Package 'NMRphasing'

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Type Package

Title Phase Error Correction and Baseline Correction for One Dimensional ('1D') 'NMR' Data

Version 1.0.5

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Depends R (>= 4.3.0),stats

Suggests knitr, rmarkdown, ggpubr

VignetteBuilder knitr

Imports baseline, splines, MassSpecWavelet

Description There are three distinct approaches for phase error correction, they are: a single linear model with a choice of optimization functions, multiple linear models with optimization function choices and a shrinkage-based method. The methodology is based on our new algorithms and various references (Binczyk et al. (2015) <doi:10.1186/1475-925X-14-S2-S5>,Chen et al. (2002) <doi:10.1016/S1090-7807(02)00069-1>, de Brouwer (2009) <doi:10.1016/j.jmr.2009.09.017>, Džakula (2000) <doi:10.1006/jmre.2000.2123>, Ernst (1969) <doi:10.1016/0022-2364(69)90003-1>, Liland et al. (2010) <doi:10.1366/000370210792434350>).

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Contents

`fdat` *This is an example data in NMRphasing*

Description

This dataset contains sample data for NMRphasing.

Usage

```
fdat
```

Format

A data frame with two columns, one is for NMR data in complex format, the other one is ppm

Author(s)

Aixiang Jiang

`MPC_AAM` *MPC_AAM*

Description

Multiple single linear models that minimize absolute area.

Usage

```
MPC_AAM(specdat, withBC = TRUE)
```

Arguments

`specdat`	A complex number vector of observed frequency domain data.
`withBC`	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is used to process phase error correction through multiple single linear models that minimize absolute area, followed by polynomial baseline correction when necessary.

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

de Brouwer, H. (2009). Evaluation of algorithms for automated phase correction of NMR spectra. J Magn Reson, 201, 230-238.

Dzakula, Z. (2000). Phase angle measurement from peak areas (PAMPAS). J Magn Reson, 146, 20-32.

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
mpc_aam_phased1 <- MPC_AAM(fdat$frequency_domain)
```

`MPC_ADSM` *MPC_ADSM*

Description

Multiple single linear models that minimize the absolute total dispersion.

Usage

```
MPC_ADSM(specdat, withBC = TRUE)
```

Arguments

`specdat`	A complex number vector of observed frequency domain data.
`withBC`	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is used to process phase error correction through multiple single linear models that minimize the absolute total dispersion, followed by polynomial baseline correction when necessary.

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Jiang, A. (2024). Phase Error Correction in Magnetic Resonance: A Review of Models, Optimization Functions, and Optimizers in Traditional Statistics and Neural Networks. Preprints. https://doi.org/10.20944/preprints202409.2252.v1

Chen, L., Weng, Z., Goh, L., & Garland, M. (2002). An efficient algorithm for automatic phase correction of NMR spectra based on entropy minimization. Journal of Magnetic Resonance, 158, 1-2.

Ernst, R. R. (1969). Numerical Hilbert transform and automatic phase correction in magnetic resonance spectroscopy. Journal of Magnetic Resonance, 1, 7-26

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
mpc_dsm_phased1 <- MPC_ADSM(fdat$frequency_domain)
```

`MPC_DANM` *MPC_DANM*

Description

Multiple linear models that minimize the difference between absolute area and net area.

Usage

```
MPC_DANM(specdat, withBC = TRUE)
```

Arguments

`specdat`	A complex number vector of observed frequency domain data
`withBC`	A logical parameter that enables/disables baseline correction after baseline correction.

Details

This function processes phase error correction through multiple linear models that minimize the difference between absolute area and net area, followed by polynomial baseline correction when necessary.

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
mpc_danm_phased1 <- MPC_DANM(fdat$frequency_domain)
```

MPC_DSM *MPC_DSM*

Description

Multiple single linear models that minimize the total dispersion.

Usage

```
MPC_DSM(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data.
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is used to process phase error correction through multiple single linear models that minimize the total dispersion, followed by polynomial baseline correction when necessary.

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Binczyk, F., Tarnawski, R., & Polanska, J. (2015). Strategies for optimizing the phase correction algorithms in Nuclear Magnetic Resonance spectroscopy. Biomedical Engineering Online, 14 Suppl 2(Suppl 2), S5. https://doi.org/10.1186/1475-925X-14-S2-S5

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
mpc_dsm_phased1 <- MPC_DSM(fdat$frequency_domain)
```

MPC_EMP *MPC_EMP*

Description

Multiple single linear models based on entropy minimization with negative peak penalty.

Usage

```
MPC_EMP(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data.
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is used to process phase error correction through multiple single linear models with entropy minimization with negative peak penalty, followed by polynomial baseline correction when necessary.

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Binczyk F, Tarnawski R, Polanska J (2015) Strategies for optimizing the phase correction algorithms in Nuclear Magnetic Resonance spectroscopy. Biomed Eng Online 14 Suppl 2:S5.

de Brouwer, H. (2009). Evaluation of algorithms for automated phase correction of NMR spectra. J Magn Reson, 201, 230-238.

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
mpc_emp_phased1 <- MPC_EMP(fdat$frequency_domain)
```

NLS *NLS*

Description

Non-linear shrinkage

Usage

```
NLS(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data.
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is used to process phase error correction through non-linear shrinkage, followed by Polynomial baseline correction when necessary.

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
nls_phased1 <- NLS(fdat$frequency_domain)
```

NMRphasing *NMRphasing*

Description

Phase error correction wrap up function

Usage

```
NMRphasing(
  specDatIn,
  absorptionOnly = FALSE,
 method = c("NLS", "MPC_DANM", "MPC_EMP", "MPC_AAM", "MPC_DSM", "MPC_ADSM", "SPC_DANM",
    "SPC_EMP", "SPC_AAM", "SPC_DSM", "SPC_ADSM"),
  withBC = TRUE
)
```

Arguments

specDatIn	Input spectrum data, which can be one of the four formats: a vector of absorption spectrum; a complex vector; a data matrix or a data frame with two columns of spectrum data, which 1st column is for absorption spectrum, and 2nd column is for dispersion spectrum
absorptionOnly	A logical variable to tell us if specDatIn is a a vector of absorption specrtrum, default is false
method	One of phase correction and baseline correction methods. There are eleven available choices, which are "NLS", "MPC_DAOM", "MPC_EMP", "MPC_AAM", "MPC_DSM", "MPC_ADSM", "SPC_DAOM", "SPC_EMP", "SPC_AAM", "SPC_DSM", "SPC_ADSM", with "NLS", non-linear shrinkage as default.
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This is a wrap function to process phase error correction and baseline correction with eleven different choices.

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Jiang, A. (2024). Phase Error Correction in Magnetic Resonance: A Review of Models, Optimization Functions, and Optimizers in Traditional Statistics and Neural Networks. Preprints. https://doi.org/10.20944/preprints202409.2252.v1

Binczyk F, Tarnawski R, Polanska J (2015) Strategies for optimizing the phase correction algorithms in Nuclear Magnetic Resonance spectroscopy. Biomed Eng Online 14 Suppl 2:S5.

Chen L, Weng Z, Goh L, Garland M (2002) An efficient algorithm for automatic phase correction of NMR spectra based on entropy minimization. J Magn Reson 158:164–168.

de Brouwer H (2009) Evaluation of algorithms for automated phase correction of NMR spectra. J Magn Reson 201:230–238.

Džakula Ž (2000) Phase Angle Measurement from Peak Areas (PAMPAS). J Magn Reson 146:20–32.

Ernst RR (1969) Numerical Hilbert transform and automatic phase correction in magnetic resonance spectroscopy. J Magn Reson 1969 1:7–26.

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
nls_phased <- NMRphasing(specDatIn = fdat$frequency_domain, method = "NLS")
```

SPC_AAM *SPC_AAM*

Description

A single linear model with minimization on absolute area.

Usage

```
SPC_AAM(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is to process phase error correction through a single linear model with minimization on absolute area, followed by polynomial baseline correction if necessary

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

de Brouwer, H. (2009). Evaluation of algorithms for automated phase correction of NMR spectra. J Magn Reson, 201, 230-238.

Dzakula, Z. (2000). Phase angle measurement from peak areas (PAMPAS). J Magn Reson, 146, 20-32.

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
spc_aam_phased1 <- SPC_AAM(fdat$frequency_domain)
```

SPC_ADSM *SPC_DSM*

Description

A single linear model with absolute dispersion summation minimization.

Usage

```
SPC_ADSM(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is to process phase error correction through a single linear model with absolute dispersion summation minimization, followed by polynomial baseline correction if necessary

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Jiang, A. (2024). Phase Error Correction in Magnetic Resonance: A Review of Models, Optimization Functions, and Optimizers in Traditional Statistics and Neural Networks. Preprints. https://doi.org/10.20944/preprints202409.2252.v1

Chen, L., Weng, Z., Goh, L., & Garland, M. (2002). An efficient algorithm for automatic phase correction of NMR spectra based on entropy minimization. Journal of Magnetic Resonance, 158, 1-2.

Ernst, R. R. (1969). Numerical Hilbert transform and automatic phase correction in magnetic resonance spectroscopy. Journal of Magnetic Resonance, 1, 7-26 Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
spc_dsm_phased1 <- SPC_ADSM(fdat$frequency_domain)
```

SPC_DANM *SPC_DANM*

Description

A single linear model with Minimization of difference between absolute area and net area

Usage

```
SPC_DANM(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is to process phase error correction through a single linear model with minimization of difference between absolute area and net area, followed by polynomial baseline correction if necessary

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
spc_danm_phased1 <- SPC_DANM(fdat$frequency_domain)
```

SPC_DSM *SPC_DSM*

Description

A single linear model with dispersion summation minimization.

Usage

```
SPC_DSM(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is to process phase error correction through a single linear model with dispersion summation minimization, followed by polynomial baseline correction if necessary

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Binczyk, F., Tarnawski, R., & Polanska, J. (2015). Strategies for optimizing the phase correction algorithms in Nuclear Magnetic Resonance spectroscopy. Biomedical Engineering Online, 14 Suppl 2(Suppl 2), S5. https://doi.org/10.1186/1475-925X-14-S2-S5

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
spc_dsm_phased1 <- SPC_DSM(fdat$frequency_domain)
```

SPC_EMP *SPC_EMP*

Description

A single linear model with entropy minimization with negative peak penalty

Usage

```
SPC_EMP(specdat, withBC = TRUE)
```

Arguments

specdat	A complex number vector of observed frequency domain data
withBC	A logical parameter that enables/disables baseline correction after baseline correction

Details

This function is to process phase error correction through a single linear model with entropy minimization with negative peak penalty, followed by polynomial baseline correction if necessary

Value

A numeric vector of phase corrected absorption spectrum

Author(s)

Aixiang Jiang

References

Binczyk F, Tarnawski R, Polanska J (2015) Strategies for optimizing the phase correction algorithms in Nuclear Magnetic Resonance spectroscopy. Biomed Eng Online 14 Suppl 2:S5.

de Brouwer, H. (2009). Evaluation of algorithms for automated phase correction of NMR spectra. J Magn Reson, 201, 230-238.

Liland KH, Almøy T, Mevik B (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, Applied Spectroscopy 64, pp. 1007-1016.

Examples

```
data("fdat")
mpc_emp_phased1 <- SPC_EMP(fdat$frequency_domain)
```

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