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Author Boxiang Wang <boxiang-wang@uiowa.edu>, Hui Zou <hzou@stat.umn.edu>

Maintainer Boxiang Wang <boxiang-wang@uiowa.edu>

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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`kerndwd-package` *Kernel Distance Weighted Discrimination*

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 `lambda` values.

The main functions of the package `kerndwd` include:
`kerndwd`
`cv.kerndwd`
`tunedwd`
`predict.kerndwd`
`plot.kerndwd`
`plot.cv.kerndwd`

Author(s)

Boxiang Wang and Hui Zou
Maintainer: Boxiang Wang <boxiang-wang@uiowa.edu>

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/10.1198/016214507000001120

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 phosphotase (ALKPHOS), alamine 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.

Author(s)

Boxiang Wang and Hui Zou
Maintainer: Boxiang Wang <boxiang-wang@uiowa.edu>

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 $j = 0, \ldots, p$. 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 $\frac{1}{u^q}\frac{q^q}{(q+1)^{(q+1)}}$ 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 ith 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 ith 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)*length(lambda) in the linear case and (N+1)*length(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.

Author(s)

Boxiang Wang and Hui Zou
Maintainer: Boxiang Wang <boxiang-wang@uiowa.edu>

References

Wang, B. and Zou, H. (2018) "Another Look at Distance Weighted Discrimination," *Journal of Royal Statistical Society, Series B*, **80**(1), 177–198.
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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 $k(x, x') = (scale < x, x' > +offset)^{degree}$
The Linear kernel $k(x, x') =< x, x' >$
The Laplacian kernel $k(x, x') = \exp(-\sigma\|x - x'\|)$
The Bessel kernel $k(x, x') = (-\text{Bessel}^n_{(\nu+1)}\sigma\|x - x'\|^2)$
The ANOVA RBF kernel $k(x, x') = \sum_{1\leq i_1 \ldots < i_D \leq N} \prod_{d=1}^{D} k(x_{id}, {x'}_{id})$ 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 cv.kerndwd object.
sign.lambda	Against log(lambda) (default) or its negative if sign.lambda=-1.
...	Other graphical parameters being passed to plot.

Details

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

Author(s)

Boxiang Wang and Hui Zou
Maintainer: Boxiang Wang <boxiang-wang@uiowa.edu>

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` *plot coefficients*

Description

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

Usage

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

Arguments

`x`	A fitted "`kerndwd`"" model.
`color`	If `TRUE`, plots the curves with rainbow colors; otherwise, with gray colors (default).
`...`	Other graphical parameters to `plot`.

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)

Boxiang Wang and Hui Zou
Maintainer: Boxiang Wang <boxiang-wang@uiowa.edu>

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` *predict class labels for new observations*

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 `kerndwd` object.
`kern`	The kernel function used when fitting the `kerndwd` object.
`x`	The predictor matrix, i.e., the `x` matrix used when fitting the `kerndwd` 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 $\beta_0 + x_i'\beta$ for the linear case and $\beta_0 + K_i'\alpha$ for the kernel case.

Value

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

Author(s)

Boxiang Wang and Hui Zou
Maintainer: Boxiang Wang <boxiang-wang@uiowa.edu>

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 $j = 0, \ldots, p$. 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 lambda 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 lambda value.
q.tune	The optimal q value.

Author(s)

Boxiang Wang and Hui Zou
Maintainer: Boxiang Wang <boxiang-wang@uiowa.edu>

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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