

# DDA5001 Machine Learning

## Unsupervised Learning: Dimensionality Reduction

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## Dimensionality Reduction

Principal Component Analysis (PCA)

Apply PCA to Real Image Dataset

# Dimensionality Reduction

- ▶ Observe samples  $x_1, \dots, x_n \in \mathbb{R}^d$ , without labels.

Dimensionality reduction: Find a **closest** point to  $x_i$  in a **lower dimensional space**, i.e.,

$$\mathbb{R}^d \ni x_i \rightarrow \tilde{x}_i \in \mathbb{R}^k,$$

where  $k \ll d$ .

- ▶ Contrary to kernel methods in supervised learning.

The motivation of dimensionality reduction:

- ▶ Reducing redundant information.
- ▶ Help algorithms to be more computationally efficient (in lower dimension).
- ▶ Preventing overfitting, especially when  $n < d$  (data preprocessing for supervised learning).

Dimensionality reduction is an important **unsupervised learning** technique. The main methods for dimensionality reduction are **feature selection** and **feature extraction**. We will focus on the later.

Dimensionality Reduction

## Principal Component Analysis (PCA)

Apply PCA to Real Image Dataset

# Principal Component Analysis

Principal component analysis (PCA): Find a low-dimensional approximation of high-dimensional data by minimizing the squared norms of distances.

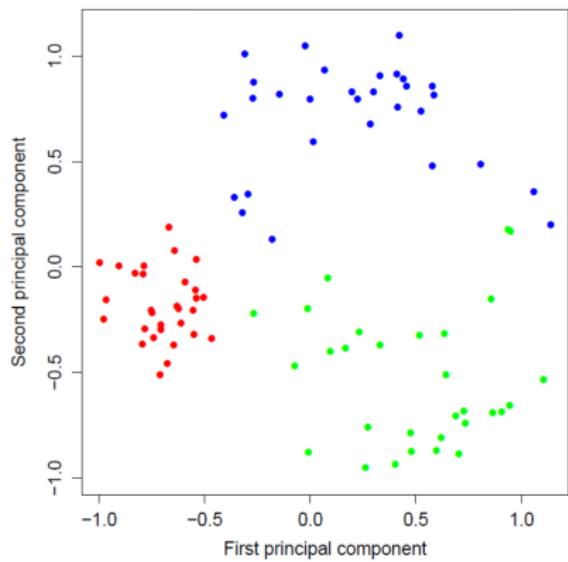
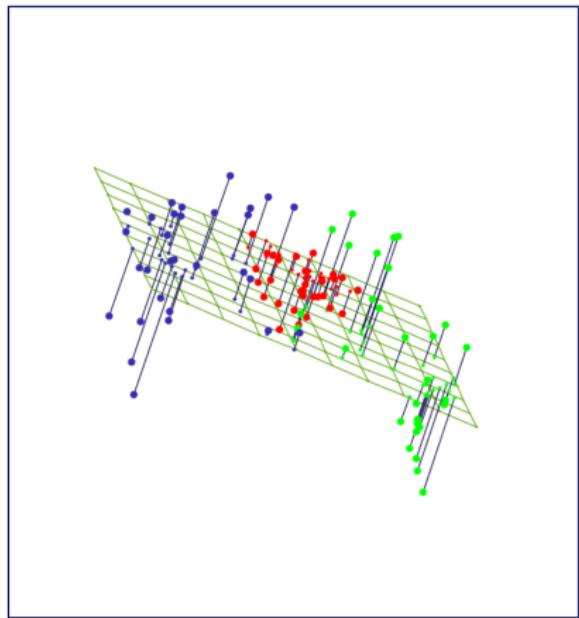
PCA modeling of data:

$$x \approx A\theta + \mu$$

- ▶  $x \in \mathbb{R}^d$  is the original sample.
- ▶  $A = [A_1, \dots, A_k] \in \mathbb{R}^{d \times k}$  with orthogonal columns, i.e., satisfying  $A^\top A = I_k$ . Matrix  $A$  is often called basis.
- ▶  $\theta \in \mathbb{R}^k$  is the principle component.
- ▶  $\mu$  is the mean of the samples.

Interpretation:  $x$  (after removing the mean  $\mu$ ) can be approximated by a  $k$ -dimensional point  $\tilde{x} = A\theta$ .

# Principal Component Analysis - Illustration



# The PCA Learning Problem

PCA boils down to

$$\underset{\mu, \{\theta_i\}, A^\top A = I_k}{\text{minimize}} \quad \frac{1}{n} \sum_{i=1}^n \|x_i - A\theta_i - \mu\|_2^2$$

- ▶ Only samples  $\{x_i\}$  are known. Others are unknowns.
- ▶ It is a **nonconvex optimization** problem.
- ▶ The hard part is to solve for  $A$ .
- ▶ Given  $A$ , finding  $\mu$  and  $\{\theta_i\}$  is easy.

## Solve for $\theta_i$

Given  $A, \mu$

$$\underset{\{\theta_i\}}{\text{minimize}} \sum_{i=1}^n \|x_i - A\theta_i - \mu\|_2^2.$$

Solution:

$$\theta_i = A^\top (x_i - \mu)$$

Why? It is just a standard least square problem with  $A$  being semi-orthogonal.

## Solve for $\mu$

Suppose given  $A$ , setting  $\theta_i = A^\top(x_i - \mu)$ , we have

$$\underset{\mu}{\text{minimize}} \sum_{i=1}^n \|x_i - AA^\top(x_i - \mu) - \mu\|_2^2.$$

It is equivalent to

$$\underset{\mu}{\text{minimize}} \sum_{i=1}^n \|(\mathbf{I} - AA^\top)(x_i - \mu)\|_2^2.$$

It is further equivalent to

$$\underset{\mu}{\text{minimize}} \sum_{i=1}^n (x_i - \mu)^\top (\mathbf{I} - AA^\top)^\top (\mathbf{I} - AA^\top)(x_i - \mu).$$

Let  $B = (\mathbf{I} - AA^\top)^\top (\mathbf{I} - AA^\top) = \mathbf{I} - AA^\top$ .

## Solve for $\mu$

Take the gradient with respect to  $\mu$  gives

$$\nabla_{\mu} = 2 \sum_{i=1}^n \mathbf{B}(\mathbf{x}_i - \mu).$$

Set the gradient to zero yields **one** solution

$$\mu = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i.$$

## Solve for $\mathbf{A}$

It remains to solve

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{minimize}} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{A}\mathbf{A}^\top(\mathbf{x}_i - \boldsymbol{\mu}) - \boldsymbol{\mu}\|_2^2$$

- We can assume  $\boldsymbol{\mu} = \mathbf{0}$  without loss of generality, as we can set  $\mathbf{x}_i = \mathbf{x}_i - \boldsymbol{\mu}$  (removing the mean from the data).

The problem reduces to

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{minimize}} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{A}\mathbf{A}^\top \mathbf{x}_i\|_2^2$$

This is one form of PCA.

- **Interpretation:** Find the **closest**  $k$ -dimensional data point  $\mathbf{A}\mathbf{A}^\top \mathbf{x}_i$  to  $\mathbf{x}_i$  (projecting  $\mathbf{x}_i$  onto the  $k$ -dimensional subspace spanned by the columns of  $\mathbf{A}$ ).

# Derivation of the Second Equivalent PCA Form

Given the PCA formulation

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{minimize}} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{A}\mathbf{A}^\top \mathbf{x}_i\|_2^2.$$

Expanding the objective function yields

$$\begin{aligned} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{A}\mathbf{A}^\top \mathbf{x}_i\|_2^2 &= \sum_{i=1}^n (\mathbf{x}_i - \mathbf{A}\mathbf{A}^\top \mathbf{x}_i)^\top (\mathbf{x}_i - \mathbf{A}\mathbf{A}^\top \mathbf{x}_i) \\ &= \sum_{i=1}^n \left( \mathbf{x}_i^\top \mathbf{x}_i - 2\mathbf{x}_i^\top \mathbf{A}\mathbf{A}^\top \mathbf{x}_i + \mathbf{x}_i^\top \mathbf{A}\mathbf{A}^\top \mathbf{A}\mathbf{A}^\top \mathbf{x}_i \right) \\ &= \sum_{i=1}^n \mathbf{x}_i^\top \mathbf{x}_i - \mathbf{x}_i^\top \mathbf{A}\mathbf{A}^\top \mathbf{x}_i. \end{aligned}$$

We reduce to the **second form** of PCA

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \sum_{i=1}^n \mathbf{x}_i^\top \mathbf{A}\mathbf{A}^\top \mathbf{x}_i = \sum_{i=1}^n \|\mathbf{A}^\top \mathbf{x}_i\|_2^2.$$

# Derivation of the Third Equivalent PCA Form

The second form is further equivalent to

$$\begin{aligned} & \underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \sum_{i=1}^n \|\mathbf{A}^\top \mathbf{x}_i\|_2^2 \\ \iff & \underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \sum_{i=1}^n \text{trace}(\mathbf{A}^\top \mathbf{x}_i \mathbf{x}_i^\top \mathbf{A}) \\ \iff & \underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \text{trace} \left( \mathbf{A}^\top \left( \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top \right) \mathbf{A} \right). \end{aligned}$$

Let

$$\mathbf{S} = \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top = \mathbf{X} \mathbf{X}^\top, \quad \text{where } \mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$$

be the **empirical covariance matrix**. We have the following **third form** of PCA

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \text{trace} \left( \mathbf{A}^\top \mathbf{S} \mathbf{A} \right).$$

We use the third form to derive the solution for  $\mathbf{A}$ . We need to consult a matrix computation tool called **eigen decomposition**.

# Eigenvalue Analysis

**Eigenvalue problem:** Given matrix  $S$ , find a vector  $u$  and a scalar  $\lambda$  such that

$$Su = \lambda u$$

- ▶  $\lambda$  characterizes the behavior of  $S$  in  $u$ .
- ▶  $u$  is called the **eigenvector**, while  $\lambda$  is called the **eigenvalue**.

## Eigen decomposition for real PSD matrix

Suppose matrix  $S \in \mathbb{R}^{d \times d}$  is **real**, **symmetric**, and **positive semidefinite (PSD)**, it always admits an eigen decomposition:

$$S = U \Lambda U^\top$$

where  $U \in \mathbb{R}^{d \times d}$  is an orthogonal matrix satisfying  $U^\top U = UU^\top = \mathbf{I}$  containing eigenvectors and  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_d)$  with  $\lambda_1 \geq \dots \geq \lambda_d \geq 0$  is a diagonal matrix containing the corresponding eigenvalues.

# Return to The Solution of PCA

Consider the third form of PCA

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \text{ trace} \left( \mathbf{A}^\top \mathbf{S} \mathbf{A} \right),$$

where  $\mathbf{S} = \mathbf{X} \mathbf{X}^\top$ .

- ▶ Note that  $\mathbf{S}$  is constructed from the data matrix  $\mathbf{X}$ , it is computable.
- ▶ Further,  $\mathbf{S}$  is real and **must be PSD** (why?).

Thus we apply eigen decomposition to  $\mathbf{S}$  to obtain

$$\mathbf{S} = \mathbf{U} \Lambda \mathbf{U}^\top.$$

The PCA problem becomes

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \text{ trace} \left( \mathbf{A}^\top \mathbf{U} \Lambda \mathbf{U}^\top \mathbf{A} \right).$$

## Return to The Solution of PCA

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \text{ trace} \left( \mathbf{A}^\top \mathbf{U} \Lambda \mathbf{U}^\top \mathbf{A} \right)$$

Let  $\Phi = \mathbf{A}^\top \mathbf{U} \in \mathbb{R}^{k \times d}$ , it is a semi-orthogonal matrix since  $\Phi \Phi^\top = \mathbf{I}$   
We can rewrite the optimization problem as

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \text{ trace} \left( \Phi \Lambda \Phi^\top \right) = \underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \text{ trace} \left( \sum_{i=1}^d \lambda_i \phi_i \phi_i^\top \right)$$

put the trace inside, we have

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}}{\text{maximize}} \sum_{i=1}^d \lambda_i \phi_i^\top \phi_i$$

**Fact:** This optimization problem has upper bound  $\leq \sum_{i=1}^k \lambda_i$ . Hence, it attains its maximum when  $\phi_i^\top \phi_i = 1, i = 1, \dots, k$  and  $\phi_i^\top \phi_i = 0, i = k+1, \dots, d$ . This is achieved by

$$\boxed{\mathbf{A} = [\mathbf{u}_1, \dots, \mathbf{u}_k]}$$

i.e., the first  $k$  eigenvectors.

# Process of Computing The PCA

Given samples  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ , without labels.

- ▶ Remove the mean

$$\mathbf{x}_i = \mathbf{x}_i - \boldsymbol{\mu},$$

where  $\boldsymbol{\mu} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$ .

- ▶ Form the empirical covariance matrix from data

$$\mathbf{S} = \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top = \mathbf{X} \mathbf{X}^\top.$$

- ▶ Compute the eigen decomposition of  $\mathbf{S}$

$$\mathbf{S} = \mathbf{U} \boldsymbol{\Lambda} \mathbf{U}^\top$$

and the PCA solution is given by

$$\mathbf{A} = [\mathbf{u}_1, \dots, \mathbf{u}_k].$$

- ▶ Compute principle component and low-dimensional sample

$$\boldsymbol{\theta}_i = \mathbf{A}^\top \mathbf{x}_i, \quad \tilde{\mathbf{x}}_i = \mathbf{A} \boldsymbol{\theta}_i = \mathbf{A} \mathbf{A}^\top \mathbf{x}_i.$$

# Connection to Singular Value Decomposition

## Singular value decomposition (SVD)

Given **any** real matrix  $\mathbf{X} \in \mathbb{R}^{d \times n}$ , there exists a 3-tuple  $(\mathbf{U}, \Sigma, \mathbf{V}) \in \mathbb{R}^{d \times d} \times \mathbb{R}^{d \times n} \times \mathbb{R}^{n \times n}$  such that

$$\mathbf{X} = \mathbf{U} \Sigma \mathbf{V}^\top,$$

where  $\mathbf{U}$  and  $\mathbf{V}$  are orthogonal and  $\Sigma$  takes the form

$$\Sigma(i, j) = \begin{cases} \sigma_i, & i = j \\ 0, & i \neq j \end{cases}$$

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0, \quad p = \min(d, n).$$

- ▶  $\sigma_i$  are called **singular value**.
- ▶  $\mathbf{u}_i$  and  $\mathbf{v}_i$  are called **left and right singular vectors**.

## PCA via SVD

Recall  $\mathbf{S} = \mathbf{X}\mathbf{X}^\top$ , the eigen decomposition is  $\mathbf{S} = \mathbf{U}\Lambda\mathbf{U}^\top$ , and the solution to the PCA problem is

$$\mathbf{A} = [\mathbf{u}_1, \dots, \mathbf{u}_k]$$

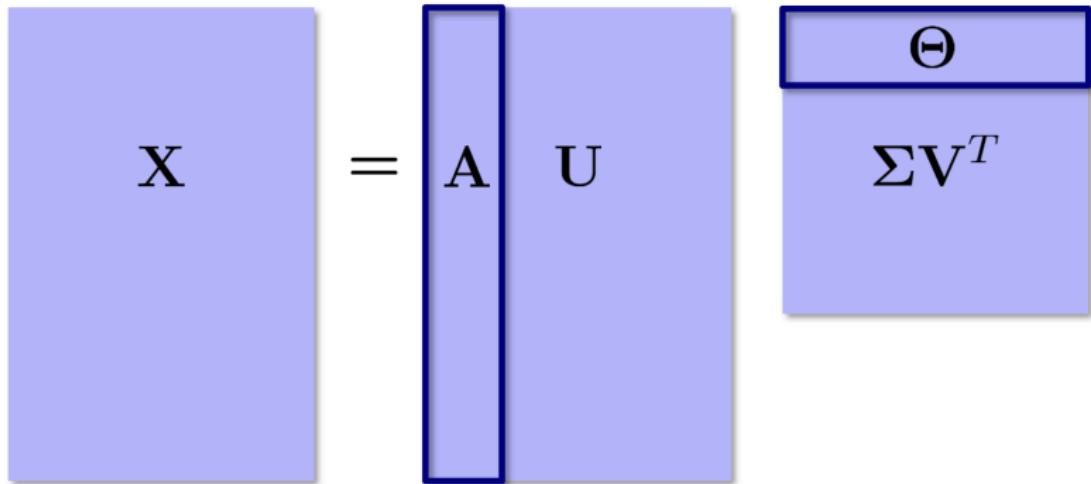
We can instead compute the SVD of matrix  $\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^\top$  and we also have

$$\mathbf{A} = [\mathbf{u}_1, \dots, \mathbf{u}_k].$$

- ▶ Computing PCA via SVD can be more favorable, as it can be more **numerically reliable** than eigen decomposition.
- ▶ It might also **save computation time** as we do not need to compute  $\mathbf{S} = \mathbf{X}\mathbf{X}^\top$ , which can be expensive when  $\mathbf{X}$  is a large matrix.

## PCA via SVD: Illustration

$$\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^T$$



# PCA From the Matrix Factorization Perspective

Recall the (first form) PCA (we assume without loss of generality that  $\mu = 0$ )

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}, \{\boldsymbol{\theta}_i\}}{\text{minimize}} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{A}\boldsymbol{\theta}_i\|_2^2.$$

It can be written in a matrix form:

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}, \boldsymbol{\Theta}}{\text{minimize}} \|\mathbf{X} - \mathbf{A}\boldsymbol{\Theta}\|_F^2$$

where  $\mathbf{A} \in \mathbb{R}^{d \times k}$  and  $\boldsymbol{\Theta} \in \mathbb{R}^{k \times n}$ , and  $\|\cdot\|_F$  is the **Frobenius norm**.

- ▶ The above problem is also called **low-rank matrix factorization**.
- ▶ **Interpretation:** Factorize  $\mathbf{X}$  into two factors' multiplication, where the latter is a **low-rank matrix**.

# PCA From the Matrix Factorization Perspective

Low-rank matrix factorization

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}, \Theta}{\text{minimize}} \|\mathbf{X} - \mathbf{A}\Theta\|_F^2$$

- ▶ Calculate the SVD of  $\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^\top$ .

Solution from PCA

- ▶ One optimal solution to the above (low-rank) matrix factorization problem is given by

$$\mathbf{A} = [\mathbf{u}_1, \dots, \mathbf{u}_k], \quad \Theta = [\sigma_1 \mathbf{v}_1, \dots, \sigma_k \mathbf{v}_k]^\top$$

- ▶ It has infinitely many equivalent optimal solutions.

It is a **closed-form solution** to a nonconvex optimization problem.

# More General Matrix Factorization

We can also remove the orthogonal constraint on  $\mathbf{A}$  to allow more flexibility

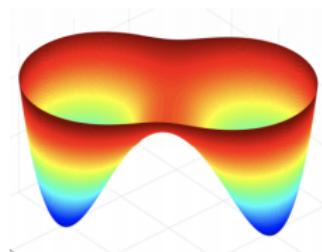
$$\underset{\mathbf{A} \in \mathbb{R}^{d \times k}, \Theta \in \mathbb{R}^{k \times n}}{\text{minimize}} \quad \|\mathbf{X} - \mathbf{A}\Theta\|_F^2.$$

One optimal solution to the above (low-rank) matrix factorization problem is given by

$$\mathbf{A} = [\sqrt{\sigma_1} \mathbf{u}_1, \dots, \sqrt{\sigma_k} \mathbf{u}_k], \quad \Theta = [\sqrt{\sigma_1} \mathbf{v}_1, \dots, \sqrt{\sigma_k} \mathbf{v}_k]^\top,$$

and it has infinitely many equivalent optimal solution.

- ▶ A nonconvex optimization problem



- ▶ Fortunately, closed-form solution exists.

# LoRA: Low-rank Adaptation

In the **post-training** stage of large models (like large language models), we often need to learn an incremental to the learned model to incorporate new knowledge. That is

$$\underset{\Delta\Theta \in \mathbb{R}^{m \times n}}{\text{minimize}} \quad \mathcal{L}(\widehat{\Theta} + \Delta\Theta)$$

**Low-rank Adaptation (LoRA)** uses the simple idea of PCA. It does not aim to learn the full  $\Delta\Theta$ , it instead learns a **PCA decomposition** of  $\Delta\Theta$ .

$$\underset{\mathbf{A} \in \mathbb{R}^{m \times r}, \mathbf{B} \in \mathbb{R}^{r \times n}}{\text{minimize}} \quad \mathcal{L}(\widehat{\Theta} + \mathbf{AB})$$

where  $r \ll \min\{m, n\}$ .

- ▶ LoRA approach can **save computation memory**.
- ▶ It is now widely utilized in large language models.
- ▶ We will use LoRA in our final project.

Dimensionality Reduction

Principal Component Analysis (PCA)

Apply PCA to Real Image Dataset

# The ORL Database of Faces



- ▶ 40 persons.
- ▶ Each has 10 distinct face images.
- ▶ Each image is of size  $92 \times 112$ .
- ▶ The images were taken at different times, varying the lighting, facial expressions (open / closed eyes, smiling / not smiling) and facial details (glasses / no glasses).

# Form the Data Matrix



vectorize  $\xrightarrow{} \mathbf{x}_i = \begin{bmatrix} \mathbf{x}_i[1] \\ \vdots \\ \mathbf{x}_i[92 \times 112] \end{bmatrix} \in \mathbb{R}^{10304}$

- ▶ Do the same thing for all the face images, we get

$$\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{d \times n},$$

where  $d = 10304$ ,  $n = 10 \times 40 = 400$ .

# Apply PCA to $\mathbf{X}$ with $k = 40$

Perform PCA, i.e., solving

$$\underset{\mathbf{A}^\top \mathbf{A} = \mathbf{I}, \Theta}{\text{minimize}} \|\mathbf{X} - \mathbf{A}\Theta\|_F^2$$

We get the **extracted features** (i.e.,  $\mathbf{A} \in \mathbb{R}^{d \times k}$ )



where we resize each column of  $\mathbf{A}$  (of dimension  $d = 10304$ ) to a  $92 \times 112$  image and show it.

# Application

$$\mathbf{x}_i = \mathbf{A}\boldsymbol{\theta}_i$$



- ▶ Each face image  $\mathbf{x}_i$  can be interpreted as a linear combination of the columns in  $\mathbf{A}$ .
- ▶ The importance of each feature is implied in  $\boldsymbol{\theta}_i$ .
- ▶  $\mathbf{x}_i \in \mathbb{R}^d$  ( $d = 10304$  here) has been nicely represented by a  $k$ -dimensional vector  $\mathbf{A}\boldsymbol{\theta}_i$  ( $k = 40$  here) — Dimensionality reduction.

~~ Next lecture: Unsupervised learning: Clustering and k-means.