UFME7K-15-M Intelligent and Adaptive Systems

Multi-Layer Perceptrons. Approximation, generalisation and validation

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Intelligent Adaptive Systems Lecture 4

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- We are focussing on function approximation tasks
  - regression
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- The same principles apply also to classification tasks (pattern recognition)
- Note that we are only considering what are now considered to be fairly small problems and other approaches (e.g. Deep Learning) are more appropriate in problems with much larger datasets

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- Therefore, they incorporate the danger of overfitting.

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  - We will try to find some **heuristics** to help design a good network

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Performance plot showing overfitting

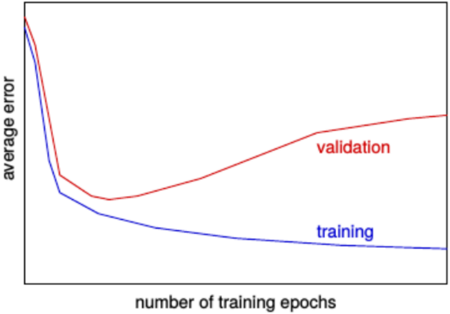

Figure 1: Overfitting

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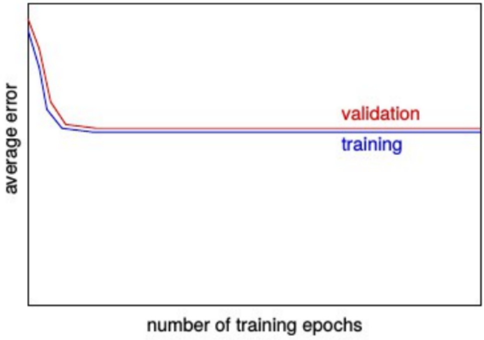

Figure 2: Underfitting

Which is a better fit to the data?

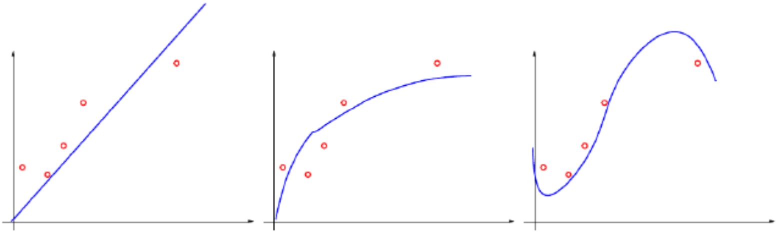

Figure 3: Some alternative curves to fit the data

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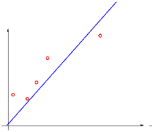
- Underfit 

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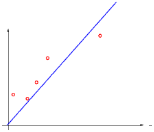
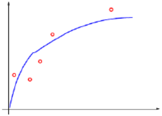
- Underfit 
- OK 

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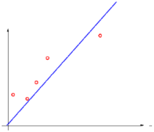
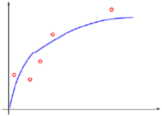
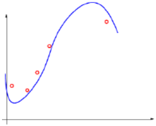
- Underfit 
- OK 
- Over-fit 

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- Note we cannot calculate the expected error since we don't know P or $f^*(\mathbf{x})$

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    - But if the learning algorithm is too flexible, it will fit each training data set differently, and hence have high variance.

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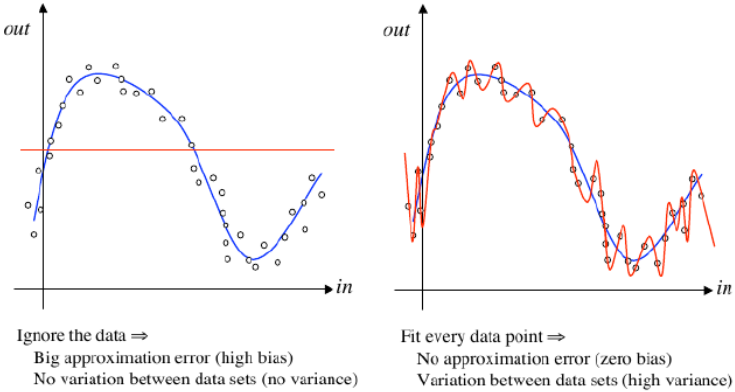
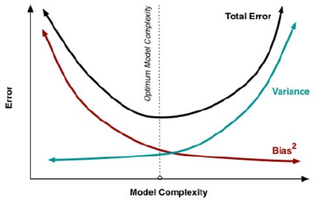


Figure 4: Bias and Variance on a Data-fitting Example

Bias/Variance Trade-off



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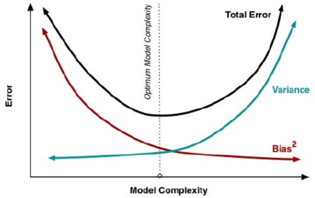

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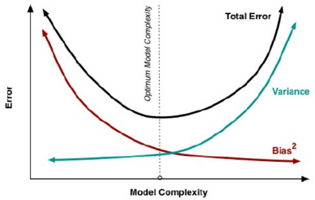

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- Bias is reduced and variance is increased in relation to model complexity.
  - As more parameters are added to a model, the complexity of the model rises and variance becomes our primary concern while bias steadily falls

Design Questions

1. How many hidden layers?
2. How many hidden nodes per layer?
3. How many training input/target pairs needed?
4. How many random initial weight trials for each hidden node configuration?

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  - However, noise may make it difficult to identify the significant error-free extrema.

Simplefit Example

2.5 local min

2.5 local max

H >= 2.5 * 2

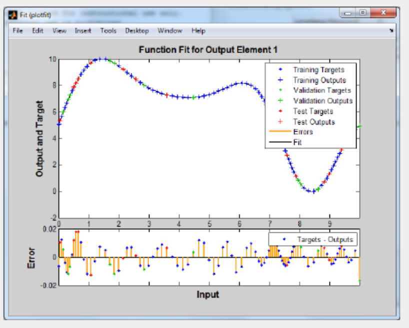

Figure 6: Simplefit function

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Error Minimization as Gradient Descent

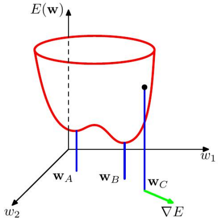

Figure 7: error surface of a network with 2 weights(Bishop, 2006)

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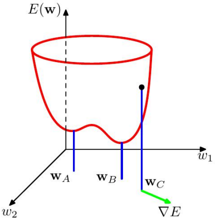

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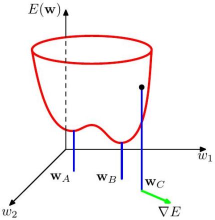

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- at any point w_c, the local gradient of the error surface is given by the vector ∇E

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  - the hypothesis set H of smaller networks is smaller than the hypothesis set of large networks
  - smaller weights should be prefered
  - neurons with logistic activation function and small weights are almost linear, networks of linear neurons can be replaced by a single neuron

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  - and Foresee and Hagan (Proceedings of the International Joint Conference on Neural Networks, June, 1997) for more detailed discussions of Bayesian regularization

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Bayesian Regularisation algorithm (Foresee and Hagan)

0. Initialize α, β and the weights
1. Take one step of the Levenberg-Marquardt algorithm to minimize the objective function
$$F(w) = \beta E_D + \alpha E_W$$
2. Compute the effective number of parameters
$$\gamma = N - 2\alpha tr(\mathbf{H})^{-1}$$
making use of the Gauss-Newton approximation to the Hessian available in the Levenberg-Marquardt training algorithm
3. Compute new estimates for the objective function parameters
$$\alpha = \frac{\gamma}{2E_w(\mathbf{w})}$$
and
$$\beta = \frac{n - \gamma}{2E_D(\mathbf{w})}$$
4. Now iterate steps 1 through 3 until convergence.

References and Further Reading

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