## Package 'SVEMnet'

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Title Self-Validated Ensemble Models with Elastic Net Regression

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Description Implements Self-Validated Ensemble Mod-

els (SVEM, Lemkus et al. (2021) <doi:10.1016/j.chemolab.2021.104439>) using Elastic Net regression via 'glmnet' (Friedman et al. <doi:10.18637/jss.v033.i01>). SVEM averages predictions from multiple models fitted to fractionally weighted bootstraps of the data, tuned with anticorrelated validation weights. Also implements the randomized permutation whole model test for SVEM (Karl (2024) <doi:10.1016/j.chemolab.2024.105122>). \Code for the whole model test was plementary material of Karl (2024). Development of this package was assisted by 'GPT o1preview' for code structure and documentation.

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SVEMnet-package

SVEMnet: Self-Validated Ensemble Models with Elastic Net Regression

## Description

The SVEMnet package implements Self-Validated Ensemble Models (SVEM) using Elastic Net (including lasso and ridge) regression via glmnet. SVEM averages predictions from multiple models fitted to fractionally weighted bootstraps of the data, tuned with anti-correlated validation weights.

## Functions

SVEMnet Fit an SVEMnet model using Elastic Net regression.

svem\_significance\_test Perform a whole-model significance test for SVEM models.

svem\_significance\_test\_parallel Perform a whole-model significance test for SVEM models. Parallelized version.

predict.svem\_model Predict method for SVEM models.

plot.svem\_model Plot method for SVEM models.

coef.svem\_model Plot method for SVEM models.

glmnet\_with\_cv Wrapper for cv.glmnet

## Acknowledgments

Development of this package was assisted by GPT o1-preview, which helped in constructing the structure of some of the code and the roxygen documentation. The code for the significance test is taken from the supplementary material of Karl (2024) (it was handwritten by that author).

#### Author(s)

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#### References

Gotwalt, C., & Ramsey, P. (2018). Model Validation Strategies for Designed Experiments Using Bootstrapping Techniques With Applications to Biopharmaceuticals. *JMP Discovery Conference*. https://community.jmp.com/t5/Discovery-Summit-2018/Model-Validation-Strategies-for-Designed-Experimeta-p/73730

Karl, A. T. (2024). A randomized permutation whole-model test heuristic for Self-Validated Ensemble Models (SVEM). *Chemometrics and Intelligent Laboratory Systems*, 249, 105122. doi:10.1016/j.chemolab.2024.105122

Karl, A., Wisnowski, J., & Rushing, H. (2022). JMP Pro 17 Remedies for Practical Struggles with Mixture Experiments. JMP Discovery Conference. doi:10.13140/RG.2.2.34598.40003/1

Lemkus, T., Gotwalt, C., Ramsey, P., & Weese, M. L. (2021). Self-Validated Ensemble Models for Design of Experiments. *Chemometrics and Intelligent Laboratory Systems*, 219, 104439. doi:10.1016/j.chemolab.2021.104439

Xu, L., Gotwalt, C., Hong, Y., King, C. B., & Meeker, W. Q. (2020). Applications of the Fractional-Random-Weight Bootstrap. *The American Statistician*, 74(4), 345–358. doi:10.1080/00031305.2020.1731599

Ramsey, P., Gaudard, M., & Levin, W. (2021). Accelerating Innovation with Space Filling Mixture Designs, Neural Networks and SVEM. *JMP Discovery Conference*. https://community.jmp.com/t5/Abstracts/Accelerating-Innovation-with-Space-Filling-Mixture-Designs/ev-p/756841

Ramsey, P., & Gotwalt, C. (2018). Model Validation Strategies for Designed Experiments Using Bootstrapping Techniques With Applications to Biopharmaceuticals. *JMP Discovery Conference -Europe*. https://community.jmp.com/t5/Discovery-Summit-Europe-2018/Model-Validation-Strategies-for-De ta-p/51286

Ramsey, P., Levin, W., Lemkus, T., & Gotwalt, C. (2021). SVEM: A Paradigm Shift in Design and Analysis of Experiments. *JMP Discovery Conference - Europe*. https://community.jmp.com/ t5/Abstracts/SVEM-A-Paradigm-Shift-in-Design-and-Analysis-of-Experiments-2021/ev-p/ 756634

Ramsey, P., & McNeill, P. (2023). CMC, SVEM, Neural Networks, DOE, and Complexity: It's All About Prediction. *JMP Discovery Conference*.

coef.svem\_model Plot Coefficient Nonzero Percentages from a SVEMnet Model

#### Description

This function calculates the percentage of bootstrap iterations in which each coefficient is nonzero.

#### Usage

```
## S3 method for class 'svem_model'
coef(object, ...)
```

glmnet\_with\_cv

## Arguments

| object | An object of class svem_model returned by the SVEMnet function. |
|--------|---|
|        | other arguments to pass.  |

## Value

Invisibly returns a data frame containing the percentage of bootstraps where each coefficient is nonzero.

## Acknowledgments

Development of this package was assisted by GPT o1-preview, which helped in constructing the structure of some of the code and the roxygen documentation. The code for the significance test is taken from the supplementary material of Karl (2024) (it was handwritten by that author).

glmnet\_with\_cv Fit a glmnet Model with Cross-Validation

## Description

A wrapper function for cv.glmnet that takes input arguments in a manner similar to SVEMnet. This function searches over multiple alpha values by running cv.glmnet() for each provided alpha, and then selects the combination of alpha and lambda with the best cross-validation performance.

## Usage

```
glmnet_with_cv(
  formula,
  data,
  glmnet_alpha = c(0, 0.5, 1),
  standardize = TRUE,
  nfolds = 10,
   ...
)
```

#### Arguments

| formula      | A formula specifying the model to be fitted.  |
|--------------|---|
| data         | A data frame containing the variables in the model.   |
| glmnet_alpha | Elastic Net mixing parameter(s) (default is $c(0, 0.5, 1)$ ). If multiple values are provided, $cv.glmnet$ is run for each alpha, and the model with the lowest cross-validation error is selected. |
| standardize  | Logical flag passed to glmnet. If TRUE (default), each variable is standardized before model fitting.   |
| nfolds       | Number of cross-validation folds (default is 10).   |
|              | Additional arguments passed to cv.glmnet.   |

## Details

This function uses cv.glmnet to fit a generalized linear model with elastic net regularization, performing k-fold cross-validation to select the regularization parameter lambda. If multiple alpha values are provided, it selects the best-performing alpha-lambda pair based on the minimal crossvalidation error.

After fitting, the function calculates a debiasing linear model (if possible). This is done by regressing the actual responses on the fitted values obtained from the selected model. The resulting linear model is stored in debias\_fit.

#### Value

A list containing:

- parms: Coefficients from the selected cv.glmnet model at lambda.min.
- debias\_fit: A linear model of the form y ~ y\_pred used for debiasing (if applicable).
- glmnet\_alpha: The vector of alpha values considered.
- best\_alpha: The selected alpha value that gave the best cross-validation result.
- best\_lambda: The lambda value chosen by cross-validation at the selected alpha.
- actual\_y: The response vector used in the model.
- training\_X: The predictor matrix used in the model.
- y\_pred: The fitted values from the final model (no debiasing).
- y\_pred\_debiased: Debiased fitted values if debias\_fit is available.
- formula: The formula used for model fitting.
- terms: The terms object extracted from the model frame.

#### References

Friedman, J., Hastie, T., & Tibshirani, R. (2010). Regularization Paths for Generalized Linear Models via Coordinate Descent. *Journal of Statistical Software*, 33(1), 1-22. doi:10.18637/jss.v033.i01

#### See Also

glmnet, cv.glmnet, SVEMnet

## Examples

```
set.seed(0)
n <- 50
X1 <- runif(n)
X2 <- runif(n)
y <- 1 + 2*X1 + 3*X2 + rnorm(n)
data <- data.frame(y, X1, X2)</pre>
```

model\_cv <- glmnet\_with\_cv(y ~ X1 + X2, data = data, glmnet\_alpha = c(0,0.5,1))
predictions <- predict\_cv(model\_cv, data)</pre>

plot.svem\_model

## Description

Plots actual versus predicted values for an svem\_model using ggplot2.

## Usage

```
## S3 method for class 'svem_model'
plot(x, plot_debiased = FALSE, ...)
```

#### Arguments

| х             | An object of class svem_model.  |
|---------------|---|
| plot_debiased | $\label{eq:logical} Logical; if \ {\tt TRUE}, includes \ debiased \ predictions \ if \ available \ (default \ is \ {\tt FALSE}).$ |
|               | Additional arguments passed to ggplot2 functions.   |

## Details

This function creates an actual vs. predicted plot for the SVEM model. If plot\_debiased is TRUE and debiased predictions are available, it includes them in the plot.

\*\*Plot Features:\*\*

- \*\*Actual vs. Predicted Points:\*\* Plots the actual response values against the predicted values from the SVEM model.
- \*\*Debiased Predictions:\*\* If available and plot\_debiased is TRUE, debiased predictions are included.
- \*\*Ideal Fit Line:\*\* A dashed line representing perfect prediction (slope = 1, intercept = 0) is included for reference.

## Value

A ggplot object showing actual versus predicted values.

#### Acknowledgments

plot.svem\_significance\_test

Plot SVEM Significance Test Results for Multiple Responses

#### Description

Plots the Mahalanobis distances for the original and permuted data from multiple SVEM significance test results.

## Usage

## S3 method for class 'svem\_significance\_test'
plot(..., labels = NULL)

## Arguments

|        | One or more objects of class <pre>svem_significance_test</pre> , which are the outputs<br>from <pre>svem_significance_test</pre> . |
|--------|--|
| labels | Optional character vector of labels for the responses. If not provided, the func-<br>tion uses the response variable names.        |

## Details

This function creates a combined plot of the Mahalanobis distances (d\_Y and d\_pi\_Y) for the original and permuted data from multiple SVEM significance test results. It groups the data by response and source type, displaying original and permutation distances side by side for each response.

\*\*Usage Notes:\*\*

- Use this function to compare the significance test results across multiple responses.
- The plot shows original and permutation distances next to each other for each response.

#### Value

A ggplot object showing the distributions of Mahalanobis distances for all responses.

#### Acknowledgments

predict.svem\_model Predict Method for SVEM Models

## Description

Generates predictions from a fitted svem\_model.

## Usage

```
## S3 method for class 'svem_model'
predict(object, newdata, debias = FALSE, se.fit = FALSE, ...)
```

## Arguments

| object  | An object of class svem_model.  |
|---------|---|
| newdata | A data frame of new predictor values.   |
| debias  | Logical; default is FALSE.  |
| se.fit  | $\label{eq:logical} \mbox{Logical; if TRUE, returns standard errors (default is FALSE)}.$ |
|         | Additional arguments.   |

## Details

A debiased fit is available (along with the standard fit). This is provided to allow the user to match the output of JMP.\https://www.jmp.com/support/help/en/18.1/?utm\_source=help&utm\_medium=redirect#page/jmp/overvie of-selfvalidated-ensemble-models.shtml. The debiasing coefficients are always calculated by SVEMnet(), and the predict() function determines whether the raw or debiased predictions are returned via the debias argument. Default is FALSE based on performance on unpublished simulation studies.

#### Value

Predictions or a list containing predictions and standard errors.

## Acknowledgments

#### Description

Generate predictions from the model fitted by glmnet\_with\_cv. This function accepts new data and returns predictions, optionally debiased if a debiasing linear model was fit.

## Usage

predict\_cv(object, newdata, debias = FALSE, ...)

## Arguments

| object  | An object returned by glmnet_with_cv.   |
|---------|---|
| newdata | A data frame of new predictor values.   |
| debias  | Logical; if TRUE, applies the debiasing linear model stored in object\$debias_fit (if available). Default is FALSE. |
|         | Additional arguments (not used).  |

## Details

Predictions are computed by forming the model matrix from newdata using the stored formula and terms in the fitted model object. The coefficients used are those stored in parms. If debias=TRUE and a debias\_fit linear model is available, predictions are adjusted by that model.

## Value

A numeric vector of predictions.

#### See Also

glmnet\_with\_cv, SVEMnet, predict.svem\_model

## Examples

```
set.seed(0)
n <- 50
X1 <- runif(n)
X2 <- runif(n)
y <- 1 + 2*X1 + 3*X2 + rnorm(n)
data <- data.frame(y, X1, X2)
model_cv <- glmnet_with_cv(y ~ X1 + X2, data = data, glmnet_alpha = c(0,0.5,1))
predictions <- predict_cv(model_cv, data)
predictions_debiased <- predict_cv(model_cv, data, debias = TRUE)</pre>
```

print.svem\_significance\_test

Print Method for SVEM Significance Test

## Description

Prints the p-value from an object of class svem\_significance\_test.

## Usage

```
## S3 method for class 'svem_significance_test'
print(x, ...)
```

## Arguments

| х | An object of class svem_significance_test. |
|---|--|
|   | Additional arguments (not used).           |

Fit an SVEMnet Model

## Description

Wrapper for 'glmnet' (Friedman et al. 2010) to fit an ensemble of Elastic Net models using the Self-Validated Ensemble Model method (SVEM, Lemkus et al. 2021). Allows searching over multiple alpha values in the Elastic Net penalty.

## Usage

```
SVEMnet(
  formula,
  data,
  nBoot = 200,
  glmnet_alpha = c(0, 0.5, 1),
  weight_scheme = c("SVEM", "FWR", "Identity"),
  objective = c("wAIC", "wSSE"),
  standardize = TRUE,
  ...
)
```

## **SVEMnet**

#### Arguments

| formula       | A formula specifying the model to be fitted.  |
|---------------|---|
| data          | A data frame containing the variables in the model.   |
| nBoot         | Number of bootstrap iterations (default is 200).  |
| glmnet_alpha  | Elastic Net mixing parameter(s) (default is $c(0, 0.5, 1)$ ). Can be a vector of alpha values, where alpha = 1 corresponds to Lasso and alpha = 0 corresponds to Ridge regression.  |
| weight_scheme | Weighting scheme for SVEM (default is "SVEM"). Valid options are "SVEM",<br>"FWR", and "Identity". "FWR" calculates the Fractional Weight Regression<br>(Xu et al., 2020) and is included for demonstration; "SVEM" generally provides<br>better performance."Identity" simply sets the training and validation weights to<br>1. Use with nBoot = 1 and objective = "wAIC" to get an elastic net fit on the<br>training data using AIC. |
| objective     | Objective function for selecting lambda (default is "wAIC"). Valid options are "wAIC" and "wSSE". The "w" refers to "weighted" validation.  |
| standardize   | logical. Passed to glmnet to control standardization (default is TRUE).   |
|               | Additional arguments passed to the underlying glmnet() function.  |

## Details

The Self-Validated Ensemble Model (SVEM, Lemkus et al., 2021) framework provides a bootstrap approach to improve predictions from various base learning models, including Elastic Net regression as implemented in 'glmnet'. SVEM is particularly suited for situations where a complex response surface is modeled with relatively few experimental runs.

In each of the 'nBoot' iterations, SVEMnet applies random exponentially distributed weights to the observations. Anti-correlated weights are used for validation.

SVEMnet allows for the Elastic Net mixing parameter ('glmnet\_alpha') to be a vector, enabling the function to search over multiple 'alpha' values within each bootstrap iteration. Within each iteration, the model is fit for each specified 'alpha', and the best 'alpha' is selected based on the specified 'objective'.

objective options:

- "wSSE" Weighted Sum of Squared Errors. Selects the lambda that minimizes the weighted validation error without penalizing model complexity. While this may lead to models that overfit when the number of parameters is large relative to the number of observations, SVEM mitigates overfitting (high prediction variance) by averaging over multiple bootstrap models. This is the objective function used by Lemkus et al. (2021) with weight\_scheme="SVEM"
- "wAIC" Weighted Akaike Information Criterion. Balances model fit with complexity by penalizing the number of parameters. It is calculated as AIC = n \\* log(wSSE / n) + 2 \\* k, where wSSE is the weighted sum of squared errors, n is the number of observations, and k is the number of parameters with nonzero coefficients. Typically used with weight\_scheme="FWR" or weight\_scheme="Identity"

weight\_scheme options:

- "SVEM" Uses anti-correlated fractional weights for training and validation sets, improving model generalization by effectively simulating multiple training-validation splits (Lemkus et al. (2021)). Published results (Lemkus et al. (2021), Karl (2024)) utilize objective="wSSE". However, unpublished simulation results suggest improved performance from using objective="wAIC" with weight\_scheme="SVEM". See the SVEMnet Vignette for details.
- "FWR" Fractional Weight Regression as described by Xu et al. (2020). Weights are the same for both training and validation sets. This method does not provide the self-validation benefits of SVEM but is included for comparison. Used with objective="wAIC".
- "Identity" Uses weights of 1 for both training and validation. This uses the full dataset for both training and validation, effectively disabling the self-validation mechanism. Use with objective="wAIC" and nBoot=1 to fit the Elastic Net on the AIC of the training data.

A debiased fit is output (along with the standard fit). This is provided to allow the user to match the output of JMP, which returns a debiased fit whenever nBoot>=10. \https://www.jmp.com/support/help/en/18.1/?utm\_source= of-selfvalidated-ensemble-models.shtml. The debiasing coefficients are always calculated by SVEM-net(), and the predict() function determines whether the raw or debiased predictions are returned via its debias argument. The default is debias=FALSE, based on performance on unpublished simulation results.

The output includes: \*\*Model Output:\*\* The returned object is a list of class svem\_model, containing the following components:

- parms: Averaged coefficients across all bootstrap iterations.
- debias\_fit: The debiasing linear model fit (if applicable). This is a linear model of the form y ~ y\_pred, used to adjust the predictions and reduce bias.
- coef\_matrix: Matrix of coefficients from each bootstrap iteration. Each row corresponds to a bootstrap iteration, and each column corresponds to a model coefficient.
- nBoot: Number of bootstrap iterations performed.
- glmnet\_alpha: The Elastic Net mixing parameter(s) used. This is the alpha parameter from glmnet.
- best\_alphas: The best alpha values selected during the fitting process for each bootstrap iteration.
- best\_lambdas: The best lambda values selected during the fitting process for each bootstrap iteration.
- weight\_scheme: The weighting scheme used in SVEM. Indicates whether "SVEM", "FWR", or "Identity" weights were used.
- actual\_y: The response vector used in the model.
- training\_X: The predictor matrix used in the model.
- y\_pred: The predicted response values from the ensemble model before debiasing.
- y\_pred\_debiased: The debiased predicted response values (if debiasing is applied). Adjusted predictions using the debias\_fit model.
- nobs: The number of observations in the dataset.
- nparm: The number of parameters (including the intercept), calculated as ncol(X) + 1.
- formula: The formula used in the model fitting.
- terms: The terms object extracted from the model frame.

## **SVEMnet**

## Value

An object of class svem\_model.

## Acknowledgments

Development of this package was assisted by GPT o1-preview, which helped in constructing the structure of some of the code and the roxygen documentation. The code for the significance test is taken from the supplementary material of Karl (2024) (it was handwritten by that author).

## References

Gotwalt, C., & Ramsey, P. (2018). Model Validation Strategies for Designed Experiments Using Bootstrapping Techniques With Applications to Biopharmaceuticals. *JMP Discovery Conference*. https://community.jmp.com/t5/Discovery-Summit-2018/Model-Validation-Strategies-for-Designed-Experimeta-p/73730

Karl, A. T. (2024). A randomized permutation whole-model test heuristic for Self-Validated Ensemble Models (SVEM). *Chemometrics and Intelligent Laboratory Systems*, 249, 105122. doi:10.1016/j.chemolab.2024.105122

Karl, A., Wisnowski, J., & Rushing, H. (2022). JMP Pro 17 Remedies for Practical Struggles with Mixture Experiments. JMP Discovery Conference. doi:10.13140/RG.2.2.34598.40003/1

Lemkus, T., Gotwalt, C., Ramsey, P., & Weese, M. L. (2021). Self-Validated Ensemble Models for Design of Experiments. *Chemometrics and Intelligent Laboratory Systems*, 219, 104439. doi:10.1016/j.chemolab.2021.104439

Xu, L., Gotwalt, C., Hong, Y., King, C. B., & Meeker, W. Q. (2020). Applications of the Fractional-Random-Weight Bootstrap. *The American Statistician*, 74(4), 345–358. doi:10.1080/00031305.2020.1731599

Ramsey, P., Gaudard, M., & Levin, W. (2021). Accelerating Innovation with Space Filling Mixture Designs, Neural Networks and SVEM. *JMP Discovery Conference*. https://community.jmp.com/t5/Abstracts/Accelerating-Innovation-with-Space-Filling-Mixture-Designs/ev-p/756841

Ramsey, P., & Gotwalt, C. (2018). Model Validation Strategies for Designed Experiments Using Bootstrapping Techniques With Applications to Biopharmaceuticals. *JMP Discovery Conference -Europe*. https://community.jmp.com/t5/Discovery-Summit-Europe-2018/Model-Validation-Strategies-for-De ta-p/51286

Ramsey, P., Levin, W., Lemkus, T., & Gotwalt, C. (2021). SVEM: A Paradigm Shift in Design and Analysis of Experiments. *JMP Discovery Conference - Europe*. https://community.jmp.com/ t5/Abstracts/SVEM-A-Paradigm-Shift-in-Design-and-Analysis-of-Experiments-2021/ev-p/ 756634

Ramsey, P., & McNeill, P. (2023). CMC, SVEM, Neural Networks, DOE, and Complexity: It's All About Prediction. *JMP Discovery Conference*.

Friedman, J. H., Hastie, T., & Tibshirani, R. (2010). Regularization Paths for Generalized Linear Models via Coordinate Descent. *Journal of Statistical Software*, 33(1), 1–22.

#### Examples

# Simulate data
set.seed(0)

```
n <- 21
X1 <- runif(n)
X2 <- runif(n)
X3 <- runif(n)
y <- 1 + 2*X1 + 3*X2 + X1*X2 + X1^2 + rnorm(n)
data <- data.frame(y, X1, X2, X3)
# Fit the SVEMnet model with a formula
model <- SVEMnet(
   y ~ (X1 + X2 + X3)^2 + I(X1^2) + I(X2^2) + I(X3^2),
   glmnet_alpha = c(1),
   data = data
)
coef(model)
plot(model)
predict(model,data)
```

svem\_significance\_test

SVEM Significance Test

## Description

Performs a whole-model significance test using the SVEM framework, handling both continuous and categorical predictors.

## Usage

```
svem_significance_test(
  formula,
  data,
  nPoint = 2000,
  nSVEM = 5,
  nPerm = 125,
  percent = 85,
  nBoot = 200,
  glmnet_alpha = c(1),
  weight_scheme = c("SVEM"),
  objective = c("wAIC", "wSSE"),
  verbose = TRUE,
  ...
)
```

## Arguments

| formula | A formula specifying the model to be tested.        |
|---------|---|
| data    | A data frame containing the variables in the model. |

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| nPoint        | The number of random points to generate in the factor space (default: 2000).                         |
|---------------|--|
| nSVEM         | The number of SVEM models to fit to the original data (default: 5).                                  |
| nPerm         | The number of SVEM models to fit to permuted data for reference distribution (default: 125).         |
| percent       | The percentage of variance to capture in the SVD (default: 85).                                      |
| nBoot         | The number of bootstrap iterations within SVEM (default: 200).                                       |
| glmnet_alpha  | The alpha parameter(s) for glmnet (default: c(1)).   |
| weight_scheme | The weight scheme to use in SVEM (default: "SVEM").  |
| objective     | Character; the objective function to use in SVEMnet. Options are "wAIC" or "wSSE" (default: "wAIC"). |
| verbose       | Logical; if TRUE, displays progress messages (default: TRUE).  |
|               | Additional arguments passed to the underlying SVEMnet() and then glmnet() functions.                 |

#### Details

The 'svem\_significance\_test' function implements a whole-model test designed to gauge the significance of a fitted SVEM model compared to the null hypothesis of a constant response surface. This method helps identify responses that have relatively stronger or weaker relationships with study factors.

The test constructs standardized predictions by centering the SVEM predictions (obtained from SVEMnet()) by the response mean and scaling by the ensemble standard deviation. A reference distribution is created by fitting the SVEM model to multiple randomized permutations of the response vector. The Mahalanobis distances of the original and permuted models are calculated using a reduced-rank singular value decomposition.

The R code to perform this test (using matrices of nSVEM and nPerm predictions) is taken from the supplementary material of Karl (2024).

This function assumes that there are no restrictions among the factors (e.g. mixture factors). The method will work with restrictions, but the code would need to be changed to ensure the nPoint points respect the factor restriction(s). For example, rdirichlet() could be used for the mixture factors.

The SVEMnet parameter debias is hard coded to FALSE for this test. Unpublished simulation work suggests that setting debias=TRUE reduces the power of the test (without affecting the Type I error rate).

#### Value

A list containing the test results.

#### Acknowledgments

## References

Karl, A. T. (2024). A randomized permutation whole-model test heuristic for Self-Validated Ensemble Models (SVEM). *Chemometrics and Intelligent Laboratory Systems*, 249, 105122. doi:10.1016/j.chemolab.2024.105122

## Examples

```
# Simulate data
set.seed(1)
n <- 30
X1 <- runif(n)</pre>
X2 <- runif(n)
X3 <- runif(n)
y < -1 + X1 + X2 + X1 + X2 + X1^{2} + rnorm(n)
data <- data.frame(y, X1, X2, X3)</pre>
# Perform the SVEM significance test
test_result <- svem_significance_test(</pre>
  y \sim (X1 + X2 + X3)^2 + I(X1^2) + I(X2^2) + I(X3^2),
  data = data,
  nPoint = 2000,
  nSVEM = 7,
  nPerm = 150,
  nBoot = 200
)
# View the p-value
print(test_result)
test_result2 <- svem_significance_test(</pre>
  y \sim (X1 + X2)^2 + I(X1^2) + I(X2^2),
  data = data,
  nPoint = 2000,
  nSVEM = 7,
  nPerm = 150,
  nBoot = 200
)
# View the p-value
print(test_result2)
# Plot the Mahalanobis distances
plot(test_result,test_result2)
```

## Description

Performs a whole-model significance test using the SVEM framework, handling both continuous and categorical predictors, with parallel computation.

## Usage

```
svem_significance_test_parallel(
 formula,
 data,
  nPoint = 2000,
 nSVEM = 7,
 nPerm = 200,
 percent = 85,
 nBoot = 200,
 glmnet_alpha = c(1),
 weight_scheme = c("SVEM"),
 objective = c("wAIC", "wSSE"),
  verbose = TRUE,
 nCore = parallel::detectCores(),
 seed = NULL,
  . . .
)
```

## Arguments

| formula       | A formula specifying the model to be tested.   |
|---------------|--|
| data          | A data frame containing the variables in the model.  |
| nPoint        | The number of random points to generate in the factor space (default: 2000).                         |
| nSVEM         | The number of SVEM models to fit to the original data (default: 7).                                  |
| nPerm         | The number of SVEM models to fit to permuted data for reference distribution (default: 200).         |
| percent       | The percentage of variance to capture in the SVD (default: 85).                                      |
| nBoot         | The number of bootstrap iterations within SVEM (default: 200).                                       |
| glmnet_alpha  | The alpha parameter(s) for glmnet (default: c(1)).   |
| weight_scheme | The weight scheme to use in SVEM (default: "SVEM").  |
| objective     | Character; the objective function to use in SVEMnet. Options are "wAIC" or "wSSE" (default: "wAIC"). |
| verbose       | Logical; if TRUE, displays progress messages (default: TRUE).  |

| nCore | The number of CPU cores to use for parallel processing (default: all available cores). |
|-------|--|
| seed  | An integer seed for random number generation (default: NULL).                          |
|       | Additional arguments passed to the underlying SVEMnet() and then glmnet() functions.   |

## Details

The 'svem\_significance\_test\_parallel' function implements a whole-model test designed to gauge the significance of a fitted SVEM model compared to the null hypothesis of a constant response surface, with parallel computation. This method helps identify responses that have relatively stronger or weaker relationships with study factors.

The test constructs standardized predictions by centering the SVEM predictions (obtained from SVEMnet()) by the response mean and scaling by the ensemble standard deviation. A reference distribution is created by fitting the SVEM model to multiple randomized permutations of the response vector. The Mahalanobis distances of the original and permuted models are calculated using a reduced-rank singular value decomposition.

The R code to perform this test (using matrices of nSVEM and nPerm predictions) is taken from the supplementary material of Karl (2024).

This function assumes that there are no restrictions among the factors (e.g. mixture factors). The method will work with restrictions, but the code would need to be changed to ensure the nPoint points respect the factor restriction(s). For example, rdirichlet() could be used for the mixture factors.

The SVEMnet parameter debias is hard coded to FALSE for this test. Unpublished simulation work suggests that setting debias=TRUE reduces the power of the test (without affecting the Type I error rate).

## Value

A list containing the test results.

#### Acknowledgments

Development of this package was assisted by GPT o1-preview, which helped in constructing the structure of some of the code and the roxygen documentation. The code for the significance test is taken from the supplementary material of Karl (2024).

## References

Karl, A. T. (2024). A randomized permutation whole-model test heuristic for Self-Validated Ensemble Models (SVEM). *Chemometrics and Intelligent Laboratory Systems*, 249, 105122. doi:10.1016/j.chemolab.2024.105122

## Examples

```
# Simulate data
set.seed(0)
n <- 30</pre>
```

```
X1 <- runif(n)
X2 <- runif(n)
X3 <- runif(n)
y <- 1 + X1 + X2 + X1 * X2 + X1^2 + rnorm(n)
data <- data.frame(y, X1, X2, X3)</pre>
#CRAN requires a max of nCore=2 for example. Recommend using default nCore to use entire CPU.
# Perform the SVEM significance test
test_result <- svem_significance_test_parallel(</pre>
  y \sim (X1 + X2 + X3)^2 + I(X1^2) + I(X2^2) + I(X3^2),
  data = data,
  nPoint = 2000,
  nSVEM = 9,
  nPerm = 250,
  nBoot = 200,
 nCore = 2
)
# View the p-value
print(test_result)
test_result2 <- svem_significance_test_parallel(</pre>
  y \sim (X1 + X2)^2 + I(X1^2) + I(X2^2),
  data = data,
  nPoint = 2000,
  nSVEM = 9,
  nPerm = 250,
  nBoot = 200,
  nCore = 2
)
# View the p-value
print(test_result2)
```

```
# Plot the Mahalanobis distances
plot(test_result,test_result2)
```

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