Adaptive Frequency Sampling using Linear Bayesian Vector Fitting

Simon De Ridder, Dirk Deschrijver, Domenico Spina, Tom Dhaene and Dries Vande Ginste

We present a novel Bayesian approach to adaptively select frequency samples to obtain a rational macromodel of device responses over a broad frequency range while performing as few electromagnetic (EM) simulations as possible. The method leverages a Bayesian approach to Vector Fitting (VF) to construct a data-driven uncertainty measure. The presented technique is demonstrated by application to a double semi-circular patch antenna and is shown to accurately and efficiently construct a rational macromodel over the frequency range of interest.

Introduction: Nowadays, computer aided design (CAD) simulations are essential tools in the design phase of modern high speed circuits, due to their increasing complexity, density and bandwidth. Since linear and passive electromagnetic (EM) systems (such as interconnections, filters, connectors) are mainly analyzed in the frequency domain, adaptive frequency sampling (AFS) schemes are of paramount importance [1, 2, 3, 4]. Indeed, simulating such systems via full-wave EM simulators is expensive, given the bandwidth needed in modern applications. AFS schemes allow one to minimize the number of required EM simulations, while simultaneously being able to describe the dynamic behavior of the system considered in an accurate way [1]. A novel macromodeling-based AFS strategy using Linear Bayesian Vector Fitting (LBVF) is proposed in this letter. It formulates the problem of computing a rational model of the frequency response of the system under study in a Bayesian framework. Numerical results confirm the accuracy and efficiency of the proposed method.

Goal statement: The goal of AFS is to construct an accurate rational model of the frequency response of the system, while performing as few (expensive) EM simulations as possible. Thus, the amount of information obtained by each EM simulation must be maximized. To achieve this, standard AFS techniques compare two or more intermediate models and add, in an ad hoc way, a new frequency sample where they disagree most, in order to reduce uncertainty [1, 2, 3, 4]. The novel proposed technique, however, uses the intrinsic uncertainty of the rational models in a Bayesian way.

Linear Bayesian Vector Fitting Framework: The use of Sanathanan-Koerner (SK) iterations for rational macromodeling of device responses has been well established as the VF method [5, 6]. In this framework, the nonlinear problem of fitting a transfer function $f(s)$ (e.g. S-parameters) with a suitable rational model is linearized by multiplying $f(s)$ with a preliminary denominator $\sigma(s)$:

$$f(s) = \frac{p(s)}{\sigma(s)} = \frac{\sum_{k=1}^{K} \frac{r_k}{s-a_k} + d}{\sum_{k=1}^{K} \frac{\widehat{r_k}}{s-a_k} + \widehat{d}}, \qquad (1)$$

where $p(s)$ is the numerator, and a_k are a set of starting poles. The linear system $\sigma(s)f(s) = p(s)$ can now be solved in a least squares sense for the residues $\widehat{r_k}$ and $\widehat{d}$ of $\sigma(s)$. Then, the zeros of $\sigma(s)$ can be computed by solving a suitable eigenvalue problem [6]. Since the zeros of $\sigma(s)$ correspond to the relocated poles of $f(s)$, this process can be iterated to convergence by replacing the a_k with these new poles. Finally, the residues in the partial fraction representation of $f(s)$ can easily be estimated via another linear system.

In the proposed LBVF framework, firstly, a final set of relocated poles is estimated using several iterations of the VF algorithm, as described above. Then, in contrast to traditional SK iteration, samples are drawn from the posterior distribution of $\widehat{r_k}$ and $\widehat{d}$, after solving the linearized pole relocation system $\sigma(s)f(s) = p(s)$ using *Bayesian* linear regression. For each of these samples, the zeros of $\sigma(s)$ and the posterior distribution of the residues of $f(s)$ are calculated using Bayesian multivariate linear regression. Finally, a set of residues is obtained by sampling the corresponding posterior distribution. Each set of the computed poles and residues describes a sample from the posterior distribution of fits to the data. We denote these samples $f^i_{\text{LBVF}}(s)$, where $i = 1, \ldots, N$ and N is the total number of samples, conditioned on the starting poles. As a result, one LBVF model consists of a distribution of rational models, from which samples can be drawn, while a traditional VF model is formed by a single set of pole/residues pairs.

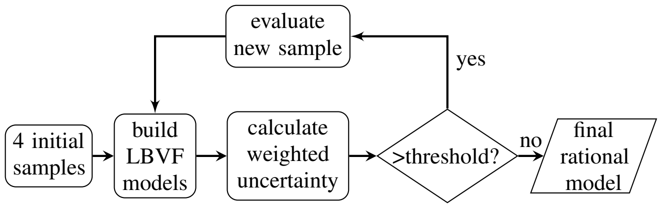

Fig. 1: *Flowchart of the proposed AFS strategy.*

A prior probability distribution on the residues of $\sigma(s)$ can be specified as a multivariate normal distribution for the residues, times an inverse Wishart distribution for the covariance, in order to yield an analytical solution for the posterior distribution. If no prior information is present, an (uninformative but improper) Jeffreys prior can be used. In that case, the mean of the posterior distribution corresponds to the solution of classical VF. Analogously, the prior for the residues of $f(s)$ can be specified as a matrix normal distribution times an inverse Wishart distribution. In this letter, we adopt uninformative priors.

Furthermore, as Bayesian linear regression allows for an analytical form of the marginal likelihood of the data, the pole relocation system can provide a likelihood of the data, conditioned only on the converged poles, and their number. Hence, the novel proposed Bayesian modeling framework offers intrinsic information on the number of poles needed to accurately describe the data. In the standard VF modeling framework, instead, the number of poles is typically chosen ad hoc or through a bottom-up strategy, where the number of poles is iteratively increased until the desired accuracy is reached.

Proposed AFS strategy: Computing the standard deviation of the aforementioned $f^i_{\text{LBVF}}(s)$ for $i = 1, \ldots, N$ gives a measure of the intrinsic model uncertainty, which naturally lends itself to an adaptive sampling scheme. Since an LBVF model is still conditioned on the number of starting poles (and their location), it is advantageous to consider several LBVF models, with different numbers of starting poles. The importance of each model can be weighted by its marginal likelihood, yielding a data-driven model selection. Hence, a more informative uncertainty measure is the weighted standard deviation of samples from multiple models, with their marginal likelihood as weights. In addition, a small Gaussian penalty is added to avoid choosing frequency points too close to each other.

The proposed adaptive sampling scheme is described in Fig. 1. An initial number of EM simulations is necessary to compute a VF model yielding the relocated poles needed by the LBVF technique, as described before. Hence, only four initial frequency points, uniformly and equidistantly spread over the considered frequency range, are chosen as initial points and LBVF models with different pole numbers are built. Note that it is not possible to use a number of poles higher than the number of frequency points considered. Then, a large number (typically > 500) of samples $f^i_{\text{LBVF}}(s)$ is drawn from each model and the corresponding uncertainty measure is calculated. If the uncertainty does not exceed a chosen threshold, the sampling stops and the best model serves as a surrogate for any other frequency. It should be noted that this threshold does not correspond to the fitting accuracy, but to a desired upper limit of the uncertainty measure. The final model is (the mean of) the LBVF model with the highest likelihood. Note that, when using uninformative priors, the mean of this model corresponds to the classical VF solution. If the threshold is surpassed, the frequency point with the maximum uncertainty is chosen and an additional EM simulation is performed for that frequency. The entire process is then iterated until the threshold is no longer exceeded. Since additional frequency points are considered, it is possible to increase the number of poles in each iteration. In order to curb computation time only the 10 highest order models are retained, while the others are discarded.

A pronounced advantage of the proposed scheme over classical AFS schemes [1, 2, 3, 4] is its capacity to sample not only where models of a different order disagree, but also where they may agree in the mean, but show a large variance. As such, this results in a more careful stopping criterion. The cost of the advantages is that for every sample of $\widehat{r_k}$

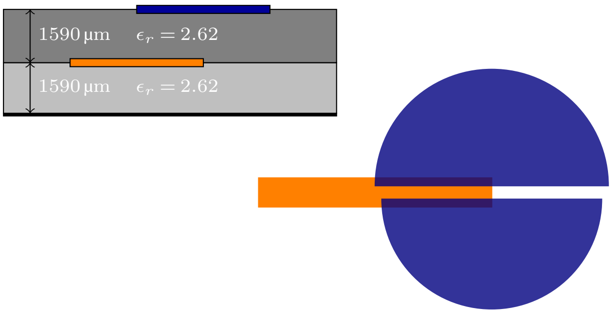

Fig. 2: *Design of the semi-circular patch antenna. Two semi-circular patches of different radii (17.5 mm and 16.5 mm, and 2 mm apart) are indirectly excited by a microstrip line of width 4.373 mm.*

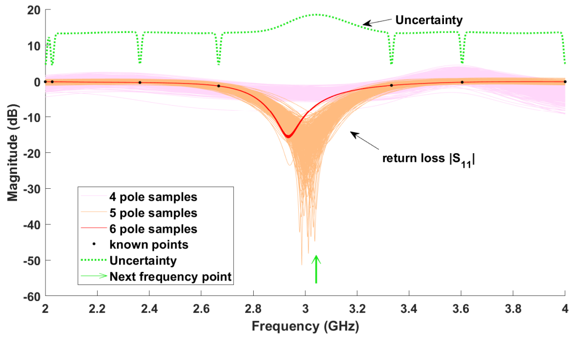

Fig. 3: *A step in the adaptive sampling scheme. The uncertainty does not conform to the vertical axis, but is rescaled and shifted for clarity.*

and $\widehat{d}$ that is drawn, an eigenvalue problem must be solved and a QR decomposition performed to find the corresponding poles and residues, though the computational cost involved is usually negligible with respect to the EM-simulation cost.

Example: The proposed method is applied to the double semi-circular patch antenna [2] shown in Fig. 2.

An example of the results obtained in one iteration of the proposed Bayesian AFS scheme is shown Fig. 3. The black points represent the known simulated points (where EM simulations have been performed). A thousand samples from LBVF models with four, five and six poles are plotted in three shades of purple, orange and red according to the likelihood of the corresponding model. Above this plot, in green, the uncertainty measure is shown (though shifted and rescaled to be discernible above the rest of the figure). The green arrow underneath indicates the maximum of the uncertainty, and thus where the next frequency point will be chosen.

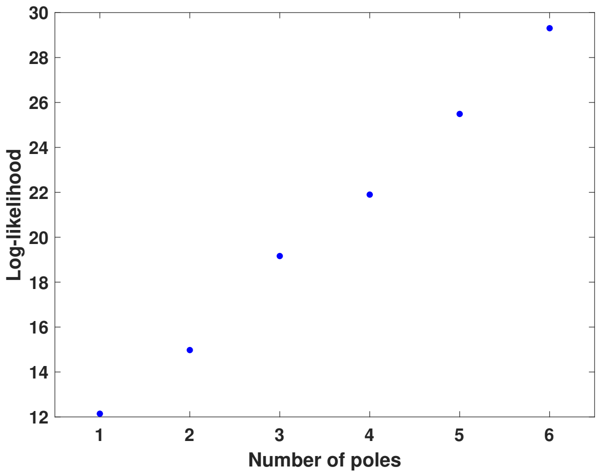

Fig. 4: *marginal log-likelihood of the data for the pole relocation system as a function of the number of poles used in each model, at the same stage as Fig. 3.*

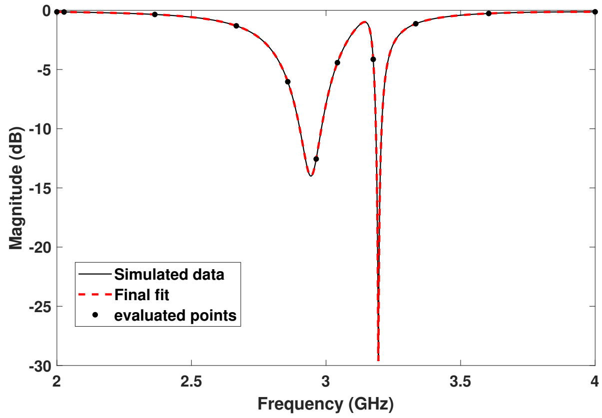

Fig. 5: *Best fit (with 10 poles) after reaching threshold.*

Fig. 4 displays the marginal log-likelihood of the pole relocation system at this step. This does not necessarily increase monotonically with the number of poles, as is the case in this intermediate stage.

In this example, a threshold of −80 dB has been chosen for the uncertainty measure. This criterion is satisfied after eleven EM simulations and the final (mean) fit is shown in Fig. 5.

The root mean square (rms) and maximum error with respect to the sampled frequency points are −138.3 dB and −130.9 dB, respectively. With respect to the antenna response calculated for 10000 frequency points in the range 2−4 GHz, the rms and maximum error are −82.1 dB and −72.8 dB, respectively. For comparison, the ad hoc method described in [2] reports a fitting error of less than −70 dB for the same example, also for eleven EM simulations.

Conclusion: This letter introduces a novel adaptive frequency sampling method, based on a Bayesian treatment of the well-established Vector Fitting method. The method makes use of samples from the posterior distribution of poles and residues to construct a probabilistic uncertainty measure. For this, it automatically weighs models of different orders by their marginal likelihood. This uncertainty measure is then used to iteratively select, in a principled way, new frequencies where additional EM simulations have to be performed.

The method is applied to an asymmetric double semi-circular patch antenna, and is shown to efficiently reach an accurate fit to the simulated data, proving its efficacy.

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