PCA

have data set $\vec{x}_1, \ldots, \vec{x}_n$ $\quad x_i \in \mathbb{R}^d$

$$X = \begin{pmatrix} - x_1 - \\ \vdots \\ - x_n - \end{pmatrix}$$

assume mean 0 $\left(\sum_{i=1}^{n} x_i = 0\right)$

Examples

- n images $\quad d$ pixels each
- n measurements $\quad d$ sensors
- n docs $\quad d$ words
- n people $\quad d$ movies
- n customers $\quad d$ products

Fix k

Find k-dimensional subspace (defined by orthonormal vectors $\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_k$)

so as to minimize $\frac{1}{n}\sum_{i=1}^{n}\left[\text{distance}\left(x_i \leftrightarrow \text{subspace } S \text{ spanned by } \vec{v}_1, v_2, \ldots, \vec{v}_k\right)\right]^2$

$\equiv$ maximizing $\underbrace{\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{k}(x_i, v_j)^2}_{\text{variance of projected pts}}$

projection of $x_i \to S$

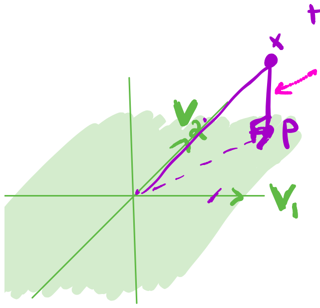
$$\sum_{j=1}^{k}(x_i, v_j)\,\vec{v}_j$$

$(x_i \cdot v_j)$

v_1

d:

find $v_1, \ldots, v_k$ to max $\frac{1}{n}\sum_{i=1}^{n}\underbrace{\boxed{\sum_{j=1}^{k}(x_i, v_j)^2}}_{\|p\|^2}$



$p = a_1 v_1 + a_2 v_2$

(x, v_1)

$(x - p, v_1) = 0$

$(x, v_1) = (p, v_1) = (a_1 v_1 + a_2 v_2, v_1)$

$= a_1$

$p = (x, v_1)\, v_1 + (x, v_2)\, v_2$

maximizing $\frac{1}{n}\sum_{i=1}^{n} \sum_{j=1}^{k} (x_i \cdot v_j)^2 = \sum_{j=1}^{k} (Xv_j)^T X v_j$

$= \frac{1}{n}\sum_{j=1}^{k} v_j^T X^T X v_j$

How to find $\vec{v}_1, \dots, \vec{v}_k$

① Compute eigendecomposition of empirical covariance matrix $X^T X$

$$A := X^T X = Q D Q^T$$

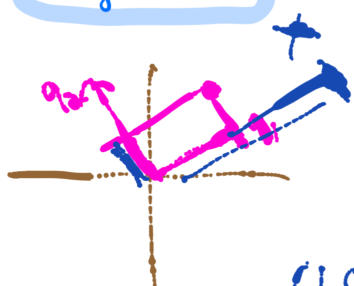
where $Q = \begin{pmatrix} | & & | \\ q_1 & \cdots & q_d \\ | & & | \end{pmatrix}$

$q_1, \dots, q_n$ orthonormal
$Q Q^T = Q^T Q = I$
$\forall w \quad \|Qw\| = \|w\|$

$D = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \ \lambda_d \end{pmatrix}$

$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$
all eigenvalues ≥ 0

$$\boxed{A q_i = \lambda_i q_i} \quad \forall i$$



$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$ $\begin{pmatrix} 3 \\ 5 \end{pmatrix}$

$$\begin{pmatrix} | & & | \\ q_1 & \cdots & q_d \\ | & & | \end{pmatrix} \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_d \end{pmatrix} \begin{pmatrix} — & q_1^T & — \\ & \vdots & \\ — & q_d^T & — \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_d \end{pmatrix}$$

$\begin{pmatrix} q_1 \cdot a \\ q_2 \cdot a \\ \vdots \\ q_d \cdot a \end{pmatrix}$

$$\begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

② Set $v_1 := q_1$
$v_2 := q_2$
$\vdots$
$v_k := q_k$

New coordinates of x_i are $\underline{(x_i \cdot v_1), (x_i \cdot v_2), \dots, (x_i \cdot v_k)}$

low dimensional representation of $\vec{x}_i$

$\Sigma = A A^T$

$$\Sigma = \underset{Q}{\begin{pmatrix} q_1 & q_2 \\ | & | \end{pmatrix}} \underset{D}{\begin{pmatrix} \lambda_1 & \\ & \lambda_2 \end{pmatrix}} \underset{Q^T}{\begin{pmatrix} — q_1^T — \\ — q_2^T — \end{pmatrix}}$$

$Q D^{k/2} D^{k/2} Q^T$

$(Q D^{k/2})(Q D^{k/2})^T$

1. Find the top component, $\mathbf{v}_1$, using power iteration.
2. Project the data matrix orthogonally to $\mathbf{v}_1$:

$$\begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \mathbf{x}_2 & - \\ & \vdots & \\ - & \mathbf{x}_m & - \end{bmatrix} \mapsto \begin{bmatrix} - & (\mathbf{x}_1 - \langle \mathbf{x}_1, \mathbf{v}_1 \rangle \mathbf{v}_1) & - \\ - & (\mathbf{x}_2 - \langle \mathbf{x}_2, \mathbf{v}_1 \rangle \mathbf{v}_1) & - \\ & \vdots & \\ - & (\mathbf{x}_m - \langle \mathbf{x}_m, \mathbf{v}_1 \rangle \mathbf{v}_1) & - \end{bmatrix}.$$

This corresponds to subtracting out the variance of the data that is already explained by the first principal component $\mathbf{v}_1$.

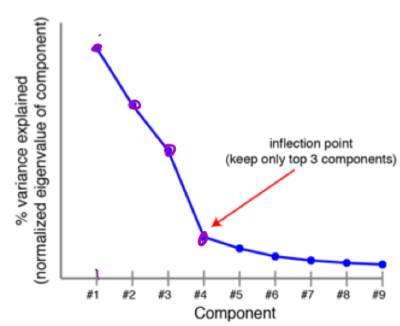
3. Recurse by finding the top $k-1$ principal components of the new data matrix.

Applications

① Visualization ② Compression ③ Learning

How to choose k?

- For data visualization: a few
- compression: Look at eigenvalues.
  As soon as small enough; happy.



k

Scree plot. Principal components are ranked by the amount of variance they capture in the original dataset, a scree plot can provide some sense of how many components are needed.

Singular Value Decomposition (SVD)

gives us best way to approximate a matrix with a "low rank" matrix

$$\begin{array}{cc} & \text{ratings} \\ \text{movies} & \begin{bmatrix} 7 & ? & ? \\ ? & 8 & ? \\ ? & 12 & 6 \\ ? & ? & 2 \\ 21 & 6 & ? \end{bmatrix}. \end{array}$$

Motivation: can we reconstruct missing entries?

Suppose I told you that all rows are multiples of each other

$$\begin{array}{cc} & \begin{matrix} 1 & 2 & 3 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} 7 & 2 & 1 \\ 28 & 8 & \boxed{4} \\ 42 & 12 & 6 \\ 14 & \boxed{4} & 2 \\ 21 & 6 & 3 \end{bmatrix} \end{array} = \begin{matrix} 1\cdot(7 & 2 & 1) \\ 4\cdot(7 & 2 & 1) \\ 6\,(7 & 2 & 1) \\ 2\,(7 & 2 & 1) \\ 3\,(7 & 2 & 1) \end{matrix}$$

$$\begin{pmatrix} 1 \\ 4 \\ 6 \\ 2 \\ 3 \end{pmatrix} \begin{pmatrix} 7 & 2 & 1 \end{pmatrix}$$

Rank 0   all 0 matrix

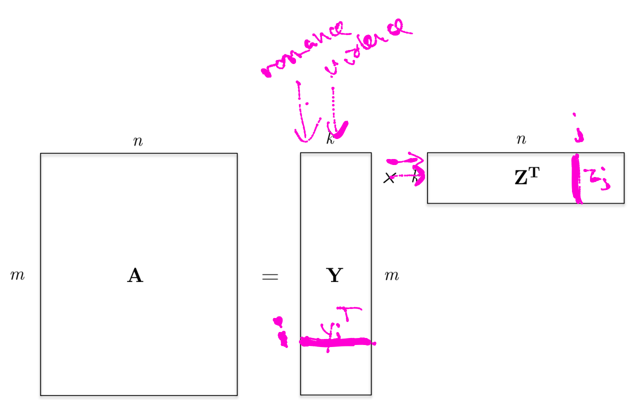
Rank 1

$$\mathbf{A} = \mathbf{u}\mathbf{v}^\top = \begin{bmatrix} — & u_1\mathbf{v}^\top & — \\ — & u_2\mathbf{v}^\top & — \\ & \vdots & \\ — & u_m\mathbf{v}^\top & — \end{bmatrix} = \begin{bmatrix} | & | & & | \\ v_1\mathbf{u} & v_2\mathbf{u} & \cdots & v_n\mathbf{u} \\ | & | & & | \end{bmatrix}$$

Rank 2

$$\mathbf{A} = \mathbf{u}\mathbf{v}^\top + \mathbf{w}\mathbf{z}^\top = \begin{bmatrix} — & u_1\mathbf{v}^\top + w_1\mathbf{z}^\top & — \\ — & u_2\mathbf{v}^\top + w_2\mathbf{z}^\top & — \\ & \vdots & \\ — & u_m\mathbf{v}^\top + w_m\mathbf{z}^\top & — \end{bmatrix} = \begin{bmatrix} | & | \\ \mathbf{u} & \mathbf{w} \\ u_i & w_i \\ | & | \end{bmatrix} \cdot \begin{bmatrix} — & \mathbf{v}^\top & v_j \\ — & \mathbf{z}^\top & z_j \end{bmatrix}$$

$u_i v_j + w_i z_j$



Find
$y_1, \ldots, y_m \in \mathbb{R}^k$
$z_1, \cdots z_n \in \mathbb{R}^k$
s.t. $a_{ij} \approx y_i \cdot z_j$

Figure 1: Any matrix $\mathbf{A}$ of rank k can be decomposed into a long and skinny matrix times a short and long one.

Why might a matrix be approximately low rank?

Example: movie ratings

Suppose each movie characterized by relatively small # of attributes

e.g. romance, violence, comedy, ...

and each person characterized by their preferences on each of these

Singular Value Decomposition (SVD)

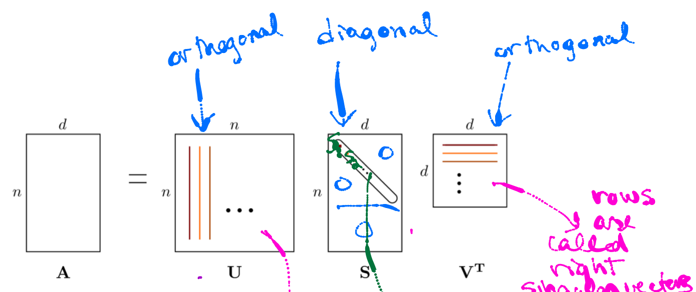


Figure 2: The singular value decomposition (SVD). Each singular value in **S** has an associated left singular vector in **U**, and right singular vector in **V**.

$UU^T = U^TU = I$

$VV^T = V^TV = I$

cols called left singular vectors

$s_1 \geq s_2 \geq \cdots \geq s_{\min(n,d)} \geq 0$

called singular values.

Running time to compute

$\min\left[O(n^2d), O(d^2n)\right]$

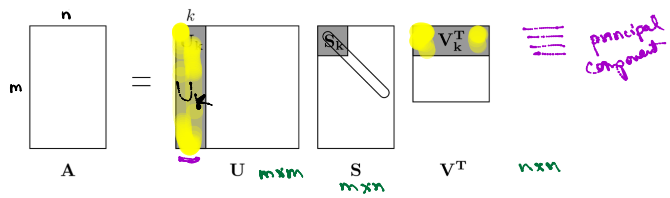


Figure 3: Low rank approximation via SVD. Recall that $\mathbf{S}$ is non-zero only on its diagonal, and the diagonal entries of S are sorted from high to low. Our low rank approximation is $\mathbf{A}_k = \mathbf{U}_k\mathbf{S}_k\mathbf{V}_k^\top$.

is optimal rank approx

Claim: $\forall$ m×n matrix A and rank target k, and rank k matrix B

$$\|A - A_k\|_F^2 \le \|A - B\|_F^2$$

$$\|M\|_F^2 = \sum_{i,j} m_{ij}^2$$

Exercise: knowing that $\vec{v}_1$ (first row) is first principal component prove this theorem for $k=1$

Relationship between SVD and PCA

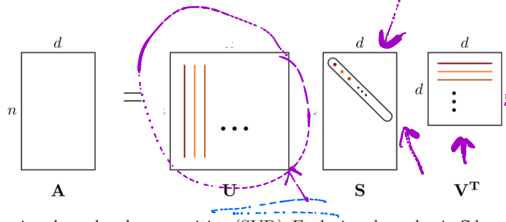


Figure 2: The singular value decomposition (SVD). Each singular value in **S** has an associated left singular vector in **U**, and right singular vector in **V**.

PCA

$$X^TX = QDQ^T$$

SVD

$$\underbrace{X}_{n \times d} = USV^T$$

$$X^TX = (USV^T)^T\, USV^T$$

$$= VS^T\underbrace{U^TU}_{I}SV^T$$

$$= VS^2V^T$$

$$\begin{pmatrix} s_1^2 & & \\ & s_2^2 & \\ & & \ddots \end{pmatrix}$$

$Q = V$

$D = S^2$

eigenvalues of X^TX are squares of singular values.

$$XX^T = US^2U^T$$

$$\begin{array}{cc} & \text{products} \\ \text{customers} & \begin{pmatrix} & & \\ & & \\ & & \end{pmatrix} \end{array}$$

X^TX covariance for products

XX^T covariance for customers

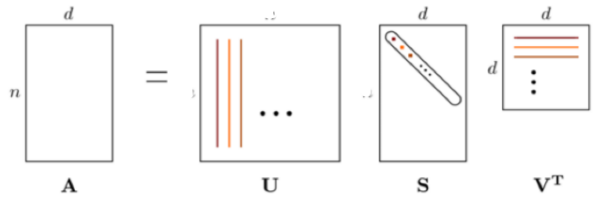


Figure 2: The singular value decomposition (SVD). Each singular value in **S** has an associated left singular vector in **U**, and right singular vector in **V**.

Application 1: Denoising

Suppose matrix A is noisy version of rank-k matrix

$$A = C + N$$

true rank k

can "reconstruct C" by taking A_k

Collaborative Filtering

recommendations: which movies to see, which products to buy

Model:

$$
\begin{array}{cc}
 & \text{movies} \\
\text{people} & \begin{bmatrix} 2.5 & 4 & 1 \\ 2.5 & 0 & 5 \\ 1 & 1 & 1 \\ 2.5 & 4 & 1 \\ 3.5 & 3 & 4 \end{bmatrix}
\end{array}
\longrightarrow
\begin{bmatrix} \boxed{2.5} & ? & ? \\ ? & 0 & ? \\ ? & 1 & 1 \\ ? & ? & 1 \\ 3.5 & 3 & ? \end{bmatrix}
$$

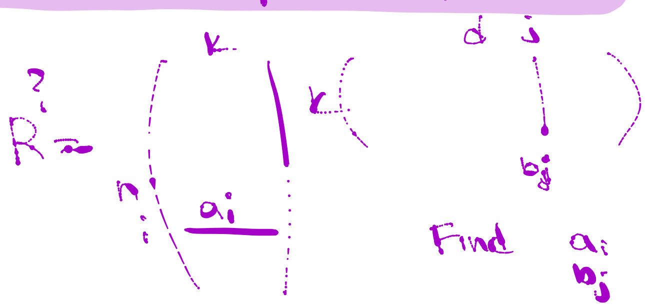
R $n \times d$ ground truth $\qquad\qquad$ $R^?$

Assumptions:

R is low rank
e.g. rank k

example: humor, violence, romance

The matrix completion problem:



Find a_i's, b_j's to min

$$\sum_{(i,j) \in R^? \text{ have entry}} (R_{ij} - a_i \cdot b_j)^2$$

Find a_i $\quad i = 1..n$
b_j $\quad j = 1..d$

s.t. if R_{ij} is present
$R_{ij} \approx \vec{a}_i \cdot \vec{b}_j$

Collaborative Filtering

recomendations: which movies to see, which products to buy

Model:

$$
\begin{array}{cc}
 & \text{movies} \\
\text{people} & \begin{bmatrix} 2.5 & 4 & 1 \\ 2.5 & 0 & 5 \\ 1 & 1 & 1 \\ 2.5 & 4 & 1 \\ 3.5 & 3 & 4 \end{bmatrix}
\end{array}
\longrightarrow
\begin{bmatrix} 2.5 & ? & ? \\ ? & 0 & ? \\ ? & 1 & 1 \\ ? & ? & 1 \\ 3.5 & 3 & ? \end{bmatrix}
$$

R $n \times d$ ground truth $\qquad$ $R^?$

Assumptions:

① R is low rank
e.g. rank k

example: humor, violence, romance

The matrix completion problem:

fill in the missing entries.

Theorem $\hat{A}$ $n \times d$ matrix of indep. r.v.s, each with variance bounded by σ^2

If $A = E(\hat{A})$ is rank k

then with high probability

$$\|A - \hat{A}_k\|_F^2 \text{ is } O(k\sigma^2(n+d))$$

avg per elt error $O\left(\frac{k\sigma^2(n+d)}{nd}\right) = o(1)$

Suppose A rank k. $\longrightarrow A^{?}$

entry (i,j) present with prob p_{ij}

$$\begin{pmatrix} ? & 5 & - & ? \\ & & & \\ & & & \end{pmatrix}$$

Let $\hat{A}_{ij} = \begin{cases} \dfrac{A^{?}_{ij}}{p_{ij}} & \text{if entry present} \\ 0 & \text{o.w.} \end{cases}$

A $\longrightarrow$ $A^{?}$

A_{ij}

rank k

entry (i,j) survives with prob p_{ij}

$$E(\hat{A}_{ij}) = \frac{A^{?}_{ij}}{p_{ij}} \cdot p_{ij} + 0 = \boxed{A_{ij}}$$

$$\underset{R^?}{\begin{bmatrix} 2.5 & ? & ? \\ ? & 0 & ? \\ ? & 1 & 1 \\ ? & ? & 1 \\ 3.5 & 3 & ? \end{bmatrix}} \longrightarrow \underset{M}{\begin{bmatrix} \quad & \quad & \quad \\ & & \\ & & \\ & & \\ & & \end{bmatrix}}$$