Zoo of Principal Component Analysis (PCA)

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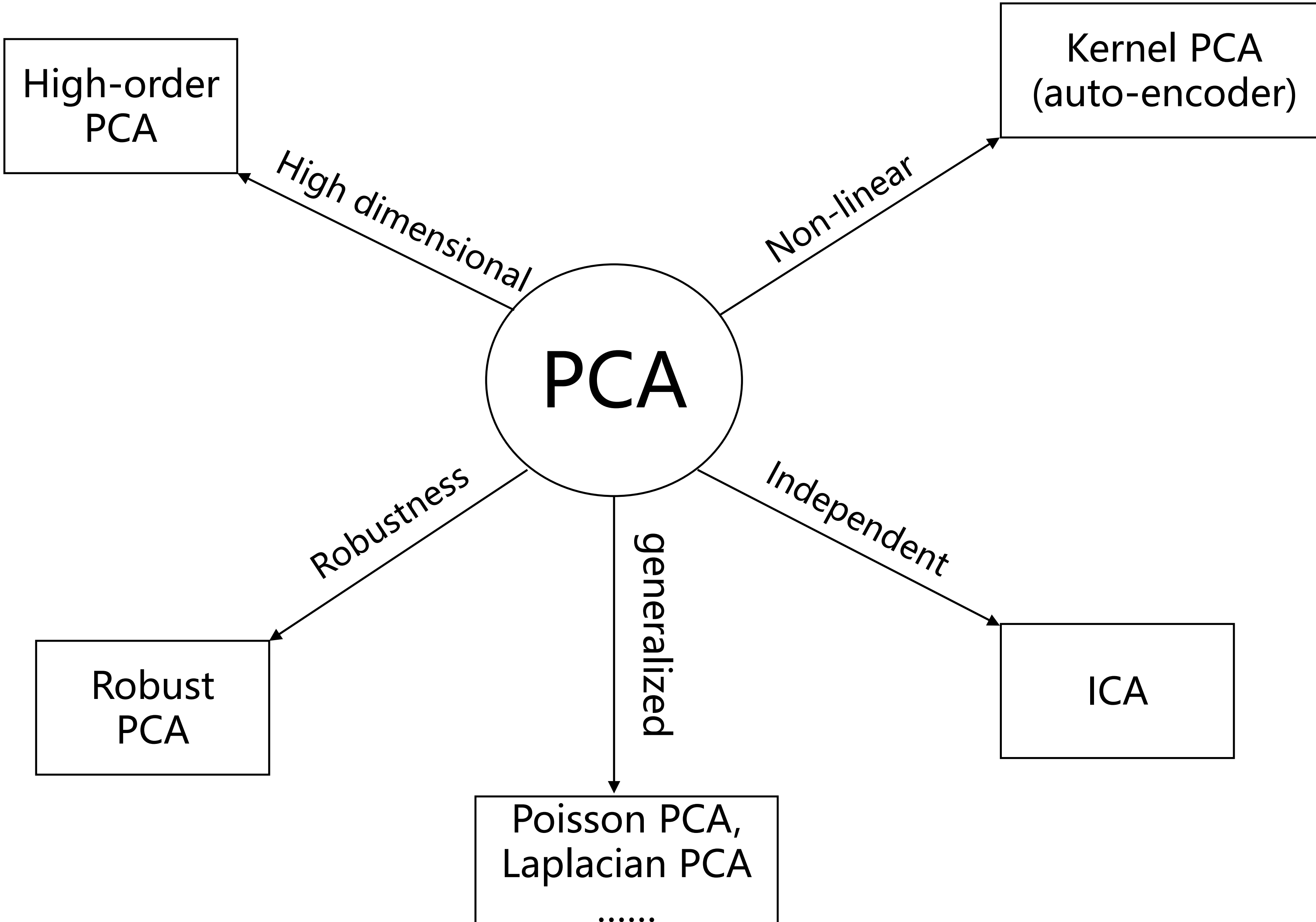


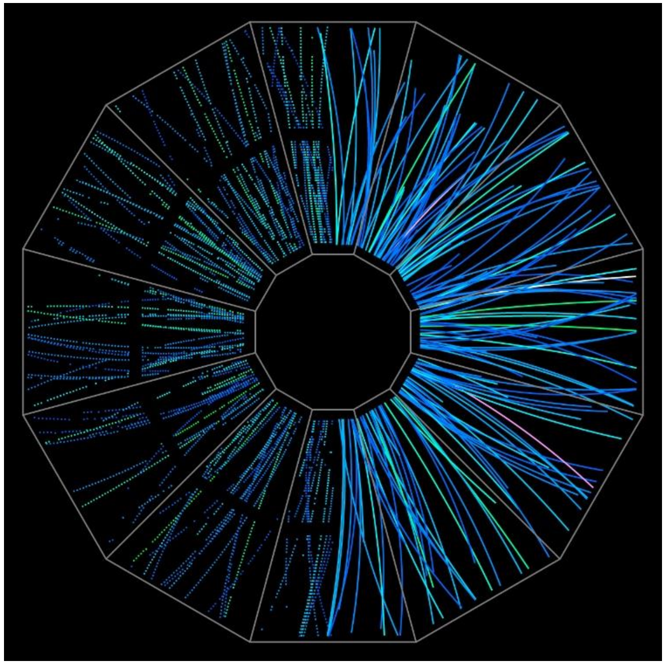
Different PCA suitable for different physics problems

1. Kernel PCA (auto-encoder)

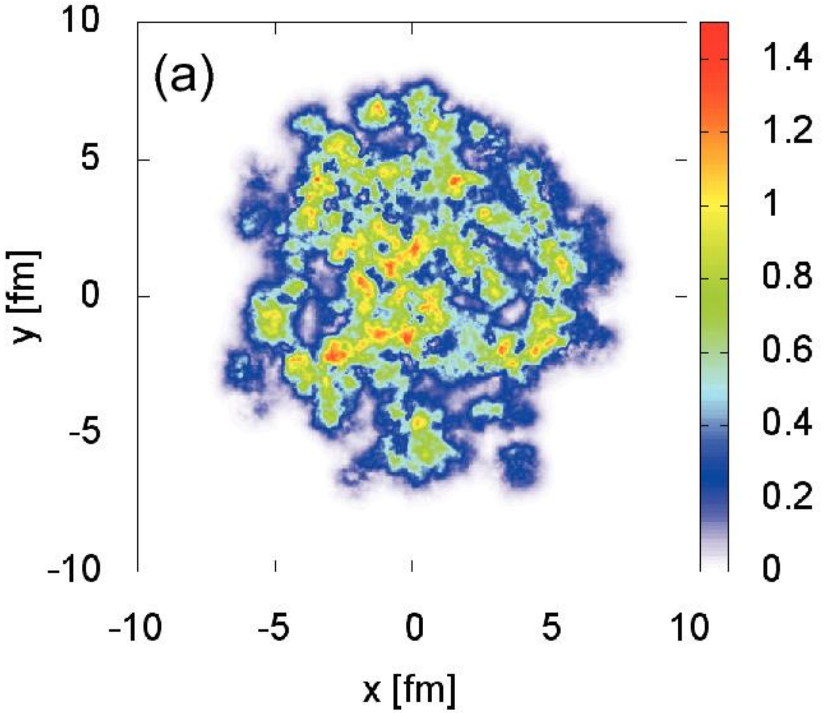
—— Learn the mapping from particle distribution to initial geometry

The wildest dream

Final Particle Tracks



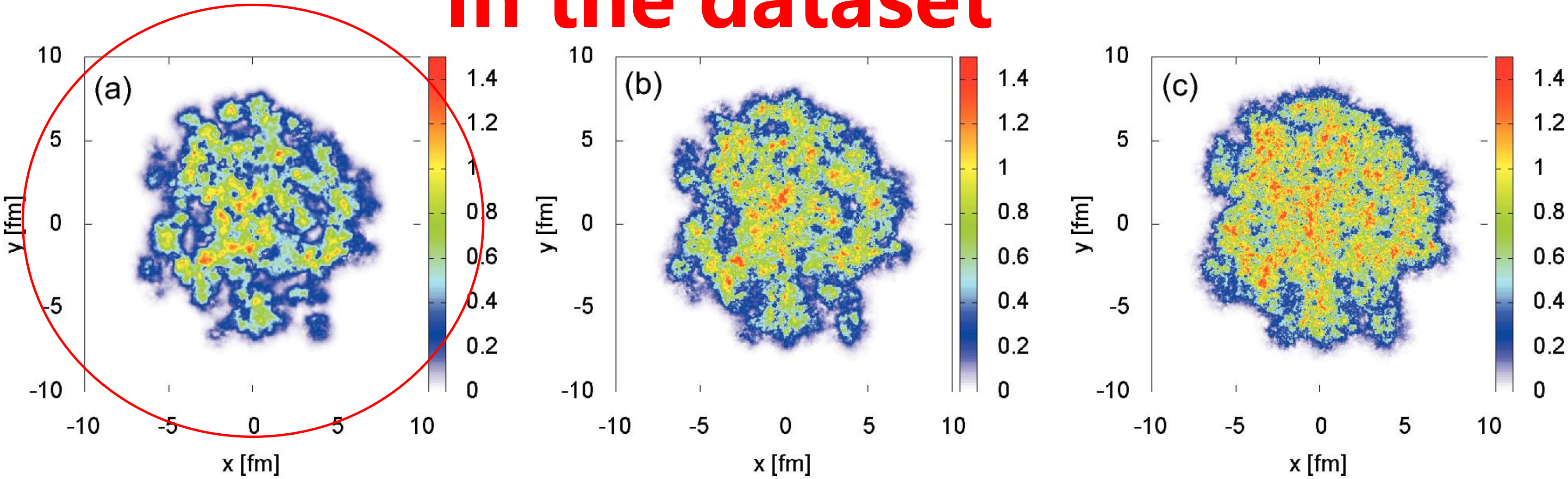
Initial fluctuations



Going back in time ?
Can learn from Monte Carlo data

Change v2 a bit, initial ?

In the dataset



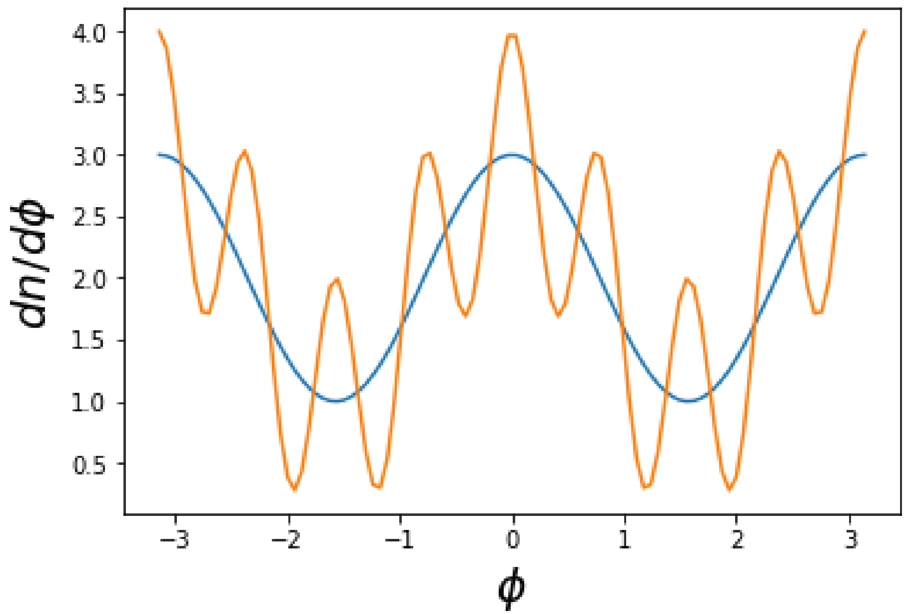
Hydro

generate

generate

V2 = 0.1 → V2 = 0.11 → V2 = 0.12

Ill-defined ?



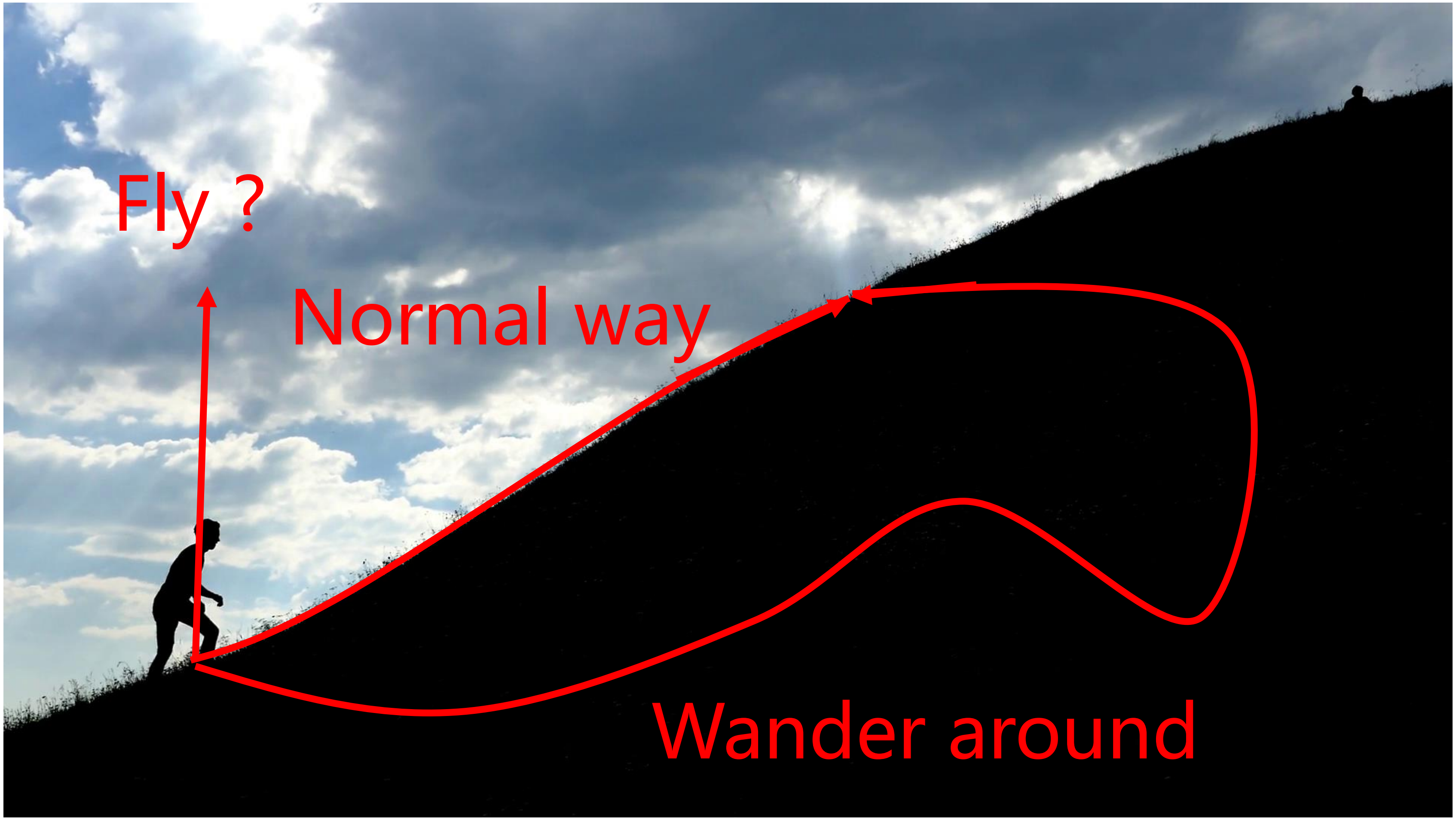
Different fluctuations size, but same v2 !

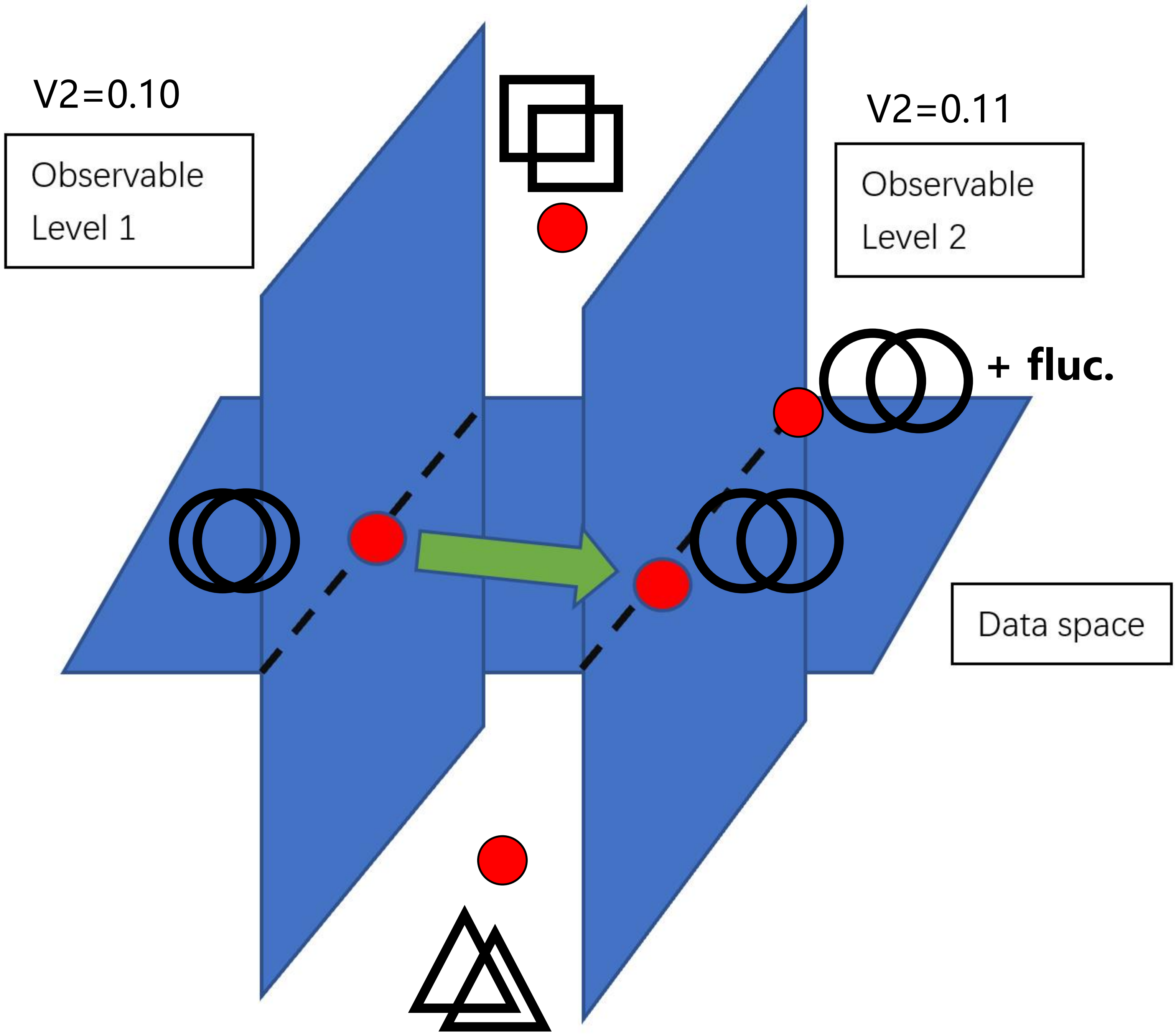
Not a one-to-one mapping problem ?!

Add constraint:

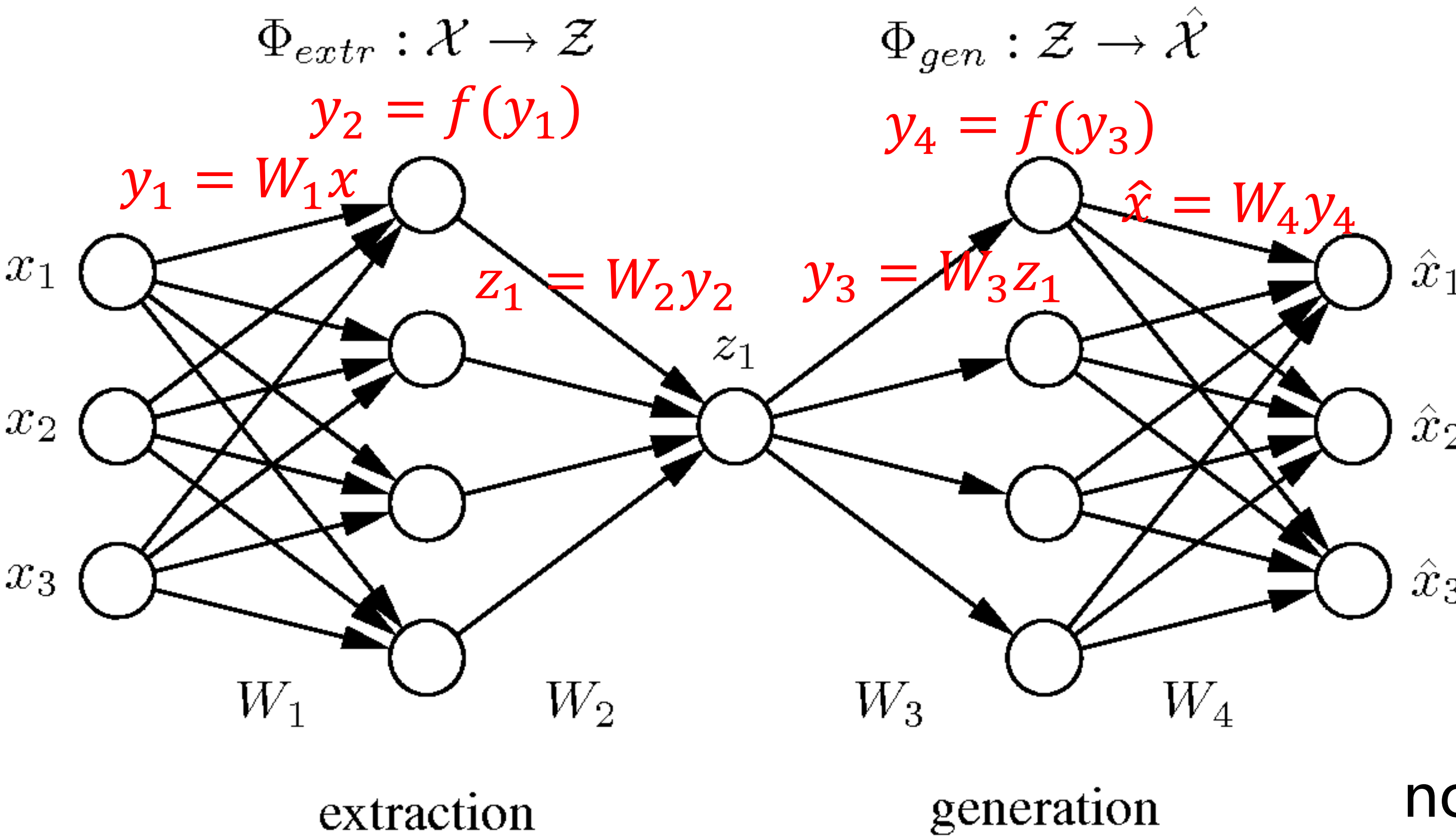
- The initial profile can be generated from the initial model – lie on "initial manifold"
- As little change as possible – "gradient"

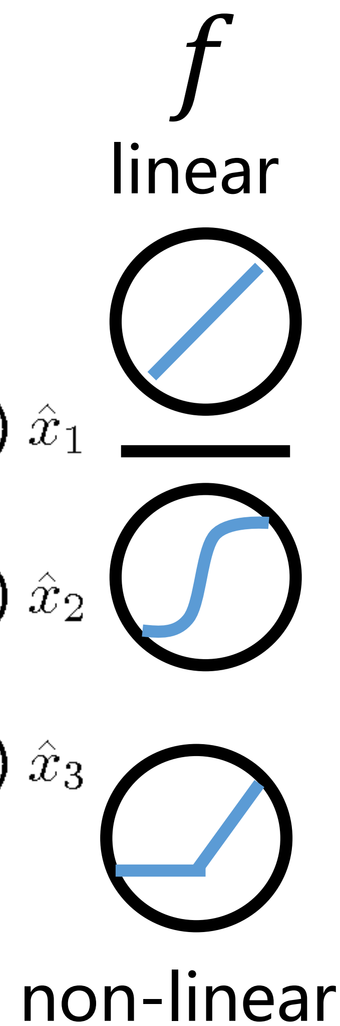
When you climb a hill ……




V2=0.10
Observable
Level 1
V2=0.11
Observable
Level 2
+ fluc.
Data space

Auto encoder

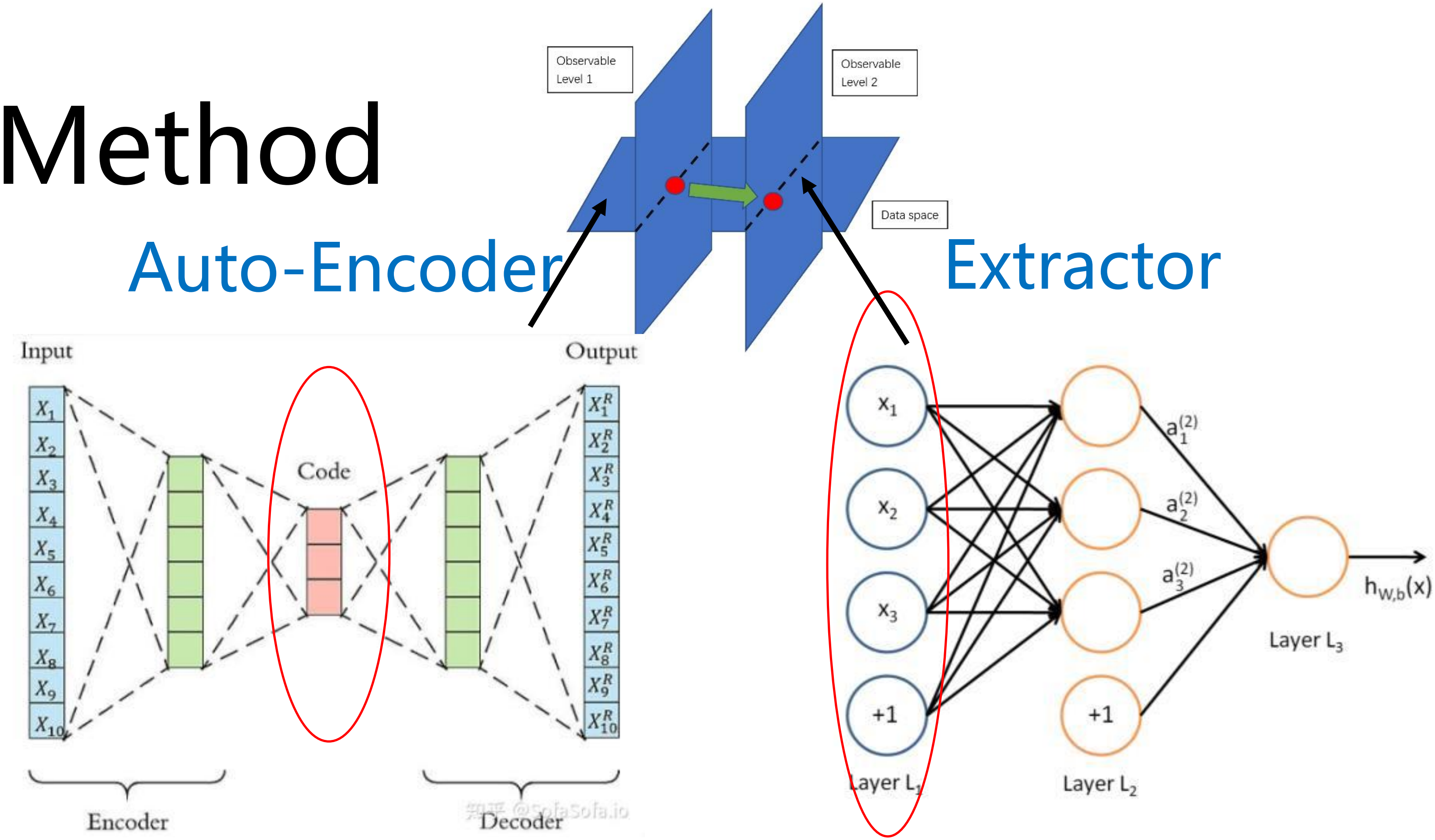




f linear: PCA

f non-linear: kernel PCA

Method



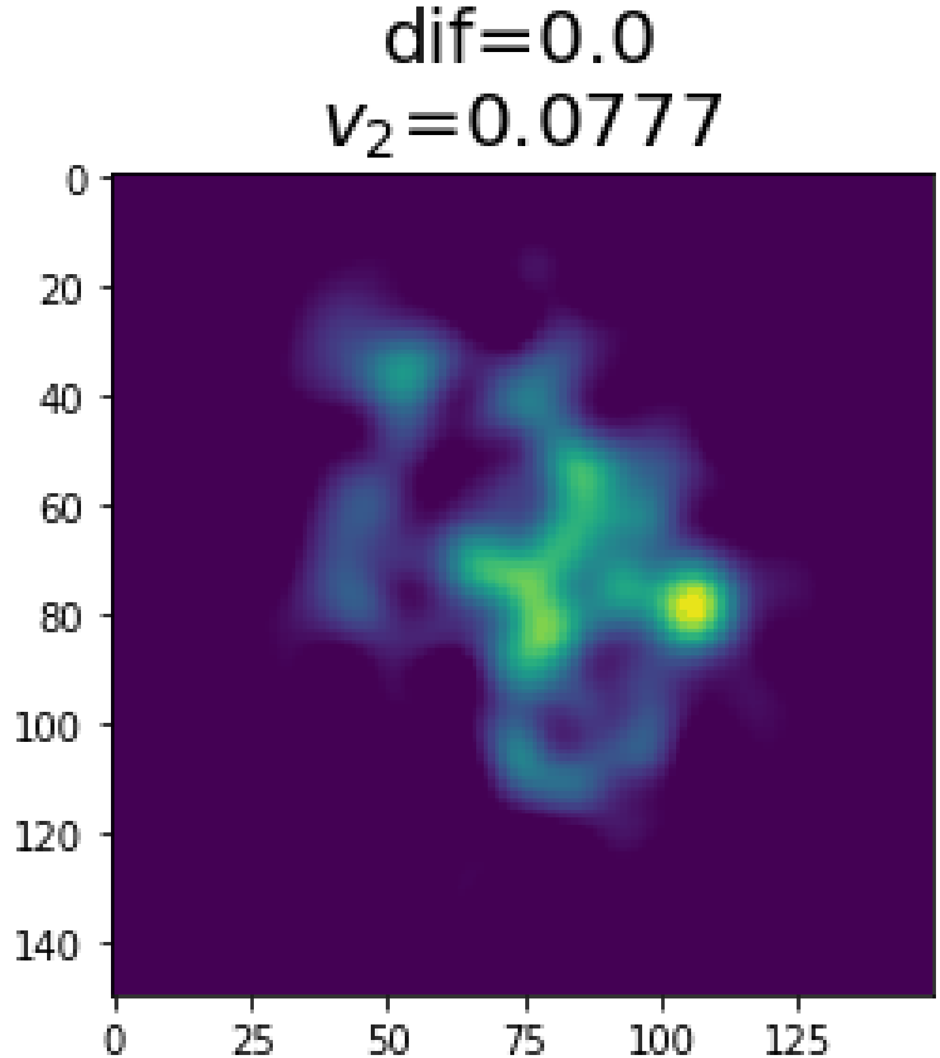
Step 1: unsupervised learning, train the autoencoder. "Code" represents the most important information.

Step 2: supervised learning. we have the "Code", and an observable. we train the neural network to fit the observable. After training, the "gradient" can be computed efficiently.

Step 3: Feed the gradient to the decoder, get the new profile.

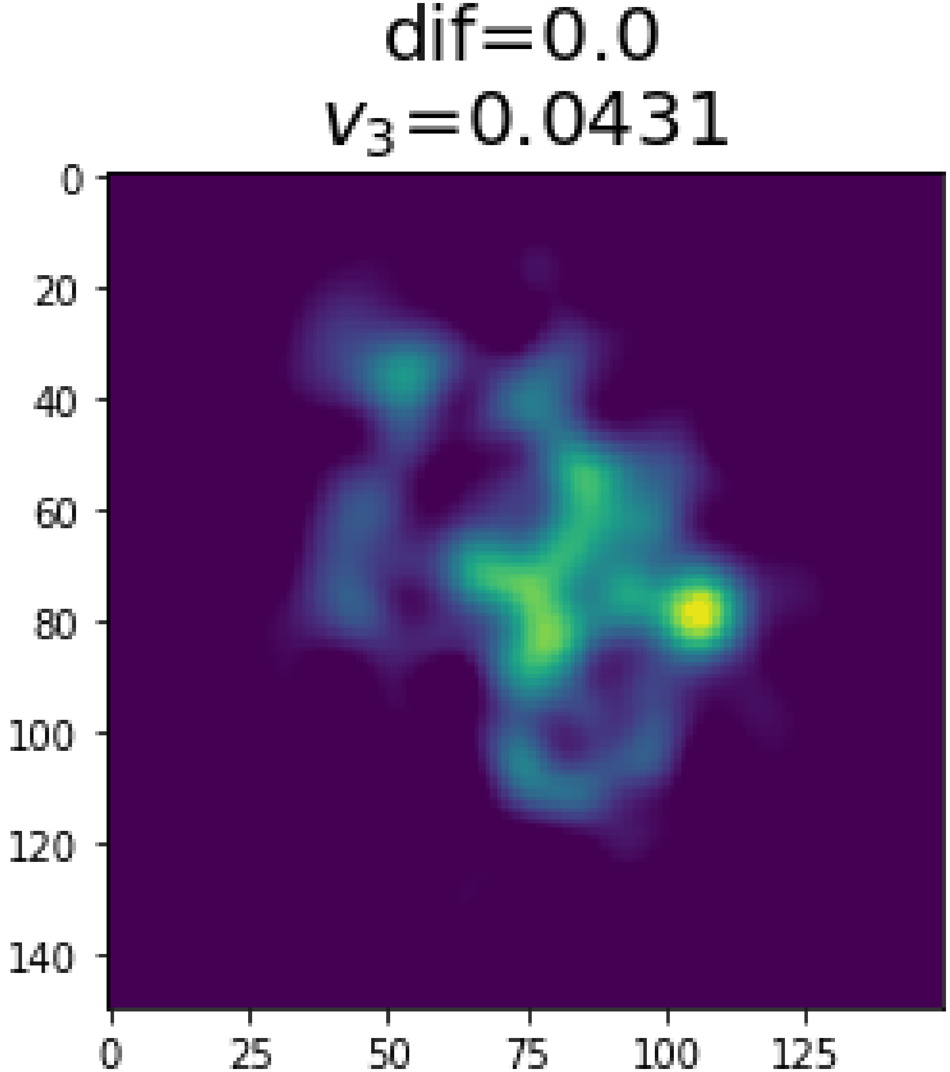
V2 Results

- Hydro data: Trento + Vishnu + iss



V3 Results

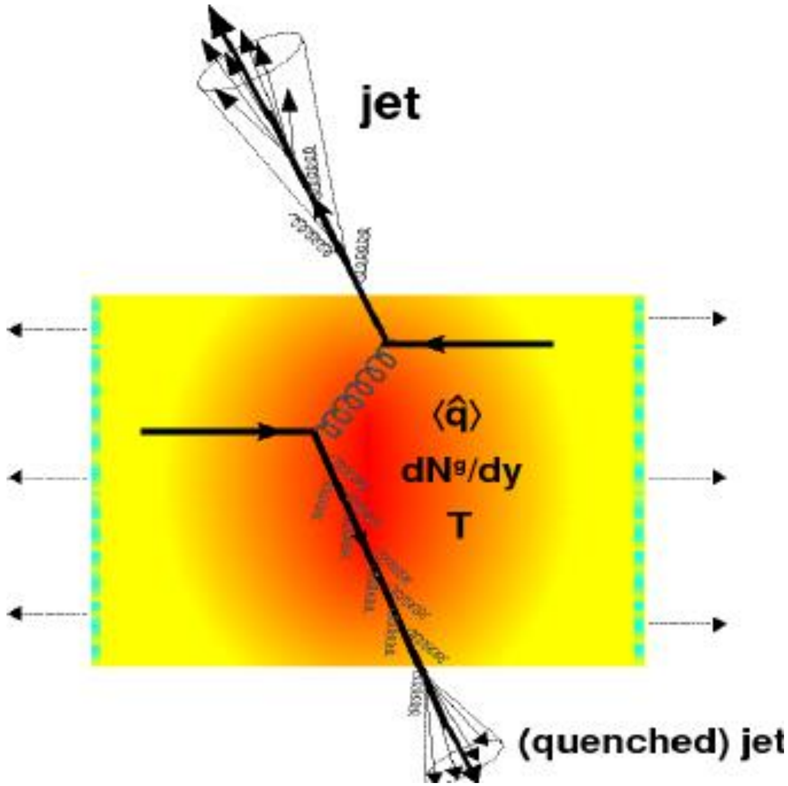
- Hydro data: Trento + Vishnu + iss



2. Robust PCA

—— automated Learning to separate flow and non-flow

Heavy-Ion collisions



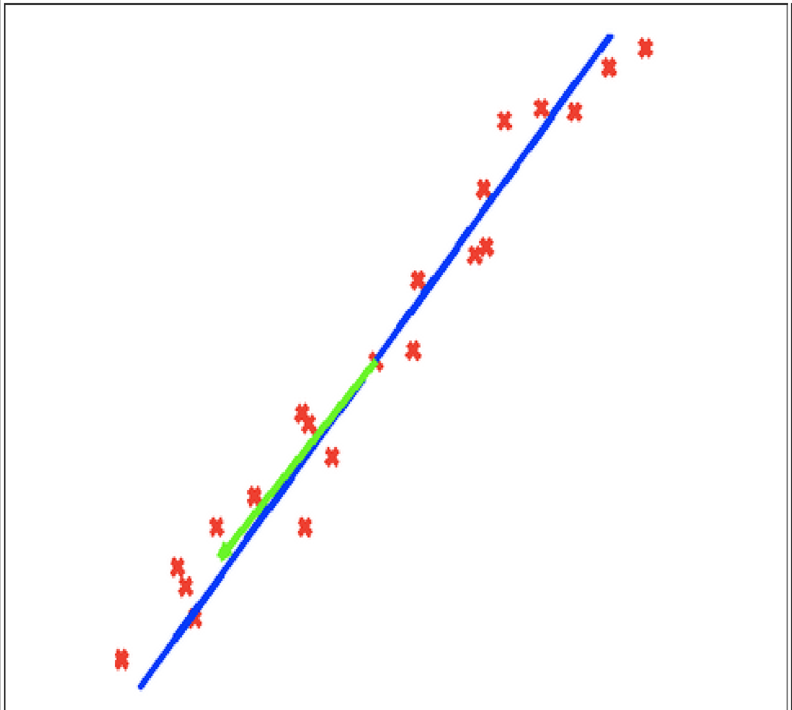
Video Surveillance

QGP	Jet	Background	Foreground
Thermalized	Not thermalized	static	moving
Long range correlation	Short range correlation	Long correlation In time	Short correlation (sparse) in time

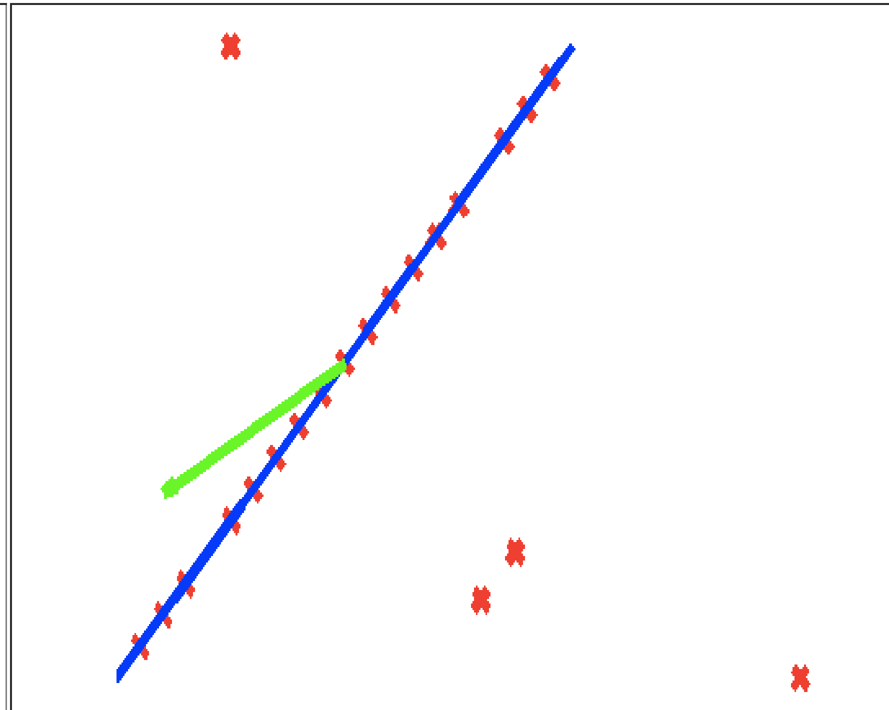
Learn Flow/Non-flow with many events of heavy-ion collisions ? Learn Background/foreground with many snapshots of a single video

What’s wrong with traditional PCA?

Blue: Robust PCA; Green: Traditional PCA

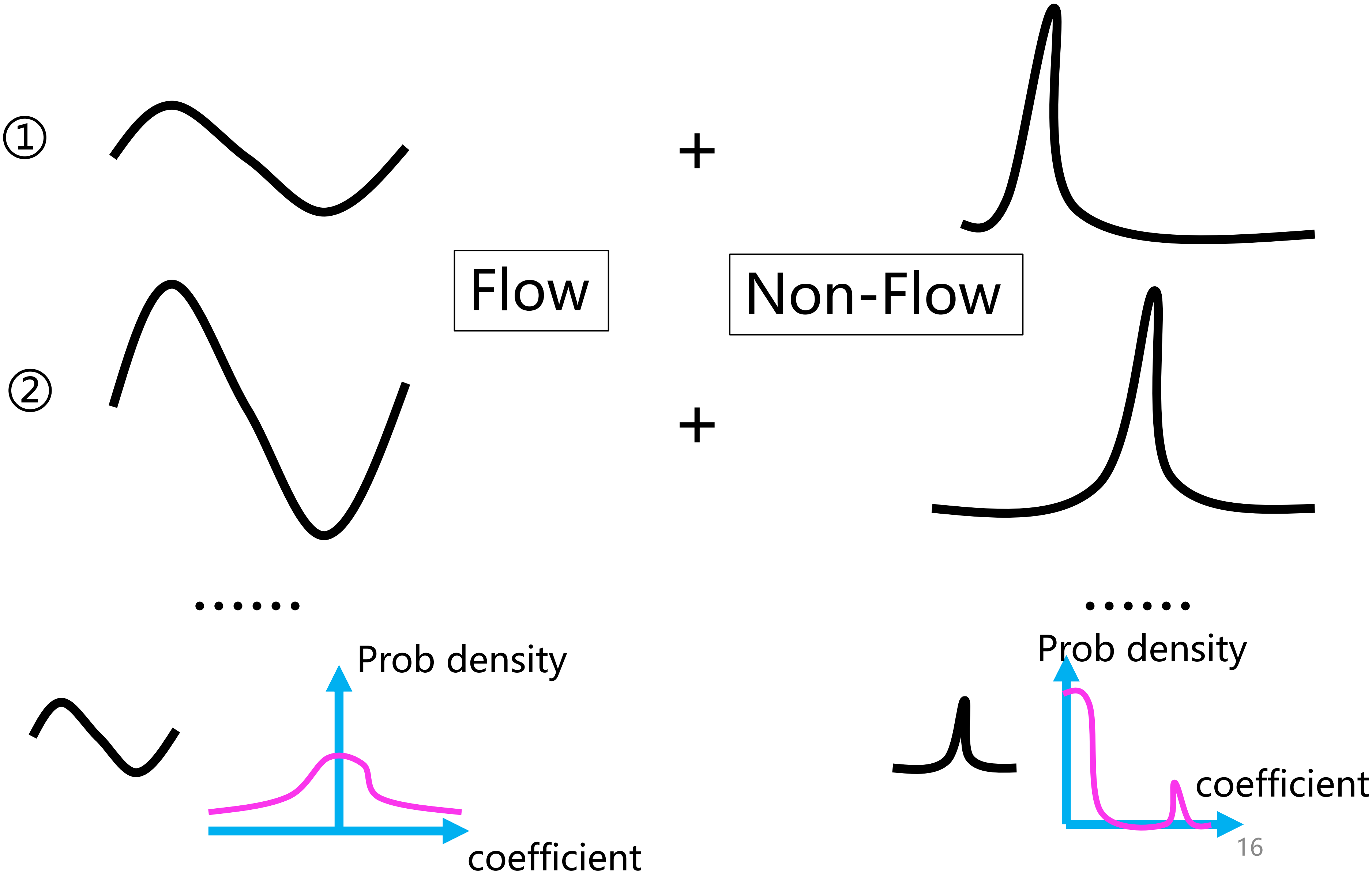


Samples (red) from a one-dimensional subspace (blue) corrupted by small Gaussian noise. The output of classical PCA (green) is very close to the true subspace despite all samples being noisy.



Samples (red) from a one-dimensional subspace (blue) corrupted by sparse, large errors. The principal component (green) is quite far from the true subspace even when over three-fourths of the samples are uncorrupted.

Why can we do this?



No free parameter !

X: input; D: low rank; X-D: sparse matrix

$$\min_{D} \quad rank(D) + \|X - D\|_0$$

$$\min_{\tilde{D}} \quad \|D\|_* + \lambda\|X - D\|_1$$

sum of singular values sum of all elements (absolute value)

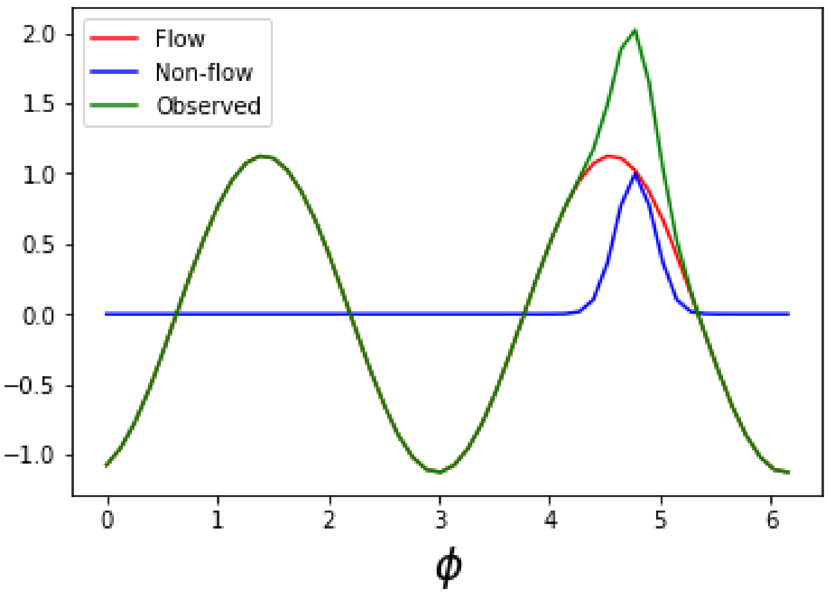
A rather remarkable fact is that there is no tuning parameter in our algorithm. Under the assumption of the theorem, minimizing

$$\|L\|_* + \frac{1}{\sqrt{n_{(1)}}}\|S\|_1, \quad n_{(1)} = \max(n_1, n_2)$$

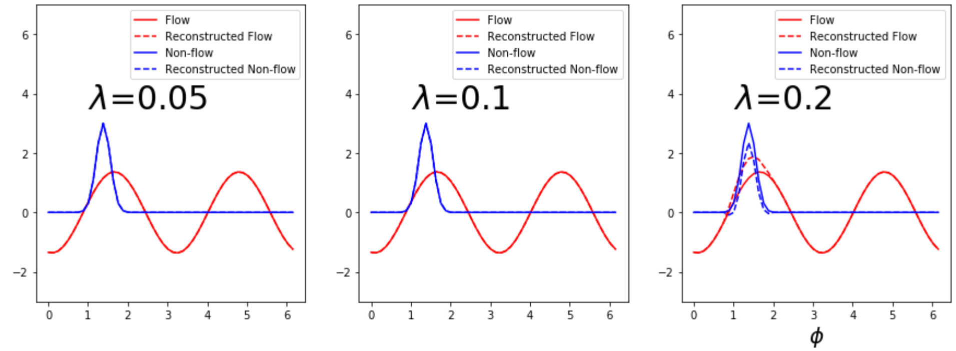
always returns the correct answer. This is surprising because one might have expected that one would have to choose the right scalar λ to balance the two terms in $\|L\|_* + \lambda\|S\|_1$ appropriately (perhaps depending on their relative size). This is, however, clearly not the case. In this sense, the choice $\lambda = 1/\sqrt{n_{(1)}}$ is universal. Further, it is not a priori very clear why $\lambda = 1/\sqrt{n_{(1)}}$ is a correct choice no matter what L_0 and S_0 are. It is the mathematical analysis which reveals the correctness of this value. In fact, the proof of the theorem gives a whole range of correct values, and we have selected a sufficiently simple value in that range.

https://statweb.stanford.edu/~candes/papers/RobustPCA.pdf

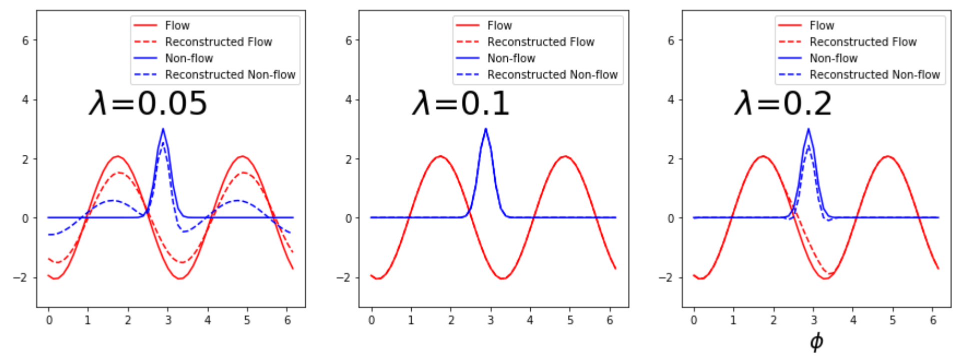
Toy model



Event 1



Event 2



Flow: elliptic $\sin(2\phi)$, $\cos(2\phi)$
Nonflow: Guassian, randomized angle
Observed: Flow+Nonflow

Robust PCA can separate flow/non-flow without any training (unsupervised) !
Comment: No physics, but very good technique :P

3. ICA

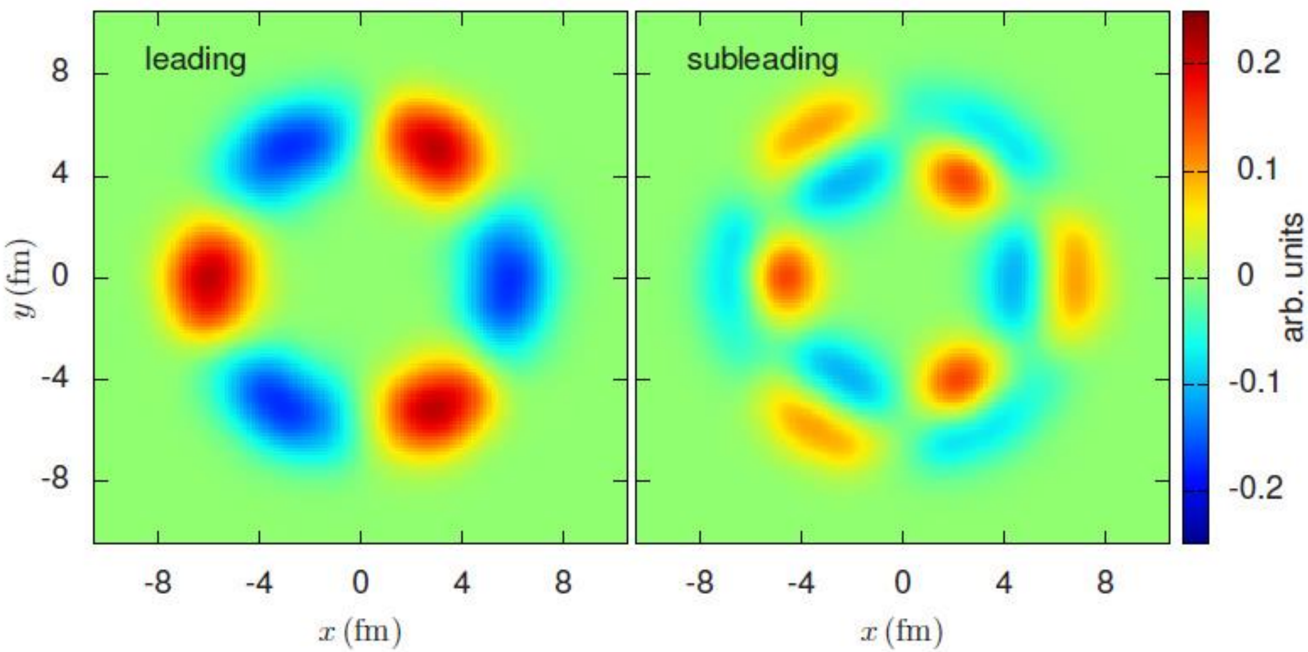
Independent Component Analysis

—— conquer limitations of PCA to study sub-leading flow

Sub-leading flow?

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

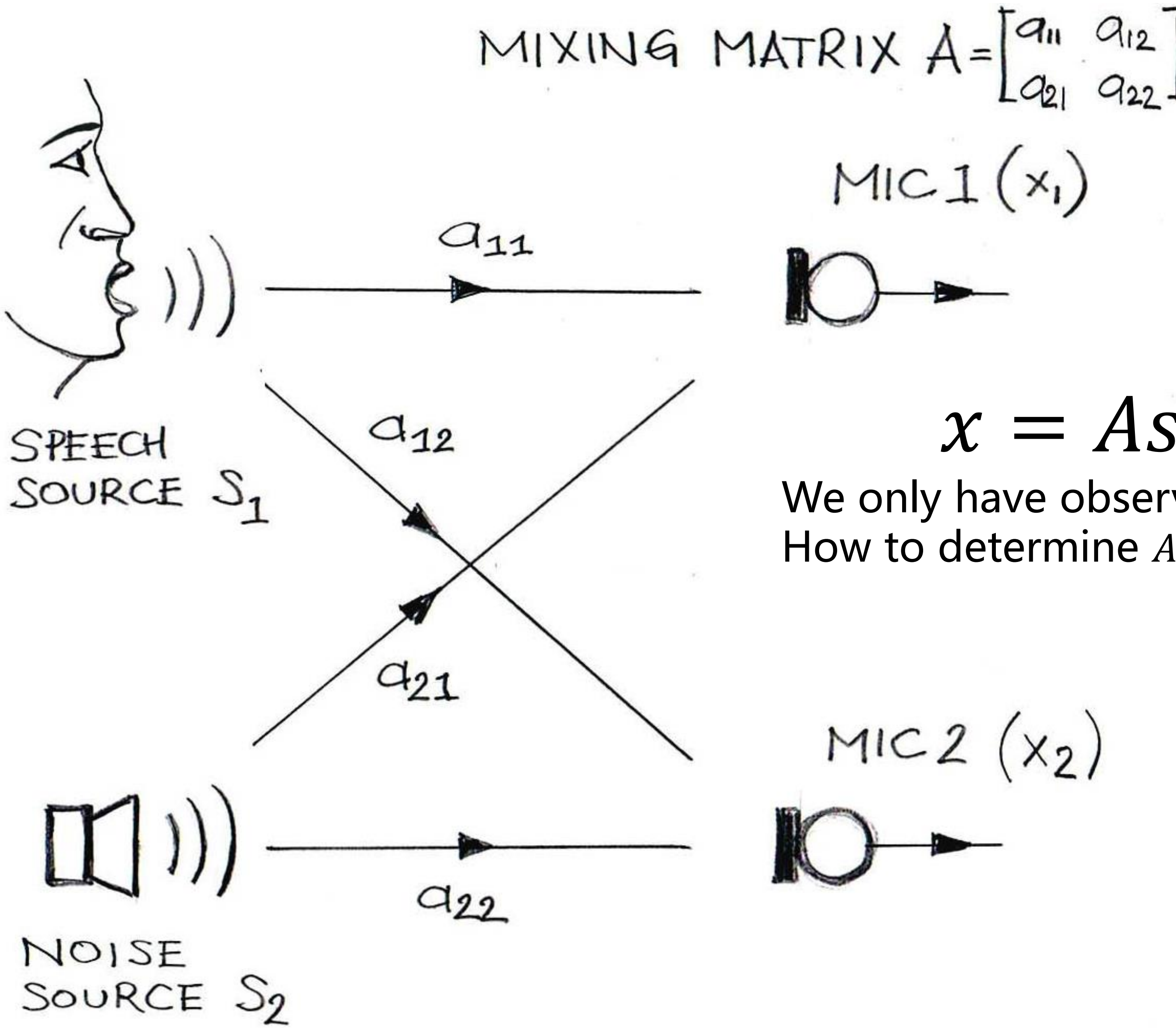
$V_3(p_T)$



Leading flow Sub-leading flow

Orthogonal? Not necessary! (PCA fails)
But independent for linear response! (ICA works)

Cocktail Party problem



$$x = As$$

We only have observation x,
How to determine A and s?

ICA

https://www.cs.helsinki.fi/u/ahyvarin/papers/NN00new.pdf

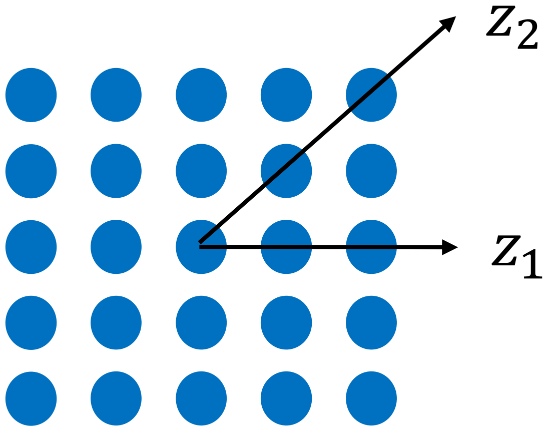
$$x = As$$

We only have observation x, how to determine A and s?

Assumption:

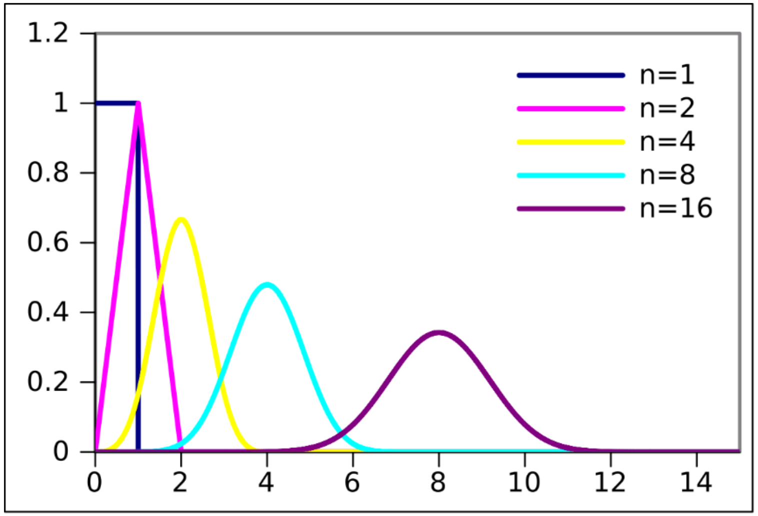
1. Sources are **independent** with each other
2. Sources should be as **non-gaussian** as possible

Why **non-gaussian**?
Central limit theorem: gaussian implies mixing!

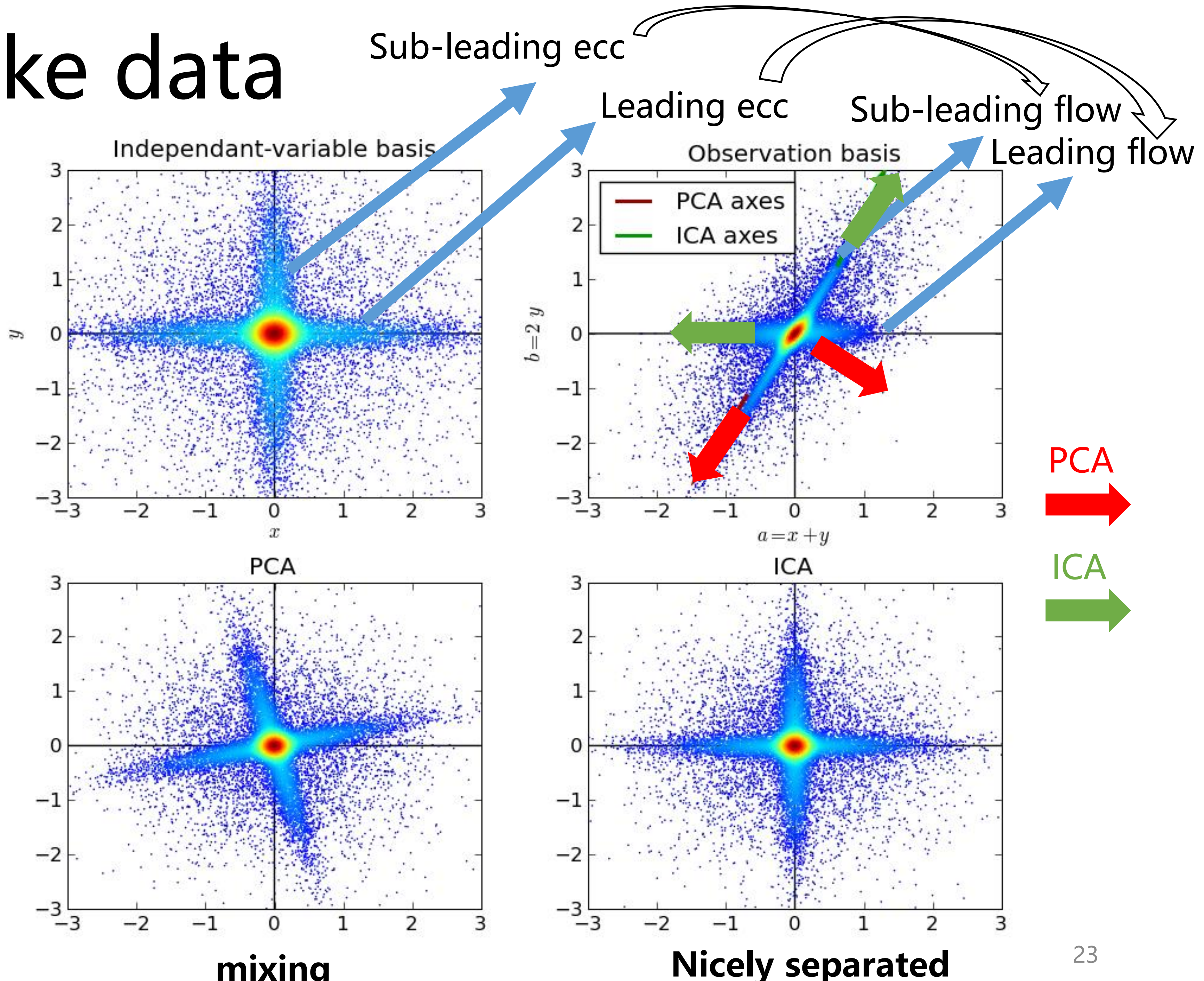


z_1: uniform distribution
z_2: sum of two uniform distribution
ICA prefers z_1 over z_2

Irwin–Hall distribution

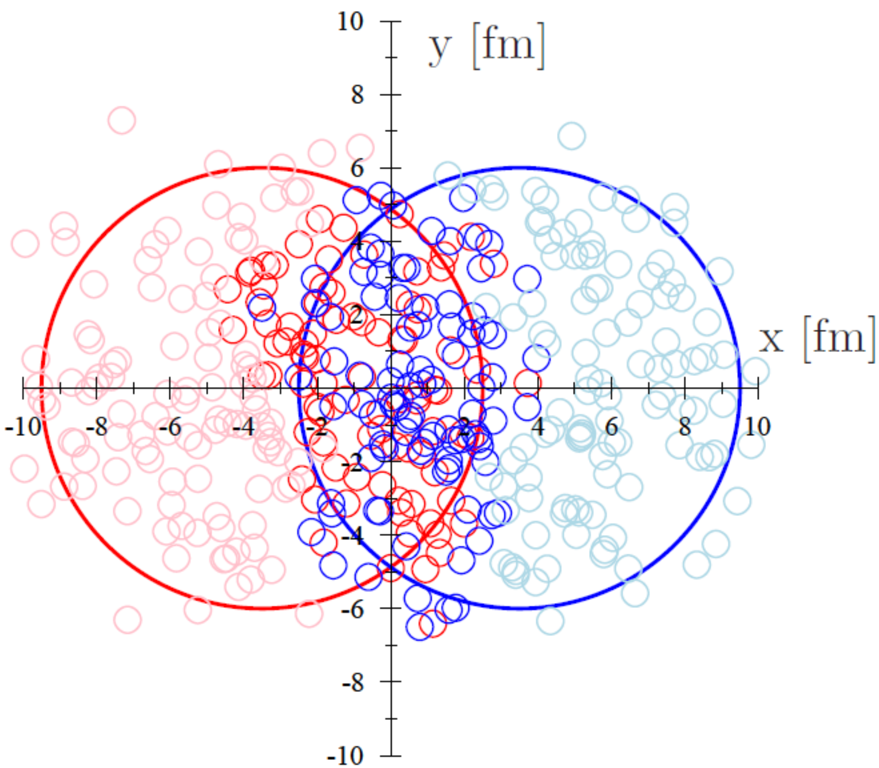


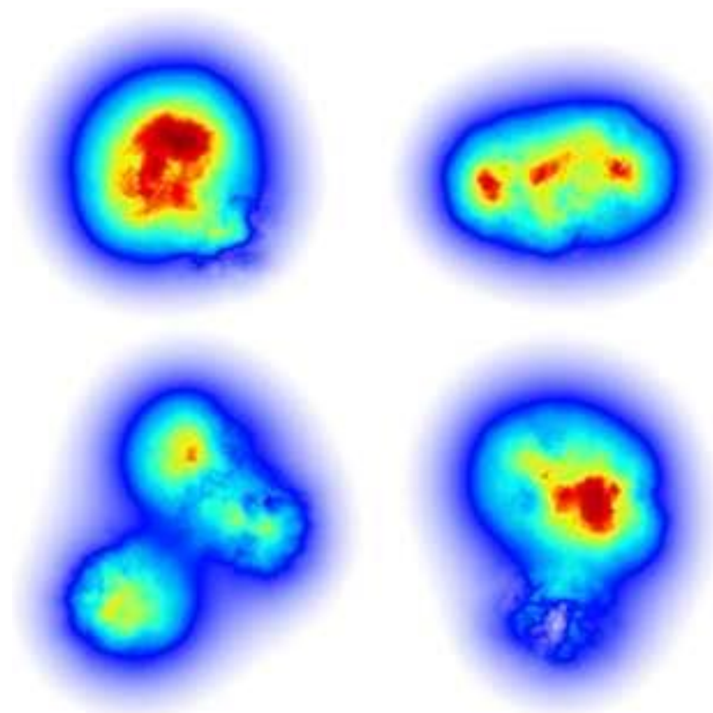
Fake data


Sub-leading ecc
Leading ecc
Sub-leading flow
Leading flow
Independant-variable basis
Observation basis
PCA axes
ICA axes
x
y
$a=x+y$
$b=2y$
PCA
ICA
PCA
ICA
mixing
Nicely separated

4. Traditional PCA

—— Probing number of initial sources





Nucleonic fluctuation

Sub-nucleonic fluctuation

Different number of initial sources?

A naïve argument:
Au+Au
197+197=394 nucleons
Each nucleon has two-dim coordinates
So we have 394*2=788 parameters
Data should lie on a 788-dim manifold
Hydrodynamics evolution is finite time
So final particle distribution is a 788-dim manifold, too
The manifold could be non-linear,

BUT

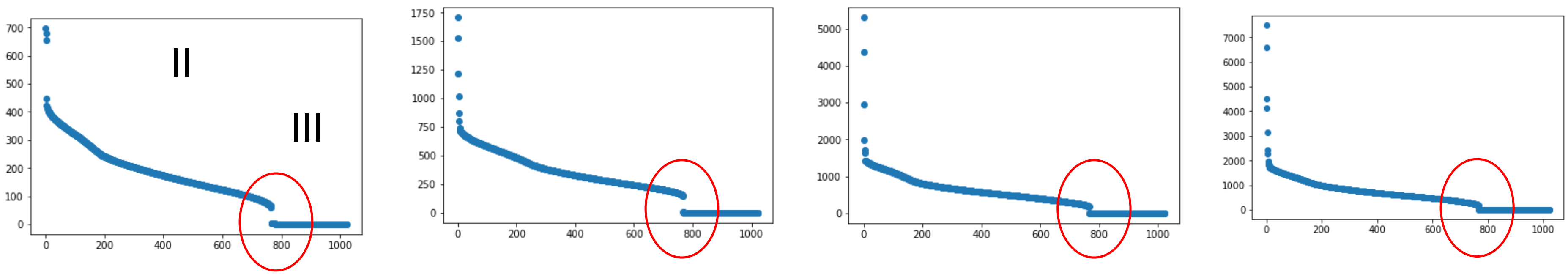
Let’s try PCA first!

PCA to two-particle data

$\frac{d^2 N_{pair}}{d\Delta\eta d\Delta\varphi}$ data, 32*32=1024 bins, 2000 events

10%-20% centrality

I ampt_39 ampt_200 hijing karpenko



For all models, the singular values show an abrupt drop at 768<~788

Guess: 768 corresponds to the mean number of participants*2

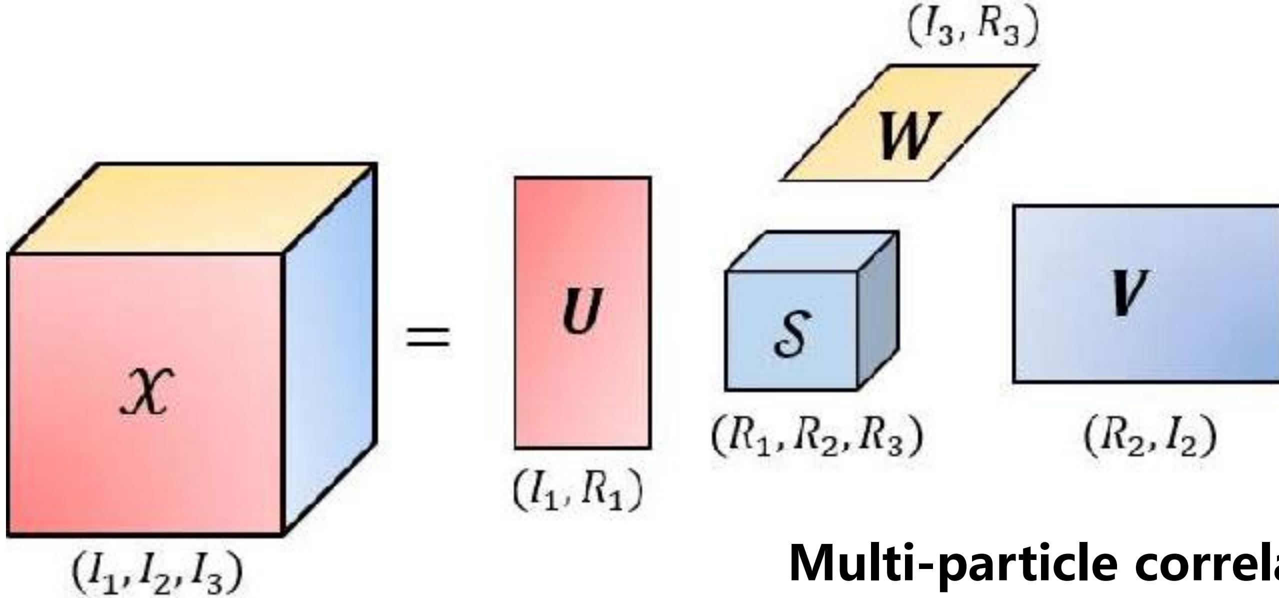
Comment:

1.Independent of collision energy? Number of events? Number of bins?
Need further check

2. May serve as an observable to measure number of sources
Can we observe such drop in experiments? Statistical errors ……

5. High-order PCA

—— For multi-particle correlation data



Multi-particle correlation data

6. Generalized PCA

—— Suitable for different data types

$$\min \left\|A - \tilde{A}\right\|_F^2 \Longleftrightarrow A = \tilde{A} + \epsilon, \epsilon \sim N(0, \sigma^2)$$

gaussian

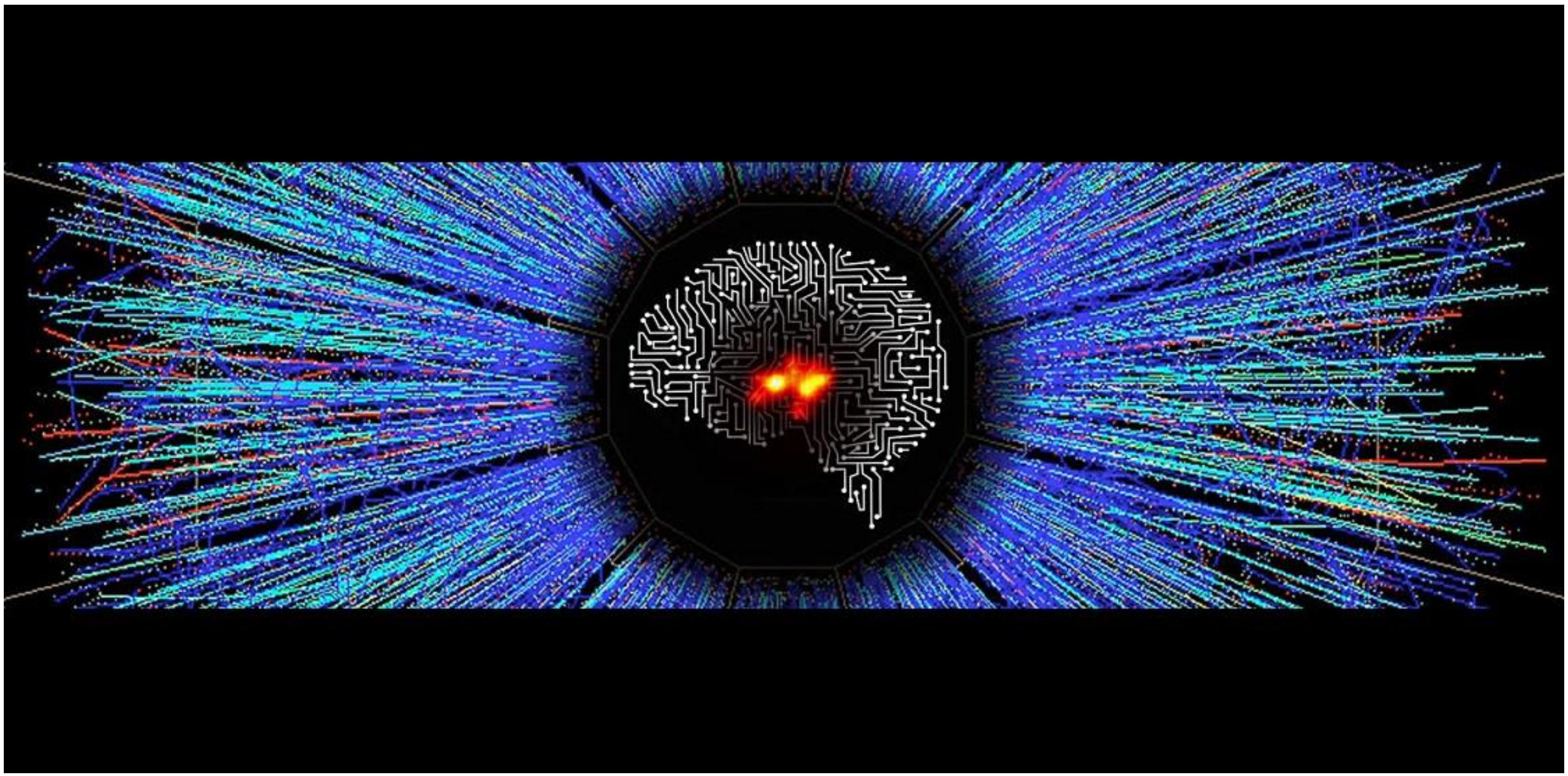
$$? \Longleftrightarrow A = \tilde{A} + \epsilon, \epsilon \sim p(\epsilon)$$

Bernoulli, Poisson, Laplacian ……

Conclusion

- PCA still has a lot to explore, at least in the application of heavy-ion physics.
- Our ultimate goal is to make PCA useful in experiments.
- But first we should publish a few method papers to elucidate the performance of these methods and arouse interests of experimentalists.

Thank you!

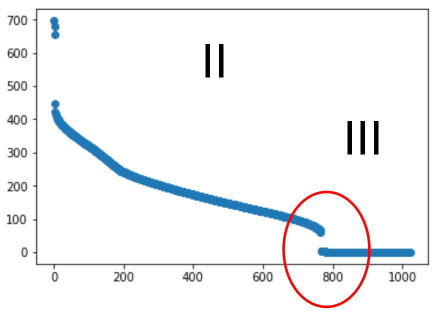


Backup

Singular values

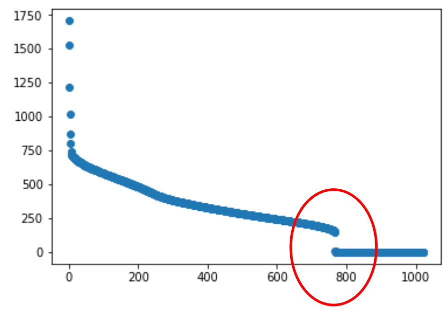
I

ampt_39

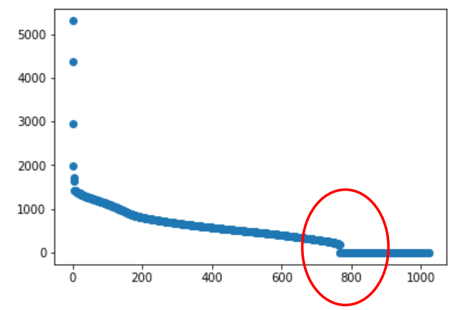


drop!

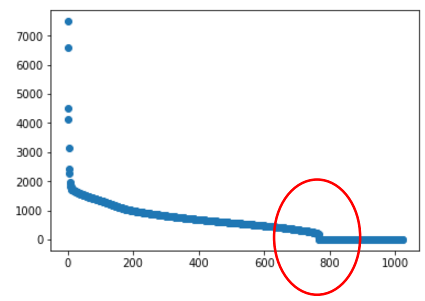
ampt_200



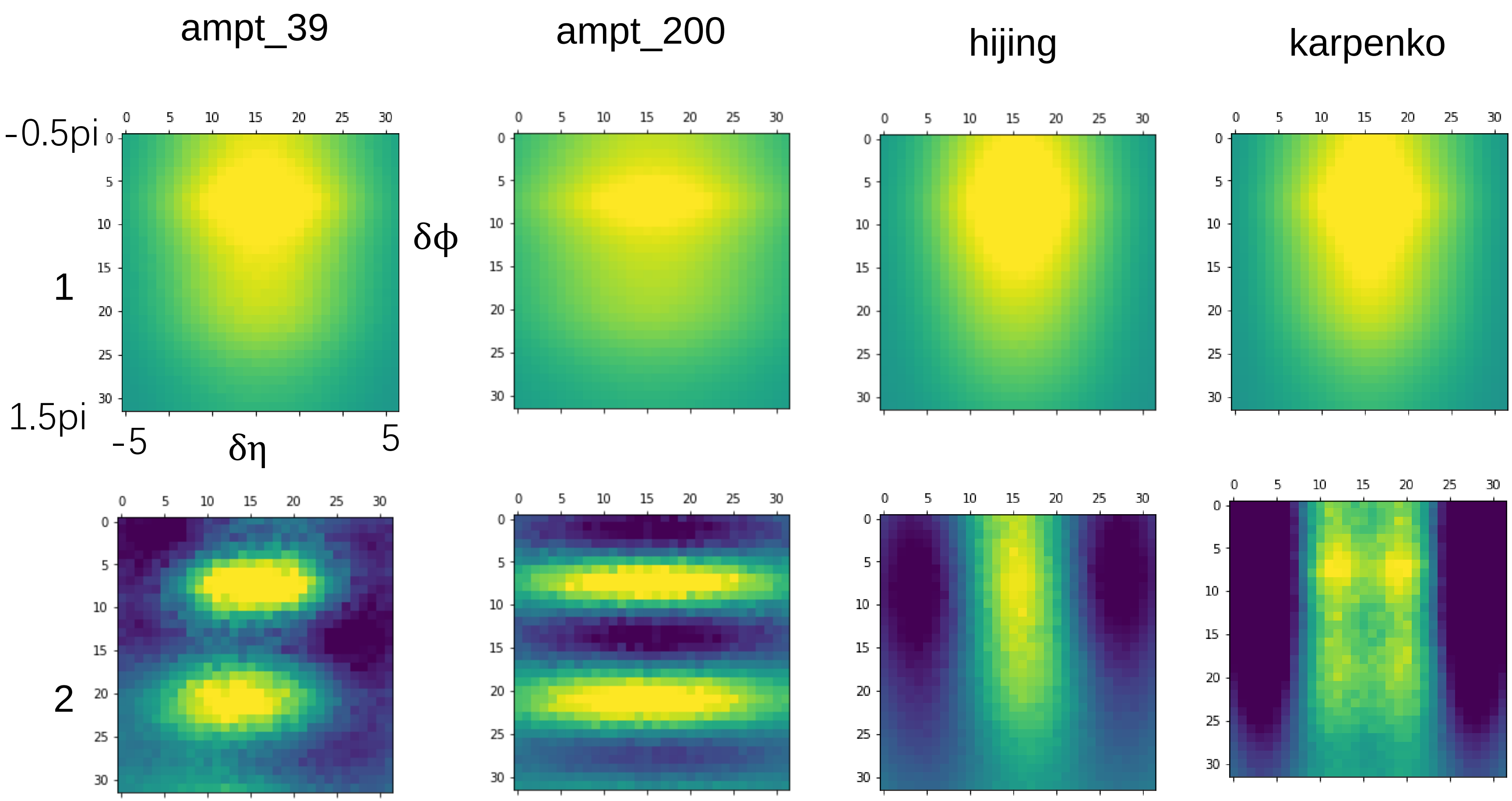
hijing



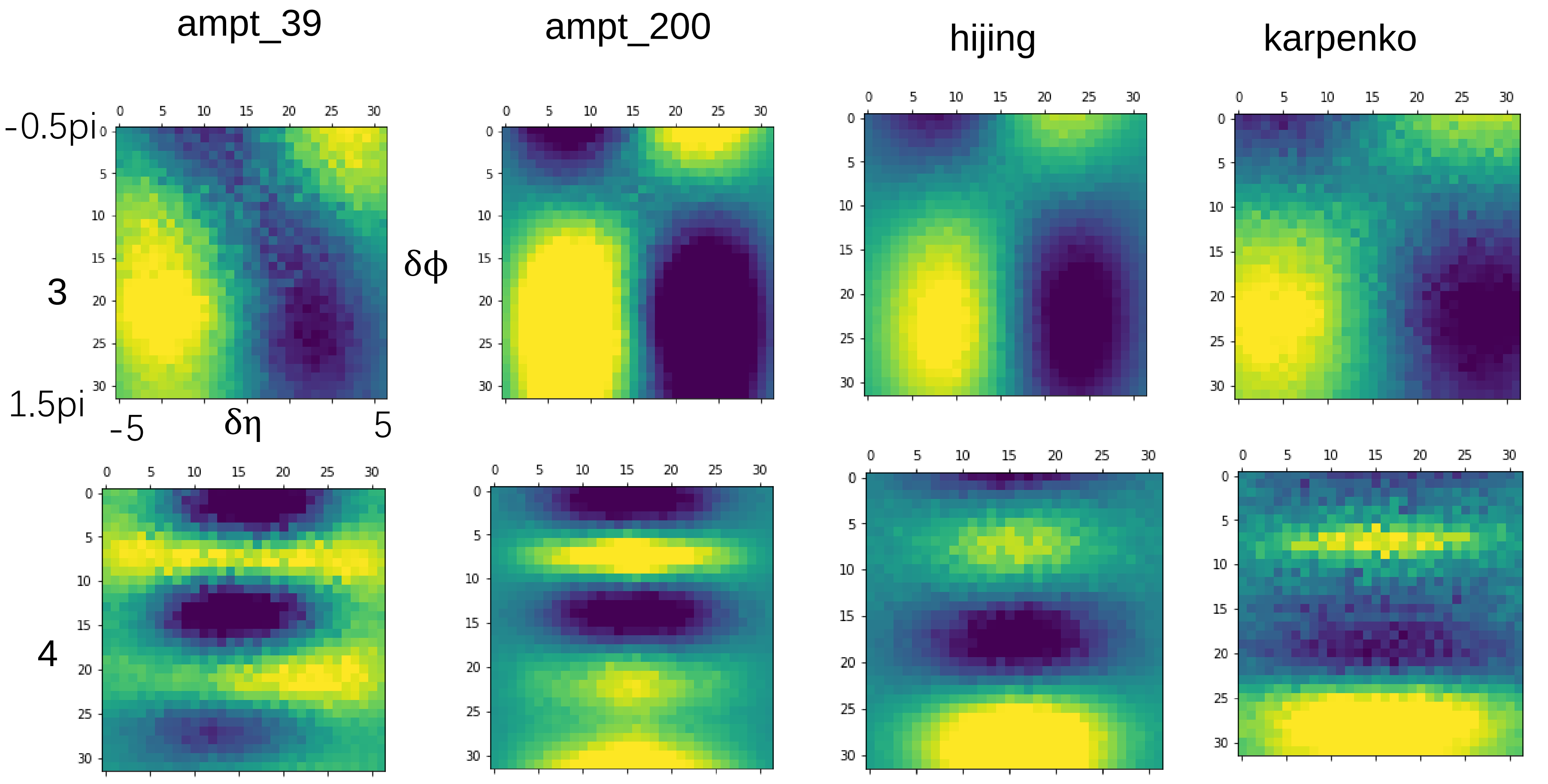
karpenko



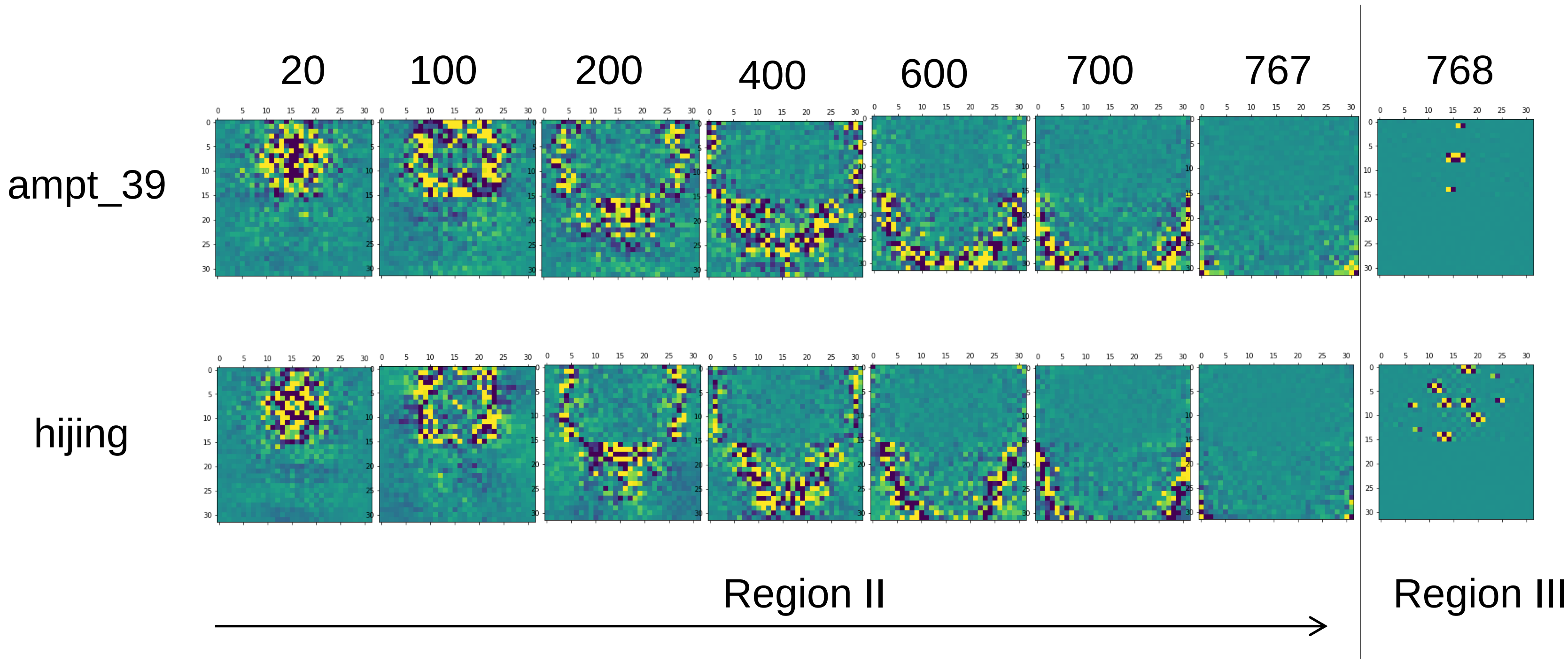
Eigenvectors in Region I



Eigenvectors in Region I



Eigenvectors in Region II and III



The bright area is “expanding” towards outside.
So in Region II, each eigenmode focuses on one local area. (In region I, the eigenmode is global)