

# Package ‘QFASA’

October 29, 2016

**Title** Quantitative Fatty Acid Signature Analysis

**Version** 1.0.2

**Description** Accurate estimates of the diets of predators are required in many areas of ecology, but for many species current methods are imprecise, limited to the last meal, and often biased. The diversity of fatty acids and their patterns in organisms, coupled with the narrow limitations on their biosynthesis, properties of digestion in monogastric animals, and the prevalence of large storage reservoirs of lipid in many predators, led us to propose the use of quantitative fatty acid signature analysis (QFASA) to study predator diets.

**Depends** R (>= 3.2)

**License** MIT + file LICENSE

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**LazyData** true

**Imports** Rsolnp, grid

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**NeedsCompilation** no

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AIT.dist	<i>Returns the distance between two compositional vectors using Aitchison's distance measure.</i>
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**Description**

Returns the distance between two compositional vectors using Aitchison's distance measure.

**Usage**

```
AIT.dist(x.1, x.2)
```

**Arguments**

x.1	compositional vector
x.2	compositional vector

**References**

Aitchison, J., (1992) On criteria for measures of compositional difference. *Mathematical Geology*, 24(4), pp.365-379.

Stewart, C. (2016) An approach to measure distance between compositional diet estimates containing essential zeros. *Journal of Applied Statistics*, 10.1080/02664763.2016.119384.

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AIT.more	<i>Used to provide additional information on various model components evaluated at the optimal solution i.e. using the QFASA diet estimates and Aitchison distance measure.</i>
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**Description**

Used to provide additional information on various model components evaluated at the optimal solution i.e. using the QFASA diet estimates and Aitchison distance measure.

**Usage**

```
AIT.more(alpha, seal, prey.quantiles)
```

**Arguments**

alpha	compositional QFASA diet estimate.
seal	fatty acid signature of predator.
prey.quantiles	matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

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AIT.obj	<i>Used in solnp() as the objective function to be minimized when Aitchison distance measure is chosen.</i>
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**Description**

Used in solnp() as the objective function to be minimized when Aitchison distance measure is chosen.

**Usage**

```
AIT.obj(alpha, seal, prey.quantiles)
```

**Arguments**

alpha	vector over which minimization takes place.
seal	fatty acid signature of predator.
prey.quantiles	matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

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CC	<i>Fatty acid calibration coefficients.</i>
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**Description**

Fatty acid calibration coefficients.

**Usage**

CC

**Format**

A data frame with 66 observations and 2 variables:

**FA** fatty acid names

**CC** calibration coefficient for corresponding fatty acid

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chisq.dist	<i>Returns the distance between two compositional vectors using the chi-square distance.</i>
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**Description**

Returns the distance between two compositional vectors using the chi-square distance.

**Usage**

```
chisq.dist(x.1, x.2, gamma)
```

**Arguments**

x.1	compositional vector
x.2	compositional vector
gamma	power transform taken to be 1.

**References**

Stewart, C., Iverson, S. and Field, C. (2014) Testing for a change in diet using fatty acid signatures. *Environmental and Ecological Statistics* 21, pp. 775-792.

Stewart, C. (2016) An approach to measure distance between compositional diet estimates containing essential zeros. *Journal of Applied Statistics*, 10.1080/02664763.2016.119384.

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CS.more	<i>Used to provide additional information on various model components evaluated at the optimal solution i.e. using the QFASA diet estimates and chi-square distance measure.</i>
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**Description**

Used to provide additional information on various model components evaluated at the optimal solution i.e. using the QFASA diet estimates and chi-square distance measure.

**Usage**

```
CS.more(alpha, seal, prey.quantiles, gamma)
```

**Arguments**

alpha	compositional QFASA diet estimate.
seal	fatty acid signature of predator.
prey.quantiles	matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.
gamma	power transform exponent (see chisq.dist).

---

CS.obj	<i>Used in solnp() as the objective function to be minimized when chi-square distance measure is chosen. Unlike AIT.obj and KL.obj, does not require modifying zeros.</i>
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**Description**

Used in solnp() as the objective function to be minimized when chi-square distance measure is chosen. Unlike AIT.obj and KL.obj, does not require modifying zeros.

**Usage**

```
CS.obj(alpha, seal, prey.quantiles, gamma)
```

**Arguments**

alpha	vector over which minimization takes place.
seal	fatty acid signature of predator.
prey.quantiles	matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.
gamma	power transform exponent (see chisq.dist).

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FAs	<i>List of fatty acids to be used for modelling.</i>
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**Description**

List of fatty acids to be used for modelling.

**Usage**

FAs

**Format**

A data frame with 39 observations and 1 variable:

**FA** Fatty acid name

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KL.dist	<i>Returns the distance between two compositional vectors using Kullback-Leibler distance measure.</i>
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**Description**

Returns the distance between two compositional vectors using Kullback-Leibler distance measure.

**Usage**

KL.dist(x.1, x.2)

**Arguments**

x.1            compositional vector

x.2            compositional vector

**References**

S.J. Iverson, C. Field, W.D. Bowen, and W. Blanchard (2004) Quantitative fatty acid signature analysis: A new method of estimating predator diets, *Ecological Monographs* 72, pp. 211-235.

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KL.more	<i>Used to provide additional information on various model components evaluated at the optimal solution i.e. using the QFASA diet estimates and Kullback-Leibler distance measure.</i>
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**Description**

Used to provide additional information on various model components evaluated at the optimal solution i.e. using the QFASA diet estimates and Kullback-Leibler distance measure.

**Usage**

```
KL.more(alpha, seal, prey.quantiles)
```

**Arguments**

alpha	compositional QFASA diet estimate.
seal	fatty acid signature of predator.
prey.quantiles	matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

---

KL.obj	<i>Used in solnp() as the objective function to be minimized when Kullback-Leibler distance measure is chosen.</i>
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---

**Description**

Used in solnp() as the objective function to be minimized when Kullback-Leibler distance measure is chosen.

**Usage**

```
KL.obj(alpha, seal, prey.quantiles)
```

**Arguments**

alpha	vector over which minimization takes place.
seal	fatty acid signature of predator.
prey.quantiles	matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

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mean.geometric	<i>Returns the geometric mean of a compositional vector</i>
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### Description

Returns the geometric mean of a compositional vector

### Usage

```
## S3 method for class 'geometric'
mean(x)
```

### Arguments

x	compositional vector
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MEANmeth	<i>Returns the multivariate mean FA signature of each prey group entered into the QFASA model. Result can be passed to prey.mat in p.QFASA().</i>
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---

### Description

Returns the multivariate mean FA signature of each prey group entered into the QFASA model. Result can be passed to prey.mat in p.QFASA().

### Usage

```
MEANmeth(preymat)
```

### Arguments

preymat	matrix containing the FA signatures of the prey. The first column indexes the prey group.
---------	---



multiplot *Multiplot*

**Description**

Multiplot

**Usage**

multiplot(..., plotlist = NULL, file, cols = 1, layout = NULL)

**Arguments**

...	TODO
plotlist	TODO
file	TODO
cols	TODO
layout	TODO

p.QFASA	<i>Computes the diet estimate for each predator in seal.mat using either the Kullback-Leibler Distance (KL), the Aitchison Distance (AIT) or the Chi-Square Distance (CS).</i>
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**Description**

Computes the diet estimate for each predator in seal.mat using either the Kullback-Leibler Distance (KL), the Aitchison Distance (AIT) or the Chi-Square Distance (CS).

**Usage**

p.QFASA(seal.mat, prey.mat, cal.mat, dist.meas, gamma, FC = rep(1, nrow(preymat)), start.val = rep(0.99999, nrow(preymat)), ext.fa)

**Arguments**

seal.mat	matrix containing the FA signatures of the predators.
prey.mat	matrix containing a representative FA signature from each prey group (usually the mean). The first column must index the prey group.
cal.mat	matrix of calibration factors where the <i>i</i> th column is to be used with the <i>i</i> th seal
dist.meas	distance measure to use for estimation: 1=KL, 2=AIT or 3=CS
gamma	parameter required for calculations using CS distance (passed to CS.obj). Currently being set to 1.
FC	vector of fat content
start.val	initial vector of parameters to be optimized
ext.fa	subset of FA's to be used to obtain QFASA diet estimates.

**Examples**

```

## Fatty Acids
data(FAs)
fa.set = as.vector(unlist(FAs))

## Predators
data(predatorFAs)
tombstone.info = predatorFAs[,1:4]
predator.matrix = predatorFAs[,5:(ncol(predatorFAs))]
npredators = nrow(predator.matrix)

## Prey
data(prexFAs)
prey.sub=(prexFAs[,4:(ncol(prexFAs))])[fa.set]
prey.sub=prey.sub/apply(prey.sub,1,sum)
group=as.vector(prexFAs$Species)
prey.matrix=cbind(group,prey.sub)
prey.matrix=MEANmeth(prey.matrix)

FC = prexFAs[,c(2,3)]
FC = as.vector(tapply(FC$lipid,FC$Species,mean,na.rm=TRUE))

## Calibration Coefficients
data(CC)
cal.vec = CC[,2]
cal.mat = replicate(npredators, cal.vec)

# Run QFASA
Q = p.QFASA(predator.matrix,
            prey.matrix,
            cal.mat,
            dist.meas=1,
            gamma=1,
            FC,
            start.val = rep(1,nrow(prey.matrix)),
            fa.set)

```

---

predatorFAs

*Predator fatty acid signatures. Each predator signature is a row with fatty acid proportions in columns.*

---

**Description**

Fatty acid signatures are subsetted for the chosen fatty acid set and renormalized during the modelling so there is no need to subset and/or renormalize prior to running p.QFASA. However, make sure that the the same fatty acids appear in the predator and prey files (if a FA appears in one but not the other the code will give you an error).

**Usage**

`predatorFAs`

**Format**

A data frame with 10 observations and 70 variables:

**SampleCode** TODO

**AnimalCode** TODO

**SampleGroup** TODO

**Biopsy** TODO

**c12.0**

**c13.0**

**Iso14**

**c14.0**

**c14.1w9**

**c14.1w7**

**c14.1w5**

**Iso15**

**Anti15**

**c15.0**

**c15.1w8**

**c15.1w6**

**Iso16**

**c16.0**

**c16.1w11**

**c16.1w9**

**c16.1w7**

**c7Mec16.0**

**c16.1w5**

**c16.2w6**

**Iso17**

**c16.2w4**

**c16.3w6**

**c17.0**

**c16.3w4**

**c17.1**

**c16.4w3**

**c16.4w1**

c18.0  
c18.1w13  
c18.1w11  
c18.1w9  
c18.1w7  
c18.1w5  
c18.2d5.11  
c18.2w7  
c18.2w6  
c18.2w4  
c18.3w6  
c18.3w4  
c18.3w3  
c18.3w1  
c18.4w3  
c18.4w1  
c20.0  
c20.1w11  
c20.1w9  
c20.1w7  
c20.2w9  
c20.2w6  
c20.3w6  
c20.4w6  
c20.3w3  
c20.4w3  
c20.5w3  
c22.1w11  
c22.1w9  
c22.1w7  
c22.2w6  
c21.5w3  
c22.4w6  
c22.5w6  
c22.4w3  
c22.5w3  
c22.6w3  
c24.1w9

**Details**

Unlike the original QFASApack code the predator data can contain as much tombstone data in columns as you wish but the predator FA signatures must be extracted as a separate input in order to run in p.QFASA.

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preyFAs	<i>Prey fatty acid signatures. Each prey signature is a row with fatty acid proportions in columns.</i>
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---

**Description**

The prey file should contain all of the individual fatty acid signatures of the prey and their lipid contents (where appropriate) - a matrix of the mean values for the FAs (prey.matrix) by the designated prey modelling group is then calculated using the MEANmeth function.

**Usage**

```
preyFAs
```

**Format**

A data frame with 302 observations and 70 variables:

**Lab.Code** TODO

**Species** TODO

**lipid** TODO

**c12.0**

**c13.0**

**Iso14**

**c14.0**

**c14.1w9**

**c14.1w7**

**c14.1w5**

**Iso15**

**Anti15**

**c15.0**

**c15.1w8**

**c15.1w6**

**Iso16**

**c16.0**

**c16.1w11**

c16.1w9  
c16.1w7  
c7Me16.0  
c16.1w5  
c16.2w6  
Iso17  
c16.2w4  
c16.3w6  
c17.0  
c16.3w4  
c17.1  
c16.3w1  
c16.4w3  
c16.4w1  
c18.0  
c18.1w13  
c18.1w11  
c18.1w9  
c18.1w7  
c18.1w5  
c18.2d5.11  
c18.2w7  
c18.2w6  
c18.2w4  
c18.3w6  
c18.3w4  
c18.3w3  
c18.3w1  
c18.4w3  
c18.4w1  
c20.0  
c20.1w11  
c20.1w9  
c20.1w7  
c20.2w9  
c20.2w6  
c20.3w6

c20.4w6  
c20.3w3  
c20.4w3  
c20.5w3  
c22.1w11  
c22.1w9  
c22.1w7  
c22.2w6  
c21.5w3  
c22.4w6  
c22.5w6  
c22.4w3  
c22.5w3  
c22.6w3  
c24.1w9

### Details

Like the predator .csv file you can have as many tombstone data columns as required but there must be at least one column that identifies the modelling group, in this case, Species.

Unlike the predator data, the prey data is not subsetted and renormalized during the modelling so the prey file needs to be subsetted for the desired fatty acid set and renormalized to sum to 1 prior to calculating the mean values.

The full FA set is extracted from the data frame (columns 4 onward), subsetted for the FA set in use and then renormalized over 1. The modelling group names (the "Species" column in this case) is then added back to the subsetted and renormalized data (as the first column) and the average values calculated using the MEANmeth function. Note that for the MEANmeth function to work the modelling group name must be in the first column.

### Description

Accurate estimates of the diets of predators are required in many areas of ecology, but for many species current methods are imprecise, limited to the last meal, and often biased. The diversity of fatty acids and their patterns in organisms, coupled with the narrow limitations on their biosynthesis, properties of digestion in monogastric animals, and the prevalence of large storage reservoirs of lipid in many predators, led us to propose the use of quantitative fatty acid signature analysis (QFASA) to study predator diets.

---

QFASA.const.eqn      *Returns sum(alpha) and used in solnp.*

---

**Description**

Returns sum(alpha) and used in solnp.

**Usage**

QFASA.const.eqn(alpha, seal, prey.quantiles, gamma)

**Arguments**

alpha	vector over which minimization takes place.
seal	fatty acid signature of predator.
prey.quantiles	matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.
gamma	power transform exponent (see chisq.dist).



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