CSE 446
Singular Value Decomposition (SVD)

Natasha Jaques

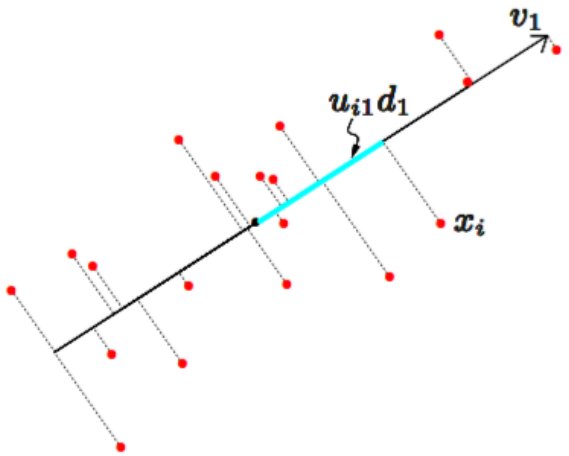
Recap: PCA = Principal Component Analysis

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

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

Minimizing the reconstruction error for a compressed representation of the data

Maximum eigen-space of Σ



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

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

Warm-up: Eigenvalue decomposition

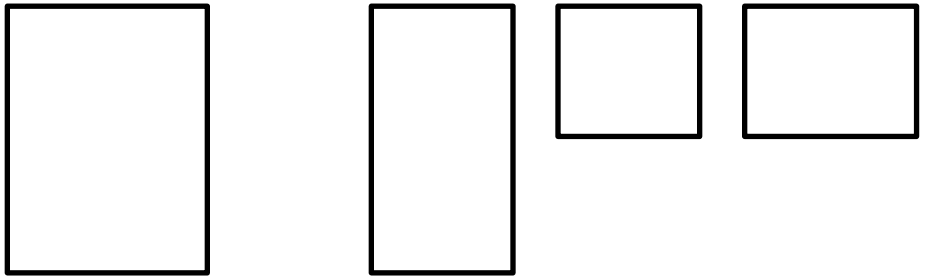
Suppose that a square matrix $A \in \mathbb{R}^{n \times n}$, has
a set of right eigen-vectors $\{v_i \in \mathbb{R}^n\}_{i=1}^n$ and corresponding eigenvalues $\{\lambda_i\}_{i=1}^n$

- $A\, v_1 \;=$
- $A\, [v_1, v_2] \;=$
- Let $V = [v_1, v_2, \ldots, v_n]$, then $A\, V \;=$
- Eigen value decomposition of A is $A \;=$

- Now, suppose A is symmetric, then its eigenvectors are orthonormal, i.e., $V^T V = V V^T = I$, which is equivalent to saying that $v_i^T v_j =$

Singular Value Decomposition (SVD): definition

Theorem [SVD]: Let $A \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $A = USV^T$ where $S \in \mathbb{R}^{r \times r}$ is diagonal with non-negative entries, $U^T U = I$, and $V^T V = I$.



What is $A^T A v_i =$

What is $A A^T u_i =$

- v_i's are the r eigen vectors of $A^T A$ with corresponding eigen values S_{ii}^2's
- u_i's are the r eigen vectors of $A A^T$ with corresponding eigen values S_{ii}^2's
- Computing SVD takes $O(mnr)$ operations

Singular Value Decomposition (SVD): definition

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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 $\text{diag}(\mathbf{S}^2)$
$\mathbf{U}$ are the first r eigenvectors of $\mathbf{A}\mathbf{A}^T$ with eigenvalues $\text{diag}(\mathbf{S}^2)$

Singular Value Decomposition (SVD): property 1

- Consider a full rank matrix $A \in \mathbb{R}^{m \times n}$ whose SVD is $A = USV^T$, and we want to find the **best rank-r approximation** of A that minimizes the error

$$\text{minimize}_{L \in \mathbb{R}^{m \times n}} \sum_{i=1}^{m} \sum_{j=1}^{n} (A_{i,j} - L_{i,j})^2$$

$$\text{subject to } \text{rank}(L) = r$$

  - The optimal rank-r approximation is $L = U_{1:r} S_{1:r,1:r} V_{1:r}^T$

Singular Value Decomposition (SVD): property 2

- Consider a full rank matrix $A \in \mathbb{R}^{m \times n}$ whose SVD is $A = USV^T$, and we want to find the best rank-r subspace Q that maximizes

$$\text{maximize}_{Q \in \mathbb{R}^{n \times r}} \quad \text{Trace}(Q^T A^T A Q) = \sum_{j=1}^{r} Q_j^T A^T A Q_j$$

$$\text{subject to} \qquad Q^T Q = I_{r \times r}$$

  - The optimal rank-r subspace is $Q = V_{1:r}$

PCA is solved using SVD

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

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

Minimizing the reconstruction error for a compressed representation of the data

Maximum eigen-space of Σ

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

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

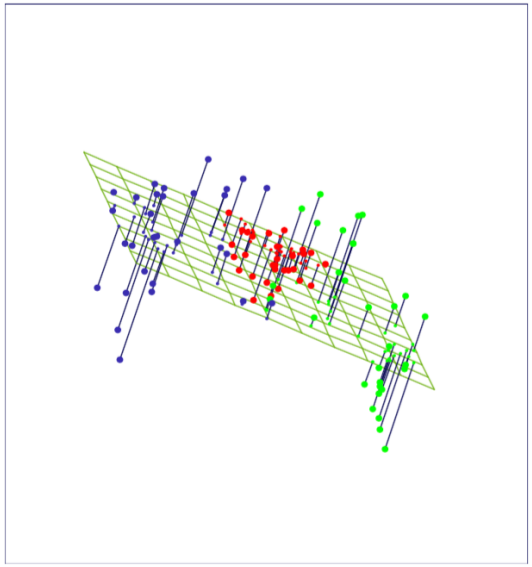
$$\max_{V_q} \quad V_q^T \Sigma V_q$$

$$\text{subject to} \quad V_q^T V_q = I$$

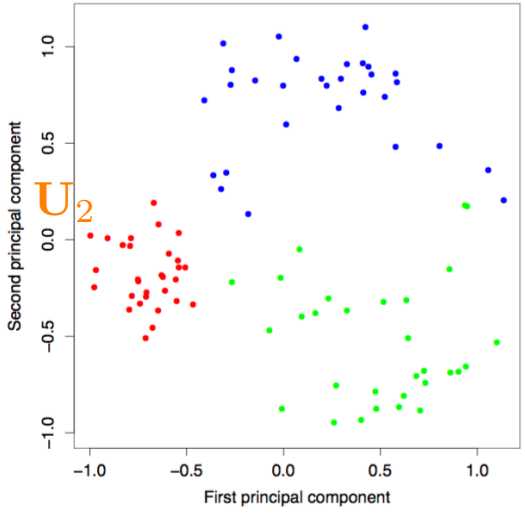
We can use SVD on the matrix $\tilde{X}$, and take the first r eigen pairs to find PCA.

Example 1: Dimensionality reduction

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



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



$\mathbf{U}_2$

$\mathbf{U}_1$

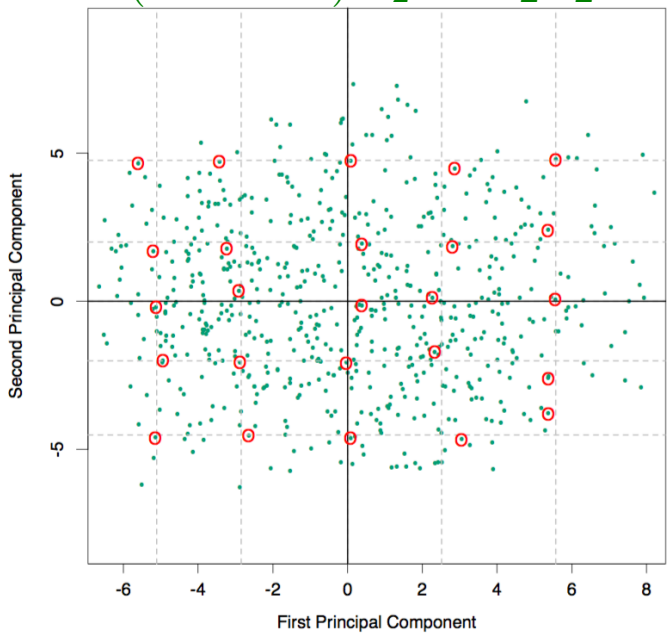
Example 2: Dimensionality reduction

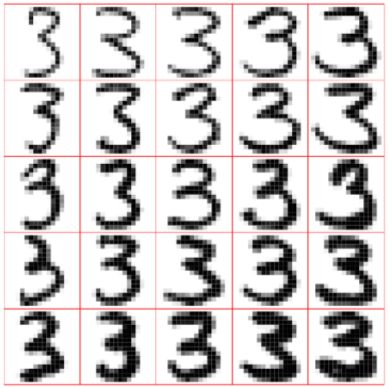
$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

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

$$\begin{aligned} \hat{f}(\lambda) &= \bar{x} + \lambda_1 v_1 + \lambda_2 v_2 \\ &= \bar{x} + \lambda_1 \cdot v_1 + \lambda_2 \cdot v_2. \end{aligned}$$

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





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

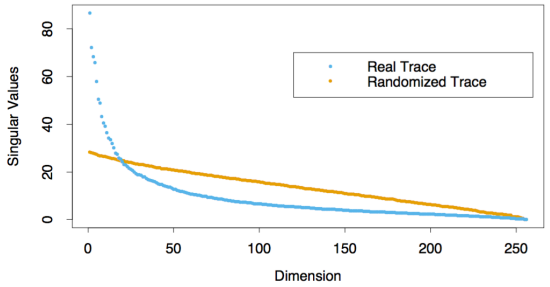


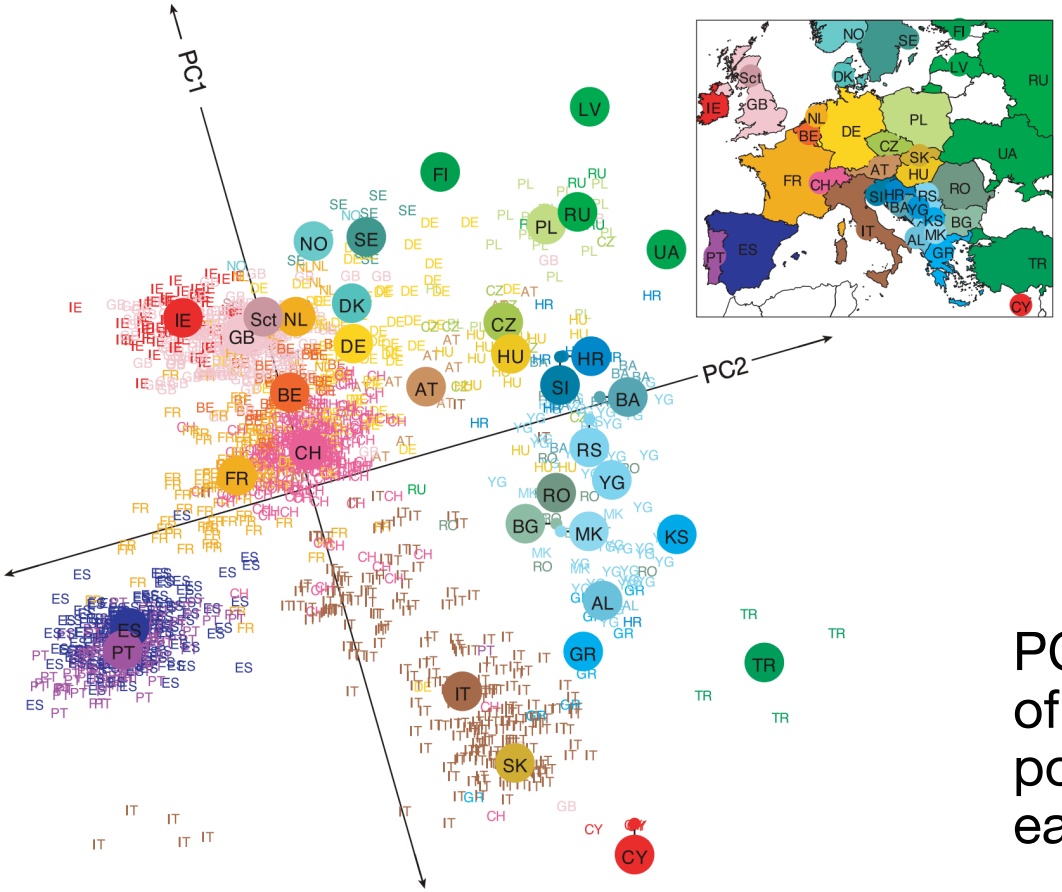
FIGURE 14.24. *The 256 singular values for the digitized threes, compared to those for a randomized version of the data (each column of* $\mathbf{X}$ *was scrambled).*

nature Vol 456|6 November 2008|doi:10.1038/nature07331

LETTERS

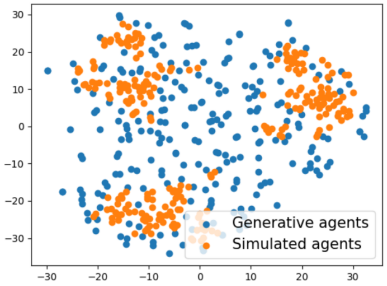
Genes mirror geography within Europe

John Novembre[1,2], Toby Johnson[4,5,6], Katarzyna Bryc[7], Zoltán Kutalik[4,6], Adam R. Boyko[7], Adam Auton[7], Amit Indap[7], Karen S. King[8], Sven Bergmann[4,6], Matthew R. Nelson[8], Matthew Stephens[2,3] & Carlos D. Bustamante[7]

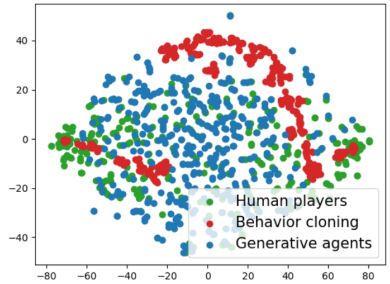


PCA on dataset consisting of 200,000 single nucleotide polymorphisms (SNPs) for each of ~1,400 individuals.

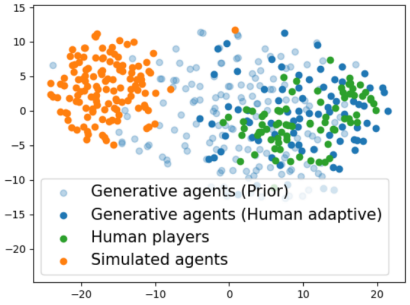
Visualization!



(a) Simulated data.



(b) Human data.



(c) Adaptive sampling.

Liang, Y., Chen, D., Gupta, A., Du, S. S., & Jaques, N. (2024). Learning to Cooperate with Humans using Generative Agents. *Neural Information Processing Systems (NeurIPS)*.

Chaudhary, P., Liang, Y., Chen, D., Du, S. S., & Jaques, N. (2025). Improving Human-AI Coordination through Adversarial Training and Generative Models. *Preprint*.

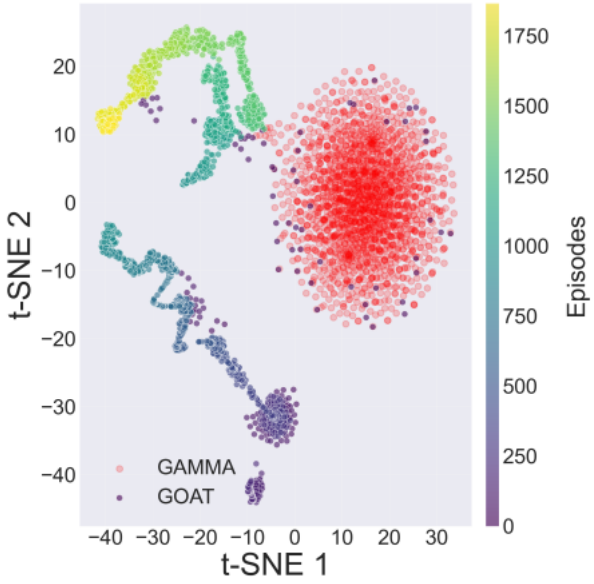


Figure 7: GOAT exploring the latent space exploration compared against GAMMA (Liang et al., 2024) in red over the whole training period.

Kernel PCA

- Assuming data is centered (i.e., zero-mean), PCA is defined by the eigenvectors corresponding to the largest eigenvalues of the covariance matrix

$$\Sigma = \frac{1}{n} X^T X = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T$$

- To apply PCA to a non-linear feature mapping $\phi : \mathbb{R}^d \to \mathbb{R}^p$, we want to use SVD on:

$$\frac{1}{n} \phi(X)^T \phi(X) = \frac{1}{n} \sum_{i=1}^{n} \phi(x_i) \phi(x_i)^T$$

- However, this is a $p \times p$ matrix, and the dimension p can be very large.
- Hence, ***Kernel PCA*** attempts to make this efficient by considering only the subspaces spanned by the data, i.e., $v_j = \sum_{i=1}^{n} \phi(x_i) \alpha_{i,j}$, now parametrized by $\alpha^{(j)} = (\alpha_{1,j}, \ldots, \alpha_{n,j})$

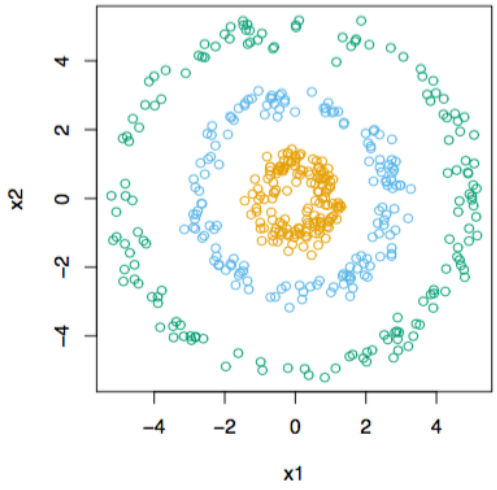
Kernel PCA

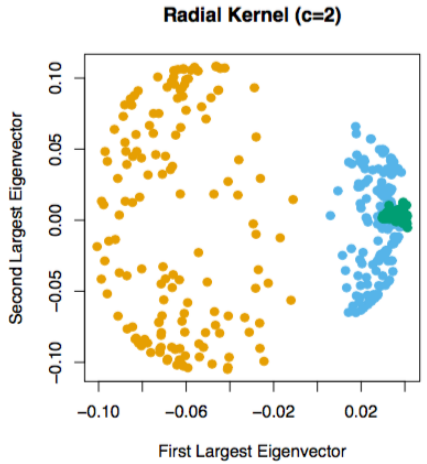
- Hence, ***Kernel PCA*** attempts to maximize

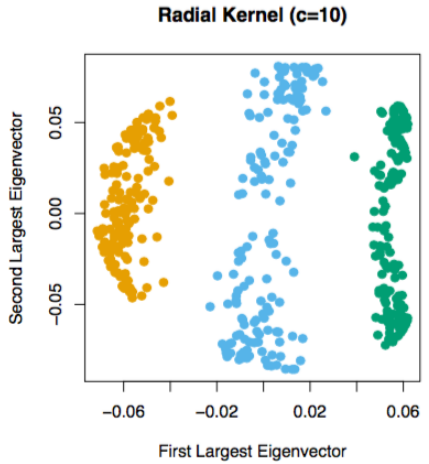
$$\max_{\alpha \in \mathbb{R}^{n \times r}} \sum_{j=1}^{r} \underbrace{(\alpha_j^T \phi(X))}_{v_j^T} \phi(X)^T \phi(X) \underbrace{(\phi(X)^T \alpha_j)}_{v_j}$$

- This is equivalent to using the eigenvectors

$$n \lambda_j K \alpha_j = K^2 \alpha_j$$







Matrix completion

Given historical data on how users rated movies in past:

NETFLIX

17,700 movies, 480,189 users, 99,072,112 ratings (Sparsity: 1.2%)

Predict how the same users will rate movies in the future (for $1 million prize)

Matrix completion problem

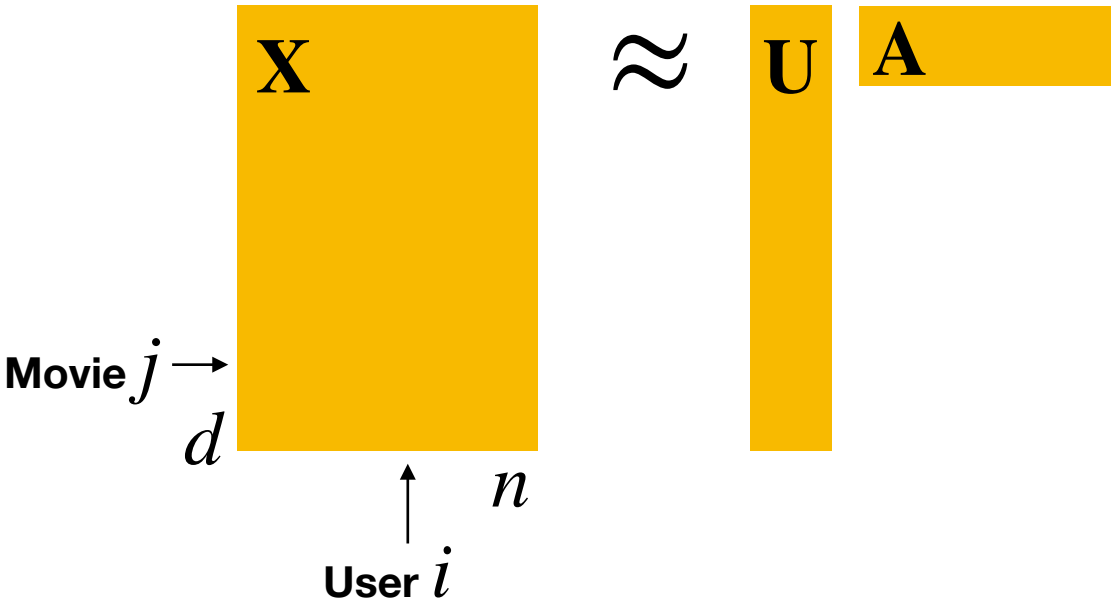
- however, the ratings are not arbitrary, but people with similar tastes rate similarly
- such structure can be modeled using low dimensional representation of the data as follows
- we will find a set of principal component vectors $\mathbf{U} = [u_1 \quad u_2 \quad \cdots \quad u_r] \in \mathbb{R}^{d \times r}$
- such that that ratings $x_i \in \mathbb{R}^d$ of user i, can be represented as

$$\begin{aligned} x_i &= a_i[1]u_1 + \cdots a_i[r]u_r \\ &= \mathbf{U}a_i \end{aligned}$$

  for some lower-dimensional $a_i \in \mathbb{R}^r$ for i-th user and some $r \ll d$
- for example, $u_1 \in \mathbb{R}^d$ means how horror movie fans like each of the d movies,
- and $a_i[1]$ means how much user i is fan of horror movies

Matrix completion

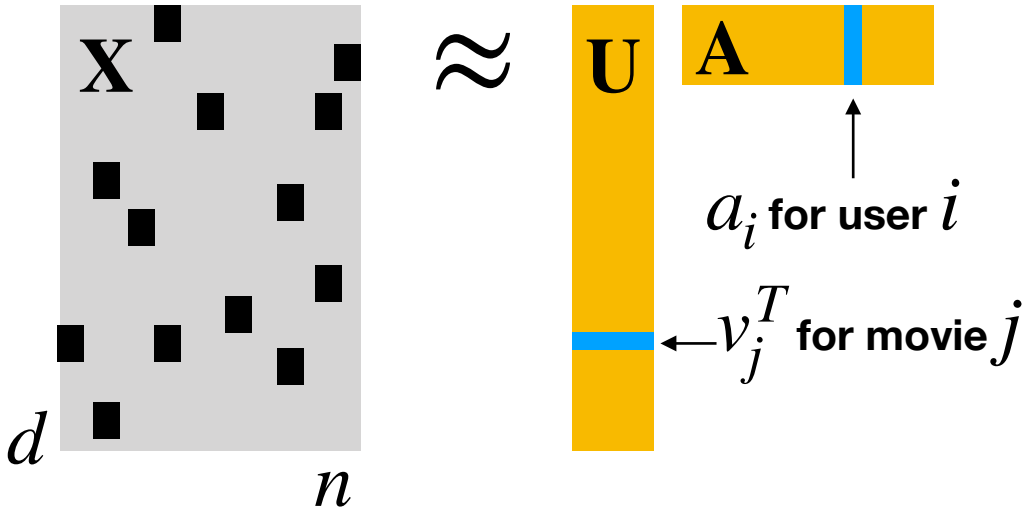
- let $\mathbf{X} = [x_1 \quad x_2 \quad \cdots \quad x_n] \in \mathbb{R}^{d \times n}$ be the ratings matrix, and assume it is fully observed, i.e. we know all the entries
- then we want to find $\mathbf{U} \in \mathbb{R}^{d \times r}$ and $\mathbf{A} = [a_1 \quad a_2 \quad \cdots \quad a_n] \in \mathbb{R}^{r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



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

Matrix completion

- in practice, we only observe $\mathbf{X}$ partially
- let $S_{\text{train}} = \{(i_\ell, j_\ell)\}_{\ell=1}^{N}$ denote N observed ratings for user i_ℓ on movie j_ℓ



- let v_j^T denote the j-th row of $\mathbf{U}$ and a_i denote i-th column of $\mathbf{A}$
- then user i's rating on movie j, i.e. $\mathbf{X}_{ji}$ is approximated by $v_j^T a_i$, which is the inner product of v_j (a column vector) and a column vector a_i
- we can also write it as $\langle v_j, a_i \rangle = v_j^T a_i$

Matrix completion

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

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

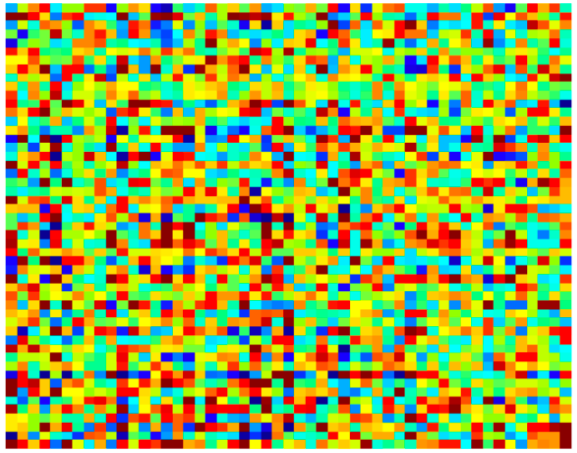
- this can be solved, for example via gradient descent or alternating minimization
- this can be quite accurate, with small number of samples

- Theorem [Keshavan,Montanari,Oh 2009]
  Assume the ground truths $\mathbf{X}$ *has rank* r*, then*
  (a variant of) gradient descent finds the optimal solution if we observe more than $c\, r\, (d+n)\, \log(dn)$ *entries at random positions*

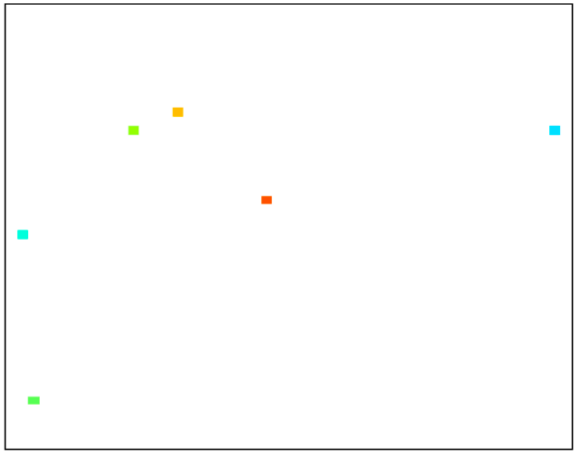
Example: 2000×2000 rank-8 random matrix

For illustration, we zoom in to a 50x50 submatrix

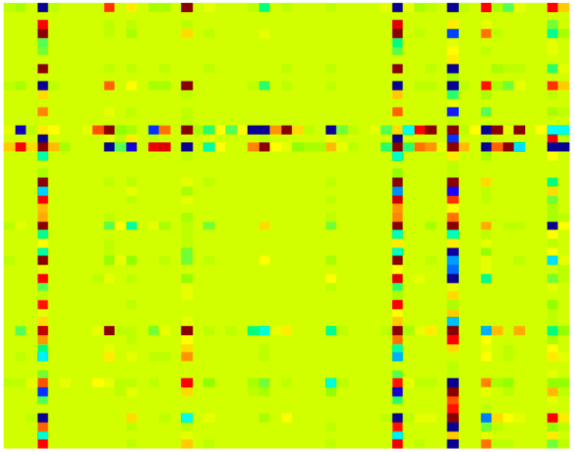
low-rank matrix $\mathbf{X}$



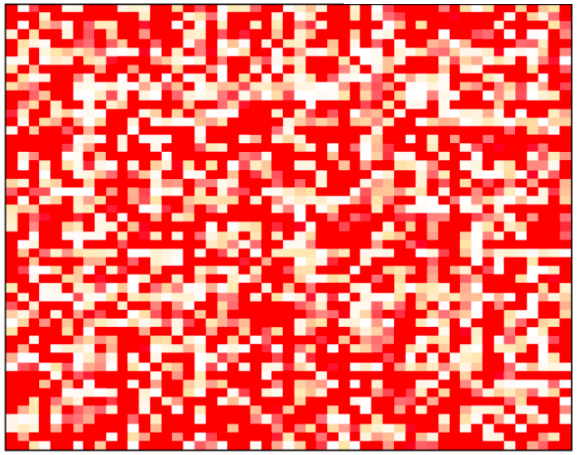
sampled matrix



Gradient descent output $\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top$



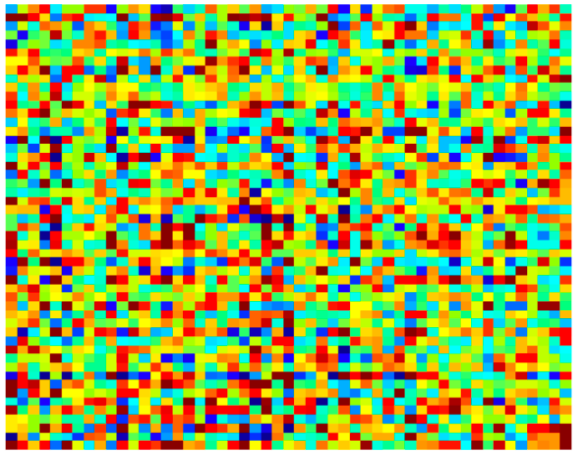
squared error $(\mathbf{X}_{ji} - (\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top)_{ji})^2$



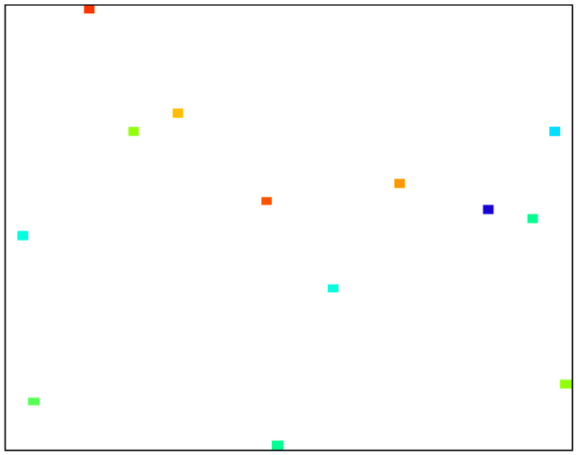
0.25% sampled

Example: 2000×2000 rank-8 random matrix

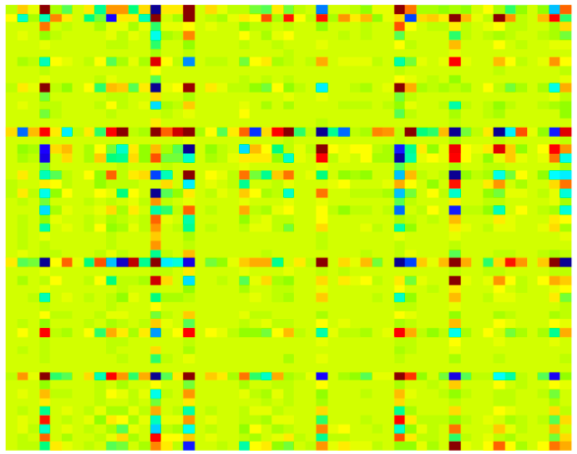
low-rank matrix $\mathbf{X}$



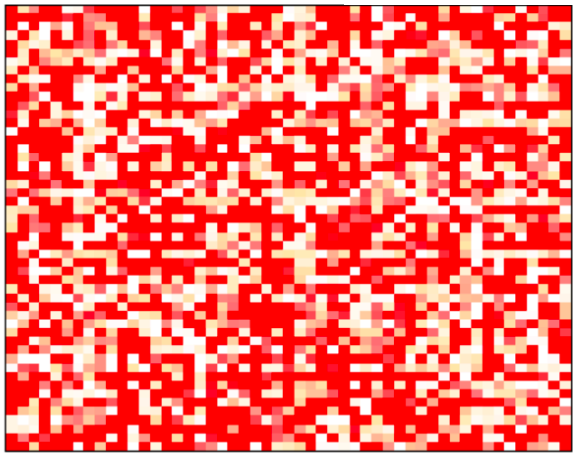
sampled matrix



Gradient descent output $\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top$



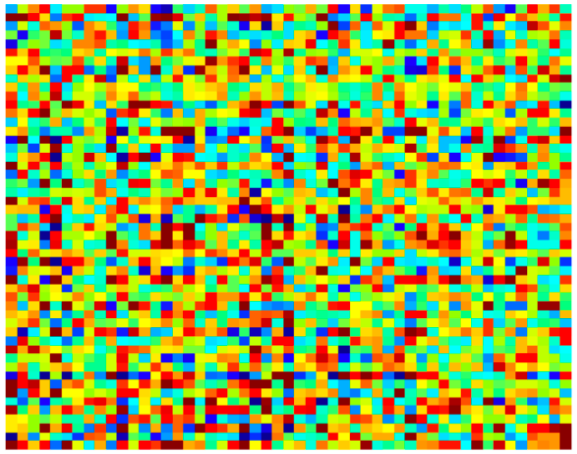
squared error $(\mathbf{X}_{ji} - (\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top)_{ji})^2$



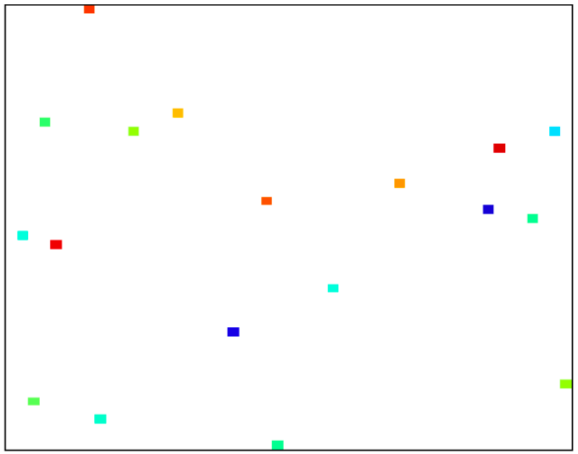
0.50% sampled

Example: 2000×2000 rank-8 random matrix

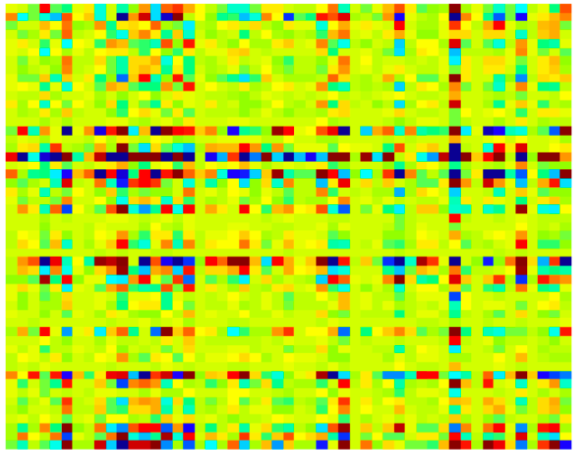
low-rank matrix $\mathbf{X}$



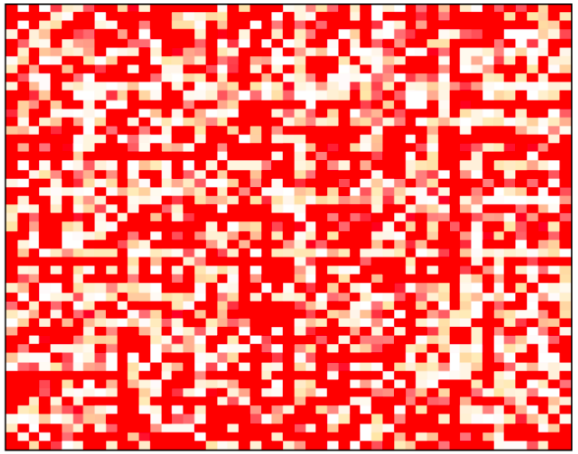
sampled matrix



Gradient descent output $\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top$



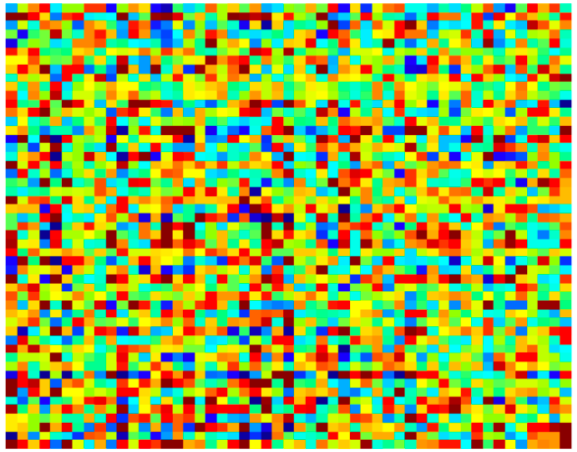
squared error $(\mathbf{X}_{ji} - (\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top)_{ji})^2$



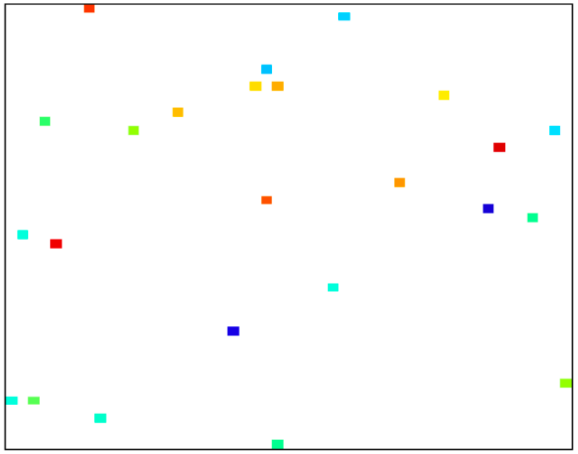
0.75% sampled

Example: 2000×2000 rank-8 random matrix

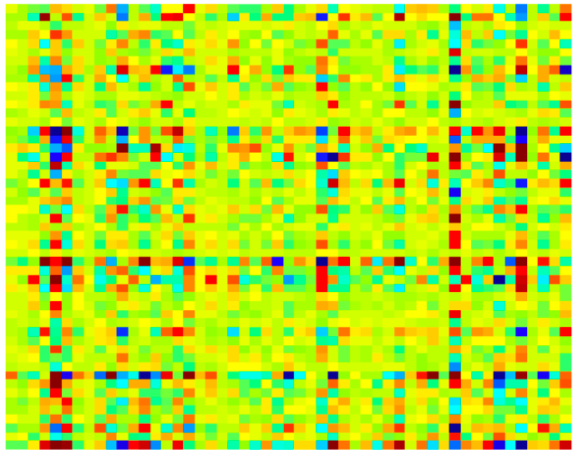
low-rank matrix $\mathbf{X}$



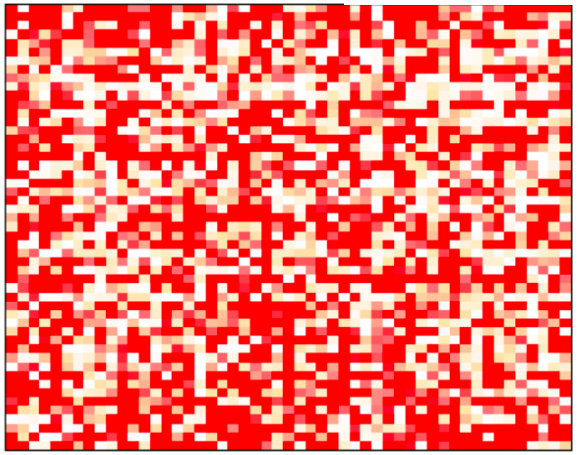
sampled matrix



Gradient descent output $\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top$



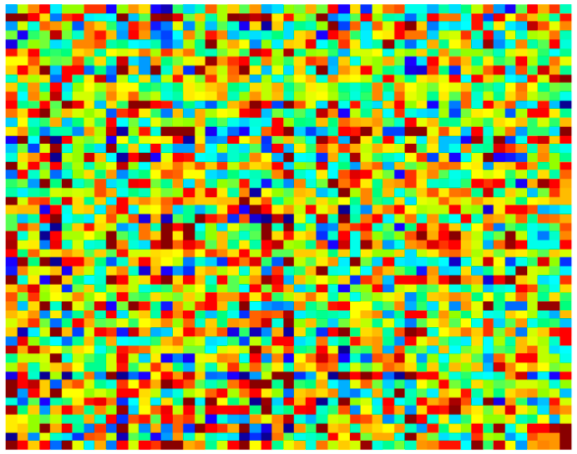
squared error $(\mathbf{X}_{ji} - (\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top)_{ji})^2$



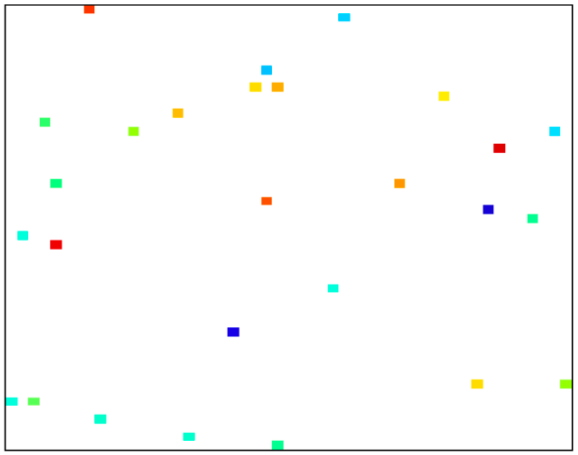
1.00% sampled

Example: 2000×2000 rank-8 random matrix

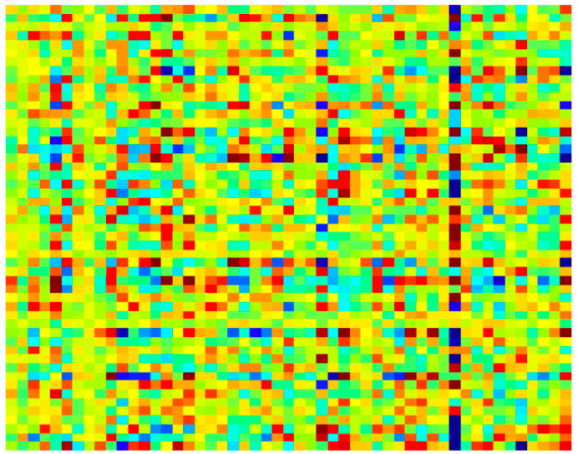
low-rank matrix $\mathbf{X}$



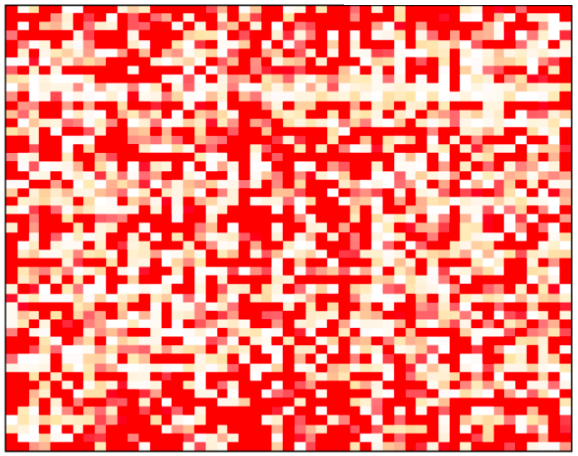
sampled matrix



Gradient descent output $\tilde{\mathbf{U}}\tilde{\mathbf{V}}^T$



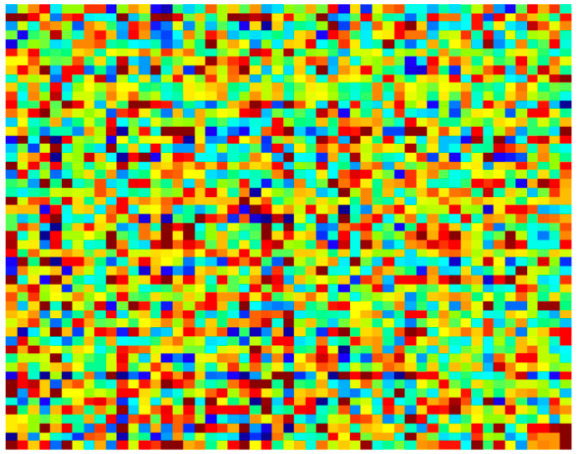
squared error $(\mathbf{X}_{ji} - (\tilde{\mathbf{U}}\tilde{\mathbf{V}}^T)_{ji})^2$



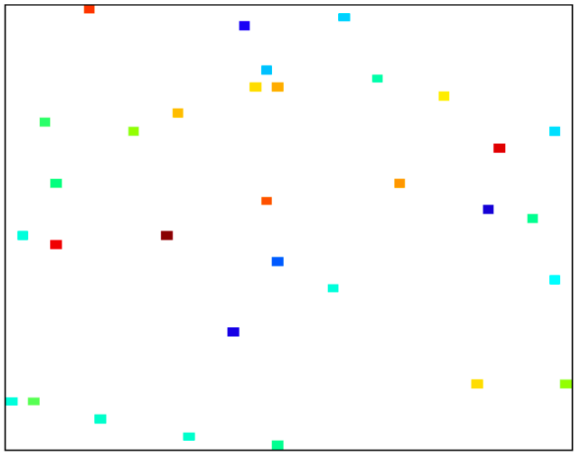
1.25% sampled

Example: 2000×2000 rank-8 random matrix

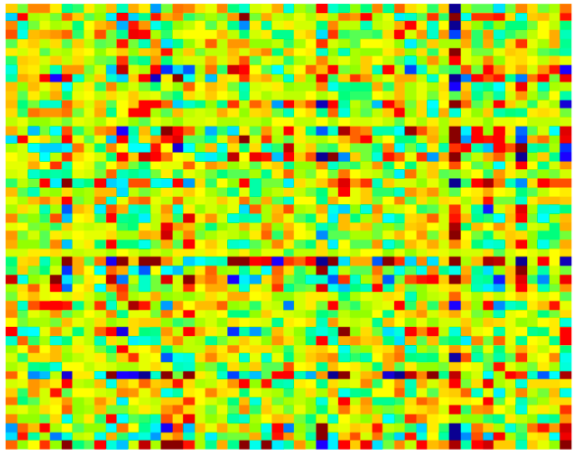
low-rank matrix $\mathbf{X}$



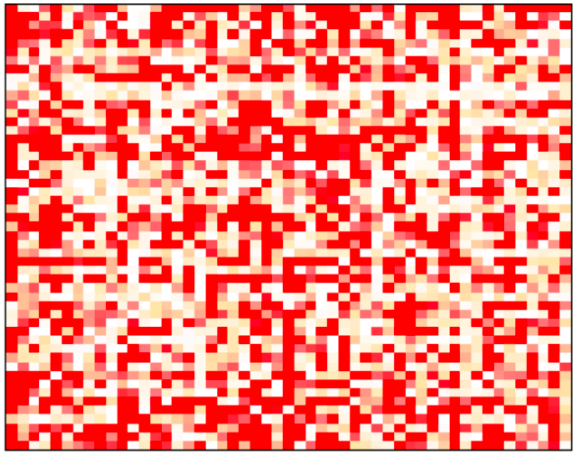
sampled matrix



Gradient descent output $\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top$



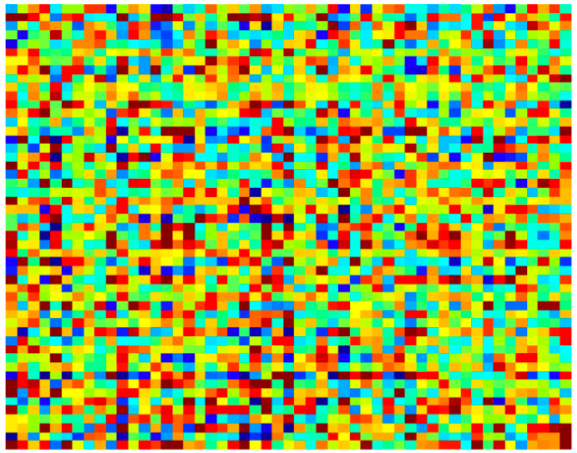
squared error $(\mathbf{X}_{ji} - (\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top)_{ji})^2$



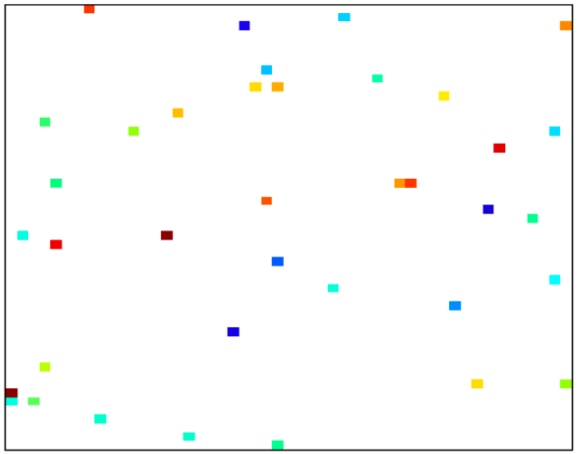
1.50% sampled

Example: 2000×2000 rank-8 random matrix

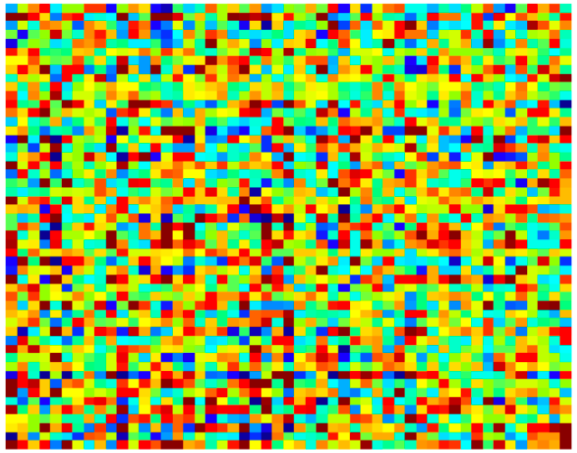
low-rank matrix $\mathbf{X}$



sampled matrix



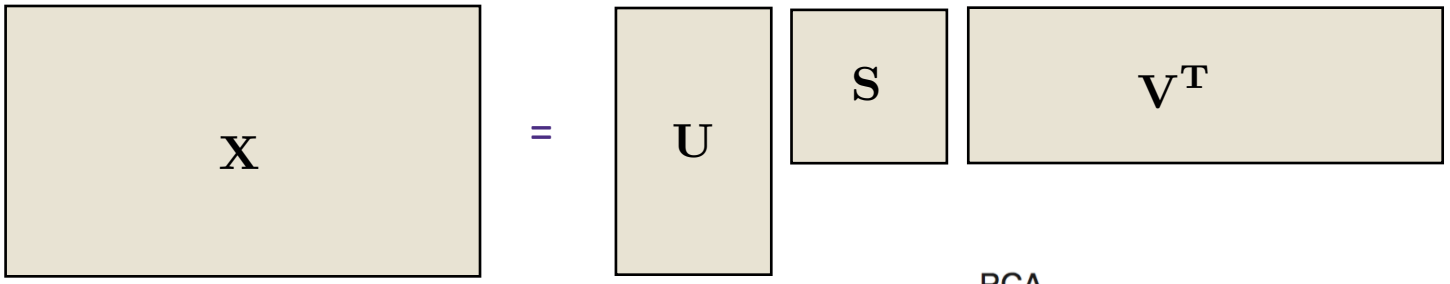
Gradient descent output $\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top$



squared error $(\mathbf{X}_{ji} - (\tilde{\mathbf{U}}\tilde{\mathbf{V}}^\top)_{ji})^2$

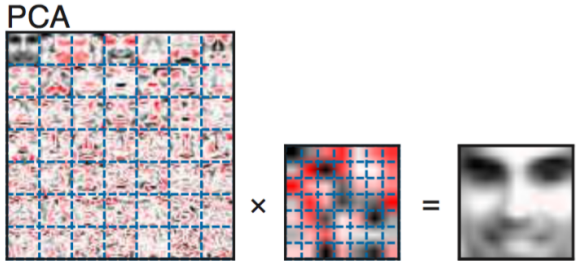
1.75% sampled

Other matrix factorizations



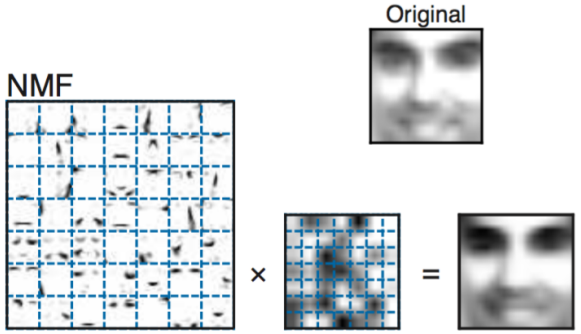
Singular value decomposition

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



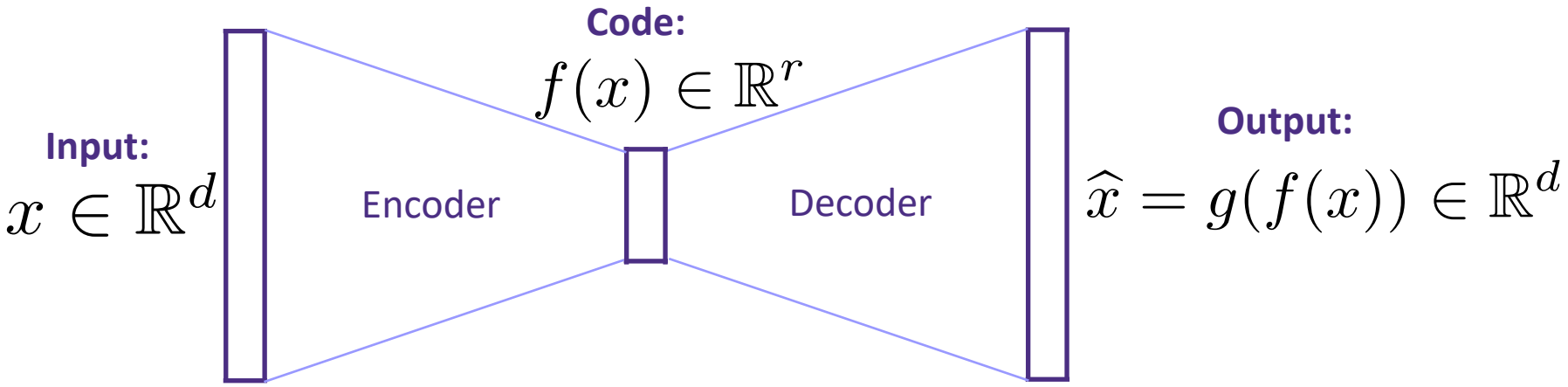
Nonnegative matrix factorization (NMF)

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



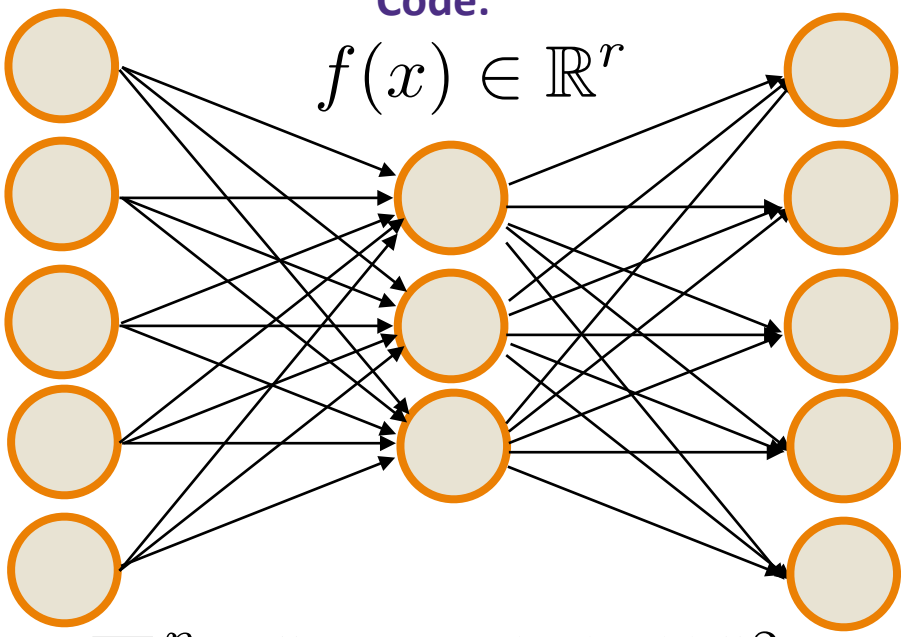
Autoencoders

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



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

Autoencoders



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 $g(y) = By$?