FOUNDATIONS
ADVANCES

Volume 75 (2019)

Supporting information for article:

Using the singular value decomposition to extract 2D correlation functions from scattering patterns

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small-angle scattering; **correlation function**; **two-dimensional Fourier transform**; **anisotropic structures**; **nanoparticles**; **singular value decomposition**; **noise filtering**

Here, we compare the results of a 2D indirect Fourier transform (IFT) using the approach for the truncated singular value decomposition (TSVD) introduced in the main manuscript, and the regularized 2D IFT from Fritz-Popovski (2013). With both approaches we derived the 2D correlation function from the scattering pattern of the aligned ellipsoids from Fig. 1(b) in the main manuscript.

With the TSVD approach the system matrix $\mathbf{K}$ (which is a $Nq \times N$ matrix, where N_q is the number of data points, and $N = N_r \cdot N_\varphi$, with N_r being the number of r-values and N_φ being the number of φ-values) is decomposed in a $N_q \times N_s$ and a $N_s \times N$ matrix as well as the vector $\mathbf{S}$ containing the N_s singular values (usually $N_s << N$, Nq). From these matrices the correlation function is computed as described in the manuscript. For the regularized 2D IFT, the two regularization matrices $\mathbf{L}_A$ and $\mathbf{L}_R$, which are both $N \times N$ matrices, are appended to the system matrix $\mathbf{K}$ ($N_q \times N$ matrix), resulting in a $(N_q + N + N) \times N$ matrix. The correlation function is then computed via a least square fit. Analysis of the computed pattern of the aligned ellipsoids (Fig. 1(b)) with both approaches results in basically identical 2D correlation functions (see Fig. 1). However, for the 2D IFT the number of data points N_q had to be reduced (here we used 6824 points instead of 30480 as done in the manuscript for the TSVD) as well as N_r (51 points instead of 101) because of memory errors (we used a normal desktop PC with 16 GB RAM). The reason for these memory errors is the significantly larger matrix $[\mathbf{K}, \mathbf{L}_R, \mathbf{L}_A]$ (which is a $(N_q+N+N) \times N$ matrix) which has to be handled, compared to the TSVD. Using the same values for N_q and N as for 2D IFT, the TSVD took around 20 s to find the solution for $N_s = 1180$. In comparison, applying a standard algorithm for the least square fit resulted in computation times of more than 250 s for the 2D IFT.

Thus, we can conclude that the TSVD can be applied for a fast determination of the underlying 2D correlation functions. Although, it has to be mentioned, that oscillations within the derived correlation function are usually present due to a restricted q-range, and which are smoothed out using the regularized IFT by Fritz-Popovski (2013). However, these oscillations could be also eliminated using the TSVD by either applying regularization schemes similar to Fritz-Popovski (2013), or by appending synthetic $\propto q^{-4}$ data in the high q-range.

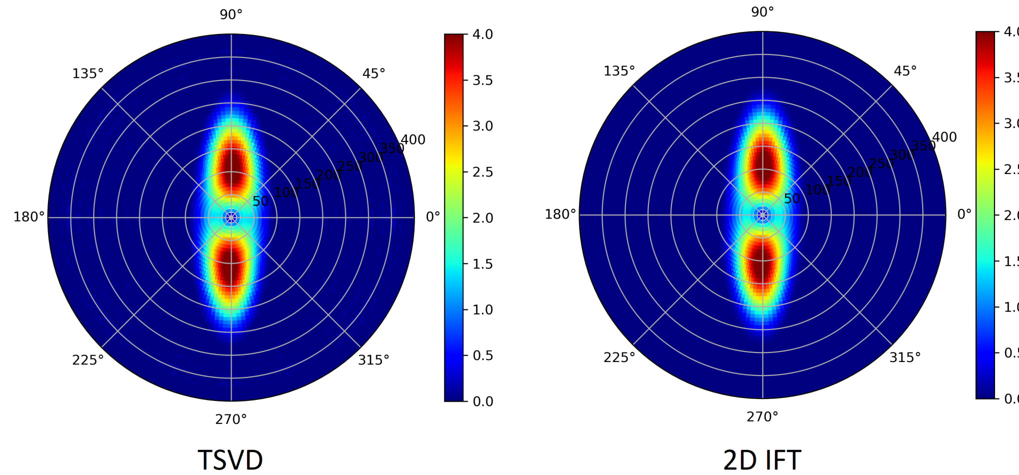

Fig. 1. Comparison of the 2D correlation functions derived from the 2D scattering pattern of the aligned elliposids (Fig. 1(b) in the main manuscript) using the TSVD and the 2D IFT proposed by Fritz-Popovski (2013).

References

Fritz-Popovski, G. (2013). *J. Appl. Crystallogr.* **46**(5), 1447–1454.