

Package ‘ppmSuite’

November 27, 2020

Type Package

Title A Collection of Models that Employ a Prior Distribution on Partitions

Version 0.1.1

Maintainer Garritt L. Page <page@stat.byu.edu>

Description Provides functions that fit hierarchical Gaussian and probit ordinal models. A (covariate dependent) product partition model is used as a prior. If a covariate dependent product partition model is selected, then all the options detailed in Page, G.L.; Quintana, F.A.; (2018) <doi:10.1007/s11222-017-9777-z> are available. In addition, a function that fits a Gaussian likelihood spatial product partition model that is detailed in Page, G.L.; Quintana, F.A.; (2016) <doi:10.1214/15-BA971> is also provided.

Depends R (>= 3.5.0)

License GPL

Encoding UTF-8

LazyData true

Suggests cluster

NeedsCompilation yes

Author Garritt L. Page [aut, cre, cph],
S. McKay Curtis [ctb, cph],
Radford M. Neal [ctb, cph]

Repository CRAN

Date/Publication 2020-11-27 02:20:09 UTC

R topics documented:

bear	2
gaussian_ppmx	2
ordinal_ppmx	7
ozone	11

rppmx	12
scallops	13
SIMCE	14
sppm	14
Index	18

bear	<i>Bear dataset</i>
------	---------------------

Description

Number of physiological measurements from 54 bears.

Format

data: A data frame with 54 rows and the following 9 variables:

age
length
sex
weight
chest
headlength
headwid
month
neck

gaussian_ppmx	<i>Function that fits Gaussian PPMx model</i>
---------------	---

Description

ppmx is the main function used to fit Gaussian PPMx model.

Usage

```

gaussian_ppmx(y, X=NULL, Xpred=NULL,
              cohesion=1,
              M=1,
              similarity_function=1,
              consim=1,
              calibrate=0,
              simParms=c(0.0, 1.0, 0.1, 1.0, 2.0, 0.1, 1),
              modelPriors=c(0, 100^2, 1, 1),
              mh=c(0.5, 0.5),
              draws=1100, burn=100, thin=1,
              verbose=FALSE)

```

Arguments

y	numeric vector for the response variable
X	a data frame whose columns consist of covariates that will be incorporated in the partition model. Those with class of "character" or "factor" will be treated as categorical covaraites. All others will be treated as continuous covariates. If NULL, then a PPM model is fit.
Xpred	a data frame containing covariate values for which out of sample predictions are desired. The format of Xpred must be the same as for X.
cohesion	Type of cohesion function to use in the PPMx prior. 1 - Dirichlet process style of cohesion $c(S) = M \times (S - 1)!$ 2 - Uniform cohesion $c(S) = 1$
M	Precision parameter. Default is 1.
similarity_function	Type of similarity function that is employed for the PPMx prior on partitions. Options are 1 - Auxilliary similarity 2 - Double dipper similarity 3 - Cluster variance or entropy for categorical covariates 4 - Mean Gower dissimilarity (this one not available if missing values are present in X)
consim	If similarity_function is either set to 1 or 2, then this specifies the type of marginal likelihood used as the similarity function. Options are 1 - N-N(m_0, s_{20}, v) (v variance of "likelihood", m_0 and s_{20} "prior" parameters), 2 - N-NIG(m_0, s_{20}, k_0, ν_0) (m_0 and s_{20} center and scale of Gaussian, k_0 and ν_0)
calibrate	Whether the similarity should be calibrated. Options are 0 - no calibration 1 - standardize similarity value for each covariate 2 - coarsening is applied so that each similarity is raised to the $1/p$ power

simParams	Vector of parameter values employed in the similarity function of the PPMx. Entries of the vector correspond to m0 - center continuous similarity with default 0, s20 - spread of 'prior' continuous similarity with default 1, v2 - spread of 'likelihood' for continuous similarity (smaller values place more weight partitions with clusters that contain homogeneous covariate values) k0 - degrees of freedom upper for v (only used for N-NIG similarity model) nu0 - scale for v (only used for N-NIG similarity model) a0 - dirichlet weight for categorical similarity with default of 0.1 (smaller more weight placed on this variable) alpha - weight associated with cluster-variance and Gower dissimilarity
modelPriors	Vector of prior parameter values used in the PPMx prior. m - prior mean for mu0 with default equal to 0, s2 - prior variance mu0 with default equal to 100^2, A - upper bound on sigma2*_j with default equal to 10 B - upper bound on sig20 with default equal to 10
mh	two dimensional vector containing values for tuning parameter associated with MH update for sigma2 and sigma20
draws	number of MCMC iterates to be collected. default is 1100
burn	number of MCMC iterates discarded as burn-in. default is 100
thin	number by which the MCMC chain is thinned. default is 1. Thin must be selected so that it is a multiple of (draws - burn)
verbose	Logical indicating if information regarding data and MCMC iterate should be printed to screen

Details

This generic function fits a Gaussian PPMx model (Muller, Quintana, and Gosner, 2011):

$$y_i | \mu^*, \sigma^{2*}, c_i \sim N(\mu_{c_i}^*, \sigma_{c_i}^{2*}), i = 1, \dots, n$$

$$\mu_j^* | \mu_0, \sigma_0^2 \sim N(\mu_0, \sigma_0^2)$$

$$\sigma_j^* | A \sim UN(0, A)$$

$$\rho | M, \xi \sim PPMx(M, \xi)$$

To complete the model specification, the following hyperpriors are assumed,

$$\mu_0 | m, s^2 \sim N(m, s^2)$$

$$\sigma_0 | B \sim UN(0, B)$$

Note that we employ uniform prior distributions on variance components as suggest in Gelman's 2006 Bayesian paper. The PPMx(M, xi) denotes the following $Pr(\rho | x, M, \xi) \propto \prod_{j=1}^k M(|S_j| - 1)! g(x_j^* | \xi)$

The computational implementation of the model is based algorithm 8 found in Neal's 2000 JCGS paper.

Value

The function returns a list containing arrays filled with MCMC iterates corresponding to model parameters and model fit metrics. In order to provide more detail, in what follows let

"T" - be the number of MCMC iterates collected,

"N" - be the number of observations,

"P" - be the number of predictions.

The output list contains the following

mu - a matrix of dimension (T, N) containing MCMC iterates associated with each subjects mean parameter ($\mu^*_{c_i}$).

sig2 - a matrix of dimension (T, N) containing MCMC iterates associated with each subjects variance parameter ($\sigma^2_{c_i}$)

Si - a matrix of dimension (T, N) containing MCMC iterates associated with each subjects cluster label.

like - a matrix of dimension (T, N) containing likelihood values at each MCMC iterate.

fitted - a matrix of dimension (T, N) containing fitted (or in sample predictions) for each subject at each MCMC iterate

ppred - a matrix of dimension (T, P) containing out of sample predictions for each "new" subject at each MCMC iterate

mu0 - vector of length T containing MCMC iterates for mu0 parameter

sig20 - vector of length T containing MCMC iterates for sig20

nclus - vector of length T containing number of clusters at each MCMC iterate

WAIC - scalar containing the WAIC value

lpml - scalar containing lpml value

Examples

```
data(bear)

# plot length, sex, and weight of bears
ck <- c(4,3,2)
pairs(bear[,ck])

# response is length
Y <- bear$weight

# Continuous Covariate is chest
# Categorical covariate is sex
X <- bear[,c("length", "sex")]
X$sex <- as.factor(X$sex)
```

```

# Randomly partition data into 44 training and 10 testing
set.seed(1)
trainObs <- sample(1:length(Y),44, replace=FALSE)

Ytrain <- Y[trainObs]
Ytest <- Y[-trainObs]

Xtrain <- X[trainObs,,drop=FALSE]
Xtest <- X[-trainObs,,drop=FALSE]

simParms <- c(0.0, 1.0, 0.1, 1.0, 2.0, 0.1)
modelPriors <- c(0, 100^2, 0.5*sd(Y), 100)
M <- 1.0

niter <- 100000
nburn <- 50000
nthin <- 50

nout <- (niter - nburn)/nthin

mh <- c(1,10)

# Run MCMC algorithm for Gaussian PPMx model
out <- gaussian_ppmx(y=Ytrain, X=Xtrain, Xpred=Xtest, M=M,
  similarity_function=1,
  consim=1,
  calibrate=0,
  simParms=simParms,
  modelPriors = modelPriors,
  draws=niter, burn=nburn, thin=nthin,
  mh=mh)

# plot MCMC iterats
plot(density(out$mu[,1:10]),type='l')
plot(density(out$sig2[,1:10]),type='l')
plot(density(out$nc),type='l')
plot(density(out$mu0), type='l')
plot(density(out$sig20), type='l')

# The first partition iterate is used for plotting
# purposes only. We recommended using the salso
# R-package to estimate the partition based on Si
pairs(bear[trainObs,ck],col=out$Si[1,], pch=out$Si[1,])

# To compare fit and predictions when covariates not included
# in the partition model, refit data with PPM rather than PPMx
out2 <- gaussian_ppmx(y=Ytrain, X=NULL, Xpred=Xtest, M=M,
  similarity_function=1,

```

```

        consim=1,
        calibrate=0,
        simParms=simParms,
        modelPriors = modelPriors,
        draws=niter, burn=nburn, thin=nthin,
        mh=mh)

oldpar <- par(no.readonly = TRUE)

par(mfrow=c(1,2))
plot(Xtrain[,1], Ytrain, ylab="weight", xlab="length", pch=20)
points(Xtrain[,1], apply(out$fitted,2,mean), col='blue',pch="+", cex=1.5)
points(Xtrain[,1], apply(out2$fitted,2,mean), col='red',pch=2, cex=1)
legend(x="topleft",legend=c("Observed","PPM","PPMx"), col=c("black","red","blue"),pch=c(20,3,2))

plot(Xtest[,1], Ytest, ylab="weight", xlab="length",pch=20)
points(Xtest[,1], apply(out$ppred,2,mean), col='blue',pch="+", cex=1.5)
points(Xtest[,1], apply(out2$ppred,2,mean), col='red',pch=2, cex=1)
legend(x="topleft",legend=c("Observed","PPM","PPMx"), col=c("black","red","blue"),pch=c(20,3,2))

par(oldpar)

```

ordinal_ppmx

Function that fits Ordinal probit model with a PPMx as a prior on partitions

Description

ordinal_ppmx is the main function used to fit ordinal probit model with a PPMx as a prior on partitions.

Usage

```

ordinal_ppmx(y, co, X=NULL,Xpred=NULL,
             cohesion=1,
             M=1,
             similarity_function=1,
             consim=1,
             calibrate=0,
             simParms=c(0.0, 1.0, 0.1, 1.0, 2.0, 0.1, 1),
             modelPriors=c(0, 10, 1, 1),
             mh=c(0.5, 0.5),
             draws=1100,burn=100,thin=1,
             verbose=FALSE)

```

Arguments

y	Response vector containing ordinal categories that have been mapped to natural numbers beginning with 0
co	Vector specifying the boundaries associated with auxiliary variables of the probit model. If the number of ordinal categories is c, then the dimension of this vector must be c+1.
X	a data frame whose columns consist of covariates that will be incorporated in the partition model. Those with class of "character" or "factor" will be treated as categorical covariates. All others will be treated as continuous covariates. If NULL, then a PPM is fit. All continuous covariates are standardized to have mean 0 and variance 1 before employing the PPMx model.
Xpred	a data frame containing covariate values for which out of sample predictions are desired. The format of Xpred must be the same as for X.
cohesion	Type of cohesion function to use in the PPMx prior. 1 - Dirichlet process style of cohesion $c(S) = M \times (S - 1)!$ 2 - Uniform cohesion $c(S) = 1$
M	Precision parameter of the PPMx if a DP style cohesion is used. See above. Default is 1.
similarity_function	Type of similarity function that is employed for the PPMx prior on partitions. Options are 1 - Auxilliary similarity 2 - Double dipper similarity 3 - Cluster variance or entropy for categorical covariates 4 - Mean Gower dissimilarity (this one not available if missing values are present in X)
consim	If similarity_function is either set to 1 or 2, then this specifies the type of marginal likelihood used as the similarity function. Options are 1 - N-N(m_0, s_{20}, v) (v variance of "likelihood", m_0 and s_{20} "prior" parameters), 2 - N-NIG(m_0, s_{20}, k_0, ν_0) (m_0 and s_{20} center and scale of Gaussian, k_0 and ν_0)
calibrate	Whether the similarity should be calibrated. Options are 0 - no calibration 1 - standardize similarity value for each covariate 2 - coarsening is applied so that each similarity is raised to the 1/p power
simParms	Vector of parameter values employed in the similarity function of the PPMx. Entries of the vector correspond to m_0 - center continuous similarity with default 0, s_{20} - spread of 'prior' continuous similarity with default 1, v_2 - spread of 'likelihood' for continuous similarity (smaller values place more weight partitions with clusters that contain homogeneous covariate values) k_0 - degrees of freedom upper for v (only used for N-NIG similarity model) ν_0 - scale for v (only used for N-NIG similarity model)

	a0 - dirichlet weight for categorical similarity with default of 0.1 (smaller more weight placed on this variable)
	alpha - weight associated with cluster-variance and Gower dissimilarity
modelPriors	Vector of prior parameter values used in the PPMx prior. m - prior mean for mu0 with default equal to 0, s2 - prior variance mu0 with default equal to 100^2, A - upper bound on sigma2*_j with default equal to 10 B - upper bound on sig20 with default equal to 10
mh	two dimensional vector containing values for tuning parameter associated with MH update for sigma2 and sigma20
draws	number of MCMC iterates to be collected. default is 1100
burn	number of MCMC iterates discarded as burn-in. default is 100
thin	number by which the MCMC chain is thinned. default is 1. Thin must be selected so that it is a multiple of (draws - thin)
verbose	Logical indicating if information regarding data and MCMC iterate should be printed to screen

Details

An ordinal probit model is fit. If covariates contain missing values, then approach employed by page et al is automatically employed. The computational implementation of the model is based algorithm 8 found in Neal's 2000 JCGS paper

Value

The function returns A list containing arrays filled with MCMC iterates corresponding to model parameters and model fit metrics. In order to provide more detail, in what follows let

"T" - be the number of MCMC iterates collected,

"N" - be the number of observations,

"P" - be the number of predictions.

The output list contains the following

mu - a matrix of dimension (T, N) containing MCMC iterates associated with each subjects mean parameter (mu*_c_i).

sig2 - a matrix of dimension (T, N) containing MCMC iterates associated with each subjects variance parameter (sigma2*_c_i)

Si - a matrix of dimension (T, N) containing MCMC iterates associated with each subjects cluster label.

like - a matrix of dimension (T, N) containing likelihood values at each MCMC iterate.

fitted - a matrix of dimension (T, N) containing fitted (or in sample predictions) for each subject at each MCMC iterate

ppred - a matrix of dimension (T, P) containing out of sample predictions for each "new" subject at each MCMC iterate

mu0 - vector of length T containing MCMC iterates for mu0 parameter

sig20 - vector of length T containing MCMC iterates for sig20
 nclus - vector of length T containing number of clusters at each MCMC iterate
 WAIC - scalar containing the WAIC value
 lpml - scalar containing lpml value

Examples

```
# Continuous Covariate
X1 <- runif(100, 0,1)

# Binary Covariate
X2 <- rbinom(100, 1, 0.5)

pi <- exp(2*X1 + -2*X2)/(exp(2*X1 + -2*X2) + 1)

# Binary response
Y <- rbinom(100, 1, pi)

keep <- sample(1:100, 75, replace=FALSE)

X <- cbind(X1, X2)

Xtn <- X[keep,]
ytn <- Y[keep]
Xtt <- X[-keep,]
ytt <- Y[-keep]

# Since Multinomial need to select boundaries of "latent states".
# For co below the latent states are < 0 and > 0
co <- c(-100000, 0, 100000)
# Their selection is arbitrary and doesn't impact things
# See Thanasis work on this.

#           m0  s20  v   k0  n0  a0
simParms <- c(0.0, 1.0, 2.0, 1.0, 2.0, 0.1)
#           m  s2  s  s  s0 s0
modelPriors <- c(0, 10, 0, 1, 0, 1)

draws <- 50000
burn <- 25000
thin <- 25
nout <- (draws - burn)/thin
```

```

# Takes about 15 seconds to run
fit <- ordinal_ppmx(y = ytn, co=co, X=Xtn, Xpred=Xtt,
                  similarity_function=1, consim=1,
                  calibrate=0,
                  simParms=c(0.0, 1.0, 0.5, 1.0, 2.0, 0.1, 1),
                  modelPriors=c(0, 1, 0, 0.5, 0, 10),
                  draws=draws, burn=burn, thin=thin, verbose=FALSE)

# The first partition iterate is used for plotting
# purposes only. We recommended using the salso
# R-package to estimate the partition based on Si
pairs(cbind(Y, X), col=fit$Si[1,])

```

ozone

Ozone data

Description

data set consists of 112 measurements of maximum daily ozone in Rennes. In addition, temperature (T), nebulosity (Ne), and projection of wind speed vectors (Vx) were measured three times daily (9:00, 12:00, and 15:00 hours) resulting in nine covariates.

Format

data: A data frame with 112 rows and the following variables:

num observed number of cancer cases

maxO3 max daily ozone

T9-T15 temperature measured at 9:00, 12:00, and 15:00 hours

Ne9-Ne15 nebulosity measured at 9:00, 12:00, and 15:00 hours

Vx9-Vx15 projection of wind speed vectors measured at 9:00, 12:00, and 15:00 hours

max03v max daily ozone of previous day.

WindDirection The wind direction

Source

Source of data: <https://github.com/njtierney/user2018-missing-data-tutorial/>

rppmx

*Function generates random realizations from a PPM or PPMx***Description**

rppmx Employs the ploya urn sampling scheme to randomly generate a partition from the PPM or PPMx.

Usage

```
rppmx(m, X=NULL,
      similarity,
      simparm,
      M=1,
      m0=0, s20=1, v=2, k0=10, v0=1, alpha=1)
```

Arguments

m	Number of unites that are allocated to partitions
X	a data frame whose columns consist of covariates that will be incorporated in the partition model. Those with class of "character" or "factor" will be treated as categorical covaraites. All others will be treated as continuous covariates. If NULL, then a PPM partition is produced.
similarity	Type of similarity function that is employed for covariates. Options are 1 - Auxilliary similarity, 2 - Double dipper similarity 3 - variance similarity
simparm	Type of similarty model employed for continuous covariates. Options are 1 - N-N(m0, s20, v) (v variance of "likelihood", m0 and s20 "prior" parameters), 2 - N-NIG(m0,k0, k0, v0, s20) (m0 and k0 center and scale of Gaussian, n0 and s20 shape and scale of IG)
M	Precision parameter. Default is 1.
m0	Continuous similarity function value (see above)
s20	Continuous similarity function value (see above)
v	Continuous similarity function value (see above)
k0	Continuous similarity function value (see above)
v0	Continuous similarity function value (see above)
alpha	Penalty value when using the variance similarity

Details

Use polya urn scheme to sample from the PPM or the PPMx

Value

The function returns randomly generated partition

Examples

```
X <- cbind(rnorm(100), rbinom(100,1,0.5))
p <- rppmx(m=100, X=X, similarity=1, simparm=1, M=1)
p
```

scallops

Scallops data

Description

Data set that provides the location and scallop catches in the Atlantic waters off the coasts of New Jersey and Long Island, New York.

Format

data: A data frame with 148 rows and the variables are the following:

strata

sample

lat

long

tcatch

prerec

recruits

Source

Banerjee, S; Carline, B. P.; Gelfand, A. E.; (2015) Hierarchical Modeling and Analysis for Spatial Data 2nd Ed. CRC. Press

SIMCE

*Standardized testing data in Chile***Description**

Average standard testing results with average mother's and father's education level for schools in the greater Santiago area of Chile. Measurements are recorded from 2005-2011 and spatial coordinates of the schools are provided.

Format

data: A data frame with 1072 rows and the following variables:

coords.x1 longitude coordinates of school

coords.x2 latitude coordinates of school

Schoole Unique school identifier

COMUNA Name of the commune in which the school resides

SIMCE05-SIMCE11 Math score of standardized test in 2005-2011

EDpad05-EDpad11 Average level of father's education of students that attended school 2005-2011

EDmad05-EDmad11 Average level of mother's education of students that attended school 2005-2011

Source

Page, G. L. and Quintana, F. A. (2016) Spatial Product Partition Models, Bayesian Anal., Volume 11, Number 1, 265-298.

sppm

*Function that fits spatial product partition model with Gaussian likelihood***Description**

sppm is the main function used to fit model with Gaussian likelihood and spatial PPM as prior on partitions.

Usage

```
sppm(y, s,
      s.pred=NULL,
      cohesion,
      M=1,
      modelPriors=c(0, 100^2, 10, 10),
      cParms=c(1, 1.5, 0, 1, 2, 2),
      mh=c(0.5, 0.5),
      draws=1100, burn=100, thin=1)
```

Arguments

y	numeric vector containing response variable
s	Two-column matrix containing spatial locations (i.e., longitude and latitude).
s.pred	Two-column matrix containing spatial locations at which out-of-sample predictions will be collected.
cohesion	Scalar that indicates which cohesion to use. <ul style="list-style-type: none"> • 1 - distance from centroids • 2 - upper bound • 3 - auxiliary similarity • 4 - double dipper similarity
M	Parameter related to Dirichlet process scale or dispersion parameter.
modelPriors	Vector containing model prior values (see below for more details)
cParms	Vector containing partition model prior values (see below for more details)
mh	Tuning standard deviations for metropolis updates for sigma2 and sigma20
draws	Number of MCMC samples to collect
burn	Number of the MCMC samples discarded in the burn-in phase of the sampler
thin	The amount of thinning desired for the chain

Details

The vector modelPriors = c(m0, s20, ms, ms0) where each prior parameter is listed in the model description below.

The cParm vector contains values associated with the cohesion function.

cParm = c(
epsilon value - cohesion 1 only,
distance bound - cohesion 2 only,
mu0 - center of NNIG for cohesion 3 and 4
k0 - scale parm of gaussian part of NNIG for cohesion 3 and 4
v0 - degrees of freedom IG part of NNIG for cohesion 3 and 4
L0 - scale parm (scalar of identity matrix) IG part of NNIG for cohesion 3 and 4).

The model this function fits is Gaussian likelihood model using the sPPM prior on partitions (Page and Quintana, 2016). Specific model details are

$$y_i | \mu^*, \sigma^{2*}, c_i \sim N(\mu_{c_i}^*, \sigma_{c_i}^{2*}), i = 1, \dots, n$$

$$\mu_j^* | \mu_0, \sigma_0^2 \sim N(\mu_0, \sigma_0^2)$$

$$\sigma_j^* | A \sim UN(0, ms)$$

$$\rho | M, \xi \sim sPPM$$

To complete the model specification, the following hyperpriors are assumed,

$$\mu_0|m, s^2 \sim N(m0, s0^2)$$

$$\sigma_0|B \sim UN(0, ms0)$$

Note that we employ uniform prior distributions on variance components as suggest in Gelman's 2006 Bayesian paper. "sPPM" in the model specificaiton denotes the the spatial product partition model. The computational implementation of the model is based algorithm 8 found in Neal's 2000 JCGS paper.

Value

This function returns in a list all MCMC iterates for each model parameter, posterior predictive, and fitted values. In addition the LPML model fit metric is provided.

Examples

```
data(scallops)

Y<-log(scallops[,5]+1)
s_coords <- scallops[,3:4] #lat and long
m <- dim(s_coords)[1]

# standardize spatial coordinates
smn <- apply(s_coords,2,mean)
ssd <- apply(s_coords,2,sd)
s_std <- t((t(s_coords) - smn)/ssd)

# Create a grid of prediction locations
np <- 10

sp <- expand.grid(seq(min(s_coords[,1]), max(s_coords[,1]),length=np),
                 seq(min(s_coords[,2]), max(s_coords[,2]), length=np))

sp_std <- t((t(sp) - smn)/ssd) # standardized prediction spatial coordinates

niter <- 20000
nburn <- 10000
nthin <- 10
nout <- (niter - nburn)/nthin

out <- sppm(y=Y,s=s_std,s.pred=sp_std,cohesion=4, M=1, draws=niter, burn=nburn, thin=nthin)
```



```
# fitted values
fitted.values <- out$fitted
fv.mn <- apply(fitted.values, 2,mean)
mean((Y - fv.mn)^2) # MSE
out$lpml #lpml value

ppred <- out$ppred
predmn <- apply(ppred,2,mean)

# The first partition iterate is used for plotting
# purposes only. We recommended using the salso
# R-package to estimate the partition based on Si
Si <- out$Si
plot(s_coords[,1], s_coords[,2], col=Si[1,])
```

Index

* **datasets**

bear, [2](#)

scallops, [13](#)

bear, [2](#)

gaussian_ppmx, [2](#)

ordinal_ppmx, [7](#)

ozone, [11](#)

rppmx, [12](#)

scallops, [13](#)

SIMCE, [14](#)

sppm, [14](#)