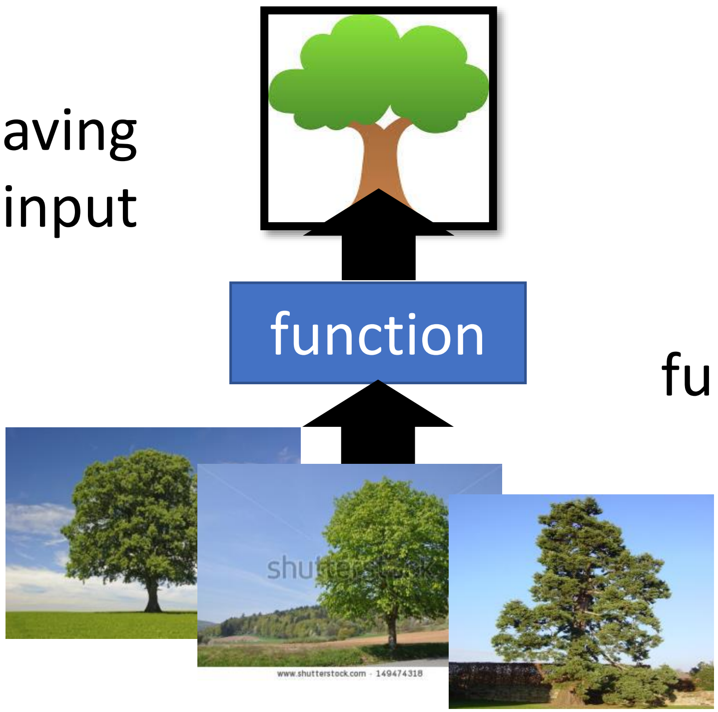
Unsupervised Learning: Principle Component Analysis

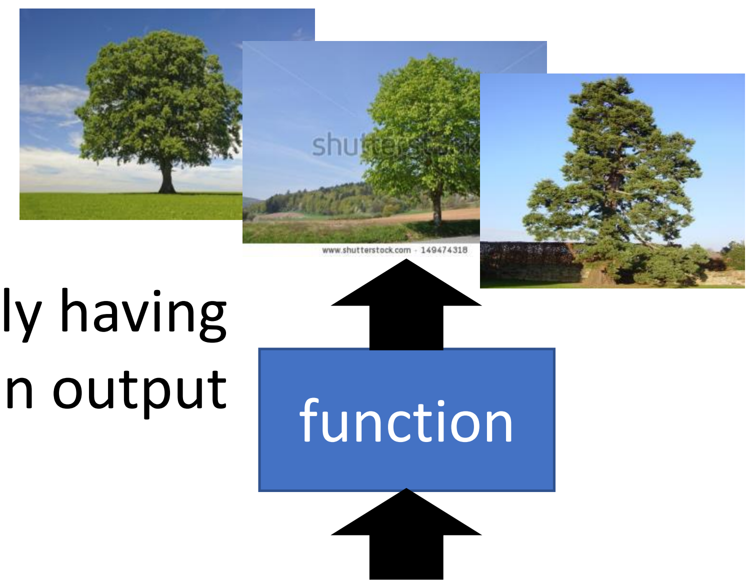
Unsupervised Learning

- Dimension Reduction (化繁為簡)
- Generation (無中生有)

only having function input

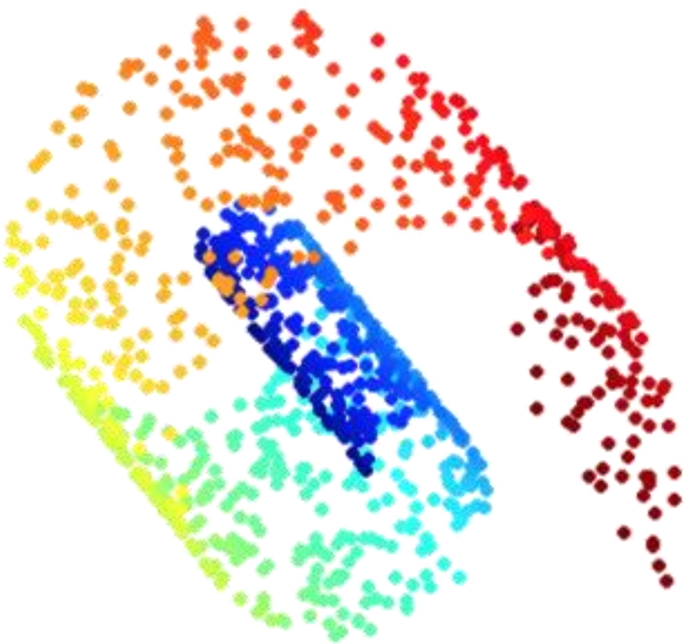


only having function output

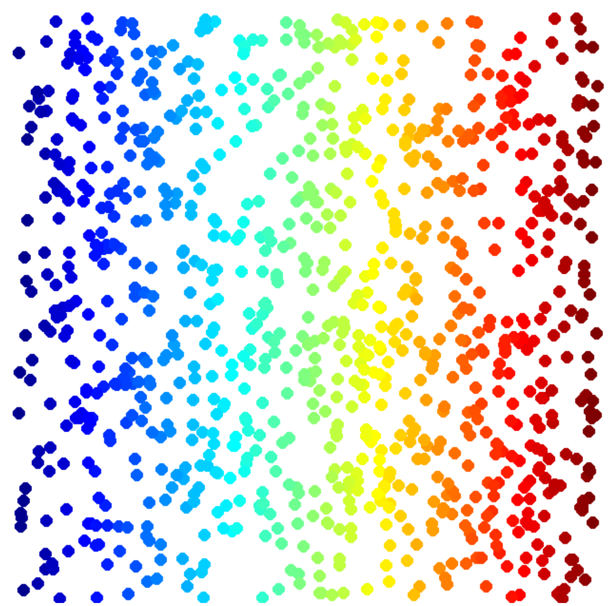


Random numbers

Dimension Reduction

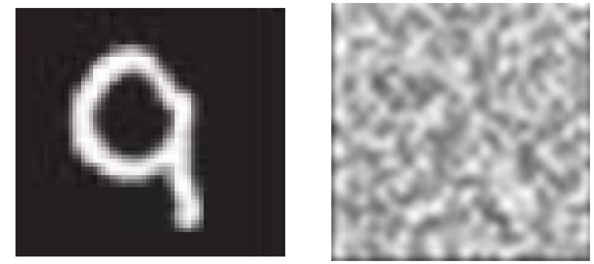


Looks like 3-D

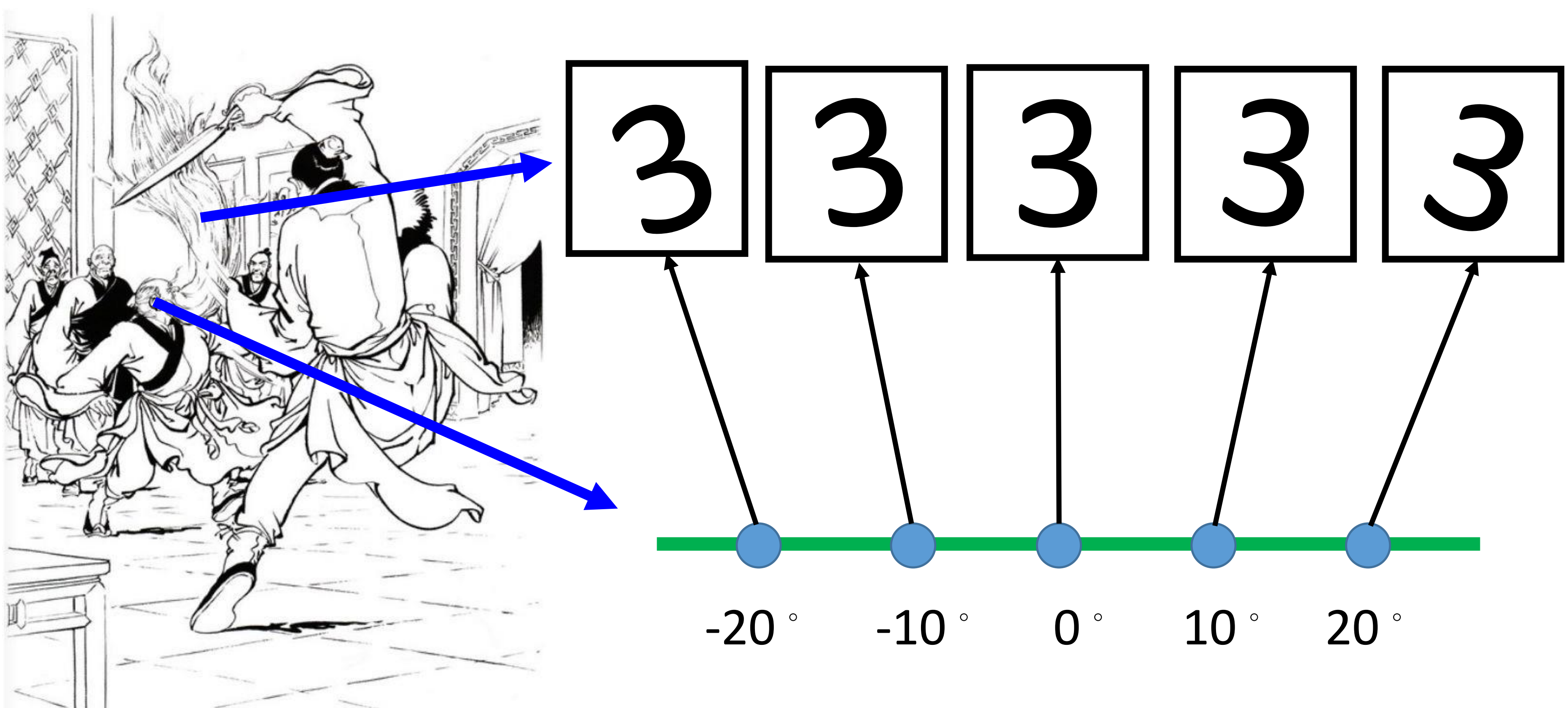


Actually, 2-D

Dimension Reduction



- In MNIST, a digit is 28 x 28 dims.
  - Most 28 x 28 dim vectors are not digits



Clustering

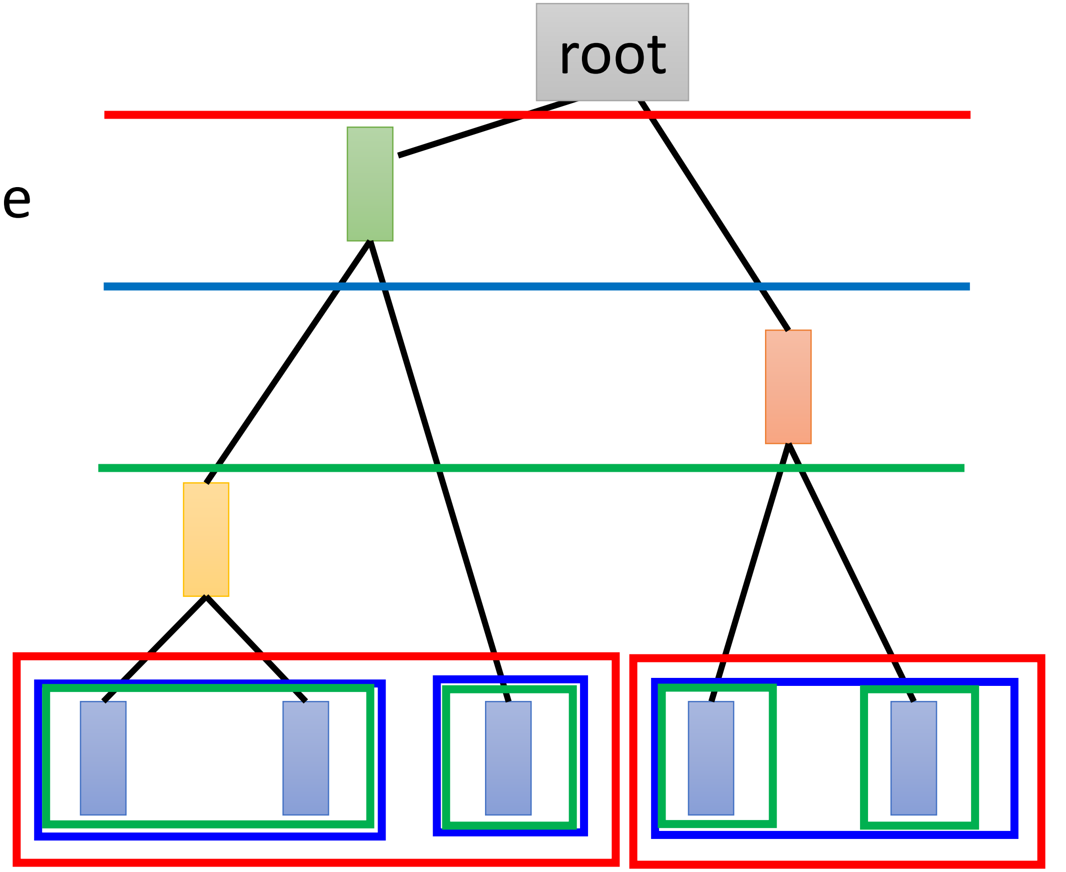
- K-means
  - Clustering $X = \{x^1, \cdots, x^n, \cdots, x^N\}$ into K clusters
  - Initialize cluster center c^i, i=1,2, ... K (K random x^n from X)
  - Repeat
    - For all x^n in X: $b_i^n \begin{cases} 1 & x^n \text{ is most "\textbf{\textit{close}}" to } c^i \\ 0 & \text{Otherwise} \end{cases}$
    - Updating all c^i: $c^i = \sum_{x^n} b_i^n x^n \Big/ \sum_{x^n} b_i^n$

Clustering

- Hierarchical Agglomerative Clustering (HAC)

Step 1: build a tree

Step 2: pick a threshold

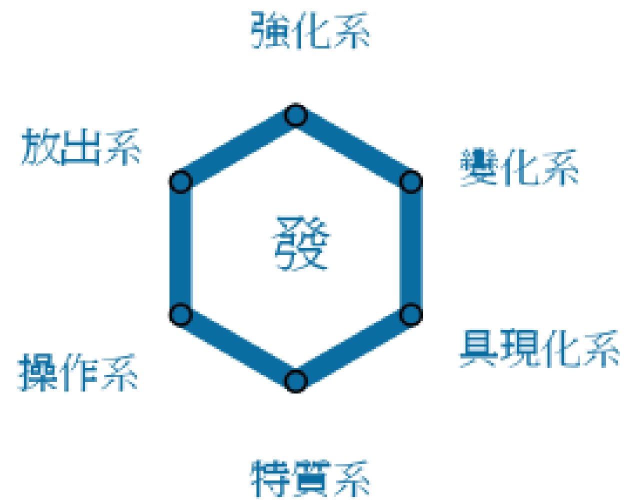


Distributed Representation

- Clustering: an object must belong to one cluster

小傑是強化系

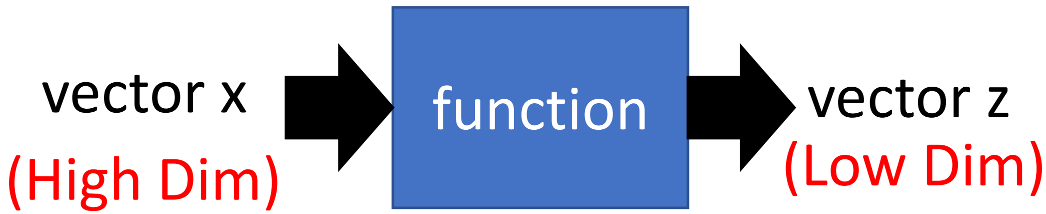
- Distributed representation



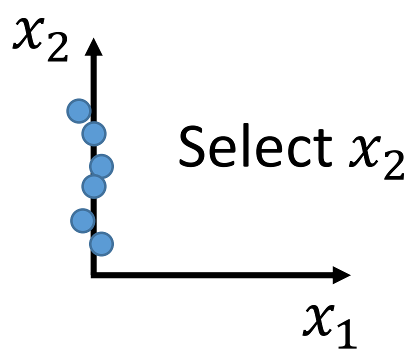
小傑是

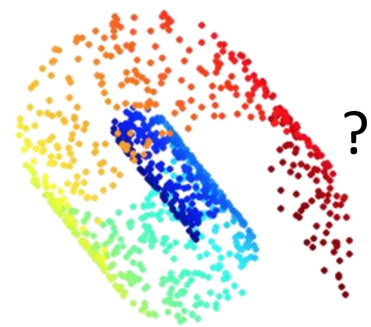
強化系	0.70
放出系	0.25
變化系	0.05
操作系	0.00
具現化系	0.00
特質系	0.00

Distributed Representation



- Feature selection



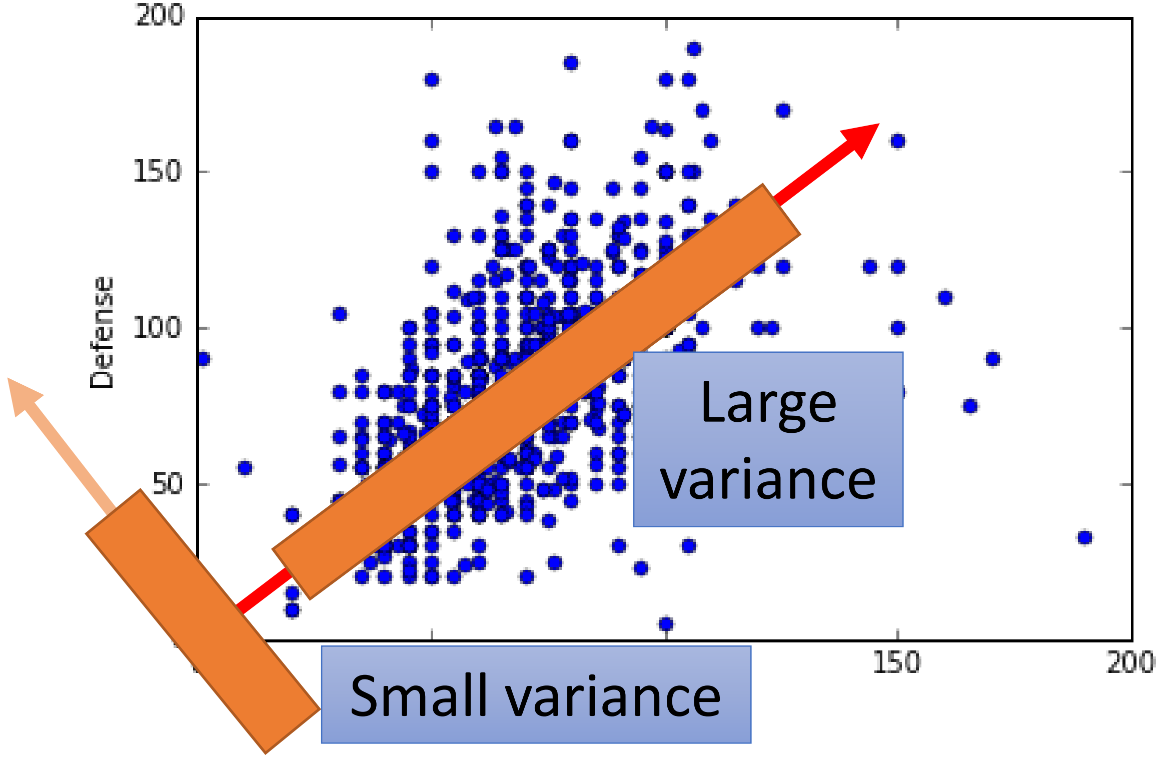


- Principle component analysis (PCA)
  [Bishop, Chapter 12]

$$z = Wx$$

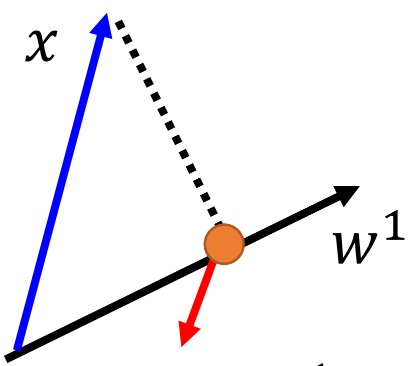
PCA

$z = Wx$



Reduce to 1-D:

$$z_1 = w^1 \cdot x$$



$$z_1 = w^1 \cdot x$$

Project all the data points x onto w^1, and obtain a set of z_1

We want the variance of z_1 as large as possible

$$Var(z_1) = \frac{1}{N}\sum_{z_1}(z_1 - \bar{z_1})^2 \quad \|w^1\|_2 = 1$$

PCA

$$z = Wx$$

Reduce to 1-D:

$$z_1 = w^1 \cdot x$$

$$z_2 = w^2 \cdot x$$

$$W = \begin{bmatrix} (w^1)^T \\ (w^2)^T \\ \vdots \end{bmatrix}$$

Orthogonal matrix

Project all the data points x onto w^1, and obtain a set of z_1

We want the variance of z_1 as large as possible

$$Var(z_1) = \frac{1}{N}\sum_{z_1}(z_1 - \bar{z_1})^2 \quad \|w^1\|_2 = 1$$

We want the variance of z_2 as large as possible

$$Var(z_2) = \frac{1}{N}\sum_{z_2}(z_2 - \bar{z_2})^2 \quad \|w^2\|_2 = 1$$

$$w^1 \cdot w^2 = 0$$

Warning of Math

PCA

$$z_1 = w^1 \cdot x$$

$$\bar{z_1} = \frac{1}{N}\sum z_1 = \frac{1}{N}\sum w^1 \cdot x = w^1 \cdot \frac{1}{N}\sum x = w^1 \cdot \bar{x}$$

$$Var(z_1) = \frac{1}{N}\sum_{z_1}(z_1 - \bar{z_1})^2$$

$$= \frac{1}{N}\sum_{x}(w^1 \cdot x - w^1 \cdot \bar{x})^2$$

$$= \frac{1}{N}\sum\left(w^1 \cdot (x - \bar{x})\right)^2$$

$$= \frac{1}{N}\sum (w^1)^T(x - \bar{x})(x - \bar{x})^T w^1$$

$$= (w^1)^T \frac{1}{N}\sum (x - \bar{x})(x - \bar{x})^T w^1$$

$$= (w^1)^T Cov(x) w^1$$

$$S = Cov(x)$$

$$(a \cdot b)^2 = (a^T b)^2 = a^T b a^T b$$

$$= a^T b (a^T b)^T = a^T b b^T a$$

Find w^1 maximizing

$$(w^1)^T S w^1$$

$$\|w^1\|_2 = (w^1)^T w^1 = 1$$

Find w^1 maximizing $(w^1)^T S w^1$ $\quad (w^1)^T w^1 = 1$

$S = Cov(x)$ Symmetric Positive-semidefinite (non-negative eigenvalues)

Using Lagrange multiplier [Bishop, Appendix E]

$$g(w^1) = (w^1)^T S w^1 - \alpha\left((w^1)^T w^1 - 1\right)$$

$$\partial g(w^1)/\partial w_1^1 = 0$$

$$\partial g(w^1)/\partial w_2^1 = 0$$

$$\vdots$$

$$S w^1 - \alpha w^1 = 0$$

$$S w^1 = \alpha w^1$$

w^1 : eigenvector

$$(w^1)^T S w^1 = \alpha (w^1)^T w^1$$

$$= \alpha$$

Choose the maximum one

w^1 is the eigenvector of the covariance matrix S

Corresponding to the largest eigenvalue λ_1

Find w^2 maximizing $(w^2)^T S w^2$ $\quad (w^2)^T w^2 = 1 \quad (w^2)^T w^1 = 0$

$$g(w^2) = (w^2)^T S w^2 - \alpha\left((w^2)^T w^2 - 1\right) - \beta\left((w^2)^T w^1 - 0\right)$$

$$\partial g(w^2)/\partial w_1^2 = 0$$

$$\partial g(w^2)/\partial w_2^2 = 0$$

$$\vdots$$

$$Sw^2 - \alpha w^2 - \beta w^1 = 0$$

$$0 - \alpha \; 0 - \beta \; 1 = 0$$

$$= \left((w^1)^T S w^2\right)^T = (w^2)^T S^T w^1$$

$$= (w^2)^T S w^1 = \lambda_1 (w^2)^T w^1 = 0$$

$$Sw^1 = \lambda_1 w^1$$

$\beta = 0$: $\quad Sw^2 - \alpha w^2 = 0 \quad Sw^2 = \alpha w^2$

w^2 is the eigenvector of the covariance matrix S

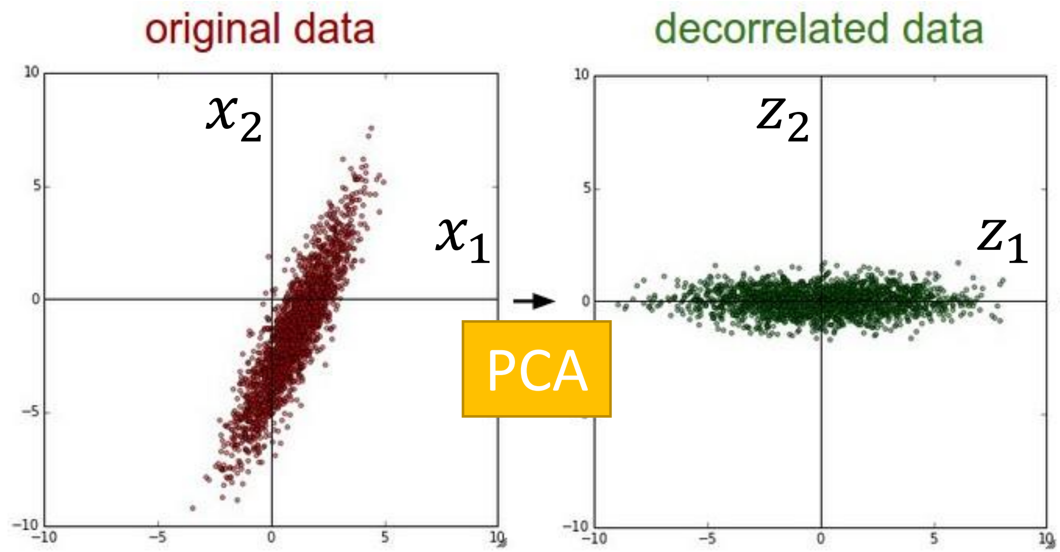
Corresponding to the 2nd largest eigenvalue λ_2

PCA - decorrelation

$$z = Wx$$

$$Cov(z) = D$$

Diagonal matrix



$$Cov(z) = \frac{1}{N}\sum(z-\bar{z})(z-\bar{z})^T = WSW^T \qquad S = Cov(x)$$

$$= WS\begin{bmatrix} w^1 & \cdots & w^K \end{bmatrix} = W\begin{bmatrix} Sw^1 & \cdots & Sw^K \end{bmatrix}$$

$$= W\begin{bmatrix} \lambda_1 w^1 & \cdots & \lambda_K w^K \end{bmatrix} = \begin{bmatrix} \lambda_1 W w^1 & \cdots & \lambda_K W w^K \end{bmatrix}$$

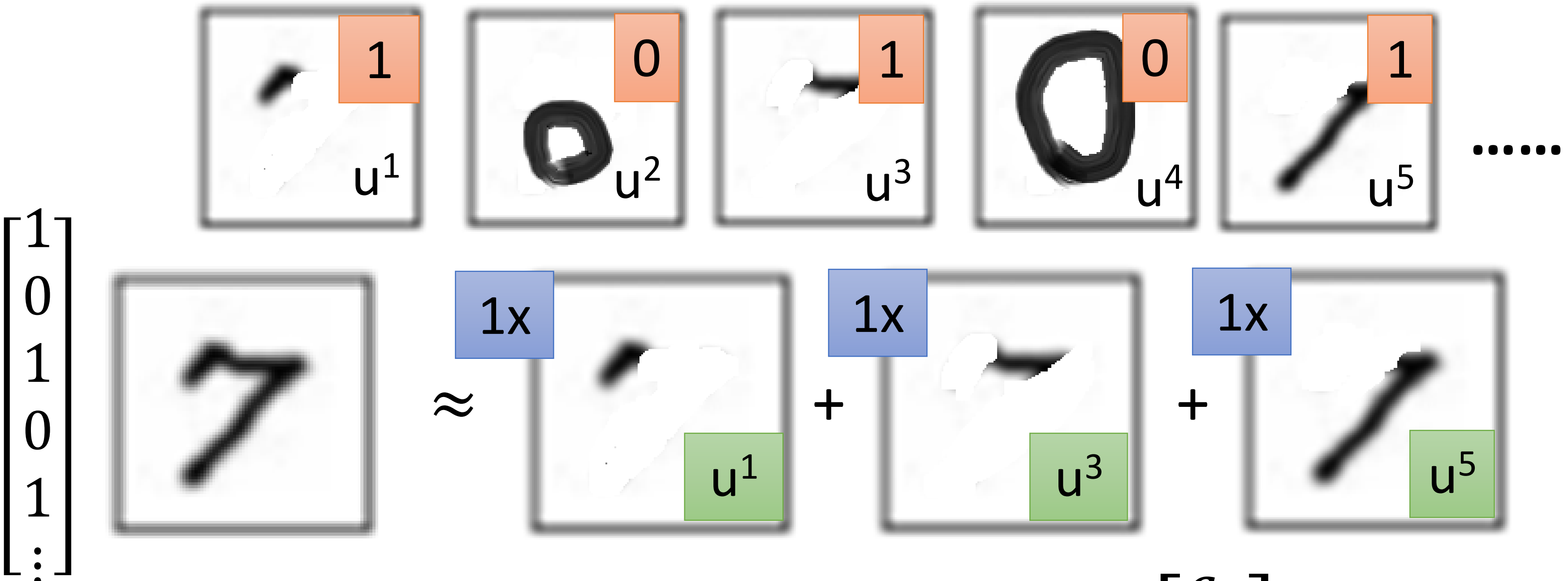
$$= \begin{bmatrix} \lambda_1 e_1 & \cdots & \lambda_K e_K \end{bmatrix} = D$$

Diagonal matrix

End of Warning

PCA – Another Point of View

Basic Component:



$$x \approx c_1 u^1 + c_2 u^2 + \cdots + c_K u^K + \bar{x}$$

Pixels in a digit image

component

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_K \end{bmatrix}$$

Represent a digit image

PCA – Another Point of View

$$x - \bar{x} \approx c_1 u^1 + c_2 u^2 + \cdots + c_K u^K \ = \hat{x}$$

Reconstruction error:
$\| (x - \bar{x}) - \hat{x} \|_2$

Find $\{u^1, \ldots, u^K\}$ minimizing the error

$$L = \min_{\{u^1,\ldots,u^K\}} \sum \left\| (x - \bar{x}) - \left(\underbrace{\sum_{k=1}^{K} c_k u^k}_{\hat{x}} \right) \right\|_2$$

PCA: $z = Wx$

$$\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_K \end{bmatrix} = \begin{bmatrix} (w_1)^{\mathrm{T}} \\ (w_2)^{\mathrm{T}} \\ \vdots \\ (w_K)^{\mathrm{T}} \end{bmatrix} x$$

$\{w^1, w^2, \ldots w^K\}$ (from PCA) is the component $\{u^1, u^2, \ldots u^K\}$ minimizing L

Proof in [Bishop, Chapter 12.1.2]

$$x - \bar{x} \approx c_1 u^1 + c_2 u^2 + \cdots + c_K u^K \quad = \hat{x}$$

Reconstruction error:
$\| (x - \bar{x}) - \hat{x} \|_2$

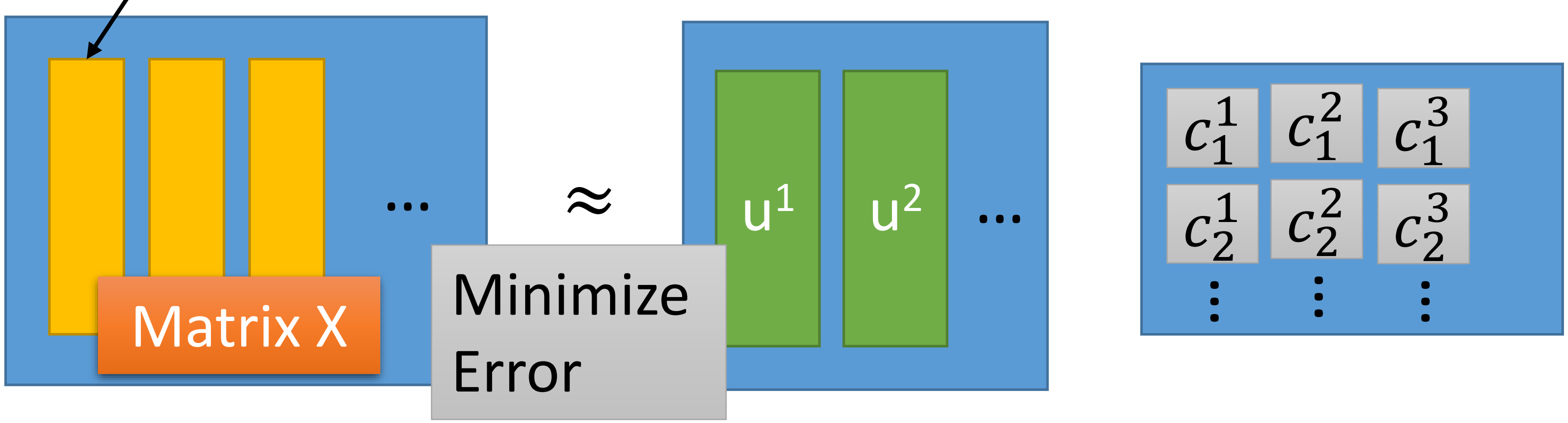
Find $\{u^1, \ldots, u^K\}$ minimizing the error

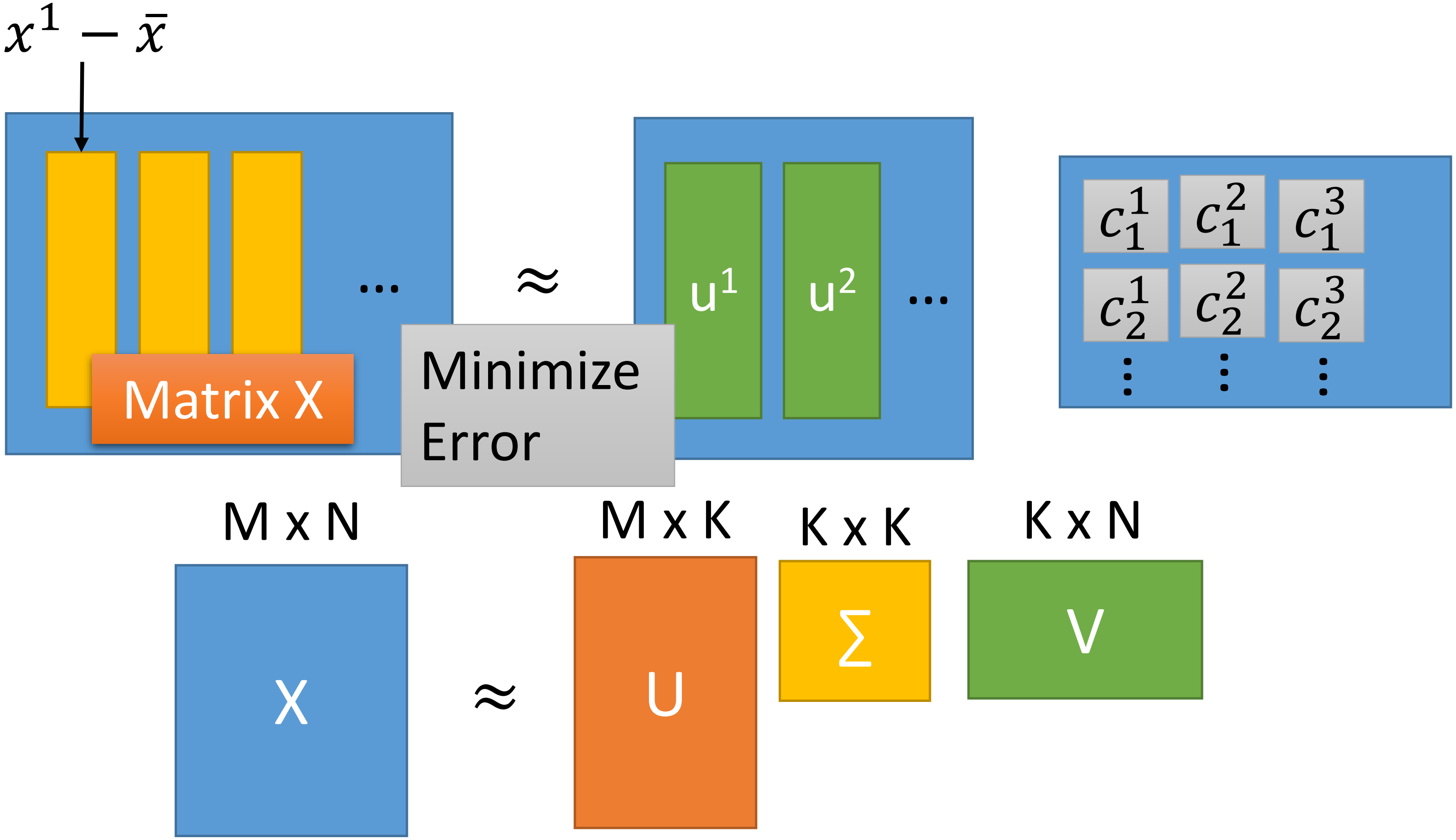
$$x^1 - \bar{x} \approx c_1^1 u^1 + c_2^1 u^2 + \cdots$$

$$x^2 - \bar{x} \approx c_1^2 u^1 + c_2^2 u^2 + \cdots$$

$$x^3 - \bar{x} \approx c_1^3 u^1 + c_2^3 u^2 + \cdots$$

$$\vdots$$





K columns of U: a set of orthonormal eigen vectors corresponding to the K largest eigenvalues of XX^T

This is the solution of PCA

SVD: http://speech.ee.ntu.edu.tw/~tlkagk/courses/LA_2016/Lecture/SVD.pdf

PCA looks like a neural network with one hidden layer (linear activation function)

Autoencoder

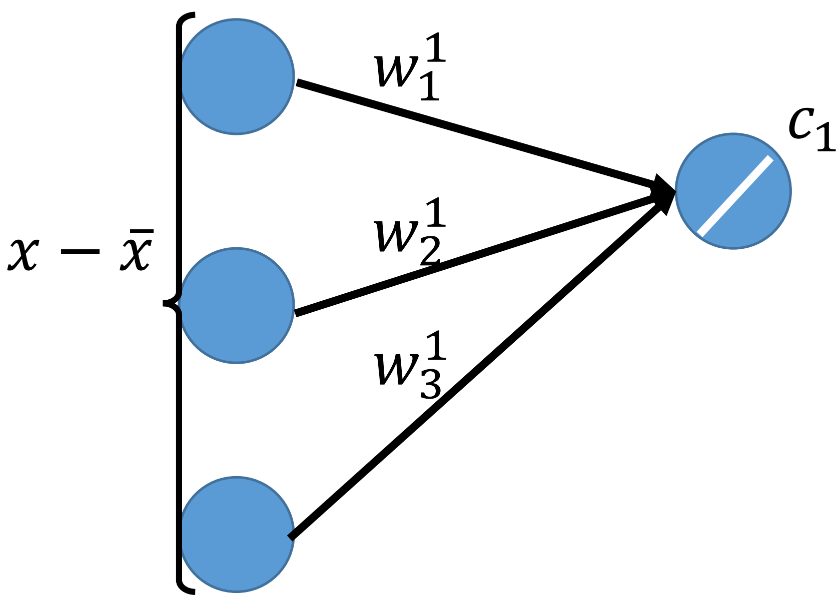
If $\{w^1, w^2, \ldots w^K\}$ is the component $\{u^1, u^2, \ldots u^K\}$

$$\hat{x} = \sum_{k=1}^{K} c_k w^k \Leftrightarrow x - \bar{x}$$

To minimize reconstruction error:

$$c_k = (x - \bar{x}) \cdot w^k$$

$K = 2$:



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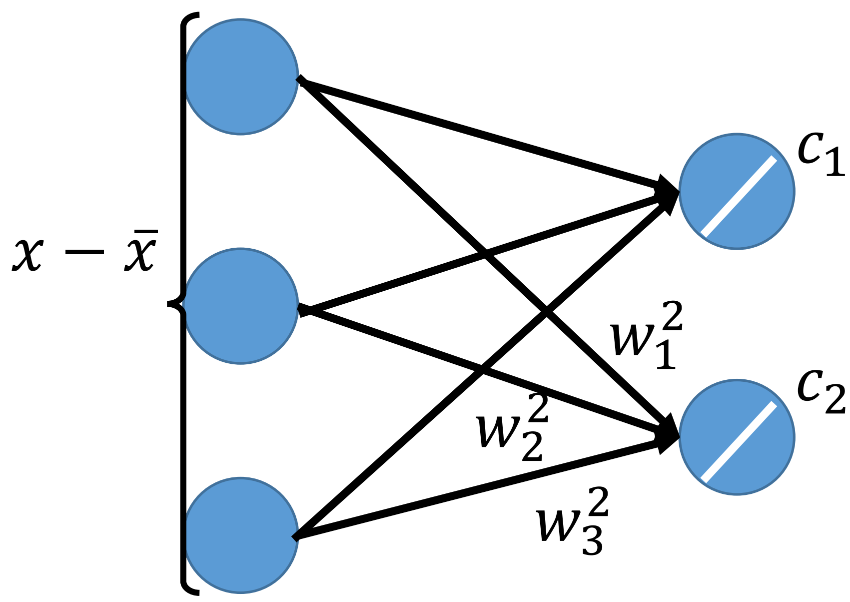

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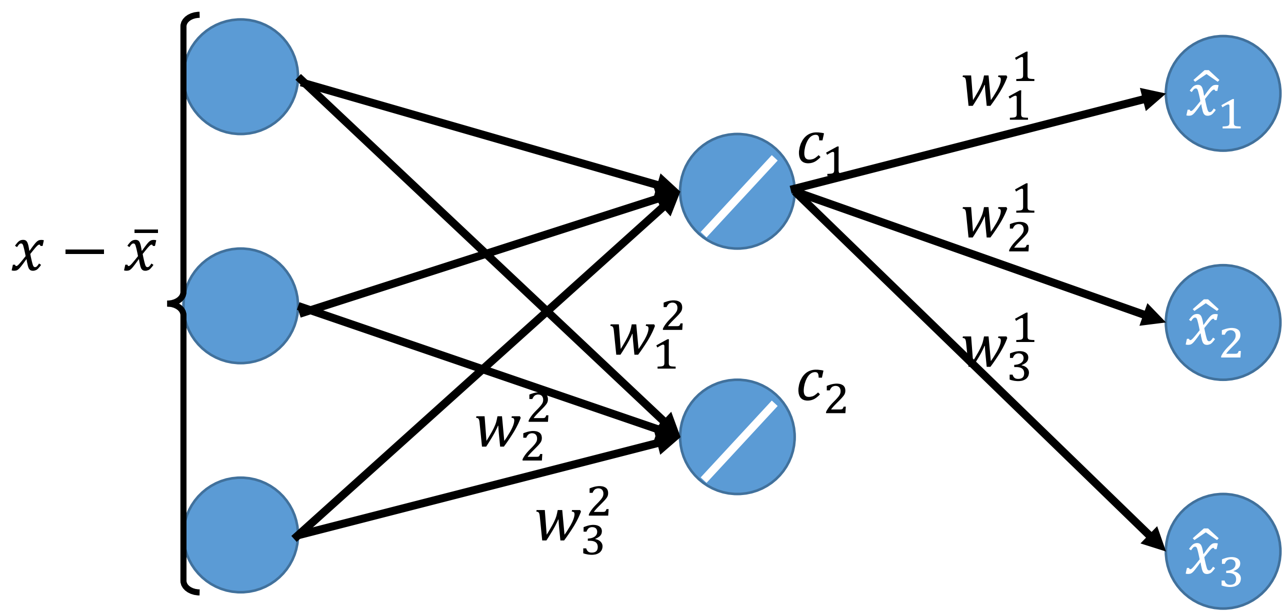

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Autoencoder

If $\{w^1, w^2, \dots w^K\}$ is the component $\{u^1, u^2, \dots u^K\}$

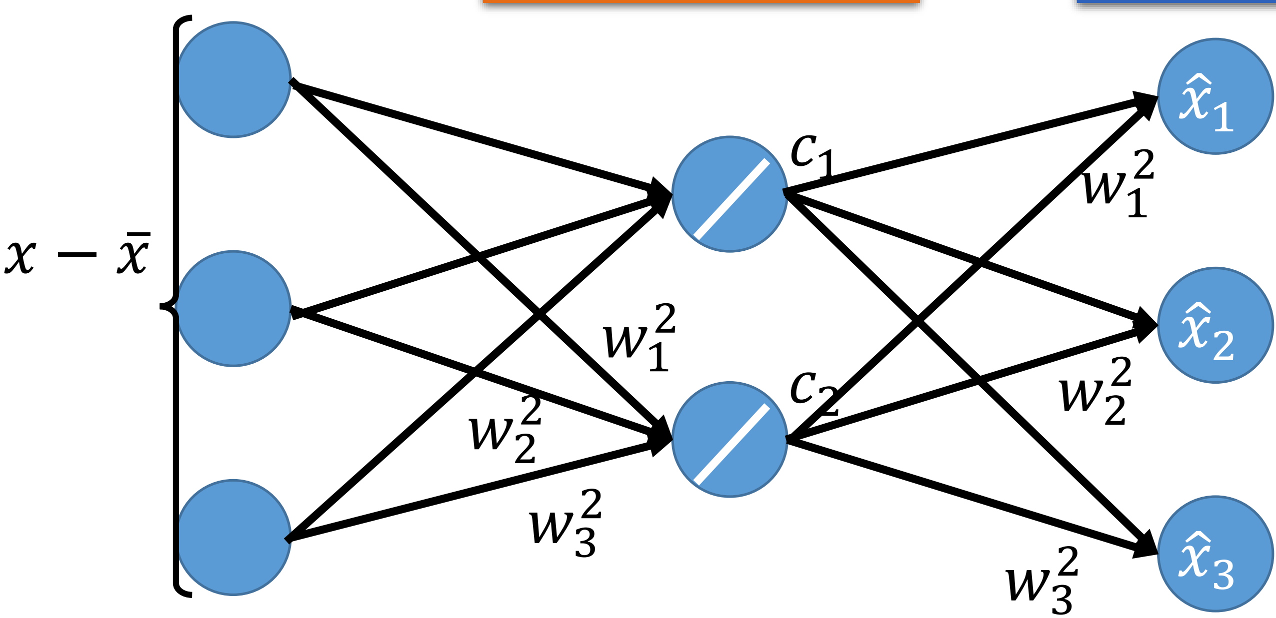
$$\hat{x} = \sum_{k=1}^{K} c_k w^k \Leftrightarrow x - \bar{x}$$

To minimize reconstruction error:

$$c_k = (x - \bar{x}) \cdot w^k$$

$K = 2$:

It can be deep. ➡ Deep Autoencoder



Minimize error ⟺ $x - \bar{x}$

Gradient Descent?

PCA - Pokémon

- Inspired from: https://www.kaggle.com/strakul5/d/abcsds/pokemon/principal-component-analysis-of-pokemon-data
- 800 Pokemons, 6 features for each (HP, Atk, Def, Sp Atk, Sp Def, Speed)
- How many principle components?

$$\frac{\lambda_i}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6}$$

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
ratio	0.45	0.18	0.13	0.12	0.07	0.04

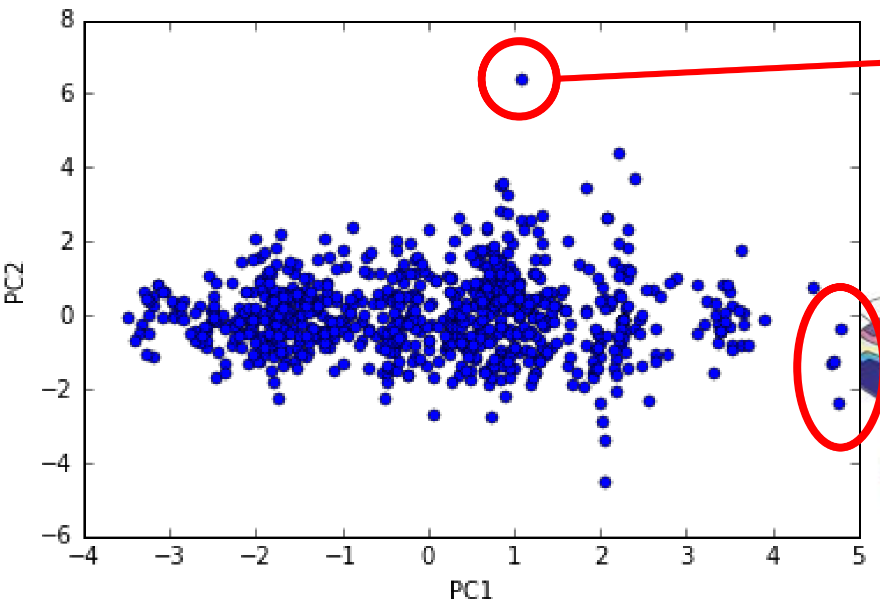
Using 4 components is good enough

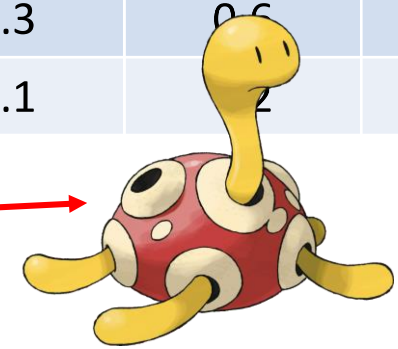
PCA - Pokémon

	HP	Atk	Def	Sp Atk	Sp Def	Speed
PC1	0.4	0.4	0.4	0.5	0.4	0.3
PC2	0.1	0.0	0.6	-0.3	0.2	-0.7
PC3	-0.5	-0.6	0.1	0.3	0.6	[illegible]
PC4	0.7	-0.4	-0.4	0.1	[illegible]	-0.3

強度

防禦(犧牲速度)



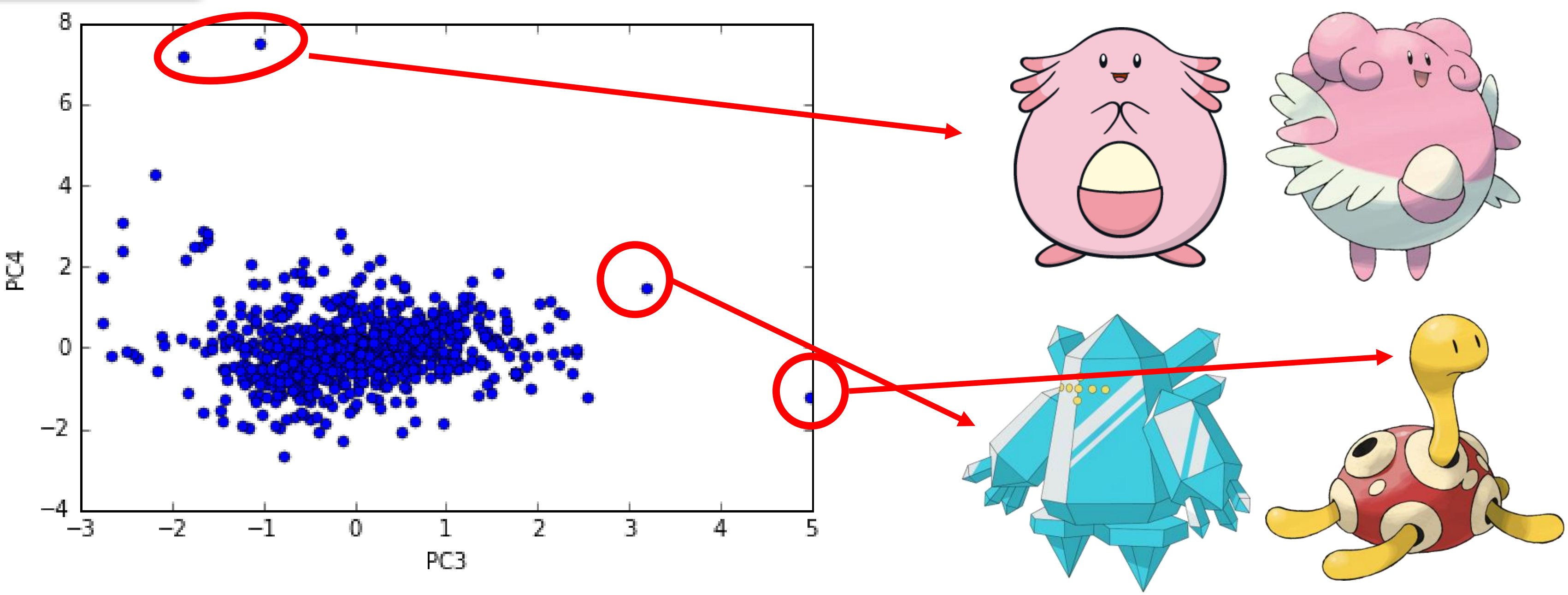


PCA - Pokémon

	HP	Atk	Def	Sp Atk	Sp Def	Speed
PC1	0.4	0.4	0.4	0.5	0.4	0.3
PC2	0.1	0.0	0.6	-0.3	0.2	-0.7
PC3	-0.5	-0.6	0.1	0.3	0.6	
	0.7	-0.4	-0.4	0.1	0.2	

生命力強

特殊防禦(犧牲攻擊和生命)



PCA - Pokémon

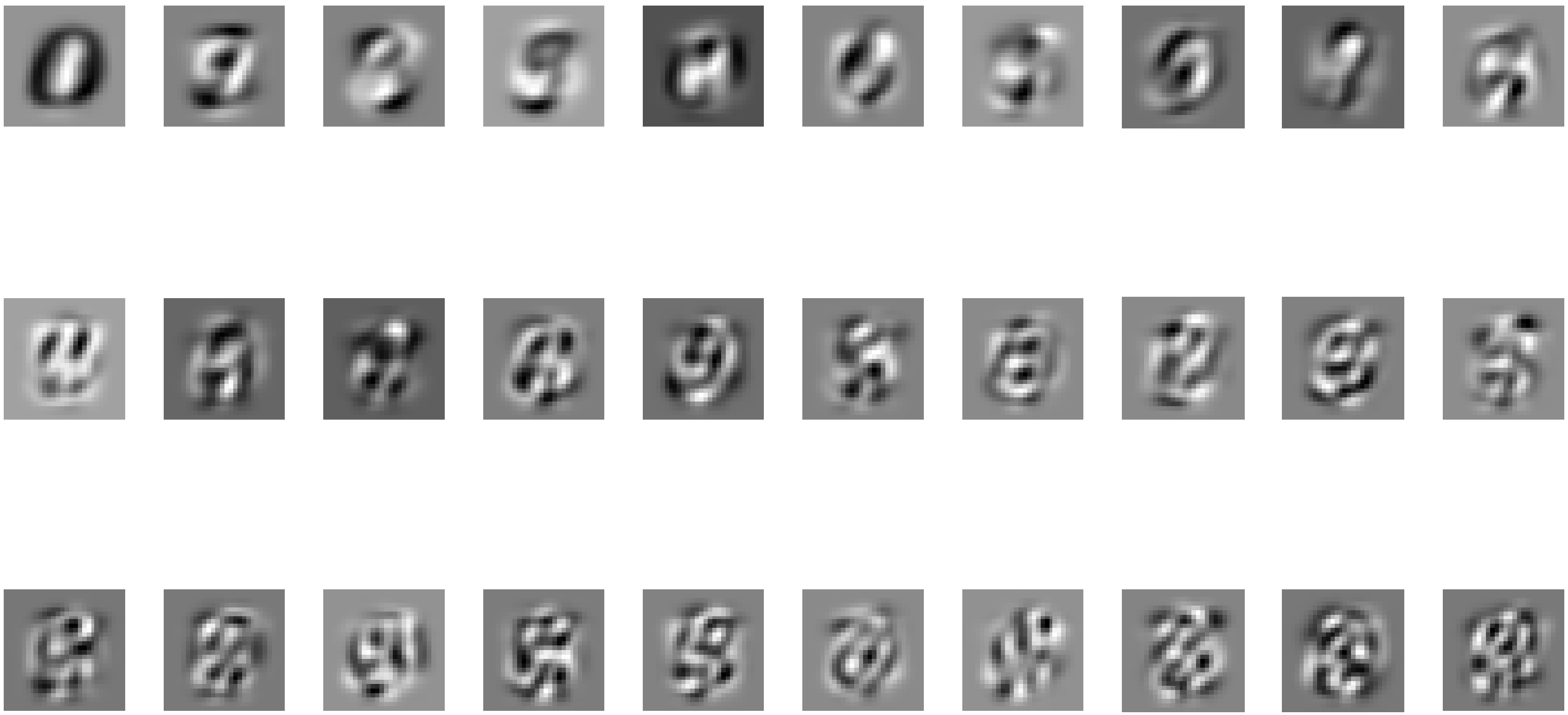
- http://140.112.21.35:2880/~tlkagk/pokemon/pca.html
- The code is modified from
    - http://jkunst.com/r/pokemon-visualize-em-all/

PCA - MNIST

$= a_1 w^1 + a_2 w^2 + \cdots$

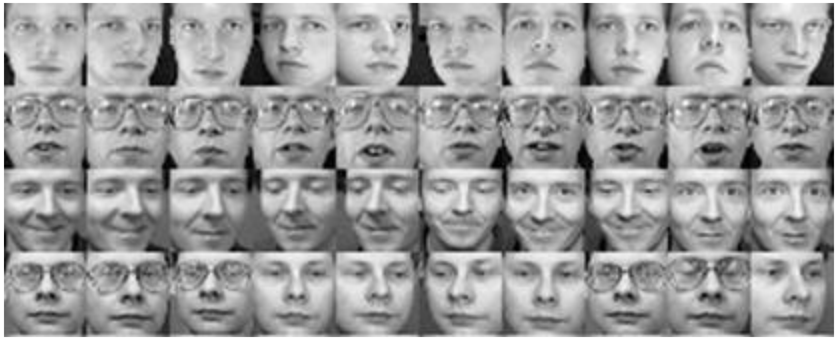
images

30 components:



Eigen-digits

PCA - Face



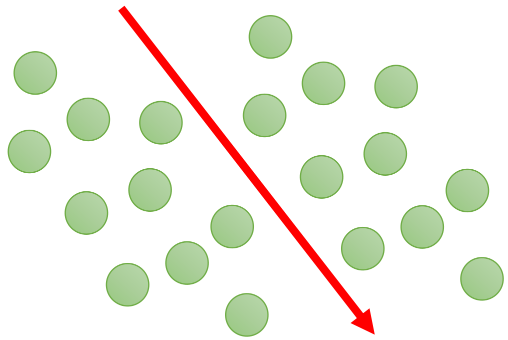
30 components:

http://www.cs.unc.edu/~lazebnik/research/spring08/assignment3.html

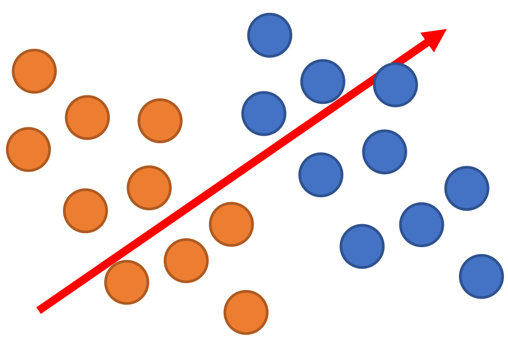
Eigen-face

Weakness of PCA

- Unsupervised

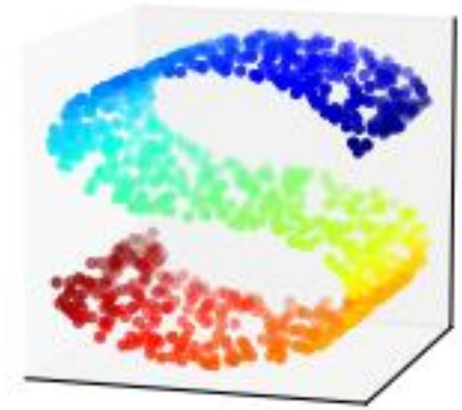


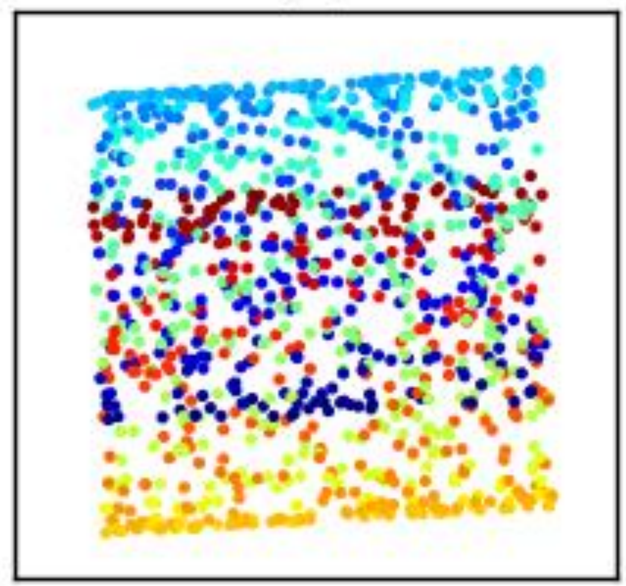
PCA



LDA

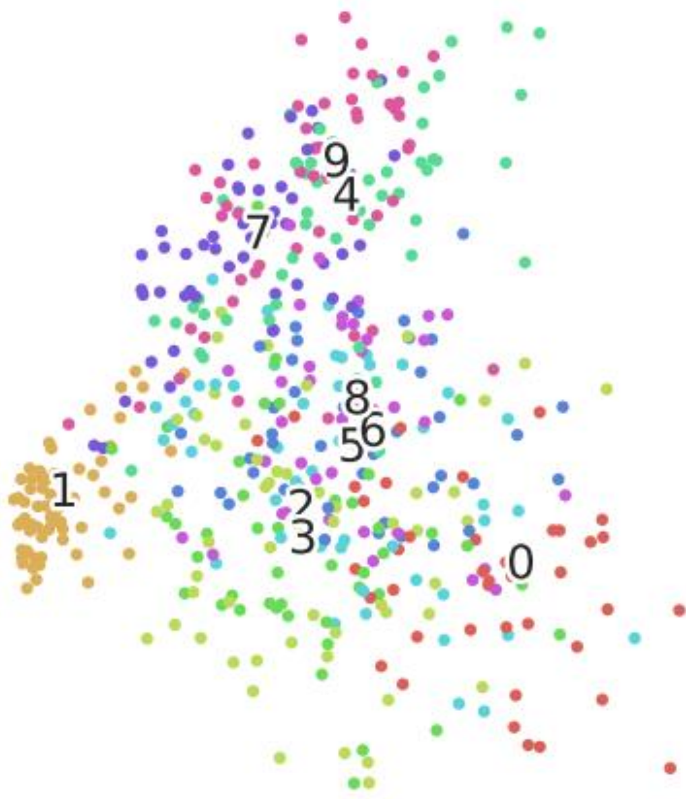
- Linear



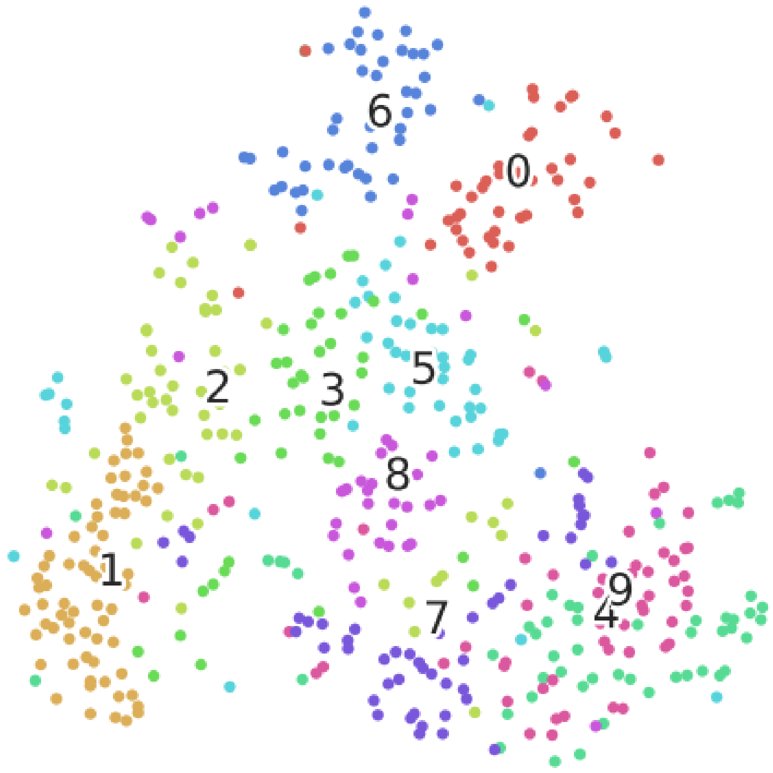


http://www.astroml.org/book_figures/chapter7/fig_S_manifold_PCA.html

Weakness of PCA



Pixel (28x28) -> PCA (2)



Pixel (28x28) -> tSNE (2)

Acknowledgement

- 感謝 彭冲 同學發現引用資料的錯誤
- 感謝 Hsiang-Chih Cheng 同學發現投影片上的錯誤

Appendix

- http://4.bp.blogspot.com/_sHcZHRnxlLE/S9EpFXYjfvI/AAAAAAAABZ0/_oEQiaR3WVM/s640/dimensionality+reduction.jpg
- https://lvdmaaten.github.io/publications/papers/TR_Dimensionality_Reduction_Review_2009.pdf