Introduction to Statistical Machine Learning

Christfried Webers

Statistical Machine Learning Group
NICTA
and
College of Engineering and Computer Science
The Australian National University

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

Outlines

Part X

Neural Networks 2

Error Backpropagation

- Goal: Efficiently update the weights in order to find a local minimum of some error function $E(\mathbf{w})$ utilizing the gradient of the error function.
- Core ideas :
  1. Propagate the errors backwards through the network to efficiently calculate the gradient.
  2. Update the weights using the calculated gradient.
- Sequential procedure : Calculate gradient and update weights for each data/target pair.
- Batch procedure : Collect gradient information for all data/target pairs for the same weight setting. Then adjust the weights.
- Main question in both cases: How to calculate the gradient of $E(\mathbf{w})$ given one data/target pair?

Error Backpropagation

- Assume the error is a sum over errors for each data/target pair

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

- After applying input $\mathbf{x}_n$ to the network, we get the output $\mathbf{y}_n$ and calculate the error $E_n(\mathbf{w})$.
- What is the gradient for one such term $E_n(\mathbf{w})$?
- Note : In the following, we will drop the n on weights $\mathbf{w}$ and targets $\mathbf{t}$ in order to unclutter the equations.
- Notation: Input pattern is $\mathbf{x}_n$.
  Scalar x_i is the i^{th} component of the input pattern $\mathbf{x}_n$.

Error Backpropagation - Simplified Model

- Simple linear model without hidden layers
- One layer only, no nonlinear activation function!

$$y_k = \sum_l w_{kl}\, x_l,$$

and error after applying input $\mathbf{x}_n$

$$E_n(\mathbf{w}) = \frac{1}{2} \sum_{k=1} (y_k - t_k)^2.$$

- The gradient with respect to w_{ji} is now

$$\begin{aligned}
\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} &= \sum_{k=1} (y_k - t_k) \frac{\partial}{\partial w_{ji}} y_k = \sum_{k=1} (y_k - t_k) \frac{\partial}{\partial w_{ji}} \sum_l w_{kl}\, x_l \\
&= \sum_{k=1} (y_k - t_k) \sum_l x_l\, \delta_{jk} \delta_{il} \\
&= (y_j - t_j)\, x_i.
\end{aligned}$$

Error Backpropagation - Simplified Model

- Do the same using the directional derivative:
  input vector $\mathbf{x} \in \mathbb{R}^{D_1}$, output vector $\mathbf{y} \in \mathbb{R}^{D_2}$

$$\mathbf{y} = \mathbf{W}^T \mathbf{x},$$

  and error after applying input training pair $(\mathbf{x}, \mathbf{t})$

$$E_n(\mathbf{W}) = \frac{1}{2}(\mathbf{y} - \mathbf{t})^T(\mathbf{y} - \mathbf{t}).$$

- The directional derivative with respect to $\mathbf{W}$ is now

$$\mathcal{D}E_n(\mathbf{W})(\xi) = \frac{1}{2}\left((\xi^T\mathbf{x})^T(\mathbf{y} - \mathbf{t}) + (\mathbf{y} - \mathbf{t})^T\xi^T\mathbf{x}\right) = (\mathbf{y} - \mathbf{t})^T\xi^T\mathbf{x}$$

- With canonical inner product $\langle A, B\rangle = \operatorname{tr}\left\{A^T B\right\}$ the gradient of $E_n(\mathbf{W})(\xi)$ is

$$\mathcal{D}E_n(\mathbf{W})(\xi) = \operatorname{tr}\left\{\underbrace{(\mathbf{y} - \mathbf{t})^T\xi^T\mathbf{x}}_{\text{just a number}}\right\} = \operatorname{tr}\left\{\xi^T\underbrace{\mathbf{x}(\mathbf{y} - \mathbf{t})^T}_{\text{gradient}}\right\}$$

Error Backpropagation

- The gradient

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = (y_j - t_j)\, x_i.$$

  looks like the product of the output error $(y_j - t_j)$ with the input x_i associated with an edge for w_{ji} in the network diagram.
- Can we generalise this idea?

Error Backpropagation

- Now consider a network with nonlinear activation functions $h(\cdot)$ composed with the sum over the inputs z_i in one layer and z_j in the next layer connected by edges with weights w_{ji}

$$a_j = \sum_i w_{ji}\, z_i$$

$$z_j = h(a_j).$$

- Use the chain rule to calculate the gradient

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = \frac{\partial E_n(\mathbf{w})}{\partial a_j}\frac{\partial a_j}{\partial w_{ji}} = \delta_j\, z_i,$$

  where we defined the error $\delta_j = \frac{\partial E_n(\mathbf{w})}{\partial a_j}$

- Same intuition as before: gradient is output error times the input associated with the edge for w_{ji}.

Error Backpropagation

- Need to calculate the errors δ in EACH layer.

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = \delta_j \, z_i \qquad\qquad \delta_j = \frac{\partial E_n(\mathbf{w})}{\partial a_j}$$

- For the output units, we have

$$\delta_k = y_k - t_k.$$

- For the hidden units we calculate

$$\delta_j = \frac{\partial E_n(\mathbf{w})}{\partial a_j} = \sum_k \frac{\partial E_n(\mathbf{w})}{\partial a_k} \frac{\partial a_k}{\partial a_j} = \sum_k \delta_k \frac{\partial a_k}{\partial a_j},$$

using the definition of δ_k.

Error Backpropagation

- Express a_k as a function of the incoming a_j

$$a_k = \sum_j w_{kj} z_j = \sum_j w_{kj} h(a_j),$$

- and differentiate

$$\frac{\partial a_k}{\partial a_j} = w_{kj} \frac{\partial h(a_j)}{\partial a_j} = w_{kj} \left. \frac{\partial h(s)}{\partial s} \right|_{s=a_j} = w_{kj}\, h'(a_j).$$

- Finally, we get for the error in the previous layer

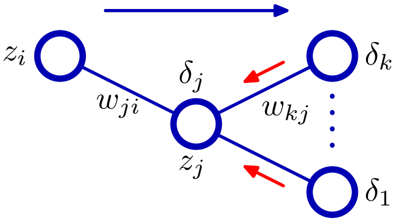
$$\delta_j = h'(a_j) \sum_k w_{kj}\, \delta_k.$$

Error Backpropagation

- The backpropagation formula

$$\delta_j = h'(a_j) \sum_k w_{kj} \delta_k.$$

- Functional form of $h'(\cdot)$ is known, because we choose the activation function $h(\cdot)$.

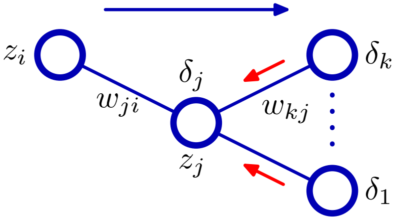


Error Backpropagation Algorithms

1. Apply the input vector $\mathbf{x}$ to the network and forward propagate through the network to calculate all activations and outputs of each unit.
2. Backpropagate the errors through the network.
3. Calculate all components of ∇E_n by

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = \delta_j \, z_i$$

4. Update the weights $\mathbf{w}$ using $\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}}$.



Error Backpropagation

- For batch processing, we repeat backpropagation for each pattern in the training set and then sum over all patterns

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

- Backpropagation can be generalised by assuming that each node has a different activation function $h(\cdot)$.

Efficieny of Error Backpropagation

- As the number of weights is usually much larger than the number of units (the network is well connected), the complexity of calculating the gradient $\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}}$ via error backpropagation is of $O(W)$ where W is the number of weights.
- Compare this to numerical differentiation using

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = \frac{E_n(w_{ji} + \epsilon) - E_n(w_{ji})}{\epsilon} + O(\epsilon)$$

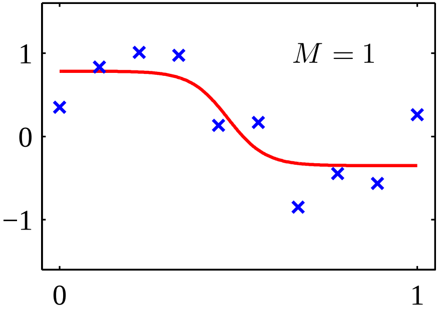
or the numerically more stable (fewer round-off errors) symmetric differences

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = \frac{E_n(w_{ji} + \epsilon) - E_n(w_{ji} - \epsilon)}{2\epsilon} + O(\epsilon^2)$$

which both need $O(W^2)$ operations.

Regularisation in Neural Networks

- Number of input and output nodes determined by the application.
- Number of hidden nodes is a free parameter.



Training a two-layer network with 1 hidden node.

Regularisation in Neural Networks

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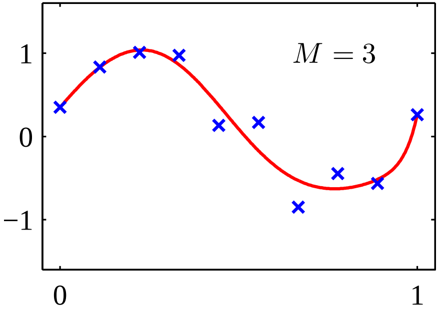
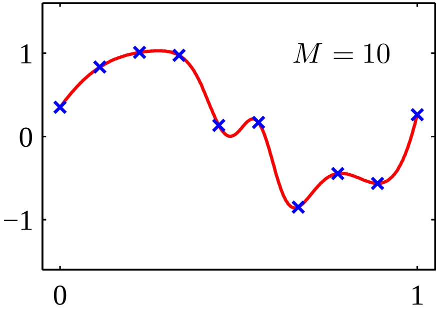


Training a two-layer network with 3 hidden nodes.

Regularisation in Neural Networks

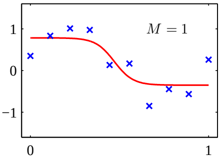
- Number of input and output nodes determined by the application.
- Number of hidden nodes is a free parameter.



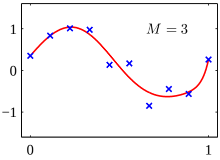
Training a two-layer network with 10 hidden nodes.

Regularisation in Neural Networks

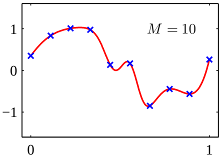
- Model complexity matters again.



$M = 1$



$M = 3$



$M = 10$

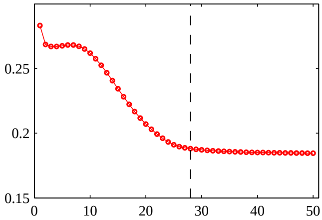
Regularisation in Neural Networks

- But the relation between generalisation error and the number of hidden units M is more complex than for fitting a polynomial. Reason : presence of local minima in the error function for the neural network.
- As before, we can use the regularised error

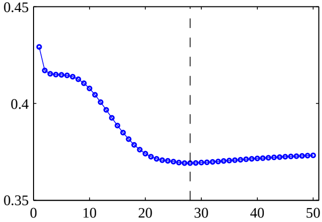
$$\widetilde{E}(\mathbf{w}) = E(\mathbf{w}) + \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

Regularisation via Early Stopping

- Stop training at the minimum of the validation set error.



Training set error.



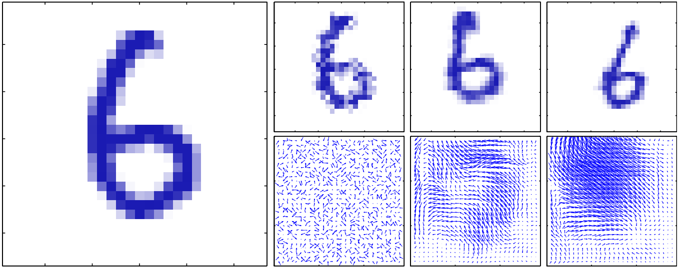
Validation set error.

Invariances

- If input data should be invariant with respect to some transformations, we can utilise this for training.
- Use training patterns including these transformations (e.g. handwritten digits translated in the input space).
- Or create extra artifical input data by applying several transformations to the original input data.
- Alternatively, preprocess the input data to remove the transformation.
- Or use convolutional neural networks (e.g. in image processing where close pixels are more correlated than far away pixels; therefore extract local features first and later feed into a network extracting higher-order features).

Synthetic Warping

- Create synthetic data by warping handwritten digits.



Left: Original digitised image. Right : Examples of warped images (above) and their corresponding displacement fields (below).

Bayesian Neural Networks

- Predict a single target t from a vector of inputs $\mathbf{x}$
- Assume conditional distribution to be Gaussian with precision β

$$p(t \mid \mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$

- Prior distribution over weights $\mathbf{w}$ is also assumed to be Gaussian

$$p(\mathbf{w} \mid \alpha) = \mathcal{N}(\mathbf{w} \mid \mathbf{0}, \alpha^{-1})$$

- For an i.i.d training data set $\{\mathbf{x}_n, t_n\}_{n=1}^{N}$, the likelihood of the targets $\mathcal{D} = \{t_1, \dots, t_N\}$ is

$$p(\mathcal{D} \mid \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n \mid y(\mathbf{x_n}, \mathbf{w}), \beta^{-1})$$

- Posterior distribution

$$p(\mathbf{w} \mid \mathcal{D}\alpha, \beta) \propto p(\mathbf{w} \mid \alpha) p(\mathcal{D} \mid \mathbf{w}, \beta)$$

Bayesian Neural Networks

- But $y(\mathbf{x}, \mathbf{w})$ is nonlinear, and therefore we can no longer calculate the posterior in closed form.
- Use Laplace approximation
  1. Find a (local) maximum $\mathbf{w}_{MAP}$ of the posterior via numerical optimisation.
  2. Evaluate the matrix of second derivatives of the negative log posterior distribution.
- Find a (local) maximum using the log-posterior

$$\ln p(\mathbf{w} \,|\, \mathcal{D}, \alpha, \beta) = -\frac{\alpha}{2} \mathbf{w}^T \mathbf{w} - \frac{\beta}{2} \sum_{n=1}^{N} \left(y(\mathbf{x}, \mathbf{w}) - t_n \right)^2 + \text{const}$$

- Find the matrix of second derivatives of the negative log posterior distribution

$$\mathbf{A} = -\nabla\nabla \ln p(\mathbf{w} \,|\, \mathcal{D}, \alpha, \beta) = \alpha \mathbf{I} + \beta \mathbf{H}$$

where $\mathbf{H}$ is the Hessian matrix of the sum-of-squares error function with respect to the components of $\mathbf{w}$.

Bayesian Neural Networks

- Having $\mathbf{w}_{MAP}$, and $\mathbf{A}$, we can approximate the posterior by a Gaussian

$$q(\mathbf{w} \,|\, \mathcal{D}, \alpha, \beta) = \mathcal{N}(\mathbf{w} \,|\, \mathbf{w}_{MAP}, \mathbf{A}^{-1})$$

- Similarly for the predictive distribution (without proof)

$$p(t \,|\, \mathbf{x}, \mathcal{D}, \alpha, \beta) = \mathcal{N}(t \,|\, y(\mathbf{x}, \mathbf{w}_{MAP}), \sigma^2(\mathbf{x}))$$

where

$$\sigma^2(\mathbf{x}) = \beta^{-1} + \mathbf{g}^T \mathbf{A}^{-1} \mathbf{g}$$

and

$$\mathbf{g} = \nabla_{\mathbf{w}} y(\mathbf{x}, \mathbf{w})|_{\mathbf{w}=\mathbf{w}_{MAP}}.$$