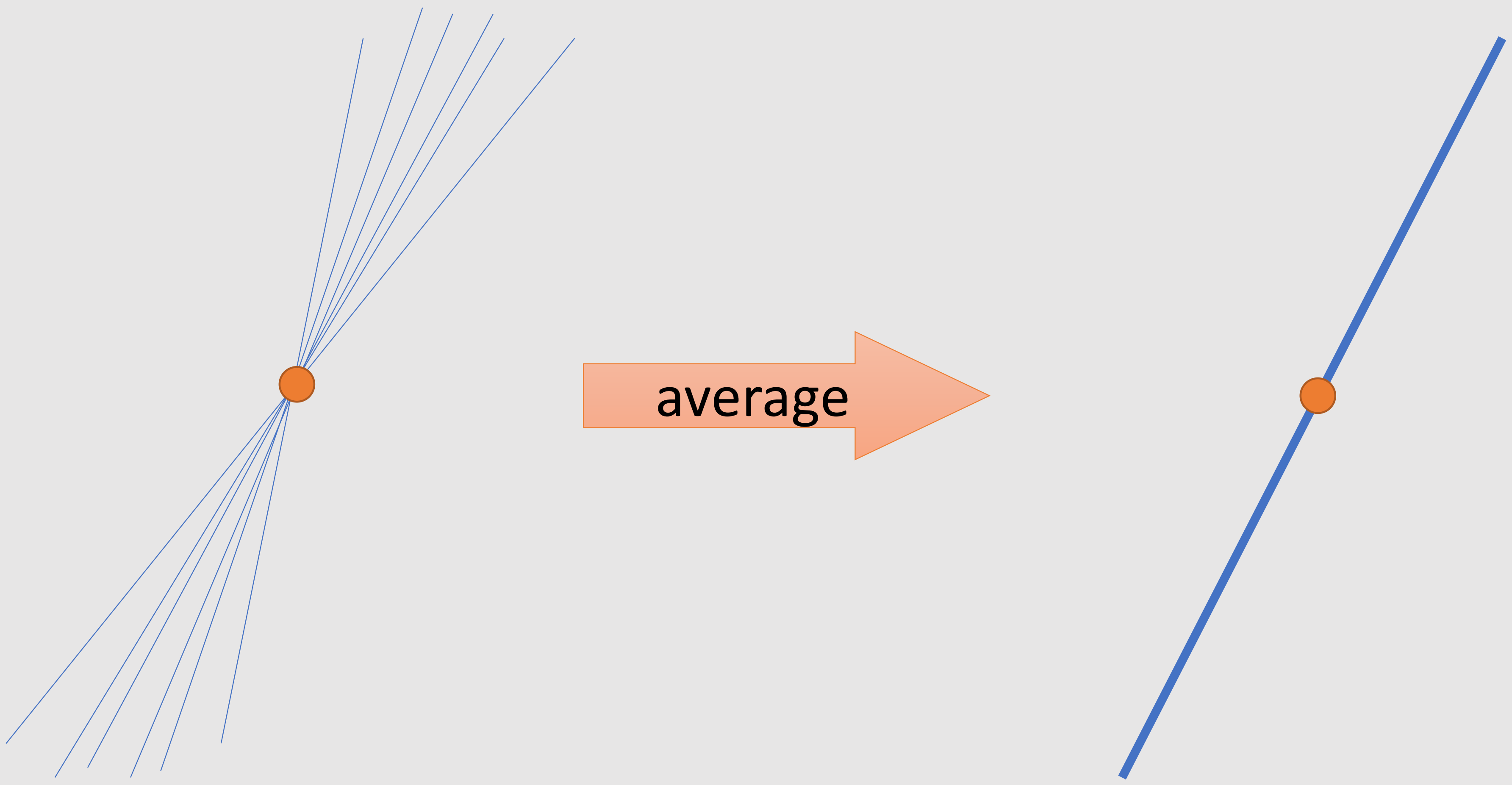
Principal Component Analysis (PCA)

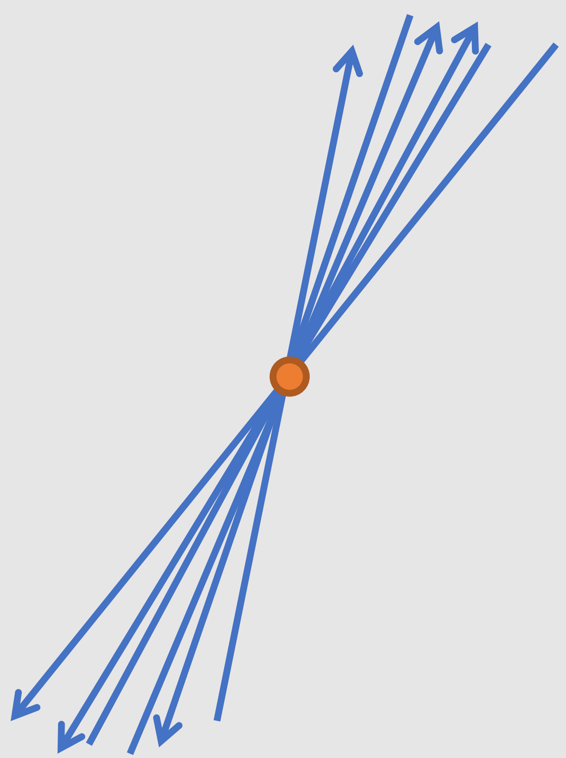
主成分分析

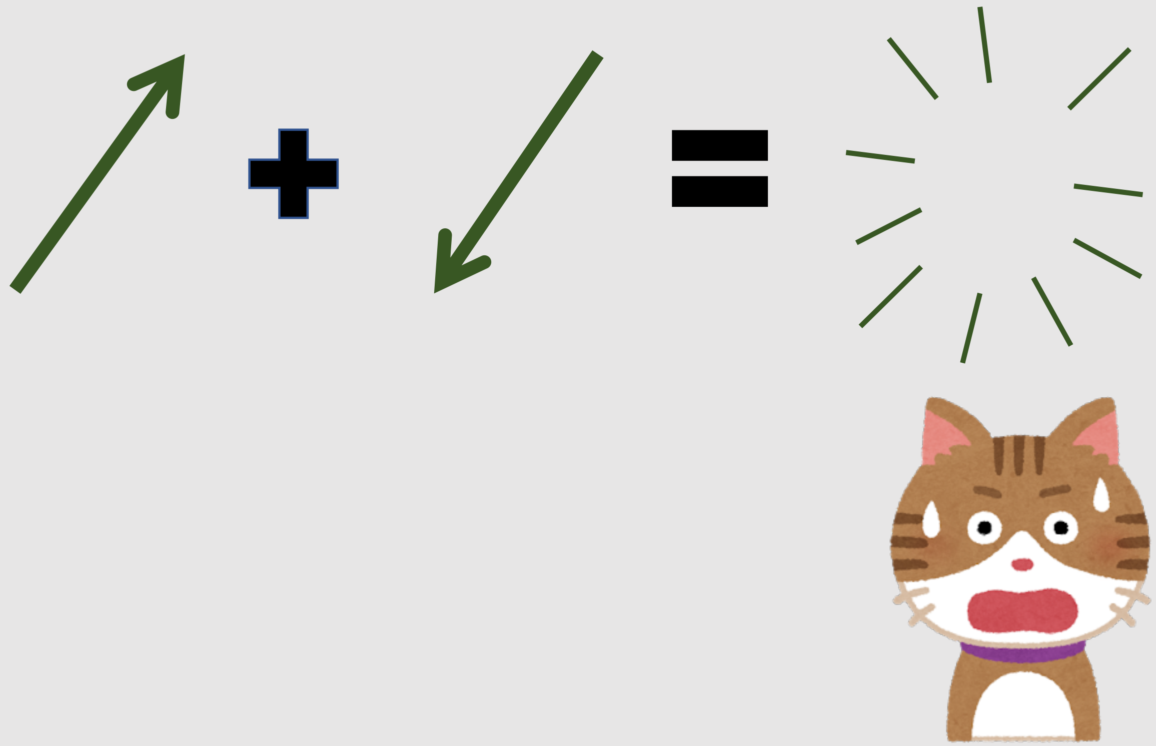
Let’s Average Orientations !



Averaging Vectors is not Straightforward

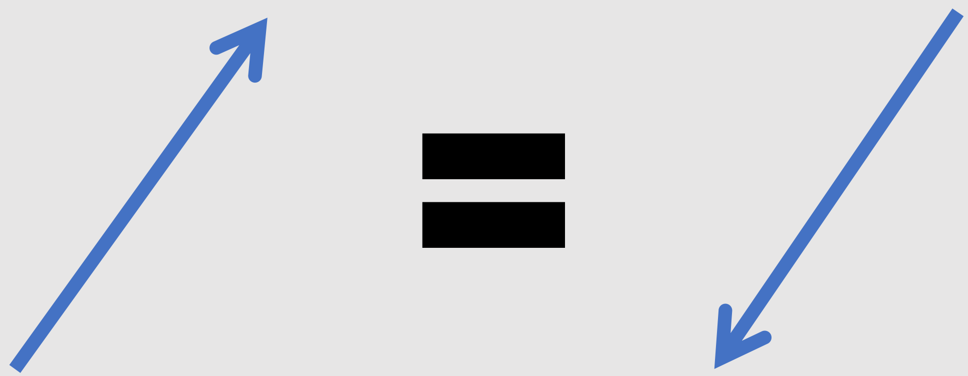
Naïve orientation representations may cancel out each other





Formulation of Add-able Orientation?

- What is the representation opposite direction is the same?
- Removing orientation information from a vector?



Matrix of Outer Product is the Solution

- Symmetric matrix from a vector

$$\vec{v} \otimes \vec{v} = \vec{v}\vec{v}^T = \begin{bmatrix} v_0 v_0 & v_0 v_1 & v_0 v_2 \\ v_1 v_0 & v_1 v_1 & v_1 v_2 \\ v_2 v_0 & v_2 v_1 & v_2 v_2 \end{bmatrix}$$

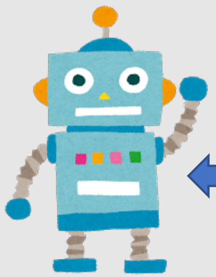
- The opposite vector gives the same matrix

$$(-\vec{v}) \otimes (-\vec{v}) = \vec{v} \otimes \vec{v}$$

Linear Form & Quadratic Form

Linear form

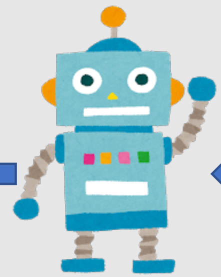
$$\vec{f} = A\vec{e}$$

vector $\vec{f}$  vector $\vec{e}$

matrix

Quadratic form

$$\mathrm{a} = \vec{e}^{T} A\vec{e}$$

scalar a  vector $\vec{e}$

vector $\vec{e}$

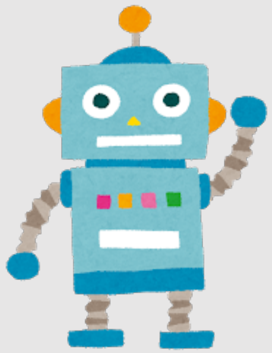
matrix

Interpretation of Quadratic Form

- Represent how much input vector $\vec{e}$ is parallel to the vector $\vec{v}$

$$\vec{e}^T A \vec{e} = \vec{e}^T (\vec{v} \otimes \vec{v}) \vec{e} = (\vec{e}^T \vec{v})(\vec{v}^T \vec{e}) = (\vec{e}^T \vec{v})^2$$

Similarity
between $\vec{e}$ and $\vec{v}$
in the range [0,1]



vector $\vec{e}$

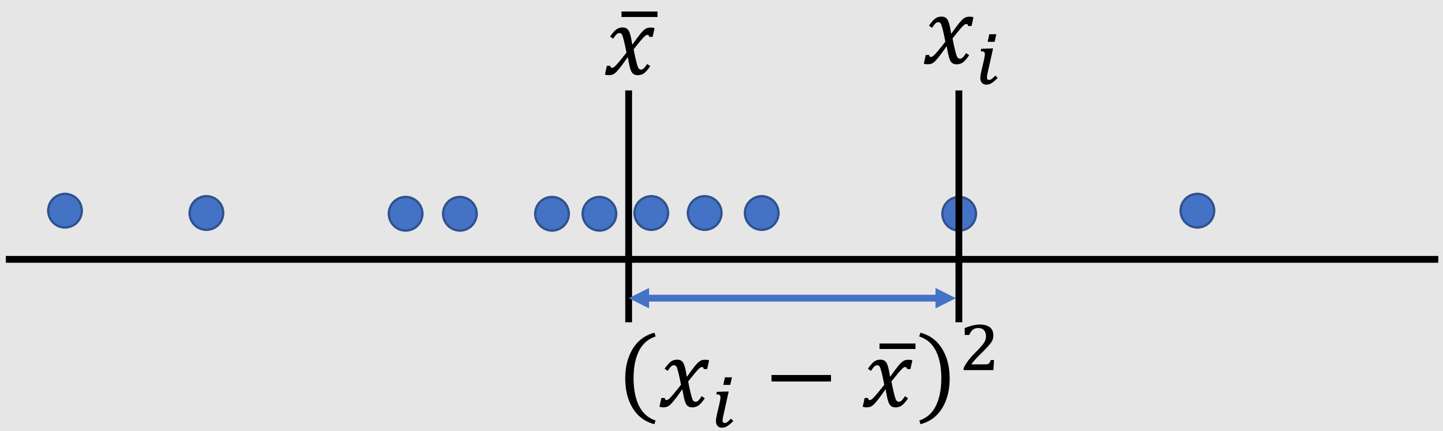
vector $\vec{e}$

matrix
$\vec{v} \otimes \vec{v}$

What is Variance?

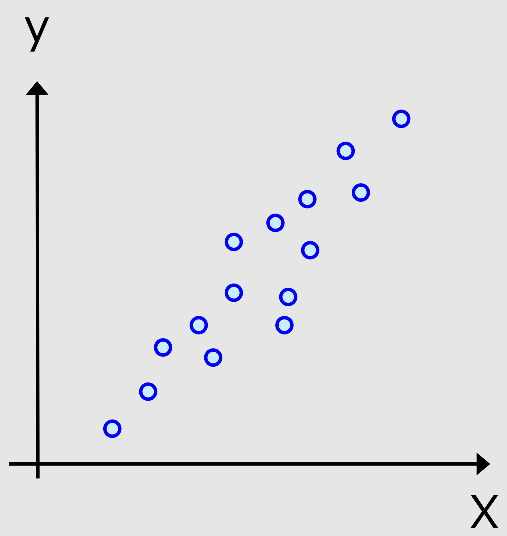
- Variance means deviation from the mean

$$\boxed{\mathrm{Var}(x) = \sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n}}$$



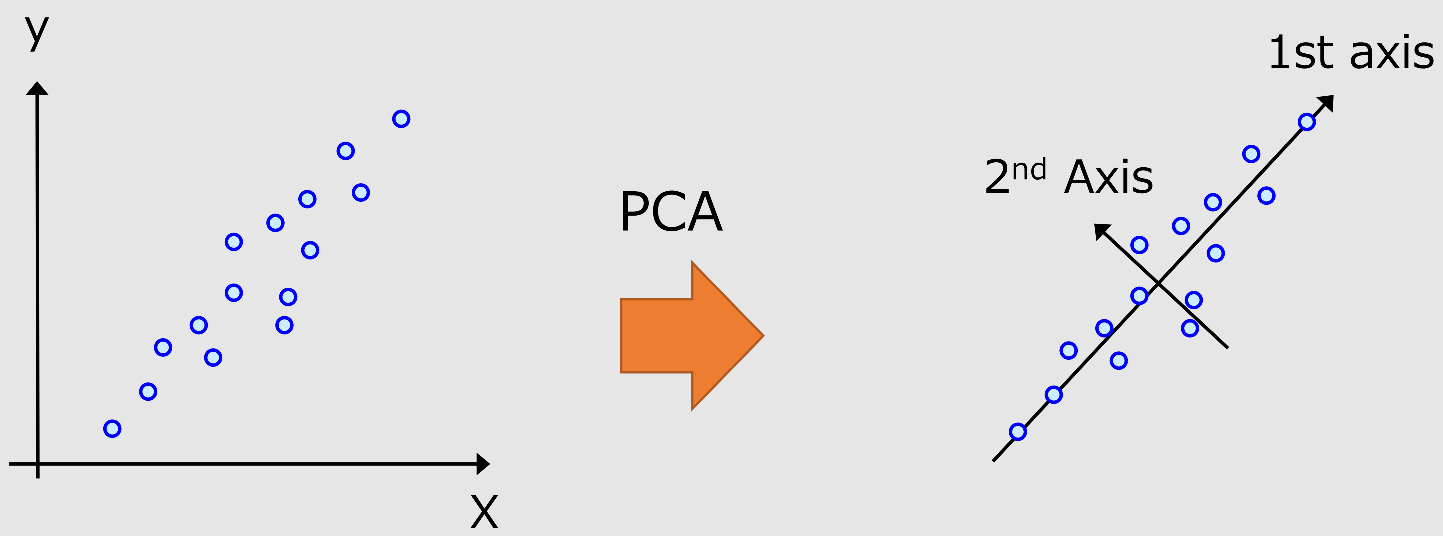
How Should We Choose Axis?

- Finding the axis with highest variance -> PCA!



What is PCA?

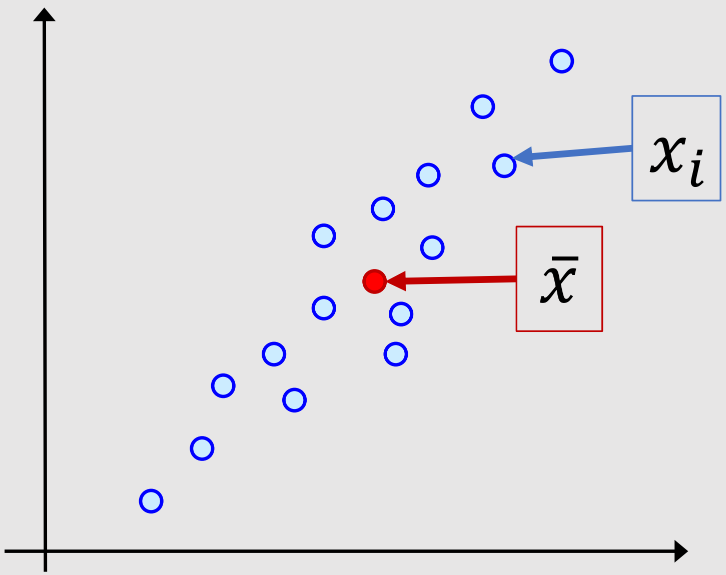
- Low-dimensional approximation of hi-dimensional data
- Find directions of large variance (the magnitude of distribution)



PCA Step 1: Averaging Points

- Adding up the multivariate value x_i and divide with #samples

$$\boxed{\bar{x} = \frac{1}{N}\sum_{i=0}^{N} x_i}$$



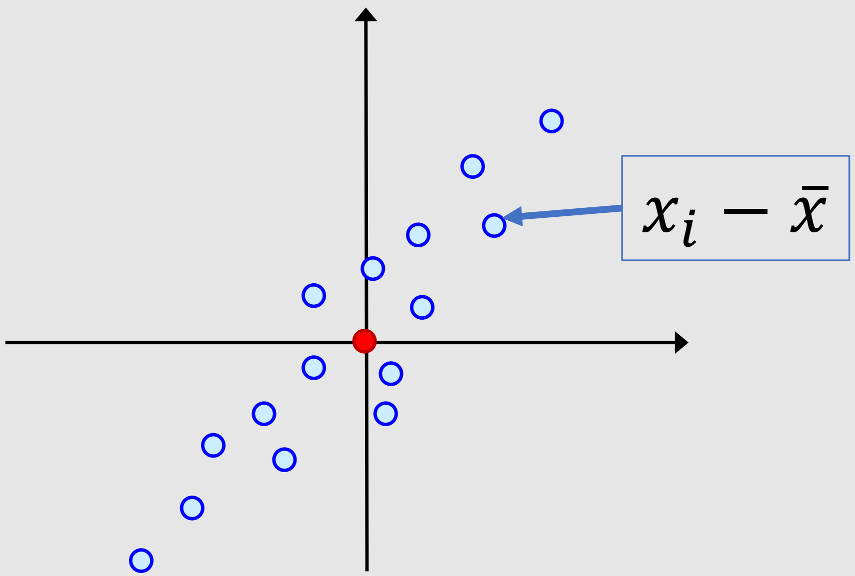
PCA Step 2：Computing Difference

- Matrix A: deviation from average

#column: number of variables in a sample

$$A = \begin{bmatrix} x_1 - \bar{x} \\ \vdots \\ x_i - \bar{x} \\ \vdots \\ x_N - \bar{x} \end{bmatrix}$$

#rows: number of sample



PCA Step 3：What is Covariance Matrix?

- $A^T A$ is called covariance matrix
- Covariance is positive (semi-)definite

$$\boxed{A = \begin{bmatrix} x_1 - \bar{x} \\ \vdots \\ x_i - \bar{x} \\ \vdots \\ x_N - \bar{x} \end{bmatrix}}$$

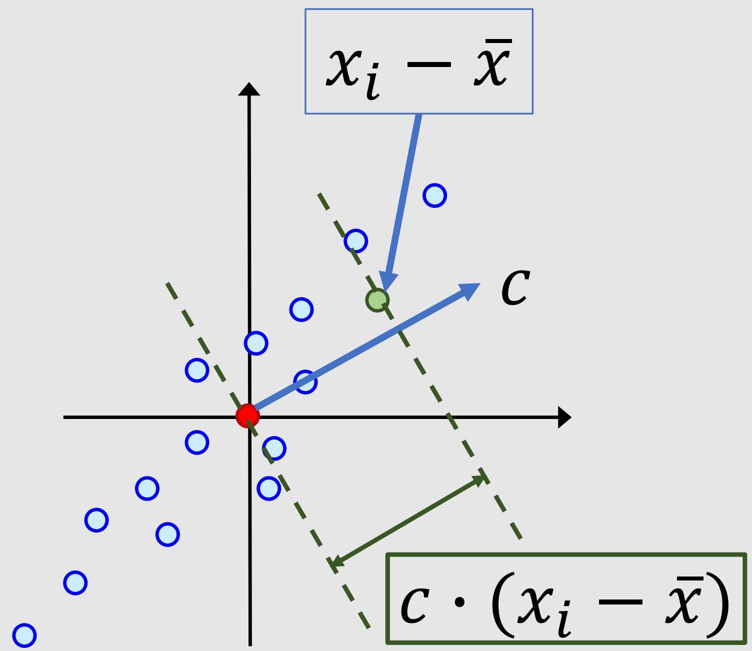
covariance matrix

$$\boxed{S = A^T A}$$

What is the Covariance Matrix?

- Variance in higher dimension
- Given direction c, the variance in that direction is $c^T S c$

$$
\begin{aligned}
&c^T S c \\
&= c^T A^T A c \\
&= \underbrace{\sum_{i=0}^{N} |c \cdot (x_i - \bar{x})|^2}_{\text{Variance in the direction of c}}
\end{aligned}
$$



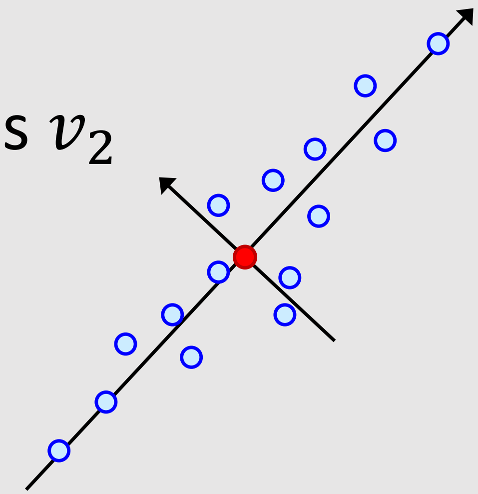
PCA Step 4：Eigen Value Decomposition

- Find the axis with large variance by eigen decomposition

$$S = \lambda_1 v_1 v_1^T + \lambda_2 v_2 v_2^T \cdots$$

1st axis v_1

2nd axis v_2



Symmetric matrix has real eigenvalues
Its eigenvectors are orthogonal

Power Method for Maximum Eigenvalues

- Iteration quickly converges into maximum eigen vector

1. $v^{i+1} = Av^i$
2. $v^{i+1} = v^{i+1} / \|v^{i+1}\|$

- Rayleigh Quotient gives maximum eigenvalue

$$\boxed{\lambda^i = \frac{(v^i \cdot Av^i)}{(v^i \cdot v^i)}}$$