Chapter 23 Deep Learning, Neural Networks



Deep learning is a special branch of machine learning using a collage of algorithms to model high-level data motifs. Deep learning resembles the biological communications of systems of brain neurons in the central nervous system (CNS), where synthetic graphs represent the CNS network as nodes/states and connections/edges between them. For instance, in a simple synthetic network consisting of a pair of connected nodes, an output sent by one node is received by the other as an input signal. When more nodes are present in the network, they may be arranged in multiple levels (like a multiscale object) where the ith layer output serves as the input of the next (i + 1)st layer. The signal is manipulated at each layer, sent as a layer output downstream, interpreted as an input to the next, (i + 1)st layer, and so forth. Deep learning relies on multipler layers of nodes and many edges linking the nodes forming input/output (I/O) layered grids representing a multiscale processing network. At each layer, linear and non-linear transformations are converting inputs into outputs.

In this chapter, we explore the R deep learning package MXNet and demonstrate state-of-the-art deep learning models utilizing CPU and GPU for fast training (learning) and testing (validation). Other powerful deep learning frameworks include *TensorFlow*, *Theano*, *Caffe*, *Torch*, *CNTK* and *Keras*.

Neural Networks vs. Deep Learning: Deep Learning is a machine learning strategy that learns a deep multi-level hierarchical representation of the affinities and motifs in the dataset. Machine learning Neural Nets tend to use shallower network models. Although there are no formal restrictions on the depth of the layers in a Neural Net, few layers are commonly utilized. Recent methodological, algorithmic, computational, infrastructure, and service advances overcome previous limitations. In addition, the rise of Big Data accelerated the evolution of classical Neural Nets to Deep Neural Nets, which can now handle lots of layers and many hidden nodes per layer. The former is a precursor to the latter; however, there are also non-neural deep learning techniques, for example, syntactic pattern recognition methods and grammar induction discover hierarchies.

23.1 Deep Learning Training

Review Chap. 11 (Black Box Machine-Learning Methods: Neural Networks and Support Vector Machines) prior to proceeding.

23.1.1 Perceptrons

A **perceptron** is an artificial analogue of a neuronal brain cell that calculates a weighted sum of the input values and outputs a thresholded version of that result. For a bivariate perceptron, P, having two inputs, (X, Y), we can denote the weights of the inputs by A and B, respectively. Then, the weighted sum could be represented as:

$$W = AX + BY$$
.

At each layer l, the weight matrix, $W^{(l)}$, has the following properties:

- The number of rows of $W^{(l)}$ equals the number of nodes/units in the previous (l-1)st layer, and
- The number of columns of $W^{(l)}$ equals the number of units in the next (l + 1)st layer.

Neuronal cells fire depending on the presynaptic inputs to the cell, which causes constant fluctuations of the neuronal membrane - depolarizing or hyperpolarizing, i.e., the cell membrane potential rises or falls. Similarly, perceptrons rely on thresholding of the weight-averaged input signal, which for biological cells corresponds to voltage increases passing a critical threshold. Perceptrons output non-zero values only when the weighted sum exceeds a certain threshold C. In terms of its input vector, (X, Y), we can describe the output of each perceptron (P) by:

$$Output(P) = \begin{cases} 1, & \text{if } AX + BY > C \\ 0, & \text{if } AX + BY \leq C \end{cases}.$$

Feed-forward networks are constructed as layers of perceptrons where the first layer ingests the inputs and the last layer generates the network outputs. The intermediate (internal) layers are not directly connected to the external world, and are called hidden layers. In *fully connected networks*, each perceptron in one layer is connected to every perceptron on the next layer enabling information "fed forward" from one layer to the next. There are no connections between perceptrons in the same layer.

Multilayer perceptrons (fully-connected feed-forward neural network) consist of several fully-connected layers representing an input matrix $X_{n \times m}$ and a generated output matrix $Y_{n \times k}$. The input $X_{n,m}$ is a matrix encoding the n cases and m features per case. The weight matrix $W_{m,k}^{(l)}$ for layer l has rows (i) corresponding to

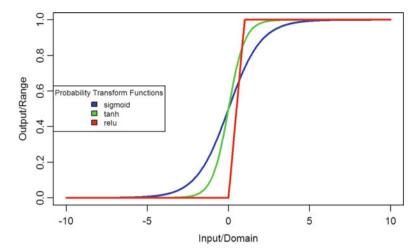


Fig. 23.1 Graphical representation of three alternative activation functions

the weights leading from all the units i in the previous layer to all of the units j in the current layer. The product matrix $X \times W$ has dimensions $n \times k$.

The hidden size parameter k, the weight matrix $W_{m \times k}$, and the bias vector $b_{n \times 1}$ are used to compute the outputs at each layer:

$$Y_{n \times k}^{(l)} = f_k^{(l)} (X_{n \times m} W_{m \times k} + b_{k \times 1}).$$

The role of the bias parameter is similar to the intercept term in linear regression and helps improve the accuracy of prediction by shifting the decision boundary along *Y* axis. The outputs are fully-connected layers that feed into an activation layer to perform element-wise operations. Examples of **activation functions** that transform real numbers to probability-like values include (Fig. 23.1):

- The sigmoid function, a special case of the logistic function, which converts real numbers to probabilities,
- The rectifier (relu, Rectified Linear Unit) function, which outputs the max(0, input),
- The tanh (hyperbolic tangent function).

The final fully-connected layer may be hidden of size equal to the number of classes in the dataset and may be followed by a softmax layer mapping the input into a probability score. For example, if a size $n \times m$ input is denoted by $X_{n \times m}$, then the probability scores may be obtained by the softmax transformation function, which maps real valued vectors to vectors of probabilities:

$$\left(\frac{e^{x_{i,1}}}{\sum_{j=1}^{m} e^{x_{i,j}}}, \dots, \frac{e^{x_{i,m}}}{\sum_{j=1}^{m} e^{x_{i,j}}}\right).$$

Fig. 23.2 A schematic of a fully-connected feed-forward neural network with two hidden layers

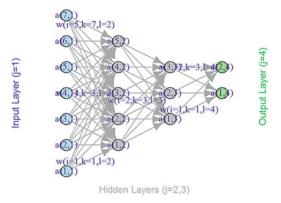


Figure 23.2 shows is a schematic of fully-connected feed-forward neural network of nodes:

$$\{a_{j=node \ index, l=layer \ index}\}_{j=1, l=1}^{n_j, 4}$$
.

The plot above illustrates the key elements in the action potential, or activation function, and the calculations of the corresponding training parameters:

$$a_{node=k,layer=l} = f\left(\sum_{i} w_{k,i}^{l} \times a_{i}^{l-1} + b_{k}^{l}\right),$$

where:

- f is the *activation function*, e.g., logistic function $f(x) = \frac{1}{1 + e^{-x}}$. It converts the aggregate weights at each node to probability values,
- $w_{k,i}^l$ is the weight carried from the *i*th element of the (l-1)th layer to the *k*th element of the current *l*th layer,
- b_k^l is the (residual) bias present in the kth element in the lth layer. This is effectively the information not explained by the training model.

These parameters may be estimated using different techniques (e.g., using least squares, or stochastically using steepest decent methods) based on the training data.

23.2 Biological Relevance

There are parallels between biology (neuronal cells) and the mathematical models (perceptrons) for neural network representation. The human brain contains about 10^{11} neuronal cells connected by approximately 10^{15} synapses forming the basis of our

functional phenotypes. Figure 23.3 illustrates some of the parallels between brain biology and the mathematical representation using synthetic neural nets. Every neuronal cell receives multi-channel (afferent) input from its dendrites, generates output signals, and disseminates the results via its (efferent) axonal connections and synaptic connections to dendrites of other neurons.

The perceptron is a mathematical model of a neuronal cell that allows us to explicitly determine algorithmic and computational protocols transforming input signals into output actions. For instance, a signal arriving through an axon x_0 is modulated by some prior weight, e.g., synaptic strength, $w_0 \times x_0$. Internally, within the neuronal cell, this input is aggregated (summed, or weight-averaged) with inputs from all other axons. Brain plasticity suggests that synaptic strengths (weight coefficients w) are strengthened by training and prior experience. This learning process controls the direction and strength of influence of neurons on other neurons. Either excitatory (w > 0) or inhibitory ($w \le 0$) influences are possible. Dendrites and axons carry signals to and from neurons, where the aggregate responses are computed and transmitted downstream. Neuronal cells only fire if action potentials exceed a certain threshold. In this situation, a signal is transmitted downstream through its axons. The neuron remains silent, if the summed signal is below the critical threshold.

Timing of events is important in biological networks. In the computational perceptron model, a first order approximation may ignore the timing of neuronal firing (spike events) and only focus on the frequency of the firing. The firing rate of a neuron with an activation function f represents the frequency of the spikes along the axon. We saw some examples of activations functions earlier.

Figure 23.3 illustrates the parallels between the brain network-synaptic organization and an artificial synthetic neural network.

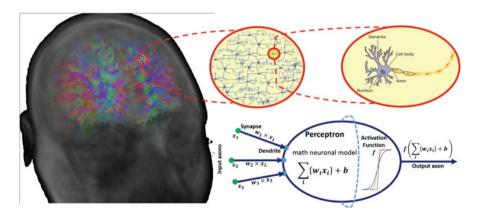


Fig. 23.3 A depiction of the parallels between a biological central nervous system network organization (human bran) and a synthetic neural network employed in deep machine learning

23.3 Simple Neural Net Examples

Before we look at some examples of deep learning algorithms applied to model observed natural phenomena. Specifically, we will develop a couple of simple networks for computing fundamental Boolean operations.

23.3.1 Exclusive OR (XOR) Operator

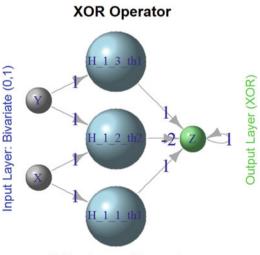
The exclusive OR (XOR) operator works as a bivariate binary-outcome function, mapping pairs of false (0) and true (1) values to dichotomous false (0) and true (1) outcomes.

We can design a simple two-layer neural network that calculates XOR. The **values listed within each neuron represent its explicit threshold**, which can be normalized so that all neurons utilize the same threshold (typically 1). The **value labels associated with network connections (edges) represent the weights of the inputs**. When the threshold is not reached, the output is 0, and when the threshold is reached, the output is correspondingly 1 (Fig. 23.4).

Let's work out manually the four possibilities (Table 23.1):

We can validate that this network indeed represents an XOR operator by plugging in all four possible input combinations and confirming the expected results at the end (Fig. 23.5).

Fig. 23.4 A neural network representation corresponding to the XOR binary function



Hidden Layers (Neurons)

Table 23.1 Exact XOR binary operator

InputX	InputY	XOR output(Z)
0	0	0
0	1	1
1	0	1
1	1	0

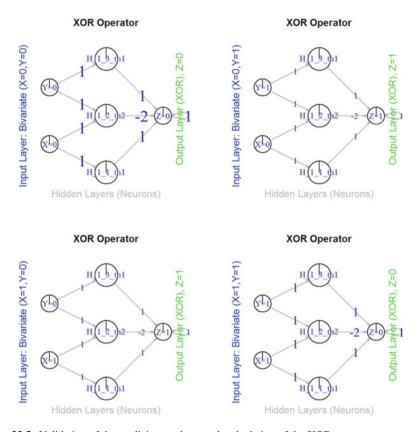


Fig. 23.5 Validation of the explicit neural network calculation of the XOR operator

23.3.2 NAND Operator

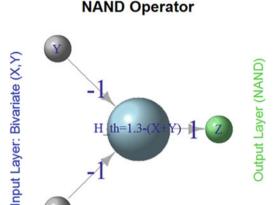
Another binary operator is NAND (negative AND, Sheffer stroke), which produces a false (0) output if and only if both of its operands are true (1), and which generates true (1), otherwise. Below is the NAND input-output table (Table 23.2).

Similarly to the XOR operator, we can design a one-layer neural network that calculates NAND. Again, the values listed within each neuron represent its explicit threshold, which can be normalized so that all neurons utilize the same threshold (typically 1). The value labels associated with network connections (edges) represent the weights of the inputs. When the threshold is not reached, the output

Table 2	3.2	Exact	NAND
binary o	pera	itor	

InputX	InputY	NAND output(Z)		
0	0	1		
0	1	1		
1	0	1		
1	1	0		

Fig. 23.6 A neural network representation corresponding to the NAND binary function



Hidden Layers (Neurons)

is trivial (0), and when the threshold is reached, the output is correspondingly 1. Here is a shorthand analytic expression for the NAND calculation:

$$NAND(X, Y) = 1.3 - (1 \times X + 1 \times Y).$$

Check that NAND(X, Y) = 0 if and only if X = 1 and Y = 1, otherwise it equals 1 (Fig. 23.6).

23.3.3 Complex Networks Designed Using Simple Building Blocks

Observe that stringing together some of these primitive networks of Boolean operators, or/and increasing the number of hidden layers, allows us to model problems with exponentially increasing complexity. For instance, constructing a 4-input NAND function would simply require repeating several of our 2-input NAND operators. This will increase the space of possible outcomes from 2^2 to 2^4 . Of course, introducing more depth in the **hidden layers** further expands the complexity of the problems that can be modeled using neural nets.

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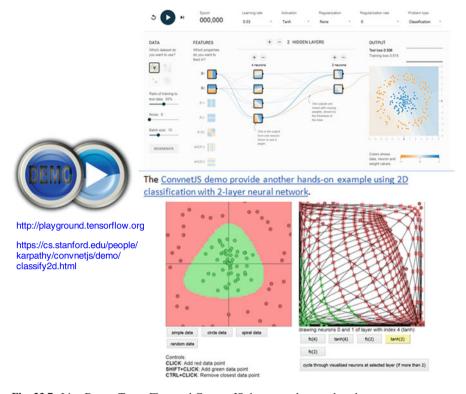


Fig. 23.7 Live Demo: TensorFlow and ConvnetJS deep neural network webapps

You can interactively manipulate Google's TensorFlow Deep Neural Network Webapp to gain additional intuition and experience with the various components of deep learning networks.

The ConvnetJS demo provide another hands-on example using 2D classification with 2-layer neural network (Fig. 23.7).

23.4 Classification

In MXNet, a Multilayer perceptron (MLP) may be defined by:

- Creating a place holder variable for the input data, data = mx.sym.Variable('data')
- Flattening the data from 4D shape space (width, height, batch_size, num_channel) into 2D (num_channel*width*height, batch_size), 'data = mx. sym.Flatten(data=data)'
- And iterating over the fully-connected layers:

- First layer, fc1 = mx.sym.FullyConnected(data=data, name='fc1', num hidden=128)
- Generate the second fully-connected layer and apply the activation function,
 fc2 = mx.sym.FullyConnected(data=act1, name='fc2',
 num_hidden = 64); act2 = mx.sym.Activation(data=fc2,
 name='relu2', act type="relu")
- Generate the third/final fully-connected layer, with a hidden size k=10, which in digit recognition tasks corresponds to the number of unique digits 0:9, fc3 = mx.sym.FullyConnected(data=act2, name='fc3', num hidden=10)
- Finally, mapping the input into a probability score using the softmax and loss layer, mlp = mx.sym.SoftmaxOutput(data=fc3, name='softmax'). See the mlp R source code here.

23.4.1 Sonar Data Example

Let's load the mlbench and mlbench packages and demonstrate the basic invocation of mxnet. The Sonar data mlbench::Sonar includes sonar signals bouncing off a metal cylinder or a roughly cylindrical rock. Each of 208 patterns includes a set of 60 numbers (features) in the range 0.0–1.0, and a label M (metal) or R (rock). Each feature represents the energy within a particular frequency band, integrated over a certain period of time. The M and R labels associated with each observation classify the record as rock or mine (metal) cylinder. The numbers in the labels are in increasing order of aspect angle, but they do not encode the angle directly.

```
# Load the required packages: mlbench and mxnet
# install.packages("mlbench"); install.packages("mxnet")
# Note mxnet requires "visNetwork"
# If it doesn't work, you may need the following lines:
# install.packages("drat", repos="https://cran.rstudio.com")
# drat:::addRepo("dmlc")
# install.packages("mxnet")

require(mLbench)
require(mxnet)
## Init Rcpp

data(Sonar, package="mlbench")

table(Sonar[,61])
```

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```
##
## M R
## 111 97

Sonar[,61] = as.numeric(Sonar[,61])-1 # R = "1", "M" = "0"
set.seed(123)
train.ind = sample(1:nrow(Sonar),0.7*nrow(Sonar))

train.x = data.matrix(Sonar[train.ind, 1:60])
train.y = Sonar[train.ind, 61]
test.x = data.matrix(Sonar[-train.ind, 1:60])
test.y = Sonar[-train.ind, 61]
```

Let's start by using a **multi-layer perceptron** as a classifier. The mxnet function mx.mlp builds a general multi-layer neural network that can be utilized to do classification or regression graph modeling. It relies on the following parameters:

- Training data and labels
- Number of hidden nodes in each hidden layers
- Number of nodes in the output layer
- Type of activation
- Type of output loss
- The device to train (GPU or CPU)
- Additional optional parameters, see mx.model.FeedForward.create

Here is one example using the *training* and *testing* data we defined above:

```
mx.set.seed(1234)
model.mx <- mx.mlp(train.x, train.y, hidden node=8, out node=2,</pre>
out_activation="softmax",
      num.round=200, array.batch.size=15, Learning.rate=0.1, momentum=0.9,
            eval.metric=mx.metric.accuracy, verbose=F)
#calculate Prediction sensitivity & specificity
preds = predict(model.mx, test.x) # these are probabilities
# You can inspect the test labels vs. assigned probabilities by
# View(data.frame(test.y, preds[2,]))
preds1 <- ifelse(preds[2,] <= 0.5, 0, 1) # dichotomize to labels</pre>
table(preds1)
## preds1
## 0 1
## 35 28
pred.label = t(preds1)
table(pred.label, test.y)
##
            test.y
## pred.label 0 1
##
   0 28 7
##
           1 6 22
Library("caret")
sensitivity(factor(preds1), factor(as.numeric(test.y)),positive = 1)
## [1] 0.7586207
specificity(factor(preds1), factor(as.numeric(test.y)), negative = 0)
## [1] 0.8235294
```

We can also use crossval::diagnosticErrors() and crossval:: confusionMatrix() to get more detailed evaluations. Similar to using the sensitivity() and specificity() methods, we should specify the *negative* and *positive* labels.

Note that you have to specify crossval::confusionMatrix() if you also have the caret package loaded, as caret also has a function called confusionMatrix().

```
Library("crossval")
diagnosticErrors(crossval::confusionMatrix(preds1, test.y, negative = 0))
## acc sens spec ppv npv Lor
## 0.7936508 0.7857143 0.8000000 0.7586207 0.8235294 2.6855773
## attr(,"negative")
## [1] 0
```

Now, we compare the results of different number of rounds, or epochs, representing the number of full (training-phase) passes through the data (cf. num. round=n).

We can plot the ROC curve and calculate the AUC (Area under the curve) (Fig. 23.8):

```
# install.packages("pROC"); install.packages("plotROC"); install.packages("r
eshape2")
Library(pROC); Library(pLotROC); Library(reshape2);
# compute AUC
get_roc = function(preds){
    roc_obj <- roc(test.y, preds[2,])
    auc(roc_obj)
}
get_roc(preds)
## Area under the curve: 0.9249
get_roc(preds100)</pre>
```

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```
## Area under the curve: 0.9209
get_roc(preds50)
## Area under the curve: 0.8824
get_roc(preds10)
## Area under the curve: 0.8022
#plot roc
dt <- data.frame(test.y, preds[2,], preds100[2,], preds50[2,], preds10[2,])</pre>
colnames(dt) <- c("D", "rounds=200", "rounds=100", "rounds=50", "rounds=10")</pre>
dt <- melt(dt,id.vars = "D")</pre>
basicplot \leftarrow qqplot(dt, qes(d = D, m = value, colour=variable)) +
geom_roc(labels = FALSE, size = 0.5, alpha.line = 0.6, linejoin = "mitre") +
  theme_bw() + coord_fixed(ratio = 1) + style_roc() + ggtitle("ROC CURVE")+
  annotate("rect", xmin = 0.4, xmax = 1, ymin = 0.2, ymax = 0.75,
  alpha = .2)+
annotate("text", x = 0.7, y = 0.5, size = 3,
           Label = "AUC: \n rounds=200: 0.9209\n rounds=100: 0.9128\n
rounds=50: 0.8824\n rounds=10: 0.8022\n " )
basicplot
```

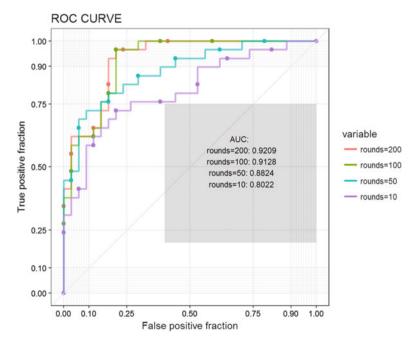


Fig. 23.8 ROC curves of multi-layer perceptron predictions (mx.mlp), using out-of-bag test-data, corresponding to different number of iterations, see Chap. 14

The plot suggests that the results stabilize after 100 training (epoch) iterations. Let's look at some visualizations of the real labels of the test data (test.y) and their corresponding ML-derived classification labels (preds [2,]) using 200 iterations (Figs. 23.9, 23.10, 23.11, 23.12, and 23.13).

```
graph.viz(model.mx$symbol)

hist(preds10[2,],main = "rounds=10")

hist(preds50[2,],main = "rounds=50")

hist(preds100[2,],main = "rounds=100")

hist(preds[2,],main = "rounds=200")

Output

O
```

Fig. 23.9 MLP model structure (the plot is rotated 90-degrees to save space)

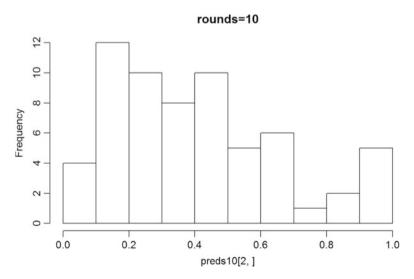


Fig. 23.10 Frequency plot of the predicted probabilities using ten epochs corresponding to ten full (training-phase) passes through the data (cf. num.round=n)

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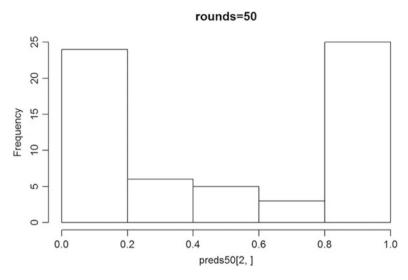


Fig. 23.11 Frequency plot of the predicted probabilities using 50 epochs, compare to Fig. 23.10

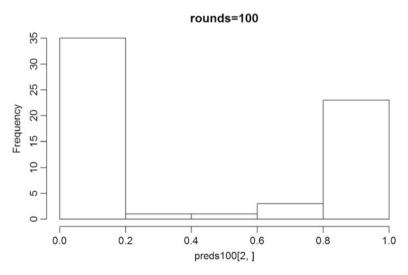


Fig. 23.12 Frequency plot of the predicted probabilities using 100 epochs, compare to Fig. 23.11

We see a significant bimodal trend when the number of rounds increases. Another plot shows more details about the agreement between the real labels and their predicted class counterparts (Fig. 23.14):

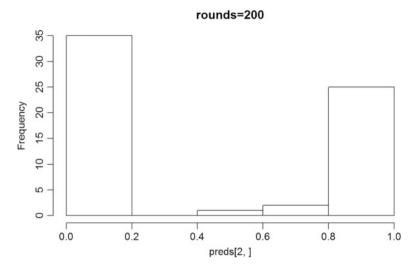


Fig. 23.13 And finally, the plot of the predicted probabilities using 200 epochs; compare to Fig. 23.12

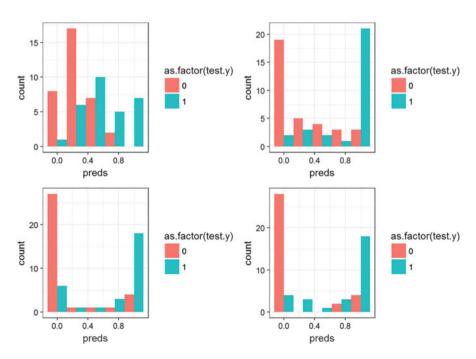


Fig. 23.14 Summary plots illustrating the progression of the neural network learning from 10 ro 200 epochs, corresponding with improved binary classification results (testing data)

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```
library(ggplot2)
get_gghist = function(preds){
    ggplot(data.frame(test.y, preds),
        aes(x=preds, group=test.y, fill=as.factor(test.y)))+
        geom_histogram(position="dodge",binwidth=0.25)+theme_bw()
}
df = data.frame(preds[2,],preds100[2,],preds50[2,],preds10[2,])
p <- lapply(df,get_gghist)
require(gridExtra) # used for arrange ggplots
grid.arrange(p$preds10.2...,p$preds50.2...,p$preds100.2...,p$preds.2...)</pre>
```

23.4.2 MXNet Notes

- The mx.mlp() function is a proxy to the more complex and laborious process of defining a neural network by using MXNet's Symbol. For instance, this call model.mx <mx.mlp(train.x, train.y, hidden node=8, out node=2, out activation="softmax", num.round=20, array.batch.size=15, learning.rate=0.1, momentum=0.9, eval.metric=mx.metric.accuracy) would be equivalent to a symbolic network definition like: data <- mx.symbol.Variable ("data"); mx.symbol.FullyConnected(data, fc1 < num hidden=128) act1 < mx.symbol.Activation(fc1, name="relu1", act type="relu"); fc2 <- mx.symbol. FullyConnected(act1, name="fc2", num hidden=64); act2 mx.symbol.Activation(fc2, name="relu2", act type="relu"); fc3 <- mx.symbol.FullyConnected(act2,</pre> name="fc3", num hidden=2); lro < -SoftmaxOutput(fc3, name="sm"); model2 <-</pre> mx.model.FeedForward.create(lro, X=train.x, y=train.y, ctx=mx. cpu(), num.round=100, array.batch.size=15, learning. rate=0.07, momentum=0.9) (see example with linear regression below).
- Layer-by-layer definitions translate inputs into outputs. At each level, the network allows for a different number of neurons and alternative activation functions. Other options can be specified by using mx.symbol:
- mx.symbol.Convolution applies convolution to the input and then adds a bias. It can create convolutional neural networks.
- mx.symbol.Deconvolution does the opposite and can be used in segmentation networks along with mx.symbol.UpSampling, e.g., to reconstruct the pixel-wise classification of an image.
- mx.symbol.Pooling reduces the data by selecting signals with the highest response.
- mx.symbol.Flatten links convolutional and pooling layers to form a fully connected network.
- mx.symbol.Dropout attempts to cope with the overfitting problem.

The function mx.mlp() is a wrapper for quick design of standard multi-layer perceptrons. For more extensive experiments, customized symbolic representation can be explicitly specified using combinations of the above methods.

```
# Example of **LeNet** network for recognizing handwritten digits:
data <- mx.symbol.Variable('data')</pre>
conv1 <- mx.symbol.Convolution(data=data, kernel=c(5,5), num_filter=20)</pre>
tanh1 <- mx.symbol.Activation(data=conv1, act type="tanh")
pool1 <- mx.symbol.Pooling(data=tanh1, pool_type="max", kernel=c(2,2),</pre>
stride=c(2,2)
conv2 <- mx.symbol.Convolution(data=pool1, kernel=c(5,5), num_filter=50)
tanh2 <- mx.symbol.Activation(data=conv2, act type="tanh")</pre>
pool2 <- mx.symbol.Pooling(data=tanh2, pool type="max", kernel=c(2,2),</pre>
stride=c(2,2)
flatten <- mx.symbol.Flatten(data=pool2)</pre>
fc1 <- mx.symbol.FullyConnected(data=flatten, num hidden=500)
tanh3 <- mx.symbol.Activation(data=fc1, act type="tanh")
fc2 <- mx.symbol.FullyConnected(data=tanh3, num_hidden=10)</pre>
lenet <- mx.symbol.SoftmaxOutput(data=fc2)</pre>
model <- mx.model.FeedForward.create(lenet, X=train.x, y=train.y, ctx=device</pre>
.cpu, num.round=5, array.batch.size=100, Learning.rate=0.05, momentum=0.9)
```

To allow smooth, fast, and consistent operation on CPU and GPU, in in mxnet, the generic R function controlling the reproducibility of stochastic results is overwritten by mx.set.seed. So can use mx.set.seed() to control random numbers in MXNet.

To examine the accuracy of the model.mx learner (trained on the training data), we can make prediction (on testing data) and evaluate the results using the provided testing labels (report the confusion matrix).

```
preds = predict(model.mx, test.x)
pred.label = max.col(t(preds))-1
table(pred.label, test.y)
## test.y
## pred.label 0 1
## 0 28 7
## 1 6 22
```

For multi-class predictions, mxnet outputs n (class) \times m (examples) confusion matrices where each row corresponds to probability of the corresponding (column-defined) class.

23.5 Case-Studies

Let's demonstrate *regression* and *prediction* deep learning examples using several complementary datasets.

23.5.1 ALS Regression Example

Let's first demonstrate a deep learning regression using the ALS data to predict ALSFRS slope, Figs. 23.15 and 23.16.

```
als <- read.csv("https://umich.instructure.com/files/1789624/download?downlo</pre>
ad_frd=1")
als <- scale(als[,-c(1,7)])
train.ind = sample(1:nrow(als), 0.7*nrow(als))
train.x = data.matrix(als[train.ind,-c(1,7)])
train.y = als[train.ind,7]
test.x = data.matrix(scale(als[-train.ind,-c(1,7)]))
test.y = als[-train.ind,7]
# Define the input data
data <- mx.symbol.Variable("data")</pre>
# A fully connected hidden layer
# data: input source
# num hidden: number of neurons in this hidden layer
fc1 <- mx.symbol.FullyConnected(data, num hidden=1)</pre>
# Use linear regression for the output layer
Lro <- mx.symbol.LinearRegressionOutput(fc1)</pre>
mx.set.seed(1234)
# Create a MXNet Feedforward neural net model with the specified training.
model <- mx.model.FeedForward.create(lro, X=train.x, y=train.y,</pre>
   ctx=mx.cpu(), num.round=1000, array.batch.size=20,
  learning.rate=2e-6, momentum=0.9, eval.metric=mx.metric.rmse, verbose=F)
```

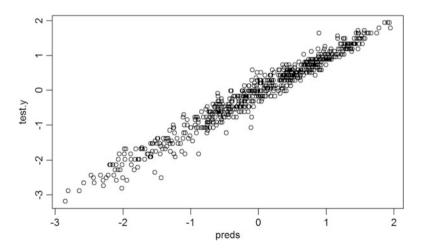
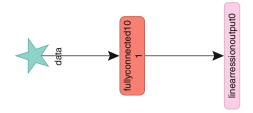


Fig. 23.15 The strong linear relation between the out-of-bag testing data continuous outcome variable (y-axis) and the corresponding predicted regression values (x-axis) suggests a good network prediction performance

Fig. 23.16 Computational graph of the neural network



The option verbose = F can suppress messages, including training accuracy reports, in each iteration. You may rerun the code with verbose = T to examine the rate of decrease of *train error* against the *number of iterations*.

You must scale data before inputting it into MXnet, which expects that the training and testing sets are normalized to the **same scale**. There are two strategies to scale the data

- Either scaling the complete data simultaneously and then splitting them into train data and test data, or
- Alternatively, scaling only the training dataset to enable model-training, but saving your protocol for data normalization, as new data (testing, validation) will need to be (pre)processed the same way as the training data.

Have a look at the Google TensorFlow API. It shows the importance of *learning* rate and the *number of rounds*. You should test different sets of parameters.

- Too small *learning rate* may lead to long computations.
- Too large *learning rate* may cause the algorithm to fail to converge, as large step size (learning rate) may by-pass the optimal solution and then oscillate or even diverge.

```
preds = predict(model, test.x)
sqrt(mean((preds-test.y)^2))
## [1] 0.2171032
range(test.y)
## [1] -3.181499  1.943890
# plot the correlation between testdata.y and testdata.predicted.y
plot(preds, test.y)
```

We can see that the *RMSE* on the test set is pretty small. To get a visual representation of the deep learning network we can also display this relatively simple computation graph (Fig. 23.16):

```
graph.viz(model$symbol)
```

23.5.2 Spirals 2D Data

We can again use the mx.mlp wrapper to construct the learning network, but we can also use a more flexible way to construct and configure the multi-layer network in mxnet. This configuration is done by using the Symbol call, which specifies the links among network nodes, the activation function, dropout ratio, and so on:

Below we show the configuration of a perceptron with one hidden layer.

```
######## Network configuration
# variables
act <- mx.symbol.Variable("data")</pre>
# affine transformation
fc <- mx.symbol.FullyConnected(act, num.hidden = 10)</pre>
# non-linear activation
act <- mx.symbol.Activation(data = fc, act_type = "relu")</pre>
# affine transformation
fc <- mx.symbol.FullyConnected(act, num.hidden = 2)</pre>
# softmax output and cross-
mlp <- mx.symbol.SoftmaxOutput(fc)</pre>
####Preparing data
set.seed(2235)
########## spirals dataset
s \leftarrow sample(x = c("train", "test"), size = 1000, prob = c(.8,.2), replace =
TRUE)
dta \leftarrow mlbench.spirals(n = 1000, cycles = 1.2, sd = .03)
dta <- cbind(dta[["x"]], as.integer(dta[["classes"]]) - 1)</pre>
colnames(dta) <- c("x", "y", "label")</pre>
####### train, validate, test
dta.train <- dta[s == "train",]</pre>
dta.test <- dta[s == "test",]</pre>
```

Let's display the data and examine its structure (Fig. 23.17).

```
dt <- as.data.frame(dta);dt[,3] <- as.factor(dt[,3])
dt.train <- dt[s == "train",]
dt.test <- dt[s == "test",]
p1 <- ggplot(dt,aes(x = x,y = y,color=label))+geom_point()+ggtitle("Whole
data structure")
p2 <- ggplot(dt.train,aes(x = x,y =
y,color=label))+geom_point()+ggtitle("Train data structure")
p3 <- ggplot(dt.test,aes(x = x,y =
y,color=label))+geom_point()+ggtitle("Test data structure")
grid.arrange(p1,p2,p3,nrow=3)</pre>
```

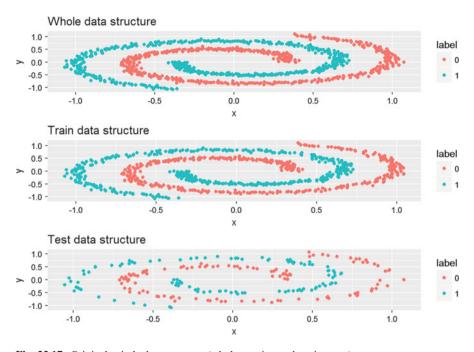


Fig. 23.17 Original spirals data structure (whole, traning and testing sets)

```
# Network training
# Feed-forward networks may be trained using iterative gradient descent algo
rithms. A **batch** is a subset of data that is used during single forward p
ass of the algorithm. An **epoch** represents one step of the iterative proc
ess that is repeated until all training examples are used.
######### basic spiral-data training
mx.set.seed(2235)
model <- mx.model.FeedForward.create(</pre>
            symbol = mlp,
            X = dta.train[, c("x", "y")],
            y = dta.train[, c("label")],
            num.round = 500,
            array.layout = "rowmajor",
            learning.rate = 1,
            eval.metric = mx.metric.accuracy, verbose = F)
preds = predict(model, dta.test[,c(1:2)])
pred.label = max.col(t(preds))-1; table(pred.label, dta.test[,3])
## pred.label 0 1
##
            0 90 30
##
            1 22 73
```

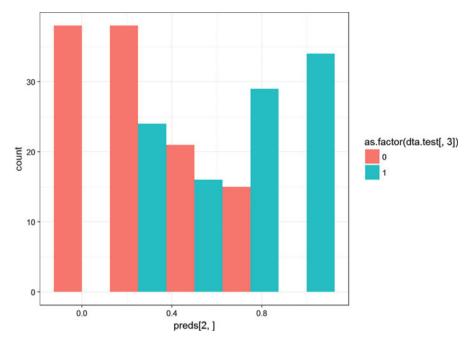


Fig. 23.18 Frequency of feed-forward neural network prediction probabilities (*x*-axis) for the spirals data relative to testing set labels (colors)

The prediction result is close to perfect, and we can inspect deeper the results using crossval::confusionMatrix (Fig. 23.18).

```
library("crossval")
diagnosticErrors(crossval::confusionMatrix(pred.label,dta.test[,3],negative
= 0))
##
         acc
                  sens
                            spec
                                       ppν
                                                  npν
                                                            Lor
## 0.7581395 0.7684211 0.7500000 0.7087379 0.8035714 2.2980293
## attr(, "negative")
## [1] 0
ggplot(data.frame(dta.test[,3], preds[2,]),
       aes(x=preds[2,], group=dta.test[,3], fill=as.factor(dta.test[,3])))+
  geom_histogram(position="dodge", binwidth=0.25)+theme_bw()
```

Once we fit a model (like the binary label classification below), we can:

- Visually inspect the quality of the ML classification.
- Display the structure of the labeled test-data objects (Fig. 23.19).

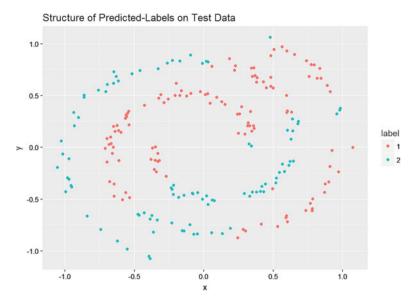


Fig. 23.19 Testing-data validation of neural network model (spirals)

```
# define a custom call-back, which stops the process of training when the pr
ogress in accuracy is below certain level of tolerance. It call is made afte
r every epoch to check the status of convergence of the algorithm.
mx.callback.train.stop <- function(tol = 1e-3, mean.n = 1e2, period = 100, m
in.iter = 100) {
   function(iteration, nbatch, env, verbose = TRUE) {
      if (nbatch == 0 & !is.null(env$metric)) {
          continue <- TRUE
          acc.train <- env$metric$get(env$train.metric)$value</pre>
          if (is.null(env$acc.log)) {
            env$acc.log <- acc.train
          } else {
            if ((abs(acc.train - mean(tail(env$acc.log, mean.n))) < tol &</pre>
                abs(acc.train - max(env$acc.log)) < tol &</pre>
                iteration > min.iter) |
                acc.train == 1) {
              cat("Training finished with final accuracy: ";
                  round(acc.train * 100, 2), " %\n", sep = "")
              continue <- FALSE
            env$acc.log <- c(env$acc.log, acc.train)</pre>
      if (iteration %% period == 0) {
        cat("[", iteration,"]"," training accuracy: "
            round(acc.train * 100, 2), " %\n", sep = "")
      return(continue)
```

```
##### training with custom stopping
mx.set.seed(2235)
model <- mx.model.FeedForward.create(</pre>
          symbol = mlp,
          X = dta.train[, c("x", "y")],
          y = dta.train[, c("Label")],
          num.round = 2000,
          array.layout = "rowmajor",
          learning.rate = 1,
          epoch.end.callback = mx.callback.train.stop(),
          eval.metric = mx.metric.accuracy,
          verbose = FALSE
## [100] training accuracy: 75.56 %
## [200] training accuracy: 76 %
## [300] training accuracy: 76 %
## [400] training accuracy: 76.45 %
## Training finished with final accuracy: 76.45 %
labeled_spiral_data <- as.data.frame(cbind(dta.test[, c("x", "y")],</pre>
as.factor(pred.label)))
colnames(labeled spiral data) <- c("x", "y", "label")</pre>
labeled_spiral_data$label <- as.factor(labeled_spiral_data$label)</pre>
p4 \leftarrow ggplot(labeled_spiral_data, aes(x = x, y = y, color=label))+
geom point()+ggtitle("Structure of Predicted-Labels on Test Data")
р4
```

23.5.3 *IBS Study*

Let's try another example using the IBS Neuroimaging study (Figs. 23.20 and 23.21).

```
# IBS NI Data
# UCLA Data
wiki url <-
read html("http://wiki.stat.ucla.edu/socr/index.php/SOCR Data April2011 NI
IBS Pain")
IBSData<- html table(html nodes(wiki url, "table")[[2]]) # table 2</pre>
set.seed(1234)
test.ind = sample(1:354, 50, replace = F) # select 50/354 of cases for
testing, train on remaining (354-50)/354 cases
# UMich Data (includes MISSING data): use `mice` to impute missing data
with mean: newData <- mice(data, m=5, maxit=50, meth='pmm', seed=500);</pre>
summary(newData)
# wiki url <-
read html("http://wiki.socr.umich.edu/index.php/SOCR Data April2011 NI IBS Pain")
# IBSData<- html_table(html_nodes(wiki_url, "table")[[1]]) # load Table 1</pre>
# set.seed(1234)
# test.ind = sample(1:337, 50, replace = F) # select 50/337 of cases for
testing, train on remaining (337-50)/337 cases
# summary(IBSData); IBSData[IBSData=="."] <- NA; newData <- mice(IBSData,</pre>
m=5,maxit=50,meth='pmm',seed=500); summary(newData)
```

```
html nodes(wiki url, "#content")
## {xml nodeset (1)}
## [1] <div id="content">\n\t\t<a name="top" id="top"></a>\n\t\t\t\t\t\h1
id= ...
# View (IBSData); dim(IBSData): Select an outcome response "DX"(3),
"FS IQ" (5)
# scale/normalize all input variables
IBSData <- na.omit(IBSData)</pre>
IBSData[,4:66] <- scale(IBSData[,4:66]) # scale the entire dataset</pre>
train.x = data.matrix(IBSData[-test.ind, c(4:66)]) # exclude outcome
train.y = IBSData[-test.ind, 3]-1
test.x = data.matrix(IBSData[test.ind, c(4:66)])
test.y = IBSData[test.ind, 3]-1
# View(data.frame(train.x, train.y))
# View(data.frame(test.x, test.y))
# table(test.y); table(train.y)
# num.round - number of iterations to train the model
act <- mx.symbol.Variable("data")</pre>
fc <- mx.symbol.FullyConnected(act, num.hidden = 10)</pre>
act <- mx.symbol.Activation(data = fc, act type = "sigmoid")</pre>
fc <- mx.symbol.FullyConnected(act, num.hidden = 2)</pre>
mlp <- mx.symbol.SoftmaxOutput(fc)</pre>
mx.set.seed(2235)
model <- mx.model.FeedForward.create(</pre>
            symbol = mlp,
            array.batch.size=20,
            X = train.x, y=train.y,
            num.round = 200,
array.layout = "rowmajor",
            learning.rate = exp(-1),
            eval.metric = mx.metric.accuracy, verbose=FALSE)
preds = predict(model, test.x)
pred.label = max.col(t(preds))-1; table(pred.label, test.y)
             test.y
## pred.label 0 1
           0 23 10
##
##
            1 10 7
library("crossval")
diagnosticErrors(crossval::confusionMatrix(pred.label,test.y,negative = 0))
                  sens
                             spec
         acc
                                        ppν
                                                   npv
## 0.6000000 0.4117647 0.6969697 0.4117647 0.6969697 0.4762342
## attr(,"negative")
## [1] 0
ggplot(data.frame(test.y, preds[2,]),
       aes(x=preds[2,], group=test.y, fill=as.factor(test.y)))+
  geom_histogram(position="dodge", binwidth=0.25)+theme_bw()
```

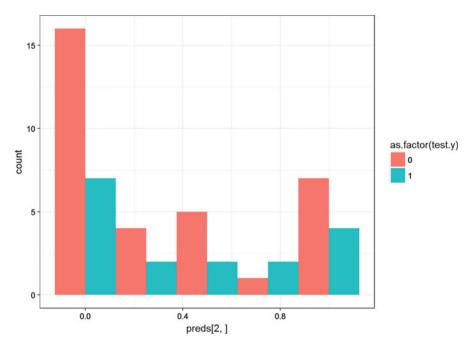


Fig. 23.20 Frequency of the feed-forward neural network prediction probabilities (*x*-axis) for the IBS data relative to testing set labels (colors)

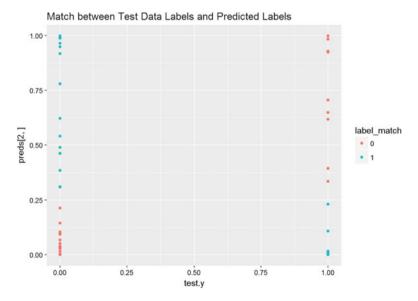


Fig. 23.21 Validation results of the binarized feed-forward neural network prediction probabilities (*y*-axis) for the IBS testing data (*x*-axis) with label-coding for match(0)/mismatch(1)

```
# convert pred-probability to binary classes threshold=0.3?
bin_preds <- ifelse (preds[2,]<0.3, 0, 1)
# get a factor variable comparing binary test-labels vs. predcted-labels
Label_match <- as.factor(ifelse (test.y==bin_preds, 0, 1))
p5 <- ggplot(data.frame(test.y, preds[2,]), aes(x = test.y, y = preds[2,],
color=Label_match))+geom_point()+ggtitle("Match between Test Data Labels and
Predicted Labels")
p5</pre>
```

This histogram plot suggests that the classification is not good (Fig. 23.20).

23.5.4 Country QoL Ranking Data

Another case study we have seen before is the country quality of life (QoL) dataset. Let's explore a new neural network model and use it to predict the overall country QoL.

```
wiki_url <-
read html("http://wiki.stat.ucla.edu/socr/index.php/SOCR Data 2008 World
CountriesRankinas")
html_nodes(wiki_url, "#content")
## {xml nodeset (1)}
## [1] <div id="content">\n\t\t<a name="top" id="top"></a>\n\t\t\t\t\t\h1
CountryRankingData<- html table(html nodes(wiki url, "table")[[2]])</pre>
# View (CountryRankingData); dim(CountryRankingData): Select an appropriate
# outcome "OA": Overall country ranking (13)
# Dichotomize outcome, Top-countries OA<20, bottom countries OA>=20
set.seed(1234)
test.ind = sample(1:100, 30, replace = F) # select 15/100 of cases for
testing, train on remaining 85/100 cases
CountryRankingData[,c(8:12,14)] <- scale(CountryRankingData[,c(8:12,14)])</pre>
# scale/normalize all input variables
train.x = data.matrix(CountryRankingData[-test.ind, c(8:12,14)]) # exclude
outcome
train.y = ifelse(CountryRankingData[-test.ind, 13] < 50, 1, 0)</pre>
test.x = data.matrix(CountryRankingData[test.ind, c(8:12,14)])
test.y = ifelse(CountryRankingData[test.ind, 13] < 50, 1, 0) # developed
(high OA rank) country
# View(data.frame(train.x, train.y)); View(data.frame(test.x, test.y))
# View(data.frame(CountryRankingData, ifelse(CountryRankingData[,13] < 20,</pre>
1, 0)))
act <- mx.symbol.Variable("data")</pre>
fc <- mx.symbol.FullyConnected(act, num.hidden = 10)</pre>
act <- mx.symbol.Activation(data = fc, act type = "sigmoid")</pre>
fc <- mx.symbol.FullyConnected(act, num.hidden = 2)</pre>
mlp <- mx.symbol.SoftmaxOutput(fc)</pre>
mx.set.seed(2235)
model <- mx.model.FeedForward.create(</pre>
            symbol = mlp,
            array.batch.size=10,
```

```
X = train.x, y=train.y,
            num.round = 15,
            array.layout = "rowmajor",
            learning.rate = exp(-1),
            eval.metric = mx.metric.accuracy)
## Start training with 1 devices
## [1] Train-accuracy=0.416666666666667
## [2] Train-accuracy=0.442857142857143
## [3] Train-accuracy=0.442857142857143
## [4] Train-accuracy=0.442857142857143
## [5] Train-accuracy=0.442857142857143
## [6] Train-accuracy=0.442857142857143
## [7] Train-accuracy=0.6
## [8] Train-accuracy=0.8
## [9] Train-accuracy=0.914285714285714
## [10] Train-accuracy=0.928571428571429
## [11] Train-accuracy=0.942857142857143
## [12] Train-accuracy=0.942857142857143
## [13] Train-accuracy=0.942857142857143
## [14] Train-accuracy=0.971428571428572
## [15] Train-accuracy=0.971428571428572
preds = predict(model, test.x); preds
##
             [,1]
                       [,2]
                                               [,4]
                                   [,3]
                                                         [,5]
                                                                    [,6]
## [1,] 0.5204602 0.8808465 0.007948651 0.009155557 0.8622462 0.8432776
## [2,] 0.4795398 0.1191535 0.992051363 0.990844429 0.1377538 0.1567224
                       [,8]
                                  [,9]
                                           [,10]
                                                      [,11]
## [1,] 0.4493238 0.6563529 0.97970927 0.7055513 0.98414272 0.9647682
## [2,] 0.5506761 0.3436471 0.02029071 0.2944487 0.01585729 0.0352319
                       [,14]
                                 [,15]
            [,13]
                                           [,16]
                                                     [,17]
## [1,] 0.6106228 0.91565907 0.8317797 0.0252018 0.7618818 0.01770884
## [2,] 0.3893772 0.08434091 0.1682204 0.9747981 0.2381181 0.98229110
              [,19]
                        [,20]
                                   [,21]
                                               [,22]
                                                          [,23]
                                                                       [,24]
## [1,] 0.007323461 0.7766624 0.94527471 0.007209368 0.09066615 0.007661197
## [2,] 0.992676497 0.2233376 0.05472526 0.992790580 0.90933383 0.992338777
                       [,26]
            [,25]
                                   [,27]
                                             [,28]
                                                        [,29]
## [1,] 0.0489373 0.009559323 0.91361207 0.1901348 0.90563852 0.97519016
## [2,] 0.9510627 0.990440726 0.08638796 0.8098652 0.09436146 0.02480989
pred.label = max.col(t(preds))-1; table(pred.label, test.y)
##
             test.y
## pred.label 0 1
            0 17 1
##
            1 1 11
```

We only need 15 rounds to achieve 97% accuracy (Figs. 23.22 and 23.23).

```
ggplot(data.frame(test.y, preds[2,]),
    aes(x=preds[2,], group=test.y, fill=as.factor(test.y)))+
    geom_histogram(position="dodge",binwidth=0.25)+theme_bw()
```

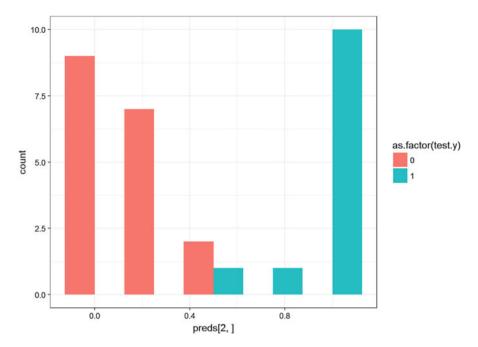


Fig. 23.22 Frequency of the feed-forward neural network prediction probabilities (*x*-axis) for the QoL data relative to testing set labels (colors)

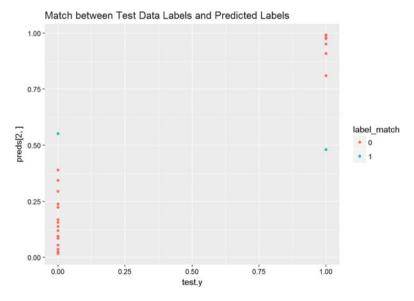


Fig. 23.23 Validation results of the binarized feed-forward neural network prediction probabilities (y-axis) for the QoL testing data with label-coding for match(0)/mismatch(1)

```
#calculate sensitivity & specificity and more
Library("crossval")
diagnosticErrors(crossval::confusionMatrix(pred.label,test.y,negative = 0))
                    sens
                               spec
                                            ppv
                                                       npν
## 0.9333333 0.9166667 0.9444444 0.9166667 0.9444444 5.2311086
## attr(, "negative")
## [1] 0
# convert pred-probability to binary classes threshold=0.5?
bin_preds <- ifelse (preds[2,]<0.5, 0, 1)
# get a factor variable comparing binary test-labels vs. predicted-labels
label_match <- as.factor(ifelse (test.y==bin_preds, 0, 1))</pre>
p6 <- ggplot(data.frame(test.y, preds[2,]), aes(x = test.y, y = preds[2,], color=Label_match))+geom_point()+ggtitle("Match between Test Data Labels
and Predicted Labels")
```

23.5.5 Handwritten Digits Classification

In Chap. 11 (ML, NN, SVM Classification) we discussed Optical Character Recognition (OCR). Specifically, we analyzed handwritten notes (unstructured text) and converted it to printed text.

MNIST includes a large set of human annotated/labeled handwritten digits imaging data set. Every digit is represented by a 28×28 thumbnail image. You can download the training and testing data from Kaggle.

The train.csv and test.csv data files contain gray-scale images of hand-drawn digits, $0, 1, 2, \ldots, 9$. Each 2D image is 28×28 in size and each of the 784 pixels has a single pixel-intensity representing the lightness or darkness of that pixel (stored as a 1 byte integer [0,255]). Higher intensities correspond to darker pixels.

The training data, train.csv, has 785 columns, where the first column, **label**, codes the actual the digit drawn by the user. The remaining 784 columns contain the $28 \times 28 = 784$ pixel-intensities of the associated 2D image. Columns in the training set have $pixel_K$ names, where $0 \le K \le 783$. To reconstruct a 2D image out of each row in the training data we use this relation between pixel-index (K) and X, Y image coordinates:

$$K = Y \times 28 + X$$

where $0 \le X$, $Y \le 27$. Thus, $pixel_K$ is located on row Y and column X of the corresponding 2D Image of size 28×28 . For instance, $pixel_{60 = (2 \times 28 + 4)} \leftrightarrow (X = 4, Y = 2)$ represents the pixel on the third row and fifth column in the image. Diagrammatically, omitting the "pixel" prefix, the pixels may be ordered to reconstruct the 2D image as follows (Table 23.3).

Note that the point-to-pixelID transformation ($K = Y \times 28 + X$) may easily be inverted as a pixelID-to-point mapping: $X = K \mod 28$ (remainder of the integer division (K/28) and Y = K (integer part of the division K/28)). For example:

Row	Col0	COl1	Col2	Col3	Col5		Col26	Co27
Row0	0	1	2	3	4		26	27
Row1	28	29	30	31	32		54	55
Row2	56	57	58	59	60		82	83
RowK								
Row26	728	729	730	731	732		754	755
Row27	756	757	758	759	760		782	783

Table 23.3 Schematic for reconstructing a 28×28 square image using a list of 784 intensities corresponding to colors in the image reflecting the manual handwritten digits

```
K <- 60
X <- K %% 28 # X= K mod 28, remainder of integer division 60/28
Y <- K%/%28 # integer part of the division
# This validates that the application of both, the back and forth
transformations, leads to an identity
K; X; Y; Y * 28 + X
## [1] 60
## [1] 4
## [1] 6</pre>
## [1] 60
```

The test data (test.csv) has the same organization as the training data, except that it does not contain the first **label** column. It includes 28,000 images and we can predict image labels that can be stored as *ImageId*, *Label* pairs, which can be visually compared to the 2D images for validation/inspection.

```
require(mxnet)
# train.csv
pathToZip <- tempfile()</pre>
download.file("http://www.socr.umich.edu/people/dinov/2017/Spring/DSPA HS650
/data/DigitRecognizer_TrainingData.zip", pathToZip)
train <- read.csv(unzip(pathToZip))</pre>
dim(train)
## [1] 42000
                785
unlink(pathToZip)
# test.csv
pathToZip <- tempfile()</pre>
download.file("http://www.socr.umich.edu/people/dinov/2017/Spring/DSPA_HS650
/data/DigitRecognizer_TestingData.zip", pathToZip)
test <- read.csv(unzip(pathToZip))</pre>
dim(test)
## [1] 28000
                784
unlink(pathToZip)
train <- data.matrix(train)</pre>
test <- data.matrix(test)</pre>
```

```
train.x <- train[,-1]
train.y <- train[,1]

# Scaling will be discussed below
train.x <- t(train.x/255)
test <- t(test/255)</pre>
```

Let's look at some of these example images (Figs. 23.24, 23.25, 23.26 and 23.27):

```
library("imager")
# first convert the CSV data (one row per image, 28,000 rows)
array_3D <- array(test, c(28, 28, 28000))
mat_2D <- matrix(array_3D[,,1], nrow = 28, ncol = 28)
plot(as.cimg(mat_2D))</pre>
```

Fig. 23.24 Image rendering of the first handwritten digit, stored as a 28×28 array of intensities

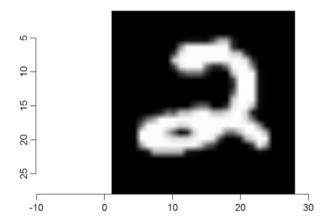


Fig. 23.25 Rendering of the fifth handwritten digit in the list of 28,000

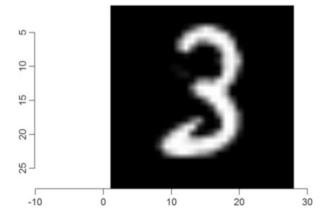


Fig. 23.26 Another strategy for indexing and plotting handwritten digits as 2D images

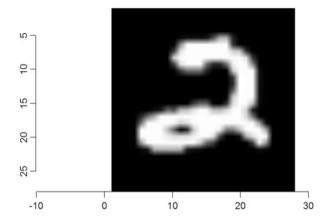


Fig. 23.27 Sequential image plot of the first four handwritten digits



```
# extract all N=28,000 images
N <- 28000
img_3D <- as.cimg(array_3D[,,], 28, 28, N)
# plot the k-th image (1<=k<=N)
k <- 5
plot(img_3D, k)

image_2D <- function(img,index){
    img[,,index,,drop=FALSE]
}
plot(image_2D(img_3D, 1))</pre>
```

```
# Plot a collage of the first 4 images
imappend(List(image_2D(img_3D, 1), image_2D(img_3D, 2), image_2D(img_3D, 3),
image_2D(img_3D, 4)), "y") %>% plot

# img <- image_2D(img_3D, 1)
# for (i in 10:20) { imappend(list(img, image 2D(img 3D, i)), "x") }</pre>
```

In these CSV data files, each 28×28 image is represented as a single row. The intensities of these greyscale images are stored as 1 byte integers, in the range [0,255], which we linearly transformed into [0, 1]. Note that we only scale the *X* input, not the output (labels). Also, we don't have manual gold-standard validation labels for the testing data, i.e., test. y is not available for the handwritten digits data.

```
# We already scaled earlier
# train.x <- t(train.x/255)
# test <- t(test/255)</pre>
```

Next, we can transpose the input matrix to n (pixels) \times m (examples), as column major format required by mxnet. The image labels are evenly distributed:

```
table(train.y); prop.table(table(train.y))
## train.y
## 0 1 2 3 4 5 6 7 8 9
## 4132 4684 4177 4351 4072 3795 4137 4401 4063 4188
## train.y
## 0 1 2 3 4 5
## 0.09838095 0.11152381 0.09945238 0.10359524 0.09695238 0.09035714
## 6 7 8 9
## 0.09850000 0.10478571 0.09673810 0.09971429
```

The majority class (1) in the training set includes 11.2% of the observations.

Configuring the Neural Network

```
data <- mx.symbol.Variable("data")
fc1 <- mx.symbol.FullyConnected(data, name="fc1", num_hidden=128)
act1 <- mx.symbol.Activation(fc1, name="relu1", act_type="relu")
fc2 <- mx.symbol.FullyConnected(act1, name="fc2", num_hidden=64)
act2 <- mx.symbol.Activation(fc2, name="relu2", act_type="relu")
fc3 <- mx.symbol.FullyConnected(act2, name="fc3", num_hidden=10)
softmax <- mx.symbol.SoftmaxOutput(fc3, name="sm")</pre>
```

data <- mx.symbol.Variable("data") represents the input layer. The first hidden layer, set by fc1 <- mx.symbol.FullyConnected(data, name="fc1", num_hidden=128), takes the data as an input, its name, and the number of hidden neurons to generate an output layer.

act1 <- mx.symbol.Activation(fc1, name="relu1", act_type="relu") sets the activation function, which takes the output from the first hidden layer "fc1" and

generates an output that is fed into the second hidden layer "fc2", which uses fewer hidden neurons (64).

The process repeats with the second activation "act2", resembling "act1" but using different input source and name. As there are only ten digits $(0, 1, \ldots, 9)$, in the last layer "fc3", we set the number of neurons to 10. At the end, we set the activation to softmax to obtain a probabilistic prediction.

Training

We are almost ready for the training process. Before we start the computation, let's decide what device we should use.

```
devices <- mx.cpu()</pre>
```

Here we assign CPU to mxnet. After all these preparation, you can run the following command to train the neural network! Note that in mxnet, the correct function to control the random process is mx.set.seed.

```
mx.set.seed(1234)
model <- mx.model.FeedForward.create(softmax, X=train.x, y=train.y,</pre>
        ctx=devices, num.round=10, array.batch.size=100,
        learning.rate=0.07, momentum=0.9, eval.metric=mx.metric.accuracy,
        initializer=mx.init.uniform(0.07),
        epoch.end.callback=mx.callback.log.train.metric(100)
## Start training with 1 devices
## [1] Train-accuracy=0.863031026252982
## [2] Train-accuracy=0.958285714285716
## [3] Train-accuracy=0.970785714285717
## [4] Train-accuracy=0.977857142857146
## [5] Train-accuracy=0.983238095238099
## [6] Train-accuracy=0.98521428571429
## [7] Train-accuracy=0.987095238095242
## [8] Train-accuracy=0.989309523809528
## [9] Train-accuracy=0.99214285714286
## [10] Train-accuracy=0.991452380952384
```

For 10 rounds, the training accuracy exceeds 99%. It may not be worthwhile trying 100 rounds, as this would increase substantially the computational complexity.

Forecasting

Now, we will demonstrate how to generate a forecasting model based on testing data, and how to evaluate its prediction performance. The preds matrix has 28,000 rows and 10 columns, containing the desired classification probabilities from the output layer of the neural net. To extract the maximum label for each row, we can use the max.col:

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```
# evaludate: "preds" is the matrix of the possibility of each of the 10
numbers
preds <- predict(model, test)</pre>
pred.label <- max.col(t(preds)) - 1</pre>
table(pred. Label)
## pred.label
## 0 1
              2 3 4 5 6 7 8
## 2774 3228 2862 2728 2781 2401 2777 2868 2826 2755
# preds1 <- ifelse(preds[2,] <= 0.5, 0, 1) # dichotomize to labels</pre>
# pred.label = t(preds1)
# table(pred.label, test.y)
# calculate sensitivity & specificity
# sensitivity(factor(preds1), factor(as.numeric(test.y)),positive = 1)
# specificity(factor(preds1), factor(as.numeric(test.y)),negative = 0)
# preds <- predict(model, test.x)</pre>
# dim(preds)
# preds1 <- ifelse(preds[2,] <= 0.5, 0, 1) # dichotomize to labels</pre>
# pred.label = t(preds1)
# table(pred.label, test.y)
```

For binary classification, mxnet outputs two prediction classes, whereas for multi-class predictions, it outputs a matrix of size n (classes) \times m (examples), where the rows correspond to the probability of the class in the specific column, so all column sums add up to 1.0.

The predictions are stored in a $28,000(rows) \times 10(colums)$ matrix, including the desired classification probabilities from the output layer. The R max.col function extracts the maximum label for each row.

```
pred.label <- max.col(t(preds)) - 1
table(pred.label)

## pred.label
## 0 1 2 3 4 5 6 7 8 9
## 2774 3228 2862 2728 2781 2401 2777 2868 2826 2755</pre>
```

We can save the predicted labels of the testing handwritten digits to CSV:

```
predicted_lables <- data.frame(ImageId=1:ncol(test), Label=pred.label)
write.csv(predicted_lables, file='predicted_lables.csv', row.names=FALSE,
quote=FALSE)</pre>
```

We can open the predicted_lables.csv file and inspect the ML-labels (saved in the 2-column ImageID and Label format CSV) assigned to the 28,000 manually drawn digits. As the **testing handwritten digits data** do not have human-provided labels, we can't quantitatively assess the validity of the algorithm on the testing data (Fig. 23.28). However, we can visually inspect random handwritten digit instances (7 in the example below, image indices 4:10) against their predictions and gain intuition of the accuracy rate of the ML classifier (Table 23.4, Fig. 23.29).

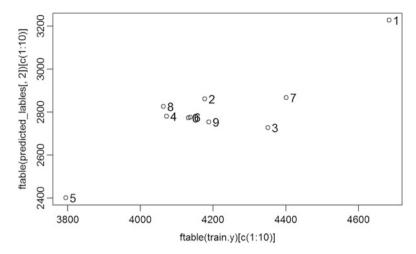
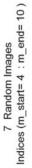


Fig. 23.28 Plot of the agreement between relative frequencies in the number of train.y labels (in range 0–9) against the testing data predicted labels. These quantities are not directly related (frequencies of digits in training.y and predicted.testing.data); we can't exlicitly validate the testing-data predicitons, as we don't have gold-standard test.y labels! However, numbers closer to the diagonal of the plot would indicate expected good classifications, whereas, off diagonal points may suggest less effective labeling

Table 23.4 Predicted labels for the set of the first 7 handwritten digits

ImageId	Label
1	2
2	0
3	9
4	9
5	3
6	7
7	0

Fig. 23.29 Visual validation of the handwritten digits (left) and their neural network prediction (right) for the set of seven images. The number and indices of these testing data images can be manually specified





L Classification Label

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```
table(train.y)
## train.v
                     3
                          4
                               5
                2
                                    6
     0
## 4132 4684 4177 4351 4072 3795 4137 4401 4063 4188
table(predicted lables[,2])
##
##
      a
          1
               2
                    3 4 5
                                    6
                                        7
                                              8
## 2774 3228 2862 2728 2781 2401 2777 2868 2826 2755
# Plot the relative frequencies between the number of train.y labels
(in range 0-9) against the testing data predicted labels.
# These are not directly related (training.y vs. predicted.testing.data!
# Remember - we don't have gold-standard test.y labels! Generally speaking,
numbers closer to the diagonal suggest expected good classifications.
Whereas, off diagonal points may suggest less effective labeling.
Label.names <- c("0", "1", "2", "3", "4", "5", "6", "7", "8", "9")
plot(ftable(train.y)[c(1:10)], ftable(predicted_lables[,2])[c(1:10)])
text(ftable(train.y)[c(1:10)]+20, ftable(predicted\ lables[,2])[c(1:10)],
labels=label.names, cex= 1.2)
# For example, the ML-classification labels assigned to the first 7 images (
from the 28,000 testing data collection) are:
head(predicted\ lables,\ n=7L)
## ImageId Label
## 1
          1
                 2
## 2
          2
                 0
          3
## 3
                 9
          4
                 9
## 4
## 5
           5
                 3
## 6
           6
                 7
## 7
Library(knitr)
kable(head(predicted_lables, n = 7L), format = "markdown")
#initialize a list of m=7 images from the N=28,000 available images
m start <- 4
m end <- 10
if (m end <= m start)</pre>
  { m_end = m_start+1 } # check that m_end > m_start
label_Ypositons <- vector() # initialize the array of label positions</pre>
on the plot
for (i in m start:m end) {
  if (i==m_start) {
    img1 <- image_2D(img_3D, m_start)</pre>
  else img1 <- imappend(list(img1, image 2D(img 3D, i)), "y")
  label.names[i+1-m_start] <- predicted_lables[i,2]</pre>
  Label_Ypositons[i+1-m_start] <- 15 + 28*(i-m_start)</pre>
plot(img1, axes=FALSE)
text(40, label_Ypositons, labels=label.names[1:(m_end-m_start)], cex= 1.2,
col="blue")
mtext(paste((m end+1-m start), " Random Images \n Indices (m start=",
m_start, " : m_end=", m_end, ")"), side=2, line=-6, col="black")
mtext("ML Classification Labels", side=4, line=-5, col="blue")
```

```
table(ftable(train.y)[c(1:10)], ftable(predicted_lables[,2])[c(1:10)])
##
        2401 2728 2755 2774 2777 2781 2826 2862 2868 3228
##
    3795
         1
            0
                  0
                      0
                          0
                              0
                                  a
                                      0
##
    4063
         0
             0
                  0
                      0
                          0
                              0
                                  1
                                      0
                                          0
                                              a
##
   4072
         0
             0
                  0
                      0
                          0
                              1
                                  0
                                      0
                                          0
                                              0
         0
   4132
             0
                 0
                      1
                          0
                              0
                                  0
                                      0
                                          0
##
   4137
             0
##
        0
                 0
                     0
                          1
                              0
                                  0
                                      0
                                          0
                                              0
                     0
##
   4177 0 0 0
                         0
                              0
                                  0
                                      1
                                         0
                                              0
##
   4188 0 0 1
                     0 0
                              a
                                  a
                                      a
                                          a
                                              a
                                      0
##
   4351 0 1 0
                     0 0
                              0
                                  0
                                          0
                                              0
##
   4401 0
              0
                  0
                      0
                          0
                              0
                                  0
                                      0
                                          1
                                              a
##
   4684
          0
              0
                  0
                      0
                          0
                              0
                                      0
                                              1
```

Examining the Network Structure Using LeNet

We can use the mxnet package LeNet convolutional neural network (CNN) protocol for learning the network.

Let's first construct the network.

```
# input
data <- mx.symbol.Variable('data')</pre>
# first conv
conv1 <- mx.symbol.Convolution(data=data, kernel=c(5,5), num filter=20)</pre>
tanh1 <- mx.symbol.Activation(data=conv1, act type="tanh")
pool1 <- mx.symbol.Pooling(data=tanh1, pool_type="max",</pre>
                            kernel=c(2,2), stride=c(2,2))
# second conv
conv2 <- mx.symbol.Convolution(data=pool1, kernel=c(5,5), num_filter=50)
tanh2 <- mx.symbol.Activation(data=conv2, act_type="tanh")</pre>
pool2 <- mx.symbol.Pooling(data=tanh2, pool_type="max",</pre>
                            kernel=c(2,2), stride=c(2,2))
# first fullc
flatten <- mx.symbol.Flatten(data=pool2)</pre>
fc1 <- mx.symbol.FullyConnected(data=flatten, num_hidden=500)</pre>
tanh3 <- mx.symbol.Activation(data=fc1, act_type="tanh")</pre>
# second fullc
fc2 <- mx.symbol.FullyConnected(data=tanh3, num_hidden=10)</pre>
lenet <- mx.symbol.SoftmaxOutput(data=fc2)</pre>
```

Next, we will reshape the matrices into arrays.

```
train.array <- train.x
dim(train.array) <- c(28, 28, 1, ncol(train.x))
test.array <- test
dim(test.array) <- c(28, 28, 1, ncol(test))</pre>
```

Compare the training speed on different devices – CPU vs. GPU. Start by defining the devices.

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```
n.gpu <- 1
device.cpu <- mx.cpu()
device.gpu <- lapply(0:(n.gpu-1), function(i) {
    mx.gpu(i)
})</pre>
```

Passing a list of devices is useful for high-end computational platforms (e.g., multi-GPU systems); mxnet can train on multiple GPUs or CPUs.

To train using the CPU, try fewer iterations as protocol is computationally very intense.

The corresponding training on GPU is similar, but it requires a separate GPU-compilation of mxnet (/mxnet/src/storage/storage.cc:78) with USE_CUDA=1 to enable GPU usage.

GPU training is faster than CPU. Everyone can submit a new classification result to Kaggle and see a ranking result for their classifier. Make sure you follow the specific result-file submission format.

```
preds <- predict(model, test.array)
pred.Label <- max.col(t(preds)) - 1
submission <- data.frame(ImageId=1:ncol(test), Label=pred.Label)
write.csv(submission, file='submission.csv', row.names=FALSE, quote=FALSE)</pre>
```

23.6 Classifying Real-World Images

A real-world example of deep learning is classification of 2D images (pictures) or 3D volumes (e.g., neuroimages).

The image classification examples below shows the use a pre-trained **Inception-BatchNorm Network** to predict a class of real world image. The network architecture is described the 2015 Ioffe and Szegedy paper. The pre-trained Inception-BatchNorm network is available online. This advanced model gives a state-of-theart prediction accuracy on imaging data. We also need the R imager package to load and preprocess the 2D images.

```
# install.packages("imager")
require(mxnet)
require(imager)
```

23.6.1 Load the Pre-trained Model

Download and unzip the pre-trained model to a working folder, and load the model and the mean image (used for preprocessing) using mx.nd.load into R. This download can either be done manually, or automated, as shown below.

23.6.2 Load, Preprocess and Classify New Images – US Weather Pattern

To classify a new image, select the image and load it in. Below, we show the classification of several alternative images (Fig. 23.30).

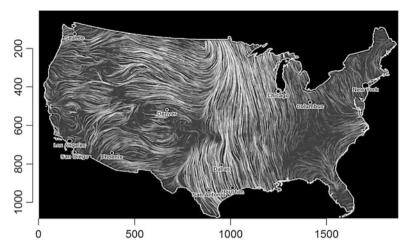


Fig. 23.30 A U.S. weather pattern map as an example image for neural network image recognition

```
Librarv("imager")
# One should be able to load the image directly from the web (but sometimes
there may be problems, in which case, we need to first download the image
and then load it in R:
# im <-
imager::load.image("http://wiki.socr.umich.edu/images/6/69/DataManagement
Fig1.png")
# download file to local working directory, use "wb" mode to avoid problems
download.file("http://wiki.socr.umich.edu/images/6/69/DataManagementFig1.png
", paste(getwd(), "results/image.png", sep="/"), mode = 'wb')
# report download image path
paste(getwd(), "results/image.png", sep="/")
img <- Load.image(paste(getwd(), "results/image.png", sep="/"))</pre>
dim(img)
## [1] 1875 1084
plot(img)
```

Before feeding the image to the deep learning network for classification, we need to do some preprocessing to make it fit the deepnet input requirements. This image preprocessing (cropping and subtraction of the mean) can be done directly in R.

```
preproc.image <-function(im, mean.image) {
    # crop the image
        shape <- dim(im)
        short.edge <- min(shape[1:2])
        xx <- floor((shape[1] - short.edge) / 2)
        yy <- floor((shape[2] - short.edge) / 2)
        cropped <- crop.borders(im, xx, yy)
    # resize to 224 x 224, needed by input of the model.</pre>
```

```
resized <- resize(cropped, 224, 224)
plot(resized)
# convert to array (x, y, channel)
arr <- as.array(resized[,,,c(1:3)]) * 255
plot(as.cimg(arr))
dim(arr) <- c(224, 224, 3)
# subtract the mean
normed <- arr - mean.img
# Reshape to format needed by mxnet (width, height, channel, num)
dim(normed) <- c(224, 224, 3, 1)
return(normed)
}</pre>
```

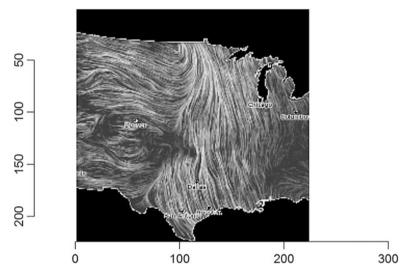


Fig. 23.31 Normalized US weather pattern map image

Call the preprocessing function with the normalized image (Fig. 23.31).

```
normed <- preproc.image(img, mean.img)
# plot(normed)</pre>
```

The image classification uses a *predict* function to get the probability over all (learned) classes.

```
prob <- predict(model, X=normed)
dim(prob)
## [1] 1000 1</pre>
```

The prob prediction generates a $1,000 \times 1$ array representing the probability of the input image to resemble (be classified as) the top 1,000 known image categories. We can report the indices of the top-10 closest image classes to the input image:

```
max.idx <- order(prob[,1], decreasing = TRUE)[1:10]
max.idx
## [1] 855 563 229 581 620 948 951 186 204 311</pre>
```

Alternatively, we can map these top-10 indices into named image-classes.

```
synsets <- readLines("synset.txt")</pre>
print(paste0("Top Predicted Image-Label Classes: Name=", synsets[max.idx], "
; Probability: ", prob[max.idx]))
## [1] "Top Predicted Image-Label Classes: Name=n04418357 theater curtain,
theatre curtain; Probability: 0.0493971668183804"
## [2] "Top Predicted Image-Label Classes: Name=n03388043 fountain;
Probability: 0.0431815795600414"
## [3] "Top Predicted Image-Label Classes: Name=n02105505 komondor;
Probability: 0.0371582210063934"
## [4] "Top Predicted Image-Label Classes: Name=n03457902 greenhouse,
nursery, glasshouse; Probability: 0.0368415862321854"
## [5] "Top Predicted Image-Label Classes: Name=n03637318 Lampshade,
Lamp shade; Probability: 0.0317880213260651"
## [6] "Top Predicted Image-Label Classes: Name=n07734744 mushroom;
Probability: 0.0292572267353535"
## [7] "Top Predicted Image-Label Classes: Name=n07747607 orange;
Probability: 0.0284675862640142"
## [8] "Top Predicted Image-Label Classes: Name=n02094114 Norfolk terrier;
Probability: 0.026896309107542"
## [9] "Top Predicted Image-Label Classes: Name=n02098286 West Highland
white terrier; Probability: 0.0257413759827614"
## [10] "Top Predicted Image-Label Classes: Name=n02219486 ant, emmet,
pismire; Probability: 0.0205500852316618"
```

Clearly, this U.S. weather pattern image is not well classified. The optimal prediction suggests this may be a *theater curtain*; however, the confidence is very low, $Prob \sim 0.049$. None of the other top-10 classes capture the type of the actual image either.

The machine learning image classifications results won't always be this poor. Let's try classifying several alternative images.

23.6.3 Lake Mapourika, New Zealand

Let's try the automated image classification of this lakeside panorama (Figs. 23.32 and 23.33).

```
download.file("https://upload.wikimedia.org/wikipedia/commons/2/23/Lake_mapo
urika_NZ.jpeg", paste(getwd(), "results/image.png", sep="/"), mode = 'wb')
im <- load.image(paste(getwd(), "results/image.png", sep="/"))
plot(im)</pre>
```

Fig. 23.32 A lakeside panorama image for neural network image recognition

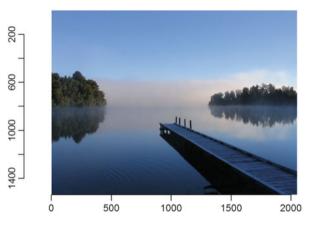


Fig. 23.33 Normalized lakeside panorama image



```
normed <- preproc.image(im, mean.img)</pre>
prob <- predict(model, X=normed)</pre>
max.idx \leftarrow order(prob[,1], decreasing = TRUE)[1:10]
print(paste0("Top Predicted Image-Label Classes: Name=", synsets[max.idx], "
; Probability: ", prob[max.idx]))
## [1] "Top Predicted Image-Label Classes: Name=n02894605 breakwater,
groin, groyne, mole, bulwark, seawall, jetty; Probability:0.648901104927063"
## [2] "Top Predicted Image-Label Classes: Name=n03216828 dock, dockage,
docking facility; Probability: 0.183006703853607"
## [3] "Top Predicted Image-Label Classes: Name=n09332890 lakeside,
Lakeshore; Probability: 0.127718329429626"
## [4] "Top Predicted Image-Label Classes: Name=n03160309 dam, dike, dyke;
Probability: 0.0115784741938114"
## [5] "Top Predicted Image-Label Classes: Name=n03095699 container ship,
containership, container vessel; Probability: 0.00913785584270954"
## [6] "Top Predicted Image-Label Classes: Name=n09428293 seashore, coast,
seacoast, sea-coast; Probability: 0.0043862983584404"
## [7] "Top Predicted Image-Label Classes: Name=n03933933 pier;
Probability: 0.00410780590027571"
## [8] "Top Predicted Image-Label Classes: Name=n02859443 boathouse;
Probability: 0.00246214028447866"
## [9] "Top Predicted Image-Label Classes: Name=n09399592 promontory,
headland, head, foreland; Probability: 0.00168424111325294"
## [10] "Top Predicted Image-Label Classes: Name=n09421951 sandbar,
sand bar; Probability: 0.00106814480386674"
```

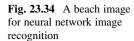
This photo does represent a lakeside, which is reflected by the top three class labels:

- Breakwater, groin, groyne, mole, bulwark, seawall, jetty.
- Dock, dockage, docking facility.
- · Lakeside, lakeshore.

23.6.4 Beach Image

Another costal boundary between water and land is represented in this beach image (Fig. 23.34).

```
download.file("https://upload.wikimedia.org/wikipedia/commons/9/90/Holloways
_beach_1920x1080.jpg", paste(getwd(), "results/image.png", sep="/"), mode = '
wb')
im <- Load.image(paste(getwd(), "results/image.png", sep="/"))
plot(im)</pre>
```





```
# normed <- preproc.image(im, mean.img)</pre>
prob <- predict(model, X=normed)</pre>
max.idx \leftarrow order(prob[,1], decreasing = TRUE)[1:10]
print(paste0("Top Predicted Image-Label Classes: Name=", synsets[max.idx],
"; Probability: ", prob[max.idx]))
## [1] "Top Predicted Image-Label Classes: Name=n09421951 sandbar,
sand bar; Probability: 0.69039398431778"
## [2] "Top Predicted Image-Label Classes: Name=n09332890 lakeside,
Lakeshore; Probability: 0.20282569527626"
## [3] "Top Predicted Image-Label Classes: Name=n09428293 seashore, coast,
seacoast, sea-coast; Probability: 0.0899285301566124"
## [4] "Top Predicted Image-Label Classes: Name=n02894605 breakwater,
groin, groyne, mole, bulwark, seawall, jetty; Probability: 0.006692836"
## [5] "Top Predicted Image-Label Classes: Name=n09399592 promontory,
headland, head, foreland; Probability: 0.00204332848079503"
## [6] "Top Predicted Image-Label Classes: Name=n02859443 boathouse;
Probability: 0.00106108584441245"
## [7] "Top Predicted Image-Label Classes: Name=n02951358 canoe;
Probability: 0.000664844119455665"
## [8] "Top Predicted Image-Label Classes: Name=n09246464 cliff, drop,
drop-off; Probability: 0.000416322873206809"
## [9] "Top Predicted Image-Label Classes: Name=n04357314 sunscreen,
sunblock, sun blocker; Probability: 0.000338666519382969"
## [10] "Top Predicted Image-Label Classes: Name=n04606251 wreck;
Probability: 0.000292503653327003"
```

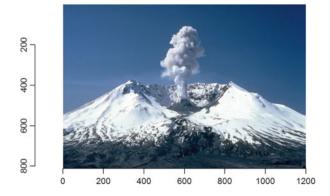
This photo was classified appropriately and with high-confidence as:

- Sandbar, sand bar.
- · Lakeside, lakeshore.
- Seashore, coast, sea-coast, sea-coast.

23.6.5 Volcano

Here is another natural image representing the Mount St. Helens Vocano (Fig. 23.35).

Fig. 23.35 A volcano image for neural network image recognition

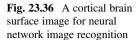


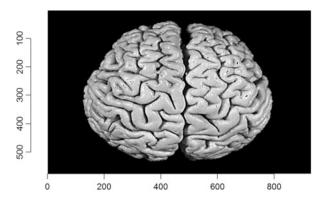
```
download.file("https://upload.wikimedia.org/wikipedia/commons/thumb/d/dc/MSH
82_st_helens_plume_from_harrys_ridge_05-19-82.jpg/1200px-MSH82_st_helens_plu
me_from_harrys_ridge_05-19-82.jpg", paste(getwd(), "results/image.png", sep="
/"), mode = 'wb')
im <- Load.image(paste(getwd(), "results/image.png", sep="/"))
plot(im)</pre>
```

```
prob <- predict(model, X=normed)</pre>
max.idx <- order(prob[,1], decreasing = TRUE)[1:10]</pre>
print(paste0("Top Predicted Image-Label Classes: Name=", synsets[max.idx],
"; Probability: ", prob[max.idx]))
## [1] "Top Predicted Image-Label Classes: Name=n09472597 volcano;
Probability: 0.993182718753815"
## [2] "Top Predicted Image-Label Classes: Name=n09288635 geyser;
Probability: 0.00681292032822967"
## [3] "Top Predicted Image-Label Classes: Name=n09193705 alp;
Probability: 4.15803697251249e-06"
## [4] "Top Predicted Image-Label Classes: Name=n03344393 fireboat;
Probability: 1.48333114680099e-07"
## [5] "Top Predicted Image-Label Classes: Name=n04310018 steam locomotive;
Probability: 1.17537313215621e-08"
## [6] "Top Predicted Image-Label Classes: Name=n03388043 fountain;
Probability: 7.4444117537098e-09"
## [7] "Top Predicted Image-Label Classes: Name=n04228054 ski;
Probability: 2.90055357510255e-09"
## [8] "Top Predicted Image-Label Classes: Name=n02950826 cannon;
Probability: 2.27150032117152e-09"
## [9] "Top Predicted Image-Label Classes: Name=n03773504 missile;
Probability: 1.69992575571598e-09"
## [10] "Top Predicted Image-Label Classes: Name=n04613696 yurt;
Probability: 1.25635490899612e-09"
```

The predicted top class labels for this image are perfect:

- Volcano.
- Geyser.
- Alp.





23.6.6 Brain Surface

The next image represents a 2D snapshot of 3D shape reconstruction of a brain cortical surface. This image is particularly difficult to automatically classify because (1) few people have ever seen a real brain, (2) the mathematical and computational models used to obtain the 2D manifold representing the brain surface do vary, and (3) the patterns of sulcal folds and gyral crests are quite inconsistent between people (Fig. 23.36).

download.file("http://wiki.socr.umich.edu/images/e/ea/BrainCortex2.png", pas

```
te(getwd(), "results/image.png", sep="/"), mode = 'wb')
im <- Load.image(paste(getwd(), "results/image.png", sep="/"))</pre>
plot(im)
# normed <- preproc.image(im, mean.img)</pre>
prob <- predict(model, X=normed)</pre>
max.idx <- order(prob[,1], decreasing = TRUE)[1:10]</pre>
print(paste0("Top Predicted Image-Label Classes: Name=", synsets[max.idx],
"; Probability: ", prob[max.idx]))
## [1] "Top Predicted Image-Label Classes: Name=n01917289 brain coral;
Probability: 0.4974305331707"
## [2] "Top Predicted Image-Label Classes: Name=n07734744 mushroom;
Probability: 0.229991897940636"
## [3] "Top Predicted Image-Label Classes: Name=n13052670 hen-of-the-woods,
hen of the woods, Polyporus frondosus, Grifola frondosa;
Probability: 0.0925175696611404"
## [4] "Top Predicted Image-Label Classes: Name=n03598930 jigsaw puzzle;
Probability: 0.0433991812169552"
## [5] "Top Predicted Image-Label Classes: Name=n07718747 artichoke,
globe artichoke; Probability: 0.0150045640766621"
## [6] "Top Predicted Image-Label Classes: Name=n07860988 dough;
Probability: 0.0124379806220531"
## [7] "Top Predicted Image-Label Classes: Name=n07715103 cauliflower;
Probability: 0.0115451859310269"
## [8] "Top Predicted Image-Label Classes: Name=n12985857 coral fungus;
Probability: 0.0109992604702711"
## [9] "Top Predicted Image-Label Classes: Name=n07714990 broccoli;
Probability: 0.00909161567687988"
## [10] "Top Predicted Image-Label Classes: Name=n03637318 Lampshade,
Lamp shade; Probability: 0.00754355266690254"
```

The top class labels for the brain image are:

- Brain coral.
- · Mushroom.
- Hen-of-the-woods, hen of the woods, Polyporus frondosus, Grifola frondosa.
- · Jigsaw puzzle.

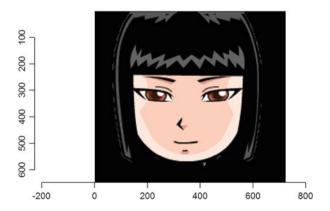
Imagine if we can train a brain image classifier that labels individuals (volunteers or patients) solely based on their brain scans into different classes reflecting their development state, clinical phenotypes, disease traits, or aging profiles. This will require a substantial amount of expert-labeled brain scans, intense model training and extensive validation. However, any progress in this direction will lead to effective computational clinical decision support systems that can assist physicians with diagnosis, tracking, and prognostication of brain growth and aging in health and disease.

23.6.7 Face Mask

The last example is a synthetic computer-generated image representing a cartoon face or a mask (Fig. 23.37).

```
download.file("http://wiki.socr.umich.edu/images/f/fb/FaceMask1.png",
paste(getwd(), "results/image.png", sep="/"), mode = 'wb')
im <- load.image(paste(getwd(), "results/image.png", sep="/"))
plot(im)</pre>
```

Fig. 23.37 A facial mask image for neural network image recognition



```
prob <- predict(model, X=normed)</pre>
max.idx <- order(prob[,1], decreasing = TRUE)[1:10]</pre>
print(paste0("Top Predicted Image-Label Classes: Name=", synsets[max.idx],
"; Probability: ", prob[max.idx]))
## [1] "Top Predicted Image-Label Classes: Name=n03724870 mask;
Probability: 0.376201003789902"
## [2] "Top Predicted Image-Label Classes: Name=n04229816 ski mask;
Probability: 0.253164798021317"
## [3] "Top Predicted Image-Label Classes: Name=n02708093 analog clock;
Probability: 0.0562068484723568"
## [4] "Top Predicted Image-Label Classes: Name=n02865351 bolo tie, bolo,
bola tie, bola; Probability: 0.029578423127532"
## [5] "Top Predicted Image-Label Classes: Name=n04192698 shield, buckler;
Probability: 0.0278499200940132"
## [6] "Top Predicted Image-Label Classes: Name=n03590841 jack-o'-lantern;
Probability: 0.0175030305981636"
## [7] "Top Predicted Image-Label Classes: Name=n02974003 car wheel;
Probability: 0.0172393135726452"
## [8] "Top Predicted Image-Label Classes: Name=n07892512 red wine;
Probability: 0.0168519839644432'
## [9] "Top Predicted Image-Label Classes: Name=n03249569 drum,
membranophone, tympan; Probability: 0.0141900414600968"
## [10] "Top Predicted Image-Label Classes: Name=n04447861 toilet seat;
Probability: 0.013601747341454"
```

The top class labels for the face mask are:

- · Mask.
- Ski mask.
- · Analog clock.

You can easily test the same image classifier on your own images and identify classes of pictures that are either well or poorly classified by the deep learning based machine learning model.

23.7 Assignment: 23. Deep Learning, Neural Networks

23.7.1 Deep Learning Classification

- Download the Alzheimer's data from the SOCR Archive.
- Properly preprocess the data and remove outliers.
- Build a multi-layer perceptron as a classifier and select proper parameters.
- Classify AD and NC and report the detailed classification accuracy metrics using cross table, accuracy, sensitivity, specificity, LOR, AUC.
- Generate some data/results visualizations, at least include histograms and model graph structures. See Chap. 23.
- Try to construct a deeper and more elaborate network model and report the prediction results.
- Compare your results with alternative data-driven methods (e.g., KNN).

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23.7.2 Deep Learning Regression

- Download the Allometric relationship data from SOCR data.
- Preprocess the data and set density as the response variable.
- Create an MXNet feedforward neural net model and properly specify the parameters.
- Train a model, predict, and report RMSE on the test data, evaluate the result, and justify your evaluation.
- Output the model's structure.

23.7.3 Image Classification

Apply the deep learning neural network techniques to classify some images using the pre-trained model as demonstrated in this chapter:

- · Google images.
- SOCR Neuroimaging data.
- Your own images.

References

Carneiro, G, Mateus, D, Loïc, P, Bradley, A, Manuel, J, Tavares, RS, Belagiannis, V, Papa, JP, Jacinto, C, Loog, M, Lu, Z, Cardoso, JS, Cornebise, J (eds). (2016) *Deep Learning and Data Labeling for Medical Applications: First International Workshop, LABELS 2016*, Springer, ISBN 3319469762, 9783319469768.

Ioffe S, Szegedy C. Batch normalization: Accelerating deep network training by reducing internal covariate shift. arXiv preprint arXiv:150203167. 2015.

Wiley, JF. (2016) *R Deep Learning Essentials*, Packt Publishing, ISBN 1785284711, 9781785284717.

Zhou, K, Greenspan, H, Shen, D. (2017) *Deep Learning for Medical Image Analysis*, Academic Press, ISBN 0128104090, 9780128104095.

MXNET R Tutorial.

Deep Learning with MXNetR.

Deep Neural Networks.

Google's TensorFlow API.

https://github.com/dmlc/mxnet/blob/master/R-package/vignettes/classifyRealImageWithPretrained Model.Rmd