

Package ‘T4transport’

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Type Package

Title Tools for Computational Optimal Transport

Version 0.1.2

Description Transport theory has seen much success in many fields of statistics and machine learning. We provide a variety of algorithms to compute Wasserstein distance, barycenter, and others. See Peyré and Cuturi (2019) <[doi:10.1561/22000000073](https://doi.org/10.1561/22000000073)> for the general exposition to the study of computational optimal transport.

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RoxygenNote 7.2.3

RdMacros Rdpack

Suggests ggplot2

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bary14C	<i>Barycenter by Cuturi & Doucet (2014)</i>
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Description

Given K empirical measures $\mu_1, \mu_2, \dots, \mu_K$ of possibly different cardinalities, wasserstein barycenter μ^* is the solution to the following problem

$$\sum_{k=1}^K \pi_k \mathcal{W}_p^p(\mu, \mu_k)$$

where π_k 's are relative weights of empirical measures. Here we assume either (1) support atoms in Euclidean space are given, or (2) all pairwise distances between atoms of the fixed support and empirical measures are given. Algorithmically, it is a subgradient method where the each subgradient is approximated using the entropic regularization.

Usage

```
bary14C(
  support,
  atoms,
  marginals = NULL,
  weights = NULL,
  lambda = 0.1,
  p = 2,
  ...
)
```

```
bary14Cdist(
  distances,
```

```

    marginals = NULL,
    weights = NULL,
    lambda = 0.1,
    p = 2,
    ...
)

```

Arguments

support	an $(N \times P)$ matrix of rows being atoms for the fixed support.
atoms	a length- K list where each element is an $(N_k \times P)$ matrix of atoms.
marginals	marginal distribution for empirical measures; if NULL (default), uniform weights are set for all measures. Otherwise, it should be a length- K list where each element is a length- N_i vector of nonnegative weights that sum to 1.
weights	weights for each individual measure; if NULL (default), each measure is considered equally. Otherwise, it should be a length- K vector.
lambda	regularization parameter (default: 0.1).
p	an exponent for the order of the distance (default: 2).
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-10).
	init.vec an initial vector (default: uniform weight).
	maxiter maximum number of iterations (default: 496).
	print.progress a logical to show current iteration (default: FALSE).
distances	a length- K list where each element is an $(N \times N_k)$ pairwise distance between atoms of the fixed support and given measures.

Value

a length- N vector of probability vector.

References

Cuturi M, Doucet A (2014). "Fast computation of wasserstein barycenters." In Xing EP, Jebara T (eds.), *Proceedings of the 31st international conference on international conference on machine learning - volume 32*, volume 32 of *Proceedings of machine learning research*, 685–693.

Examples

```

#-----
#   Wasserstein Barycenter for Fixed Atoms with Two Gaussians
#
# * class 1 : samples from Gaussian with mean=(-4, -4)
# * class 2 : samples from Gaussian with mean=(+4, +4)
# * target support consists of 7 integer points from -6 to 6,
#   where ideally, weight is concentrated near 0 since it's average!
#-----
## GENERATE DATA

```

```

# Empirical Measures
set.seed(100)
ndat = 100
dat1 = matrix(rnorm(ndat*2, mean=-4, sd=0.5), ncol=2)
dat2 = matrix(rnorm(ndat*2, mean=+4, sd=0.5), ncol=2)

myatoms = list()
myatoms[[1]] = dat1
myatoms[[2]] = dat2
mydata = rbind(dat1, dat2)

# Fixed Support
support = cbind(seq(from=-8, to=8, by=2),
                seq(from=-8, to=8, by=2))
## COMPUTE
comp1 = bary14C(support, myatoms, lambda=0.5, maxiter=10)
comp2 = bary14C(support, myatoms, lambda=1, maxiter=10)
comp3 = bary14C(support, myatoms, lambda=5, maxiter=10)

## VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3))
barplot(comp1, main="lambda=0.5")
barplot(comp2, main="lambda=1")
barplot(comp3, main="lambda=5")
par(opar)

```

bary15B

Barycenter by Benamou et al. (2015)

Description

Given K empirical measures $\mu_1, \mu_2, \dots, \mu_K$ of possibly different cardinalities, Wasserstein barycenter μ^* is the solution to the following problem

$$\sum_{k=1}^K \pi_k \mathcal{W}_p^p(\mu, \mu_k)$$

where π_k 's are relative weights of empirical measures. Here we assume either (1) support atoms in Euclidean space are given, or (2) all pairwise distances between atoms of the fixed support and empirical measures are given. Authors proposed iterative Bregman projections in conjunction with entropic regularization.

Usage

```

bary15B(
  support,
  atoms,

```

```

    marginals = NULL,
    weights = NULL,
    lambda = 0.1,
    p = 2,
    ...
)

```

```

bary15Bdist(
  distances,
  marginals = NULL,
  weights = NULL,
  lambda = 0.1,
  p = 2,
  ...
)

```

Arguments

support	an $(N \times P)$ matrix of rows being atoms for the fixed support.
atoms	a length- K list where each element is an $(N_k \times P)$ matrix of atoms.
marginals	marginal distribution for empirical measures; if NULL (default), uniform weights are set for all measures. Otherwise, it should be a length- K list where each element is a length- N_i vector of nonnegative weights that sum to 1.
weights	weights for each individual measure; if NULL (default), each measure is considered equally. Otherwise, it should be a length- K vector.
lambda	regularization parameter (default: 0.1).
p	an exponent for the order of the distance (default: 2).
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-10).
	init.vec an initial vector (default: uniform weight).
	maxiter maximum number of iterations (default: 496).
	print.progress a logical to show current iteration (default: FALSE).
distances	a length- K list where each element is an $(N \times N_k)$ pairwise distance between atoms of the fixed support and given measures.

Value

a length- N vector of probability vector.

References

Benamou J, Carlier G, Cuturi M, Nenna L, Peyré G (2015). "Iterative Bregman Projections for Regularized Transportation Problems." *SIAM Journal on Scientific Computing*, **37**(2), A1111–A1138. ISSN 1064-8275, 1095-7197.

Examples

```

#-----
#   Wasserstein Barycenter for Fixed Atoms with Two Gaussians
#
# * class 1 : samples from Gaussian with mean=(-4, -4)
# * class 2 : samples from Gaussian with mean=(+4, +4)
# * target support consists of 7 integer points from -6 to 6,
#   where ideally, weight is concentrated near 0 since it's average!
#-----
## GENERATE DATA
# Empirical Measures
set.seed(100)
ndat = 500
dat1 = matrix(rnorm(ndat*2, mean=-4, sd=0.5),ncol=2)
dat2 = matrix(rnorm(ndat*2, mean=+4, sd=0.5),ncol=2)

myatoms = list()
myatoms[[1]] = dat1
myatoms[[2]] = dat2
mydata = rbind(dat1, dat2)

# Fixed Support
support = cbind(seq(from=-8,to=8,by=2),
                seq(from=-8,to=8,by=2))

## COMPUTE
comp1 = bary15B(support, myatoms, lambda=0.5, maxiter=10)
comp2 = bary15B(support, myatoms, lambda=1,   maxiter=10)
comp3 = bary15B(support, myatoms, lambda=5,   maxiter=10)

## VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3))
barplot(comp1, main="lambda=0.5")
barplot(comp2, main="lambda=1")
barplot(comp3, main="lambda=5")
par(opar)

```

digit3

MNIST Images of Digit 3

Description

digit3 contains 2000 images from the famous MNIST dataset of digit 3. Each element of the list is an image represented as an (28×28) matrix that sums to 1. This normalization is conventional and it does not hurt its visualization via a basic `image()` function.

Usage

```
data(digit3)
```

Format

a length-2000 named list "digit3" of (28×28) matrices.

Examples

```
## LOAD THE DATA
data(digit3)

## SHOW A FEW
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,4), pty="s")
for (i in 1:8){
  image(digit3[[i]])
}
par(opar)
```

digits

MNIST Images of All Digits

Description

digits contains 5000 images from the famous MNIST dataset of all digits, consisting of 500 images per digit class from 0 to 9. Each digit image is represented as an (28×28) matrix that sums to 1. This normalization is conventional and it does not hurt its visualization via a basic image() function.

Usage

```
data(digits)
```

Format

a named list "digits" containing

image length-5000 list of (28×28) image matrices.

label length-5000 vector of class labels from 0 to 9.

Examples

```
## LOAD THE DATA
data(digits)

## SHOW A FEW
# Select 9 random images
subimgs = digits$image[sample(1:5000, 9)]

opar <- par(no.readonly=TRUE)
par(mfrow=c(3,3), pty="s")
```

```

for (i in 1:9){
  image(subings[[i]])
}
par(opar)

```

ecdfbary

Barycenter of Empirical CDFs

Description

Given a collection of empirical cumulative distribution functions $F^i(x)$ for $i = 1, \dots, N$, compute the Wasserstein barycenter of order 2. This is obtained by taking a weighted average on a set of corresponding quantile functions.

Usage

```
ecdfbary(ecdfs, weights = NULL, ...)
```

Arguments

ecdfs	a length- N list of "ecdf" objects by <code>stats::ecdf()</code> .
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	maxiter maximum number of iterations (default: 496).

Value

an "ecdf" object of the Wasserstein barycenter.

Examples

```

#-----
#                               Two Gaussians
#
# Two Gaussian distributions are parametrized as follows.
# Type 1 : (mean, var) = (-4, 1/4)
# Type 2 : (mean, var) = (+4, 1/4)
#-----
# GENERATE ECDFs
ecdf_list = list()
ecdf_list[[1]] = stats::ecdf(stats::rnorm(200, mean=-4, sd=0.5))
ecdf_list[[2]] = stats::ecdf(stats::rnorm(200, mean=+4, sd=0.5))

# COMPUTE THE BARYCENTER OF EQUAL WEIGHTS
emean = ecdfbary(ecdf_list)

```



```

# QUANTITIES FOR PLOTTING
x_grid = seq(from=-8, to=8, length.out=100)
y_type1 = ecdf_list[[1]](x_grid)
y_type2 = ecdf_list[[2]](x_grid)
y_bary = emean(x_grid)

# VISUALIZE
opar <- par(no.readonly=TRUE)
plot(x_grid, y_bary, lwd=3, col="red", type="l",
     main="Barycenter", xlab="x", ylab="Fn(x)")
lines(x_grid, y_type1, col="gray50", lty=3)
lines(x_grid, y_type2, col="gray50", lty=3)
par(opar)

```

ecdfmed

Wasserstein Median of Empirical CDFs

Description

Given a collection of empirical cumulative distribution functions $F^i(x)$ for $i = 1, \dots, N$, compute the Wasserstein median. This is obtained by a functional variant of the Weiszfeld algorithm on a set of quantile functions.

Usage

```
ecdfmed(ecdfs, weights = NULL, ...)
```

Arguments

ecdfs	a length- N list of "ecdf" objects by <code>stats::ecdf()</code> .
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	maxiter maximum number of iterations (default: 496).

Value

an "ecdf" object of the Wasserstein median.

Examples

```

#-----
#                               Tree Gaussians
#
# Three Gaussian distributions are parametrized as follows.
# Type 1 : (mean, sd) = (-4, 1)
# Type 2 : (mean, sd) = ( 0, 1/5)
# Type 3 : (mean, sd) = (+6, 1/2)
#-----
# GENERATE ECDFs
ecdf_list = list()
ecdf_list[[1]] = stats::ecdf(stats::rnorm(200, mean=-4, sd=1))
ecdf_list[[2]] = stats::ecdf(stats::rnorm(200, mean=+4, sd=0.2))
ecdf_list[[3]] = stats::ecdf(stats::rnorm(200, mean=+6, sd=0.5))

# COMPUTE THE MEDIAN
emeds = ecdfmed(ecdf_list)

# COMPUTE THE BARYCENTER
emean = ecdfbary(ecdf_list)

# QUANTITIES FOR PLOTTING
x_grid = seq(from=-8, to=10, length.out=500)
y_type1 = ecdf_list[[1]](x_grid)
y_type2 = ecdf_list[[2]](x_grid)
y_type3 = ecdf_list[[3]](x_grid)

y_bary = emean(x_grid)
y_meds = emeds(x_grid)

# VISUALIZE
opar <- par(no.readonly=TRUE)
plot(x_grid, y_bary, lwd=3, col="orange", type="l",
     main="Wasserstein Median & Barycenter",
     xlab="x", ylab="Fn(x)", lty=2)
lines(x_grid, y_meds, lwd=3, col="blue", lty=2)
lines(x_grid, y_type1, col="gray50", lty=3)
lines(x_grid, y_type2, col="gray50", lty=3)
lines(x_grid, y_type3, col="gray50", lty=3)
legend("topleft", legend=c("Median","Barycenter"),
      lwd=3, lty=2, col=c("blue","orange"))
par(opar)

```

Description

Given a collection of Gaussian distributions $\mathcal{N}(\mu_i, \sigma_i^2)$ for $i = 1, \dots, n$, compute the Wasserstein barycenter of order 2. For the barycenter computation of variance components, we use a fixed-point algorithm by Álvarez-Esteban et al. (2016).

Usage

```
gaussbary1d(means, vars, weights = NULL, ...)
```

Arguments

means	a length- n vector of mean parameters.
vars	a length- n vector of variance parameters.
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- n vector of nonnegative weights.
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	maxiter maximum number of iterations (default: 496).

Value

a named list containing

mean mean of the estimated barycenter distribution.

var variance of the estimated barycenter distribution.

References

Álvarez-Esteban PC, del Barrio E, Cuesta-Albertos JA, Matrán C (2016). “A Fixed-Point Approach to Barycenters in Wasserstein Space.” *Journal of Mathematical Analysis and Applications*, **441**(2), 744–762. ISSN 0022247X.

See Also

[gaussbarypd\(\)](#) for multivariate case.

Examples

```
#-----
#                               Two Gaussians
#
# Two Gaussian distributions are parametrized as follows.
# Type 1 : (mean, var) = (-4, 1/4)
# Type 2 : (mean, var) = (+4, 1/4)
#-----
# GENERATE PARAMETERS
par_mean = c(-4, 4)
par_vars = c(0.25, 0.25)
```

```

# COMPUTE THE BARYCENTER OF EQUAL WEIGHTS
gmean = gaussbary1d(par_mean, par_vars)

# QUANTITIES FOR PLOTTING
x_grid = seq(from=-6, to=6, length.out=200)
y_dist1 = stats::dnorm(x_grid, mean=-4, sd=0.5)
y_dist2 = stats::dnorm(x_grid, mean=+4, sd=0.5)
y_gmean = stats::dnorm(x_grid, mean=gmean$mean, sd=sqrt(gmean$var))

# VISUALIZE
opar <- par(no.readonly=TRUE)
plot(x_grid, y_gmean, lwd=2, col="red", type="l",
      main="Barycenter", xlab="x", ylab="density")
lines(x_grid, y_dist1)
lines(x_grid, y_dist2)
par(opar)

```

gaussbarypd

Barycenter of Gaussian Distributions in \mathbf{R}^p

Description

Given a collection of n -dimensional Gaussian distributions $\mathcal{N}(\mu_i, \Sigma_i^2)$ for $i = 1, \dots, n$, compute the Wasserstein barycenter of order 2. For the barycenter computation of variance components, we use a fixed-point algorithm by Álvarez-Esteban et al. (2016).

Usage

```
gaussbarypd(means, vars, weights = NULL, ...)
```

Arguments

means	an $(n \times p)$ matrix whose rows are mean vectors.
vars	a $(p \times p \times n)$ array where each slice is covariance matrix.
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- n vector of nonnegative weights.
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	maxiter maximum number of iterations (default: 496).

Value

a named list containing

mean a length- p vector for mean of the estimated barycenter distribution.

var a $(p \times p)$ matrix for variance of the estimated barycenter distribution.

References

Álvarez-Esteban PC, del Barrio E, Cuesta-Albertos JA, Matrán C (2016). “A Fixed-Point Approach to Barycenters in Wasserstein Space.” *Journal of Mathematical Analysis and Applications*, **441**(2), 744–762. ISSN 0022247X.

See Also

[gaussbary1d\(\)](#) for univariate case.

Examples

```
#-----
#                               Two Gaussians in R^2
#-----
# GENERATE PARAMETERS
# means
par_mean = rbind(c(-4,0), c(4,0))

# covariances
par_vars = array(0,c(2,2,2))
par_vars[, ,1] = cbind(c(4,-2),c(-2,4))
par_vars[, ,2] = cbind(c(4,+2),c(+2,4))

# COMPUTE THE BARYCENTER OF EQUAL WEIGHTS
gmean = gaussbarypd(par_mean, par_vars)

# GET COORDINATES FOR DRAWING
pt_type1 = gaussvis2d(par_mean[1,], par_vars[, ,1])
pt_type2 = gaussvis2d(par_mean[2,], par_vars[, ,2])
pt_gmean = gaussvis2d(gmean$mean, gmean$var)

# VISUALIZE
opar <- par(no.readonly=TRUE)
plot(pt_gmean, lwd=2, col="red", type="l",
     main="Barycenter", xlab="", ylab="",
     xlim=c(-6,6))
lines(pt_type1)
lines(pt_type2)
par(opar)
```

gaussmed1d

Wasserstein Median of Gaussian Distributions in R

Description

Given a collection of Gaussian distributions $\mathcal{N}(\mu_i, \sigma_i^2)$ for $i = 1, \dots, n$, compute the Wasserstein median.

Usage

```
gaussmed1d(means, vars, weights = NULL, ...)
```

Arguments

means a length- n vector of mean parameters.

vars a length- n vector of variance parameters.

weights a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- n vector of nonnegative weights.

... extra parameters including

abstol stopping criterion for iterations (default: 1e-8).

maxiter maximum number of iterations (default: 496).

Value

a named list containing

mean mean of the estimated median distribution.

var variance of the estimated median distribution.

See Also

[gaussmedpd\(\)](#) for multivariate case.

Examples

```
#-----
#                               Tree Gaussians
#
# Three Gaussian distributions are parametrized as follows.
# Type 1 : (mean, sd) = (-4, 1)
# Type 2 : (mean, sd) = ( 0, 1/5)
# Type 3 : (mean, sd) = (+6, 1/2)
#-----
# GENERATE PARAMETERS
par_mean = c(-4, 0, +6)
par_vars = c(1, 0.04, 0.25)

# COMPUTE THE WASSERSTEIN MEDIAN
gmeds = gaussmed1d(par_mean, par_vars)

# COMPUTE THE BARYCENTER
gmean = gaussbary1d(par_mean, par_vars)

# QUANTITIES FOR PLOTTING
x_grid = seq(from=-6, to=8, length.out=1000)
y_dist1 = stats::dnorm(x_grid, mean=par_mean[1], sd=sqrt(par_vars[1]))
y_dist2 = stats::dnorm(x_grid, mean=par_mean[2], sd=sqrt(par_vars[2]))
y_dist3 = stats::dnorm(x_grid, mean=par_mean[3], sd=sqrt(par_vars[3]))
```

```

y_gmean = stats::dnorm(x_grid, mean=gmean$mean, sd=sqrt(gmean$var))
y_gmeds = stats::dnorm(x_grid, mean=gmeds$mean, sd=sqrt(gmeds$var))

# VISUALIZE
opar <- par(no.readonly=TRUE)
plot(x_grid, y_gmeds, lwd=3, col="red", type="l",
      main="Three Gaussians", xlab="x", ylab="density",
      xlim=range(x_grid), ylim=c(0,2.5))
lines(x_grid, y_gmean, lwd=3, col="blue")
lines(x_grid, y_dist1, lwd=1.5, lty=2)
lines(x_grid, y_dist2, lwd=1.5, lty=2)
lines(x_grid, y_dist3, lwd=1.5, lty=2)
legend("topleft", legend=c("Median", "Barycenter"),
      col=c("red", "blue"), lwd=c(3,3), lty=c(1,2))
par(opar)

```

gaussmedpd

Wasserstein Median of Gaussian Distributions in \mathbf{R}^p

Description

Given a collection of p -dimensional Gaussian distributions $\mathcal{N}(\mu_i, \sigma_i^2)$ for $i = 1, \dots, n$, compute the Wasserstein median.

Usage

```
gaussmedpd(means, vars, weights = NULL, ...)
```

Arguments

means	an $(n \times p)$ matrix whose rows are mean vectors.
vars	a $(p \times p \times n)$ array where each slice is covariance matrix.
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- n vector of nonnegative weights.
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	maxiter maximum number of iterations (default: 496).

Value

a named list containing

mean a length- p vector for mean of the estimated median distribution.

var a $(p \times p)$ matrix for variance of the estimated median distribution.

See Also

[gaussmed1d\(\)](#) for univariate case.

Examples

```

#-----
#                               Three Gaussians in R^2
#-----
# GENERATE PARAMETERS
# means
par_mean = rbind(c(-4,0), c(0,0), c(5,-1))

# covariances
par_vars = array(0,c(2,2,3))
par_vars[,,1] = cbind(c(2,-1),c(-1,2))
par_vars[,,2] = cbind(c(4,+1),c(+1,4))
par_vars[,,3] = diag(c(4,1))

# COMPUTE THE MEDIAN
gmeds = gaussmedpd(par_mean, par_vars)

# COMPUTE THE BARYCENTER
gmean = gaussbarypd(par_mean, par_vars)

# GET COORDINATES FOR DRAWING
pt_type1 = gaussvis2d(par_mean[1,], par_vars[,,1])
pt_type2 = gaussvis2d(par_mean[2,], par_vars[,,2])
pt_type3 = gaussvis2d(par_mean[3,], par_vars[,,3])
pt_gmean = gaussvis2d(gmean$mean, gmean$var)
pt_gmeds = gaussvis2d(gmeds$mean, gmeds$var)

# VISUALIZE
opar <- par(no.readonly=TRUE)
plot(pt_gmean, lwd=2, col="red", type="l",
     main="Three Gaussians", xlab="", ylab="",
     xlim=c(-6,8), ylim=c(-2.5,2.5))
lines(pt_gmeds, lwd=2, col="blue")
lines(pt_type1, lty=2, lwd=5)
lines(pt_type2, lty=2, lwd=5)
lines(pt_type3, lty=2, lwd=5)
abline(h=0, col="grey80", lty=3)
abline(v=0, col="grey80", lty=3)
legend("topright", legend=c("Median", "Barycenter"),
     lwd=2, lty=1, col=c("blue", "red"))
par(opar)

```


Description

This function samples points along the contour of an ellipse represented by mean and variance parameters for a 2-dimensional Gaussian distribution to help ease manipulating visualization of the specified distribution. For example, you can directly use a basic `plot()` function directly for drawing.

Usage

```
gaussvis2d(mean, var, n = 500)
```

Arguments

<code>mean</code>	a length-2 vector for mean parameter.
<code>var</code>	a (2×2) matrix for covariance parameter.
<code>n</code>	the number of points to be drawn (default: 500).

Value

an $(n \times 2)$ matrix.

Examples

```
#-----
#                               Three Gaussians in R^2
#-----
# MEAN PARAMETERS
loc1 = c(-3,0)
loc2 = c(0,5)
loc3 = c(3,0)

# COVARIANCE PARAMETERS
var1 = cbind(c(4,-2),c(-2,4))
var2 = diag(c(9,1))
var3 = cbind(c(4,2),c(2,4))

# GENERATE POINTS
visA = gaussvis2d(loc1, var1)
visB = gaussvis2d(loc2, var2)
visC = gaussvis2d(loc3, var3)

# VISUALIZE
opar <- par(no.readonly=TRUE)
plot(visA[,1], visA[,2], type="l", xlim=c(-5,5), ylim=c(-2,9),
      lwd=3, col="red", main="3 Gaussian Distributions")
lines(visB[,1], visB[,2], lwd=3, col="blue")
lines(visC[,1], visC[,2], lwd=3, col="orange")
legend("top", legend=c("Type 1","Type 2","Type 3"),
      lwd=3, col=c("red","blue","orange"), horiz=TRUE)
par(opar)
```

 histbary14C

Barycenter of Histograms by Cuturi & Doucet (2014)

Description

Given multiple histograms represented as "histogram" S3 objects, compute Wasserstein barycenter. We need one requirement that all histograms in an input list `hists` must have **same breaks**. See the example on how to construct a histogram on predefined breaks/bins.

Usage

```
histbary14C(hists, p = 2, weights = NULL, lambda = NULL, ...)
```

Arguments

<code>hists</code>	a length- N list of histograms ("histogram" object) of same breaks.
<code>p</code>	an exponent for the order of the distance (default: 2).
<code>weights</code>	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
<code>lambda</code>	a regularization parameter; if NULL (default), a paper's suggestion would be taken, or it should be a nonnegative real number.
<code>...</code>	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	init.vec an initial weight vector (default: uniform weight).
	maxiter maximum number of iterations (default: 496).
	nthread number of threads for OpenMP run (default: 1).
	print.progress a logical to show current iteration (default: TRUE).

Value

a "histogram" object of barycenter.

References

Cuturi M, Doucet A (2014). "Fast computation of wasserstein barycenters." In Xing EP, Jebara T (eds.), *Proceedings of the 31st international conference on international conference on machine learning - volume 32*, volume 32 of *Proceedings of machine learning research*, 685–693.

See Also

[bary14C](#)

Examples

```

#-----
#                               Binned from Two Gaussians
#
# EXAMPLE : Very Small Example for CRAN; just showing how to use it!
#-----
# GENERATE FROM TWO GAUSSIANS WITH DIFFERENT MEANS
set.seed(100)
x = stats::rnorm(1000, mean=-4, sd=0.5)
y = stats::rnorm(1000, mean=+4, sd=0.5)
bk = seq(from=-10, to=10, length.out=20)

# HISTOGRAMS WITH COMMON BREAKS
histxy = list()
histxy[[1]] = hist(x, breaks=bk, plot=FALSE)
histxy[[2]] = hist(y, breaks=bk, plot=FALSE)

# COMPUTE
hh = histbary14C(histxy, maxiter=5)

# VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2))
barplot(histxy[[1]]$density, col=rgb(0,0,1,1/4),
        ylim=c(0, 0.75), main="Two Histograms")
barplot(histxy[[2]]$density, col=rgb(1,0,0,1/4),
        ylim=c(0, 0.75), add=TRUE)
barplot(hh$density, main="Barycenter",
        ylim=c(0, 0.75))
par(opar)

```

 histbary15B

Barycenter of Histograms by Benamou et al. (2015)

Description

Given multiple histograms represented as "histogram" S3 objects, compute Wasserstein barycenter. We need one requirement that all histograms in an input list `hists` must have **same breaks**. See the example on how to construct a histogram on predefined breaks/bins.

Usage

```
histbary15B(hists, p = 2, weights = NULL, lambda = NULL, ...)
```

Arguments

hists	a length- N list of histograms ("histogram" object) of same breaks.
p	an exponent for the order of the distance (default: 2).
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
lambda	a regularization parameter; if NULL (default), a paper's suggestion would be taken, or it should be a nonnegative real number.
...	extra parameters including abstol stopping criterion for iterations (default: 1e-8). init.vec an initial weight vector (default: uniform weight). maxiter maximum number of iterations (default: 496). nthread number of threads for OpenMP run (default: 1). print.progress a logical to show current iteration (default: TRUE).

Value

a "histogram" object of barycenter.

References

Benamou J, Carlier G, Cuturi M, Nenna L, Peyré G (2015). "Iterative Bregman Projections for Regularized Transportation Problems." *SIAM Journal on Scientific Computing*, **37**(2), A1111–A1138. ISSN 1064-8275, 1095-7197.

See Also

[bary15B](#)

Examples

```
#-----
#                               Binned from Two Gaussians
#
# EXAMPLE : Very Small Example for CRAN; just showing how to use it!
#-----
# GENERATE FROM TWO GAUSSIANS WITH DIFFERENT MEANS
set.seed(100)
x = stats::rnorm(1000, mean=-4, sd=0.5)
y = stats::rnorm(1000, mean=+4, sd=0.5)
bk = seq(from=-10, to=10, length.out=20)

# HISTOGRAMS WITH COMMON BREAKS
histxy = list()
histxy[[1]] = hist(x, breaks=bk, plot=FALSE)
histxy[[2]] = hist(y, breaks=bk, plot=FALSE)

# COMPUTE
hh = histbary15B(histxy, maxiter=5)
```

```

# VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2))
barplot(histxy[[1]]$density, col=rgb(0,0,1,1/4),
        ylim=c(0, 0.75), main="Two Histograms")
barplot(histxy[[2]]$density, col=rgb(1,0,0,1/4),
        ylim=c(0, 0.75), add=TRUE)
barplot(hh$density, main="Barycenter",
        ylim=c(0, 0.75))
par(opar)

```

histmed22Y

Wasserstein Median of Histograms by You et al. (2022)

Description

Given multiple histograms represented as "histogram" S3 objects, compute the Wasserstein median of order 2. We need one requirement that all histograms in an input list `hists` must have **same breaks**. See the example on how to construct a histogram on predefined breaks/bins.

Usage

```
histmed22Y(hists, weights = NULL, lambda = NULL, ...)
```

Arguments

<code>hists</code>	a length- N list of histograms ("histogram" object) of same breaks.
<code>weights</code>	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
<code>lambda</code>	a regularization parameter; if NULL (default), a paper's suggestion would be taken, or it should be a nonnegative real number.
<code>...</code>	extra parameters including <ul style="list-style-type: none"> abstol stopping criterion for iterations (default: 1e-8). init.vec an initial weight vector (default: uniform weight). maxiter maximum number of iterations (default: 496). nthread number of threads for OpenMP run (default: 1). print.progress a logical to show current iteration (default: FALSE).

Value

a "histogram" object of the Wasserstein median histogram.

Examples

```

#-----
#                               Binned from Two Gaussians
#
# EXAMPLE : small example for CRAN for visualization purpose.
#-----
# GENERATE FROM TWO GAUSSIANS WITH DIFFERENT MEANS
set.seed(100)
x = stats::rnorm(1000, mean=-4, sd=0.5)
y = stats::rnorm(1000, mean=+4, sd=0.5)
bk = seq(from=-10, to=10, length.out=20)

# HISTOGRAMS WITH COMMON BREAKS
histxy = list()
histxy[[1]] = hist(x, breaks=bk, plot=FALSE)
histxy[[2]] = hist(y, breaks=bk, plot=FALSE)

# COMPUTE
hmean = histbary15B(histxy)
hmeds = histmed22Y(histxy)

# VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3))
barplot(histxy[[1]]$density, col=rgb(0,0,1,1/4),
        ylim=c(0, 1.05), main="Two Histograms")
barplot(histxy[[2]]$density, col=rgb(1,0,0,1/4),
        ylim=c(0, 1.05), add=TRUE)
barplot(hmean$density, main="Barycenter",
        ylim=c(0, 1.05))
barplot(hmeds$density, main="Wasserstein Median",
        ylim=c(0, 1.05))
par(opar)

```

imagebary14C

Barycenter of Images according to Cuturi & Doucet (2014)

Description

Using entropic regularization for Wasserstein barycenter computation, `imagebary14C` finds a *barycentric* image X^* given multiple images X_1, X_2, \dots, X_N . Please note the followings; (1) we only take a matrix as an image so please make it grayscale if not, (2) all images should be of same size - no resizing is performed.

Usage

```
imagebary14C(images, p = 2, weights = NULL, lambda = NULL, ...)
```

Arguments

images	a length- N list of same-size image matrices of size $(m \times n)$.
p	an exponent for the order of the distance (default: 2).
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
lambda	a regularization parameter; if NULL (default), a paper's suggestion would be taken, or it should be a nonnegative real number.
...	extra parameters including <ul style="list-style-type: none"> abstol stopping criterion for iterations (default: 1e-8). init.image an initial weight image (default: uniform weight). maxiter maximum number of iterations (default: 496). nthread number of threads for OpenMP run (default: 1). print.progress a logical to show current iteration (default: TRUE).

Value

an $(m \times n)$ matrix of the barycentric image.

References

Cuturi M, Doucet A (2014). "Fast computation of wasserstein barycenters." In Xing EP, Jebara T (eds.), *Proceedings of the 31st international conference on international conference on machine learning - volume 32*, volume 32 of *Proceedings of machine learning research*, 685–693.

See Also

[bary14C](#)

Examples

```
## Not run:
#-----
#                               MNIST Data with Digit 3
#
# EXAMPLE 1 : Very Small Example for CRAN; just showing how to use it!
# EXAMPLE 2 : Medium-size Example for Evolution of Output
#-----
# EXAMPLE 1
data(digit3)
datsmall = digit3[1:2]
outsmall = imagebary14C(datsmall, maxiter=3)

# EXAMPLE 2 : Barycenter of 100 Images
# RANDOMLY SELECT THE IMAGES
data(digit3)
dat2 = digit3[sample(1:2000, 100)] # select 100 images

# RUN SEQUENTIALLY
```

```

run10 = imagebary14C(dat2, maxiter=10)           # first 10 iterations
run20 = imagebary14C(dat2, maxiter=10, init.image=run10) # run 40 more
run50 = imagebary14C(dat2, maxiter=30, init.image=run20) # run 50 more

# VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,3), pty="s")
image(dat2[[sample(100,1)]], axes=FALSE, main="a random image")
image(dat2[[sample(100,1)]], axes=FALSE, main="a random image")
image(dat2[[sample(100,1)]], axes=FALSE, main="a random image")
image(run10, axes=FALSE, main="barycenter after 10 iter")
image(run20, axes=FALSE, main="barycenter after 20 iter")
image(run50, axes=FALSE, main="barycenter after 50 iter")
par(opar)

## End(Not run)

```

imagebary15B

Barycenter of Images according to Benamou et al. (2015)

Description

Using entropic regularization for Wasserstein barycenter computation, imagebary15B finds a *barycentric* image X^* given multiple images X_1, X_2, \dots, X_N . Please note the followings; (1) we only take a matrix as an image so please make it grayscale if not, (2) all images should be of same size - no resizing is performed.

Usage

```
imagebary15B(images, p = 2, weights = NULL, lambda = NULL, ...)
```

Arguments

images	a length- N list of same-size image matrices of size $(m \times n)$.
p	an exponent for the order of the distance (default: 2).
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
lambda	a regularization parameter; if NULL (default), a paper's suggestion would be taken, or it should be a nonnegative real number.
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	init.image an initial weight image (default: uniform weight).
	maxiter maximum number of iterations (default: 496).
	nthread number of threads for OpenMP run (default: 1).
	print.progress a logical to show current iteration (default: TRUE).

Value

an $(m \times n)$ matrix of the barycentric image.

References

Benamou J, Carlier G, Cuturi M, Nenna L, Peyré G (2015). “Iterative Bregman Projections for Regularized Transportation Problems.” *SIAM Journal on Scientific Computing*, **37**(2), A1111–A1138. ISSN 1064-8275, 1095-7197.

See Also

[bary15B](#)

Examples

```
#-----
#                               MNIST Data with Digit 3
#
# EXAMPLE 1 : Very Small Example for CRAN; just showing how to use it!
# EXAMPLE 2 : Medium-size Example for Evolution of Output
#-----
# EXAMPLE 1
data(digit3)
datsmall = digit3[1:2]
outsmall = imagebary15B(datsmall, maxiter=3)

## Not run:
# EXAMPLE 2 : Barycenter of 100 Images
# RANDOMLY SELECT THE IMAGES
data(digit3)
dat2 = digit3[sample(1:2000, 100)] # select 100 images

# RUN SEQUENTIALLY
run05 = imagebary15B(dat2, maxiter=5) # first 5 iterations
run10 = imagebary15B(dat2, maxiter=5, init.image=run05) # run 5 more
run50 = imagebary15B(dat2, maxiter=40, init.image=run10) # run 40 more

# VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,3), pty="s")
image(dat2[[sample(100,1)]], axes=FALSE, main="a random image")
image(dat2[[sample(100,1)]], axes=FALSE, main="a random image")
image(dat2[[sample(100,1)]], axes=FALSE, main="a random image")
image(run05, axes=FALSE, main="barycenter after 05 iter")
image(run10, axes=FALSE, main="barycenter after 10 iter")
image(run50, axes=FALSE, main="barycenter after 50 iter")
par(opar)

## End(Not run)
```

 imagemed22Y

 Wasserstein Median of Images by You et al. (2022)

Description

Given multiple images X_1, \dots, X_N , the Wasserstein median of order 2 is computed. The proposed method relies on a choice of barycenter computation in that we opt for an algorithm of [imagebary15B](#), which uses entropic regularization for barycenter computation. Please note the followings; (1) we only take a matrix as an image so please make it grayscale if not, (2) all images should be of same size - no resizing is performed.

Usage

```
imagemed22Y(images, weights = NULL, lambda = NULL, ...)
```

Arguments

images	a length- N list of same-size image matrices of size $(m \times n)$.
weights	a weight of each image; if NULL (default), uniform weight is set. Otherwise, it should be a length- N vector of nonnegative weights.
lambda	a regularization parameter; if NULL (default), a paper's suggestion would be taken, or it should be a nonnegative real number.
...	extra parameters including
	abstol stopping criterion for iterations (default: 1e-8).
	init.image an initial weight image (default: uniform weight).
	maxiter maximum number of iterations (default: 496).
	nthread number of threads for OpenMP run (default: 1).
	print.progress a logical to show current iteration (default: TRUE).

Value

an $(m \times n)$ matrix of the Wasserstein median image.

Examples

```
## Not run:
#-----
#                               MNIST Data with Digit 3
#
# EXAMPLE : Very Small Example for CRAN; just showing how to use it!
#-----
# LOAD THE DATA
data(digit3)
datsmall = digit3[1:10]

# COMPUTE
```

```

outsmall = imagemed22Y(datsmall, maxiter=5)

# VISUALIZE
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,4), pty="s")
image(outsmall, xaxt='n', yaxt='n', main="Wasserstein Median")
image(datsmall[[3]], xaxt='n', yaxt='n', main="3rd image")
image(datsmall[[6]], xaxt='n', yaxt='n', main="6th image")
image(datsmall[[9]], xaxt='n', yaxt='n', main="9th image")
par(opar)

## End(Not run)

```

Description

Due to high computational cost for linear programming approaches to compute Wasserstein distance, Cuturi (2013) proposed an entropic regularization scheme as an efficient approximation to the original problem. This comes with a regularization parameter $\lambda > 0$ in the term

$$\lambda h(\Gamma) = \lambda \sum_{m,n} \Gamma_{m,n} \log(\Gamma_{m,n}).$$

IPOT algorithm is known to be relatively robust to the choice of regularization parameter λ . Empirical observation says that very small number of inner loop iteration like $L=1$ is sufficient.

Usage

```
ipot(X, Y, p = 2, wx = NULL, wy = NULL, lambda = 1, ...)
```

```
ipotD(D, p = 2, wx = NULL, wy = NULL, lambda = 1, ...)
```

Arguments

X	an $(M \times P)$ matrix of row observations.
Y	an $(N \times P)$ matrix of row observations.
p	an exponent for the order of the distance (default: 2).
wx	a length- M marginal density that sums to 1. If NULL (default), uniform weight is set.
wy	a length- N marginal density that sums to 1. If NULL (default), uniform weight is set.
lambda	a regularization parameter (default: 0.1).
...	extra parameters including

maxiter maximum number of iterations (default: 496).
abstol stopping criterion for iterations (default: 1e-10).
L small number of inner loop iterations (default: 1).
D an $(M \times N)$ distance matrix $d(x_m, y_n)$ between two sets of observations.

Value

a named list containing

distance \mathcal{W}_p distance value

iteration the number of iterations it took to converge.

plan an $(M \times N)$ nonnegative matrix for the optimal transport plan.

References

Xie Y, Wang X, Wang R, Zha H (2020). “A fast proximal point method for computing exact wasserstein distance.” In Adams RP, Gogate V (eds.), *Proceedings of The 35th Uncertainty in Artificial Intelligence Conference*, volume 115 of *Proceedings of machine learning research*, 433–453.

Examples

```

#-----
# Wasserstein Distance between Samples from Two Bivariate Normal
#
# * class 1 : samples from Gaussian with mean=(-1, -1)
# * class 2 : samples from Gaussian with mean=(+1, +1)
#-----
## SMALL EXAMPLE
set.seed(100)
m = 20
n = 30
X = matrix(rnorm(m*2, mean=-1),ncol=2) # m obs. for X
Y = matrix(rnorm(n*2, mean=+1),ncol=2) # n obs. for Y

## COMPARE WITH WASSERSTEIN
outw = wasserstein(X, Y)
ipt1 = ipot(X, Y, lambda=1)
ipt2 = ipot(X, Y, lambda=10)

## VISUALIZE : SHOW THE PLAN AND DISTANCE
pmw = paste0("wasserstein plan ; dist=",round(outw$distance,2))
pm1 = paste0("ipot lbd=1 ; dist=",round(ipt1$distance,2))
pm2 = paste0("ipot lbd=10; dist=",round(ipt2$distance,2))

opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3))
image(outw$plan, axes=FALSE, main=pmw)
image(ipt1$plan, axes=FALSE, main=pm1)
image(ipt2$plan, axes=FALSE, main=pm2)
par(opar)

```

sinkhorn

*Wasserstein Distance by Entropic Regularization***Description**

Due to high computational cost for linear programming approaches to compute Wasserstein distance, Cuturi (2013) proposed an entropic regularization scheme as an efficient approximation to the original problem. This comes with a regularization parameter $\lambda > 0$ in the term

$$\lambda h(\Gamma) = \lambda \sum_{m,n} \Gamma_{m,n} \log(\Gamma_{m,n}).$$

As $\lambda \rightarrow 0$, the solution to an approximation problem approaches to the solution of a true problem. However, we have an issue with numerical underflow. Our implementation returns an error when it happens, so please use a larger number when necessary.

Usage

```
sinkhorn(X, Y, p = 2, wx = NULL, wy = NULL, lambda = 0.1, ...)
```

```
sinkhornD(D, p = 2, wx = NULL, wy = NULL, lambda = 0.1, ...)
```

Arguments

X	an $(M \times P)$ matrix of row observations.
Y	an $(N \times P)$ matrix of row observations.
p	an exponent for the order of the distance (default: 2).
wx	a length- M marginal density that sums to 1. If NULL (default), uniform weight is set.
wy	a length- N marginal density that sums to 1. If NULL (default), uniform weight is set.
lambda	a regularization parameter (default: 0.1).
...	extra parameters including maxiter maximum number of iterations (default: 496). abstol stopping criterion for iterations (default: 1e-10).
D	an $(M \times N)$ distance matrix $d(x_m, y_n)$ between two sets of observations.

Value

a named list containing

distance \mathcal{W}_p distance value.

iteration the number of iterations it took to converge.

plan an $(M \times N)$ nonnegative matrix for the optimal transport plan.

References

Cuturi M (2013). “Sinkhorn distances: Lightspeed computation of optimal transport.” In *Proceedings of the 26th international conference on neural information processing systems - volume 2*, NIPS’13, 2292–2300.

Examples

```

#-----
# Wasserstein Distance between Samples from Two Bivariate Normal
#
# * class 1 : samples from Gaussian with mean=(-1, -1)
# * class 2 : samples from Gaussian with mean=(+1, +1)
#-----
## SMALL EXAMPLE
set.seed(100)
m = 20
n = 10
X = matrix(rnorm(m*2, mean=-1),ncol=2) # m obs. for X
Y = matrix(rnorm(n*2, mean=+1),ncol=2) # n obs. for Y

## COMPARE WITH WASSERSTEIN
outw = wasserstein(X, Y)
skh1 = sinkhorn(X, Y, lambda=0.05)
skh2 = sinkhorn(X, Y, lambda=0.10)

## VISUALIZE : SHOW THE PLAN AND DISTANCE
pm1 = paste0("wasserstein plan ; distance=",round(outw$distance,2))
pm2 = paste0("sinkhorn lbd=0.05; distance=",round(skh1$distance,2))
pm5 = paste0("sinkhorn lbd=0.1 ; distance=",round(skh2$distance,2))

opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3))
image(outw$plan, axes=FALSE, main=pm1)
image(skh1$plan, axes=FALSE, main=pm2)
image(skh2$plan, axes=FALSE, main=pm5)
par(opar)

```

swdist

Sliced Wasserstein Distance

Description

Sliced Wasserstein (SW) Distance (Rabin et al. 2012) is a popular alternative to the standard Wasserstein distance due to its computational efficiency on top of nice theoretical properties. For the d -dimensional probability measures μ and ν , the SW distance is defined as

$$SW_p(\mu, \nu) = \left(\int_{\mathbf{S}^{d-1}} \mathcal{W}_p^p(\langle \theta, \mu \rangle, \langle \theta, \nu \rangle) d\lambda(\theta) \right)^{1/p},$$

where \mathbf{S}^{d-1} is the $(d-1)$ -dimensional unit hypersphere and λ is the uniform distribution on \mathbf{S}^{d-1} . Practically, it is computed via Monte Carlo integration.

Usage

```
swdist(X, Y, p = 2, ...)
```

Arguments

X an $(M \times P)$ matrix of row observations.
Y an $(N \times P)$ matrix of row observations.
p an exponent for the order of the distance (default: 2).
... extra parameters including
nproj the number of Monte Carlo samples for SW computation (default: 496).

Value

a named list containing

distance \mathcal{SW}_p distance value.

projdist a length- n vector of projected univariate distances.

References

Rabin J, Peyré G, Delon J, Bernot M (2012). “Wasserstein Barycenter and Its Application to Texture Mixing.” In Bruckstein AM, ter Haar Romeny BM, Bronstein AM, Bronstein MM (eds.), *Scale Space and Variational Methods in Computer Vision*, volume 6667, 435–446. Springer Berlin Heidelberg, Berlin, Heidelberg.

Examples

```
#-----
# Sliced-Wasserstein Distance between Two Bivariate Normal
#
# * class 1 : samples from Gaussian with mean=(-1, -1)
# * class 2 : samples from Gaussian with mean=(+1, +1)
#-----
# SMALL EXAMPLE
set.seed(100)
m = 20
n = 30
X = matrix(rnorm(m*2, mean=-1),ncol=2) # m obs. for X
Y = matrix(rnorm(n*2, mean=+1),ncol=2) # n obs. for Y

# COMPUTE THE SLICED-WASSERSTEIN DISTANCE
outsw <- swdist(X, Y, nproj=100)

# VISUALIZE
# prepare ingredients for plotting
plot_x = 1:1000
```

```

plot_y = base::cumsum(outsw$projdist)/plot_x

# draw
opar <- par(no.readonly=TRUE)
plot(plot_x, plot_y, type="b", cex=0.1, lwd=2,
      xlab="number of MC samples", ylab="distance",
      main="Effect of MC Sample Size")
abline(h=outsw$distance, col="red", lwd=2)
legend("bottomright", legend="SW Distance",
      col="red", lwd=2)
par(opar)

```

wasserstein

Wasserstein Distance between Empirical Measures

Description

Given two empirical measures μ, ν consisting of M and N observations on \mathcal{X} , p -Wasserstein distance for $p \geq 1$ between two empirical measures is defined as

$$\mathcal{W}_p(\mu, \nu) = \left(\inf_{\gamma \in \Gamma(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{X}} d(x, y)^p d\gamma(x, y) \right)^{1/p}$$

where $\Gamma(\mu, \nu)$ denotes the collection of all measures/couplings on $\mathcal{X} \times \mathcal{X}$ whose marginals are μ and ν on the first and second factors, respectively. Please see the section for detailed description on the usage of the function.

Usage

```
wasserstein(X, Y, p = 2, wx = NULL, wy = NULL)
```

```
wassersteinD(D, p = 2, wx = NULL, wy = NULL)
```

Arguments

- | | |
|----|--|
| X | an $(M \times P)$ matrix of row observations. |
| Y | an $(N \times P)$ matrix of row observations. |
| p | an exponent for the order of the distance (default: 2). |
| wx | a length- M marginal density that sums to 1. If NULL (default), uniform weight is set. |
| wy | a length- N marginal density that sums to 1. If NULL (default), uniform weight is set. |
| D | an $(M \times N)$ distance matrix $d(x_m, y_n)$ between two sets of observations. |

Value

a named list containing

distance \mathcal{W}_p distance value.

plan an $(M \times N)$ nonnegative matrix for the optimal transport plan.

Using wasserstein() function

We assume empirical measures are defined on the Euclidean space $\mathcal{X} = \mathbf{R}^d$,

$$\mu = \sum_{m=1}^M \mu_m \delta_{X_m} \quad \text{and} \quad \nu = \sum_{n=1}^N \nu_n \delta_{Y_n}$$

and the distance metric used here is standard Euclidean norm $d(x, y) = \|x - y\|$. Here, the marginals $(\mu_1, \mu_2, \dots, \mu_M)$ and $(\nu_1, \nu_2, \dots, \nu_N)$ correspond to `wx` and `wy`, respectively.

Using wassersteinD() function

If other distance measures or underlying spaces are one's interests, we have an option for users to provide a distance matrix `D` rather than vectors, where

$$D := D_{M \times N} = d(X_m, Y_n)$$

for flexible modeling.

References

Peyré G, Cuturi M (2019). "Computational Optimal Transport: With Applications to Data Science." *Foundations and Trends® in Machine Learning*, **11**(5-6), 355–607. ISSN 1935-8237, 1935-8245.

Examples

```
#-----
# Wasserstein Distance between Samples from Two Bivariate Normal
#
# * class 1 : samples from Gaussian with mean=(-1, -1)
# * class 2 : samples from Gaussian with mean=(+1, +1)
#-----
## SMALL EXAMPLE
m = 20
n = 10
X = matrix(rnorm(m*2, mean=-1), ncol=2) # m obs. for X
Y = matrix(rnorm(n*2, mean=+1), ncol=2) # n obs. for Y

## COMPUTE WITH DIFFERENT ORDERS
out1 = wasserstein(X, Y, p=1)
out2 = wasserstein(X, Y, p=2)
out5 = wasserstein(X, Y, p=5)

## VISUALIZE : SHOW THE PLAN AND DISTANCE
pm1 = paste0("plan p=1; distance=", round(out1$distance, 2))
```

```

pm2 = paste0("plan p=2; distance=",round(out2$distance,2))
pm5 = paste0("plan p=5; distance=",round(out5$distance,2))

opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3))
image(out1$plan, axes=FALSE, main=pm1)
image(out2$plan, axes=FALSE, main=pm2)
image(out5$plan, axes=FALSE, main=pm5)
par(opar)

## Not run:
## COMPARE WITH ANALYTIC RESULTS
# For two Gaussians with same covariance, their
# 2-Wasserstein distance is known so let's compare !

niter = 1000          # number of iterations
vdist = rep(0,niter)
for (i in 1:niter){
  mm = sample(30:50, 1)
  nn = sample(30:50, 1)

  X = matrix(rnorm(mm*2, mean=-1),ncol=2)
  Y = matrix(rnorm(nn*2, mean=+1),ncol=2)

  vdist[i] = wasserstein(X, Y, p=2)$distance
  if (i%%10 == 0){
    print(paste0("iteration ",i,"/", niter," complete."))
  }
}

# Visualize
opar <- par(no.readonly=TRUE)
hist(vdist, main="Monte Carlo Simulation")
abline(v=sqrt(8), lwd=2, col="red")
par(opar)

## End(Not run)

```

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