Causal or Not? A Definite Answer for Frequency-Response Data

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***Abstract*—This paper poses the question of whether a dataset can be identified to be causal by employing rational function fitting techniques. Specifically, overfitting is considered to be a factor that could prevent the user from correctly identifying causality. Without the emphasis on overfitting, we show that every frequency-response data is causal. The ability of the adaptive generation (AG) scheme in highlighting an ideal model order is used as an example where the fit may inform the user about the causal quality of the data.**

***Index Terms*—rational function approximation, blackbox macromodeling, causality, measurement data**

I. Introduction

There is increasing interest in verifying the integrity of scattering parameters obtained from electromagnetic simulators or vector network analyzers (VNA). A primary concern is the causality of the time-domain response when the scattering parameters are used as blocks in a system-level circuit simulation. If the system-level simulation consists of linear elements, convolution or Fourier techniques can be used. Otherwise, an equivalent circuit model needs to be generated from the scattering parameters. Such a lumped-element model has an exact rational function representation. Frequency response data with causality issues results in a rational function, or equivalently a circuit model, with unstable poles. This is an unacceptable error that warrants discarding the data and repeating the simulation or the measurement. Repeating a measurement is especially a severe problem, as there is usually a time gap between measurement and the use of that data in circuit simulation, and these steps are usually the responsibility of different groups in the semiconductor industry.

Causality requires that the response cannot precede the input. This is expressed in terms of the system's impulse response as $h(t) = 0$ for $t < 0$. The implication for its Fourier transform $H(\omega) = R(\omega) + jX(\omega)$ is that $R(\omega)$ and $X(\omega)$ have to be a Hilbert transform pair (also called Kramers-Kronig or dispersion relation.) The difficulty of verifying causality in VNA measurements is that what is measured are the samples H_i of $H(\omega)$ at the frequency points $\omega = \omega_i$, and not $h(t)$, and numerical calculation of Hilbert or Fourier transforms suffer from the inherent bandlimited and discrete nature of the measured data [1]–[4]. Worst-case error bounds are presented in [5], where the data is confirmed as noncausal if it is outside worst-case error bounds. Such techniques become more accurate as the measured data becomes densely sampled and linearly spaced. Fast, discrete transforms are readily available and robust; however, they do not work for a general-purpose methodology where the frequency sweep for measurement is selected by the user and could be narrowband, not linearly spaced, etc. This makes checking the causality of measured frequency responses by discrete Fourier or Hilbert transforms or numerical integration impractical.

There is, however, a more fundamental issue in certifying the causality of frequency-response data. A common intuition is that the data can be certified to be causal if we can interpolate it with a causal function. We show in this paper that this intuition is misleading. As proof, we present a causal function that interpolates random data. This fundamental result obviates the causality checks for frequency-response data. We instead propose a causal quality definition to account for causality issues in the practical use of frequency-response data.

II. Are All Frequency-Response Data Causal?

Assume that an interpolating rational function $r(s)$ could be found that would precisely match the measured data as $r(j\omega_i) = H_i$ at all the frequency points $s_i = j\omega_i$. If $r(s)$ is a causal function, then the measurement can be verified as causal.

A rational transfer function with poles on the left-half plane, which implies bounded-input bounded-output stability, represents a causal system [6]. There is, in fact, always an interpolating function with stable poles for arbitrary data on the imaginary axis. The proposed interpolating function for n arbitrary data points is:

$$r(s) = \frac{\sum_{i=1}^{n} sc_i \frac{R_i + X_i s/\omega_i}{s^2+\omega_i^2}}{c_0 + \sum_{i=1}^{n} \frac{sc_i}{s^2+\omega_i^2}} \tag{1}$$

Equation (1) represents $r(s)$ in barycentric form. It interpolates the data $R_i + jX_i$ at the given frequency points $s = j\omega_i$ similar to a Lagrangian interpolation as long as the weights c_i are nonzero [7], [8]. Assume that the weights are all positive; for example, $c_i = 1$ for all i. The denominator of $r(s)$ is a positive-real function consisting of the summation

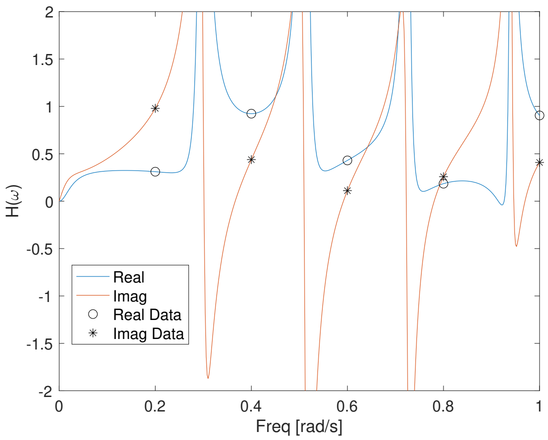

Fig. 1. A rational function interpolating random data points. The poles are all stable; therefore, the rational function represents a causal system.

of the positive constant 1 and the impedance of a lossless LC network. Therefore, its zeros, the poles of $r(s)$, lie in the left half plane. In fact, $r(s)$ interpolates any data provided at n frequencies with the same set of poles. It is easy to see that $r(s)$ reduces to a rational function, as the $s^2 + \omega_i^2$ terms are common in the denominators and cancel out. As a result, (1) is a rational function with stable poles; therefore, it represents a causal system, interpolating arbitrary complex data points.

An example is shown in Fig. 1 for 5 data points. The prior intuition would be that the Kramers-Kronig relations would not hold, as the real and imaginary parts of the data are independently, actually randomly, generated. However, it is interpolated with a stable rational function, confirming the causality of the data. The implication is that there is no noncausal measured or simulated data – all data are causal, satisfying Kramers-Kronig relations.

III. Causal Quality of Measured Data

The results of the previous section are certainly not validated by everyday engineering practice, where "bad data" frequently results in modeling and simulation difficulties. This contradiction is resolved with consideration of practical issues caused by so-called noncausal data. The causality of measured data needs a definition beyond Kramers-Kronig relation (which can always be satisfied with an interpolating causal function). The definition of causality needs to be accompanied by the assumption made for the behavior of frequency response between the data points. For example, the interpolating rational function in (1) has $2n$ poles for n data points. This rational function is certainly overfitting the data. Such interpolation methods tend to have large fluctuations between the interpolation nodes [9] as can also be seen in Figure 1. As a result, there is very low confidence in this interpolating rational function to recover the original transfer function from its discrete points. What is needed is a rational function approximation, rather than interpolation, based on a methodology to prevent overfitting. The proposed definition for causality of data is:

Definition 1: Frequency-response data has good causal quality if it can be approximated well with a causal function without overfitting.

A causality metric can now be determined based on the quality of the fit, for example, using a rational function with stable poles. We note that application of the vector fitting algorithm [6], [10] to assess the causality of the data would be in the spirit of this definition. However, vector fitting is not the best choice, as it does not directly address the overfitting problem.

IV. Adaptive Generation of Rational Approximations

In [12] we have presented the adaptive generation (AG) algorithm for gradually building up a rational approximation. In AG, we find the rational function $r(s) = b(s)/a(s)$ that minimizes least-squares residual error from measurement data H, so that $b(j\omega)/a(j\omega) \approx H$. This is a non-linear least-squares problem due to the unknown coefficients of the denominator polynomial $a(s)$, which must be a Hurwitz polynomial for $r(s)$ to represent a causal system. We solve the linearized version $b(j\omega)/\hat{a}(j\omega) \approx Ha(j\omega)/\hat{a}(j\omega)$ iteratively in a heuristic approach, where we start with $\hat{a}(s) = 1$. At each iteration, we take the order of $a(s)$ to be one larger than $\hat{a}(s)$, and start the next iteration with $\hat{a}(s) = a(s)$ until convergence. This allows to add one pole at a time to the rational function approximation.

Measured data of a common-mode filter per the design in [11] was used to test how AG would be able to detect over-fitting and causality. AG was run in stable mode, which indicated that it was conducting pole-flipping for unstable poles, and in an unstable mode where this was turned off. The original measurement data has good causal quality as shown in Fig. 2 and Fig. 4. To obtain an example with low causal quality, an additional $j0.05$ term was added to each datapoint. As shown in Fig. 3 and Fig. 5, the error in fitting data is now higher with a stable fit than with the unstable option, indicating low causal quality of the modified data.

V. Conclusion

In this paper, the question was posed about whether causality can be identified from the data alone. It was shown that we can always find an interpolating rational function with stables poles, representing a causal function. The implication is that if there is overfitting, it may be not possible to discern if the original data points were causal or not. AG is presented as an algorithm which, due to its ability to adaptively determine the model order, may prevent overfitting, and therefore provide an indication as to whether the original data indeed has good causal quality. This is shown in an example using measurement data from a VNA. To compare the outcome when the data has low causal quality, an addition of a purely imaginary term and a comparison of the resulting error with and without stable poles were performed.

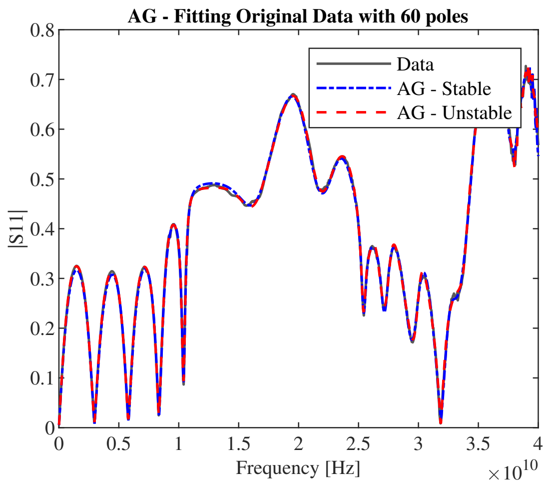

Fig. 2. A comparison of the fit on measured data from a common-mode filter in [11] using AG with 60 poles. The function visibly fits the data.

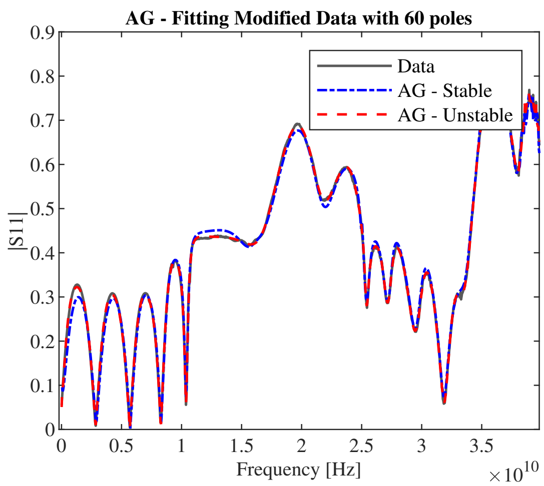

Fig. 3. A comparison of the fit on measured data from a common-mode filter in [11] using AG with 60 poles with the addition of a $j0.05$ term for the comparison of the fit of AG to data with low causal quality.

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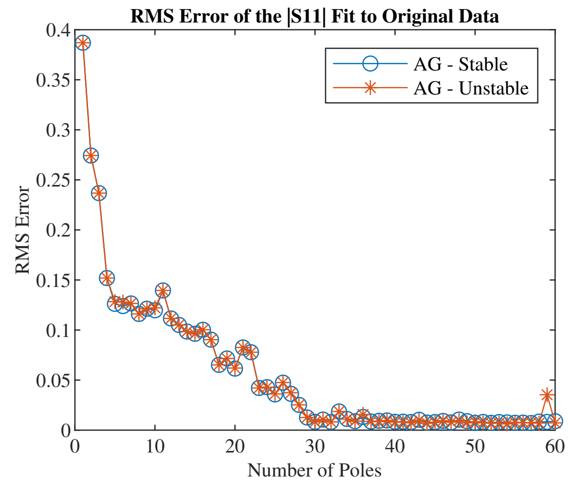

Fig. 4. A comparison of the RMS error from measured data from a common-mode filter in [11] using AG with 60 poles. Enforcing stability of poles does not increase the residual error, indicating data with high causal quality.

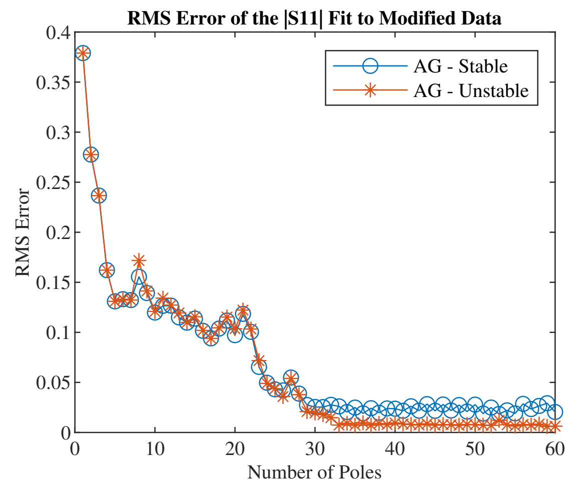

Fig. 5. A comparison of the RMS error from measured data from a common-mode filter in [11] using AG with 60 poles with the addition of a $j0.05$ term for the comparison of the fit of AG to data with low causal quality.

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