

Package ‘CoOL’

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Type Package

Title Causes of Outcome Learning

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URL <https://bioconductor.org>

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CoOL_0_binary_encode_exposure_data
Binary encode exposure data

Description

This function binary encodes the exposure data set so that each category is coded 0 and 1 (e.g. the variable sex will be two variables men (1/0) and women (0/1)).

Usage

```
CoOL_0_binary_encode_exposure_data(exposure_data)
```

Arguments

exposure_data The exposure data set.

Value

Data frame with the expanded exposure data, where all variables are binary encoded.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

```
CoOL_0_common_simulation  
    Common example
```

Description

To reproduce the common causes example.

Usage

```
CoOL_0_common_simulation(n)
```

Arguments

n number of observations for the synthetic data.

Value

A data frame with the columns Y, A, B, C, D, E, F and n rows.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

CoOL_0_complex_simulation

Complex example

Description

To reproduce the complex example.

Usage

```
CoOL_0_complex_simulation(n)
```

Arguments

n number of observations for the synthetic data.

Value

A data frame with the columns Y, Physically_active, Low_SES, Mutation_X, LDL, Night_shifts, Air_pollution and n rows.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

CoOL_0_confounding_simulation

Confounding example

Description

To reproduce the confounding example.

Usage

```
CoOL_0_confounding_simulation(n)
```

Arguments

n number of observations for the synthetic data.

Value

A data frame with the columns Y, A, B, C, D, E, F and n rows.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

CoOL_0_mediation_simulation

Mediation example

Description

To reproduce the mediation example.

Usage

CoOL_0_mediation_simulation(n)

Arguments

n number of observations for the synthetic data.

Value

A data frame with the columns Y, A,B ,C, D, E, F and n rows.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

CoOL_0_working_example

CoOL working example with sex, drug A, and drug B

Description

To reproduce the CoOL working example with sex, drug A, and drug B.

Usage

CoOL_0_working_example(n)

Arguments

n number of observations for the synthetic data.

Value

A data frame with the columns Y, sex, drug_a, drug_b and rows equal to n.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
while (FALSE) {
  library(CoOL)
  set.seed(1)
  data <- CoOL_0_working_example(n=10000)
  outcome_data <- data[,1]
  exposure_data <- data[,-1]
  exposure_data <- CoOL_0_binary_encode_exposure_data(exposure_data)
  model <- CoOL_1_initiate_neural_network(inputs=ncol(exposure_data),
  output = outcome_data,hidden=5)
  model <- CoOL_2_train_neural_network(lr = 1e-4,X_train=exposure_data,
  Y_train=outcome_data,X_test=exposure_data, Y_test=outcome_data,
  model=model, epochs=1000,patience = 200, input_parameter_reg = 1e-3
  ) # Train the non-negative model (The model can be retrained)
  model <- CoOL_2_train_neural_network(lr = 1e-5,X_train=exposure_data,
  Y_train=outcome_data,X_test=exposure_data, Y_test=outcome_data, model=model,
  epochs=1000,patience = 100, input_parameter_reg = 1e-3)
  # Train the non-negative model (The model can be retrained)
  model <- CoOL_2_train_neural_network(lr = 1e-6,X_train=exposure_data,
  Y_train=outcome_data,X_test=exposure_data, Y_test=outcome_data, model=model,
  epochs=1000,patience = 50, input_parameter_reg = 1e-3
  ) # Train the non-negative model (The model can be retrained)
  plot(model$train_performance,type='l',yaxs='i',ylab="Mean squared error",
  xlab="Epochs",main="A) Performance during training\n\n",
  ylim=quantile(model$train_performance,c(0,.975))) # Model performance
  CoOL_3_plot_neural_network(model,names(exposure_data),5/max(model[[1]]),
  title = "B) Model connection weights\nand intercepts") # Model visualization
  CoOL_4_AUC(outcome_data,exposure_data,model,
  title = "C) Receiver operating\ncharacteristic curve") # AUC
  risk_contributions <- CoOL_5_layerwise_relevance_propagation(exposure_data,model
  ) # Risk contributions
  CoOL_6_dendrogram(risk_contributions,number_of_subgroups = 3,
  title = "D) Dendrogram with 3 sub-groups") # Dendrogram
  sub_groups <- CoOL_6_sub_groups(risk_contributions,number_of_subgroups = 3
  ) # Assign sub-groups
  CoOL_7_prevalence_and_mean_risk_plot(risk_contributions,sub_groups,
  title = "E) Prevalence and mean risk of sub-groups") # Prevalence and mean risk plot
  CoOL_8_mean_risk_contributions_by_sub_group(risk_contributions,
  sub_groups,outcome_data = outcome_data,exposure_data = exposure_data,
  model=model,exclude_below = 0.01) # Mean risk contributions by sub-groups
}
```

 CoOL_1_initiate_neural_network

Initiates a non-negative neural network

Description

This function initiates a non-negative neural network. The one-hidden layer non-negative neural network is designed to resemble a DAG with hidden synergistic components. With the model, we intend to learn the various synergistic interactions between the exposures and outcome. The model needs to be non-negative and estimate the risk on an additive scale. Neural networks include hidden activation functions (if the sum of the input exceeds a threshold, information is passed on), which can model minimum threshold values of interactions between exposures. We need to specify the upper limit of the number of possible hidden activation functions and through model fitting, the model may be able to learn both stand-alone and synergistically interacting factors.

Usage

```
CoOL_1_initiate_neural_network(inputs, output, hidden = 10)
```

Arguments

inputs	The number of exposures.
output	The output variable is used to calculate the mean of it used to initiate the baseline risk.
hidden	Number of hidden nodes.

Details

The non-negative neural network can be denoted as:

$$P(Y = 1|X^+) = \sum_j \left(w_{j,k}^+ ReLU_j \left(\sum_i (w_{i,j}^+ X_i^+) + b_j^- \right) \right) + R^b$$

Value

A list with connection weights, bias weights and meta data.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

 CoOL_2_train_neural_network

Training the non-negative neural network

Description

This function trains the non-negative neural network. Fitting the model is done in a step-wise procedure one individual at a time, where the model estimates individual's risk of the disease outcome, estimates the prediction's residual error and adjusts the model parameters to reduce this error. By iterating through all individuals for multiple epochs (one complete iterations through all individuals is called an epoch), we end with parameters for the model, where the errors are smallest possible for the full population. The model fit follows the linear expectation that synergism is a combined effect larger than the sum of independent effects. The initial values, derivatives, and learning rates are described in further detail in the Supplementary material. The non-negative model ensures that the predicted value cannot be negative. The model does not prevent estimating probabilities above 1, but this would be unlikely, as risks of disease and mortality even for high risk groups in general are far below 1. The use of a test dataset does not seem to assist deciding on the optimal number of epochs possibly due to the constrains due to the non-negative assumption. We suggest splitting data into a train and test data set, such that findings from the train data set can be confirmed in the test data set before developing hypotheses.

Usage

```
CoOL_2_train_neural_network(
  X_train,
  Y_train,
  X_test,
  Y_test,
  model,
  lr = c(1e-04, 1e-05, 1e-06),
  epochs = 2000,
  patience = 100,
  monitor = TRUE,
  plot_and_evaluation_frequency = 50,
  input_parameter_reg = 0.001,
  spline_df = 10,
  restore_par_options = TRUE,
  drop_out = 0
)
```

Arguments

X_train	The exposure data for the training data.
Y_train	The outcome data for the training data.
X_test	The exposure data for the test data (currently the training data is used).
Y_test	The outcome data for the test data (currently the training data is used).

model	The fitted non-negative neural network.
lr	Learning rate (several LR can be provided, such that the model training will train for each LR and continue to the next).
epochs	Epochs.
patience	The number of epochs allowed without an improvement in performance.
monitor	Whether a monitoring plot will be shown during training.
plot_and_evaluation_frequency	The interval for plotting the performance and checking the patience.
input_parameter_reg	Regularisation decreasing parameter value at each iteration for the input parameters.
spline_df	Degrees of freedom for the spline fit for the performance plots.
restore_par_options	Restore par options.
drop_out	To drop connections if their weights reaches zero.

Value

An updated list of connection weights, bias weights and meta data.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

```
CoOL_3_plot_neural_network
      Plotting the non-negative neural network
```

Description

This function plots the non-negative neural network

Usage

```
CoOL_3_plot_neural_network(
  model,
  names,
  arrow_size = NA,
  title = "Model connection weights and intercepts",
  restore_par_options = TRUE
)
```

Arguments

model	The fitted non-negative neural network.
names	Labels of each exposure.
arrow_size	Define the arrow_size for the model illustration in the reported training progress.
title	Title on the plot.
restore_par_options	Restore par options.

Value

A plot visualizing the connection weights.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

CoOL_4_AUC

Plot the ROC AUC

Description

Plot the ROC AUC

Usage

```
CoOL_4_AUC(
  outcome_data,
  exposure_data,
  model,
  title = "Receiver operating\ncharacteristic curve",
  restore_par_options = TRUE
)
```

Arguments

outcome_data	The outcome data.
exposure_data	The exposure data.
model	The fitted the non-negative neural network.
title	Title on the plot.
restore_par_options	Restore par options.

Value

A plot of the ROC and the ROC AUC value.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

CoOL_4_predict_risks *Predict the risk of the outcome using the fitted non-negative neural network*

Description

Predict the risk of the outcome using the fitted non-negative neural network.

Usage

```
CoOL_4_predict_risks(X, model)
```

Arguments

X	The exposure data.
model	The fitted the non-negative neural network.

Value

A vector with the predicted risk of the outcome for each individual.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

CoOL_5_layerwise_relevance_propagation

Layer-wise relevance propagation of the fitted non-negative neural network

Description

Calculates risk contributions for each exposure and a baseline using layer-wise relevance propagation of the fitted non-negative neural network and data.

Usage

CoOL_5_layerwise_relevance_propagation(X, model)

Arguments

X The exposure data.
 model The fitted the non-negative neural network.

Details

For each individual:

$$P(Y = 1|X^+) = R^b + \sum_i R_i^X$$

The below procedure is conducted for all individuals in a one by one fashion. The baseline risk, R^b , is simply parameterised in the model. The decomposition of the risk contributions for exposures, R^X , takes 3 steps:

Step 1 - Subtract the baseline risk, R^b :

$$R_k^X = P(Y = 1|X^+) - R^b$$

Step 2 - Decompose to the hidden layer:

$$R_j^X = \frac{H_j w_{j,k}}{\sum_j (H_j w_{j,k})} R_k^X$$

Where H_j is the value taken by each of the $\text{ReLU}(\cdot)_j$ functions for the specific individual.

Step 3 - Hidden layer to exposures:

$$R_i^X = \sum_j \left(\frac{X_i^+ w_{i,j}}{\sum_i (X_i^+ w_{i,j})} R_j^X \right)$$

This creates a dataset with the dimensions equal to the number of individuals times the number of exposures plus a baseline risk value, which can be termed a risk contribution matrix. Instead of exposure values, individuals are given risk contributions, R^X .

Value

A data frame with the risk contribution matrix [number of individuals, risk contributors + the baseline risk].

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

CoOL_6_dendrogram	<i>Dendrogram and sub-groups</i>
-------------------	----------------------------------

Description

Calculates presents a dendrogram coloured by the pre-defined number of sub-groups and provides the vector with sub-groups.

Usage

```
CoOL_6_dendrogram(  
  risk_contributions,  
  number_of_subgroups = 3,  
  title = "Dendrogram",  
  colours = NA  
)
```

Arguments

<code>risk_contributions</code>	The risk contributions.
<code>number_of_subgroups</code>	The number of sub-groups chosen (Visual inspection is necessary).
<code>title</code>	The title of the plot.
<code>colours</code>	Colours indicating each sub-group.

Value

A dendrogram illustrating similarities between individuals based on their risk contributions.

Examples

```
#See the example under CoOL_0_working_example
```

CoOL_6_individual_effects_matrix

Risk contribution matrix based on individual effects (had all other exposures been set to zero)

Description

Estimating the risk contribution for each exposure if each individual had been exposed to only one exposure, with the value the individual actually had.

Usage

```
CoOL_6_individual_effects_matrix(X, model)
```

Arguments

X	The exposure data.
model	The fitted the non-negative neural network.

Value

A matrix [Number of individuals, exposures] with the estimated individual effects by each exposure had all other values been set to zero.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

CoOL_6_sub_groups *Assign sub-groups*

Description

Calculates presents a dendrogram coloured by the pre-defined number of sub-groups and provides the vector with sub-groups.

Usage

```
CoOL_6_sub_groups(risk_contributions, number_of_subgroups = 3)
```

Arguments

`risk_contributions`
The risk contributions.

`number_of_subgroups`
The number of sub-groups chosen (Visual inspection is necessary).

Value

A vector [number of individuals] with an assigned sub-group.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

#See the example under `CoOL_0_working_example`

`CoOL_6_sum_of_individual_effects`

Predict the risk based on the sum of individual effects

Description

By summing the through the risk as if each individual had been exposed to only one exposure, with the value the individual actually had.

Usage

`CoOL_6_sum_of_individual_effects(X, model)`

Arguments

`X` The exposure data.

`model` The fitted the non-negative neural network.

Value

A value the sum of individual effects, had there been no interactions between exposures.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

```
CoOL_7_prevalence_and_mean_risk_plot  
Prevalence and mean risk plot
```

Description

This plot shows the prevalence and mean risk for each sub-group. Its distribution hits at sub-groups with great public health potential.

Usage

```
CoOL_7_prevalence_and_mean_risk_plot(  
  risk_contributions,  
  sub_groups,  
  title = "Prevalence and mean risk\nof sub-groups",  
  y_max = NA,  
  restore_par_options = TRUE,  
  colours = NA  
)
```

Arguments

<code>risk_contributions</code>	The risk contributions.
<code>sub_groups</code>	The vector with the sub-groups.
<code>title</code>	The title of the plot.
<code>y_max</code>	Fix the axis of the risk of the outcome.
<code>restore_par_options</code>	Restore par options.
<code>colours</code>	Colours indicating each sub-group.

Value

A plot with prevalence and mean risks by sub-groups.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

CoOL_8_mean_risk_contributions_by_sub_group
Mean risk contributions by sub-groups

Description

Table with the mean risk contributions by sub-groups.

Usage

```
CoOL_8_mean_risk_contributions_by_sub_group(  
  risk_contributions,  
  sub_groups,  
  exposure_data,  
  outcome_data,  
  model,  
  exclude_below = 0.001,  
  restore_par_options = TRUE,  
  colours = NA  
)
```

Arguments

<code>risk_contributions</code>	The risk contributions.
<code>sub_groups</code>	The vector with the sub-groups.
<code>exposure_data</code>	The exposure data.
<code>outcome_data</code>	The outcome data.
<code>model</code>	The trained non-negative model.
<code>exclude_below</code>	A lower cut-off for which risk contributions shown.
<code>restore_par_options</code>	Restore par options.
<code>colours</code>	Colours indicating each sub-group.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
#See the example under CoOL_0_working_example
```

 CoOL_default

The default analysis for computational phase of CoOL

Description

The analysis and plots presented in the main paper. We recommend using `View(CoOL_default)` and `View()` on the many sub-functions to understand the steps and modify to your own research question. 3 sets of training will run with a learning rate of $1e-4$ and a patience of 200 epochs, a learning rate of $1e-5$ and a patience of 100 epochs, and a learning rate of $1e-6$ and a patience of 50 epochs.

Usage

```
CoOL_default(
  data,
  sub_groups = 3,
  exclude_below = 0.01,
  input_parameter_reg = 0.001,
  hidden = 10,
  monitor = TRUE,
  epochs = 10000
)
```

Arguments

<code>data</code>	A <code>data.frame(cbind(outcome_data,exposure_data))</code> .
<code>sub_groups</code>	Define the number of expected sub-groups.
<code>exclude_below</code>	Risk contributions below this value are not shown in the table.
<code>input_parameter_reg</code>	The regularization of the input parameters.
<code>hidden</code>	The number of synergy-functions.
<code>monitor</code>	Whether monitoring plots will be shown in R.
<code>epochs</code>	The maximum number of epochs.

Value

A series of plots across the full Causes of Outcome Learning approach.

References

Rieckmann, Dworzynski, Arras, Lapuschkin, Samek, Arah, Rod, Ekstrom. Causes of outcome learning: A causal inference-inspired machine learning approach to disentangling common combinations of potential causes of a health outcome. medRxiv (2020) <doi:10.1101/2020.12.10.20225243>

Examples

```
# Not run
while (FALSE) {
#See the example under CoOL_0_working_example for a more detailed tutorial
library(CoOL)
data <- CoOL_0_working_example(n=10000)
CoOL_default(data)
}
```

cpp_train_network_relu

Function used as part of other functions

Description

Non-negative neural network

Usage

```
cpp_train_network_relu(
  x,
  y,
  testx,
  testy,
  W1_input,
  B1_input,
  W2_input,
  B2_input,
  lr = 0.01,
  maxepochs = 100,
  input_parameter_reg = 1e-06,
  drop_out = 0L
)
```

Arguments

x	A matrix of predictors for the training dataset of shape (nsamples, nfeatures)
y	A vector of output values for the training data with a length similar to the number of rows of x
testx	A matrix of predictors for the test dataset of shape (nsamples, nfeatures)
testy	A vector of output values for the test data with a length similar to the number of rows of x
W1_input	Input-hidden layer weights of shape (nfeatures, hidden)
B1_input	Biases for the hidden layer of shape (1, hidden)
W2_input	Hidden-output layer weights of shape (hidden, 1)

B2_input	Bias for the output layer (the baseline risk) af shape (1, 1)
lr	Initial learning rate
maxepochs	The maximum number of epochs
input_parameter_reg	Regularisation decreasing parameter value at each iteration for the input parameters
drop_out	To drop connections if their weights reaches zero.

Value

A list of class "SCL" giving the estimated matrices and performance indicators

Author(s)

Andreas Rieckmann, Piotr Dworzynski, Leila Arras, Claus Ekstrøm

random	<i>Function used as part of other functions</i>
--------	---

Description

Function used as part of other functions

Usage

random(r, c)

Arguments

r	rows in matrix
c	columns in matrix

rcpprelu	<i>Function used as part of other functions</i>
----------	---

Description

relu-function

Usage

rcpprelu(x)

Arguments

x	input in the relu function
---	----------------------------

rcpprelu_neg	<i>Function used as part of other functions</i>
--------------	---

Description

negative relu-function

Usage

```
rcpprelu_neg(x)
```

Arguments

x	input in the negative relu-function
---	-------------------------------------

relu	<i>Function used as part of other functions</i>
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Description

Function used as part of other functions

Usage

```
relu(input)
```

Arguments

input	input in the relu function
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