Principal Component Analysis

Motivation: dimensionality reduction

- It takes $n \times d$ memory to store data $\{x_i\}_{i=1}^n$ with $x_i \in \mathbb{R}^d$
- But many real data have patterns that repeat over samples. Can we find some patterns and use them?

d=32x32pixels per image

n images

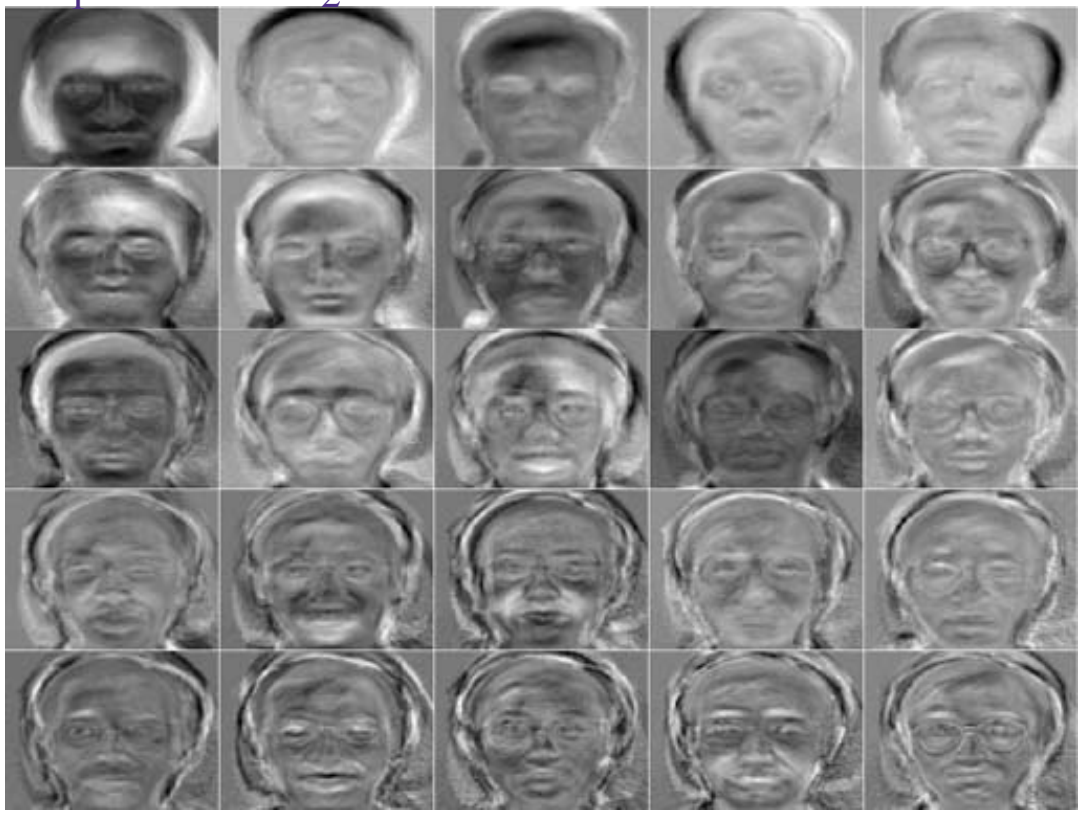
$d \times n$ real values to store the data

Principal component analysis finds a compact linear representation

- patterns that capture the distinct features of the samples is called **principal component** (to be formally defined later)
-

Principal components:

$u_1 \in \mathbb{R}^d$ u_2



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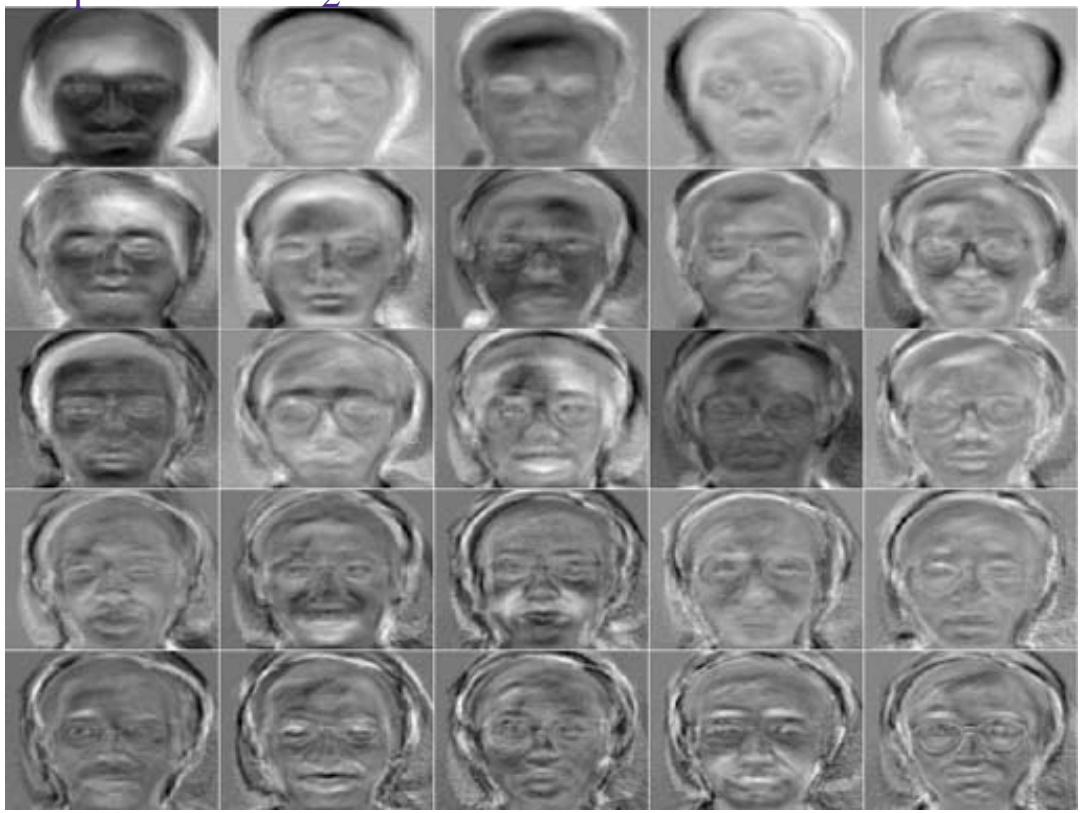

$$\approx a[1]u_1 + a[2]u_2 + \cdots + a[25]u_{25}$$

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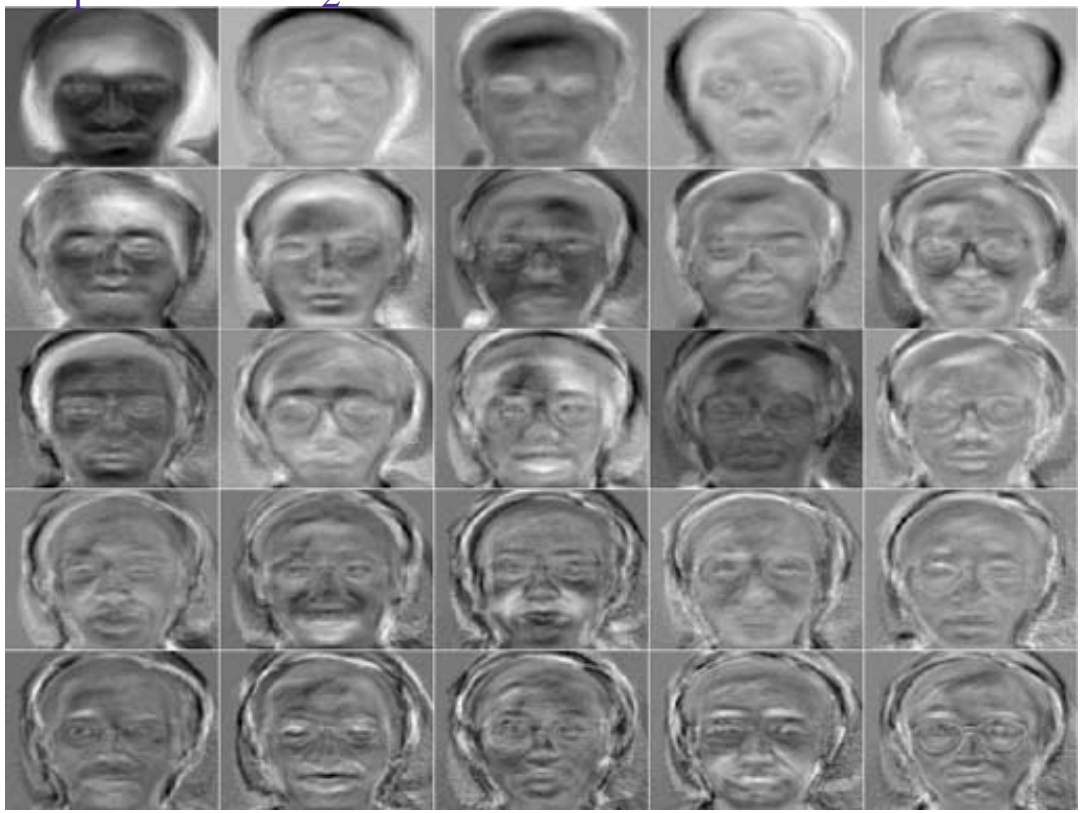

$$\approx a[1]u_1 + a[2]u_2 + \cdots + a[25]u_{25}$$

- With q=25, to store n images, it requires memory of only $d \times q + q \times n \ll d \times n$

10 principal components give a pretty good reconstruction of a face

average face $\bar{x} + a[1]u_1$ $\bar{x} + a[1]u_1 + a[2]u_2$

Ground truths real face

PCA: a high-fidelity linear projection

$V_q : d \times q$

Given $x_1, \ldots, x_n \in \mathbb{R}^d$, for $q \ll d$ find a compressed representation with $\lambda_1, \ldots, \lambda_n \in \mathbb{R}^q$ such that $x_i \approx \mu + \mathbf{V}_q \lambda_i$ and $\mathbf{V}_q^T \mathbf{V}_q = I$

$$\min_{\mu, \mathbf{V}_q, \{\lambda_i\}_i} \sum_{i=1}^{n} \|x_i - \mu - \mathbf{V}_q \lambda_i\|_2^2$$

PCA: a high-fidelity linear projection

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$$\mu = \bar{x} = \tfrac{1}{n} \textstyle\sum_{i=1}^{n} x_i$$

$$\lambda_i = \mathbf{V}_q^T (x_i - \bar{x})$$

$$\widehat{x}_i := \bar{x} + \mathbf{V}_q \mathbf{V}_q^\top (x_i - \bar{x}) = \bar{x} + \sum_{j=1}^{q} v_j \langle v_j, x_i - \bar{x} \rangle$$

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$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

$\mathbf{V}_q \mathbf{V}_q^T$ is a *projection matrix* that minimizes error in basis of size q

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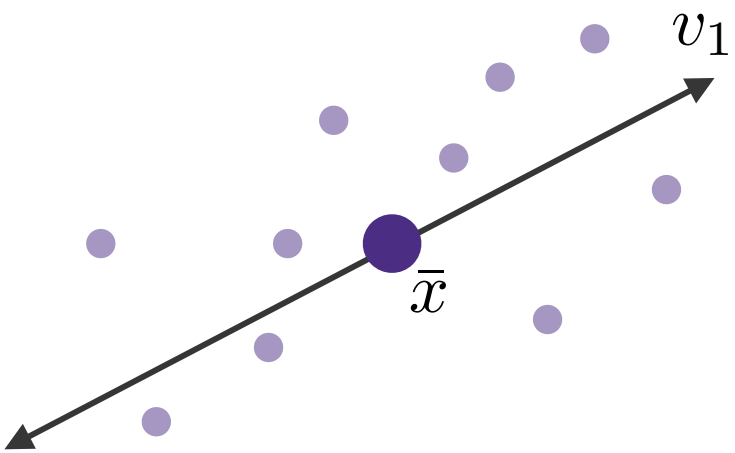
Case when $q = 1$

$$v_1 = \arg \min_{v : \|v\|_2 = 1} \sum_{i=1}^{N} \|(x_i - \bar{x}) - v v^\top (x_i - \bar{x})\|_2^2$$



PCA: a high-fidelity linear projection

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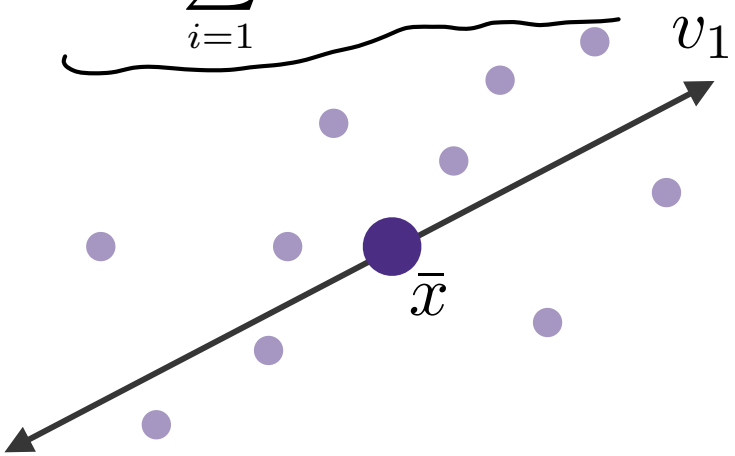
$$= \arg \min_{v:\|v\|_2=1} \sum_{i=1}^{N} \|x_i - \bar{x}\|_2^2 - 2(x_i - \bar{x})^\top vv^\top (x_i - \bar{x}) + (x_i - \bar{x})^\top vv^\top vv^\top (x_i - \bar{x})$$

$$= \arg \min_{v:\|v\|_2=1} \sum_{i=1}^{N} \|x_i - \bar{x}\|_2^2 - \sum_{i=1}^{N} (x_i - \bar{x})^\top vv^\top (x_i - \bar{x})$$

$$= \arg \max_{v:\|v\|_2=1} \sum_{i=1}^{N} (x_i - \bar{x})^\top vv^\top (x_i - \bar{x})$$

$$= \arg \max_{v:\|v\|_2=1} v^\top \Sigma v$$

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$



power method
conjugate gradient

PCA: a high-fidelity linear projection

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

$\mathbf{V}_q \mathbf{V}_q^T$ is a *projection matrix* that minimizes error in basis of size q

$$\widehat{x}_i := \bar{x} + \mathbf{V}_q \mathbf{V}_q^\top (x_i - \bar{x}) = \bar{x} + \sum_{j=1}^{q} v_j \langle v_j, x_i - \bar{x} \rangle$$

$\Leftarrow$ $\max Tr(V_q^T \Sigma V_q)$

General $q \geq 1$

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2 = \min_{\mathbf{V}_q} Tr(\Sigma) - Tr(\mathbf{V}_q^T \Sigma \mathbf{V}_q)$$

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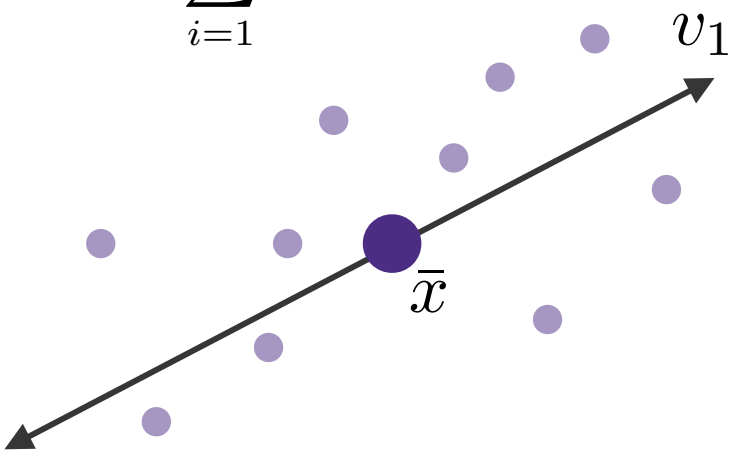


$\mathbf{V}_q$ are the first q eigenvectors of Σ

Minimize reconstruction error and capture the most variance in your data.

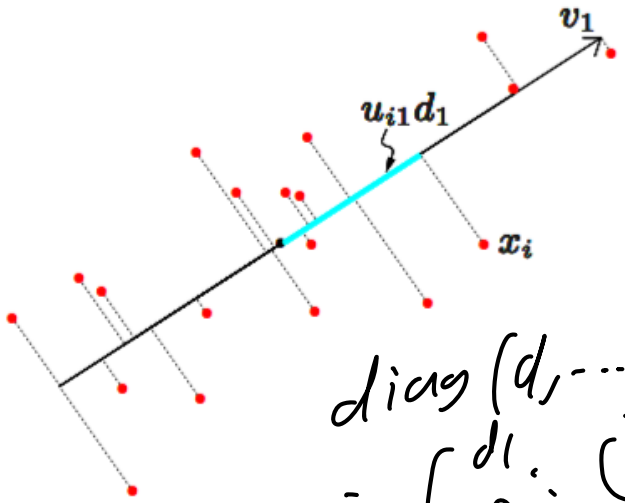
PCA: a high-fidelity linear projection

Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

where $\mathbf{V}_q = [v_1, v_2, \ldots, v_q]$ is orthonormal:

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$



$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

Principal Component Analysis (PCA) projects $(\mathbf{X} - \mathbf{1}\bar{x}^T)$ down onto $\mathbf{V}_q$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U}_q \mathrm{diag}(d_1, \ldots, d_q) \qquad \mathbf{U}_q^T \mathbf{U}_q = I_q$$

$\mathbf{X}$: n x d

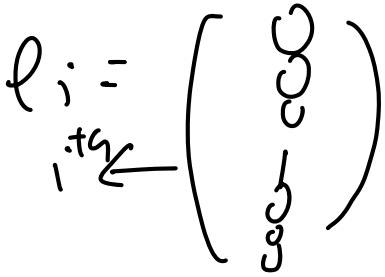
$\mathbf{V}_q$: d x q: top q eigenvectors of Σ

$\mathbf{U}_q$: n x q: top q eigenvectors of $(\mathbf{X}-\mathbf{1}\bar{x}^T)(\mathbf{X}-\mathbf{1}\bar{x}^T)^T$ (n x n)

$\mathbf{U}_q$: n x q

$\mathrm{diag}(d_1, \ldots d_q) = \begin{pmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_q \end{pmatrix}$: q x q

Singular Value Decomposition (SVD)



$S^2 = \begin{pmatrix} s_{11}^2 & & 0 \\ & \ddots & \\ 0 & & s_{rr}^2 \end{pmatrix}$ $\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$ U: $m \times r$, V: $n \times r$

Theorem (SVD): Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $\mathbf{A} = \mathbf{USV}^T$ where $\mathbf{S} \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

$r \times r$ $r \times r$

$A = X - 1\bar{x}^T$, $X - 1\bar{x}^T = U_q \begin{pmatrix} d_1 & & \\ & \ddots & \\ & & d_q \end{pmatrix} V_q^T$

$\mathbf{A}^T\mathbf{A}v_i = (USV^T)^T(USV^T) \cdot v_i = VSU^TUSV^T v_i$

v_i: i^{th} column of V

$= VS^2V^Tv_i$

$= VS^2 e_i$

$= V \cdot e_i \cdot s_{ii}^2 = s_{ii}^2 \cdot v_i$

$\mathbf{AA}^T u_i = s_{ii}^2 u_i$

scalar

def of eigenvector of Σ

$\Sigma v = \lambda \cdot v$

λ: scalar

Singular Value Decomposition (SVD)

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$$\mathbf{A}^T\mathbf{A}v_i = \mathbf{S}_{i,i}^2 v_i$$

$$\mathbf{A}\mathbf{A}^T u_i = \mathbf{S}_{i,i}^2 u_i$$

$\mathbf{V}$ are the first r eigenvectors of $\mathbf{A}^T\mathbf{A}$ with eigenvalues $\text{diag}(\mathbf{S})$
$\mathbf{U}$ are the first r eigenvectors of $\mathbf{A}\mathbf{A}^T$ with eigenvalues $\text{diag}(\mathbf{S})$

Linear projections

Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

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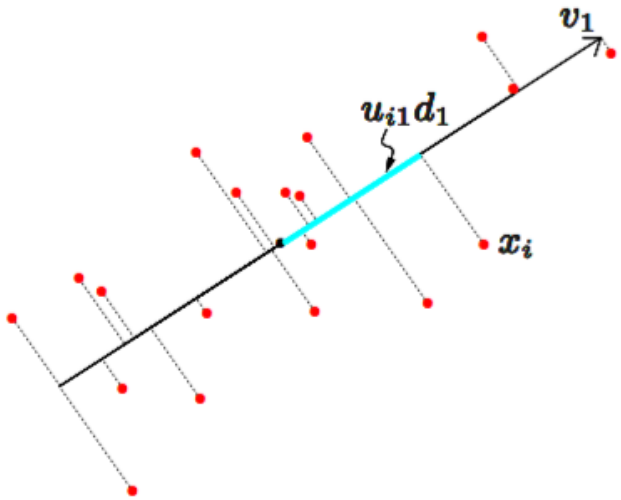

where $\mathbf{V}_q = [v_1, v_2, \ldots, v_q]$ is orthonormal:

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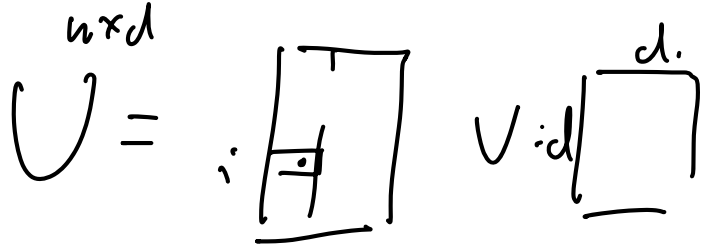
Singular Value Decomposition defined as

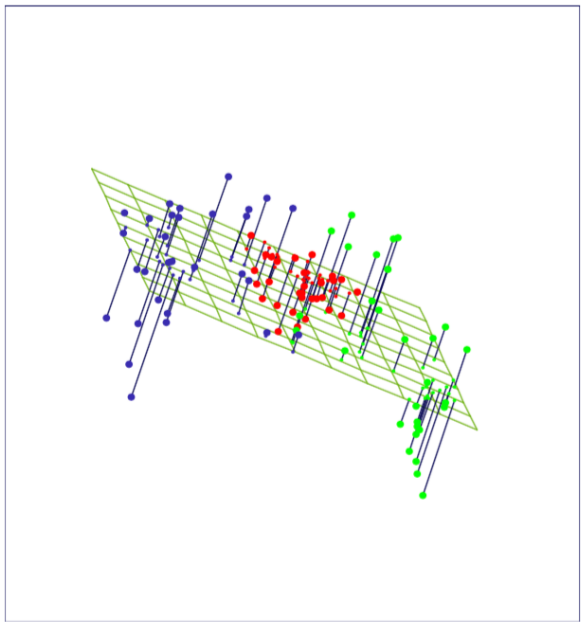
$$\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$$

Dimensionality reduction



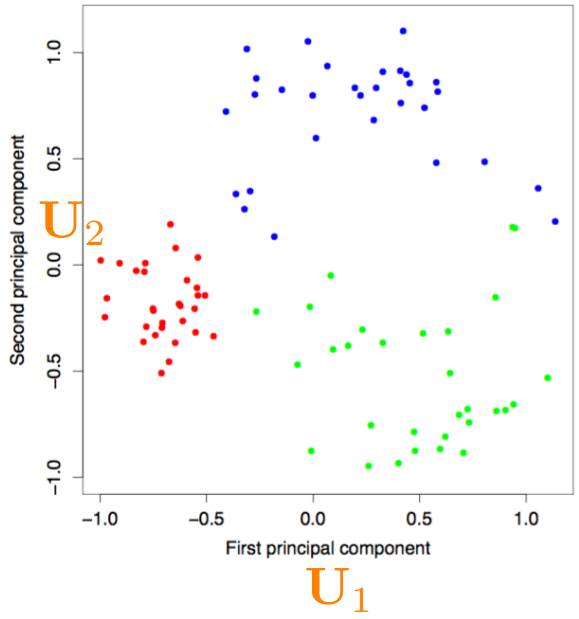
$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{USV}^T$

$x_i \approx \bar{x} + U_{1i} \cdot S_{11} \cdot V_1 + U_{2i} S_{22} \cdot V_2$



$\mathbf{X} - \mathbf{1}\bar{x}^T$

3D



→ 2D

Dimensionality reduction

choose r PC

$$\frac{\sum_{i=1}^{r} S_{ii}}{\sum_{i=1}^{d} S_{ii}} \geq 80\%$$

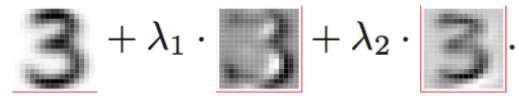
$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{USV}^T$

Handwritten 3's, 16x16 pixel image so that $x_i \in \mathbb{R}^{256}$

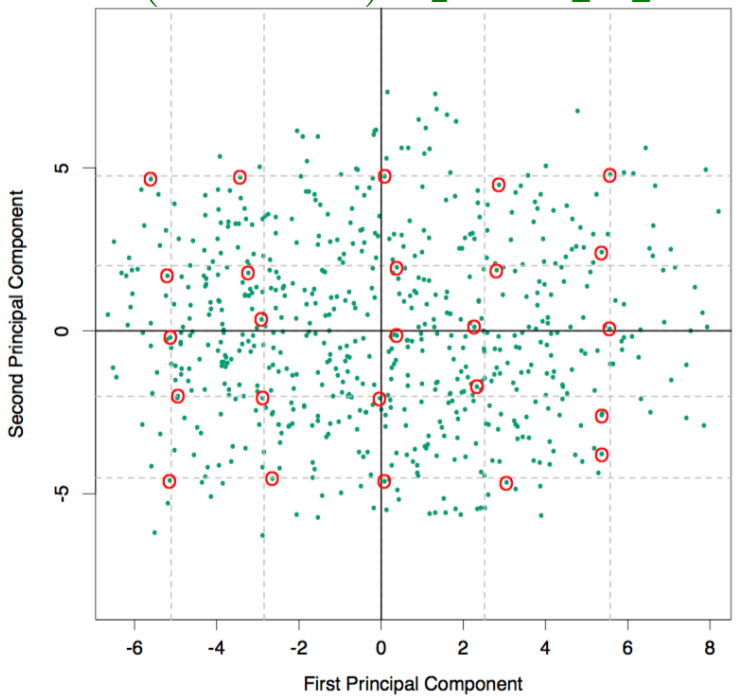
random X

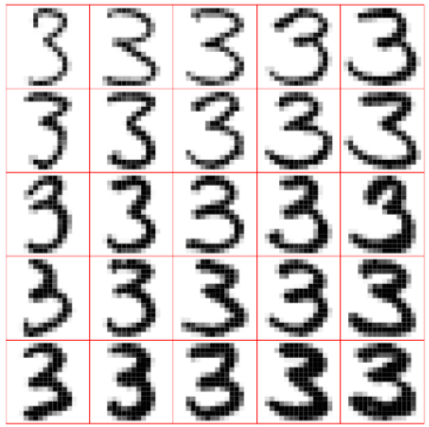
$X_{ij} \sim N(0,1)$

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$



$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_2 = \mathbf{U}_2\mathbf{S}_2 \in \mathbb{R}^{n\times 2}$$





$\mathrm{diag}(\mathbf{S})$

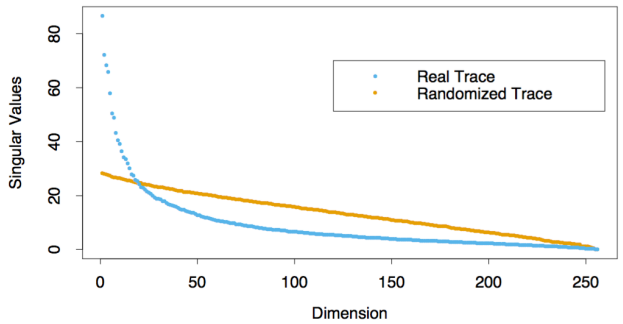
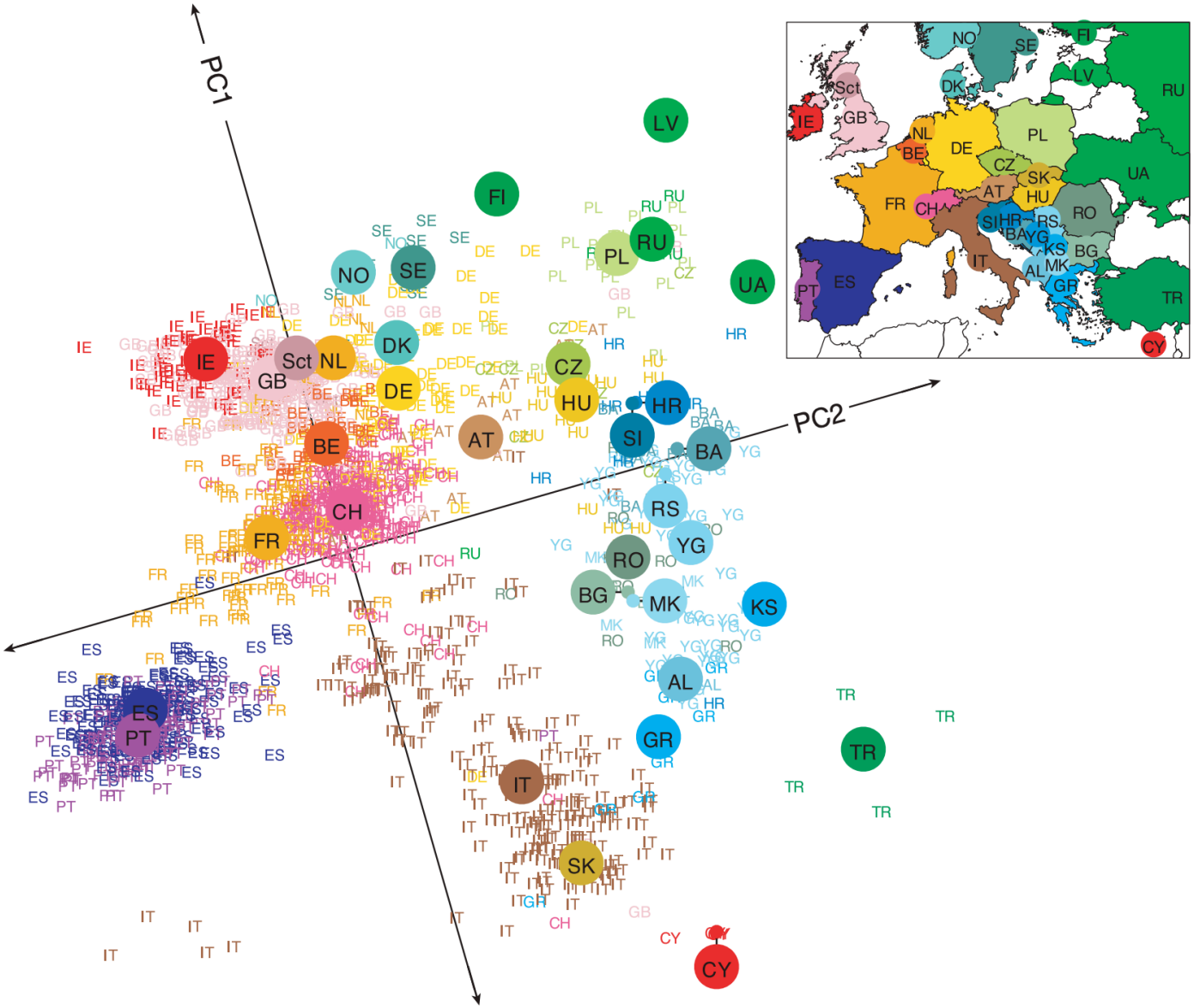


FIGURE 14.24. *The 256 singular values for the digitized threes, compared to those for a randomized version of the data (each column of* $\mathbf{X}$ *was scrambled).*

Dimensionality reduction



Novembre, et al, “Genes mirror geography within Europe” Nature 2008.

Kernel PCA

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U_q}\mathbf{S_q} \in \mathbb{R}^{n \times q}$$

$\langle x_i, x_j \rangle \rightarrow K(x_i, x_j)$

$(I - \frac{2\mathbf{1}^T}{n})X = X - \mathbf{1}\cdot\frac{\mathbf{1}^T X}{n}$

$= X - \mathbf{1}\cdot\bar{x}$

$\mathbf{JX} = \mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T \qquad \mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n$

$(\mathbf{JX})(\mathbf{JX})^T = JXX^TJ$

$XX^T \rightarrow K \in \mathbb{R}^{n \times n}$

$K_{ij} = K(x_i, x_j)$

$\rightarrow JKJ$

$= JUSV^TV^TSUJ$

$= JUS^2UJ$

Kernel PCA

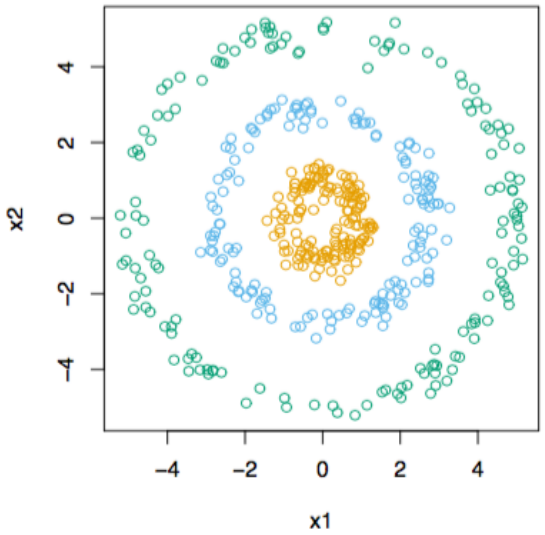
$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

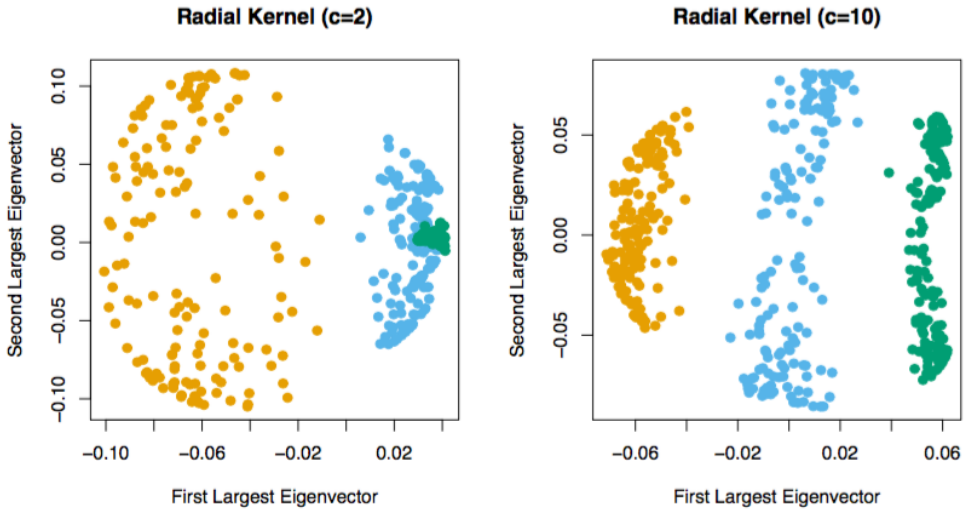
$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U_q}\mathbf{S_q} \in \mathbb{R}^{n \times q}$$

$$\mathbf{J}\mathbf{X} = \mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T \qquad \mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n$$

$$(\mathbf{J}\mathbf{X})(\mathbf{J}\mathbf{X})^T = \mathbf{U}\mathbf{S}^2\mathbf{U}^T$$

$$K(x_i, x_j) = e^{-\frac{\|x_i - x_j\|_2^2}{2\sigma^2}}$$





Random projections

PCA finds a low-dimensional representation that reduces population variance

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

$\mathbf{V}_q \mathbf{V}_q^T$ is a *projection matrix* that minimizes error in basis of size q

$\mathbf{V}_q$ are the first q eigenvectors of Σ

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

But what if I care about the reconstruction of the *individual* points?

$$\min_{\mathbf{W}_q} \max_{i=1,\ldots,n} ||(x_i - \bar{x}) - \mathbf{W}_q \mathbf{W}_q^T (x_i - \bar{x})||^2$$

Random projections

$$\min_{\mathbf{W}_q} \max_{i=1,\ldots,n} ||(x_i - \bar{x}) - \mathbf{W}_q \mathbf{W}_q^T (x_i - \bar{x})||^2$$

$d \gg k$

Johnson-Lindenstrauss (1983)

Theorem 1.1. *(Johnson-Lindenstrauss) Let* $\epsilon \in (0, 1/2)$. *Let* $Q \subset \mathbb{R}^d$ *be a set of* n *points and* $k = \frac{20 \log n}{\epsilon^2}$. *There exists a Lipshcitz mapping* $f : \mathbb{R}^d \to \mathbb{R}^k$ *such that for all* $u, v \in Q$:

(independent of d)

$$(1 - \epsilon)\|u - v\|^2 \leq \|f(u) - f(v)\|^2 \leq (1 + \epsilon)\|u - v\|^2$$

Random projections

$$\min_{\mathbf{W}_q} \max_{i=1,\ldots,n} ||(x_i - \bar{x}) - \mathbf{W}_q \mathbf{W}_q^T (x_i - \bar{x})||^2$$

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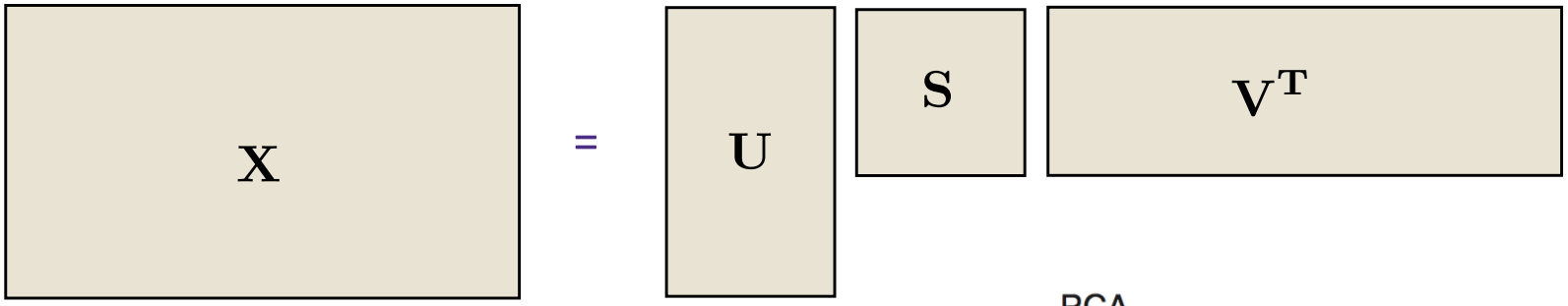
$$(1 - \epsilon)\|u - v\|^2 \leq \|f(u) - f(v)\|^2 \leq (1 + \epsilon)\|u - v\|^2$$

Theorem 1.2. *(Norm preservation) Let* $x \in \mathbb{R}^d$. *Assume that the entries in* $A \subset \mathbb{R}^{k \times d}$ *are sampled independently from* $N(0, 1)$. *Then,*

$$\Pr((1 - \epsilon)\|x\|^2 \leq \|\frac{1}{\sqrt{k}} Ax\|^2 \leq (1 + \epsilon)\|x\|^2) \geq 1 - 2e^{-(\epsilon^2 - \epsilon^3)k/4}$$

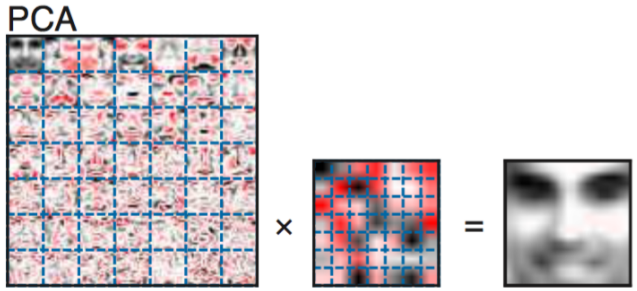
$$f(x) = \frac{1}{\sqrt{k}} A \cdot x$$

Other matrix factorizations



Singular value decomposition

Elements of $\mathbf{U}, \mathbf{S}, \mathbf{V}$ in $\mathbb{R}$



Nonnegative matrix factorization (NMF)

Elements of $\mathbf{U}, \mathbf{S}, \mathbf{V}$ in $\mathbb{R}_+$

S: diagonal.

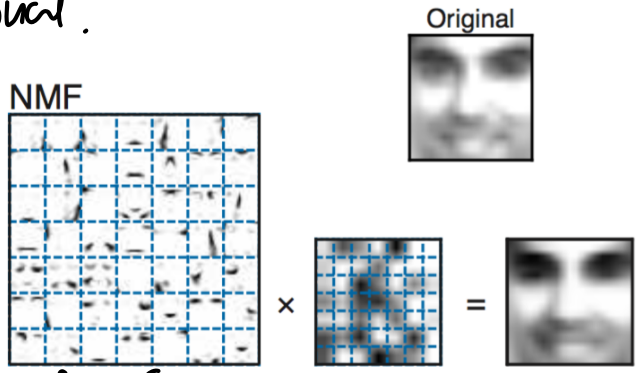
$X \approx U S V^T$,

CX- decomposition

$X \approx C \cdot M$, C: columns of X

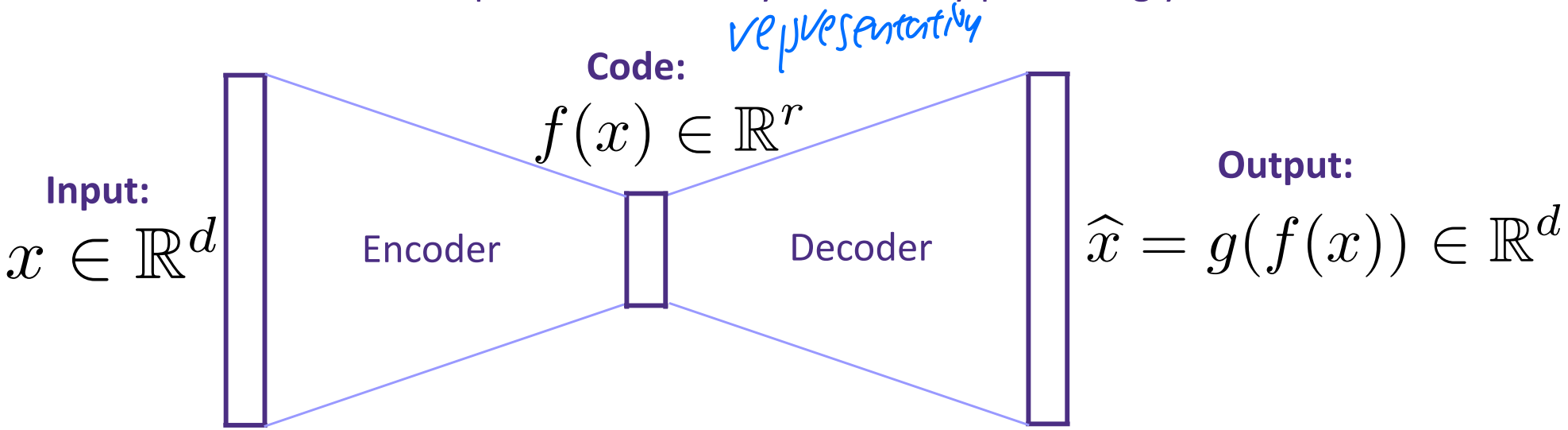
CUR decomposition

$X \approx CUR$



Autoencoders

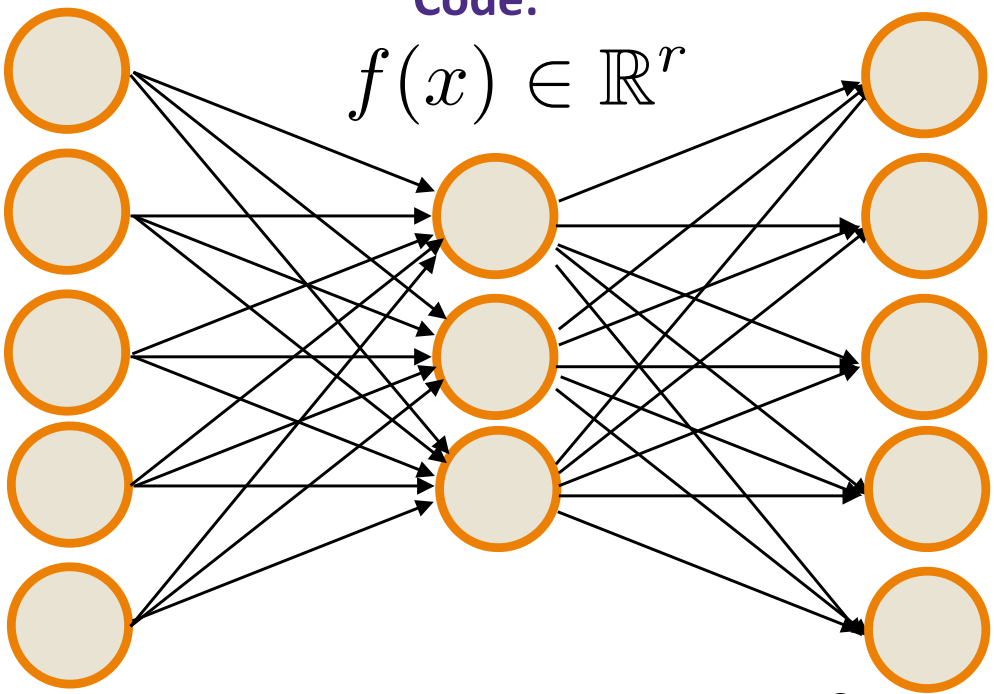
Find a low dimensional representation for your data by predicting your data



$$\underset{f,g}{\text{minimize}} \sum_{i=1}^{n} \|x_i - g(f(x_i))\|_2^2$$

f, g : deep neural network

Autoencoders



Code:

$f(x) \in \mathbb{R}^r$

Input:

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

Output:

$\widehat{x} = g(f(x)) \in \mathbb{R}^d$

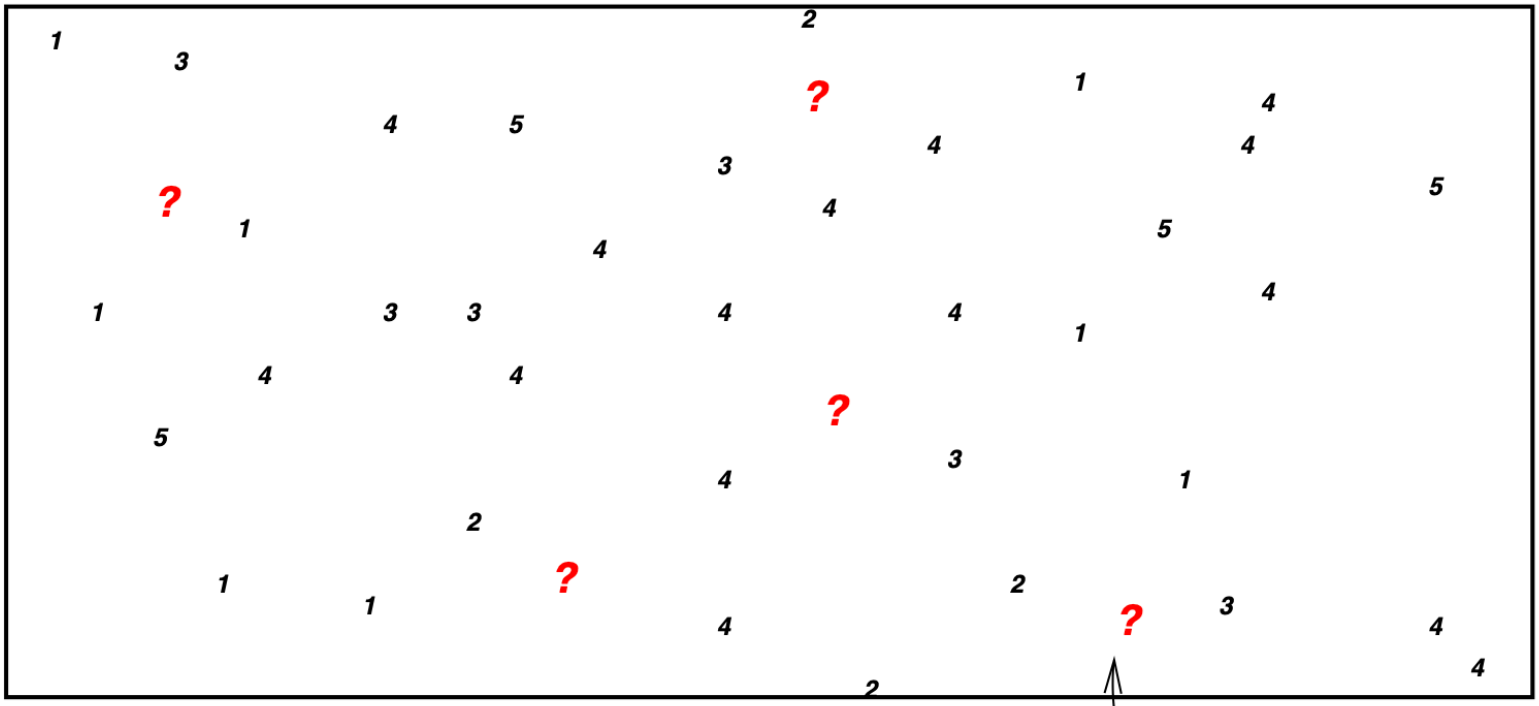
$$\underset{f,g}{\text{minimize}} \sum_{i=1}^{n} \|x_i - g(f(x_i))\|_2^2$$

What if $f(X) = Ax$ and $g(y) = By$?

Matrix Completion

Matrix completion for recommendation systems

Netflix challenge dataset

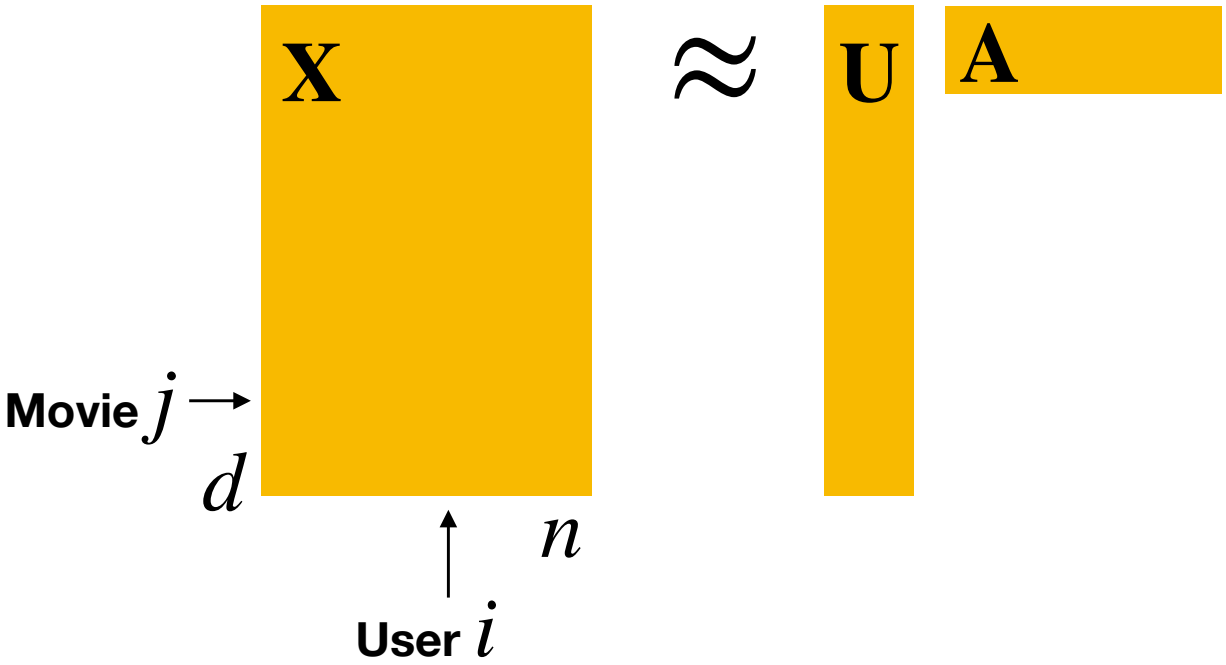


- users provide ratings on a few movies, and we want to predict the missing entries in this ratings matrix, so that we can make recommendations
- without any assumptions, the missing entries can be anything, and no prediction is possible

Matrix completion problem

Matrix completion

- let $\mathbf{X} = [x_1 \quad x_2 \quad \cdots \quad x_n] \in \mathbb{R}^{d \times n}$ be the ratings matrix, and assume it is fully observed, i.e. we know all the entries
- then we want to find $\mathbf{U} \in \mathbb{R}^{d \times r}$ and $\mathbf{A} = [a_1 \quad a_2 \quad \cdots \quad a_n] \in \mathbb{R}^{r \times n}$ that approximates $\mathbf{X}$



- if we **observe all entries** of $\mathbf{X}$, then we can find the best rank-r approximation with SVD

Optimization for Matrix Completion

- a natural approach to fit v_j's and $a_i's$ to given training data is to solve

$$\text{minimize}_{\mathbf{U},\mathbf{A}} \sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} - v_j^T a_i)^2$$

- this can be solved, for example via gradient descent or alternating minimization

Matrix Recovery

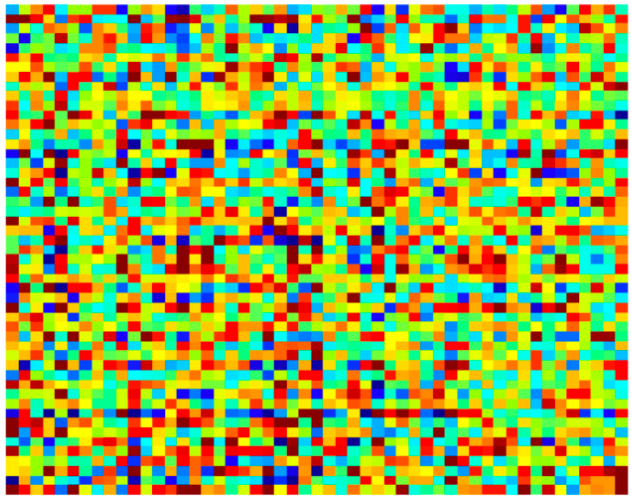
- a natural approach to fit v_j's and $a_i's$ to given training data is to solve

$$\text{minimize}_{\mathbf{U},\mathbf{A}} \sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} - v_j^T a_i)^2$$

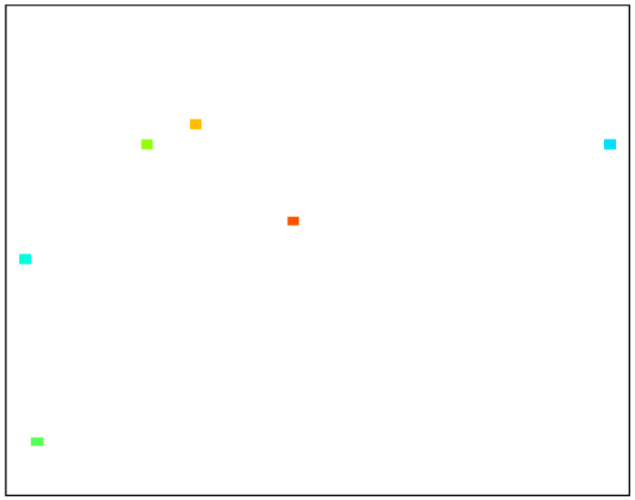
- If X is low rank, why only observe a few (<< dn) entries, we can recover X?

Example: 2000×2000 rank-8 random matrix

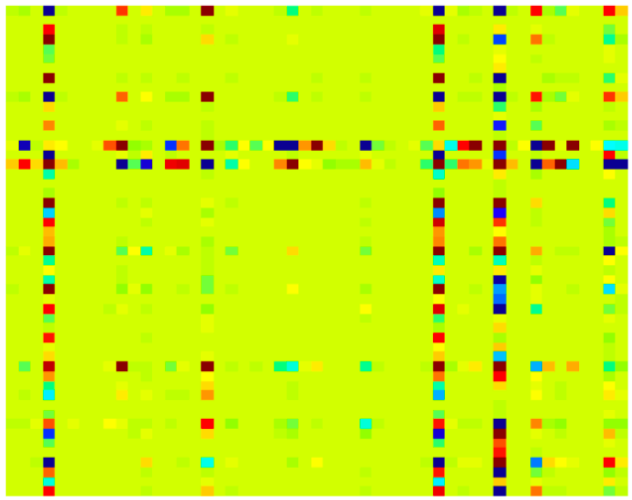
low-rank matrix $\mathbf{X}$



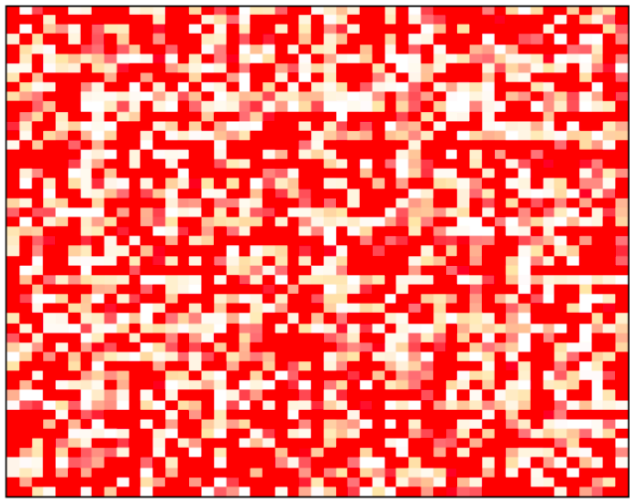
sampled matrix



Gradient descent output $\mathbf{UA}$



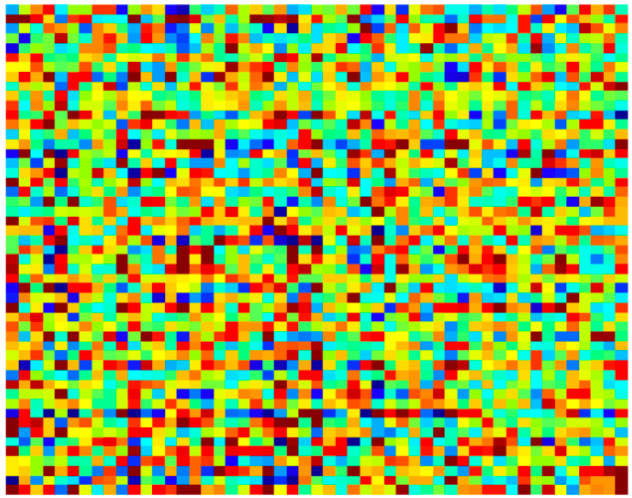
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



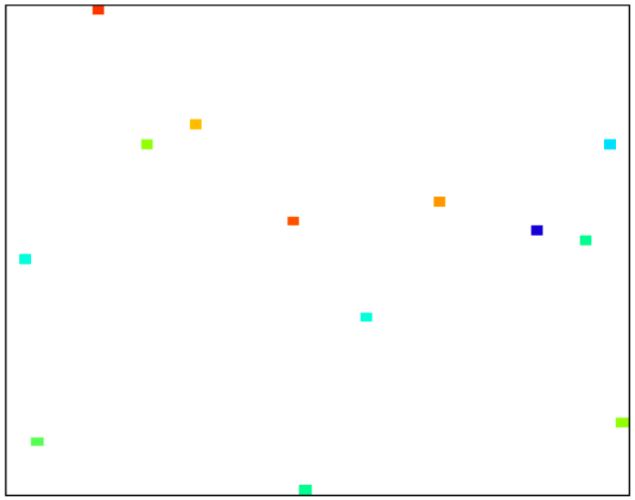
0.25% sampled

Example: 2000×2000 rank-8 random matrix

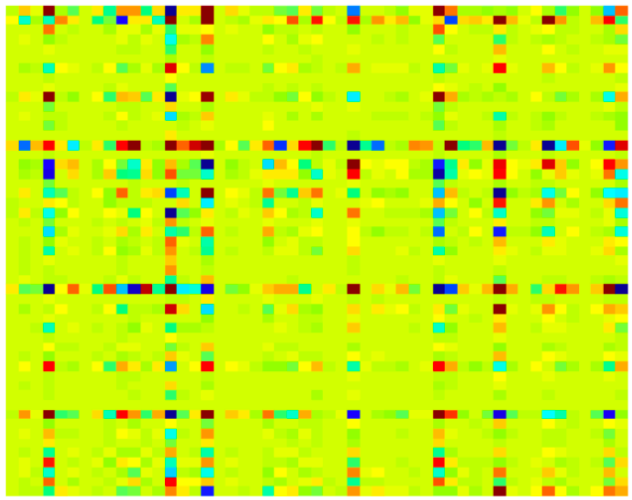
low-rank matrix $\mathbf{X}$



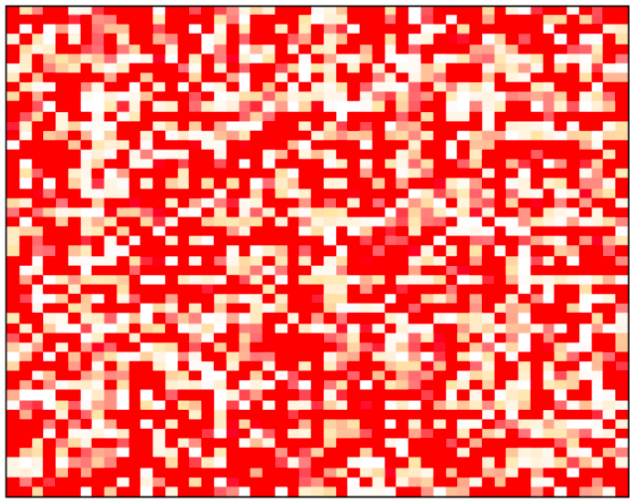
sampled matrix



Gradient descent output $\mathbf{UA}$



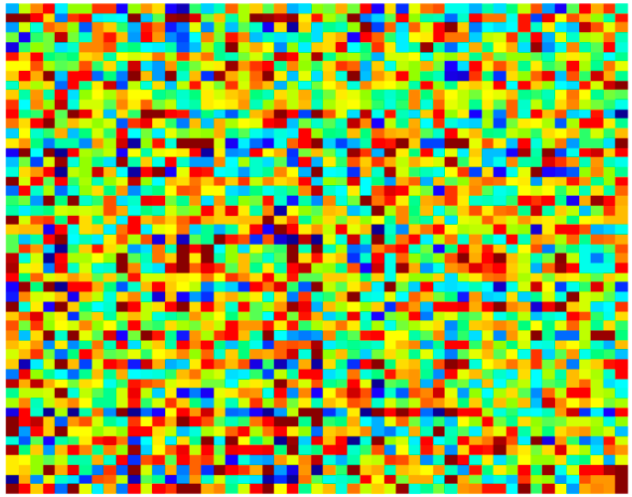
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



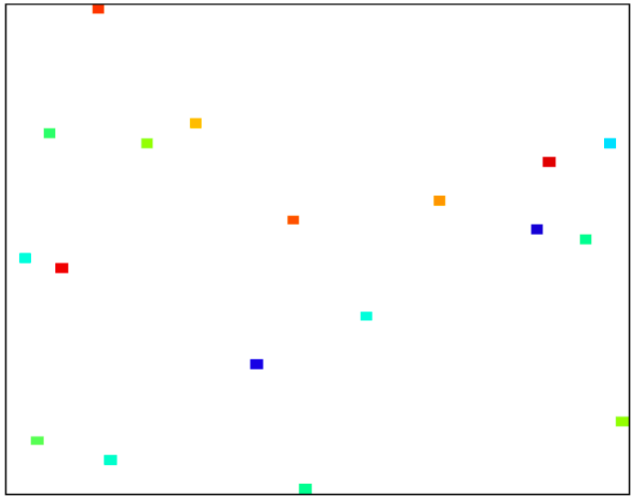
0.50% sampled

Example: 2000×2000 rank-8 random matrix

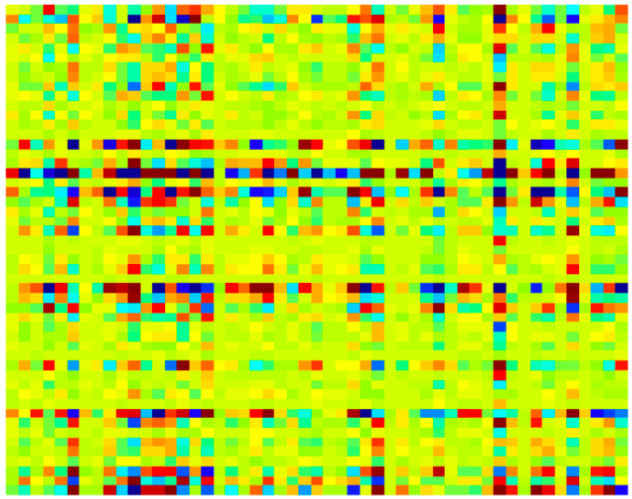
low-rank matrix $\mathbf{X}$



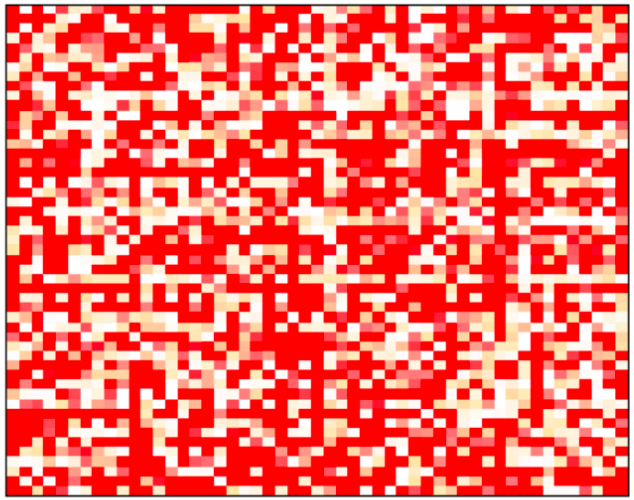
sampled matrix



Gradient descent output $\mathbf{UA}$



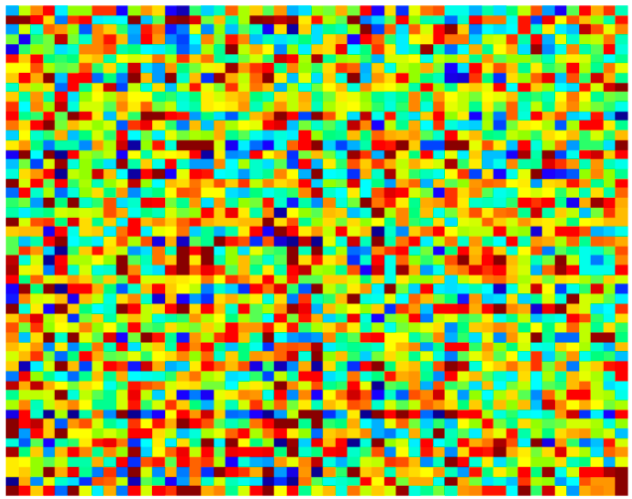
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



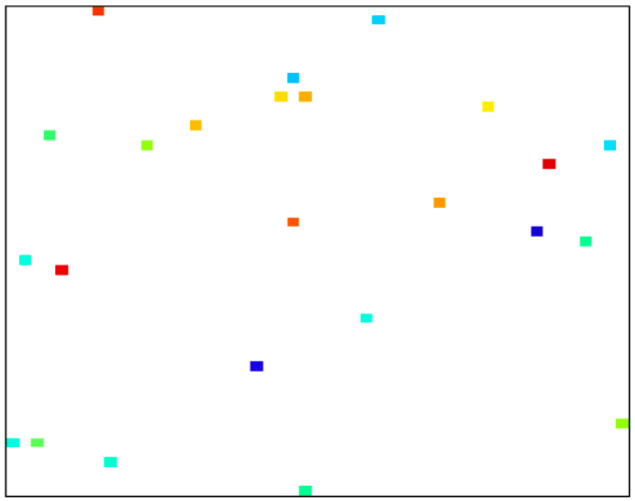
0.75% sampled

Example: 2000×2000 rank-8 random matrix

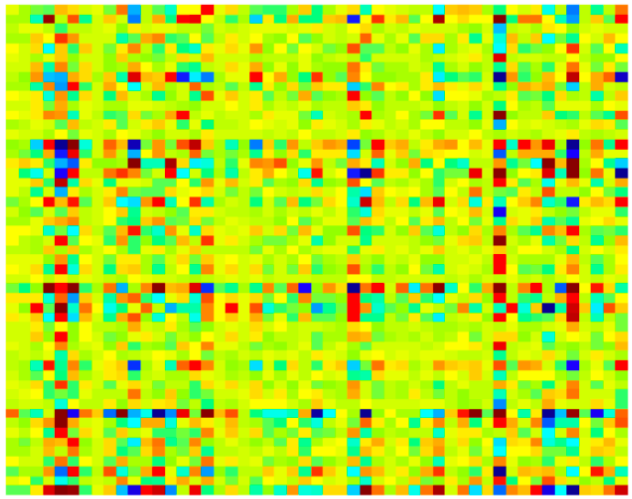
low-rank matrix $\mathbf{X}$



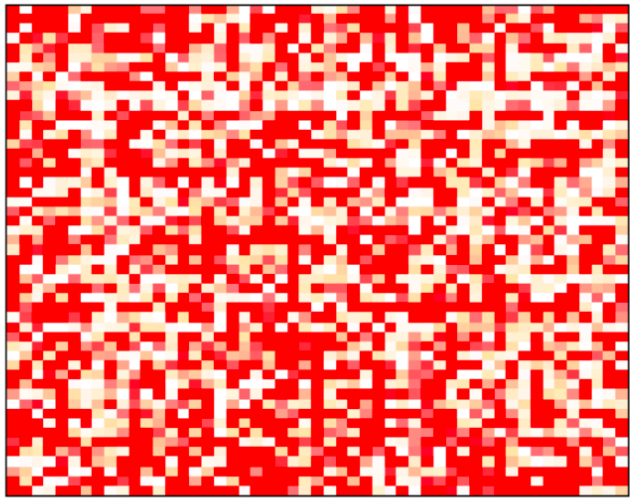
sampled matrix



Gradient descent output $\mathbf{UA}$



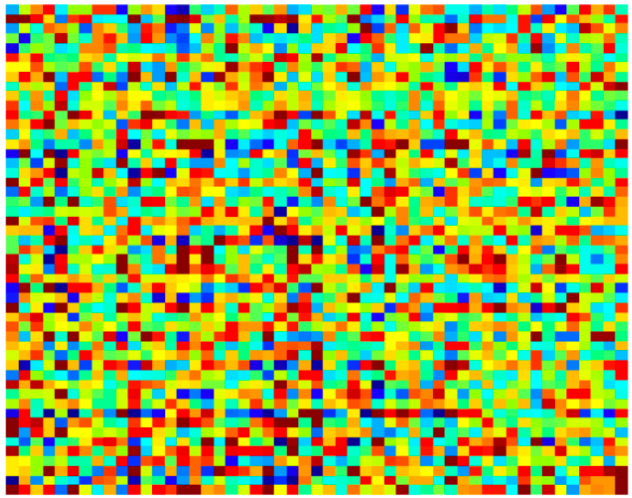
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



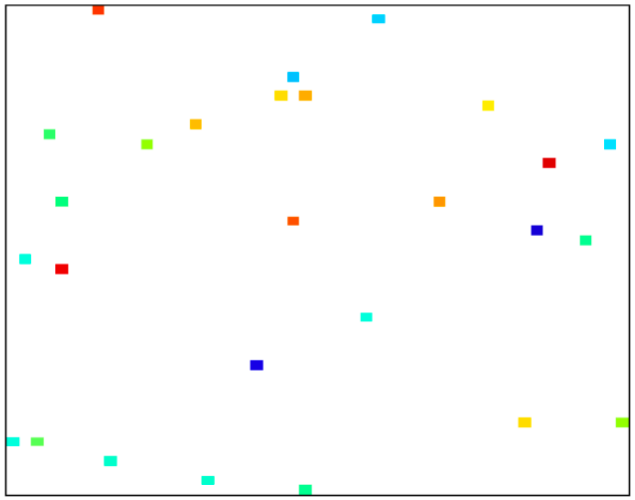
1.00% sampled

Example: 2000×2000 rank-8 random matrix

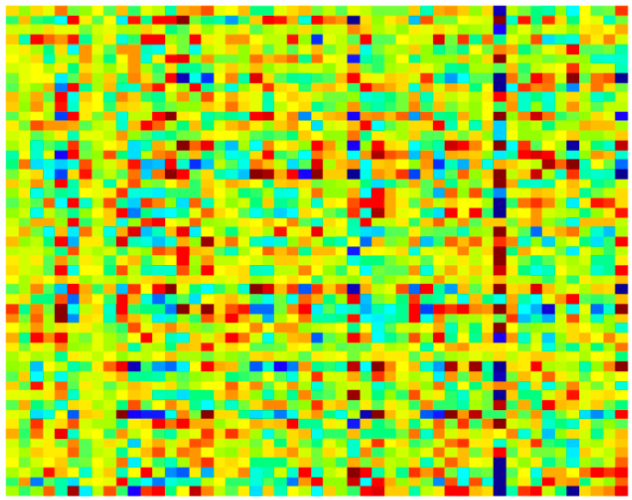
low-rank matrix $\mathbf{X}$



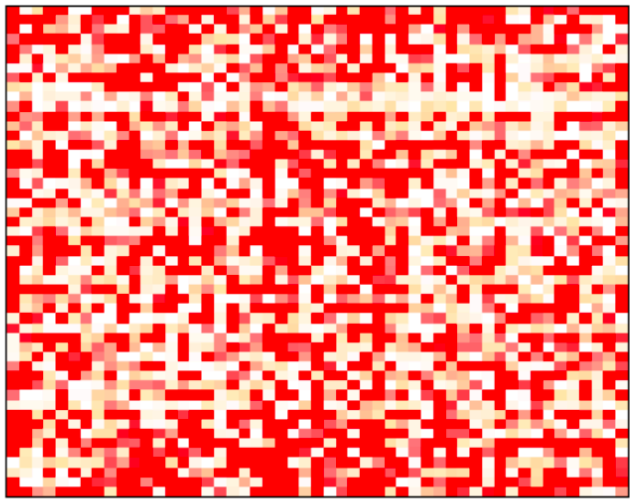
sampled matrix



Gradient descent output $\mathbf{UA}$



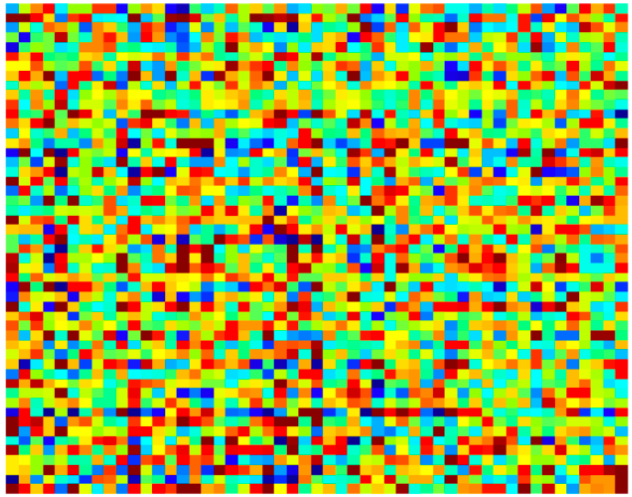
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



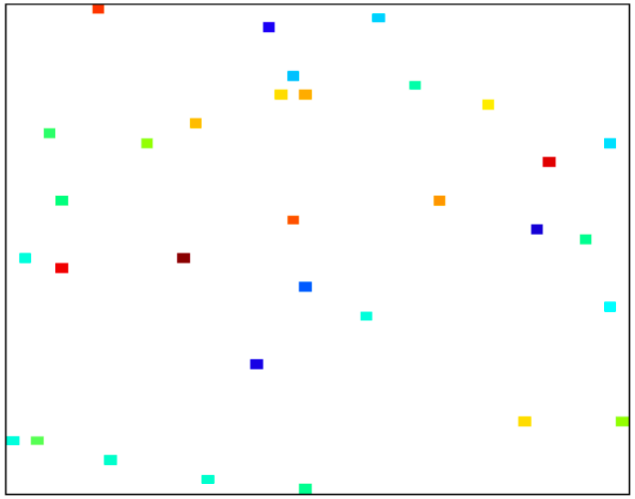
1.25% sampled

Example: 2000×2000 rank-8 random matrix

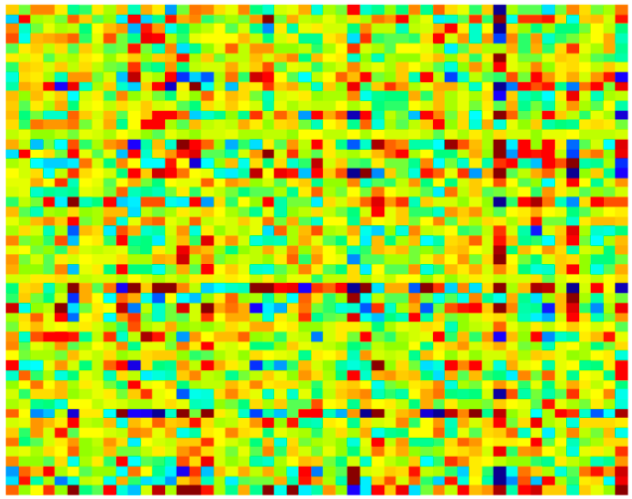
low-rank matrix $\mathbf{X}$



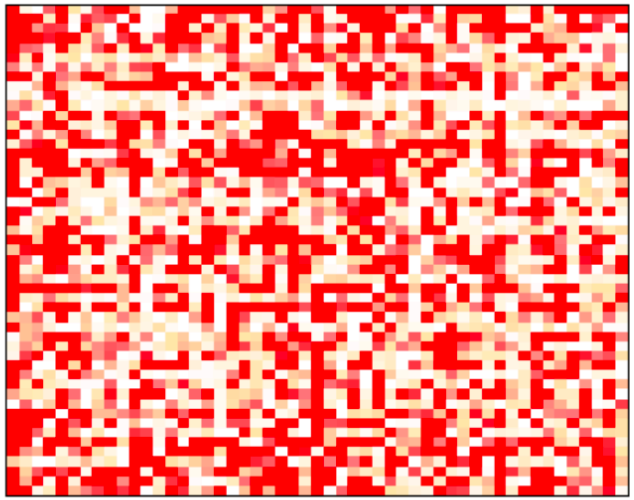
sampled matrix



Gradient descent output $\mathbf{UA}$



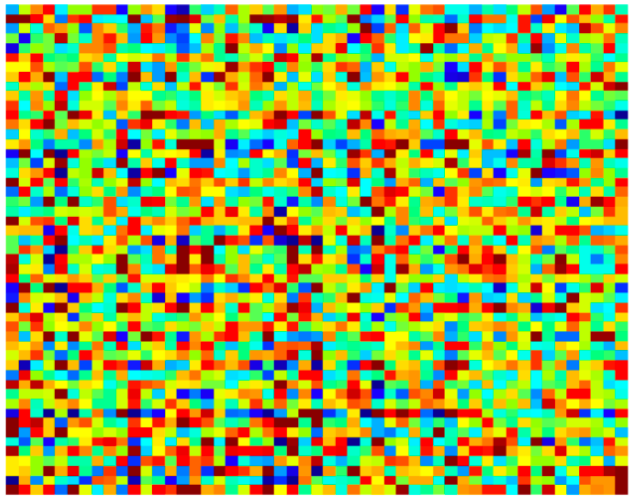
squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



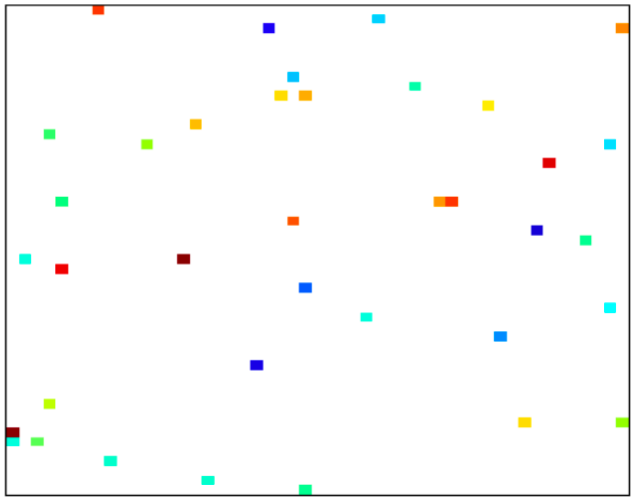
1.50% sampled

Example: 2000×2000 rank-8 random matrix

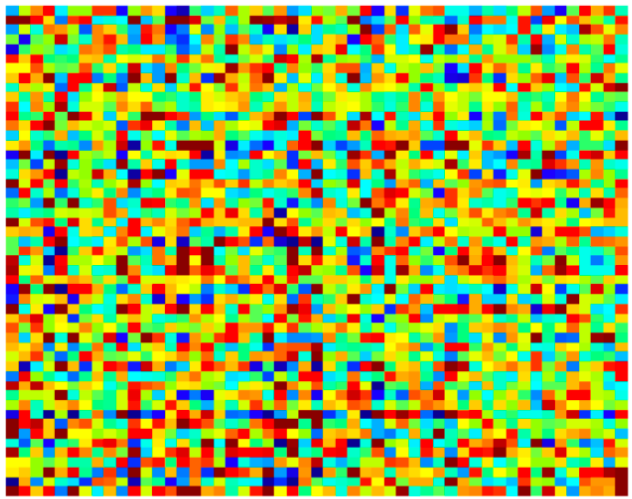
low-rank matrix $\mathbf{X}$



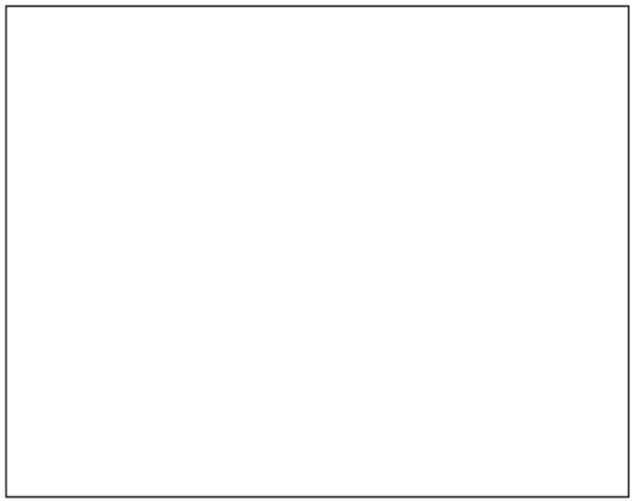
sampled matrix



Gradient descent output $\mathbf{UA}$



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



1.75% sampled