Package 'ADPF'

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Title Use Least Squares Polynomial Regression and Statistical Testing to Improve Savitzky-Golay

Version 0.0.1

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Description This function takes a vector or matrix of data and smooths the data with an improved Savitzky Golay transform. The Savitzky-Golay method for data smoothing and differentiation calculates convolution weights using Gram polynomials that exactly reproduce the results of least-squares polynomial regression. Use of the Savitzky-Golay method requires specification of both filter length and polynomial degree to calculate convolution weights. For maximum smoothing of statistical noise in data, polynomials with low degrees are desirable, while a high polynomial degree is necessary for accurate reproduction of peaks in the data. Extension of the least-squares regression formalism with statistical testing of additional terms of polynomial degree to a heuristically chosen minimum for each data window leads to an adaptive-degree polynomial filter (ADPF). Based on noise reduction for data that consist of pure noise and on signal reproduction for data that is purely signal, ADPF performed nearly as well as the optimally chosen fixed-degree Savitzky-Golay filter and outperformed sub-optimally chosen Savitzky-Golay filters. For synthetic data consisting of noise and signal, ADPF outperformed both optimally chosen and sub-optimally chosen fixed-degree Savitzky-Golay filters. See Barak, P. (1995) <doi:10.1021/ac00113a006> for more information.

Depends R (>= 3.2.4), stats, utils

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1

NeedsCompilation no

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Contents

ADPF *Adaptive Degree Polynomial Filter [ADPF]*

Description

ADPF outputs a `data.frame` containing a column for the original data, the polynomial degree used to smooth it, and the requested derivative(s).

Usage

```
ADPF(YData, SthDeriv,MaxOrder,FilterLength, DeltaX, WriteFile)
```

Arguments

`YData`	a numeric `data.frame`, `matrix` or `vector` to transform
`SthDeriv`	differentiation order
`MaxOrder`	maximum polynomial order
`FilterLength`	window size (must be odd)
`DeltaX`	optional sampling interval
`WriteFile`	a boolean that writes a `data.frame` to the working directory if true

Details

This is a code listing of a smoothing algorithm published in 1995 and written by Phillip Barak. ADPF modifies the Savitzky-Golay algorithm with a statistical heurism that increases signal fidelty while decreasing statisical noise. Mathematically, it operates simply as a weighted sum over a given window:

$$f_t^{n,s} = \sum_{i=-m}^{m} h_i^{n,s,t} y_i$$

Where $h_i^{n,s,t}$ is the convolution weight of the ith point to the evaluate the sth derivative at point t using a polynomial of degree n on $2m+1$ data points, y. These convolution weights h are calculated using Gram polynomials which are optimally selected using a F_{chi} test. This improves upon the signal fidelity of Savitzky-Golay by optimally choosing the Gram polynomial degree between zero and the max polynomial order give by the user while removing statistical noise. The sampling interval specified with the `DeltaX` argument is used for scaling and get numerically correct derivatives. For more details on the statistical heurism see the Barak, 1995 article. This can be found at http://soils.wisc.edu/facstaff/barak/ under the publications section.

Author(s)

Phillip Barak

Samuel Kruse

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Examples

```
ADPF::CHROM

smooth<-ADPF(CHROM[,6],0,9,13)
numpoints=length(CHROM[,6])
plot(x=1:numpoints,y=CHROM[,6]);lines(x=1:numpoints, y=smooth[,3])
```

CHROM *Data frame of Chromatogram values*

Description

This file contains a `data.frame` of sample chromotography data. The 6th column is data without noise and the first five all have some gaussian noise added; these data sets showcase the advantages of ADPF over Savitzky-Golay.

Usage

```
data("CHROM")
```

Format

A data frame with 201 observations on the following 6 variables.

`CHROM1` a numeric vector

`CHROM2` a numeric vector

`CHROM3` a numeric vector

`CHROM4` a numeric vector

`CHROM5` a numeric vector

`CHROM6` a numeric vector

Source

Barak, P., 1995. Smoothing and Differentiation by and Adaptive-Degree Polynomial filter; Anal. Chem. 67, 2758-2762.

Examples

```
ADPF::CHROM

smooth<-ADPF(CHROM[,6],0,9,13)
numpoints=length(CHROM[,6])
plot(x=1:numpoints,y=CHROM[,6]);lines(x=1:numpoints, y=smooth[,3])
```

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