

Package ‘BayesFluxR’

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Type Package

Title Implementation of Bayesian Neural Networks

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Description Implementation of 'BayesFlux.jl' for R; It extends the famous 'Flux.jl' machine learning library to Bayesian Neural Networks. The goal is not to have the fastest production ready library, but rather to allow more people to be able to use and research on Bayesian Neural Networks.

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.install_pkg	<i>Installs Julia packages if needed</i>
--------------	--

Description

Installs Julia packages if needed

Usage

```
.install_pkg(...)
```

Arguments

... strings of package names

`.julia_project_status` *Obtain the status of the current Julia project*

Description

Obtain the status of the current Julia project

Usage

`.julia_project_status()`

`.set_seed` *Set a seed both in Julia and R*

Description

Set a seed both in Julia and R

Usage

`.set_seed(seed)`

Arguments

seed seed to be used

Value

No return value, called for side effects.

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
.set_seed(123)  
  
## End(Not run)
```

<code>.using</code>	<i>Loads Julia packages</i>
---------------------	-----------------------------

Description

Loads Julia packages

Usage

```
.using(...)
```

Arguments

... strings of package names

<code>BayesFluxR_setup</code>	<i>Set up of the Julia environment needed for BayesFlux</i>
-------------------------------	---

Description

This will set up a new Julia environment in the current working directory or another folder if provided. This environment will then be set with all Julia dependencies needed.

Usage

```
BayesFluxR_setup(
  pkg_check = TRUE,
  nthreads = 4,
  seed = NULL,
  env_path = getwd(),
  installJulia = FALSE,
  ...
)
```

Arguments

<code>pkg_check</code>	(Default=TRUE) Check whether needed Julia packages are installed
<code>nthreads</code>	(Default=4) How many threads to make available to Julia
<code>seed</code>	Seed to be used.
<code>env_path</code>	The path to where the Julia environment should be created. By default, this is the current working directory.
<code>installJulia</code>	(Default=TRUE) Whether to install Julia
...	Other parameters passed on to <code>julia_setup</code>

Value

No return value, called for side effects.

Examples

```
## Not run:
## Time consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)

## End(Not run)
```

bayes_by_backprop	<i>Use Bayes By Backprop to find Variational Approximation to BNN.</i>
-------------------	--

Description

This was proposed in Blundell, C., Cornebise, J., Kavukcuoglu, K., & Wierstra, D. (2015, June). Weight uncertainty in neural network. In International conference on machine learning (pp. 1613-1622). PMLR.

Usage

```
bayes_by_backprop(
  bnn,
  batchsize,
  epochs,
  mc_samples = 1,
  opt = opt.ADAM(),
  n_samples_convergence = 10
)
```

Arguments

bnn	a BNN obtained using BNN
batchsize	batch size
epochs	number of epochs to run for
mc_samples	samples to use in each iteration for the MC approximation usually one is enough.
opt	An optimiser. These all start with 'opt.'. See for example opt.ADAM
n_samples_convergence	At the end of each iteration convergence is checked using this many MC samples.

Value

a list containing

- ‘juliavar’ - julia variable storing VI
- ‘juliacode’ - julia representation of function call
- ‘params’ - variational family parameters for each iteration
- ‘losses’ - BBB loss in each iteration

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(RNN(5, 1))
like <- likelihood.seqtone_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
data <- matrix(rnorm(10*1000), ncol = 10)
# Choosing sequences of length 10 and predicting one period ahead
tensor <- tensor_embed_mat(data, 10+1)
x <- tensor[1:10, , , drop = FALSE]
# Last value in each sequence is the target value
y <- tensor[11,,]
bnn <- BNN(x, y, like, prior, init)
vi <- bayes_by_backprop(bnn, 100, 100)
vi_samples <- vi.get_samples(vi, n = 1000)

## End(Not run)
```

BNN

Create a Bayesian Neural Network

Description

Create a Bayesian Neural Network

Usage

BNN(x, y, like, prior, init)

Arguments

x For a Feedforward structure, this must be a matrix of dimensions variables x observations; For a recurrent structure, this must be a tensor of dimensions sequence_length x number_variables x number_sequences; In general, the last dimension is always the dimension over which will be batched.

y	A vector or matrix with observations.
like	Likelihood; See for example likelihood.feedforward_normal
prior	Prior; See for example prior.gaussian
init	Initialiser; See for example initialise.allsame

Value

List with the following content

- ‘juliavar’ - the julia variable containing the BNN
- ‘juliacode’ - the string representation of the BNN
- ‘x’ - x
- ‘juliax’ - julia variable holding x
- ‘y’ - y
- ‘juliay’ - julia variable holding y

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.SGLD()
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

BNN.totparams

Obtain the total parameters of the BNN

Description

Obtain the total parameters of the BNN

Usage

BNN.totparams(bnn)

Arguments

bnn A BNN formed using [BNN](#)

Value

The total number of parameters in the BNN

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
BNN.totparams(bnn)

## End(Not run)
```

Chain

Chain various layers together to form a network

Description

Chain various layers together to form a network

Usage

Chain(...)

Arguments

... Comma separated layers

Value

List with the following content

- juliavar - the julia variable containing the network
- specification - the string representation of the network
- nc - the julia variable for the network constructor

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
Chain(LSTM(5, 5))
Chain(RNN(5, 5, "tanh"))
Chain(Dense(1, 5))

## End(Not run)
```

Dense	<i>Create a Dense layer with ‘in_size’ inputs and ‘out_size’ outputs using ‘act’ activation function</i>
-------	--

Description

Create a Dense layer with ‘in_size’ inputs and ‘out_size’ outputs using ‘act’ activation function

Usage

```
Dense(in_size, out_size, act = c("identity", "sigmoid", "tanh", "relu"))
```

Arguments

in_size	Input size
out_size	Output size
act	Activation function

Value

A list with the following content

- in_size - Input Size
- out_size - Output Size
- activation - Activation Function
- julia - Julia code representing the Layer

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 5, "relu"))

## End(Not run)
```

find_mode

Find the MAP of a BNN using SGD

Description

Find the MAP of a BNN using SGD

Usage

```
find_mode(bnn, optimiser, batchsize, epochs)
```

Arguments

bnn	a BNN obtained using BNN
optimiser	an optimiser. These start with 'opt.'. See for example opt.ADAM
batchsize	batch size
epochs	number of epochs to run for

Value

Returns a vector. Use [posterior_predictive](#) to obtain a prediction using this MAP estimate.

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
find_mode(bnn, opt.RMSProp(), 10, 100)

## End(Not run)
```

Gamma	<i>Create a Gamma Prior</i>
-------	-----------------------------

Description

Creates a Gamma prior in Julia using Distributions.jl

Usage

```
Gamma(shape = 2, scale = 2)
```

Arguments

shape	shape parameter
scale	scale parameter

Value

A list with the following content

- juliavar - julia variable containing the distribution
- juliacode - julia code used to create the distribution

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(Dense(5, 1))  
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))  
  
## End(Not run)
```

get_random_symbol	<i>Creates a random string that is used as variable in julia</i>
-------------------	--

Description

Creates a random string that is used as variable in julia

Usage

```
get_random_symbol()
```

<code>initialise.allsame</code>	<i>Initialises all parameters of the network, all hyper parameters of the prior and all additional parameters of the likelihood by drawing random values from 'dist'.</i>
---------------------------------	---

Description

Initialises all parameters of the network, all hyper parameters of the prior and all additional parameters of the likelihood by drawing random values from 'dist'.

Usage

```
initialise.allsame(dist, like, prior)
```

Arguments

<code>dist</code>	A distribution; See for example Normal
<code>like</code>	A likelihood; See for example likelihood.feedforward_normal
<code>prior</code>	A prior; See for example prior.gaussian

Value

A list containing the following

- 'juliavar' - julia variable storing the initialiser
- 'juliacode' - julia code used to create the initialiser

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(Dense(5, 1))  
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))  
prior <- prior.gaussian(net, 0.5)  
init <- initialise.allsame(Normal(0, 0.5), like, prior)  
x <- matrix(rnorm(5*100), nrow = 5)  
y <- rnorm(100)  
bnn <- BNN(x, y, like, prior, init)  
BNN.totparams(bnn)  
  
## End(Not run)
```

InverseGamma	<i>Create an Inverse-Gamma Prior</i>
--------------	--------------------------------------

Description

Creates and Inverse Gamma prior in Julia using Distributions.jl

Usage

```
InverseGamma(shape = 2, scale = 2)
```

Arguments

shape	shape parameter
scale	scale parameter

Value

A list with the following content

- juliavar - julia variable containing the distribution
- juliacode - julia code used to create the distribution

See Also

[Gamma](#)

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(Dense(5, 1))  
like <- likelihood.feedforward_normal(net, InverseGamma(2.0, 0.5))  
  
## End(Not run)
```

likelihood.feedforward_normal

Use a Normal likelihood for a Feedforward network

Description

This creates a likelihood of the form

$$y_i \sim \text{Normal}(\text{net}(x_i), \sigma) \forall i = 1, \dots, N$$

where the x_i is fed through the network in a standard feedforward way.

Usage

```
likelihood.feedforward_normal(chain, sig_prior)
```

Arguments

chain	Network structure obtained using <code>link{Chain}</code>
sig_prior	A prior distribution for sigma defined using <code>Gamma</code> , <code>link{InverGamma}</code> , <code>Truncated</code> , <code>Normal</code>

Value

A list containing the following

- juliavar - julia variable containing the likelihood
- juliacode - julia code used to create the likelihood

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
BNN.totparams(bnn)

## End(Not run)
```

likelihood.feedforward_tdist

Use a t-Distribution likelihood for a Feedforward network

Description

This creates a likelihood of the form

$$\frac{y_i - net(x_i)}{\sigma} \sim T_\nu \quad \forall i = 1, \dots, N$$

where the x_i is fed through the network in the standard feedforward way.

Usage

```
likelihood.feedforward_tdist(chain, sig_prior, nu = 30)
```

Arguments

chain	Network structure obtained using <code>link{Chain}</code>
sig_prior	A prior distribution for sigma defined using Gamma , <code>link{InverGamma}</code> , Truncated, Normal
nu	DF of TDist

Value

see [likelihood.feedforward_normal](#)

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_tdist(net, Gamma(2.0, 0.5), nu=8)
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
BNN.totparams(bnn)

## End(Not run)
```

likelihood.seqtoone_normal

Use a Normal likelihood for a seq-to-one recurrent network

Description

This creates a likelihood of the form

$$y_i \sim \text{Normal}(\text{net}(x_i), \sigma), i = 1, \dots, N$$

Here x_i is a subsequence which will be fed through the recurrent network to obtain the final output $\text{net}(x_i) = \hat{y}_i$. Thus, if one has a single time series, and splits the single time series into subsequences of length K which are then used to predict the next output of the time series, then each x_i consists of K consecutive observations of the time series. In a sense one constrains the maximum memory length of the network this way.

Usage

```
likelihood.seqtoone_normal(chain, sig_prior)
```

Arguments

chain	Network structure obtained using <code>link{Chain}</code>
sig_prior	A prior distribution for sigma defined using Gamma , <code>link{InverGamma}</code> , Truncated , Normal

Value

see [likelihood.feedforward_normal](#)

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(RNN(5, 1))
like <- likelihood.seqtoone_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- array(rnorm(5*100*10), dim=c(10,5,100))
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
BNN.totparams(bnn)

## End(Not run)
```

`likelihood.seqtoone_tdist`*Use a T-likelihood for a seq-to-one recurrent network.*

Description

See [likelihood.seqtoone_normal](#) and [likelihood.feedforward_tdist](#) for details,

Usage

```
likelihood.seqtoone_tdist(chain, sig_prior, nu = 30)
```

Arguments

<code>chain</code>	Network structure obtained using <code>link{Chain}</code>
<code>sig_prior</code>	A prior distribution for sigma defined using Gamma , <code>link{InverGamma}</code> , Truncated, Normal
<code>nu</code>	DF of TDist

Value

see [likelihood.feedforward_normal](#)

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(RNN(5, 1))
like <- likelihood.seqtoone_tdist(net, Gamma(2.0, 0.5), nu=5)
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- array(rnorm(5*100*10), dim=c(10,5,100))
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
BNN.totparams(bnn)

## End(Not run)
```

LSTM	<i>Create an LSTM layer with 'in_size' input size, and 'out_size' hidden state size</i>
------	---

Description

Create an LSTM layer with 'in_size' input size, and 'out_size' hidden state size

Usage

```
LSTM(in_size, out_size)
```

Arguments

in_size	Input size
out_size	Output size

Value

A list with the following content

- in_size - Input Size
- out_size - Output Size
- julia - Julia code representing the Layer

See Also

[Dense](#)

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(LSTM(5, 5))  
  
## End(Not run)
```

madapter.DiagCov	<i>Use the diagonal of sample covariance matrix as inverse mass matrix.</i>
------------------	---

Description

Use the diagonal of sample covariance matrix as inverse mass matrix.

Usage

```
madapter.DiagCov(adapt_steps, windowlength, kappa = 0.5, epsilon = 1e-06)
```

Arguments

adapt_steps	Number of adaptation steps
windowlength	Lookback window length for calculation of covariance
kappa	How much to shrink towards the identity
epsilon	Small value to add to diagonal so as to avoid numerical non-pos-def problem

Value

list containing 'juliavar' and 'juliacode' and all given arguments.

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
madapter <- madapter.DiagCov(100, 10)
sampler <- sampler.GGMC(madapter = madapter)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

```
madapter.FixedMassMatrix
      Use a fixed mass matrix
```

Description

Use a fixed mass matrix

Usage

```
madapter.FixedMassMatrix(mat = NULL)
```

Arguments

mat (Default=NULL); inverse mass matrix; If 'NULL', then identity matrix will be used

Value

list with 'juliavar' and 'juliacode' and given matrix or 'NULL'

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
madapter <- madapter.FixedMassMatrix()
sampler <- sampler.GGMC(madapter = madapter)
ch <- mcmc(bnn, 10, 1000, sampler)

# Providing a non-sense weight matrix
weight_matrix <- matrix(runif(BNN.totparams(bnn)^2, 0, 1),
                        nrow = BNN.totparams(bnn))
madapter2 <- madapter.FixedMassMatrix(weight_matrix)
sampler2 <- sampler.GGMC(madapter = madapter2)
ch2 <- mcmc(bnn, 10, 1000, sampler2)

## End(Not run)
```

madapter.FullCov	<i>Use the full covariance matrix as inverse mass matrix</i>
------------------	--

Description

Use the full covariance matrix as inverse mass matrix

Usage

```
madapter.FullCov(adapt_steps, windowlength, kappa = 0.5, epsilon = 1e-06)
```

Arguments

adapt_steps	Number of adaptation steps
windowlength	Lookback window length for calculation of covariance
kappa	How much to shrink towards the identity
epsilon	Small value to add to diagonal so as to avoid numerical non-pos-def problem

Value

see [madapter.DiagCov](#)

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(Dense(5, 1))  
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))  
prior <- prior.gaussian(net, 0.5)  
init <- initialise.allsame(Normal(0, 0.5), like, prior)  
x <- matrix(rnorm(5*100), nrow = 5)  
y <- rnorm(100)  
bnn <- BNN(x, y, like, prior, init)  
madapter <- madapter.FullCov(100, 10)  
sampler <- sampler.GGMC(madapter = madapter)  
ch <- mcmc(bnn, 10, 1000, sampler)  
  
## End(Not run)
```

madapter.RMSProp *Use RMSProp to adapt the inverse mass matrix.*

Description

Use RMSProp as a preconditions/mass matrix adapter. This was proposed in Li, C., Chen, C., Carlson, D., & Carin, L. (2016, February). Preconditioned stochastic gradient Langevin dynamics for deep neural networks. In Thirtieth AAAI Conference on Artificial Intelligence for the use in SGLD and related methods.

Usage

```
madapter.RMSProp(adapt_steps, lambda = 1e-05, alpha = 0.99)
```

Arguments

adapt_steps	number of adaptation steps
lambda	see above paper
alpha	see above paper

Value

list with 'juliavar' and 'juliacode' and all given arguments

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
madapter <- madapter.RMSProp(100)
sampler <- sampler.GGMC(madapter = madapter)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

mcmc

*Sample from a BNN using MCMC***Description**

Sample from a BNN using MCMC

Usage

```
mcmc(
  bnn,
  batchsize,
  numsamples,
  sampler = sampler.SGLD(stepsize_a = 1),
  continue_sampling = FALSE,
  start_value = NULL
)
```

Arguments

bnn	A BNN obtained using BNN
batchsize	batchsize to use; Most samplers allow for batching. For some, theoretical justifications are missing (HMC)
numsamples	Number of mcmc samples
sampler	Sampler to use; See for example sampler.SGLD and all other samplers start with 'sampler.' and are thus easy to identify.
continue_sampling	Do not start new sampling, but rather continue sampling For this, numsamples must be greater than the already sampled number.
start_value	Values to start from. By default these will be sampled using the initialiser in 'bnn'.

Value

a list containing the 'samples' and the 'sampler' used.

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
```

```
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.SGNHTS(1e-3)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

Normal

Create a Normal Prior

Description

Creates a Normal prior in Julia using Distributions.jl. This can then be truncated using [Truncated](#) to obtain a prior that could then be used as a variance prior.

Usage

```
Normal(mu = 0, sigma = 1)
```

Arguments

mu	Mean
sigma	Standard Deviation

Value

see [Gamma](#)

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Truncated(Normal(0, 0.5), 0, Inf))

## End(Not run)
```

opt.ADAM	<i>ADAM optimiser</i>
----------	-----------------------

Description

ADAM optimiser

Usage

```
opt.ADAM(eta = 0.001, beta = c(0.9, 0.999), eps = 1e-08)
```

Arguments

eta	stepsize
beta	momentum decays; must be a list of length 2
eps	Flux does not document this

Value

see [opt.Descent](#)

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(Dense(5, 1))  
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))  
prior <- prior.gaussian(net, 0.5)  
init <- initialise.allsame(Normal(0, 0.5), like, prior)  
x <- matrix(rnorm(5*100), nrow = 5)  
y <- rnorm(100)  
bnn <- BNN(x, y, like, prior, init)  
find_mode(bnn, opt.ADAM(), 10, 100)  
  
## End(Not run)
```

opt.Descent	<i>Standard gradient descent</i>
-------------	----------------------------------

Description

Standard gradient descent

Usage

```
opt.Descent(eta = 0.1)
```

Arguments

eta stepsize

Value

list containing

- ‘julivar’ - julia variable holding the optimiser
- ‘juliocode’ - string representation

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(Dense(5, 1))  
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))  
prior <- prior.gaussian(net, 0.5)  
init <- initialise.allsame(Normal(0, 0.5), like, prior)  
x <- matrix(rnorm(5*100), nrow = 5)  
y <- rnorm(100)  
bnn <- BNN(x, y, like, prior, init)  
find_mode(bnn, opt.Descent(1e-5), 10, 100)  
  
## End(Not run)
```

opt.RMSProp	<i>RMSProp optimiser</i>
-------------	--------------------------

Description

RMSProp optimiser

Usage

```
opt.RMSProp(eta = 0.001, rho = 0.9, eps = 1e-08)
```

Arguments

eta	learning rate
rho	momentum
eps	not documented by Flux

Value

see [opt.Descent](#)

Examples

```
## Not run:  
## Needs previous call to `BayesFluxR_setup` which is time  
## consuming and requires Julia and BayesFlux.jl  
BayesFluxR_setup(installJulia=TRUE, seed=123)  
net <- Chain(Dense(5, 1))  
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))  
prior <- prior.gaussian(net, 0.5)  
init <- initialise.allsame(Normal(0, 0.5), like, prior)  
x <- matrix(rnorm(5*100), nrow = 5)  
y <- rnorm(100)  
bnn <- BNN(x, y, like, prior, init)  
find_mode(bnn, opt.RMSProp(), 10, 100)  
  
## End(Not run)
```

posterior_predictive *Draw from the posterior predictive distribution*

Description

Draw from the posterior predictive distribution

Usage

```
posterior_predictive(bnn, posterior_samples, x = NULL)
```

Arguments

bnn a BNN obtained using `link{BNN}`

posterior_samples a vector or matrix containing posterior samples. This can be obtained using [mcmc](#), or [bayes_by_backprop](#) or [find_mode](#).

x input variables. If 'NULL' (default), training values will be used.

Value

A matrix whose columns are the posterior predictive draws.

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.SGLD()
ch <- mcmc(bnn, 10, 1000, sampler)
pp <- posterior_predictive(bnn, ch$samples)

## End(Not run)
```

prior.gaussian *Use an isotropic Gaussian prior*

Description

Use a Multivariate Gaussian prior for all network parameters. Covariance matrix is set to be equal 'sigma * I' with 'I' being the identity matrix. Mean is zero.

Usage

```
prior.gaussian(chain, sigma)
```

Arguments

chain	Chain obtained using Chain
sigma	Standard deviation of Gaussian prior

Value

a list containing the following

- 'juliavar' the julia variable used to store the prior
- 'juliacode' the julia code

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.SGLD()
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

prior.mixturescale *Scale Mixture of Gaussian Prior*

Description

Uses a scale mixture of Gaussian for each network parameter. That is, the prior is given by

$$\pi_1 \text{Normal}(0, \text{sigma1}) + (1 - \pi_1) \text{Normal}(0, \text{sigma2})$$

Usage

```
prior.mixturescale(chain, sigma1, sigma2, pi1)
```

Arguments

chain	Chain obtained using Chain
sigma1	Standard deviation of first Gaussian
sigma2	Standard deviation of second Gaussian
pi1	Weight of first Gaussian

Value

a list containing the following

- ‘juliavar’ the julia variable used to store the prior
- ‘juliacode’ the julia code

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.mixturescale(net, 10, 0.1, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.SGLD()
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

prior_predictive	<i>Sample from the prior predictive of a Bayesian Neural Network</i>
------------------	--

Description

Sample from the prior predictive of a Bayesian Neural Network

Usage

```
prior_predictive(bnn, n = 1)
```

Arguments

bnn	BNN obtained using BNN
n	Number of samples

Value

matrix of prior predictive samples; Columns are the different samples

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
pp <- prior_predictive(bnn, n = 10)

## End(Not run)
```

RNN	<i>Create a RNN layer with 'in_size' input, 'out_size' hidden state and 'act' activation function</i>
-----	---

Description

Create a RNN layer with 'in_size' input, 'out_size' hidden state and 'act' activation function

Usage

```
RNN(in_size, out_size, act = c("sigmoid", "tanh", "identity", "relu"))
```

Arguments

in_size	Input size
out_size	Output size
act	Activation function

Value

A list with the following content

- in_size - Input Size
- out_size - Output Size
- activation - Activation Function
- julia - Julia code representing the Layer

See Also

[Dense](#)

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(RNN(5, 5, "tanh"))

## End(Not run)
```

sadapter.Const	<i>Use a constant stepsize in mcmc</i>
----------------	--

Description

Use a constant stepsize in mcmc

Usage

```
sadapter.Const(1)
```

Arguments

1	stepsize
---	----------

Value

list with ‘juliavar’, ‘juliacode’ and the given arguments

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sadapter <- sadapter.Const(1e-5)
sampler <- sampler.GGMC(sadapter = sadapter)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

sadapter.DualAverage *Use Dual Averaging like in STAN to tune stepsize*

Description

Use Dual Averaging like in STAN to tune stepsize

Usage

```
sadapter.DualAverage(
  adapt_steps,
  initial_stepsize = 1,
  target_accept = 0.65,
  gamma = 0.05,
  t0 = 10,
  kappa = 0.75
)
```

Arguments

adapt_steps	number of adaptation steps
initial_stepsize	initial stepsize
target_accept	target acceptance ratio
gamma	See STAN manual NUTS paper

t0 See STAN manual or NUTS paper
 kappa See STAN manual or NUTS paper

Value

list with ‘juliavar’, ‘juliacode’, and all given arguments

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sadapter <- sadapter.DualAverage(100)
sampler <- sampler.GGMC(sadapter = sadapter)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

sampler.AdaptiveMH *Adaptive Metropolis Hastings as introduced in*

Description

Haario, H., Saksman, E., & Tamminen, J. (2001). An adaptive Metropolis algorithm. *Bernoulli*, 223-242.

Usage

```
sampler.AdaptiveMH(bnn, t0, sd, eps = 1e-06)
```

Arguments

bnn BNN obtained using [BNN](#)
 t0 Number of iterators before covariance adaptation will be started. Also the look-back period for covariance adaptation.
 sd Tuning parameter; See paper
 eps Used for numerical reasons. Increase this if pos-def-error thrown.

Value

a list with ‘juliavar’, ‘juliacode’, and all given arguments

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.AdaptiveMH(bnn, 10, 1)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

sampler.GGMC

Gradient Guided Monte Carlo

Description

Proposed in Garriga-Alonso, A., & Fortuin, V. (2021). Exact langevin dynamics with stochastic gradients. arXiv preprint arXiv:2102.01691.

Usage

```
sampler.GGMC(
  beta = 0.1,
  l = 1,
  sadapter = sadapter.DualAverage(1000),
  madapter = madapter.FixedMassMatrix(),
  steps = 3
)
```

Arguments

beta	See paper
l	stepsize
sadapter	Stepsize adapter; Not used in original paper
madapter	Mass adapter; Not used in original paper
steps	Number of steps before accept/reject

Value

a list with ‘juliavar’, ‘juliacode’ and all provided arguments.

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sadapter <- sadapter.DualAverage(100)
sampler <- sampler.GGMC(sadapter = sadapter)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

sampler.HMC

Standard Hamiltonian Monte Carlo (Hybrid Monte Carlo).

Description

Allows for the use of stochastic gradients, but the validity of doing so is not clear.

Usage

```
sampler.HMC(
  l,
  path_len,
  sadapter = sadapter.DualAverage(1000),
  madapter = madapter.FixedMassMatrix()
)
```

Arguments

l	stepsize
path_len	number of leapfrog steps
sadapter	Stepsize adapter
madapter	Mass adapter

Details

This is motivated by parts of the discussion in Neal, R. M. (1996). Bayesian Learning for Neural Networks (Vol. 118). Springer New York. <https://doi.org/10.1007/978-1-4612-0745-0>

Value

a list with 'juliavar', 'juliacode', and all given arguments

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sadapter <- sadapter.DualAverage(100)
sampler <- sampler.HMC(1e-3, 3, sadapter = sadapter)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

sampler.SGLD

Stochastic Gradient Langevin Dynamics as proposed in Welling, M., & Teh, Y. W. (n.d.). Bayesian Learning via Stochastic Gradient Langevin Dynamics. 8.

Description

Stepsizes will be adapted according to

$$a(b+t)^{-\gamma}$$

Usage

```
sampler.SGLD(
  stepsize_a = 0.1,
  stepsize_b = 0,
  stepsize_gamma = 0.55,
  min_stepsize = -Inf
)
```

Arguments

stepsize_a See eq. above
 stepsize_b See eq. above
 stepsize_gamma see eq. above
 min_stepsize Do not decrease stepsize beyond this

Value

a list with 'juliavar', 'juliacode', and all given arguments

Examples

```

## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.SGLD()
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)

```

sampler.SGNHTS

Stochastic Gradient Nose-Hoover Thermostat as proposed in

Description

Proposed in Leimkuhler, B., & Shang, X. (2016). Adaptive thermostats for noisy gradient systems. SIAM Journal on Scientific Computing, 38(2), A712-A736.

Usage

```

sampler.SGNHTS(
  1,
  sigmaA = 1,
  xi = 1,
  mu = 1,
  madapter = madapter.FixedMassMatrix()
)

```

Arguments

l	Stepsize
sigmaA	Diffusion factor
xi	Thermostat
mu	Free parameter of thermostat
madapter	Mass Adapter; Not used in original paper and thus has no theoretical backing

Details

This is similar to SGNHT as proposed in Ding, N., Fang, Y., Babbush, R., Chen, C., Skeel, R. D., & Neven, H. (2014). Bayesian sampling using stochastic gradient thermostats. *Advances in neural information processing systems*, 27.

Value

a list with 'juliavar', 'juliacode' and all arguments provided

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
x <- matrix(rnorm(5*100), nrow = 5)
y <- rnorm(100)
bnn <- BNN(x, y, like, prior, init)
sampler <- sampler.SGNHTS(1e-3)
ch <- mcmc(bnn, 10, 1000, sampler)

## End(Not run)
```

tensor_embed_mat	<i>Embed a matrix of timeseries into a tensor</i>
------------------	---

Description

This is used when working with recurrent networks, especially in the case of seq-to-one modelling. Creates overlapping subsequences of the data with length 'len_seq'. Returned dimensions are seq_len x num_vars x num_subsequences.

Usage

```
tensor_embed_mat(mat, len_seq)
```

Arguments

mat	Matrix of time series
len_seq	subsequence length

Value

A tensor of dimension: len_seq x num_vars x num_subsequences

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(RNN(5, 1))
like <- likelihood.seqtone_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
data <- matrix(rnorm(5*1000), ncol = 5)
# Choosing sequences of length 10 and predicting one period ahead
tensor <- tensor_embed_mat(data, 10+1)
x <- tensor[1:10, , , drop = FALSE]
# Last value in each sequence is the target value
y <- tensor[11,1,]
bnn <- BNN(x, y, like, prior, init)
BNN.totparams(bnn)

## End(Not run)
```

Truncated

Truncates a Distribution

Description

Truncates a Julia Distribution between ‘lower‘ and ‘upper‘.

Usage

```
Truncated(dist, lower, upper)
```

Arguments

dist	A Julia Distribution created using Gamma , InverseGamma ...
lower	lower bound
upper	upper bound

Value

see [Gamma](#)

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(Dense(5, 1))
like <- likelihood.feedforward_normal(net, Truncated(Normal(0, 0.5), 0, Inf))

## End(Not run)
```

<code>vi.get_samples</code>	<i>Draw samples form a variational family.</i>
-----------------------------	--

Description

Draw samples form a variational family.

Usage

```
vi.get_samples(vi, n = 1)
```

Arguments

<code>vi</code>	obtained using bayes_by_backprop
<code>n</code>	number of samples

Value

a matrix whose columns are draws from the variational posterior

Examples

```
## Not run:
## Needs previous call to `BayesFluxR_setup` which is time
## consuming and requires Julia and BayesFlux.jl
BayesFluxR_setup(installJulia=TRUE, seed=123)
net <- Chain(RNN(5, 1))
like <- likelihood.seqtoone_normal(net, Gamma(2.0, 0.5))
prior <- prior.gaussian(net, 0.5)
init <- initialise.allsame(Normal(0, 0.5), like, prior)
data <- matrix(rnorm(10*1000), ncol = 10)
# Choosing sequences of length 10 and predicting one period ahead
tensor <- tensor_embed_mat(data, 10+1)
x <- tensor[1:10, , , drop = FALSE]
```

```
# Last value in each sequence is the target value
y <- tensor[11,,]
bnn <- BNN(x, y, like, prior, init)
vi <- bayes_by_backprop(bnn, 100, 100)
vi_samples <- vi.get_samples(vi, n = 1000)
pp <- posterior_predictive(bnn, vi_samples)

## End(Not run)
```

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