Principal component analysis applied to time-of-flight pictures of an ultracold Fermi gas

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1 Introduction

Consider a set of random variables $\boldsymbol{x} = (x_1, x_2, ..., x_n)$. For us, x_i would be any 2D (or 1D) density distribution.

Idea of principal-component analysis: Find a basis of vectors $\boldsymbol{\alpha}_i$, $i \in \{1, ..., n\}$ such that $x_j = \sum \alpha_{1i} s_i \;\; \forall j = 0, ..., n$. This basis has to maximize the variance, so maximizing

$$\mathrm{var}(\boldsymbol{\alpha}_1 \boldsymbol{x}) = \boldsymbol{\alpha}_1^T \Sigma \boldsymbol{\alpha}_1, \tag{1}$$

where $\Sigma_{ij} = \mathrm{cov}(x_i, x_j)$ is the covariance matrix of $\boldsymbol{x}$. The principal component z_1 is then given by

$$z_1 = \boldsymbol{\alpha}_1^T \boldsymbol{x}.$$

Higher order PCs are found by looking for the next vector $\boldsymbol{\alpha_i}$, $1 < i$ — uncorrelated to $\boldsymbol{\alpha_j}$, $j < i$ — that again maximizes the variance $\mathrm{var}(\boldsymbol{\alpha_i x})$. One can show that the $\boldsymbol{\alpha_i}$ are the eigenvectors of Σ [Jol02], and the variance $\mathrm{var}(\boldsymbol{\alpha_i x})$ is the corresponding eigenvalue λ_i. So by solving the eigensystem

$$\Sigma \boldsymbol{v} = \lambda \boldsymbol{v} \tag{2}$$

one obtains the principal component analysis.

Implementation Consider a discrete 1D density distribution $\boldsymbol{n} = (n_{y_0}, n_{y_1}, ..., n_{y_n})$ as an array of n random variables corresponding to the n pixels of our region of interest (ROI). Now we realize k different versions of this density distributions (e.g. taking several images for statistical averaging, or a data set with different atom numbers / temperatures), labeled as $\boldsymbol{n_k}$. Now we want to construct the covariance matrix of this data. To that end we subtract the mean value of each random variable:

$$\bar{\boldsymbol{n}} = \frac{1}{n} \sum_{i=0}^{n} \boldsymbol{n_i}, \tag{3}$$

$$\tilde{\boldsymbol{n}}_{\boldsymbol{i}} = \boldsymbol{n_i} - \bar{\boldsymbol{n}}. \tag{4}$$

Then we define the matrix $\boldsymbol{B}$ $(k \times n)$ whose columns are the $\tilde{\boldsymbol{n}}_{\boldsymbol{i}}$:

$$\boldsymbol{B} = \begin{pmatrix} \tilde{\boldsymbol{n}}_{\boldsymbol{0}}^{\mathrm{T}} & \tilde{\boldsymbol{n}}_{\boldsymbol{1}}^{\mathrm{T}} & \cdots & \tilde{\boldsymbol{n}}_{\boldsymbol{k}}^{\mathrm{T}} \end{pmatrix} \tag{5}$$

Thus each row represents k realization of one random variable. The covariance matrix is then readily obtained using for example **np.cov(B)**. The eigenvalues λ_i and eigenvectors $\boldsymbol{\alpha_i}$ can then be found using **np.linalg.eigh(np.cov(B))**.

Generally the idea is that few PCs are responsible for most of the variation in a data set. Assuming the first m PCs explain most of the variation, one can then project the original data $\tilde{\boldsymbol{n}}_{\boldsymbol{i}}$ on the subspace spanned by this subset of basis vectors.

$$\tilde{\boldsymbol{n}}_{\boldsymbol{i}}^{\boldsymbol{m}} \coloneqq \sum_{i=0}^{m} (\tilde{\boldsymbol{n}}_{\boldsymbol{i}} \cdot \boldsymbol{\alpha_i}) \boldsymbol{\alpha_i} \approx \tilde{\boldsymbol{n}}_{\boldsymbol{i}}. \tag{6}$$

2 Application: 1D atom density

We look at a density profile along the experimental $y-$direction, where $x-$ and $z-$directions are integrated out by line summing (x) and imaging (z). That way we obtain 1D-density profiles as exemplary shown in Fig. 1, with the axis indicating position along y in µm.

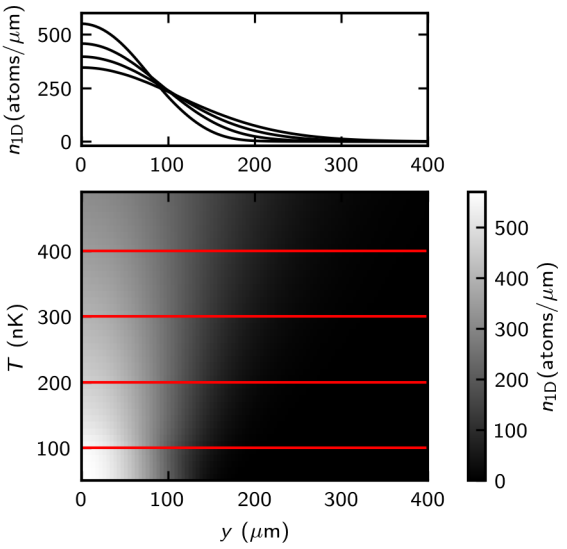

FIGURE 1: 1D density profiles along longitudinal $y-$direction (see Eq. (7)) for a cloud of 100'000 atoms at various temperatures T. The upper part shows few exemplary curve indicated as red lines in the lower plot.

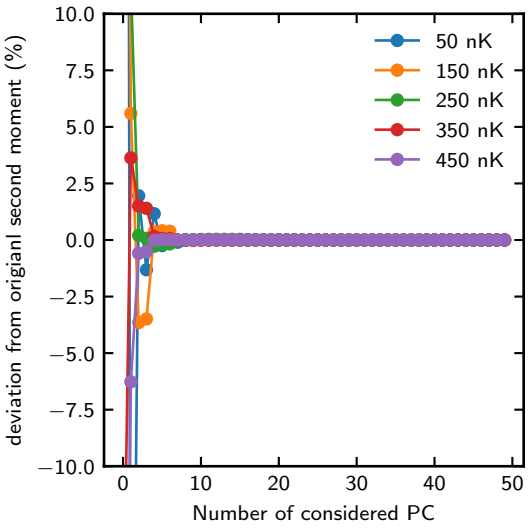

FIGURE 2: Deviation of the second moments obtained form density profiles reconstructed from a various number of principal components (see also Eq. (9)).

The ones shown in Fig. 1 are artificial profiles created from the equation in [Gua13]

$$n(y) = \frac{2\pi}{m_{\mathrm{Li}}\omega_r^2}\frac{k_{\mathrm{B}}T}{\lambda_T^3} f_p\left(q_0 - \frac{1}{2k_{\mathrm{B}}T} m_{\mathrm{Li}}\omega_y^2 y^2\right) \tag{7}$$

where m_{Li} is the mass of Lithium 6, ω_r the geometric mean of the transverse trapping frequencies ω_x and ω_z, λ_T the thermal de-Broglie wavelength, q_0 the reduced chemical potential $\mu/k_{\mathrm{B}}T$ in the trap center, and ω_y the longitudinal trap frequency. Here we varied the temperature T while keeping the atom number $N = 100'000$ fixed (so the chemical potential changes accordingly, as described by the EoS).

Performing a PCA on the data shown in Fig. 1 we find the eigenvalues shown in Fig. 3 and the according eigenvectors shown in Fig. 4. As can be seen the main structures of the profiles is given by the first few components.

We can now reduce the dimensionality and reconstruct the density profiles from the m largest principal components (see Eq. (6)). Ultimately we want to know how the value of the second moment

$$\left\langle y^2 \right\rangle = \int_{-\infty}^{\infty} \mathrm{d}y\; n(y) y^2 \tag{8}$$

changes when using an increasing number of PCs. When all principal components are included in the reconstruction, the picture should be the original, and so should be the value of the second moment (can be used as a consistency check). We define the second moment obtained form density profile reconstruction $\boldsymbol{n}^{\boldsymbol{m}} = \tilde{\boldsymbol{n}}^{\boldsymbol{m}} + \bar{\boldsymbol{n}}$ using the m larges PCs as $\langle y_m^2 \rangle$ (here we have suppressed the index i for better readability). The deviation of this second moment value (in percent) from the original value is plotted in Fig. 2:

$$\text{plotted deviation } (\%) = \left(\frac{\langle y_m^2 \rangle}{\langle y^2 \rangle} - 1\right) \cdot 100 \tag{9}$$

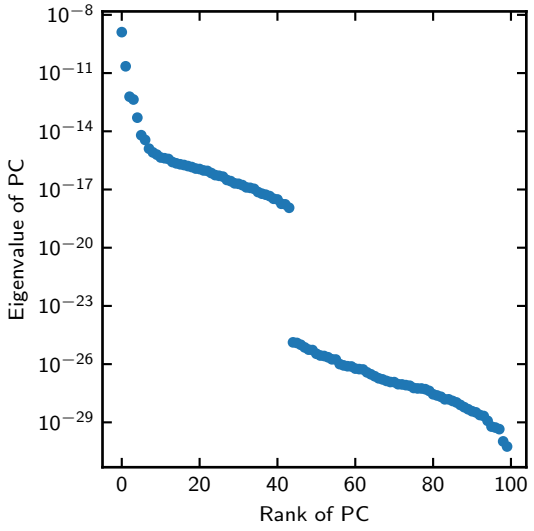

FIGURE 3: Eigenvalues of the covariance matrix, sorted in descending order.

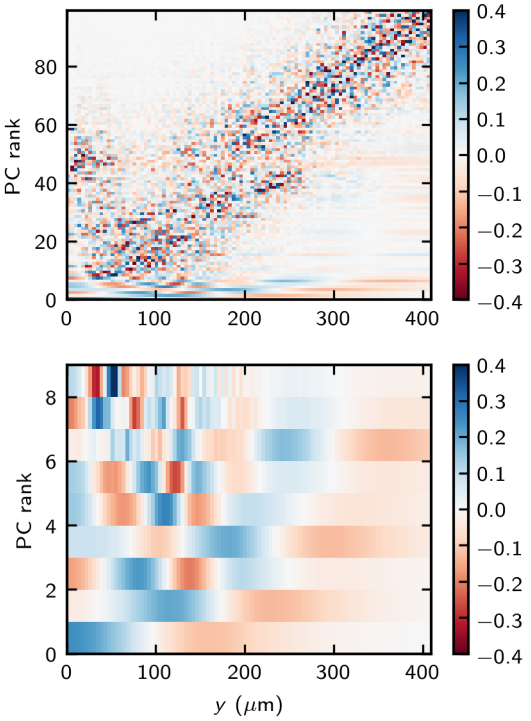

FIGURE 4: Eigenvectors of the covariance matrix. The lower part shows a zoom into the first 10 EVs.

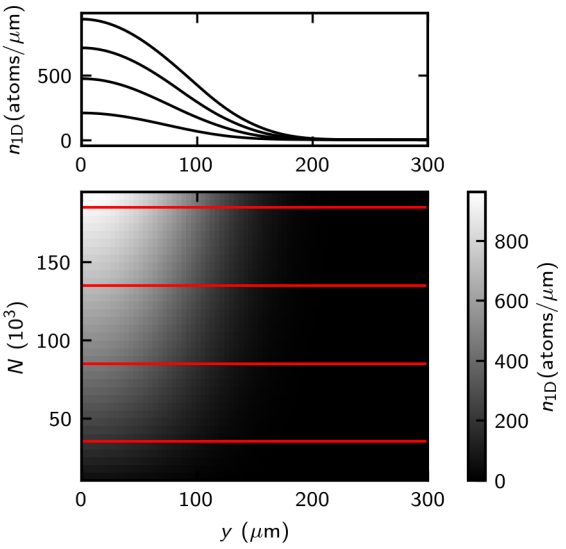

FIGURE 5: 1D density profiles along longitudinal $y-$direction (see Eq. (7)) for a cloud of temperature $T = 100\,\mathrm{nK}$ and atom numbers varying from $10^4 - 2 \cdot 10^5$ atoms. The upper part shows an exemplary curve for $T = 200\,\mathrm{nK}$. The upper part shows few exemplary curve indicated as red lines in the lower plot.

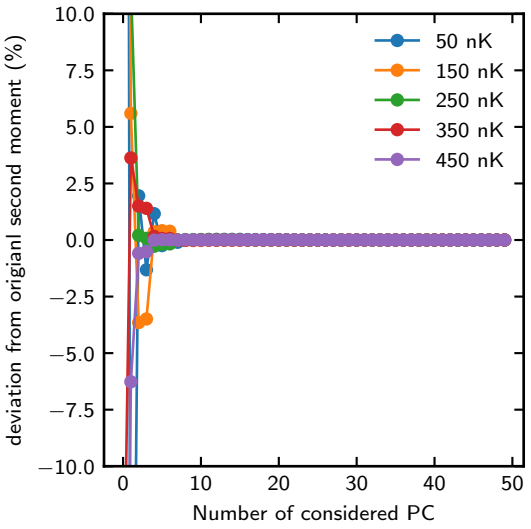

FIGURE 6: Deviation of the second moments obtained form density profiles reconstructed from a various number of principal components (see also Eq. (9)) at fixed temperature $T = 100\,\mathrm{nK}$.

The fast convergence confirms that only few PCs are required to fully describe the data and specifically the second moment.

Constant temperature We repeat the analysis while fixing the temperature to $T = 100\,\mathrm{nK}$ and varying the particle number. The density profiles are shown in Fig. 5. The results of the analysis are shown in Fig. 6, 7 and 8.

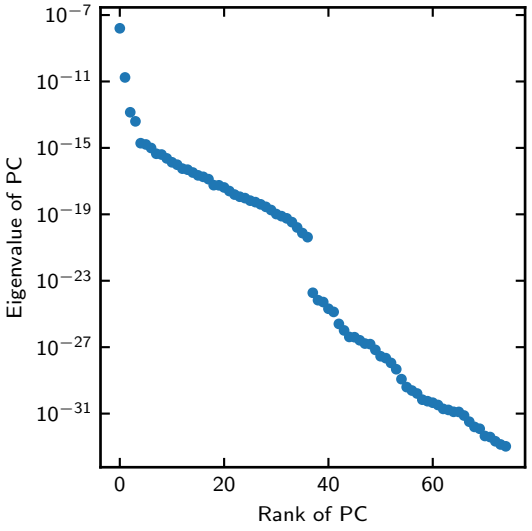

FIGURE 7: Eigenvalues of the covariance matrix, sorted in descending order.

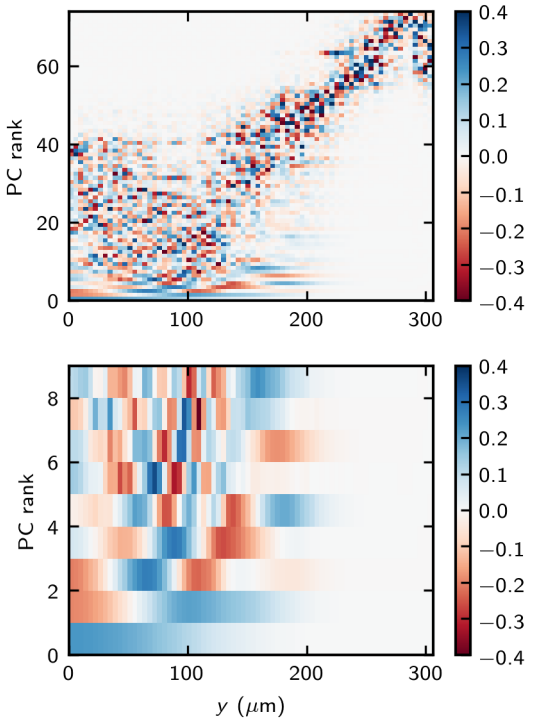

FIGURE 8: Eigenvectors of the covariance matrix. The lower part shows a zoom into the first 10 EVs.

Density profiles with noisy data Now we want to get to a situation closer to what is encountered in the experiment, namely we add random noise to our density pictures. Here the noise amplitude s_0 is quantified as fraction of the maximal signal from the density profile (the central peak). We accordingly modify the density profiles by adding this noise:

$$\boldsymbol{n} \to \boldsymbol{n} + \boldsymbol{\delta n} \tag{10}$$

where $\boldsymbol{\delta n} = s_0 \boldsymbol{s}$ and $\boldsymbol{s}$ is a vector of random numbers between -0.5 and 0.5, and s_0 indicates the magnitude of the error.

A simple repetition of PC analysis gives sobering results.

References

[Gua13] E. R. S. Guajardo, M. K. Tey, L. A. Sidorenkov, and R. Grimm, *Higher-nodal collective modes in a resonantly interacting Fermi gas*, Physical Review A **87**, 063601 (2013) (cit. on p. 3).

[Jol02] I. T. Jolliffe, *Principal Component Analysis*, en, 2nd ed., Springer Series in Statistics (Springer-Verlag, New York, 2002) (cit. on p. 2).