基礎機器學習與深度學習-2

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基礎機器學習

針對前述的介紹，每個topic都介紹一個演算算法

1. Regression: Linear regression & Regularization

2. Classification: Linear and Quadratic Discriminant Analysis

3. Clustering: K-means (Unsupervised learning)

4. Dimension Reduction: PCA (Unsupervised learning)

5. Ensemble learning: 不介紹。

k-means Clustering(Unsupervised learning)

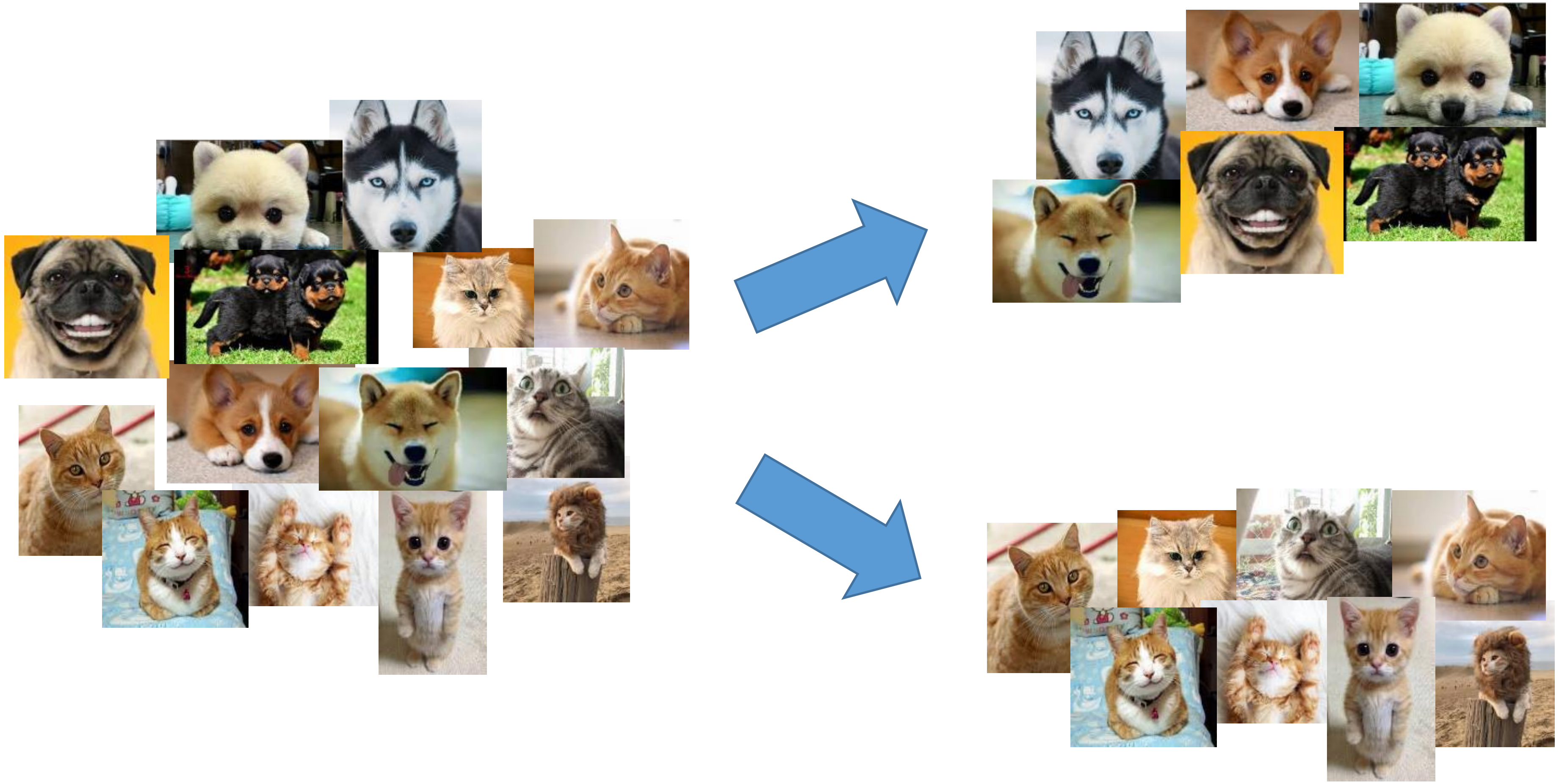
- *k*-means Clustering: 物以類聚 (類似歸納法)

不斷學習(iteration)，直到收斂為止。

為什麼叫*k*-means顧名思義就是有*k*個群心，我們將資料學習後判斷這些資料屬於哪個群心。

EX: 給你一組身高和體重資料，但我沒有跟你說這組資料哪些是男生哪些是女生。我希望你用這組資料分出兩群，這種時候就是用非監督式學習。→ 2-means clustering

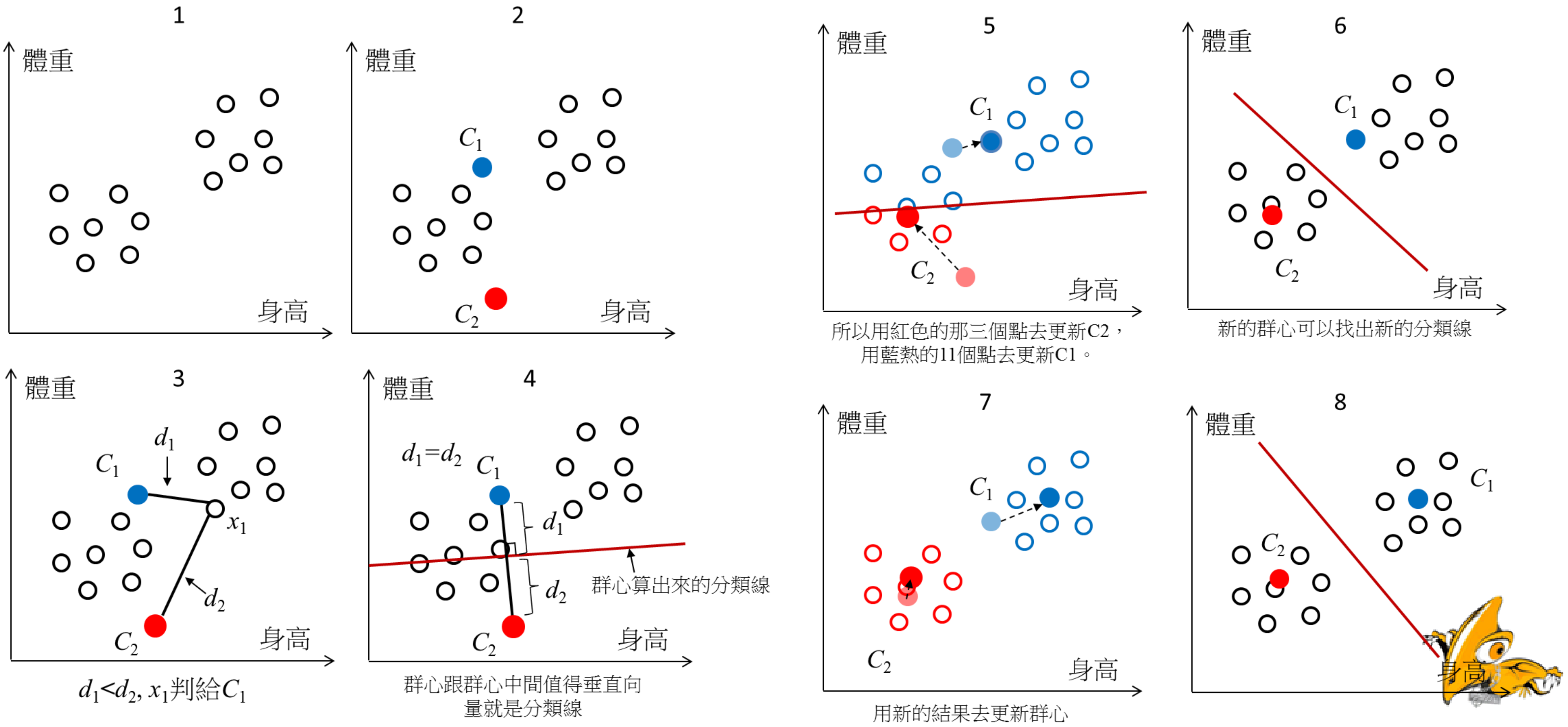
k-means Clustering(Unsupervised learning)



k-means Clustering(Unsupervised learning)

- *k*-means: with a name “means”.
- Most important information is “mean vector”.
- *k*-means is based on learning the mean vector for each cluster.
- Number of cluster is setting by user.

k-means Clustering(Unsupervised learning)

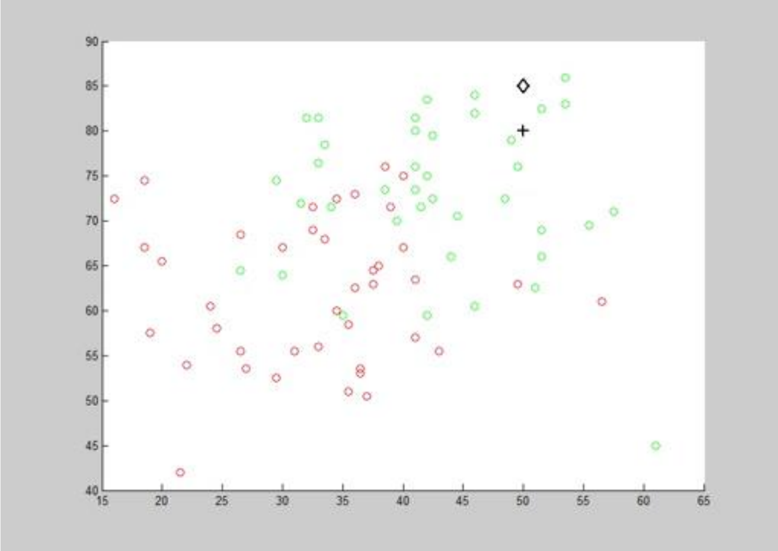


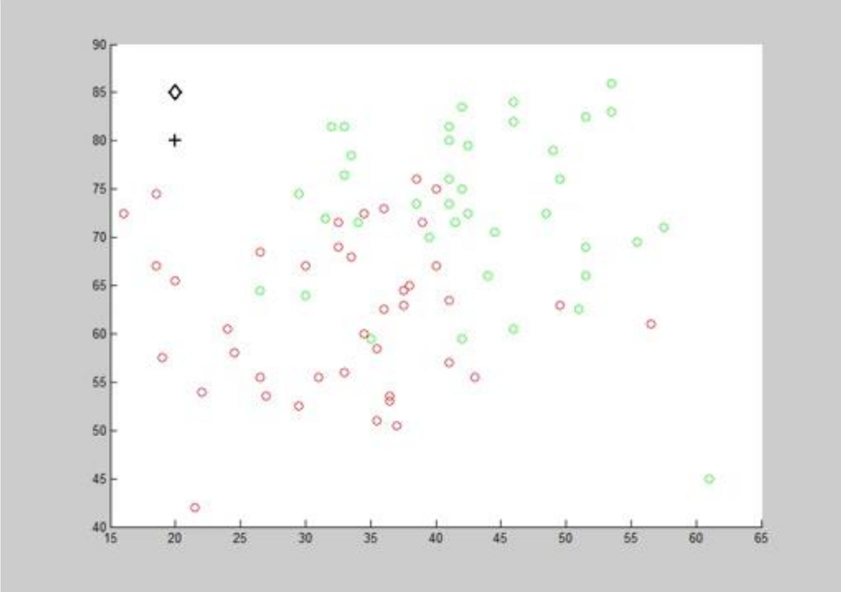
k-means Clustering(Unsupervised learning)

- 設定有k(必須$\leq n$)個Clusters {**S**1,**S**2, ...,**S**k}，k-means clustering就是希望可以最小化群內的資料和群心的誤差平方和越小越好，數學公式如下:

$$\underset{\mu}{\arg\min} \sum_{c=1}^{K} \sum_{i=1}^{n_c} \|x_i - \mu_c\|^2 \Big|_{x_i \in S_c}$$

k-means Clustering





1. 初始隨機設定k個群心.

$$\mu_c^{(0)} \in R^d, c = 1,2,\dots,K$$

2. 計算分類到每一群體的樣本，(t)為第t次運算

$$S_c^{(t)} = \left\{x_i : \left\|x_i - \mu_c^{(t)}\right\| \le \left\|x_i - \mu_{c^*}^{(t)}\right\|, \forall i = 1,\dots,n\right\}$$

3. 更新群心(nc個資料在第c群內。)

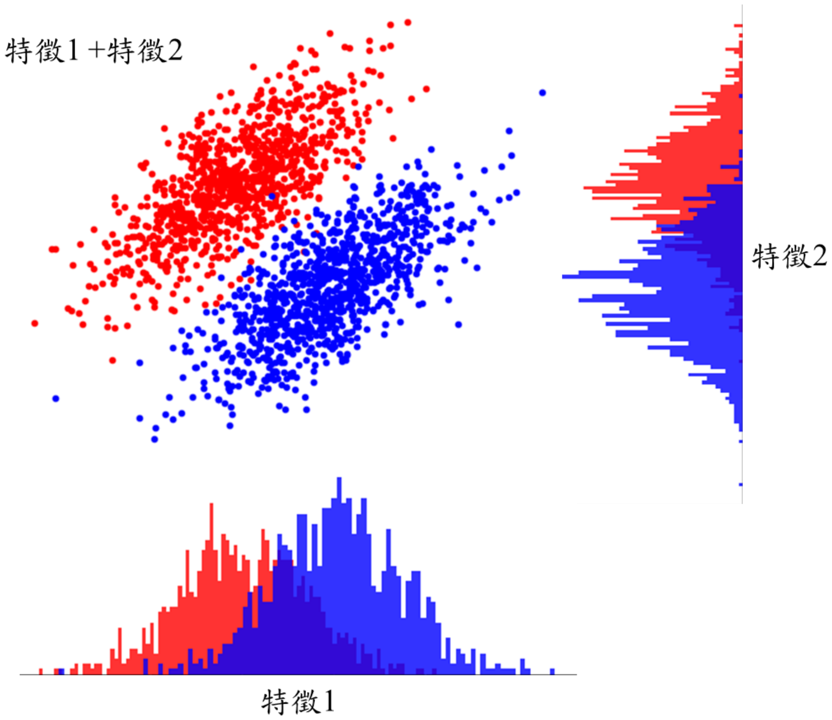
$$\mu_c^{(t+1)} = \frac{sum(S_c^{(t)})}{n_c} = \sum_{i=1}^{n_c} x_i \Big|_{x_i \in S_c^{(t)}}$$

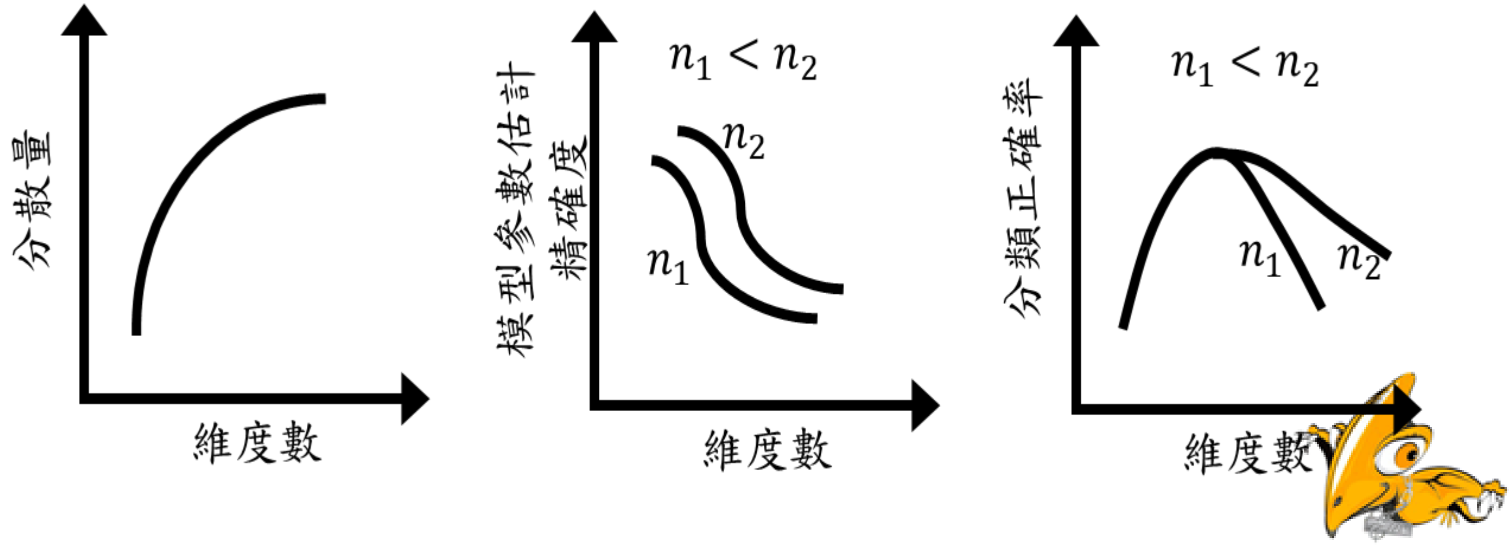
4. 重複2–3，直到群心不變動，也就是

$$S_c^{(t+1)} = S_c^{(t)}, \forall c = 1,\dots,K$$

Dimension Reduction

在建立預測模型時，容易因為**特徵數大於資料樣本數**造成模型參數估計錯誤，導致模型無法有效進行任務預測，在機器學習稱此現象為「休斯現象(Hughes phenomenon)」，也稱為「維度詛咒(Curse of dimensionality)」，





Dimension Reduction

Example:

Model 1: “body fat (bf)”

Model 2: “body fat (bf)”, “weight (w)”, “hair length (hl)”

$$\operatorname{cov}(\text{model1}) = \left[\operatorname{cov}(bf, bf)\right]$$

$$\operatorname{cov}(\text{model2}) = \begin{bmatrix} \operatorname{cov}(bf, bf) & \operatorname{cov}(w, bf) & \operatorname{cov}(hl, bf) \\ \operatorname{cov}(bf, w) & \operatorname{cov}(w, w) & \operatorname{cov}(hl, w) \\ \operatorname{cov}(bf, hl) & \operatorname{cov}(w, hl) & \operatorname{cov}(hl, hl) \end{bmatrix}$$

Example for single variable

If we only get one sample, and try to calculate covariance.

$$\mu = x_i$$

$$cov(model\ 1) = \sigma = \frac{1}{1}\sum_{i=1}^{1}(x_i - \mu_x)^2 = 0$$

$$f(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Example for multi-variables

If we only get two sample, and try to calculate covariance matrix.

$$\Sigma = \begin{bmatrix} \operatorname{cov}(bf, bf) & \operatorname{cov}(w, bf) & \operatorname{cov}(hl, bf) \\ \operatorname{cov}(bf, w) & \operatorname{cov}(w, w) & \operatorname{cov}(hl, w) \\ \operatorname{cov}(bf, hl) & \operatorname{cov}(w, hl) & \operatorname{cov}(hl, hl) \end{bmatrix}$$

The elements in covariance matrix are larger than 0, but the covariance matrix would be singular.

$$f(\boldsymbol{x}|\boldsymbol{\mu}, \Sigma) = (2\pi)^{-d/2}|\Sigma|^{-0.5} exp\{-0.5(\boldsymbol{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}-\mu)\}$$

Dimension Reduction

- Dimension Reduction is proposed to overcome this issue.

1. Feature selection

   Using only “import” features.

2. Feature extraction

   Feature Fusion.

Feature Selection

In statistics,

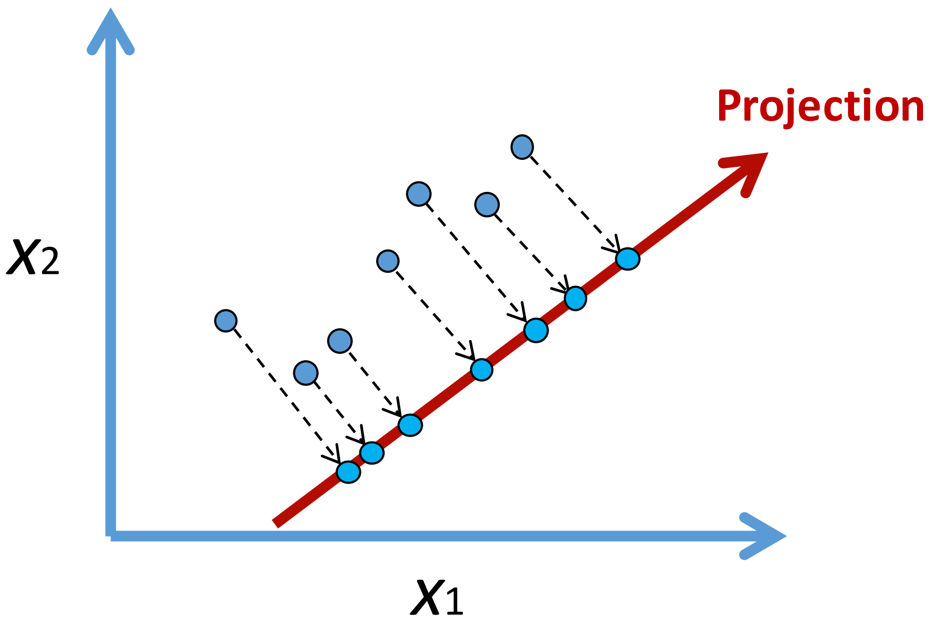
- Forward sequential feature selection
- Backward sequential feature selection
- Stepwise feature selection
- LASSO

In machine learning,

- Random subspace.

Feature Extraction

- Feature Fusion (Projection)



Feature extraction:
Just finding the projection vectors for input features.

Feature Extraction

- **Principal component analysis (PCA)**
- Independent component analysis (ICA)
- Canonical component analysis (CCA)
- Non-negative matrix factorization
- Discriminant Analysis Feature Extraction(DAFE)
- Neural Network

Principal component analysis (PCA)

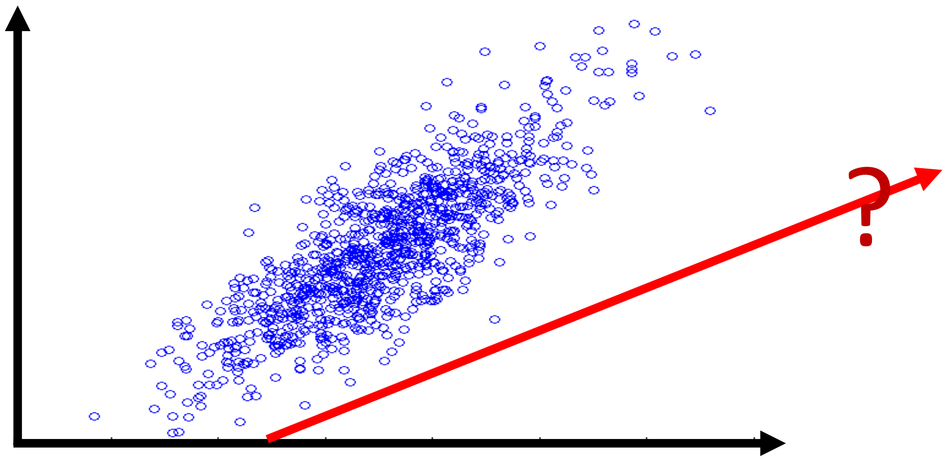
Why do I introduce PCA?

1. Stronger knowledge.
2. Unsupervised.
3. Most popular
4. Basic

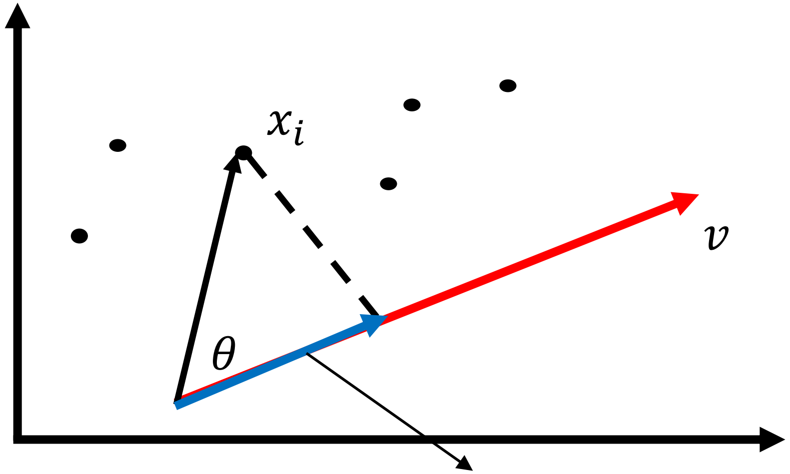
Principle Component Analysis

DL/ML/Statistics are developed by a given goal.

- PCA aims to find a set of vector containing the maximum amount of variance in the data.



Principle Component Analysis



$$\|x_i\| \cos\theta$$

$$\cos\theta = \frac{\langle x_i, v \rangle}{\|x_i\| \|v\|}$$

$$\|x_i\| \cos\theta \frac{v}{\|v\|}$$

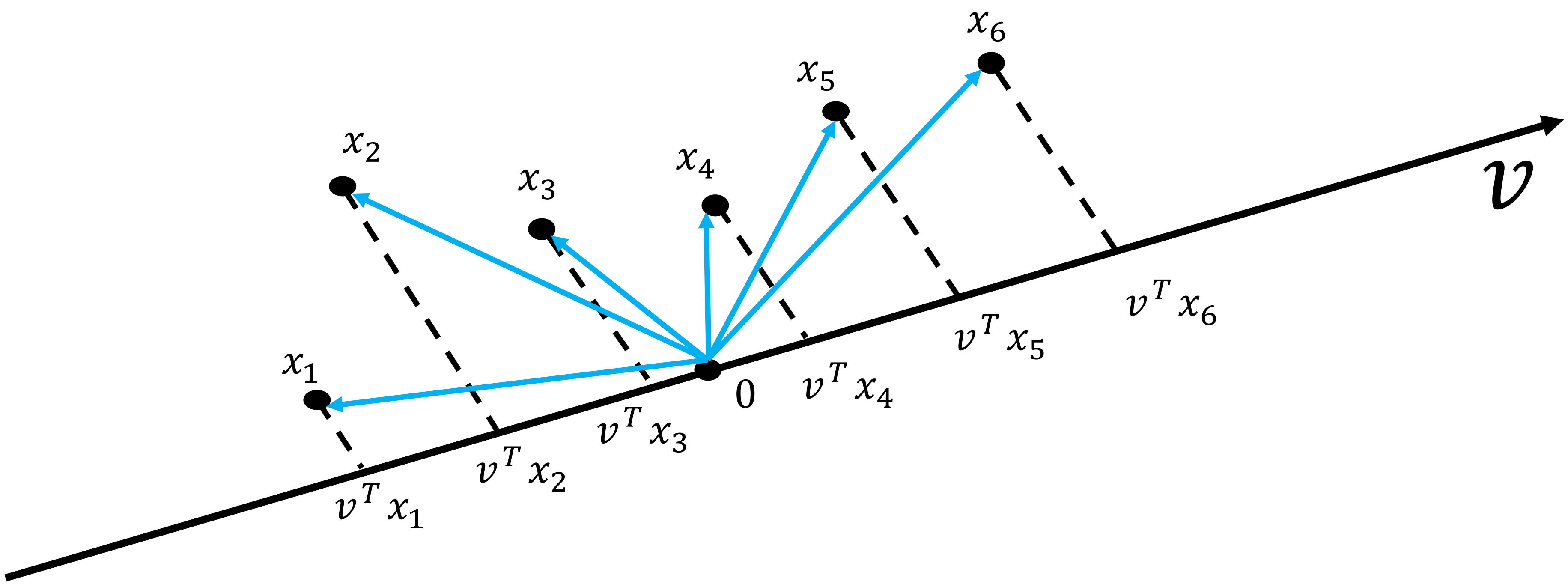
$$= \|x_i\| \frac{\langle x_i, v \rangle}{\|x_i\| \|v\|} \frac{v}{\|v\|} = \frac{\langle x_i, v \rangle}{\|v\|^2} v$$

- If $\|v\|$ is unit, then $\langle x_i, v \rangle v$

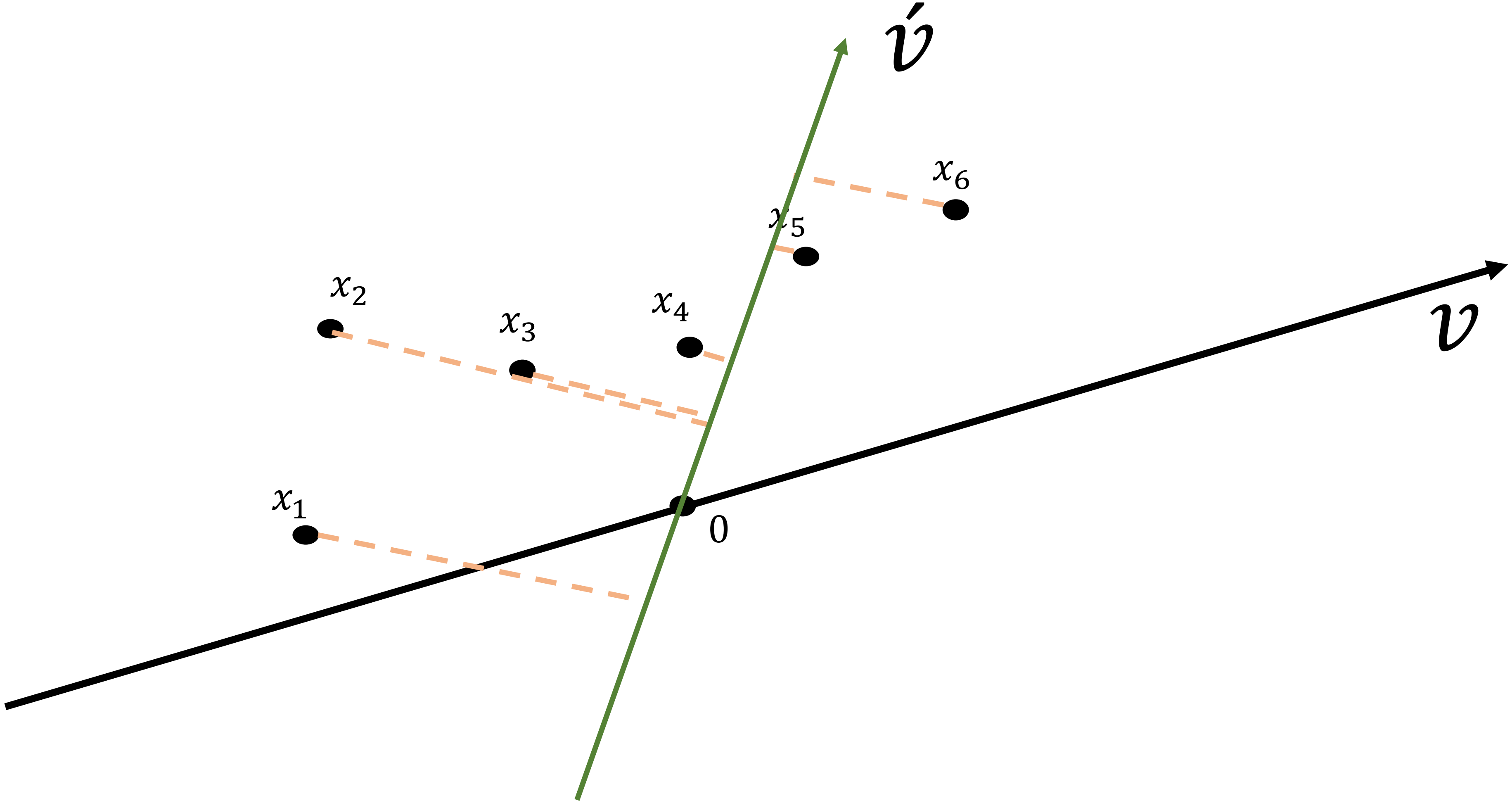
$$\langle x_i, v \rangle = x_i^T v = v^T x_i$$

$$y_i = v^T x_i$$

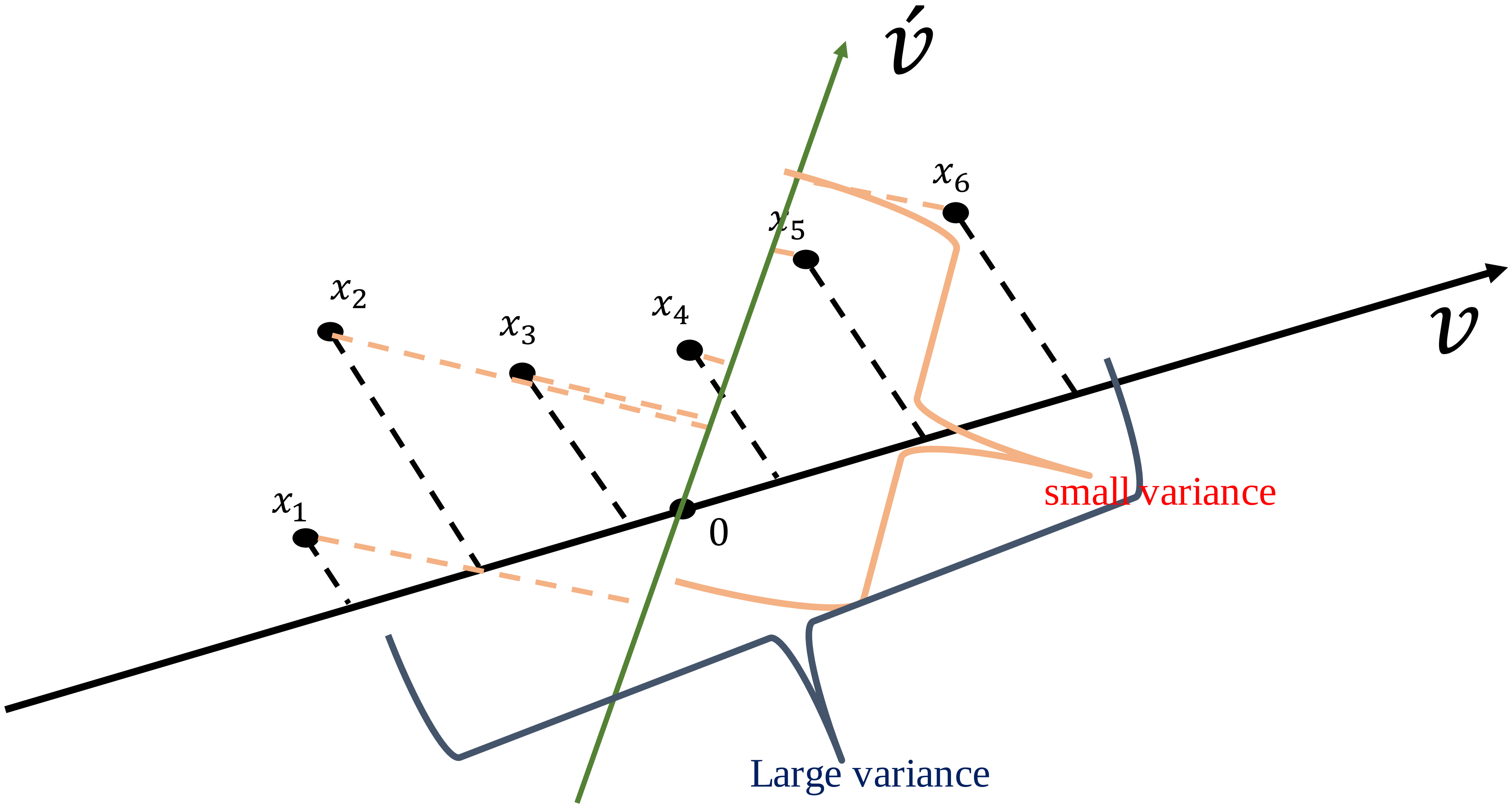
Principle Component Analysis



Principle Component Analysis



Principle Component Analysis



Principle Component Analysis

- The projections of the all points x_i into the direction v are

$$v^T x_1, v^T x_2, \dots, v^T x_N$$

The variance of the projections is

$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(v^T x_i - \mu)^2 = \frac{1}{N}\sum_{i=1}^{N}(v^T x_i - 0)^2 = \frac{1}{N}\sum_{i=1}^{N}(v^T x_i)^2$$

$$\Sigma = \frac{1}{N}\sum_{i=1}^{N}(v^T x_i)(v^T x_i)^T = \frac{1}{N}\sum_{i=1}^{N}(v^T x_i x_i^T v) = v^T\left(\frac{1}{N}\sum_{i=1}^{N} x_i x_i^T\right)v$$

$$= v^T C v$$

C covariance matrix

Principle Component Analysis

- The first principal vector can be found by the following equation:

$$v = \underset{v \in R^d, \|v\|=1}{\arg\max}\, v^T C v$$

Principle Component Analysis

$$v = \underset{v \in R^d,\ \|v\|=1}{\arg\max}\, v^T C v$$

Lagrange function:

$$f(v,\lambda) = v^T C v - \lambda(v^T v - 1)$$

$$\frac{\partial f(v,\lambda)}{\partial v} = 0 \Rightarrow 2Cv - \lambda v = 0 \Rightarrow Cv = \lambda v$$

$$\frac{\partial f(v,\lambda)}{\partial \lambda} = 0 \Rightarrow v^T v - 1 = 0 \Rightarrow v^T v = 1$$

Principle Component Analysis

- The first principal vector can be found by the following equation:

$$v = \underset{v \in R^d,\ \|v\|=1}{\operatorname{argmax}} (v^T C v)$$

- This is equivalent to find the largest eigenvalue of the following eigenvalue problem:

$$Cv = \lambda v$$
$$\|v\| = 1$$

$$C = \frac{1}{N}\sum_{i=1}^{N} x_i x_i^T = \frac{1}{N}[x_1 \ \ldots \ x_N]\begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = \frac{1}{N} X^T X$$

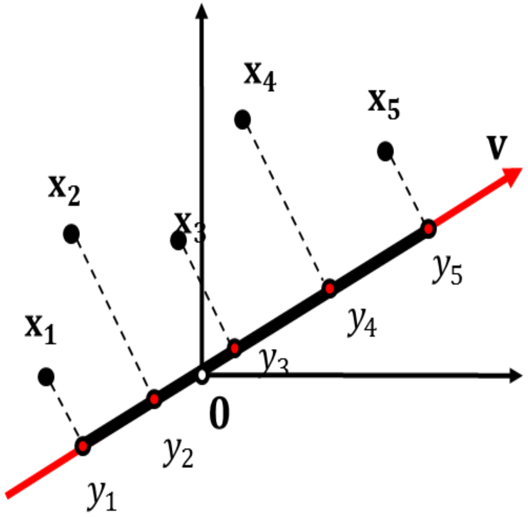
Principle Component Analysis

Eigenvalue vector is the corresponding variance vector.

$$v^T C v = \sigma^2$$

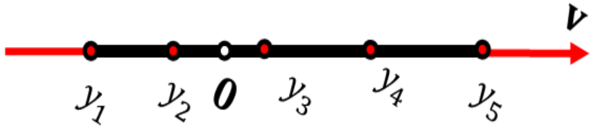
$$\Rightarrow v^T \lambda v = \lambda v^T v = \lambda = \sigma^2$$

Projection



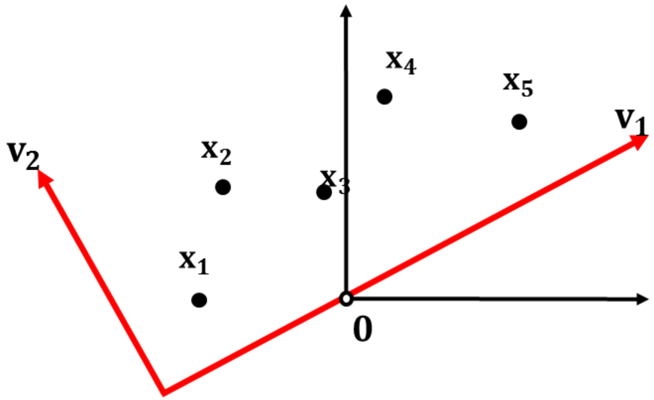
X空間轉換到特徵空間

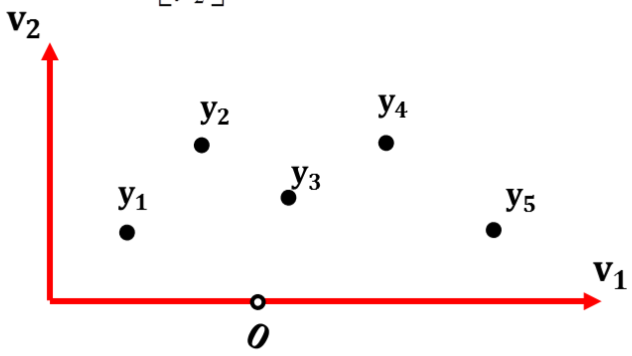
$$y = \mathbf{v}^T \mathbf{x}$$



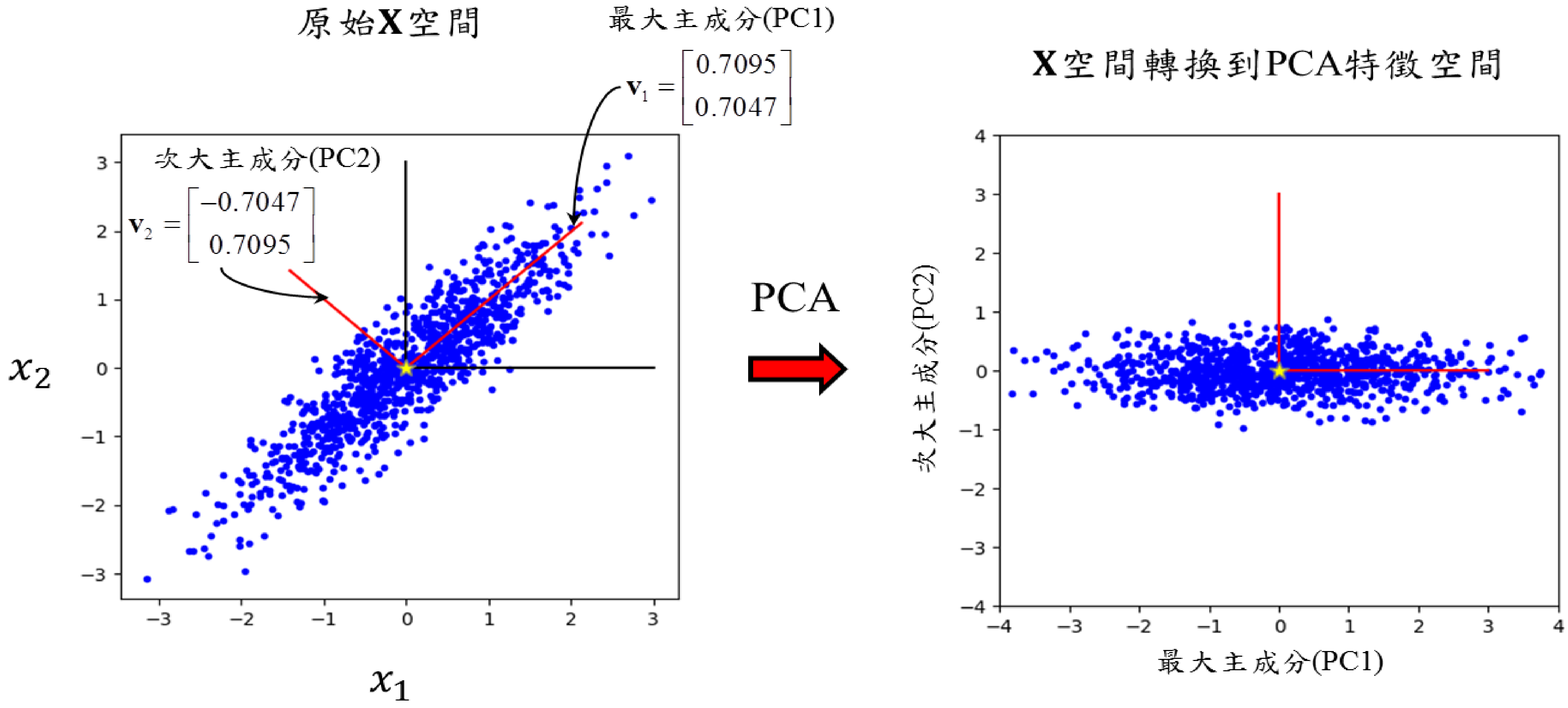
X空間轉換到Y空間

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \mathbf{V}^T \mathbf{x} = [\mathbf{v}_1 \quad \mathbf{v}_2]\mathbf{x}$$





Exercise



原始X空間
最大主成分(PC1)
$\mathbf{v}_1 = \begin{bmatrix} 0.7095 \\ 0.7047 \end{bmatrix}$
次大主成分(PC2)
$\mathbf{v}_2 = \begin{bmatrix} -0.7047 \\ 0.7095 \end{bmatrix}$
x_2
x_1
PCA
X空間轉換到PCA特徵空間
次大主成分(PC2)
最大主成分(PC1)