Improved Maximum Entropy Analysis with an Extended Search Space

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I propose an improvement to the implementation of the well established Maximum Entropy Method by departing from Bryan’s concept $^1$ of singular search space. Working with numerical data from Lattice QCD $^2$ I found that in cases where prior information is scarce and the number of data-points small, extension of the search space can dramatically improve the reconstructed spectra. The reason for the inadequacy of Bryan’s method and a remedy are discussed based on the shape of the basis functions of the search space and results from a mock data analysis. In order to adequately approach problems where an exponentially damped Kernel is used, I provide an implementation using the C/C++ language that utilizes high precision arithmetic adjustable at run-time $^3$. The LBFGS algorithm is included in the code in order to attack problems without the need to resort to a particular search space restriction.

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I. INTRODUCTION

In this paper I would like to discuss an improvement to the implementation of the Maximum Entropy Method (MEM). This algorithm allows to address the generally ill-defined problem of determining the inverse Laplace Transform from a discrete and noisy set of data-points using Bayesian inference. In the present case the bilateral Laplace transform is investigated, which connects the positive definite spectrum $\rho(\omega) \geq 0$ with the data $D(\tau)$ via an integral convolution

$$ D(\omega) = \int_{-\infty}^{\infty} K(\tau, \omega) \rho(\omega). \hspace{1cm} (1) $$

In the following I will restrict myself to the exponentially damped Kernel $K(\tau, \omega) = \exp(-\tau \omega)$.

In practice the data is obtained by an experimental apparatus or a numerical simulation and thus is known only at $N_\tau$ discrete points $D(\tau_i) = D_i$ and up to a given uncertainty given by an error matrix

$$ C_{ij} = \frac{1}{N_c(N_c-1)} \sum_{k=1}^{N_c} (D_i^k - D_i)(D_j^k - D_j), \hspace{1cm} (2) $$

where $D_i^k$ denotes one of the $N_c$ individual measurements of the data-point at $\tau_i$.

In addition, to carry out the task of determining the spectrum from data, we discretize $\rho(\omega_i) = \rho_i$ in the integral over the frequencies $\omega_i$ using $N_\omega$ points between an upper and lower cutoff $\omega_{\max}$ and $\omega_{\min}$, i.e with a spacing of $\Delta \omega = \frac{\omega_{\max} - \omega_{\min}}{N_\omega}$.

This is the first time we use prior information about our system, since $\omega_{\max}$ and $\omega_{\min}$ need to be chosen such that all relevant frequencies of the spectrum encoded in the data can be accounted for. Such prior information can often be derived from sampling theorems in the case of an experimental apparatus or the finite size of the underlying numerical simulation that produces the data-points.

Thus the fully discretized equation we are to supposed to invert reads

$$ D_i = \Delta \omega \sum_{l=1}^{N_\omega} K_{il} \rho_l = \rho_i \hspace{1cm} (3) $$

It can happen that one is faced with the situation that the number of data-points $N_\tau$ is significantly smaller than the number of points one wishes to reconstruct in the spectrum. In such cases the inversion of Eq.(3) is an inherently ill-defined problem even if perfect data were available. Imagine performing a simple $\chi^2$ fitting, i.e. finding a set of points $\rho_l$ that reproduces the data $D_i$, within the errors $\sigma_i = \sqrt{C_{ii}}$. In such as case many degenerate solutions exist, none of which is superior to any other. The reason for this is that the finite number of data-points can only constrain parts of the spectrum, but at this stage we have no way to decide which of the reconstructed features in $\rho$ these correspond to.

Let me note on another aspect, in that the problem at hand is not a linear problem as might be assumed from Eq.(3). The underlying physics required the values of $\rho_i$ to be positive definite, which corresponds to an additional constraint equation to be met. Therefore even in the case that $N_\tau = N_\omega$ one cannot directly argue for the existence of a unique solution for the inversion of Eq.(3).

To address the challenges posed by both finite accuracy and finite resolution in the data, one can introduce a regularization for the $\chi^2$ fitting procedure, which is motivated by arguments from Bayesian inference. This allows one to understand the above inversion problem as a test of hypotheses, in the sense of answering the...
question: How probable is it that a chosen test-function \( \rho_t \) is the correct spectral function, given the measured data \( D_1 \) and any other prior knowledge available about the system. I.e. one rephrases the problem in terms of probability distributions (Note that at this point \( \rho \) itself does not need to be a probability distribution).

The ingredients to our problem so far are measured data \( D_1 \) and prior knowledge \( I \). The latter is encoded in the formalism through a function \( m(\omega) \), which by definition corresponds to the correct spectral function in the absence of data. If such prior knowledge is interpreted as a sort of additional data available to us, one can construct from the joint probability function \( P(\rho, D, I(m)) \) the following expressions

\[
P(\rho, D, I(m)) = P[\rho | D, I(m)]P[D | I(m)]P[I(m)]
\]

\[
= P[D | \rho, I(m)]P[\rho | I(m)]P[I(m)]
\]

\[
= P[I(m) | \rho, D]P[D | \rho]P[\rho]
\]

\[
\vdots
\]

(7)

from which the following relation can be obtained

\[
P[\rho | D, I(m)] = \frac{P[D | \rho]P[\rho | I(m)]P[I(m) | D, \rho]}{P[D | I(m)]P[I(m)]}.
\]

(8)

In the case that our prior information is exactly known, the above term should simplify to the form usually used in the MEM

\[
P_{\text{MEM}}[\rho | D, I(m)] = \frac{P[D | \rho]P[\rho | I(m)]}{P[D | I(m)]P[I(m)]}.
\]

(9)

It is thus necessary to find the most probable spectral function, i.e. a function \( \rho_{\text{MEM}} \), which maximizes Eq. (9)

\[
\frac{\delta}{\delta \rho_t} P_{\text{MEM}}[\rho | D, I(m)] \bigg| _{\rho = \rho_{\text{MEM}}} = 0.
\]

(10)

\[
\text{II. STANDARD IMPLEMENTATION}
\]

In order for Eq. (7) to be of use, we need to state the explicit form of the factors appearing within. In the following we neglect the denominator as it does not depend on the spectral function itself. This leaves us with the so called Likelihood probability

\[
P[D | \rho] = e^{-L} = \exp \left[ - \frac{1}{2} \sum_{i,j=1}^{N_x} (D_1 - D_1^\rho)C^{-1}_{ij} (D_1 - D_1^\rho) \right],
\]

(11)

which contains nothing but the usual \( \chi^2 \) fitting term and a regulator, the so called prior probability.

\[
P[\rho | I(m)] = e^{\alpha S} = \exp \left[ \alpha \sum_{l=1}^{N_\omega} \left( \rho_1 - m_l - \rho_1 \log \left( \frac{\rho_1}{m_l} \right) \right) \right]
\]

(12)

\( S \) corresponds to the so called Shannon-Janes entropy, which assumes the spectrum \( \rho \) to be positive definite. Whereas Eq. (11) quantifies how well the current test-function \( \rho \) reproduces the measured data, Eq. (12) tells us how well it agrees with our prior knowledge. In the optimization task of Eq. (10) these two terms compete in the determination of the extremum of \( P_{\text{MEM}}[\rho | D, I(m)] \).

Since the exponential function of real numbers is a monotonous function one usually uses the negative of the argument in a numerical implementation, i.e. one attempts to find the minimum of the functional

\[
Q(\rho, D, m) = L(D, \rho) - \alpha S(m, \rho)
\]

(13)

Three comments are in order. First, one has introduced an additional parameter into the formalism, called \( \alpha \), which however is integrated out self consistently at the end of the MEM procedure [1, 4–6]. Its meaning is actually closely related to the confidence placed in the prior information, since it weights the importance of the likelihood against the entropy term. In this context it should be understood to quantify how certain we are about the information encoded by the prior function \( m \).

Secondly, the Likelihood probability \( P[D | \rho] \) does not depend on any prior information, which is why it is distinct from the quantity \( P[D | \rho, I] \) appearing in the usual formulation of the MEM [1, 4–6].

Most importantly one should note that there exist a proof [6], which shows that if we supply in addition to our measured \( N_x \) data-points additional \( N_\omega \) points of information by introducing the function \( m_\ell \), the functional \( Q(\rho, D, m) \) does possess a unique extremum in the \( N_\omega \) dimensional space of functions \( \rho_\ell \), if such a minimum exists. At this true global extremum, the likelihood \( L \) will be of comparable size to the entropy term \( \alpha S \), all of them being of order \( O(1 - 10)^1 \).

Conversely, if we use a restricted search space, e.g. in Bryan’s approach, we have to make sure that the obtained extremum is actually a global extremum and not just a local extremum in the chosen subspace.

Taken together the above statements tell us that by supplementing the measured data \( D_1 \) by some form of additional data-points, called prior information \( m_\ell \), the standard \( \chi^2 \) fitting procedure is regularized to give a unique solution. This solution is characterized by having maximum entropy in the sense of maximizing Eq. (12) and minimizing Eq. (11).

In regularizing the usual \( \chi^2 \) fitting we are now able to extract in a meaningful way those parts of the spectrum that are actually encoded by the given data. I.e. wherever the data is not capable of constraining the spectrum, our choice of prior function will select the corre-

\[1\] If in the numerical implementation the most probable spectrum still remains at values of \( L \) larger than \( \sim 100 \) the discretization in frequency space in chosen too coarse.
Bryan’s Search Space

Through the stationary condition

$$\frac{\delta Q}{\delta \rho_l} = 0$$

one is lead to the expression

$$-\alpha \log \left[ \frac{\rho_l}{m_l} \right] = \sum_{i=1}^{N_l} K_{li} \frac{dL}{d\rho_i}.$$ (15)

The fraction in the logarithm invites us to make the positive definiteness of the spectrum and the prior explicit by using the general parametrization \( \rho_l = m_l \exp[\alpha_l] \), which gives in vector notation

$$-\alpha \vec{a} = K^t \frac{d\vec{L}}{d\vec{D}}.$$ (16)

Bryan’s proposal refers to the introduction of the Singular Value Decomposition (SVD) of the transposed kernel

$$-\alpha \vec{a} = \mathbf{U} \Sigma V^t \frac{d\vec{L}}{d\vec{D}}.$$ (17)

Note that the matrix \( \mathbf{U} \) contains a full orthonormal basis of the \( \mathbb{R}^{N_{\omega}} \). \( \Sigma \) on the other hand is a diagonal matrix, which contains only \( N_{\tau} \) entries different from zero. The above (implicit) expression leads Bryan to the incorrect (as will be shown in the next section) assumption that the vector \( \vec{a} \) characterizing the global extremum always has to lie in the subspace spanned by the first \( N_{\tau} \) columns of the matrix \( \mathbf{U} \). Thus his spectral function is parametrized using the \( N_{\tau} \) values \( b_j \)

$$\rho_l = m_l \exp[\sum_j U_{lj} b_j].$$ (18)

Mock data analysis

The exponentially damped Kernel

$$K(\tau, \omega) = \exp[-\tau \omega]$$ (19)

is used to reconstruct an a priori known function \( \rho_{mock} \). A discrete mock spectrum is calculated from an analytic expression containing the sum of four Gaussian peaks with parameters as shown in Tab. I. From it a set of data-points is generated via Eq. (16) and after distorting these through Gaussian noise they are fed to the MEM code as input measurements. We use \( N_{\omega}^{mock} = 5000 \) to construct ideal data \( D^{ideal} \), to which we add Gaussian noise at each individual \( \tau \) with variance \( \delta D_{lj}^{mock} \). The strength of the disturbance is controlled by the parameter \( \eta \):

$$\delta D_{lj}^{mock} = \eta D_{lj}^{ideal}, \quad j \in \{1, \cdots, N_{\tau}\}$$ (20)

We choose as prior the function

$$m(\omega) = \frac{1}{\omega + \omega_0},$$

even though the original spectral function did not in fact contain such a behavior. Note that by using this function along the full frequency interval we explicitly acknowledge that wrong prior information is supplied. To facilitate the reconstruction the prior function is normalized such that the area under it coincides with the integral over the mock spectral function.

As discretization for the reconstruction we choose the frequency range \( \omega \in [-10, 20] \) divided into \( N_{\omega} = 1500 \) points, whereas \( \tau \in [0, 6.1] \) with \( N_{\tau} = 12 \). To capture the large dynamic range of the kernel, resulting from the inclusion of negative frequencies, the internal arithmetic is set to use 384 bits of precision. We wish to separate the question of successful reconstruction from the quality of data, hence a small noise \( \eta = 0.0001 \) is used to only slightly distort the ideal mock data.

When performing the MEM reconstruction of the mock spectrum based on Bryan’s search space, we find the following problem

- The spectral features are only poorly reproduced. Both at positive and negative frequencies peaks are missing or washed out. (see top left panel in Fig. 4 and Fig. 5)
- Even the mock data itself is not reproduced within its error-bars, i.e. the final value of \( Q \simeq 10^4 \) (see top left panel in Fig. 3)

III. INADEQUACY OF THE SVD SEARCH SPACE

In order to illustrate that restricting one’s test functions to Bryan’s singular subspace can lead to an incorrect result for the extremum of Eq. (13) and that extending the search space can remedy such artifacts, I perform a mock data analysis using the code given in [3].
FIG. 1: Reconstruction of the mock function $\rho_{\text{mock}}$ for different values of $N_{\text{ext}}$. Negative frequency structures are too small to see and are thus shown separately in Fig. 2.

FIG. 2: The negative frequency part of the reconstructions of the mock function $\rho_{\text{mock}}$ for different values of $N_{\text{ext}}$. 

We can understand this failure if we look at the available basis functions in the top left panel of Fig. 4. Based on Eq. (17), the SVD search space is solely determined by the number of data-points $N_\tau$ and the values for $\omega_{\text{max}}$ and $\omega_{\text{min}}$. Hence we are left with 12 basis functions in the present case.

For our choice of $\omega_{\text{min}} = -10$, Fig. 4 shows that the available basis functions oscillate mostly in the negative frequency range and almost no structure remains at $\omega > 0$. It is therefore very difficult to reproduce any sharply peaked spectral structure in the positive domain. Note that the mock spectrum includes peaks that are located widely apart, which prevents us from remediating the problem by just shifting the overall frequency interval towards positive frequencies.

Bryan’s prescription to select the SVD search space in general does not make any reference to our choice of $\omega_{\text{min}}$. I.e. we are allowed to set its value arbitrarily large and negative. Since his basis functions are obtained from the first $N_\tau$ columns of the SVD matrix $U$, their oscillating behavior always starts at the most negative frequency as shown in Fig. 3. Hence it is always possible to make the MEM fail within Bryan’s search space by just extending the frequency interval to larger negative values of $\omega$.

IV. EXTENSION OF THE SEARCH SPACE

The reason for the popularity of Bryan’s approach is that it apparently offers a dramatic decrease in computational cost from $N_\omega$ to $N_\tau$ degrees of freedom. However the proof on the existence and uniqueness of an MEM solution in [6] applies only to the full $\mathbb{R}^{N_\omega}$ search space. In addition, as we have seen above, the reconstruction in the SVD subspace can always be made to fail by choosing $\omega_{\text{min}}$ large and negative.

Therefore I propose to systematically enlarge the search space starting from Bryan’s SVD subspace with the prospect of locating the correct global extremum of the functional $Q(\rho, D, m)$ already with a number of $N_{\text{ext}} < N_\omega$ basis functions.

As an arbitrary choice, I decide to extend the search space by including more and more of the columns of the matrix $U$ in the parametrization of the spectrum, so that now

$$\rho_l = \exp\left[\sum_{k=1}^{N_{\text{ext}}} U^*_k b_k\right]$$

(21)

with $N_\tau < N_{\text{ext}} < N_\omega$.

The number of basis vectors required to adequately determine the global extremum can then be determined by increasing the number $N_{\text{ext}}$ until the minimal value of $Q(\rho, D, m)$ does not decrease when adding an additional basis function. In the worst case this process has to be continued until $N_{\text{ext}} = N_\omega$ since only the full set of columns of $U$ encodes a complete set of basis vectors for the $\mathbb{R}^{N_\omega}$.

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2 Keeping $\Delta\omega$ in the discretization fixed while sending $\omega_{\text{min}} \rightarrow -\infty$ guarantees that in the full search space the correct extremum can still be found.
Mock data analysis with extended search space

The improvement in the reconstruction of the mock spectrum of section III after increasing the number of basis vectors is clearly seen in the various panels of Fig.1 and Fig.2. With Bryan’s approach (in the top left panel), we are not able to capture the \( \omega < 0 \) peak at all and the positive frequency peaks are severely washed out. Increasing the number of basis vectors (their number being denoted by the subscript in \( \rho_{N_{\text{ext}}} \)) the reconstructed spectra improve even though no additional data has been included. Nevertheless in the present case of only \( N_t = 12 \) data-points, we find that only the lowest lying peak on the positive frequency side is reconstructed in a stable manner. All higher lying structures show a significant amount of variation when changing between different basis sets.

A more quantitative indicator for improvement of the method is the reduction of the value of the most probable \( Q \) in the extended space compared to Bryan’s prescription. The most probable spectral function \( \rho_{\text{MEM}}^l \) is obtained at the global extremum of the functional \( Q \), which as we can see in Fig.3, clearly lies outside the SVD space.

Small values of \( Q \) also correspond to a successful reproduction of the supplied data-set by \( D^\rho \). If we take a look at the result using Bryan’s approach in Fig.3 (the left panel of the first row), we can see that the data-points between \( 4.5 < \tau < 6 \) do not match within the small error bars. This leads to a large value of \( Q \) where \( L \gg S \). Only when we go to the extended search spaces are \( L \) and thus \( Q \) able to decrease, such that their value actually stabilizes around the same order of magnitude as \( S \).

V. CONCLUSION

The Maximum Entropy method offers a solution to the question of how to bring meaning to the ill-defined problem of inferring the values \( \rho_l \) from a noisy and finite data-set \( D_i \). Instead of maximizing only the likelihood probability with a test spectral function \( \rho_l \), one regularizes the process by including the prior probability. The function \( \rho_{\text{MEM}}^l \) that represents the extremum of (10) is hence the most probable answer in the Bayesian
Since the choice of the SVD basis functions does not depend on the choice of \(\omega_{\min}\) and their number is fixed by the supplied number of data-points, I argued that Bryan’s search space does not in general contain the correct global extremum of the functional \(Q(\rho, D, m)\). Numerical evidence was presented to support this conclusion. I thus propose to systematically expand the search space to \(N_\tau < N_{\text{ext}} < N_\omega\) dimensions until the correct global extremum of the functional has been found.

Introducing a large number of basis functions inevitably leads to the appearance of “wiggly” structures in the reconstructed spectral function \(\rho_{\text{MEM}}(\omega)\). Since they are not constrained by the data, such artifacts can be identified through a variation of the prior function. In turn, those features of \(\rho_{\text{MEM}}(\omega)\) that are reliably encoded in the data do not suffer from such variations of \(m_t\).

### A. Recipe for a consistent MEM

1. Measure the data points with as small error as possible.
2. Construct a set of prior functions that vary significantly in the region where one expects the data to encode a spectral signal.
3. Search for the global maximum of \(p[\rho|D|m]\): Start with Bryan’s search space and increase the number of basis vectors until the extremal value of \(Q(\rho)\) does not change appreciably when adding an additional basis vector.
4. For the spectral structures obtained in this way, carry out the determination of the intrinsic error according to [6].
5. Repeat from step 3 after changing to another prior function of the set chosen in step 2.
6. By identifying those spectral features that remain unchanged under the variation of the prior and that show small errors from step 4., locate the structures that are truly constrained by the data.

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### Appendix A: Efficient marginalization of \(\alpha\)

In this appendix I would like to mention a technical detail regarding the implementation of the procedure to marginalize the artificial parameter \(\alpha\) inserted in Eq. (12). To this end one calculates the maximum \(\rho^\alpha\) of \(Q(\rho, D, m, \alpha)\) for many different values of \(\alpha\) and then self consistently averages the results [1] [5] [2] using the following relation

\[
\rho_{\text{MEM}}^\alpha(\omega) = \int D\rho \left| \frac{\delta^2 L}{\delta \rho \delta \rho^\alpha} \right|_{\rho = \rho^\alpha} \sqrt{\rho_{\text{MEM}}^\alpha} P[\rho|D, I|m] \quad (A1)
\]

\[
\simeq \int d\alpha \rho^\alpha(\omega) P[\rho|D, I|m] \quad (A2)
\]

The explicit expression of \(P[\alpha|D, I|m]\) has been shown to be

\[
P[\alpha|D, I|m] \propto \exp \left[ Q[D, \rho^\alpha, I|m] \right] + \frac{1}{2} \sum_{k=0}^{N_\tau - 1} \log \left( \frac{\alpha}{\alpha + \Delta \omega \lambda_k} \right) \quad (A3)
\]

where \(\lambda_k\) are the \(N_\tau\) non-zero eigenvalues of the matrix

\[
\Lambda^\alpha_{\alpha i} = \sqrt{\rho_{\text{MEM}}^\alpha} \left| \frac{\delta^2 L}{\delta \rho \delta \rho^\alpha} \right|_{\rho = \rho^\alpha} \sqrt{\rho_{\text{MEM}}^\alpha} \quad (A4)
\]

Let us see why this symmetric \(N_\omega \times N_\omega\) matrix only contains such a small number of nonzero eigenvalues. Using the Singular Value Decomposition of \(K^t = \overline{U} \Sigma \overline{V}^t\) (\(\overline{U}\) is the \(N_\omega \times N_\omega\) sized matrix consisting of the first \(N_\tau\) columns of the matrix \(U\) in Eq. (17) and \(\Sigma\) and \(\overline{V}\) the corresponding matrices of size \(N_\tau \times N_\tau\)) we can rewrite \((\sqrt{\rho_{\text{MEM}}})^\alpha\) as

\[
\Lambda^\alpha = \sqrt{\rho_{\text{MEM}}} \overline{U} \overline{V}^t \left| \frac{\delta^2 L}{\delta \rho \delta \rho^\alpha} \right|_{\rho = \rho^\alpha} \overline{V} \overline{\Sigma} \overline{V}^t \sqrt{\rho^\alpha} \quad (A5)
\]

With the additional definition of the two symmetric \(N_\tau \times N_\tau\) matrices

\[
M = \overline{V} \overline{\Sigma} \overline{V}^t \left| \frac{\delta^2 L}{\delta \rho \delta \rho^\alpha} \right|_{\rho = \rho^\alpha} \overline{V} \overline{\Sigma} \quad (A6)
\]

\[
T = \overline{U} \overline{\Sigma} \overline{U}^t \text{diag}[\rho] \overline{U} \quad (A7)
\]

and an application of Sylvester’s determinant theorem we can rewrite the Eigenvalue equation for the matrix \(\Lambda\) as

\[
0 = \det \left[ \Lambda - \lambda_k I_{N_\omega \times N_\omega} \right] \quad (A8)
\]

\[
= \det \left[ \sqrt{\rho_{\text{MEM}}} \overline{U} \overline{V}^t \left| \frac{\delta^2 L}{\delta \rho \delta \rho^\alpha} \right|_{\rho = \rho^\alpha} \overline{V} \overline{\Sigma} \overline{V}^t \sqrt{\rho^\alpha} - \lambda_k I_{N_\omega \times N_\omega} \right] \quad (A9)
\]

\[
= \det \left[ \overline{V} \overline{U}^t \left| \frac{\delta^2 L}{\delta \rho \delta \rho^\alpha} \right|_{\rho = \rho^\alpha} \overline{V} \overline{\Sigma} \overline{V}^t \sqrt{\rho^\alpha} \overline{U} - \lambda_k I_{N_\tau \times N_\tau} \right] \quad (A10)
\]

\[
= \det \left[ MT - \lambda_k I_{N_\tau \times N_\tau} \right] \quad (A11)
\]
Here it is important to realize that the product of two symmetric matrices is not necessarily symmetric, i.e. $M \neq T M$, so that algorithms for Hermitian matrices cannot be used. Of course, since the spectrum of the original matrix $\Lambda$ is real, the matrix $M T$ does not harbor any complex eigenvalues. In addition we see that the matrix $\Lambda$ contains two factors of the Kernel $K$, which, in the case of a large dynamical range in $K$, requires arithmetic of around twice the precision compared to the rest of the procedure to yield correct values.

The reader should also be aware that the above manipulations are independent from our choice of search space. The matrix $\Lambda$ always has $N_\tau$ non-zero eigenvalues even if we choose a search space with a different dimensionality. Furthermore we note that if one artificially restricts the SVD space by taking only a number of singular values larger than a certain small value into account, one has to ensure that the corresponding eigenvalues of the Matrix $\Lambda$ that one discards are small in comparison to the values $\alpha$.

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