Comment on “Benchmarking Compressed Sensing, Super-Resolution, and Filter Diagonalization”

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In a recent paper [Int. J. Quant. Chem. (2016) DOI: 10.1002/qua.25144] Markovich, Blau, Sanders, and Aspuru-Guzik presented a numerical evaluation and comparison of three methods, Compressed Sensing (CS), Super-Resolution (SR), and Filter Diagonalization (FDM), on their ability of “recovering information” from time signals, concluding that CS and RS outperform FDM. We argue that this comparison is invalid for the following reasons. FDM is a well established method designed for solving the harmonic inversion problem or, similarly, for the problem of spectral estimation, and as such should be applied only to problems of this kind. The authors incorrectly assume that the problem of data fitting is equivalent to the spectral estimation problem, regardless of what parametric form is used, and, consequently, in all five numerical examples FDM is applied to the wrong problem. Moreover, the authors’ implementation of FDM turned out to be incorrect, leading to extremely bad results, caused by numerical instabilities. As we demonstrate here, if implemented correctly, FDM could still be used for fitting the data, at least for the time signals composed of damped sinusoids, resulting in superior performance. In addition, we show that the published article is full of inaccuracies, mistakes and incorrect statements.

Given a (generally complex-valued) time signal sampled on an equidistant time grid \( f_n := f(n\tau) \), the Filter Diagonalization Method (FDM) is designed to solve the Harmonic Inversion Problem (HIP),

\[
\sum_{j=1}^{K} \lambda_j u_j^n = f_n, \quad (n = 0, \ldots, N - 1),
\]

for the unknown (generally complex) amplitudes \( \lambda_j \) and poles \( u_j \equiv e^{-i\tau_\omega_0 \gamma_j} \), where \( \omega_j \) are frequencies and \( \gamma_j \) are the decay parameters. (It is usually assumed that all \( \gamma_j \geq 0 \), so that the time signal does not increase exponentially with \( n \).)

In FDM the seemingly nonlinear fitting problem \([1]\) is solved by mapping it to a generalized eigenvalue problem with data matrices defined by the sequence \( \{f_n\} \). If the condition (the information uncertainty principle)

\[
N \geq 2K
\]

is satisfied with exact arithmetics, then FDM provides the exact solution of HIP \([1]\). To a certain extent, this property of FDM is shared with other linear algebraic methods (Linear Regression, Linear Prediction, Matrix Pencil, etc.), with the differences buried in the details. From a numerical/algorismic perspective, FDM is perhaps the best such method that combines numerical efficiency with robustness and accuracy, and as such demonstrates nearly optimal performance. One important and distinct feature of FDM is the use of a Fourier basis, which allows for the reduction of a large and often ill-conditioned generalized eigenvalue problem to a set of small and well-conditioned problems, effectively reducing the global parametric fit \([1]\) to a local spectral analysis. Consequently, in practice condition \([2]\) holds in a weak sense, especially for large data sets, when only local spectral analysis can be performed, in which case it reads as

\[
N \geq 4\pi \rho / \tau,
\]

where \( \rho \) is the local density of states (i.e., the density of frequencies \( \omega_j \)).

Consider the infinite-time discrete Fourier transform (FT) of the time signal \( f_n \) satisfying Eq. \([1]\)

\[
I(\omega) := \tau \sum_{n=0}^{\infty} f_n z^{-n} = \tau \sum_{j} \frac{\lambda_j}{1 - u_j / z}; \quad (z := e^{-i\tau \omega})
\]

This function of frequency has peaks centered at \( \omega = \omega_j \) with amplitudes given by \( \lambda_j \), and as such provides the information related to the “line list” \( \{\lambda_j, u_j\} \). (Note also that for a “phased” signal, e.g., assuming all the amplitudes \( \lambda_j \) being real, the absorption mode spectrum, \( \text{Re}\ I(\omega) \), has line shapes superior to those of the absolute value spectrum \(|I(\omega)|\).) Consequently, the parametric fit problem \([1]\) is related to the spectral estimation problem, i.e., given a finite sequence \( \{f_n\} \) (\( n = 0, \ldots, N - 1 \)) estimate its infinite-time FT \( I(\omega) \).

The conventional way to estimate \( I(\omega) \) is to use the finite-time FT

\[
I^{(\text{FT})}(\omega) := \tau \sum_{n=0}^{N-1} f_n g_n z^{-n}
\]

where \( g_n \) is a suitable apodization function. As is well known, the main drawback of Eq. \([5]\) is its slow convergence with respect to the data size \( N \), often referred to as the FT uncertainty principle for the spectral resolution \( \delta \omega \) as a function of signal size:

\[
\delta \omega \sim 2\pi / N \tau.
\]

According to Eq. \([5]\) the line list determined from solving HIP \([1]\) can be used to estimate \( I(\omega) \) directly. Consequently, the FDM spectral estimate may result in high
(or even infinite) resolution (depending on how well condition (3) is satisfied), while the resolution of the finite FT spectrum is still limited by the uncertainty principle [6].

Importantly, FDM never attempts to solve the spectral estimation problem by first extrapolating the time signal \( f_n \) to longer times \( (n > N) \) followed by its Fourier transformation. In fact, the extrapolation problem is generally much harder than the problem of spectral estimation.

All of the above has been explained and demonstrated in a number of publications (see, e.g., refs. [12] to mention just a few). Of course, things become much more complicated and less straightforward when the data in question has imperfections, i.e., when the benefits from the solution of HIP (1) become unclear. In this regard we note ref [3] in which FDM performance was critically assessed by applying it to noisy data, both synthesized and experimental.

Quite surprisingly, the authors of the recent publication [2], which from now on we refer to as the Paper, managed to ignore all of the knowledge accumulated since 1997, when the FDM algorithm in its present form was first introduced [9]. It reports a study comparing three methods: Super-Resolution (SR), Compressed Sensing (CS), and FDM. The Paper is full of various inaccuracies, mistakes, and incorrect statements and assumptions, starting already in the abstract: “Signal processing techniques have been developed that use different strategies to bypass the Nyquist sampling theorem in order to recover more information than a traditional discrete Fourier transform.” In light of what we have discussed above, in the abstract and later in the Paper the authors probably mean the FT uncertainty principle [6], which is indeed the main motivation for developing various super-resolution techniques, such as FDM, while the mentioned “sampling theorem” simply refers to the relationship between the time interval \( \tau \) for a uniformly sampled data, \( f_n = f(n\tau) \), and the range of recoverable frequencies (the Nyquist range):

\[
[\omega_{\text{min}}, \omega_{\text{max}}] = [-\pi/\tau; \pi/\tau]
\] (7)

The corresponding phenomenon associated with this theorem is often referred to as “aliasing” or “folding”, and the only way to circumvent it with uniformly sampled data is to reduce the sampling time \( \tau \).

A comparison of FDM with any other signal processing technique would be meaningful only within the framework discussed above, i.e., by comparing the performance of the methods as either parameter estimators or spectral estimators. It may appear that the authors’ original intention was to carry out such a comparison, but instead they decided to solve the problem of data-fitting without addressing either HIP (1) or the spectral estimation problem. In one sentence, the Paper demonstrates that a violin (FDM) is not good for chopping vegetables. In order to justify their way to assess the performance of the three methods the authors refer to “Parseval’s theorem” (page 4), claiming that a good fit in the time domain implies a good fit in the frequency domain. This statement is incorrect. In fact, even a perfect fit of the data within a finite time interval does not solve the FT spectral estimation problem, unless a very specific parametrization, directly related to the latter is used, and FDM is designed to accomplish this goal, while neither of the five numerical examples in the Paper test the methods in question for their ability in spectral estimation.

The first numerical example is the most extreme in terms of its irrelevance to the problem of spectral estimation. It considers a Gaussian time signal (Eq. 24 in the Paper), i.e., a time signal with no spectral features. Both CS and SR then attempt to expand \( f(t) \) as a linear combination of 10,000 Gaussian basis functions with one of the basis functions being identical to \( f(t) \). Not surprisingly, the resulting fit of \( f(t) \) as a “linear combination of Gaussians” is perfect! The question is: what goal has been accomplished by fitting a single Gaussian with itself?

Interestingly, on several occasions, including the corresponding statement in the abstract, the authors try to compliment FDM on “providing the best results for Lorentzian signals”, however, their numerical examples prove the opposite: the error estimates for FDM, in all five numerical examples, are so big compared to that for CS and SR, that a logarithmic scale is required, even for the time signals exactly satisfying the form of HIP (1), for which, according to all our experience, FDM should provide numerically exact results. (Plotting the results obtained by CS and SR in the same plot with the authors’ version of the FDM results achieved only one goal: they made both SR and CS look very good, even when their errors were not small.)

On page 3 the authors describe Filter Diagonalization. Several mathematical expressions contain unrecognized symbols. Before Eq. 11, they incorrectly call the evolution operator unitary. Most of the citations in this section are incorrect. For example, the “2D filter diagonalization” was not introduced in [R. Chen, H. Guo, J. Chem. Phys. 1999, 111, 464], and “multi-resolution filter diagonalization” claimed to be introduced in [K. Aizikov, P. B. O’Conner, J. Am. Soc. Mass Spectrom. 2006, 17, 836] does not exist. The “adaptive frequency grid” was proposed in ref [2] but was not recommended in our later publications. In fact, a very simple uniform grid with spacings given by

\[
\Delta \nu = 4 \pi/(N \tau)
\] (8)
defines the Fourier basis with optimal performance (see e.g. ref. [15]). Apparently, in their implementation of FDM these authors used a frequency grid in the range of 0 to 20 kHz (or even 0 to 200kHz), while according to the Nyquist criterion (7) the maximum meaningful frequency would be \( \omega_{\text{max}} = 4095 \pi \text{ rad/s} \) (\( \tau = 1/4095 \text{ s} \)), i.e. they used the frequency range an order of magnitude larger than the correct range. (For the undersampled data (see below) the discrepancy is even greater.) Moreover, they
then attempted to use an adaptive frequency grid. We believe that this poor choice of the frequency grid defining the FT basis was the main reason for the numerical instabilities (mentioned on page 8) encountered by these authors. In light of this instability, it is unclear how they “ensured the robustness of their results” (as they mentioned on page 4).

There are many other inconsistencies and/or mistakes and/or inaccuracies in the Paper. In the remaining part of this Comment we mention the ones which are most striking.

Eq. 28 in the Paper with 20 random damped cosines

\[ f(t) = \sum_{n=1}^{20} e^{-\gamma_n t} \cos \omega_n t \quad (\text{Eq. 28 in the Paper}) \]  

(9)

is supposed to define the time signal shown in Fig. 5a of the Paper. The description of this time signal says that the frequencies \( \omega_n \) are drawn randomly from the range between 0 to 50 rad/s. Here in Fig. 1 we reproduce this time signal. By examining the plot of \( f(t) \) we find that \( f(0) = 15 \), and not 20! That is, the data shown in the Paper is not consistent with its description. The power spectrum in Fig. 5b of the Paper does have about 20 peaks, but the spectral range is [0; 2048] Hz rather than [0; 50 rad/s]. Table I lists the parameters \( \{ \omega_n, \gamma_n \} \) \((n = 1, ..., 15)\) of \( f(t) \) shown in the figure, and the maximum frequency, \( \omega_{15} = 304.95 \text{ rad/s} \), is outside of the range ([0; 50 rad/s]) indicated in the Paper. Regardless of all these inconsistencies, the time signal from Fig. 1 with the frequencies \( \omega_n \) and decays \( \gamma_n \) from the table represents an easy toy problem for our old FDM code written in Fortran 77 in 1997. (Note that the sum of 15 damped cosines corresponds to a sum of 30 damped complex exponentials.)

Here is how the authors describe their numerical protocol (page 4): “For each sparse signal processing method, we varied how many of the 4096 time points we sampled (in increments of 64) and investigated the dependence of the recovery error on the extent of undersampling.” Then later on the same page: “Because super-resolution requires a grid of equally spaced sample points, we began our analysis by examining the full signal and computing the errors. We then repeated our analysis for the signal by successively undersampling in powers of two, taking care to ensure that our sample points were always equally spaced.”

These two contradictory statements do not explain how the data was actually “undersampled”. Thus, we make a reasonable assumption and apply FDM to the signal from Fig. 1 using only 128 points, i.e., taking every 32nd point (as shown by blue dots). This corresponds to the time step \( \tau = 1/127s \) and the Nyquist range \([\omega_{\min} = -127\pi; 127\pi]\), i.e., just enough to correctly reconstruct the spectrum. A solution of the small generalized eigenvalue problem then gave exactly 30 complex frequencies and amplitudes that agreed with those in the table to many significant figures. That is, we confirmed once again, that the solution of HIP by FDM in the case of perfect Lorentzian signal is numerically exact. As expected, no numerical instability has been encountered. We then used the computed line list to construct the spectrum \( \text{Re} \{ I(\omega) \} \) as shown in Fig. 2. Moreover, nearly the same spectral estimate (not shown) is obtained by using only the first \( N = 64 \) data points (out of 128) of the same subset, although in the latter case some of the entries in the line list were not extremely accurate. Note that the FT spectrum computed using all the 4096 signal points shows some artifacts (Gibbs oscillations) around the narrow feature at \( \omega = 48.82 \text{ rad/s} \).

In conclusion, we have demonstrated that the Paper cannot be considered a valid “benchmarking” of any of the methods in question. Based on the critical mass of direct and indirect evidence described above, we conclude that the numerical implementation of FDM by these authors was done poorly, ignoring most of the “know how” accumulated in a number of publications since 1997. While FDM has already established itself as an efficient spectral estimator, both CS and RS still require a proper investigation. Note that two earlier papers by related groups of authors presented CS and RS as methods for FT spectral reconstruction of time signals using data from molecular dynamics simulations. That is, unlike the Paper these two publications were concerned with a correct problem. In ref[1] the authors concluded that CS beats FT by a factor of five and in ref[3] they gave a slightly less optimistic factor (four) by which RS beats FT. Both conclusions were made based on a single application of the method in question to irreproducible short-time data, and most importantly, with the converged spectrum unavailable. (In both cases, all of the spectra involved in the comparisons were not con-

![FIG. 1. The time signal \( f(t) \) from Fig 5a from the Paper, defined here in the caption of Table I. The 128 blue dots indicate the data points used to process \( f_n = f(n\tau) \) by FDM with \( \tau = 1/127s \).](image)
TABLE I. The frequencies $\omega_n$ and decays $\gamma_n$ (in rad/s) of the time signal, $f(t) = \sum_{n=1}^{15} e^{-\gamma_n t} \cos \omega_n t$, shown in Fig. 1.

| $\omega_n$ | 32.85 | 36.51 | 38.29 | 48.82 | 105.63 | 146.96 | 183.24 | 191.10 | 217.34 | 241.39 | 253.59 | 283.60 | 298.20 | 299.85 | 304.95 |
|-------------|-------|-------|-------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| $\gamma_n$  | 4.61  | 9.44  | 12.95 | 0.09  | 9.24   | 14.88  | 10.19  | 7.46   | 11.21  | 7.46   | 11.21  | 2.18   | 11.03  | 9.64   | 4.42   |

FIG. 2. The FT and FDM spectral estimates of $\text{Re}I(\omega)$ of the time signal $f(t)$ shown in Fig 5a in the Paper and here in Fig. 1. The FT is evaluated using the entire data set consisting of 4096 points, and the FDM spectrum (which coincides with the exact spectrum) is computed using the 128 points indicated in Fig. 1 by blue dots. The FDM spectrum using only 64 first data points (out of 128) would also be indistinguishable from the exact result if shown in this plot.

verged.) Therefore, the usefulness of either CS or SR for spectral reconstruction remains to be demonstrated.

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