

Package ‘kerndwd’

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Title Distance Weighted Discrimination (DWD) and Kernel Methods

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Description

A novel implementation that solves the linear distance weighted discrimination and the kernel distance weighted discrimination. Reference: Wang and Zou (2018) <doi:10.1111/rssb.12244>.

Depends methods

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Description

Extremely novel efficient procedures for solving linear generalized DWD and kernel generalized DWD in reproducing kernel Hilbert spaces for classification. The algorithm is based on the majorization-minimization (MM) principle to compute the entire solution path at a given fine grid of regularization parameters.

Details

Suppose x is predictor and y is a binary response. The package computes the entire solution path over a grid of λ values.

The main functions of the package `kerndwd` include:

```
kerndwd
cv.kerndwd
tunedwd
predict.kerndwd
plot.kerndwd
plot.cv.kerndwd
```

Author(s)

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References

- Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.
<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>
- Karatzoglou, A., Smola, A., Hornik, K., and Zeileis, A. (2004) "kernlab – An S4 Package for Kernel Methods in R", *Journal of Statistical Software*, **11**(9), 1–20.
<https://www.jstatsoft.org/v11/i09/paper>
- Marron, J.S., Todd, M.J., Ahn, J. (2007) "Distance-Weighted Discrimination", *Journal of the American Statistical Association*, **102**(408), 1267–1271.
<https://www.tandfonline.com/doi/abs/10.1198/01621450700001120>

BUPA

BUPA's liver disorders data

Description

BUPA's liver disorders data: 345 male individuals' blood test result and liver disorder status.

Usage

```
data(BUPA)
```

Details

This data set consists of 345 observations and 6 predictors representing the blood test result liver disorder status of 345 patients. The three predictors are mean corpuscular volume (MCV), alkaline phosphatase (ALKPHOS), alanine aminotransferase (SGPT), aspartate aminotransferase (SGOT), gamma-glutamyl transpeptidase (GAMMAGT), and the number of alcoholic beverage drinks per day (DRINKS).

Value

A list with the following elements:

X	A numerical matrix for predictors: 345 rows and 6 columns; each row corresponds to a patient.
y	A numeric vector of length 305 representing the liver disorder status.

Source

The data set is available for download from UCI machine learning repository.

Examples

```
# load data set
data(BUPA)

# the number of samples predictors
dim(BUPA$X)

# the number of samples for each class
sum(BUPA$y == -1)
sum(BUPA$y == 1)
```

cv.kerndwd

*cross-validation***Description**

Carry out a cross-validation for [kerndwd](#) to find optimal values of the tuning parameter lambda.

Usage

```
cv.kerndwd(x, y, kern, lambda, nfolds=5, foldid, wt, ...)
```

Arguments

x	A matrix of predictors, i.e., the matrix x used in kerndwd .
y	A vector of binary class labels, i.e., the y used in kerndwd . y has to be two levels.
kern	A kernel function.
lambda	A user specified lambda candidate sequence for cross-validation.
nfolds	The number of folds. Default value is 5. The allowable range is from 3 to the sample size.
foldid	An optional vector with values between 1 and nfold, representing the fold indices for each observation. If supplied, nfold can be missing.
wt	A vector of length n for weight factors. When wt is missing or wt=NULL, an unweighted DWD is fitted.
...	Other arguments being passed to kerndwd .

Details

This function computes the mean cross-validation error and the standard error by fitting [kerndwd](#) with every fold excluded alternatively. This function is modified based on the cv function from the glmnet package.

Value

A [cv.kerndwd](#) object including the cross-validation results is return..

lambda	The lambda sequence used in kerndwd .
cvm	A vector of length length(lambda): mean cross-validated error.
cvsd	A vector of length length(lambda): estimates of standard error of cvm.
cvupper	The upper curve: cvm + cvsd.
cvlower	The lower curve: cvm -cvsd.
lambda.min	The lambda incurring the minimum cross validation error cvm.
lambda.1se	The largest value of lambda such that error is within one standard error of the minimum.
cvm.min	The cross-validation error corresponding to lambda.min, i.e., the least error.
cvm.1se	The cross-validation error corresponding to lambda.1se.

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References

Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.
<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>
 Friedman, J., Hastie, T., and Tibshirani, R. (2010), "Regularization paths for generalized linear models via coordinate descent," *Journal of Statistical Software*, **33**(1), 1–22.
<https://www.jstatsoft.org/v33/i01/paper>

See Also

[kerndwd](#) and [plot.cv.kerndwd](#)

Examples

```
set.seed(1)
data(BUPA)
BUPA$X = scale(BUPA$X, center=TRUE, scale=TRUE)
lambda = 10^(seq(3, -3, length.out=10))
kern = rbfdot(sigma=sigest(BUPA$X))
m.cv = cv.kerndwd(BUPA$X, BUPA$y, kern, qval=1, lambda=lambda, eps=1e-5, maxit=1e5)
m.cv$lambda.min
```

kerndwd

solve Linear DWD and Kernel DWD

Description

Fit the linear generalized distance weighted discrimination (DWD) model and the generalized DWD on Reproducing kernel Hilbert space. The solution path is computed at a grid of values of tuning parameter lambda.

Usage

```
kerndwd(x, y, kern, lambda, qval=1, wt, eps=1e-05, maxit=1e+05)
```

Arguments

x	A numerical matrix with N rows and p columns for predictors.
y	A vector of length N for binary responses. The element of y is either -1 or 1.
kern	A kernel function; see dots .
lambda	A user supplied lambda sequence.
qval	The exponent index of the generalized DWD. Default value is 1.

wt	A vector of length n for weight factors. When wt is missing or wt=NULL, an unweighted DWD is fitted.
eps	The algorithm stops when (i.e. $\sum_j (\beta_j^{new} - \beta_j^{old})^2$ is less than eps, where $j = 0, \dots, p$. Default value is 1e-5.
maxit	The maximum of iterations allowed. Default is 1e5.

Details

Suppose that the generalized DWD loss is $V_q(u) = 1 - u$ if $u \leq q/(q + 1)$ and $\frac{1}{w^q} \frac{q^q}{(q+1)^{(q+1)}}$ if $u > q/(q + 1)$. The value of λ , i.e., lambda, is user-specified.

In the linear case (kern is the inner product and $N > p$), the `kerndwd` fits a linear DWD by minimizing the L2 penalized DWD loss function,

$$\frac{1}{N} \sum_{i=1}^n V_q(y_i(\beta_0 + X_i' \beta)) + \lambda \beta' \beta.$$

If a linear DWD is fitted when $N < p$, a kernel DWD with the linear kernel is actually solved. In such case, the coefficient β can be obtained from $\beta = X' \alpha$.

In the kernel case, the `kerndwd` fits a kernel DWD by minimizing

$$\frac{1}{N} \sum_{i=1}^n V_q(y_i(\beta_0 + K_i' \alpha)) + \lambda \alpha' K \alpha,$$

where K is the kernel matrix and K_i is the i th row.

The weighted linear DWD and the weighted kernel DWD are formulated as follows,

$$\frac{1}{N} \sum_{i=1}^n w_i \cdot V_q(y_i(\beta_0 + X_i' \beta)) + \lambda \beta' \beta,$$

$$\frac{1}{N} \sum_{i=1}^n w_i \cdot V_q(y_i(\beta_0 + K_i' \alpha)) + \lambda \alpha' K \alpha,$$

where w_i is the i th element of wt. The choice of weight factors can be seen in the reference below.

Value

An object with S3 class `kerndwd`.

alpha	A matrix of DWD coefficients at each lambda value. The dimension is $(p+1) \times \text{length}(\text{lambda})$ in the linear case and $(N+1) \times \text{length}(\text{lambda})$ in the kernel case.
lambda	The lambda sequence.
npass	Total number of MM iterations for all lambda values.
jerr	Warnings and errors; 0 if none.
info	A list including parameters of the loss function, eps, maxit, kern, and wt if a weight vector was used.
call	The call that produced this object.

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References

- Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.
<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>
- Karatzoglou, A., Smola, A., Hornik, K., and Zeileis, A. (2004) "kernlab – An S4 Package for Kernel Methods in R", *Journal of Statistical Software*, **11**(9), 1–20.
<https://www.jstatsoft.org/v11/i09/paper>
- Friedman, J., Hastie, T., and Tibshirani, R. (2010), "Regularization paths for generalized linear models via coordinate descent," *Journal of Statistical Software*, **33**(1), 1–22.
<https://www.jstatsoft.org/v33/i01/paper>
- Marron, J.S., Todd, M.J., and Ahn, J. (2007) "Distance-Weighted Discrimination", *Journal of the American Statistical Association*, **102**(408), 1267–1271.
<https://www.tandfonline.com/doi/abs/10.1198/016214507000001120>
- Qiao, X., Zhang, H., Liu, Y., Todd, M., Marron, J.S. (2010) "Weighted distance weighted discrimination and its asymptotic properties", *Journal of the American Statistical Association*, **105**(489), 401–414.
<https://www.tandfonline.com/doi/abs/10.1198/jasa.2010.tm08487>

See Also

[predict.kerndwd](#), [plot.kerndwd](#), and [cv.kerndwd](#).

Examples

```
data(BUPA)
# standardize the predictors
BUPA$X = scale(BUPA$X, center=TRUE, scale=TRUE)

# a grid of tuning parameters
lambda = 10^(seq(3, -3, length.out=10))

# fit a linear DWD
kern = vanilladot()
DWD_linear = kerndwd(BUPA$X, BUPA$y, kern,
  qval=1, lambda=lambda, eps=1e-5, maxit=1e5)

# fit a DWD using Gaussian kernel
kern = rbfdot(sigma=1)
DWD_Gaussian = kerndwd(BUPA$X, BUPA$y, kern,
  qval=1, lambda=lambda, eps=1e-5, maxit=1e5)

# fit a weighted kernel DWD
kern = rbfdot(sigma=1)
weights = c(1, 2)[factor(BUPA$y)]
```

```
DWD_wtGaussian = kerndwd(BUPA$X, BUPA$y, kern,
  qval=1, lambda=lambda, wt = weights, eps=1e-5, maxit=1e5)
```

kernel functions *Kernel Functions*

Description

Kernel functions provided in the R package kernlab. Details can be seen in the reference below.

The Gaussian RBF kernel $k(x, x') = \exp(-\sigma \|x - x'\|^2)$

The Polynomial kernel $k(x, x') = (\text{scale} \langle x, x' \rangle + \text{offset})^{\text{degree}}$

The Linear kernel $k(x, x') = \langle x, x' \rangle$

The Laplacian kernel $k(x, x') = \exp(-\sigma \|x - x'\|)$

The Bessel kernel $k(x, x') = (-\text{Bessel}_{\nu+1}^n \sigma \|x - x'\|^2)$

The ANOVA RBF kernel $k(x, x') = \sum_{1 \leq i_1, \dots, i_D \leq N} \prod_{d=1}^D k(x_{id}, x'_{id})$ where $k(x, x')$ is a Gaussian RBF kernel.

The Spline kernel $\prod_{d=1}^D 1 + x_i x_j + x_i x_j \min(x_i, x_j) - \frac{x_i + x_j}{2} \min(x_i, x_j)^2 + \frac{\min(x_i, x_j)^3}{3}$. The parameter sigma used in rbfdot can be selected by sigest().

Usage

```
rbfdot(sigma = 1)
polydot(degree = 1, scale = 1, offset = 1)
vanilladot()
laplacedot(sigma = 1)
besseldot(sigma = 1, order = 1, degree = 1)
anovadot(sigma = 1, degree = 1)
splinedot()
sigest(x)
```

Arguments

sigma	The inverse kernel width used by the Gaussian, the Laplacian, the Bessel, and the ANOVA kernel.
degree	The degree of the polynomial, bessel or ANOVA kernel function. This has to be an positive integer.
scale	The scaling parameter of the polynomial kernel function.
offset	The offset used in a polynomial kernel.
order	The order of the Bessel function to be used as a kernel.
x	The design matrix used in kerndwd when sigest is called to estimate sigma in rbfdot().

Details

These R functions and descriptions are directly duplicated and/or adapted from the R package kernlab.

Value

Return an S4 object of class `kernel` which can be used as the argument of `kern` when fitting a `kerndwd` model.

References

Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.

<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>

Karatzoglou, A., Smola, A., Hornik, K., and Zeileis, A. (2004) "kernlab – An S4 Package for Kernel Methods in R", *Journal of Statistical Software*, **11**(9), 1–20.

<https://www.jstatsoft.org/v11/i09/paper>

Examples

```
data(BUPA)
# generate a linear kernel
kfun = vanilladot()

# generate a Laplacian kernel function with sigma = 1
kfun = laplacedot(sigma=1)

# generate a Gaussian kernel function with sigma estimated by sigest()
kfun = rbfdot(sigma=sigest(BUPA$X))

# set kern=kfun when fitting a kerndwd object
data(BUPA)
BUPA$X = scale(BUPA$X, center=TRUE, scale=TRUE)
lambda = 10^(seq(-3, 3, length.out=10))
m1 = kerndwd(BUPA$X, BUPA$y, kern=kfun,
             qval=1, lambda=lambda, eps=1e-5, maxit=1e5)
```

plot.cv.kerndwd

plot the cross-validation curve

Description

Plot cross-validation error curves with the upper and lower standard deviations versus log lambda values.

Usage

```
## S3 method for class 'cv.kerndwd'
plot(x, sign.lambda, ...)
```

Arguments

x	A fitted <code>cv.kerndwd</code> object.
sign.lambda	Against $\log(\lambda)$ (default) or its negative if <code>sign.lambda=-1</code> .
...	Other graphical parameters being passed to <code>plot</code> .

Details

This function plots the cross-validation error curves. This function is modified based on the `plot.cv` function of the `glmnet` package.

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References

Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.

<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>

Friedman, J., Hastie, T., and Tibshirani, R. (2010), "Regularization paths for generalized linear models via coordinate descent," *Journal of Statistical Software*, **33**(1), 1–22.

<https://www.jstatsoft.org/v33/i01/paper>

See Also

[cv.kerndwd](#).

Examples

```
set.seed(1)
data(BUPA)
BUPA$X = scale(BUPA$X, center=TRUE, scale=TRUE)
lambda = 10^(seq(-3, 3, length.out=10))
kern = rbfdot(sigma=sigest(BUPA$X))
m.cv = cv.kerndwd(BUPA$X, BUPA$y, kern,
  qval=1, lambda=lambda, eps=1e-5, maxit=1e5)
m.cv
```

plot.kerndwd	<i>plot coefficients</i>
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Description

Plot the solution paths for a fitted `kerndwd` object.

Usage

```
## S3 method for class 'kerndwd'  
plot(x, color=FALSE, ...)
```

Arguments

<code>x</code>	A fitted “ <code>kerndwd</code> ” model.
<code>color</code>	If TRUE, plots the curves with rainbow colors; otherwise, with gray colors (default).
<code>...</code>	Other graphical parameters to <code>plot</code> .

Details

Plots the solution paths as a coefficient profile plot. This function is modified based on the `plot` function from the `glmnet` package.

Author(s)

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References

Wang, B. and Zou, H. (2018) “Another Look at Distance Weighted Discrimination,” *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.
<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>
Friedman, J., Hastie, T., and Tibshirani, R. (2010), “Regularization paths for generalized linear models via coordinate descent,” *Journal of Statistical Software*, **33**(1), 1–22.
<https://www.jstatsoft.org/v33/i01/paper>

See Also

`kerndwd`, `predict.kerndwd`, `coef.kerndwd`, `plot.kerndwd`, and `cv.kerndwd`.

Examples

```

data(BUPA)
BUPA$X = scale(BUPA$X, center=TRUE, scale=TRUE)
lambda = 10^(seq(-3, 3, length.out=10))
kern = rbfdot(sigma=sigest(BUPA$X))
m1 = kerndwd(BUPA$X, BUPA$y, kern, qval=1,
             lambda=lambda, eps=1e-5, maxit=1e5)
plot(m1, color=TRUE)

```

predict.kerndwd	<i>predict class labels for new observations</i>
-----------------	--

Description

Predict the binary class labels or the fitted values of an `kerndwd` object.

Usage

```

## S3 method for class 'kerndwd'
predict(object, kern, x, newx, type=c("class", "link"), ...)

```

Arguments

object	A fitted <code>kerndwd</code> object.
kern	The kernel function used when fitting the <code>kerndwd</code> object.
x	The predictor matrix, i.e., the x matrix used when fitting the <code>kerndwd</code> object.
newx	A matrix of new values for x at which predictions are to be made. We note that newx must be a matrix, predict function does not accept a vector or other formats of newx.
type	"class" or "link"? "class" produces the predicted binary class labels and "link" returns the fitted values. Default is "class".
...	Not used. Other arguments to predict.

Details

If "type" is "class", the function returns the predicted class labels. If "type" is "link", the result is $\beta_0 + x_i^t \beta$ for the linear case and $\beta_0 + K_i^t \alpha$ for the kernel case.

Value

Returns either the predicted class labels or the fitted values, depending on the choice of type.

Author(s)

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References

Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.
<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>

See Also

[kerndwd](#)

Examples

```
data(BUPA)
BUPA$X = scale(BUPA$X, center=TRUE, scale=TRUE)
lambda = 10^(seq(-3, 3, length.out=10))
kern = rbfdot(sigma=sigest(BUPA$X))
m1 = kerndwd(BUPA$X, BUPA$y, kern,
  qval=1, lambda=lambda, eps=1e-5, maxit=1e5)
predict(m1, kern, BUPA$X, tail(BUPA$X))
```

tunedwd

fast tune procedure for DWD

Description

A fast implementaiton of cross-validation for [kerndwd](#) to find the optimal values of the tuning parameter lambda.

Usage

```
tunedwd(x, y, kern, lambda, qvals=1, eps=1e-5, maxit=1e+5, nfolds=5, foldid=NULL)
```

Arguments

x	A matrix of predictors, i.e., the matrix x used in kerndwd .
y	A vector of binary class labels, i.e., the y used in kerndwd . y has two levels.
kern	A kernel function.
lambda	A user specified lambda candidate sequence for cross-validation.
qvals	A vector containing the index of the generalized DWD. Default value is 1.
eps	The algorithm stops when (i.e. $\sum_j (\beta_j^{new} - \beta_j^{old})^2$ is less than eps, where $j = 0, \dots, p$. Default value is 1e-5.
maxit	The maximum of iterations allowed. Default is 1e5.
nfolds	The number of folds. Default value is 5. The allowable range is from 3 to the sample size.
foldid	An optional vector with values between 1 and nfold, representing the fold indices for each observation. If supplied, nfold can be missing.

Details

This function returns the best tuning parameters q and λ by cross-validation. An efficient tune method is employed to accelerate the algorithm.

Value

A `tunedwd.kerndwd` object including the cross-validation results is return.

`lam.tune` The optimal λ value.

`q.tune` The optimal q value.

Author(s)

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References

Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.

<https://rss.onlinelibrary.wiley.com/doi/10.1111/rssb.12244>

Friedman, J., Hastie, T., and Tibshirani, R. (2010), "Regularization paths for generalized linear models via coordinate descent," *Journal of Statistical Software*, **33**(1), 1–22.

<https://www.jstatsoft.org/v33/i01/paper>

See Also

[kerndwd](#).

Examples

```
set.seed(1)
data(BUPA)
BUPA$X = scale(BUPA$X, center=TRUE, scale=TRUE)
lambda = 10^(seq(-3, 3, length.out=10))
kern = rbfdot(sigma=sigest(BUPA$X))
ret = tunedwd(BUPA$X, BUPA$y, kern, qvals=c(1,2,10), lambda=lambda, eps=1e-5, maxit=1e5)
ret
```

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