STATS 235: Modern Data Analysis
Neural Networks

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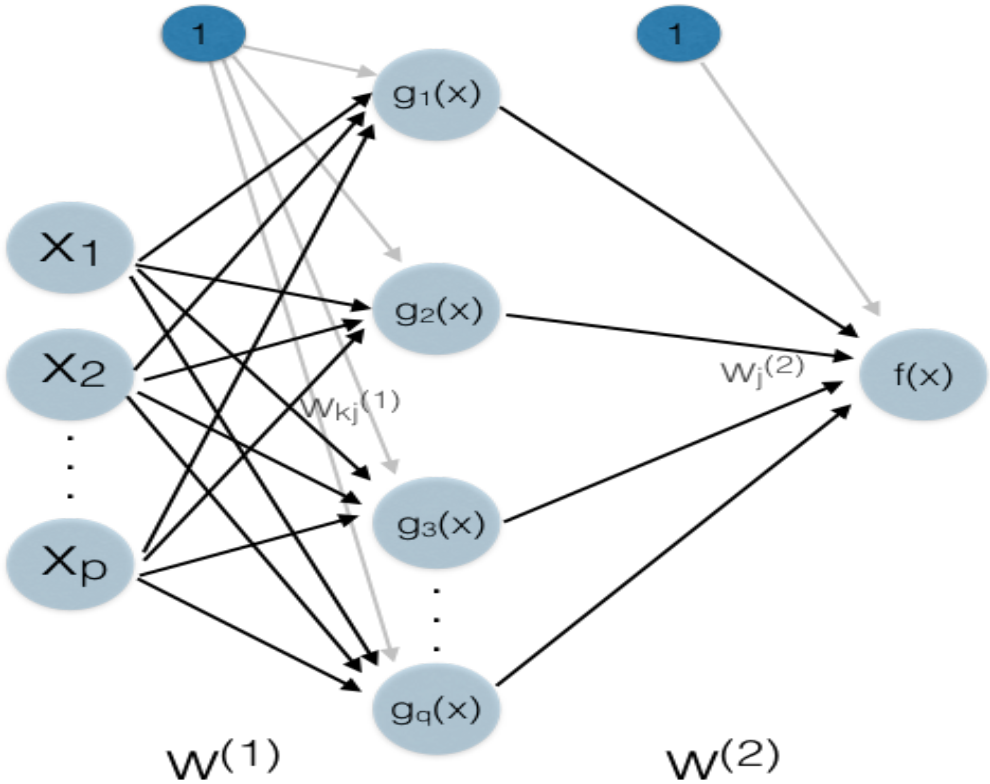
Neural Networks (NN)



Multilayer perceptron (MLP) with p input variables, one hidden layer with q hidden units, and a single output. Here, $w^{(1)}$ represents the connection weight matrix between the input layer and the hidden layer, and $w^{(2)}$ is the vector of connection weights between the hidden layer and the output.

Neural Networks (NN)

- A multilayer perceptron (MLP, aka feedforward NN) is comprised of an input layer, output layer and a number of hidden layers in between
- The hidden layers creates a set of basis by applying nonlinear transformations, g, to their input and pass their results to the next layer until we reach the output layer.
- We refer to g as the activation or transfer function, which is usually set to the sigmoid (aka logistic) function

$$\text{sigm}(a) = \frac{1}{1 + e^{-a}}$$

or the hyperbolic tangent function

$$\tanh(a) = \frac{e^{a} - e^{-a}}{e^{a} + e^{-a}}$$

Neural Networks (NN)

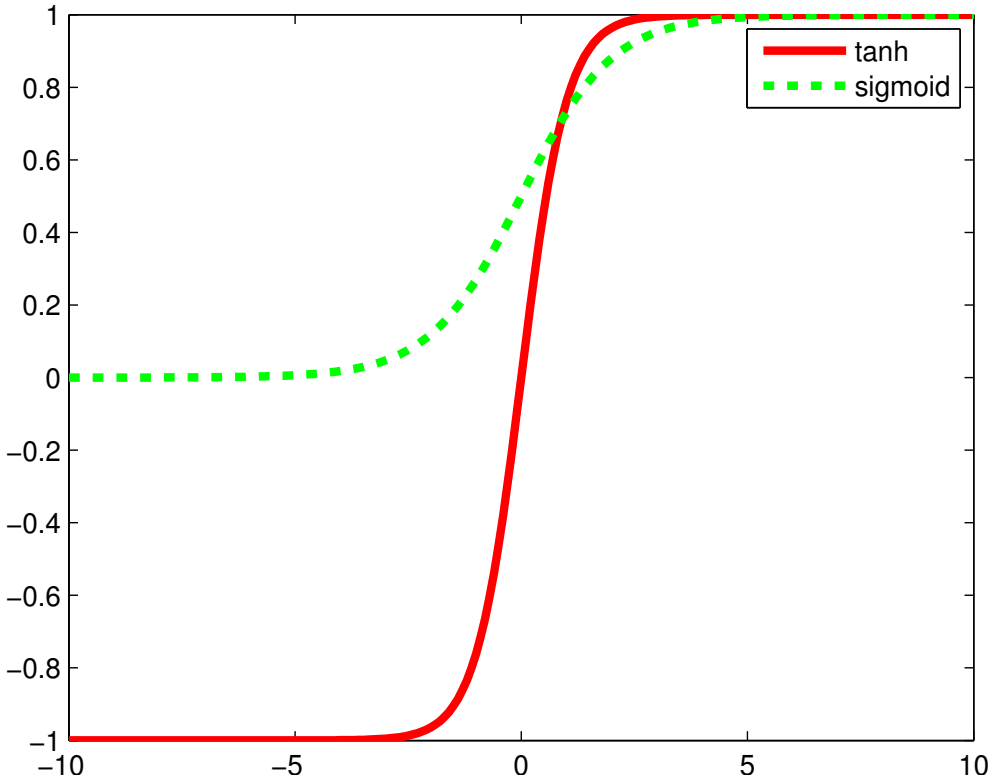


Figure 16.6 in Murphy (2012).

Neural Networks (NN)

- The output $f(x)$, which is a function used to approximate y, is a linear combination of basis defined by the hidden layers
- For linear regression models (continuous outcome)

$$P(y|x, w) = N(y|f(x), \sigma^2)$$

- For logistic regression models (binary outcome)

$$P(y|x, w) = \mathrm{Ber}(y|\mathrm{sigm}(f(x)))$$

- For multiple categories, we use the multinomial logit model, which is also known as the softmax function

Neural Networks (NN)

- For a MLP with one hidden layer and tanh activation function, we have

$$
\begin{aligned}
g_j(x) &= \tanh[w_{0j}^{(1)} + \sum_{k=1}^{p} w_{kj}^{(1)} x_k], \qquad \text{for } j = 1, \ldots, q \\
f(x) &= w_0^{(2)} + \sum_{j=1}^{q} w_j^{(2)} g_j(x)
\end{aligned}
$$

- Here w_0's, which play the role of the intercept in regression models, are called biases

Learning

- To train a MLP, we first need to specify the negative log-likelihood, which is also known as the energy function, E
- For regression, we have (squared error)

$$E = \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

for binary classification models, we have (cross entropy)

$$E = -\sum_{i=1}^{n} y_i [\log \operatorname{sigm}(f(x_i))] + (1 - y_i)[\log(1 - \operatorname{sigm}(f(x_i)))]$$

- To estimate the weights, we minimize the energy function with respect to w

Learning

- The parameters of a neural network model are not identifiable
  - Permuting the order of hidden units does not change the model
  - If we change the sign of weights entering a hidden unit, the model remains the same as long as we also change the sign of the weights going out of that unit since $\tanh(-a) = -\tanh(a)$
- Also, in general the energy function for MLP is non-convex
- Nevertheless, we can still use common iterative optimization methods (e.g., gradient descent algorithms) to obtain locally optimal estimates
- Using the chain rule, it is easy to find the gradient

Backpropagation

- For learning (i.e., estimating the weights), we start with initializing the weights (including the biases) to some random numbers (all different values) and iteratively perform the following steps
  - At each iteration, we use *forward propagation* to find the values going to each unit, before and after transformation, until we reach the output layer
  - We find the derivatives of E with respect to each unit starting from the output and *backpropagate* using the chain rule to find the derivatives with respect to hidden units
  - Using the chain rule again, we find the derivatives with respect to the weights
  - We then update the weights by moving in the direction of the negative gradient (see the notes on optimization)
  - We repeat the above steps until some stopping criterion is reached

Backpropagation

- For a MLP with one hidden layer and tanh activation function, given the current weights, forward propagation involves finding the following values at each hidden unit before and after transformation

$$\begin{aligned} z_j &= w_{0j}^{(1)} + \sum_{k=1}^{p} w_{kj}^{(1)} x_k \\ g_j &= \tanh(z_j) \end{aligned}$$

- For the output unit, we hve

$$f = w_0^{(2)} + \sum_{j=1}^{q} w_j^{(2)} g_j$$

Backpropagation

- Backpropagation starts with finding $\partial E/\partial f$; For regression model

$$\frac{\partial E}{\partial f} = -\frac{1}{\sigma^2}\sum_{i=1}^{n}(y - f(x_i))$$

- Next, using the chain rule we have

$$\frac{\partial E}{\partial g_j} = \frac{\partial E}{\partial f}\frac{\partial f}{\partial g_j} = w_j^{(2)}\frac{\partial E}{\partial f}$$

- We then find the derivatives with respect to z_j

$$\frac{\partial E}{\partial z_j} = \frac{\partial E}{\partial g_j}\frac{\partial g_j}{\partial z_j} = (1 - g_j^2)\frac{\partial E}{\partial g_j}$$

Recall that $\frac{d}{da}\tanh(a) = 1 - \tanh^2(a)$

Backpropagation

- Finally, we find the derivatives with respect to the weights
- For connection weights between the hidden layer and output we have

$$\frac{\partial E}{\partial w_j^{(2)}} = \frac{\partial E}{\partial f}\frac{\partial f}{\partial w_j^{(2)}} = g_j \frac{\partial E}{\partial f}$$

Note that $g_0 = 1$ when evaluating $\partial E / \partial w_0^{(2)}$

- For the weights connecting the input layer to the hidden layer we have

$$\frac{\partial E}{\partial w_{kj}^{(1)}} = \frac{\partial E}{\partial z_j}\frac{\partial z_j}{\partial w_{kj}^{(1)}} = x_k \frac{\partial E}{\partial z_j}$$

$x_0 = 1$ when evaluating $\partial E / \partial w_0^{(1)}$

Backpropagation

- After we find the gradient ∇E, we update the parameters by taking a step in a direction of negative gradient, with stepsize t

$$\begin{aligned} \Delta w &= -\nabla E \\ w &\leftarrow w + t\Delta w \end{aligned}$$

- The stepsize (aka learning rate) is found by trial-and-error
- We could run the algorithm until the approximation error falls below a desired threshold; however, this could lead to *overfitting*
- Two common strategies to avoid this issue are *early stopping* and *weight decay*

Early stopping

- Overfitting occurs when the model performs well on the training data and performs poorly on the test (future) data
- In the "early stopping" method, we start with some initial weights close to zero and monitor the performance of the neural network model throughout the training process based on an independent *validation set* (usually 20% of the data; this is separate from any test set used for model evaluation); we stop the algorithm when the model's performance on the validation set starts to decline substantially (a sign of overfitting)
- We can use the prediction error or average log probability on the validation set as a measure of performance
- This method could be very successful for avoiding overfitting; however it is *ad hoc* and wasteful since some of the data points are not used in the training directly

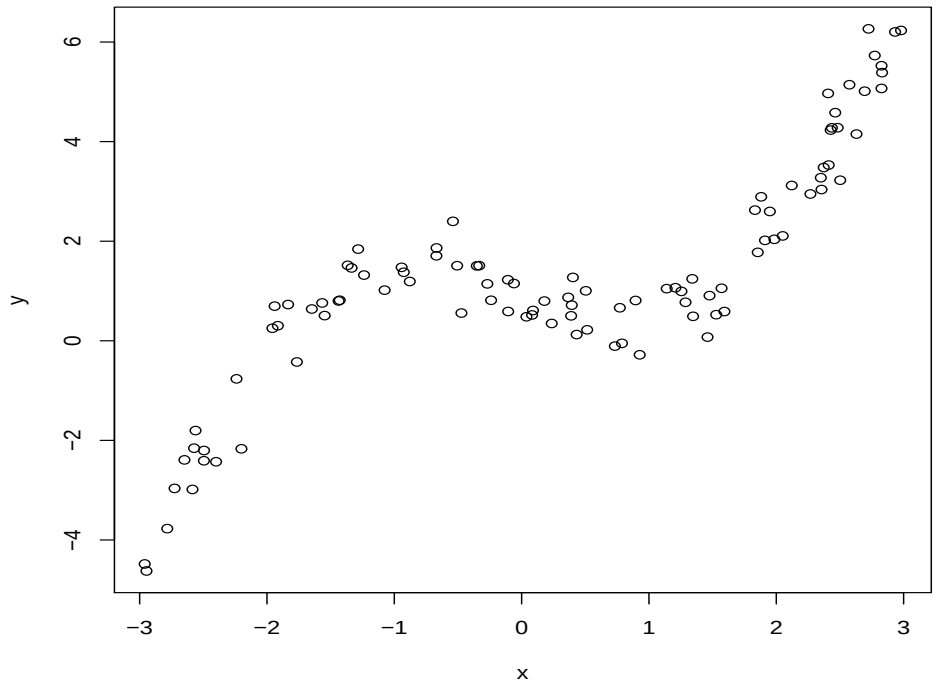
Weight decay

- Alternatively, to avoid overfitting, we can penalize models agains complexity (similar to ridge regression and Lasso)
- To this end, instead of minimizing the energy function, we minimize the penalized version of it by adding the following penalty terms:

$$\lambda_1 \sum_{k=1}^{p} \sum_{j=1}^{q} [w_{kj}^{(1)}]^2 + \lambda_2 \sum_{j=1}^{q} [w_j^{(2)}]^2$$

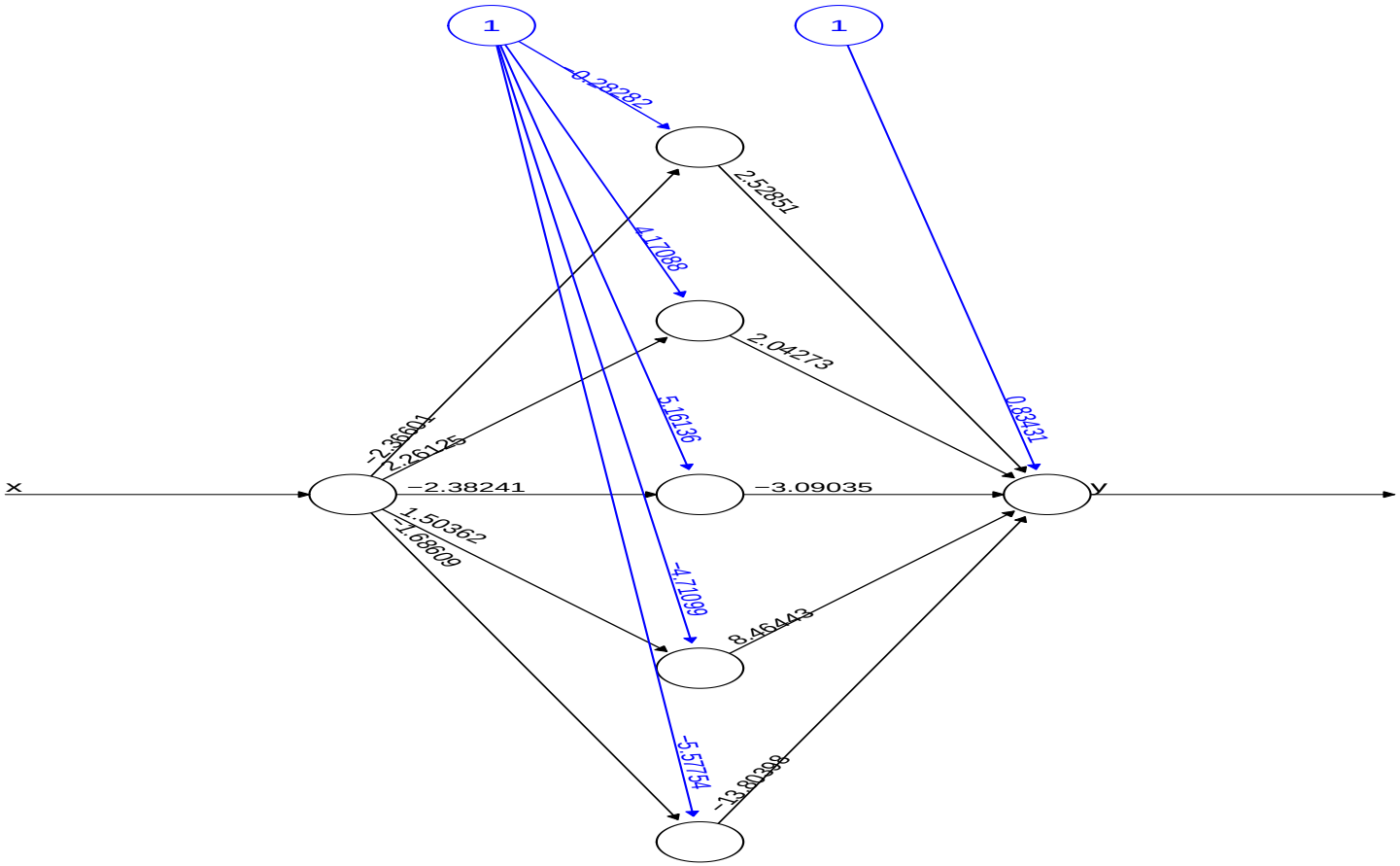
- This is known as "weight decay" since it shrinks the weights towards zero to encourage simpler models
- To set the values of λ_1 and λ_2, we can use an independent validation set as before or use cross-validation when the sample size is small

Illustrative Example



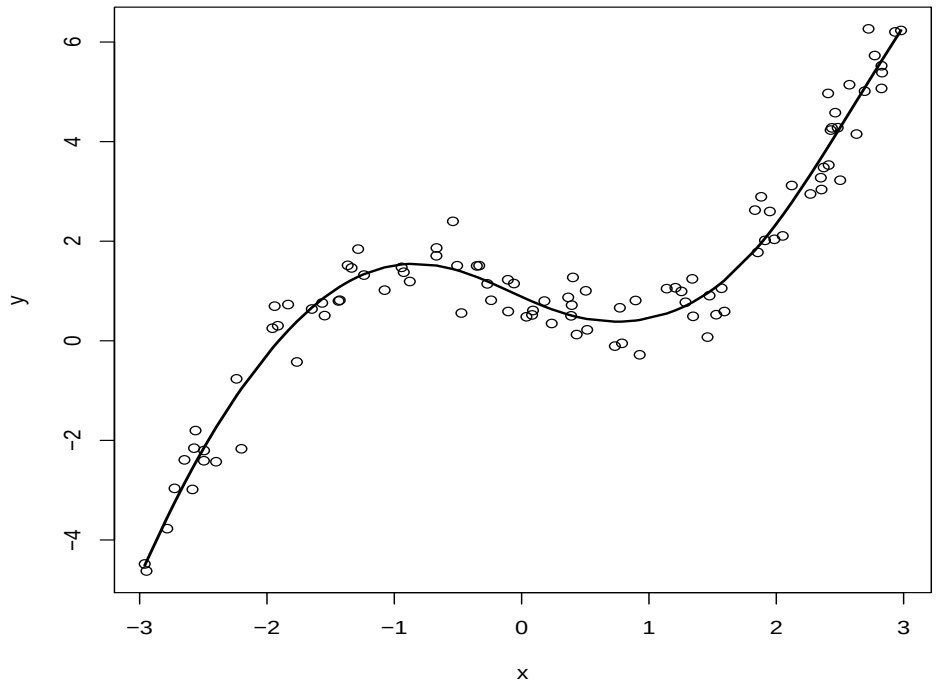
Observed data

Illustrative Example



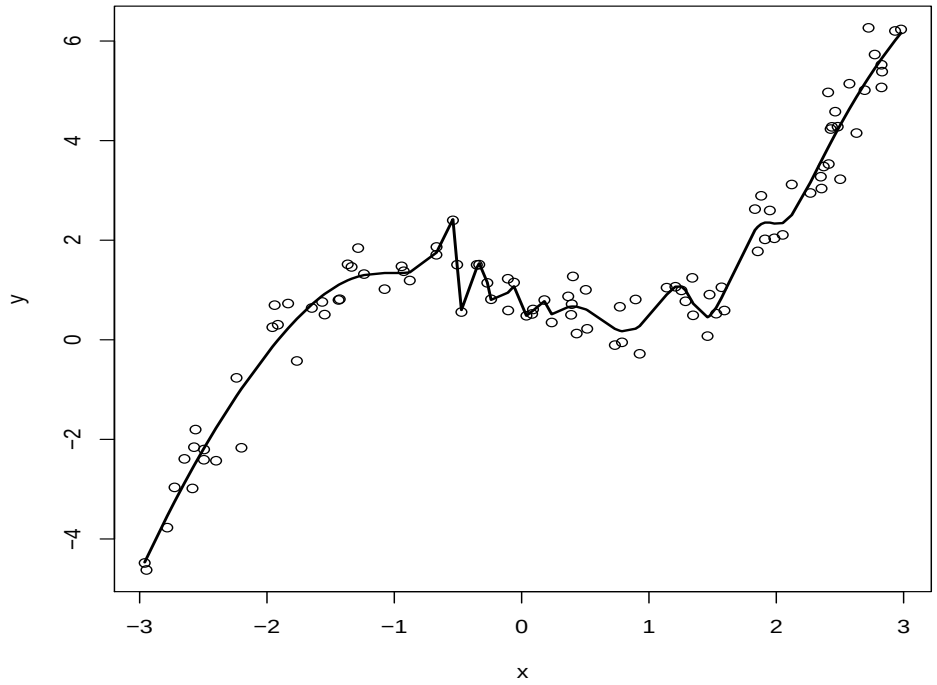
A neural network with 5 hidden units

Illustrative Example



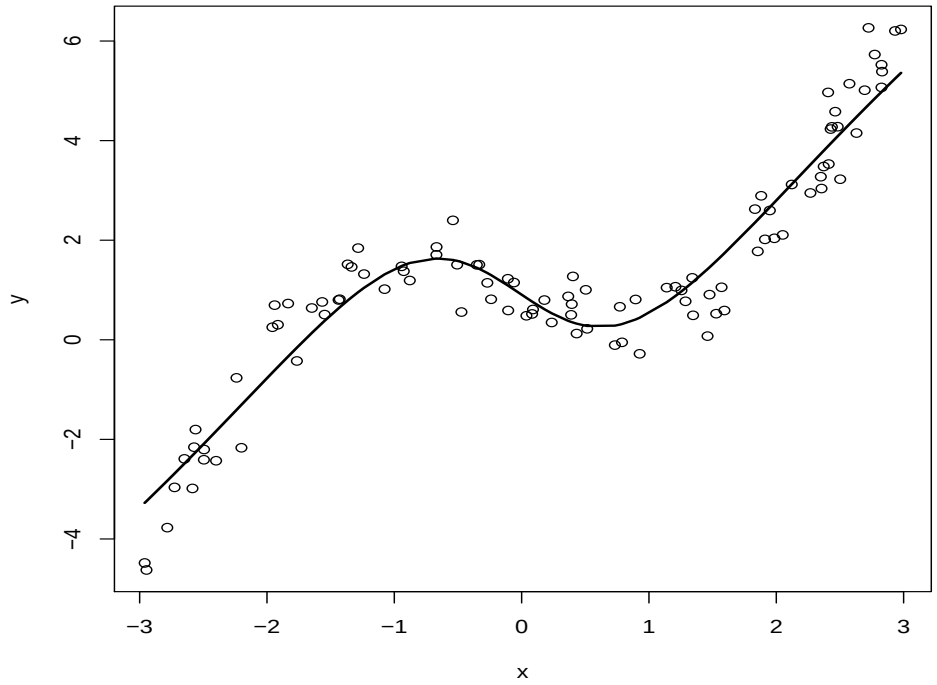
Estimated function, $f(x)$, with 5 hidden units

Illustrative Example



Estimated function, $f(x)$, with 50 hidden units

Illustrative Example



Estimated function, $f(x)$, with 50 hidden units using weight decay