Supplementary Material : Fast methods for estimating the Numerical rank of large matrices

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1. Additional Details

In this supplementary material, we give additional details on the two polynomial filters discussed in the main paper. First, we give an example to illustrate how the choice of the degree in the extend McWeeny filter method affects the inflexion point and the rank estimated. Next, we discuss some details on the practical implementation of the Chebyshev polynomial filter method. In section 4, we propose an alternate method for the threshold ε selection using multiple filters. Finally, we present some additional numerical experiments and an application from signal processing where our rank estimation methods can be useful.

2. McWeeny filter: An example

In the main paper, we discussed how the cut-off or the inflexion point of the extended McWeeny filter depends on the choice of the degree m_1. We also know that a higher degree m_1 implies a better filter (captures the relevant eigenvalues better) as depicted in figure 1 of the main paper. Here we give a small toy example to illustrate the performance of the four filters from figure 1 of the main paper. We consider a random matrix X_0 of size 25×15 and rank exactly 5 to which we add noise to obtain the matrix $X = X_0 + 0.1 \times randn(m, n)$ (matlab notation used). The 15 nonzero exact singular values after division by the largest one and squaring are :

$$1.0000,\ 0.7919,\ 0.4774,\ 0.3639,\ 0.3499,$$
$$0.0098,\ 0.0083,\ \cdots, \cdots, 0.0004.$$

The exact rank is 15 but there is a sharp drop after the fifth eigenvalue suggesting that the data we have is the result of perturbing a matrix of rank 5, as is indeed the case. The traces of $\psi(A)$ obtained for each of the cases shown in figure 1 of the main paper are :

Trace$(\Theta_{2,2}(A)) = 2.9375$, Trace$(\Theta_{2,6}(A)) = 4.4811$,
Trace$(\Theta_{2,10}(A)) = 4.8936$, Trace$(\Theta_{2,14}(A)) = 4.9991$.

The $\Theta_{2,2}$ polynomial misses the desired rank by about 2. This is because the only singular values that are moved really close to one are those close to 0.8 and higher. The cut-off here is $1/2$ and is is not adequate for this case. The second polynomial $\Theta_{2,6}$ gives slightly better result. The traces of both $\Theta_{2,10}(A)$ and $\Theta_{2,14}(A)$ are rather close to the exact value of 5. To estimate the trace, we have used the Hutchinson's trace estimator. Using just 20 random vectors, the trace of $\Theta_{2,14}(A)$ was evaluated to be 5.02 while that of $\Theta_{2,10}(A)$ was evaluated to 4.9, though these estimates show some small variance between different runs. In the main paper, we saw how the choice of m_1 affected the inflexion point and how a dichotomy method can be used to choose appropriate τ_1 and m_1 to get the ideal filter for a given threshold ε.

Though we have not analyzed the rounding error or the stability of the scheme based on Hermite polynomials, we observed that even when very high degree polynomials are used (a few hundreds) no numerical difficulties of any sort were encountered.

3. Pacticalities with Chebyshev Filters

In this section, we discuss some details on the practical implementation of the Chebyshev polynomial filter method.

Damping. When we expand discontinuous functions using Chebyshev polynomials, oscillations known as *Gibbs Phenomenon (Oscillations)* appear near the discontinuities. To suppress this behavior or limit its extent, damping multipliers are included, i.e., we replace eq. (11) in the main paper by

$$P \approx \psi_m(A) = \sum_{k=0}^{m} g_k^m \gamma_k T_k(A).$$

In effect, each γ_k is multiplied by a smoothing factor g_k^m and this factor tends to be quite small for larger k, i.e., for the highly oscillatory terms in the expansion. In the simplest case where no damping is applied we set $g_k^m = 1$. The most popular damping used in the literature is called Jackson smoothing whereby the coefficients g_k^m are given

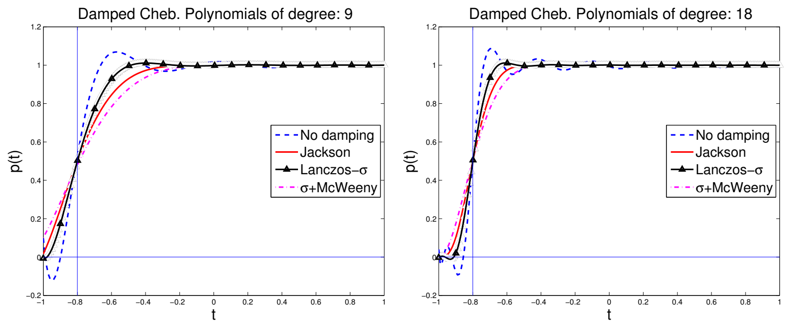

Figure 1. Four different ways of dampening Gibbs oscillations for Chebyshev approximation. All the final polynomials have the same degree (9 on the left and 18 on the right).

by the formula

$$g_k^m = \frac{\sin(k+1)\alpha_m}{(m+2)\sin(\alpha_m)} + \left(1 - \frac{k+1}{m+2}\right)\cos(k\alpha_m),$$

where $\alpha_m = \frac{\pi}{m+2}$. Details on this expression can be found in (Di Napoli et al., 2013). Another form of smoothing proposed by Lanczos (see Chap. 4 in (Lanczos, 1956)) which is referred to as σ-smoothing can also be used. It uses simpler damping coefficients called σ factors given by:

$$\sigma_0^m = 1; \quad \sigma_k^m = \frac{\sin(k\theta_m)}{k\theta_m}, \quad k = 1, \ldots, m$$

with $\theta_m = \frac{\pi}{m+1}$.

The damping factors are small for larger values of k and this has the effect of reducing the oscillations. The Jackson polynomials have a much stronger damping effect on these last terms than the Lanczos σ factors. For example the very last factors, and their approximate values for large m's, are in each case:

$$g_m^m = \frac{2\sin^2(\alpha_m)}{m+2} \approx \frac{2\pi^2}{(m+2)^3}; \qquad \sigma_m^m = \frac{\sin(\theta_m)}{m\theta_m} \approx \frac{1}{m}.$$

Jackson coefficients tend to over-damp the oscillations at the expense of sharpness of the approximation. Thus, the Lanczos smoothing can be viewed as an intermediate form of damping between no damping and Jackson damping. A comparison of the three forms of damping is shown in Figure 1. To the three forms of damping just discussed (no-damping, Jackson, σ-damping) we have added a fourth one which consists of compounding the degree 3 McWeeny filter with the Chebyshev filter. In the numerical experiments presented in the main paper and here, Lanczos σ-smoothing were used.

Recurrence. In general, since the input matrix A does not necessarily have eigenvalues between -1 and 1, we will transform A linearly into the matrix :

$$B = \frac{A - cI}{h} \qquad \text{with} \quad c = \frac{\lambda_1 + \lambda_n}{2}, \quad h = \frac{\lambda_1 - \lambda_n}{2} \tag{1}$$

whose spectrum is included in $[-1,\ 1]$. In practice, λ_1 and λ_n in the above formulas are replaced by upper and lower bounds respectively obtained from the Lanczos process, see for e.g., (Saad, 2011) for details. Note that the interval $[\varepsilon,\ \lambda_1]$ must be mapped to $[\hat{\varepsilon},\ 1]$, where $\hat{\varepsilon}$ is the linear transformation of ε using (1).

Another important practical consideration is that Chebyshev polynomials obey a three term recurrence which allows an economical computation of vectors of the form $T_k(B)v$. Indeed,

$$T_{k+1}(t) = 2tT_k(t) - T_{k-1}(t)$$

with $T_0(t) = 1, T_1(t) = t$. This results in the following iteration for computing $w_k = T_k(B)v$;

$$w_{k+1} = 2Bw_k - w_{k-1}, k = 1, 2, \ldots, m; \quad .$$

with $w_0 = v;\ w_1 = Bv$.

Remark 1 *If the input matrix X is rectangular or non symmetric, we can consider B to be of the form $B = Y^\top Y$, where Y is a linear transformation of the data matrix X using the mapping (1). This matrix B need not be computed explicitly since only matrix-vector product operations are required.*

4. Threshold selection: An alternate method

In the main paper, we presented a threshold selection method based on the spectral density plots and used the Lanczos spectroscopic method (LSM) to estimate these spectral densities. Here we present an alternate method to estimate the threshold ε using multiple filters.

Let us consider the Chebyshev polynomial rank expression given by

$$r_\varepsilon = \eta_{[\varepsilon,\lambda_1]} \approx \frac{n}{\mathrm{n_v}} \sum_{l=1}^{\mathrm{n_v}} \left[\sum_{k=0}^{m} \gamma_k (v_l)^\top T_k(A) v_l \right]. \quad (2)$$

We observe that the only terms in the above expression that depend on the choice of ε are the γ_k's and the expensive computations $(v_l)^\top T_k(A)v_l$ remain the same for any ε chosen. So, once the scalars $(v_l)^\top T_k(A)v_l$ are computed, we can define any number of filters (defined over different intervals $[a,\ b]$) with no additional cost. Hence, an alternate method for threshold selection/rank estimation is to define several filters and count the eigenvalues by setting $a = \lambda_n$ and incrementing b from λ_n to λ_1 with a small step-size. The eigenvalue counts obtained by these filters will be increasing and in the region of a gap in the spectrum, this count will remain the same. That is, the plot of the eigenvalue-counts obtained by the multiple filters will be an increasing function with plateaus in the region of gaps. We know that the threshold ε must be located at the first gap encountered this way. Thus, we can select the threshold as *the value of* b *for which the first plateau in the eigenvalue count plot occurs*, and the corresponding rank will be the difference between the matrix size and the value of the eigencount at this plateau. From another viewpoint, if we consider the differences between the eigen-counts obtained by these filters, then the threshold ε can be selected as *the value of* b *for which the eigencount difference plot becomes zero for the first time*.

As an illustration, let us consider the numerically rank deficient matrix discussed in the threshold selection section (sec. 4.2) of the main paper. The eigenvalue count plot for this matrix obtained using Chebyshev filters of degree $m = 50$ is given in the left plot of fig. 2. The step size for incrementing b was chosen to be 0.01. We see that the plot increases from 0 to 0.1 indicating the existence of a large number of smaller noise related eigenvalues. Next, there is a plateau between $0.1-0.5$. This region corresponds to the gap in the spectrum and we can select the threshold and the corresponding rank in this region. The differences between the eigencounts are plotted in the right plot of fig. 2. We see that the difference plot goes to zero at the gap, and we can choose the corresponding b value as the threshold.

Interestingly, we note that the eigencount difference plot appears similar to the spectral density plot obtained for the matrix (see right plot of fig. 2 in the main paper). Indeed the eigencount difference plot is equivalent to the spectral density plot, since the eigencount over an interval $[a,\ b]$ is just the integration of the spectral density function over the interval. So, in a sense, the two threshold selection methods are equivalent. However, in the multiple filter method, we need to select an incremental step size for b. Experiments show that the spectral density plot method performs better than the multiple filter method for threshold selection.

5. Additional Experiments

In the main paper, we presented several numerical experiments to illustrate the performances of the two rank estimation methods proposed. In this section, we give some additional numerical experimental results. We also give an application from signal processing where our rank estimation methods can be useful.

5.1. Threshold ε and the gap

In the first experiment, we examine whether the threshold ε selected by the spectral density plot method discussed in the main paper is indeed located in the gap of the matrix spectrum. We consider two matrices namely `deter3` and `dw4096` from UFL database, the matrices consdiered in rows 2 and 3 of table 1 in the main paper. Figure 3 plots their spectra and the corresponding spectral densities obtained by LSM using Chebyshev polynomial of degree $m = 50$. In the first spectrum (of deter3 matrix), there are around 7056 eigenvalues between 0 to 8 followed by a gap in the region 8 to 20. Ideally, the threshold ε should be in this gap. The DOS plot shows a high value between 0 to 8 indicating the presents of the large number of noise related eigenvalues and drops to zero near 10 depicting the gap. The threshold selected by the spectral density plot method was 10.01 (see table 1, main paper) and clearly this value is in the gap.

Similarly, in the second spectrum (third plot of figure 3, of matrix dw4096), after several smaller eigenvalues, there is a gap in the spectrum from 20 to 100. The threshold selected by the spectral density plot method was 79.13 (see table 1, main paper). These two examples not only show us that the thresholds selected are indeed in the gap of the matrix spectra, but also let us visualize the connection between the actual matrix spectra and the corresponding spectral density plots.

In the next two sections, we shall consider two applications and illustrate how the rank estimation methods based on polynomial filtering perform on these application matrices.

5.2. Matérn covariance matrices

The first application is with the Matérn covariance functions, that are commonly used in statistical analysis applications such as Machine Learning (Rasmussen & Williams, 2006). We demonstrate the performance of the two rank estimator techniques on two such covariance matrices ob-

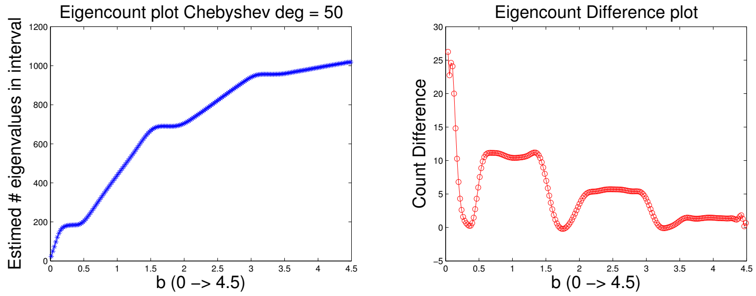

Figure 2. Eigenvalue count plot for the numerically low rank matrix by Chebyshev filters (left) and the eigencount difference plot (right).

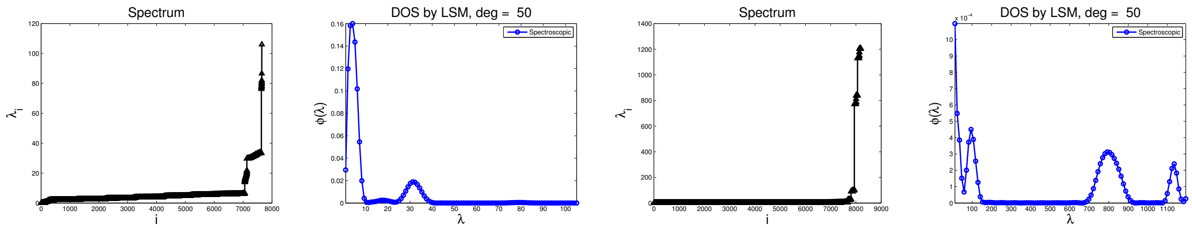

Figure 3. The sprectra and the corresponding spectral densities obtained by LSM.

tained for a 1D and a 2D regular grids[1]. It is found that such covariance matrices are numerically low rank and a low rank approximations of the matrices suffices in many applications.

First, we consider a 1D regular grid of dimension 1024 and define its covariance matrix using a Matern scaling factor $\ell = 7$ (Chen et al., 2013). The covariance matrix will be a 1024×1024 PSD matrix. The approximate rank estimated for this matrix by the extended McWeeny filter method of degree $[2, 42]$ and 30 samples was 16.74. The actual count above the threshold selected is 17. The approximate rank computed by Chebyshev filter method with degree 50 and $\mathrm{n_v} = 30$ was 17.10.

Next, we consider a 2D regular grid with dimension 32×32. The corresponding Matern covariance matrix will be of size 1024×1024. The approximate rank estimated by the extended McWeeny filter method of degree $[2, 48]$ and 30 samples was 64.21. The actual count above the threshold is 65. The approximate rank estimated by Chebyshev filter method with degree 50 and 30 samples was 68.20.

5.3. Estimation of the number of signals

The second application we will consider here comes from Signal Processing. The objective is to detect the number of signals r embedded in the noisy signals received by a collection of n sensors (equivalent to estimating the number of transmitting antennas). This can be achieved by finding the numerical rank of the corresponding sample covariance matrix of the received signals. Here we demonstrate how the rank estimation techniques discussed in the main paper can be employed to estimate the number of signals r, by computing the numerical rank of the sample output covariance matrix.

We consider $n = 1000$ element sensor array receiving $r = 8$ interference signals incident at angles $[-90^0, 90^0, -45^0, 45^0, 60^0, -30^0, 30^0, 0^0]$. The output signal $y(t)$ can be represented as

$$y(t) = \sum_{i=1}^{r} s_i(t)a_i + \eta(t) = As(t) + \eta(t), \qquad (3)$$

where $A = [a_1(\theta_1), a_2(\theta_2), \ldots, a_r(\theta_r)]$ is an $n \times r$ mixing matrix, $s(t) = [s_1(t), s_2(t), \ldots, s_r(t)]$ an $r \times 1$ signal vector (signals sent from the transmitters) and $\eta(t)$ is a white noise vector, with the noise power set to $-10DB$. The covariance matrix $C = \mathbb{E}[y(t)y(t)^\top]$ is a numerically rank deficient matrix. That is, the matrix is a noisy version of a low rank r matrix. Hence, we can employ the rank estimation methods to estimate the numerical rank of this matrix, in turn estimating the number of signals r in the received signals.

Figure 4 (left) shows the spectral density obtained using Chebyshev polynomial of degree $m = 50$ and number of samples $\mathrm{n_v} = 30$. The threshold ε was estimated by the method described in the main paper using this spectral density plot. Figure 4 (middle) shows the estimated numerical rank by the extended Mc-Weeny filter method with 30 samples. The degree of Hermite polynomial estimated was $[m_0, m_1] = [2, 44]$. The average of approximate ranks estimated over 30 sample vectors was equal to 8.07. The actual count in the interval is 8 (we know there are 8 signals).

[1]These matrices were generated using the codes available at http://press3.mcs.anl.gov/scala-gauss/.

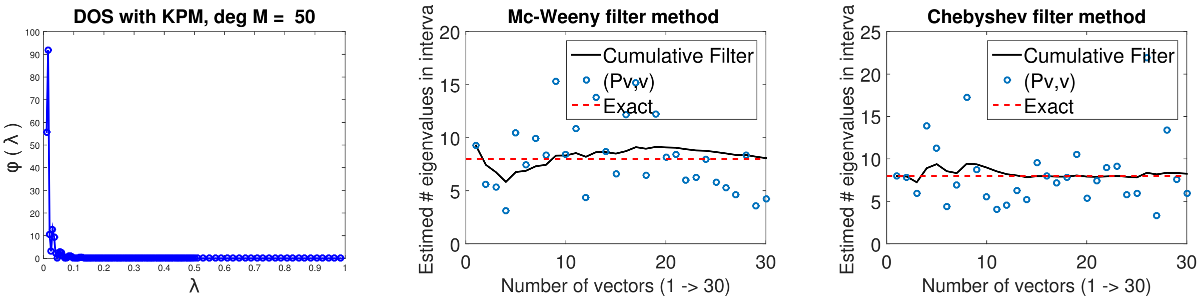

Figure 4. (Left): The spectral density found by KPM. (Middle) Approximate rank estimation by Mc-Weeny filter method for the adaptive beamforming example. (Right) Approximate rank estimation by Chebyshev filtering.

Similarly, figure 4 (right) shows the estimated numerical rank by the Chebyshev filtering method using degree $m = 50$ and $\mathrm{n_v} = 30$. The average of approximate ranks estimated over 30 sample vectors was equal to 8.25. Clearly, both the methods have accurately estimated the number of interference signals embedded in the received signals.

It is observed that the accuracy of these rank estimation techniques in the estimation of the number of signals depends on the interference signal strength and noise power used. There exists a gap between signal related eigenvalues and eigenvalues due to noise in the covariance matrix only when the signal strength is high and noise power is low. In practice the rank estimation will be affected by factors such as the angle of incidence, the number of arrays, the surrounding noise and others.

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