ML01 – Introduction to Machine Learning

Neural Networks

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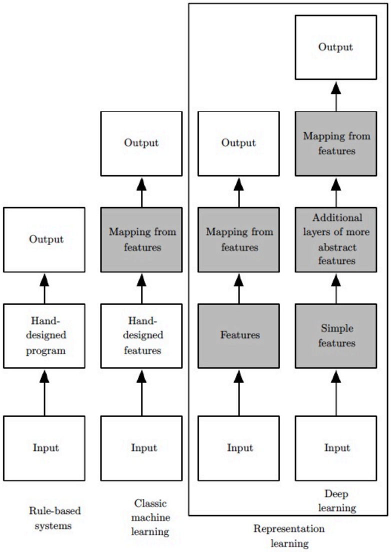
Neural networks

- A class of learning methods that was developed in AI with inspiration from neuroscience.
- The central idea is to learn simultaneously
  - New predictors (activation of "hidden neurons") and
  - A linear regressor or classifier in the predictor space.
- The result is a powerful learning method, with widespread applications in many fields.
- In recent years, there has been a surge of interest in deep networks/learning, with applications to computer vision and natural language processing.
- There exist many neural network models. In this chapter we describe the most widely used multilayer feedforward neural networks.

Neural networks within AI

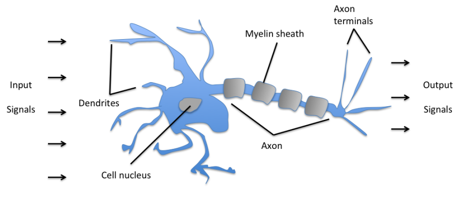


Historical perspective

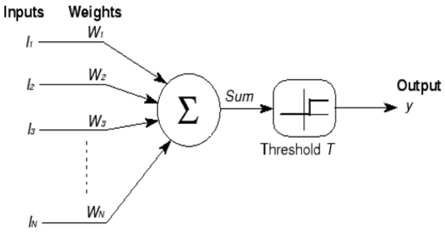
- Three main phases:
  1. Perceptron (1955-1965)
  2. Multi-layer neural networks (1985-1995)
  3. Deep networks (2010-)
- The history can be summarized by a list of 4 influential papers.

McCulloch-Pitts Model

- W. S. McCulloch and W. Pitts. A logical calculus of the ideas immanent in nervous activity. *The Bulletin of Mathematical Biophysics*, 5(4):115-133, 1943.
- Main idea: biological neurons modeled as simple logic gates with binary outputs.



Schematic of a biological neuron.



McCulloch-Pitts neuron as a logic gate

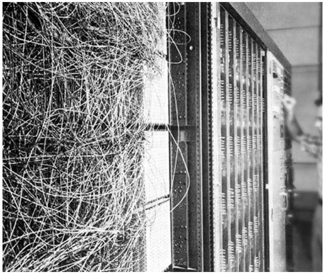
- Assume
  - The inputs I_j take values in $\{0,1\}$ for $j=1,\ldots,N$ (1 codes for "TRUE" and 0 for "FALSE")
  - The weights W_j are all equal to 1, and
  - The threshold is $T = N$
- Then the output is

$$y = \begin{cases} 1 & \text{if } \sum_{j=1}^{N} I_j - N \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

  It is equal to 1 iff $I_j = 1$ for all j: the neuron computes a logical AND.
- If $T = 1$, $y = 1$ iff $I_j = 1$ for some j: the neuron computes a logical OR.

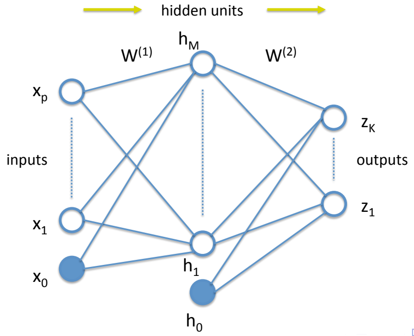
Perceptron

- F. Rosenblatt. *The perceptron, a perceiving and recognizing automaton (Project PARA)*. Cornell Aeronautical Laboratory, 1957.
- Main idea: an algorithm to learn the weights of a McCulloch-Pitts neuron. Implementation in a machine call the “Mark 1 perceptron”.
- The algorithm worked only for two linearly separable classes and it was very slow.



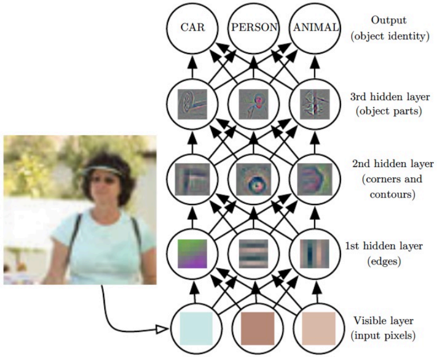
Multilayer neural networks

- D. E. Rumelhart, G. E. Hinton and R. J. Williams (1986). Learning representations by back-propagating errors. *Nature*, 323 (6088):533–536.
- Main ideas: train neural networks with (one or two) hidden layers using an efficient algorithm for computing the gradient of the error (back-propagation algorithm).



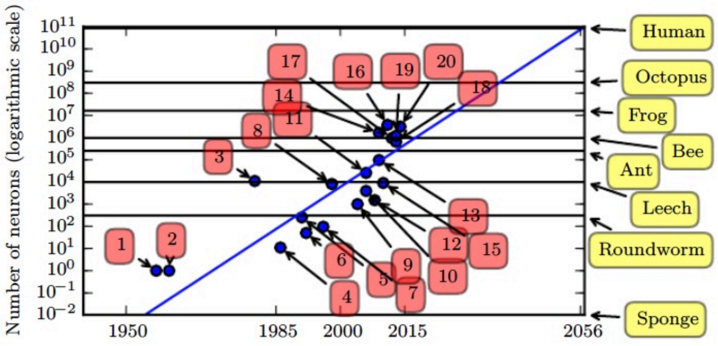
Deep networks

- Y. LeCun, Y. Bengio and G. Hinton (2015). Deep learning. *Nature*, 521:436–444.
- Main idea: train neural networks with many hidden layers that encode more and more abstract features.



Increase of neural network size

Since the introduction of hidden units, artificial neural networks have doubled in size roughly every 2.4 years.

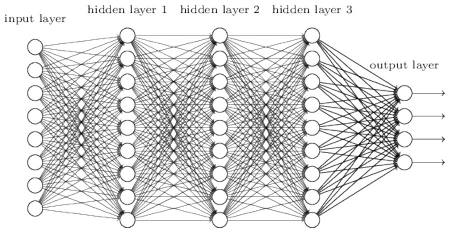


1: Perceptron; 4: Early back-propagation network; 8: LeNet-5 (LeCun et al., 1998b); 20: GoogLeNet

Overview

Definition

- A multilayer feedforward neural network (multilayer perceptron, MLP) is composed of computational units (neurons) arranged in layers: one input layer, one or several hidden layers and one output layer
- Neurons in each layer (expect the input one) are connected to all neurons in the previous layers through weighted connections.
- The information flows from the input layer to the output layer.



Overview

Equation of hidden units

- Each hidden neuron m computes a weighted sum of its inputs

$$z_m = \sum_{j=1}^{p} w_{mj} x_j + w_{m0} = w_m^T x + w_{m0}$$

  where w_{mj} is the connection weight between input unit j and hidden unit m, w_m is the vector of weights of unit m, and w_{m0} is a bias term (which may be seen as the weight of a connection from an input unit with constant input 1).

- The output of unit m is

$$h_m = g(z_m),$$

  where g is a nonlinear activation function.

Sigmoid activation functions

- The first generation of multi-layer networks used the logistic activation function

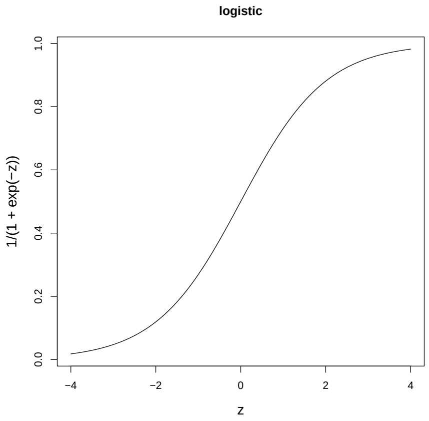
$$g(z) = \Lambda(z) = \frac{1}{1+e^{-z}} \in [0,1]$$

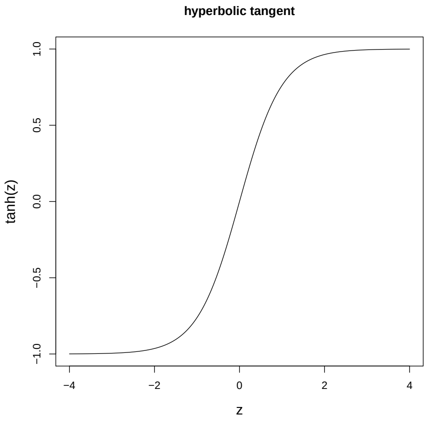
taking values in $[0,1]$, or the hyperbolic tangent activation function

$$g(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} = 2\Lambda(2z) - 1 \in [-1,1]$$

- These activation functions are said to be “sigmoid” (S-shaped).
- Sigmoid units saturate across most of their domain, and are only strongly sensitive to their input when z is near 0. This can make gradient-based learning very difficult. For this reason, their use as hidden units in feedforward networks is now discouraged.

Sigmoid activation functions





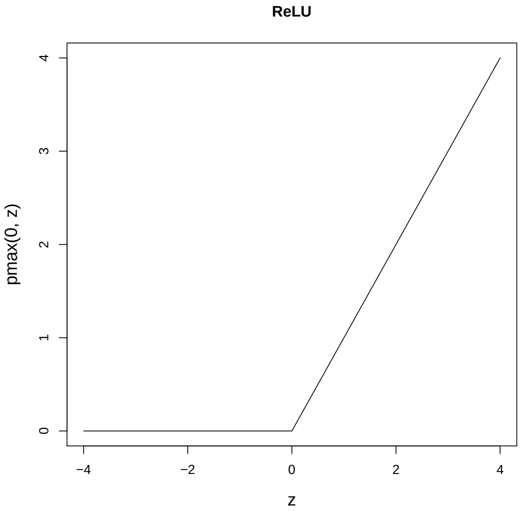
Rectified linear units

- Rectified linear units (ReLU) use the activation function

$$g(z) = \max(0, z).$$

- Rectified linear units are easy to optimize because they are similar to linear units: the only difference is that a rectified linear unit outputs zero across half its domain.
- This makes the derivatives through a rectified linear unit remain large whenever the unit is active.

Rectified linear unit activation functions



Overview

Output units for regression

- A neural network can be used for regression or classification.
- For regression, there is only one linear output unit ($K = 1$). However, we can easily generalize the model to $K > 1$ outputs.
- The k-th output is computed as

$$z_k = \sum_{m=1}^{M} w_{km} h_m + w_{k0} = w_k^T h + w_{k0}$$

- The output units are similar to hidden units, except that their activation function is linear.

Output units for binary classification

- For binary classification, we usually have one output unit with a sigmoid activation function:

$$\widehat{y} = \Lambda\left(\sum_{m=1}^{M} w_m h_m + w_0\right) = \Lambda(w^T h + w_0) \in [0,1]$$

  This output can be made to approximate the conditional probability $P(x) = \mathbb{P}(Y = 1|x)$.

- When there is no hidden layer, the input-output equation is

$$\widehat{y} = \Lambda(w^T x + w_0)$$

  It is exactly the binomial logistic regression model.

Output units for c-class classification

- For c-class classification, there are $K = c$ output units with the kth unit modeling the probability of class k. We use the softmax function

$$\widehat{y}_k = g_k(z) = \frac{\exp(z_k)}{\sum_{\ell=1}^K \exp(z_\ell)}$$

  with $z_k = w_k^T h + w_{k0}$ and $z = (z_1, \ldots, z_K)$.
- This is exactly the transformation used in the multinomial logistic regression model; it produces positive probability estimates that sum to one.

Overview

Architecture design

- A key design consideration for neural networks is determining the architecture, i.e., the overall structure of the network: how many units it should have and how these units should be connected to each other.
- In multilayer feedforward networks, groups of units (layers) are arranged in a chain structure, with each layer being a function of the layer that preceded it. The vector of outputs from the 1st layer is

$$\underbrace{h^{(1)}}_{M_1\times 1} = g^{(1)}(\underbrace{W^{(1)}}_{M_1\times p}\underbrace{x}_{p\times 1} + \underbrace{w_0^{(1)}}_{M_1\times 1}),$$

the second-layer output vector is

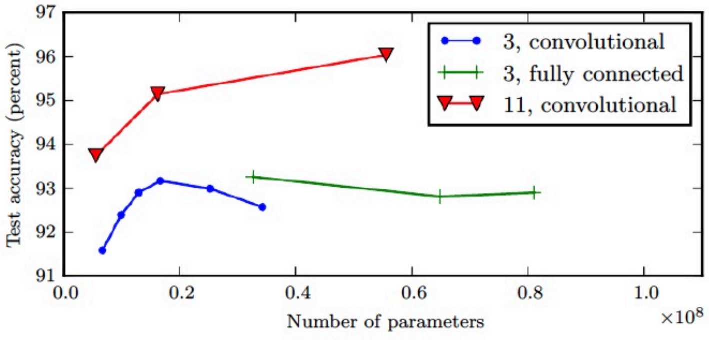
$$\underbrace{h^{(2)}}_{M_2\times 1} = g^{(2)}(\underbrace{W^{(2)}}_{M_2\times M_1}\underbrace{h^{(1)}}_{M_1\times 1} + \underbrace{w_0^{(2)}}_{M_2\times 1}),$$

and so on. Here, $W^{(l)}$ is the matrix of weights for connections into hidden layer l.

How many layers?

- It can be shown that neural networks with only one hidden layer of nonlinear units are universal approximators: they can approximate any sufficiently smooth (e.g., continuous) function at any desired accuracy.
- However, the hidden layer may be infeasibly large and may fail to learn and generalize correctly.
- In many circumstances, using deeper models can reduce the number of units required to represent the desired function and can reduce the amount of generalization error.
- Empirical results show that deeper models tend to perform better, not merely because the model is larger.

Example



This experiment from Goodfellow et al. (2014) shows that increasing the number of parameters in layers of convolutional networks without increasing their depth is not nearly as effective at increasing test set performance. We observe that shallow models in this context overfit at around 20 million parameters while deep ones can benefit from having over 60 million.

Overview

Overview

Gradient-based learning

- Designing and training a neural network is not much different from training any other machine learning model by minimizing a loss (cost, error) function.
- The largest difference between the models we have seen so far and neural networks is that the nonlinearity of a neural network causes most interesting loss functions to become non-convex.
- This means that neural networks are usually trained using iterative, gradient-based optimization algorithms that merely drive the cost function to a local minimum.

Loss function

- We first need to define a loss function $\mathcal{L}(\widehat{y}, y)$.
- Given a learning set $\{(x_i, y_i)\}_{i=1}^n$, we then minimize the average loss

$$\boxed{J(\theta) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}(f(x_i;\theta), y_i),}$$

  where
  - θ denote the vector of all connection weights (the learnable parameters) and
  - $f(x;\theta)$ the vector of outputs for input vector x.
- This is an estimate of the expected loss

$$\boxed{\mathbb{E}_{X,Y}\mathcal{L}(f(X;\theta), Y)}$$

Loss function for regression

- For regression, we often use the sum-of-squares loss function:

$$\mathcal{L}(f(x;\theta),y) = \|y - f(x;\theta)\|^2 = \sum_{k=1}^{K} (y_k - f_k(x;\theta))^2$$

- Minimizing $J(\theta)$ is equivalent to maximizing the conditional likelihood, assuming a Gaussian error model

$$Y = f(x;\theta) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_K)$$

(see next slide).

Sum-of-squares loss and Gaussian error assumption

- Assuming $\epsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_K)$, the conditional likelihood is

$$L(\theta) = \prod_{i=1}^{n} p(y_i \mid x_i) \propto \prod_{i=1}^{n} \exp\left(-\frac{1}{2\sigma^2}\|y_i - f(x_i;\theta)\|^2\right)$$

$$\propto \exp\left(-\frac{1}{2\sigma^2} \underbrace{\sum_{i=1}^{n} \|y_i - f(x_i;\theta)\|^2}_{\mathcal{L}(f(x_i;\theta),y_i)}\right)$$

- Maximizing the conditional likelihood is equivalent to minimizing the average sum-of-squares loss.

Loss function for classification

- For classification we use cross-entropy (deviance) loss function:

$$\mathcal{L}(f(x;\theta),y) = -\sum_{k=1}^{c} y_k \log f_k(x;\theta),$$

where $y_k = I(y=k)$. The corresponding classifier is

$$C(x) = \arg\max_k f_k(x;\theta).$$

- If $f_k(x;\theta)$ is a model of $P_k(x) = \mathbb{P}(Y=k \mid X=x)$, then $J(\theta)$ equals minus the log-likelihood $\ell(\theta)$ (see next slide).

Cross-entropy and conditional likelihood

- The conditional likelihood is

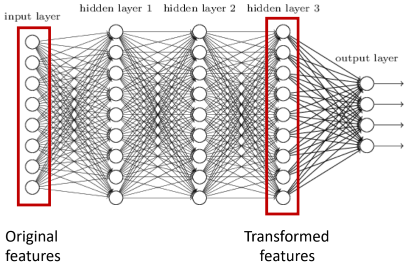
$$\begin{aligned} L(\theta) &= \prod_{i=1}^{n} \mathbb{P}(Y_i = y_i \mid X_i = x_i) \\ &= \prod_{i=1}^{n} \prod_{k=1}^{c} f_k(x_i;\theta)^{y_{ik}} \end{aligned}$$

- The conditional log-likelihood is

$$\ell(\theta) = \sum_{i=1}^{n} \underbrace{\sum_{k=1}^{c} y_{ik} f_k(x_i;\theta)}_{-\mathcal{L}(f(x_i;\theta),y_i)}$$

Relation with logistic regression

- With the logistic ($c = 2$) or softmax ($c > 2$) activation function and the cross-entropy error function, the neural network model is exactly a logistic regression model in which the hidden unit outputs are the predictors.
- All the parameters are estimated by maximum likelihood.
- Training a neural network is equivalent to learning a transformation from the input space to a feature space, and learning a logistic regression classifier in the feature space at the same time.



Overview

Principle

- The vector θ^* minimizing $J(\theta)$ does not have a closed-form expression: we need to use an iterative optimization algorithm.
- Most optimization algorithms require to compute the gradient of $J(\theta)$ at each step.
- The gradient of $J(\theta)$ can be easily derived using the chain rule for differentiation.
- The corresponding algorithm is called back-propagation (BP).
- For ease of exposition, we present the BP algorithm in the case of two hidden layers. Generalization to any number of hidden layers is straightforward.

Propagation equations and loss function

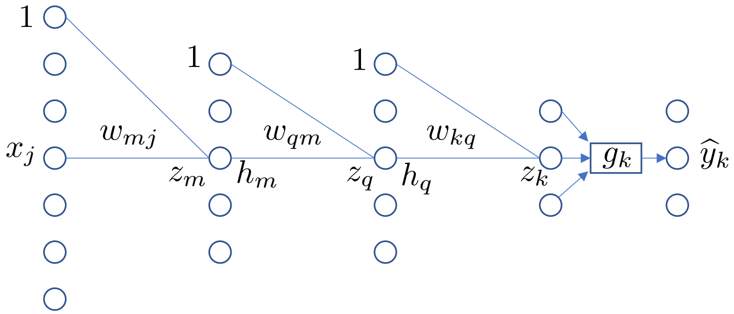
- Propagation equations (see next slide):

$$
\begin{aligned}
z_m &= \sum_j w_{mj} x_j + w_{m0}, \quad h_m = g(z_m), \quad m = 1, \ldots, M \\
z_q &= \sum_m w_{qm} h_m + w_{q0}, \quad h_q = g(z_q), \quad q = 1, \ldots, Q \\
z_k &= \sum_q w_{kq} h_q + w_{k0}, \quad k = 1, \ldots, K \\
\widehat{y}_k &= g_k(z_1, \ldots, z_K) = f_k(x, \theta), \quad k = 1, \ldots, K
\end{aligned}
$$

- Loss function:

$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(f(x_i; \theta), y_i).$$

Notations



Derivatives w.r.t to the w_{kq}

- We compute the gradient of $\mathcal{L}(f(x;\theta),y)$.
- The derivatives w.r.t to the weights w_{kq} can be computed as

$$\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial w_{kq}} = \underbrace{\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial z_k}}_{\delta_k} \underbrace{\frac{\partial z_k}{\partial w_{kq}}}_{h_q}$$

with

$$\delta_k = \sum_{k'=1}^{K} \frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial \widehat{y}_{k'}} \frac{\partial \widehat{y}_{k'}}{\partial z_k}$$

- With the sum-of-squares criterion and linear output units, we have $\mathcal{L}(f(x;\theta),y) = (\widehat{y}_k - y_k)^2$ and $\widehat{y}_k = z_k$, so

$$\delta_k = 2(\widehat{y}_k - y_k)$$

Derivatives w.r.t to the w_{qm}

The derivatives w.r.t to the weights w_{qm} can be computed as

$$\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial w_{qm}} = \underbrace{\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial z_q}}_{\delta_q} \underbrace{\frac{\partial z_q}{\partial w_{qm}}}_{h_m}$$

with

$$\delta_q = \sum_k \underbrace{\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial z_k}}_{\delta_k} \underbrace{\frac{\partial z_k}{\partial h_q}}_{w_{kq}} \underbrace{\frac{\partial h_q}{\partial z_q}}_{g'(z_q)}$$

$$\delta_q = g'(z_q) \sum_k \delta_k w_{kq}$$

Derivatives w.r.t to the w_{mj}

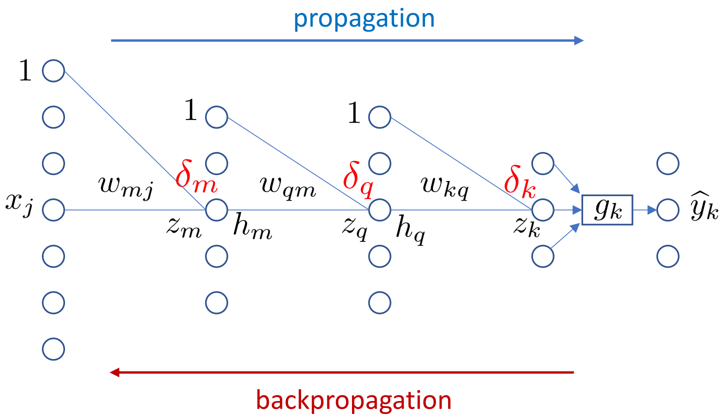
The derivatives w.r.t to the weights w_{mj} can be obtained as

$$\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial w_{mj}} = \underbrace{\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial z_m}}_{\delta_m} \underbrace{\frac{\partial z_m}{\partial w_{mj}}}_{x_j}$$

with

$$\begin{aligned}\delta_m &= \sum_q \underbrace{\frac{\partial \mathcal{L}(f(x;\theta),y)}{\partial z_q}}_{\delta_q} \underbrace{\frac{\partial z_q}{\partial h_m}}_{w_{qm}} \underbrace{\frac{\partial h_m}{\partial z_m}}_{g'(z_m)} \\ &= g'(z_m) \sum_q \delta_q w_{qm}\end{aligned}$$

Back-propagation algorithm



Advantage of back-propagation

- The advantage of back-propagation is its local nature: each hidden unit passes and receives information only to and from units that share a connection.
- Hence it can be implemented efficiently on a parallel architecture computer.
- Each gradient evaluation requires $O(N)$ operations, where N is the number of weights in the network. Consequently, the algorithm can be applied to large networks.

Overview

Batch learning with gradient descent

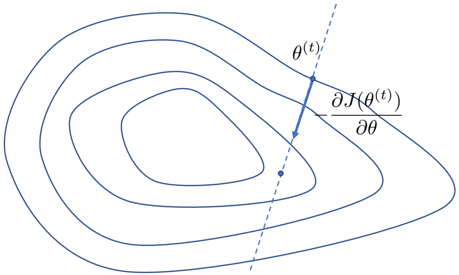
- The simplest approach to using gradient information is gradient descent: we choose the weight update to comprise a small step in the direction of the negative gradient, so that

$$\begin{aligned}\theta^{(t+1)} &= \theta^{(t)} - \eta_t \frac{\partial J(\theta^{(t)})}{\partial \theta} \\ &= \theta^{(t)} - \eta_t \frac{1}{n} \sum_{i=1}^{n} \frac{\partial \mathcal{L}(f(x_i, \theta^{(t)}), y_i)}{\partial \theta}\end{aligned}$$

  Coefficient η_t is called the learning rate.
- The error function is the average loss over the training set, and so each step requires that the entire training set be processed in order to evaluate the gradient. This is called called batch learning.

Batch gradient descent with line search

The learning rate η_t for batch learning was originally taken to be a constant; it can also be optimized by a line search, which minimizes the error function at each update.



Quasi-Newton methods

- Faster learning can be achieved using more powerful optimization algorithms.
- The Newton-Raphson method cannot be used, because the second derivative matrix of J (the Hessian) can be very large.
- Quasi-Newton methods are based on approximations of the Hessian. For instance, a diagonal approximation can be computed in $O(N)$ time. Other methods like the BFGS algorithm update the Hessian estimate by analyzing successive gradient vectors.

Stochastic gradient descent

- Batch learning is not feasible with very large learning sets. Learning can then be carried out online – processing each observation one at a time, updating the gradient after each training case, and cycling through the training cases many times.
- In this case, the update equation become

$$\theta^{(t+1)} = \theta^{(t)} - \eta_t \frac{\partial \mathcal{L}(f(x_t, \theta^{(t)}), y_t)}{\partial \theta}$$

  where (x_t, y_t) is the training example presented at iteration t.
- Here, $\frac{\partial \mathcal{L}(f(x_t,\theta^{(t)}),y_t)}{\partial \theta}$ can be seen as an estimate of $\frac{\partial \mathbb{E}\mathcal{L}(f(X,\theta^{(t)}),Y)}{\partial \theta}$
- Online training (also called stochastic gradient descent – SGD) allows the network to handle very large training sets, and also to update the weights as new observations come in.

Minibatch

- In practice, we often average the gradient over a randomly selected subset of $\nu \ll n$ learning examples $\{(x_{i_1}, y_{i_1}), \ldots, (x_{i_n}, y_{i_\nu})\}$ called a minibatch.
- The update equation is then

$$\theta^{(t+1)} = \theta^{(t)} - \eta_t \frac{1}{\nu} \sum_{j=1}^{\nu} \frac{\partial \mathcal{L}(f(x_{i_j}, \theta^{(t)}), y_{i_j})}{\partial \theta}$$

- A minibatch is randomly selected before each weight update.

SGD algorithm with a fixed learning rate

```
Require: Learning rate $\eta$
Require: Initial parameter $\theta$
  while stopping criterion not met do
    Sample a minibatch $\{(x_{i_1}, y_{i_1}), \ldots, (x_{i_n}, y_{i_\nu})\}$ of $\nu$ examples from the training set
    Compute gradient estimate $\widehat{\boldsymbol{g}} = \frac{1}{n} \sum_{j=1}^{\nu} \frac{\partial \mathcal{L}(f(x_{i_j}, \theta), y_{i_j})}{\partial \theta}$
    Apply update: $\theta \leftarrow \theta - \eta \widehat{\boldsymbol{g}}$
  end while
```

Learning rate

- In practice, it is necessary to gradually decrease the learning rate over time, so we now denote the learning rate at iteration t as η_t.
- The decrease should be neither too fast, nor too slow to guarantee convergence.
- In practice, it is common to decay the learning rate linearly until some iteration τ:

$$\eta_t = \begin{cases} \left(1 - \frac{t}{\tau}\right)\eta_0 + \frac{t}{\tau}\eta_\tau & \text{if } t < \tau \\ \eta_\tau & \text{if } t \geq \tau \end{cases}$$

- Usually τ may be set to the number of iterations required to make a few hundred passes through the training set.
- While SGD remains a very popular optimization strategy, learning with it can sometimes be slow, and several accelerated learning algorithms have been proposed.

The RMSprop algorithm

- The RMSprop algorithm uses a separate learning rate for each parameter and automatically adapts these learning rates throughout the course of learning.
- Idea: the parameters with smaller partial derivative of the loss should have a correspondingly larger learning rate.
- RMSprop adapts the learning rates of all model parameters by scaling them inversely proportional to the square root of an exponentially decaying average of historical squared values of the gradient.
- RMSProp is currently one of the most widely used methods for training deep neural networks.

RMSprop algorithm

```
Require: Global learning rate $\epsilon$, decay rate $\rho$
Require: Initial parameter $\theta$
Require: Small constant $\delta$, usually $10^{-6}$ used to stabilize division by small numbers
  Initialize accumulation variables $\mathbf{r} = 0$
  while stopping criterion not met do
    Sample a minibatch $\{(x_{i_1}, y_{i_1}), \ldots, (x_{i_n}, y_{i_\nu})\}$ of $\nu$ examples from the training set
    Compute gradient estimate $\widehat{\mathbf{g}} = \frac{1}{n}\sum_{j=1}^{\nu} \frac{\partial \mathcal{L}(f(x_{i_j}, \theta^{(t)}), y_{i_j})}{\partial \theta}$
    Accumulate squared gradient: $\mathbf{r} \leftarrow \rho \mathbf{r} + (1-\rho)\widehat{\mathbf{g}} \odot \widehat{\mathbf{g}}$ (multiplication applied element-wise)
    Compute parameter update: $\Delta\theta = -\frac{\epsilon}{\sqrt{\delta + \mathbf{r}}} \odot \widehat{\mathbf{g}}$ (division and square root applied element-wise)
    Apply update: $\theta \leftarrow \theta + \Delta\theta$
  end while
```

Importance of starting values

- Most learning algorithms are strongly affected by the choice of initialization. The initial point can determine whether the algorithm converges at all, as well as the speed of convergence.
- The initial parameters need to "break symmetry" between different units: If two hidden units with the same activation function are connected to the same inputs, then these units must have different initial parameters.
- Typically, we set the biases for each unit to heuristically chosen constants, and initialize only the weights randomly.

Some heuristics

- Some heuristics are available for choosing the initial scale of the weights.
- One heuristic is to initialize the weights of a fully connected layer with m inputs and n outputs by sampling each weight from

$$\mathcal{U}\left(-\frac{1}{\sqrt{m}}, +\frac{1}{\sqrt{m}}\right).$$

- Other authors suggest using the normalized initialization:

$$w_{ij} \sim \mathcal{U}\left(-\sqrt{\frac{6}{m+n}}, +\sqrt{\frac{6}{m+n}}\right).$$

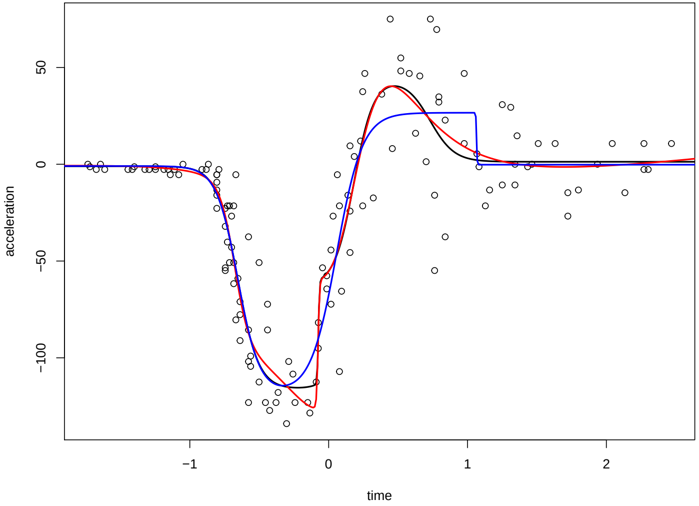
- It is best to standardize all inputs to have mean zero and standard deviation one, or to belong to $[-1, 1]$.

Overview

Shallow NN training using the nnet package

```
library('MASS')
mcycle.data<-data.frame(mcycle,x=scale(mcycle$times))
test.data<-data.frame(x=seq(-2,3,0.01))

library('nnet')

nn1<- nnet(accel ~ x, data=mcycle.data, size=5, linout = TRUE)
pred1<- predict(nn1,newdata=test.data)

nn2<- nnet(accel ~ x, data=mcycle.data, size=5, linout = TRUE)
pred2<- predict(nn2,newdata=test.data)

nn3<- nnet(accel ~ x, data=mcycle.data, size=5, linout = TRUE)
pred3<- predict(nn3,newdata=test.data)
```

Results

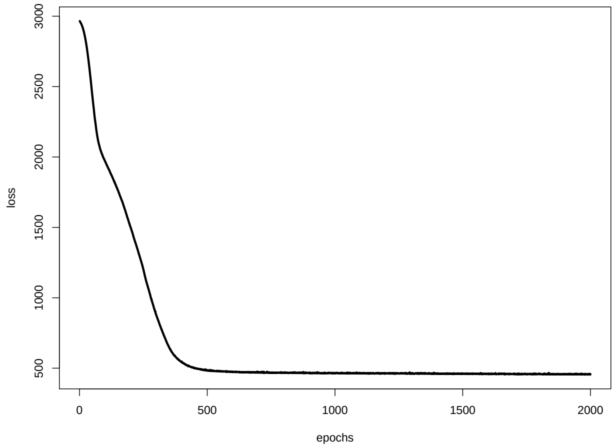


Deep NN training using the keras package

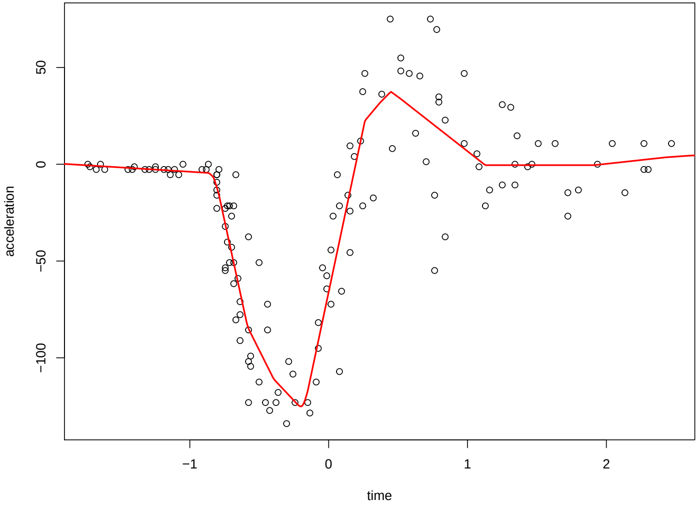
```
library(keras)

model <- keras_model_sequential()

model %>% layer_dense(units = 30, activation = 'relu', input_shape = 1) %>%
layer_dense(units = 20, activation = 'relu') %>%
layer_dense(units = 5, activation = 'relu') %>%
layer_dense(units = 1, activation = 'linear')


model %>% compile(loss = 'mean_squared_error', optimizer = optimizer_rmsprop())

history <- model %>% fit(mcycle.data$x, mcycle.data$accel,
           epochs = 2000, batch_size = 30)

x=seq(-2,3,0.01)
pred <- predict(model, x)
```

Training error

```
plot(history$metrics$loss,type="l",lwd=3,,xlab="epochs",ylab="loss")
```



Result



Overview

Necessity of complexity control

- Because of the universal approximation property of neural networks, the training error can, in principle, be made arbitrarily small by increasing the number of hidden units.
- However, a large neural network will be prone to overfitting and will typically have bad generalization performance.
- We need to control the complexity of the model. Many approaches have been proposed. We will review two approaches:
  1. Regularization
  2. Early stopping

Overview

Weight decay

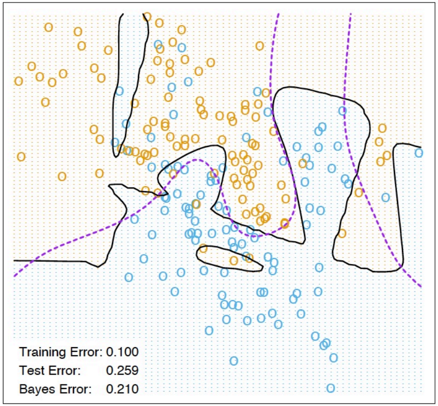
- An approach to control the complexity of a neural network is to choose a relatively large value for M and to add a norm penalty term (regularizer) to the error function.
- The simplest regularizer is the quadratic (L_2), giving a regularized error

$$\widetilde{J}(\theta) = J(\theta) + \lambda \theta^T \theta$$

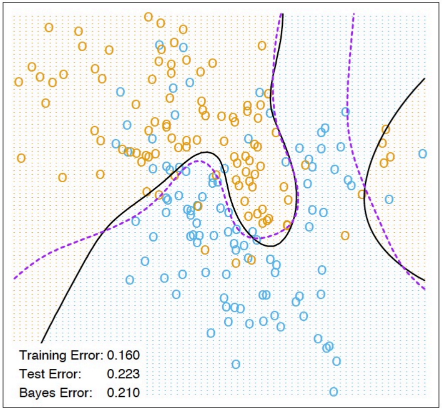
- This regularizer is also as weight decay. It is similar to ridge regression. The regularization coefficient λ is usually determined by cross-validation.
- This regularizer can be interpreted as the negative logarithm of a zero-mean Gaussian prior distribution over the weight vector θ.
- Other regularizer choices, such as L_1 (Lasso) correspond to a different prior (Laplace).

Example 1: classification

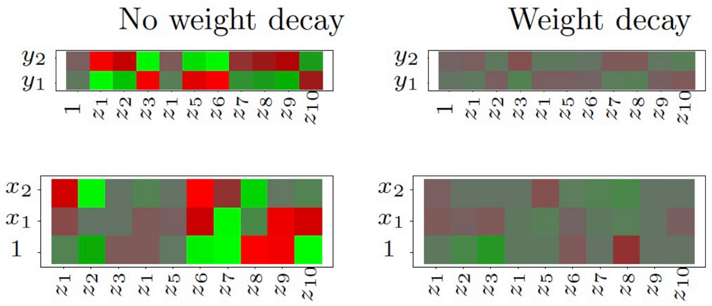
Neural Network - 10 Units, No Weight Decay



Neural Network - 10 Units, Weight Decay=0.02



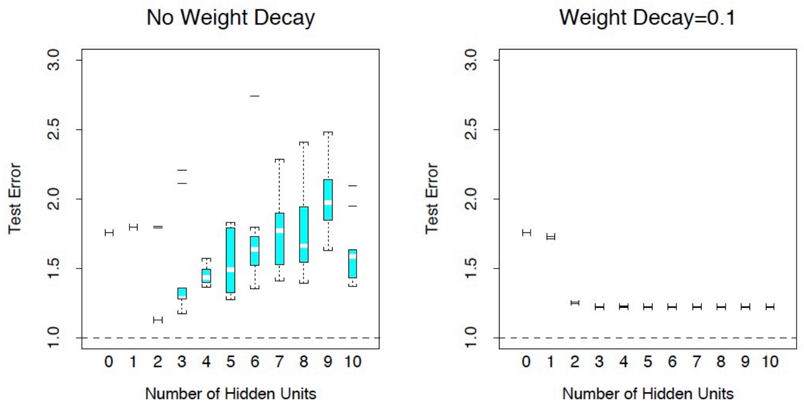
Heat maps of estimated weights



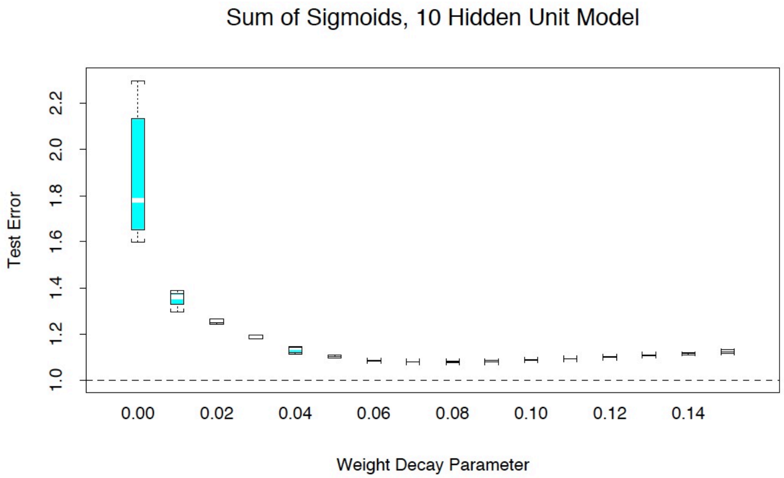
Example 2: regression

- Model $Y = f(X) + \varepsilon$ with
$$f(X) = \Lambda(a_1^T X) + \Lambda(a_2^T X),$$
$X = (X_1, X_2)$, $a_1 = (3, 3)$, $a_2 = (3, -3)$, $\mathrm{Var}(f(X))/\mathrm{Var}(\varepsilon) = 4$.
- Training sample of size 100, a test sample of size 10,000.
- Neural networks with weight decay and various numbers of hidden units.
- 10 random starting weights for each configutation.

Results without and with weight decay



Influence of the weight decay hyper-parameter



Generalization

- More generally, we can penalize each layer of weights with a different coefficient.
- For instance, in the case of one hidden layer, we have

$$\lambda_1 \sum_{m=1}^{M} \sum_{j=1}^{p} w_{mj}^2 + \lambda_2 \sum_{k=1}^{K} \sum_{m=1}^{M} w_{km}^2$$

- This corresponds to the Gaussian prior

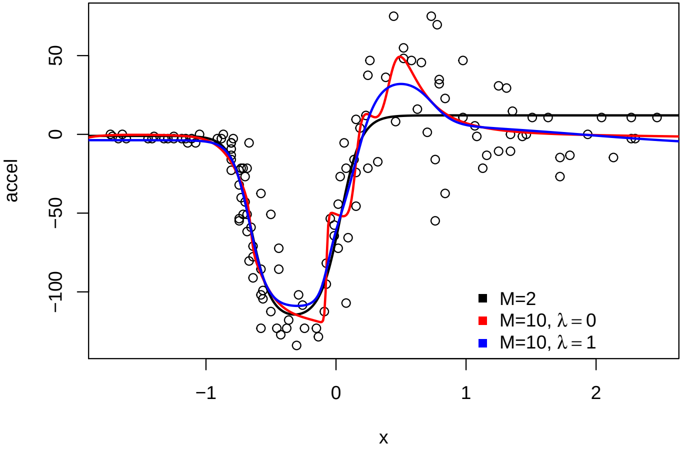
$$p(\mathbf{w} \mid \lambda_1, \lambda_2) \propto \exp\left(-\lambda_1 \sum_{m=1}^{M} \sum_{j=1}^{p} w_{mj}^2 - \lambda_2 \sum_{k=1}^{K} \sum_{m=1}^{M} w_{km}^2 \right)$$

- This approach has some theoretical advantages (it makes the regularizer invariant under linear transformations of the inputs and outputs), but we now have two (or more) hyperparameters to fix.

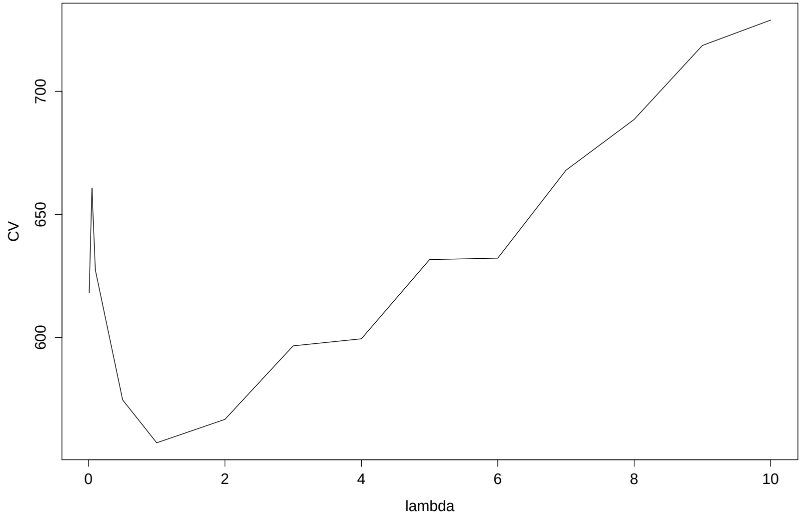
Shallow NN training with weight decay using nnet

```
library('MASS')
mcycle.data<-data.frame(mcycle,x=scale(mcycle$times))
test.data<-data.frame(x=seq(-2,3,0.01))

library('nnet')

nn1<- nnet(accel ~ x, data=mcycle.data, size=2, linout = TRUE, decay=0)
pred1<- predict(nn1,newdata=test.data)

nn2<- nnet(accel ~ x, data=mcycle.data, size=10, linout = TRUE, decay=0)
pred2<- predict(nn2,newdata=test.data)

nn3<- nnet(accel ~ x, data=mcycle.data, size=10, linout = TRUE, decay=1)
pred3<- predict(nn3,newdata=test.data)
```

Results



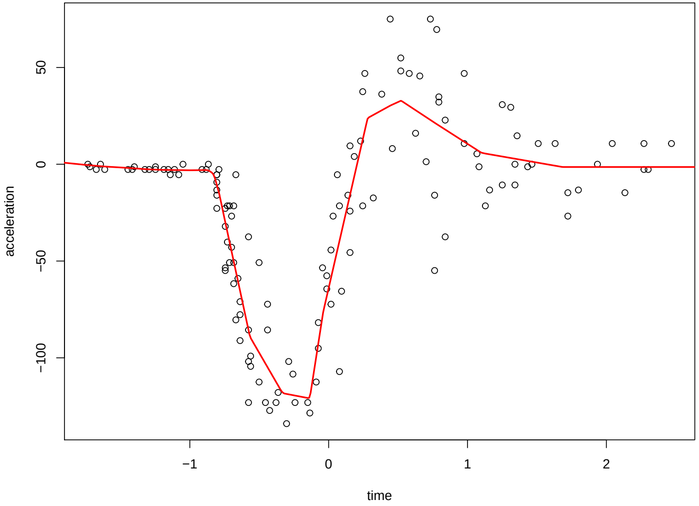
Selection of λ by 10-fold cross-validation



Deep NN training with weight decay using keras

```
library('keras')

model <- keras_model_sequential()
model %>%
layer_dense(units = 50, activation = 'relu', input_shape = 1,
kernel_regularizer = regularizer_l2(l=0.1)) %>%
layer_dense(units = 30, activation = 'relu',
kernel_regularizer = regularizer_l2(l=0.1)) %>%
layer_dense(units = 20, activation = 'relu',
kernel_regularizer = regularizer_l2(l=0.1)) %>%
layer_dense(units = 1, activation = 'linear')

model %>% compile(loss = 'mean_squared_error',optimizer = optimizer_rmsprop())
history <- model %>% fit(mcycle.data$x, mcycle.data$accel, epochs = 2000,
           batch_size = 30)
pred <- predict(model, x)
```

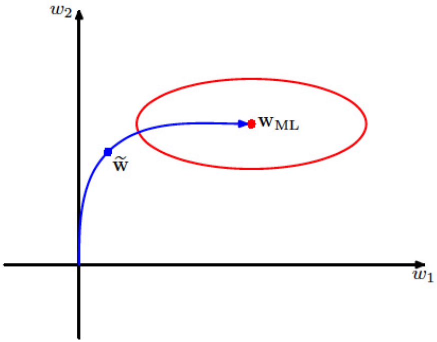
Results



Overview

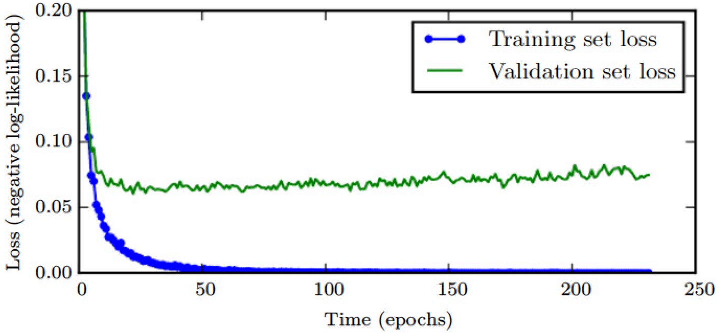
Early stopping

- An alternative to regularization as a way of controlling the effective complexity of a network is early stopping: we train the model only for a while, and stop well before we approach the global minimum.



- Since the weights start at a highly regularized (linear) solution, this has the effect of shrinking the final model toward a linear model.
- A validation dataset is useful for determining when to stop, since we expect the validation error to start increasing.

Example



Learning curves showing how the negative log-likelihood loss changes over time (indicated as number of training iterations over the dataset, or epochs). The training loss decreases consistently over time, but the validation loss eventually begins to increase again, forming an asymmetric U-shaped curve.