On feasibility of azimuthal flow studies with Principal Component Analysis

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Abstract.
It is shown that the Principal Component Analysis applied to azimuthal single-particle distributions allows to perform flow analysis in ways that are analogous to the traditional approaches based on multi-particle correlations. In particular, symmetric cumulants are considered. It is demonstrated also that statistical fluctuations due to a finite number of particles per event practically do not play a role for higher order PCA-based cumulants.

1. Introduction
Principal Component Analysis (PCA) is a method for decorrelation of multivariate data. PCA finds the most optimal basis for a given problem and thus reduces its dimensionality. Recently, it was suggested to apply PCA to heavy-ion collisions data on two-particle azimuthal correlations [1], in order to reveal hidden patterns of the collective behaviour of the hadronic medium. In [2] it was shown that PCA applied directly to single-particle azimuthal ($\phi$) distributions in A–A collisions reveals Fourier harmonics as the natural and the most optimal basis.

In the latter approach, technically, one needs to take distributions of particles in $M$ bins in each out of $N$ events, normalize them and subtract the mean, and then apply PCA to the obtained $N \times M$ matrix (see more details in [2, 3]). As an output from PCA, we have a set of orthonormal eigenvectors ($e_i$, $i = 1, ..., M$), and also a set of coefficients $\alpha_i^k$ ($k = 1, ..., N$) of PCA decomposition, such that the particle distribution in $k$-th event (denoted as $x^{(k)}$ that is a vector with $M$ elements) can be written as

$$x^{(k)} = \sum_{i=1}^{M} \alpha_i^k e_i.$$  

(1)

By construction, the first $K$ components ($K < M$) contain the most of the total variance of a dataset.

The azimuthal flow in heavy-ion collisions is typically studied using expansion of particle azimuthal probability density in a series:

$$f(\phi) = \frac{1}{2\pi} \left[ 1 + 2 \sum_{n=1}^{\infty} v_n \cos \left(n(\phi - \Psi_n)\right) \right],$$  

(2)
where \( v_n \) are the flow coefficients. As mentioned above, PCA applied to event-by-event azimuthal single-particle distributions reveals the Fourier basis, and thus coefficients of the PCA decomposition gain a definite meaning. If the decomposition (2) is applied event-by-event, values of \( \hat{v}_n \) observed in the \( k \)-th event are related to the PCA coefficients (assuming that the elliptic flow dominates, and the next is the triangular flow) as follows: 
\[
\hat{v}_2^{(k)} = \sqrt{\frac{M}{2}} \sqrt{\alpha_2^2 + \alpha_3^2}, \\
\hat{v}_3^{(k)} = \sqrt{\frac{M}{2}} \sqrt{\alpha_3^2 + \alpha_4^2},
\]
and so on.

In this paper, it is demonstrated that the coefficients of the PCA decomposition can be combined into expressions that are equivalent to the multi-particle cumulants used in the flow studies. The first observable considered in Section 2 is the flow amplitude calculated via two- and four-particle correlations. So-called symmetric cumulants that measure correlations between amplitudes of flow harmonics of different orders are studied in Section 3. It is estimated also how the statistical fluctuations contribute to the values extracted using PCA.

2. Higher-order cumulants from PCA

In flow studies, the simplest way to get an estimate for the amplitudes \( v_n \) is to use the two-particle cumulants \( c_n \{2\} \):
\[
v_n \{2\} = \sqrt{c_n \{2\}} = \sqrt{\langle v_n^2 \rangle}.
\]

It is well-known that this quantity suffers from the so called non-flow contributions coming from e.g. resonance decays and jets. Suppression of the non-flow is typically done by utilizing the multi-particle cumulants. For example, the amplitude of the \( n \)-th harmonic can be estimated from the fourth-order cumulant \( c_n \{4\} \) [4] as
\[
v_n \{4\} = \sqrt{-c_n \{4\}} = \sqrt{2\langle v_n^2 \rangle^2 - \langle v_n^4 \rangle}.
\]

We may try to adopt (3) and (4) for the flow studies with the PCA. When one deals with event-by-event particle distributions (like in the present application of the PCA), it is essential to investigate the influence of the statistical fluctuations due to a limited number of particles per event. Following the approach used, for instance, in [5,6], we denote a true amplitude of the \( n \)-th Fourier harmonic in a given event as \( v_n \), and an amplitude of the statistical noise as \( a_n \). If \( \hat{v}_n \) is the observed amplitude, extracted by PCA in a given event, projections of the corresponding flow vector on \( x \) and \( y \) axes in the transverse plane are
\[
\hat{v}_{n,x} = v_{n,x} + a_{n,x}, \quad \hat{v}_{n,y} = v_{n,y} + a_{n,y},
\]
The squares of the \( v_n \), \( a_n \) and \( \hat{v}_n \) are
\[
v_n^2 = v_{n,x}^2 + v_{n,y}^2, \quad a_n^2 = a_{n,x}^2 + a_{n,y}^2, \quad \hat{v}_n^2 = \hat{v}_{n,x}^2 + \hat{v}_{n,y}^2 = v_n^2 + a_n^2 + 2(v_{n,x}a_{n,x} + v_{n,y}a_{n,y}).
\]
After averaging (8) over events, we get
\[
\langle \hat{v}_n^2 \rangle = \langle v_n^2 \rangle + \langle a_n^2 \rangle + 2\langle v_{n,x}a_{n,x} \rangle + 2\langle v_{n,y}a_{n,y} \rangle
\]
If we assume that signal and the statistical noise are uncorrelated, the last two terms factorize:
\[
\langle v_{n,x}a_{n,x} \rangle = \langle v_{n,x} \rangle \langle a_{n,x} \rangle \quad \text{and} \quad \langle v_{n,y}a_{n,y} \rangle = \langle v_{n,y} \rangle \langle a_{n,y} \rangle.
\]
Since event-averaged values of the \( x \)- and \( y \)-components of \( v_n \) and \( a_n \) are zero, (9) becomes
\[
\langle \hat{v}_n^2 \rangle = \langle v_n^2 \rangle + \langle a_n^2 \rangle,
\]
and the true value $v_n$ is found by inverting (10):

$$\langle v_n^2 \rangle = \langle \hat{v}_n^2 \rangle - \langle a_n^2 \rangle. \quad (11)$$

This result was obtained in [2] and can be used to get an estimation of the Fourier amplitudes $v_n\{2\}$ using (3). Values $\langle a_n^2 \rangle$ measure the statistical fluctuations. They can be calculated by applying PCA to the same events, but with randomized $\phi$-angles.

The effect from the statistical noise correction on the $v_2$ is shown in Figure 1 for Pb-Pb events simulated in AMPT event generator. Uncorrected raw $\hat{v}_2$ values (upper gray diamonds), extracted directly from PCA, after the correction become blue open circles. These circles are on top of the values obtained with the traditional two-particle cumulant method (full circles). It can be seen that effect from the correction is more pronounced for the peripheral events, where a number of particles per event is lower.

For the fourth power of the observed magnitude, we can use (8) again:

$$\hat{v}_n^4 = \left[ v_n^2 + a_n^2 + 2(v_{n,x}a_{n,x} + v_{n,y}a_{n,y}) \right]^2. \quad (12)$$

Averaging (12) over events and taking into account that $x$ and $y$ components of the noise are independent and their variances are equal, $\langle a_{n,x}a_{n,y} \rangle = \langle a_{n,x}^2 \rangle \langle a_{n,y}^2 \rangle$ and $\langle a_{n,x}^2 \rangle = \langle a_{n,y}^2 \rangle$, we get

$$\langle \hat{v}_n^4 \rangle = \langle v_n^4 \rangle + \langle a_n^4 \rangle + 4\langle v_n^2 \rangle \langle a_n^2 \rangle. \quad (13)$$

From (11) and (13),

$$2(\hat{v}_n^2)^2 - \langle \hat{v}_n^4 \rangle = 2(v_n^2)^2 - \langle v_n^4 \rangle + 2\langle a_n^2 \rangle^2 - \langle a_n^4 \rangle, \quad (14)$$

and, inverting (14) and substituting into (4), we get the following estimation for the $v_n$:

$$v_n\{4\} = \sqrt{2(\hat{v}_n^2)^2 - \langle \hat{v}_n^4 \rangle - (2\langle a_n^2 \rangle^2 - \langle a_n^4 \rangle)}. \quad (15)$$

**Figure 1.** Amplitudes $v_2$ of the second Fourier harmonic as a function of centrality in Pb-Pb collisions at 5 TeV in AMPT. Values extracted by PCA are shown by open markers: circles – $v_2\{2\}$, squares – $v_2\{4\}$. Small full markers show calculations using standard 2- and 4-particle cumulant methods. Gray diamonds denote PCA values before the correction on the statistical noise. Analysis is performed for charged particles with pseudorapidity $|\eta| < 0.8$ within transverse momentum ($p_T$) range is 0.2–5 GeV/c. Number of $\varphi$ bins used for PCA is $M = 48$. 
From this expression, one may note that when \( v_n \gg a_n \), values of \( v_n \{4\} \) are remarkably insensitive to the statistical noise. Indeed, for a hypothetical case of constant magnitudes of the flow and the statistical noise, \( v_n \{4\} = \sqrt{\hat{v}_n^4 - a_n^4} \), while \( v_n \{2\} = \sqrt{\hat{v}_n^2 - a_n^2} \).

In Figure 1, open squares correspond to estimations of \( v_n \{4\} \) based on PCA coefficients, formula (15). They match small closed squares that stand for \( v_n \{4\} \) calculated with the traditional approach using four-particle correlations. At the same time, it can be seen that the raw values \( \hat{v}_n \{4\} \) (diamonds), calculated by (15) without taking into account the statistical term, are almost on top of the squares even for peripheral events. This indicates that the correction for statistical fluctuations is almost irrelevant for the \( v_n \{4\} \) as soon as the number of particles in events is large enough. Toy studies showed that this is the case when the flow magnitude is \( v_n \sim 0.1 \) and a number of particles is \( \gtrsim 100 \).

3. Symmetric cumulants with PCA

Following the same strategy, we can investigate feasibility of the studies of the so-called symmetric cumulants [7] with the PCA. This observable measures correlations between the amplitudes of the \( n \)-th and \( m \)-th Fourier harmonics and is defined as

\[
\text{SC}(n,m) = \langle v_n^2 v_m^2 \rangle - \langle v_n^2 \rangle \langle v_m^2 \rangle. \tag{16}
\]

Previous attempt to study the symmetric cumulants with the PCA was done in a paper [3]. Since the PCA basis obtained in [3] was somehow distorted (i.e. not identical to the Fourier harmonics), extracted SC in this paper values did not match the “truth” values.

We start with the single-event raw quantity:

\[
\hat{v}_n^2 \hat{v}_m^2 = (\hat{v}_{n,x}^2 + \hat{v}_{n,y}^2)(\hat{v}_{m,x}^2 + \hat{v}_{m,y}^2) = \frac{[v_{n,x}^2 + (v_{n,y} + a_{n,y})^2][v_{m,x}^2 + (v_{m,y} + a_{m,y})^2]}{[v_n^2 + a_n^2 + 2(v_{n,x}a_{n,x} + v_{n,y}a_{n,y})][v_m^2 + a_m^2 + 2(v_{m,x}a_{m,x} + v_{m,y}a_{m,y})]}.
\tag{17}
\]

Figure 2. Centrality dependence of the symmetric cumulants SC(3,2) and SC(4,2) in Pb-Pb collisions from AMPT. Open markers – values are extracted from PCA, closed markers – by traditional method of multi-particle correlations. Particles within \(|\eta| < 2.4\), \( p_T \) range 0.2–5 GeV/c.
Averaging over events and taking into account $\langle v_{n,x} \rangle = \langle v_{n,y} \rangle = \langle a_{n,x} \rangle = \langle a_{n,y} \rangle = 0$ (the same for the $m$-th harmonic), and also the factorization of the noise harmonics $\langle a_{n}^{2} a_{m}^{2} \rangle = \langle a_{n}^{2} \rangle \langle a_{m}^{2} \rangle$ as well as the noise and the signal $\langle v_{n}^{2} a_{m}^{2} \rangle = \langle v_{n}^{2} \rangle \langle a_{m}^{2} \rangle$, we obtain

$$\langle \hat{v}_{n}^{2} \hat{v}_{m}^{2} \rangle = \langle v_{n}^{2} v_{m}^{2} \rangle + \langle v_{n}^{2} \rangle \langle a_{m}^{2} \rangle + \langle v_{m}^{2} \rangle \langle a_{n}^{2} \rangle + \langle a_{n}^{2} \rangle \langle a_{m}^{2} \rangle.$$  \hspace*{1cm} (18)

Using (11) and (18), the desired term $\langle v_{n}^{2} v_{m}^{2} \rangle$ can be expressed via “measurable” quantities as

$$\langle v_{n}^{2} v_{m}^{2} \rangle = \langle \hat{v}_{n}^{2} \hat{v}_{m}^{2} \rangle - \langle \hat{v}_{n}^{2} \rangle \langle \hat{v}_{m}^{2} \rangle - \langle \hat{v}_{n}^{2} \rangle \langle \hat{v}_{m}^{2} \rangle + \langle \hat{v}_{n}^{2} \rangle \langle \hat{v}_{m}^{2} \rangle.$$

(19)

The final expression for the SC$(n, m)$ is thus

$$\text{SC}(n, m) = \langle v_{n}^{2} v_{m}^{2} \rangle - \langle v_{n}^{2} \rangle \langle v_{m}^{2} \rangle = \langle \hat{v}_{n}^{2} \hat{v}_{m}^{2} \rangle - \langle \hat{v}_{n}^{2} \rangle \langle \hat{v}_{m}^{2} \rangle.$$ \hspace*{1cm} (20)

It is remarkable that all terms related to the statistical noise are canceled.

Figure 2 shows centrality dependence of the symmetric cumulants SC(3,2) and SC(4,2) in Pb-Pb collisions from AMPT. It can be seen that values extracted from PCA (open markers) match with calculations using multi-particle correlations (closed markers). For SC(4,2), there are slight deviations in peripheral centrality classes, a possible reason is the event-plane correlation of these two harmonics. Detailed investigation of this is out of the scope of this article.

4. Summary

It was shown that the Principal Component Analysis applied to event-by-event azimuthal single-particle distributions allows to perform flow analyses that are analogous to the traditional approaches based on multi-particle correlations. As the first example, flow amplitudes based on the fourth-order cumulant were considered. As the second case, correlations between flow amplitudes in terms of symmetric cumulants were calculated. Using realistic events from the AMPT generator, PCA results were directly compared to calculations using the traditional techniques, a good correspondence was obtained. It was demonstrated also that a contribution from statistical fluctuations due to a finite number of particles per event to the higher-order PCA-based cumulants is small.

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