Title: Public report on electro-thermal fitting and Volterra analysis
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1 Introduction

This deliverable is related to a detailed distortion analysis algorithm called Volterra on Harmonic Balance (VoHB) [1, 2]. It breaks the total nonlinear distortion given by Harmonic Balance into a vector sum of smaller components so that the dominant causes, mixing and cancelling mechanisms can be easily seen. This is done so that for each nonlinear element, a polynomial presentation is first fitted in the frequency domain. These polynomial expansions are then used in Volterra analysis to calculate different mixing mechanisms from one tone to another. Both for the fitting and the expansion, frequency domain convolution is used.

Fitting the polynomial model is one of the major problems in VoHB, as such models are not commonly available. Several approaches to build polynomial models have been found in the literature, and these are briefly reviewed here. Specifically, the current version of VoHB fits the model in the frequency domain by using simulated voltage and current spectra (see Section 3.4). The pros and cons of this fitting technique are studied in more detail, and the numerically more robust solutions are sought out.

The polynomials used in Volterra calculations have several specific features that complicate the fitting.

- First, polynomial models themselves are known to result in an ill-conditioned fitting matrix (called Vandermonde matrix), the inversion of which is sensitive to errors.
- Second, the used models are often bivariate or even multivariate – for example, the electro-thermal model of the I-V function of a transistor has 3-4 inputs: 2-3 voltages and one temperature node. The need for several input variables is especially true with devices with low output impedance, while BJTs, for example, are quite sensitive to self-heating effects.
- This leads to the third and most serious complication: in normal operating mode, the different inputs often correlate strongly – for example, the input and output voltages of a linear amplifier correlate perfectly. Unfortunately, this immensely complicates the fitting of the Ids-Vgs-Vds source if the only data we have is from in-situ simulations.
- Fourth, we are usually interested in the behavior of small distortion components that are by no means dominant when fitting the model. Hence, we may need to weight the response of the distortion components, but then we need to worry about how the weighting affects the fitting result.
- Fifth, the fitting results are also functions of the test signals, as different signal amplitude distribution functions by nature excite non-linearities in different operating regions. Hence, we need to be careful when extrapolating simulations from 1- or 2-tone simulations to modulated data.
2 A circuit example

As a typical example, the distortion analysis of a linear class AB linear amplifier is shown next. The capacitances in the LDMOS MET model are 1-dimensional and hence very easy to fit, but the Ids VCCS source is 3-dimensional, controlled by gate and drain voltages vgs and vds and the time-varying junction temperature t. Marking the polynomial coefficient of a term vgs*\textit{vds}*t\textit{c} by \textit{k}_{abc}, the 3rd-degree expansion of Ids source can be written as

\[ \text{Ids} = k_{100}\text{vgs} + k_{200}\text{vgs}^2 + k_{300}\text{vgs}^3 \ldots + k_{010}\text{vds} + k_{020}\text{vds}^2 + k_{030}\text{vds}^3 \ldots + k_{110}\text{vgs*vds} + k_{210}\text{vgs}^2\text{vds} + k_{120}\text{vgs*vgs*vds}^2 \ldots + k_{001}\text{t} + k_{101}\text{vgs*}\text{t} + k_{011}\text{vds*}\text{t} \ldots \]

Here the 1st row is a function of the vgs only, 2nd of vds only, 3rd row consists of input-output cross-terms (of vgs and vds), and 4th row contains the electro-thermal terms.

In a normal linear amplifier, vgs and vds correlate strongly, making it difficult to separate which one is causing the nonlinearity. However, the output-related terms are increasingly important in modern transistors that have a low output-impedance and operate near the drain break-through where the Ids-Vds curvature is high. Hence, the output-related effects are truly needed.

To illustrate the scope of the problem, Fig.1a shows the vgs-vds trajectory in a normal 2-tone test to indicate, that in a normal operating mode we have very little data of the overall ids-vgs-vds function. Plots b and c show some approaches to employ a separate test signal in the output node to broaden the vds variability. For a while, however, we will see what can be done with the 2-tone test data.

![Figure 1. Vgs-Vds correlation in an LDMOS amplifier driven by a) a normal 2-tone test, b) a 1-tone input, 1-tone output test, c) a 2-tone input – 1-tone output test. [3]](image_url)
The 2-sided spectra of Figure 2 show the similarity of $v_{gs}$ and $v_{ds}$ in the frequency domain. Fundamental tones are normalised to equal amplitude, and also the IM3 level is pretty similar. The output node ($V_o$) has high IM2 and 2nd harmonic content. Due to capacitive coupling to the gate, the 2nd harmonic is much stronger than the low-frequency IM2 in the input node $V_i$. It is also obvious that all distortion components are relatively weak (20-30 dB below the fundamentals), which means that the fitting will be dominated by the compression/expansion of the fundamental tones.

The strength of the input-output correlation depends on the used technology. In BJTs and HBTs the base node is highly nonlinear, and is often more distorted than the output, which simplifies the fitting. In FETs all the nonlinear elements connected at the gate are capacitive, and this causes distortion at gate to be proportional to the frequency of the distortion tone. Many high-power devices are relatively slow, and the excess transit delay causes frequency dependent phase shift in the output tones, which also somewhat breaks the input-output correlation. Finally, thermal effects are strong in BJTs and HBTs, and here especially the temperature-dependent gain (i.e. $v_{be^t}$ term) may be important.

![Figure 2](image2.png)

Figure 2. Two-sided spectra of the input and output voltages ($V_{gs}$ and $V_{ds}$).

To go to extremes, Figures 3 and 4 show the correlation matrix of all up to 5th degree electrical and electro-thermal spectra in the above LDMOS amplifier. In the matrix each number corresponds to a term, 7 being $V_o$, and 22 the junction temperature $n_T$, for example, and e.g. $V_o3$ means the spectrum of a $v_o^3$ term, i.e. $V_o$ spectra in Fig.2 convolved twice by itself. From the cross-correlation plot below we notice, that the most similar model functions are the 5th-order input-output cross-terms $V_i2V_o3$ (i.e., $V_i^2 V_o^3$), $V_i3V_o2$, and $V_iV_o4$. Strong correlation can also be found between $V_i5$ and $V_o$ that correlate with all odd-order spectra, and between $V_iT$ and $V_oT$. Higher-order electro-thermal terms are even worse and most likely to be dropped, leaving just the $V_iT$ term.
Figure 3. Correlation of model functions when fitting Ids-Vgs-Vds-T function (orange means >0.9, blue low, self-correlation of diagonal elements is 1).

Figure 4 is drawn so that model functions (spectra) are added one by one, and the condition number of the model matrix is calculated at each step. Altogether, the model functions seem to correlate heavily, and e.g. the term ViVo2 raises the condition number beyond $10^8$. Obviously, we can not include all the 5$^{th}$-order terms. A typical model of the studies made so far has used the following model complexity:

- 5$^{th}$-degree model for the input vgs as the dominant and strongest nonlinearity
- 3$^{rd}$-degree model for output input-output cross terms to model the Ids-Vds curvature
- minimal self-heating effects, at minimum term ViT.

The above will be called the 5+3+3+2 model according to the degrees of input, output, cross-terms, and electro-thermal terms, respectively. Figures 3 and 4 show a full 5+5+5+5 model.
3 Existing fitting techniques

Earlier methods for fitting polynomial models to available data are studied e.g. in [1, Chapter 4]. Their properties are briefly repeated here. Before going to the actual fitting methods, we review the various effects that affect the fitting result and the required model order.

3.1 Effects affecting the fitting results

There are many things that affect the result of the polynomial fitting. These include:

- The chosen operating point. For this purpose, it is important to use the real large-signal operating point, as especially BJT’s and circuits with DC feedback from a heavily distorted node suffer from quite heavy self-biasing.
- The fitting range. It is important that the polynomial is fitted with the same range signal varies, and this is again one good reason to combine the fitting to a real large-signal simulation.
• The degree of the polynomial. Using a too low-order polynomial forces the polynomial coefficients to be heavily signal-dependent. However, the detailed analysis is usually limited to relatively low order, and in that sense it may be better to force the model to a fixed, given order as well. The 5th-order analysis currently implemented in VoHB supports quite heavy non-linearities.
• The amplitude distribution of the signal used for fitting. A 1-tone signal has a high probability of the peak amplitudes, while most modulated signal mostly dwell at the centre and have the peak values very seldom. It is shown in [1] that 1-tone signal exaggerates the nonlinearity, and it would be wise to use at least a 2-tone signal to characterise the polynomial nonlinearity.

3.2 Small-signal derivatives

Many symbolic analyses and e.g. [4] employ symbolically solved Nth-order small-signal partial derivatives of the I-V and Q-V sources. This method is often used without any large-signal analysis, which makes the estimation of the large signal operating point problematic (especially BJTs suffer from self-biasing). Further, the derivative functions are quite complicated to derive and need to be written into the device model. New versions of device model are complex and needed quickly, and hence we would like to avoid serious rewriting of the device models themselves.

3.3 Fitting using I-V data

The simplest methods to fit a polynomial to measured data $y$ is to build a Vandermonde matrix $M$ of the model functions of form $x^i$ and solve the coefficient vector $C$ from equation $MC = I$ in the least square sense.

\[
M = \begin{bmatrix}
1 & x_1 & x_1^2 & x_1^3 \\
1 & x_2 & x_2^2 & x_2^3 \\
\vdots & \vdots & \vdots & \vdots \\
1 & x_n & x_n^2 & x_n^3 \\
\end{bmatrix}
\quad C = \begin{bmatrix}
c_0 \\
c_1 \\
c_2 \\
c_3 \\
\end{bmatrix}
\quad I = \begin{bmatrix}
i_1 \\
i_2 \\
i_3 \\
i_n \\
\end{bmatrix}
\]

\[
C = (M^T \cdot M)^{-1} \cdot (M^T \cdot I)
\]

This can achieve a better large-signal fit than fixed number of derivatives in a given bias point, but now we have an additional degree of freedom to worry about: we need to know the signal amplitudes and trajectories to choose the fitting range. As a free benefit, however, we can imitate any real amplitude density distribution by proper weighting of the rows of the equations.
3.4 Frequency domain fitting

It is easier to get frequency domain than time domain data from harmonic balance. As time-domain multiplication corresponds to a frequency domain convolution, it is possible to perform the fitting also by using frequency spectra: time domain term $v^k$ can be replaced by $V_k$, where the original spectrum $V_1$ of $v(t)$ is convolved $(k-1)$ times by itself.

The frequency domain fitting brings us some new properties:

- The transit delay of the device is easily compensated by frequency dependent phase shift
- Now there is one equation per frequency, and we can choose at what frequencies we perform the fitting, and also weight a chosen frequency.
- However, the amplitude of interesting distortion components like IM3 tone is very small, and their effect to the fitting matrix is small without any additional scaling.

3.5 Utilizing the frequency conversion matrix within HB

The ultimate use of the polynomial model in VoHB is simply to calculate the frequency conversion gain from one frequency to another – this information tells us how much from IM3 distortion is down-converted from the second harmonic band, for example. The frequency conversion gains, however, are also used to find the convergence of the harmonic balance: the Jacobian of normal HB consists of a matrix that describes the transformation from one sinusoidal signal to another.

While the Jacobian is a completely free side-product of solving harmonic balance, its use is not entirely simple. First, the Jacobian is usually calculated as a sum of all VCCS connected to one node, complicating the analysis of a single non-linearity [5]. Second, the relationship between the Jacobian and the polynomial coefficients varies depending on the number of tones and harmonics. Third, the Jacobian is used only to steer the iteration, and may contain some simplifications.

The use of Jacobian for building the polynomial models was tested with a circuit with one 1-dimensional polynomial nonlinearity only. The extraction of the coefficients seemed to vary slightly from term to term, and a few percent variation (most probably due to the iterative update of the Jacobian) can be seen e.g. in k20 terms extracted from two different tones.
4 Numerical techniques for aiding the LMS fit

4.1 Chebychev polynomials

Chebychev polynomials $T_n(x)$ [6] are orthogonal polynomials that are built up by a recursion formula

$$T_{n+1}(x) = 2 \cdot x \cdot T_n(x) - T_{n-1}(x) = 2 \cdot T_1(x) \cdot T_n(x) - T_{n-1}(x)$$

When properly normalized and weighted, Chebychev polynomials are orthogonal. Even when they are not completely orthogonal, they can largely relax the numerical properties of model fitting. If a Vandermonde matrix is converted into a Chebychev polynomial base $T_0 = 1, T_1 = x, T_2 = 2x^2 - 1, T_3 = 4x^3 - 3x, \ldots$, it is usually not completely orthogonal, but the condition number of the model matrix is still considerably smaller, and hence the fitting of the coefficients is less sensitive to small numerical errors. This property is used also in practice, to speed up the adaptation of polynomial predistortion devices, for example [6].

Chebychev polynomial results into orthogonality also in the frequency domain. A one-tone input normalized to amplitude of 1 results in a fully orthogonal series of harmonic frequencies, as all lower frequency components are cancelled by the $T_{n-1}$ term. In a case of multi-tone or otherwise broader spectrum the effect is not so striking, but with carefull amplitude normalization, signals of different order can be quite well separated to different harmonic bands. This is illustrated in the following example.

Figure 5 compares a 2-tone test signal in a 5+3+3+2 model, when fitted in the frequency domain without and with Chebychev type processing ($V_{k+1} = 2\text{conv}(V_k, V_1) - V_{k-1}$). Chebychev polynomials to large extent seem to break up the correlation between $V_i1-V_i5$ (condition number of these terms alone drops from 20000 to 400). Still, the strong input-output correlation causes $V_i$ and $V_o$, and $V_i3, V_o3$, and $V_i2V_o$ to be very similar, and this maintains the total condition number of the model very high.

The conclusion is that Chebychev polynomials reduce a lot of correlation between higher-order spectra derived from the same input signal, but can not break the correlation of strongly correlated input and output voltages.
Figure 5. Comparison of models for spectral fitting. Top: Using normal polynomial functions, bottom: using Chebychev polynomial base.
4.2 Normalization and weighting

Normalization of the fitted signals usually improves the numerical properties of the fitting, and for example with the use of Chebychev polynomials it is a necessity: it inherently assumes that the input signal is limited to range from -1 to +1. In spectral fitting with Chebychev polynomials it is essential to assure, that the maximum amplitude of the higher order spectra does not increase, rather decrease slightly compared to the original spectrum.

In non-linear circuits the amplitude scaling affects the result, and the fitted parameters must naturally be de-normalized after the fitting. If the gate and drain voltages \( v_g \) and \( v_d \), the junction temperature \( t \) and the drain current \( i_d \) are normalized by dividing them by maximum values \( v_{gA}, v_{dA}, t_A, \) and \( i_{dA} \), respectively,

\[
v_d = v_d/v_{dA}; \quad v_g = v_g/v_{gA}; \quad t = t/t_A; \quad i_d = i_d/i_{dA};
\]

then the fitted polynomial coefficients must be scaled, too. For a term

\[
p(i,j) = k_{ij}*(v_g^i)*(v_d^j)
\]

must correct the polynomial coefficient by scaling it as

\[
k_{ij} = k_{ij} / (v_{gA}^i * v_{dA}^j)
\]

Equation-wise weighting is another possibility. With time-domain i-v data pairs this gives a possibility to imitate a given amplitude density function: by weighting the points near the operating point we get a situation that resembles the real input drive better than evenly distributed data points. In the spectral fitting, each equation corresponds to a built-up of a given tone, and by equation-wise weighting we can increase the importance of a given tone. For example, we can remove the highest harmonics altogether from the LMS fit, or increase the weight of the IM3 tones. This may be needed, as the LMS solution essentially calculates the total power of each spectra, and this is heavily dominated by the fundamental tones (and their expansion or compression), while IM3 tones almost never contribute more than 1% to the total power. In the examples used, IM3 and IM2 tones have been weighted by multiplying these equations by a factor of 5-60.

Figures 6 and 7 show the fitting results of the Ids-Vgs-Vds-T model, when the equations are not weighted and then weighted. Most clearly the effect is seen in the error plots (real minus fitted) in lower-left corner. When no weighting is applied, the relative error of IM3 and IM5 tones is -20 dB (1:10), while by weighting these tones in the fitting process it can be forced below – 50 dB. We will return to curvature seen the top Ids-Vds plots in the next section.
Figure 6. Fitting results of the $I_{ds}$-$V_{gs}$-$V_{ds}$ function, with no equation-wise scaling. Top plot $I_{ds}$-$V_{ds}$ (vertical $I_{ds}$, horizontal $V_{ds}$), center $I_{ds}$ mag and phase spectra, bottom fitting error mag and phase spectra.
As seen from Figures 6 and 7, one of most attractive features of the spectral fitting is that one can decide which tones are modeled accurately. With sufficient number of parameters the precision can be improved arbitrarily. However, we need to consider if the resulting model is physically meaningful, and this will be studied in Section 4.5.
4.3 Use of QR factoring, pseudoinverse, etc.

LMS solutions are seldom sought by plain matrix inversion, but more advanced matrix operations are usually used. QR factorization and Moore-Penrose pseudoinverse techniques have been experimented here. The orthogonalization done by these techniques is important when dealing with limited numerical precision. However, in the tests made with matlab (employing double-precision floating point numbers and virtually noise-free input data), very little difference was seen between the techniques.

4.4 Recognizing a bad fit

With the statistical F-test outlined e.g. in [8] (using ANOVA techniques from statistics) one can verify if the change in the sum-square error due to one added or removed term is significant or not. The following, simplified code does the following: the error of the estimate is used to calculate the sum-square value of the fitting error. When multiplied by $\text{MMI} = \text{inv}(M'*M)$ where $M$ is the matrix of model basis functions, we get matrix $\hat{V}$, whose diagonals directly give the variance of each fitted parameter. The value $\text{rel}(i)$ is the ratio of the fitted parameter divided by corresponding std deviation, and a threshold of 3.0, for example, can be used to judge if a fitted parameter is significant or not.

```matlab
MMI = inv(M'*M); % c contains fitted coeff for basis functions in M
est = M*c; err = I-est; % fitted estimate and fitting error
SSR = err'*err;
[mx,nx] = size(M1); m_n = mx-nx; % degrees of freedom
sig_2 = SSR/m_n; % estimate to sigma^2
V = sig_2*MMI; sig = []; rel = [];
for i=1:length(c)
    sig(i) = sqrt(abs(V(i,i)));
    rel(i) = abs(c(i)/sig(i));
end
```

The above method can be automated so that after the first full fit, insignificant model functions are removed and the model is re-fitted. When testing this manually it was found out that, unfortunately, it does not automatically guarantee that the model would be physically meaningful, as described next.

The main fitting problem in the above drain current model is that although the input-output cross-mixing results are important, these correlate heavily and are difficult to separate from purely input or output related non-linearities. Hence, a poor value-to-deviation ratio does not mean that the effect would be insignificant, but with the data available it can not be separated from other effects.

Such a situation often results in an over-trained fit that has several very large but mutually canceling cross-product terms that are not physically meaningful or even possible. Mathematically speaking, the model order is higher than the data supports.
A graphical method for verifying the physical correctness of the model is simply to plot the fitted function over a slightly larger range than used for the fitting. This is illustrated in Fig. 8, where Ids-Vds curves are plotted, when fitted using the three characterization setups shown in Figure 1. The model should follow the shape of the full Ids model (high output impedance with very weak curvature), and all the models seem to fit nicely between the two straight lines, that show the limits of the trajectory of input data for setup A. Outside this region, curve A (corresponding to a input-driven 2-tone setup with very narrow input-output trajectory) bends heavily, departing seriously from the shape of the physically motivated I-V curve. This results in excess input-output mixing gains, and hence it also overestimates the significance of these effects. Curves B and C behave a bit better, as more VDS data was available for the fitting. The same effect is seen in Figs. 6 and 7: the Ids-Vds curves have some non-physical curvature.

The problem caused by heavily correlating control signals was eventually solved by AWR-APLAC propriety technique that allows to modify the characterization signals of sources that are found to be hard to fit otherwise.

5 Main results and conclusions

The ease or difficulty of the fit depends on the underlying circuit. HBT VBIC models have been very easy to fit, but the LDMOS amplifier used as an example has such a high correlation between input and output signal that it is already quite difficult to fit properly.

The input-output correlation can always be broken by employing a separate characterisation setup with a non-correlated test signal at the output. However, whenever possible we would like to avoid this and use only the data available from the underlying HB simulation. To improve fitting in such a situation, various mathematical techniques were experimented, but none alone proved to be fool-proof. The problem compared to normal principal component analysis is, that due to physical reasons we are interested in a given set of functions and would not like to alter them. Hence, eliminating e.g. the
output–related effects is equivalent of saying that these do not exist, while the truth is that they can not be detected from the data available.

The most promising techniques experimented were the following:

- **Re-shaping the model functions.** Chebychev-like expansion seems to break the correlation of the higher-order spectra of one input signal, and the fitted Chebychev base is relatively easy to convert back to polynomials. However, this does not solve the input-output correlation problem.
- **Calculating the conversion gains from the frequency conversion Jacobian looks tempting, but also it suffers from the limited data provided by heavily correlated control signal.**
- **So far the most reliable solution seems to de-correlate the controlling signals of a poorly fitting VCCS.** In APLAC this can be done for a single VCCS by driving it separately with a new set of excitations, and this was eventually chosen for the implementation (see [9]).

Regarding the self-heating effects, the following issues need to be remembered: The original device model needs to be able to calculate thermally-induced distortion – otherwise it is pointless to calculate its portion in the total distortion. Also, one needs to take care that we do not unnecessarily complicate the fitting of the polynomial mixing gains by too many electro-thermal terms.

The minimum requirement for electro-thermal distortion simulations is that the original device model calculates real-time self-heating and has a proper model for the thermal impedance, that low-pass filters the thermal fluctuations. Unfortunately, many device models use the self-heating only for setting the bias point, and the bandwidth of the thermal network is so narrow, that no thermally-induced distortion is visible. Hence, the thermal impedance model necessarily needs to have a multi-pole response that allows realistic amount of fast temperature variations in the sub-MHz range.

Inclusion of the thermal effects in the polynomial model further complicates the fitting, as many of the terms seem to correlate strongly. The dominant and hence most obvious term to be included in the polynomial model is $V_i T$, which describes the thermally induced gain variations.

Thermally induced gain variations are very often compensated by a proper biasing circuitry, and this leads us to the third problem: also the thermal coupling between the strongly heating device and the temperature sensing component in the biasing network needs to be modelled correctly. Tight and broadband coupling can compensate some nonlinear effects, while slow heat transfer corrects the DC bias, but leaves room for distortion caused by rapid thermal fluctuations.
6 Summary

The VoHB analysis needs polynomial models to calculate mixing gains from one tone to another. The techniques for fitting polynomials are reviewed, concentrating on the spectral fitting technique employed in the VoHB prototype.

Various numerical methods were presented and tested, but none of them fully avoids the problem of heavily correlating input variables. Hence, as a brute-force solution one can limit the model order so that the input may be up to 5\textsuperscript{th}-degree, while output, input-output, and temperature related terms are to at most 3\textsuperscript{rd}-degree terms. Some diagnostic measures to aid the model order reduction were experimented.

Inclusion of electro-thermal effects complicates the fitting process, but not intolerably. However, it is vitally important to ensure that the electro-thermal modeling in general is sufficient. In many devices the bandwidth of the thermal impedance is extremely narrow, in which case there is no ac temperature variations and no thermally induced distortion, either.

7 References