Eigenvalues and Singular Values

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[1]Course MATH-UA.0252/MA-UY_4424, Spring 2021

Spring 2021

Outline

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The need for iterative algorithms

- The eigenvalues are roots of the **characteristic polynomial** of **A**, which is generally of order n.
- According to Abel's theorem, there is no closed-form (rational) solution for $n \geq 5$.
  All eigenvalue algorithms must be iterative!
- There is an important distinction between iterative methods to:
  - Compute **all eigenvalues** (similarity transformations). These are based on dense-matrix factorizations such as the QR factorization, with total cost $O(n^3)$.
  - Compute **only one or a few eigenvalues**, typically the smallest or the largest one (e.g., power method). These are similar to iterative methods for solving linear systems.

Sparse Matrices

- Recall that for a diagonalizable matrix

$$\mathbf{A}^n = \mathbf{X}\mathbf{\Lambda}^n\mathbf{X}^{-1}$$

  and **assume well-separated eigenvalues** $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \cdots |\lambda_n|$, and that the columns of $\mathbf{X}$ are normalized, $\|\mathbf{x}_j\| = 1$.
- For sparse matrices we sometimes only need to know a **few of the eigenvalues**/vectors, not all of them.
- Notably, knowing the eigenvector corresponding to the **smallest and largest (in magnitude) eigenvalues** is often most important (see Google Page Rank algorithm).

Iterative Method

- Any **initial guess** vector $\mathbf{q}_0$ can be represented in the linear basis formed by the eigenvectors

$$\mathbf{q}_0 = \mathbf{X}\mathbf{a}$$

- Recall iterative methods for linear systems: **Multiply a vector with the matrix A** many times:

$$\mathbf{q}_{k+1} = \mathbf{A}\mathbf{q}_k$$

$$\mathbf{q}_n = \mathbf{A}^n\mathbf{q}_0 = \left(\mathbf{X}\boldsymbol{\Lambda}^n\mathbf{X}^{-1}\right)\mathbf{X}\mathbf{a} = \mathbf{X}\left(\boldsymbol{\Lambda}^n\mathbf{a}\right)$$

Power Method

- As $n \to \infty$, the **eigenvalue of largest modulus** λ_0 will dominate,

$$\boldsymbol{\Lambda}^n = \lambda_1^n \text{Diag}\left\{1, \left(\frac{\lambda_2}{\lambda_1}\right)^n, \ldots\right\} \to \text{Diag}\left\{\lambda_1^n, 0, \ldots, 0\right\}$$

$$\mathbf{q}_n = \mathbf{X}\left(\boldsymbol{\Lambda}^n \mathbf{a}\right) \to \lambda_1^n \mathbf{X} \begin{bmatrix} a_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \lambda_1^n \mathbf{x}_1$$

- Therefore the **normalized iterates** converge to the eigenvector:

$$\tilde{\mathbf{q}}_n = \frac{\mathbf{q}_n}{\|\mathbf{q}_n\|} \to \mathbf{x}_1$$

- The **Rayleigh quotient** converges to the eigenvalue:

$$r_A\left(\mathbf{q}_n\right) = \frac{\mathbf{q}_n^\star \mathbf{A} \mathbf{q}_n}{\mathbf{q}_n \cdot \mathbf{q}_n} = \tilde{\mathbf{q}}_n^\star \mathbf{A} \tilde{\mathbf{q}}_n \to \lambda_1$$

An alternative derivation

$$q_0 = \sum_n a_i \cdot x_i$$

$$q_n = A^n q_0 = \sum_n a_i (A^n x_i)$$

$$= \sum a_i (\lambda_i^n x_i) =$$

$$= \sum_n a_i \lambda_1 \left(\frac{\lambda_i}{\lambda_1}\right)^n \cdot x_i \xrightarrow[n\to\infty]{\text{as}} a_1 \lambda_1^n x_1 + O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^n\right)$$

$$\Rightarrow \boxed{\tilde{q}_n \to x_1 + O(\varepsilon)\, x_2 + O(\varepsilon) x_3 + \cdots \quad \text{where} \quad \varepsilon = \left|\frac{\lambda_2}{\lambda_1}\right|^n}$$

Now $\tilde{q}_n^* A \tilde{q}_n = x_1^* A x_1 + O(\varepsilon^2) \sum_{i,j\neq 1} x_i^* A x_j$

$$\Rightarrow \boxed{\hat{\lambda}_n'' = \lambda_1 + O(\varepsilon^2)}$$

Power Iteration

Start with an initial guess $\mathbf{q}_0$, and then iterate:

1. Compute **matrix-vector product** and normalize it:

$$\mathbf{q}_k = \frac{\mathbf{A}\mathbf{q}_{k-1}}{\left\|\mathbf{A}\mathbf{q}_{k-1}\right\|}$$

2. Use Raleigh quotient to obtain **eigenvalue estimate**:

$$\hat{\lambda}_k = \mathbf{q}_k^{\star}\mathbf{A}\mathbf{q}_k$$

3. **Test for convergence**: Evaluate the residual

$$\mathbf{r}_k = \mathbf{A}\mathbf{q}_k - \hat{\lambda}_k\mathbf{q}_k$$

and terminate if the residual norm is smaller than some tolerance, e.g., for tolerance $\epsilon \ll 1$,

$$\|\mathbf{r}_k\| \approx \left|\lambda_1 - \hat{\lambda}_k\right| \leq \epsilon\hat{\lambda}_k.$$

Convergence Estimates

- The normalized iterates converge to the eigenvector **linearly**:

$$\left\|\mathbf{q}_k - (\pm\mathbf{x}_1)\right\| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

- Typically the eigenvalue estimate converges **quadratically**:

$$\left\|\hat{\lambda}_k - \lambda_1\right\| \sim O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k}\right)$$

- The power method is fast when the **dominant eigenvalue is well-separated from the rest** (even if it is degenerate).
- This conclusion is rather general for all iterative methods: Convergence is good for **well-separated** eigenvalues, bad otherwise.

Eigenvalues in MATLAB

- The **Schur decomposition** is provided by $[U, T] = schur(A)$.
- In MATLAB, sophisticated variants of the **QR algorithm** (LAPACK library) are implemented in the function *eig*:

$$\Lambda = eig(A)$$

$$[X, \Lambda] = eig(A)$$

- For large or sparse matrices, iterative methods based on the **Arnoldi iteration** (ARPACK library), can be used to obtain a **few** of the largest eigenvalues:

$$\Lambda = eigs(A, n_{eigs})$$

$$[X, \Lambda] = eigs(A, n_{eigs})$$

Outline

Sensitivity (conditioning) of the SVD

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\star}$$

- Since unitary matrices have unit 2-norm,

$$\|\delta\Sigma\|_2 \approx \|\delta A\|_2 \,.$$

- The SVD computation is always **perfectly well-conditioned**!
- However, this refers to absolute errors: The **relative error** of small singular values will be large.
- The **power of the SVD** lies in the fact that it always exists and can be computed stably...but it is somewhat **expensive to compute**.

Computing the SVD

- The SVD can be computed by performing an eigenvalue computation for the **normal matrix $\mathbf{A}^{\star}\mathbf{A}$** (a positive-semidefinite matrix).
- This squares the condition number for small singular values and is **not numerically-stable**.
- Instead, modern algorithms use an algorithm based on computing eigenvalues / eigenvectors using the QR factorization.
- The cost of the calculation is $\sim O(mn^2)$, of the same order as eigenvalue calculation if $m \sim n$.

Reduced SVD

The **full (standard) SVD**

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\star} = \sum_{i=1}^{p} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\star}$$
$$[m \times n] = [m \times m]\,[m \times n]\,[n \times n]\,,$$

is in practice often computed in **reduced (economy) SVD** form, where $\boldsymbol{\Sigma}$ is $[p \times p]$:

$$\begin{aligned} [m \times n] &= [m \times n]\,[n \times n]\,[n \times n] \quad \text{for} \quad m > n \\ [m \times n] &= [m \times m]\,[m \times m]\,[m \times n] \quad \text{for} \quad n > m \end{aligned}$$

This contains all the information as the full SVD but can be **cheaper to compute** if $m \gg n$ or $m \ll n$.

In MATLAB

- $[U, \Sigma, V] = svd(A)$ for **full SVD**, computed using a QR-like method.
- $[U, \Sigma, V] = svd(A,' econ')$ for **economy SVD**.
- The **least-squares solution** for square, overdetermined, underdetermined, or even rank-defficient systems can be computed using *svd* or *pinv* (pseudo-inverse, see homework).
- The q largest singular values and corresponding approximation can be computed efficiently for **sparse matrices** using

$$[U, \Sigma, V] = svds(A, q).$$

Outline

Rank-Revealing Properties

- Assume the rank of the matrix is r, that is, the dimension of the range of $\mathbf{A}$ is r and the dimension of the null-space of $\mathbf{A}$ is $n-r$ (recall the fundamental theorem of linear algebra).
- The SVD is a **rank-revealing** matrix factorization because only r of the singular values are nonzero,

$$\sigma_{r+1} = \cdots = \sigma_p = 0.$$

- The left singular vectors $\{\mathbf{u}_1, \ldots, \mathbf{u}_r\}$ form an **orthonormal basis for the range** (column space, or image) of $\mathbf{A}$.
- The right singular vectors $\{\mathbf{v}_{r+1}, \ldots, \mathbf{v}_n\}$ form an **orthonormal basis for the null-space** (kernel) of $\mathbf{A}$.

The matrix pseudo-inverse

- For square non-singular systems, $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$. Can we generalize the matrix inverse to non-square or rank-deficient matrices?
- Yes: **matrix pseudo-inverse** (Moore-Penrose inverse):

$$\mathbf{A}^{\dagger} = \mathbf{V}\boldsymbol{\Sigma}^{\dagger}\mathbf{U}^{\star},$$

where

$$\boldsymbol{\Sigma}^{\dagger} = \text{Diag}\left\{\sigma_1^{-1}, \sigma_2^{-1}, \ldots, \sigma_r^{-1}, 0, \ldots, 0\right\}.$$

- In numerical computations very small singular values should be considered to be zero (see homework).
- The least-squares solution to over- or under-determined linear systems $\mathbf{A}\mathbf{x} = \mathbf{b}$ can be obtained from:

$$\mathbf{x} = \mathbf{A}^{\dagger}\mathbf{b}.$$

Proof of Least-Squares (1)

$$\min_{x} \|Ax - b\|_2 \leftarrow \text{LEAST SQUARES}$$

SUCH THAT $\|x\|_2$ IS MINIMAL

$$(Ax-b)^*(Ax-b) = x^*(A^*A)x - 2x^*A^*b + \ldots$$

USING SVD: $x^*A^*Ax = x^*V\Sigma^2 \underline{\underline{V^*x}}$

AND $x^*A^*b = b^*(Ax) = (U^*b)\Sigma\underline{\underline{(V^*x)}}$

DENOTING $\begin{cases} V^*x = w & \leftarrow \text{NEW VARIABLE} \\ U^*b = c & \leftarrow \text{CONSTANT} \end{cases}$

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Proof of Least-Squares (2)

$$\|Ax-b\|_2^2 = w^* \Sigma^2 w - 2 c^* \Sigma w + \dots$$

$$= \sum_{i=1}^{r} \sigma_i^2 |w_i|^2 - 2 \sum_{i=1}^{r} (\sigma_i w_i) c_i^*$$

$$= \sum_{i=1}^{r} |\sigma_i w_i - c_i|^2 + \text{CONSTANTS}$$

WHICH IS MINIMIZED IF

$$\sigma_i w_i = c_i \Rightarrow w_i = \frac{c_i}{\sigma_i}$$

or

$$\boxed{(V^* x)_i = \frac{(U^* b)_i}{\sigma_i}, \quad i \leq r}$$

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Proof of Least-Squares (3)

HOW ABOUT $w_{r+1}, \dots, w_m$?

$$\|x\|_2^2 = \|Vw\|_2^2 = w^*(V^*V)w^*$$
$$= \|w\|_2^2 = \sum |w_i|^2$$

SO THE NORM OF x IS MINIMIZED IF THE NORM OF w IS MINIMIZED.

$$\Rightarrow \boxed{w_{r+1} = \dots = 0}$$

$$\Rightarrow \quad x = Vw = V\Sigma^{\dagger}c =$$
$$= (V\Sigma^{\dagger}U^*)b = A^{\dagger}b$$

$\boxed{\text{QED}}$ ③

Low-rank approximations

- The SVD is a decomposition into **rank-1 outer product matrices**:

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\star} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\star} = \sum_{i=1}^{r} \mathbf{A}_i$$

- The rank-1 components $\mathbf{A}_i$ are called **principal components**, the most important ones corresponding to the larger σ_i.
- Ignoring all singular values/vectors except the first q, we get a **low-rank approximation**:

$$\mathbf{A} \approx \hat{\mathbf{A}}_q = \mathbf{U}_q \boldsymbol{\Sigma}_q \mathbf{V}_q^{\star} = \sum_{i=1}^{q} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\star}.$$

- Theorem: This is the **best approximation** of rank-q in the Euclidian and Frobenius norm:

$$\left\| \mathbf{A} - \hat{\mathbf{A}}_q \right\|_2 = \sigma_{q+1}$$

Applications of SVD

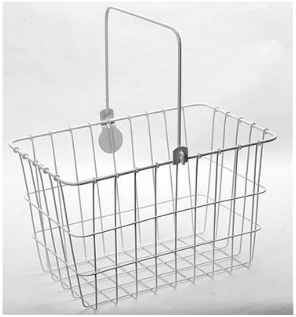
- **Statistical analysis** (e.g., DNA microarray analysis, clustering), often called **Principal Component Analysis (PCA)**
- Data **compression** (e.g., image compression, explained next).
- **Feature extraction**, e.g., face or character recognition (see Eigenfaces on Wikipedia).
- **Latent semantic indexing** for context-sensitive searching (see Wikipedia).
- **Noise reduction** (e.g., weather prediction).

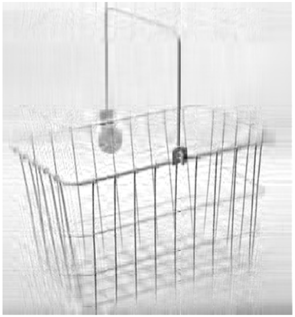
Image Compression

```
>> A=rgb2gray(imread('basket.jpg'));
>> imshow(A);
>> [U,S,V]=svd(double(A));
>> r=25; % Rank-r approximation
>> Acomp=U(:,1:r)*S(1:r,1:r)*(V(:,1:r))';
>> imshow(uint8(Acomp));
```

Compressing an image of a basket

We used only 25 out of the ~ 400 singular values to construct a rank 25 approximation:





Outline

Estimating all eigenvalues / eigenvectors

- Iterative methods akin the power method are not suitable for estimating all eigenvalues.
- Basic idea: Build a sequence of matrices $\mathbf{A}_k$ that all share eigenvalues with $\mathbf{A}$ via **similarity transformations**:

$$\mathbf{A}_{k+1} = \mathbf{P}^{-1}\mathbf{A}_k\mathbf{P}, \text{ starting from } \mathbf{A}_1 = \mathbf{A}.$$

- The goal is to reduce the matrix $\mathbf{A}_{k\to\infty}$ to as close to diagonal as possible.
- A numerically stable and good way to do this is to use the *QR* factorization:

$$\mathbf{A}_k = \mathbf{Q}_{k+1}\mathbf{R}_{k+1}$$

$$\mathbf{A}_{k+1} = \mathbf{Q}_{k+1}^{-1}\mathbf{A}_k\mathbf{Q}_{k+1} = \left(\mathbf{Q}_{k+1}^{-1}\mathbf{Q}_{k+1}\right)\mathbf{R}_{k+1}\mathbf{Q}_{k+1} = \mathbf{R}_{k+1}\mathbf{Q}_{k+1}.$$

The basic *QR* method

- The behavior of the QR iteration can be understood most transparently as follows [following Trefethen and Bau]:
- Observation: The range of the matrix $\mathbf{A}^k$ converges to the space spanned by the eigenvectors of $\mathbf{A}$,
  with the eigenvectors corresponding to the largest eigenvalues dominating as $k \to \infty$ (so this is ill-conditioned).
- Recall: The columns of $\mathbf{Q}$ in $\mathbf{A} = \mathbf{QR}$ form an **orthonormal basis** for the range of $\mathbf{A}$.
- Idea: Form a **well-conditioned basis for the eigenspace** of $\mathbf{A}$ by factorizing:

$$\mathbf{A}^k = \tilde{\mathbf{Q}}_k \tilde{\mathbf{R}}_k$$

  and then calculate

$$\mathbf{A}_k = \tilde{\mathbf{Q}}_k^{-1} \mathbf{A} \tilde{\mathbf{Q}}_k = \tilde{\mathbf{Q}}_k^{\star} \mathbf{A} \tilde{\mathbf{Q}}_k.$$

- It is not too hard to show that this produces the **same sequence** of matrices $\mathbf{A}_k$ as the QR algorithm.

Why the *QR* algorithm works

- Summary: The columns of $\tilde{\mathbf{Q}}_k$ converge to the eigenvectors, and

$$\mathbf{A}_k = \tilde{\mathbf{Q}}_k^{\star} \mathbf{A} \tilde{\mathbf{Q}}_k .$$

- We can recognize the above as a matrix of Rayleigh quotients, which for diagonalizable matrices

$$(\mathbf{A}_k)_{ij} = \tilde{\mathbf{q}}_i^{\star} \mathbf{A} \tilde{\mathbf{q}}_j \to \lambda_i \delta_{ij} = \begin{cases} \lambda_i & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

showing that (under suitable assumptions):

$$\mathbf{A}_k \to \mathbf{\Lambda}$$

- It can also be shown that

$$\tilde{\mathbf{Q}}_k = \mathbf{Q}_1 \mathbf{Q}_2 \cdots \mathbf{Q}_k \to \mathbf{X}$$

More on *QR* algorithm

- The convergence of the basic *QR* algorithm is closely related to that of the power method: It is only fast if all eigenvalues are **well-separated**.
- For more general (non-diagonalizable) matrices in complex arithmetic, the algorithm converges to the **Schur decomposition** $\mathbf{A} = \mathbf{U}\mathbf{T}\mathbf{U}^{\star}$,

$$\mathbf{A}_k \to \mathbf{T} \text{ and } \tilde{\mathbf{Q}}_k \to \mathbf{U}.$$

- It is possible to implement the algorithm entirely using real arithmetic (no complex numbers).
- There are several key improvements to the basic method that make this work in practice: **Hessenberg matrices** for faster *QR* factorization, **shifts** and **deflation** for acceleration.
- There are other sophisticated algorithms as well, such as the **divide-and-conquer algorithm**, and the best are implemented in the library LAPACK (MATLAB).