A harmonic analysis of exponential decay

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Abstract

We analyse the decay of a single exponential function of the form, $C_k e^{-\lambda_k}$, and develop an algorithm to determine the exponent and the constant C_k . In essence this approach involves ‘transforming’ exponential functions into harmonic functions, i.e. $A'_k \sin \lambda_k t$ and $B'_k \cos \lambda_k t$. This manoeuvre allows techniques that are used to analyse functions to be used to characterise decaying exponential functions.

Introduction

Exponentials arise in a wide range of contexts, and thus it is desirable to be able to unambiguously identify and characterise them.

Analysing and characterising exponentials is of great biomedical interest as people use a wide variety of fitting techniques in several areas to analyse and characterise their data. Examples include: fluorescence lifetime imaging microscopy, e.g. Lakowicz (2006) [1]; MRI, (Magnetic resonance imaging) Storås et al (2008) [2]; PET (Positron emission tomography), Valk (2003)[3]; analysing the concentration of compounds in the bloodstream and various organs Baxter et al (1994)[4] and (1995)[5], Lubic (2001)[6]. Several approaches have been used to extract information on the exponents, and the constants that multiply the exponential functions, $C_k \exp(-\lambda_k)$. Istratov and Vyvenko (1999) have given an informative presentation and discussion of some of the issues that arise when attempting to fit exponential functions to noisy data sets.

A particularly scathing critique of inappropriate usage of the algorithms used to identify the exponential functions that characterise a decaying process is given by [7]:

“The answer to this problem lies in the chemical rather than the computer laboratory and the sooner the hopeful innocent can be sent there and away from the computer room the better off everyone will be. For it is well known that an exponential problem of this type in which all four parameters are to be fitted is extremely ill conditioned. That is there are many combinations of $(\alpha_k \text{ and } A_k)$ that will fit most exact data quite well indeed (will you believe four significant figures?)”

In essence it is important to be aware that the problem can be challenging as there may be several ‘good answers’ that do not correspond to the real parameters that produced the signal, that nonetheless provide a “good fit” to the data.

Interpolation

The data is interpolated using Chebyshev polynomials. The underlying ideas are similar to those used in the NAG Fortran subroutine **E02ADF**. We implemented the Chebyshev interpolation code with the algorithm presented in Mason (1984)[8], and Powell (1981)[9].

It is possible to obtain a set of basis functions with the property that satisfies the orthogonality relationship

$$\sum_{i=1}^m g_j(x_i)g_k(x_i) = \begin{cases} 1 & j=k \\ 0 & j \neq k \end{cases} \quad (1)$$

for a set of data points $\{x_i\}$. The polynomials can be obtained by making use of the following relationships, Mason(1984)[8], Powell (1981)[9]

$$\begin{aligned} g_1(x) &= 1 \\ g_{j+1}(x) &= (x - B_j)g_j(x) + C_j \\ g_{j+1}(x) &= (x - B_j)g_j(x) + C_j g_{j-1}(x) \quad (j = 1, 2, \dots) \end{aligned} \quad (2)$$

where C_j is a constant.

Interpolation of data points is a useful and robust way of obtaining a good approximation of a data set that correspond to a discrete set of points in terms of a continuous function. It provides us with a way of dealing with a

data set corresponding to a set of measurements corresponding to a signal representing a decaying phenomenon in terms of a continuous function. Clenshaw [10] developed a modification of the basic approach illustrated above in terms of the generalised orthogonal polynomials. This involved expressing the polynomials in terms of Chebyshev polynomials. This is significant as it has benefits in terms of storage efficiency and the favourable stability properties that Chebyshev polynomials have over the general polynomials $g_i(x)$, when used as a basis set to approximate a function. In practice powers of x can be expressed in terms of Chebyshev polynomials, and more generally it can be shown that the k th power of x is given by

$$x^n = \frac{1}{2^{k-1}} \sum_{k=0}^{\lfloor n/2 \rfloor} \left(\begin{matrix} n \\ k \end{matrix} \right) T_{n-2k}(x) \quad (3)$$

where the dash $\sum'$ denotes that the k th term in the sum is to be halved if n is even and $k = n/2$, Mason and Handscomb (2002)[11].

In addition when evaluating Chebyshev polynomials the standard Chebyshev recurrence relation was used

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \quad (4)$$

together with the initial input expressions

$$T_0(x) = 1 \quad (5)$$

and

$$T_1(x) = x \quad (6)$$

Numerical: exponential fitting

The techniques that are developed in this article are concerned with the analysis and characterisation of data of the form

$$f(t) = \sum_{j=1}^{\infty} C_j e^{-\lambda_j t} + n(t) \quad (7)$$

The noise is expressed by the term $n(t)$. This term or function can be thought of as a stochastic function of the time. We begin the analysis by

utilising some properties of Chebyshev polynomials. It can be shown that the Chebyshev expansion of an exponential function has the form

$$e^{-\alpha x} = 2I_0(\alpha)T_0(\alpha x) + 2 \sum_{j=1}^{\infty} T_j(\alpha x)I_j(\alpha)(-1)^j \quad (8)$$

Arfken and Weber, (2000) where I_m represents modified Bessels functions of order m . The Chebyshev expansion occurs over an interval, $-1 \leq x \leq 1$. In practice when data has been collected over an interval such that $x_{min} \leq x \leq x_{max}$, this interval can be converted to the *normalised* interval $-1 \leq \bar{x} \leq 1$ by using the transformation

$$\bar{x} = \frac{2x - x_{min} - x_{max}}{x_{max} - x_{min}} \quad (9)$$

Thus the Chebyshev expansion for an exponential function can be generalised to an exponential function that is defined in the finite interval, e.g. $-1 \leq x \leq 1$.

Consider a signal, $g(t)$, consisting of an exponential function and some noise, where

$$f(t) = Ce^{-\lambda t} + n(t) \quad (10)$$

The noise is expressed by the stochastic function $n(t)$.

The function $f(t)$, can be expressed as a series of Chebyshev polynomials, where

$$f(t) = \sum_{n=0}^{\infty} A_n T_n(x) \quad (11)$$

In practice the sum will of course be done over a finite number of terms, and so the function $f(t)$ will be represented by an approximation of the form

$$f(t) \approx \sum_{n=0}^{N_{max}} A_n T_n(x) \quad (12)$$

where N_{max} is the highest order term used in the Chebyshev expansion for $f(t)$.

Relating a series of exponential functions in a noisy environment to a series of harmonic functions in a noisy environment can be achieved by converting a series of Chebyshev polynomials, $T_n(x)$, to a power series in x .

Consider an exponential function, this can be expressed in terms of a power series

$$e^{ax} = \sum_{n=0}^{\infty} \frac{(ax)^n}{n!} \quad (13)$$

This can of course be approximated by

$$e^{ax} \approx \sum_{n=0}^{N_{max}} \frac{(ax)^n}{n!} \quad (14)$$

where the N_{max} th order term i.e. $x^{N_{max}}$, is the highest order term that is used in the approximation. The expansion for $\sin(ax)$, is given by

$$\sin(ax) \approx \sum_{n=0}^{N_{max}} \frac{(-1)^n (ax)^{2n+1}}{(2n+1)!} \quad (15)$$

similarly the expansion for $\cos(ax)$ is given by

$$\cos(ax) \approx \sum_{n=0}^{N_{max}} \frac{(-1)^n (ax)^{2n}}{2n!} \quad (16)$$

Where the sum $\sum_{n=0}^{N_{max}}$ corresponds to a sum with an upper limit of either N_{max} or $N_{max} - 1$. The even upper limit applies to the cosine power series, and the odd upper is used with the sine power series.

In essence the algorithm for converting an exponential function into harmonic function involves expanding the exponential in terms of some polynomials e.g. generalised orthogonal polynomials, $g_i(x)$.

The odd order terms in the expansion are separated from the even order terms. The odd polynomials are then expanded out into a set of terms that consist of powers of x , and similarly the even terms can also be expanded into a power series.

One way of converting the power series of an exponentially decaying signal where noise is not present to a power series for cosine and sine functions is to multiply all of the negative terms in the power series that is obtained for e^{-ax} by -1 , i.e. terms of the form x^r , are multiplied by -1 . This yields the power series for, e^{ax} . Now consider the odd order terms in the power series,

i.e. terms where the power in, x^r , satisfies, $r = 2q + 1$. If $\frac{r-1}{2}$, is even or equal to zero, the term is left untouched. However if $\frac{r-1}{2}$, is odd the term is multiplied by -1 . This yields the power series for $\sin(ax)$. Consider the even order terms in the power series. If $\frac{r}{2}$, is even or equal to zero, the term is left untouched. If $\frac{r}{2}$, is odd the term is multiplied by -1 . This yields the power series for $\cos(ax)$. Thus the even powers of the expansion of the function, $f(x) = e^{ax}$, when processed as above will yield the function $\cos(ax)$. This process can be thought of in terms of obtaining a power series in x and then replacing x by the imaginary number $z = ix$, where $i = \sqrt{-1}$. Thus
In effect the transformation

$$e^{ax} \xrightarrow{\text{Is transformed to}} \cos ax + i \sin ax = e^{iax} \quad (17)$$

The harmonic functions that are generated from the exponentially decaying signals can of course be processed by a range of standard techniques such as Fourier based techniques, e.g. the fast Fourier transform, if the resulting harmonics have been collected over a time interval that spans at the very least a full cycle. In practice the user may only have a small section of the harmonic signal, that spans less than a full periodic cycle of the harmonic functions that are generated by the above process. One way of overcoming this limitation is to multiply the expansions for $\cos(ax)$ and $\sin(ax)$ by a suitable harmonic function and then to recombine them. Consider the following trigonometric relationship

$$s(x) = \cos(\alpha x) \cos(\Omega x) - \sin(\alpha x) \sin(\Omega x) \equiv \cos(\Omega x + \alpha x) \quad (18)$$

This is generated by multiplying the term $\cos(\alpha x)$, by $\cos(\Omega x)$, and the term, $\sin(\alpha x)$, by $\sin(\Omega x)$. If Ω , is chosen so that it varies by at least one cycle over the interval in which the power series approximations for $\sin(\alpha x)$ and $\cos(\alpha x)$ were generated, it should result in there being more than one cycle of the function $s(x)$ over the interval of the variable x in which we have generated the approximate power series for, $e^{\alpha x}$. Several *convenient* expressions for harmonic functions that can be generated from the power series for $\cos(\alpha x)$ and $\sin(\alpha x)$, with the aid of the standard trigonometric identities, e.g.

$$\sin([\Omega \pm \alpha]x) \equiv \sin(\Omega x) \cos(\alpha x) \pm \cos(\Omega x) \sin(\alpha x) \quad (19)$$

and

$$\cos([\Omega \mp \alpha]x) \equiv \cos(\Omega x) \cos(\alpha x) \pm \sin(\Omega x) \sin(\alpha x) \quad (20)$$

If Ω is chosen appropriately this process results in the generation of one or more cycles of a harmonic function.

The functions $\sin([\Omega \pm \alpha]x)$ and $\cos([\Omega \pm \alpha]x)$ can then be analysed by using a suitable harmonic analysis technique e.g. the periodogram or a fast Fourier transform.

Spectral analysis

An FFT implementation of the discrete Fourier transform is a simple route to performing a spectral analysis on the harmonic data that is generated from interpolated exponential functions.

In practice however, sometimes important features of a signal's spectrum fall at frequencies between the discrete Fourier transform bin frequencies which can result in these features having an ambiguous nature, which could make it difficult to identify them properly. This phenomenon is sometimes called the '*picket fence effect*'.

One approach for overcoming the issues that can arise due to the picket fence effect involves padding the input data for the discrete Fourier transform with a number of zero-valued samples in order to generate a longer discrete Fourier transform with more finely spaced frequency bins can be used. This approach is called '*zero-padding*'.

Zero padding can of course generate artefacts that are not consistent with the input data for example the observed amplitude of the peak in the zero-padded discrete Fourier transform will probably be incorrect. It's important to note that zero padding does not improve on the resolution of a discrete Fourier transform, as zero-padding will not improve the quality of the measurements of the input sequence.

One limitation of the FFT algorithm is that it requires evenly spaced time series. However in practice a time series may consist of unevenly spaced data. It follows that another limitation of the FFT algorithm is that it will

not tolerate ‘missing values’. These omissions could arise due to data omission during an analysis of a data set or from failure to make an observation at the required time.

The LombScargle periodogram is an approach to dealing with a real data set where the points are not necessarily equispaced. It is widely used to analyse astrophysical data, Lomb (1976)[12], Scargle (1982)[13]. Generally astronomers are not in a position to have absolute control over viewing times, telescope availability and the position of an objects in the sky.

The Lomb-Scargle periodogram analysis can be thought of as a least-square fitting of sine waves to a data set. It is important to note that least squares fitting is intimately tied to the assumption about Gaussian errors and measurement uncertainties in the data.

According to Hansen et al [14], when the probability distribution for the noise in the data has tails that are larger than the Gaussian probability distribution the least squares fit may not be particularly useful. In addition when the probability distribution has a ‘thick’ tail, the data might contain outliers, i.e., observations with exceptionally large errors and residuals. The presence of outliers is another factor that can undermine the usefulness of a least squares fit, and can lead to the presence of spurious peaks in a Lomb Scargle periodogram, Schimmel (2001), in [15] and [16].

The Lomb-Scargle periodogram is a very general mathematical technique that can be thought of as an extension of Fourier analysis to unevenly spaced data. However in addition to this it can also be viewed as a least squares spectral fitting method or a statistical spectral analysis technique that can be formulated in terms of Bayesian probability theory, [17], [18]. The Bayesian approach is a useful alternative in many settings to a classical statistical approach when analysing uncertainty in a measurement and standards laboratory setting, Lira (2002)[19]. This arises from the systematic way that it treats areas such as parameter marginalisation, the inclusion of prior knowledge in a statistical analysis and the impact of the propagation of uncertainty on a statistical analysis of a series of measurements, Lira (2002)[19], and Agostini (2003) [20]. Despite the obvious differences in approaches between classical and Bayesian statistical techniques in many areas they appear to be in reasonable agreement Morgan (2001) and Davison (2003), though the Bayesian approach tends to give a tighter measure of the uncertainty associated with a quantity of interest, Lira (2002)[19]. In general this is likely to arise because of the systematic way in which prior knowledge can be incorporated into a

Bayesian framework.

The Bayesian approach has an in built Ockham’s razor, [18], Ruanaidh and Fitzgerald (1996)[21]. This effect penalises model complexity, unless it is justified by prior information associated with the data. Ruanaidh and Fitzgerald[21] described the Ockham factor as being proportional to the volume of space being occupied by the posterior density divided by the volume occupied by the prior.

Another important consideration is that makes the Bayesian approach attractive is that it is easier to integrate a wide range of noise types with the analysis, and the Bayesian approach provides a systematic approach to the uncertainty analysis that is required for when ascertaining the output parameters. It is also important to note that with a Bayesian approach the probabilities connected with the uncertainty due to noise and measurement are built into the analysis, Ruanaidh and Fitzgerald (1996)[21], whereas with the conventional periodogram the uncertainty analysis is somewhat more convoluted, VanderPlas (2018)[22].

The exponential data analysis technique was analysed by investigating a simulated data set. The input signal $s(t)$ was an exponential of the form

$$s(t) = e^{-kt} + n(t) \quad (21)$$

where $n(t)$ is normally distributed noise with a mean $\mu = 0$ Units and standard deviation $\sigma = 0.01$ Units.

The noisy exponential was used as input, the resulting Chebyshev series that was generated is used to generate the corresponding harmonic expressions e.g. 19 and 20 which are the output harmonics functions.

An issue that might arise in practice is that the harmonic signal isn’t necessarily going to span a full cycle over the time interval of measurement.

One way of overcoming this, when both the sine and cosine of a signal at the frequency of interest is to use the harmonic addition formulae. This approach permits the generation of a harmonic function $\sin(\alpha + \Omega)t$ which undergoes several cycles of oscillation over the time interval over which the signal is measured, whereas the signals $\sin \alpha t$ or $\cos \alpha t$ may not have completed a cycle over this interval.

This manoeuvre generates a signal that can be processed by standard harmonic analysis techniques such as the FFT and the periodogram.

Analysis of the simulated exponential function in a noisy environment, illustrates that it is possible to recover the decay constant k from a decay of

the form e^{-kt} .

Figure (1) illustrates the simulated input data. It is a noisy exponential function, where the decay constant k has a value of $2.0 \times \pi \times (0.1)$ units. The normally distributed noise has a standard deviation of 0.01 Units, and a mean of 0.0 units.

The processing of the data is illustrated in figures (1) to (6). Starting with a decaying exponential as input. The input can be interpolated to generate a Chebyshev series. The Chebyshev expansion of the noisy exponential is used to generate a noisy harmonic signal that spans more than one cycle over the time interval that the input signal was observed. This signal was analysed using the Lomb - Scargle periodogram. The peak in the periodogram occurred at a frequency of 2.2 units. The frequency of signal that spans several cycles over the time at which the exponential decay is measured is 2.1 units. This approach allows the recovery of the frequency associated with the exponential decay, e.g. 2.1 units. The periodogram used was the *PyAstronomy* Lomb Scargle Python code for periodogram analysis, Zechmeister and Kürster (2009)[23].

Interpreting the false alarm probability in the periodogram can be a subtle process, VanderPlas (2018)[22], and requires some care. The periodogram gave a result of a single sinusoid with a frequency of 2.200 (Units) and an amplitude of 0.993 (Units). According to this program the probability of obtaining a power greater than this level from the noise, which is assumed to be Gaussian was 0.0.

Discussion

In this article, we demonstrated that it is viable to convert an exponential signal of the form e^{-kx} into its associated harmonic functions $\cos kx$ and $\sin kx$. When dealing with noisy data the Chebyshev expansion was used as a starting point as in practice it is more stable numerically than an attempt at a direct expansion in a power series. This analysis was demonstrated using a single exponential function and a moderate level of noise.

From a review of the literature, e.g. the discussion from Acton, [7] the algorithms for analysing harmonic signals and the associated uncertainty analysis is generally more robust than the corresponding techniques for analysing decaying exponential signals. Thus a conversion of the problem from an exponential decay analysis to a harmonic frequency analysis will

generally result in much more robust and reproducible quantitative output. When using conventional approaches to analyse a harmonic signal this approach could produce output that is potentially problematic. For example if the harmonic signal that is produced by this process doesn't undergo one or more cycles over the time interval, leading to a fraction of a full cycle over the interval of observation. One way around this is to use the cos and sin components of the signal and the addition formulae for cosines and sines to generate a signal that undergoes one or more oscillatory cycles over the observation time interval. Thus potentially enabling the technique to access decay constants when the associated harmonic functions do not undergo a full cycle of oscillation over the time interval of observation. A key feature of this analysis is the use of interpolation using Chebyshev polynomials. This approach comes with a number of advantages as it provides the basis for transforming the initial input signal into another signal based on the input by using the mathematical properties of exponential functions and harmonic functions. This approach can be thought of as a '*toolbox approach*' to analysing harmonic signals, as it makes it easier to combine the original data set with harmonic / exponential functions.

These tools can provide a method for developing robust mathematical approaches to test the output from an analysis by using the fundamental properties of harmonic functions. Another useful tool to keep in mind when performing a harmonic analysis is the Hilbert transform. This can be useful when more than a full harmonic cycle of a signal is present, e.g. the Hilbert transform of $\sin \omega x$ is given by

$$\sin(\omega x) \rightarrow -\operatorname{sgn}(\omega) \cos(\omega x) \quad (22)$$

and the corresponding Hilbert transform of $\cos \omega x$ is given by

$$\cos(\omega x) \rightarrow \operatorname{sgn}(\omega) \sin(\omega x) \quad (23)$$

Thus if information is available on the (symmetric— asymmetric) component of a harmonic signal is available the corresponding (asymmetric— symmetric) signal can be obtained from the Hilbert transform, if a full cycle or more of the input harmonic is available.

A toolbox approach using interpolation provides a robust basis for using the analytic properties of harmonic and exponential signals, and thus in practice it can provide a mechanism for using the original signal to generate

new signals through well defined mathematical processes such as integration; use of the Hilbert transform; etc.

In addition the flexibility of the toolbox approach can be beneficial for reducing the impact of noise on the data. For example the sine series could be generated from a sinh expansion instead of obtaining it directly from the exponential. This approach could potentially reduce the weighting of the tail on the noisy exponential, thus potentially improving the uncertainty bounds on the final estimates of the parameters of interest.

Conclusion

A technique for analysing noisy exponentials has been developed. This is a problematic area as many of the approaches in the literature for obtaining numerical information about the parameters that characterise the exponentials are not particularly robust. In this study we looked at a single exponential in a noisy environment, though in principle the same approach should be readily applicable when more than one exponential signal is present. This approach uses interpolation based on Chebyshev polynomials. There are several benefits to this approach. The use of Chebyshev polynomials makes it easier to exploit the mathematical properties of harmonic functions and exponential functions, this can help to generate an output signal in a form that is convenient for extracting the information of interest, e.g. converting a harmonic signal that doesn't undergo a full cycle over the measurement interval into a signal that undergoes one or more complete cycles over the measurement interval. This manoeuvre could start with a signal that isn't accessible to standard harmonic analysis techniques as input, and would produce an output signal that could be used to characterise the output signal using standard approaches to analysing harmonic signals.

To summarise, an approach has developed that enables a harmonic analysis techniques to be used to characterise exponentially decaying signals. This approach should be more robust than many of the techniques that are currently widely used when attempting to characterise an exponential decay.

From a practical standpoint, this approach has potential utility in several fields as decaying exponentials arise in a wide range of contexts, e.g. MRI, radioactive decay and FLIM microscopy.

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Figures

Figure (1) is the input data. It is a noisy exponential function, where the decay constant k has a value of $2.0 \times \pi \times (0.1)$ units.

Figure (2) is a plot of a Chebyshev interpolation of the input data.

Figure (3) is the even function (cosine) obtained from the input data. It's worth noting that the resulting cosine function has a low frequency, ($2.0 \times \pi \times (0.1)$ units) and that it doesn't undergo a full oscillation over the time interval over which the exponential decay was measured.

Figure (4) is the corresponding odd function (sine) obtained from the input data. Similarly this will not undergo a full cycle over the measurement time interval, with a frequency of ($2.0 \times \pi \times (0.1)$ units).

Figure (5) illustrates a situation where the low frequency harmonic functions, e.g. ($\cos \alpha t$, and $\sin \alpha t$) are combined with higher frequency sine and cosine functions ($\cos \Omega t$, and $\sin \Omega t$, using the formula $\cos(\Omega + \alpha t) = \cos \alpha \cos \Omega - \sin \alpha \sin \Omega$. In this example $\alpha = 2.0 \times \pi \times (0.1)$ units

and

$\Omega = 2.0 \times \pi \times (2.1)$ units

It follows that the frequency of the resulting cosine function should be

$\Omega = 2.0 \times \pi \times (2.2)$ units

Figure (6) is a periodogram of the noisy harmonic functions that have been combined with higher frequency harmonic functions in order to produce a signal that undergoes one more complete oscillatory over the time interval which the exponential decay data was originally collected. A peak is obtained at a frequency of $\Omega = 2.0 \times \pi \times (2.2)$ units.

Figure 1: The input data $e^{-kt} + n(t)$

Figure 2: Interpolating the input data with Chebyshev polynomials

Figure 3: The cosine obtained from the exponential data

Figure 4: The sine obtained from the exponential data

Figure 5: Constructing a high frequency cosine function

Figure 6: A spectral analysis with the periodogram

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