# Principal Component Analysis And its application to Relativistic Heavy-Ion Collisions

For Initial Stages 2019

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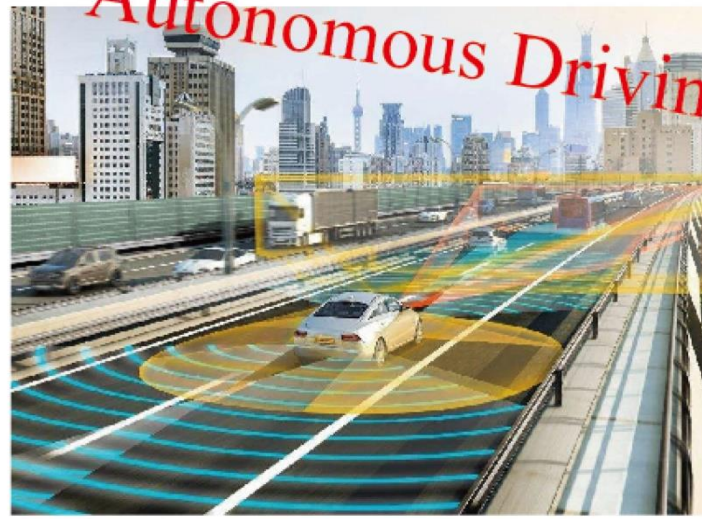
# Overview

- Introduction to PCA
- Paper I:
  PCA Analysis of Collective Flow
- Paper II:
  PCA Analysis of flow factorization breaking

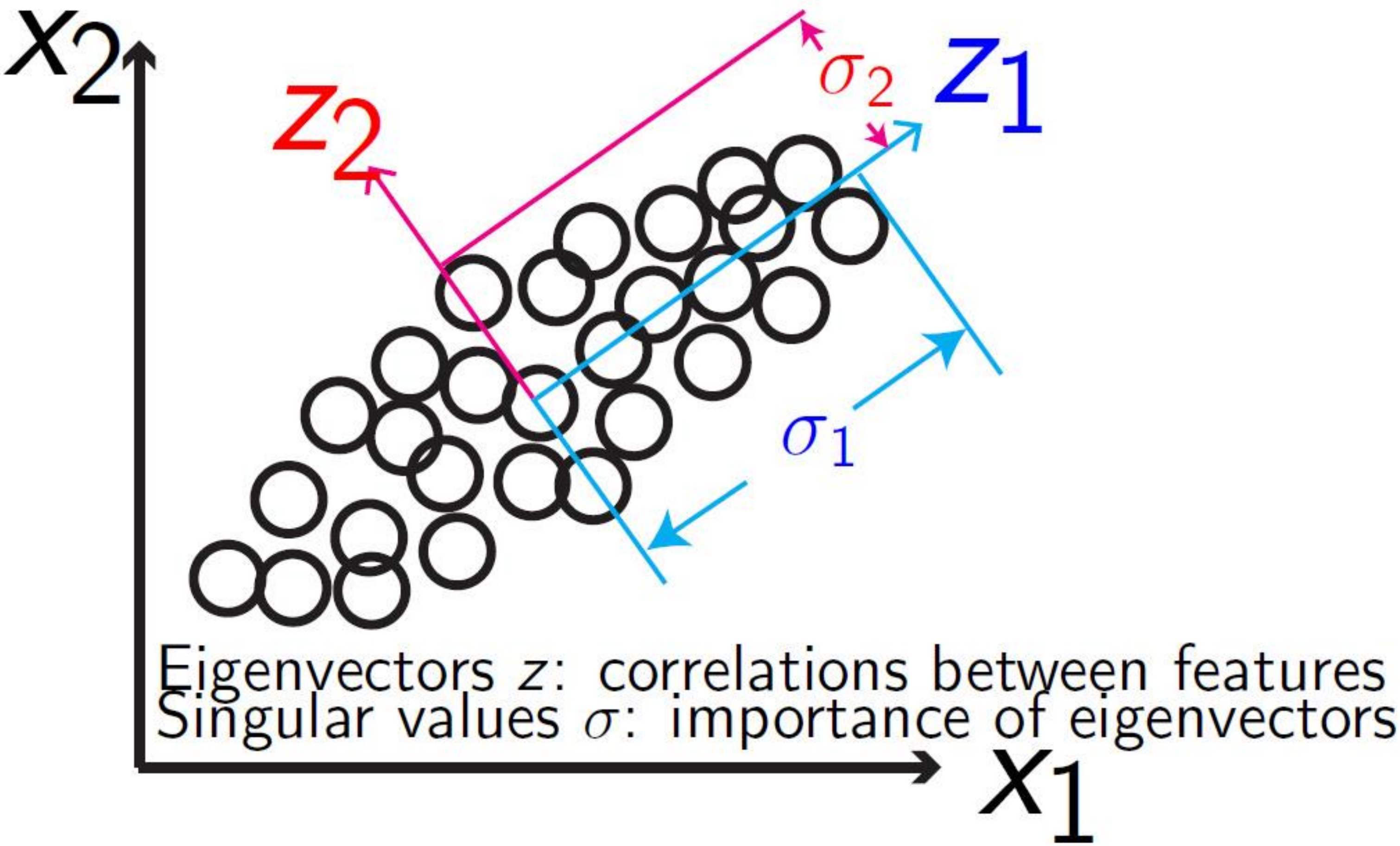
# Machine learning



# What is PCA?

# An intuitive way for PCA

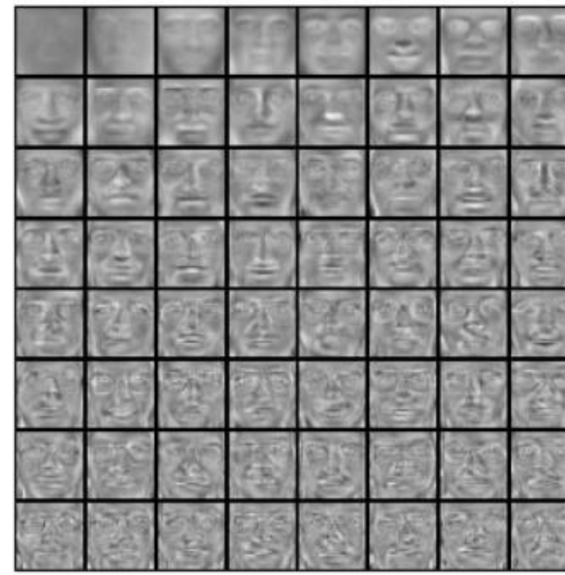


# Principal component analysis ——Application

Dataset:Faces of different people

Mean: μ

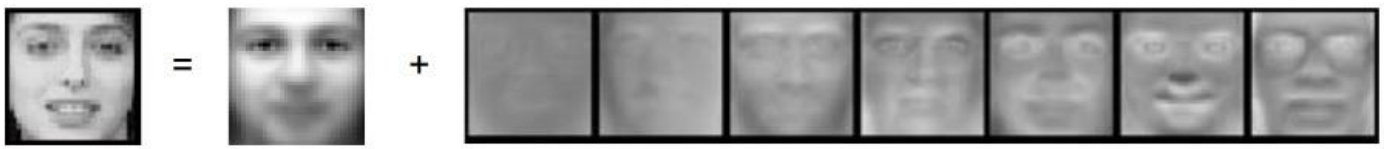
Top eigenvectors: $u_1, \ldots u_k$



Eigenfaces

# Principal component analysis ——Application

- Each face is decomposed into superposition of eigenfaces.



$$\hat{x} = \mu + w_1u_1 + w_2u_2 + w_3u_3 + w_4u_4 + \ldots$$

- We can drop unimportant high order eigenfaces. So we can use a few coefficients and corresponding eigenfaces to reconstruct original faces. (**Image compression**)

# Principal component analysis --math

**Theorem: SVD(Singular Value Decomposition)**

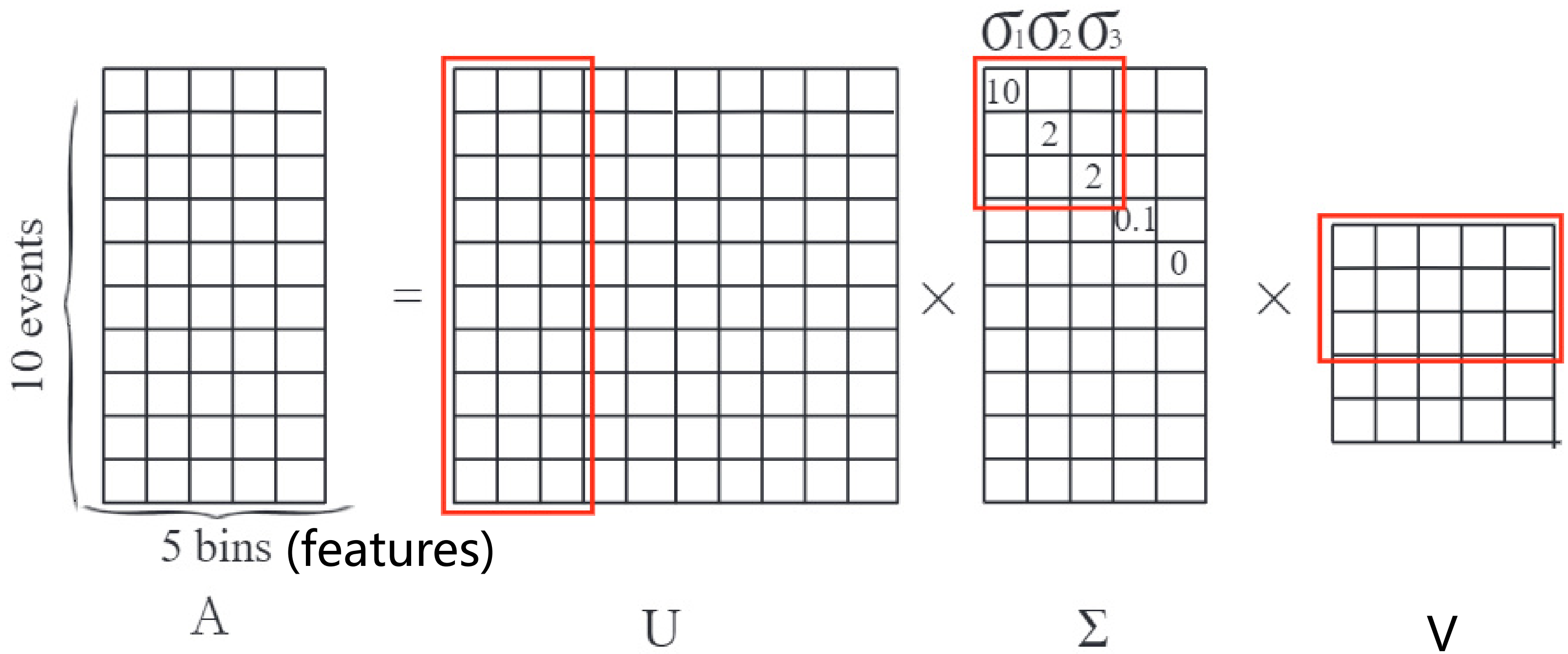
For a complex (real) matrix $A \in R^{n\times m}$, $\exists$ unitary (orthogonal) matrices $U_{n\times n}$ and $V_{m\times m}$, along with a sub-diagonal matrix $\Sigma_{n\times m}$ such that

$$A = U\Sigma V$$

Where $\Sigma = diag(\sigma_1, \sigma_2, \dots,)$ such that $\sigma_1 \geq \sigma_2 \geq= \cdots \geq 0$

$\sigma$: singular values

$v_{i,:}$: eigenmodes/ eigenvectors/principal components

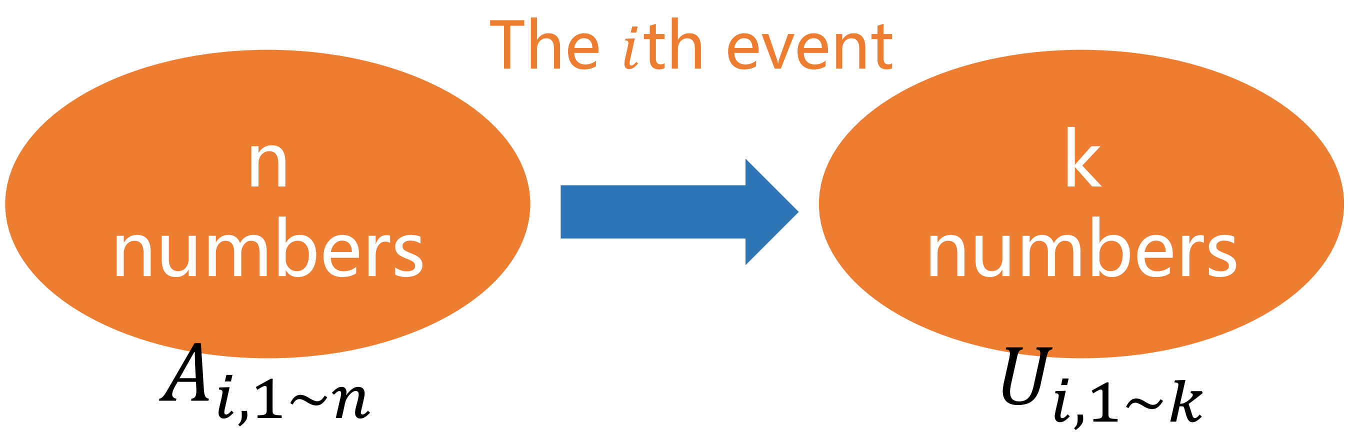


# Principal component analysis --math

Now, the $i$th event can be decomposed as summation of eigenvectors $z_j$ :

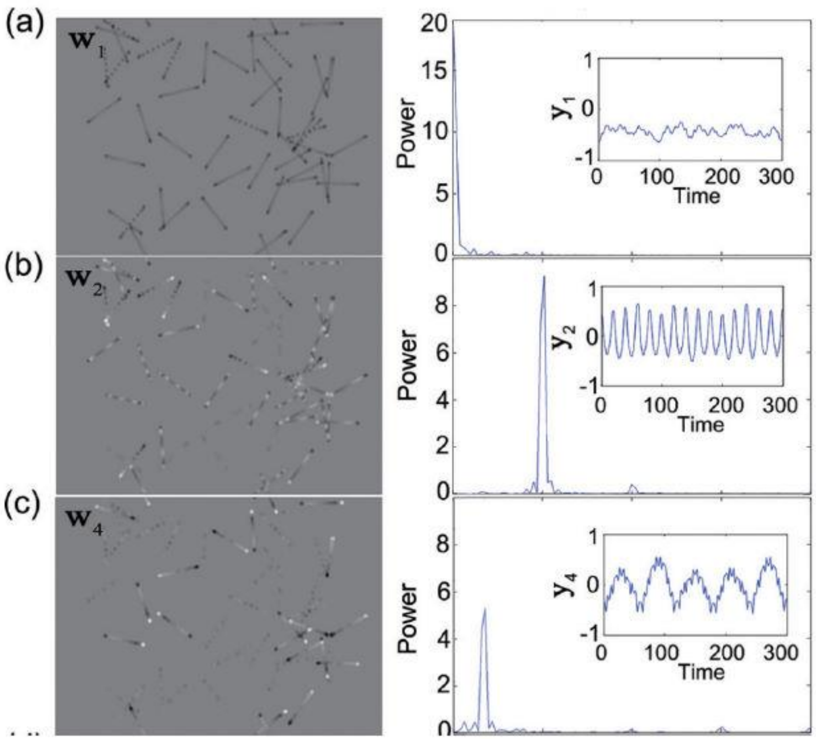
$$A_{i,:} \approx \sum_{j=1,2,\ldots,k} \sigma_j u_{i,j} v_{:,j}$$

$k$ is the cut we choose to drop out minor modes.

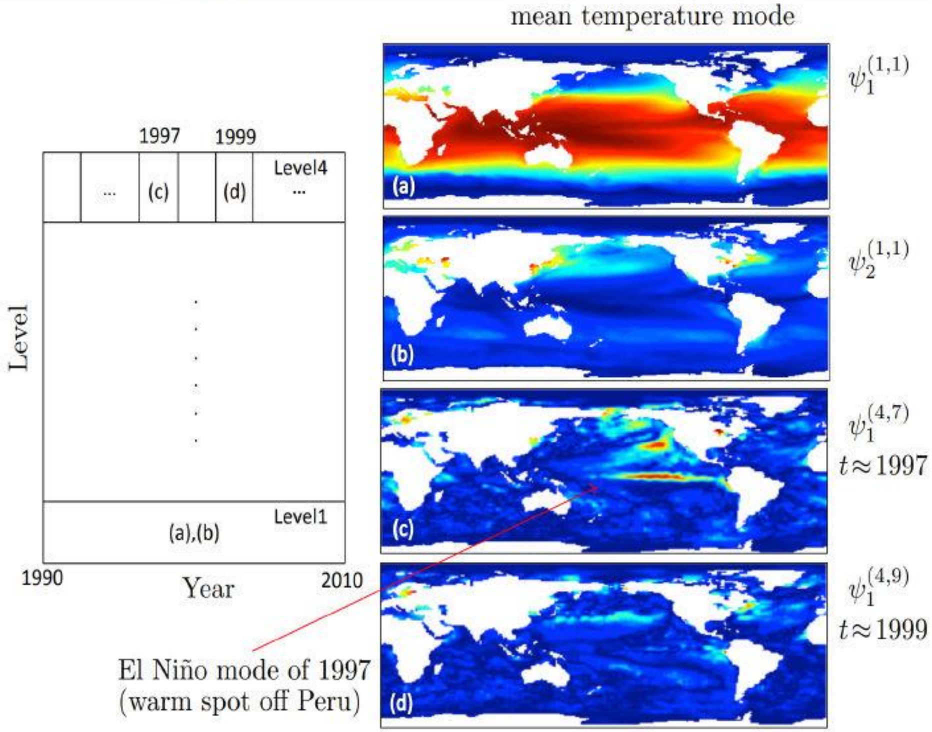


# PCA in physics

- eigenfrequencies in particle motion




- Multi-resolution PCA to discover El Nino.




H. Y. Chen, Raphal Ligeois, John R. de Bruyn, and Andrea Soddu Phys. Rev. E 91, 042308 Published 15 April 2015

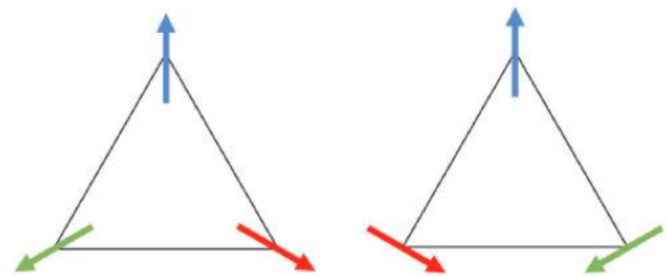
https://arxiv.org/pdf/1506.00564.pdf

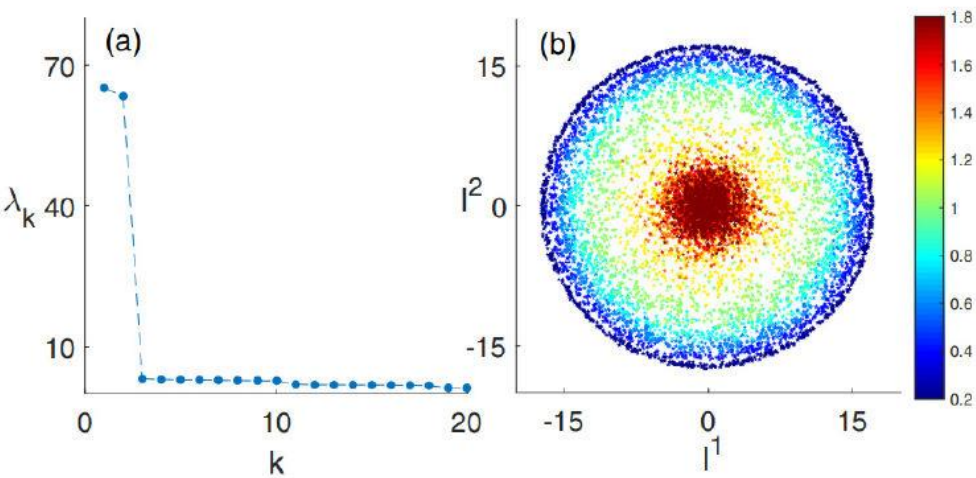
# PCA in physics

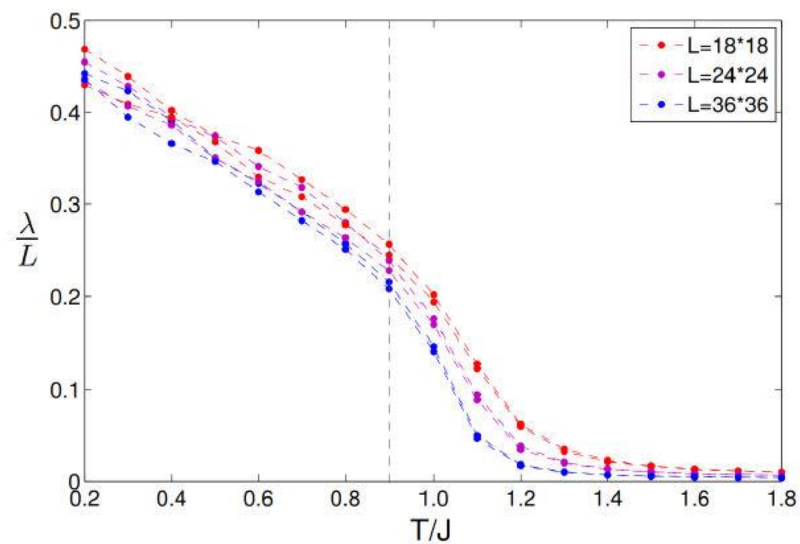
Machine learning helps discover

- Correlations between spin configurations
- Phase transition

$$\mathcal{H} = J \sum_{\langle i j \rangle} \cos(\theta_i - \theta_j)$$



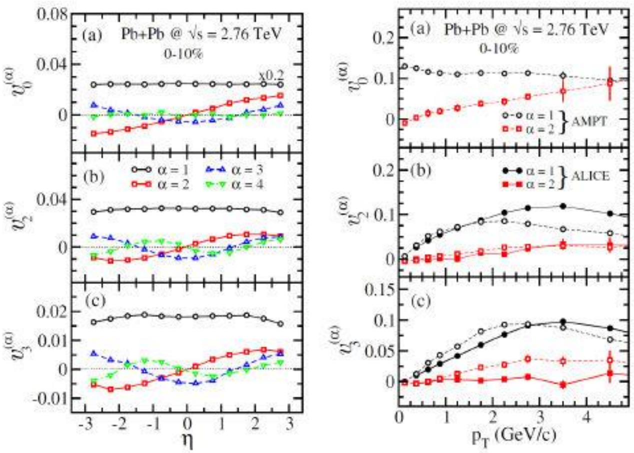



C Wang, H Zhai - Physical Review B,**96(2017)**,14,144432

# PCA in Heavy-Ion

- subleading modes of factorization breaking



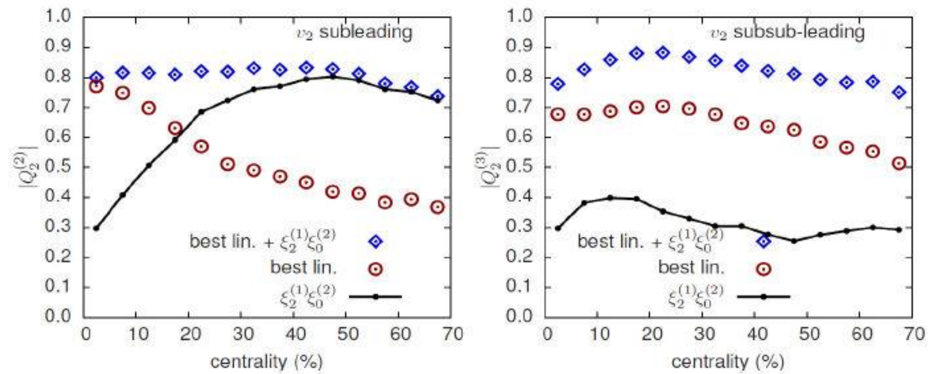

Rajeev S. Bhalerao, Jean-Yves Ollitrault, Subrata Pal, Derek Teaney Phys.Rev.Lett. **114** (2015) no.15, 152301

- Nonlinear response coefficients

Piotr Bozek, Phys.Rev. **C97** (2018) no.3, 034905

- Best linear descriptor

$$\zeta^{(a)}_{n,pred} = \varepsilon_{n,n} + c_1 \varepsilon_{n,n+2}$$




Aleksas Mazeliauskas, Derek Teaney Phys.Rev.**C93** (2016) no.2, 024913

- Experimental data

**CMS** collaboration, Phys.Rev. **C96** (2017) no.6, 064902

# Principal Component Analysis(PCA) in Heavy-ion Physics

arXiv: 1903.09833
Ziming Liu, Wenbin Zhao, **Huichao Song**
Principal Component Analysis (PCA) of Collective Modes in Relativistic Heavy-Ion Collisions

Recent work, paper in preparation
Ziming Liu, Arabinda Behera, **Huichao Song, and Jiangyong Jia**
Reconsideration on studying sub-leading flow with PCA

# Can a machine automatically discover flow?

arXiv: 1903.09833

Ziming Liu, Wenbin Zhao, **Huichao Song**

Principal Component Analysis (PCA) of Collective Modes in Relativistic Heavy-Ion Collisions

Previous work utilizes Fourier Transformation in the $\phi$ direction:

$$\frac{dN}{dp} = \sum_{n=-\infty}^{+\infty} V_n(p) e^{in\phi} \quad p = (p_t, \eta)$$

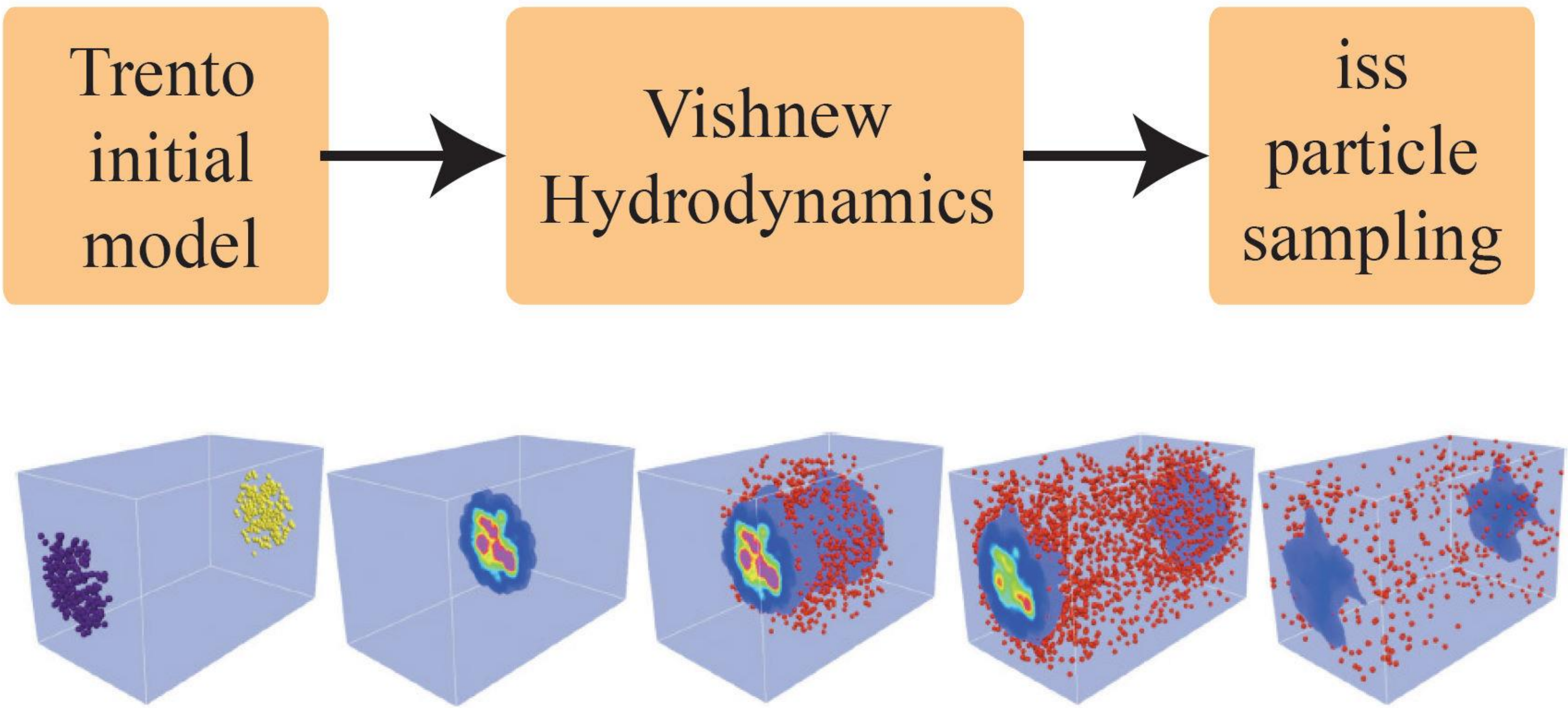
PCA decomposes $V_n(p)$ into eigenmodes:

$$V_n(p) = \sum_{\alpha=1}^{k} \xi^{(\alpha)} V_n^{(\alpha)}(p)$$

However, we apply PCA directly to $dN/d\phi$ data without FT:

$$\frac{dN}{d\phi} = \sum_{\alpha=1}^{k} \xi^{(\alpha)} \left(\frac{dN}{d\phi}\right)^{(\alpha)}$$

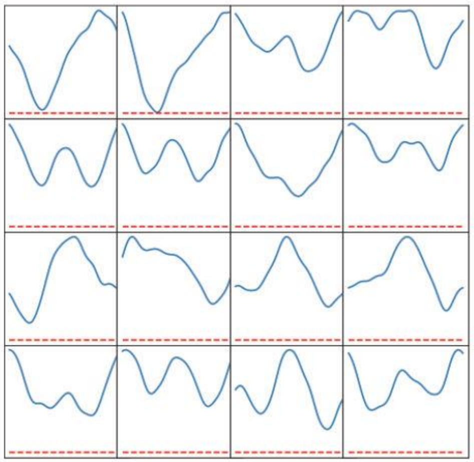
Pb+Pb collisions at 2.76 A TeV




No hadron rescattering or resonance decays to simplify problem settings.

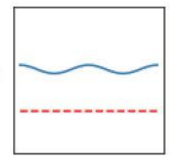
# PCA for flow analysis

Data sets: $\frac{dN}{d\varphi}$

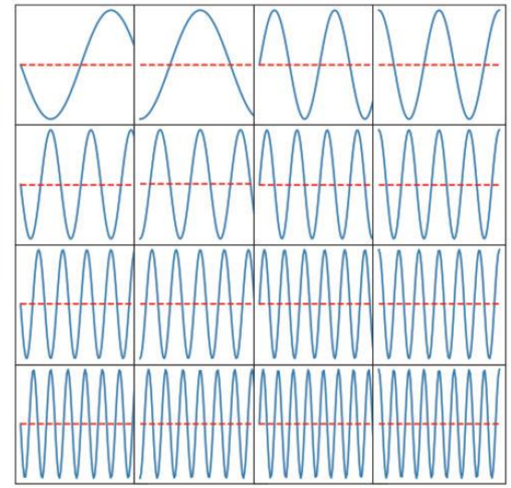


PCA

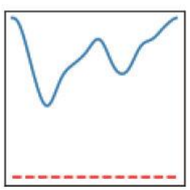
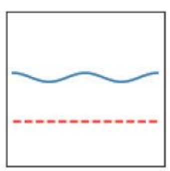
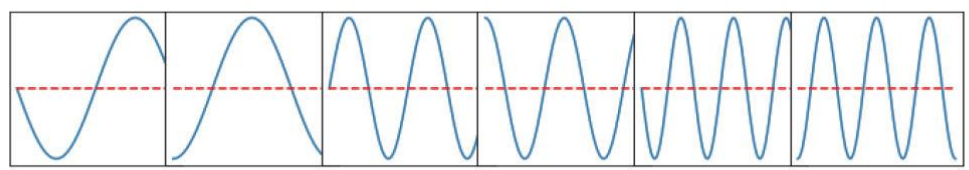
mean $\mu$



top eigenvectors: $\sigma_1, \sigma_2, \sigma_3 \ldots\ldots$

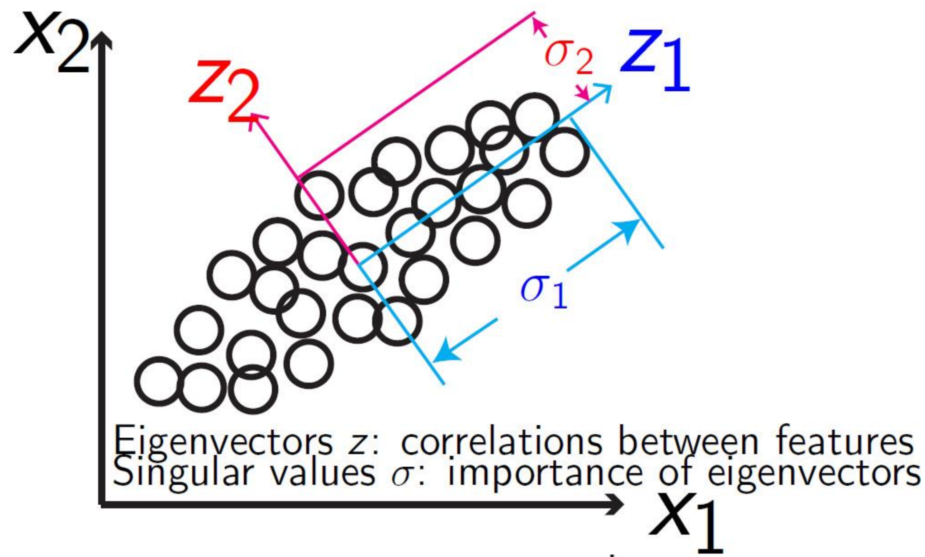


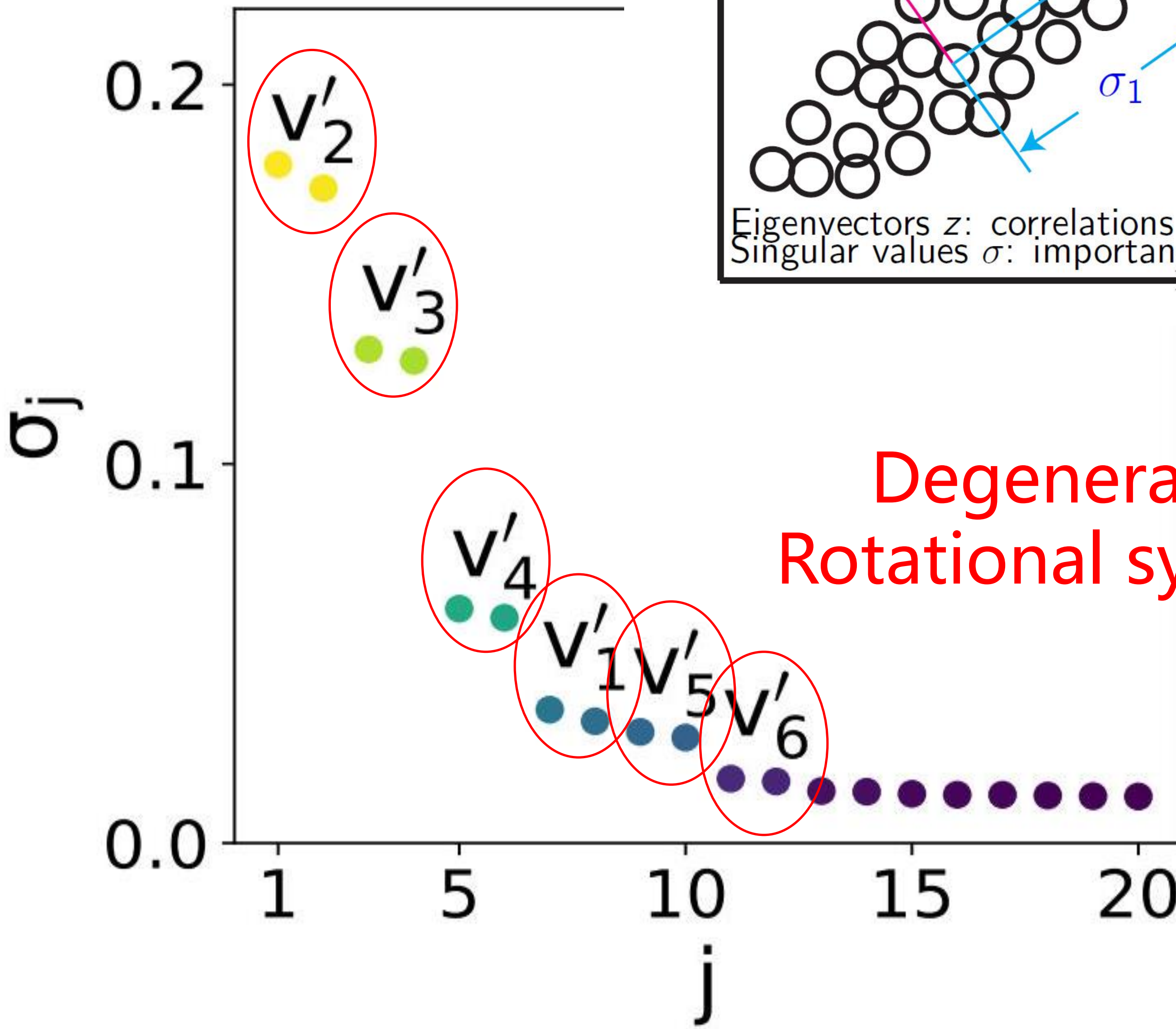
With PCA, each flow distribution is decomposed into superposition of eigenmodes.

 =  + 

$$\frac{dN}{d\varphi} = \mu + x_1 z_1 + x_2 z_2 + x_3 z_3 + \ldots\ldots$$

## Singular values

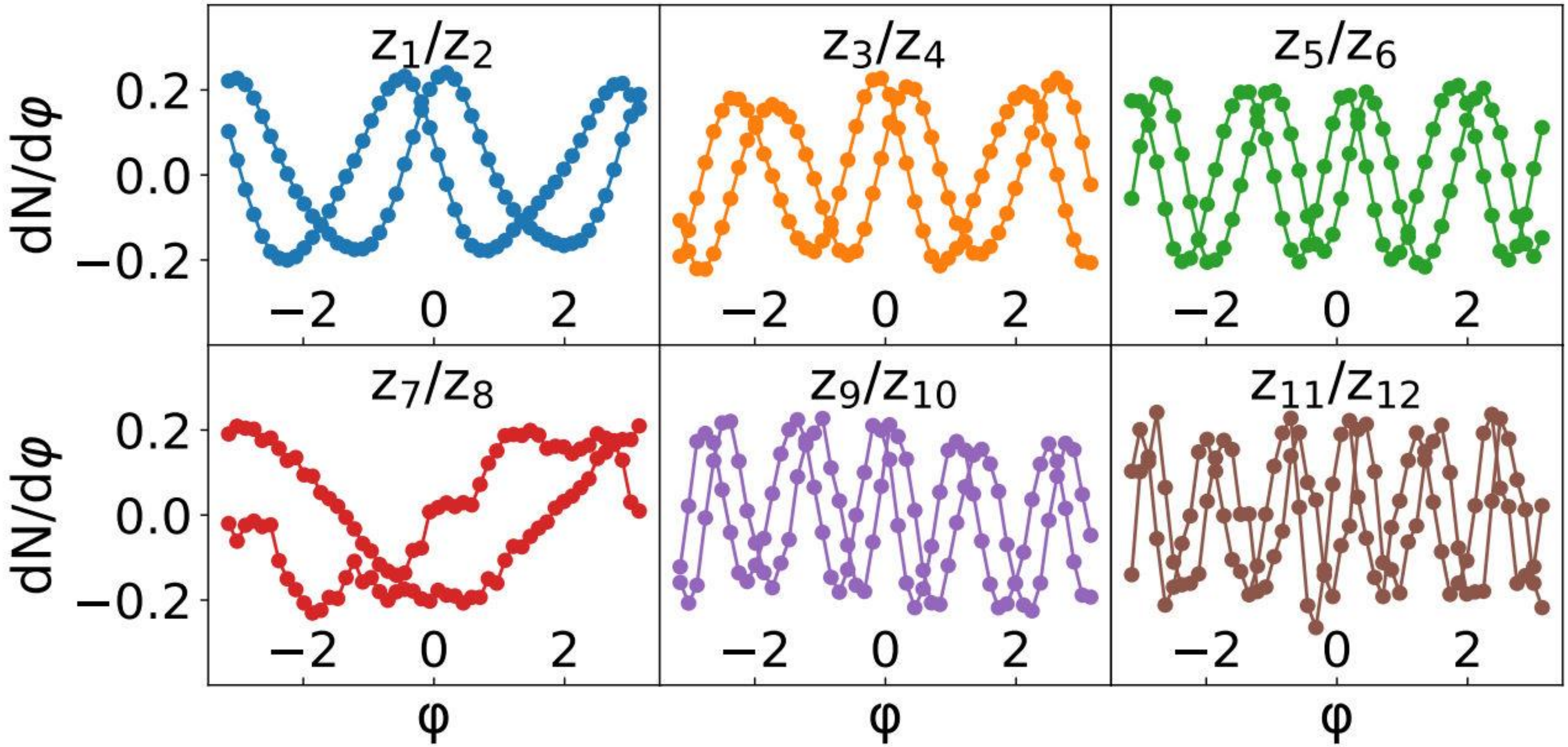



Degeneracy → Rotational symmetry

Eigenvectors/ Principal components

Elliptic flow  Triangular flow  ……




Machines can automatically discover flow without any guidance from human beings!

Define flow harmonics with PCA

$$\frac{dN}{d\phi} = \mu + \sum_{i=1}^{k} x_k z_k$$

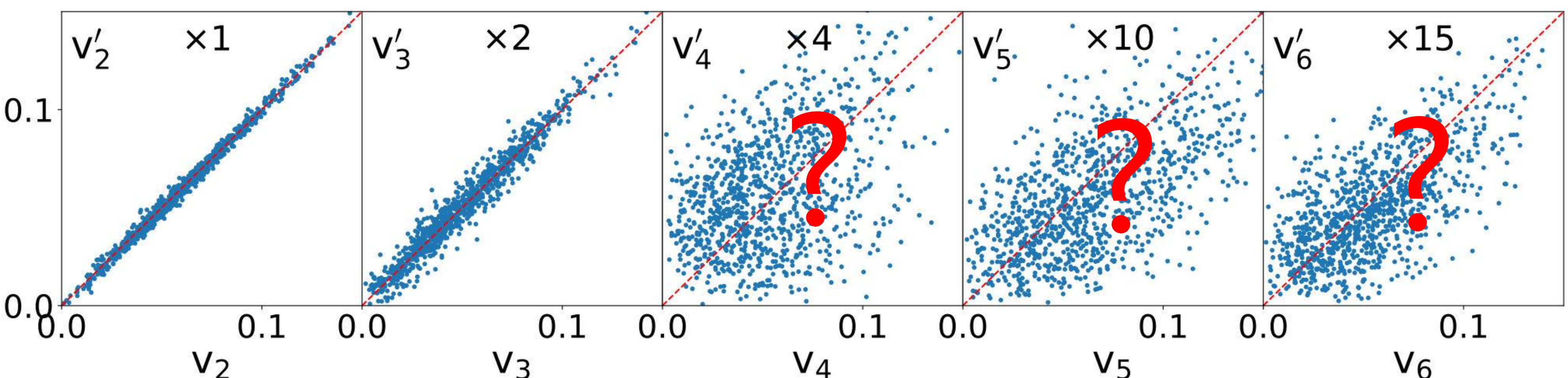
# Event average comparisons

Define flow harmonics with Fourier (Tradition)

| $n$ | $v'_n$ | $\overline{v'_n} \times 10^2$ | $\overline{v_n} \times 10^2$ |
|---|---|---|---|
| 2 | $\sqrt{\frac{m}{2}}\sqrt{x_1^2 + x_2^2}$ | 6.03 | 6.08 |
| 3 | $\sqrt{\frac{m}{2}}\sqrt{x_3^2 + x_4^2}$ | 2.57 | 2.53 |
| 4 | $\sqrt{\frac{m}{2}}\sqrt{x_5^2 + x_6^2}$ | 1.21 | 1.25 |
| 5 | $\sqrt{\frac{m}{2}}\sqrt{x_9^2 + x_{10}^2}$ | 0.57 | 0.66 |
| 6 | $\sqrt{\frac{m}{2}}\sqrt{x_{11}^2 + x_{12}^2}$ | 0.26 | 0.37 |

PCA flow harmonics
≈
Traditional flow harmonics

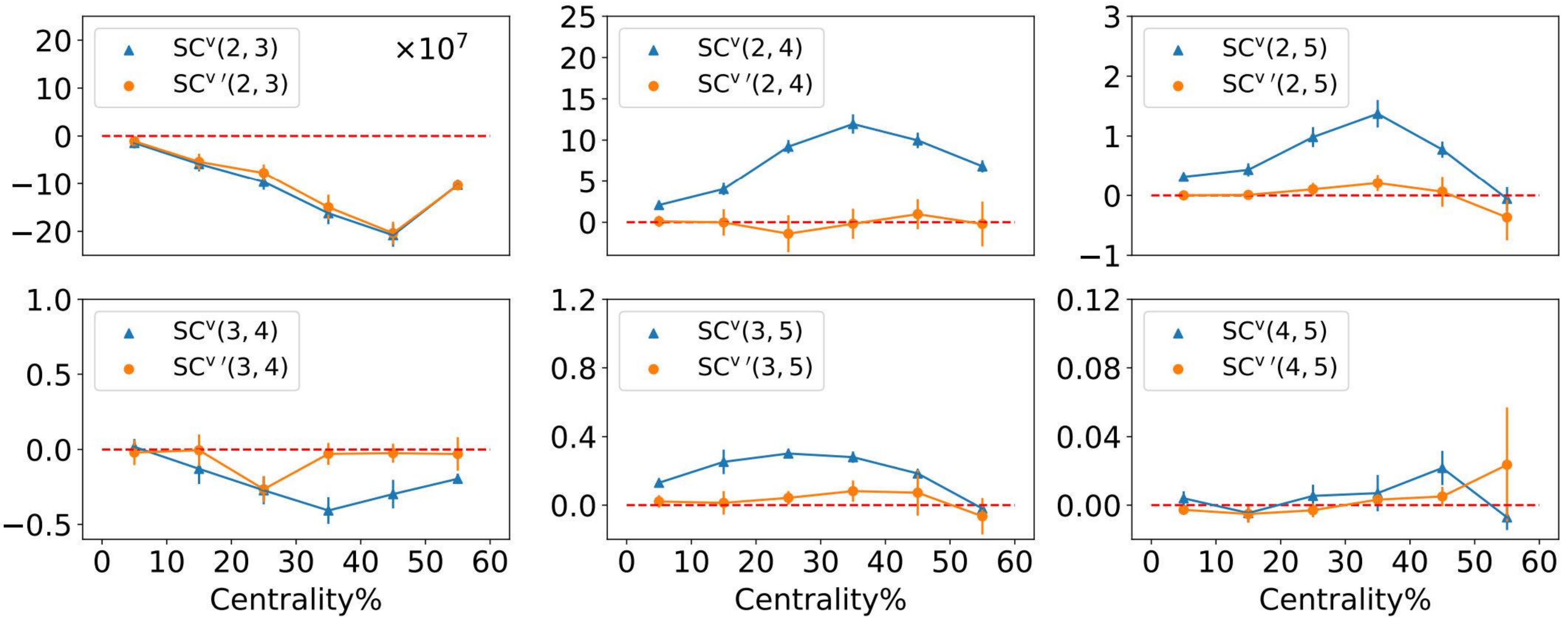
# Event-by-event comparisons



# Symmetric cumulants

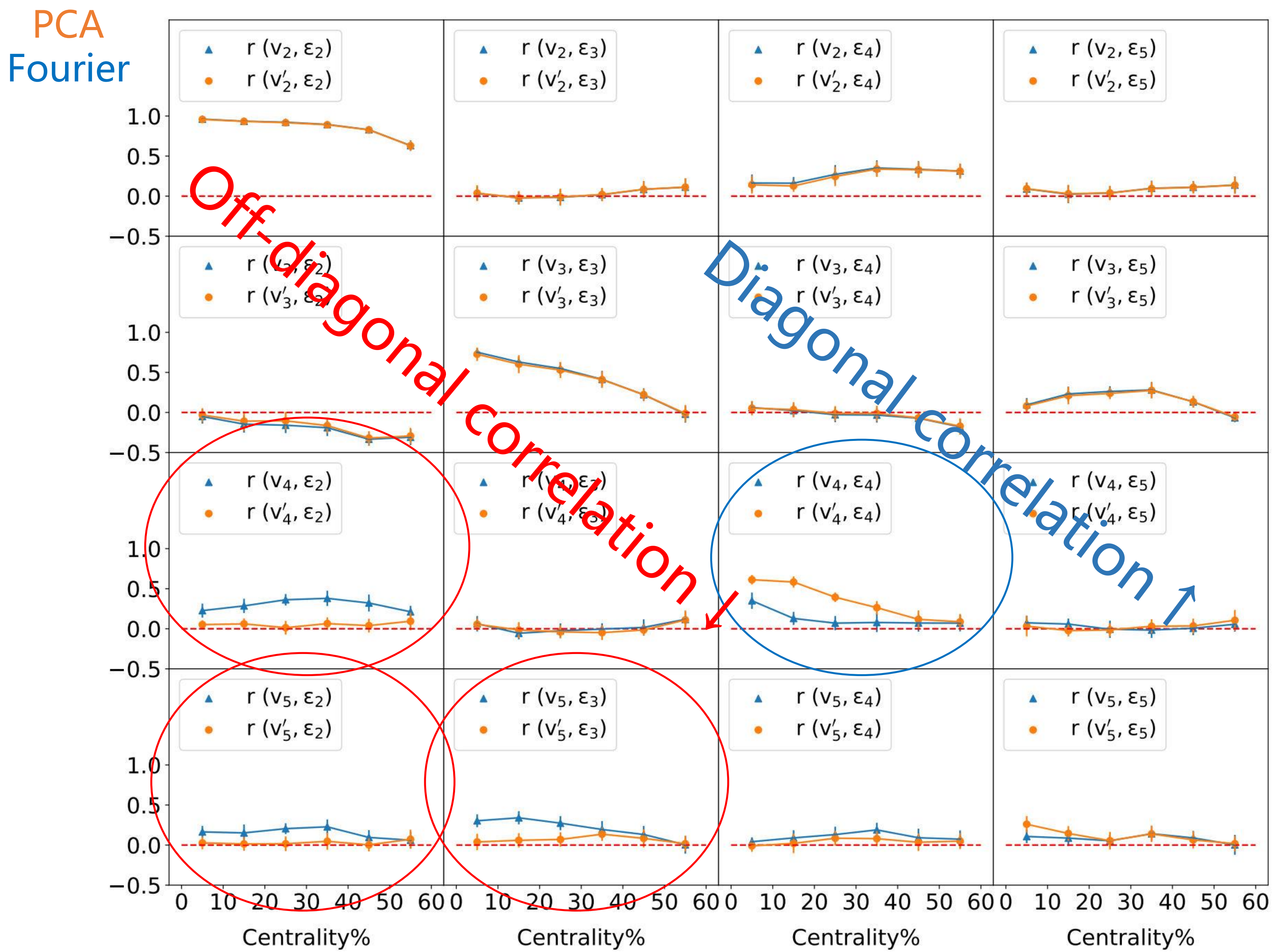
Fourier : $SC^v(m,n) = \langle v_m^2 v_n^2 \rangle - \langle v_m^2 \rangle \langle v_n^2 \rangle$

PCA : $SC^{v'}(m,n) = \left\langle {v'}_m^2 {v'}_n^2 \right\rangle - \left\langle {v'}_m^2 \right\rangle \left\langle {v'}_n^2 \right\rangle$




Correlation between different harmonics decrease for PCA !

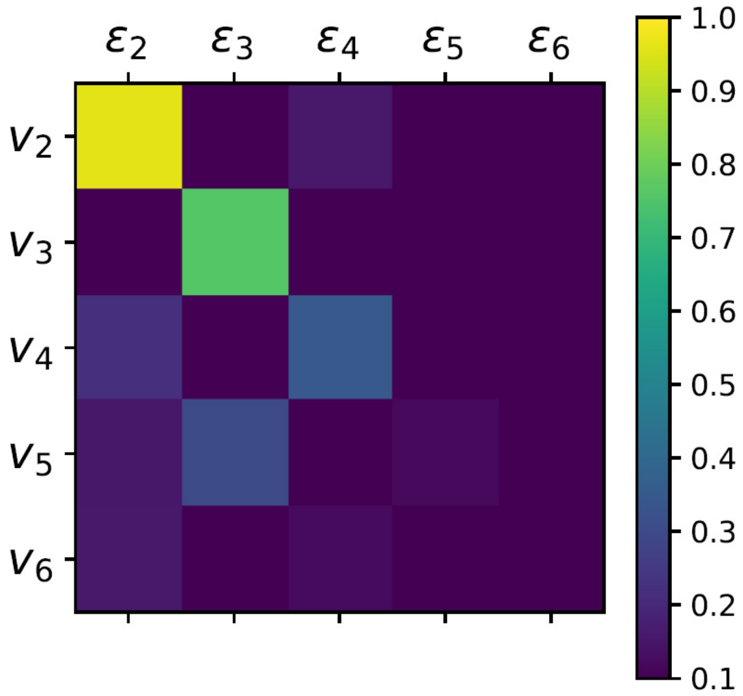
# Pearson correlation between initial and final



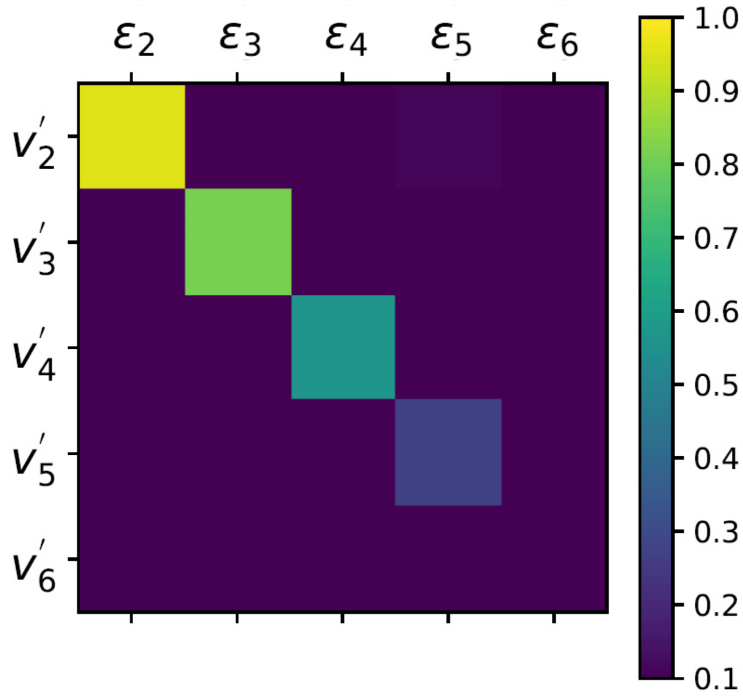
# Pearson correlation between initial and final

## 20%-30% centrality data

Fourier:




PCA:




PCA has a more diagonal pattern!

# Conclusion for paper 1

- Without defining Fourier bases, PCA can automatically discover flow.
- We use PCA bases to re-define flow harmonics and find that
  - PCA bases lead to less correlations between different flow harmonics.
  - PCA flow harmonics have a more diagonal pattern with initial eccentricities as compared to traditional one.

# The limitation of studying sub-leading flow with PCA

Recent work, paper in preparation
Ziming Liu, Arabinda Behera, **Huichao Song, and Jiangyong Jia**
Reconsideration on studying sub-leading flow with PCA

# Principal component analysis of event-by-event fluctuations

PRL 114, 152301 (2015)

Rajeev S. Bhalerao, Jean-Yves Ollitrault, Subrata Pal, and Derek Teaney

**Single particle distribution**

$$\frac{dN}{dp} = \sum V_n(p) e^{-in\phi}$$

**Two-particle correlation**

$$\langle V_{n\Delta}(p_a, p_b) \rangle = \langle V_n(p_a) V_n^*(p_b) \rangle$$

⇩ diagonalization

**Decompose $V_n(p_T)$ with PCA modes**

$$V_n(p_T) = \zeta_n^{(1)} V_n^{(1)}(p_T) + \zeta_n^{(2)} V_n^{(2)}(p_T) + \zeta_n^{(3)} V_n^{(3)}(p_T) + \cdots + \zeta_n^{(k)} V_n^{(k)}(p_T)$$

⇩ Leading flow

⇩ Sub-leading flow

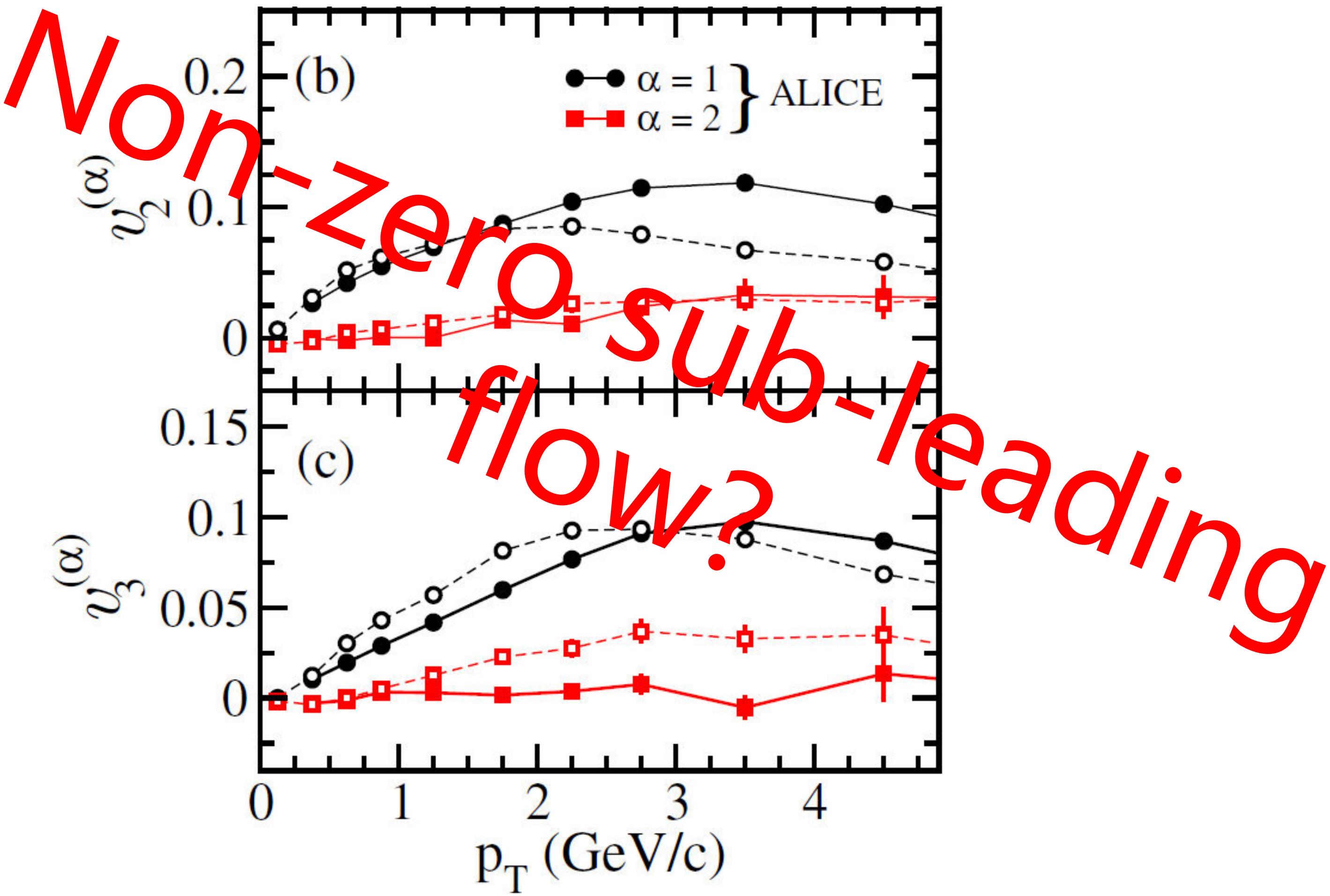
⇩ Sub-sub-leading flow

⇩ k-th mode

# Principal component analysis of event-by-event fluctuations

PRL 114, 152301 (2015)

Rajeev S. Bhalerao, Jean-Yves Ollitrault, Subrata Pal, and Derek Teaney

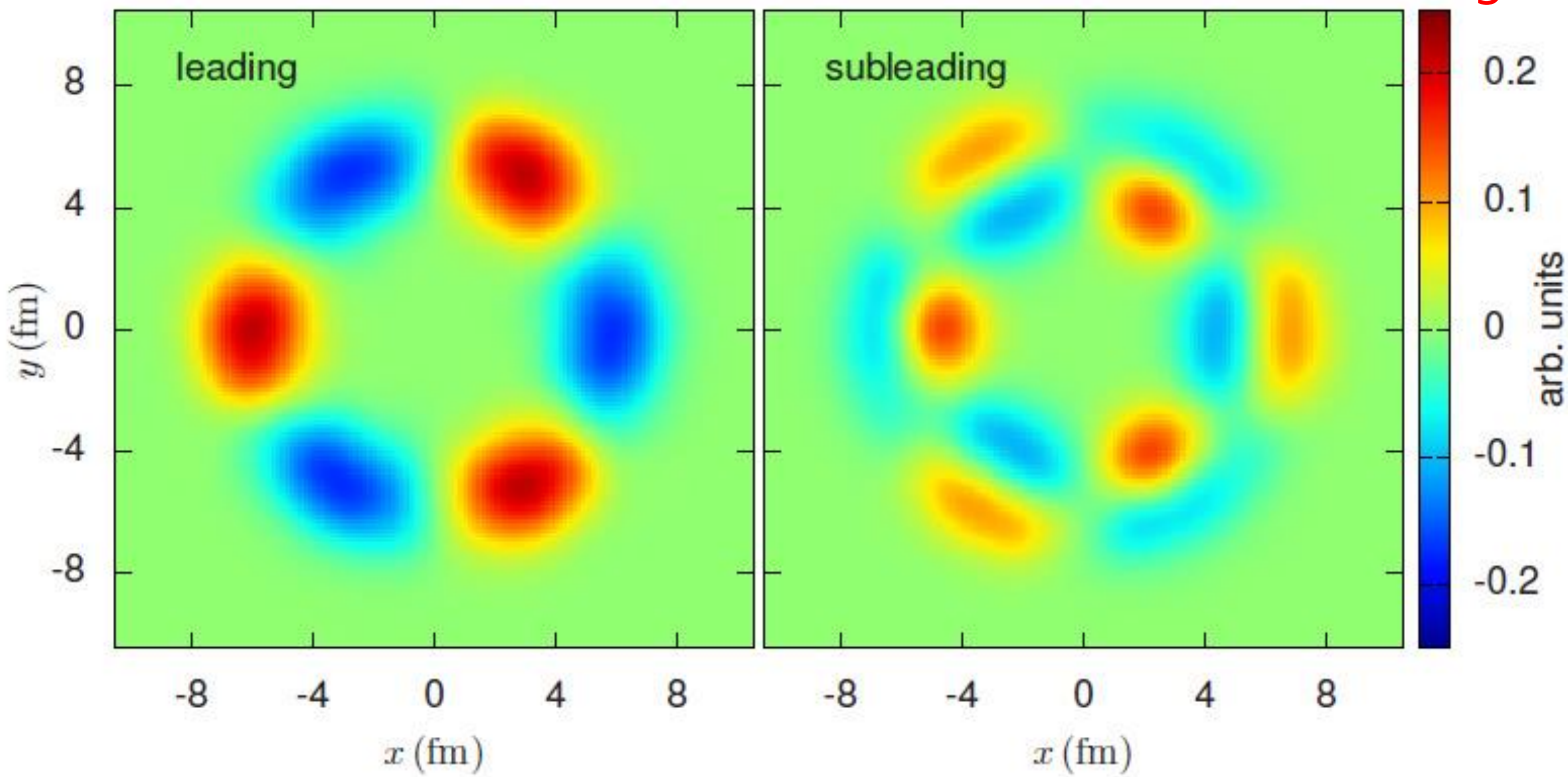


# Cause for Sub-leading flow

Phys.Rev. C91 (2015) no.4, 044902
Aleksas Mazeliauskas, Derek Teany

$V_3(p_T)$

Radial excitation leads to sub-leading flow!



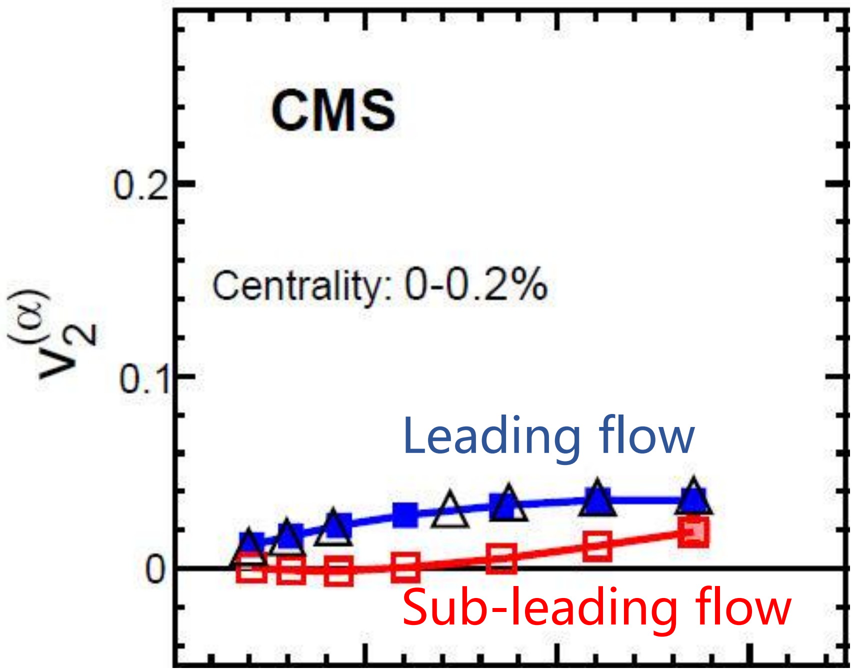

Sub-leading flow is theoretically important!!!

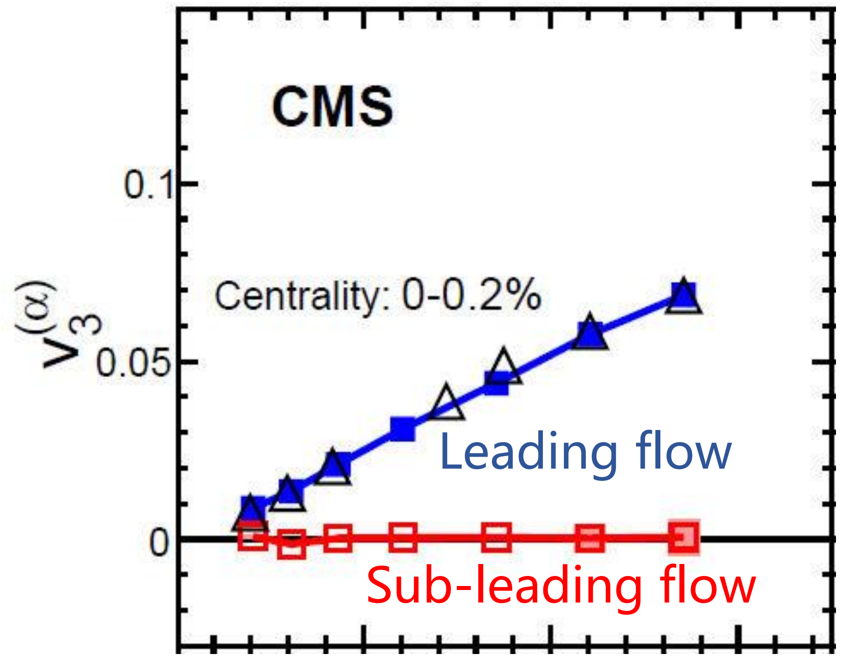
# Experimental results

Phys. Rev. C 96, 064902
The CMS Collaboration

▲ $v_3\{|\Delta\eta| > 2.0\}$, CMS

★ $v_3\{|\Delta\eta| > 0.8\}$, ALICE



# Think more about it.

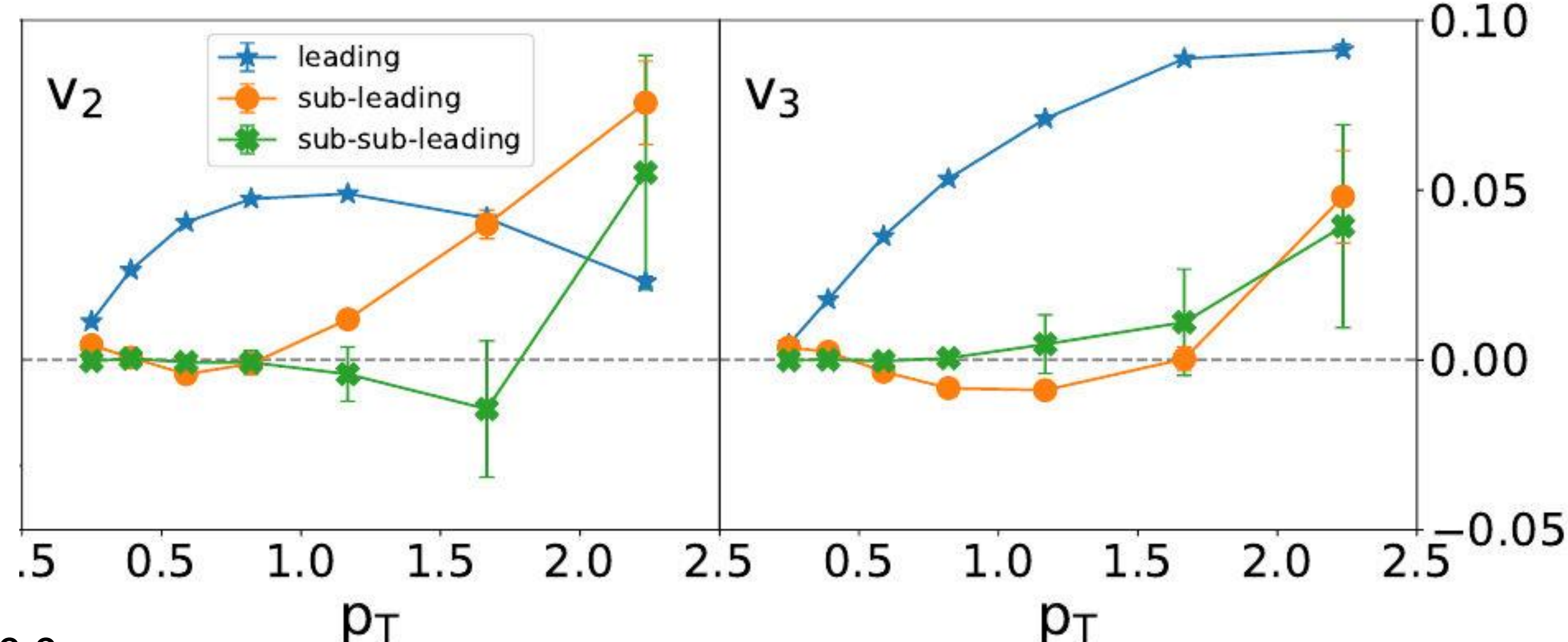
Model setup:

- AMPT model
- 1M UCC events
- subevent method

(paper in preparation)

Ziming Liu, Arabinda Behera, Huichao Song, and Jiangyong Jia

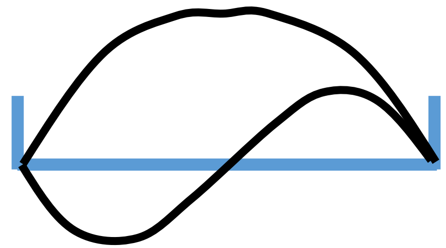
# Reproduce CMS results



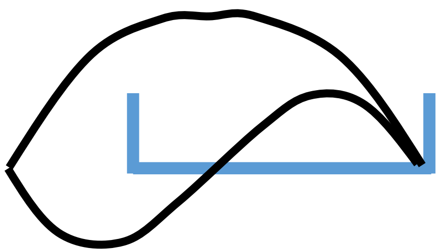

0.0

Same $p_T$ cut and proper $\eta$ gap $|\Delta\eta| < 0.8$ .
Our model can properly reproduce the results @CMS

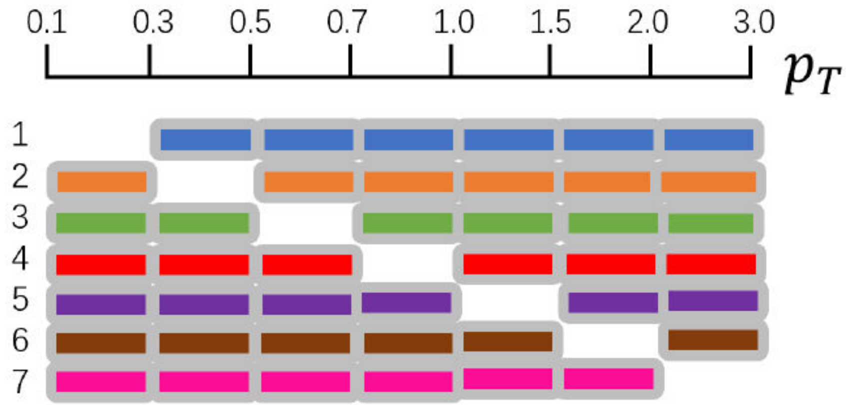
# Problem 1: How to choose $p_T$ bins?



Orthogonal on this large interval



Not orthogonal on this small interval

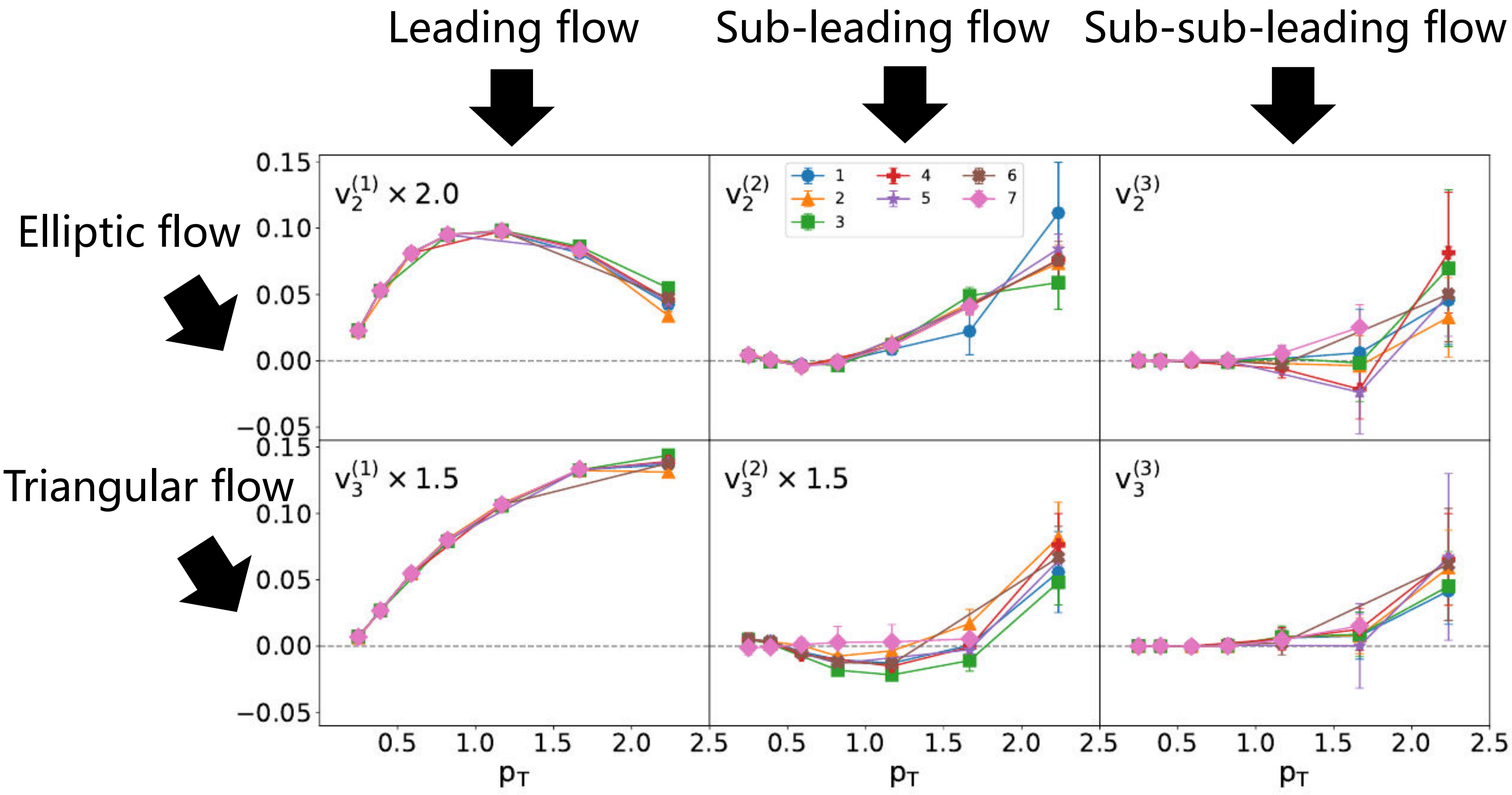



Drop one $p_T$ bin each time,
and redo the PCA

PCA will try to mix these two modes!

Will the modes still be stable?

# Problem 1: How to choose $p_T$ bins?




Different choice of $p_T$ bins can introduce systematic errors!
PCA modes are sensitive to our choice of $p_T$ bins!

# Problem 2 : Normalization

**Traditional PCA**

$$\langle V_{n\Delta}(p_a, p_b)\rangle = \langle V_n(p_a) V_n^*(p_b)\rangle$$

⇓ PCA

$$V_n(p_T) = \zeta_n^{(1)} V_n^{(1)}(p_T) + \zeta_n^{(2)} V_n^{(2)}(p_T) + \zeta_n^{(3)} V_n^{(3)}(p_T) + \cdots + \zeta_n^{(k)} V_n^{(k)}(p_T)$$

⇓ Normalize with $\langle M(p_T)\rangle$

$$v_n^{(\alpha)}(p_T) = \frac{V_n^{(\alpha)}(p_T)}{\langle M(p_T)\rangle}$$

**New PCA**

$$\langle V_{n\Delta}(p_a, p_b)\rangle = \langle V_n(p_a) V_n^*(p_b)\rangle$$

⇓ Normalize with $\langle M(p_T)\rangle$

$$v_{n\Delta}(p_a, p_b) = \frac{\langle V_{n\Delta}(p_a, p_b)\rangle}{\langle M(p_a)\rangle\langle M(p_b)\rangle}$$

$$\tilde{v}_n(p_T) = \frac{V_n(p_T)}{\langle M(p_T)\rangle}$$

⇓ PCA

$$\tilde{v}_n(p_T) = \zeta_n^{(1)} \tilde{v}_n^{(1)}(p_T) + \zeta_n^{(2)} \tilde{v}_n^{(2)}(p_T) + \zeta_n^{(3)} \tilde{v}_n^{(3)}(p_T) + \cdots + \zeta_n^{(k)} \tilde{v}_n^{(k)}(p_T)$$

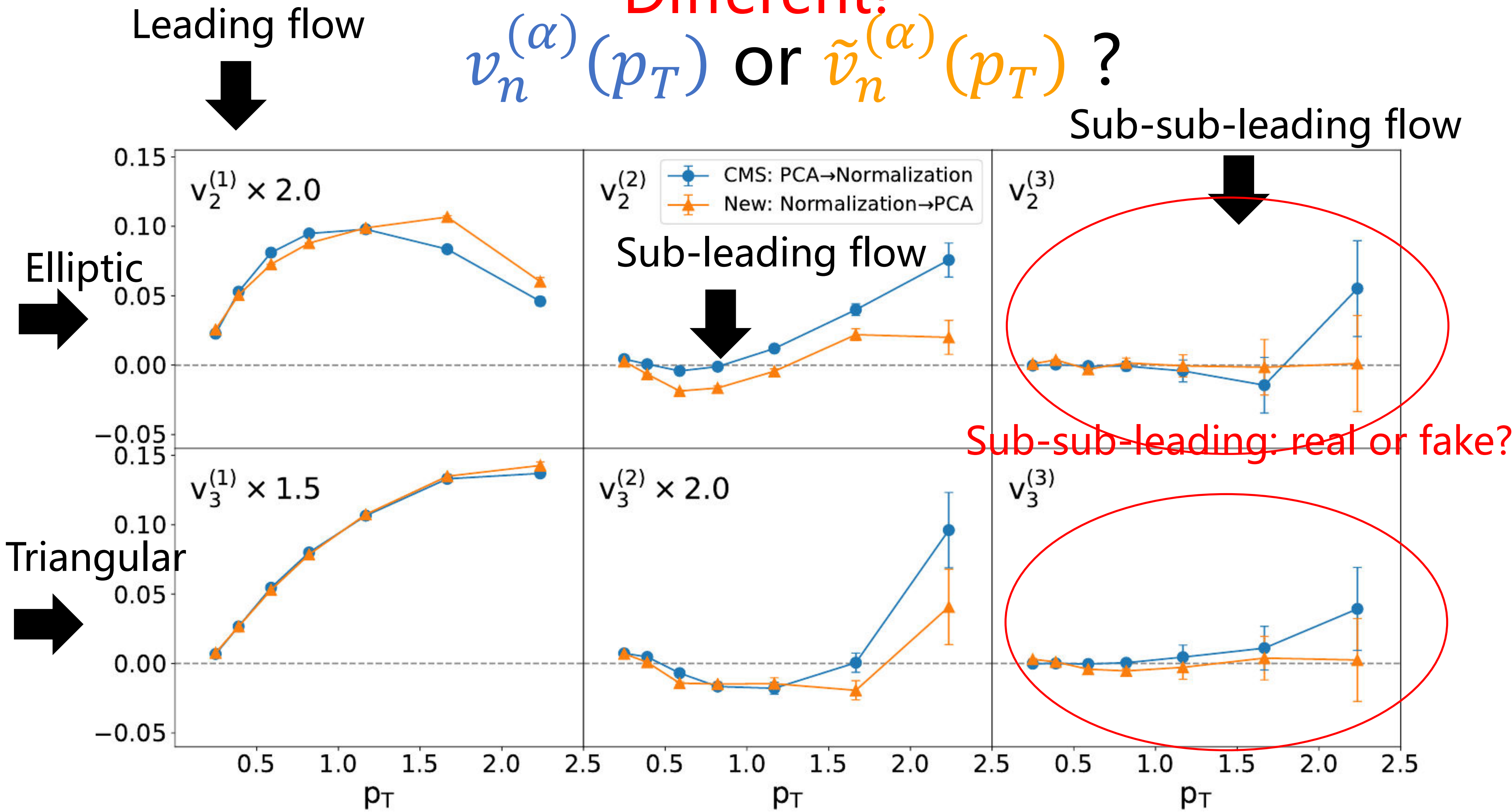
$$\tilde{v}_n^{(\alpha)}(p_T)$$

$v_n^{(\alpha)}(p_T)$ ⟷ $\tilde{v}_n^{(\alpha)}(p_T)$: Different?

# Problem 2 : Normalization

Different!

$v_n^{(\alpha)}(p_T)$ or $\tilde{v}_n^{(\alpha)}(p_T)$ ?




But which scheme can reveal more physics about initial profiles?
More analysis should be done to fully unravel the mystery of PCA!

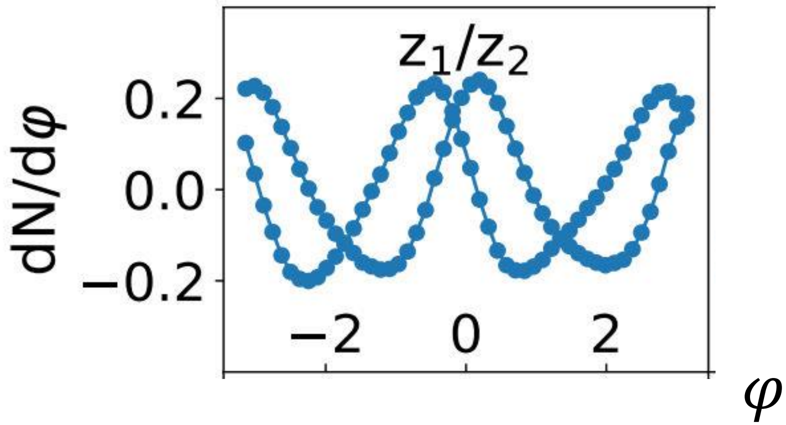
# Conclusion for paper 2

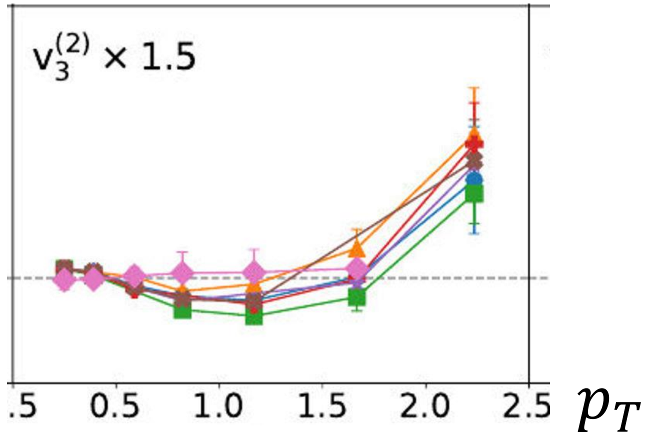
- The choice of $p_T$ bins introduces systematic errors, but we have no guidance from physics about how to choose them
- Technically, the normalization procedure before/after PCA also lead to different results. Which is the real physics? Need more discussion.

# Summary & Outlook

# Principal Component Analysis:

- Unsupervised learning (dimensionality reduction)
- Good at discovering hidden correlations in data




PCA for flow discovery

- Integrate $p_T$, so stable
- discover flow automatically
- Reduce mode coupling

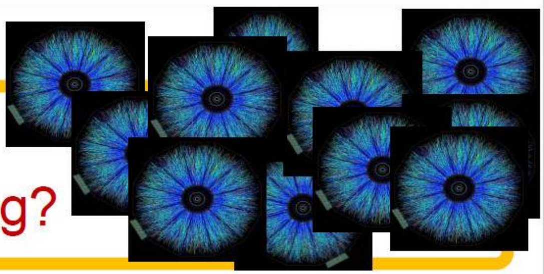
PCA for sub-leading flow

- $p_T$ differential, sensitive to $p_T$ bins
- Ambiguity in normalization

All in all, PCA is a transparent yet powerful machine learning tool to extract main information/ hidden correlations in data! But we should also be more careful about its results.

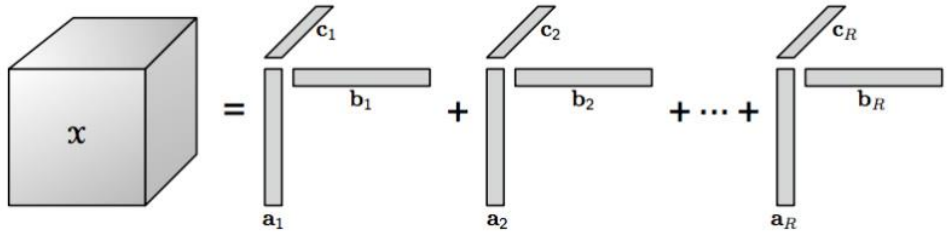
## Outlook

Can PCA detect modes or structures from the massive data that is not realized or easily defined by human being?



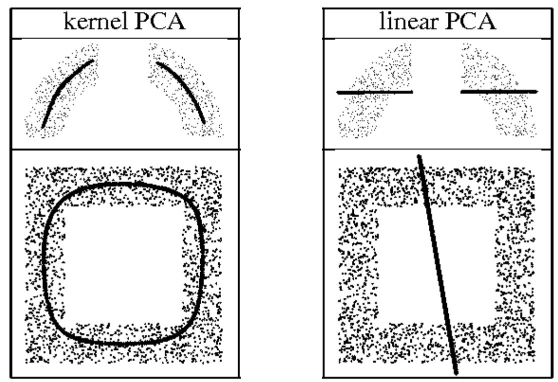
# More advanced PCAs ......

- High-order PCA




Suitable for high-order data, not constrained to 2-part correlation matrix

- Kernel PCA




Able to capture non-linearity. Hope can help study non-linearity in hydro.

- Robust PCA


Hope: Eliminate non-flow in the single particle distribution level, without the trouble to construct 2-part data.

Observed = Collective Flow + non-flow

Thank you
for your attention!

# VI. Back up

# Model Details

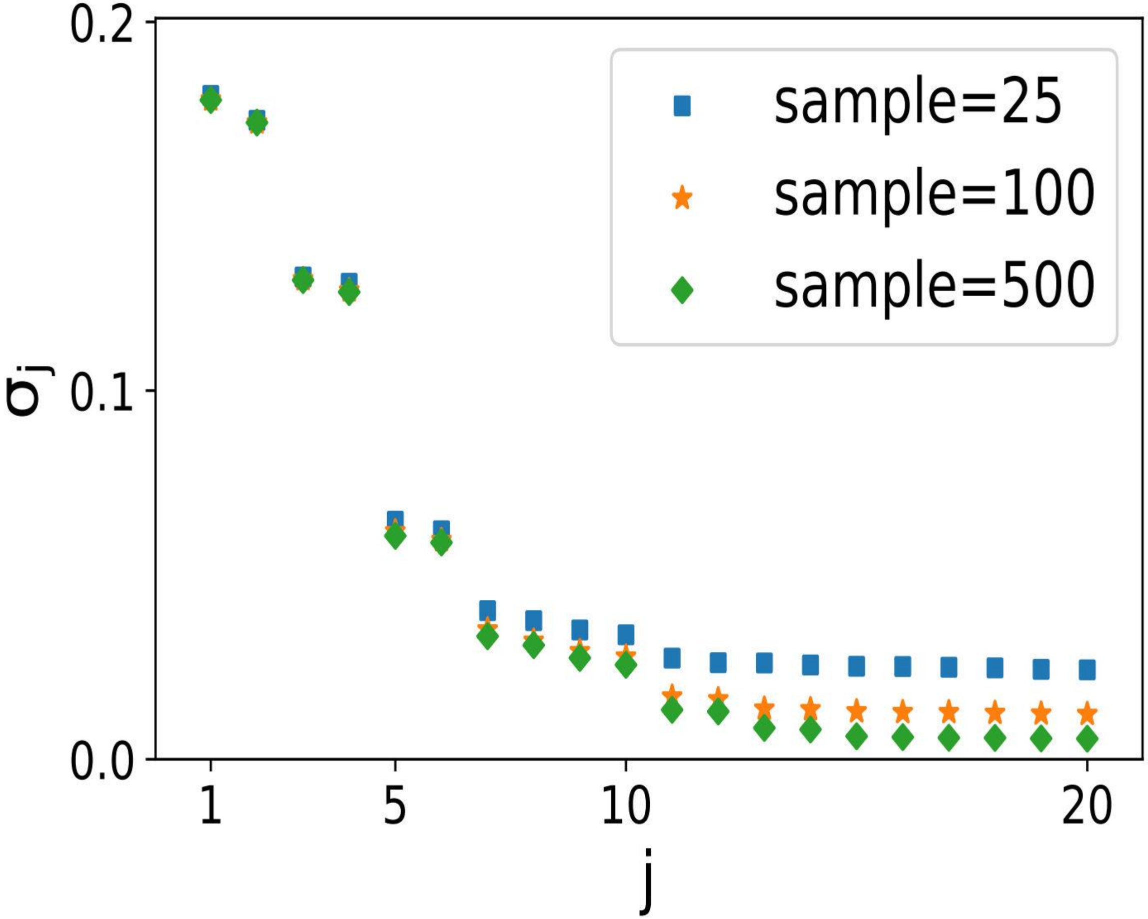
- 2.76 A TeV Pb+Pb
- Viscous Hydro: VISH2+1
- EOS: s95-PCE
- Initial condition: TRENTo
- Hydrodynamic starting time $\tau_0 = 0.6fm/c$
- Decoupling temperature $T_{sw} = \frac{148MeV}{c}$
- $0.3 < p_T < 3GeV$, Pions only
- 0%-10%,……,50%-60% totally 6 centrality bins, 2000 events for each bin

# PCA Implementation

- Python – sklearn
- From sklearn.decomposition import PCA
- Mode cut $k = 12$
- https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html

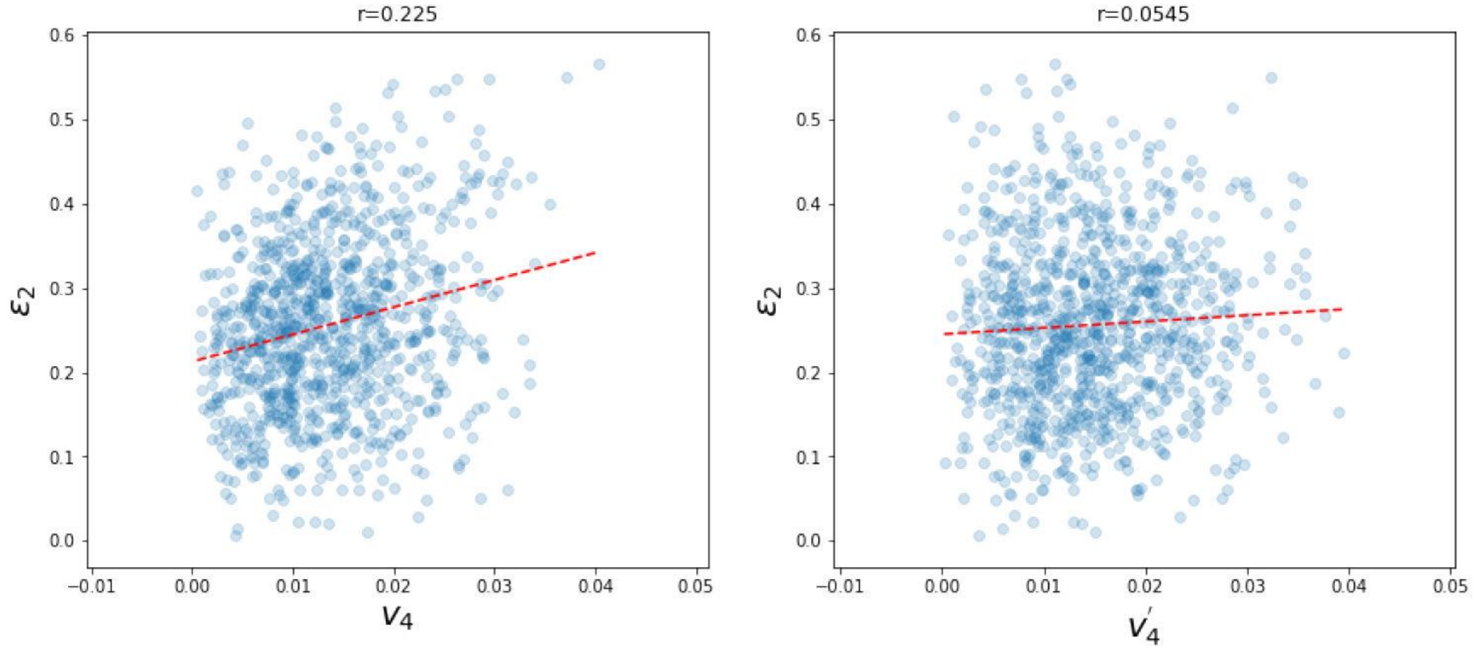
# Signal & Noise

Copper-Fryer: $$\frac{dN}{dy p_T dp_T d\varphi} = \int_\Sigma \frac{g}{(2\pi)^3} p^\mu d^3\sigma_\mu f(x,p)$$



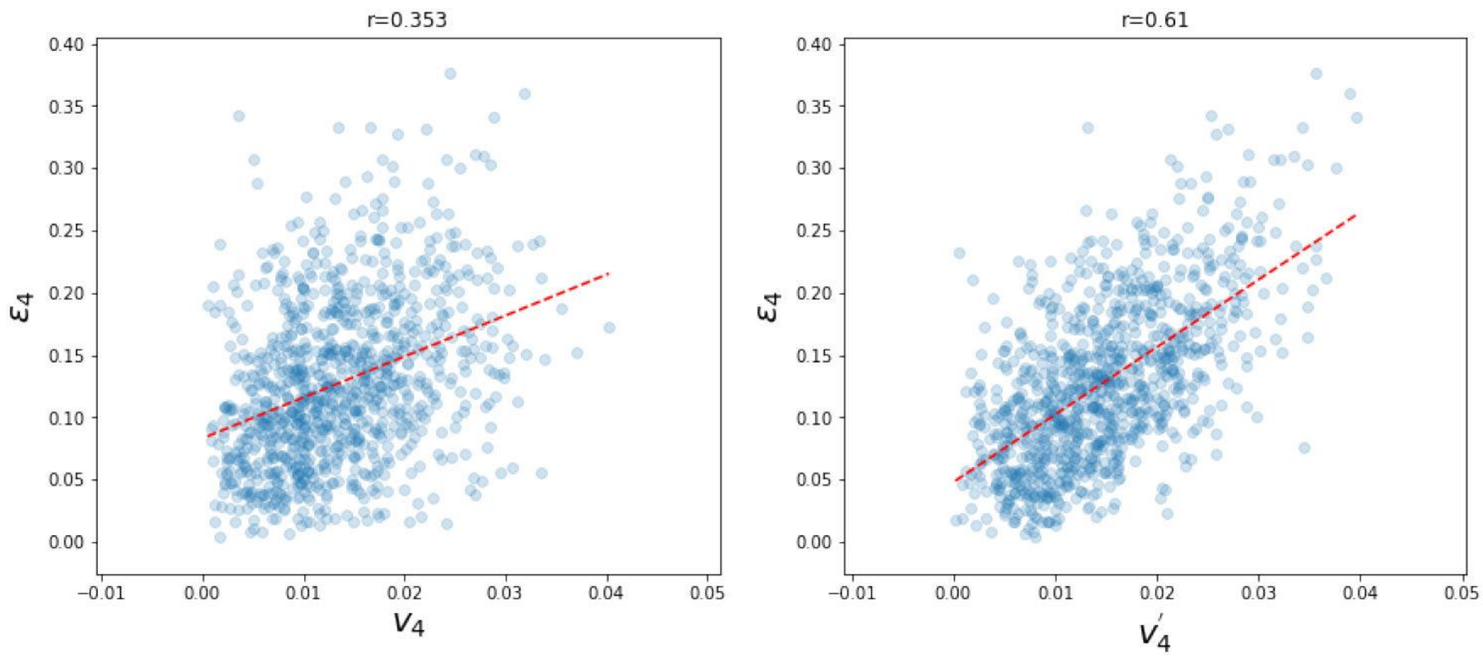
# Bases Mixing ($2^{nd}$ and $4^{th}$)

- Left : Fourier, $v_4 \sim \varepsilon_2$
- Right : PCA, $v_4' \sim \varepsilon_2$



# Bases Mixing ($2^{nd}$ and $4^{th}$)

- Left : Fourier, $v_4 \sim \varepsilon_4$
- Right : PCA, $v_4^{'} \sim \varepsilon_4$

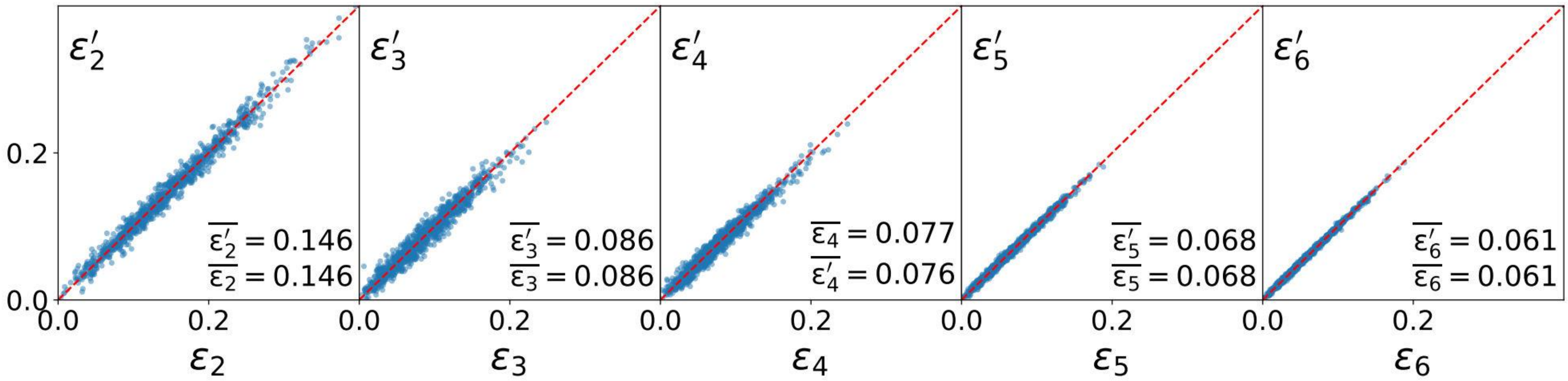


# PCA for Initial Profiles

## Smoothing Procedure

$$\left(\frac{dS}{d\varphi}\right)_{smooth} = \int K(\varphi', \varphi)\frac{dS}{d\varphi'}d\varphi'$$

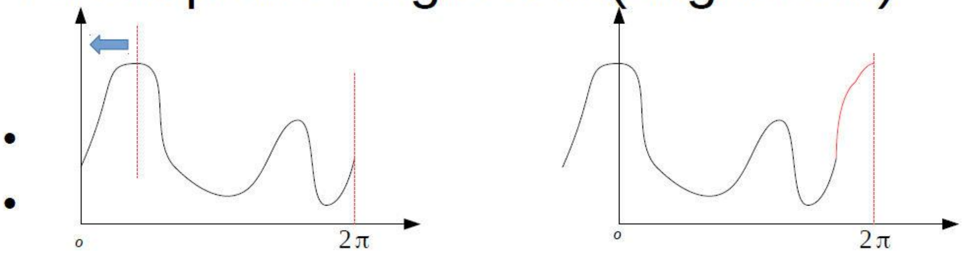
$$K(\varphi', \varphi) = \frac{1}{\sqrt{2\pi}a}e^{-\frac{(\varphi'-\varphi)^2}{2a^2}}, a = 0.251\, rad$$

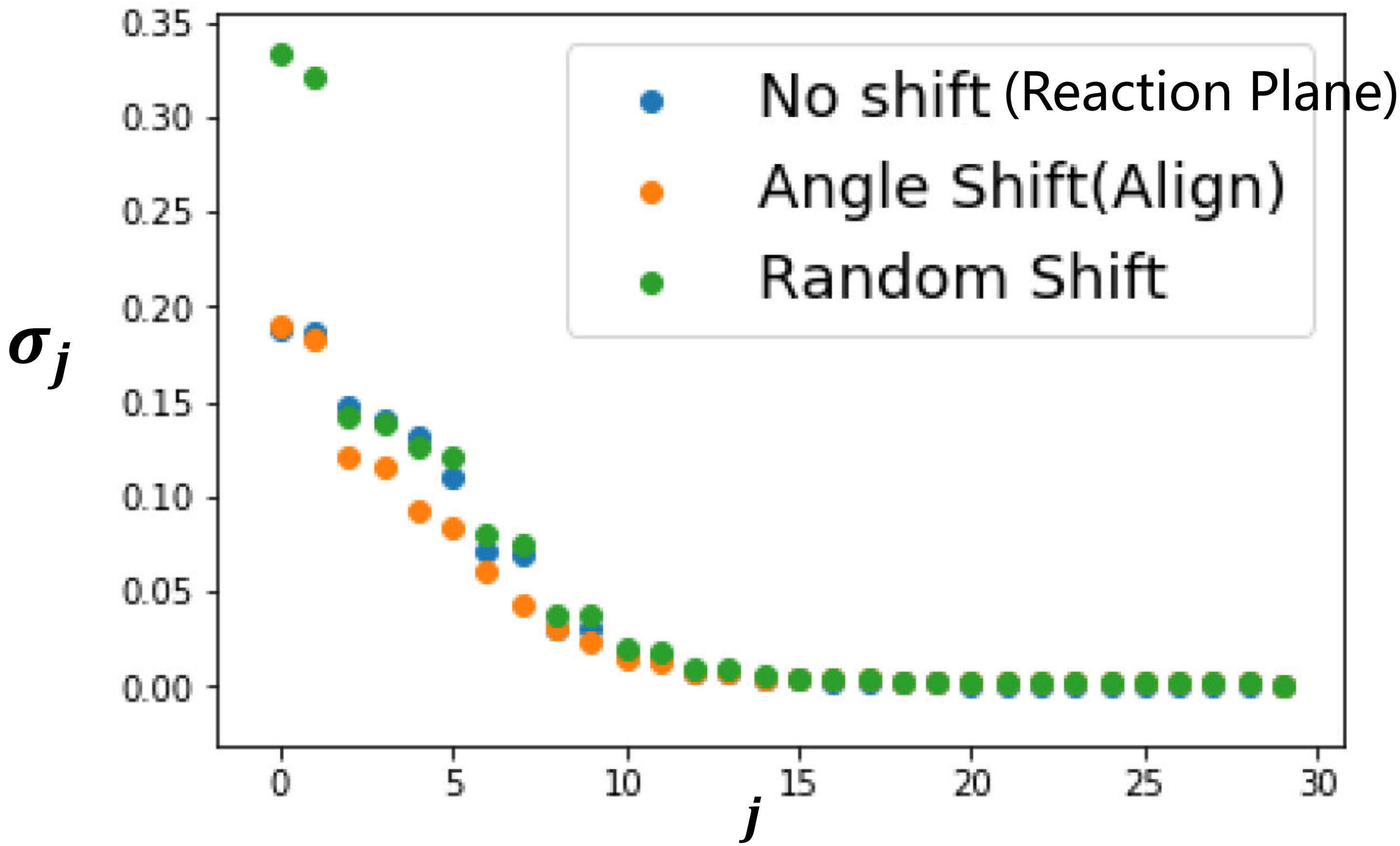



For initial states, PCA=Fourier

# Angle shift

Event plane Angle shift(alignment)



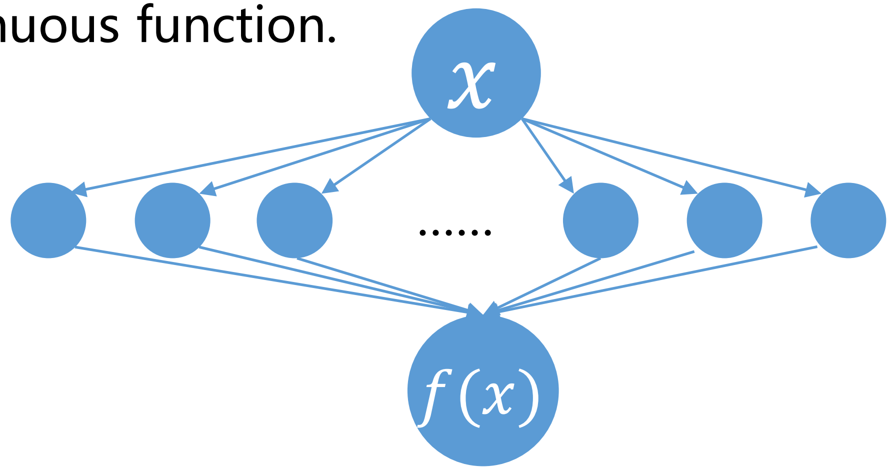
# Angle Shift

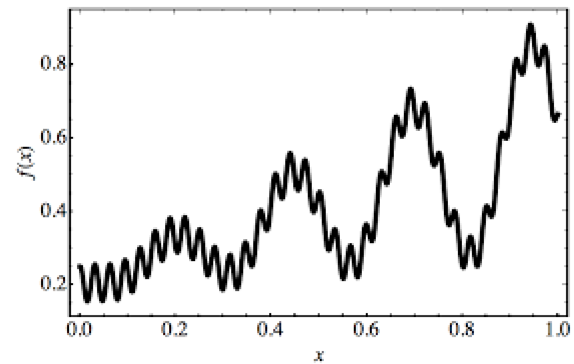
- The PCA is implemented in the reaction plane, so that eigenvectors mix 2nd and 4th flow harmonics.
- If randomly shifting every event (as in experiments), the bases will be exact Fourier bases due to rotational symmetry.

# Good about Neural Networks

## Universal Approximation Theorem:

A neural network with one layer but infinitely many neurons can approximate any continuous function.

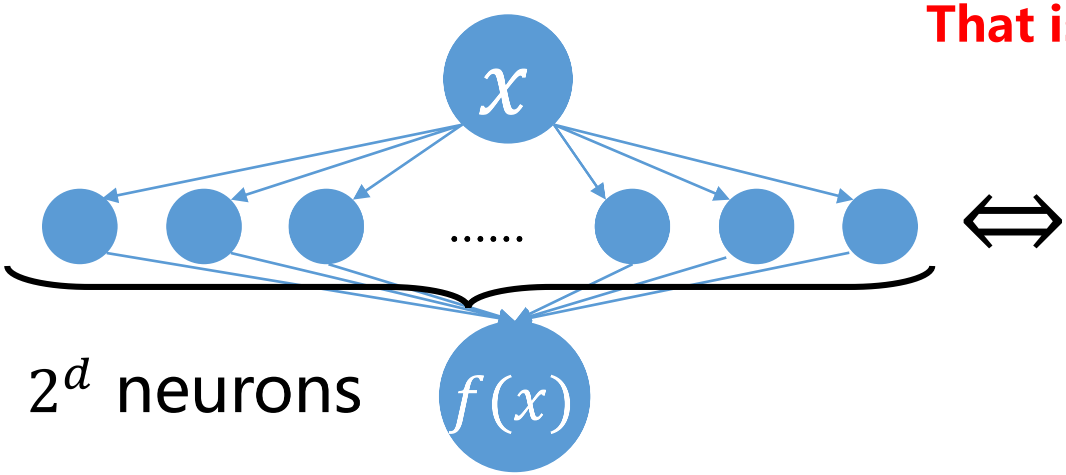


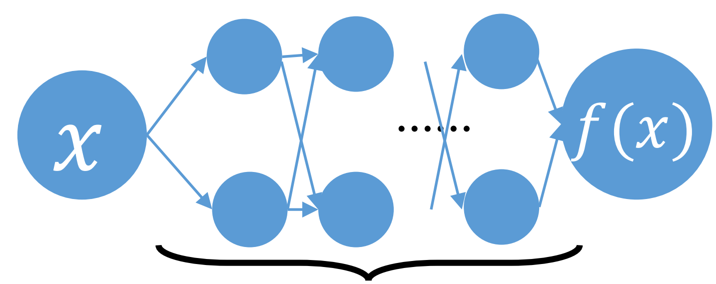

## Width v.s. Deep Theorem:

An exponentially number of neurons in one layer = linear number of layers

**That is why we need DEEP learning!**




$2^d$ neurons




$d$ layers, $2d$ neurons

# How to train a model?

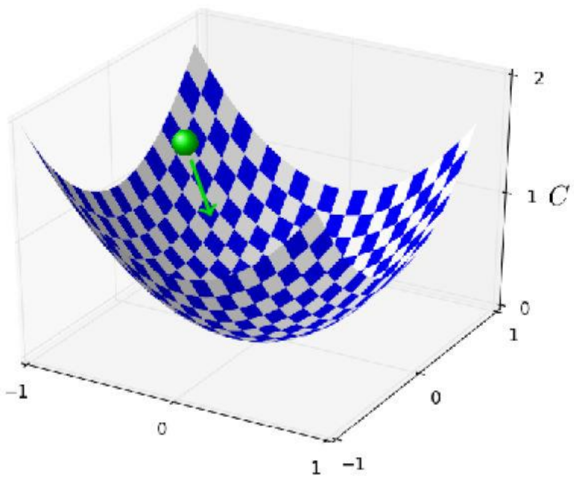
# Train/Evaluate a model

- The evaluation is to evaluate the difference between the network's outputs and learning targets. — loss function

For supervised learning, since there has been a target $y(x)$, loss function can be defined as

- $\ell(\theta) = \frac{1}{2n} \sum_x [y(x) - \hat{y}(x)]^2$
- $\ell(\theta) = -\frac{1}{n} \sum_x [y(x) \ln \hat{y}(x) - (1 - y(x)) \ln(1 - \hat{y}(x))]$

Train a model ⇔ Minimize the loss function




**Stochastic Gradient Descent**

$$\theta' = \theta - \epsilon \frac{\partial \ell(\theta)}{\partial \theta}$$

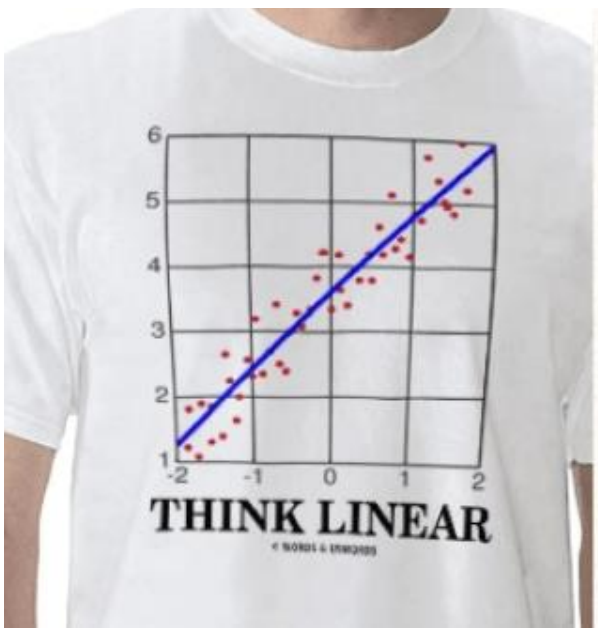
Ian Goodfellow, Yoshua Bengio, and Aaron Courville, http://www.deeplearningbook.org MIT Press, 2016

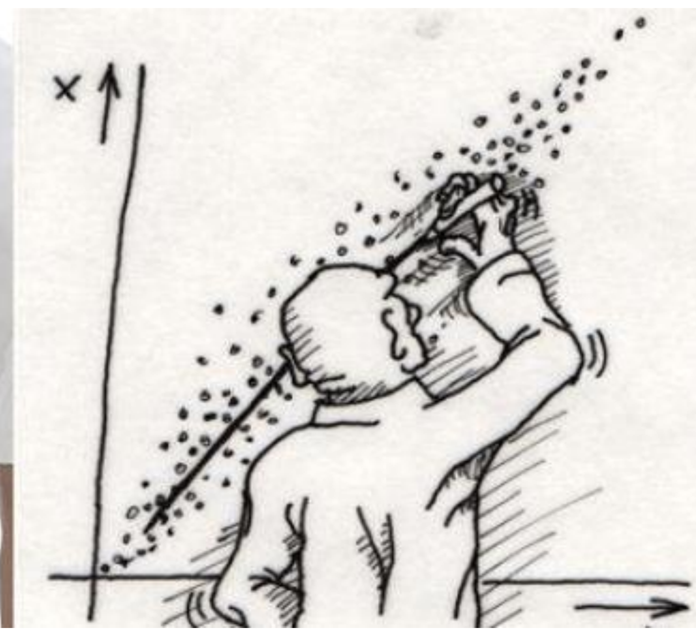
# What is Machine Learning?

**Machine learning** (**ML**) is the scientific study of algorithms and statistical models that computer systems use to effectively perform a specific task without using explicit instructions.

——wikipedia

Linear Regression is also Machine Learning!



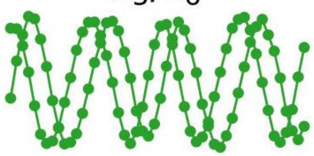



# How PCA bases mix Fourier bases?

# Bases Mixing (2nd and 4th)

$z_1/z_2$

$z_5/z_6$



$z$: PCA eigenmodes

$$\begin{pmatrix} z_1 \\ z_2 \\ z_5 \\ z_6 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \begin{pmatrix} \cos(2\phi) \\ \sin(2\phi) \\ \cos(4\phi) \\ \sin(4\phi) \end{pmatrix}$$

If the eigenmodes of PCA is the same as fourier bases, the mixing matrix $A$ should be identity. But actually, the matrix is not diagonal. Take data from centrality $30\% - 40\%$ for example

$$A = \begin{pmatrix} 0.956 & 0.295 & 0.213 & 0.053 \\ -0.295 & 0.956 & -0.057 & 0.215 \\ -0.217 & -0.041 & 0.960 & 0.209 \\ 0.035 & -0.215 & -0.219 & 0.951 \end{pmatrix}$$

# Bases Mixing ($2^{nd}$ and $4^{th}$)

It is interesting to find that the mixing matrix $A$ follows the form below for all centrality classes. The parameters do not hold, but the form does.

$$A = \begin{pmatrix} \cos(\theta_2) & \sin(\theta_2) & a\cos(\theta_2) & a\sin(\theta_2) \\ -\sin(\theta_2) & \cos(\theta_2) & -a\sin(\theta_2) & a\cos(\theta_2) \\ -a\cos(\theta_4) & -a\sin(\theta_4) & \cos(\theta_4) & \sin(\theta_4) \\ a\sin(\theta_4) & -a\cos(\theta_4) & -\sin(\theta_4) & \cos(\theta_4) \end{pmatrix}$$

To make notations easier, we denote

$$U_1 = \begin{pmatrix} \cos(\theta_2) & \sin(\theta_2) \\ -\sin(\theta_2) & \cos(\theta_2) \end{pmatrix}, U_2 = \begin{pmatrix} \cos(\theta_4) & \sin(\theta_4) \\ -\sin(\theta_4) & \cos(\theta_4) \end{pmatrix}$$

Note that $U_1$ and $U_2$ are just rotation matrix in 2-d Cartesian coordinate.

# Bases Mixing ($2^{nd}$ and $4^{th}$)

$$A = \begin{pmatrix} U_1 & aU_1 \\ -aU_2 & U_2 \end{pmatrix}$$

It is interesting to note that $A$ can be decomposed into multiplication of simpler matrices.

$$A = \begin{pmatrix} U_1 & 0 \\ 0 & I_2 \end{pmatrix} \begin{pmatrix} I_1 & 0 \\ 0 & U_2 \end{pmatrix} \begin{pmatrix} I_2 & a \\ -a & I_2 \end{pmatrix}$$

A new observable defined by PCA to characterize v2/v4 correlation

If we sees matrix as an operation, then the operation was decomposed into three steps:

- First, PCA mixed 2nd harmonic flow and 4th harmoninc flow, by adjusting $a$.
- Second, PCA mixed within $4th$ order plane by adjusting $\theta_4$.
- Third, PCA mixed within $2nd$ order plane by adjusting $\theta_2$.