PARAFAC3W

Fits a PARAFAC model of rank F to a 3-way array[6].

Requirements:

Matlab 6.5 and the 'N-way toolbox'[1].

Fitting the PARAFAC model

To fit a rank F model to a given the three-way array **X**, one can use the following algorithms (and calls):

ALS   Alternating Least Squares[1,2]
```
Options = ParOptions('algorithm','ALS');
[A,B,C,Diag] = Parafac3W(X,F,Options);
```

dGN   damped Gauss-Newton[5,6]
```
Options = ParOptions('algorithm','dGN');
[A,B,C,Diag] = Parafac3W(X,F,Options);
```

PMF3   Positive Matrix Factorization for 3-way arrays[5,6]
```
Options = ParOptions('algorithm','PMF3');
[A,B,C,Diag] = Parafac3W(X,F,Options);
```

SWATLD   Self-Weighted Alternating Trilinear Decomposition[4,6]
```
Options = ParOptions('algorithm','SWATLD');
[A,B,C,Diag] = Parafac3W(X,F,Options);
```

In addition, it is possible to compress the array prior to fitting to reduce the computational expense (NB that a refining step using ALS always follows the fitting to a compressed array)[3,6].

Notes.

This implementation does not handle missing values, weighted least squares criteria or the general N-way case.

The PMF3 algorithm as implemented here cannot enforce non-negativity.

Options

Several options are available and can be set using the function ParOptions.

ParOptions generates a structure holding all the parameters necessary to the different algorithms. Some options (e.g. cc_par) are specific to some fitting algorithms.
If an Options structure is already present (Options_old), any options can be changed providing the existing Options structure as the first input to ParOptions followed by the name(s) of the option(s) and the new value(s).

```
Options_new =
ParOptions(Options_old,'algorithm','ALS','display','none');
```

If initial estimates for the loading matrices are available

Initial estimates for the loading matrices ($\mathbf{A}^0$, $\mathbf{B}^0$, and $\mathbf{C}^0$) shall follow the Options parameters when calling Parafac3w. Thus:

```
[A,B,C,Diag] = Parafac3w(X,F,Options,A0,B0,C0);
```

How to change relative fit decrease convergence criterion to (e.g.) 1e-8:

All the options' names pertaining to convergence criteria start with 'cc_'. Specifically, the relative fit decrease convergence criterion has name 'cc_relfit'. Thus:

- if an Options structure already exist (Options_old)
  ```
  Options_new = ParOptions(Options_old, 'cc_relfit', 1e-8);
  ```

- if several options are set at once (e.g. the ALS algorithm)
  ```
  Options_new = ParOptions('algorithm','ALS','algorithm',1e-8);
  ```

How to display some diagnostics:

```
Options = ParOptions('diagnostics','on');
```

Note that the diagnostics can change depending on the algorithm.

How to display some information during the fitting (e.g. every 10 iterations):

```
Options = ParOptions('display',10);
```

Display information every 10 iterations (both in fitting and refining).

How to activate or deactivate compression.

Compression is applied by default. It can be activated/deactivated using the option 'compress':

- to activate compression

  ```
  Options = ParOptions('compress','on');
  ```

- to deactivate compression

  ```
  Options = ParOptions('compress','off');
  ```

For bug reports and problems, please contact the authors:

Giorgio Tomasi. E-mail: gt@kvl.dk

Rasmus Bro. E-mail: rb@kvl.dk

Reference List

1. C. A. Andersson, R. Bro, *Chemometrics and Intelligent Laboratory Systems* **52**, 1 (2000).

2. R. Bro, *Multi-way Analysis in the Food Industry. Models, Algorithms, and Applications*, Ph.D. dissertation, University of Amsterdam (1998).

3. R. Bro, C. A. Andersson, *Chemometr. Intell. Lab. Syst.* **42**, 105 (1998).

4. Z. P. Chen, H. L. Wu, J. H. Jiang, Y. Li, R. Q. Yu, *Chemometr. Intell. Lab. Syst.* **52**, 75 (2000).

5. P. Paatero, *Chemometr. Intell. Lab. Syst.* **38**, 223 (1997).

6. Tomasi G., R. Bro, *Computational Statistics & Data Analysis*, in press.