Unsupervised Feature Learning

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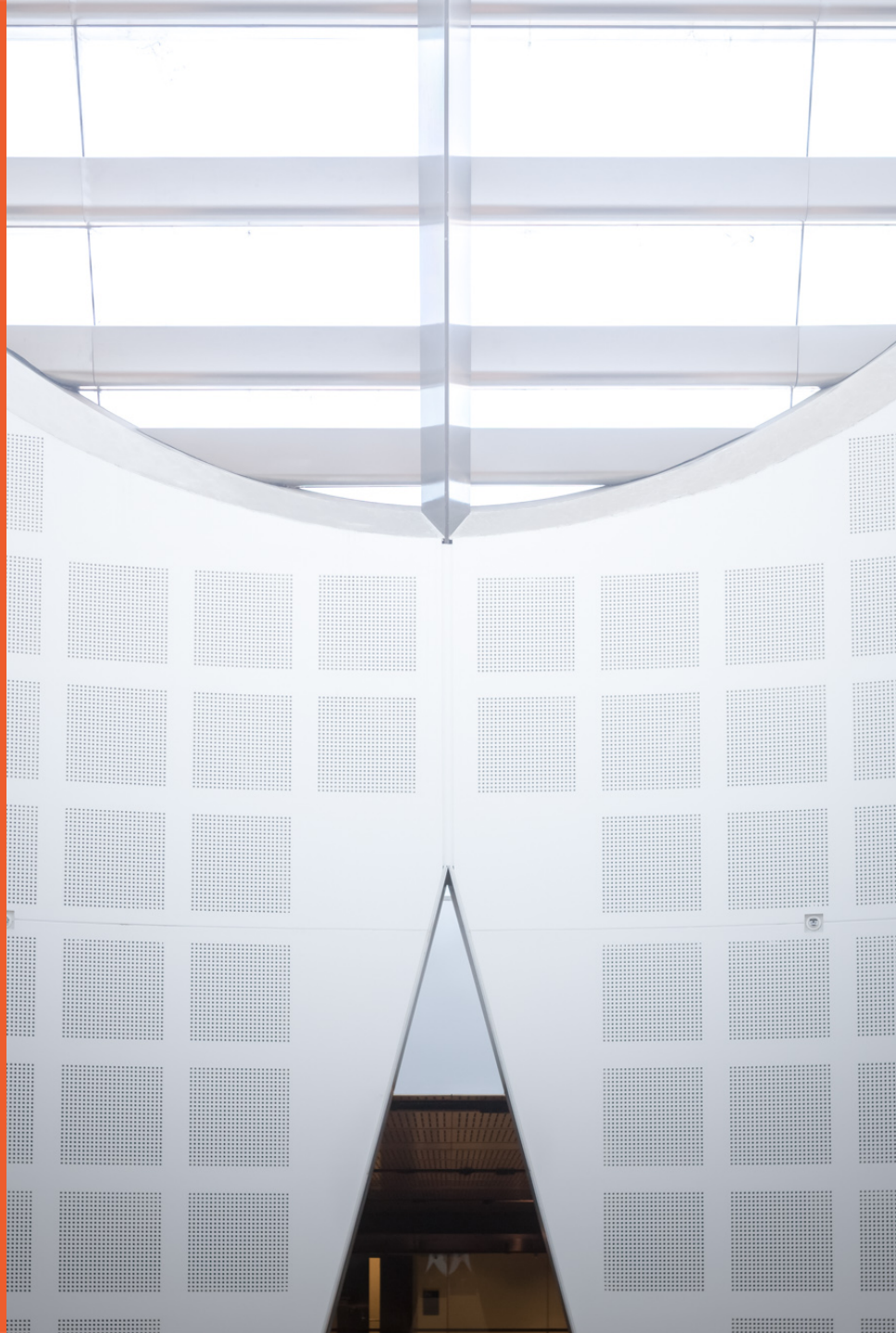
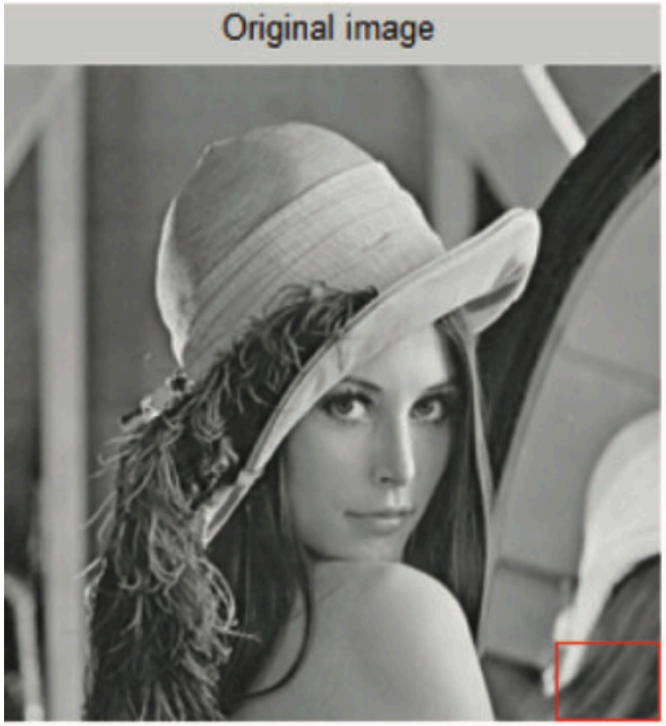


Data Representation



(a)

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148	161	164	185	206	215	219	214	208	197	169	134	116	111	109	103	100	93	90	96	102	97	91	80	76	86	101	111	107	100	98	90	88	91	95	98	94	98	96	83
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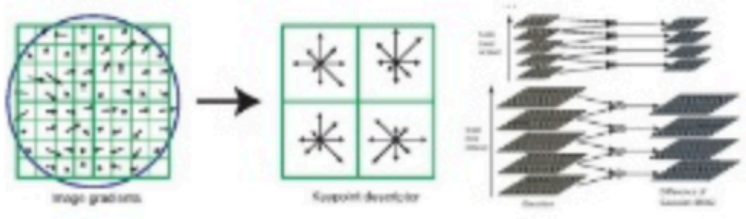
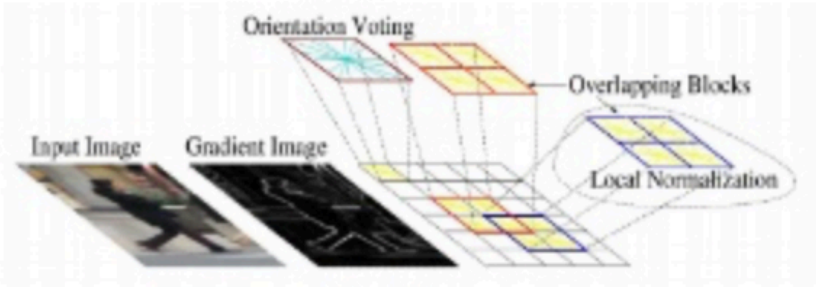
(b)

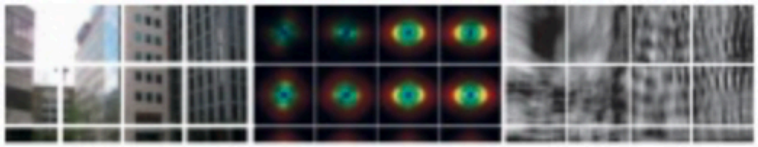
Hand-crafted features



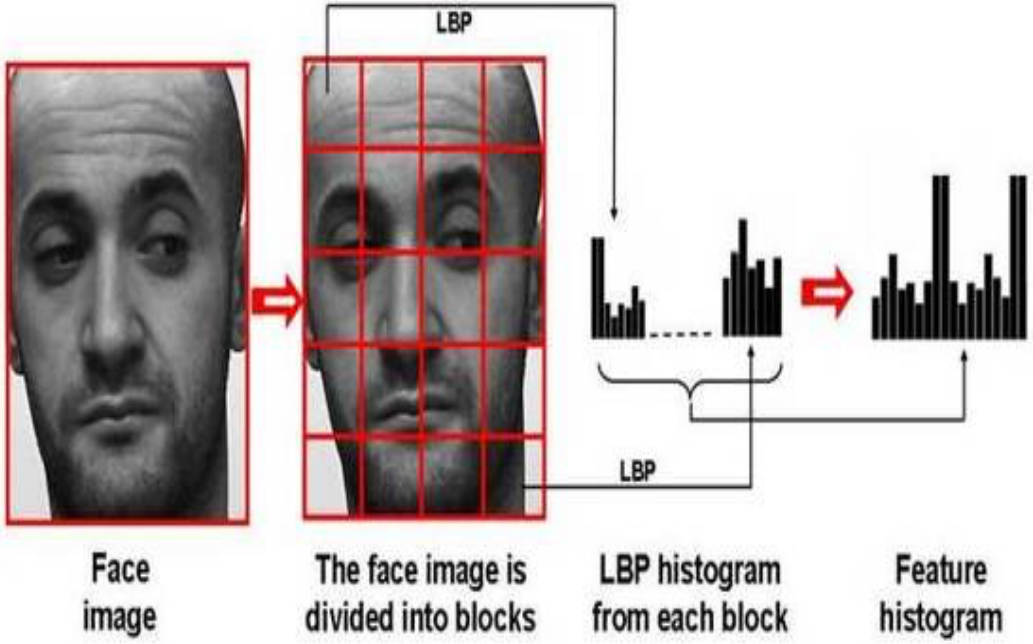
SIFT



HoG



GIST



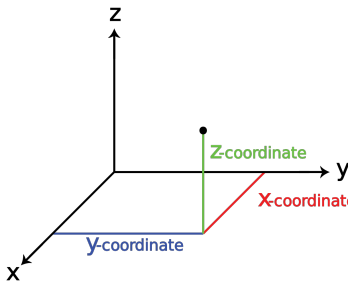
Outline

1. Background
2. Principal Component Analysis (PCA)
3. Autoencoder (AE)
4. Sparse Coding (SC)

Unsupervised feature learning

For raw data $\boldsymbol{x} \in \boldsymbol{R}^d$, we try to find an approximation in a space:

$$\hat{\boldsymbol{x}} = \sum_{i=1}^{k} \alpha_i \phi_i$$



where ϕ_i, $1 \leq i \leq k$, are basis vectors of the space; and α_i, $1 \leq i \leq k$, are features or representations in the space.

Over-complete representation: if $k > d$, i.e., The dimension of features (the number of basis vectors) is larger than that of raw data.
Under-complete representation: if $k < d$, i.e., the dimension of features is smaller than that of raw data.

Constraints such as sparsity, low-rankness, orthogonality, linear independence on the basis or features can lead to different models.

Principal Component Analysis (PCA)

Principal Component Analysis (PCA)

- A technique widely used for
  --Dimension reduction
  --Data compression
  --Feature extraction
  --Data visualization

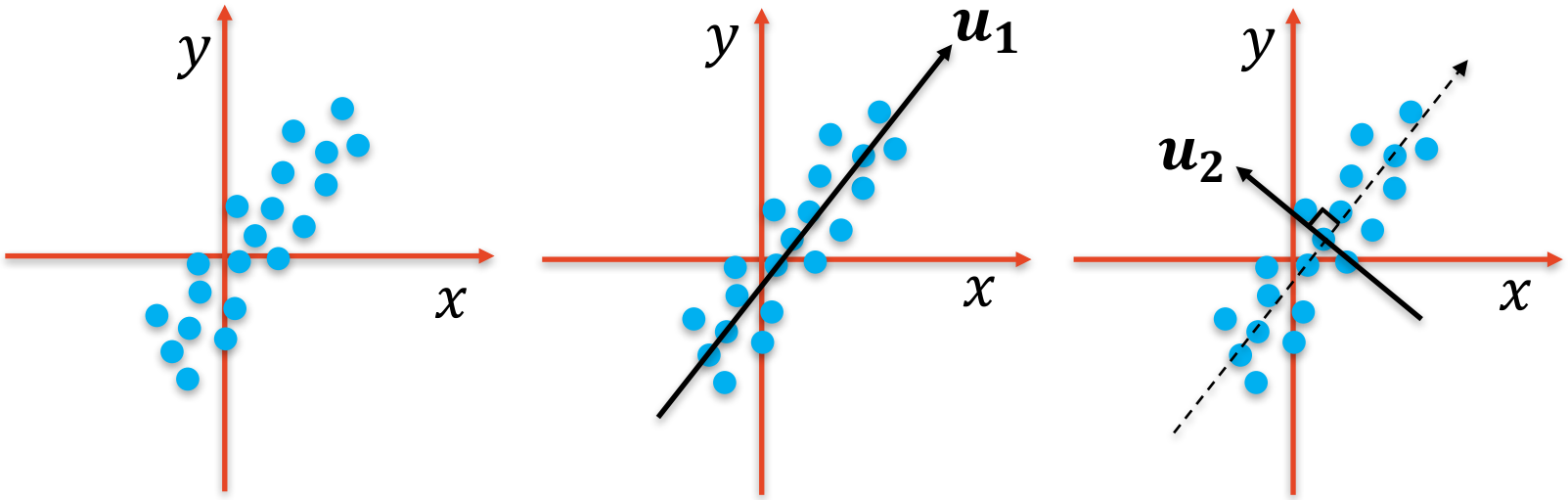
- Two equivalent definitions of PCA:

[Maximum Variance Formulation] Project the data onto a lower dimensional space such that the variance of the projected data is maximized.

[Minimum Error Formulation] Project the data onto a lower dimensional space such that the mean squared distance between data points and their projections (average projection cost) is minimized.

PCA Cont'd

Maximum Variance Formulation



data

The first principal component

The second principal component

PCA Cont'd

Let $\boldsymbol{X} = \{\boldsymbol{x}_i \in \boldsymbol{R}^d\}_{1 \le i \le n}$ be a set of observations.

PCA: project $\boldsymbol{X}$ onto a k dimensional subspace ($k < d$) such that the variance of the projected data is maximized.

We first let $k = 1$, then generalize it to the case $k > 1$.

Let $\boldsymbol{u}_1$ be the basis of the 1 dimensional subspace, and $\boldsymbol{u}_1^\top \boldsymbol{u}_1 = 1$.

$$\widehat{Var} = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{u}_1^\top \boldsymbol{x}_i - \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{u}_1^\top \boldsymbol{x}_i)^2$$

PCA Cont'd

Let $\bar{\boldsymbol{x}} = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{x}_i$ and $\boldsymbol{S} = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{x}_i - \bar{\boldsymbol{x}})(\boldsymbol{x}_i - \bar{\boldsymbol{x}})^\top$.

$$\widehat{Var} = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{u}_1^\top(\boldsymbol{x}_i - \bar{\boldsymbol{x}}))^2 = \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{u}_1^\top(\boldsymbol{x}_i - \bar{\boldsymbol{x}})(\boldsymbol{x}_i - \bar{\boldsymbol{x}})^\top\boldsymbol{u}_1 = \boldsymbol{u}_1^\top\boldsymbol{S}\boldsymbol{u}_1$$

where $\boldsymbol{S}$ is the scatter matrix.

Then, the problem becomes

$$\max_{\boldsymbol{u}_1} \boldsymbol{u}_1^\top\boldsymbol{S}\boldsymbol{u}_1 \quad s.t. \quad \boldsymbol{u}_1^\top\boldsymbol{u}_1 = 1.$$

PCA Cont'd

$$\min_{\boldsymbol{u}_1} -\boldsymbol{u}_1^\top \boldsymbol{S}\boldsymbol{u}_1 \quad s.t. \quad \boldsymbol{u}_1^\top \boldsymbol{u}_1 = 1.$$

Lagrangian function:

$$L = -\boldsymbol{u}_1^\top \boldsymbol{S}\boldsymbol{u}_1 + \lambda_1(\boldsymbol{u}_1^\top \boldsymbol{u}_1 - 1)$$

where λ_1 is the Lagrangian multiplier.

According to KKT conditions,

$$\frac{\partial L}{\partial \boldsymbol{u}_1} = -\boldsymbol{S}\boldsymbol{u}_1 + \lambda_1 \boldsymbol{u}_1 = 0$$

$$\boldsymbol{S}\boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1$$

PCA Cont'd

$$\boldsymbol{S}\boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1$$

Thus, $\boldsymbol{u}_1$ is a eigenvector of $\boldsymbol{S}$ and λ_1 is its eigenvalue. Note that

$$-\boldsymbol{u}_1^\top \boldsymbol{S}\boldsymbol{u}_1 = -\lambda_1 \boldsymbol{u}_1^\top \boldsymbol{u}_1 = -\lambda_1$$

λ_1 is the largest eigenvalue of $\boldsymbol{S}$.

$$\min_{\boldsymbol{u}_1} -\boldsymbol{u}_1^\top \boldsymbol{S}\boldsymbol{u}_1 \quad s.t. \quad \boldsymbol{u}_1^\top \boldsymbol{u}_1 = 1.$$

PCA Cont'd

$$\boldsymbol{S}\boldsymbol{u} = \lambda \boldsymbol{u}$$

For $k < d$ dimensions:
-- $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k$ are the eigenvectors corresponding to the largest eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of the scatter matrix $\boldsymbol{S}$.

Then, the i-th principal component of $\boldsymbol{X}$ is $\boldsymbol{u}_i^\top \boldsymbol{X}$ and $var\left(\boldsymbol{u}_i^\top \boldsymbol{X}\right) = \lambda_i$.

PCA Cont'd

Proof for $k = 2$ (the proof for $k \geq 3$ is similar).

$$\min_{\boldsymbol{u}_2} -\boldsymbol{u}_2^\top \boldsymbol{S}\boldsymbol{u}_2\,, \qquad s.t.\ \ \boldsymbol{u}_2^\top \boldsymbol{u}_2 = 1, \qquad \boldsymbol{u}_1^\top \boldsymbol{u}_2 = 0$$

Lagrangian function:

$$L = -\boldsymbol{u}_2^\top \boldsymbol{S}\boldsymbol{u}_2 + \lambda_2(\boldsymbol{u}_2^\top \boldsymbol{u}_2 - 1) + \theta \boldsymbol{u}_1^\top \boldsymbol{u}_2$$

According to KKT conditions,

$$\frac{\partial L}{\partial \boldsymbol{u}_2} = -\boldsymbol{S}\boldsymbol{u}_2 + \lambda_2 \boldsymbol{u}_2 + \theta \boldsymbol{u}_1 = 0$$

PCA Cont'd

$$\frac{\partial L}{\partial \boldsymbol{u}_2} = -\boldsymbol{S}\boldsymbol{u}_2 + \lambda_2 \boldsymbol{u}_2 + \theta \boldsymbol{u}_1 = 0$$

$$\Downarrow \boldsymbol{u}_1^\top \times$$

$$-\boldsymbol{u}_1^\top \boldsymbol{S}\boldsymbol{u}_2 + \lambda_2 \boldsymbol{u}_1^\top \boldsymbol{u}_2 + \theta \boldsymbol{u}_1^\top \boldsymbol{u}_1 = 0$$

$$\Downarrow \boldsymbol{u}_1^\top \boldsymbol{S}\boldsymbol{u}_2 = \lambda_1 \boldsymbol{u}_1^\top \boldsymbol{u}_2 = 0$$

$$\theta = 0$$

$$\Downarrow$$

$$-\boldsymbol{S}\boldsymbol{u}_2 + \lambda_2 \boldsymbol{u}_2 = 0$$

$$\Downarrow$$

λ_2 can not be the largest eigenvalue of $\boldsymbol{S}$. Then it is the second largest. Proof completed.

PCA Cont'd

Algorithm

- Step 1: Substract the mean data $\overline{\boldsymbol{x}}$ from original data, i.e., $\boldsymbol{z} = \boldsymbol{x} - \overline{\boldsymbol{x}}$;
- Step 2: Compute the scatter matrix $\boldsymbol{S} = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{z}_i \boldsymbol{z}_i^\top$;
- Step 3: Compute the eigenvectors $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k$ and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ by using Singular Value Decomposition (SVD) of $\boldsymbol{S}$. Then $\boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k]$ is the projection matrix.
- Step 4: $\boldsymbol{y}_i = \boldsymbol{U}^\top \boldsymbol{x}_i$

PCA Cont'd

Minimum Error Formulation

$\boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \dots, \boldsymbol{u}_k]$ is the projection matrix, where $\boldsymbol{U}^\top \boldsymbol{U} = \boldsymbol{I}$.
Assume $\overline{\boldsymbol{x}} = 0$, then for any data $\boldsymbol{x}_i$, the projected data is $\boldsymbol{y}_i = \boldsymbol{U}^\top \boldsymbol{x}_i$.

The reconstructed data $\widehat{\boldsymbol{x}_i} = \boldsymbol{U}\boldsymbol{y}_i = \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{x}_i$.

$$\min_{\boldsymbol{U}} \frac{1}{n} \sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{x}_i\|^2 \qquad s.t. \quad \boldsymbol{U}^\top \boldsymbol{U} = \boldsymbol{I}$$

$$\frac{1}{n} \sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{x}_i\|^2 = \frac{1}{n} \sum_{i=1}^{n} (-\boldsymbol{x}_i^\top \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{x}_i + \boldsymbol{x}_i^\top \boldsymbol{x}_i) = \frac{1}{n} \sum_{i=1}^{n} \mathrm{tr}(-\boldsymbol{U}^\top \boldsymbol{x}_i \boldsymbol{x}_i^\top \boldsymbol{U} + \boldsymbol{x}_i^\top \boldsymbol{x}_i)$$

$$\min_{\boldsymbol{U}} -\mathrm{tr}(\boldsymbol{U}^\top \boldsymbol{S}\boldsymbol{U}) \qquad s.t. \quad \boldsymbol{U}^\top \boldsymbol{U} = \boldsymbol{I}$$

PCA Q&A

Q: How to determine k?

A: Percentage of variance retained: $P(k) = \frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{n} \lambda_i} \geq t$ (say, t=0.95).

Q: How about $d \gg n$?

A: Assume that data has zero mean and $\boldsymbol{X} = [\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n]^\top \in \boldsymbol{R}^{n \times d}$, then $\boldsymbol{S} = \frac{1}{n}\boldsymbol{X}^\top \boldsymbol{X}$. If λ_k and $\boldsymbol{u}_k$ are the k-th eigenvalue and eigenvector of $\boldsymbol{S}$ ($k < n$), then λ_k and $\lambda_k^{-1/2}\boldsymbol{X}\boldsymbol{u}_k$ are the k-th eigenvalue and eigenvector of $\frac{1}{n}\boldsymbol{X}\boldsymbol{X}^\top$. Thus, we can decompose $\frac{1}{n}\boldsymbol{X}\boldsymbol{X}^\top$ to save computations.

PCA Cont'd

$$\hat{\boldsymbol{x}} = \sum_{i=1}^{k} \alpha_i \phi_i$$

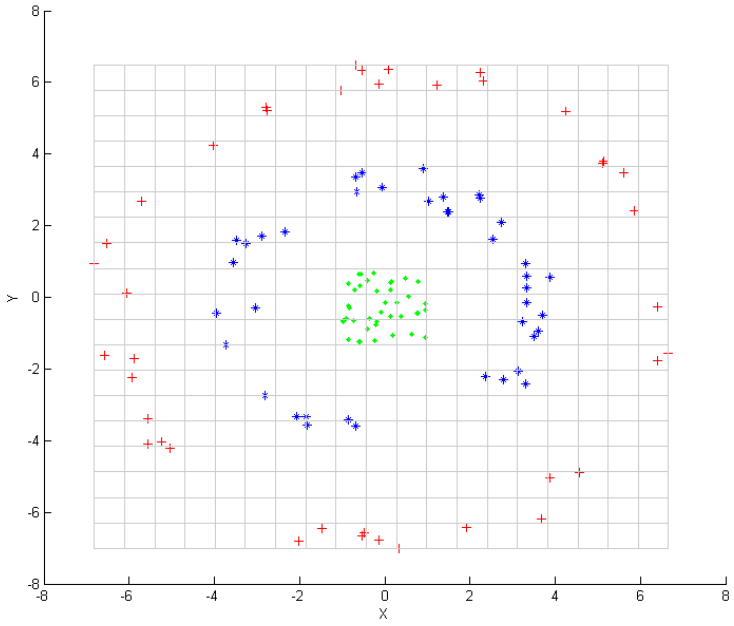
where ϕ_i, $1 \leq i \leq k$, are basis vectors of the space; and α_i, $1 \leq i \leq k$, are features or representations in the space.

For PCA:

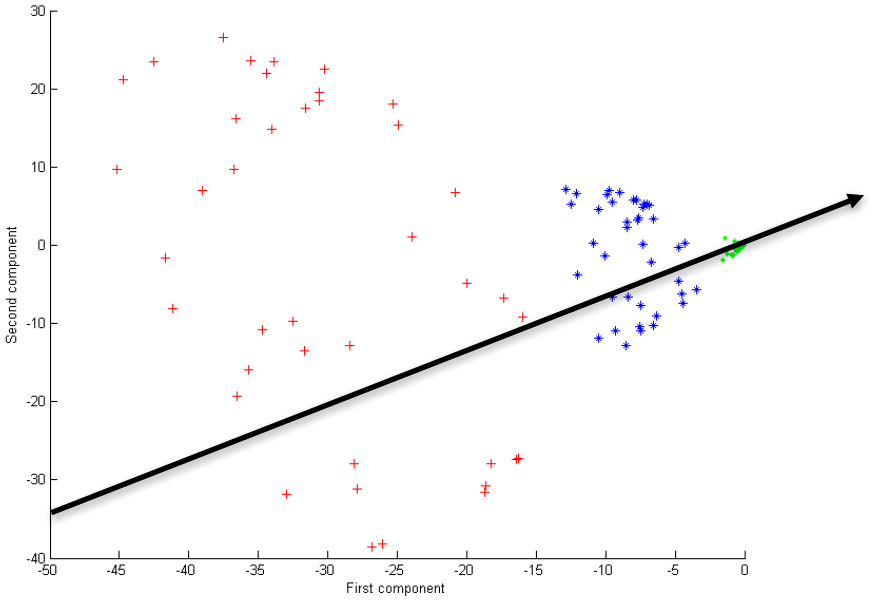
$$\hat{\boldsymbol{x}}_i = \boldsymbol{U}\boldsymbol{y}_i = \sum_{j=1}^{k} y_{ij}\boldsymbol{u}_j$$

- Under-complete representation, $k < d$
- Orthogonality constraints

Kernel PCA



Input points before kernel PCA



Output points after kernel PCA with kernel $k(\boldsymbol{x}_1, \boldsymbol{x}_2) = (\boldsymbol{x}_1^\top \boldsymbol{x}_2 + 1)^2$.

Images credit: https://en.wikipedia.org/wiki/Kernel_principal_component_analysis

Kernel PCA Cont'd

We assume the data $\boldsymbol{x}_i$ is first mapped to a feature space $\psi(\boldsymbol{x}_i)$, and the mean feature has been subtracted. $k(\boldsymbol{x}_1, \boldsymbol{x}_2) = \psi(\boldsymbol{x}_1)^\top \psi(\boldsymbol{x}_2)$ is the kernel function defined in the feature space.

$$\boldsymbol{S} = \frac{1}{n}\sum_{i=1}^{n} \psi(\boldsymbol{x}_i)\psi(\boldsymbol{x}_i)^\top$$

Follow the standard PCA, the projection vectors $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m$ statisfy:

$$\boldsymbol{S}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$$

The problem is: ψ is unknown to us!

Kernel PCA Cont'd

$$\boldsymbol{S} = \frac{1}{n}\sum_{j=1}^{n} \psi(\boldsymbol{x}_j)\psi(\boldsymbol{x}_j)^\top \qquad \boldsymbol{S}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$$

$$\frac{1}{n}\sum_{j=1}^{n} \psi(\boldsymbol{x}_j)\{\psi(\boldsymbol{x}_j)^\top \boldsymbol{v}_i\} = \lambda_i \boldsymbol{v}_i$$

Assume that $\boldsymbol{v}_i = \sum_{j=1}^{n} \alpha_{ij}\psi(\boldsymbol{x}_j)$

$$\frac{1}{n}\sum_{j=1}^{n} \psi(\boldsymbol{x}_j)\left\{\psi(\boldsymbol{x}_j)^\top \sum_{m=1}^{n} \alpha_{im}\psi(\boldsymbol{x}_m)\right\} = \lambda_i \sum_{j=1}^{n} \alpha_{ij}\psi(\boldsymbol{x}_j)$$

Kernel PCA Cont'd

$$\frac{1}{n}\sum_{j=1}^{n}\psi(\boldsymbol{x}_j)\left\{\psi(\boldsymbol{x}_j)^\top\sum_{m=1}^{n}\alpha_{im}\psi(\boldsymbol{x}_m)\right\}=\lambda_i\sum_{j=1}^{n}\alpha_{ij}\psi(\boldsymbol{x}_j)$$

Multiplying both sides by $\psi(\boldsymbol{x}_l)^\top$,

$$\frac{1}{n}\sum_{j=1}^{n}\psi(\boldsymbol{x}_l)^\top\psi(\boldsymbol{x}_j)\left\{\sum_{m=1}^{n}\alpha_{im}\psi(\boldsymbol{x}_j)^\top\psi(\boldsymbol{x}_m)\right\}=\lambda_i\sum_{j=1}^{n}\alpha_{ij}\psi(\boldsymbol{x}_l)^\top\psi(\boldsymbol{x}_j)$$

$$\frac{1}{n}\sum_{j=1}^{n}k(\boldsymbol{x}_l,\boldsymbol{x}_j)\left\{\sum_{m=1}^{n}\alpha_{im}k(\boldsymbol{x}_j,\boldsymbol{x}_m)\right\}=\lambda_i\sum_{j=1}^{n}\alpha_{ij}k(\boldsymbol{x}_l,\boldsymbol{x}_j)$$

Kernel PCA Cont'd

$$\frac{1}{n}\sum_{j=1}^{n} k(\boldsymbol{x}_l, \boldsymbol{x}_j)\left\{\sum_{m=1}^{n} \alpha_{im} k(\boldsymbol{x}_j, \boldsymbol{x}_m)\right\} = \lambda_i \sum_{j=1}^{n} \alpha_{ij} k(\boldsymbol{x}_l, \boldsymbol{x}_j)$$

Let $\boldsymbol{K}$ be the kernel matrix, where $\boldsymbol{K}_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$ and $\boldsymbol{K}_{l.}$ is the l-th row of $\boldsymbol{K}$.

$$\frac{1}{n}\boldsymbol{K}_{l.}\boldsymbol{K}\boldsymbol{\alpha}_i = \lambda_i \boldsymbol{K}_{l.}\boldsymbol{\alpha}_i$$

For $l = 1, \cdots, n$, we have

$$\frac{1}{n}\boldsymbol{K}^2\boldsymbol{\alpha}_i = \lambda_i \boldsymbol{K}\boldsymbol{\alpha}_i$$

Kernel PCA Cont'd

$$\frac{1}{n}\boldsymbol{K}^2\boldsymbol{\alpha}_i = \lambda_i \boldsymbol{K}\boldsymbol{\alpha}_i$$

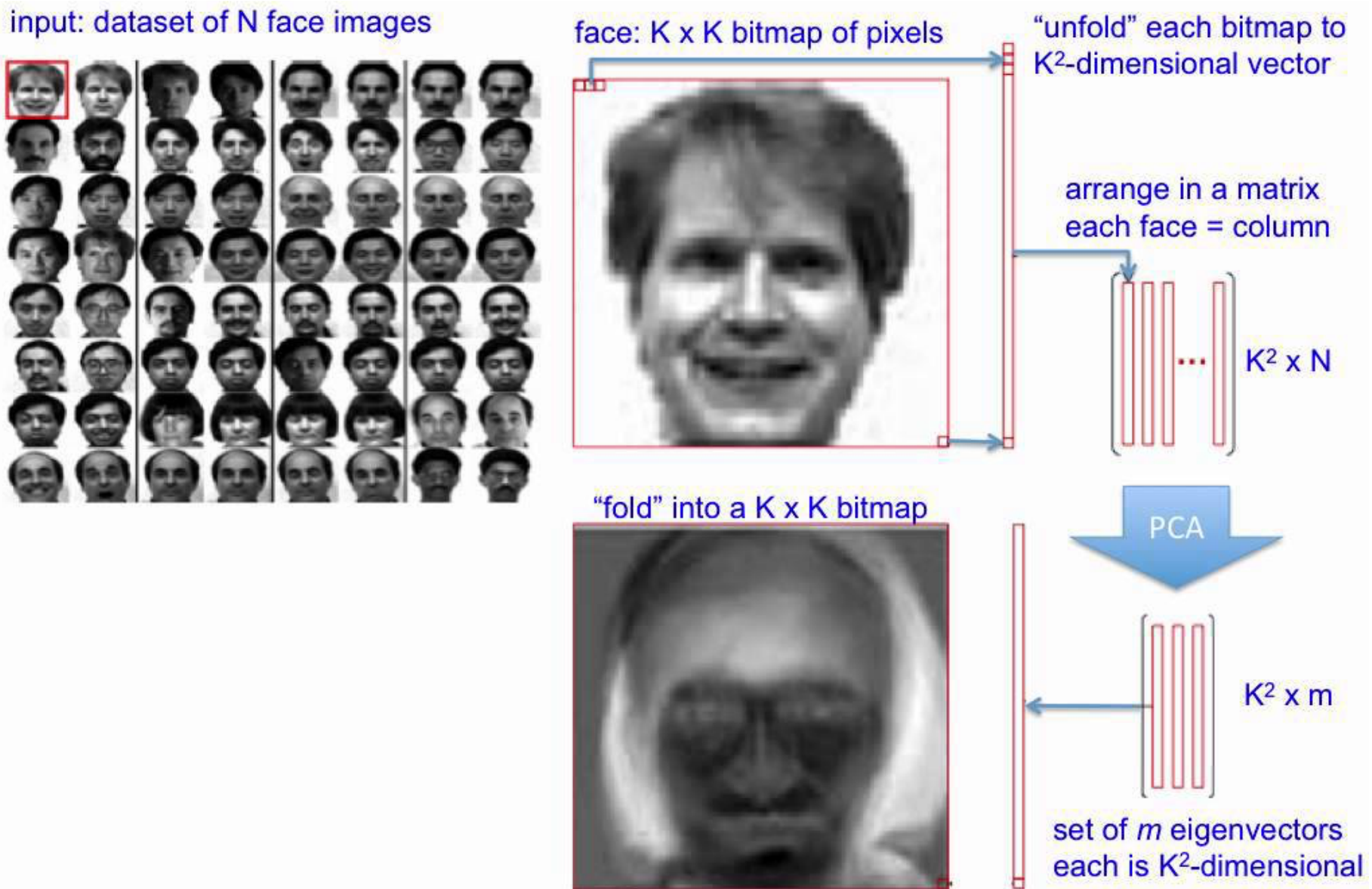
$$\boldsymbol{K}\boldsymbol{\alpha}_i = n\lambda_i \boldsymbol{\alpha}_i$$

$\boldsymbol{\alpha}_i$ is the eigenvector of $\boldsymbol{K}$.

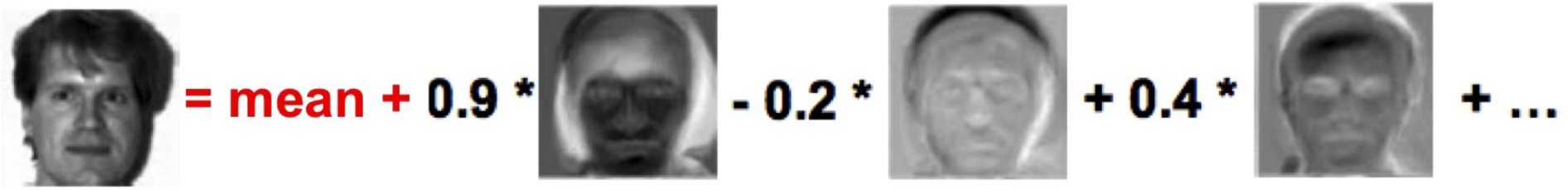
Recall that $\boldsymbol{v}_i = \sum_{j=1}^{n} \alpha_{ij}\psi(\boldsymbol{x}_j)$

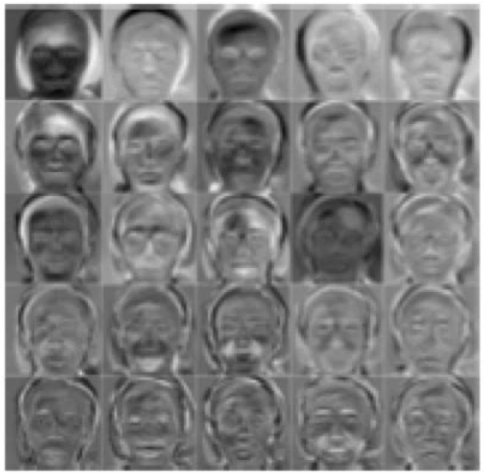
$$y = \psi(\boldsymbol{x})^\top \boldsymbol{v}_i = \sum_{j=1}^{n} \alpha_{ij}\psi(\boldsymbol{x})^\top \psi(\boldsymbol{x}_j) = \sum_{j=1}^{n} \alpha_{ij} k(\boldsymbol{x},\boldsymbol{x}_j)$$

Face Recognition

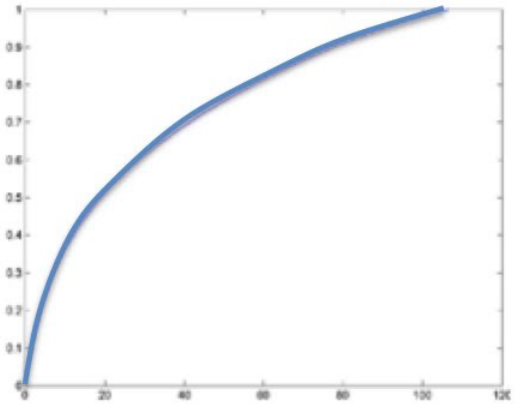


Face Recognition





- Project new face to space of eigen-faces
- Represent vector as a linear combination of principal components
- How many do we need?



Autoencoder (AE)

Autoencoder (AE)

Autoencoder aims to learn discriminative representations $\mathbf{y}$ which capture the main factors of variation in input data.

Encoder: mapping the input data $\boldsymbol{x}$ to a hidden representation $\boldsymbol{y}$ via:

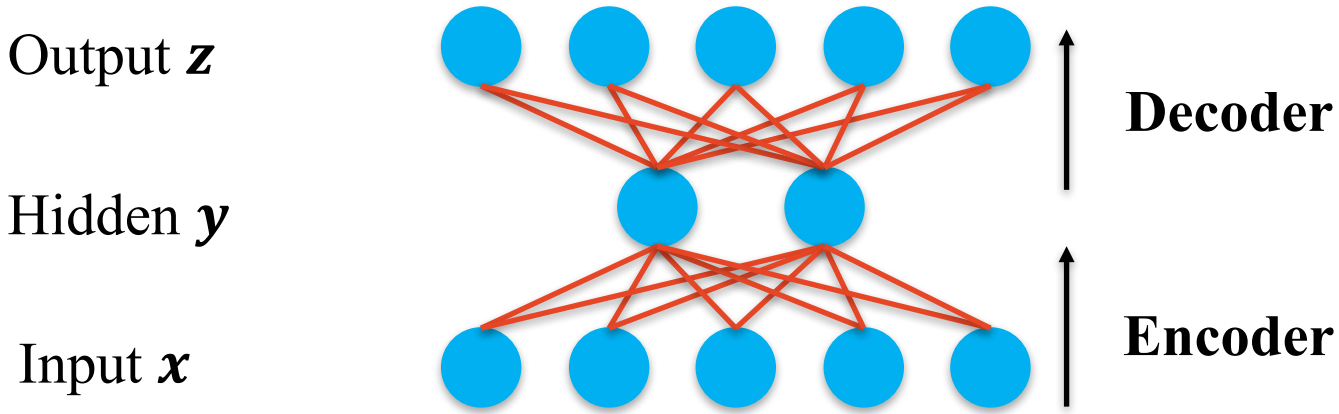
$$\boldsymbol{y} = f\left(\boldsymbol{W}^{(1)}\boldsymbol{x} + \boldsymbol{b}^{(1)}\right),$$

Decoder: mapping the hidden representation back into a reconstruction $\boldsymbol{z}$ of the same shape as $\boldsymbol{x}$,

$$\boldsymbol{z} = f\left(\boldsymbol{W}^{(2)}\boldsymbol{y} + \boldsymbol{b}^{(2)}\right).$$

where f denotes the activation function, such as sigmoid.

Target: $\boldsymbol{z}$ reconstruct $\boldsymbol{x}$.



AE Cont'd

The objective function measures the reconstruction error:

- Square loss: $J(\theta) = \|\boldsymbol{x} - \boldsymbol{z}\|^2$, $\theta = \{\boldsymbol{W}^{(1)}, \boldsymbol{b}^{(1)}, \boldsymbol{W}^{(2)}, \boldsymbol{b}^{(2)}\}$
- Cross-entropy: $J(\theta) = -\sum_{i=1}^{d} x_i \log(z_i) + (1 - x_i)\log(1 - z_i)$

We can constrain the weight matrix $\boldsymbol{W}^{(2)}$ of the reverse mapping to be the transpose of the forward mapping: $\boldsymbol{W}^{(1)} = \boldsymbol{W}$, and $\boldsymbol{W}^{(2)} = \boldsymbol{W}^{\top}$, referred to as **tied weights**.

Regularization term, such as l_1 norm and l_2 norm of $\boldsymbol{W}^{(1)}$ and $\boldsymbol{W}^{(2)}$, is often added.

AE Cont'd

Backpropagation (BP) algorithm is often applied to optimize AE. Take the objective function $J(\theta) = \frac{1}{n}\sum_{i=1}^{n}\|\boldsymbol{x}_i - \boldsymbol{z}_i\|^2 + \lambda\sum_{l=1}^{2}\left\|\boldsymbol{W}^{(l)}\right\|_F^2$ as an example:

One iteration of gradient descent updates the parameters as follows:

$$\boldsymbol{W}^{(l)} = \boldsymbol{W}^{(l)} - \alpha\frac{\partial}{\partial \boldsymbol{W}^{(l)}}J(\theta)$$

$$\boldsymbol{b}^{(l)} = \boldsymbol{b}^{(l)} - \alpha\frac{\partial}{\partial \boldsymbol{b}^{(l)}}J(\theta)$$

Where α is the learning rate. The detail of BP algorithm will be introduced in another class.

AE Cont'd

A special case: We choose f as the identity mapping, $\mathbf{y} \in \boldsymbol{R}^k$ resides in a lower dimensional space ($k < d$), and ignore the bias term. We apply the squared loss and tied weights into AE:

$$J(\boldsymbol{x}, \boldsymbol{z}) = \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{W}^\top \boldsymbol{W}\boldsymbol{x}_i\|^2$$

PCA:

$$\min_{\boldsymbol{U}} \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{x}_i\|^2 \qquad s.t. \quad \boldsymbol{U}^\top \boldsymbol{U} = \boldsymbol{I}$$

Differences between AE and PCA are the nonlinearity in AE and the orthogonality constraint in PCA.

AE Cont'd

Without any regularization, AE tends to learn the identity function.

Thus, many regularizations have been added to AE. Beside that the code $\mathbf{y}$ has a lower dimension, there are another two popular regularizations:

- Sparse AE requires the code $\mathbf{y}$ to be sparse.
- Denoising AE: adds noises to input data, uses this corrupted data as input of AE, and then reconstructs the original input $\boldsymbol{x}$.

$$\boldsymbol{y} = f\left(\boldsymbol{W}^{(1)}\boldsymbol{x} + \boldsymbol{b}^{(1)}\right),$$
$$\boldsymbol{z} = f\left(\boldsymbol{W}^{(2)}\boldsymbol{y} + \boldsymbol{b}^{(2)}\right).$$

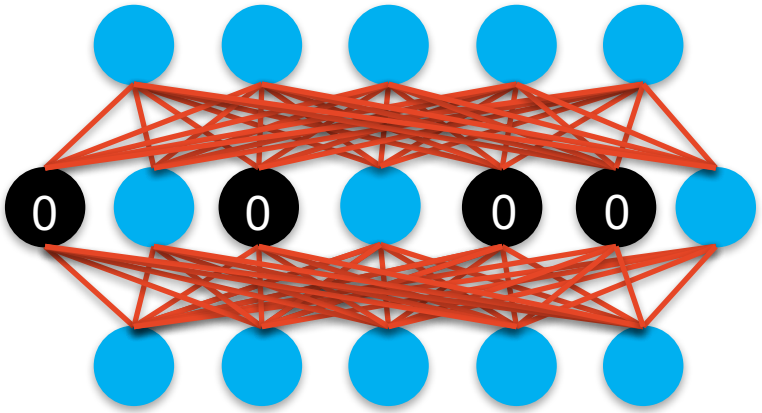
Sparse AE

An illustration of sparse autoencoder ($k > d$):

$\boldsymbol{z} \in \boldsymbol{R}^d$

$\boldsymbol{y} \in \boldsymbol{R}^k$

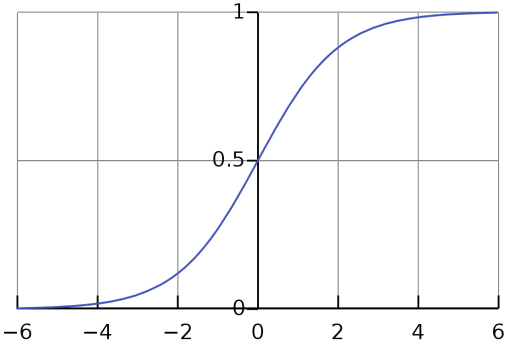
$\boldsymbol{x} \in \boldsymbol{R}^d$



$\boldsymbol{W}^{(2)} \in \boldsymbol{R}^{d \times k}$

$\boldsymbol{W}^{(1)} \in \boldsymbol{R}^{k \times \boldsymbol{d}}$

We choose sigmoid as the activation functions of sparse AE.



Sparse AE Cont'd

Compute the average activation of **each neuron** $j, \forall j \in \{1, \cdots, k\}$, on the hidden layer w.r.t. the training examples $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\}$:

$$\hat{\rho}_j = \frac{1}{n}\sum_{i=1}^{n} y_j(\boldsymbol{x}_i), y_j = \boldsymbol{y}[j], \boldsymbol{y} \in \boldsymbol{R}^k$$

We would like the average activation of each neuron to be low and close to a sparsity parameter ρ, say, 0.05, such that only a few neurons activate.

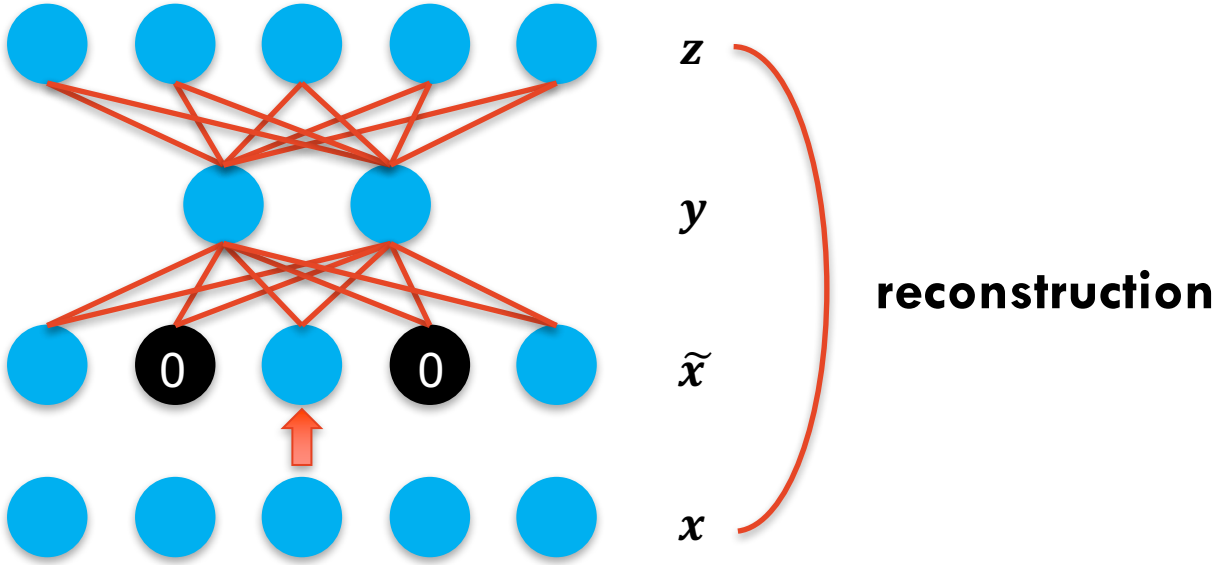
$$J_{sparse}(\theta) = J(\theta) + \beta \sum_{j=1}^{k} KL(\rho || \hat{\rho}_j),$$

where β controls the weight of sparsity penalty term and $\mathrm{KL}(\rho||\hat{\rho}_j) = \rho \log\left(\frac{\rho}{\hat{\rho}_j}\right) + (1-\rho)\log(\frac{1-\rho}{1-\hat{\rho}_j})$.

Denoising AE

To learn representations which are robust to partial destruction of the inputs. We need to add a stochastic corruption step on the input. Here is an example:

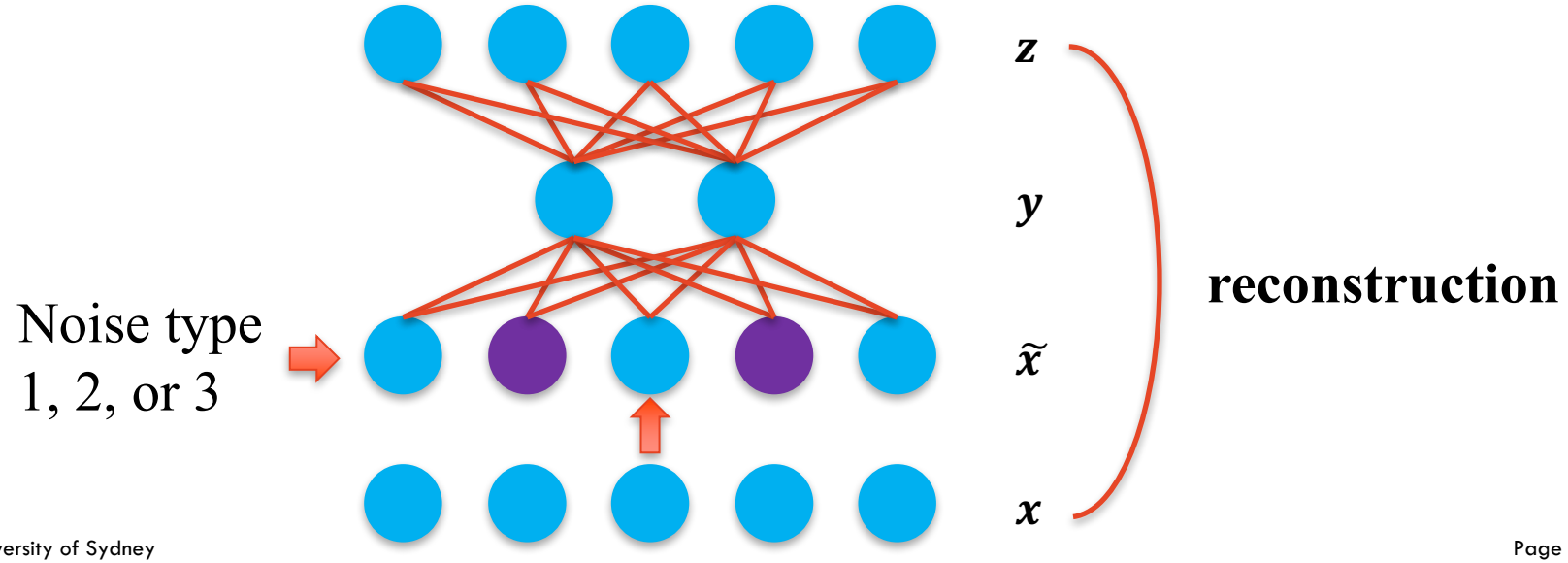
- Step 1: Choose a desired proportion ρ of destruction;
- Step 2: Select $\rho \times d$ components of $\boldsymbol{x}$ randomly and set them to 0;
- Step 3: Use the corrupted $\tilde{\boldsymbol{x}}$ as input, and train the AE.



Denoising AE

Noise types usually considered for corrupting the input data:

1. Additive Gaussian noise;
2. Multiplicative 0-1 noise or masking noise, seen in the previous slide.
3. Salt-and-pepper noise: a fraction ρ of the elements of $\boldsymbol{x}$ (chosen at random for each example) is set to their minimum or maximum possible value (typically 0 or 1) according to a fair coin flip.



AE Cont'd

$$\hat{\boldsymbol{x}} = \sum_{i=1}^{k} \alpha_i \phi_i$$

where ϕ_i, $1 \leq i \leq k$, are basis vectors of the space; and α_i, $1 \leq i \leq k$, are features or representations in the space.

In AE, assume f is identity function, and ignore the bias term, then

$$\hat{\boldsymbol{x}}_i = \boldsymbol{W}^{(2)} \boldsymbol{y}_i = \sum_{j=1}^{k} y_{ij} \boldsymbol{W}_{\cdot j}^{(2)}$$

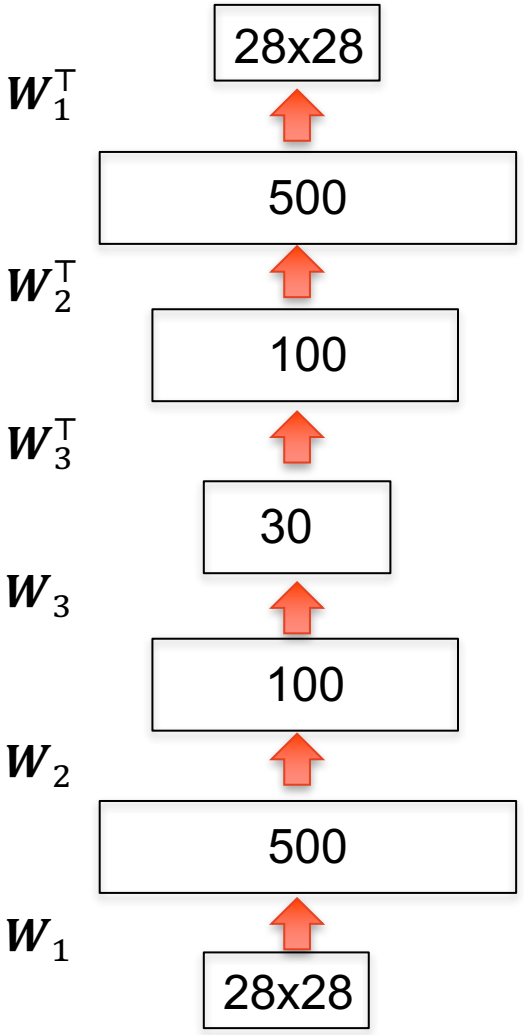
Classical AE: Under-complete representation

Sparse AE: Over-complete representation and sparsity on features

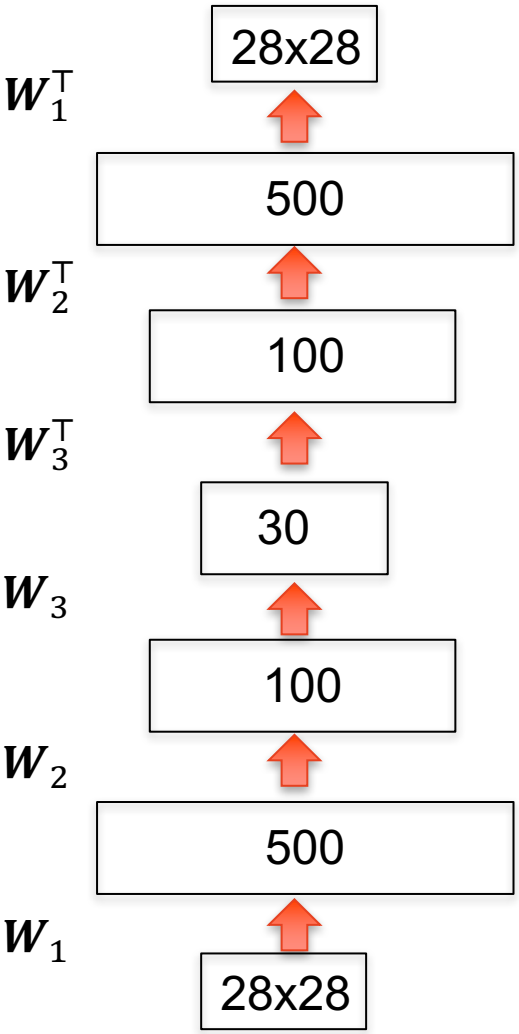
Stacked AE

A stacked autoencoder enjoys all the benefits of any deep network of greater expressive power, and tends to learn higher-order features.

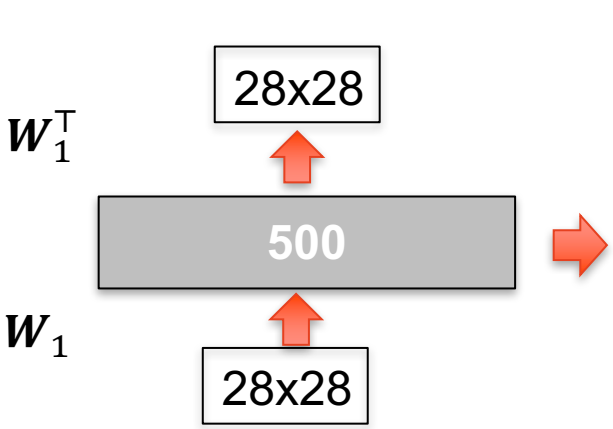
The problem is that it is very difficult to optimize directly using backpropagation (BP).

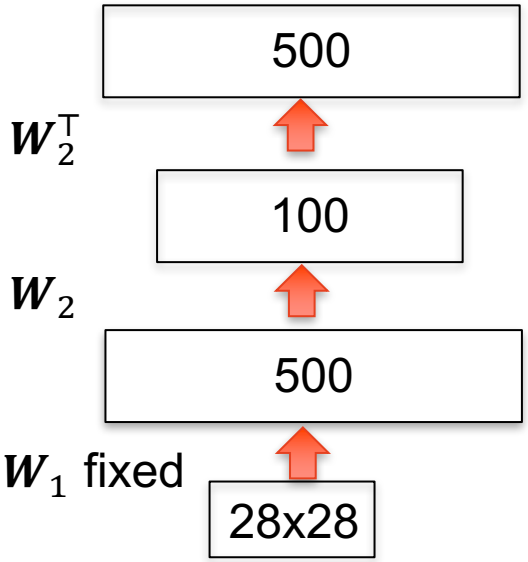


Stacked AE Cont'd



Method: Greedy layer-wise training + fine-tuning using BP.



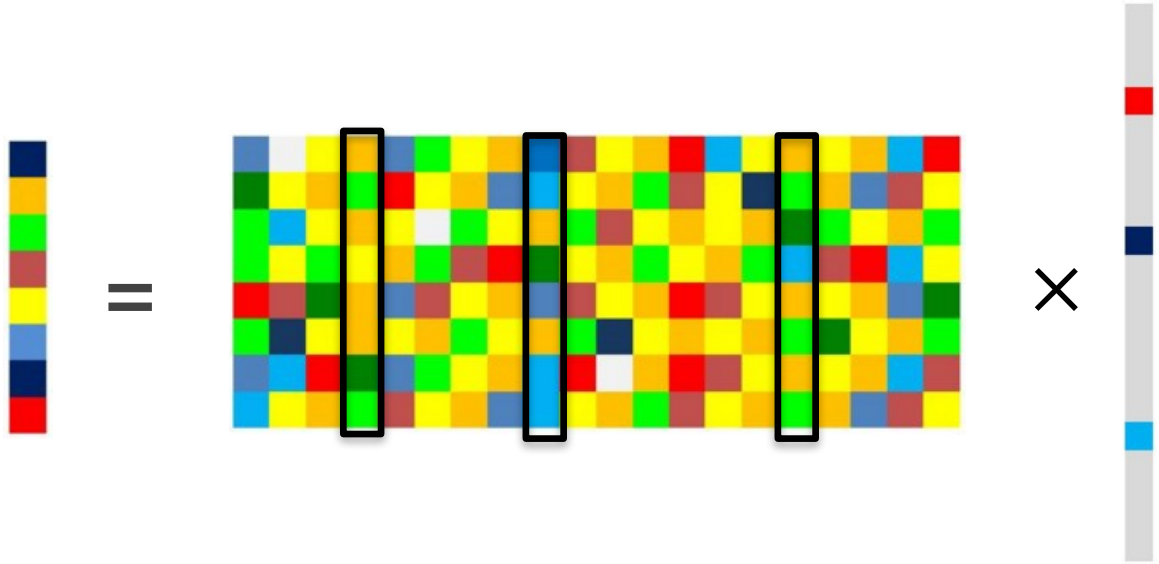


Sparse Coding (SC)

Sparse Coding (SC)

Given a set of input data, sparse coding learns a possibly over-complete set of basis vectors $\{\phi_i\}$ and features $\boldsymbol{\alpha}$.

But not all basis vectors are necessarily needed to approximate the input data $\boldsymbol{x}$. We thus add the sparsity constraint.



Data x

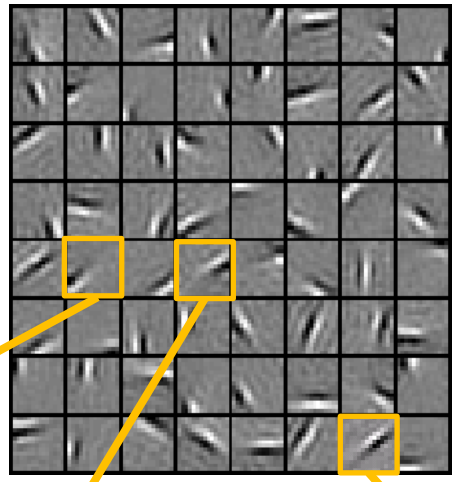
Basis vectors: Over-complete

Features: Sparse

SC Cont'd

Natural Images

Learned bases $(f_1, \ldots, f_{64})$: "Edges"



Test example

$$x = 0.8 * f_{36} + 0.3 * f_{42} + 0.5 * f_{63}$$

Feature: $[0, 0, \ldots, 0, \mathbf{0.8}, 0, \ldots, 0, \mathbf{0.3}, 0, \ldots, 0, \mathbf{0.5}, \ldots] = [\alpha_1, \ldots, \alpha_{64}]$

Slide credit: Andrew Ng

SC Cont'd

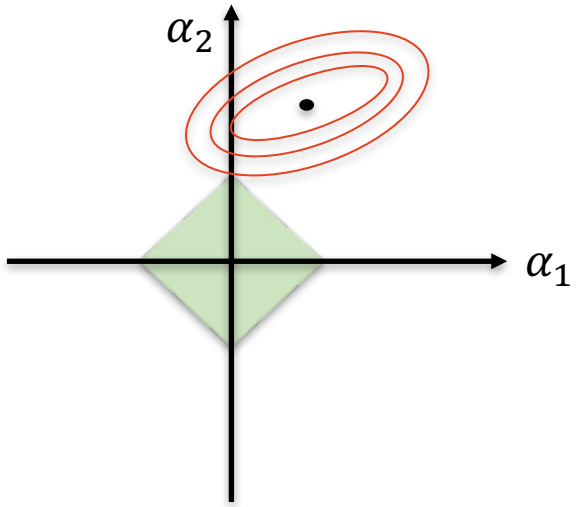
Let $\boldsymbol{X} = \{\boldsymbol{x}_i \in \boldsymbol{R}^d\}_{1 \le i \le n}$ be a set of observations. The cost function becomes the reconstruction error + sparsity term:

$$J(\theta) = \sum_{i=1}^{n} \left(\left\| \boldsymbol{x}_i - \sum_{j=1}^{k} \alpha_{ij} \phi_j \right\|^2 + \beta \sum_{j=1}^{k} s(\alpha_{ij}) \right)$$

Sparsity function $s(\alpha_j)$:

L0: $s(\alpha_j) = 1(\alpha_j \neq 0)$;

L1: $s(\alpha_j) = |\alpha_j|$;



SC Cont'd

Without regularization on the basis vector, the sparsity term can be arbitrarily small by rescaling α and ϕ.

$$\min_{\alpha,\phi} J(\theta) = \sum_{i=1}^{n} \left(\left\| \boldsymbol{x}_i - \sum_{j=1}^{k} \alpha_{ij} \phi_j \right\|^2 + \beta \sum_{j=1}^{k} s(\alpha_{ij}) \right)$$

$$\text{s.t. } \|\phi_j\|^2 \leq 1, \forall j = 1, \ldots, k$$

$$\min_{\alpha,\phi} J(\theta) = \sum_{i=1}^{n} \left(\left\| \boldsymbol{x}_i - \sum_{j=1}^{k} \alpha_{ij} \phi_j \right\|^2 + \beta \sum_{j=1}^{k} s(\alpha_{ij}) \right) + \gamma \sum_{j=1}^{k} \|\phi_j\|^2$$

SC Cont'd

$$\min_{\alpha,\phi} J(\theta) = \sum_{i=1}^{n} \left(\left\| \boldsymbol{x}_i - \sum_{j=1}^{k} \alpha_{ij} \phi_j \right\|^2 + \beta \sum_{j=1}^{k} s(\alpha_{ij}) \right) + \gamma \sum_{j=1}^{k} \|\phi_j\|^2$$

Vectorization: $\boldsymbol{\phi} = [\phi_1, \dots, \phi_k]$, $\boldsymbol{A} = [\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_n]$.

$$\min_{\alpha,\phi} J(\theta) = \|\boldsymbol{X} - \boldsymbol{\phi A}\|^2 + \beta s(\boldsymbol{A}) + \gamma \|\boldsymbol{\phi}\|^2$$

Alternating optimization:

1. Fix the basis (dictionary) $\boldsymbol{\phi}$, optimize $\boldsymbol{A}$ (a standard LASSO problem).
2. Fix $\boldsymbol{A}$, optimize $\boldsymbol{\phi}$ (a convex QP problem).

Outline

1. Background
2. Principal Component Analysis (PCA)
3. Autoencoder (AE)
4. Sparse Coding (SC)