Fast and Reliable Passivity Assessment and Enforcement with Extended Hamiltonian Pencil

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ABSTRACT

Passivity is an important property for a macro-model generated from measured or simulated data. Existence of purely imaginary eigenvalues of a Hamiltonian matrix provides useful information in assessing and correcting the passivity of a system. Since direct computation of eigenvalues is very expensive for large-scale systems, several authors have proposed to solve iteratively for a subset of the eigenvalues based on heuristic sampling along the imaginary axis. However, completeness is not guaranteed in such methods and thus potential risk of missing important eigenvalues is difficult to avoid. In this paper we are aiming at finding all eigenvalues efficiently to avoid both the high cost and the potential risk of missing important eigenvalues. The idea of the proposed method is to convert the Hamiltonian matrix to an equivalent sparse form, termed the "extended Hamiltonian pencil", and solve for its eigenvalues efficiently using a special eigensolver. Experiments on several realistic systems demonstrate an 80X speed-up compared with standard direct eigensolvers.

1. INTRODUCTION

Passivity-constrained macro-modeling based on approximation to tabulated data has been a hot topic for many years. Devices such as spiral inductors, baluns, SAW filters, transmission lines, etc, are commonly described using tabulated s-parameter data obtained either by measurement or through numerical simulation. Although some of the existing circuit simulators can take this data as input directly, the supported types of analysis are very limited.

In order to generate a model that supports all different modes of the simulation from the tabulated data, a practical method is via rational fitting [1] or vector fitting [2]. One main difficulty that must be faced during the process of generating these macro-models is passivity enforcement. Passivity can be viewed as the inability of a given system to generate energy. Models generated for passive systems are required to retain this property. Otherwise they can be troublesome when used in numerical simulation, since convergence issues and/or unstable transient simulations may occur.

Mathematically, passivity requires that the transfer matrix under investigation be positive real (in the case of hybrid representations such as Y- or Z- parameters) or bounded real (in the case of scattering representations such as S-parameters). One of the methods to test or enforce passivity of a system is to check and enforce it for discrete sampling frequency points [3]. While these methods are straightforward, they do not provide any guarantee of the passivity in the whole frequency range.

Fortunately, algebraic tests for passivity exist. One way to test and enforce passivity is based on the positive real lemma, which reveals the equivalence between passivity and the existence of solution for an LMI equation [4]. Based on this theory, convex semi-definite programming (SDP) [5] can be performed to generate passive models with global optimality in accuracy. However, the computational complexity, $O(n^3)$ with large constants, limits its application for even medium-size problems.

More recently, methods based on the Hamiltonian matrix become more attractive [6–11] because they possess much lower cost. Hamiltonian matrix is a frequency independent matrix derived from the state space representation of a system. The passivity can be determined by the absence of purely imaginary eigenvalues of the Hamiltonian matrix. The essence of methods based on Hamiltonian matrix is to first find those imaginary eigenvalues and then use some techniques to move these eigenvalues away from the imaginary axis.

The most demanding task in these methods is to find the eigenvalues of the Hamiltonian matrix. Direct computation with $O(n^3)$ complexity is prohibitive for large scale problems, thus [8-11] propose to compute only a subset of the eigenvalues with iterative methods, and sample around the imaginary axis based on heuristics. Such methods have shown promising results for some problems. However, they may potentially suffer from the risk of missing important eigenvalues due to their incompleteness. Therefore, a complete and efficient method is required. A relatively minor issue with current Hamiltonian-based methods is that construction of Hamiltonian matrix requires that the matrix $D + D^T$ matrix in the state space model to be non-singular. This is not always true in practice. Systems with singular or even zero D matrix are often seen in practical circuits.

This paper presents a new method for passivity testing based on an extended version of the Hamiltonian matrix [12]. The extended Hamiltonian pencil is sparse and has a very special structure that facilitates a highly efficient solver for computing its eigenvalues. As a by-product, construction of the extended Hamiltonian pencil does not require non-singular $D + D^T$ and thus is more general compared to those in literature.

The rest of this paper is organized as follows. In Section 2 we introduce the mathematical background of the problem, and review exiting methods based on Hamiltonian matrix. Section 3 presents our proposed method based on extended Hamiltonian pencil and an efficient eigensolver, and introduces how to do the passivity en-

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forcement in this framework. Results and conclusions will be given in Sections 4 and 5.

2. BACKGROUND

In this section we review some of the main procedures for passivity test. For the sake of simplicity, we only consider the hybrid case (Y- or Z- form). For the scattering case (S- form), parallel derivations can be easily obtained.

The linear system under investigation is described in the frequency domain using the following transfer function

$$H(s) = C(sI - A)^{-1}B + D \tag{1}$$

where $A \in \mathcal{R}^{n\times n}$, $B \in \mathcal{R}^{n\times m}$, $C \in \mathcal{R}^{m\times n}$, $D \in \mathcal{R}^{m\times m}$ are system matrices. n is the number of states and m is the number of input/output ports. Generally $m \ll n$.

Throughout the following we will assume that the system is strictly stable, which means that all its poles are located in the left half plane. Moreover, we will assume, without loss of generality, that matrix A is *diagonal*. These assumptions are naturally guaranteed in rational fitting or vector fitting.

2.1 Passivity Test

A system is passive if it it not able to generate energy. This is crucial since the interconnection of passive system is guaranteed to be stable. It is always required that the macro-model for a passive system also be passive. Mathematically passivity requires that the Hermitian part of the transfer matrix must be positive semi-definite on the imaginary axis, i.e.

$$G(s) = H(s) + H^H(s) \geq 0, \quad s = j\omega \tag{2}$$

A practical way to test the passivity of a system is to verify the eigenvalues of the Hamiltonian matrix [7]

$$M = \begin{bmatrix} A + BR^{-1}C & BR^{-1}B^H \\ C^H R^{-1}C & -A^H + C^H R^{-1}B^H \end{bmatrix} \tag{3}$$

where $R = D + D^H$. A system is non-passive if and only if the Hamiltonian matrix has purely imaginary eigenvalues. Once these eigenvalues are found, they can be displace away from the imaginary axis to enforce the passivity. For details of the enforcement one may refer to [7].

The most demanding portion in methods based on Hamiltonian matrix is the calculation for the eigenvalues of the Hamiltonian matrix. The rest of this paper is focusing on efficient and reliable computation of the eigenvalues of the Hamiltonian matrix.

2.2 Existing Methods

Existing methods for calculating the eigenvalues of a Hamiltonian matrix include direct methods and iterative methods. Direct methods solve for all the eigenvalues and are of $O(n^3)$ cost, which is too expensive when dealing with large scale problems.

Another existing alternative is to adopt iterative methods such as the tuned versions of the Arnoldi's method [8, 9]. Such methods aim at computing a carefully selected subset of the eigenvalues. To ensure that this kind of method works well in most cases, considerable effort is required in implementing complex heuristics that choose the sampling points to capture all the important eigenvalues, as has been done in [8, 9]. In our experience it is difficult to implement robust heuristics, so there is a significant risk of encountering extreme cases that can cause failures of such methods.

3. THE PROPOSED METHOD

In this section we propose an efficient method for computing all the eigenvalues of the Hamiltonian matrix. The idea of the new algorithm is to compute the eigenvalues of an equivalent form, which is termed the Extended Hamiltonian Pencil. Due to the special structure of the Extended Hamiltonian Pencil, the eigenvalues of the Extended Hamiltonian Pencil can be computed efficiently with a special polynomial root findings algorithm.

We need to emphasis that it is always critical to avoid the potential numerical instabilities possible with using a polynomial root-finding technique. This is difficult in general. However, as will be presented in this section, with properly exploiting the special structure of the extended Hamiltonian matrix, the computation can be done in a stable way.

3.1 The Extended Hamiltonian Pencil

The extended Hamiltonian pencil is defined as [12]

$$Mv = sNv \tag{4}$$

where

$$M = \begin{bmatrix} A & & B \\ & -A^H & -C^H \\ C & B^H & D + D^H \end{bmatrix}, \quad N = \begin{bmatrix} I & & \\ & I & \\ & & \end{bmatrix} \tag{5}$$

It can be easily verified that the extended Hamiltonian pencil is equivalent to the Hamiltonian matrix for assessing passivity, since they have the same eigenvalues. A key observation on the extended Hamiltonian pencil is that it is a sparse matrix with very special structure. The majority of the matrix is diagonal since matrix A is assumed to be diagonal. Only the last m columns and m rows are non-zeros. In the next subsections we will propose an algorithm for calculating the eigenvalues of the extended Hamiltonian pencil efficiently.

3.2 Laguerre's Method

Laguerre's method [14, 15] is a simple yet stable method for numerically computing the roots of an arbitrary polynomial. The method has exhibited good performance in solving eigenvalues for matrices with some special structure [16]. It is fairly simple, and can be shown to converge at a cubic rate, except in the vicinity of a multiple root, where it has only linear convergence. It almost guarantees to converge to a root of a polynomial no matter from what point the iteration is started. Although variations with improved convergence exist [17], for the sake of clarity in this paper we will still use the original form of Laguerre's method.

With dropping the derivations, Laguerre's method can be described as performing an iterative calculation for the root of a polynomial $p(x)$ of order n by

$$x_{k+1} = x_k - a \tag{6}$$

where a is defined as

$$a = \frac{n}{G \pm \sqrt{(n-1)(nH - G^2)}} \tag{7}$$

and G and H are defined as

$$G = \frac{p'(x)}{p(x)}, \quad H = G^2 - \frac{p''(x)}{p(x)} \tag{8}$$

where $p'(x)$ and $p''(x)$ are the first and the second derivatives of $p(x)$ with respect to x.

The sign in (7) is chosen to give the largest absolute value for the denominator. The iteration stops when the magnitude of a is smaller than some given tolerance, and thus a root is found.

Once a root is found, it can be removed and the polynomial is deflated. Further computations can then be performed in a similar manner to find the remaining roots of the polynomial until all roots have been found. The removal of known roots is rather simple. All

that is required is to replace (8) with the following ones

$$G = \frac{p'(x)}{p(x)} - \sum_{i=1}^{n_1} \frac{1}{x - r_i} \tag{9}$$

$$H = G^2 - \frac{p''(x)}{p(x)} + \sum_{i=1}^{n_1} \frac{1}{(x - r_i)^2} \tag{10}$$

assuming that r_i are the roots that have already been found, and n_1 is the number of them.

The symmetry of the roots can be exploited efficiently to further reduce the cost. Once a root is found, its symmetrical counterparts can also be removed in the same way as described above when finding the rest roots. With this trick, the efficiency can be improved by a factor of 4 in the specific problem of solving eigenvalues of Hamiltonian matrices, since the eigenvalues of a Hamiltonian matrix are symmetric with respect to both real and imaginary axes.

The remaining issue when applying Laguerre's method to a specific problem is thus how to calculate the ratios $p'(x)/p(x)$ and $p''(x)/p(x)$.

We should emphasize that here we want to avoid calculating the value of the polynomial and its derivatives, i.e. $p(x)$, $p'(x)$, $p''(x)$ directly. This is critical when applying this method to calculate roots for high order polynomials or the eigenvalue of a matrix, since eigenvalues of a matrix M correspond to the roots of the determinant polynomial, and the value of a determinant usually grows (or vanishes) exponentially and quickly it will cause floating point overflow or underflow in finite precision computations. Fortunately, and this is a key point, the computation of the ratios between the derivatives and the polynomial does not have this issue.

3.3 Solving Eigenvalues for the Extended Hamiltonian Pencil

In order to use Laguerre's method to calculate the eigenvalues of a matrix, first let's review some useful identities related to determinant. In the following, all derivatives are with respect to variable λ, e.g. $X' = \frac{dX}{d\lambda}$, if without further notice.

The first identity reveals the derivative of the determinant [18],

$$\frac{|X|'}{|X|} = \mathbf{tr}\left(X^{-1}X'\right) \tag{11}$$

where $|X|$ denotes the determinant of X and '$\mathbf{tr}$' denotes the trace of a matrix, i.e. sum of all diagonal entries.

The second derivative of the determinant is given as

$$\frac{|X|''}{|X|} = \mathbf{tr}^2\left(X^{-1}X'\right) + \mathbf{tr}\left[-\left(X^{-1}X'\right)^2 + X^{-1}X''\right] \tag{12}$$

The derivation involves (11) and the following identity

$$d\mathbf{tr}(X) = \mathbf{tr}(dX) \tag{13}$$

It is worth noticing in both (11) and (12), the left hand sides are the ratios that we want to obtain in Laguerre's method, and the right hand sides are quantities that can be calculated efficiently and stably. *There is no need to calculate the determinant itself.* This is consistent with the aforementioned avoidance of calculating the value of polynomials.

Now it is enough for us to calculate the eigenvalues of the extended Hamiltonian pencil. The characteristic polynomial of the extended Hamiltonian pencil (4) is

$$\begin{aligned} p(\lambda) &= |M - \lambda N| \\ &= \begin{vmatrix} A - \lambda I & & B \\ & -A^H - \lambda I & -C^H \\ C & B^H & D + D^H \end{vmatrix} \end{aligned} \tag{14}$$

Now let

$$P = \begin{bmatrix} A & \\ & -A^H \end{bmatrix} \tag{15}$$

$$Q = \begin{bmatrix} B \\ -C^H \end{bmatrix} \tag{16}$$

$$R = \begin{bmatrix} C & B^H \end{bmatrix} \tag{17}$$

$$S = D + D^H \tag{18}$$

Then (14) becomes

$$p(\lambda) = \begin{vmatrix} (P - \lambda I) & Q \\ R & S \end{vmatrix} \tag{19}$$

$$= |P - \lambda I| \cdot |S - R(P - \lambda I)^{-1}Q| \tag{20}$$

$$= |Y(\lambda)| \cdot |Z(\lambda)| \tag{21}$$

$$= y(\lambda)z(\lambda) \tag{22}$$

where $Y = P - \lambda I$, $Z = S - R(P - \lambda I)^{-1}Q$, and y and z are the determinants of Y, Z correspondingly.

To apply Laguerre's method, the following quantities are required to be calculated for any root candidate λ

$$\frac{p'(\lambda)}{p(\lambda)} = \frac{y'(\lambda)}{y(\lambda)} + \frac{z'(\lambda)}{z(\lambda)} \tag{23}$$

$$\frac{p''(\lambda)}{p(\lambda)} = \frac{y''}{y} + \frac{z''}{z} + 2\frac{y'}{y} \cdot \frac{z'}{z} \tag{24}$$

Applying (11) gives

$$\frac{y'}{y} = -\mathbf{tr}(Y^{-1}) \tag{25}$$

$$\frac{z'}{z} = \mathbf{tr}\left(Z^{-1}Z'\right) = -\mathbf{tr}\left(Z^{-1}RY^{-2}Q\right) \tag{26}$$

Applying (12) gives

$$\frac{y''}{y} = \mathbf{tr}^2(Y^{-1}) - \mathbf{tr}(Y^{-2}) \tag{27}$$

$$\begin{aligned} \frac{z''}{z} &= \mathbf{tr}^2\left(Z^{-1}RY^{-2}Q\right) \\ &\quad + \mathbf{tr}\left[-(Z^{-1}RY^{-2}Q)^2 - Z^{-1}RY^{-3}Q\right] \end{aligned} \tag{28}$$

Notice that the cost of (25-28) is $O(n)$, considering P is diagonal and Z is with size m, and $m \ll n$. Further improvement is possible, considering the sparsity of the matrix B.

Possible instability issues may occur if care is not taken when numerically calculating (25-28), due to the inversion of Y and Z. Matrix Y is easily handled since it is diagonal, and the inverse of it is just to calculate the inverse of each diagonal entries. Z is usually a dense matrix and in practice it could be very ill-conditioned. Fortunately Z is a small matrix with the size equal to the number of ports, thus more stable algorithms can be adopted. A good candidate for stably computing the inverse of a matrix is through SVD decomposition. The cost of SVD decomposition is $O(m^3)$ and this operation needs to be performed $O(n)$ times. This cost is usually ignorable if $m \ll n$, considering the overall cost is $O(n^2)$.

Now since all the quantities needed can be computed efficiently and stably, Laguerre's method that has been introduced in the previous section can be adopted readily to compute the eigenvalues of the extended Hamiltonian pencil.

Once eigenvalues are found, the eigenvectors corresponding to those purely imaginary eigenvalues can be computed using a standard algorithm such as inverse iteration. The number of such eigenvalues are usually small, thus this can be done without much effort.

With knowing the passivity violating eigenvalues and the corresponding eigenvectors, the rest of the passivity enforcement is similar to that in existing literature. Interested readers are referred to [7].

4. RESULTS

This section illustrates the performance of the passivity check and enforcement using the proposed algorithms. All the experiments were done with a machine with a 3.2 GHz CPU and 4GB memory.

4.1 Validity

The first example illustrates the validity of the proposed generalized Hamiltonian matrix as well as the Laguerre's method. The network to be studied is a system generated for a 3-port balun measurement data using vector fitting. The number of poles is 300. Figure 1 shows the eigenvalues of the Hamiltonian matrix defined by (3) and calculated using Matlab eig function, and correspondingly the eigenvalues of the generalized eigenvalue problem defined by (4) and calculated using the Laguerre's method proposed in this paper. The eigenvalues from both methods are on top of each other. Closer examination shows that the errors are generally smaller than 10^{-12}.

Figure 2 shows the eigenvalues of the transfer function changing with respect to the frequency for the systems before and after the passivity enforcement described in [7]. It takes 4 iterations for this problem to find a passive solution. Figure 3 shows the statistics, in terms of a histogram, of iteration count for the Laguerre's method in finding the eigenvalues of the extended Hamiltonian pencil. The relative error in the stopping criteria of Laguerre's method is set to $tol = 10^{-12}$, which is sufficiently small for identifying passivity violating eigenvalues. From the histogram it can be seen that in most cases, the algorithm converges to an eigenvalue within 15 iterations, and on average the number of iterations is 7.5. We have tested the convergence for a large variety of systems, and the mean values are very similar to this number for the same error tolerance, indicating the stability and efficiency of Laguerre's method.

4.2 Efficiency

To verify the efficiency of the proposed eigensolver introduced in Section 3, we use a set of large scale problems. As shown in Table 1, the number of poles of the tested problems n varies from 600 to 8000. The number of ports m varies from 3 to 20. The sizes of the Hamiltonian matrix and the extended Hamiltonian pencil are $2n$ and $2n + m$ respectively. We do the comparison by solving for the eigenvalues of the extended Hamiltonian pencil using the method proposed in Section 3 and solving for the eigenvalues of the regular Hamiltonian matrix using the general-purpose eigensolver from LAPACK [19].

The results are compared in Table 2, where it is shown that the proposed method possesses a 33X∼80X speed-up over a general purpose eigensolver, and the speed-up increases as the size of the problems grows. This is reasonable since the cost of using a general-purpose eigensolver is $O(n^3)$ and the cost for the proposed method is $O(n^2)$. For the largest problem where there are 8000 poles and the size of the matrix to be solved is 16000, the general-purpose eigensolver failed to proceed due to memory overflow. Another thing that is worth noticing is the convergence rate. Although the iteration number for solving different eigenvalues could vary from 4 to 20, the average iteration number is very stable–it depends only on the accuracy tolerance and not on the size of the problem.

Now we would like to compare our method with [8, 9] in an indirect way–we use the cost of the general-purpose eigensolver as a reference and compare the speed-up factors of various methods. From Table 2 it can be seen that for the problem with 2000 poles, the speed-up of the proposed method is about 40X. This is less than the maximum speed-up $147X$ shown in [9] for similar size problem, but we should mention that the speed-up in [9] tightly depends on the problem. For the worst case problem, the speed-up in [9] is only 7.5X. So we can expect that the proposed method wins for badly conditioned problems in terms of efficiency. We should emphasize again that the methods in [8, 9] only solve for a subset of the eigenvalues, and they may suffer from the potential risk of missing critical ones. As a contrast, our method solves for all the eigenvalues and therefore does not have similar problems.

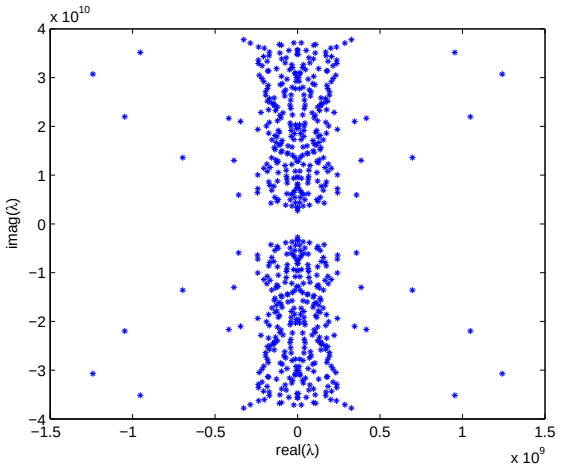

Figure 1: Eigenvalues of Hamiltonian Matrix for a System with 300 Poles

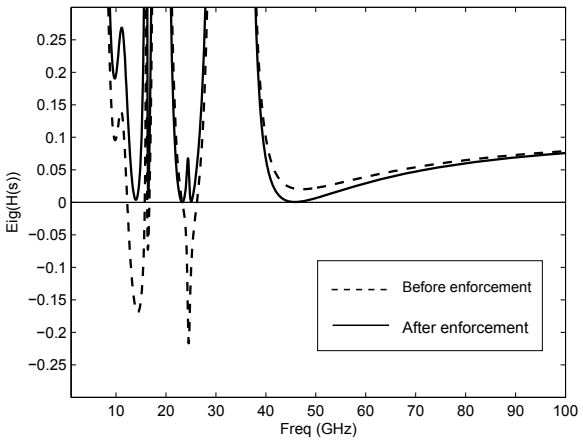

Figure 2: Eigenvalues of the transfer matrix $H(s)$ before and after passivity enforcement. Negative values indicate violation of passivity condition.

5. CONCLUSIONS

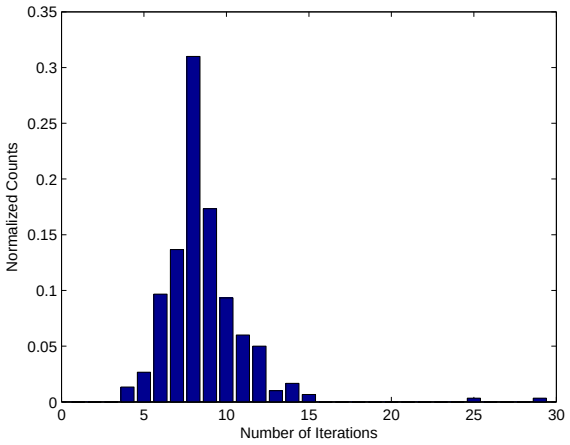

Figure 3: Statistics of Iteration for Laguerre's Method

Table 1: Summary of Test Cases

Problem	#poles	#ports	problem size
#1	600	3	1203
#2	1000	5	2005
#3	2000	10	4010
#4	4000	20	8020
#5	1200	3	2403
#6	2000	5	4005
#7	4000	10	8010
#8	8000	20	16020

In this paper, we have proposed a new method for assessing and enforcing the passivity of a linear system generated via rational or vector fitting. The new method is based on computing eigenvalues of the extended version of the Hamiltonian matrix, termed extended Hamiltonian pencil, with exploiting the special matrix structure. A special eigensolver for the extended Hamiltonian pencil shows $O(n^2)$ complexity for typical cases in computing all the eigenvalues, thus the proposed method avoids the issues with existing iterative methods regarding the potential risk of missing important eigenvalues. Besides this advantage, the efficiency of the proposed method is in general better than existing iterative methods that compute only a subset of the eigenvalues except for some well-conditioned problems. As a limitation of the proposed method, here we require that the number of ports is much less than the dimension of the system, which prevents its usage for some applications with many ports, such as power grids.

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Table 2: Comparison of CPU time for LAPACK and this work.

Problem	#Iter	LAPACK	This work	Speed-up
#1	6	20	0.6	33X
#2	6	90	2.2	41X
#3	7	633	13	49X
#4	7	4592	95	48X
#5	6	153	2.5	61X
#6	7	624	8.7	71X
#7	7	4238	53	80X
#8	8	–	409	–

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