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Implementation of the Prony Method for Signal Deconvolution ⋆

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Abstract: Modern implementations of the Prony method have been used in the statistical analysis of sinusoidal and/or exponential signals distorted with noise. Modern implementations are auto-regressive, using a series of matrix calculations and least-squares to calculate the values of interest from a signal; the frequency, decay constant, initial amplitude, and phase. In cavity ring-down spectroscopy, the frequency and decay constant of an exponentially decaying sinusoidal signal need to be obtained, in order to identify molecules and the chirality of these molecules, which may be applied in, for instance, development of pharmaceuticals. This method is applicable to signals from other fields - signals which are sinusoidal or exponential in nature. An implementation of the Prony method for cavity ring-down spectroscopy has been developed and characterised in Python.

Keywords: Statistical data analysis, Modeling and identification, Errors in variables identification, Time series modeling, Software for system identification

1. INTRODUCTION

The *chirality* of a molecule in a substance can be of vital importance in determining the action of that substance. If a molecule is not the same as its mirror image, it is chiral; a chiral molecule cannot be superimposed on to its mirror image. The chiral molecule and its mirror image are called *enantiomers*. An example from pharmacology is that of penicillamine: one enantiomer is a treatment for rheumatoid arthritis, Wilson's disease and as an antidote for heavy metal poisoning; the other enantiomer is highly toxic, causing nerve inflammation and bone infections (He et al. (2006)). Therefore the identification of the chirality of molecules is highly important in pharmacology and multiple other fields such as analytical chemistry, cosmetics, and biology.

Cavity ring-down signals can be used to identify the chirality of a substance. In such an investigation, a laser is used to illuminate an optical cavity, which contains the substance of interest in gaseous form. The laser light is reflected between two mirrors in the cavity, and can be detected using micro-channel plate detectors. When the laser is switched off, the light decays in the form of a exponentially-decaying sinusoid

$$e^{-\frac{t}{\tau}}(X\sin(\omega t+\varphi)+Z)+S(t),$$

where the signal S stands for the measurement noise. The frequency, ω, and decay constant, τ of this signal need to be measured to a high level of speed and accuracy, in order to measure the chirality of the substance. The decay constant determines the concentration of substance of interest in the cavity, and the frequency is indicative of the chirality.

The Ultrachiral collaboration is in the process of developing a highly sensitive method of determining chirality using cavity ring-down spectroscopy, with the signal being detected by photon detectors such as photo-multiplier tubes and avalanche photo-diodes (Sofikitis et al. (2014)). Current chirality measurements are hindered by weak signals, which may be further obscured by spurious birefringence and imperfect background subtraction. The Ultrachiral collaboration has developed a cavity-enhanced optical method to amplify weak signals; this method uses a pulsed-laser bowtie cavity ring-down polarimeter with counter propagating beams, which enhances the signal by a factor equal to the number of cavity passes. The effects of birefringence are suppressed and the need for background subtraction eliminated. Two laser beams travelling in opposite directions within the cavity are used to obtain the chirality; one beam is right-handed circularly polarised, while the other is left-handed circularly polarised. The frequencies of these beams are used to obtain the chirality of the substance of interest.

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Determining, however, all relevant parameters of the signal, that is its frequencies and the decay constants, is a challenging technical problem due to the presence of measurement noise and the requirements to produce estimates in near-real time. The problem of inferring parameters of signals has been the subject of intensive research in signal processing, identification, applied mathematics, and control community (see e.g. classical books (Ljung (1998)), (Tarantola (2005)), (Aster et al. (2005)) and references therein). More recently, observer-based approaches were shown to be efficient in this problem too (Aranovskiy et al. (2016)), (Na et al. (2015)), including for sums of non-harmonic signals (Tyukin et al. (2003)) and those whose models are non-linearly parameterised (Tyukin et al. (2013)).

Despite these theoretical successes, industrial and practical applications demand increased efficiency of estimation, with high computational scalability and reduced costs. As a response to these demands, recent years have seen increased interest in simple classical methods such as e.g. the method of Prony (de Prony (1795)) due to their low computational complexity and high scalability. This leads to a possibility to develop a one-shot estimation procedure as opposed to the asymptotic ones stemming from the observer-based approaches.

In this contribution we demonstrate that, remarkably, simple auto-regression methods like the Prony method, can deliver a surprisingly high efficiency and accuracy if coupled with suitable pre-processing and statistical analysis. This is consistent with previous studies which used the Prony approach to e.g. signal analysis (Kumaresan et al. (1982)), high energy physics (Cushman and Fleming (2018)), biomedical science (Fernández Rodríguez et al. (2018)), and to power system oscillation analysis (Arpanahi et al. (2019)). In addition, by exploring various combinations of sampling rates and parameters of noise, we propose a procedure for finding optimal sampling rates delivering most robust and accurate estimates.

The paper is organized as follows. In section 2 we present a background of the Prony method, Sections 3-5 describe our procedure for determining relevant parameters of the measurement data, and Section 6 concludes the paper.

2. THE PRONY ALGORITHM

Prony's original algorithm was designed for processing discrete time signals that are superpositions of exponentially decaying sinusoids. It is also applicable to continuous signals upon their discretisation at a generic sample rate. Since the original signal satisfies an ordinary differential equation with constant coefficients, the discretised signal solves a finite difference equation facilitating Prony's approach.

The original algorithm solved a linear system of equations to exactly match the curve produced by the expansion of gases. Modern implementations of Prony's method extract information from a signal, providing a statistical estimate of frequency, initial amplitude, phase, and damping components of that signal.

The application of Prony's method consists of three steps:

(1) Build an autoregressive model that explains the measurements.
(2) Recover the roots of polynomials built from the model.
(3) Use the roots to determine the characteristics of the signal.

Discrete time measurement of a mixture of exponentially decaying sinusoidal signals satisfying an auto-regressive model of order p has p past values, and assumes that the value of y_k depends linearly on the past p values in $\mathbf{y}$ in the relation:

$$y_k = -\sum_{j=0}^{p-1} \alpha_{p-j} y_{k-j} \qquad k \geq p \tag{1}$$

To begin, the coefficient α is found by combining p copies of this equation with different $k-$values into a $n \times p$, $n \geq p$ system of linear equations:

$$\begin{bmatrix} y_0 & y_1 & y_2 & \cdots & y_{p-1} \\ y_1 & y_2 & y_3 & \cdots & y_p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_{n-1} & y_p & y_{p+1} & \cdots & y_{n+p-1} \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{p-1} \end{bmatrix} = - \begin{bmatrix} y_p \\ y_{p-1} \\ \vdots \\ y_{2p-1} \end{bmatrix} \tag{2}$$

The matrix on the left, if $n = p$, is a Hankel matrix. Equation 2 can also be written as:

$$\mathbf{H}\boldsymbol{\alpha} = -\mathbf{h} \tag{3}$$

Where $\mathbf{H}$ is substituted for the data matrix, $\boldsymbol{\alpha}$ is the matrix of coefficients, and $\mathbf{h}$ is the vector of sampled measurements.

The second step recovers the exponential parameters (i.e. the rates of decay and frequencies) from $\boldsymbol{\alpha} = -(\mathbf{H}'\mathbf{H})^{-1}\mathbf{H}'\mathbf{h}$, by finding the roots (eigenvalues) of the following characteristic polynomial equation:

$$q(z) = z^p + \alpha_{p-1} z^{p-1} + ... + \alpha_1 z + \alpha_0 = \sum_k (z - \lambda_k)_k^r \qquad , \tag{4}$$

where $\sum_k r_k = p$ and λ_k are the roots of $q(z)$ (see Hokanson (2013)).

Observe that the minimal number of data points is $n \geq p$, which in the case of a single sinusoid and $Z = 0$ is 3. The number of data points affects computational costs of the implementation, and we will exploit this later on in the paper.

When implemented as an algorithm, the Prony method is of the following form:

Algorithm 1. To implement the Prony method:

for each data point **do** generate discrete matrices **H**
  for each matrix **H do** least squares fit
    for each output **do** find roots
    end for
  end for
end for

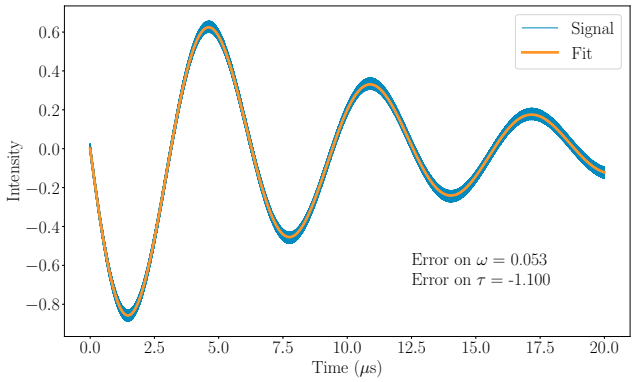

Fig. 1. The simulated signal, with 3% uniform noise, ω= 1 MHz, and τ = 10 μs, from a cavity ring-down spectroscopy experiment, and a fit using the Prony method. The fit obtains values of $\omega = 1.000530$ MHz and $\tau = 9.888738$ μs.

Briefly, the data points on a signal are sampled at equally-spaced intervals, and these points are used to generate an $n \times p$ matrix (**H** in equation 3) and an associated $p \times 1$ matrix ($\boldsymbol{\alpha}$ in equation 3). Solutions of these matrices are found using the least squares fit method, and solved as a polynomial (cubic) equation. These roots, which are found though finding the eigenvalues of the companion matrix, can then be simply manipulated to obtain the sought characteristics of the signal. If the sample rate is equal to ω/π, the covariance matrix participating in least squaring fails to be invertible, and the method is not applicable. This manifests as the singularity at ω/π in figure 2, to be discussed in greater detail in section 4.

3. ANALYSIS OF SIMULATED SIGNALS FROM CHIRAL EXPERIMENTS

The form of signals from cavity ring-down spectroscopy experiments is that of an exponentially decaying sinusoid, as shown in figure 1. This is of the form:

$$V(t) = e^{-t/\tau}(X\cos(\omega t) + Y\sin(\omega t) + Z) \tag{5}$$

Here, X, Y, and Z are known constants, t is the time, τ is the damping component, ω is the frequency, and S is the noise. In these simulations, a range of values for ω, τ, and the noise were suggested, based on discussions with the Ultrachiral collaboration. The range of values for ω was between 1 and 10 MHz, for τ between 1 and 10 μs, and a normal noise distribution of between 0% and 5%.

Although this signal is time continuous, it becomes discrete upon sampling at equidistant time moments. Not all sample rates are admissible, so we process the signal at various sample rates simultaneously, to determine the valid region and do additional statistical processing, making use of a weak dependence of the result of the sample rate in a "good" region. When applied to a continuous signal, a sample rate is utilised in order to approximate a discrete signal. As Prony analysis is a sub-Nyquist method, this periodic, discrete sampling is required in order to obtain accurate results. The Nyquist frequency is the minimum sampling frequency of a sinusoidal function, in order to regenerate the function without the loss of information (Colarusso et al. (1999)), which is not applicable to the Prony method due to the satisfaction the full spark condition (or full Kruskal rank) (see Kruskal (1977); Ye et al. (2017)). The Nyquist sampling limit is twice the waveform frequency.

Using the trigonometric identity:

$$a\cos(\theta) + b\sin(\theta) = c\sin(\theta + \varphi) \tag{6}$$

where $c = \sqrt{(a^2 + b^2)}$ and $\varphi = \arctan\left(\frac{b}{a}\right)$, the signal can be rearranged as:

$$V(t) = e^{-t/\tau}(X_2\sin(\omega t + \varphi) + Z) \tag{7}$$

Then, using the identity:

$$\sin\theta = -\cos\left(\theta + \frac{\pi}{2}\right) \tag{8}$$

The form of the signal can be further rearranged as:

$$V(t) = e^{-t/\tau}\left(-X_2\cos(\omega t + \varphi + \frac{\pi}{2}) + Z\right). \tag{9}$$

Fix a sampling time interval T. Then, with the use of the Euler identity

$$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}, \tag{10}$$

equation (9) translates to

$$V(nT) = e^{-\frac{nT}{\tau}}\left(Z_+ e^{i\omega nT} + Z_- e^{-i\omega nT} + Z\right) \tag{11}$$

where $Z_\pm = -\frac{X_2}{2}e^{\pm i\left(\varphi + \frac{\pi}{2}\right)}$ and $n = 0, 1, \ldots$. The sequence $V(nT)$ satisfies the auto-regression relation of order 3. Once the roots $u_0 = e^{-\frac{T}{\tau}}$, $u_\pm = e^{-\frac{T}{\tau}}e^{\pm i\omega T}$ of its characteristic equation have been found via the Cardano formulas, values of ω_0' and τ' can be obtained:

$$\tau' = -\ln(u_0)/T, \tag{12}$$

$$\omega' = Im\ln(u_+)/T. \tag{13}$$

Remark that the estimates ω' and τ' can be alternatively determined directly from any pair of coefficients of the characteristic polynomial, but the difference in the results is found statistically insignificant.

4. PERFORMANCE OF PRONY'S METHOD FOR A SIGNAL WITH NOISE

The range of parameters for which this implementation of the Prony method works well was investigated. This included modelling a signal, of the form of equation 7, with a range of values of ω, between 1 and 10 MHz, a range of values of τ , between 1 and 10 μs, and a range of values of uniform noise, between 0 and 5%.

It was found that the product of the values of ω and τ gives a good indication of how well the fit using the Prony method would perform; when $\omega\tau \leq 2$, the error seen on the fit is significantly greater than when $\omega\tau > 2$. This inequality is only applicable for a signal of the form

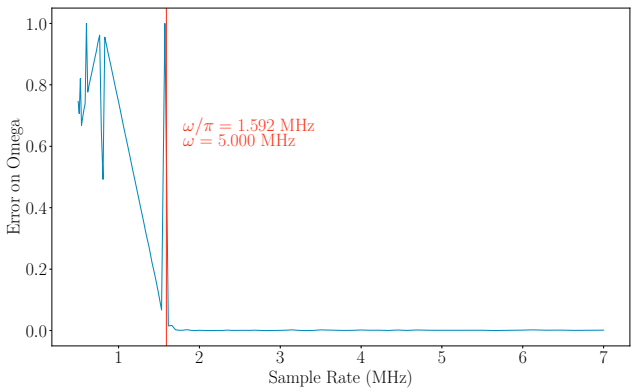

Fig. 2. Showing the error on ω at different values of the sample rate. The input value of ω is 5 MHz, with ω/π being 1.592 MHz. Where the sample rate is less than ω/π, indicated by the red vertical line, the error on ω becomes significant. At values of the sample rate greater than ω/π, the error on ω is close to zero.

discussed here, and with 3% uniform noise (that is, the noise is 3% of the initial amplitude of the signal). Below this boundary the signal decays so fast that oscillations are suppressed by the noise and the frequency cannot be reliably determined.

Also of importance in indicating how well the fit would perform is a relation between the sample rate R and ω. Both are measured in MHz, and if $R < \omega/\pi$, then the error on the fit can be significant (due to symmetries of the cosine function the phase a root cannot be uniquely determined from the characteristic polynomial). An example of this is shown in figure 2, wherein the difference in the error on ω is clearly delineated at $R = \omega/\pi$. This is due to the covariance matrix degenerating, as mentioned previously. In order to process a signal with noise, an initial calculation based on an assumed maximum value of ω is used.

In the case of the experimental work performed by the Ultrachiral collaboration the signal is processed at a grid of sample rates. Since the assumed maximum value of ω is 10 MHz, the initial approximation ω_{init} of ω with a margin error of $< 20\%$ is derived at a sample rate greater than $10/\pi$ MHz. From this estimate the singularity ω/π is approximated. Then all the rates below ω_{init}/π are discarded and only the rates above ω_{init}/π are utilized and averaged over to obtain final calculations of ω and τ.

In most cases, with 3% uniform noise, the code fits well, with calculations of ω having an error of within 0.2%, and calculations of τ within 2%. As ω is of greater interest in obtaining the chirality of a substance, this is a positive indication of the Prony method's applicability to this work.

5. IMPLEMENTATIONS OF PRONY'S METHOD IN PYTHON

Given the nature of cavity ring-down spectroscopy experiments, the fast calculation of ω and τ is required. To that end, different methods of implementing the Prony method in Python were investigated. This includes implementations in pure python, as well as using different Python packages in order to speed up the computation. These included NumPy (van der Walt et al. (2011)), Numba (Lam et al. (2015)), Cython (Behnel et al. (2011)), and the asynchronous, parallel computation package trio (Smith (2017)).

5.1 Comparison of Python Implementations

Table 1. Summarising the time taken and rate of each implementation of the Prony method, with different Python packages, as well as the fast Fourier transform, implemented in Python with NumPy (indicated by '*').

Package(s) Used	Time (μs)	Rate (kHz)
Pure Python	20000	0.005
NumPy	6000	0.2
Numba	35	28.6
Cython	60	16.7
trio	1000	1.0
NumPy and Numba	27	37.0
FFT*	59	16.8

The slowest implementation of the Prony method was the pure Python implementation. The quickest was a combination of NumPy and Numba - this combination of highly optimised operations and *jit* compilation resulted in a rate of around 37 kHz, or a signal fitting time of 27 μs. This allows for sustained calculations with this method at a laser switch off frequency in cavity ring-down spectroscopy of around 37 kHz . A summary of these implementations, and the time and rate for each, are shown in table 1.

Also of interest are alternative methods of implementing more widely-used methods which can be used to obtain the properties of the signals, such as the discrete fast Fourier transform. In order to recover the parameters of interest, the Prony method requires the fewest data points, on balance comparing favourably with the fast Fourier transform, and the adaptive observer method; while the fast Fourier transform may be more accurate, the larger number of points required to accurately recover parameters mean that these require greater computational resources. For instance, the most computationally intensive part of the Prony method is finding the matrix inverse, but since this is only for a 3×3 matrix, this is not as onerous as, for example, the adaptive observer method.

6. CONCLUSION

The development of a quick algorithm for obtaining the frequency and damping components of a signal produced during cavity ring-down spectroscopy is of great importance for obtaining the chirality of a substance. The Prony method is shown to calculate the frequency and damping components of a signal to a good degree of accuracy, to within 0.2% and 2% respectively, for a signal with uniform noise of 3% of the initial amplitude of the signal.

Several different implementations of this using different Python packages were performed, of which the quickest was found to be a combination of NumPy and Numba, with a peak rate of 37 kHz.

The Prony method has a speed advantage over other methods such as performing a least squares fit or Fourier transform on the full signal, since it requires fewer data points. Unlike the other two methods, the Prony method requires fewer data points than the Nyquist frequency (Nyquist (1928); Shannon (1949)); the Prony method is a *sub-Nyquist method*. The Nyquist frequency is the minimum sampling frequency of a sinusoidal function, in order to regenerate the function without the loss of information (Colarusso et al. (1999)). That the Prony method does not require so high a sample rate is due to the satisfaction of an algebraic condition, the full spark condition (or full Kruskal rank) (see Kruskal (1977); Ye et al. (2017)). The result of the Prony method being sub-Nyquist is that it has the potential to be quicker than a fit to a full signal, for example in a least square fit or Fourier transform (see Gherasim (2006)).

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