Package ‘autoencoder’

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Title Sparse Autoencoder for Automatic Learning of Representative Features from Unlabeled Data

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Description Implementation of the sparse autoencoder in R environment, following the notes of Andrew Ng (http://www.stanford.edu/class/archive/cs/cs294a/cs294a.1104/sparseAutoencoder.pdf). The features learned by the hidden layer of the autoencoder (through unsupervised learning of unlabeled data) can be used in constructing deep belief neural networks.

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autoencoder-package

Implementation of sparse autoencoder for automatic learning of representative features from unlabeled data.

Description

The package implements a sparse autoencoder, described in Andrew Ng’s notes (see the reference below), that can be used to automatically learn features from unlabeled data. These features can then be used, e.g., for weight initialization in hidden layers of deep-belief neural networks.

Details

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The current version of the package consists of two main functions: autoencode() and predict(). See help for autoencode() and predict.autoencoder() for more details on how to use them.

Author(s)

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References

Andrew Ng. Sparse autoencoder (Lecture notes) http://www.stanford.edu/class/archive/cs/cs294a/cs294a.1104/sparseAutoencoder.pdf

See Also

autoencode, predict.autoencoder

Examples

## Train the autoencoder on unlabeled set of 5000 image patches of
## size Nx.patch by Ny.patch, randomly cropped from 10 nature photos:
## Load a training matrix with rows corresponding to training examples,
## and columns corresponding to input channels (e.g., pixels in images):
data('training_matrix_N=5e3_Ninput=100') ## the matrix contains 5e3 image
## patches of 10 by 10 pixels

## Set up the autoencoder architecture:
nl=3  ## number of layers (default is 3: input, hidden, output)
unit.type = "logistic"  ## specify the network unit type, i.e., the unit's
## activation function ("logistic" or "tanh")
Nx.patch=10  ## width of training image patches, in pixels
Ny.patch=10  ## height of training image patches, in pixels
N.input = Nx.patch*Ny.patch  ## number of units (neurons) in the input layer (one unit per pixel)
N.hidden = 5*5  ## number of units in the hidden layer
lambda = 0.0002  ## weight decay parameter
beta = 6  ## weight of sparsity penalty term
rho = 0.01  ## desired sparsity parameter
epsilon <- 0.001  ## as small as small gaussian random numbers sampled from N(0,epsilon^2)
max.iterations = 2000  ## number of iterations in optimizer

## Train the autoencoder on training.matrix using BFGS optimization method
## (see help("optim") for details):
## WARNING: the training can take as long as 20 minutes for this dataset!
## Not run:
autoencoder.object <- autoencode(X.train=training.matrix,nl=nl,N.hidden=N.hidden,
unit.type=unit.type,lambda=lambda,beta=beta,rho=rho,epsilon=epsilon,
optim.method="BFGS",max.iterations=max.iterations,
rescale.flag=TRUE,rescaling.offset=0.001)
## End(Not run)
## N.B.: Training this autoencoder takes a long time, so in this example we do not run the above
## autoencode function, but instead load the corresponding pre-trained autoencoder.object.

## Report mean squared error for training and test sets:
cat("autoencode(): mean squared error for training set: ",
round(autoencoder.object$mean.error.training.set,3),"\n")

## Visualize hidden units' learned features:
visualize.hidden.units(autoencoder.object,Nx.patch,Ny.patch)

## Compare the output and input images (the autoencoder learns to approximate
## inputs in outputs using features learned by the hidden layer):
## Evaluate the output matrix corresponding to the training matrix
## (rows are examples, columns are input channels, i.e., pixels)
X.output <- predict(autoencoder.object, X.input=training.matrix, hidden.output=FALSE)$X.output

## Compare outputs and inputs for 3 image patches (patches 7,26,16 from
## the training set) - outputs should be similar to inputs:
op <- par(no.readonly = TRUE)  ## save the whole list of settable par's.
par(mfrow=c(3,2),mar=c(2,2,2,2))
for (n in c(7,26,16))
  ## input image:
  image(matrix(training.matrix[n,],nrow=Ny.patch,ncol=Nx.patch),axes=FALSE,main="Input image",
  col=gray((0:32)/32))
  ## output image:
  image(matrix(X.output[n,],nrow=Ny.patch,ncol=Nx.patch),axes=FALSE,main="Output image",
  col=gray((0:32)/32))
autoencode implements the sparse autoencoder (described in Andrew Ng’s lecture notes [http://www.stanford.edu/class/archive/cs/cs294a/cs294a.1104/sparseAutoencoder.pdf](http://www.stanford.edu/class/archive/cs/cs294a/cs294a.1104/sparseAutoencoder.pdf)). The features learned by the autoencoder trained on unlabeled data are available through weights of the trained autoencoder object. These automatically learned features are useful, e.g., in constructing deep belief networks.

**Usage**

```r
autoencode(X.train, X.test = NULL, nl = 3, N.hidden, unit.type = c("logistic", "tanh"), lambda, beta, rho, epsilon, optim.method = c("BFGS", "L-BFGS-B", "CG"), rel.tol=sqrt(.Machine$double.eps), max.iterations = 2000, rescale.flag = c(F, T), rescaling.offset = 0.001)
```

**Arguments**

- `X.train`: a matrix of training data, with rows corresponding to training examples, and columns corresponding to input channels. For example, if training data consists of 10x10-pixel images, then `X.train` has 100 columns corresponding to each pixel.
- `X.test`: an optional matrix of test data in the same format as `X.train`, used for testing of the trained autoencoder by evaluating the squared error for the test data set.
- `nl`: number of layers in the autoencoder (default is 3 layers: input, hidden, output).
- `N.hidden`: a vector of numbers of units (neurons) in each of the hidden layers. For `nl=3` (default architecture) this is just the number of units in the single hidden layer of the autoencoder.
- `unit.type`: type of units used in the autoencoder, defined by the activation function of the units (‘logistic’ or ‘tanh’).
- `lambda`: weight decay parameter controlling the relative importance of the regularization term in the autoencoder’s cost function.
- `beta`: weight of sparsity penalty term.
- `rho`: sparsity parameter, constrains the average (over training examples) activation of hidden units. Typically should be a small value close to zero (hence sparse autoencoder).
- `epsilon`: a small parameter for initialization of autoencoder weights as small gaussian random numbers sampled from the normal distribution $N(0,\epsilon^2)$.
- `optim.method`: the optimization method to be used for searching the minimum of the cost function. See `method` in `help('optim')` for details.
rel.tol  relative convergence tolerance determining the convergence of optim() optimizer. The algorithm stops if it is unable to reduce the value by a factor of reltol * (abs(value) + reltol) at a step. Defaults to sqrt(.Machine$double.eps), typically about 1e-8.

max.iterations  maximum number of iterations in searching for cost function minimum. Defaults to 2000.

rescale.flag  a logical flag indicating whether to uniformly rescale the training matrix to make sure the values of all input channels are within the range of unit outputs (the range is [0,1] for 'logistic' units, and [-1,1] for 'tanh' units).

rescaling.offset  a small non-negative value used in rescaling to [offset,1-offset] for 'logistic' units, and to [-1+offset,1-offset] for 'tanh' units. Defaults to 0.001.

Details

An autoencoder neural network is an unsupervised learning algorithm that applies backpropagation to adjust its weights, attempting to learn to make its target values (outputs) to be equal to its inputs. In other words, it is trying to learn an approximation to the identity function, so as its output is similar to its input, for all training examples. With the sparsity constraint enforced (requiring that the average, over training set, activation of hidden units be small), such autoencoder automatically learns useful features of the unlabeled training data, which can be used for, e.g., data compression (with losses), or as features in deep belief networks.

The training is performed by optimizing the autoencoder’s cost function \( J(W,b) \) that depends on the autoencoder’s weights \( W \) and biases \( b \). The optimization (searching for a local minimum) is performed with the \texttt{optim} function using one of the three methods: 'BFGS', 'L-BFGS-B', or 'CG' (see details in help(optim)).

After the optimization converges, the mean squared error between the output and input matrix (either the training matrix, or a test matrix) is evaluated as a measure of goodness of fit of the autoencoder.

For the autoencoder to work well, one must rescale, if necessary, the training matrix to make sure all the input channels (and hence all the output channels) have values within the range of unit activation function values: [0,1] for 'logistic' units, [-1,1] for 'tanh' units. If rescaling flag is true (\texttt{rescale.flag=TRUE}), the input matrix is rescaled uniformly using its minimum and maximum elements \( \min(X.train) \) and \( \max(X.train) \) as

\[
X.train.rescaled=(X.train-min(X.train))/(max(X.train)-min(X.train)) \quad \text{for 'logistic' units, and}
\]

\[
X.train.rescaled=2*(X.train-min(X.train))/(max(X.train)-min(X.train))-1 \quad \text{for 'tanh' units.}
\]

The minimum and maximum elements of the training matrix are then passed to the object returned by the function, to be used for rescaling input data in predict.autoencode function, for compatibility with the rescaling of the data used for training the autoencoder.

Value

An object of class autoencoder, containing a list with the following components:

\( W \)  a list of weight matrices in the format \( W[[l]][i,j] \), where \( l \) is the number of the layer, \( i \) and \( j \) are the row and column indices. An element \( W[[l]][i,j] \) is
the weight associated with a connection between unit j in layer l and unit i in layer l+1.

b a list of biases; b[[1]][i] is the bias associated with unit i in layer l+1.

unit.type type of units used in the autoencoder, the value if the same as unit.type argument.

rescaling a list with elements rescale.flag (a logical flag indicating whether rescaling was applied to the training matrix before training the autoencoder), rescaling.min, and rescaling.max (the minimum and maximum elements of the training matrix used for rescaling - see 'Details').

mean.error.training.set average, over all training matrix rows (training examples), sum of (X.output-X.train)^2, where X.output is the matrix of autoencoder outputs corresponding to the training matrix X.train (i.e., each row in X.output is a result of the feed-forward pass of the corresponding training example through the trained autoencoder).

mean.error.test.set average, over all test matrix rows (test examples), sum of (X.output-X.test)^2, where X.output is the matrix of autoencoder outputs corresponding to the test matrix X.test (i.e., each row in X.output is a result of the feed-forward pass of the corresponding test example through the trained autoencoder).

Author(s)

Eugene Dubossarsky (project leader, chief designer), Yuriy Tyshetskiy (design, implementation, testing)

References

See Andrew Ng’s lecture notes at http://www.stanford.edu/class/archive/cs/cs294a/cs294a.1104/sparseAutoencoder.pdf

See Also

predict.autoencoder

Examples

```r
## Train the autoencoder on unlabeled set of 5000 image patches of
## size Nx.patch by Ny.patch, randomly cropped from 10 nature photos:
## Load a training matrix with rows corresponding to training examples,
## and columns corresponding to input channels (e.g., pixels in images):
data('training_matrix_N=5e3_Ninput=100') ## the matrix contains 5e3 image
## patches of 10 by 10 pixels

## Set up the autoencoder architecture:
nl=3 ## number of layers (default is 3: input, hidden, output)
unit.type = "logistic" ## specify the network unit type, i.e., the unit's
## activation function ("logistic" or "tanh")
Nx.patch=10 ## width of training image patches, in pixels
Ny.patch=10 ## height of training image patches, in pixels
```
autoencoder_Ninput=100_Nhidden=100_rho=1e-2

N.input = Nx.patch*Ny.patch ## number of units (neurons) in the input layer (one unit per pixel)
N.hidden = 10*10 ## number of units in the hidden layer
lambda = 0.0002 ## weight decay parameter
beta = 6 ## weight of sparsity penalty term
rho = 0.01 ## desired sparsity parameter
epsilon <- 0.001 ## as small gaussian random numbers sampled from N(0,epsilon^2)
max.iterations = 2000 ## number of iterations in optimizer

## Train the autoencoder on training.matrix using BFGS optimization method
## WARNING: the training can take a long time (~1 hour) for this dataset!
## Not run:
autoencoder.object <- autoencode(X.train=training.matrix,nl=nl,N.hidden=N.hidden,
unit.type=unit.type,lambda=lambda,beta=beta,rho=rho,epsilon=epsilon,
optim.method="BFGS",max.iterations=max.iterations,
rescale.flag=TRUE,rescaling.offset=0.001)
## End(Not run)
## N.B.: Training this autoencoder takes a long time, so in this example we do not run the above
## autoencode function, but instead load the corresponding pre-trained autoencoder.object.

## Report mean squared error for training and test sets:
cat("autoencode(): mean squared error for training set: ",
round(autoencoder.object$mean.error.training.set,3),"\n")

## Extract weights W and biases b from autoencoder.object:
W <- autoencoder.object$W
b <- autoencoder.object$b
## Visualize hidden units' learned features:
visualize.hidden.units(autoencoder.object,Nx.patch,Ny.patch)

autoencoder_Ninput=100_Nhidden=100_rho=1e-2
A trained autoencoder example with 100 hidden units

Description

autoencoder.object is an example object of class autoencoder containing the weights, biases
and other parameter of a sparse autoencoder with N.input=100, N.hidden=100, with sparsity pa-
rameter rho=0.01, trained on a dataset of 5000 image patches of 10 by 10 pixels, randomly cropped
from decoloured nature photos.

Usage
data('autoencoder_Ninput=100_Nhidden=100_rho=1e-2')
autoencoder_Ninput=100_Nhidden=25_rho=1e-2

Format

The format is: chr "autoencoder_Ninput=100_Nhidden=100_rho=1e-2"

Examples

## Load a pre-trained autoencoder object with N.input=100 and N.hidden=10*10, 
## trained on unlabeled set of 5000 image patches of size Nx.patch by Ny.patch, 
## randomly picked from 10 nature photos, and visualize the features 
## learned by its hidden units:

data('autoencoder_Ninput=100_Nhidden=100_rho=1e-2')

## Visualize hidden units' learned features:
visualize.hidden.units(autoencoder.object,Nx.patch=10,Ny.patch=10)

autoencoder_Ninput=100_Nhidden=25_rho=1e-2

A trained autoencoder example with 25 hidden units

Description

autoencoder.object is an example object of class autoencoder containing the weights, biases 
and other parameter of a sparse autoencoder with N.input=100, N.hidden=25, with sparsity pa-
rameter rho=0.01, trained on a dataset of 5000 image patches of 10 by 10 pixels, randomly cropped 
from decoloured nature photos.

Usage

data('autoencoder_Ninput=100_Nhidden=25_rho=1e-2')

Format

The format is: chr "autoencoder_Ninput=100_Nhidden=25_rho=1e-2"

Examples

## Load a pre-trained autoencoder object with N.input=100 and N.hidden=5*5, 
## trained on unlabeled set of 5000 image patches of size Nx.patch by Ny.patch, 
## randomly picked from 10 nature photos, and visualize the features 
## learned by its hidden units:

data('autoencoder_Ninput=100_Nhidden=25_rho=1e-2')

## Visualize hidden units' learned features:
visualize.hidden.units(autoencoder.object,Nx.patch=10,Ny.patch=10)
**predict**

Predict outputs of a sparse autoencoder

**Description**

Predict outputs for a given set of inputs, and estimate mean squared error between inputs and outputs of a sparse autoencoder network trained using `autoencode` function. Optionally, predict outputs of units in the hidden layer of the autoencoder instead of outputs of units in the output layer.

**Usage**

```r
## S3 method for class 'autoencoder'
predict(object, X.input=NULL, hidden.output = c(F, T), ...)
```

**Arguments**

- `object`: an object of class `autoencoder` produced by the `autoencode` function.
- `X.input`: a matrix of inputs, with columns corresponding to the columns of the training matrix used in training the autoencoder object, and an arbitrary number of rows corresponding to the number of inputs.
- `hidden.output`: a logical switch telling whether to produce outputs of units in the output layer (for `hidden.output=FALSE`) or of units in the hidden layer (for `hidden.output=TRUE`). The latter can be used for stacked autoencoders.
- `...`: not used.

**Details**

All the information about the autoencoder (weights and biases, unit type, rescaling data) is contained in object of class `autoencoder` produced by `autoencode` function. See `autoencode` for details about the `autoencoder` class object.

**Value**

A list with elements:

- `X.output`: output matrix with rows corresponding to outputs corresponding to examples (rows) in `X.input`. Depending on the value of `hidden.output`, these are outputs of units in the hidden layer (for `hidden.output=TRUE`) or in the output layer (for `hidden.output=FALSE`).
- `hidden.output`: (same as `hidden.output` in the arguments) logical flag telling whether the outputs are generated by units in the hidden layer (for `hidden.output=TRUE`) or in the output layer (for `hidden.output=FALSE`) of the autoencoder.
- `mean.error`: average, over rows, sum of `(X.output - X.input)^2`. 
Author(s)

Eugene Dubossarsky (project leader, chief designer), Yuriy Tyshetskiy (design, implementation, testing)

Examples

## Train the autoencoder on unlabeled set of 5000 image patches of size Nx.patch by Ny.patch, randomly cropped from 10 nature photos:

## Load a training matrix with rows corresponding to training examples, and columns corresponding to input channels (e.g., pixels in images):

data('training_matrix_N=5e3_Ninput=100') ## the matrix contains 5e3 image patches of 10 by 10 pixels

## Set up the autoencoder architecture:

nl=3 ## number of layers (default is 3: input, hidden, output)
unit.type = "logistic" ## specify the network unit type, i.e., the unit's activation function ("logistic" or "tanh")
Nx.patch=10 ## width of training image patches, in pixels
Ny.patch=10 ## height of training image patches, in pixels
N.input = Nx.patch*Ny.patch ## number of units (neurons) in the input layer (one unit per pixel)
N.hidden = 10*10 ## number of units in the hidden layer
lambda = 0.0002 ## weight decay parameter
beta = 6 ## weight of sparsity penalty term
rho = 0.01 ## desired sparsity parameter
epsilon <- 0.001 ## a small parameter for initialization of weights as small gaussian random numbers sampled from N(0,epsilon^2)
max.iterations = 2000 ## number of iterations in optimizer

## Train the autoencoder on training.matrix using BFGS optimization method (see help('optim') for details):

## Not run:
autoencoder.object <- autoencode(X.train=training.matrix,nl=nl,N.hidden=N.hidden,unit.type=unit.type,lambda=lambda,beta=beta,rho=rho,epsilon=epsilon,optim.method="BFGS",max.iterations=max.iterations,rescale.flag=TRUE,rescaling.offset=0.001)

## End(Not run)

## N.B.: Training this autoencoder takes a long time, so in this example we do not run the above autoencode function, but instead load the corresponding pre-trained autoencoder.object.

## Report mean squared error for training and test sets:

cat("autoencode(): mean squared error for training set: ",round(autoencoder.object$mean.error.training.set,3),"\n")

## Visualize hidden units' learned features:
visualize.hidden.units(autoencoder.object,Nx.patch,Ny.patch)

## Compare the output and input images (the autoencoder learns to approximate inputs in its outputs using features learned by the hidden layer):

## Predict the output matrix corresponding to the training matrix
## (rows are examples, columns are input channels, i.e., pixels)

```
X.output <- predict(autoencoder.object, X.input=training.matrix, hidden.output=FALSE)$X.output
```

## Compare outputs and inputs for 3 image patches (patches 7, 26, 16 from
## the training set) - outputs should be similar to inputs:
```
op <- par(no.readonly = TRUE) ## save the whole list of settable par's.
par(mfrow=c(3,2),mar=c(2,2,2,2))
for (n in c(7,26,16)){
  ## input image:
  image(matrix(training.matrix[n,],nrow=Ny.patch,ncol=Nx.patch),axes=FALSE,main="Input image",
col=gray((0:32)/32))
  ## output image:
  image(matrix(X.output[n,],nrow=Ny.patch,ncol=Nx.patch),axes=FALSE,main="Output image",
col=gray((0:32)/32))
}
par(op) ## restore plotting par's
```

---

An example training set of images for training sparse autoencoder

### Description

This is an example set `training.matrix` of 5000 image patches of 10 by 10 pixels, randomly
cropped from a set of 10 decoloured nature photos. The rows of `training.matrix` correspond to
the training examples, the columns correspond to pixels of the image patches.

### Usage

```
data('training_matrix_N=5e3_Ninput=100')
```

### Format

The format is: chr "training_matrix_N=5e3_Ninput=100"

### Examples

```
data('training_matrix_N=5e3_Ninput=100') ## load the example training.matrix

## Set up the autoencoder architecture:
nl=3  ## number of layers (default is 3: input, hidden, output)
unit.type = "logistic"  ## specify the network unit type, i.e., the unit's
## activation function ("logistic" or "tanh")
Nx.patch=10  ## width of training image patches, in pixels
Ny.patch=10  ## height of training image patches, in pixels
N.input = Nx.patch*Ny.patch  ## number of units (neurons) in the input layer (one unit per pixel)
N.hidden = 10*10  ## number of units in the hidden layer
lambda = 0.0002  ## weight decay parameter
beta = 6  ## weight of sparsity penalty term
rho = 0.01  ## desired sparsity parameter
```
epsilon <- 0.001 ## a small parameter for initialization of weights
## as small gaussian random numbers sampled from N(0,epsilon^2)
max.iterations = 2000 ## number of iterations in optimizer

## Train the autoencoder on training.matrix using BFGS optimization method
## (see help('optim') for details):

## Not run:
autoencoder.object <- autoencode(X.train=training.matrix,nl=nl,N.hidden=N.hidden,
  unit.type=unit.type,lambda=lambda,beta=beta,rho=rho,epsilon=epsilon,
  optim.method="BFGS",max.iterations=max.iterations,
  rescale.flag=TRUE,rescaling.offset=0.001)
## End(Not run)

## Extract weights W and biases b from autoencoder.object:
W <- autoencoder.object$W
b <- autoencoder.object$b
## Visualize learned features of the autoencoder:
visualize.hidden.units(autoencoder.object,Nx.patch,Ny.patch)

visualize.hidden.units

Visualize features learned by a sparse autoencoder

Description

Visualizes features learned by a sparse autoencoder, by plotting (norm bounded) input images that
maximally activate each of the hidden units of the trained autoencoder. Here it is assumed that the
autoencoder is trained on a set of images of size Nx.patch by Ny.patch (in pixels).

Usage

visualize.hidden.units(object, Nx.patch, Ny.patch)

Arguments

object an object of class autoencoder produced by the autoencode function, and con-
taining information (architecture, weights, biases, unit type, etc.) about the au-
toencoder network.

Nx.patch width (in pixels) of images in data set used for training the autoencoder. See 'Examples'.

Ny.patch height (in pixels) of images in data set used for training the autoencoder. See 'Examples'.
Value

A figure in which each square shows the (norm bounded) input image of size \(N_x,\text{patch}\) by \(N_y,\text{patch}\) (in pixels) that maximally activates each of the hidden units. These squares represent the features learned by the autoencoder from the unlabeled data used for its training.

Author(s)

Yuriy Tyshetskiy

Examples

```r
## Load a pre-trained autoencoder object with \(N_{\text{input}}=100\) and \(N_{\text{hidden}}=10 \times 10\),
## trained on unlabeled set of 5000 image patches of size
## \(N_x,\text{patch}=10\) by \(N_y,\text{patch}=10\) pixels,
## randomly cropped from 10 nature photos, and visualize the features
## learned by its hidden units:

data('autoencoder_Ninput=100_Nhidden=100_rho=1e-2')

## Visualize hidden units' learned features:
visualize.hidden.units(autoencoder.object,Nx,patch=10,Ny,patch=10)
```
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