Users' guide to *FAC-PACK*

A software for the computation of multi-component factorizations and the area of feasible solutions

Software version 1.0

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FAC-PACK is a software for the computation of nonnegative multi-component factorizations and for the numerical approximation of the area of feasible solutions (AFS). ***FAC-PACK*** comes with a graphical user interface (GUI) in MatLab. The GUI provides the functionality for computing a low rank approximation of the data matrix, for determining an initial nonnegative matrix factorization, for approximating the AFS by the polygon inflation method, as well as for graphically representing the admissible spectral and concentration factors. Currently, ***FAC-PACK*** can be applied to two- and three-component systems.

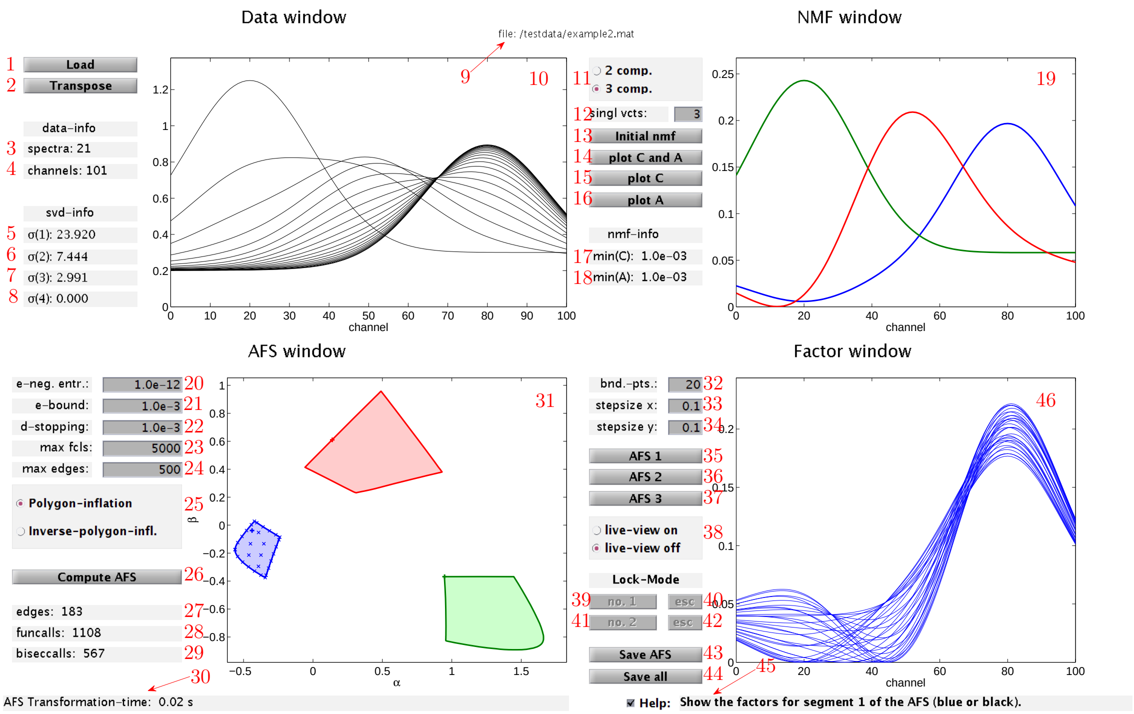
A special feature of the AFS representation is its live-view mode which allows an interactive visual inspection of the spectra or concentration profiles while moving the mouse pointer through the AFS. For two-component systems the full solution is presented in the live-view mode. For three-component systems the GUI provides a further functionality: If a certain point of the AFS is locked (i.e. some known spectrum has been detected or some additional information on the system has been used), then the associated reduced and smaller AFS can be computed. This locking-and-AFS-reduction procedure can be repeated.

The ***FAC-PACK*** GUI has been implemented on MatLab. No additional packages or MatLab-toolboxes are needed. The computational core of ***FAC-PACK*** is written in C which includes an implementation of the polygon inflation procedure.

Contents

1 Quick reference

A screen-shot of the ***FAC-PACK*** GUI:



file: /testdata/example2.mat

spectra: 21
channels: 101

σ(1): 23.920
σ(2): 7.444
σ(3): 2.991
σ(4): 0.000

singl vcts: 3

min(C): 1.0e–03
min(A): 1.0e–03

e–neg. entr.: 1.0e–12
e–bound: 1.0e–3
d–stopping: 1.0e–3
max fcls: 5000
max edges: 500

edges: 183
funcalls: 1108
bisectcalls: 567

AFS Transformation–time: 0.02 s

bnd.–pts.: 20
stepsize x: 0.1
stepsize y: 0.1

☑ Help: Show the factors for segment 1 of the AFS (blue or black).

The GUI buttons, data fields and figures:

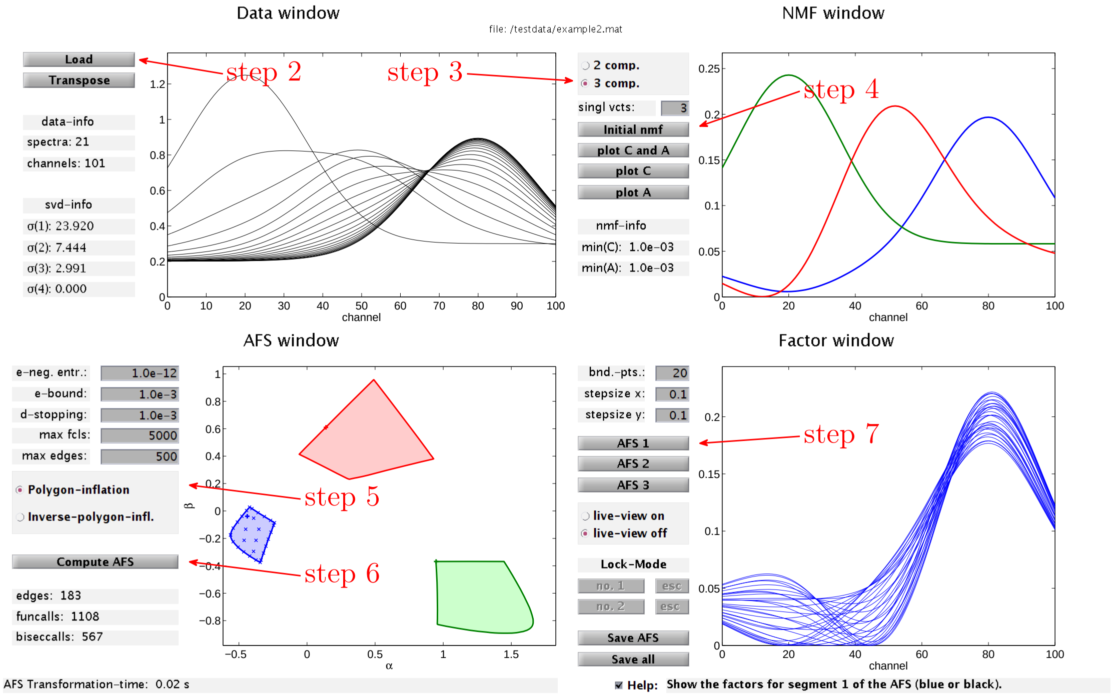
1 Load button
2 Transpose button
3 # rows of data matrix D
4 # columns in D
5 Singular value 1 of D
6 Singular value 2 of D
7 Singular value 3 of D
8 Singular value 4 of D
9 File name
10 Data - axes
11 Input # components
12 # of singular values used for initial NMF
13 Compute NMF
14 Plot factors C and A
15 Plot factor C
16 Plot factor A
17 Minimal matrix elements of C in the NMF
18 Minimal matrix elements of A in the NMF
19 NMF - axes
20 Acceptable negativeness for the NMF
21 Precision at the boundary
22 Stopping precision
23 Maximal # calls of the target function
24 Maximal # of edges
25 Select type of polygon inflation
26 Compute AFS
27 # edges
28 # calls of target function
29 No. used function calls for the boundary-precision
30 Output on the numerical computation
31 AFS-axes
32 # of boundary points for the factor representation
33 Step size x direction for the factor representation
34 Step size y direction for the factor representation
35 Plot factors for segment 1 of the AFS
36 Plot factors for segment 2 of the AFS
37 Plot factors for segment 3 of the AFS
38 Activate live-view mode
39 Compute AFS for 1 selected point
40 Reset 1. restricted AFS
41 Compute AFS for 2 selected points
42 Reset 2. restricted AFS
43 Save button (AFS)
44 Save button (all)
45 Help field
46 Axes of factor window

2 Quick start - for the impatient user

Step 1: Download the ***FAC-PACK*** software from

http://www.math.uni-rostock.de/facpack/

Extract the software package FACPACK.zip. Open a MatLab desktop window and start facpack.m.



data-info
spectra: 21
channels: 101

svd-info
σ(1): 23.920
σ(2): 7.444
σ(3): 2.991
σ(4): 0.000

singl vcts: 3

nmf-info
min(C): 1.0e-03
min(A): 1.0e-03

e-neg. entr.: 1.0e-12
e-bound: 1.0e-3
d-stopping: 1.0e-3
max fcls: 5000
max edges: 500

edges: 183
funcalls: 1108
biseccalls: 567

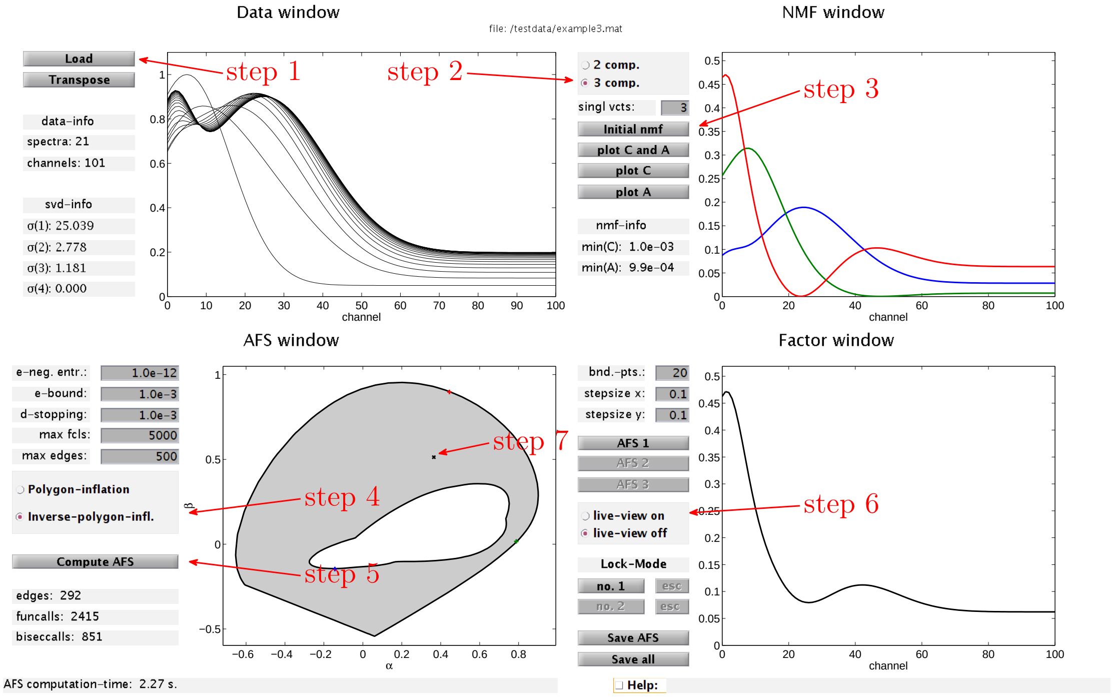
AFS Transformation-time: 0.02 s

bnd.-pts.: 20
stepsize x: 0.1
stepsize y: 0.1

☑ Help: Show the factors for segment 1 of the AFS (blue or black).

Step 2: Select example2 as the data matrix.
Step 3: Select 3 as the number of components.
Step 4: Compute an initial nonnegative matrix factorization (NMF).
Step 5: Choose Polygon inflation.
Step 6: Compute the AFS which consists of three segments (a blue, red and green segment).
Step 7: Plot the range of spectral factors associated with segment 1 (blue segment) of the AFS.

A second test problem:



file: /testdata/example3.mat

data-info
spectra: 21
channels: 101

svd-info
σ(1): 25.039
σ(2): 2.778
σ(3): 1.181
σ(4): 0.000

○ 2 comp.
● 3 comp.
singl vcts: 3

nmf-info
min(C): 1.0e-03
min(A): 9.9e-04

e-neg. entr.: 1.0e-12
e-bound: 1.0e-3
d-stopping: 1.0e-3
max fcls: 5000
max edges: 500

○ Polygon-inflation
● Inverse-polygon-infl.

edges: 292
funcalls: 2415
bisectcalls: 851

bnd.-pts.: 20
stepsize x: 0.1
stepsize y: 0.1

○ live-view on
● live-view off

AFS computation-time: 2.27 s.

Figure 1: Quickstart with live-view mode in 7 steps.

Step 1: Select example3 as the data matrix.
Step 2: Select 3 as the number of components.
Step 3: Compute an initial nonnegative matrix factorization (NMF).
Step 4: Choose Inverse polygon inflation. The AFS consists of only one segment with a hole.
Step 5: Compute the AFS.
Step 6: Select live-view on.
Step 7: Move the mouse pointer through the AFS and watch the interactively computed solutions.

If you like these appetizers you might want to read more in the following sections.

Enjoy working with ***FAC-PACK***!

3 Introduction to *FAC-PACK*

FAC-PACK is a software for the computation of nonnegative multi-component factorizations and for the numerical approximation of the area of feasible solutions (AFS). Currently, the software can be applied to systems with $s = 2$ or $s = 3$ components.

Given a nonnegative matrix $D \in \mathbb{R}^{k \times n}$, which may even be perturbed in a way that some of its entries are slightly negative, a multivariate curve resolution (MCR) technique can be used to find nonnegative matrix factors $C \in \mathbb{R}^{k \times s}$ and $A \in \mathbb{R}^{s \times n}$ so that

$$D \approx CA. \tag{1}$$

Some references on MCR techniques are [5, 8–10, 13]. Typically the factorization (1) does not result in unique nonnegative matrix factors C and A. Instead a continuum of possible solutions exists [6, 10, 18]; this non-uniqueness is called the rotational ambiguity of MCR solutions. Sometimes additional information can be used to reduce this rotational ambiguity, see [7, 14] for the use of kinetic models.

The most rigorous approach is to compute the complete continuum of nonnegative matrix factors (C, A) which satisfy (1). In 1985 Borgen and Kowalski [3] found an approach for a low dimensional representation of this continuum of solutions by the so-called area of feasible solutions (AFS). For instance, for a three-component system ($s = 3$) the AFS is a two-dimensional set. Further references on the AFS are [1, 12, 17, 18]. For a numerical computation of the AFS two methods have been developed: the triangle-boundary-enclosure scheme [4] and the polygon inflation method [16]. ***FAC-PACK*** uses the polygon inflation method.

FAC-PACK works as follows: First the data matrix D is loaded. The singular value decomposition (SVD) is used to determine the number s of independent components underlying the spectral data in D. ***FAC-PACK*** can be applied to systems with $s = 2$ or $s = 3$ predominating components. Noisy data is not really a problem for the algorithm as far as the SVD is successful in separating the characteristic system data (larger singular values and the associated singular vectors) from the smaller noise-dependent singular values. Then the SVD is used to compute a low rank approximation of D. After this an initial nonnegative matrix factorization (NMF) is computed from the low rank approximation of D. This NMF is the starting point for the polygon inflation algorithm since it supplies two or three points within the AFS. From these points an initial polygon can be constructed, which is a first coarse approximation of the AFS. The initial polygon is inflated to the AFS by means of an adaptive algorithm. This algorithm allows to compute all three segments of an AFS separately. Sometimes the AFS is a single topologically connected set with a hole. Then an "inverse polygon inflation" scheme is applied. The program allows to compute from the AFS the continuum of admissible spectra. The concentration profiles can be computed if the whole algorithm is applied to the transposed data matrix D^T.

FAC-PACK provides a live-view mode which allows an interactive visual inspection of the spectra (or concentration profiles) while moving the mouse pointer through the AFS.

Within the live-view mode the user might want to lock a certain point of the AFS, for instance, if a known spectrum has been found. Then a reduced and smaller AFS can be computed, which makes use of the fact that one spectrum is locked. For a three-component system this locking-and-AFS-reduction can be applied to a second point of the AFS.

4 Get ready to start

Please download ***FAC-PACK*** from

http://www.math.uni-rostock.de/facpack/

Then extract the file FACPACK.zip. Open a MatLab desktop and run facpack.m.

This software can be used for academic, research and other similar noncommercial uses. In all other cases (e.g. commercial use) please contact the authors.

FAC-PACK does not make guarantee that the software is free of errors and that it can successfully be used for a particular purpose.

4.1 Program structure

The graphical user interface of ***FAC-PACK*** is written in MatLab. The main file is PolygonInflation.m which handles all functionalities in a joint GUI. No additional MatLab toolboxes are required to run ***FAC-PACK***.

The GUI is built around four windows:

1. Data window (Upper-left window): The data window shows the k rows (spectra) of the data matrix $D \in \mathbb{R}^{k \times n}$ in a 2D-plot. The number of spectra k is printed together with the number of spectral channels n. The four largest singular values of D are shown. By transposing the data matrix D it is possible to compute the AFS for the concentration factor C (instead of the AFS for the spectral factor A).
2. NMF window (Upper-right window): This window allows to set the number of components to $s = 2$ or $s = 3$ and to compute an initial NMF. The smallest minimal components of C and A are printed. The figure shows the profiles of the so-called abstract matrix factors. The buttons allow to compute the profiles of C and/or A.
3. AFS window (Lower-left window): Various control parameters allow to make certain settings for the AFS computation in order to control the approximation quality or maximal number of edges. Pressing the Compute AFS button starts the AFS computation. The live-view mode is active after the AFS has been drawn. Just move the mouse pointer to (and through) the AFS.
4. Factor window (Lower-right window): This window shows the spectral factors (or concentration profiles if the transpose option has been activated in the first window) for the grid points shown in the AFS window.

4.2 External C-routine

All time-consuming numerical computations are externalized to a C-routine in order to accelerate ***FAC-PACK***. This C-routine is AFScomputationSYSTEMNAME.exe, wherein SYSTEMNAME stands for your system including the bit-version. For example AFScomputationWINDOWS64.exe is used on a 64 bit windows system. The external routine is called if any of the buttons **Initial nmf** (13), **Compute AFS** (26), **no. 1** (40) or **no. 2** (42) is pressed. Pre-compiled version of the C-routine for the following systems are parts of the ***FAC-PACK*** distribution:

- Windows 32/64 bit,
- Unix 32/64 bit and
- Mac 64 bit.

The execution of the external routine can always be stopped by CTRL + C in the command window. If the C-routine is running and takes too much computation time, the reason for this can be too large values for k, n, max fcls (23) or max edges (24) or too small values for ε-bound (21) or δ-stopping (22).

4.3 Further included libraries

The C-routine AFScomputationSYSTEMNAME.exe includes the netlib library lapack and the ACM routine nl2sol. Any use of ***FAC-PACK*** must respect
the lapack license, see http://www.netlib.org/lapack/LICENSE.txt, and
the nl2sol license, see http://www.acm.org/publications/policies/softwarecrnotice.

5 Warming-up: Initial steps

This section describes how to use the data window and the NMF window of ***FAC-PACK***. An initial NMF of the data matrix is a necessary prerequisite for the AFS computation which is explained in Section 6.

5.1 Load problem data

To load the spectral data matrix D press the **Load** button (1). The data must be given in the form of a MAT-file whose file name is $*$.mat. The MAT-file must contain the matrix $D \in \mathbb{R}^{k \times n}$ whose rows are the k spectra. Each spectrum contains absorption values at n frequencies. The file may also contain a vector x with n components representing the wave-numbers/frequencies of the spectral channels and a vector t with k components containing the time coordinates. The loading process is automatically followed by a singular value decomposition (SVD) of the data matrix. The computing time is printed in the field **Computing time info** (30). The dimensions of D are shown in the data window together with the singular values $\sigma_1, \ldots, \sigma_4$. These singular values allow to determine the "numerical rank" of the data matrix and are the basis for assigning the number of components s in the NMF window.

5.1.1 Test data

FAC-PACK provides some test data matrices. You can load these matrices by pressing the Load button (1) and by selecting one of the following files:

example1.mat: $k = 51$ spectra, $n = 101$ channels, $s = 2$ components.

example2.mat: $k = 21$ spectra, $n = 101$ channels, $s = 3$ components, the AFS has three clearly separated segments.

example3.mat: $k = 21$ spectra, $n = 101$ channels, $s = 3$ components, the AFS is one topologically connected set with a hole.

example4.mat: some random noise has been added to data matrix D given in example2.mat, the AFS has three clearly separated segments.

Figure 2 shows the data window with the data from example2.mat. Three clearly nonnegative singular values indicate a three-component system.

5.2 Transposing the problem

FAC-PACK computes and displays the spectral matrix factor A, see (1), together with its AFS. In order to compute the first matrix factor C and its AFS, press the **Transpose** button (2) to transpose the matrix D and to interchange x and t.

5.3 Initial NMF

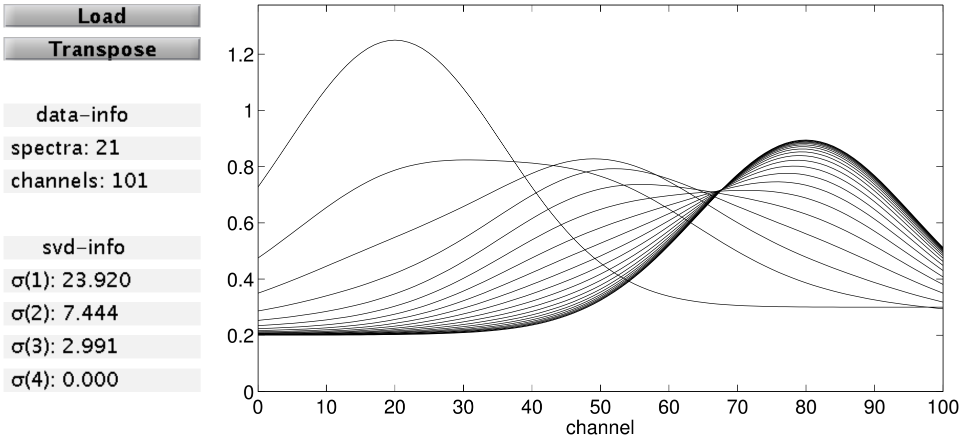
To run the polygon inflation algorithm an initial NMF is required. First the number of components (either $s = 2$ or $s = 3$) is to be assigned. In the case of noisy data additional singular vectors can be used for the decomposition by selecting a larger number of **singl vcts** (12). For details on this option see [11], wherein the variable z equals **singl vcts**.

The initial NMF is computed by pressing the button **Initial nmf** (13). The NMF uses a genetic algorithm and a least-squares minimizer. The smallest relative entries in the columns of C and rows of A, see [16] for the normalization of the columns of C and rows of A, are also shown in the NMF window, see (17) and (18). These quantities are used to define an appropriate noise-level ε; see Equation (6) in [16] for details.

The initial NMF provides a number of s interior points of the AFS; see Equations (3) and (5) in [16].

The buttons **plot C and A** (14), **plot C** (15) and **plot A** (16) serve to display the factors C and A together or separately. Note that these abstract factors are associated with the current NMF. After an NMF computation the A factor is displayed automatically.

Figure 3 shows the factor A for an NMF for example2.mat. The relative minimal components in both factors are greater than zero ($9.9 \cdot 10^{-4}$ and 10^{-3}). So the noise-level **e-neg. entr.:** (20) can be set to the lower bound **e-neg. entr.:** $1 \cdot 10^{-12}$.



spectra: 21

channels: 101

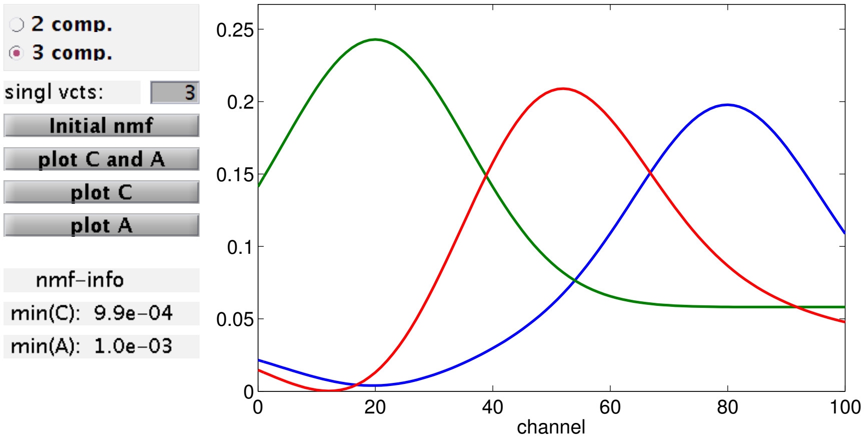
σ(1): 23.920

σ(2): 7.444

σ(3): 2.991

σ(4): 0.000

Figure 2: Test matrix example2.mat loaded by pressing the **Load** button (1).



○ 2 comp.

● 3 comp.

singl vcts: 3

min(C): 9.9e−04

min(A): 1.0e−03

Figure 3: The initial NMF for example2.mat with $s = 3$ components.

6 Computation of the AFS

For two-component systems ($s = 2$) ***FAC-PACK*** represents the AFS by rectangles. Their rectangular sides are the intervals of admissible values for α and β where

$$T = \begin{pmatrix} 1 & \alpha \\ 1 & \beta \end{pmatrix}$$

is the transformation matrix which constitutes the rotational ambiguity. See [1, 2] for the AFS for the case $s = 2$. However in [1], see Equation (6), the entries of the second row of T are interchanged.

For three-component systems ($s = 3$) the AFS is formed by all points (α, β) so that

$$T = \begin{pmatrix} 1 & \alpha & \beta \\ 1 & s_{11} & s_{12} \\ 1 & s_{21} & s_{22} \end{pmatrix}$$

is a transformation which is associated with nonnegative factors C and A, see [16]. A permutation argument shows that with (α, β) the points (s_{11}, s_{12}) and (s_{21}, s_{22}) belong to the AFS, too.

The initial NMF is the starting point for the numerical computation of the AFS since it provides first α and β in the AFS.

Next various control parameters for the numerical computation of the AFS are explained. Further two ways of computing different kinds of the AFS are introduced.

6.1 Control parameters

Five control parameters are used to steer the adaptive polygon inflation algorithm. ***FAC-PACK*** aims at the best possible approximation of the AFS with the smallest computational costs. Default values are pre-given for these control parameters.

- The parameter **e-neg. entr.** (20) is the noise level control parameter which is denoted by ε in [16]. Negative matrix elements of C and A do not contribute to the penalization functional if their relative magnitude is larger than $-\varepsilon$. In other words, an NMF with such slightly nonnegative matrix elements is accepted as valid.
- The parameter **e-bound** (21) controls the precision of the boundary approximation and is denoted by ε_b in [16]. Decreasing the value ε_b improves the accuracy of the positioning of new vertices of the polygon.
- The parameter **d-stopping** (22) controls the termination of the adaptive polygon inflation procedure. This parameter is denoted by δ in Section 3.5 of [16] and is an upper bound for change-of-area which can be gained by a further subdivision of any of the edges of the polygon.

- **max fcls.** (23) and **max edges** (24) are upper bounds for the number of function-calls and for the number of vertices of the polygon.

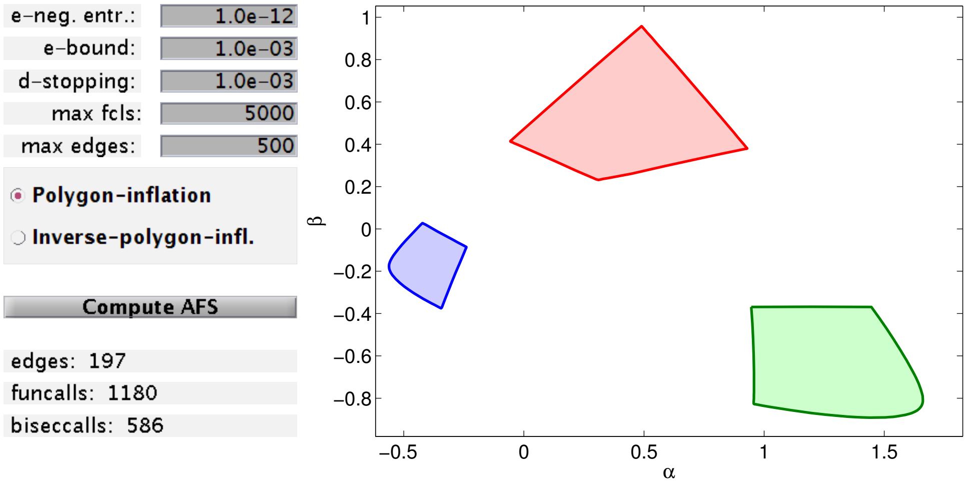
6.2 Type of polygon inflation

FAC-PACK offers two possibilities to apply the polygon inflation method for systems with three components ($s = 3$). The user should select the proper method according to the following explanations:

1. The "classical" version of the polygon inflation algorithm is introduced in [16] and applies best to an AFS which consists of three clearly separated segments. Select **Polygon inflation** by pressing the upper button (25). A typical example is shown in Figure 4 for the test problem example2.mat. In each of the segments an initial polygon has been inflated from the interior. Interior points are accessible from an initial NMF.
2. Alternatively, the **Inverse polygon inflation** procedure is activated by pressing the lower button in (25). This should be done if the AFS is only one topologically connected set (with a hole) or if the isolated segments of AFS are in close neighborhood. See Figure 5 for an example.

   The inverse polygon inflation method is more expensive than the classical version. First the complement of the AFS is computed and then some superset of the AFS is computed. A set subtraction results in the desired AFS. The details are to be explained in a forthcoming paper of the authors of ***FAC-PACK***.

The user should always try the second variant of the polygon inflation algorithm if the results of the first variant are not satisfying or if something appears to be doubtful.

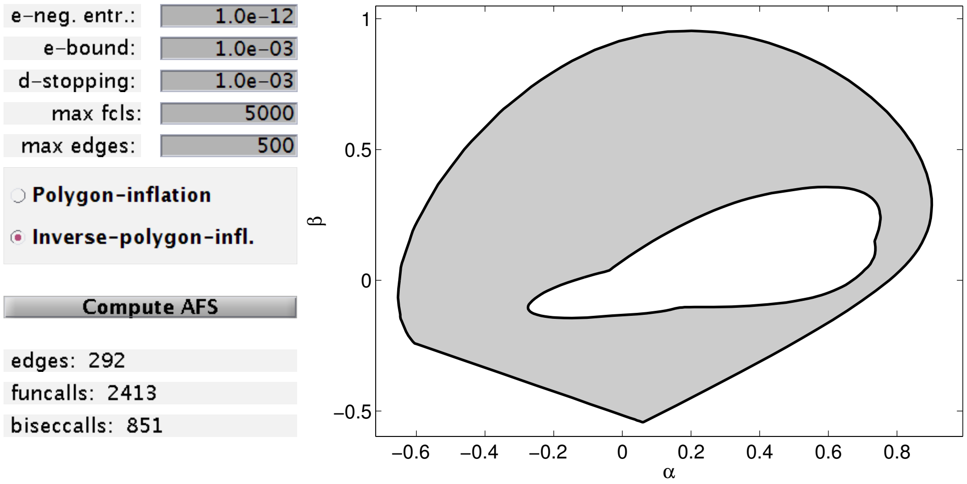


e-neg. entr.: 1.0e-12
e-bound: 1.0e-03
d-stopping: 1.0e-03
max fcls: 5000
max edges: 500

● Polygon-inflation
○ Inverse-polygon-infl.

edges: 197
funcalls: 1180
biseccalls: 586

Figure 4: An AFS with three clearly separated segments as computed by the "classical" polygon inflation algorithm. Data: example2.mat.



e-neg. entr.: 1.0e-12
e-bound: 1.0e-03
d-stopping: 1.0e-03
max fcls: 5000
max edges: 500

○ Polygon-inflation
● Inverse-polygon-infl.

edges: 292
funcalls: 2413
biseccalls: 851

Figure 5: An AFS which consists of only one segment with a hole. For the computation the inverse polygon inflation algorithm has been applied to example3.mat.

7 Factor representation & live-view mode

Next the plotting of the spectra and/or concentration profiles is described. These factors can be computed from the AFS by certain linear combinations of the right and/or left singular vectors. The live-view mode allows an interactive representation of the factors by moving the mouse pointer through the AFS.

7.1 Two-component systems

For two-component systems a full and simultaneous representation of the factors C and A is possible. In order to get an overview of the range of possible spectra one can discretize the AFS-intervals equidistantly. For each point of the resulting 2D discrete grid the associated spectral line is plotted in the factor window. The discretization parameter (subinterval length) is selected in the field (33) and/or (34). The plot of the spectra is activated by pressing button **AFS 1** (35) or button **AFS 2** (36).

Live-view mode: The live-view mode can be activated in the field (38). By moving the pointer through the AFS the associated solutions are shown interactively. Figure 6 shows a typical screenshot. The y-axis labels are turned off.

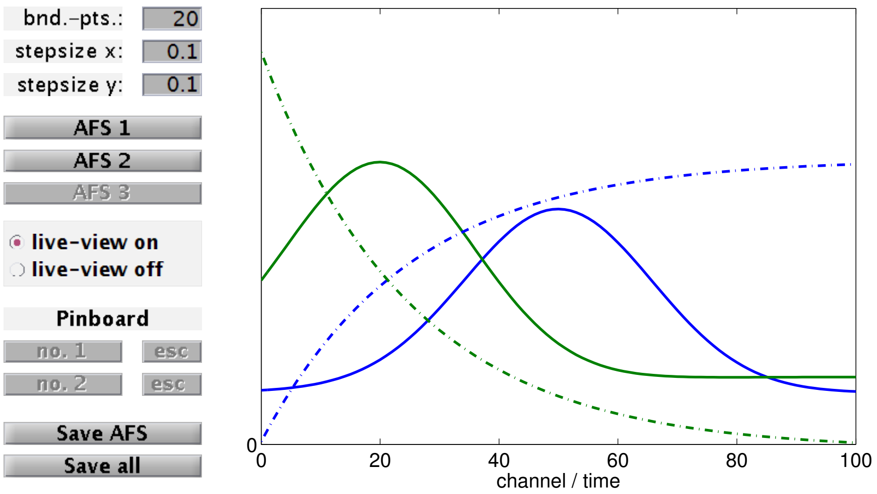
7.2 Three component systems

For three-component systems the range of possible solutions is presented for each segment of the AFS separately. The user can select with the buttons **AFS 1** (35), **AFS 2** (36) and **AFS 3** (37) a specific AFS which is then covered by a grid. First the boundary of the AFS segment (which is a closed curve) is discretized by a number of **bnd-pts** nodes. The discretization parameters for the interior of this AFS segment are **step size x** (33) and **step size y** (34); the interior points are constructed line by line. The resulting nodes are shown in the AFS window by symbols × in the color of the AFS segment. For each of these nodes the associated spectrum is drawn in the factor window. For the test problem example2.mat the bundle of spectra is shown in Figure 7. The resolution can be refined by increasing the number of points on the boundary or by decreasing the step size in the direction of x or y.

If the admissible concentration profiles are to be printed, then the whole procedure is to be applied to the transposed data matrix D; activate the **Transpose** button (2) at the beginning and recompute everything.

Live-view mode: The live-view mode can be activated in the field (38). By moving the pointer through the AFS, the associated solutions are shown interactively. An example is shown in Figure 8.

Additionally, a certain point in the AFS can be locked by clicking the left mouse button; then the AFS for the remaining two components is re-computed. The resulting AFS is a smaller subset of the original AFS, which reflects the fact that some additional



bnd.-pts.: 20

stepsize x: 0.1

stepsize y: 0.1

● live-view on

○ live-view off

Figure 6: The live-view mode for the two-component system example1.mat. By moving the mouse pointer through the AFS the transformation to the factors C and A is computed interactively and all results are plotted in the factor window. The spectra are drawn by solid lines and the concentration profiles are represented by dash-dotted lines.

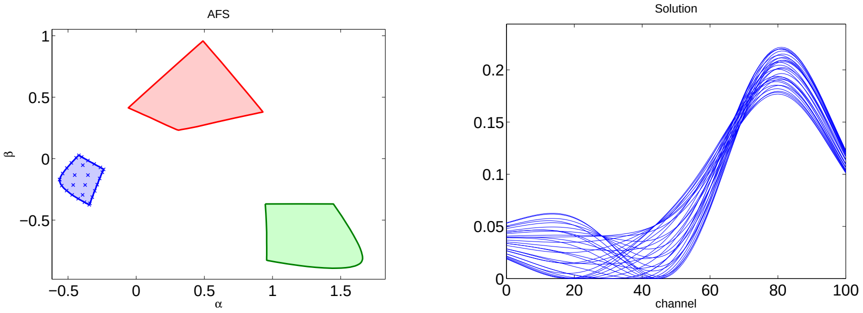


Figure 7: The AFS for the problem example2.mat consists of three separated segments. The blue segment of the AFS is covered with grid points (dark blue points). For each of these points the associated spectral line is plotted in the right figure.

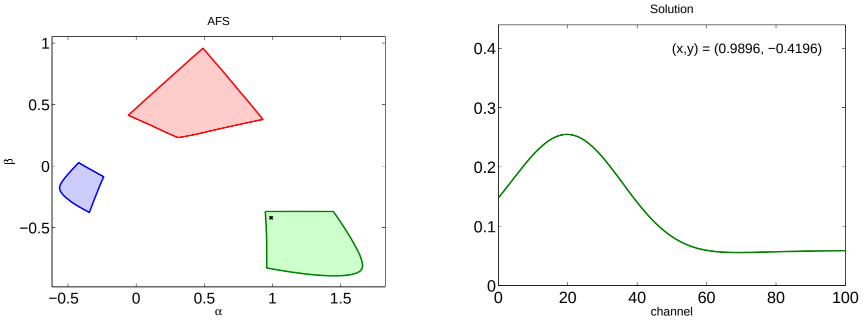


Figure 8: The live-view mode is active for the 3 component system example2.mat. In the green AFS-segment the mouse pointer is positioned in the left upper corner at the coordinates $(0.9896, -0.4196)$. The associated spectrum is shown in the right figure together with the mouse pointer coordinates.

information is added by locking a certain point of the AFS. See Section 8 for further explanations.

8 Reduction of the rotational ambiguity

With the computation of the AFS ***FAC-PACK*** provides a continuum of admissible matrix factorizations. All these factorizations are mathematically correct in the sense that they represent nonnegative matrix factors, whose product reproduces the original data matrix D. However, the user aims at the *one* solution which is believed to represent the chemical system correctly. Additional information on the system can help to reduce the so-called rotational ambiguity. ***FAC-PACK*** supports the user in this way. If, for instance one spectrum within the continuum of possible spectra is detected, which can be associated with a known chemical compound, then this spectrum can be locked and the resulting restrictions can be used to reduce the AFS for the remaining components.

8.1 Locking a first spectrum

After computing the AFS, activate the **live-view** mode (38). While moving the mouse pointer through any segment of the AFS, the factor window shows the associated spectra. If a certain (known) spectrum is found, then the user can lock this spectrum by clicking the left mouse button. A × is plotted into the AFS and the button **no. 1** (39) becomes active. By pressing this button a smaller subset of the original AFS is drawn by solid black lines in the AFS window. This smaller AFS reflects the fact that some additional information on the system has been added. The button **esc** (40) can be used for unlocking any previously locked point.

8.2 Locking a second spectrum

Having locked a first spectrum and having computed the reduced AFS the **live-view** mode can be reactivated. Then a second point within the reduced AFS can be locked. By pressing button **no. 2** (41) the AFS for the remaining component is reduced for a second time and is shown as a black broken line. Once again, the button **esc** (42) can be used for unlocking the second point.

Figure 9 shows the result of such a locking-and-AFS-reduction procedure for the test problem example2.mat. For this problem the AFS consists of three clearly separated segments and the final reduction of the AFS is shown by the black broken line in the red segment of the AFS. The live-view mode allows to display the possible spectra along this

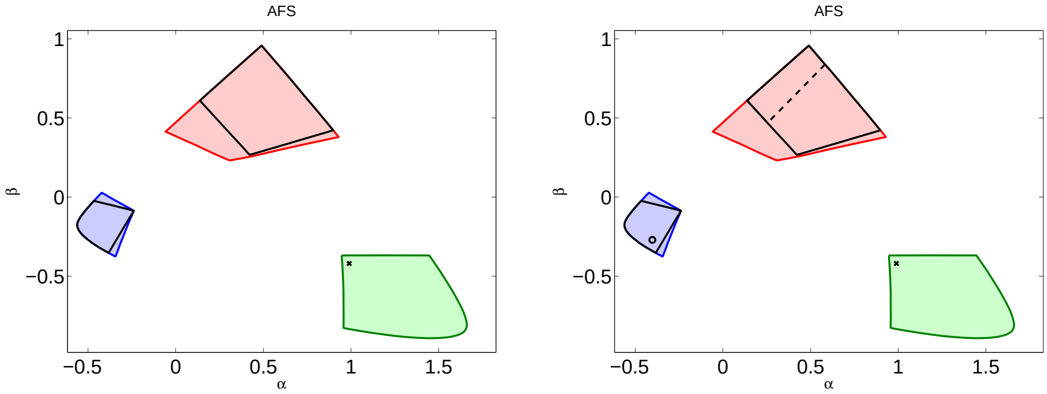


Figure 9: Reduction of the AFS for the test problem example2.mat. Left: the reduced AFS is shown by black solid lines after locking a first spectrum (marker ×). Right: The AFS of the remaining third component is shown by a black broken line.

line. Here we do not show the resulting restrictions on the complementary concentration factor C; this will be the topic of some future work, cf. [15].

9 Appendix

9.1 Save data and extract axes

To save the results in a MatLab *.mat file press either **Save AFS** (43) or **Save all** (44). A proper file name is suggested.

Save AFS saves the data D, the factors U, S, V of the singular value decomposition, the factors $Cinit$, $Ainit$ of the initial NMF and the AFS. The AFS has the data format of a structure which contains the following variables:

- For $s = 2$ the AFS consists of two segments: $AFS\{1\} \in \mathbb{R}^2$ and $AFS\{2\} \in \mathbb{R}^2$ with $\alpha \in [AFS\{1\}(1),\ AFS\{1\}(2)]$ and $\beta \in [AFS\{2\}(1),\ AFS\{2\}(2)]$ and vice versa.
- For $s = 3$ and an AFS consisting of three segments: $AFS\{i\} \in \mathbb{R}^{m_i \times 2}$ with $i = 1, 2, 3$ is a polygon whose x-coordinates are $AFS\{i\}(:, 1)$ and whose y-coordinates are $AFS\{i\}(:, 2)$.
- For $s = 3$ and an AFS consisting of one segment with a hole: $AFS\{1\} \in \mathbb{R}^{m \times 2}$ is the outer polygon ($AFS\{1\}(:, 1)$ the x-coordinates and $AFS\{1\}(:, 2)$ the y-coordinates) and $AFS\{2\} \in \mathbb{R}^{\ell \times 2}$ is the inner polygon surrounding the hole.

If the lock-mode has been used, see Section 8, then the results are saved in $AFSLockMode1$ and $LockPoint2$ (case of one locked spectrum) as well as $AFSLockMode2$ and $LockPoint1$ (case of two locked spectra).

The user can get access to all figures. Therefore click the right mouse button in the desired figure. Then a separate MatLab figure opens. The figure can now be modified, printed or exported in the usual way.

9.2 Cancellation of the program

Whenever the buttons **Initial nmf** (13), **Compute AFS** (26), **no. 1** (40) or **no. 2** (42) are pressed, an external C-routine is called, see Section 4.2. The GUI does not respond during the execution of the C-routine. Therefore, in case of any problems or in case of too long program runtimes, the C-routine cannot be canceled from the GUI. The termination can be enforced by typing CTRL + C in the MatLab command window. Time consuming processes can be avoided if all the parameters are adjusted to reasonable (default) values.

9.3 How to get help

If the **Help** box (45) is checked and the mouse pointer is moved over a button, a text field or an axis, then a short explanation appears right next to **Help** field. Further, a small pop-up window opens if the mouse pointer rests for more than one second on a button.

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