Eigenvalues and eigenvectors. Singular values and singular vectors. CP tensor decomposition. PCA

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Eigenvalues and eigenvectors

Eigenvectors and eigenvalues

A scalar value λ is an eigenvalue of the $n \times n$ matrix A if there is a nonzero vector q such that

$$Aq = \lambda q.$$

he vector q is called an eigenvector of A. The matrix A is nonsingular if none of its eigenvalues are zero. The eigenvalues of symmetric matrices are all real numbers, while nonsymmetric matrices may have imaginary eigenvalues. If the matrix is positive definite as well as symmetric, its eigenvalues are all positive real numbers.

Eigenvectors and eigenvalues

Theorem

$$A \succeq (\succ) 0 \Leftrightarrow \text{all eigenvalues of } A \text{ are } \geq (>) 0$$

Proof

1. $\rightarrow$ Suppose some eigenvalue λ is negative and let x denote its corresponding eigenvector. Then

$$Ax = \lambda x \rightarrow x^T Ax = \lambda x^T x < 0$$

which contradicts the condition of $A \succeq 0$.

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   which contradicts the condition of $A \succeq 0$.
2. $\leftarrow$ For any symmetric matrix, we can pick a set of eigenvectors $v_1, \ldots, v_n$ that form an orthogonal basis of $\mathbb{R}^n$. Pick any $x \in \mathbb{R}^n$.

$$\begin{aligned} x^T Ax &= (\alpha_1 v_1 + \ldots + \alpha_n v_n)^T A(\alpha_1 v_1 + \ldots + \alpha_n v_n) \\ &= \sum \alpha_i^2 v_i^T A v_i = \sum \alpha_i^2 \lambda_i v_i^T v_i \geq 0 \end{aligned}$$

   here we have used the fact that $v_i^T v_j = 0$, for $i \neq j$.

Eigendecomposition (spectral decomposition)

Suppose $A \in S_n$, i.e., A is a real symmetric $n \times n$ matrix. Then A can be factorized as

$$A = Q\Lambda Q^T,$$

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where $Q \in \mathbb{R}^{n\times n}$ is orthogonal, i.e., satisfies $Q^TQ = I$, and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. The (real) numbers λ_i are the eigenvalues of A and are the roots of the characteristic polynomial $\det(A - \lambda I)$. The columns of Q form an orthonormal set of eigenvectors of A. The factorization is called the spectral decomposition or (symmetric) eigenvalue decomposition of A. [1]

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We usually order the eigenvalues as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. We use the notation $\lambda_i(A)$ to refer to the i-th largest eigenvalue of $A \in S$. We usually write the largest or maximum eigenvalue as $\lambda_1(A) = \lambda_{\mathsf{max}}(A)$, and the least or minimum eigenvalue as $\lambda_n(A) = \lambda_{\mathsf{min}}(A)$.

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Eigenvalues

The largest and smallest eigenvalues satisfy

$$\lambda_{\min}(A) = \inf_{x \neq 0} \frac{x^T A x}{x^T x}, \qquad \lambda_{\max}(A) = \sup_{x \neq 0} \frac{x^T A x}{x^T x}$$

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If we use spectral matrix norm, we can get:

$$\kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$$

If, moreover, $A \in \mathbb{S}^n_{++}$: $\kappa(A) = \dfrac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$

SVD

Singular value decomposition

Suppose $A \in \mathbb{R}^{m \times n}$ with rank $A = r$. Then A can be factored as

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This factorization is called the **singular value decomposition (SVD)** of A. The columns of U are called left singular vectors of A, the columns of V are right singular vectors, and the numbers σ_i are the singular values. The singular value decomposition can be written as

$$A = \sum_{i=1}^{r} \sigma_i u_i v_i^T,$$

where $u_i \in \mathbb{R}^m$ are the left singular vectors, and $v_i \in \mathbb{R}^n$ are the right singular vectors.

Singular value decomposition

Question

Suppose, matrix $A \in \mathbb{S}^n_{++}$. What can we say about the connection between its eigenvalues and singular values?

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How do the singular values of a matrix relate to its eigenvalues, especially for a symmetric matrix?

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Simple, yet very interesting decomposition is Skeleton decomposition, which can be written in two forms:

$$A = UV^T \quad A = \hat{C}\hat{A}^{-1}\hat{R}$$

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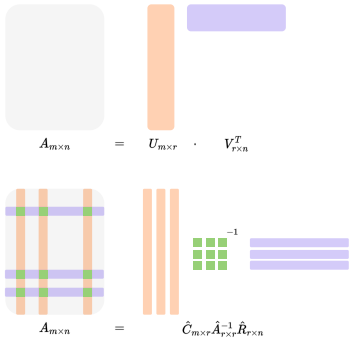
Use cases for Skeleton decomposition are:

- Model reduction, data compression, and speedup of computations in numerical analysis: given rank-r matrix with $r \ll n, m$ one needs to store $\mathcal{O}((n+m)r) \ll nm$ elements.



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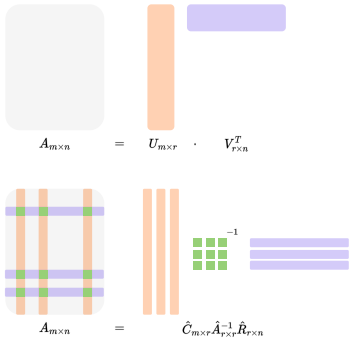

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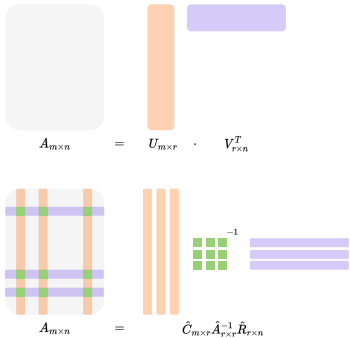
- All applications where SVD applies, since Skeleton decomposition can be transformed into truncated SVD form.



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Canonical tensor decomposition

One can consider the generalization of Skeleton decomposition to the higher order data structure, like tensors, which implies representing the tensor as a sum of r primitive tensors.

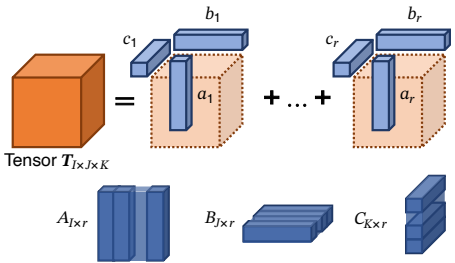

Figure 2: Illustration of Canonical Polyadic decomposition

Example

Note, that there are many tensor decompositions: Canonical, Tucker, Tensor Train (TT), Tensor Ring (TR), and others. In the tensor case, we do not have a straightforward definition of *rank* for all types of decompositions. For example, for TT decomposition rank is not a scalar, but a vector.

Determinant and trace

The determinant and trace can be expressed in terms of the eigenvalues

$$\det A = \prod_{i=1}^{n} \lambda_i, \qquad \operatorname{tr} A = \sum_{i=1}^{n} \lambda_i$$

The determinant has several appealing (and revealing) properties. For instance,

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Don't forget about the cyclic property of a trace for arbitrary matrices A, B, C, D (assuming, that all dimensions are consistent):

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Question

How does the determinant of a matrix relate to its invertibility?

First-order Taylor approximation

The first-order Taylor approximation, also known as the linear approximation, is centered around some point x_0. If $f : \mathbb{R}^n \to \mathbb{R}$ is a differentiable function, then its first-order Taylor approximation is given by:

$$f^I_{x_0}(x) = f(x_0) + \nabla f(x_0)^T (x - x_0)$$

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It is very usual to replace the $f(x)$ with $f^I_{x_0}(x)$ near the point x_0 for simple analysis of some approaches.

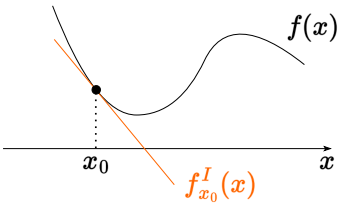

Figure 3: First order Taylor approximation near the point x_0

Second-order Taylor approximation

The second-order Taylor approximation, also known as the quadratic approximation, includes the curvature of the function. For a twice-differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, its second-order Taylor approximation centered at some point x_0 is:

$$f_{x_0}^{II}(x) = f(x_0) + \nabla f(x_0)^T (x - x_0) + \frac{1}{2}(x - x_0)^T \nabla^2 f(x_0)(x - x_0)$$

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When using the linear approximation of the function is not sufficient one can consider replacing the $f(x)$ with $f_{x_0}^{II}(x)$ near the point x_0. In general, Taylor approximations give us a way to locally approximate functions. The first-order approximation is a plane tangent to the function at the point x_0, while the second-order approximation includes the curvature and is represented by a parabola. These approximations are especially useful in optimization and numerical methods because they provide a tractable way to work with complex functions.

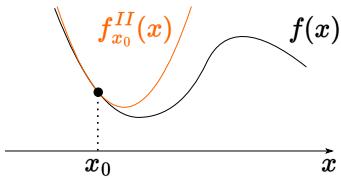

Figure 4: Second order Taylor approximation near the point x_0

Exercises

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- How to calculate minimum and maximum eigenvalue of the hessian matrix of linear least squares problem? What about binary logistic regression?