Lecture 17: Neural Networks

Reading: Chapter 11

GU4241/GR5241 Statistical Machine Learning

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Overview

- A neural network is a supervised learning method. It can be applied to both regression and classification problems.
- The central idea is to extract linear combinations of the inputs as derived features, and then model the target as a nonlinear function of these features.
- The nonlinear transformation contributes to the model flexibility.
- We will focus on the most widely used "vanilla" neural net, also called the single hidden layer feedforward neural networks.

General Description

- Derived features Z_m are obtained by applying the *activation function* σ to linear combinations of the inputs:

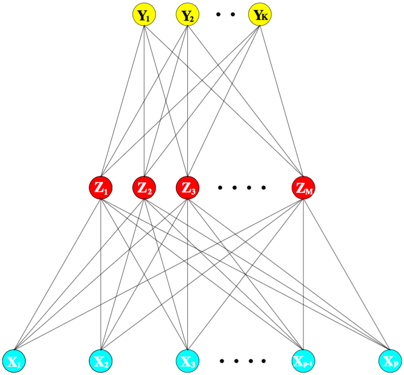
$$Z_m = \sigma(\alpha_{0m} + \alpha_m^T X), m = 1, \ldots, M.$$

- The target Y_k (or T_k in the figure) is modeled as a function of linear combinations of the Z_m:

$$T_k = \beta_{0k} + \beta_k^T Z, \quad k = 1, \ldots, K.$$

- The output function $g_k(T)$ allows a final transformation of the vector of outputs T:

$$f_k(X) = g_k(T), \quad k = 1, \ldots, K.$$



Schematic of a single hidden layer, feed-forward neural network

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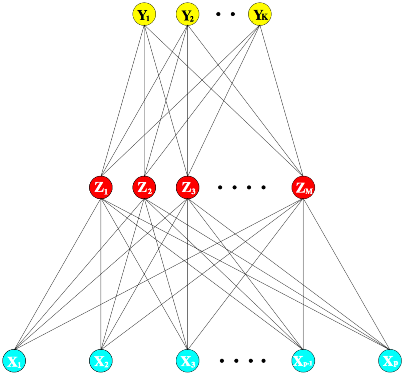
- For regression, we typically choose the identity function

$$g_k(T) = T_k.$$



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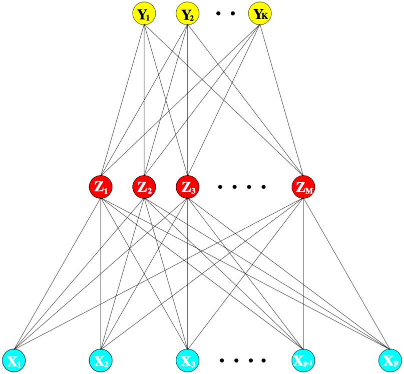
$$T_k = \beta_{0k} + \beta_k^T Z, \quad k = 1, \dots, K.$$

- For K-class classification, we use the *softmax* function

$$g_k(T) = \frac{e^{T_k}}{\sum_{l=1}^{K} e^{T_l}}$$



Schematic of a single hidden layer, feed-forward neural network

The activation function

- The activation function σ is usually chosen to be the *sigmoid* $\sigma(v) = 1/(1+e^{-v})$.
- Notice that is σ is the identity function, then the entire modle collapses to a linear model in the inputs.
- The rate of activation of the sigmoid depends on the norm of α_m.
- We can also choose other σ, like Gaussian radial basis functions.

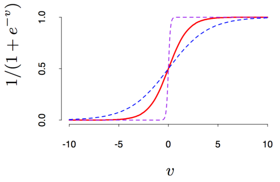


FIGURE 11.3. *Plot of the sigmoid function* $\sigma(v) = 1/(1+\exp(-v))$ *(red curve), commonly used in the hidden layer of a neural network. Included are* $\sigma(sv)$ *for* $s = \frac{1}{2}$ *(blue curve) and* $s = 10$ *(purple curve). The scale parameter* s *controls the activation rate, and we can see that large* s *amounts to a hard activation at* $v = 0$. *Note that* $\sigma(s(v - v_0))$ *shifts the activation threshold from* 0 *to* v_0.

Fitting Neural Networks

Recall our model is:

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\begin{aligned}
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f_k(X) &= g_k(T), \quad k = 1, \ldots, K.
\end{aligned}
$$

The unknow parameters of the model are often called *weights*. We denote the complete set of weights by θ, which consists of

$$
\begin{aligned}
\{\alpha_{0m}, \alpha_m;\ m = 1, 2, \ldots, M\} &\qquad M(p+1) \text{ weights,} \\
\{\beta_{0k}, \beta_k;\ k = 1, 2, \ldots, K\} &\qquad K(M+1) \text{ weights.}
\end{aligned}
$$

For regression, we use the squared error loss

$$
R(\theta) = \sum_{k=1}^{K} \sum_{i=1}^{n} (y_{ik} - f_k(x_i))^2.
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For classification we use either squared error or corss-entropy

$$R(\theta) = -\sum_{i=1}^{n} \sum_{k=1}^{K} y_{ik} \log f_k(x_i),$$

and the correponding classifier is $G(x) = \text{argmax}_k f_k(x)$.

Gradient Descent

Assume we use squared error loss. Let $z_{mi} = \sigma(\alpha_{0m} + \alpha_m^T x_i)$ and let $z_i = (z_{1i}, z_{2i}, \ldots, z_{Mi})$. Then we have

$$R(\theta) \equiv \sum_{i=1}^{n} R_i = \sum_{i=1}^{n} \sum_{k=1}^{K} (y_{ik} - f_k(x_i))^2,$$

where

$$f_k(x_i) = g_k(\beta_{0k} + \beta_k^T z_i) = g_k\left(\beta_{0k} + \sum_{m=1}^{M} \beta_{km}\sigma(\alpha_{0m} + \alpha_m^T x_i)\right).$$

The derivatives are

$$\begin{aligned}
\frac{\partial R_i}{\partial \beta_{km}} &= -2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)z_{mi}, \\
\frac{\partial R_i}{\partial \alpha_{ml}} &= -\sum_{k=1}^{K} 2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)\beta_{km}\sigma'(\alpha_m^T x_i)x_{il},
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A gradient update at the $(r+1)$st iteration has the form

$$\begin{aligned}
\beta_{km}^{(r+1)} &= \beta_{km}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \beta_{km}^{(r)}}, \\
\alpha_{ml}^{(r+1)} &= \alpha_{ml}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \alpha_{ml}^{(r)}}.
\end{aligned}$$

Back-propagation

If we write the gradients as

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If we write the gradients as

$$\begin{aligned}\frac{\partial R_i}{\partial \beta_{km}} &= \delta_{ki} z_{mi}, \\ \frac{\partial R_i}{\partial \alpha_{ml}} &= s_{mi} x_{il}.\end{aligned}$$

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In some sense, δ_{ki} and s_{mi} are "errors" at the output and hidden layer units. The errors satisfy

$$s_{mi} = \sigma'(\alpha_m^T x_i) \sum_{k=1}^{K} \beta_{km} \delta_{ki}.$$

They are called the *back-propagation equations*. The updates can be implemented with a two-pass algorithm:

- *forward pass*: fix weights, compute the predicted values $\hat{f}_k(x_i)$.
- *backward pass*: errors δ_{ki} are computed, and back-propagated to give the errors s_{mi}. Then use both sets of errors to compute the gradients.

Alternative Algorithm

A gradient update at the $(r+1)$st iteration has the form

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\end{aligned}$$

This algorithm is a kind of *batch learning*.

We compute the gradients as a sum over all the training cases.

We can use an alternative algorithm in which the learning is carried out online.

Starting Values

- If the weights are near zero, then the operative part of the sigmoid is roughly zero.
- Usually starting values for weights are chosen to be random values near zero.
- Hence the model starts out nearly linear, and becomes nonlinear as the weights increases.

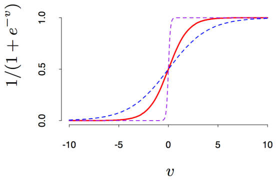


FIGURE 11.3. *Plot of the sigmoid function* $\sigma(v) = 1/(1+\exp(-v))$ *(red curve), commonly used in the hidden layer of a neural network. Included are* $\sigma(sv)$ *for* $s = \frac{1}{2}$ *(blue curve) and* $s = 10$ *(purple curve). The scale parameter* s *controls the activation rate, and we can see that large* s *amounts to a hard activation at* $v = 0$*. Note that* $\sigma(s(v - v_0))$ *shifts the activation threshold from* 0 *to* v_0*.*

Multiple Minima

The error function $R(\theta)$ is nonconvex, possessing many local minima.

The solution we obtained from back-propagation is a local minimum.

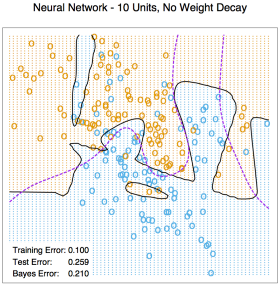
Usually, we try a number of random starting configuration, and choose the solution giving lowest error, or use the average predictions over the collection of networks as the final prediction.

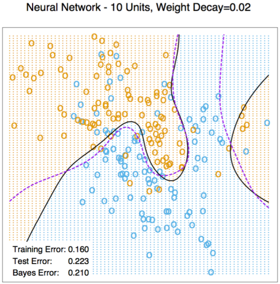
Regularization

- Often neural networks have too many weights and will overfit the data at the global minimum of R.
- A regularization method is *weight decay*. We add a penalty to the error function $R(\theta) + \lambda J(\theta)$, where

$$J(\theta) = \sum_{k,m} \beta_{km}^2 + \sum_{m,l} \alpha_{ml}^2.$$

- $\lambda \geq 0$ is a tuning parameter, can be chosen by cross-validation.





Example: Simulated Data

We generate data from two additive error models $Y = f(X) + \epsilon$:

$$\begin{aligned} \text{Sum of sigmoids: } Y &= \sigma(a_1^T X) + \sigma(a_2^T X)\epsilon_1; \\ \text{Radial: } Y &= \prod_{m=1}^{10} \phi(X_m) + \epsilon_2. \end{aligned}$$

Here $X^T = (X_1, X_2, \ldots, X_p)$, each X_j being a standard Gaussian variate, with $p = 2$ in the first model, and $p = 10$ in the second.

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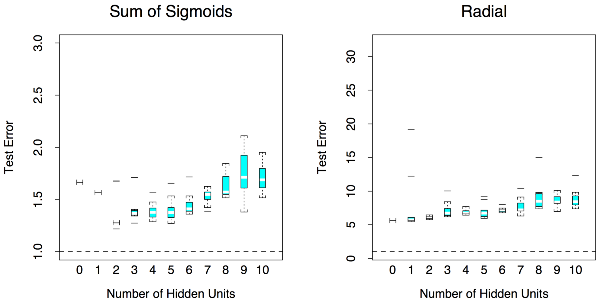

Boxplots of test error

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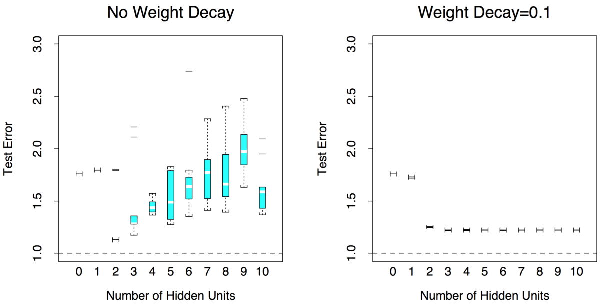

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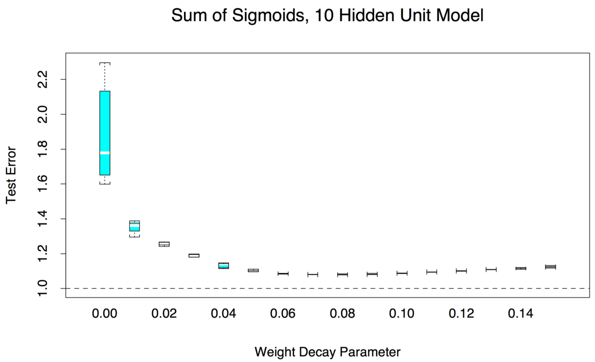
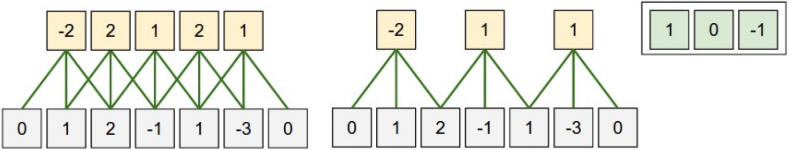


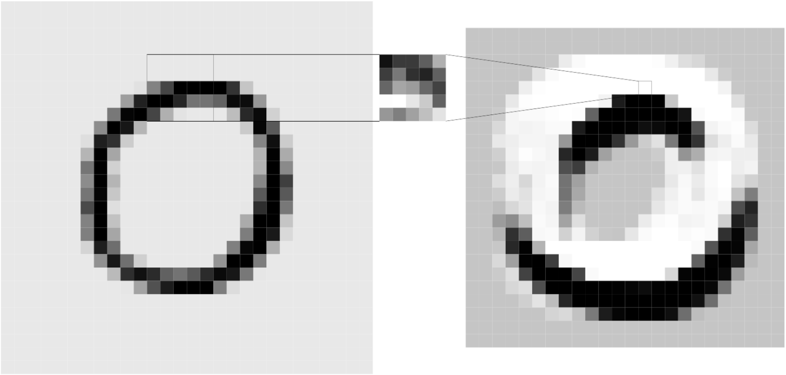
Convolutional Neural Networks: Sharing the Weights

- Convolutional Neural Networks (CNN) have been widely used in image analysis.
- They are similar to the neural networks we discussed before. The difference is that they force the derived features for different hidden units to be computed by the *same* linear functional, or in other words, the hidden units *share* the weights.



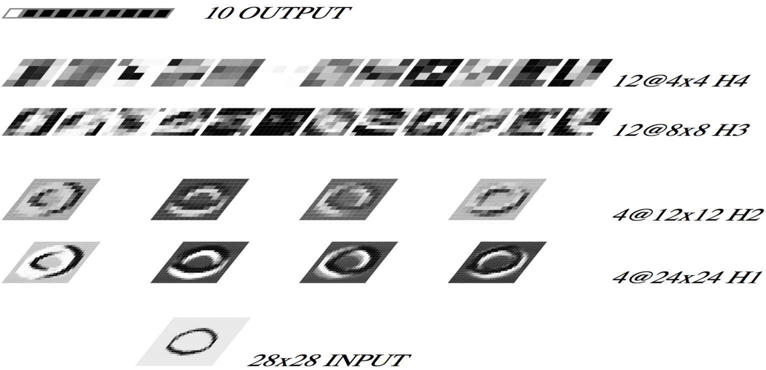
The weights are (1, 0, -1) (shown on top right), and the bias is zero. These weights are shared across all yellow neurons.

Convolutional Neural Networks: Sharing the Weights



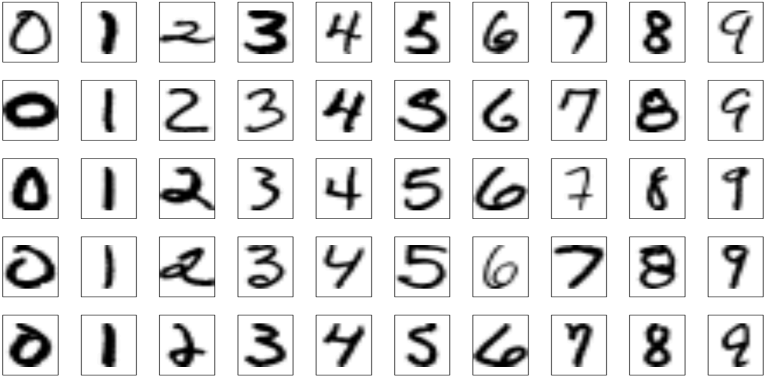
Input image (left), weight vector, and the resulting feature map (right). White represents corresponds to intensity -1.

Convolutional Neural Networks



Network Architecture with 5 layers of fully adaptive connections (Le Cun, 1989).

Example: ZIP Code Data



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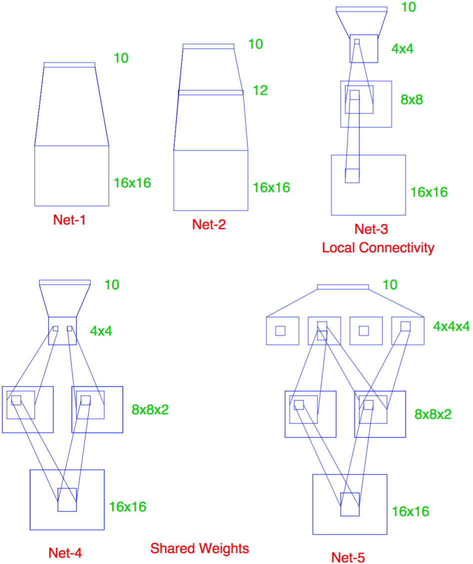

FIGURE 11.10. *Architecture of the five networks used in the ZIP code example.*

Example: ZIP Code Data