Notes on the Ward Johnson Problem

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Contents

1 The Ultrasonic Resonance System

A block diagram of the ultrasonic resonance system is shown in Figure 1. The gated

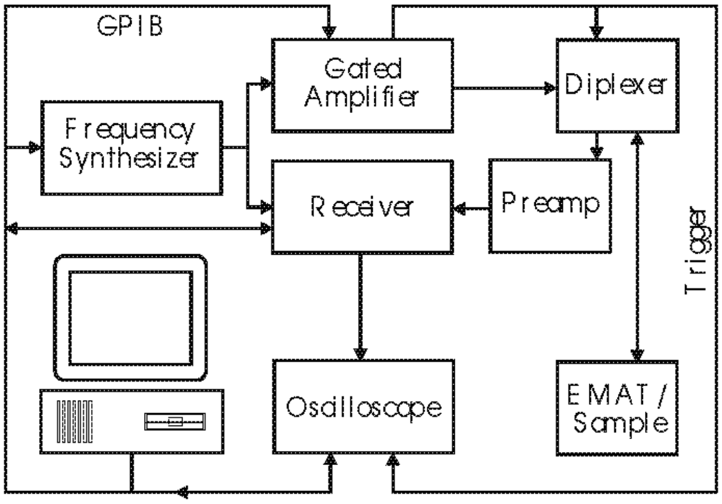

Figure 1: The ultrasonic resonance system

amplifier creates a tone burst of typically 3 ms from the continuous sinewave reference (ω_0, normally in the range 0.3-3 MHz) of the frequency synthesizer. The reference is given by

$$V(t) = A \sin(\omega_0 t) \ . \tag{1}$$

The tone burst drives the sample into resonance if ω_0 is sufficiently close to an acoustic resonance. "Sufficiently close" is defined by the bandwidth of the tone burst (the Fourier transform of the tone burst); the effective bandwidth is several times the inverse of the pulse width, so, typically, on the order of 1 kHz.

The transduction is electromagnetic. There is a coil surrounding the sample, which is usually cylindrical, and the coil and sample are in a static magnetic field. (This constitutes an "electromagnetic-acoustic transducer" or EMAT.) An oscillating current in the coil induces eddy currents in the sample, and this current, in combination with the static B, results in Lorentz forces on the sample with a symmetry determined by the coil geometry.

After the driving tone burst, there is a resonant ringdown of the sample, and the transducer operates in reverse to detect the vibrations. The signal from the transducer is passed to a receiver. (The diplexer in the figure performs the switching between the gated amp and the receiver.) If a single resonance is excited, the signal is given approximately by

$$V(t) = B\exp(-\alpha t) sin(\omega t) \ , \tag{2}$$

where ω is the acoustic resonant frequency.

The receiver contains two mixers that manipulate the received signal in a manner similar to a lock-in amplifier. (The RITEC is actually significantly more complicated than a lock-in amp, because it's a superheterodyne receiver, but it's functionally equivalent.) One of the mixers essentially multiplies the signal and the reference and has an output V_1:

$$\begin{aligned} V_1(t) &= AB\exp(-\alpha t)\sin(\omega t)\sin(\omega_0 t) && (3) \\ &= \frac{AB}{2}\exp(-\alpha t)\left\{\cos\left[(\omega-\omega_0)\,t\right] - \cos\left[(\omega+\omega_0)\,t\right]\right\} \ . && (4) \end{aligned}$$

This is passed through a low-pass filter, producing y_1 as an output from the instrument:

$$y_1(t) = \frac{AB}{2}\exp(-\alpha t)\cos\left[(\omega-\omega_0)\,t\right] \ . \tag{5}$$

The second mixer shifts the phase of the reference by $\pi/2$ before the multiplication and has an output V_2:

$$\begin{aligned} V_2(t) &= AB\exp(-\alpha t)\sin(\omega t)\cos(\omega_0 t) && (6) \\ &= \frac{AB}{2}\exp(-\alpha t)\left\{\sin\left[(\omega-\omega_0)\,t\right] + \sin\left[(\omega+\omega_0)\,t\right]\right\} \ . && (7) \end{aligned}$$

which, after low-pass filtering becomes

$$y_2(t) = \frac{AB}{2}\exp(-\alpha t)\sin\left[(\omega-\omega_0)\,t\right] \ . \tag{8}$$

The advantage of this technique is that digitizing the signals y_1 and y_2 gives all of the useful information about the resonant ringdown (the frequency and the damping coefficient) in a relatively small number of data points. That is, instead of digitizing and analyzing a 1 MHz signal over tens of milliseconds (requiring on the order of 100,000 data points), one can digitize much more slowly varying signals (with typically 1000 data points).

2 The Mathematical Model

We need a transition section here where we introduce the notion of signals which are superpositions of several damped frequencies and also allow for (explain) the DC components in the measured signals. We also need to explain how the phase shifts get into the picture, i.e., how we get from $\sin\left[\left(\omega-\omega_0\right)t\right]$ to $\sin\left(C_i t + D_i\right)$ and etc. for the cos's.

We also need to make the notation consistent. I'm quite willing to give up the $(A_j, B_j, C_j, D_j, E_j, F_j)$'s. In fact, I sort of like α's for the damping constants and think that f's would be more natural for frequencies than C's. But I sort of like A's for amplitudes. I don't have any strong feelings about what to use for the phase shifts D_j, or for the E_j, F_j's. It would also simplify the notation to use angular frequencies ω_j's rather than $2\pi C_j$'s though the final results should probably be in units of natural frequency.

We should try to establish as much of the notation as possible in this section so the following sections will be easier to write.

3 The Nonlinear Regression Model

We are given two simultaneously measured time series, $y_1(t_i)$ and $y_2(t_i)$ which are measured at equally spaced times $t_1, t_2, \ldots, t_m$. We believe that these two time series represent discrete samples from the two mathematical functions

$$y_1(t) = E_0 + \sum_{j=1}^{N} A_j \exp\left(-B_j t\right) \cos\left[2\pi\left(C_j t + D_j\right)\right] \ , \tag{9}$$

$$y_2(t) = F_0 + \sum_{j=1}^{N} A_j \exp\left(-B_j t\right) \sin\left[2\pi\left(C_j t + D_j\right)\right] \ , \tag{10}$$

where $E_0, F_0, A_1, \ldots, A_N, B_1, \ldots, B_N, C_1, \ldots, C_N, D_1, \ldots, D_N$ are constants to be determined by least squares fitting. The statistical regression model can thus be written

$$y_1(t_i) = E_0 + \sum_{j=1}^{N} A_j e^{-B_j t_i} \cos\left[2\pi\left(C_j t_i + D_j\right)\right] + \epsilon_{1,i} \ , \quad i = 1, \ldots, m \ , \tag{11}$$

$$y_2(t_i) = F_0 + \sum_{j=1}^{N} A_j e^{-B_j t_i} \sin\left[2\pi\left(C_j t_i + D_j\right)\right] + \epsilon_{2,i} \ , \quad i = 1, \ldots, m \ , \tag{12}$$

where the $\epsilon_{1,i}$ and $\epsilon_{2,i}$ are random measurement errors which are assumed to be independently, indentically, normally distributed with mean 0 and unknown variance σ^2.

Note that the model is linear in $E_0, F_0, A_1, \ldots, A_N$, but it is nonlinear in the parameters $B_1, \ldots, B_N, C_1, \ldots, C_N, D_1, \ldots, D_N$ so a nonlinear regression will be required to determine the best fit.

It will simplify the nonlinear least squares calculation if we substitute the trigonometric identities

$$\cos\left[2\pi\left(C_j t_i + D_j\right)\right] = \cos\left(2\pi C_j t_i\right)\cos\left(2\pi D_j\right) - \sin\left(2\pi C_j t_i\right)\sin\left(2\pi D_j\right) \ , \tag{13}$$

$$\sin\left[2\pi\left(C_j t_i + D_j\right)\right] = \sin\left(2\pi C_j t_i\right)\cos\left(2\pi D_j\right) + \cos\left(2\pi C_j t_i\right)\sin\left(2\pi D_j\right) \ , \tag{14}$$

into Eqs. (11) and (12), and define new parameters

$$E_j = A_j \cos\left(2\pi D_j\right) \ , \quad F_j = A_j \sin\left(2\pi D_j\right) \ , \quad j = 1, 2, \ldots, N \ , \tag{15}$$

so that the regression equations can be written in the form

$$y_1(t_i) = E_0 + \sum_{j=1}^{N} e^{-B_j t_i}\left[E_j \cos\left(2\pi C_j t_i\right) - F_j \sin\left(2\pi C_j t_i\right)\right] + \epsilon_{1,i} \ , \tag{16}$$

$$y_2(t_i) = F_0 + \sum_{j=1}^{N} e^{-B_j t_i}\left[E_j \sin\left(2\pi C_j t_i\right) + F_j \cos\left(2\pi C_j t_i\right)\right] + \epsilon_{2,i} \ . \tag{17}$$

This form for the regression model is better than that given by Eqs. (11) and (12) because it has only $2N$ nonlinear parameters $B_1, \ldots, B_N$ and $C_1, \ldots, C_N$ while the earlier form has $3N$ nonlinear parameters. Once the estimates of the E_j and F_j have been determined by the fitting program, the values of the original parameters A_j and D_j can be computed from the inverse transformations

$$A_j = \sqrt{E_j^2 + F_j^2} \ , \qquad D_j = \tfrac{1}{2\pi}\tan^{-1}\left(\tfrac{F_j}{E_j}\right) \ , \qquad j = 1, 2, \ldots, N \ . \tag{18}$$

4 The VARPRO Nonlinear Least Squares Code

To simplify the notation let us define the two N-vectors $\mathbf{B}$ and $\mathbf{C}$ and the two $(N+1)$-vectors $\mathbf{E}$ and $\mathbf{F}$ by

$$\mathbf{B} = \begin{bmatrix} B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \\ B_N \end{bmatrix} , \quad \mathbf{C} = \begin{bmatrix} C_1 \\ C_2 \\ \cdot \\ \cdot \\ \cdot \\ C_N \end{bmatrix} , \quad \mathbf{E} = \begin{bmatrix} E_0 \\ E_1 \\ E_2 \\ \cdot \\ \cdot \\ \cdot \\ E_N \end{bmatrix} , \quad \mathbf{F} = \begin{bmatrix} F_0 \\ F_1 \\ F_2 \\ \cdot \\ \cdot \\ \cdot \\ F_N \end{bmatrix} . \tag{19}$$

Then the residual functions for the regression model can be written

$$r_1\left(t_i, \mathbf{B}, \mathbf{C}, \mathbf{E}, \mathbf{F}\right) = y_1\left(t_i\right) - E_0 - \sum_{j=1}^{N} e^{-B_j t_i}\left[E_j \cos\left(2\pi C_j t_i\right) - F_j \sin\left(2\pi C_j t_i\right)\right] \;, \quad (20)$$

$$r_2\left(t_i, \mathbf{B}, \mathbf{C}, \mathbf{E}, \mathbf{F}\right) = y_2\left(t_i\right) - F_0 - \sum_{j=1}^{N} e^{-B_j t_i}\left[E_j \sin\left(2\pi C_j t_i\right) + F_j \cos\left(2\pi C_j t_i\right)\right] \;, \quad (21)$$

and the sum of squared residuals becomes

$$\rho^2\left(\mathbf{B}, \mathbf{C}, \mathbf{E}, \mathbf{F}\right) = \sum_{i=1}^{m}\left[r_1^2\left(t_i, \mathbf{B}, \mathbf{C}, \mathbf{E}, \mathbf{F}\right) + r_2^2\left(t_i, \mathbf{B}, \mathbf{C}, \mathbf{E}, \mathbf{F}\right)\right] \;. \quad (22)$$

The nonlinear least squares estimates of the unknown parameters are obtained by minimizing this function with respect to $\mathbf{B}, \mathbf{C}, \mathbf{E}$, and $\mathbf{F}$. Since it is nonlinear in the unknown parameters, it is not possible to find closed form expressions for the estimates or the minimum value. Instead, it is necessary to start with initial estimates $\mathbf{B}^{(0)}, \mathbf{C}^{(0)}, \mathbf{E}^{(0)}$, and $\mathbf{F}^{(0)}$ and to march iteratively to the minimum.

Before 1973, it would have been necessary to provide initial estimates for all $4N+2$ of the unknown parameters and to iterate on all of them to find the minimum value of ρ^2. But then, along came Golub and Pereyra [2], etc., etc., etc, ...

$$\left[\begin{array}{c} y_1\left(t_1\right) \\ y_1\left(t_2\right) \\ \cdot \\ \cdot \\ \cdot \\ y_1\left(t_m\right) \\ \hline y_2\left(t_1\right) \\ y_2\left(t_2\right) \\ \cdot \\ \cdot \\ \cdot \\ y_2\left(t_m\right) \end{array}\right] = \left[\begin{array}{cccc} 1 & 0 & e^{-B_1 t_1}\cos\left(2\pi C_1 t_1\right) & -e^{-B_1 t_1}\sin\left(2\pi C_1 t_1\right) \\ 1 & 0 & e^{-B_1 t_2}\cos\left(2\pi C_1 t_2\right) & -e^{-B_1 t_2}\sin\left(2\pi C_1 t_2\right) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & e^{-B_1 t_m}\cos\left(2\pi C_1 t_m\right) & -e^{-B_1 t_m}\sin\left(2\pi C_1 t_m\right) \\ \hline 0 & 1 & e^{-B_1 t_1}\sin\left(2\pi C_1 t_1\right) & e^{-B_1 t_1}\cos\left(2\pi C_1 t_1\right) \\ 0 & 1 & e^{-B_1 t_2}\sin\left(2\pi C_1 t_2\right) & e^{-B_1 t_2}\cos\left(2\pi C_1 t_2\right) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & e^{-B_1 t_m}\sin\left(2\pi C_1 t_m\right) & e^{-B_1 t_m}\cos\left(2\pi C_1 t_m\right) \end{array}\right] \left[\begin{array}{c} E_0 \\ F_0 \\ E_1 \\ F_1 \end{array}\right] + \left[\begin{array}{c} \epsilon_{1,1} \\ \epsilon_{1,2} \\ \cdot \\ \cdot \\ \cdot \\ \epsilon_{1,m} \\ \hline \epsilon_{2,1} \\ \epsilon_{2,2} \\ \cdot \\ \cdot \\ \cdot \\ \epsilon_{2,m} \end{array}\right]$$

5 Finding Initial Estimates $\mathbf{B}^{(0)}$ and $\mathbf{C}^{(0)}$

Introduce a real data set here (with graphs) and show the complex Fourier amplitude (or power) spectrum.

6 Fitting the Model to the Data

Show the results of fitting the data set introduced in the previous section.

7 Residual Diagnostics

- Show in detail how to analyze the residuals for the fits obtained in the previous section.
- Refer to appendices to explain the various statistical and time-series test that will be used here.
- Introduce the notion that a model is acceptable only when it gives residuals that are statistically consistent with white noise and show how to iterate (repeat) the fitting step to incorporate new damped waves when they are found to be statistically significant. (It might be better to put the iteration procedure in another section.)

8 Appendix A. The Residual Periodogram

9 Appendix B. The Cumulative Periodogram

10 Appendix C. The χ^2 Test for Normality

Acknowledgements

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