Package ‘T4transport’

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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:10.1561/2200000073> for the general exposition to the study of computational optimal transport.
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Wasserstein Barycenter via Entropic Regularization by Cuturi & Doucet (2014)

Description

Given $K$ empirical measures $\mu_1, \mu_2, \ldots, \mu_K$, wasserstein barycenter $\mu^*$ is the solution to the following problem

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

where $\pi_k$'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. Here the subgradient is approximated using the entropic regularization.

Usage

```r
barysinkhorn14(
  support,
  measures,
  marginals = NULL,
  weights = NULL,
  lambda = 0.1,
  p = 2,
  ...
)

barysinkhorn14D(
  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.
- **measures**: 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 $(N \times N_i)$ pairwise distance between atoms of the fixed support and given measures.

References


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)
dat1 = matrix(rnorm(sample(20:50, 1)*2, mean=-4, sd=0.5),ncol=2)
dat2 = matrix(rnorm(sample(20:50, 1)*2, mean=+4, sd=0.5),ncol=2)
measures = list()
measures[[1]] = dat1
measures[[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 = barysinkhorn14(support, measures, lambda=0.5, maxiter=10)
comp2 = barysinkhorn14(support, measures, lambda=1, maxiter=10)
comp3 = barysinkhorn14(support, measures, 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")
digit3 contains 2000 images from the famous MNIST dataset of digit 3. Each element of the list is an image represented as an $(28 \times 28)$ matrix that sums to 1. This normalization is conventional and it does not hurt its visualization via a basic `image()` function.

**Usage**

```r
data(digit3)
```

**Format**

A length-2000 named list “digit3” of $(28 \times 28)$ matrices.

**Examples**

```r
## 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)
```

Using entropic regularization for Wasserstein barycenter computation, `image14C` finds a barycentric image $X^*$ given multiple images $X_1, X_2, \ldots, X_N$. 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**

```r
image14C(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


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 = image14C(datsmall, maxiter=3)
## Not run:
# EXAMPLE 2 : Barycenter of 100 Images
# RANDOMLY SELECT THE IMAGES
dat2 = digit3[sample(1:2000, 100)] # select 100 images

# RUN SEQUENTIALLY
run10 = image14C(dat2, maxiter=10) # first 10 iterations
run20 = image14C(dat2, maxiter=10, init.image=run10) # run 40 more
run50 = image14C(dat2, maxiter=30, init.image=run20) # run 50 more
sinkhorn

Sinkhorn Distance by Cuturi (2013)

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 $\lambda \to 0$, 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
sinkhorn

**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**


**Examples**

```r
#-------------------------------------------------------------------
# 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)
```
**Wasserstein Distance between Empirical Measures**

**Description**

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

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

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

**Usage**

```r
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** $W_p$ distance value
- **plan** an $(M \times N)$ nonnegative matrix for the optimal transport plan.

**Usage**

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

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

and the distance metric used here is standard Euclidean norm $d(x, y) = ||x - y||$. Here, the marginals $(\mu_1, \mu_2, \ldots, \mu_M)$ and $(\nu_1, \nu_2, \ldots, \nu_N)$ 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


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 = 5000  # 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.\n"))
    }
}

# 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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