

Effective Phase Transition Identification with Dimensional Reduction Techniques on the Muon Spectroscopy Data

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Thanks to our collaborator

Effective Phase Transition Identification with Dimensional Reduction Techniques on the Muon Spectroscopy Data

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This presentation is based on the submitted paper (under review) in Physical Review B

Outline

- Introduction: Our Group & μ -SR
- Dimensional Reduction Techniques: PCA & t-SNE
- The Experiments
- Results
- Summary & Outlook

Introduction

First, Please Allow Me to Introduce Our Research Group:

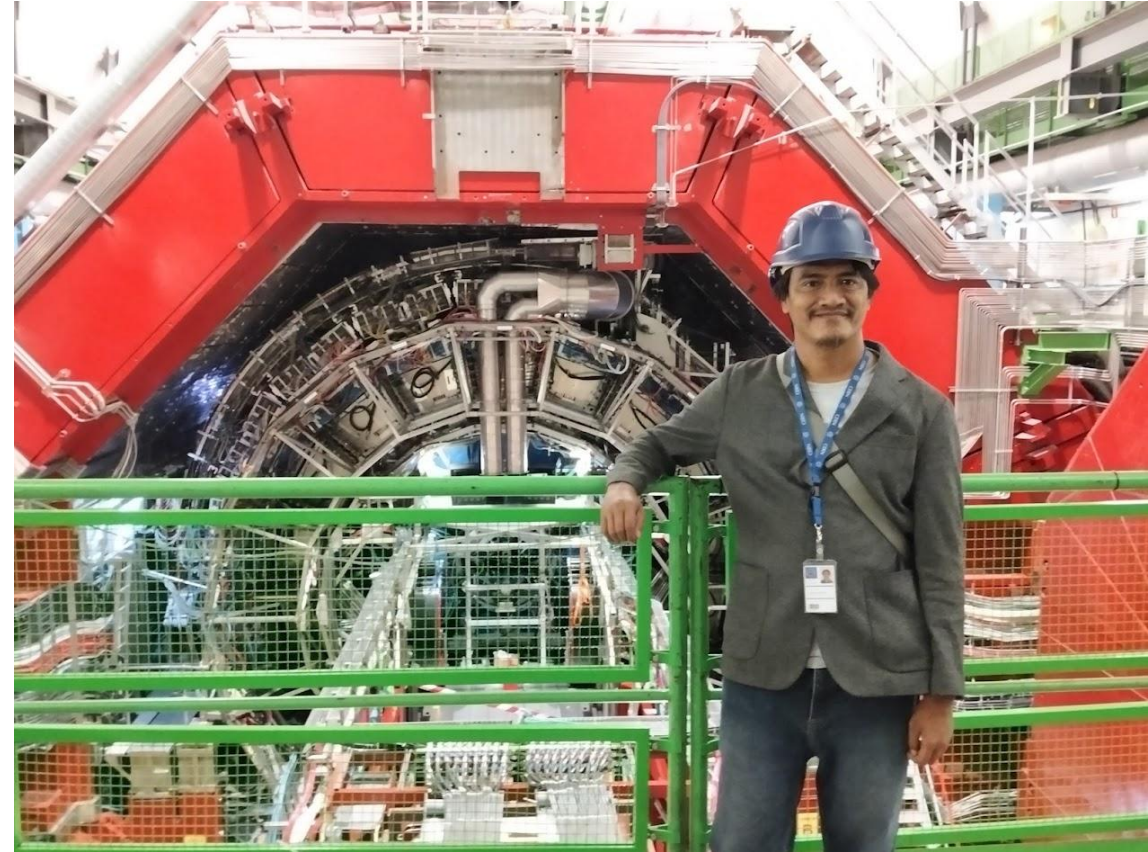
Experimental High Energy Physics Group @BRIN

Our group (which is relatively new):

- Currently Member of **ALICE Experiment @ CERN**
- 4 Scientists with previous collaboration in: Fermilab, Jefferson Lab, KEK and CERN
- 1 Engineer
- 10 Students and Postdoc

Main Research activities:

- Involved in RICH (Ring Imaging Cherenkov Detector) upgrade of ALICE detector @ CERN
- Detector & Instrumentation: SiPM based photodetector, DAQ, FPGA
- Machine-Learning application in Physics
- **Muon Tomography**



3D MUON TRACK THROUGH TWO POINTS INSIDE THE DETECTOR AND INTERSECTION WITH COORDINATE PLANE

Muon telescope placed at an angle, facing Monas (Monumen Nasional), Jakarta.

The two points P_1 and P_2 are inside the detector (blue layers).

Plane $x = x_0$ crosses Monas. The intersection point is obtained by extrapolating the muon track line.

Plane $x = x_0$ (constant)

Two points measured inside the detector (blue layers)

$P_1 (x_1, y_1, z_1)$

$P_2 (x_2, y_2, z_2)$

— Line through P_1 and P_2 (extrapolated)

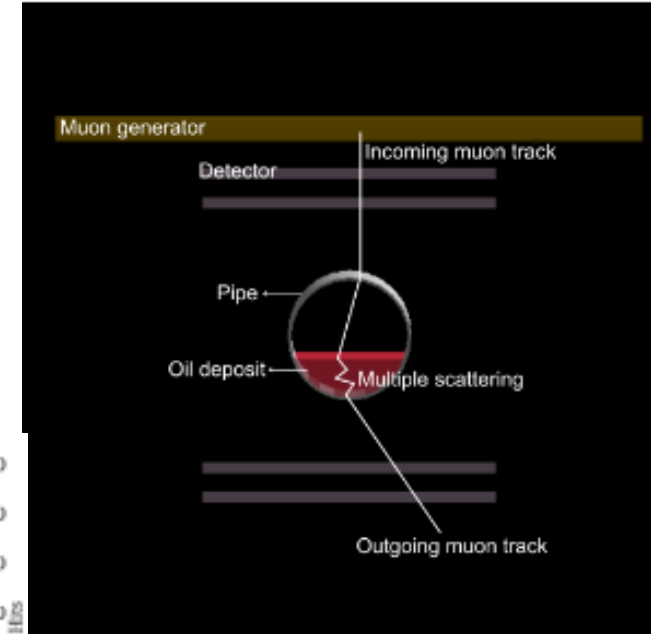
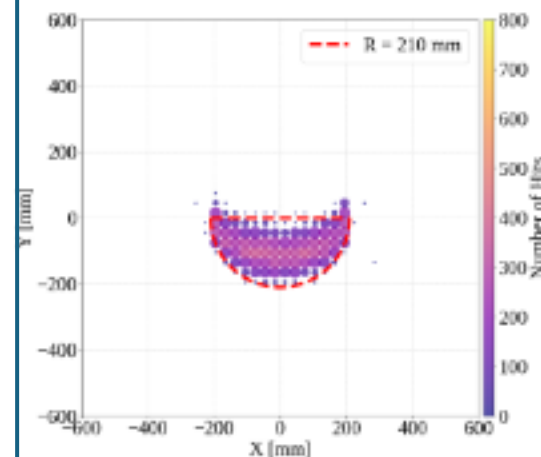
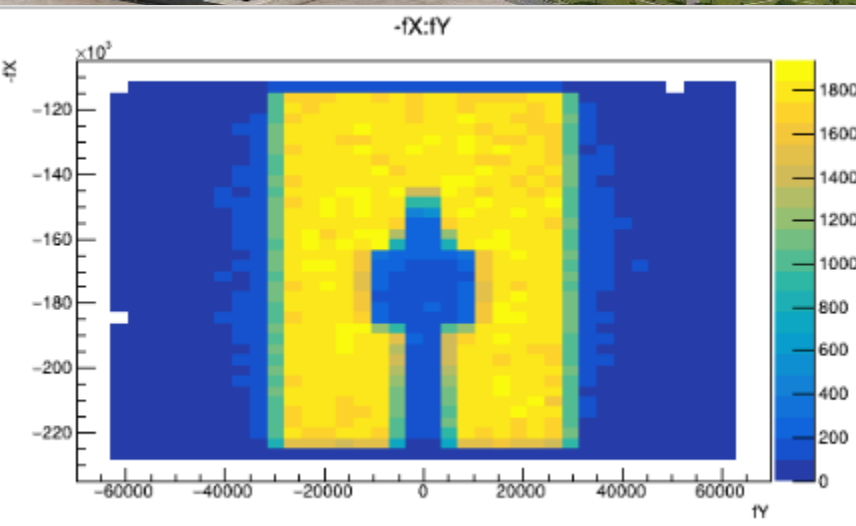
- - Intersection with plane $x = x_0$

$$t = \frac{x_0 - x_1}{x_2 - x_1}$$

$$P_{int} = (x_0, y_1 + t(y_2 - y_1), z_1 + t(z_2 - z_1))$$

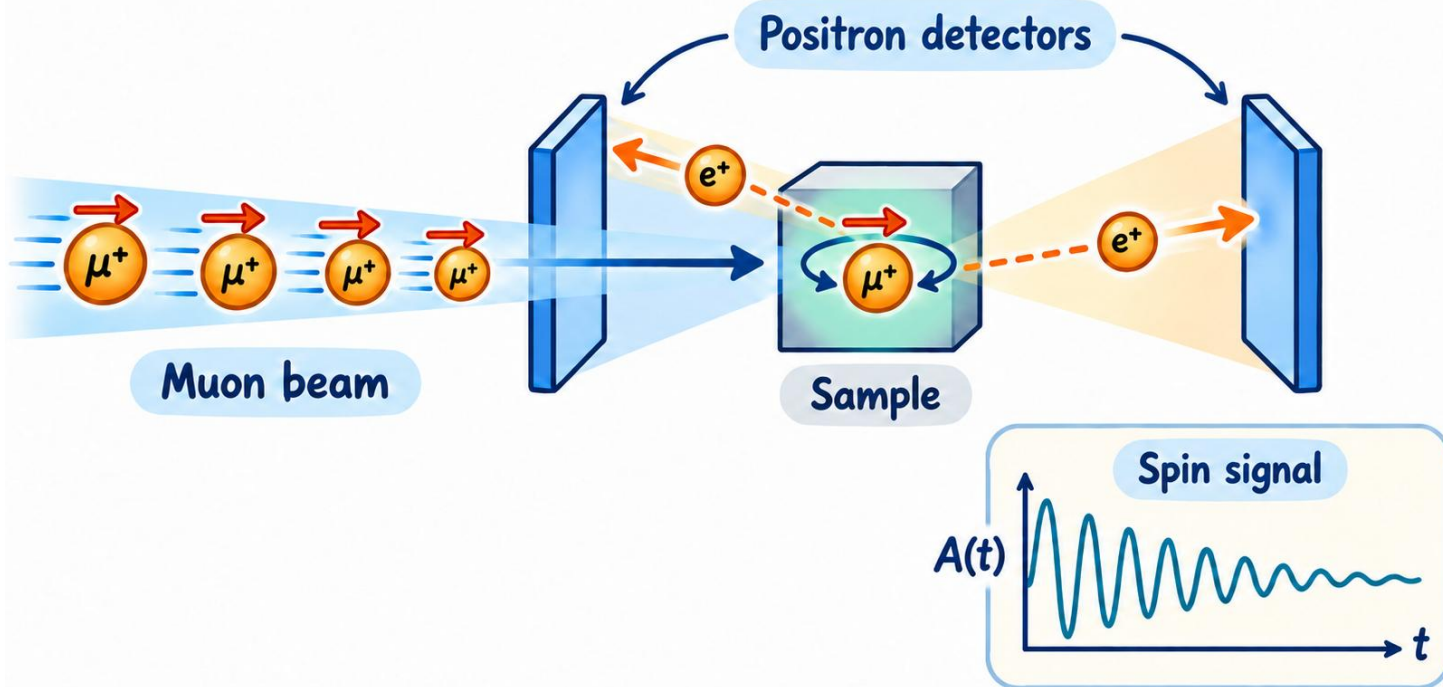
$t < 0 \rightarrow$ intersection is to the left of both points (extrapolated)

$t > 1 \rightarrow$ intersection is to the right of both points (extrapolated)



Our muon telescope will arrive next month. Over the past two years, we did extensive **Geant4 simulation** and developed **machine learning** methods for **muon reconstruction and imaging** and conducted **feasibility studies** for applications ranging from imaging Indonesia's National Monument (Monas) to detecting deposits inside oil and gas pipelines.

Muon Spin Spectroscopy (μ SR)

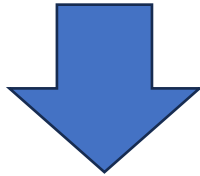


- Muon produced from the pion decay is 100% polarized (the spins are aligned in one direction)
- When the muons pass the sample material, the local magnetic field in the sample induce Larmor precession of the muons
- Muons then decay into positron
- Due to the Muon precession, the detected positrons are uneven between the forward and backward detectors
- Therefore, using the Asymmetry of the detected muon we could probe the Magnetic properties of the materials

Challenge in the data analysis

Typical analysis:

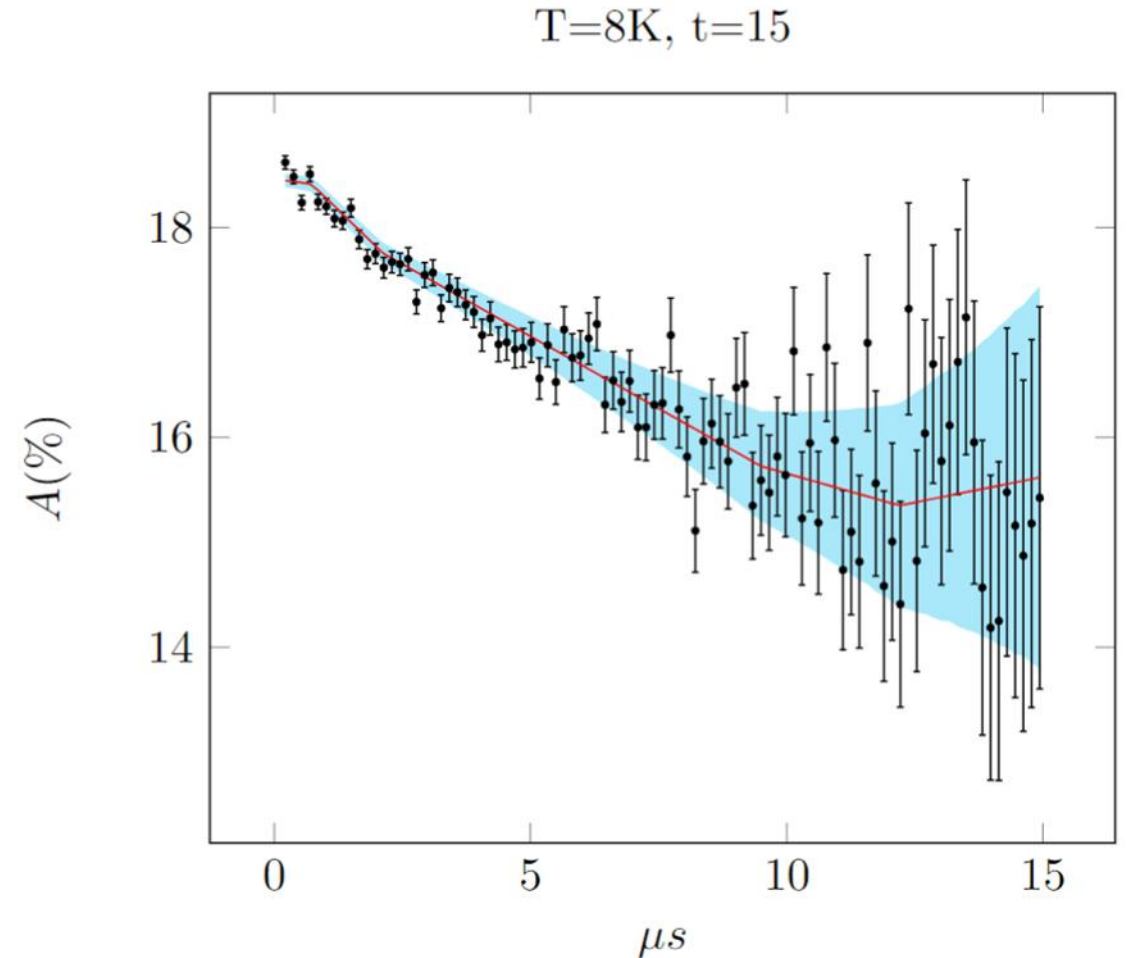
- Guessing what function best describe the data manually by eyes
- Fit with that function to obtain the important parameters
- This is very challenging, especially in the region where the phase transition happens since the fit function will be different for the data before and after the transition



Can we use Machine Learning for:

- **Help to decide where the transition happens.**
- Avoid Fitting functions

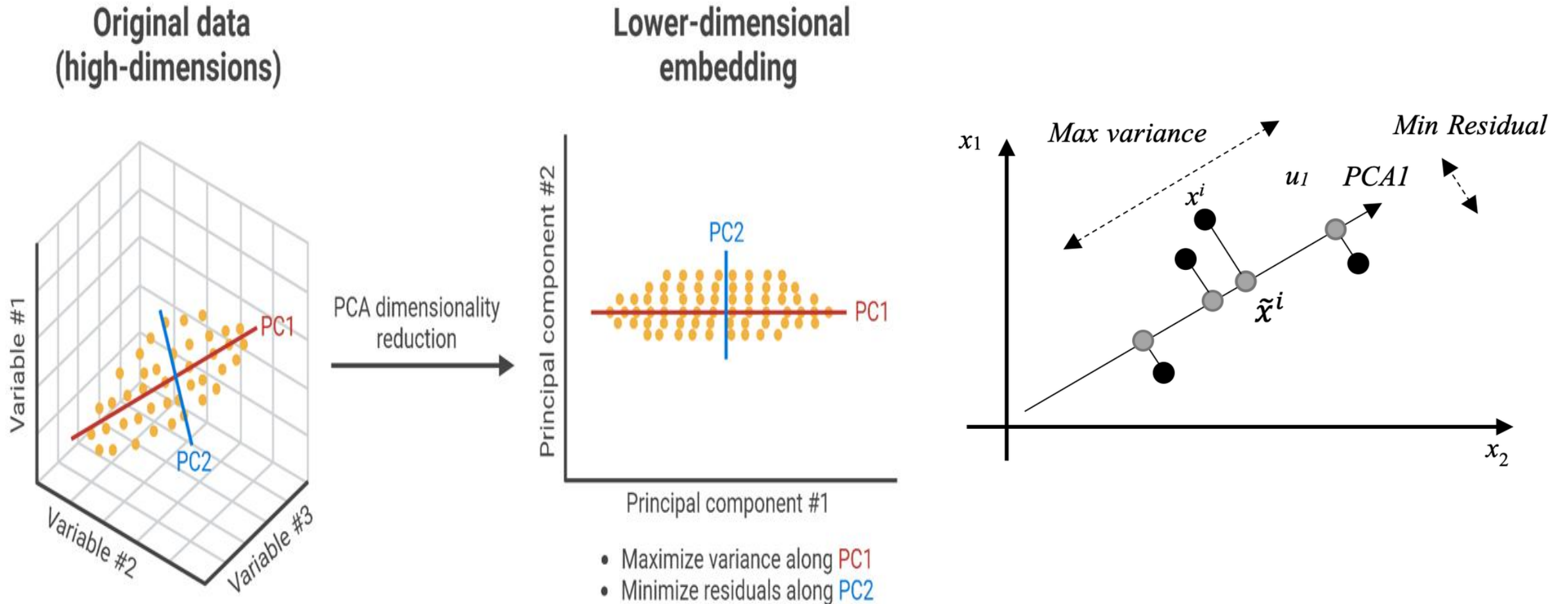
Challenge: Noisy data



Dimensional Reduction Techniques

PCA & t-SNE

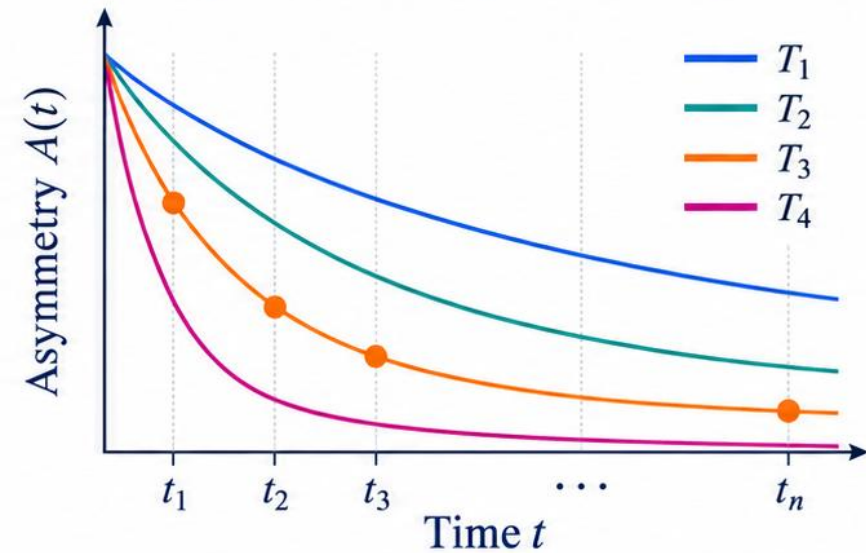
PRINCIPLE COMPONENT ANALYSIS (PCA)



Principal Component Analysis (PCA) is a statistical technique used for **dimensionality reduction** and data visualization. It works by transforming high-dimensional data into a lower-dimensional space while preserving the most important information

One spectrum, one point

1. Temperature-dependent spectra

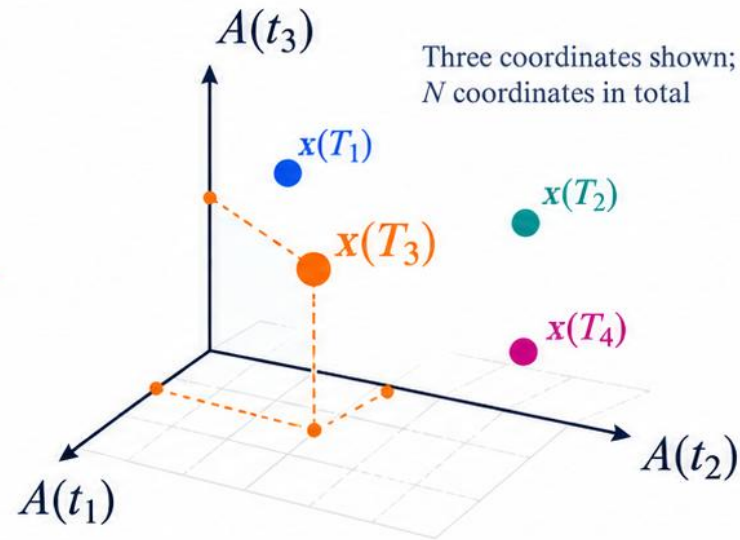


$$\mathbf{x}(T_3) = [A(t_1, T_3), A(t_2, T_3), \dots, A(t_n, T_3)]$$

Sample at
 N time bins

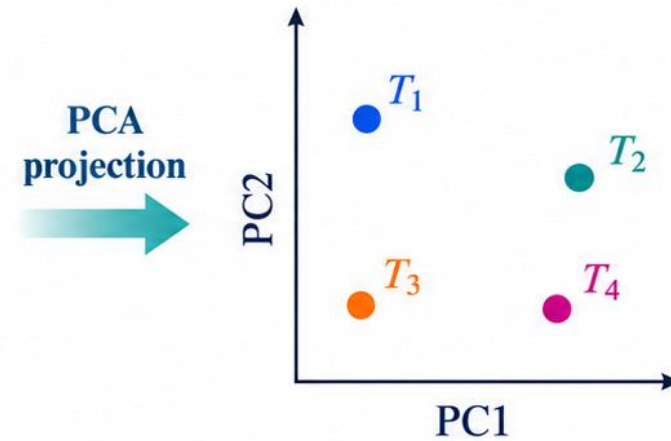


2. A point in N -dimensional space



Each temperature gives ONE point

3. Low-dimensional view



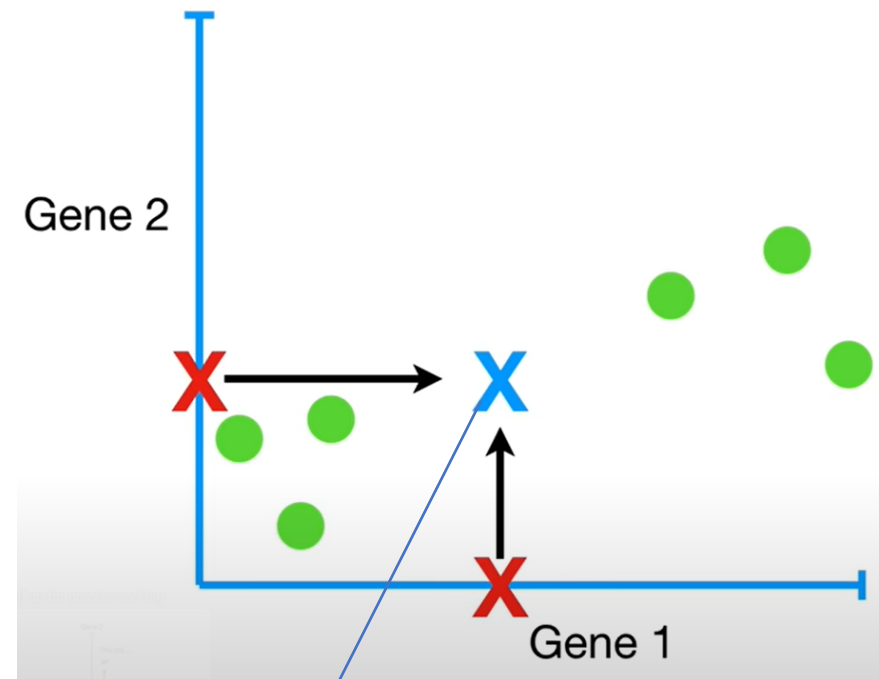
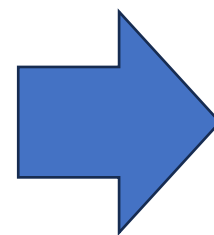
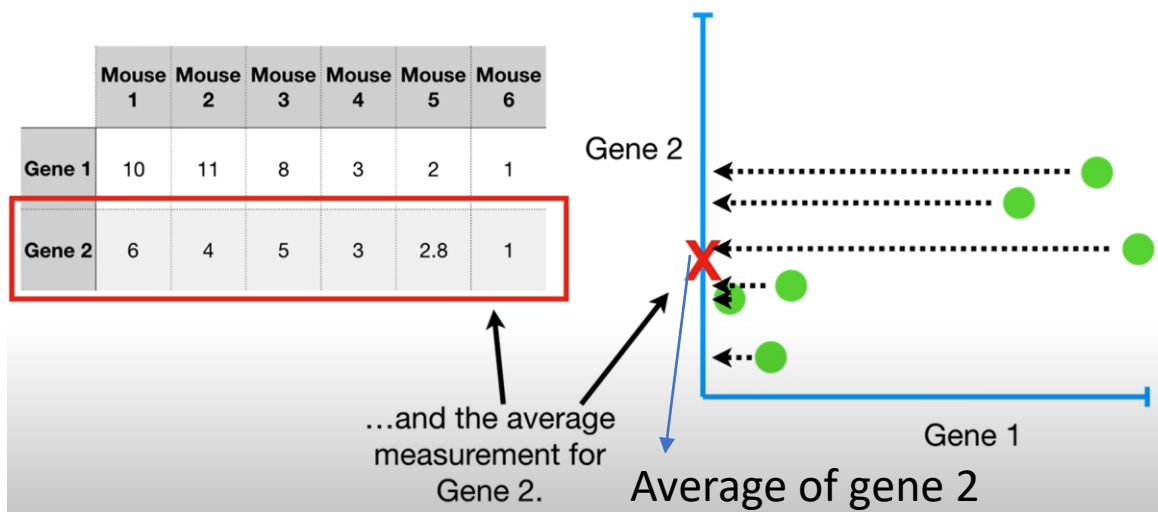
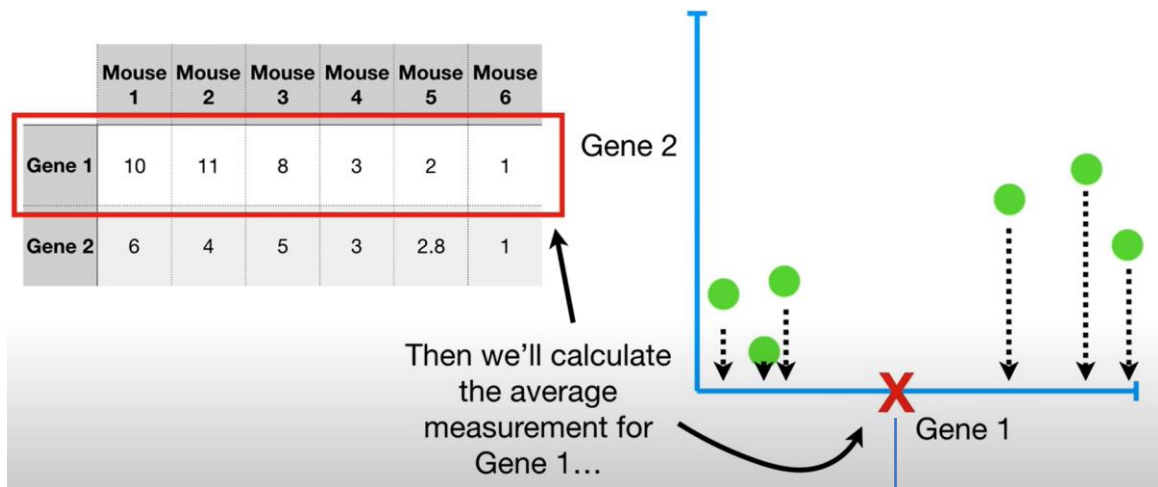
N features $\rightarrow$ 2 PCA scores

M temperatures $\times N$ time bins = M points in an N -dimensional feature space

Each two-dimensional plot of asymmetry versus time, $A(t)$ is represented as a point in an N -dimensional space, with the coordinate along axis i being the measured asymmetry, A_i . Consequently, for M different temperature measurements, we will have M points in this N -dimensional space

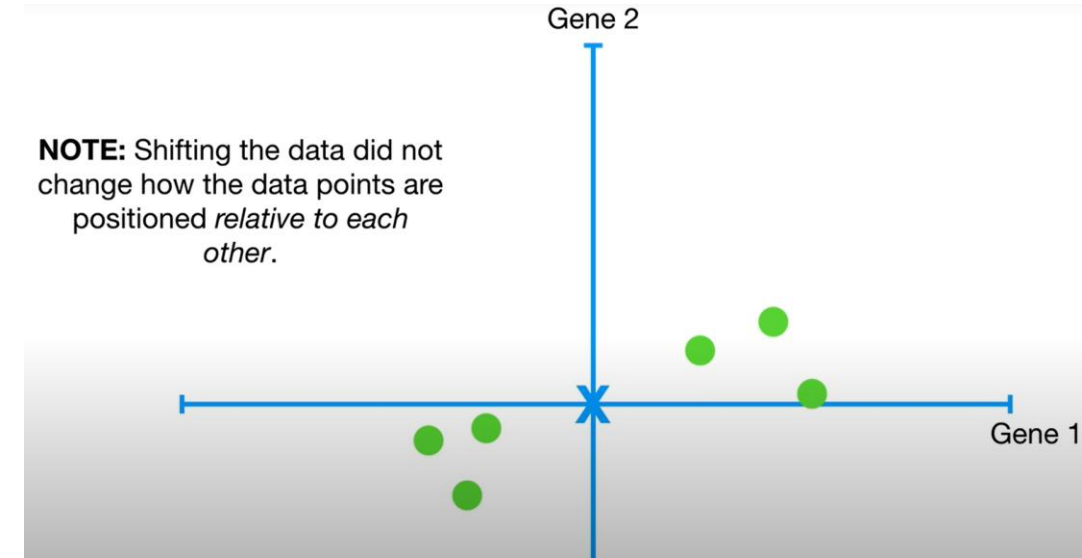
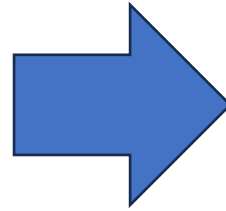
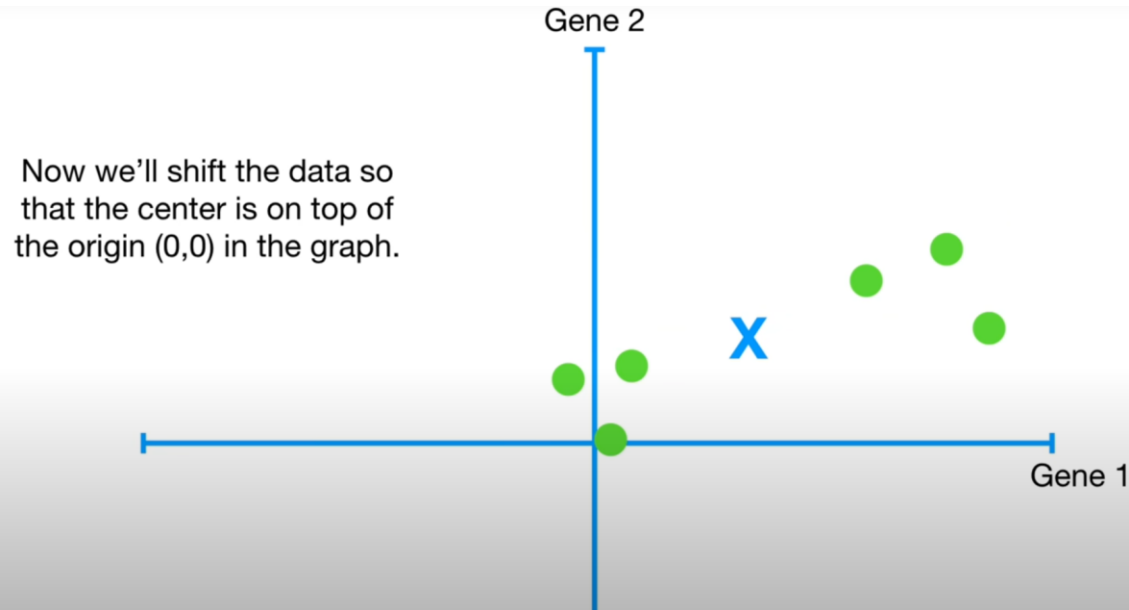
Step-1: Calculate the **average** measurement of all variables (gene 1 and gene 2)

Simple Illustration on how PCA works

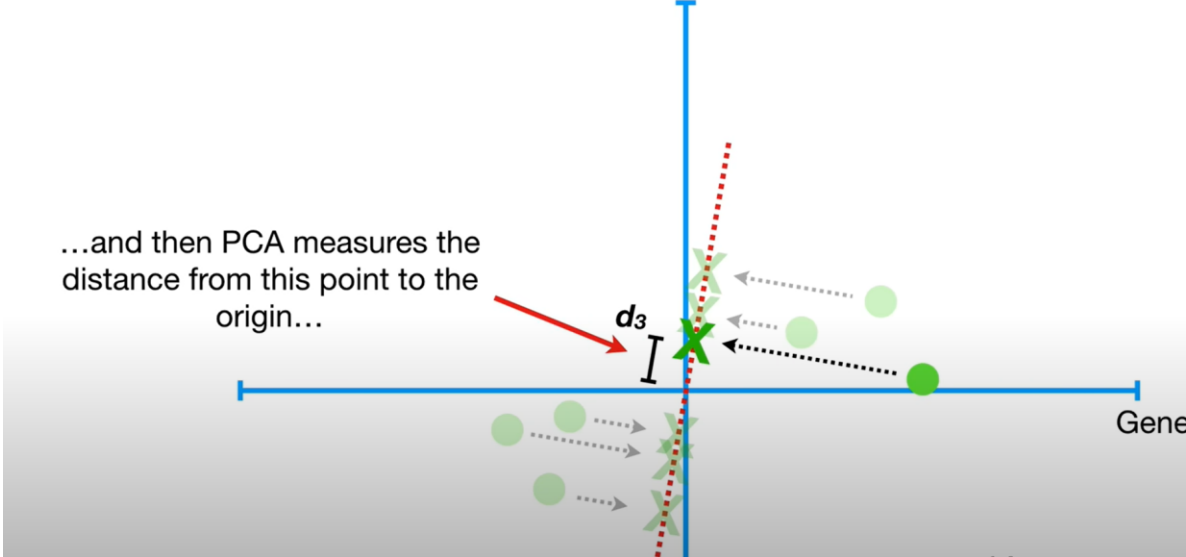
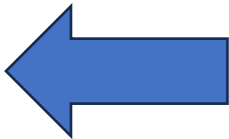
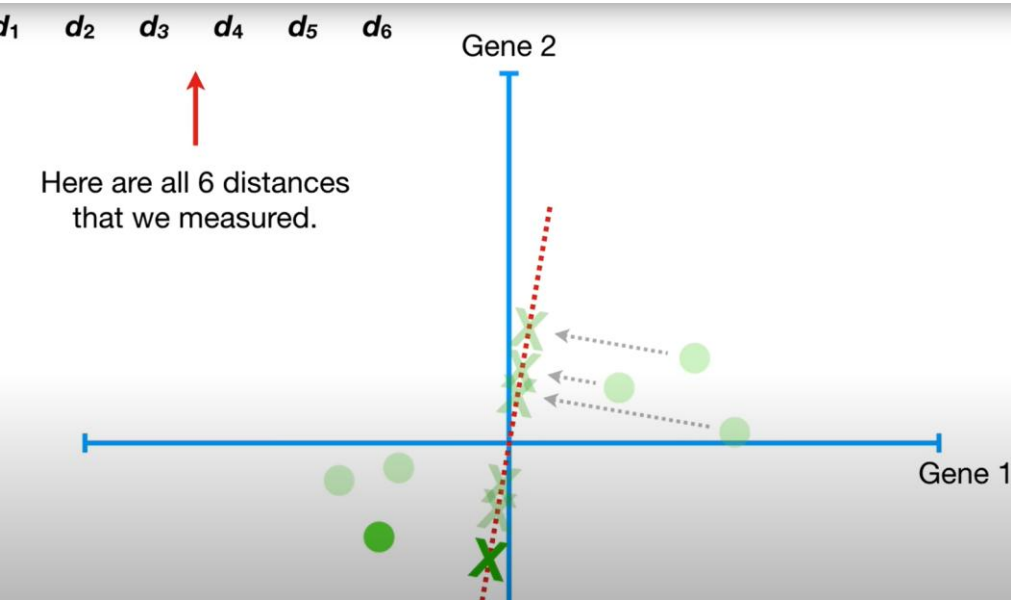
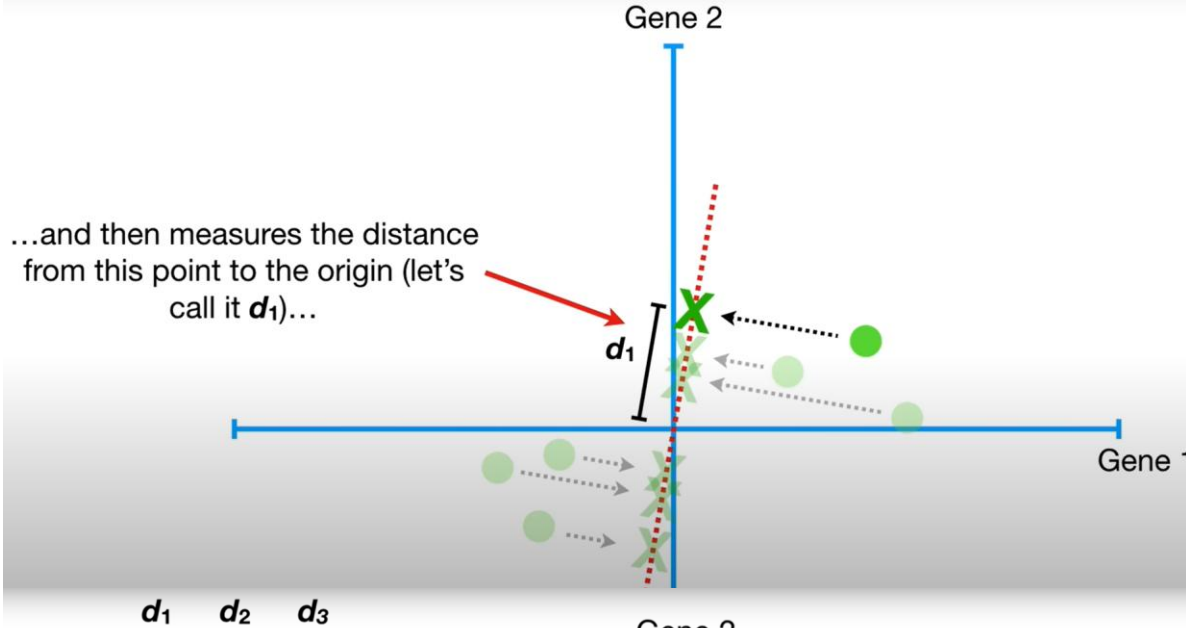
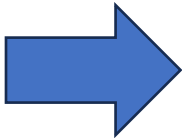
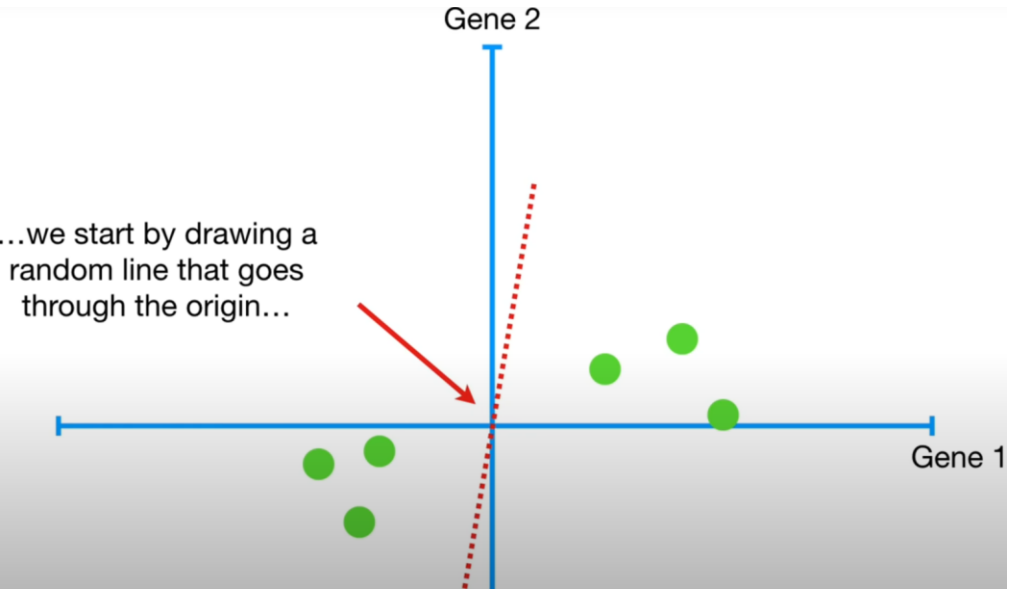


For simplicity, we illustrate how PCA reduces the dimensionality of data which was originally described by two variables (2 dimensions) into One dimension

Step-2: Subtract all data by the average to shift the mean of the data to the coordinate center (0,0)



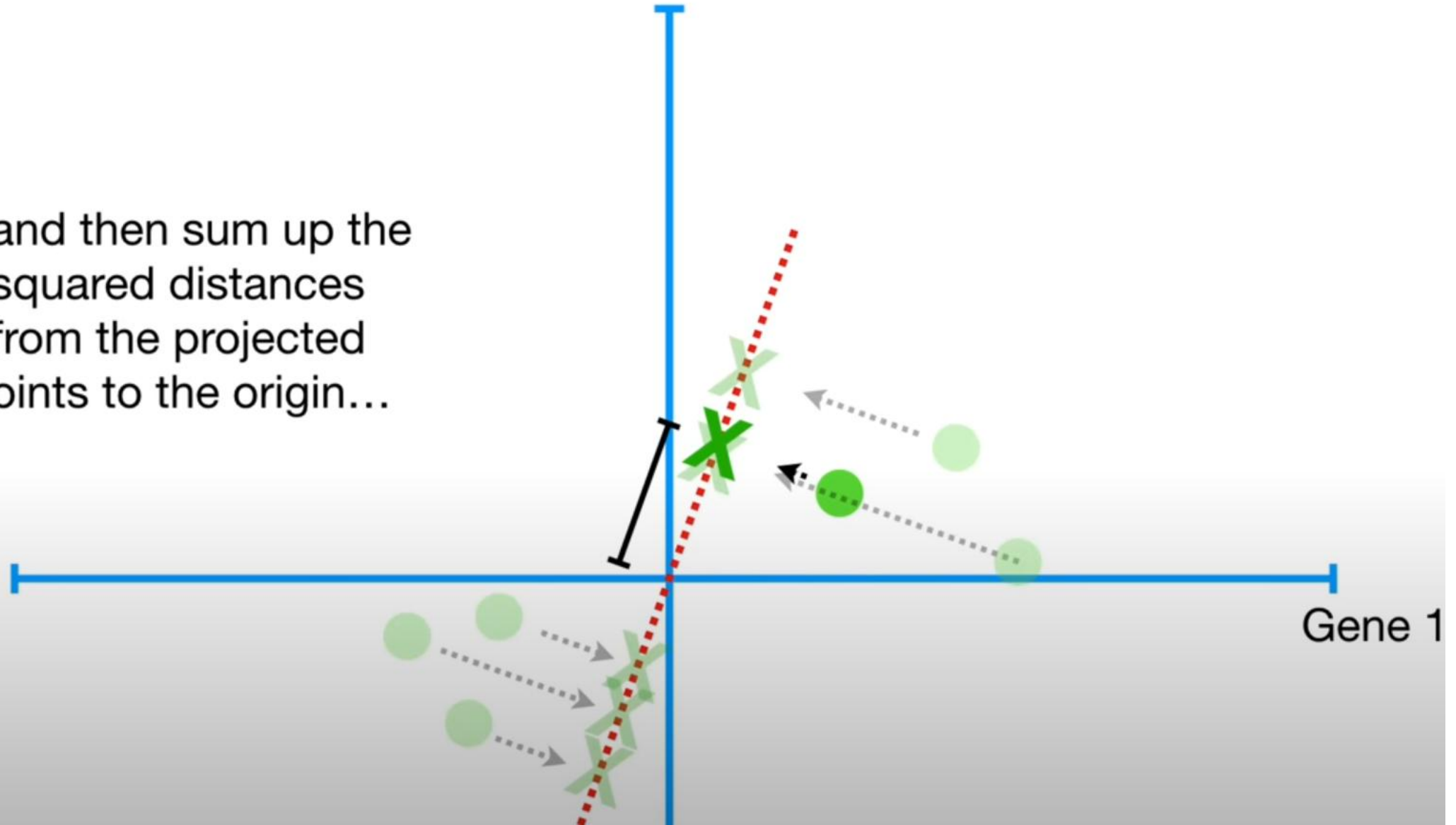
Step-3: Draw a random line through the origin and find the projected distance of all data to this line



Step-4: Calculate the sum of the distance square

$$d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2 = \text{sum of squared distances} = \text{SS}(\text{distances})$$

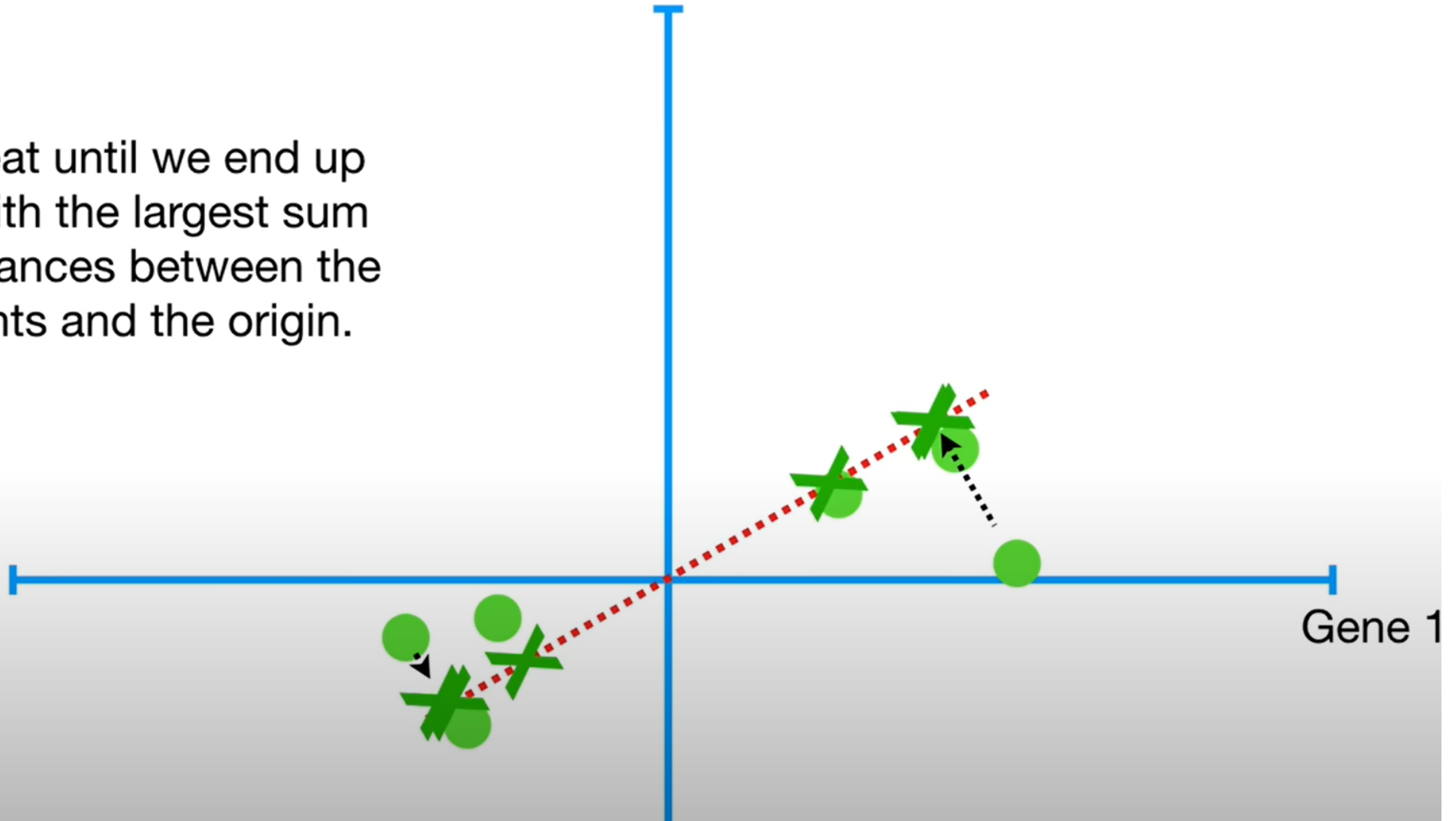
...and then sum up the squared distances from the projected points to the origin...



Step-5: Repeat the step. Draw another random line through the origin and calculate the projected distance

$$d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2 = \text{sum of squared distances} = \text{SS}(\text{distances})$$

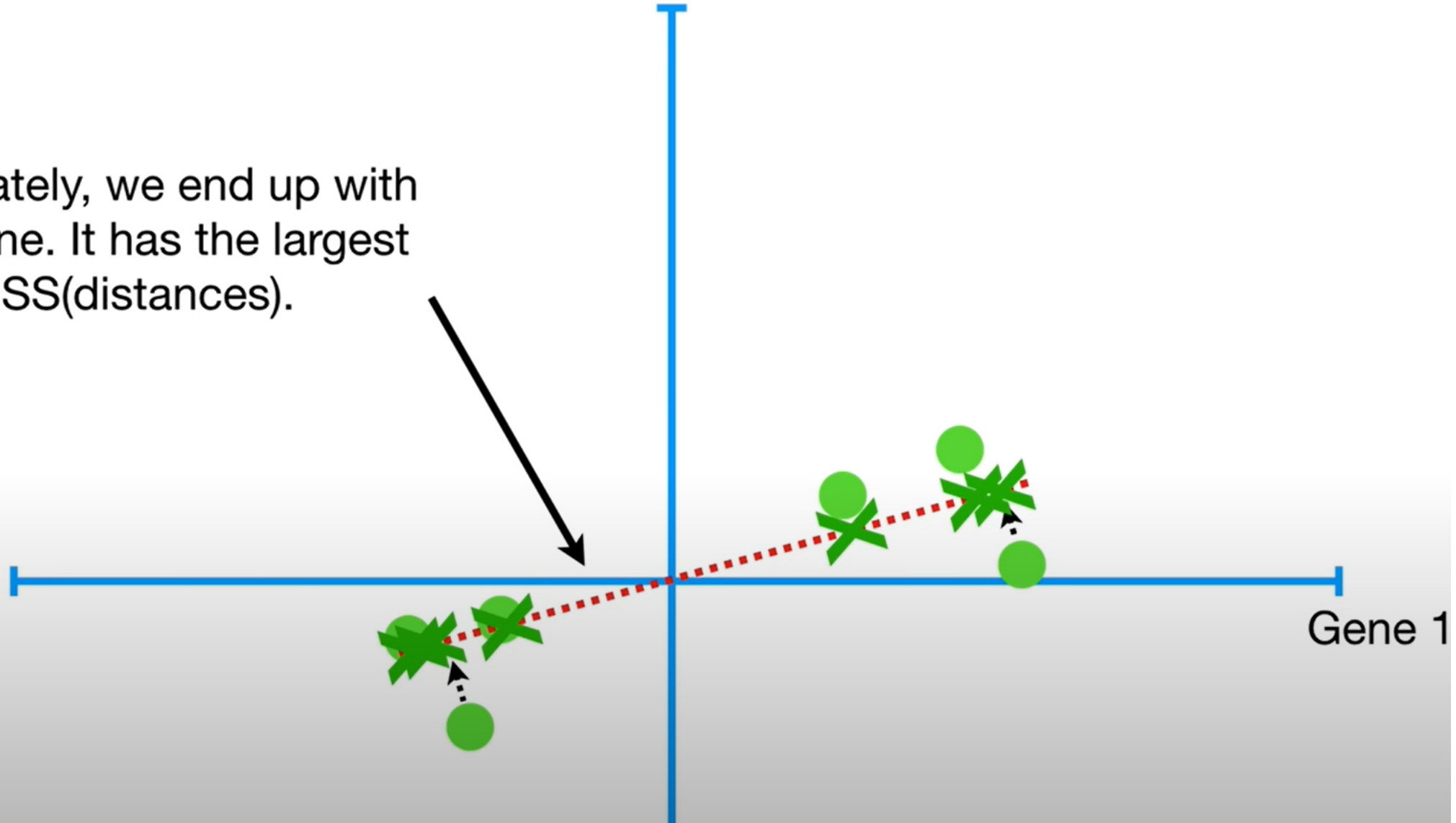
...and we repeat until we end up with the line with the largest sum of squared distances between the projected points and the origin.



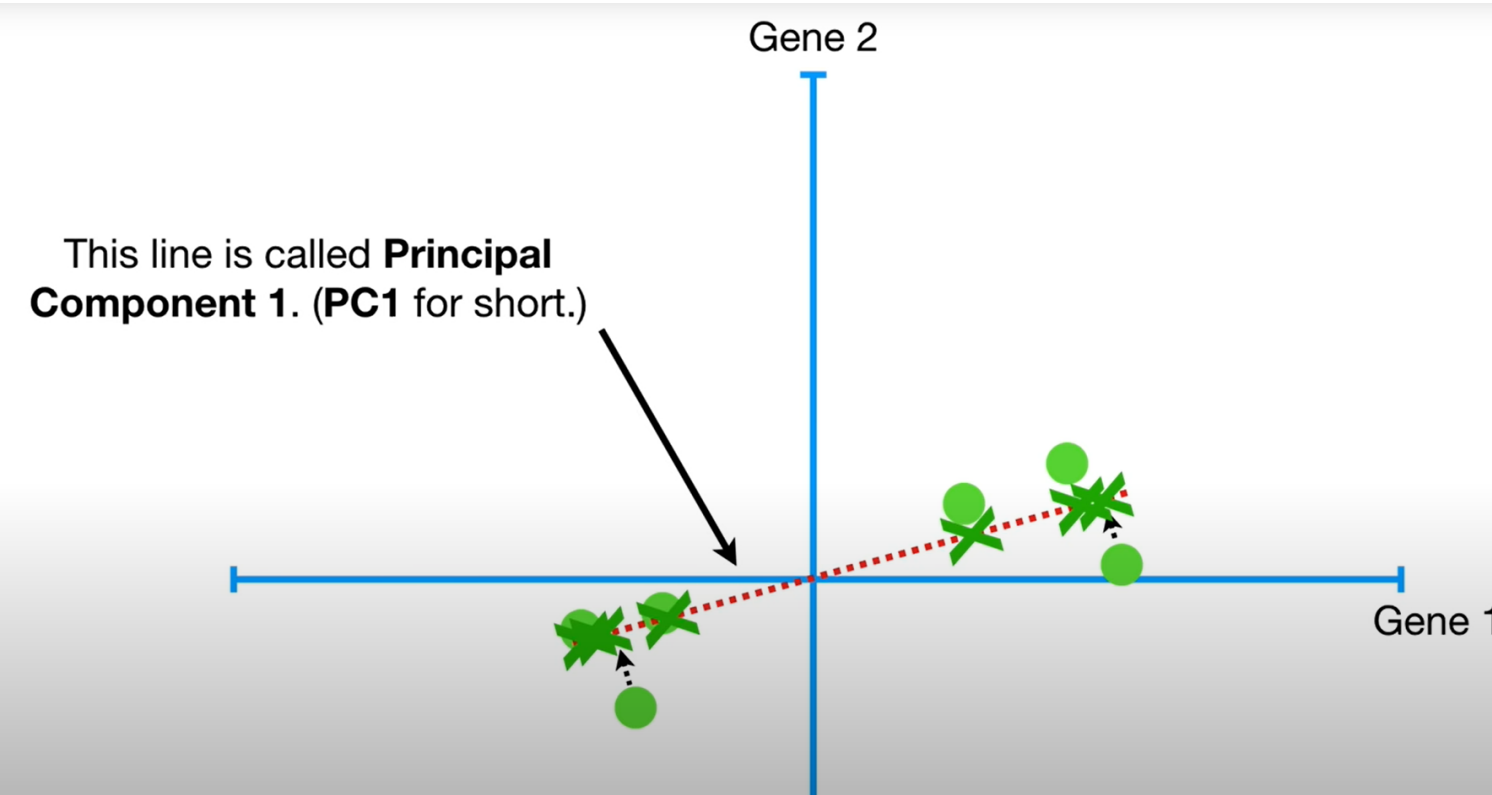
Step-6: Draw more lines until we end up with a line that provide the **Largest** sum of squared distance

$$d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2 = \text{sum of squared distances} = \text{SS}(\text{distances})$$

Ultimately, we end up with this line. It has the largest SS(distances).



Step-7: This line (with the largest sum of squared distance) is called Principal Component 1 (PC1)

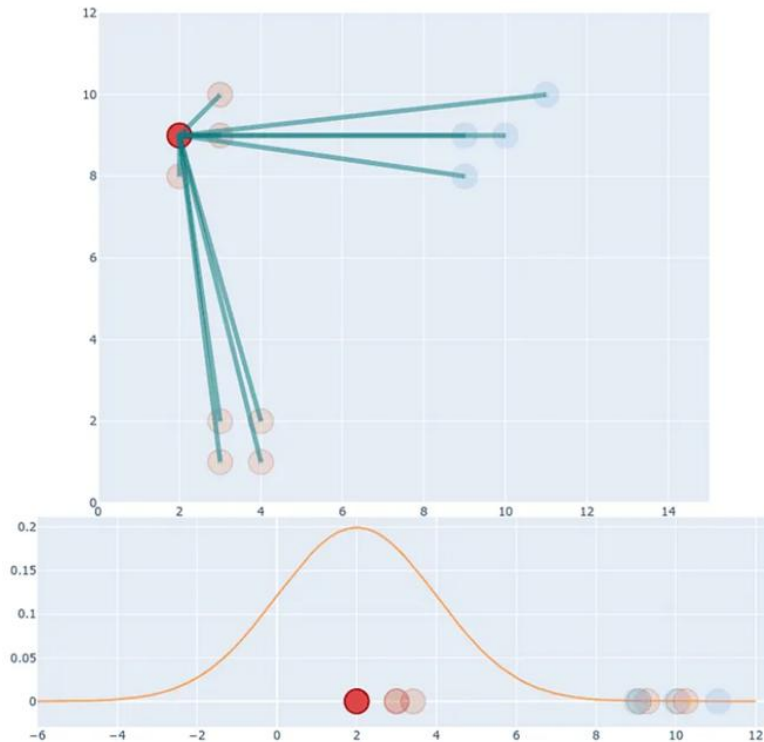


And the projected distance in this axis (d1, d2, d3, d4, d5, d6) are called PC1-score for each data points

The second component (PC2 line) is formed orthogonal from the PC1 line. But most information to identify phase transition is in the first component (PC1). Therefore, currently we are only focus on the first component (PC1)

t-SNE

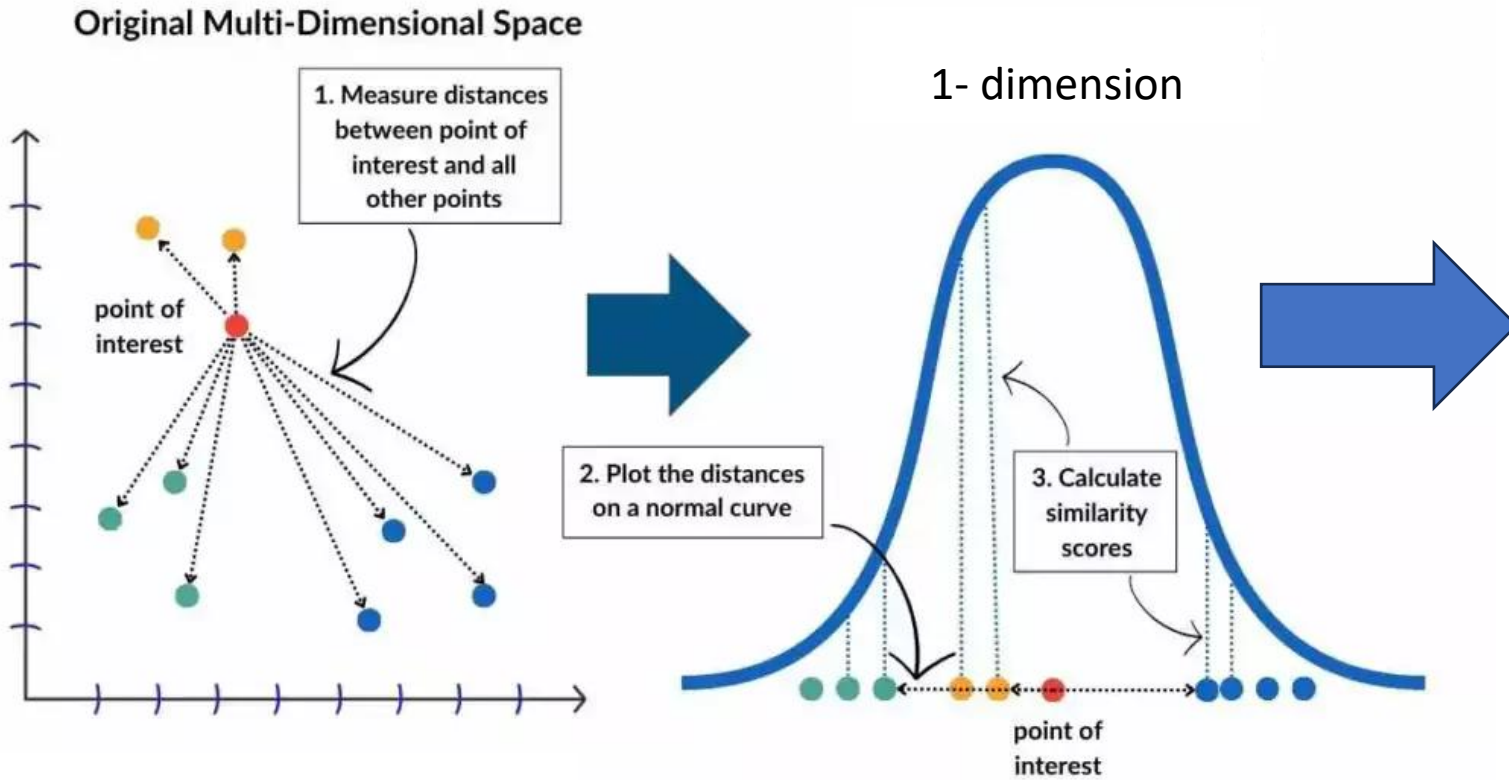
- t-SNE follows the logic and similar step with PCA
- But instead of finding a line that provides the **Largest sum of squared distance (as in PCA)**, t-SNE will find a line that **preserves the similarities between data points** in lower dimensions



The similarities between two points (i and j) in high/original dimension are calculated using gaussian probability distribution:

$$P_{j|i} = \frac{\exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma_i^2}\right)}{\sum_{k \neq i} \exp\left(-\frac{\|x_i - x_k\|^2}{2\sigma_i^2}\right)}$$

t-SNE



The goal is to project all data points in high-dimension space to one- or lower-dimension line in such a way that P_{ij} is equal to Q_{ij} for all i and j

Function to minimize:

$$P_{j|i} = \frac{\exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma_i^2}\right)}{\sum_{k \neq i} \exp\left(-\frac{\|x_i - x_k\|^2}{2\sigma_i^2}\right)}$$

The similarities between 2 points in lower dimension:

$$Q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|y_k - y_l\|^2)^{-1}}$$

$$KL(P||Q) = \sum_i \sum_j P_{ij} \log \frac{P_{ij}}{Q_{ij}}$$

The Experiments

λ -(BETS)₂GaCl₄ AND Bi2201-Fe9

Published TF- μ SR measurements of λ -(BETS) $_2$ GaCl $_4$

PHYSICAL REVIEW B **104**, 224506 (2021)

Distorted superconducting nodal line on a single Fermi surface in the anisotropic organic superconductor λ -(BETS) $_2$ GaCl $_4$

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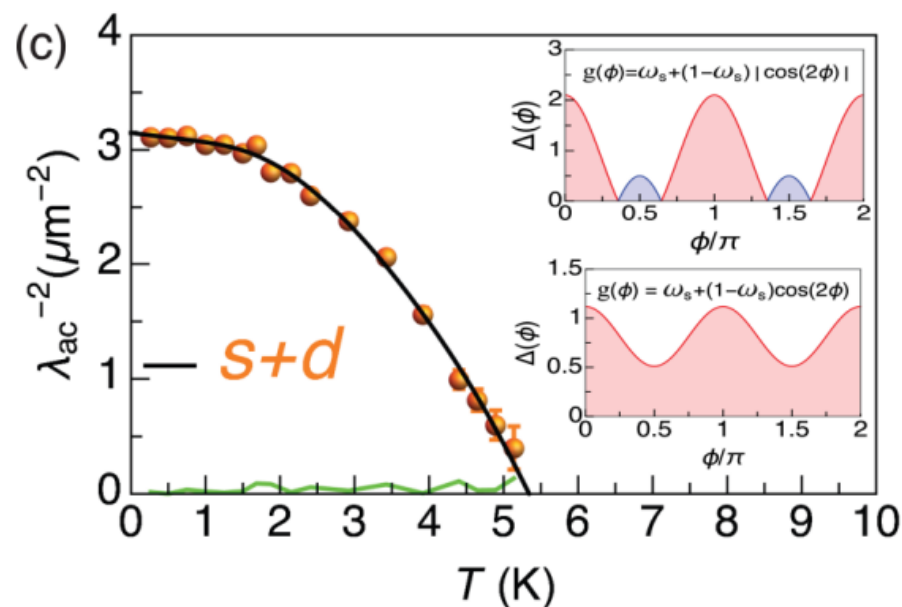
⁵*College of Engineering, Shibaura Institute of Technology, Saitama 337-8570, Japan*

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Published TF- μ SR measurements of λ -(BETS) $_2$ GaCl $_4$

The superconducting (SC) gap structure appearing in systems with single Fermi surface (FS) is generally described by the single gap function with s - or d -wave symmetry. The organic superconductor λ -(BETS) $_2$ GaCl $_4$ [BETS = (CH $_2$) $_2$ S $_2$ Se $_2$ C $_6$ Se $_2$ S $_2$ (CH $_2$) $_2$] endeavors to examine a novel SC gap structure on the distorted single cylindrical FS. Here, we show an example of the formation of the distorted SC nodal line by using the positive muon spin rotation (μ^+ SR) spectroscopy on λ -(BETS) $_2$ GaCl $_4$. Our analysis method of the μ^+ SR data reveals that the nodal line has a narrower width than that of the traditional d -wave by the steepness factor of 4.6(2.1), and a flat part with the maximum gap exists. We found that the amplitude of the SC gap is $2\Delta/k_B T_c = 3.9(2)$ and the in-plane penetration depth is $\lambda_{ac}(0) = 560(5)$ nm. Our present study gives insight into the relation of the FS distortion and the unusual Cooper pair formation mediated by the anisotropic spin fluctuations.

- ARGUS and MuSR, RIKEN-RAL/ISIS, UK
- TF perpendicular to initial muon polarization
- Temperature: 0.3 K – 10 K
- Metal to SC Transition at $T_c = 5.3$ K



ZF- μ SR experiment on Bi2201-Fe9 Unpublished experimental data

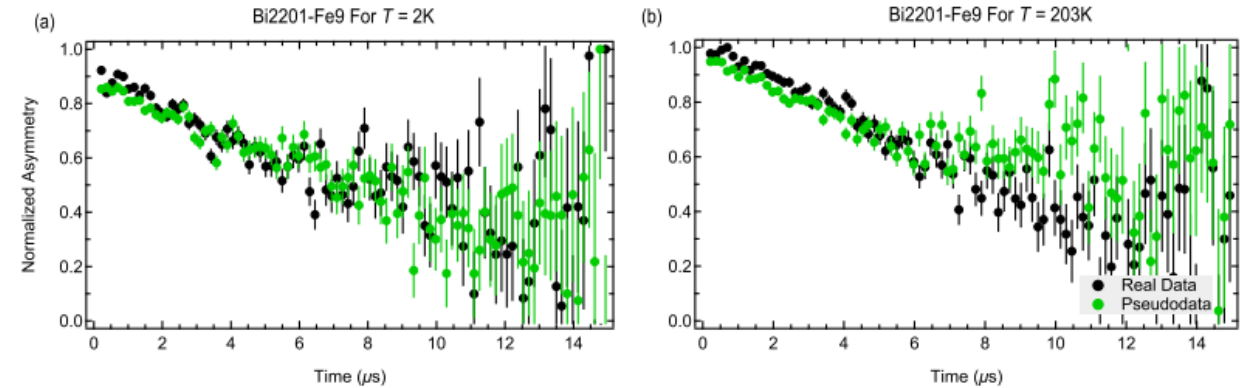
Experimental setup

- ARGUS, RIKEN-RAL/ISIS, UK
- Zero-field μ SR: no applied magnetic field
- Temperature range: 2 K to room temperature

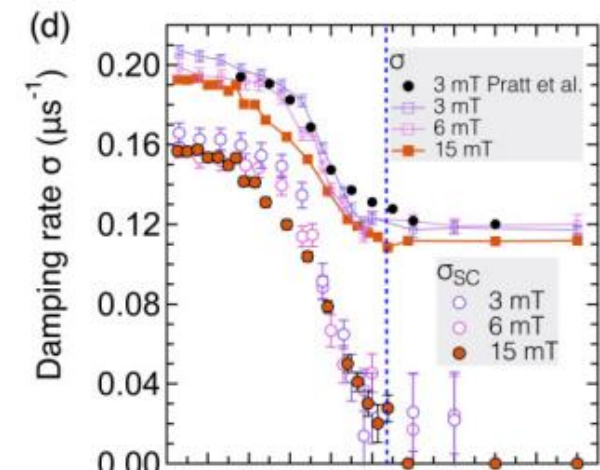
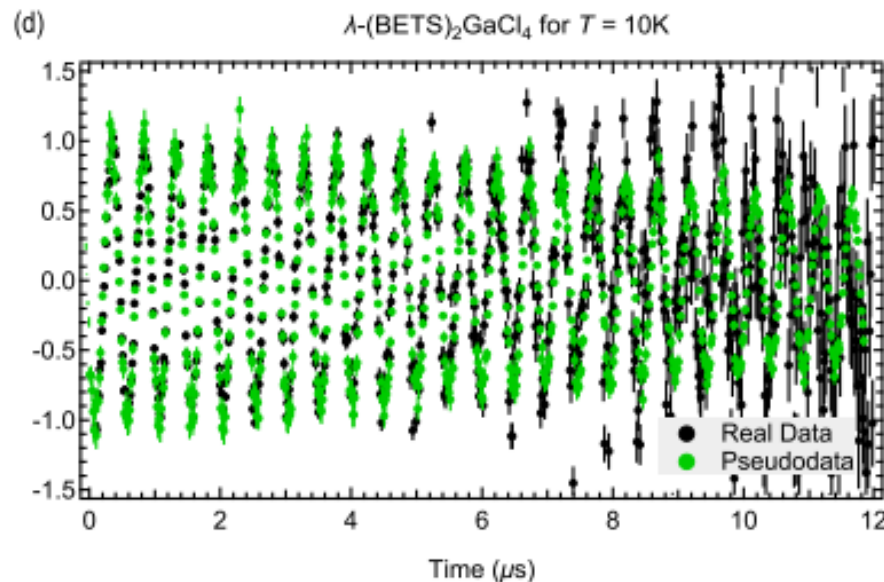
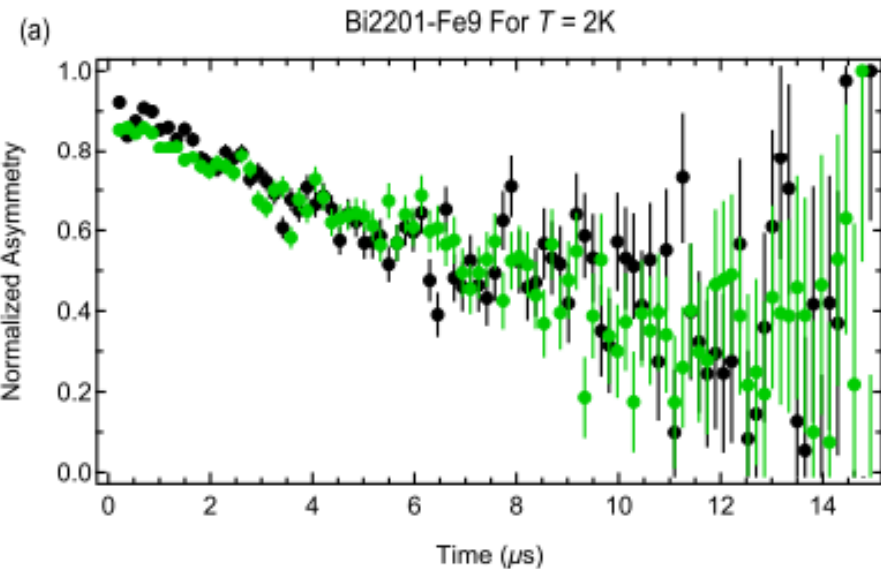
Sample and physics goal

- $(\text{Bi,Pb})_2\text{Sr}_2\text{Cu}_{1-\gamma}\text{Fe}_\gamma\text{O}_{6+\delta}$, $\gamma = 0.09$
- 9% Fe substitution on Cu sites
- Single crystals grown by floating-zone method
- Probe spin correlations and spin freezing

Example spectra: 2 K and 203 K



Pseudo-data generation and Gaussian smearing



- First, we tested the methods (PCA & t-SNE) on the generated pseudo-data
- Two sets of pseudo data: Large set (10 times Temperature measurement) and Normal set (The temperature measurement match with the real data)
- The pseudo-data are generated as close as possible with the real data
- Gaussian smearing for the uncertainty

As an example, for λ -(BETS)₂GaCl₄ the pseudo-data is generated using

$$A_0(t, T) = A_1 e^{-\sigma^2 t^2} \cos(\gamma_\mu B_1 t + \phi) + A_2 \cos(\gamma_\mu B_2 t + \phi)$$

- And we know that there is **transition** in the pseudo-data
- We want to know if PCA and t-SNE can reveal the transition

Results

PCA and t-SNE on Pseudo-data and Experimental Data

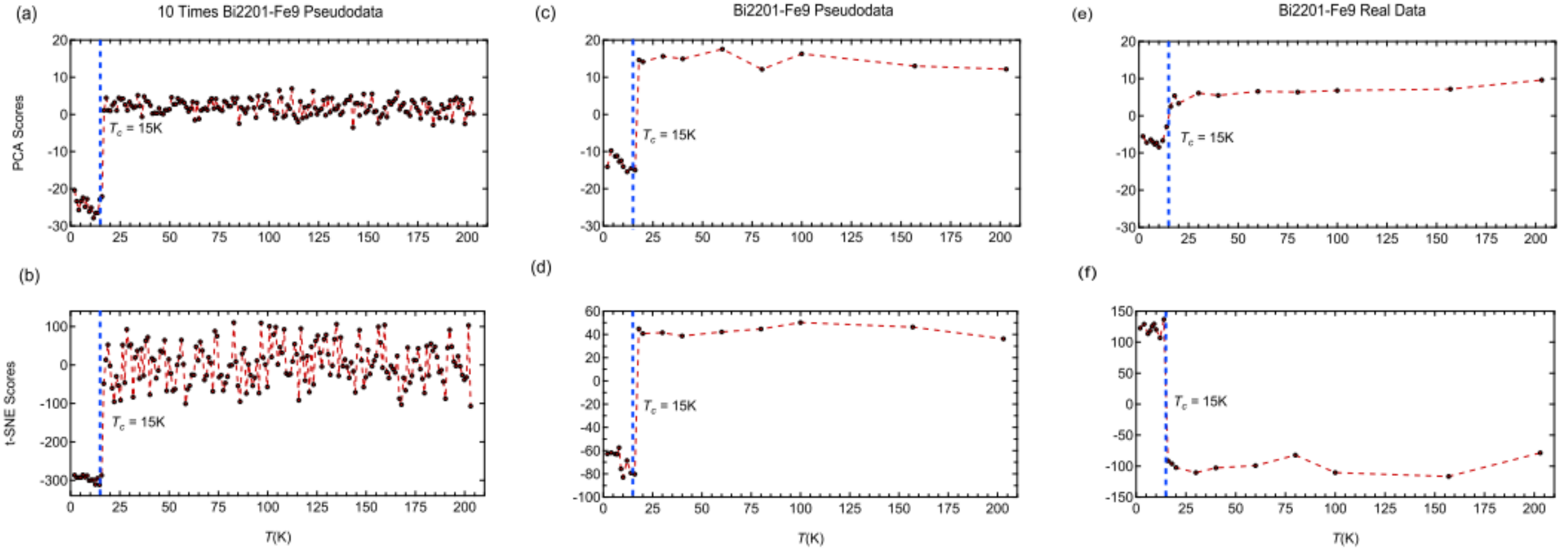


FIG. 3. The first component results of Bi2201-Fe9. The first component scores from PCA (top) and t-SNE (bottom) are shown for the large pseudo data set (left), the normal pseudo data set (middle), and the real experimental data (right). Both PCA and t-SNE successfully identify the phase transition at the expected critical temperature indicated by the solid line for the pseudodata at $T_c = 15$ K for the experimental data. The t-SNE method offers greater separation between the two phases compared to PCA.

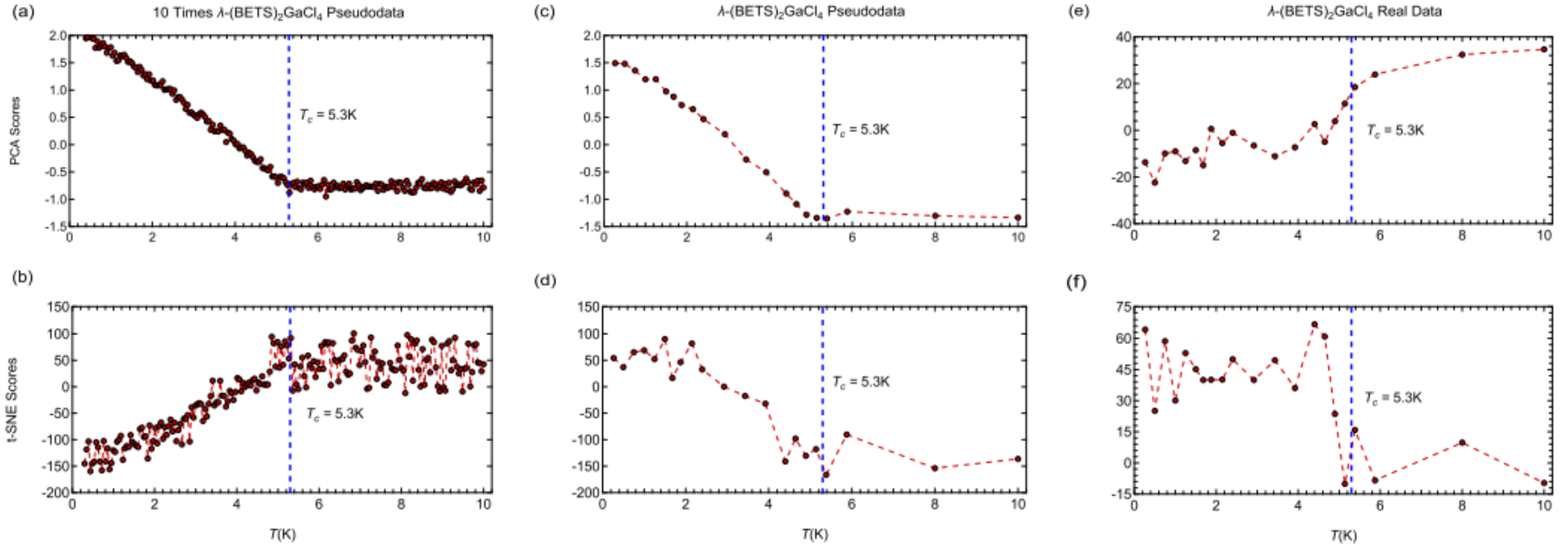
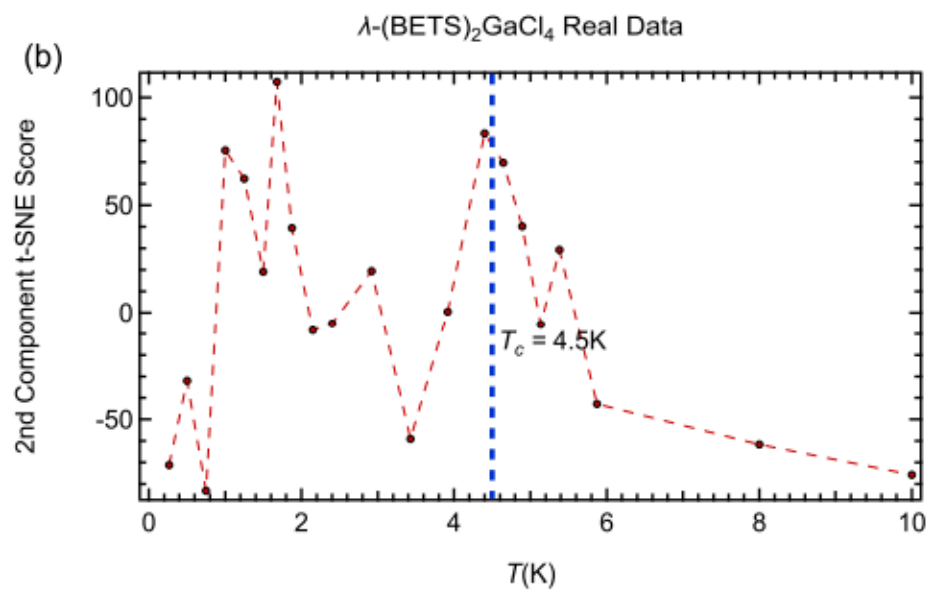
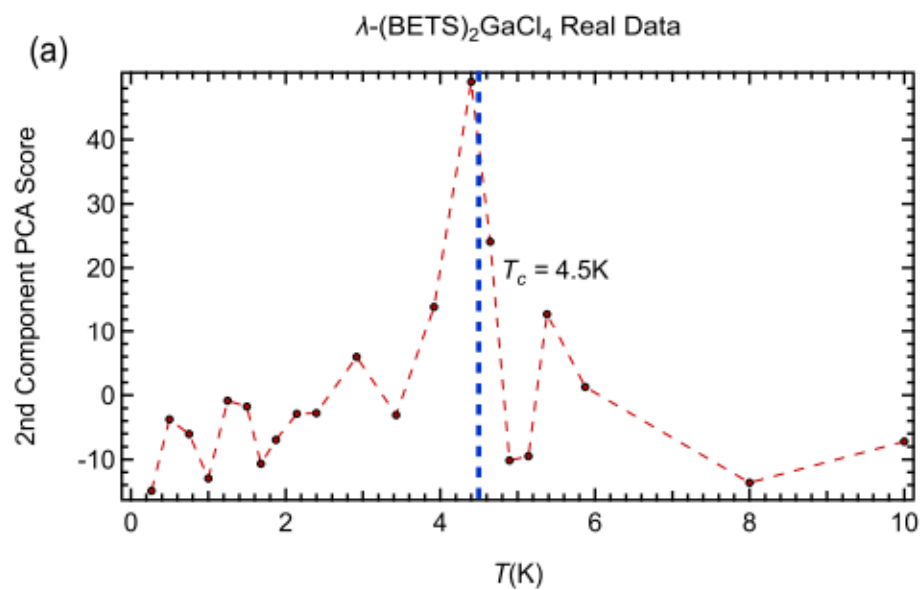
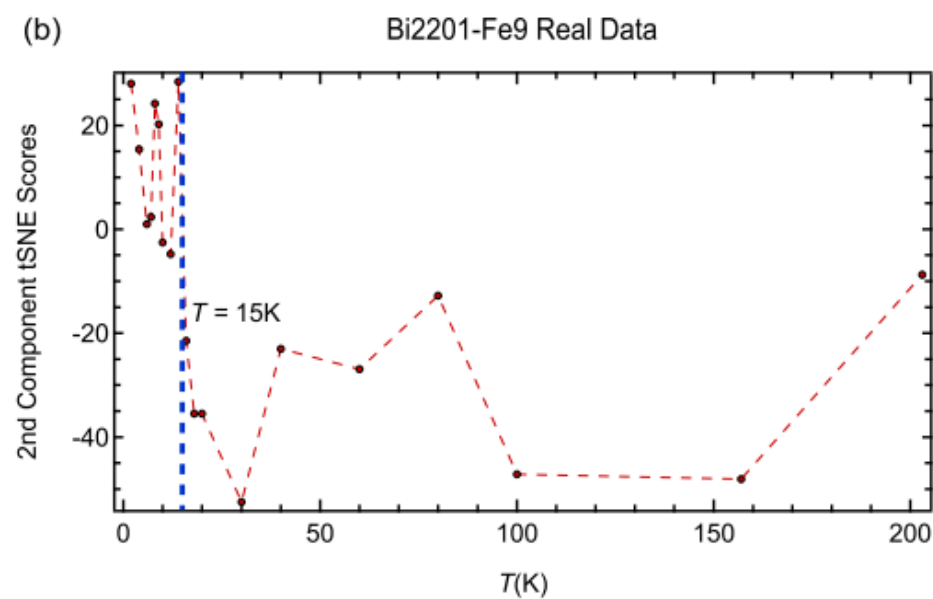
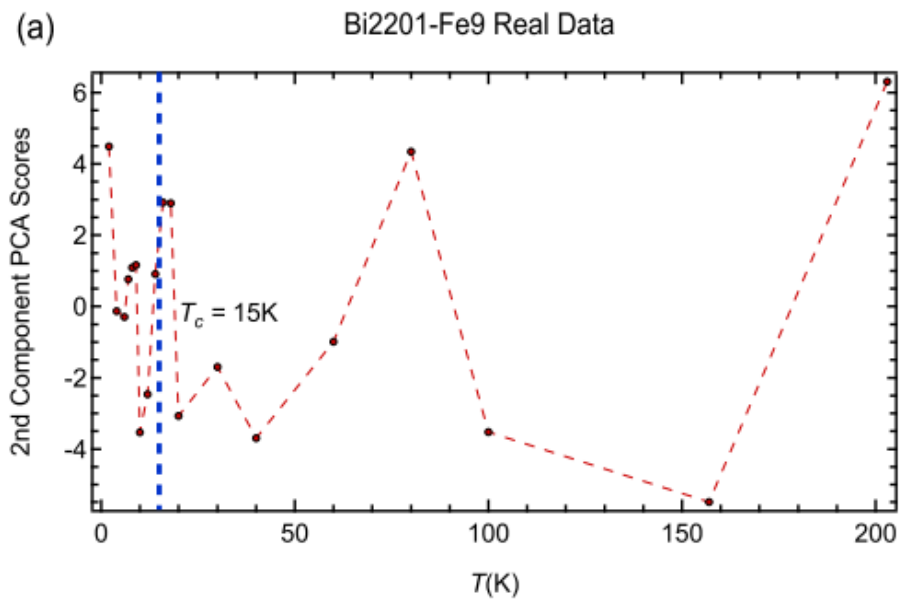


FIG. 4. The first component results of λ -(BETS) $_2$ GaCl $_4$. The first component scores from PCA (top) and t-SNE (bottom) for the large pseudo-data set (left), the normal pseudo-data set (middle), and the real experimental data (right). In the large pseudo-data set, a clear transition is observed at the expected temperature. t-SNE shows a broader range of component scores, resulting in greater separation between the two phases compared to PCA.

Second Component



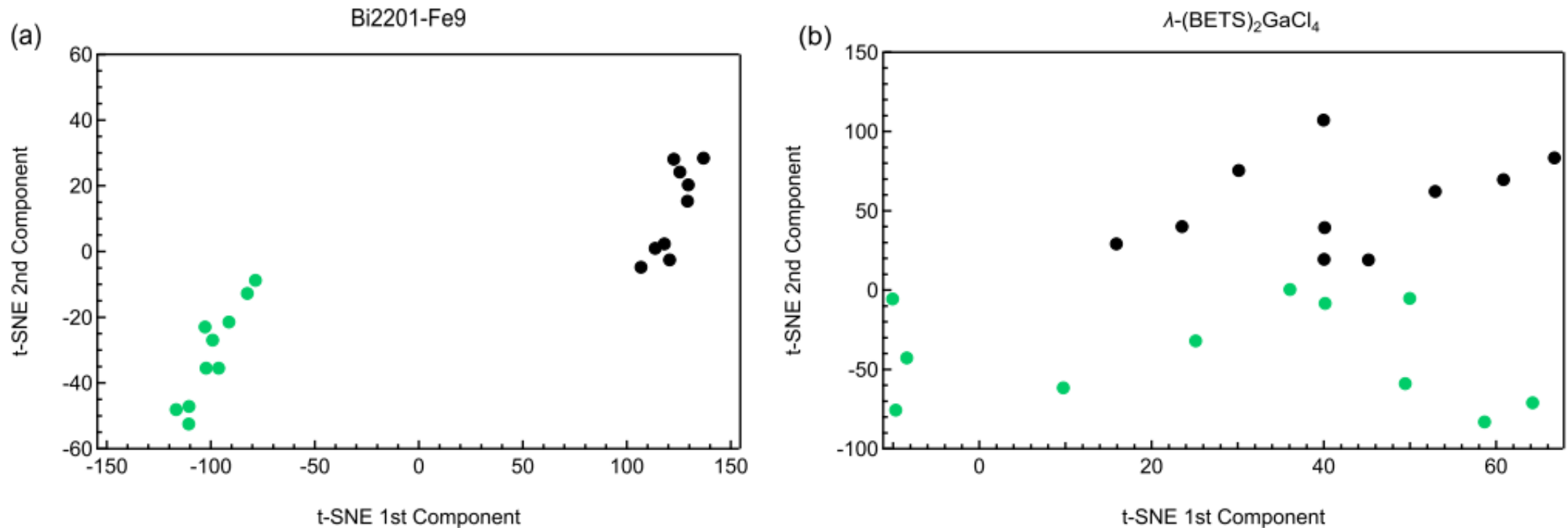


FIG. 8. Two-dimensional t-SNE embeddings of the experimental μ SR datasets for (a) Bi2201-Fe9 and (b) λ -(BETS)₂GaCl₄. Each point represents a temperature-dependent μ SR spectrum projected into the two-dimensional embedding space. Bi2201-Fe9 exhibits two clearly separated clusters associated with the low- and high-temperature regimes, whereas λ -(BETS)₂GaCl₄ displays a more continuous distribution consistent with a gradual superconducting transition.

Summary & Outlook

- **Dimensional reduction techniques are complementary approach to conventional μ SR fitting**
- These methods can identify or provide signatures of phase transitions
- Further exploration using extensive phase-transition datasets is required (Need a lot more data)
- I believe that applying **pattern recognition algorithms** to **PCA and t-SNE scores** will yield significant insights, making this an excellent project for student

Thank You