Statistical Machine Learning

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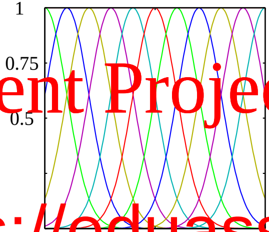
(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Outlines

Part VII

Basis Functions



- Play a crucial role in the algorithms explored so fa
- Previously (*e.g.* Linear Regression and Lin Classification): were fixed before learning sta
- Now for Neural Networks: number of basis functions fixed, parameters of the basis functions are adaptive
- Later in kernel methods: center basis functions on the data / have an infinite number of effective basis functions (*e.g.* Support Vector Machines).

Outline

- The functional form of the network model (including special parametrisation of the basis functions).
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- Error backpropagation : efficiently evaluate t
  of the log likelihood function with respect to the ne
  parameters.

- Various approaches to regularise neural net

Feed-forward Network Functions

- Same goal as before: *e.g.* for regression, decompose

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

  where ϵ is the noise.

- (Ge

$$j=0$$

  where $\phi = (\phi_0, \ldots, \phi_M)^T$ is the fixed mode
  $\mathbf{w} = (w_0, \ldots, w_M)^T$ are the model paramete

- 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.
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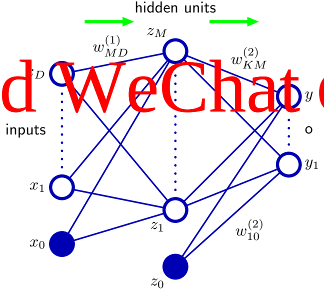

Functional Transformations

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

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)} \qquad j = 1, \dots, M$$

activations   weights   bias

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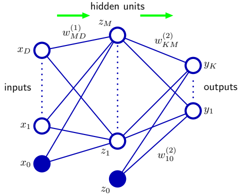
- $h(\cdot)$ is typically sigmoid, $\tanh$, or more rec
ReLU$(x) = \max(x, 0)$

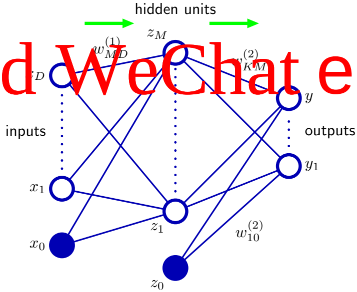


Functional Transformations

- Outputs of the hidden units are again linearly combined

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

- Ap
  $g(\cdot)$



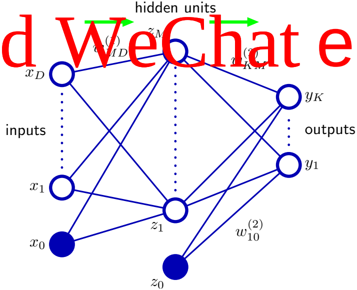
Functional Transformations

- 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 so $y_k = a_k$.
- For multiple binary classification, $g(\cdot)$ is a logistic sigmoid:

$$y_k = \sigma(a_k) = \frac{1}{[illegible]}$$

- Re [illegible]

$$\frac{[illegible]}{p(\mathbf{x}, \mathcal{C}_{k_2})}$$

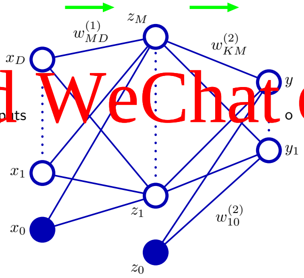


Functional Transformations

- Combine all transformations into one formula

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

wh

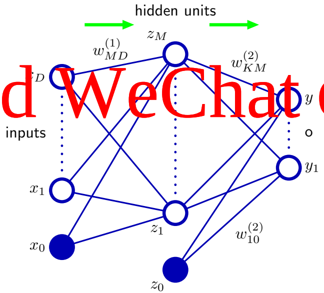


Functional Transformations

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

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

wh



Comparison to Perceptron

- A neural network looks like a multilayer perceptron.
- But perceptron's nonlinear activation function was a step function — neither smooth nor differentiable.

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

- The
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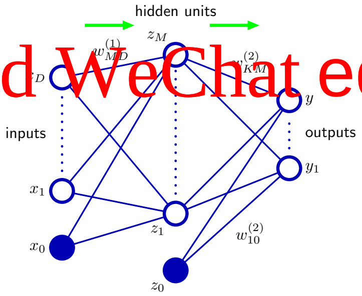

Linear Activation Functions

- 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 t
  tha
  line

- Dimensionality reduction.
- *c.f.* Principal Component Analysis (upcomi

- Generally, most neural networks use nonline functions as the goal is to approximate a nonline mapping from the input space to the outputs.

Neural Networks as Universal Function Approximators

- Feed-forward neural networks are universal app
- Exa
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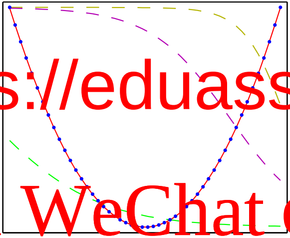
  co
  enough hidden units.
- Holds for a wide range of hidden unit activation fu
- Remaining big question : Where do we get the ap settings for the weights from? With other words we learn the weights from training examples?

Aproximation Capabilities of Neural Networks

- Neural network approximating

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



Two-layer network with 3 hidden units (
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

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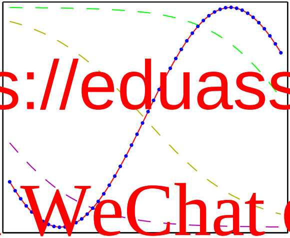
- Neural network approximating

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



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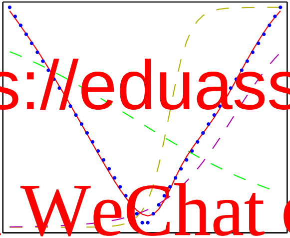
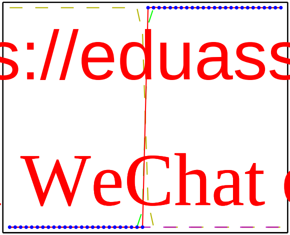


Two-layer network with 3 hidden units (functions) and linear outputs trained on 50 data points sampled from the interval $(-1, 1)$. Red: resulting output. Dashed: Output of the hidden units.

Aproximation Capabilities of Neural Networks

- Neural network approximating Heaviside function

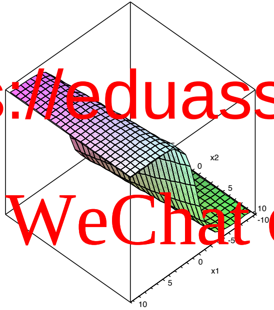
$$f(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$



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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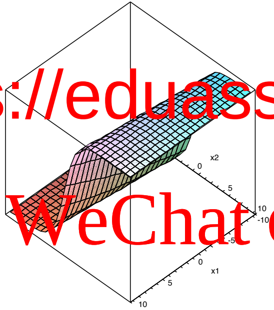

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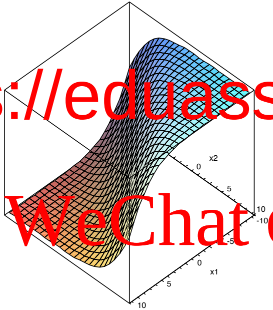

$z = \sigma(w_0 + w_1 x_1 + w_2 x_2)$ for $(w_0, w_1, w_2) = (0.0, -0.5, 0.5)$

Variable Basis Functions in a Neural Networks

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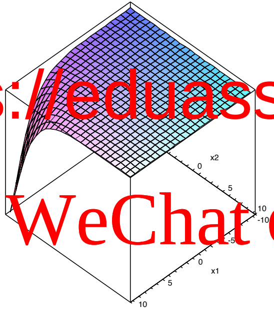

$z = \sigma(w_0 + w_1 x_1 + w_2 x_2)$ for $(w_0, w_1, w_2) = (10.0, -0.5, 0.5)$

Aproximation Capabilities of Neural Networks

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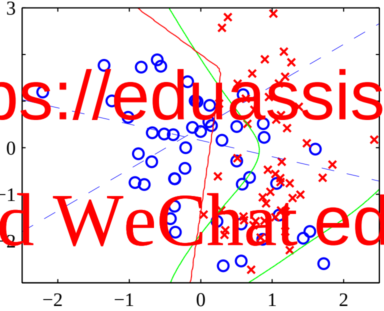
- Neural network for two-class classification.
- 2 inputs, 2 hidden units with $\tanh$ activation function, 1 output with logistic sigmoid activation function.



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 $\tan$
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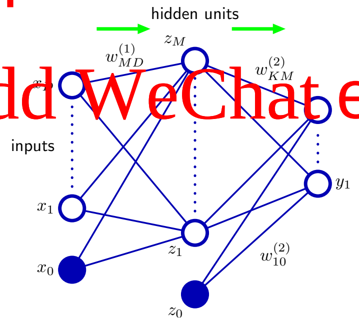

Weight-space Symmetries

- 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.
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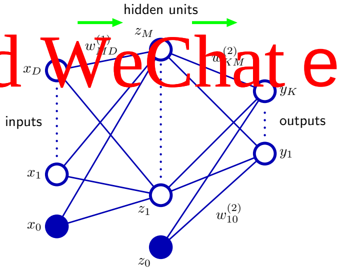
M							



- Assume the error $E(\mathbf{w})$ is a smooth function of the weights.
- Sm

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

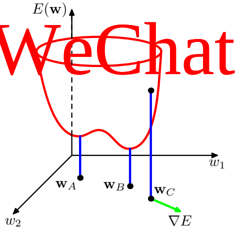
Definition (Global Minimum)

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

Definitio

A point

error $E($



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 local minimum).
- Error functions for neural networks are not convex (sy
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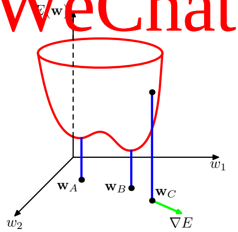
- Us find

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



Local Quadratic Approximation

- Around a stationary point $\mathbf{w}^*$ 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 $\mathbf{w}^*$ so that

- Usi $\{\ _i\}$

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

to expand

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

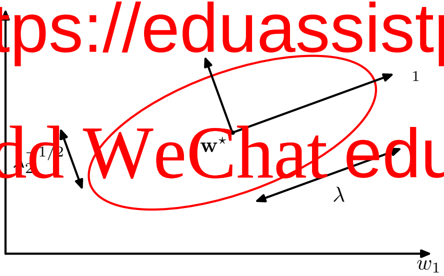
- We get

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

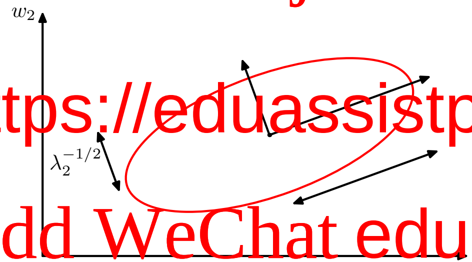
Local Quadratic Approximation

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

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



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



- This explains why the Laplace approximation always yields a valid covariance matrix.

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.

- If we use function evaluations only:
  - 2

- If we
  - Surprisingly the gradient ∇E also costs although it provides W pieces of informa
  - We now need only $O(W)$ steps, so the o complexity is reduced to $O(W^2)$.

FYI only: In general we have the "cheap gradient principle". See (Griewank, A., 2000. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*, Section 5.1).

Gradient Descent Optimisation

- Batch processing : Update the weight vector with a small ste

  where η is the learning rate.
- After each step, re-evaluate the gradient
- Gradient Descent has problems in long valley

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.
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  He
  usu
- Us
  calculates an estimate of the inverse Hessian w
  iterating.
- Even simpler are *momentum* based stra
- Run the algorithm from a set of starting points to fin
  smallest local minimum.

- 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

$$n=1$$

we can use on-line gradient descent (also called sequential gradient descent or stochastic gradient descent) to update the weights by one data point

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

FYI Only: NN Extensions

- Add more hidden layers (deep learning). To make it work we need many of the following tricks:
- Clever weight initialisation to ensure the gradient is flowing through the entire network.
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  sub
- Fav
  gra
- Clever regularisation methods such as dropo
- Specific architectures, not further considere
  - Parameters may be shared, notably as in conv neural networks for images.
  - A state space model with neural network transitions is a recurrent neural network.
  - Attention mechanisms learn to focus on specific parts of an input.