Package ‘meshed’

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meshed-package

Methods for fitting models based on Meshed Gaussian Processes (MGPs)

Description

Meshed is a flexible package for Bayesian regression analysis on spatial or spatiotemporal datasets. The main function for fitting regression models is `spmeshed`, which outputs posterior samples obtained from Markov chain Monte Carlo which can be summarised using standard tools. The package also provides a function `rmeshedgp` for quickly simulating correlated spatial or spatiotemporal data at a very large number of locations.

Details

The functions `rmeshedgp` and `spmeshed` are provided for prior and posterior sampling (respectively) of Bayesian spatial or spatiotemporal multivariate regression models based on Meshed Gaussian Processes as introduced by Peruzzi, Banerjee, and Finley (2020). Posterior sampling via `spmeshed` proceeds by default via GriPS as detailed in Peruzzi, Banerjee, Dunson, and Finley (2021). When at least one outcome is not modeled with Gaussian errors, sampling proceeds taking advantage of Metropolis-adjusted Langevin dynamics.

Author(s)

Michele Peruzzi

References


See Also

`spmeshed`, `rmeshedgp`
**predict.spmeshed**

*Posterior predictive sampling for models based on MGP*

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**Description**

Sample from the posterior predictive distribution of the outcomes at new spatial or spatiotemporal locations after MCMC.

**Usage**

```r
## S3 method for class 'spmeshed'
predict(object, newx, newcoords,
        n_threads=4, verbose=FALSE, ...)
```

**Arguments**

- `object`: Object output from `spmeshed` with option `settings$saving=TRUE`.
- `newx`: matrix of covariate values at the new coordinates.
- `newcoords`: matrix of new coordinates.
- `n_threads`: integer number of OpenMP threads. This is ineffective if `spmeshed` was not compiled with OpenMP support.
- `verbose`: boolean for progress messaging.
- `...`: other arguments (unused).

**Details**

While this function can always be used to make predictions, in most cases it is more efficient to just include the prediction locations in the main data as NA values; `spmeshed` will sample from the posterior predictive distribution at those locations while doing MCMC. The `predict` method is only recommended when all 4 of the following are true:

1. `spmeshed` was run with `settings$forced_grid=FALSE` and
2. the prediction locations are uniformly scattered on the domain (or rather, they are not clustered as a large empty area) and
3. the number of prediction locations is a large portion of the number of observed data points and
4. the prediction locations are not on a grid.

In all other cases the main `spmeshed` function is setup to be more efficient in automatically performing predictions during MCMC.

**Value**

- `coords_out`: matrix with the prediction location coordinates (order updated after predictions).
- `preds_out`: array of dimension \((n_o, q, m)\) where \(n_o\) is the number of prediction locations, \(q\) is the output dimension, and \(m\) is the number of MCMC samples.
Author(s)

Michele Peruzzi <michele.peruzzi@duke.edu>

References


Examples

# toy example with tiny dataset and short MCMC
# on a univariate outcome
library(magrittr)
library(dplyr)
library(meshed)

set.seed(2021)

SS <- 12
n <- SS^2 # total n. locations, including missing ones

coords <- data.frame(Var1=runif(n), Var2=runif(n)) %>% as.matrix()

# generate data
sigmasq <- 2.3
phi <- 6
tausq <- .1
B <- c(-1,.5,1)

CC <- sigmasq * exp(-phi * as.matrix(dist(coords)))
LC <- t(chol(CC))
w <- LC %*% rnorm(n)
p <- length(B)
X <- rnorm(n * p) %>% matrix(ncol=p)
y_full <- X %*% B + w + tausq*5 * rnorm(n)

set_missing <- rbinom(n, 1, 0.1)

simdata <- data.frame(coords,
  y_full = y_full,
  w_latent = w) %>%
  mutate(y_observed = ifelse(set_missing==1, NA, y_full))

# MCMC setup
mcmc_keep <- 500
mcmc_burn <- 100
mcmc_thin <- 2

y <- simdata$y_observed
ybar <- mean(y, na.rm=TRUE)

# training set
y_in <- (y-ybar)[!is.na(y)]
X_in <- X[!is.na(y),]
coords_in <- coords[!is.na(y),]

# suppose we don't want to have gridded knots
# i.e. we are fixing the MGP reference set at the observed locations
# (this may be inefficient in big data settings)
meshout <- spmeshed(y_in, X_in, coords_in,
  axis_partition=c(4,4),
  n_samples = mcmc_keep,
  n_burn = mcmc_burn,
  n_thin = mcmc_thin,
  settings = list(forced_grid=FALSE, cache=FALSE),
  prior=list(phi=c(1,15)),
  verbose = 0,
  n_threads = 1)

# test set
coords_out <- coords[is.na(y),]
X_out <- X[is.na(y),]

df_predict <- predict(meshout, newx=X_out, newcoords=coords_out)

y_posterior_predictive_mean <- df_predict$preds_out[,1] %>%
  apply(1, mean) %>% add(ybar)
df_predicted <- df_predict$coords_out %>% cbind(y_posterior_predictive_mean)

---

**rmeshedgp**

*Prior sampling from a Meshed Gaussian Process*

**Description**

Generates samples from a (univariate) MGP assuming a cubic directed acyclic graph and axis-
parallel domain partitioning.

**Usage**

rmeshedgp(coords, theta,
  axis_partition = NULL, block_size = 100,
  n_threads=1, cache=TRUE, verbose=FALSE, debug=FALSE)
Arguments

coords  matrix of spatial or spatiotemporal coordinates with \( d = 2 \) or \( d = 3 \) columns for spatial or spatiotemporal data, respectively.

theta  vector with covariance parameters. If \( d = 2 \) and theta is a 2-dimensional vector then \( \theta = (\phi, \sigma^2) \) where \( \phi \) is the spatial decay and \( \sigma^2 \) is the spatial variance in the exponential covariance model. If \( d = 2 \) and theta is a 3-dimensional vector then \( \theta = (\phi, \nu, \sigma^2) \) and a Matern model with smoothness \( \nu \) is used instead. If \( d = 3 \), theta must be a 4-dimensional vector and \( \theta = (a, \phi, b, \sigma^2) \) using Gneiting’s non-separable spatiotemporal covariance detailed below.

axis_partition  integer vector of length \( d \) with the number of intervals along which each axis should be partitioned. The domain will be partitioned into \( \prod(\text{axis}\_\text{partition}) \) blocks. This argument can be left blank when using block_size.

block_size  integer specifying the (approximate) size of the blocks, i.e. how many spatial or spatiotemporal locations should be included in each block. Note: larger values correspond to an MGP that is closer to a full GP, but require more expensive computations.

n_threads  integer number of OpenMP threads. This is ineffective if meshed was not compiled with OpenMP support.

cache  bool: whether to use cache. Some computational speedup is associated to cache=TRUE if coords are a grid.

verbose  bool: print some messages.

debug  bool: print more messages.

Details

Gaussian processes (GPs) lack in scalability to big datasets due to the assumed unrestricted dependence across the spatial or spatiotemporal domain. Meshed GPs instead use a directed acyclic graph (DAG) with patterns, called mesh, to simplify the dependence structure across the domain. Each DAG node corresponds to a partition of the domain. MGPs can be interpreted as approximating the GP they originate from, or as standalone processes that can be sampled from. This function samples random MGPs and can thus be used to generate big spatial or spatiotemporal data. The only requirement to sample from a MGP compared to a standard GP is the specification of the domain partitioning strategy. Here, either axis_partition or block_size can be used; the default block_size=100 can be used to quickly sample smooth surfaces at millions of locations.

Just like in a standard GP, one needs a covariance function or kernel which can be set as follows. For spatial data \((d = 2)\), the length of theta determines which model is used (see above). Letting \( h = \|s - s'\| \) where \( s \) and \( s' \) are locations in the spatial domain, the exponential covariance is defined as:

\[
C(h) = \sigma^2 \exp\{-\phi h\},
\]

whereas the Matern model is

\[
C(h) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \phi^\nu h^\nu K_\nu(\phi h),
\]

where \( K_\nu \) is the modified Bessel function of the second kind of order \( \nu \). For spatiotemporal data \((d = 3)\) the covariance function between locations \((s, t)\) and \((s', t')\) with distance \( h = \|s - s'\| \) and
time lag \( u = \|t - t'\| \) is defined as
\[
C(h, u) = \sigma^2/(\alpha u + 1) \exp\{\phi h(\alpha u + 1)^{-b/2}\},
\]
which is a special case of non-separable spacetime covariance as introduced by Gneiting (2002).

Value
data.frame with the (reordered) supplied coordinates in the first \( d \) columns, and the MGP sample in the last column, labeled \( w \).

Author(s)
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References


Examples

```r
library(ggplot2)
library(magrittr)
library(meshed)

# spatial domain (we choose a grid to make a nice image later)
# this generates a dataset of size 6400
xx <- seq(0, 1, length.out=80)
coords <- expand.grid(xx, xx) %>%
  as.matrix()

raster_plot <- function(df){
  ggplot(df, aes(Var1, Var2, fill=w)) + geom_raster() +
  scale_fill_viridis_c() +
  theme_minimal() }

# spatial data, exponential covariance
# phi=14, sigma^2=2
simdata <- rmeshedgp(coords, c(14, 2))
raster_plot(simdata)

# spatial data, matern covariance
# phi=14, nu=1, sigma^2=2
simdata <- rmeshedgp(coords, c(14, 1, 2))
raster_plot(simdata)
```
# spacetime data, gneiting's covariance
# 64000 locations
stcoords <- expand.grid(xx, xx, seq(0, 1, length.out=10))

# it should take less than a couple of seconds
simdata <- rmeshedgp(stcoords, c(1, 14, .5, 2))
# plot data at 7th time period
raster_plot(simdata %>% dplyr::filter(Var3==unique(Var3)[7]))

---

spmeshed

**Posterior sampling for models based on MGPs**

### Description

Fits Bayesian multivariate spatial or spatiotemporal regression models with latent MGPs via Markov chain Monte Carlo.

### Usage

```
spmeshed(y, x, coords, k=NULL,
          family = "gaussian",
          axis_partition = NULL,
          block_size = 30,
          grid_size = NULL,
          grid_custom = NULL,
          n_samples = 1000,
          n_burnin = 100,
          n_thin = 1,
          n_threads = 4,
          verbose = 0,
          predict_everywhere = FALSE,
          settings = list(adapting=TRUE, forced_grid=NULL,
                           cache=NULL, ps=TRUE, saving=TRUE, low_mem=FALSE, hmc=4),
          prior = list(beta=NULL, tausq=NULL, sigmasq = NULL,
                        phi=NULL, a=NULL, nu = NULL,
                        toplim = NULL, btmlim = NULL, set_unif_bounds=NULL),
          starting = list(beta=mean(y), tausq=mean(y), theta=mean(y), lambda=mean(y), v=mean(y),
                          a=NULL, nu = NULL,
                          mcmcsd=.05,
                          mcmc_startfrom=0),
          debug = list(sample_beta=TRUE, sample_tausq=TRUE,
                        sample_theta=TRUE, sample_w=TRUE, sample_lambda=TRUE,
                        verbose=FALSE, debug=FALSE),
          indpart=FALSE
)
```
Arguments

- **y**: matrix of multivariate outcomes with \(n\) rows and \(q\) columns. Each row of \(y\) corresponds to a row of \(\text{coords} \). NA values are accepted in any combination and will be predicted via MCMC.

- **x**: matrix of covariates with \(n\) rows and \(p\) columns.

- **coords**: matrix of coordinates with \(n\) rows and \(d=2\) or \(d=3\) columns for spatial or spacetime regression, respectively.

- **k**: integer \(k \leq q\), number of latent processes to use for the linear model of coregionalization. If unspecified, this is set to \(q=\text{ncol}(y)\).

- **family**: a vector with length 1 or \(q\) whose elements corresponds to the data types of columns of \(y\). Available choices are \text{gaussian}, \text{poisson}, \text{binomial}, \text{beta} for outcomes that are continuous, count, binary, or \((0,1)\) proportions.

- **axis_partition**: integer vector of size \(d\): number of intervals each coordinate axis is split into.

- **block_size**: integer approximate size of the blocks after domain partitioning. Only used if \(\text{axis_partition} \) is not specified.

- **grid_size**: integer vector of size \(d\): number of 'knots' of the reference grid along each axis. This grid is then partitioned using either \(\text{axis_partition}\) or \(\text{block_size}\). If unspecified, this is set so that the eventual grid size is close to \(n\). This parameter is ignored if \(\text{settings$forced_grid=FALSE}\) in which case the data are assumed to be on a grid.

- **grid_custom**: list with elements \(\text{grid}\) and \(\text{axis_interval_partition}\). \(\text{grid}\) is a data.frame with the user supplied grid of knots. It is possible to include covariate values for the grid locations as additional columns, as long as their number matches \(\text{ncol}(x)\) - this is useful to make raster images of predictions. \(\text{axis_interval_partition}\) is the user supplied set of cuts for each coordinate axis (Note: these are the actual cutpoints along the axes, not the number of cuts). If left empty, \(\text{axis_partition}\) will be used to partition the custom grid. No checks are made on the validity of this grid. This parameter is ignored if \(\text{settings$forced_grid=FALSE}\) in which case the data are assumed to be on a grid.

- **n_samples**: integer number of MCMC samples at which all the unknowns are stored (including the latent effects).

- **n_burnin**: integer number of MCMC samples to discard at the beginning of the chain.

- **n_thin**: integer thinning parameter for the MCMC chain. Only the chain of latent effects \((w)\) is thinned to save memory in big data problems. Chains for other unknowns are not thinned and thus will be of length \(n\_\text{thin} \times n\_\text{samples}\).

- **n_threads**: integer number of OpenMP threads. This is ineffective if \text{meshed} was not compiled with OpenMP support.

- **verbose**: integer. If \(\text{verbose}=10\), then this is the number of times a message is displayed during MCMC. If \(\text{verbose}>20\), then this is the number of MCMC iterations to wait until the next message update. If \(\text{verbose}=\text{Inf}\), then a message will be printed at each MCMC iteration.

- **predict_everywhere**: bool used if \(\text{settings$forced_grid=T}\). Should predictions be made at the reference grid locations? If not, predictions will be made only at the supplied NA values of \(Y\).
settings list: settings$adapting turns the adaptation of MCMC on/off, settings$forced_grid determines whether or not to use the data grid or a forced grid; if unspecified, the function will try to see what the data look like. Note: if forced_grid=FALSE and \( n \) is very large and coords are irregularly spaced, then expect slowdowns in preprocessing and consider using forced_grid=TRUE instead. settings$saving will save model data if set to TRUE. settings$low_mem will only save beta_mcmc, lambda_mcmc, \( v \_mcmc \), tausq_mcmc (and not \( w \_mcmc \) and lp_mcmc, which can be recovered from the others), thereby using less memory. All fitted predictions remain available in yhat_mcmc for convenience. settings$ps (default TRUE) determines whether to use the PS parametrization (Peruzzi et al 2021). settings$hmc, used if any outcome is not Gaussian, (1: MALA, 2: NUTS, 3: RM-MALA, 4: Simplified manifold preconditioning (default))

prior list: setup for priors of unknown parameters. prior$phi needs to be specified as the support of the Uniform prior for \( \phi \). There is currently limited functionality here and some inputs are currently ignored. Defaults are: a vague Gaussian for \( \beta, \tau^2 \sim IG(2,1), \theta_j \sim IG(2,2) \), all subject to change.

starting list: setup for starting values of unknown parameters. starting$mcmcsd is the initial standard deviation of proposals. starting$mcmc_startfrom is input to the adaptive MCMC and can be used to manually restart MCMC. There is currently limited functionality here and some parameters may be ignored.

default list: setup for debugging things. Some parts of MCMC can be turned off here.

indpart bool defaults to FALSE. If TRUE, this computes an independent partition model.

Details

This function targets the following model:

\[
y(s) = x(s)^T \beta + \Lambda v(s) + \epsilon(s),
\]

where \( y(s) \) is a \( q \)-dimensional vector of outcomes at spatial location \( s \), \( x(s) \) is a \( p \)-dimensional vector of covariates with static coefficients \( \beta \), \( \Lambda \) is a matrix of factor loadings of size \( (q,k) \), \( v(s) \) is a \( k \)-dimensional vector which collects the realization of independent Gaussian processes \( v_j \sim spmeshed(0,C_j) \) for \( j = 1, \ldots, k \) and where \( C_j(s,s') \) is a correlation function. \( s \) is a coordinate in space \( (d = 2) \) or space plus time \( (d = 3) \). The Meshed GP implemented here associates an axis-parallel tessellation of the domain to a cubic directed acyclic graph (mesh).

Value

coordsdata data.frame including the original \( n \) coordinates plus the \( n_g \) knot coordinates if the model was run on a forced grid. The additional column forced_grid has value 1 if the corresponding coordinate is a knot in the forced grid. See examples.

savedata Available if settings$saving==TRUE. Needed for making predictions using predict() after MCMC. Note: NA values of the output are automatically and more efficiently predicted when running spmeshed.

yhat_mcmc list of length \( n \_samples \) whose elements are matrices with \( n + n_g \) rows and \( q \) columns. Each matrix in the list is a posterior predictive sample of the latent spatial process. \( n_g = 0 \) if the data grid is being used. Given the possibly large \( n \), only the thinned chain is output for \( y \).
spmeshed

v_mcmc list of length n_samples whose elements are matrices with \( n + n_g \) rows and \( k \) columns. Each matrix in the list is a posterior sample of the \( k \) latent spatial process. \( n_g = 0 \) if the data grid is being used. Given the possibly large \( n \), only the thinned chain is output for \( v \).

w_mcmc list of length n_samples whose elements are matrices with \( n + n_g \) rows and \( q \) columns. Each matrix in the list is a posterior sample of \( w = \Lambda v \). \( n_g = 0 \) if the data grid is being used. Given the possibly large \( n \), only the thinned chain is output for \( w \).

lp_mcmc list of length n_samples whose elements are matrices with \( n + n_g \) rows and \( q \) columns. Each matrix in the list is a posterior sample of the linear predictor \( X\beta + \Lambda v \). \( n_g = 0 \) if the data grid is being used. Given the possibly large \( n \), only the thinned chain is output for \( w \).

beta_mcmc array of size \((p, q, n\_thin*n\_samples)\) with the posterior sample for the static regression coefficients \( \beta \). The \( j \)th column of each matrix \((p \text{ rows and } q \text{ columns})\) corresponds to the \( p \) linear effects on the \( j \)th outcome. The full chain minus burn-in is returned NOT thinned since \( p \) and \( q \) are relatively small.

tausq_mcmc matrix of size \((q, n\_thin*n\_samples)\). Each row corresponds to the full MCMC chain for the nugget \( \tau^2 \) of the \( j \)th outcome in the coregionalization/factor model. The full chain minus burn-in is returned NOT thinned since \( q \) is relatively small.

theta_mcmc array of size \((h, k, n\_thin*n\_samples)\) with the posterior sample for the correlation function parameters \( \theta \). \( h \) is 2 for spatial data (corresponding to the spatial decay of the exponential covariance \( (\phi_i, i = 1, \ldots, k) \)), and the variance \( \sigma^2_i, i = 1, \ldots, k \), 4 for spacetime data (corresponding to temporal decay, spatial decay, and separability – these are referred to as \( a_i, \phi_i, \) and \( \beta_i, i = 1, \ldots, k \), in Gneiting (2002), see doi: 10.1198/016214502760047113, plus the variance \( a^2_i, i = 1, \ldots, k \). The full chain minus burn-in is returned NOT thinned since \( h \) and \( k \) are relatively small. If settings$ps=TRUE$, the MCMC output for \( a^2_i \) (last row of theta_mcmc) should be discarded and \( \Lambda \) used instead.

lambda_mcmc array of size \((q, k, n\_thin*n\_samples)\). Each matrix (of size \((q, k)\)) is a posterior sample for \( \Lambda \) in the coregionalization/factor model. In univariate models, this is usually called \( \sigma \). The full chain minus burn-in is returned NOT thinned since \( q \) and \( k \) are relatively small.

paramsd Cholesky factorization of the proposal covariance for adaptive MCMC, after adaptation.

mcmc Total number of MCMC iterations performed.

mcmc_time Time in seconds taken for MCMC (not including preprocessing).

Author(s)

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References

Examples

# toy example with tiny dataset and short MCMC
# on a univariate outcome
library(magrittr)
library(dplyr)
library(ggplot2)
library(meshed)

set.seed(2021)
SS <- 12
n <- SS^2 # total n. locations, including missing ones
coords <- expand.grid(xx <- seq(0,1,length.out=SS), xx) %>% as.matrix()

# generate data
sigmasq <- 2.3
phi <- 6
tausq <- .1
B <- c(-1,.5,1)

CC <- sigmasq * exp(-phi * as.matrix(dist(coords)))
LC <- t(chol(CC))
w <- LC %*% rnorm(n)
p <- length(B)
X <- rnorm(n * p) %>% matrix(ncol=p)
y_full <- X %*% B + w + tausq^.5 * rnorm(n)

set_missing <- rbinom(n, 1, 0.1)
simdata <- data.frame(coords,
                     y_full = y_full,
                     w_latent = w) %>%
                     mutate(y_observed = ifelse(set_missing==1, NA, y_full))

# MCMC setup
mcmc_keep <- 500
mcmc_burn <- 100
mcmc_thin <- 2

y <- simdata$y_observed
ybar <- mean(y, na.rm=TRUE)
meshout <- spmeshed(y-ybar, X, coords,  
axis_partition=c(4,4),  
n_samples = mcmc_keep,  
n_burn = mcmc_burn,  
n_thin = mcmc_thin,  
prior=list(phi=c(1,15)),  
verbose = 0,  
n_threads = 1)

# posterior means
best_post_mean <- meshout$beta_mcmc %>% apply(1:2, mean)

# process means
wmesh <- data.frame(w_mgp = meshout$w_mcmc %>% summary_list_mean())
# predictions
ymesh <- data.frame(y_mgp = meshout$yhat_mcmc %>% summary_list_mean())

outdf <-  
  meshout$coordsdata %>%  
  cbind(ymesh, wmesh)

# plot predictions
pred_plot <- outdf %>%
  ggpplot(aes(Var1, Var2, color=y_mgp)) +
  geom_point() +
  scale_color_viridis_c()

# plot latent process
latent_plot <- outdf %>%
  ggpplot(aes(Var1, Var2, color=w_mgp)) +
  geom_point() +
  scale_color_viridis_c()

# estimation of regression coefficients
plot(density(meshout$beta_mcmc[1,1,]))
abline(v=B[1], col="red")

---

### summary_list_mean

**Arithmetic mean of matrices in a list**

**Description**

For a list of matrices \(\{X^{(1)}, \ldots, X^{(L)}\}\), all of the same dimension, this function computes the matrix \(\bar{X}\) with \(i, j\) entry \(\bar{X}_{ij} = \frac{1}{L} \sum_{l=1}^{L} X_{ij}^{(l)}\). This function does not run any check on the dimensions and uses OpenMP if available.

**Usage**

```
summary_list_mean(x, n_threads=1)
```
summary_list_q

Arguments

x
A list of matrices of the same dimension

n_threads
integer number of OpenMP threads. This is ineffective if meshed was not compiled with OpenMP support.

Value

The matrix of mean values.

Author(s)

Michele Peruzzi <michele.peruzzi@duke.edu>

Examples

# make some data into a list
set.seed(2021)
L <- 200
x <- lapply(1:L, function(i) matrix(runif(300), ncol=3))
mean_done <- summary_list_mean(x)

# summary_list_q

summary_list_q

Quantiles of elements of matrices in a list

Description

For a list of matrices \( \{X^{(1)}, \ldots, X^{(L)}\} \), all of the same dimension, this function computes the matrix \( \hat{X} \) with \( i,j \) entry \( \hat{X}_{i,j} = \text{quantile} \left( \{X_{i,j}^{(l)}\}_{l=1}^{L}, q \right) \). This function does not run any check on the dimensions and uses OpenMP if available. This is only a convenience function that is supposed to speed up quantile computation for very large problems. The results may be slightly different from R’s `quantile` which should be used for small problems.

Usage

summary_list_q(x, q, n_threads=1)

Arguments

x
A list of matrices of the same dimension.

q
A number between 0 and 1.

n_threads
integer number of OpenMP threads. This is ineffective if meshed was not compiled with OpenMP support.

Value

The matrix of quantiles.
Author(s)
Michele Peruzzi <michele.peruzzi@duke.edu>

Examples

```r
# make some data into a list
set.seed(2021)
L <- 200
x <- lapply(1:L, function(i) matrix(runif(300), ncol=3))
quant_done1 <- summary_list_q(x, .9)
```
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