Adaptive frequency sampling using linear Bayesian vector fitting

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The authors 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
simulations as possible. The method leverages a Bayesian approach
to vector fitting 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 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, and connectors) are mainly analysed in the frequency domain,
adaptive frequency sampling (AFS) schemes are of paramount impor-
tance [1–4]. Indeed, simulating such systems through full-wave EM
simulators is expensive, given the bandwidth needed in modern appli-
cations. AFS schemes allow one to minimise the number of required
EM simulations, while simultaneously being able to describe the
dynamic behaviour of the system considered in an accurate way [1].
A novel macromodelling-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 the 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 maximised. To
achieve this, standard AFS techniques compare two or more inter-
mediate models and add, in an ad hoc way, a new frequency sample
where they disagree most, in order to reduce uncertainty [1–4]. The
novel proposed technique, however, uses the intrinsic uncertainty of
the rational models in a Bayesian way.

LBVF framework: The use of Sanathanan–Koerner (SK) iterations for
rational macromodelling of device responses has been well established
as the vector fitting (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 linearised by multiplying $f(s)$ with a pre-
liminary denominator $\sigma(s)$

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

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 a_k with these new poles. Finally, the resi-
dues in the partial fraction representation of $f(s)$ can easily be estimated
through 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 linearised
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 $f_{\mathrm{LBVF}}^i(s)$, 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/residue pairs.

A prior probability distribution on the residues of $\sigma(s)$ can be speci-
fied as a multivariate normal distribution for the residues, times an
inverse Wishart distribution for the covariance, in order to yield an
analytical solution to 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 the 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 modelling
framework offers intrinsic information on the number of poles needed to
accurately describe the data. In the standard VF modelling 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 $f_{\mathrm{LBVF}}^i(s)$ 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 choos-
ing 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 equidis-
tantly 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 $f_{\mathrm{LBVF}}^i(s)$ 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. To curb
computation time, only the ten highest order models are retained, while
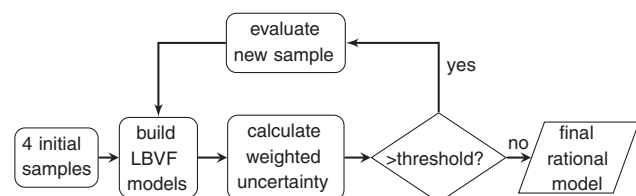the others are discarded.

Fig. 1 *Flowchart of proposed AFS strategy*

A pronounced advantage of the proposed scheme over classical AFS
schemes [1–4] 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 stop-
ping criterion. The cost of the advantages is that for every sample of
$\widehat{r_k}$ 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
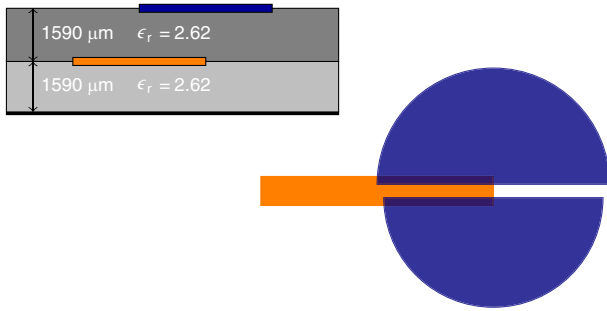with respect to the EM-simulation cost.

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

Example: The proposed method is applied to the double semi-circular patch antenna [2, 7] shown in Fig. 2.

An example of the results obtained in one iteration of the proposed Bayesian AFS scheme is shown in Fig. 3. The black points represent the known simulated points (where EM simulations have been performed). A thousand samples from the 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.
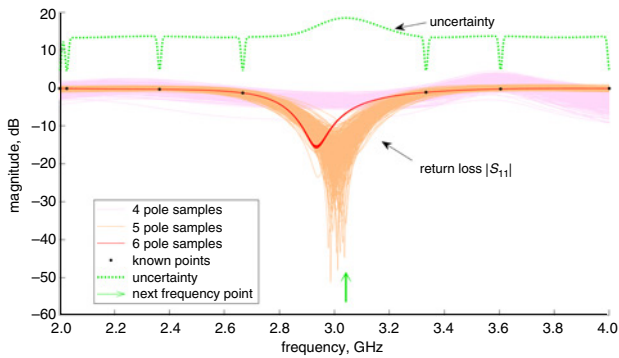

Fig. 3 *Step in adaptive sampling scheme. Uncertainty does not conform to vertical axis, but is rescaled and shifted for clarity*

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.
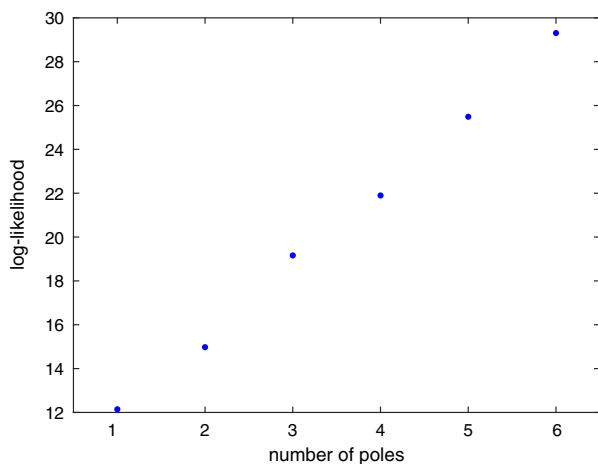

Fig. 4 *Marginal log-likelihood of data for pole relocation system as function of number of poles used in each model, at same stage as Fig. 3*

In this example, a threshold of −80 dB has been chosen for the uncertainty measure. This criterion is satisfied after 11 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 and −130.9 dB, respectively. With respect to the antenna response calculated for 10,000 frequency points in the range of 2–4 GHz, the rms and maximum error are −82.1 and −72.8 dB, respectively. For comparison, the ad hoc method described in [2] reports a fitting error of < −70 dB for the same example, also for 11 EM simulations.
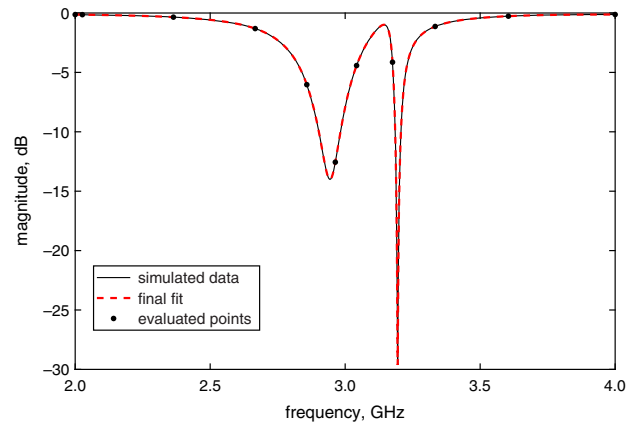

Fig. 5 *Best fit (with ten poles) after reaching threshold*

Conclusion: This Letter introduces a novel AFS method, based on a Bayesian treatment of the well-established VF 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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