Package ‘ISEtools’

April 1, 2020

Type Package

Title Tools for Ion Selective Electrodes

Version 3.1.1.1

Date 2018-12-31

Author Peter Dillingham [aut, cre],
       Christina McGraw [ctb],
       Aleksandar Radu [ctb],
       Basim Alsaedi [ctb]

Maintainer Peter Dillingham <peter.dillingham@otago.ac.nz>

Description Characterisation and calibration of single or multiple Ion Selective Electrodes (ISEs); activity estimation of experimental samples. Implements methods described in:

Depends Xmisc, coda

Imports graphics, stats, utils

Suggests R2WinBUGS, BRugs, boot, rjags, R.rsp

VignetteBuilder R.rsp

SystemRequirements OpenBUGS (>=3.0) OR jags (>=4.0.0)

License GPL-2

URL http://www.maths.otago.ac.nz/~dillingh/software.html

RoxygenNote 6.0.0

NeedsCompilation no

Repository CRAN

Date/Publication 2020-04-01 05:38:09 UTC
R topics documented:

ISEtools-package .................................................. 2
analyseISE ............................................................... 3
carbonate ............................................................... 6
describeISE ............................................................. 6
LeadStdAdd ........................................................... 9
loadISEdata ........................................................... 10
plot.analyseISE ....................................................... 12
plot.ISEdata .......................................................... 13
plot.ISEdescription ............................................... 14
print.analyseISE ...................................................... 15
print.ISEdata ........................................................ 15
print.ISEdescription .............................................. 16
summary.analyseISE ............................................... 17
summary.ISEdata .................................................... 17
summary.ISEdescription ........................................ 18

Index ................................................................. 20

ISEtools-package  Analysis tools for ion selective electrodes (ISEs)

Description

Bayesian calibration for single or multiple ISEs using R and OpenBUGS. Estimation of analyte activities using single ISEs or ISE arrays.

Details

Package: ISEtools
Type: Package
Version: 2.5.2
Depends: R (>2.13.0), R2OpenBUGS (>3.0)
Date: 2018-10-15
License: GPL-2
SystemRequirements: OpenBUGS (>3.0)

The primary functions are loadISEdata (which loads calibration and experimental data from tab-delimited text files), describeISE (uses Bayesian calibration to estimate ISE parameters from calibration data), and analyseISE (combines calibration data with experimental data in basic or standard addition format to estimate analyte concentrations).

Author(s)

Peter Dillingham [aut, cre], Christina McGraw [ctb], Aleksandar Radu [ctb], Basim Alsaedi [ctb]
**analyseISE**

Ion selective electrode characterisation and estimation of sample concentrations

---

**Description**

Use Bayesian calibration to estimate parameters for \( y = a + b \log(x + c) + \text{error} \), where error follows a normal distribution with mean 0 and standard deviation \( \sigma \). The limit of detection (false positive/negative method or S/N=3 method) is also estimated. These values are then used to the estimate sample concentrations.

**Usage**

```r
analyseISE(data, model.path=NA, model.name=NA, Z=NA, temperature = 21,
burnin=25000, iters = 50000, chains=4, thin = 1,
a.init= NA, b.init=NA, cstar.init=NA, logc.limits = c(-8.9, -1.9),
sigma.upper = 5, diagnostic.print=F, offset = 1,
alpha = 0.05, beta = 0.05, SN = NA, program="OpenBUGS")
```
Arguments

data
model.path
model.name
Z
temperature
burnin
iters
chains
thin
a.init
b.init
cstar.init
logc.limits
sigma.upper
diagnostic.print
offset
alpha
beta
SN
program

analyseISE returns a list of class 'analyseISE'. Individual components include:

SampleID
log10x.exp
ahat
bhat
chat
**analyseISE**

- **cstarhat** Estimated value for cstar (from the median of the posterior distribution)
- **sigmahat** Estimated value for cstar (from the median of the posterior distribution)
- **LOD.info** List describing LOD method (alpha, beta or S/N) and corresponding values (alpha, beta, SN)
- **LOD.hat** Estimated value for the limit of detection (from the median of the posterior distribution)
- **<parametername>.lcl** Lower limit for the above parameters (e.g. ahat.lcl, bhat.lcl, ...) (from the 2.5th percentile of the posterior distribution)
- **<parametername>.ucl** Upper limit for the above parameters (from the 97.5th percentile of the posterior distribution)
- **LOD.Q1** 25th percentile estimated value of the limit of detection
- **LOD.Q3** 75th percentile estimated value of the limit of detection

**Author(s)**

Peter Dillingham, <peter.dillingham@otago.ac.nz>

**References**


**Examples**

- Fast-running example with only 100 MCMC iterations for testing:
  ```r
data(LeadStdAdd)
example2test = analyseISE(LeadStdAdd, Z = 2, temperature = 21,
                         burnin=100, iters=200, chains=1, a.init=c(176, 146, -112),
                         b.init=c(29, 30, 31), cstar.init=c(0.26, 0.27, 0.22), program="jags")
print(example2test)
summary(example2test)
plot(example2test, ylim = c(-7, -3), xlab = "ID (Sample)",
     ylab = expression(paste(log[10], " " , Pb^{paste("2","+",sep="") } )))
```

- Full example with 100,000 iterations (25,000 by 4 chains):
  ```r
data(LeadStdAdd)
example2 = analyseISE(LeadStdAdd, Z = 2, temperature = 21)
print(example2)
summary(example2)
plot(example2, ylim = c(-7, -3), xlab = "ID (Sample)",
     ylab = expression(paste(log[10], " " , Pb^{paste("2","+",sep="") } )))
```
**carbonate**  
*ISE measurements of carbonate in seawater*

**Description**
A data set containing emf responses for 8 ISEs measuring carbonate in seawater

**Usage**
```r
data(carbonate)
```

**Format**
Load example carbonate data as an object of type ISEdata (see function loadISEdata)

**References**

**Examples**
```r
data(carbonate)
print(carbonate)
plot(carbonate)
```

**describeISE**  
*Ion selective electrode characterisation*

**Description**
Use Bayesian calibration to estimate parameters for \( y = a + b \log(x + c) + \text{error} \), where error follows a normal distribution with mean 0 and standard deviation sigma. The limit of detection is also estimated.

**Usage**
```r
describeISE(data, model.path=NA, model.name = NA, Z=NA, temperature = 21, burnin=25000, iters = 50000, chains=4, thin = 1, a.init= NA, b.init=NA, cstar.init=NA, logc.limits = c(-8.9, -1.9), sigma.upper = 5, diagnostic.print=F, offset = 1, alpha = 0.05, beta = 0.05, SN = NA, keep.coda=T, coda.n=1000, program="OpenBUGS")
```
describeISE returns a list of class 'ISEdescription'. Individual components are:

ahat Estimated value for a (from the median of the posterior distribution)
bhat Estimated value for b (from the median of the posterior distribution)
chat
- Estimated value for c (from the median of the posterior distribution)

cstarhat
- Estimated value for cstar (c to the 0.1 power) (from the median of the posterior distribution)

sigmahat
- Estimated value for cstar (from the median of the posterior distribution)

LOD.info
- List describing LOD method (alpha, beta or S/N) and corresponding values (alpha, beta, SN)

LOD.hat
- Estimated value for the limit of detection (from the median of the posterior distribution)

<parametername>.lcl
- Lower limit for the above parameters (e.g. ahat.lcl, bhat.lcl, ...) (from the 2.5th percentile of the posterior distribution)

<parametername>.ucl
- Upper limit for the above parameters (from the 95.5th percentile of the posterior distribution)

LOD.Q1
- 25th percentile estimated value of the limit of detection

LOD.Q3
- 75th percentile estimated value of the limit of detection

If keep.coda = TRUE, then these additional items are returned:

ahat.coda
- Random sample (without replacement) of length coda.n from the Markov Chain Monte Carlo simulations for a

bhat.coda
- Random sample (without replacement) of length coda.n from the Markov Chain Monte Carlo simulations for b

chat.coda
- Random sample (without replacement) of length coda.n from the Markov Chain Monte Carlo simulations for c

sigmahat.coda
- Random sample (without replacement) of length coda.n from the Markov Chain Monte Carlo simulations for sigma

cstarhat.coda
- Random sample (without replacement) of length coda.n from the Markov Chain Monte Carlo simulations for cstar

LOD.coda
- Random sample (without replacement) of length coda.n from the Markov Chain Monte Carlo simulations for LOD

**Author(s)**

Peter Dillingham, <peter.dillingham@otago.ac.nz>

**References**


Examples

# Fast-running example with only 100 MCMC iterations for testing:
data(carbonate)
example3test = describeISE(carbonate, Z = -2, SN = 3.6,
burnin=100, iters=200, chains=1,
a.init= c(-50, 180, 140, 65, 100, 170, 100, 130),
b.init= rep(-20, 8), cstar.init= rep(0.2, 8), program="jags")
print(example3test)
summary(example3test)
plot(example3test)

# Full example with 100,000 iterations (25,000 by 4 chains):
data(carbonate)
example3 = describeISE(carbonate, Z = -2, SN = 3.6)
print(example3)
summary(example3)
plot(example3)

---

LeadStdAdd
ISE measurements of lead in soil

Description
A data set containing emf responses for 3 ISEs measuring lead in soil at Silvermines, Ireland. Calibration data and experimental data for 17 samples (in standard addition format) are included.

Usage
data(LeadStdAdd)

Format
Load example lead data as an object of type ISEdata (see function loadISEdata)

References

Examples
data(LeadStdAdd)
print(LeadStdAdd)
summary(LeadStdAdd)
plot(LeadStdAdd)
### Not run:
# Additional usage of this dataset with describeISE and analyseISE:
example1 = describeISE(LeadStdAdd, Z = 2, temperature = 21)
```r
print(example1)
summary(example1)
plot(example1)
example2 = analyseISE(LeadStdAdd, Z = 2, temperature = 21)
print(example2)
summary(example2)
plot(example2, ylim = c(-7, -3), xlab = "ID (Sample)",
 ylab = expression(paste(log[10], " \times \ Pb\"{\(2\"^{+}\"{,sep=""})} )))
```

---

**loadISEdata**  
*Load ISE calibration and experimental data.*

### Description

Loads tab-delimited calibration and (if it exists) experimental sample data.

### Usage

```r
loadISEdata(filename.calibration, filename.experimental = NA)
```

### Arguments

- `filename.calibration`
  
The name and location of the tab-delimited calibration file. It should have the following structure:

  - First line (header row): ISEID log10x emf
  - Remaining lines (data): ISEID is an identifier for the ISE. The ISEID variables should be integers, with the lowest value equal to 1, and no gaps. That is, if there are four ISEs, they must be labeled 1, 2, 3, and 4. log10x is the log10 concentration (mol/l) of the calibration samples. The emf readings (in mV) follow.

- `filename.experimental`
  
The experimental file (if there is one, otherwise keep the default filename.experimental=NA) should have one of the following structures:

  - **basic model:** The header row will include ISEID, SampleID, and emf. ISEID is defined the same way as in the calibration file. SampleID is an integer indicating which sample is being measured, and must follow the same numbering rules as ISEID. Finally, emf is the mV reading of the experimental samples for each ISE.
  - **or**
    - **standard addition:** When using the standard addition model, the experimental file will contain ISEID and SampleID as before. Two emf values are recorded: emf1 is the mV reading of the sample, and emf2 is the mV reading of the sample plus the addition. Additionally, V.s is the volume of the sample, V.add is the volume of the addition, and conc.add is the concentration (mol/l) of the addition. The units of V.s and V.add do not matter as long as they are the same.
loadISEdata

Details

Internally calls 'ISEdata.calibration' if there is no experimental data.

Value

loadISEdata returns the following values in a list of class ISEdata:

Calibration variables:

N  Total number of calibration measurements (e.g. for 5 calibration points measured with 3 ISEs, N = 15)
R  Number of ISEs
ISEID  Identifier for the ISE
log10x  log concentration (mol/l) of calibration data
emf  emf (mV) for calibration data

Experimental variables:

M  Number of experimental samples
M.obs  Total number of experimental measurements. E.g. for 4 samples each measured by 3 ISEs, M.obs = 12. Only returned if R > 1
ISEID.exp  Identifier for the ISE for the experimental data (returned if R > 1)
x.exp  Identifier for the experimental (returned if R > 1)

Basic format only:

emf.exp  emf (mV) for experimental data

Standard addition format only:

delta.emf  difference between emf1 and emf2 (mV) for experimental data
V.s  Sample volume (any units allowed but must be consistent)
V.add  Volume added to the sample
conc.add  Concentration added.

Summary variables of calibration and experimental data:

calibration.only  Indicates whether there was only calibration data (TRUE) or calibration and experimental data (FALSE)
stdadd  Indicates whether standard addition was used. Returns NA (calibration data only), FALSE (basic experimental data), or TRUE (standard addition experimental data)
data.calib  The loaded calibration data frame
data.exp  The loaded experimental data frame
Author(s)

Peter Dillingham <peter.dillingham@otago.ac.nz>

Examples

```r
###
# Loading the example tab-delimited text files for the lead data
###

# 1. Find pathnames for the lead example txt files:
path.calib = paste(path.package('ISEtools'), "/extdata", "/Lead_calibration.txt", sep="")
path.basic = paste(path.package('ISEtools'), "/extdata", "/Lead_experimentalBasic.txt", sep="")
path.sa = paste(path.package('ISEtools'), "/extdata", "/Lead_experimentalSA.txt", sep="")
# Load the calibration data
lead.example1 = loadISEdata(filename.calibration = path.calib)
print(lead.example1)

# ... and with experimental data, Basic format
lead.example2 = loadISEdata(filename.calibration = path.calib,
filename.experimental = path.basic)
print(lead.example2)

# ... and with experimental data, Standard Addition format
lead.example3 = loadISEdata(filename.calibration = path.calib,
filename.experimental = path.sa)
print(lead.example3)
```

---

**plot.analyseISE**

Plot function for ion selective electrode characterisation and estimation of sample concentrations

### Description

Plots sample concentration estimates derived from Bayesian calibration. E.g. analyseISE uses Bayesian calibration to estimate parameters for $y = a + b \log(x + c) + \text{error}$, where error follows a normal distribution with mean 0 and standard deviation sigma. These values are combined with experimental data to estimate sample concentrations.

### Usage

```r
## S3 method for class 'analyseISE'
plot(x, xlab = "Sample ID",
ylab = expression(paste(log[10], " (", italic(x), " )")), xlim = NA,
ylim = c(-15, 0), x.ticks = NA, y.ticks = NA, x.ticks.label = TRUE,
y.ticks.label = TRUE, y.las = 2, col = 1, x.shift = 0, xaxs = "r",
yaxs = "r", add.box = TRUE, ...)
```
plot.ISEdata

Arguments

- **x**: Calibration and experimental sample results (of class 'analyseISE'; see analyseISE)
- **xlab**: Label for the x-axis
- **ylab**: Label for the y-axis
- **xlim**: Limits for the x-axis. Automatically calculated if xlim = NA.
- **ylim**: Limits for the y-axis.
- **x.ticks**: Location of tickmarks for the x-axis. Automatically calculated if x.ticks = NA.
- **y.ticks**: Location of tickmarks for the y-axis. Automatically calculated if y.ticks = NA.
- **x.ticks.label**: Labels associated with x-axis tickmarks for the x-axis. Automatically calculated labels (TRUE), no labels (FALSE), or a column of text specifying custom labels (e.g. x.ticks.label = c("A", "B", "C") or similar, of the same length as x.ticks).
- **y.ticks.label**: Labels associated with y-axis tickmarks for the y-axis. See x.ticks.label for details.
- **y.las**: Indicates whether y-axis labels be perpendicular to the y-axis (2) or parallel to it (0).
- **col**: Colour for the field of the plot.
- **x.shift**: Shifts the plots to the left (- values) or right (+ values); useful for overlaying figures.
- **xaxs**: The style of x-axis interval. See par for further details, but "r" adds 4 percent padding, "i" has no padding.
- **yaxs**: The style of y-axis interval. See xaxs above.
- **add.box**: Indicates whether a box should be drawn around the plot (TRUE) or not (FALSE).
- **...**: Other arguments to be passed through to plotting functions.

Author(s)

Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also

analyseISE

---

plot.ISEdata  
*Basic plot of ion selective electrode calibration data*

Description

Plots raw ISE calibration data; data should follow a hockey stick pattern coinciding with the equation \( y = a + b \log(x + c) + \) error, where error follows a normal distribution with mean 0 and standard deviation sigma.
Usage

## S3 method for class 'ISEdata'
plot(x, xlab = expression(paste(log[10], " { ", italic(x), " }")), ylab = "emf", pch = 20, ...)

Arguments

- **x**: ISE calibration data
- **xlab**: Label for the x-axis
- **ylab**: Label for the y-axis
- **pch**: Plotting symbol for data
- **...**: Other arguments to be passed through to plotting functions.

Author(s)

Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also

- `loadISEdata`

Examples

```r
data(LeadStdAdd)
plot(LeadStdAdd)
```

---

plot.ISEdescription  
*Plot ISE parameter values*

Description

Plots histograms of ISE parameter values a, b, c, sigma, and LOD (alpha, beta or S/N) for the equation \( y = a + b \log(x + c) + \text{error} \), where error follows a normal distribution with mean 0 and standard deviation sigma.

Usage

## S3 method for class 'ISEdescription'
plot(x, breaks = 20, ...)

Arguments

- **x**: ISE description (e.g. object of class ISEdescription)
- **breaks**: Approximate number of bins for histograms, defaults to 20
- **...**: Other arguments to be passed through to plotting (histogram) functions
print.analyseISE

Author(s)
Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also
describeISE

print.analyseISE
Prints tables of ISE parameters and estimated sample concentrations.

Description
Prints tables of ISE parameters and estimated sample concentrations.

Usage
## S3 method for class 'analyseISE'
print(x, ...)

Arguments

x
ISE analysis results (e.g. object of class analyseISE)

... Other objects passed through.

Author(s)
Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also
analyseISE

print.ISEdata
Prints ISE data

Description
Prints tables of calibration data and experimental data (if present).

Usage
## S3 method for class 'ISEdata'
print(x, ...)

### S3 method for class 'analyseISE'
print(x, ...)

Arguments

x
ISE analysis results (e.g. object of class analyseISE)

... Other objects passed through.

Author(s)
Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also
analyseISE

print.ISEdata
Prints ISE data
print.ISEdescription

Arguments

  x ISE data (e.g. object of class ISEdata)
  ... Other objects passed through.

Author(s)

  Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also

  loadISEdata

Examples

  data(LeadStdAdd)
  print(LeadStdAdd)

print.ISEdescription  Prints tables of ISE parameters.

Description

  Prints tables of ISE parameters for one or multiple ISEs.

Usage

  ## S3 method for class 'ISEdescription'
  print(x, ...)

Arguments

  x ISE analysis results (e.g. object of class analyseISE)
  ... Other objects passed through.

Author(s)

  Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also

  describeISE
Summary of estimates for ISE parameter values and experimental sample concentrations.

**Description**

`summary.analyseISE` takes an object of class `analyseISE` and produces summary tables.

**Usage**

```r
## S3 method for class 'analyseISE'
summary(object, ...)
```

**Arguments**

- `object`: Data set of class `ISEdata`
- `...`: Other objects passed through.

**Value**

- `tables`: Two tables (table1 and table2) are returned as a list.
  - `table1`: A table of ISE parameter values (see `summary.describeISE` for details)
  - `table2`: A table of estimated analyte concentrations for experimental samples

**Author(s)**

Peter Dillingham, <peter.dillingham@otago.ac.nz>

**See Also**

- `analyseISE`
- `summary.ISEdescription`

---

**Summary ISE Data**

Summarises ISE data

**Description**

`summary.ISEdata` takes an object of class `ISEdata` (e.g. see `loadISEdata`) and produces metadata for it.

**Usage**

```r
## S3 method for class 'ISEdata'
summary(object, ...)
```
summary.ISEdescription

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>object</td>
<td>Data set of class ISEdata</td>
</tr>
<tr>
<td>...</td>
<td>Other objects passed through.</td>
</tr>
</tbody>
</table>

Value

metadata: Metadata for the ISEs, a list with N, R, calibration.only, M, and stdadd

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>Total number of calibration observations</td>
</tr>
<tr>
<td>R</td>
<td>Number of ISEs</td>
</tr>
<tr>
<td>calibration.only</td>
<td>Indicates calibration only data (T), or calibration and experimental data (F)</td>
</tr>
<tr>
<td>M</td>
<td>Number of experimental samples (NA if no experimental data were loaded)</td>
</tr>
<tr>
<td>stdadd</td>
<td>Indicates whether standard addition used for experimental samples (T) or the basic model was used (F), or no experimental data (NA)</td>
</tr>
</tbody>
</table>

Author(s)

Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also

loadISEdata

Examples

data(LeadStdAdd)
summary(LeadStdAdd)

Description

summary.ISEdescription takes an object of class ISEdescription and prints a table of parameter values for \( y = a + b \log(x + c) + \text{error} \), with the errors following a Normal distribution with mean 0 and standard deviation sigma. Also calculates LOD using the conditional analytic method (alpha, beta, or S/N).

Usage

```r
## S3 method for class 'ISEdescription'
summary(object, ...)
```
Arguments

object object of class ISEdescription
... Other objects passed through.

Value

table1: A matrix with parameter values for each ISE

Author(s)

Peter Dillingham, <peter.dillingham@otago.ac.nz>

See Also

describeISE
Index

*Topic **datasets**
  carbonate, 6
  LeadStdAdd, 9
*Topic **package**
  ISEtools-package, 2
analyseISE, 3, 13, 15, 17
carbonate, 6
describeISE, 6, 15, 16, 19
ISEtools (ISEtools-package), 2
ISEtools-package, 2
LeadStdAdd, 9
loadISEdata, 10, 14, 16, 18
plot.analyseISE, 12
plot.ISEdata, 13
plot.ISEdescription, 14
print.analyseISE, 15
print.ISEdata, 15
print.ISEdescription, 16
summary.analyseISE, 17
summary.ISEdata, 17
summary.ISEdescription, 17, 18