Scientific Computing: Eigen and Singular Values

Aleksandar Donev
Courant Institute, NYU[1]
donev@courant.nyu.edu

[1]Course MATH-GA.2043 or CSCI-GA.2112, Fall 2020

October 1st, 2020

Outline

Outline

Eigenvalue Decomposition

- For a square matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$, there exists at least one λ such that

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \quad \Rightarrow \quad (\mathbf{A} - \lambda\mathbf{I})\,\mathbf{x} = \mathbf{0}$$

- Putting the **eigenvectors** $\mathbf{x}_j$ as columns in a matrix $\mathbf{X}$, and the **eigenvalues** λ_j on the diagonal of a diagonal matrix $\mathbf{\Lambda}$, we get

$$\mathbf{A}\mathbf{X} = \mathbf{X}\mathbf{\Lambda}.$$

- A matrix is **non-defective** or **diagonalizable** if there exist n **linearly independent eigenvectors**, i.e., if the matrix $\mathbf{X}$ is invertible:

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

  leading to the **eigen-decomposition** of the matrix

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

Unitarily Diagonalizable Matrices

- A **unitary** or **orthogonal** matrix $\mathbf{U}$ has orthogonal colums each of which has unit L_2 norm:
$$\mathbf{U}^{-1} = \mathbf{U}^{\star}.$$
Unitary is used for complex matrices and is more general than orthogonal, reserved for real matrices.
Recall that star denotes **adjoint** (conjugate transpose).
- Unitary matrices are important because they are **always well-conditioned**, $\kappa_2(\mathbf{U}) = 1$.
- A matrix is **unitarily diagonalizable** if there exist n linearly independent **orthogonal eigenvectors**, $\mathbf{X} \equiv \mathbf{U}$,
$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\star}.$$
- Theorem: **Hermitian matrices**, $\mathbf{A}^{\star} = \mathbf{A}$, are unitarily diagonalizable and have **real eigenvalues**.
For real matrices we use the term **symmetric**.

Non-diagonalizable Matrices

- For matrices that are not diagonalizable, one can use **Jordan form factorizations**, or, more relevant to numerical mathematics, the **Schur factorization** (decomposition):

$$\mathbf{A} = \mathbf{U}\mathbf{T}\mathbf{U}^{\star},$$

  where $\mathbf{T}$ is **upper-triangular** (unlike **Jordan form** where only nonzeros are on super-diagonal).
- The eigenvalues are on the diagonal of $\mathbf{T}$, and in fact if $\mathbf{A}$ is unitarily diagonalizable then $\mathbf{T} \equiv \mathbf{\Lambda}$.
- The Schur decomposition is **not unique** but it is the best generalization of the eigenvalue (spectral) decomposition to general matrices.

Singular Value Decomposition (SVD)

Every matrix has a **singular value decomposition (SVD)**

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

where **U** and **V** are **unitary matrices** whose columns are the left, $\mathbf{u}_i$, and the right, $\mathbf{v}_i$, **singular vectors**, and

$$\mathbf{\Sigma} = \mathrm{Diag}\left\{\sigma_1, \sigma_2, \ldots, \sigma_p\right\}$$

is a **diagonal matrix** with real positive diagonal entries called **singular values** of the matrix

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0,$$

and $p = \min(m, n)$ is the maximum possible rank of the matrix.

Comparison to eigenvalue decomposition

- Recall the eigenvector decomposition for diagonalizable matrices

$$\mathbf{AX} = \mathbf{X\Lambda}.$$

- The singular value decomposition can be written similarly to the eigenvector one

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

and they both **diagonalize A**, but there are some important **differences**:

1. The SVD exists for any matrix, not just diagonalizable ones.
2. The SVD uses different vectors on the left and the right (different basis for the domain and image of the linear mapping represented by **A**).
3. The SVD always uses orthonormal basis (unitary matrices), not just for unitarily diagonalizable matrices.

Relation to Eigenvalues

- For **Hermitian (symmetric) matrices**, there is **no fundamental difference** between the SVD and eigenvalue decompositions (and also the Schur decomposition).
- The squared singular values are **eigenvalues of the normal matrix**:

$$\sigma_i(\mathbf{A}) = \sqrt{\lambda_i(\mathbf{A}\mathbf{A}^\star)} = \sqrt{\lambda_i(\mathbf{A}^\star\mathbf{A})}$$

  since

$$\mathbf{A}^\star\mathbf{A} = (\mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^\star)(\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\star) = \mathbf{V}\boldsymbol{\Sigma}^2\mathbf{V}^\star$$

- Similarly, the singular vectors are eigenvectors of $\mathbf{A}^\star\mathbf{A}$ or $\mathbf{A}\mathbf{A}^\star$.

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):

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

where

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

- 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:

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

Outline

Sensitivity of Eigenvalues

- Now consider a perturbation of a diagonalizable matrix $\delta\mathbf{A}$ and see how perturbed the similar matrix becomes:

$$\mathbf{X}^{-1}\left(\mathbf{A}+\delta\mathbf{A}\right)\mathbf{X}=\boldsymbol{\Lambda}+\delta\boldsymbol{\Lambda}\quad\Rightarrow$$

$$\delta\boldsymbol{\Lambda}=\mathbf{X}^{-1}\left(\delta\mathbf{A}\right)\mathbf{X}\quad\Rightarrow$$

$$\left\|\delta\boldsymbol{\Lambda}\right\|\leq\left\|\mathbf{X}^{-1}\right\|\left\|\delta\mathbf{A}\right\|\left\|\mathbf{X}\right\|=\kappa\left(\mathbf{X}\right)\left\|\delta\mathbf{A}\right\|$$

- Conclusion: The conditioning of the eigenvalue problem is related to the **conditioning of the matrix of eigenvectors**.

Conditioning of Eigenvalue problems

$$\|\delta \boldsymbol{\Lambda}\| \leq \kappa\left(\mathbf{X}\right)\|\delta \mathbf{A}\|$$

- If $\mathbf{X}$ is unitary then $\|\mathbf{X}\|_2 = 1$ (from now on we exclusively work with the 2-norm): **Unitarily diagonalizable matrices are always perfectly conditioned!**
- Warning: The **absolute error** in all eigenvalues is of the same order, meaning that the **relative error will be very large** for the smallest eigenvalues.
- The conditioning number for computing eigenvectors is inversely proportional to the **separation between the eigenvalues**

$$\kappa\left(\mathbf{x}, \mathbf{A}\right) = \left(\min_j |\lambda - \lambda_j|\right)^{-1}.$$

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:

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

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 $\epsilon \ll 1$,

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

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

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

- 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**

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

is in practice often computed in **reduced (economy) SVD** form, where $\mathbf{\Sigma}$ 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

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/PCA

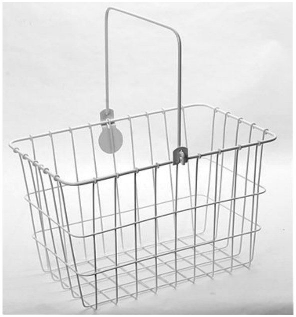
- **Statistical analysis** (e.g., DNA microarray analysis, clustering).
- Data **compression** (e.g., image compression, explained next).
- **Feature extraction**, e.g., face or character recognition (see Eigenfaces on Wikipedia).
- **Latent semantic indexing** for context-sensitive searching (see Wikipedia).
- **Noise reduction** (e.g., weather prediction).
- One example concerning language analysis given in homework.

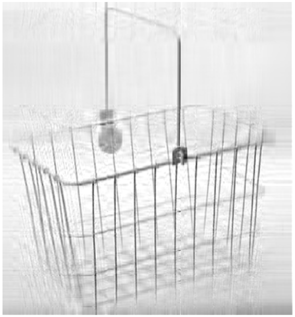
Image Compression

```
>> 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:

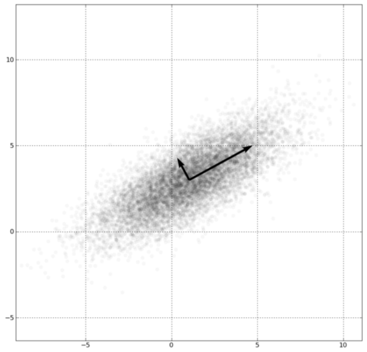




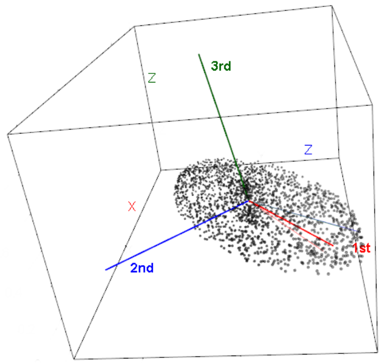
Principal Component Analysis

- **Principal Component Analysis** (PCA) is a term used for low-rank approximations in statistical analysis of data.
- Consider having m empirical data points or **observations** (e.g., daily reports) of n **variables** (e.g., stock prices), and put them in a **data matrix** $\mathbf{A} = [m \times n]$.
- Assume that each of the variables has **zero mean**, that is, the empirical mean has been subtracted out.
- It is also useful to choose the units of each variable (normalization) so that the **variance is unity**.
- We would like to find an **orthogonal transformation** of the original variables that accounts for as much of the variability of the data as possible.
- Specifically, the first principal component is the direction along which the variance of the data is largest.

PCA and Variance



PCA applied to an ellipsoidically shaped point cloud



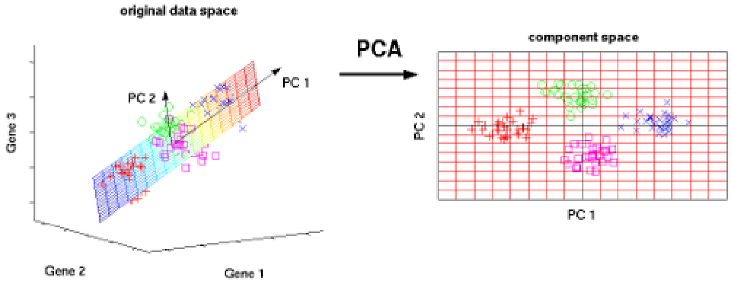
more information: www.joyofdata.de/blog/illustration-of-principal-component-analysis-pca

PCA and SVD

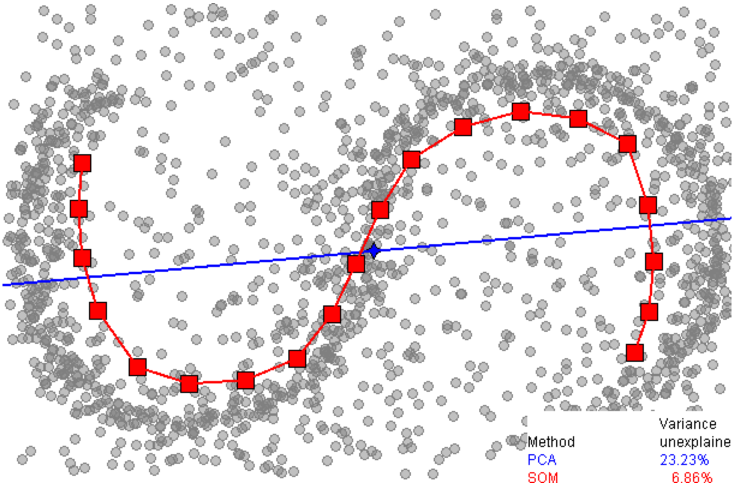
- The **covariance matrix** of the data tells how correlated different pairs of variables are:
$$\mathbf{C} = \mathbf{A}^T\mathbf{A} = [n \times n]$$
- The largest eigenvalue of $\mathbf{C}$ is the direction (line) that minimizes the sum of squares of the distances from the points to the line, or equivalently, **maximizes the variance** of the data projected onto that line.
- The SVD of the data matrix is $\mathbf{A} = \mathbf{U\Sigma V}^\star$.
- The eigenvectors of $\mathbf{C}$ are in fact the columns of $\mathbf{V}$, and the eigenvalues of $\mathbf{C}$ are the squares of the singular values,
$$\mathbf{C} = \mathbf{A}^T\mathbf{A} = \mathbf{V\Sigma}\left(\mathbf{U}^\star\mathbf{U}\right)\mathbf{\Sigma V}^\star = \mathbf{V\Sigma}^2\mathbf{V}^\star.$$

Note: the eigenvalues values are necessarily real and positive since $\mathbf{C}$ is positive semi-definite.

Dimensionality reduction via PCA



Nonlinear "PCA"



Outline

Summary for Eigenvalues

- Eigenvalues are **well-conditioned** for **unitarily diagonalizable matrices** (includes Hermitian matrices), but ill-conditioned for nearly non-diagonalizable matrices.
- Eigenvectors are **well-conditioned** only when **eigenvalues are well-separated**.
- Eigenvalue algorithms are **always iterative**.
- Estimating **all eigenvalues and/or eigenvectors** can be done by using iterative QR factorizations, with cost $O(n^3)$.
- Iterative algorithms are used to obtain only a **few eigenvalues/vectors** for sparse matrices.
- MATLAB has high-quality implementations of sophisticated variants of these algorithms.

Summary for SVD

- The **singular value decomposition** (SVD) is an alternative to the eigenvalue decomposition that is **better for rank-defficient and ill-conditioned matrices** in general.
- Computing the SVD is **always numerically stable** for any matrix, but is typically more expensive than other decompositions.
- The SVD can be used to compute **low-rank approximations** to a matrix via the principal component analysis (PCA).
- PCA has many practical applications and usually **large sparse matrices** appear.