Package ‘VPdtw’

January 20, 2025

Type Package

Title Variable Penalty Dynamic Time Warping

Version 2.2.1

Date 2024-08-27

Description Variable Penalty Dynamic Time Warping (VPdtw) for aligning chromatographic signals. With an appropriate penalty this method performs good alignment of chromatographic data without deforming the peaks (Clifford, D., Stone, G., Montoliu, I., Rezzi S., Martin F., Guy P., Bruce S., and Kochhar S.(2009) <doi:10.1021/ac802041e>; Clifford, D. and Stone, G. (2012) <doi:10.18637/jss.v047.i08>).

License GPL-2

URL `https://github.com/ethanbass/VPdtw/`

BugReports `https://github.com/ethanbass/VPdtw/issues`

RoxygenNote 7.3.0

Encoding UTF-8

Suggests testthat (>= 3.0.0), vdiffr

Config/testthat/edition 3

NeedsCompilation yes

Author David Clifford [aut],
Glenn Stone [aut],
Ethan Bass [ctb, cre] (<`https://orcid.org/0000-0002-6175-6739`>)

Maintainer Ethan Bass <`ethanbass@gmail.com`>

Repository CRAN

Date/Publication 2024-08-29 07:30:09 UTC

Contents

`dilation` *Compute a morphological dilation of a signal*

Description

A dilation is a moving local maximum over a window of specific fixed width specified by `span`. This dilation is computed first in one direction and then in the other.

Usage

```
dilation(y, span)
```

Arguments

`y`	Signal (as a numeric vector).
`span`	An integer specifying the width of the moving window.

Details

A dilation is a method often used in mathematical morphology and image analysis (Soille 1999). This function is for vectors not matrices or images though applying it to rows and columns of a matrix will give the corresponding results.

An erosion of a vector or image can also be computed easily from this by computing the dilation of -1 times the vector and transforming back.

We recommend using a dilation to form a `penalty` for use in `VPdtw`.

Value

`res`	Dilation of `y` with width specified by `span`

Author(s)

David Clifford

References

Soille, P. Morphological Image Analysis: Principles and Applications; Springer: New York, 1999.

Examples

```
## Example 1 - dilation of a signal
data(reference)
dref <- dilation(reference, 150)
plot(reference, log = "y", type = "l")
lines(dref, col = 2)

## Example 2 - dilation of an image
BIN <- (volcano > 177)
dBIN <- t(apply(BIN, 1, dilation, span = 5))
dBIN <- apply(dBIN, 2, dilation, span = 5)
oldpar <- par(no.readonly = TRUE)
par(mfrow=c(2, 2))
image(volcano)
image(BIN)
image(dBIN)
par(oldpar)
```

`plot.VPdtw` *Plot VPdtw object*

Description

Plot VPdtw object

Usage

```
## S3 method for class 'VPdtw'
plot(
  x,
  type = c("All", "Before", "After", "Shift", "Chromatograms"),
  xlim = NULL,
  ...
)
```

Arguments

`x`	A VPdtw object generated by `VPdtw`.
`type`	What to plot.
`xlim`	Numeric vector specifying x-axis limits.
`...`	Additional arguments

Value

No return value, called for side effects.

Side effects

Plots information about alignment according to value of `type`: either unaligned query and reference (`"Before"`), aligned query and reference (`"After"`), shift at each index (`"Shift"`), a three-panel plot containing all three of these options (`"All"`), or a two-panel plot with unaligned and aligned query (`"Chromatograms"`).

Examples

```
query <- c(1,5,4,3,9,8,5,2,6,5,4)
reference <- c(rnorm(5), query, rnorm(5))
lambda <- rep(0, length(reference))
maxshift <- 11
res <- VPdtw(reference, query, lambda, maxshift)
plot(res)
```

`print.VPdtw` *Print VPdtw*

Description

Print VPdtw

Usage

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

Arguments

`x`	A VPdtw object generated by `VPdtw`.
`...`	Additional argument.

Value

Numeric vector from the `summary` slot in the `VPdtw` object specified by `x`.

Examples

```
query <- c(1,5,4,3,9,8,5,2,6,5,4)
reference <- c(rnorm(5), query, rnorm(5))
lambda <- rep(0, length(reference))
maxshift <- 11
res <- VPdtw(reference, query, lambda, maxshift)
print(res)
```

`reference` *GC-MS Chromatogram*

Description

GC-MS chromatogram from a wine sample

Format

A numeric vector of length 10018

Details

This together with the `query` data are used in the VPdtw examples. The alignment of these two signals is usually carried out on the log scale. Plotting of this signal is best done also on the log scale (see example below).

Source

Amalia Berna, Stephen Trowell, CSIRO Food Futures Flagship

References

Amalia Z. Berna, Stephen Trowell, David Clifford, Wies Cynkar, Daniel Cozzolino, Geographical origin of Sauvignon Blanc wines predicted by mass spectrometry and metal oxide based electronic nose, Analytica Chimica Acta, Volume 648, Issue 2, 26 August 2009, Pages 146-152, ISSN 0003-2670, DOI: 10.1016/j.aca.2009.06.056. Keywords: Sauvignon Blanc; Electronic nose; Gas chromatography-mass spectrometry; Prediction

Examples

```
data(reference)
data(query)
plot(reference, log="y", type="l", main = "Gas Chromatogram",
  ylab = "log(intensity)", lwd = 2, col = 1)
lines(query, col = 2)
```

`VPdtw` *Variable Penalty Dynamic Time Warping function*

Description

Use variable penalty dynamic time warping to align one (or many) query signal(s) to a master signal. Penalties are incurred whenever a non-diagonal move is taken.

Usage

```
VPdtw(
  reference,
  query,
  penalty = 0,
  maxshift = 50,
  Reference.type = c("random", "median", "mean", "trimmed")
)
```

Arguments

`reference`	Reference signal, NULL or a vector, see details.
`query`	Query signal, a vector or matrix, see details
`penalty`	Penalty term, a vector of same length as reference (not checked) or a matrix. See details. Default is 0 repeated to the length of reference
`maxshift`	Maximum allowable shift, an integer
`Reference.type`	Choices for `reference` if NULL is input

Details

Performs variable penalty dynamic time warping of `query` to `reference`. Sakoe Chiba dtw used with width `maxshift`.

The basic operation aligns a `query` vector to a `reference` vector.

If `reference` is not specified and `query` is a matrix then the `reference` is created based on the value of `Reference.type`. The four choices are `random`, `median`, `mean` and `trimmed`. These choose a column of `query` at random as a reference, or the piecewise median, mean or trimmed mean (with `trim = 0.1`) with missing values removed.

If `query` is a matrix and `penalty` is a vector then the same penalty is used to align each column of `query` to the `reference`. Different alignment paths are chosen for each column of the `query` matrix.

If `query` is a vector and `penalty` is a matrix then the `query` is aligned to the `reference` several times, using each column of the `penalty` matrix in turn as the penalty for the alignment.

If `query` and `penalty` are matrices then nothing happens. If you wish to align many query vectors and test many penalty vectors at the same time then do the appropriate looping (over queries, or penalties) outside of `VPdtw`.

Value

`xVals`	For plotting everything to correct index
`reference`	reference vector used by VPdtw expanded by NAs for plotting.
`query`	query passed to VPdtw
`penalty`	penalty passed to VPdtw
`warpedQuery`	result of alignment, same class as query
`shift`	shifts required to achieve alignment
`summary`	Summary information about the alignment. Used for `print.VPdtw`
`information`	Information about the alignment. Used for `print.VPdtw`

Author(s)

David Clifford, Glenn Stone

References

Alignment Using Variable Penalty Dynamic Time Warping by Clifford, D; Stone, G; Montoliu, I; et al. Analytical Chemistry Volume: 81 Issue: 3 Pages: 1000-1007 Published: 2009

See Also

Also check out the `dtw` package by Toni Giorgino which covers many variations of dynamic time warping.

Examples

```
## Citation
citation("VPdtw")

## Basic Examples of zero-penalty DTW

## Example of exact fit in the middle
query <- c(1,5,4,3,9,8,5,2,6,5,4)
reference <- c(rnorm(5), query, rnorm(5))
lambda <- rep(0, length(reference))
maxshift <- 11
res <- VPdtw(reference, query, lambda, maxshift)
plot(res)
res

## Example of exact fit on one side
reference <- c(1,5,4,3,9,8,5,2,6,5,4)
query <- c(rnorm(5), reference)
reference <- c(reference, rnorm(5))
lambda <- rep(0, length(reference))
maxshift <- 6
res <- VPdtw(reference, query, lambda, maxshift)
plot(res)
res
```

```
  ## Example of exact fit on the other side
  reference <- c(1,5,4,3,9,8,5,2,6,5,4)
  query <- c(reference, rnorm(5))
  reference <- c(rnorm(5), reference)
  lambda <- rep(0, length(reference))
  maxshift <- 6
  res <- VPdtw(reference, query, lambda, maxshift)
  plot(res)
  res

  ## Example of exact fit except where one query gets dropped and its all on one side
  reference <- c(1,5,4,3,9,8,5,2,6,5,4)
  query <- c(reference[1:5], 20, reference[6:11])
  reference <- c(rnorm(5), reference)
  query <- c(query, rnorm(5))
  lambda <- rep(0, length(reference))
  maxshift <- 6
  res <- VPdtw(reference, query, lambda, maxshift)
  plot(res)
  res

## Examples that use penalty term. Examples with long signals

data(reference)
data(query)
## Do alignment on log scale
reference <- log(reference)
query <- log(query)

## VPdtw
result <- VPdtw(reference=reference[1:2500], query = query[1:2500],
                penalty = dilation(reference[1:2500], 150)/4, maxshift=150)
plot(result)
result

## Zero penalty DTW
result2 <- VPdtw(reference = reference[1:2500], query = query[1:2500],
                 penalty = rep(0, length(reference)), maxshift = 150)
plot(result2)

## Try both penalties at the same time
penalty <- dilation(reference, 350)/5
penalty <- cbind(penalty, rep(0, length(penalty)))

result <- VPdtw(reference, query, penalty = penalty, maxshift = 350)
plot(result, "After")
plot(result, "Shift")
result

## All three plots at once
plot(result)
```

Index