Application of Principal Component Analysis to Establish a Proper Basis for Flow Studies in Heavy-Ion Collisions

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Abstract—It is shown that Principal Component Analysis (PCA) applied to event-by-event single-particle distributions in A–A collisions allows establishing the most optimal basis for anisotropic flow studies from data itself, in contrast to manual selection of the basis functions. PCA coefficients for azimuthal particle distributions are identical to Fourier coefficients from a conventional analysis techniques. PCA applied in longitudinal dimension reveals optimal basis that is similar to Legendre polynomial series. Analysis in both dimensions simultaneously allows studying the coupling of the longitudinal structure of events with the azimuthal anisotropy of particle emission.

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INTRODUCTION

Principal Component Analysis (PCA) is a method for decorrelation of multivariate data by finding the most optimal basis for a given problem and thus reducing its dimensionality. PCA is widely applied in industry, in particular, for image compression, classification and recognition tasks [1], and many branches of science, see a short overview, for example, in [2]. It was suggested to apply PCA to heavy-ion collisions data to bring out substructures from two-particle azimuthal correlations [3].

In this article, PCA is applied directly to single-particle distributions in A–A collisions, namely, to azimuthal (ϕ) distribution, distribution in pseudorapidity (η) and to two-dimensional distribution η–ϕ. Mathematically, this means that we take distribution of particles in M bins in each out of N events, normalize with a number of particles in a given event, subtract in each bin an event-averaged value (in order to have zero mean in each bin) and apply PCA to the obtained N × M matrix (PCA is most often done through the singular value decomposition). As an output from PCA, we have a set of orthonormal eigenvectors (e_i, i = 1,..., M), each of the length M itself, which are ordered in such a way that corresponding variances (σ_i, i = 1,..., M) ascend from the largest to the smallest values. We get also coefficients c^{(k)}_i (k = 1,..., N) of PCA decomposition so that the particle distribution in k-th event (denote it as x^{(k)} that is a vector with M elements) can be written as

\[ x^{(k)} = \sum_{i=1}^{M} c^{(k)}_i \sigma_i e_i = \sum_{i=1}^{M} a^{(k)}_i e_i, \]

where in the last equality the variances are absorbed into coefficients: a^{(k)}_i ≡ c^{(k)}_i \sigma_i. So, the first benefit of PCA is that the data matrix N × M is projected on a set of eigenvectors e_i that are the most optimal basis for given data. As the second benefit, we can keep only the first K components (K < M) in order to have a good approximation for the data. An exact value of K can be understood after a closer look at the PCA output.

Single particle distribution, denoted by x^{(k)}, can actually be ϕ, η or η–ϕ distributions—results of the PCA applied in all the three cases are discussed below.

1. APPLICATION OF PCA TO AZIMUTHAL DISTRIBUTIONS

PCA was applied to 1.5 mln Pb–Pb events at √s_{NN} = 5 TeV simulated in the AMPT event generator [4]. Event-by-event ϕ-distributions in M = 48 bins were taken for particles within |η| < 0.8 and transverse momentum range 0.2 < p_T < 5.0 GeV/c. The first eight eigenvectors are shown in Fig. 1, and one may immediately notice that they correspond to pairs of the cosine and sine functions, i.e. the Fourier basis (with arbitrary common phase shifts with respect to 0). In order to demonstrate this better, the eigenvectors
are fitted with a cosine function (shown as lines)—the phase shift between the pairs of the functions in each panel equals $\pi/2$ with 0.01% precision.

Fractions of explained variances associated to obtained eigenvectors are shown in Fig. 2. Pairing of variances for eigenvectors again confirms the validity of association of eigenvectors with the Fourier basis. Eigenvectors with $i \geq 10$ are just a statistical noise. It should be noted here that similar PCA analysis was performed recently in [5], where eigenvectors resembles Fourier harmonics but shapes of them are somehow distorted\(^1\).

The PCA reveals the Fourier basis from event-by-event $\phi$-distributions independently of centrality class and number of bins $M$. The explanation why PCA finds this basis as the optimal one is in the fact that a set of sine and cosine functions is a natural basis for periodic or rotationally invariant problems: events with similar characteristic structures like elliptic flow or jets may appear at various event plane angles, and the Fourier basis allows “capturing” this information in the most optimal way.

2. FLOW COEFFICIENTS FROM PCA AND CORRECTION FOR STATISTICAL NOISE

After the basic functions are established and interpreted, coefficients of PCA decomposition also gain a definite meaning. Recall that flow phenomenon in heavy-ion collisions is usually studied using expansion of particle azimuthal probability density in a series:

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

where $v_n$ are the flow coefficients. If the decomposition (2) is applied event-by-event, values of $v_n$ observed in the $k$th event according to results shown above, are related to the PCA coefficients (associated to eigenvectors shown above) as follows:

$$v_{2,i}^{\text{obs}(k)} = \sqrt{\frac{M}{2}} \sqrt{a_1^2 + a_2^2}, \quad v_{3,i}^{\text{obs}(k)} = \sqrt{\frac{M}{2}} \sqrt{a_3^2 + a_4^2},$$

and so on for $v_1$ and $v_4$.

However, since $v_n^{\text{obs}}$ coefficients are extracted event-by-event and a number of particles in each event is finite, they contain statistical fluctuations inside, while the task is to extract “true” $v_n$ averaged over dataset. It can be shown that these fluctuations can be subtracted in the following way:

$$\langle v_n^{\text{corr}} \rangle = \langle v_n^{\text{obs}} \rangle - \langle v_n^{\text{rand}} \rangle, \quad (3)$$

where $v_n^{\text{rand}}$ corresponds to Fourier coefficients extracted by applying PCA to events with randomized

\(^1\)Possible explanations for such a distortion of the eigenvectors in [5] could be a small number of events ($N = 2000$) used for PCA or some peculiarities in event simulation process.
φ-angles. In case of small flow fluctuations and absence of non-flow effects, the true \( v_n \) can thus be estimated as \( \sqrt{\left(v_n^{corr}\right)^2} \).

Performance of the correction procedure (3) is tested using a toy model with flow, where particles are distributed according to (2) with some “typical” values of \( v_n \). Analysis is done with different number of φ-bins, results are shown in Fig. 3. Different φ-binnings allow one to investigate when PCA results become reliable for various harmonic orders \( n \). It can be seen that corrected values (red circles) stabilize at true values at \( n_\phi \approx 30 \) for \( v_2 \), \( v_3 \) and \( v_4 \), while the true value of \( v_1 \) is reached somewhat earlier (since \( v_1 \) measures just an overall shift of the event in azimuthal dimension that is “captured” already with a very few φ-bins).

In order to test robustness of \( v_n \) extracted with PCA, this analysis was applied to Pb–Pb events at \( \sqrt{s_{NN}} = 5 \text{ TeV} \) simulated in AMPT event generator (Fig. 4, corrected PCA results for \( v_2 \), \( v_3 \) and \( v_4 \) are shown as open circles) and compared to calculations with the traditional two-particle cumulant method (\( v_n^2 \), full circles). Correspondence between the values justifies again the possibility to extract \( v_n \) with PCA. It is important to note also that other conventional analyses, like symmetric cumulants and event-plane correlations, are also possible with the azimuthal PCA.

3. LONGITUDINAL HARMONICS FROM PCA

While the Fourier basis as the best option for azimuthal distributions was somewhat expected, it is not so obvious which basis is optimal for longitudinal (\( \eta \)) dimension. It was suggested to quantify longitudinal structure of events using Chebyshev [8] or Legendre polynomials [6] in some pseudorapidity range \([-Y, Y]\), without a strong motivation for a particular choice.
The question of a proper basis for $\eta$-dimension can be addressed using PCA. First of all, when does this or that polynomial basis appear in PCA? To answer that, let us take a toy model of “random parabola”, where the particle $\eta$-density in each event is sampled according to expression $\rho(\eta) \sim A(\eta - B)^2$ with $A$ and $B$ being random numbers. It turns out that PCA reveals the basis of $P_1(\eta) = \eta$ and $P_2(\eta) = \frac{1}{2}(3\eta^2 - 1)$, which are the first two Legendre polynomials. This is demonstrated in the left panel in Fig. 5.

However, in a more realistic case of AMPT events eigenvectors from PCA have different shapes (right panel in Fig. 5). Mathematically, this indicates that a set of these orthonormal polynomials has its own unique weight function (recall, that for the Legendre polynomials the weight function equals 1). Moreover, it can be shown that, unlike azimuthal case, PCA basis in $\eta$-dimension depends on kinematic cuts ($\eta$- and $\phi$-ranges) and physics of the collisions (for example, results differ between AMPT and HIJING event generators). It is interesting to get PCA eigenvectors from real A–A events and compare with model results.

4. TWO-DIMENSIONAL CASE

Finally, the PCA can be straightforwardly applied for single-particle densities in two dimensions, in particular, to $\eta$–$\phi$ distributions. Eigenvectors for AMPT semi-central collisions (centrality 20–30%) are shown in Fig. 6 for the case of $M = \eta \times \phi = 10 \times 48 = 480$ bins. We may note the pairs of “azimuthal” harmonics $(1, 2)$, $(3, 4)$, etc. that are nearly uniform in $\eta$; it was checked...
that corresponding event-averaged $v_n$ values agree with purely azimuthal PCA presented above. Longitudinal eigenvectors 7 and 10 are uniform in $\phi$, their shapes are the same as in the right panel in Fig. 5. Finally, “mixed” (or “twisted”) $\eta$–$\phi$ harmonics appear, namely, pairs (5, 6), (8, 9), (11, 12). A closer look shows that these mixed eigenvectors can be factorized into $\phi$- and $\eta$-parts (since PCA components must be able to capture different structures in $\eta$ at any azimuthal rotation). Thus, event-by-event particle densities can be decomposed according to

$$\rho(\eta, \phi) = \frac{1}{2\pi} \sum_{k=0}^{K_\phi} \sum_{l=0}^{K_\eta} a_{k,l} \Phi_k(\phi) H_l(\eta),$$

where $\Phi_k(\phi)$ denotes the azimuthal part (it can be written as $2\cos[k(\phi - \Psi_k)]$), the longitudinal part is denoted as $H_l(\eta)$. $a_{k,l}$ are the decomposition coefficients, $K_\phi$ and $K_\eta$ stand for cut-off numbers of harmonics to consider. This decomposition could be used, for instance, in studies of the longitudinal decorrelation of harmonic flow as an alternative to other methods like those described in [9, 10]. Another possible application of this 2D-analysis is the study of rapidity dependence of the directed flow. Detailed discussion of the two-dimensional PCA is out of scope of the present paper.

5. CONCLUSIONS

Application of PCA to single-particle distributions in A–A collisions gives a hint how a proper (most optimal) basis should look like. It was shown how PCA coefficients could be corrected for statistical noise. For azimuthal dimension, PCA confirms that the basis of Fourier harmonics is a proper choice, since it is natural for rotationally invariant problems. In case of longitudinal dimension, a set of PCA eigenvectors is not a “standard” one—the most optimal basis of orthogonal functions depends on given data (collision system, energy, acceptance). Finally, PCA was applied to two-dimensional $\eta$–$\phi$ distributions, where “twisted” harmonics are revealed. This approach may be of practical use in studies of longitudinal decorrelation of collective flow.

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