Package 'support'

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e_dist

support-package

Support Points

Description

The 'support' package provides functions for computing support points.

Details

Package: support
Type: Package
Version: 0.1.4
Date: 2019-07-15
License: GPL (>= 2)

The 'support' package provides the functions sp() and sp_seq() for computing the support points in Mak and Joseph (2018) <DOI:10.1214/17-AOS1629>. Support points can be used as a representative sample of a desired distribution, or a representative reduction of a big dataset (e.g., an "optimal" thinning of Markov-chain Monte Carlo sample chains). This work was supported by USARO grant W911NF-14-1-0024 and NSF DMS grant 1712642.

Author(s)

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References

Mak, S. and Joseph, V. R. (2018). Support points. Annals of Statistics, 46(6A):2562-2592.

e_dist

Computes the energy distance of a point set

Description

e_dist computes the energy distance between points D and a target distribution (or big dataset) F. The cross-term E[||X-X'||], X,X' F is NOT computed in e_dist for computational efficiency, since this is not needed for optimizing D. The target distribution or big dataset can be set using dist.str or dist.samp, respectively.

Usage

e_dist

Arguments

D An $n \times p$ point set.

dist.str A p-length string vector for target distribution (assuming independence). Cur-

rent options include uniform, normal, exponential, gamma, lognormal, student-t, weibull, cauchy and beta. Exactly one of dist.str or dist.samp should be NA.

dist.param A p-length list for desired distribution parameters in dist.str. The following parameters are supported:

• Uniform: Minimum, maximum;

• Normal: Mean, standard deviation;

• Exponential: Rate parameter;

• Gamma: Shape parameter, scale parameter;

• Lognormal: Log-mean, Log-standard deviation;

• Student-t: Degree-of-freedom;

• Weibull: Shape parameter, scale parameter;

• Cauchy: Location parameter, scale parameter;

• **Beta**: Shape parameter 1, shape parameter 2.

nsamp Number of samples to draw from dist.str for comparison.

dist.samp An $N \times p$ matrix for the target big dataset (e.g., MCMC chain). Exactly one of dist.str or dist.samp should be NA.

References

Szekely, G. J. and Rizzo, M. L. (2013). Energy statistics: A class of statistics based on distances. *Journal of Statistical Planning and Inference*, 143(8):1249-1272.

Examples

```
## Not run:
 # Generate 25 SPs for the 2-d i.i.d. N(0,1) distribution
 n <- 25 #number of points
 p <- 2 #dimension
 D <- sp(n,p,dist.str=rep("normal",p))</pre>
 Drnd <- matrix(rnorm(n*p),ncol=p)</pre>
 e_dist(D$sp,dist.str=rep("normal",p)) #smaller
 e_dist(Drnd, dist.str=rep("normal",p))
 # Support points for big data reduction: Franke's function
 # library(MHadaptive) # Package archived, but you can use your favorite MCMC sampler
# #Generate MCMC samples
# li_func <- franke2d #Desired log-posterior</pre>
# ini \leftarrow c(0.5,0.5) #Initial point for MCMc
```

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```
# NN <- 1e5 #Number of MCMC samples desired
 # burnin <- NN/2 #Number of burn-in runs</pre>
    mcmc_franke <- Metro_Hastings(li_func, pars=ini, prop_sigma=0.05*diag(2),</pre>
                               iterations=NN, burn_in=burnin)
   data(mcmc_franke) # Loading MCMC sample from data
    #Use modified Franke's function as posterior
    franke2d <- function(xx){</pre>
      if ((xx[1]>1)||(xx[1]<0)||(xx[2]>1)||(xx[2]<0)){
        return(-Inf)
      }
      else{
        x1 \leftarrow xx[1]
        x2 \leftarrow xx[2]
        term1 <- 0.75 * exp(-(9*x1-2)^2/4 - (9*x2-2)^2/4)
        term2 <- 0.75 * exp(-(9*x1+1)^2/49 - (9*x2+1)/10)
        term3 <- 0.5 * exp(-(9*x1-7)^2/4 - (9*x2-3)^2/4)
        term4 <- -0.2 * exp(-(9*x1-4)^2 - (9*x2-7)^2)
        y <- term1 + term2 + term3 + term4
        return(2*log(y))
      }
   }
    #Generate ncur SPs
   ncur <- 50
   D <- sp(ncur,2,dist.samp=mcmc_franke$trace)$sp</pre>
   Drnd <- mcmc_franke$trace[sample(1:nrow(mcmc_franke$trace),n,F),]</pre>
   e\_dist(D,dist.samp=mcmc\_franke\$trace) \ \#smaller
   e_dist(Drnd,dist.samp=mcmc_franke$trace)
## End(Not run)
```

mcmc_franke

MCMC sample from the modified Franke function

Description

MCMC sample from the modified Franke function using the package MHadaptive (which is currently archived).

Usage

```
data(mcmc_franke)
```

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Computing support points using difference-of-convex programming

sp

Description

sp is the main function for computing the support points in Mak and Joseph (2018). Current options include support points on standard distributions (specified via dist.str) or support points for reducing big data (specified via dist.samp). For big data reduction, weights on each data point can be specified via wts.

Usage

```
sp(n, p, ini=NA,
   dist.str=NA, dist.param=vector("list",p),
   dist.samp=NA, scale.flg=TRUE, wts=NA, bd=NA,
   num.subsamp=ifelse(any(is.na(dist.samp)),
   max(10000,10*n),min(10000,nrow(dist.samp))),
   rnd.flg=ifelse(any(is.na(dist.samp)),
   TRUE,ifelse(num.subsamp<=10000,FALSE,TRUE)),
   iter.max=max(250,iter.min), iter.min=50,
   tol=1e-10, par.flg=TRUE, n0=n*p)</pre>
```

Arguments

n Number of support points.

p Dimension of sample space.

ini An $n \times p$ matrix for initialization.

dist.str A p-length string vector for desire

A p-length string vector for desired distribution (assuming independence). Current options include uniform, normal, exponential, gamma, lognormal, student-t, weibull, cauchy and beta. Exactly one of dist.str or dist.samp should be NA.

dist.param A p-length list for desired distribution parameters in dist.str. The following parameters are supported:

Uniform: Minimum, maximum;

• Normal: Mean, standard deviation;

• Exponential: Rate parameter;

• Gamma: Shape parameter, scale parameter;

• Lognormal: Log-mean, Log-standard deviation;

• Student-t: Degree-of-freedom;

• Weibull: Shape parameter, scale parameter;

• Cauchy: Location parameter, scale parameter;

• Beta: Shape parameter 1, shape parameter 2.

dist.samp

An $N \times p$ matrix for the big dataset (e.g., MCMC chain) to be reduced. Exactly one of dist.str or dist.samp should be NA.

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scale.flg	Should the big data dist.samp be normalized to unit variance before processing?
wts	Weights on each data point in dist.samp. Uniform weights are assigned if NA.
bd	A $p \times 2$ matrix for the lower and upper bounds of each variable.
num.subsamp	Batch size for resampling. For distributions, the default is max(10000,10*n). For data reduction, the default is min(10000,nrow(dist.samp)).
rnd.flg	Should the big data be randomly subsampled?
iter.max	Maximum iterations for optimization.
iter.min	Minimum iterations for optimization.
tol	Error tolerance for optimization.
par.flg	Should parallelization be used?

Value

n0

sp An $n \times p$ matrix for support points. ini An $n \times p$ matrix for initial points.

References

Mak, S. and Joseph, V. R. (2018). Support points. Annals of Statistics, 46(6A):2562-2592.

Momentum parameter for optimization.

Examples

```
## Not run:
# Support points on distributions
#Generate 25 SPs for the 2-d i.i.d. N(0,1) distribution
n <- 25 #number of points
p <- 2 #dimension
D <- sp(n,p,dist.str=rep("normal",p))</pre>
x1 \leftarrow seq(-3.5, 3.5, length.out=100) #Plot contours
x2 < - seq(-3.5, 3.5, length.out=100)
z \leftarrow \exp(-\text{outer}(x1^2, x2^2, \text{FUN}="+")/2)
contour.default(x=x1,y=x2,z=z,drawlabels=FALSE,nlevels=10)
points(D$sp,pch=16,cex=1.25,col="red")
# Generate 50 SPs for the 2-d i.i.d. Beta(2,4) distribution
n <- 50
p <- 2
dist.param <- vector("list",p)</pre>
for (l in 1:p){
 dist.param[[1]] \leftarrow c(2,4)
```

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```
D <- sp(n,p,dist.str=rep("beta",p),dist.param=dist.param)
 x1 <- seq(0,1,length.out=100) #Plot contours
 x2 \leftarrow seq(0,1,length.out=100)
 z <- matrix(NA,nrow=100,ncol=100)</pre>
 for (i in 1:100){
   for (j in 1:100){
     z[i,j] \leftarrow dbeta(x1[i],2,4) * dbeta(x2[j],2,4)
 }
 contour.default(x=x1,y=x2,z=z,drawlabels=FALSE,nlevels=10\ )
 points(D$sp,pch=16,cex=1.25,col="red")
 # Generate 100 SPs for the 3-d i.i.d. Exp(1) distribution
 n <- 100
 p < -3
 D <- sp(n,p,dist.str=rep("exponential",p))</pre>
 pairs(Dsp,xlim=c(0,5),ylim=c(0,5),pch=16)
 # Support points for big data reduction: Franke's function
 #Use modified Franke's function as posterior
 franke2d <- function(xx){</pre>
   if ((xx[1]>1)||(xx[1]<0)||(xx[2]>1)||(xx[2]<0)){
     return(-Inf)
   }
   else{
     x1 \leftarrow xx[1]
     x2 \leftarrow xx[2]
     term1 <- 0.75 * exp(-(9*x1-2)^2/4 - (9*x2-2)^2/4)
     term2 <- 0.75 * exp(-(9*x1+1)^2/49 - (9*x2+1)/10)
     term3 <- 0.5 * exp(-(9*x1-7)^2/4 - (9*x2-3)^2/4)
     term4 <- -0.2 * exp(-(9*x1-4)^2 - (9*x2-7)^2)
     y <- term1 + term2 + term3 + term4
     return(2*log(y))
   }
 }
# library(MHadaptive) # Package archived, but you can use your favorite MCMC sampler
# #Generate MCMC samples
# li_func <- franke2d #Desired log-posterior</pre>
# ini <- c(0.5,0.5) #Initial point for MCMc \,
# NN <- 1e5 #Number of MCMC samples desired
# burnin <- NN/2 #Number of burn-in runs</pre>
# mcmc_franke <- Metro_Hastings(li_func, pars=ini, prop_sigma=0.05*diag(2),</pre>
```

sp_seq

```
iterations=NN, burn_in=burnin)
   data(mcmc_franke) # Loading MCMC sample from data
    #Compute n SPs
   n <- 100
   D <- sp(n,2,dist.samp=mcmc_franke$trace)</pre>
    #Plot SPs
   oldpar <- par(mfrow=c(1,2))</pre>
   x1 <- seq(0,1,length.out=100) #contours
   x2 \leftarrow seq(0,1,length.out=100)
   z <- matrix(NA,nrow=100,ncol=100)</pre>
    for (i in 1:100){
      for (j in 1:100){
        z[i,j] \leftarrow franke2d(c(x1[i],x2[j]))
    }
   plot(mcmc_franke$trace,pch=4,col="gray",cex=0.75,
      xlab="",ylab="",xlim=c(0,1),ylim=c(0,1)) #big data
   points(D$sp,pch=16,cex=1.25,col="red")
    contour.default(x=x1,y=x2,z=z,drawlabels=TRUE,nlevels=10) #contour
   points(D$sp,pch=16,cex=1.25,col="red")
   par(oldpar)
## End(Not run)
```

sp_seq

Computing (batch) sequential support points using difference-ofconvex programming

Description

sp_seq computes (batch) sequential support points to add onto a current point set D. Current options include sequential support points on standard distributions (specified via dist.str) or sequential support points for reducing big data (specified via dist.samp).

Usage

```
sp_seq(D, nseq, ini=NA, num.rep=1,
    dist.str=NA, dist.param=vector("list",p),
    dist.samp=NA, scale.flg=TRUE, bd=NA,
    num.subsamp=ifelse(any(is.na(dist.samp)),
    max(10000,10*(nseq+nrow(D))),
    min(10000,nrow(dist.samp))),
    iter.max=max(200,iter.min), iter.min=50,
    tol=1e-10, par.flg=TRUE)
```

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Arguments

D	An $n \times p$ matrix for the current point set.
nseq	Number of support points to add to D.
ini	An $nseq \times p$ matrix for initialization.
num.rep	Number of random restarts for optimization.
dist.str	A <i>p</i> -length string vector for desired distribution (assuming independence). Current options include uniform, normal, exponential, gamma, lognormal, student-t, weibull, cauchy and beta. Exactly one of dist.str or dist.samp should be NA.
dist.param	A p -length list for desired distribution parameters in dist.str. The following parameters are supported:
	• Uniform: Minimum, maximum;
	• Normal: Mean, standard deviation;
	• Exponential: Rate parameter;
	• Gamma: Shape parameter, scale parameter;
	• Lognormal: Log-mean, Log-standard deviation;
	• Student-t: Degree-of-freedom;
	• Weibull: Shape parameter, scale parameter;
	• Cauchy: Location parameter, scale parameter;
	• Beta : Shape parameter 1, shape parameter 2.
dist.samp	An N x p matrix for the big dataset (e.g., MCMC chain) to be reduced. Exactly one of dist.str or dist.samp should be NA.
scale.flg	Should the big data dist.samp be normalized to unit variance before processing?
bd	A $p \times 2$ matrix for the lower and upper bounds of each variable.
num.subsamp	Batch size for resampling. For distributions, the default is max(10000,10*n).

For data reduction, the default is min(10000, nrow(dist.samp)).

iter.max Maximum iterations for optimization.

iter.min Minimum iterations for optimization.

tol Error tolerance for optimization.
par.flg Should parallelization be used?

Value

D An $n \times p$ matrix for the current point set.

seq An $nseq \times p$ matrix for the additional nseq support points.

References

Mak, S. and Joseph, V. R. (2018). Support points. Annals of Statistics, 46(6A):2562-2592.

Examples

```
## Not run:
 # Generate 50 SPs for the 2-d i.i.d. N(0,1) distribution
 cur.sp <- sp(ncur,2,dist.str=rep("normal",2))$sp</pre>
 #Add 50 sequential SPs
 nseq <- 50
 seq.sp <- sp_seq(cur.sp,nseq,dist.str=rep("normal",2))$seq</pre>
 x1 \leftarrow seq(-3.5, 3.5, length.out=100) #Plot contours
 x2 < - seg(-3.5, 3.5, length.out=100)
 z \leftarrow \exp(-\text{outer}(x1^2, x2^2, \text{FUN}="+")/2)
 contour.default(x=x1,y=x2,z=z,drawlabels=FALSE,nlevels=10)\\
 points(cur.sp,pch=4,cex=1.25,col="black",lwd=2) # (current in black)
 points(seq.sp,pch=16,cex=1.25,col="red")
                                            # (new SPs in red)
 # Support points for big data reduction: Franke distribution
 #Use modified Franke's function as posterior
 franke2d <- function(xx){</pre>
   if ((xx[1]>1)||(xx[1]<0)||(xx[2]>1)||(xx[2]<0)){
     return(-Inf)
   }
   else{
     x1 < -xx[1]
     x2 <- xx[2]
     term1 <- 0.75 * exp(-(9*x1-2)^2/4 - (9*x2-2)^2/4)
     term2 <- 0.75 * exp(-(9*x1+1)^2/49 - (9*x2+1)/10)
     term3 <- 0.5 * exp(-(9*x1-7)^2/4 - (9*x2-3)^2/4)
     term4 <- -0.2 * exp(-(9*x1-4)^2 - (9*x2-7)^2)
     y <- term1 + term2 + term3 + term4
     return(2*log(y))
   }
 }
# library(MHadaptive) # Package archived, but you can use your favorite MCMC sampler
# #Generate MCMC samples
# li_func <- franke2d #Desired log-posterior</pre>
# ini <- c(0.5,0.5) #Initial point for MCMc
# NN <- 1e5 #Number of MCMC samples desired
# burnin <- NN/2 #Number of burn-in runs</pre>
# mcmc_franke <- Metro_Hastings(li_func, pars=ini, prop_sigma=0.05*diag(2),</pre>
```

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```
iterations=NN, burn_in=burnin)
   data(mcmc_franke) # Loading MCMC sample from data
    #Generate ncur SPs
    ncur <- 50
    cur.sp <- sp(ncur,2,dist.samp=mcmc_franke$trace)$sp</pre>
    #Add nseq sequential SPs
    nseq <- 50
    seq.sp <- sp_seq(cur.sp,nseq,dist.samp=mcmc_franke$trace)$seq</pre>
    #Plot SPs
    par(mfrow=c(1,2))
    x1 \leftarrow seq(0,1,length.out=100) #contours
    x2 <- seq(0,1,length.out=100)</pre>
    z <- matrix(NA,nrow=100,ncol=100)</pre>
    for (i in 1:100){
      for (j in 1:100){
        z[i,j] \leftarrow franke2d(c(x1[i],x2[j]))
    }
   plot(mcmc_franke$trace,pch=4,col="gray",cex=0.75,
      xlab="",ylab="",xlim=c(0,1),ylim=c(0,1))
                                                      #big data
    points(cur.sp,pch=4,cex=1.25,col="black",lwd=2) # (current in black)
                                                      # (new SPs in red)
   points(seq.sp,pch=16,cex=1.25,col="red")
    contour.default(x=x1,y=x2,z=z,
      drawlabels=TRUE,nlevels=10)
                                                      #contour
    points(cur.sp,pch=4,cex=1.25,col="black",lwd=2) # (current in black)
    points(seq.sp,pch=16,cex=1.25,col="red")
                                                      # (new SPs in red)
## End(Not run)
```

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