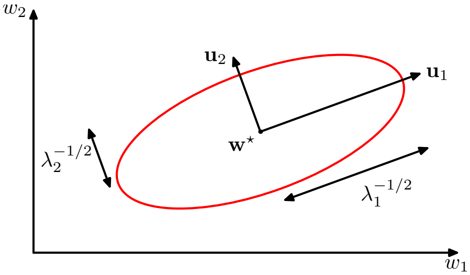
- We get

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2} \sum_i \lambda_i \alpha_i^2.$$

Local Quadratic Approximation

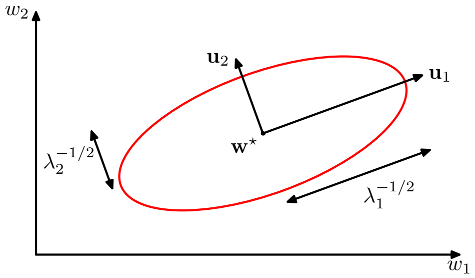
- Around a minimum $\mathbf{w}^*$ we can approximate

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2} \sum_i \lambda_i \alpha_i^2.$$



Local Quadratic Approximation

- Around a minimum $\mathbf{w}^*$, the Hessian $\mathbf{H}$ must be positive definite if evaluated at $\mathbf{w}^*$.



Gradient Information improves Performances

- Hessian is symmetric and contains $W(W+1)/2$ independent entries where W is the total number of weights in the network.
- Need to gather this $O(W^2)$ pieces of information by doing $O(W)$ function evaluations if nothing else is know. Get order $O(W^3)$.
- The gradient ∇E provides W pieces of information at once. Still need $O(W)$ steps, but the order is now $O(W^2)$.

Gradient Descent Optimisation

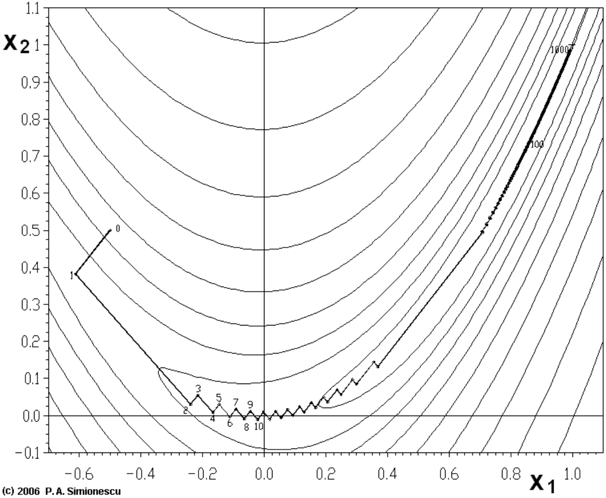
- Batch processing : Update the weight vector with a small step in the direction of the negative gradient

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E(\mathbf{w}^{(\tau)})$$

  where η is the learning rate.
- After each step, re-evaluate the gradient $\nabla E(\mathbf{w}^{(\tau)})$ again.
- Gradient Descent has problems in 'long valleys'.

Gradient Descent Optimisation

- Gradient Descent has problems in 'long valleys'.



Example of zig-zag of Gradient Descent Algorithm.

Nonlinear Optimisation

- Use Conjugate Gradient Descent instead of Gradient Descent to avoid zig-zag behaviour.
- Use Newton method which also calculates the inverse Hessian in each iteration (but inverting the Hessian is usually costly).
- Use Quasi-Newton methods (e.g. BFGS) which also calculates an estimate of the inverse Hessian while iterating.
- Run the algorithm from a set of starting points to find the smallest local minimum.

Nonlinear Optimisation

- Remaining big problem: Error function is defined over the whole training set. Therefore, need to process the whole training set for each calculation of the gradient $\nabla E(\mathbf{w}^{(\tau)})$.
- If the error function is a sum of errors for each data point

$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

we can use on-line gradient descent (also called sequential gradient descent or stochastic gradient descent updating the weights by one data point at a time

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n(\mathbf{w}^{(\tau)}).$$