Padé–Laplace analysis of signal averaged voltage decays obtained from a simple circuit

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The Padé–Laplace method is an interesting yet relatively unknown method for determining the exponential time constants in a decaying signal. We apply it to data from a simple electronic circuit specifically designed for investigations of signal averaging. Possible decays of the voltage include single, multi-exponential, and predominantly logarithmic. Students in our computer-interfacing course write a LABVIEW program that collects the data and performs the signal averaging.

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I. INTRODUCTION

In this paper we apply the Padé–Laplace method of curve fitting to decaying voltages obtained from a simple circuit designed specifically for investigations of signal averaging. The Padé–Laplace method is an interesting alternative to commonly used nonlinear curve-fitting methods that are based on the minimization of the sum of the squares of the errors.[1] It incorporates Laplace transforms, function approximation (using Padé approximants), Taylor series expansion, matrix inversion, and finding the zeroes of polynomials. Its effectiveness is similar to nonlinear least-squares methods for resolving multi-exponential decays.[2,3] The fact that it is not a significant improvement probably explains why Padé–Laplace is not widely known. However, readers who are familiar with standard curve-fitting methods will likely find the Padé–Laplace method intriguing.

The problem of resolving a multi-exponential decay arises in a variety of phenomena, including fluorescence lifetime and nuclear magnetization relaxation.[2–5] In the presence of a moderate amount of noise it can be very difficult to determine even the correct number of decay constants, much less to resolve them if they are closely spaced. The proper identification of the number of exponentials often is crucial for the accurate interpretation of data in terms of physical characteristics such as molecular conformations and dynamics. Padé–Laplace provides an alternative approach for addressing this problem.

The versatile circuit presented in Sec. III is designed specifically for investigations of signal averaging. The circuit's output is a decaying voltage combined with noise generated by the breakdown of a reverse biased emitter-base junction. The form of the decay and the magnitude of the noise are easily controlled. The signal-to-noise ratio is typically set close to one so that the decaying signal is obscured by the noise. In this way it is particularly satisfying to see the signal emerge from the noise as signal averaging progresses.

We use LABVIEW to construct a data acquisition and analysis program that performs the signal averaging. Alternatively, an instrument such as an oscilloscope with built-in signal averaging capabilities can be used to collect data.

II. PADÉ–LAPLACE ANALYSIS METHOD

The Padé–Laplace method has the attractive feature that the number of exponential decay constants is not assumed. The method determines the number of decay constants by evaluating successive Padé approximants of the Laplace transform of the data. The poles of the Padé approximants give the decay constants. The number of decay constants is found when successive Padé approximants produce no new poles. For a detailed explanation of Padé approximants and the Padé–Laplace method, see Refs. 1 and 6. Our intention is to show enough detail to apply the method to the data in this paper.

A Padé approximant $P_{n,m}(p)$ is a rational function expressed as a fraction, where the numerator and denominator are polynomial functions of p with degree n and m, respectively. A Padé approximant of a function $F(p)$ is constructed by requiring that the power series expansion of $P_{n,m}(p)$ be identical to the power series expansion of $F(p)$ up to the p^{n+m} term. In our case $F(p)$ is the Laplace transform $L(p)$ of the data $f(t)$. Formally, the Laplace transform of a function $f(t)$ is

$$L(p)=\int_0^\infty e^{-pt}f(t)dt. \tag{1}$$

In reality the data are a finite set of values so the integral must be evaluated numerically. The trapezoid rule for M data points (t_j,f_j) at equal time intervals Δt, gives

$$L(p)=\Delta t\left(\frac{1}{2}(e^{(-pt_1)}f_1+e^{(-pt_M)}f_M)+\sum_{j=2}^{M-1}e^{(-pt_j)}f_j\right). \tag{2}$$

The summation approximates the integral in Eq. (1) as long as the data are close to zero by the last data point.

The key idea of Padé–Laplace is that if the time dependence of the decay is a sum of n exponentials, then the Padé approximant $P_{n-1,n}(p)$ is an exact analytic expression for $L(p)$ so that the poles of $P_{n-1,n}(p)$ give the decay constants, and the residues give their amplitudes.

Problem 1. Integrate Eq. (1) for the case $f(t)=Ae^{-\lambda t}$ to see why the poles of $P_{n-1,n}(p)$ give the decay constants and the residues give the amplitudes for a decay of n exponentials.

We are interested in finding the Padé approximants $P_{n-1,n}(p)$ of $L(p)$,

$$P_{n-1,n}(p)=L(p). \tag{3}$$

The right-hand side of Eq. (3) is expressed as the Taylor series expansion about some point p_0 up to degree $2n-1$

and the left-hand side is expressed as a fraction comprised of polynomial functions of $(p-p_0)$,

$$\frac{a_0+a_1(p-p_0)+\cdots+a_{n-1}(p-p_0)^{n-1}}{1+b_1(p-p_0)+\cdots+b_n(p-p_0)^n} = d_0+d_1(p-p_0)+\cdots+d_{2n-1}(p-p_0)^{2n-1}. \tag{4}$$

The coefficients of the Taylor series expansion are

$$d_i=\frac{1}{i!}\left(\frac{d^{(i)}L}{dp^{(i)}}\right)_{p=p_0} \qquad (i=0,...,2n-1). \tag{5}$$

The derivatives of the Laplace transform are obtained by taking derivatives of Eq. (2):

$$\left(\frac{d^{(i)}L}{dp^{(i)}}\right)_{p=p_0} = \Delta t\left(\frac{1}{2}((-t_1)^i e^{(-p_0t_1)}f_1 + (-t_M)^i e^{(-p_0t_M)}f_M) + \sum_{j=2}^{M-1}(-t_j)^i e^{(-p_0t_j)}f_j\right). \tag{6}$$

Note that Eq. (2) is the $i=0$ case of Eq. (6).

The procedure is to start with $n=1$ and use the data (t_j,f_j) in Eq. (6) to generate d_i from Eq. (5). The d_i are put into Eq. (4), thus determining the a and b coefficients. The n poles and residues of the left-hand side of Eq. (4) are calculated. The value of n is then increased by 1, and the procedure is repeated until no new poles are found (the new poles have residues with values close to zero).

Equation (6) requires numerical evaluation at a point p_0. A good choice for p_0 is the inverse of the time it takes for the data to decay to $\frac{1}{2}$ its initial value. As described in Sec. V other values for p_0 are used as part of the evaluation of the results. Note that p_0 is the only input parameter for the Padé–Laplace method. Unlike standard least-squares methods, Padé–Laplace requires no initial guesses for the fitting parameters.

A set of $2n$ equations for the unknowns $a_0,\ldots,a_{n-1}$, $b_1,\ldots,b_n$ is found by multiplying both sides of Eq. (4) by the denominator on the left-hand side, and then setting the coefficients of like powers of $(p-p_0)$ on each side equal, up to power $2n-1$. (Note that for powers n to $2n-1$, the resulting coefficients on the right-hand side must equal zero, because the numerator of the left-hand side only has powers up to $n-1$.) The set of $2n$ equations can be reduced to solving a $n\times n$ matrix problem for $b_1,\ldots,b_n$:

$$\begin{pmatrix} d_{n-1} & \cdots & d_1 & d_0 \\ d_n & \cdots & d_2 & d_1 \\ \vdots & \cdot^{\cdot^{\cdot}} & \vdots & \vdots \\ d_{2(n-1)} & \cdots & d_n & d_{n-1} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = \begin{pmatrix} -d_n \\ -d_{n+1} \\ \vdots \\ -d_{2n-1} \end{pmatrix}. \tag{7}$$

Then n equations for the values $a_0,\ldots,a_{n-1}$ are

$$a_i=d_i+d_{i-1}b_1+\ldots+d_0b_i \qquad (i=0,...,n-1). \tag{8}$$

Problem 2: Derive Eqs. (7) and (8) from Eq. (4).

The steps for the Padé–Laplace method for a particular n and p_0 are summarized as follows:

1. Perform the $2n-1$ summations in Eq. (6) to obtain the d_i in Eq. (5).
2. Invert the $n\times n$ matrix in Eq. (7) to obtain the b_i.
3. Solve Eq. (8) for the n values of a_i.
4. Construct the Padé approximant [the left-hand side of Eq. (4)] and find its poles and residues.

The poles of the Padé approximant give the decay constants and the residues give the amplitudes. The poles are easily found by standard numerical methods to find the zeroes of the polynomial in the denominator of Eq. (4). The residue is what remains of the fraction in Eq. (4) evaluated at a pole when the factor containing the pole is removed. (It is the coefficient of the -1 power term of a Laurent series expansion.) For example if $n=2$ and the coefficients 1, b_1, and b_2 are the input to a function that outputs s_1 and s_2 as the zeros of a polynomial in $s=(p-p_0)$, then the Padé approximant is reexpressed as:

$$\frac{a_0+a_1(p-p_0)}{b_2(p-(s_1+p_0))(p-(s_2+p_0))}. \tag{9}$$

The poles give the decay constants, $-(s_1+p_0)$ and $-(s_2+p_0)$, and the residues are their associated amplitudes

$$\frac{a_0+a_1(s_1)}{b_2(s_1-s_2)}, \quad \frac{a_0+a_1(s_2)}{b_2(s_2-s_1)}. \tag{10}$$

As described here the method requires that the data have essentially decayed to zero by the last data point $(j=M)$, so that the Laplace transform and its derivatives are accurately calculated by Eq. (6).

III. DESCRIPTION OF CIRCUIT

Figure 1 shows the circuit used to generate decaying voltage signals in the presence of noise. The signal is the sum of two decaying exponentials provided by the RC circuits R_1C_1 and R_2C_2. A low output from the 555 turns on the 2N3906 transistors attached to the RC circuits, causing the capacitors to charge quickly. The fully charged voltage is reached when the transistor's collector and emitter voltages are equal. When the 555 output goes high, the transistors turn off, allowing each capacitor to discharge through its adjacent resistor. The voltage dividers that make up R_1 and R_2 provide a fraction of these decaying voltages to the unity gain op amps U1A and U2A. These voltages are then added together by U1B prior to addition of the noise. In this configuration the periodic output of the 555 causes repeated decays. Figure 2 shows how to configure the 555 so that voltage decay is initiated from an external positive-going trigger pulse.

Problem 3: Show that the predicted decay signal for the circuit in Fig. 1 is

$$V(t)=A_1\exp(-\lambda_1 t)+A_2\exp(-\lambda_2 t), \tag{11}$$

where the decay constants λ are 2000 and 200 s^{-1}, and the amplitudes A are about 50 mV each. (Hint: when the capacitors are fully charged, the transistors are saturated so that the collector and emitter voltages are equal and about 0.7 V above the base voltage.)

All the characteristics of the decay signal are easy to adjust. The amplitude of each exponential may be varied by adjusting the voltage dividers that make up R_1 and R_2. The amplitude of the noise is controlled by the gain of the non-

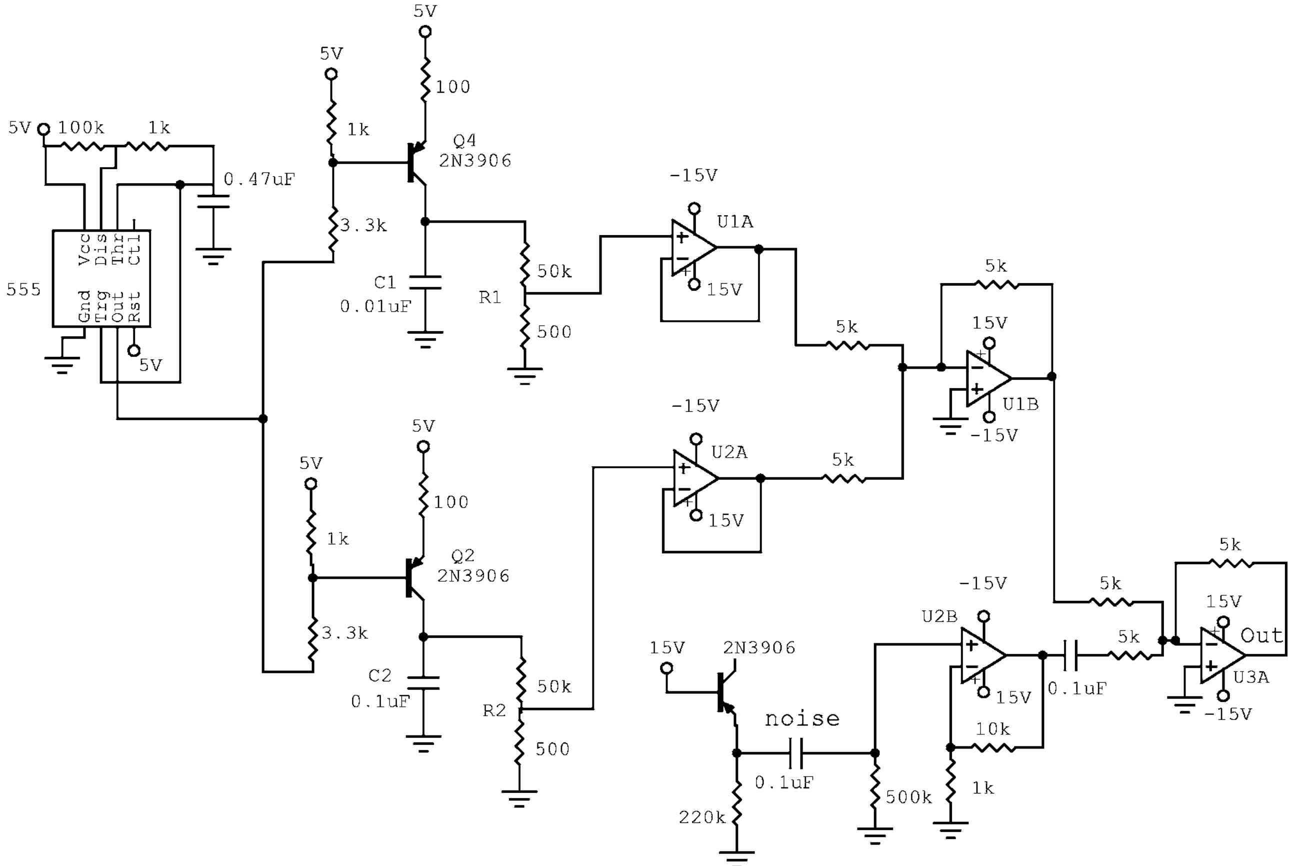

Fig. 1. Circuit for generating voltage decays in the presence of noise. The 555 is configured as an astable timer to produce periodic voltage decays initiated by the rising edge of the 555 output. The resulting decay is a sum of two exponentials with time constants R_1C_1 and R_2C_2.

inverting amplifier U2B. The RC time constants also may be adjusted easily. The use of two RC circuits as in Fig. 1 makes this circuit useful for investigations in resolving multi-exponential decays. It becomes increasingly difficult to resolve two decay constants as their values become closer. Note that Eq. (11) requires that any offset from zero has been subtracted from the data. Subtraction of a background signal such as an offset is standard procedure.

Noise is generated by breakdown of a reverse biased emitter-base junction, in this case a 2N3906 transistor. Breakdown for this junction occurs at about 10 V. Note that the collector is unconnected. The magnitude of the noise varies significantly from one transistor to another even of the same type. For ten different 2N3906 transistors the rms noise varied from 20 to 35 mV. (Any bipolar junction transistor can be used. Reverse biasing the emitter-base of a 2N3904 results in a breakdown at about 7 V, but with a much smaller magnitude noise than for the 2N3906.) The noise is amplified by U2B and added to the decay signal by U3A. ac coupling of the noise avoids addition of a dc offset to the decay signal. The resulting output is a 100 mV decay that is barely noticeable due to the noise.

A simple way to produce a decaying voltage that is not a finite sum of exponentials is to replace the RC circuits by a diode-capacitor circuit. We have shown that the voltage decay for a capacitor discharging through a diode is predominantly a logarithmic function of time.[7] In this case a voltage divider should not be used to sample a fraction of the capacitor voltage because the resistance of the voltage divider would disrupt the logarithmic behavior of the decay.

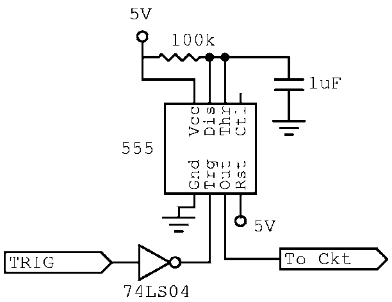

Fig. 2. Configuration of the 555 as a monostable timer for external triggering of voltage decays. A positive pulse at the TRIG input initiates a voltage decay.

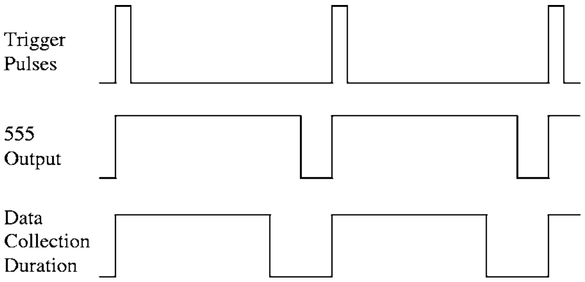

Fig. 3. Signal timing for external triggering of voltage decays using the circuit in Fig. 2.

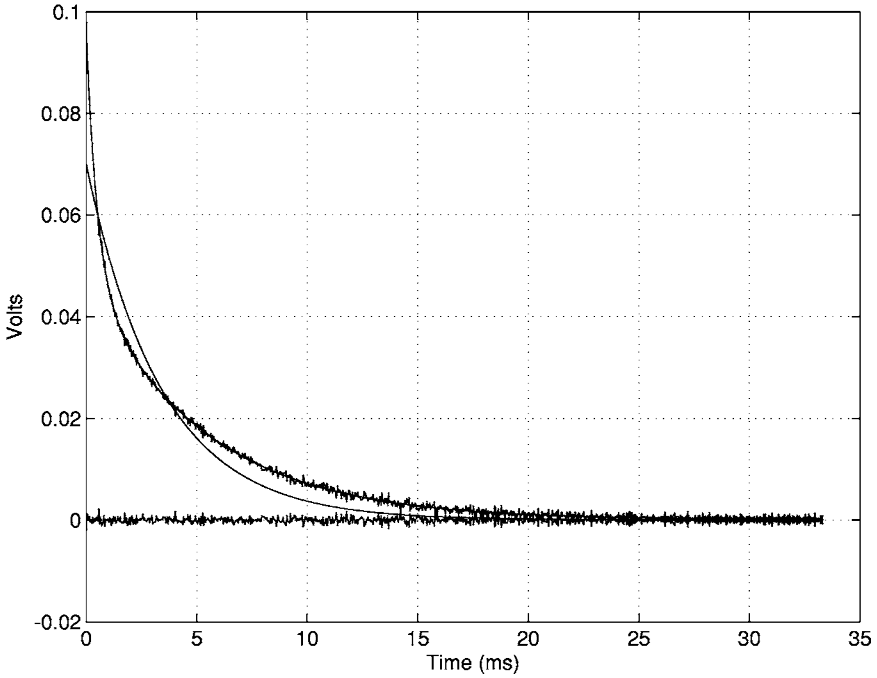

Fig. 4. Signal average of 10 000 voltage decays. Also shown are the Padé–Laplace curve fits for $n=1$ and $n=2$, and the residuals for $n=2$. The curve fit for $n=2$ is excellent, as indicated by the flat residuals.

IV. SIGNAL AVERAGED DATA COLLECTION

Signal averaging is an important technique for increasing the signal-to-noise ratio (SNR) of an inherently noisy signal. The idea is that by adding the results of N experiments performed under identical conditions, the SNR increases by a factor of $\sqrt{N}$ over the value for a single experiment. The reason is that the total signal is proportional to N, and the standard deviation (the statistical noise) increases as $\sqrt{N}$. Thus when the signal average is formed by dividing the total signal by N, the magnitude of the averaged signal remains constant whereas its noise decreases by $\sqrt{N}$. So an inherently noisy experiment with a hopelessly small SNR for analysis may achieve a large SNR if it can be repeated enough times.

Data collection may be accomplished in two ways depending on how the 555 is used. The data acquisition program (a LABVIEW program in our case) must either monitor its own trigger input for a signal generated by the decay circuit, or it must send out a trigger signal that initiates a decay. Both scenarios are important for students in a computer-interfacing course to understand and accomplish.

In the first mode the 555 is configured as an astable timer (as in Fig. 1) so that its periodic output at pin 3 initiates the decays. Each decay begins when the 555 output goes high, so the rising edge of the 555 output is used to trigger data acquisition by connecting it to the TRIG input of the data acquisition card. In our case the LABVIEW program specifies that the data collection begins on a rising edge at the TRIG input.

In the second mode the data acquisition program generates trigger pulses that initiate decays and data acquisition. To accomplish this the LABVIEW program configures a counter output of the data acquisition card to generate a pulse train that is connected to the TRIG inputs of the circuit shown in Fig. 2 and the data acquisition card. The 555 is configured as a monostable timer. Note that it is triggered by bringing pin 2 momentarily low from its normally high state, so the 7404 is used to invert the positive going trigger pulses. When triggered, the output of the 555 goes high for a duration determined by the resistor and capacitor connected to it, about 100 ms for the values shown in Fig. 2. Care must be taken to be sure that the 555 output high duration is longer than the data collection duration, but shorter than the trigger pulse train period as shown in Fig. 3.

The LABVIEW program performs signal averaging by updating the average after data from each run is collected:

$$\langle S_N \rangle = \frac{1}{N} S_N + \frac{N-1}{N} \langle S_{N-1} \rangle. \tag{12}$$

Here N is the total number of runs and S_N is the data from the Nth run. Figure 4 shows the result of averaging 10 000 runs. A single decay had a SNR close to 2 (55 mV noise, 100 mV decay), so for the signal averaged decay in Fig. 4 the SNR is about 200.

Table I. Padé–Laplace analysis. Decay constants λ and amplitudes A obtained from poles and residues of Padé approximants $P_{n-1,n}$ for signal averages of 100, 1000, and 10 000 voltage decays. In all three cases the number of decay constants is found to be 2 since the decay constants (λ_1 and λ_2) and amplitudes (A_1 and A_2) are repeated when n goes from 2 to 3 and λ_3 has negligible amplitude. The units of λ are s^{-1} and the units of A are V.

Padé–Laplace		100 runs	1000 runs	10 000 runs
$n=1$	λ_1	298	293	294
	A_1	0.0707	0.0698	0.0699
$n=2$	λ_1	197	194	189
	A_1	0.0486	0.0490	0.0474
	λ_2	1920	2377	2006
	A_2	0.0459	0.0506	0.0486
$n=3$	λ_1	196	194	192
	A_1	0.0485	0.0490	0.0525
	λ_2	1890	2382	1975
	A_2	0.0457	0.0506	0.0486
	λ_3	-840	-521	243
	A_3	-1.8×10^{-6}	2.9×10^{-9}	-0.0053

Table II. Nonlinear least-squares analysis. Decay constants λ and amplitudes A and their uncertainties obtained from commercial curve-fitting routines (GRAPHICAL ANALYSIS, LABVIEW, and SIGMAPLOT gave the same results) for signal averages of 100, 1000, and 10 000 voltage decays. A reduced-chi-squared value χ_v^2 close to one indicates an acceptable fit.

Nonlinear least squares		100 runs	1000 runs	10 000 runs
One exponential	λ_1	270±7	261±3	261±3
	A_1	0.068±0.001	0.0665±0.0006	0.0666±0.0005
	χ_v^2	1.30	3.6	27
Two exponential	λ_1	202±8	191±2	189±1
	A_1	0.050±0.002	0.0482±0.0006	0.0474±0.0002
	λ_2	2400±300	2120±80	2000±24
	A_2	0.048±0.003	0.049±0.001	0.0486±0.0003
	χ_v^2	1.10	0.98	1.10

V. DATA ANALYSIS

Signal averaged voltage decays using 100, 1000, and 10 000 runs were collected. Table I shows the results from a MATLAB program that applies the Padé–Laplace analysis to these data sets. The value for p_0 was chosen to be 400 s^{-1}. The decay constants (negative of the poles) and amplitudes (residues) are shown for $n=1$, 2, and 3. The increase of n from 1 to 2 produced two decay constants, each different from the $n=1$ case. The increase of n to 3 produced the same two poles as $n=2$, with the third pole having negligible amplitude (about a tenth or less of the size of the other amplitudes). Varying p_0 from 200 to 600 s^{-1} for $n=2$ resulted in about a 1% variation in the decay constants. These results clearly indicate that the voltage decay data are comprised of two exponential decays of about 200 and 2000 s^{-1} with equal amplitudes of about 50 mV (as predicted in Problem 3). Figure 4 shows the Padé–Laplace fits of 10 000 averaged decays for $n=1$ (single exponential) and $n=2$ (double exponential). The $n=2$ fit follows the data, as indicated by its flat residuals (also shown).

Next we applied standard nonlinear least-squares curve-fitting routines[8,9] to the same data analyzed in Table I. These methods may be found in many software packages including GRAPHICAL ANALYSIS, LABVIEW, and SIGMAPLOT. The results from these packages agreed and are shown in Table II for one and two exponential decay functions. For averages of 100 runs the value of the reduced chi square, χ_v^2, indicates that a single exponential gives an acceptable fit. However as the number of averaged runs increases, χ_v^2 for the single exponential fit increases to unacceptable values, whereas χ_v^2 for the two exponential fit remains close to one. Thus, we can conclude that the voltage decay is a sum of two exponentials. The rms noise for a single decay was 55 mV and was used along with the sum of the square of the errors in determining the reduced χ_v^2. The calculation of χ_v^2 requires knowledge of the expected error, which is not always well known. The results in Tables I and II demonstrate that Padé–Laplace and the standard curve-fitting methods both find the correct parameters.

What happens when the Padé–Laplace method is applied to a decay that cannot be expressed as a finite number of exponentials? We investigated this question by analyzing the predominantly logarithmic voltage decay obtained from the diode-capacitor circuit.[7] The Padé–Laplace method found new poles each time n was increased, and the values of the poles depended strongly on the choice of p_0. These results indicate correctly that the diode-capacitor decay is not a finite sum of exponentials (at least up to three, the maximum n used).

VI. CONCLUSION

We applied the Padé–Laplace method of analyzing multiexponential decays to signal-averaged voltages obtained from a simple electronic circuit. This interesting alternative to nonlinear least-squares methods is a valuable computational project. The versatile circuit we described is useful for investigations of signal averaging. These methods may be incorporated into an investigation in which different decaying signals that appear indistinguishable due to noise are resolved by using signal averaging and Padé–Laplace analysis.

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[1] E. Yeramian and P. Claverie, "Analysis of multiexponential functions without a hypothesis as to the number of components," Nature (London) **326**, 169–174 (1987).

[2] Z. Bajzer, J. C. Sharp, S. S. Sedarous, and F. G. Prendergast, "Padé-Laplace method for analysis of fluorescence intensity decay," Eur. Biophys. J. **18**, 101–115 (1990).

[3] N. J. Clayden, "Padé-Laplace analysis in the fitting of multi-exponential nuclear magnetic resonance relaxation decay curves," J. Chem. Soc., Faraday Trans. **88**, 2481–2486 (1992).

[4] A. A. Istratov and O. F. Vyvenko, "Exponential analysis in physical phenomena," Rev. Sci. Instrum. **70**, 1233–1257 (1999). An extensive review on exponential analysis.

[5] D. P. O'Leary, "Fitting exponentials: An interest in rates," Comput. Sci. Eng. **6**, 66–72 (2004).

[6] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in Fortran* (Cambridge U.P., Cambridge, 1994), 2nd ed., Chap. 5, p. 194.

[7] E. H. Hellen, "Verifying the diode-capacitor circuit voltage decay," Am. J. Phys. **71**, 797–800 (2003).

[8] D. C. Baird, *Experimentation: An Introduction to Measurement Theory and Experiment Design* (Prentice–Hall, Englewood Cliffs, 1988).

[9] P. R. Bevington and D. K. Robinson, *Data Reduction and Error Analysis* (McGraw-Hill, Boston, 2003), 3rd ed.