Generalised Modal Analysis with the Padé-Laplace transform

C. Tannous

Laboratoire de Magnétisme de Bretagne, CNRS/UMR 6135 6 avenue Le Gorgeu BP: 809, 29285 Brest CEDEX, France

We present the G-MAPLE (Generalised Modal Analysis from the Poles of the Laplace Expansion) software that allows decomposing data depending on a single parameter (such as time series data) into a set of exponential functions having complex amplitudes and arguments. The novelty is that G-MAPLE determines the unknown number of exponentials in the data along with the corresponding complex amplitudes and arguments.

I. INTRODUCTION

Decomposing a series of data points depending on a single parameter (that might be time, temperature, pressure...) is an important problem in Science and Technology.

The data might be conductivity, chemical concentration, stock market volume, a communication signal etc... It is required that the data is suspected to contain an unknown number of exponential components possessing complex amplitudes and having complex arguments linear functions of the single parameter at hand [1, 2, 3].

The important point is that we do not have to specify the number of exponential components: the Padé-Laplace algorithm finds it. This means, the algorithm performs Fourier analysis in the case of periodic or multiperiodic input data, decomposes a purely decaying function into a set of exponentials having real arguments in contrast to Fourier analysis where the arguments are pure imaginary, and finally analyses a function that decays while simultaneously oscillating as consisting of a set of exponentials having complex arguments. In all three cases the amplitudes are determined in complex form. It is a well-known fact that Fourier/spectral analysis breaks down when dealing with exponentially decaying functions and numerical analysis or standard fitting techniques fail when dealing with functions of that sort, because of the ill-posed nature of the problem of exponential fitting [4]. G-MAPLE circumvents ill-posedness and successfully gives, not only the number of exponential components in the function, but also the corresponding amplitudes and arguments.

The applications of Generalised Modal analysis are numerous. Some of the fields of applications are:

1. Numerical fitting software:
   Exponential and trigonometric fitting of functions as used in the general Padé rational approximation approach encountered in Quantum Mechanics [5], Particle physics, statistical physics [6]....

2. Time series software:
   Determination of time constants in arbitrary profiles of use in general diagnosis, seasonal trends, forecasting etc... [6].

3. Communications engineering:
   Separation of a signal from its echoes in telephone lines, multipath links (line of sight microwave propagation or mobile outdoor/in door); traffic analysis requiring the determination of different parameters yielding traffic volume such as mean arrival times at a given channel [4].

4. Chemical engineering, oil, gas, pharmaceutical...:
   Determination of the order of a given chemical reaction, detection of intermediate reactions, help in the finding of intermediate reactants or processes etc... here, one expects exponential functions of temperature as well, due to the various thermal activation or propagation processes [6].

5. Control systems:
   Detection of the optimal or hidden number of parameters governing the behaviour of a complex system or plant...

6. Mechanical engineering:
   Determination of the number of degrees of freedom (linear or angular displacements or velocities) in the the response of mechanical system such as a robot, mechanical arm, calculation of friction constants controlling the motion etc...
7. Population models in economics, biology, ecology:  
   Determination of number and type of species (biological or economic entities) and understanding the underlying  
   dynamics giving rise to the overall observed population or stock market volume at any given time... For instance,  
   it is used in fluorescence decay studies in Biochemistry [10, 11].

8. Speech and acoustic engineering:  
   Determination of basic components of a phoneme in the time domain, in contrast to the windowed spectral  
   analysis method that is usually performed. Echo and reverberation investigation in concert halls...

9. Geophysical prospection and seismic data processing:  
   Separation of the various echoes produced by a shock wave, seism and identification of the various types and  
   spatial extent of different layers of materials, strata... [12].

10. Micro-electronics industry:  
   Determination of types of impurities or dopants when one monitors the total current versus temperature or the  
   time dependent capacitance in DLTS (Deep Level Transient Spectroscopy) studies...

   More recently, it was applied to gene sequencing where exponential functions are used in the calculation of partition  
   functions of DNA loop sequences [13, 14].

II. SOFTWARE PRESENTATION

G-MAPLE is a software that decomposes the given data in a set of exponential functions having complex  
   amplitudes and arguments. The novelty is that G-MAPLE determines the unknown number of exponentials in the  
   data along with their complex amplitudes and arguments [15].  

G-MAPLE does a Taylor expansion of the Laplace transform of the data around a selected point in the complex  
   plane, fits the expansion to a rational approximation, finds its poles and infers from them the arguments of the  
   exponential components and the values of their corresponding amplitudes. The number of exponential components  
   is found by increasing steadily the degree of the rational approximation. Presumably a set of poles will appear beyond  
   a certain degree and keep appearing later on, regardless of the degree. The number of stable poles is the number of  
   exponential components sought. These stable poles and their associated amplitudes give the exponential functions  
   the sum of which is the best fit to the initial data.

Hence the plan of the G-MAPLE strategy [16] is:

- Preprocessing of the data: Filtering/Estimating the noise contained in the data or/and altering the sampling  
   rate of the data.

- Determination of the optimal point $p_0$ for the Taylor expansion of the Laplace transform of the data.

- Padé rational approximation to the Taylor expansion.

- Inspection of pole stability.

- Consistency analysis.

A. Preprocessing of the data:

This is performed with a spline program. Once the data is entered an an estimate of the noise and a smoothing  
   parameter are provided. Altering and trying several sampling rates is done because it is important for the accuracy  
   required in the calculation of the Taylor coefficients.

B. Determination of the optimal expansion point $p_0$:

1. Initial study of the approximate locations of the poles from the Laplace transform of the data.

2. Performing the Taylor expansion for a given degree around several expansion points and examining the behaviour  
   of the coefficients with the degree.
The estimation of the Taylor coefficients of the Laplace transform of the data is done for several trial p value. An acceptable value for the expansion point $p_0$ should yield a set of coefficients whose magnitude decrease smoothly with their algebraic normalised value staying at about the same level. This is done by a simple inspection of the plots of the above sets of coefficients versus the various expansion points. Once the point $p_0$ is found one can start the rational approximation analysis. By the same token the damping coefficient is calculated as well. This is required for rapidly varying data. It is possible sometimes to alter slightly the damping coefficient in order to get a better expansion point.

C. Rational approximation procedure:

Once the Taylor coefficients of the Laplace transform have been determined about the optimal expansion point $p_0$, one has to vary the degree of the rational approximation to the Taylor expansion. One selects a high degree (5...12) and calculates the rational approximation for all degrees: beginning from degree 2 to the highest possible degree. One repeats for every degree between 2 and the largest one the calculation of the Taylor expansion and the rational approximation. All poles and corresponding amplitudes for every degree are calculated and stored them in a master pole file. The latter is required for the stability analysis. Regarding this procedure, two comments are in order:

1. It is is very important to choose carefully the expansion point $p_0$ of the Taylor expansion. Once it is chosen the Taylor coefficients will be determined and from them the poles of the Laplace transform are obtained along with the corresponding amplitudes.

2. When the poles and amplitudes are found one has to assess the implications of the signs of the amplitudes and poles. For example: If the data shows a monotonic falloff, then the poles should all be real negative. If the data show oscillatory behaviour, then one must expect imaginary or complex poles. The poles and amplitudes stored in pole file for all degrees calculated, from 2 to the highest one (5..12) will be analysed by a stability check procedure that will establish the history of occurrence of each pole as the degree has been varied.

D. Pole stability analysis:

After poles and amplitudes are calculated from the Laplace and rational approximation, one has to study the number of occurrence of each pole with its corresponding amplitude. Since we are looking at the frequency of occurrence of poles in the two-dimensional complex plane, we have to look at small areas where a given pole keeps showing up persistently beyond a certain degree. For a given rough estimate of the size of the area in which the occurrence of poles is confined (an interactive test is provided for the size of the radius of the circular area). The sensitivity analysis of the presumed stable poles and their occurrence in that small area is performed in order to evaluate the robustness of the poles found.

E. Consistency analysis:

As a final analysis of the soundness of the results, the software provides three capabilities:

1. The sequence of ratios of the Taylor coefficients should converge towards the smallest modulus of the poles found. This is a test of the accuracy of the calculation of the Taylor coefficients.

2. Once the stable amplitudes and poles are found and have passed all tests described above, one can define an analytical function from them that can generate data to be compared with the initial input data.

3. If the analysis fails or one wishes to perform a robustness analysis, it is required that the Taylor coefficients are well calculated since all the subsequent analysis is based on them. The software allows the selection of several integration techniques along with several possible interpolation routes for the data to analyse. One may compare the values of the coefficients under the different assumptions and choose the satisfactory ones.

III. DETAILED DESCRIPTION OF THE PROCESSING STEPS:

1. Preprocessing:
   Performing the smoothing of the data, estimating the noise contained in it and altering the sampling rate at will for accuracy considerations during the calculation of the Taylor coefficients.
2. Finding the optimal expansion point $p_0$:
   Two procedures are used:
   
   (a) The Laplace transform of the data is performed in order to find the approximate locations of the poles. The optimal expansion point $p_0$ should be larger than the largest pole found.
   
   (b) Determination of the optimal point: This performs the Taylor expansion of the Laplace transform of the data and estimates the damping coefficient required for rapidly varying data values. The Taylor coefficients are plotted as a function of their order for the given degree and set of points chosen.

3. Rational approximation to the Taylor expansion of the Laplace transform of the data:
   This step is to perform the rational approximation and find the poles and amplitudes for all degrees starting from 2 up to the highest degree chosen.

4. Stability Analysis:
   This step performs the stability analysis. The stable poles and amplitudes are found and stored.

5. Consistency and final checks:
   
   (a) Generating an analytical function from the stable poles and amplitudes found. The accuracy of the Taylor coefficients is being granted by the graph showing whether their ratios approach the minimal pole modulus or not as their order increases.
   
   (b) Generating data points from the constructed analytical function and adding synthetic noise. One might even add Gaussian or Uniform noise in order to make it as similar as possible to the initial data.
   
   (c) Accuracy testing: This consists in obtaining the Taylor coefficients with various methods depending on the data available and the accuracy needed. It is advised to see how the various ways of calculating the coefficients alters the final results (poles and amplitudes).

IV. PROCEDURE SUMMARY:

The summary reviews every step and indicates how the required input data is processed and how the results obtained at every step described previously are checked:

1. Preprocessing: The user has to provide the data file name, the number of data points and how the file is organized (data only, index and data or x, y data). In the filtering step, an estimate of the noise contained in the data as well as a smoothing parameter should be provided. The spline procedure returns an estimate of the noise and if the smoothing parameter is well chosen the initial estimate of the noise and the returned noise figure should be roughly in agreement. Finally it is possible to choose a different sampling rate of the data once it has been smoothed and splined. This has implications on the accuracy of the Taylor coefficients and a test exists in the software to check this accuracy.

2. Optimal expansion point: Assuming a range of points about which the Taylor coefficients are calculated for a chosen degree, the software returns the graphs and values of these coefficients versus the degree.

3. Rational approximation: Providing an upper value of the degree for which the analysis is performed, the software returns all poles and amplitudes for all degrees between degree 2 and the largest degree chosen. It returns also a consistency graph showing the sequence of ratios of Taylor coefficients for increasing order versus the minimal modulus of the poles found.

4. Stability Analysis: For a given radius (within bounds) of the circular neighborhood about which the frequency of occurrence of a given pole is examined, this analysis is done. The software returns the history of occurrences of the poles and determines the stable ones.

5. Consistency Analysis: This is done automatically through the display of the graph of the ratios of the Taylor coefficients versus order with respect to the smallest modulus of the poles found with the Padé-Laplace rational approximation. A new set of data from the stable poles and amplitudes found can be generated and compared it to the initial input data. It is advised to examine the sensitivity of the Taylor coefficients with respect to the various ways of calculating them, depending on the type of data available.
V. EXAMPLES:

A. Synthetic example: Degree 12 Lanczos

We start first with a synthetic example. The parameters are:

Amplitudes:
3.00000
0.400000
3.40000
6.20000

Corresponding exponential arguments (poles):
(-1.0000000000000, 0.)
(-3.0000000000000, 0.)
(-5.0000000000000, 0.)

Damping parameter: -4.16

1. Determination of the optimal expansion point and the damping coefficient:
   the taylor expansion coefficients c(r) are listed according to their absolute values whereas r!c(r) are given in
   algebraic values:

   \[ p = 1.000D-01, \]

   \[
   c(1)= 2.6760968316948 \\
   c(2)= -0.92274649709482 \\
   c(3)= 0.46139353620293 \\
   c(4)= -0.31918555072345 \\
   c(5)= 0.26204150623143 \\
   c(6)= -0.22997288909213 \\
   c(7)= 0.20656813173070 \\
   c(8)= -0.1870154280649 \\
   c(9)= 0.1697702984234 \\
   c(10)= -0.15425931881287 \\
   c(11)= 0.14021104327295 \\
   c(12)= -0.12745666366475 \\
   c(13)= 0.11586714821751 \\
   c(14)= -0.10533295150486
   \]

   **********************************************  c(1)
   *********  c(2)
   ********  c(3)
   **  c(4)
   **  c(5)
   **  c(6)
   *  c(7)
   *  c(8)
   *  c(9)
   *  c(10)
   *  c(11)
   *  c(12)
   *  c(13)
   c(14)
Optimal expansion point $p_0=0.4$

2. Laplace and rational approximation calculations for degrees $= 2...12$

3. Stability study of the poles versus radius:

radius = 1
number of stable poles = 8
pole # 1 (-4.0787128997673, 0.) appeared 11 times
pole # 2 (-1.0821008803446, 0.) appeared 14 times
pole # 3 (-3.0000000476863, 0.) appeared 10 times
pole # 4 (3.8482758680100, 0.) appeared 3 times
pole # 5 (-8.6468139578141, 0.) appeared 2 times
pole # 6 (1.8636510844379, 0.) appeared 6 times
pole # 7 (-6.3269596366764D-02, -0.66701505012643) appeared 26 times
pole # 8 (-6.3269590975568D-02, 0.66701507038499) appeared 5 times
the number of occurrences of some pole is larger than the highest degree = 12

Going to a smaller radius $= 10^{-2}$

Number of stable poles = 10

pole # 1 (-4.9999999672223, 0.) appeared 10 times
pole # 2 (-3.0000000476863, 0.) appeared 10 times
pole # 3 (-0.99999996721772, 0.) appeared 10 times
pole # 4 (3.8482758680100, 0.) appeared 2 times
pole # 5 (-8.6468139578141, 0.) appeared 2 times
pole # 6 (1.8636510844379, 0.) appeared 2 times
pole # 7 (-6.3269596366764D-02, -0.66701505012643) appeared 2 times
pole # 8 (-6.3269590975568D-02, 0.66701507038499) appeared 2 times
pole # 9 (2.7049633928318, -1.6749074721005D-09) appeared 2 times
pole # 10 (0.40001532007036, 2.9758199321717D-03) appeared 2 times

4. Consistency check:
   Occurrence of the poles versus degree (1 for occurrence and 0 for no-occurrence):

   pole # 1: 0 1 1 1 1 1 1 1 1 1 1 1
   pole # 2: 0 1 1 1 1 1 1 1 1 1 1 1
pole # 3: 0 1 1 1 1 1 1 1 1 1
pole # 4: 0 0 1 0 0 0 0 1 0 0
pole # 5: 0 0 0 1 0 0 0 1 0 0
pole # 6: 0 0 0 1 0 0 0 1 0 0
pole # 7: 0 0 0 1 0 0 0 1 0 0
pole # 8: 0 0 0 1 0 0 0 1 0 0
pole # 9: 0 0 0 1 0 0 0 1 0 0
pole # 10: 0 0 0 0 0 1 0 0 0 0

After reducing radius to $10^{-5}$

Number of stable poles= 3
pole # 1 (-4.9999999672223, 0.) appeared 10 times
pole # 2 (-3.0000000476863, 0.) appeared 10 times
pole # 3 (-0.99999996721772, 0.) appeared 10 times
pole # 1: 0 1 1 1 1 1 1 1 1 1
pole # 2: 0 1 1 1 1 1 1 1 1 1
pole # 3: 0 1 1 1 1 1 1 1 1 1
Conclusion of the analysis:
Rational approximation degree= 12
Expansion point: 0.400000, Damping parameter= -4.16000

5. Stable poles and their corresponding amplitudes:

amplitude # 1 (6.1999983164819, -9.6235532915790D-10)
pole # 1 (-5.0000004239243, -1.1584249121758D-11)
amplitude # 2 (3.4000016676147, 1.2316899810646D-08)
pole # 2 (-3.0000003747023, 9.9268993397018D-12)
amplitude # 4 (0.3999998529666, -1.8860442419695D-07)
pole # 4 (-0.9999997587661, 2.7211949994764D-10)
for comparison, the input amplitudes and arguments are:

3

0.400000
3.400000
6.200000

(-1.0000000000000, 0.)
(-3.0000000000000, 0.)
(-5.0000000000000, 0.)

B. Decaying only exponentials

5

(200.000,0.)
(1000.000,0.)
(500.000,0.)
(800.000,0.)
(300.000,0.)

(-50.0000000000000, 0.)
(-5.0000000000000, 0.)
Damping parameter= -5.00

Expansion point $p_0 = 1.2$, damping parameter=-5.

amplitude # 1 ( 200.44842041705, -6.4297285954932D-08)
pole # 1 ( -50.199847855334, 1.7266006542437D-09)

amplitude # 2 ( 1000.06460142389, -5.7036189955559D-06)
pole # 2 ( -5.0002454942104, -1.3064326900177D-08)

amplitude # 3 ( 499.40738201272, 1.3497166341200D-05)
pole # 3 ( -0.50015131820020, 0.17487380533828)

amplitude # 4 ( 798.94082988133, 2.3349965623979D-05)
pole # 4 ( -0.25024465114282, 0.)

amplitude # 5 ( 301.65857589825, 9.1799870303999D-06)
pole # 5 ( -0.15016920303216, 0.)

amplitude # 6 ( -6.8688938206640D-08, -3.5775972803453D-08)
pole # 6 ( 0.51069582321812, 0.17487380533828)

amplitude # 7 ( -6.8686582230124D-08, 3.5777421059967D-08)
pole # 7 ( 0.51069582321812, -0.17487380533828)

amplitude # 8 ( 3.98289888025503D-05, -1.2554952329213D-05)
pole # 8 ( 2.0290173507300, 1.2045224512252)

amplitude # 9 ( -2.3797048952317D-05, -2.7704251925653D-05)
pole # 9 ( 2.0290173521374, -1.2045224398712)

amplitude # 10 ( 5.4490417778712D-07, 3.4864743102636D-14)
pole # 10 ( 2.6347983285165, 0.)

Rational approximation degree= 10

Damping parameter= -5.00, Expansion point $p_0$: 1.20

Stable poles:

amplitude # 1 = ( 200.44842041705, -6.4297285954932D-08)
pole # 1 = ( -51.104140221450, 0.)

amplitude # 2 = ( 1000.06460142389, -5.7036189955559D-06)
pole # 2 = ( -5.3490716102094, 0.)

amplitude # 3 = ( 499.40738201272, 1.3497166341200D-05)
pole # 3 = ( -0.50758978101004, 0.)

amplitude # 4 = ( 798.94082988133, 2.3349965623979D-05)
pole # 4 = ( -0.26205674432617, 0.)
amplitude # 5 = (301.65857589825, 9.1799870303999D-06)
pole # 5 = (-0.15111811290477, 0.)

C. Oscillating and decaying exponentials

5
(400.000,0.)
(175.000,0.)
(175.000,0.)
(-500.000,0.)
(250.000,0.)
(-2.0000000000000D-03, 0.)
(-8.0000000000000D-03, 3.0000000000000D-02)
(-8.0000000000000D-03, -3.0000000000000D-02)
(-2.0000000000000D-02, 0.)
(-0.2000000000000, 0.)

Stability radius = 10^{-2}
Number of stable poles = 5

Stable poles and amplitudes:
amplitude # 1 = (250.00011450201, 9.2737811992658D-07)
pole # 1 = (-0.20001227827931, 0.)
amplitude # 2 = (-499.99976169965, -8.0435000145924D-04)
pole # 2 = (-2.0047256715262D-02, 4.362439471021D-13)
amplitude # 3 = (175.00010854502, -8.5323335360501D-05)
pole # 3 = (-8.0240426328942D-03, -2.9980187019490D-02)
amplitude # 4 = (175.00006247227, 2.3514996070493D-04)
pole # 4 = (-8.0240426329283D-03, 2.9980187019495D-02)
amplitude # 5 = (399.99945705790, 6.6704669352807D-04)
pole # 5 = (-1.9888744154064D-03, 0.)

D. Experimental example borrowed from fast spectroscopy

The example below Fig.1 shows an experimental noisy signal borrowed from fast laser spectroscopy. After preprocessing the data and estimating the value of the noise present in the data, we perform the Padé-Laplace analysis and the results are displayed in Fig.2. The difficulty in fitting this example is due not only to the presence of noise but also of the large initial value in the data. Despite these difficulties, G-MAPLE was able to extract the exponential arguments and corresponding amplitudes successfully for a rough value of $p_0$. Slightly changing $p_0$ gave a minor improvement of the fitting. The obstacle in finding a better fit stems from the fact it is harder to find a good expansion point $p_0$ for real noisy data. The challenge is to find a better automatic procedure for the determination of $p_0$ in the case of noisy data. In that case, least-squares [2] or fast least-squares estimation methods provide better answers [17].

Acknowledgements
The author wishes to acknowledge helpful discussions with Randy Borle and Art Monk that helped improve substantially the graphical user interface of the software. He also thanks Daniel Houde for kindly providing two fast spectroscopy data sets for testing the software, and P. Rasolofoosaon for providing reprints/preprints of his work.
[1] D. W. Tufts and R. Kumaresan: Proceedings of the IEEE, 70, 975 (1982).
[2] J. A. Cadzow: IEEE ASSP Magazine, 12 (October 1990).
[3] B. D. Rao and K. S. Arun: Proceedings of the IEEE, 80, 283 (1992).
[4] F. S. Acton: "Numerical methods that work", Harper and Row, New-York (1990).
[5] C.N. Leung, Y. Y. Y. Wong: Am. J. Physics 70, 1020 (2002).
[6] N. S. Wittle, L. C. L. Hollenberg and Z. Weihong: Phys. Rev. B 55, 10412 (1997).
[7] L. L. Scharf: "Statistical signal processing: Detection, Estimation and Time series analysis", Addison-Wesley, New-York (1991).
[8] T. K. Sarkar and O. Pereira: IEEE Antennas and Propagation Magazine 37, 48 (1995).
[9] P.N.J. Rasolofosaon: J. Acoust. Soc. Am. 89, 1532 (1991).
[10] G. Foucault, M. Vacher, S. Cribiero and M. Arrio-Dupont: Biochem. J. 346, 127 (2000).
[11] M. L. Scala!ey, Q. Yi, H. Gu, A. McCormack, J. R. Yates III and D. Baker: Biochemistry, 36 3373 (1997).
[12] C.H. Mehta, B.S. Goel, D. D. Bhatta and S. Radhakrishnan: IEEE Trans. Signal Proc. 38, 512 (1991).
[13] A.N. Gorban, A.Yu. Zinovyev and T.G Popova: Institut des Hautes Etudes Scientifiques preprint (France), [http://www.ihes.fr/PREPRINTS/M01/Resu/resu-M01-34.html](http://www.ihes.fr/PREPRINTS/M01/Resu/resu-M01-34.html).
[14] E. Yeramian: Gene 255, 139 (2000).
[15] E. Yeramian and P. Claverie: Nature Vol. 326, 169 (1987)
[16] P. Claverie, A. Denis and E. Yeramian: Comp. Phys. Rep. 9, 247 (1989).
[17] C. J. Demeure: Signal Processing 21, 107 (1990).

![FIG. 1: Fast spectroscopy raw data set # 67](image-url)
FIG. 2: G-Maple result for the fast spectroscopy data set # 67