Low Rank Approximation
Lecture 1

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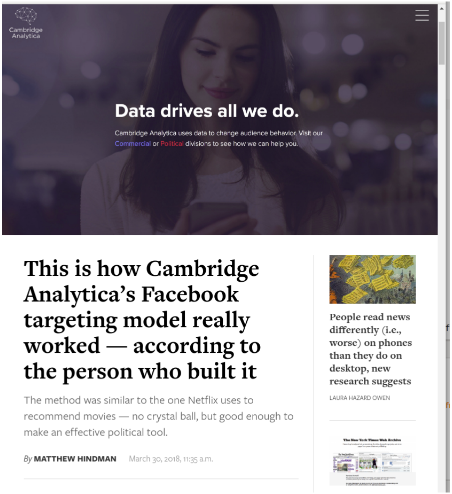
Organizational aspects

- Lecture dates: 16.4., 23.4., 30.4., 14.5., 28.5., 4.6., 11.6., 18.6., 25.6., 2.7. (tentative)
- Exam: To be discussed next week (most likely oral exam).
- Webpage: `https://www5.in.tum.de/wiki/index.php/Low_Rank_Approximation`
  Slides on `http://anchp.epfl.ch`.
- EFY = Exercise For You.

From http://www.niemanlab.org



Cambridge Analytica

Data drives all we do.

Cambridge Analytica uses data to change audience behavior. Visit our Commercial or Political divisions to see how we can help you.

This is how Cambridge Analytica's Facebook targeting model really worked — according to the person who built it

The method was similar to the one Netflix uses to recommend movies — no crystal ball, but good enough to make an effective political tool.

By MATTHEW HINDMAN March 30, 2018, 11:35 a.m.

People read news differently (i.e., worse) on phones than they do on desktop, new research suggests

LAURA HAZARD OWEN

... his [Aleksandr Kogan's] message went on to confirm that his approach was indeed similar to SVD or other matrix factorization methods, like in the Netflix Prize competition, and the Kosinki-Stillwell-Graepel Facebook model. Dimensionality reduction of Facebook data was the core of his model.

Rank and matrix factorizations

For field F, let $A \in F^{m\times n}$. Then

$$\text{rank}(A) := \dim(\text{range}(A)).$$

For simplicity, $F = \mathbb{R}$ throughout the lecture and often $m \geq n$.

Let $\mathcal{B} = \{b_1, \ldots, b_r\} \subset \mathbb{R}^m$ with $r = \text{rank}(A)$ be basis of range(A).
Then each of the columns of $A = \begin{pmatrix} a_1, a_2, \ldots, a_n \end{pmatrix}$ can be expressed as linear combination of $\mathcal{B}$:

$$a_j = \sum_{j=1}^{r} b_i c_{ij} \quad \text{for some coefficients } c_{ij} \in \mathbb{R},\ i = 1, \ldots, r,\ j = 1, \ldots, n.$$

Defining $B = \begin{pmatrix} b_1, b_2, \ldots, b_r \end{pmatrix} \in \mathbb{R}^{m\times r}$:

$$a_j = B \begin{pmatrix} c_{j1} \\ \vdots \\ c_{jr} \end{pmatrix} \quad \rightsquigarrow \quad A = B \begin{pmatrix} c_{11} & \cdots & c_{n1} \\ \vdots & & \vdots \\ c_{1r} & \cdots & c_{nr} \end{pmatrix}$$

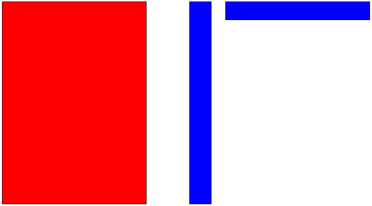
Rank and matrix factorizations

Lemma. A matrix $A \in \mathbb{R}^{m\times n}$ of rank r admits a factorization of the form

$$A = BC^T, \quad B \in \mathbb{R}^{m\times r}, \quad C \in \mathbb{R}^{n\times r}.$$

We say that A has low rank if $\operatorname{rank}(A) \ll m, n$.

Illustration of low-rank factorization:



	A	BC^T
#entries	mn	$mr + nr$

- Generically (and in most applications), A has full rank, that is, $\operatorname{rank}(A) = \min\{m, n\}$.
- Aim instead at approximating A by a low-rank matrix.

Questions addressed in lecture series

What? Theoretical foundations of low-rank approximation.

When? A priori and a posteriori estimates for low-rank approximation. Situations that allow for low-rank approximation techniques.

Why? Applications in engineering, scientific computing, data analysis, ... where low-rank approximation plays a central role.

How? State-of-the-art algorithms for performing and working with low-rank approximations.

Will cover both, matrices and tensors.

Contents of Lecture 1

1. Fundamental tools (SVD, relation to eigenvalues, norms, best low-rank approximation)
2. Overview of applications
3. Fundamental tools (Stability, QR)
4. Extensions (weighted approximation, bivariate functions)
5. Subspace iteration

Literature for Lecture 1

Golub/Van Loan'2013 Golub, Gene H.; Van Loan, Charles F. Matrix computations. Fourth edition. Johns Hopkins University Press, Baltimore, MD, 2013.

Horn/Johnson'2013 Horn, Roger A.; Johnson, Charles R. Matrix analysis. Second edition. Cambridge University Press, 2013.

\+ References on slides.

1. Fundamental tools

- SVD
- Relation to eigenvalues
- Norms
- Best low-rank approximation

The singular value decomposition

Theorem (SVD). Let $A \in \mathbb{R}^{m\times n}$ with $m \geq n$. Then there are orthogonal matrices $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ such that

$$A = U\Sigma V^T, \quad \text{with} \quad \Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{pmatrix} \in \mathbb{R}^{m\times n}$$

and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.

- $\sigma_1, \ldots, \sigma_n$ are called singular values
- $u_1, \ldots, u_m$ are called *left* singular vectors
- $v_1, \ldots, v_n$ are called *right* singular vectors
- $Av_i = \sigma_i u_i$, $A^T u_i = \sigma_i v_i$ for $i = 1, \ldots, n$.
- Singular values are always uniquely defined by A.
- Singular values are *never* unique. If $\sigma_1 > \sigma_2 > \cdots \sigma_n > 0$ then unique up to $u_i \leftarrow \pm u_i$, $v_i \leftarrow \pm v_i$.

SVD: Sketch of proof

Induction over n. $n = 1$ trivial.

For general n, let v_1 solve $\max\{\|Av\|_2 : \|v\|_2 = 1\} =: \|A\|_2$. Set $\sigma_1 := \|A\|_2$ and $u_1 := Av_1/\sigma_1$.[1] By definition,

$$Av_1 = \sigma_1 u_1.$$

After completion to orthogonal matrices $U_1 = \begin{pmatrix} u_1, & U_\perp \end{pmatrix} \in \mathbb{R}^{m\times m}$ and $V_1 = \begin{pmatrix} v_1, & V_\perp \end{pmatrix} \in \mathbb{R}^{n\times n}$:

$$U_1^T A V_1 = \left(\begin{array}{c|c} u_1^T A v_1 & u_1^T A V_\perp \\ \hline U_\perp^T A v_1 & U_\perp^T A V_\perp \end{array}\right) = \left(\begin{array}{c|c} \sigma_1 & w^T \\ \hline 0 & A_1 \end{array}\right),$$

with $w := V_\perp^T A^T u_1$ and $A_1 = U_\perp^T A V_\perp$. $\|\cdot\|_2$ invariant under orthogonal transformations $\rightsquigarrow$

$$\sigma_1 = \|A\|_2 = \|U_1^T A V_1\|_2 = \left\| \left(\begin{array}{c|c} \sigma_1 & w^T \\ \hline 0 & A_1 \end{array}\right) \right\|_2 \geq \sqrt{\sigma_1^2 + \|w\|_2^2}.$$

Hence, $w = 0$. Proof completed by applying induction to A_1.

[1] If $\sigma_1 = 0$, choose arbitrary u_1.

Very basic properties of the SVD

- $r = \text{rank}(A)$ is number of nonzero singular values of A.
- $\text{kernel}(A) = \text{span}\{v_{r+1}, \ldots, v_n\}$
- $\text{range}(A) = \text{span}\{u_1, \ldots, u_r\}$

SVD: Computation (for small dense matrices)

Computation of SVD proceeds in two steps:

1. Reduction to bidiagonal form: By applying n Householder reflectors from left and $n-1$ Householder reflectors from right, compute orthogonal matrices U_1, V_1 such that

$$U_1^T A V_1 = B = \begin{pmatrix} B_1 \\ 0 \end{pmatrix} = \begin{pmatrix} \diagdown\!\diagdown \\ 0 \end{pmatrix},$$

   that is, $B_1 \in \mathbb{R}^{n \times n}$ is an upper bidiagonal matrix.

2. Reduction to diagonal form: Use Divide&Conquer to compute orthogonal matrices U_2, V_2 such that $\Sigma = U_2^T B_1 V_2$ is diagonal.

   Set $U = U_1 U_2$ and $V = V_1 V_2$.

Step 1 is usually the most expensive. Remarks on Step 1:

- If m is significantly larger than n, say, $m \geq 3n/2$, first computing QR decomposition of A reduces cost.
- Most modern implementations reduce A successively via banded form to bidiagonal form.[2]

[2] Bischof, C. H.; Lang, B.; Sun, X. A framework for symmetric band reduction. ACM Trans. Math. Software 26 (2000), no. 4, 581–601.

SVD: Computation (for small dense matrices)

In most applications, vectors $u_{n+1}, \dots, u_m$ are not of interest. By omitting these vectors one obtains the following variant of the SVD.

Theorem (Economy size SVD). Let $A \in \mathbb{R}^{m\times n}$ with $m \geq n$. Then there is a matrix $U \in \mathbb{R}^{m\times n}$ with orthonormal columns and an orthonormal matrix $V \in \mathbb{R}^{n\times n}$ such that

$$A = U\Sigma V^T, \quad \text{with} \quad \Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \in \mathbb{R}^{n\times n}$$

and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.

Computed by MATLAB's `[U,S,V] = svd(A,'econ')`.

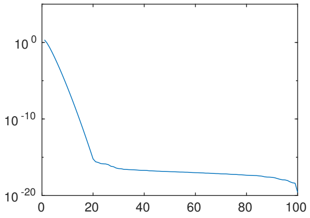
Complexity:

	memory	operations
singular values only	$\mathcal{O}(mn)$	$\mathcal{O}(mn^2)$
economy size SVD	$\mathcal{O}(mn)$	$\mathcal{O}(mn^2)$
(full) SVD	$\mathcal{O}(m^2 + mn)$	$\mathcal{O}(m^2 n + mn^2)$

SVD: Computation (for small dense matrices)

Beware of roundoff error when interpreting singular value plots.

Exmaple: `semilogy(svd(hilb(100)))`



- Kink is caused by roundoff error and does not reflect true behavior of singular values.
- Exact singular values are known to decay exponentially.[3]
- *Sometimes* more accuracy possible.[4].

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[3] Beckermann, B. The condition number of real Vandermonde, Krylov and positive definite Hankel matrices. Numer. Math. 85 (2000), no. 4, 553–577.

[4] Drmač, Z.; Veselić, K. New fast and accurate Jacobi SVD algorithm. I. SIAM J. Matrix Anal. Appl. 29 (2007), no. 4, 1322–1342

Singular/eigenvalue relations: symmetric matrices

Symmetric $A = A^T \in \mathbb{R}^{n \times n}$ admits spectral decomposition

$$A = U \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) U^T$$

with orthogonal matrix U.

After reordering may assume $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$. Spectral decomposition can be turned into SVD $A = U \Sigma V^T$ by defining

$$\Sigma = \operatorname{diag}(|\lambda_1|, \ldots, |\lambda_n|), \quad V = U \operatorname{diag}(\operatorname{sign}(\lambda_1), \ldots, \operatorname{sign}(\lambda_n)).$$

Remark: This extends to the more general case of normal matrices (e.g., orthogonal or symmetric) via complex spectral or real Schur decompositions.

Singular/eigenvalue relations: general matrices

Consider SVD $A = U\Sigma V^T$ of $A \in \mathbb{R}^{m\times n}$ with $m \geq n$. We then have:

1. Spectral decomposition of Gramian
   $A^TA = V\Sigma^T\Sigma V^T = V\,\mathrm{diag}(\sigma_1^2, \dots, \sigma_n^2)V^T \rightsquigarrow$
   A^TA has eigenvalues $\sigma_1^2, \dots, \sigma_n^2$,
   right singular vectors of A are eigenvectors of A^TA.
2. Spectral decomposition of Gramian
   $AA^T = U\Sigma\Sigma^TU^T = U\,\mathrm{diag}(\sigma_1^2, \dots, \sigma_n^2, 0, \dots, 0)U^T \rightsquigarrow$
   AA^T has eigenvalues $\sigma_1^2, \dots, \sigma_n^2$ and, additionally, $m - n$ zero eigenvalues,
   first n left singular vectors A are eigenvectors of AA^T.
3. Decomposition of Golub-Kahan matrix

$$\mathcal{A} = \begin{pmatrix} 0 & A \\ A^T & 0 \end{pmatrix} = \begin{pmatrix} U & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} 0 & \Sigma \\ \Sigma^T & 0 \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & V \end{pmatrix}^T.$$

EFY. Prove that $\mathcal{A}$ has eigenvalues $\pm\sigma_j$ with eigenvectors $\frac{1}{\sqrt{2}}\begin{pmatrix} \pm u_j \\ v_j \end{pmatrix}$.

Norms: Spectral and Frobenius norm

Given SVD $A = U\Sigma V^T$, one defines:

- Spectral norm: $\|A\|_2 = \sigma_1$.
- Frobenius norm: $\|A\|_F = \sqrt{\sigma_1^2 + \cdots + \sigma_n^2}$.

Basic properties:

- $\|A\|_2 = \max\{\|Av\|_2 \,:\, \|v\|_2 = 1\}$ (see proof of SVD).
- $\|\cdot\|_2$ and $\|\cdot\|_F$ are both (submultiplicative) matrix norms.
- $\|\cdot\|_2$ and $\|\cdot\|_F$ are both unitarily invariant, that is

$$\|QAZ\|_2 = \|A\|_2, \qquad \|QAZ\|_F = \|A\|_F$$

  for any orthogonal matrices Q, Z.
- $\|A\|_2 \le \|A\|_F \le \|A\|_2/\sqrt{r}$
- $\|AB\|_F \le \min\{\|A\|_2\|B\|_F, \|A\|_F\,\|B\|_2\}$

EFY. Prove these two inequalities. Hint for the second inequality: Use the relations on the next slide to first show that $\|B\|_F = \|(\|b_1\|_2, \ldots, \|b_n\|_2)\|_F$.

EFY. Find a matrix $A \in \mathbb{R}^{m_1 \times n}$ and a *nonzero* matrix $B \in \mathbb{R}^{m_2 \times n}$ such that $\|A\|_2 = \left\|\begin{pmatrix} A \\ B \end{pmatrix}\right\|_2$. Classify the set of matrices $A \in \mathbb{R}^{m_1 \times n}$ such that $\|A\|_2 < \left\|\begin{pmatrix} A \\ B \end{pmatrix}\right\|_2$ for *every* nonzero matrix $B \in \mathbb{R}^{m_2 \times n}$.
Investigate analogous questions for the Frobenius norm.

Euclidean geometry on matrices

Let $B \in \mathbb{R}^{n \times n}$ have eigenvalues $\lambda_1, \ldots, \lambda_n \in \mathbb{C}$. Then

$$\operatorname{trace}(B) := b_{11} + \cdots + b_{nn} = \lambda_1 + \cdots + \lambda_n.$$

In turn,

$$\|A\|_F^2 = \operatorname{trace} A^T A = \operatorname{trace} AA^T = \sum_{i,j} a_{ij}^2.$$

Two simple consequences:

- $\|\cdot\|_F$ is the norm induced by the matrix inner product

$$\langle A, B\rangle := \operatorname{trace}(AB^T), \qquad A, B \in \mathbb{R}^{m \times n}.$$

- Partition $A = \big(a_1, a_2, \ldots, a_n\big)$ and define vectorization

$$\operatorname{vec}(A) = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} \in \mathbb{R}^{mn}.$$

Then $\langle A, B\rangle = \langle \operatorname{vec}(A), \operatorname{vec}(B)\rangle$ and $\|A\|_F = \|\operatorname{vec}(A)\|_2$.

Von Neumann's trace inequality

Theorem

For $m \geq n$, let $A, B \in \mathbb{R}^{m \times n}$ have singular values $\sigma_1(A) \geq \cdots \geq \sigma_n(A)$ and $\sigma_1(B) \geq \cdots \geq \sigma_n(B)$, respectively. Then

$$|\langle A, B \rangle| \leq \sigma_1(A)\sigma_1(B) + \cdots + \sigma_n(A)\sigma_n(B).$$

Consequence:

$$\begin{aligned} \|A - B\|_F^2 &= \langle A - B, A - B \rangle = \|A\|_F^2 - 2\langle A, B \rangle + \|B\|_F^2 \\ &\geq \|A\|_F^2 - 2\sum_{i=1}^{n} \sigma_i(A)\sigma_i(B) + \|B\|_F^2 \\ &= \sum_{i=1}^{n} (\sigma_i(A) - \sigma_i(B))^2. \end{aligned}$$

EFY. Use Von Neumann's trace inequality and the SVD to show for $1 \leq k \leq n$ that

$$\max\{ |\langle A, PQ^T \rangle| : P \in \mathbb{R}^{m \times k}, Q \in \mathbb{R}^{n \times k}, P^T P = Q^T Q = I_k \} = \sigma_1(A) + \cdots + \sigma_k(A).$$

Proof of Von Neumann's trace inequality[5]

Singular value vector $\sigma(A)$ can be written as convex combination

$$\sigma(A) = \sigma_n(A) f_n + (\sigma_{n-1}(A) - \sigma_n(A)) f_{n-1} + \cdots$$

with $f_j = e_1 + \cdots + e_j$. Decompose A analogously via its SVD $A = U_A \Sigma_A V_A^T$:

$$A = \sigma_n(A) A_n + (\sigma_{n-1}(A) - \sigma_n(A)) A_{n-1} + \cdots , \quad A_j := U_A \mathrm{diag}(f_j) V_A^T$$

Insert in lhs of trace inequality:

$$|\langle A, B\rangle| \le \sigma_n(A) |\langle A_n, B\rangle| + (\sigma_{n-1}(A) - \sigma_n(A)) |\langle A_{n-1}, B\rangle| + \cdots .$$

Rhs is linear wrt $\sigma(A)$ $\rightsquigarrow$ May assume $A = A_k$ for $k = 1, \ldots, n$. Analogously for B.

[5] This proof follows [Grigorieff, R. D. Note on von Neumann's trace inequality. Math. Nachr. 151 (1991), 327–328]. For Mirsky's ingenious proof based on doubly stochastic matrices; see Theorem 8.7.6 in [Horn/Johnson'2013].

Proof of Von Neumann's trace inequality

Let $A = U_A \text{diag}(f_k) V_A^T$, $B = U_B \text{diag}(f_\ell) V_B^T$, and $k \leq \ell$. Then

$$\begin{aligned}
\langle A, B \rangle &= \text{trace}\left(\sum_{i=1}^{k} v_{A,i} u_{A,i}^T \sum_{j=1}^{\ell} u_{B,j} v_{B,j}^T \right) \\
&= \sum_{i=1}^{k} \sum_{j=1}^{\ell} \text{trace}\left(v_{A,i} u_{A,i}^T u_{B,j} v_{B,j}^T \right) \\
&= \sum_{i=1}^{k} \sum_{j=1}^{\ell} (u_{A,i}^T u_{B,j})(v_{B,j}^T v_{A,i})
\end{aligned}$$

Cauchy-Schwartz$\rightsquigarrow$

$$|\langle A, B \rangle| \leq \sum_{i=1}^{k} \| U_B^T u_{A,i} \|_2 \| V_B^T v_{A,i} \|_2 = k,$$

which completes the proof.

Schatten norms

There are other unitarily invariant matrix norms.[6]

Let $s(A) = (\sigma_1, \ldots, \sigma_n)$. The p-Schatten norm defined by

$$\|A\|_{(p)} := \|s(A)\|_p$$

is a matrix norm for any $1 \le p \le \infty$.

$p = \infty$: spectral norm, $p = 2$: Frobenius norm, $p = 1$: nuclear norm.

EFY. What is $\lim_{p \to 0+} \|A\|_{(p)}$?

Definition

The dual of a matrix norm $\|\cdot\|$ on $\mathbb{R}^{m \times n}$ is defined by

$$\|A\|^D = \max\{\langle A, B\rangle : \ \|B\| = 1\}.$$

Lemma

Let $p, q \in [1, \infty]$ such that $p^{-1} + q^{-1} = 1$. Then

$$\|A\|^D_{(p)} = \|A\|_{(q)}.$$

EFY. Prove this lemma for $p = \infty$. Hint: Von Neumann's trace inequality.

[6] Complete characterization via symm gauge functions in [Horn/Johnson'2013].

Best low-rank approximation

Consider $k < n$ and let

$$U_k := \begin{pmatrix} u_1 & \cdots & u_k \end{pmatrix}, \quad \Sigma_k := \operatorname{diag}(\sigma_1, \ldots, \sigma_k), \quad V_k := \begin{pmatrix} u_1 & \cdots & u_k \end{pmatrix}.$$

Then

$$\mathcal{T}_k(A) := U_k \Sigma_k V_k^T$$

has rank at most k. For any unitarily invariant norm $\|\cdot\|$:

$$\|\mathcal{T}_k(A) - A\| = \big\|\operatorname{diag}(0, \ldots, 0, \sigma_{k+1}, \ldots, \sigma_n)\big\|$$

In particular, for spectral norm and the Frobenius norm:

$$\|A - \mathcal{T}_k(A)\|_2 = \sigma_{k+1}, \qquad \|A - \mathcal{T}_k(A)\|_F = \sqrt{\sigma_{k+1}^2 + \cdots + \sigma_n^2}.$$

Nearly equal if and only if singular values decay sufficiently quickly.

Best low-rank approximation

Theorem (Schmidt-Mirsky). Let $A \in \mathbb{R}^{m\times n}$. Then

$$\|A - \mathcal{T}_k(A)\| = \min\left\{\|A - B\| : \ B \in \mathbb{R}^{m\times n} \text{ has rank at most } k\right\}$$

holds for any unitarily invariant norm $\|\cdot\|$.

Proof[7] *for* $\|\cdot\|_F$: Follows directly from consequence of Von Neumann's trace inequality.

Proof for $\|\cdot\|_2$: For any $B \in \mathbb{R}^{m\times n}$ of rank $\leq k$, kernel(B) has dimension $\geq n-k$. Hence, $\exists w \in \text{kernel}(B) \cap \text{range}(V_{k+1})$ with $\|w\|_2 = 1$. Then

$$\begin{aligned}
\|A - B\|_2^2 &\geq \|(A-B)w\|_2^2 = \|Aw\|_2^2 = \|AV_{k+1}V_{k+1}^T w\|_2^2 \\
&= \|U_{k+1}\Sigma_{k+1}V_{k+1}^T w\|_2^2 \\
&= \sum_{j=1}^{r+1} \sigma_j |v_j^T w|^2 \geq \sigma_{k+1} \sum_{j=1}^{r+1} |v_j^T w|^2 = \sigma_{k+1}.
\end{aligned}$$

[7] See Section 7.4.9 in [Horn/Johnson'2013] for the general case.

Best low-rank approximation

Uniqueness:

- If $\sigma_k > \sigma_{k+1}$ best rank-k approximation with respect to Frobenius norm is unique.
- If $\sigma_k = \sigma_{k+1}$ best rank-k approximation never unique. For example I_3 has several best rank-two approximations:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

- With respect to spectral norm best rank-k approximation only unique if $\sigma_{k+1} = 0$. For example, $\mathrm{diag}(2, 1, \epsilon)$ with $0 < \epsilon < 1$ has infinitely many best rank-two approximations:

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 2-\epsilon/2 & 0 & 0 \\ 0 & 1-\epsilon/2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 2-\epsilon/3 & 0 & 0 \\ 0 & 1-\epsilon/3 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ldots.$$

EFY. Given a symmetric matrix $A \in \mathbb{R}^{n \times n}$ and $1 \leq k < n$, show that there is always a best rank-k approximation that is symmetric. Is every best rank-k approximation (with respect to Frobenius norm) symmetric? What about the spectral norm?

Approximating the range of a matrix

Aim at finding a matrix $Q \in \mathbb{R}^{m \times k}$ with orthonormal columns such that

$$\operatorname{range}(Q) \approx \operatorname{range}(A).$$

$I - QQ^T$ is orthogonal projector onto $\operatorname{range}(Q)^\perp \rightsquigarrow$
Aim at minimizing

$$\|(I - QQ^T)A\| = \|A - QQ^T A\|$$

for unitarily invariant norm $\|\cdot\|$. Because $\operatorname{rank}(QQ^T A) \le k$,

$$\|A - QQ^T A\| \ge \|A - \mathcal{T}_k(A)\|.$$

Setting $Q = U_k$ one obtains

$$U_k U_k^T A = U_k U_k^T U \Sigma V^T = U_k \Sigma_k V_k^T = \mathcal{T}_k(A).$$

$\rightsquigarrow Q = U_k$ is optimal.

Approximating the range of a matrix

Variation:

$$\max\{\|Q^T A\|_F : \; Q^T Q = I_k\}.$$

Equivalent to

$$\max\{|\langle AA^T, QQ^T\rangle| : \; Q^T Q = I_k\}.$$

By Von Neumann's trace inequality and equivalence between eigenvectors of AA^T and left singular vectors of A, optimal Q given by U_k.

EFY. When replacing the Frobenius norm by the spectral norm in this formulation, does one obtain the same result?

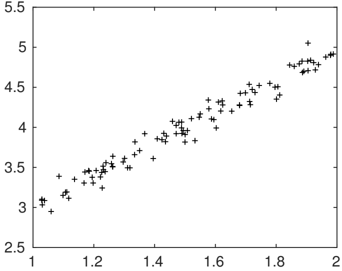
2. Applications

- Principal Component Analysis
- Matrix Completion
- Some other applications

Principal Component Analysis (PCA)

- Most popular method for dimensionality reduction in statistics, data science, ...

Consider N independently drawn observations for K random variables $X_1, \ldots, X_K$. Illustration of $N = 100$ observations for $K = 2$:



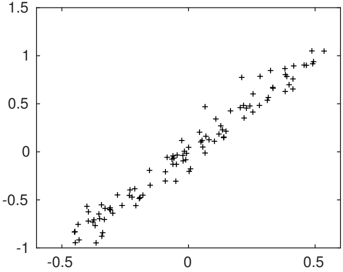
Principal Component Analysis (PCA)

Each of the observations is arranged in a vector $x_j \in \mathbb{R}^K$ with $j = 1, \ldots, N$.

Subtract sample mean

$$\overline{x} := \frac{1}{N}(x_1 + \cdots + x_N)$$

Date with mean subtracted:



Principal Component Analysis (PCA)

Covariance matrix

$$C := \frac{1}{N-1} \sum_{j=1}^{N} (x_j - \overline{x})(x_j - \overline{x})^T.$$

Diagonal entry c_{ii} estimates variance of X_i, while off-diagonal entry c_{ik} estimates covariance between X_i and X_k.

Defining $A := \left[x_1 - \overline{x},\ \ldots,\ x_N - \overline{x}\right] \in \mathbb{R}^{K \times N}$, we can equivalently write

$$C = \frac{1}{N-1} AA^T.$$

Principal Component Analysis (PCA)

Reduce data to dimension 1:
Find linear combination $Y_1 = w_1 X_1 + \cdots + w_K X_K$ with $w_1, \ldots, w_K \in \mathbb{R}$ and $w_1^2 + \cdots + w_K^2 = 1$ that captures most of the observed variation.

Maximize variance of new variable Y_1.

Corresponding observations of Y_1 given by $w^T x_1, \ldots, w^T x_N$ with sample mean $w^T \overline{x}$ $\rightsquigarrow$ maximization of variance corresponds to

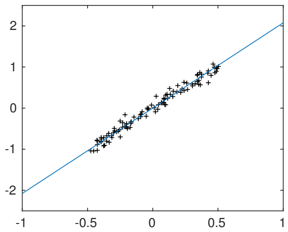
$$\max_{\substack{w \in \mathbb{R}^N \\ \|w\|_2 = 1}} \sum_{j=1}^{N} (w^T x_j - w^T \overline{x})^2 = \max_{\substack{w \in \mathbb{R}^N \\ \|w\|_2 = 1}} \|w^T A\|_2^2.$$

Optimal vector w given by dominant left singular vector of A!
(Corresponds to eigenvector for largest eigenvalue of AA^T.)

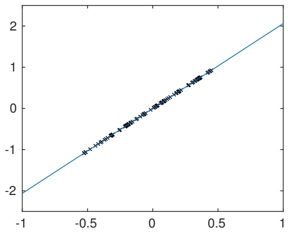
This is the first principal vector.

Principal Component Analysis (PCA)

Data with first principal vector:



Projection of data onto first principal vector:



Principal Component Analysis (PCA)

- Analogously, first k principal vectors given by dominant k left singular vectors $u_1, \ldots, u_k$. Equivalent to best rank-k approximation of data matrix:

$$\min_{U^T U = I_k} \|A - UC^T\|$$

- PCA not robust wrt outliers in data. Robust PCA[8] uses model

$$A \approx \text{low rank} + \text{sparse}.$$

Obtained via solution of

$$\min\{\|L\|_{(1)} + \lambda\|S\|_1 : A = L + S\},$$

for multiplier $\lambda > 0$ and $\|S\|_1 =$ 1-norm of vec(S).

[8] Emmanuel J. Candes; Xiaodong Li; Yi Ma; John Wright. Robust Principal Component Analysis?

Matrix Completion

				
Alice	4			4
Bob		5	4	
Joe		5		
Sam	5			

Assume that data matrix is modeled by (low) rank k. Two popular approaches to deal with missing entries:

1. Impute data (insert 0 or row/column means in missing entries). Apply SVD to get best low-rank approximation BC^T of imputed data matrix.
2. Find rank-k matrix BC^T that fits known entries best; measured in (weighted) Euclidean norm.

Predict unknown entries from BC^T.

Netflix prize won by combination of matrix completion with other techniques.

Applications in Scientific Computing and Engineering

- POD, reduced basis method, reduced-order modelling.
- High-dimensional integration.
- Solution of large-scale matrix equations. Optimal control.
- Solution of high-dimensional PDEs.
- Uncertainty quantification.
- ...

Several of these will be covered in later parts of the course.

3. Fundamental Tools

- Stability of SVD
- Canonical angles
- Stability of low-rank approximation
- QR decomposition

Stability of SVD

What happens to SVD if A is perturbed by noise?

Lemma

Let $A, E \in \mathbb{R}^{m\times n}$. Then

$$|\sigma_i(A+E) - \sigma_i(A)| \le \|E\|_2.$$

Proof.

Using the characterization

$$\sigma_i(A+E) = \min\{\|B\|_2 : \mathrm{rank}(A+E-B) \le i-1\}$$

and setting $B = A - \mathcal{T}_{i-1}(A) + E$, we obtain

$$\sigma_i(A+E) \le \|B\|_2 \le \|A - \mathcal{T}_{i-1}(A)\|_2 + \|E\|_2 = \sigma_i(A) + \|E\|_2,$$

which implies the result. □

Result also special case of famous Weyl's inequality.

EFY. Show that the matrix rank is a lower semi-continuous function.

Stability of SVD

Singular values are perfectly well conditioned.

Singular vectors tend to be less stable! Example:

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1+\varepsilon \end{pmatrix}, \qquad E = \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & -\varepsilon \end{pmatrix}.$$

- A has right singular vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.
- $A + E$ has right singular vectors $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

To formulate perturbation bound, need to measure distances between subspaces.

Canonical angles

Let columns of $X, Y \in \mathbb{C}^{n \times k}$ contain orthonormal bases of two k-dimensional subspaces $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^n$, respectively. Denote singular values (in reverse order) of $X^T Y$:

$$0 \leq \sigma_1 \leq \cdots \leq \sigma_p \leq 1.$$

We call

$$\theta_i(\mathcal{X}, \mathcal{Y}) := \arccos \sigma_i, \quad i = 1, \ldots, k,$$

the canonical angles between $\mathcal{X}$ and $\mathcal{Y}$. Note: For $k = 1$, θ_1 is the usual angle $\theta(x, y)$ between vectors.

Geometric characterization:

$$\theta_1(\mathcal{X}, \mathcal{Y}) = \max_{\substack{x \in \mathcal{X} \\ x \neq 0}} \min_{\substack{y \in \mathcal{Y} \\ y \neq 0}} \theta(x, y).$$

It follows that $\theta_1(\mathcal{X}, \mathcal{Y}) = 0$ if and only if $\mathcal{X} \cap \mathcal{Y}^\perp \neq \{0\}$.

Canonical angles

Note that XX^T and YY^T are orthogonal projectors on $\mathcal{X}$ and $\mathcal{Y}$, respectively.

Lemma (Projector characterization)

Define $\sin\Theta(\mathcal{X},\mathcal{Y}) = \mathrm{diag}(\sin\theta_1(\mathcal{X},\mathcal{Y}),\dots,\sin\theta_p(\mathcal{X},\mathcal{Y}))$. *Then*

$$\sin\theta_1(\mathcal{X},\mathcal{Y}) = \|\sin\Theta(\mathcal{X},\mathcal{Y})\|_2 = \|XX^T - YY^T\|_2.$$

Proof. See Theorem I.5.5 in [Stewart/Sun'1990].

Lemma

Let $Q \in \mathbb{R}^{(n-k)\times k}$, *and* $\mathcal{X} = \mathrm{range}\begin{pmatrix} I_k \\ 0 \end{pmatrix}$, $\mathcal{Y} = \mathrm{range}\begin{pmatrix} I_p \\ Q \end{pmatrix}$.

Then $\theta_1(\mathcal{X},\mathcal{Y}) = \arctan\|Q\|_2$.

Proof.

The columns of $\binom{I_p}{Q}(I+Q^TQ)^{-1/2}$ form an orthonormal basis of $\mathcal{Y}$. By definition, this implies that $\cos\theta_1(\mathcal{X},\mathcal{Y})$ is the smallest singular value of $(I+Q^TQ)^{-1/2}$. By the SVD of Q, it follows that

$$\cos\theta_1(\mathcal{X},\mathcal{Y}) = \frac{1}{\sqrt{1+\|Q\|_2^2}}.$$

Stability of SVD

Theorem (Wedin). Let $k < n$ and assume

$$\delta := \sigma_k(A + E) - \sigma_{k+1}(A) > 0.$$

Let $\mathcal{U}_k/\tilde{\mathcal{U}}_k/\mathcal{V}_k/\tilde{\mathcal{V}}_k$ denote subspaces spanned by first k left/right singular vectors of A / $A + E$. Then

$$\sqrt{\|\sin\Theta(\mathcal{U}_k, \tilde{\mathcal{U}}_k)\|_F^2 + \|\sin\Theta(\mathcal{V}_k, \tilde{\mathcal{V}}_k)\|_F^2} \leq \sqrt{2}\frac{\|E\|_F}{\delta}. \tag{1}$$

Θ: diagonal matrix containing canonical angles between two subspaces.

- Perturbation on input multiplied by $\delta^{-1} \approx [\sigma_k(A) - \sigma_{k+1}(A)]^{-1}$.
- Bad news for stability of low-rank approximations?

Stability of low-rank approximation

Lemma. Let $A \in \mathbb{R}^{m\times n}$ have rank $\leq k$. Then

$$\|\mathcal{T}_k(A+E) - A\| \leq C\|E\|$$

holds with $C = 2$ for any unitarily invariant norm $\|\cdot\|$. For the Frobenius norm, the constant can be improved to $C = (1+\sqrt{5})/2$.

Proof. Schmidt-Mirsky gives $\|\mathcal{T}_k(A+E) - (A+E)\| \leq \|E\|$. Triangle inequality implies

$$\|\mathcal{T}_k(A+E) - (A+E) + (A+E) - A\| \leq 2\|E\|.$$

Second part is result by Hackbusch[9]. □

Implication for general matrix A:

$$\begin{aligned} \|\mathcal{T}_k(A+E) - \mathcal{T}_k(A)\| &= \big\|\mathcal{T}_k\big(\mathcal{T}_k(A) + (A - \mathcal{T}_k(A)) + E\big) - \mathcal{T}_k(A)\big\| \\ &\leq C\|(A - \mathcal{T}_k(A)) + E\| \leq C(\|A - \mathcal{T}_k(A)\| + \|E\|). \end{aligned}$$

Perturbations on the level of truncation error pose no danger.

---

[9] Hackbusch, W. New estimates for the recursive low-rank truncation of block-structured matrices. Numer. Math. 132 (2016), no. 2, 303–328

Stability of low-rank approximation: Application

Consider partitioned matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \qquad A_{ij} \in \mathbb{R}^{m_i \times n_j},$$

and desired rank $k \le m_i, n_j$. Let $\varepsilon := \|\mathcal{T}_k(A) - A\|$.

$$E_{ij} := \mathcal{T}_k(A_{ij}) - A_{ij} \qquad \Rightarrow \qquad \|E_{ij}\| \le \varepsilon.$$

By stability of low-rank approximation,

$$\left\| \mathcal{T}_k \begin{pmatrix} \mathcal{T}_k(A_{11}) & \mathcal{T}_k(A_{12}) \\ \mathcal{T}_k(A_{21}) & \mathcal{T}_k(A_{22}) \end{pmatrix} - A \right\|_F = \left\| \mathcal{T}_k \left(A + \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix} \right) - A \right\|_F \le C\varepsilon,$$

with $C = \frac{3}{2}(1 + \sqrt{5})$.

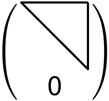
This allows, e.g., to perform truncations in parallel.

The QR decomposition

Theorem

Let $X \in \mathbb{R}^{m\times n}$ with $m \geq n$. Then there is an orthogonal matrix $Q \in \mathbb{R}^{m\times m}$ such that

$$X = QR, \quad \text{with} \quad R = \begin{pmatrix} R_1 \\ 0 \end{pmatrix} =$$



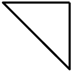
,

that is, $R_1 \in \mathbb{R}^{n\times n}$ is an upper triangular matrix.

MATLAB: `[Q,R] = qr(X)`.

Will use economy size QR decomposition instead: Letting $Q_1 \in \mathbb{C}^{m\times n}$ contain first n columns of Q, one obtains

$$X = Q_1 R_1 = Q_1 \cdot$$



.

MATLAB: `[Q,R] = qr(X,0)`.

EFY. Let $A = (a_1, a_2, \ldots, a_n)$ with $a_j \in \mathbb{R}^m$. Using the QR decomposition, show *Hadamard's inequality*:

$$|\det(A)| \leq \|a_1\|_2 \cdot \|a_2\|_2 \cdots \|a_n\|_2 .$$

Characterize the set of all $m \times n$ matrices A for which equality holds.

QR for recompression

Suppose that

$$A = BC^T, \quad \text{with} \quad B \in \mathbb{R}^{m \times K}, C \in \mathbb{R}^{n \times K}. \tag{2}$$

Goal: Compute best rank-k approximation of A for $k < K$.
Typical example: Sum of J matrices of rank k:

$$A = \sum_{j=1}^{J} \underbrace{B_i}_{\in \mathbb{R}^{m \times k}} \underbrace{C_i}_{\in \mathbb{R}^{n \times k}}{}^T = \underbrace{\begin{pmatrix} B_1 & \cdots & B_J \end{pmatrix}}_{\mathbb{R}^{m \times Jk}} \underbrace{\begin{pmatrix} C_1 & \cdots & C_J \end{pmatrix}}_{\mathbb{R}^{m \times Jk}}{}^T. \tag{3}$$

Algorithm to recompress A:

1. Compute (economic) QR decomps $B = Q_B R_B$ and $C = Q_C R_C$.
2. Compute truncated SVD $\mathcal{T}_k(R_B R_C^T) = \tilde{U}_k \Sigma_k \tilde{V}_k^T$.
3. Set $U_k = Q_B \tilde{U}_k$, $V_k = Q_C \tilde{V}_k$ and return $\mathcal{T}_k(A) := U_k \Sigma_k V_k^T$.

Returns best rank-k approximation of A with $O((m+n)K^2)$ ops.

4. Extensions

- Weighted and structured low-rank approximation
- Semi-separable approximation of bivariate functions

Weighted low-rank approximation

If some columns or rows are more important than others (e.g., they are known to be less corrupted by noise), replace low-rank approximation problem by

$$\min\left\{\|D_R(A-B)D_C\| : \ B \in \mathbb{R}^{m\times n} \text{ has rank at most } k\right\}$$

with suitably chosen pos def diagonal matrices D_R, D_C. More general:

Given invertible matrices $W_R \in \mathbb{R}^{m\times m}$, $W_C \in \mathbb{R}^{n\times n}$, weighted low-rank approximation problem consists of

$$\min\left\{\|W_R(A-B)W_C\| : \ B \in \mathbb{R}^{m\times n} \text{ has rank at most } k\right\}.$$

Solution given by

$$B = W_R^{-1} \cdot \mathcal{T}_k(W_R A W_C) \cdot W_C^{-1}$$

Proof: EFY.

Remark: Numerically more stable approach via generalized SVD [Golub/Van Loan'2013] .

Limit case: Infinite weights

Choosing diagonal weights that converge to $\infty \rightsquigarrow$ rows/columns remain unperturbed.

Case of fixed columns: Consider block column partition

$$A = \begin{pmatrix} A_1 & A_2 \end{pmatrix}.$$

Consider

$$\min \left\{ \|A_2 - B_2\| : \begin{pmatrix} A_1 & B_2 \end{pmatrix} \text{ has rank at most } k \right\}$$

No/trivial solution if $\text{rank}(A_1) \geq k$. Assume $\ell := \text{rank}(A_1) < k$ and let $X_1 \in \mathbb{R}^{n \times \ell}$ contain orthonormal basis of range(A_1). Then[10]

$$B_2 = X_1 X_1^T A_2 + \mathcal{T}_{k-\ell}\big((I - X_1 X_1^T) A_2\big).$$

[10] Golub, G. H.; Hoffman, A.; Stewart, G. W. A generalization of the Eckart-Young-Mirsky matrix approximation theorem. Linear Algebra Appl. 88/89 (1987), 317–327.

General weights

Given an $mn \times mn$ symmetric pos def matrix W, define

$$\|A\|_W = \sqrt{\mathrm{vec}(A)^T W \,\mathrm{vec}(A)}$$

Equals Frobenius norm for $W = I$. General weighted low-rank approximation problem:

$$\min \left\{ \|A - B\|_W : \; B \in \mathbb{R}^{m \times n} \text{ has rank at most } k \right\}.$$

EFY. Show that this problem can be rephrased as the previously considered (standard) weighted low-rank approximation problem for the case of a Kronecker product $W = W_2 \otimes W_1$. Hint: Cholesky decomposition.

- For general W no expression in terms of SVD available $\rightsquigarrow$ need to use general optimization method.
- Similarly, imposing general structures on A (such as nonnegativity, fixing individual entries, ...) usually does not admit solutions in terms of SVD. Often end up with NP-hard problems.

Separable approximation of bivariate functions

Given $\Omega_x \subset \mathbb{R}^{d_x}$ and $\Omega_y \subset \mathbb{R}^{d_y}$ aim at finding semi-separable approximation of $f \in L^2(\Omega_x \times \Omega_y) \cong L^2(\Omega_x) \otimes L^2(\Omega_y)$:

$$f(x,y) \approx g_1(x)h_1(y) + \cdots + g_r(x)h_r(y)$$

for $g_1, \ldots, g_r \in L^2(\Omega_x)$, $h_1, \ldots, h_r \in L^2(\Omega_y)$

Application to higher-dimensional integrals:

$$\begin{aligned}
& \int_{\Omega_x} \int_{\Omega_y} f(x,y) \mathrm{d}\mu_y(y)\, \mathrm{d}\mu_x(x) \\
\approx \quad & \sum_{i=1}^{r} \int_{\Omega_x} \int_{\Omega_y} g_i(x) h_i(y)\, \mathrm{d}\mu_y(y)\, \mathrm{d}\mu_x(x) \\
= \quad & \sum_{i=1}^{r} \Big[\int_{\Omega_x} g_i(x)\, \mathrm{d}\mu_x(x) \Big] \Big[\int_{\Omega_y} h_i(y)\, \mathrm{d}\mu_y(y) \Big]
\end{aligned}$$

$\rightsquigarrow$ semi-separable approximation breaks down dimensionality of integrals (for separable measures).

Separable approximation of bivariate functions

Given $f \in L^2(\Omega_x \times \Omega_y)$, consider linear operator

$$L_f : L^2(\Omega_x) \to L^2(\Omega_y), \quad w \mapsto \int_{\Omega_x} w(x) f(x, y) \, \mathrm{d}x.$$

Admits SVD

$$L_f(\cdot) = \sum_{i=1}^{\infty} \sigma_i u_i \langle v_i, \cdot \rangle$$

with L^2 orthonormal bases $u_1, u_2, \dots$ and $v_1, v_2, \dots$.
Best semi-separable approximation of f (in $L^2(\Omega_x \times \Omega_y)$) given by

$$f_r(x, y) = \sum_{i=1}^{r} \sigma_i u_i(x) v_i(y),$$

provided that $\sum_{i=1}^{\infty} \sigma_i^2 < \infty$ (Hilbert-Schmidt).

$$\|f - f_r\|_{L^2} = \sigma_{r+1}^2 + \sigma_{r+2}^2 + \cdots .$$

Separable and low-rank approximation

Choose discretization $x_1, \dots, x_m \in \Omega_x$, $y_1, \dots, y_m \in \Omega_y$. Define

$$F = \begin{pmatrix} f(x_1, y_1) & f(x_1, y_2) & \cdots & f(x_1, y_n) \\ f(x_2, y_1) & f(x_2, y_2) & \cdots & f(x_2, y_n) \\ \vdots & \vdots & & \vdots \\ f(x_m, y_1) & f(x_m, y_2) & \cdots & f(x_m, y_n) \end{pmatrix}$$

and

$$F_r = \begin{pmatrix} f_r(x_1, y_1) & f_r(x_1, y_2) & \cdots & f_r(x_1, y_n) \\ f_r(x_2, y_1) & f_r(x_2, y_2) & \cdots & f_r(x_2, y_n) \\ \vdots & \vdots & & \vdots \\ f_r(x_m, y_1) & f_r(x_m, y_2) & \cdots & f_r(x_m, y_n) \end{pmatrix} = \sum_{i=1}^{r} \begin{pmatrix} g_i(x_1) \\ g_i(x_2) \\ \vdots \\ g_i(x_m) \end{pmatrix} \begin{pmatrix} h_i(y_1) \\ h_i(y_2) \\ \vdots \\ h_i(y_n) \end{pmatrix}^T$$

F_r has rank at most r.

EFY. Prove $\|F - F_r\|_F^2 \leq \sigma_{r+1}^2 + \sigma_{r+2}^2 + \cdots$.

5. Subspace Iteration

Subspace iteration and low-rank approximation

Subspace iteration $=$ extension of power method.

Input: Matrix $A \in \mathbb{R}^{m \times n}$.

```
Choose starting matrix X^(0) ∈ R^{m×k} with (X^(0))^T X^(0) = I_k.
j = 0.
repeat
    Set j := j + 1.
    Compute Y^(j) := A A^T X^(j−1).
    Compute economy size QR factorization: Y^(j) = QR.
    Set X^(j) := Q.
until convergence is detected
```

Choose starting matrix $X^{(0)} \in \mathbb{R}^{m \times k}$ with $\left(X^{(0)}\right)^T X^{(0)} = I_k$.
$j = 0$.
repeat
  Set $j := j + 1$.
  Compute $Y^{(j)} := AA^T X^{(j-1)}$.
  Compute economy size QR factorization: $Y^{(j)} = QR$.
  Set $X^{(j)} := Q$.
until convergence is detected

As will soon be seen, converges to basis of dominant subspace $\mathcal{U}_k$.

Low-rank approximation obtained from

$$\mathcal{T}_k(A) \approx X^{(j)} \left(X^{(j)}\right)^T A.$$

Convergence of subspace iteration

Theorem

Consider SVD $A = U\Sigma V^T$ *and, for* $k < n$*, let* $\mathcal{U}_k = \operatorname{span}\{u_1, \dots, u_k\}$*. Assume that* $\sigma_{k+1} > \sigma_k$ *and* $\theta_1(\mathcal{U}_k, \mathcal{X}^{(0)}) < \pi/2$*. Then the iterates* $\mathcal{X}^{(j)} = \operatorname{range}(X^{(j)})$ *of the subspace iteration satisfy*

$$\tan\theta_1(\mathcal{U}_k, \mathcal{X}^{(j)}) = \left|\frac{\sigma_{k+1}}{\sigma_k}\right|^{2j} \tan\theta_1(\mathcal{U}_k, \mathcal{X}^{(0)}).$$

Sketch of proof. As angles do not depend on choice of bases, may omit QR decompositions $\rightsquigarrow X^{(j)} = (AA^T)^j X^{(0)}$. By SVD of A, may set $A = \Sigma$ and hence $\mathcal{U}_k = \operatorname{span}\{e_1, \dots, e_k\}$. Partition

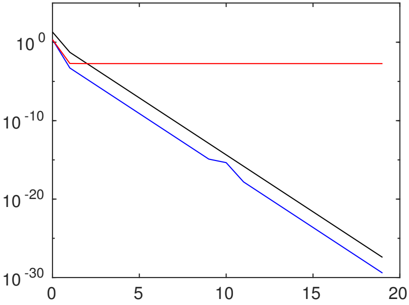
$$\Sigma = \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix}, \quad X^{(0)} = \begin{pmatrix} X_1^{(0)} \\ X_2^{(0)} \end{pmatrix}, \quad \Sigma_1, X_1^{(0)} \in \mathbb{R}^{k\times k}.$$

Result follows from applying expression for tangent of θ_1. □

EFY. Complete details of proof.

Numerical experiments

Convergence of subspace iteration for 100×100 Hilbert matrix.
$k = 5 \rightsquigarrow \sigma_{k+1}/\sigma_k = 0.188$. Random starting guess.



Black curve:
$\tan \theta_1(\mathcal{U}_k, \mathcal{X}^{(j)})$

Blue curve:
$\|\mathcal{T}_7(A) - X^{(j)}\big(X^{(j)}\big)^T A\|_2$

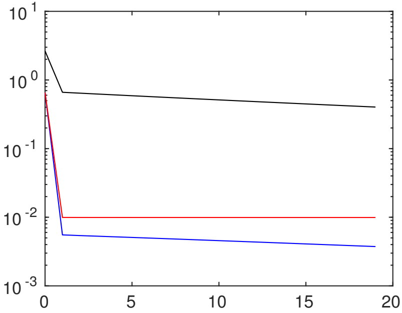
Red curve:
$\|A - X^{(j)}\big(X^{(j)}\big)^T A\|_2$

Numerical experiments

Convergence of subspace iteration for matrix with singular values

$$1, 0.99, 0.98, \frac{1}{10}, \frac{0.99}{10}, \frac{0.98}{10}, \frac{1}{100}, \frac{0.99}{100}, \frac{0.98}{100}, \ldots$$

$k = 7 \rightsquigarrow \sigma_{k+1}/\sigma_k = 0.99$. Random starting guess.



Black curve:
$\tan \theta_1(\mathcal{U}_k, \mathcal{X}^{(j)})$

Blue curve:
$\|\mathcal{T}_7(A) - X^{(j)}\left(X^{(j)}\right)^T A\|_2$

Red curve:
$\|A - X^{(j)}\left(X^{(j)}\right)^T A\|_2$

Numerical experiments

Observations:

- Low-rank approximation sufficiently good (for most purposes) already after 1 iteration.
- Convergence to dominant subspace arbitrarily slow, but not relevant.
- Classical, asymptotic convergence analysis insufficient.
- Pre-asymptotic analysis needs to take randomization of starting guess into account.