Singular Value Decomposition and Linear Least Squares

CSE 6367: Computer Vision

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Introduction

- The **singular value decomposition** (SVD) efficiently organizes any given matrix
- It is useful for several purposes:
  - It explains clearly the action of the matrix (as a linear operator) and it can be used to reestablish many elementary properties of matrices
  - It can efficiently compress a matrix with the least loss of information (in a **least squares** sense) by summarizing only the most relevant features and suppressing unnecessary information (e.g. SVD is used for dimensionality reduction by projecting a dataset onto a lower dimensional subspace)

Eigenvalue Decomposition of Symmetric Matrices

- The **eigenvalue decomposition** (EVD) of a symmetric matrix $A \in \mathbb{R}^{n \times n}$ is

$$A = U \Lambda U^T \tag{1}$$

  where $\Lambda \in \mathbb{R}^{n \times n}$ is diagonal, $U \in \mathbb{R}^{n \times n}$, and $UU^T = I$ (i.e. U is orthogonal)

- We denote the eigenvalues of $\Lambda_{n \times n}$ by $\lambda_1, \ldots, \lambda_n$ and the columns of U by $\mathbf{u}_1, \ldots, \mathbf{u}_n$

EVD Formulation

- Let $\{\mathbf{u}_i\}_{i=1}^{n}, \forall\, 1 \leq i \leq n$ be an orthonormal basis for $\mathbb{R}^n$, then the EVD can be formulated as

$$A\mathbf{u}_i = \lambda_i \mathbf{u}_i \tag{2}$$

where $\lambda_i \in \mathbb{R}$

EVD Formulation

- Thus, $A = U\Lambda U^T$ iff $AU = U\Lambda$, that is

$$A \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_n \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

  or equivalently

$$\begin{bmatrix} A\mathbf{u}_1 & \dots & A\mathbf{u}_n \end{bmatrix} = \begin{bmatrix} \lambda_1\mathbf{u}_1 & \dots & \lambda_n\mathbf{u}_n \end{bmatrix}$$

- $\{\mathbf{u}_i\}_{i=1}^n$ is an orthonormal basis for $\mathbb{R}^n$, and is equivalent with the fact that U is an orthogonal matrix

EVD Formulation

- Another equivalent formulation of the EVD is

$$A = \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^T \tag{3}$$

where $\{\mathbf{u}_i\}_{i=1}^n$ is as in (2) and $\{\lambda_i\}_{i=1}^n \subset \mathbb{R}$

Proof of EVD Formulation Equivalence

- To prove the equivalence of (1) and (3) we use the following basic identity for multiplying a row of column vectors with a column of row vectors

$$\begin{bmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_n \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_n^T \end{bmatrix} = \sum_{i=1}^{n} \mathbf{v}_i \mathbf{u}_i^T \tag{4}$$

- We express the equality in (1) as follows

$$A = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_n^T \end{bmatrix} \tag{5}$$

Proof of EVD Formulation Equivalence

- By applying direct multiplication with a diagonal matrix and then the identity (4), we expand the expression in (5) as follows

$$A = \begin{bmatrix} \lambda_1 \mathbf{u}_1 & \dots & \lambda_n \mathbf{u}_n \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_n^T \end{bmatrix} = \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^T$$

and this establishes the equivalence of (1) and (3)

Eigenvalues of Symmetric Matrices

- The eigenvalues of symmetric matrices are real, however they can be negative
- In the special case where a symmetric matrix has the form $A^T A$ (A is a rectangular matrix) the eigenvalues are nonnegative
- Thus if $A^T A\mathbf{v} = \lambda\mathbf{v}$, then $\mathbf{v}^T A^T A\mathbf{v} = \lambda\mathbf{v}^T\mathbf{v}$ and consequently

$$\lambda = \frac{\mathbf{v}^T A^T A\mathbf{v}}{\mathbf{v}^T\mathbf{v}} = \frac{||A\mathbf{v}||_2^2}{||\mathbf{v}||_2^2} = ||A\mathbf{v}||_2 \geq 0$$

- Recall that the Euclidean norm of a vector $\mathbf{y} \in \mathbb{R}^k, k \in \mathbb{N}$ is $||\mathbf{y}||_2 = \sqrt{\mathbf{y}^T\mathbf{y}}$

The Thin SVD

- Let $A \in \mathbb{R}^{m\times n}$ and assume that $m \geq n$ (otherwise we consider A^T), then the **thin** SVD of A is

$$A_{m\times n} = U_{m\times n}\Sigma_{n\times n}V^T_{n\times n}$$

where Σ is a digaonal matrix with nonnegative elements, V is orthongonal (i.e. $VV^T = V^TV = I$) and U satisfies $U^T_{m\times n}U_{m\times n} = I_{n\times n}$ iff $m = n$

The Thin SVD

- We refer to the diagonal elements of Σ, denoted by $\{\sigma_i\}_{i=1}^{n}$, as the singular values of A and order them so that $\sigma_1 \geq \cdots \geq \sigma_n \geq 0$
- We denote the columns of V by $\mathbf{v}_1, \ldots, \mathbf{v}_n$ and refer to them as right singular vectors
- Similarly, the columns of U are denoted by $\mathbf{u}_1, \ldots, \mathbf{u}_n$ and are called left singular vectors

The Full SVD

- The **full** SVD of A takes the form

$$A_{m\times n} = U_{m\times m}\Sigma_{m\times n}V^T_{n\times n}$$

where U and V are orthogonal matrices and $\Sigma_{m\times n}$ is obtained from $\Sigma_{n\times n}$ of the thin SVD by padding it with an $(m-n)\times n$ bock of zeros, i.e.

$$\Sigma_{m\times n} = \begin{bmatrix} \Sigma_{n\times n} \\ \mathbf{0}_{(m-n)\times n} \end{bmatrix}$$

The Compressed SVD

- The **compressed** SVD is even thinner than the thin SVD
- Let $r = r(A)$ be the number of nonzero singular values of A (note that $\sigma_1 \geq \ldots \geq \sigma_r > \sigma_{r+1} = \ldots = \sigma_n = 0$), the compressed SVD of A has the form

$$A_{m\times n} = U_{m\times r}\Sigma_{r\times r}V_{n\times r}^T$$

where $\Sigma_{r\times r}$ is diagonal (with positive elements), $U_{m\times r}^T U_{m\times r} = I_{r\times r}$ and $V_{n\times r}^T V_{n\times r} = I_{r\times r}$

The Full, Thin, and Compressed SVDs

- The full SVD is common in pure mathematics (due to its use of two orthogonal transformations) and is the default for the MATLAB `svd` command
- In practice the thin SVD is more economical and avoids redundant space, it can be obtained from the MATLAB `svd` command by choosing the option 0
- The compressed SVD is even more economical, however the problem is that it is difficult to precisely determine r (a smaller estimate for r may be used)

SVD Formulation (Thin)

- Similar to the three equivalent formulations of the EVD, the SVD has three equivalent formulations
- For simplicity, we formulate them for the thin SVD

$$A_{m\times n} = U_{m\times n}\Sigma_{n\times n}V_{n\times n}^T \tag{6}$$

where Σ is diagonal with nonnegative elements, $U^TU = I_{n\times n}$, and $V^TV = I_{n\times n}$

SVD Formulation (Thin)

- Let $\{\mathbf{v}_i\}_{i=1}^n, i = 1, \ldots, n$ be an orthonormal basis for $\mathbb{R}^n$ and $\{\mathbf{u}\}_{i=1}^n$ be an orthonormal system for $\mathbb{R}^m$, $\sigma_1 \geq \ldots \geq \sigma_n \geq 0$, then

$$A\mathbf{v}_i = \sigma_i \mathbf{u}_i \tag{7}$$

and

$$A = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i {\mathbf{v_i}}^T \tag{8}$$

where $\{\mathbf{u}_i\}_{i=1}^n$, $\{\mathbf{v}_i\}_{i=1}^n$, and $\{\sigma_i\}_{i=1}^n$ are as in (2)

- The equivalence of (6)-(8) is proved similarly to the equivalence of (1)-(3)

Example: Computing the SVD

- Let

$$A_{3\times 2} = \begin{bmatrix} 2 & -1 \\ 1 & 2 \\ 1 & 1 \end{bmatrix}$$

and form $A^T A = \begin{bmatrix} 6 & 1 \\ 1 & 6 \end{bmatrix}$

- Since the trace of this matrix is 12 and the determinant is 35, its eigenvalues are $\lambda_1 = 7$ and $\lambda_2 = 5$ and therefore $\sigma_1 = \sqrt{7}$ and $\sigma_2 = \sqrt{5}$

Example: Computing the SVD

- Next, we need to compute the eigenvectors of $A^T A$
- One may quickly notice that $[1, 1]^T$ is an eigenvector with eigenvalue 7, the other eigenvector needs to be orthogonal to it and thus $[1, -1]^T$ is an eigenvector with eigenvalue 5
- To form an orthonormal basis we normalize these vectors and obtain $\mathbf{v}_1 = [1/\sqrt{2}, 1/\sqrt{2}]^T$ and $\mathbf{v}_2 = [1/\sqrt{2}, -1/\sqrt{2}]^T$
- Finally, $\mathbf{u}_1 = \frac{A\mathbf{v}_1}{\sigma_1} = [1/\sqrt{14}, 3/\sqrt{14}, 2/\sqrt{14}]^T$ and $\mathbf{u}_2 = \frac{A\mathbf{v}_2}{\sigma_2} = [3/\sqrt{10}, -1/\sqrt{10}, 0]^T$

Example: Computing the SVD

- Since there are no zero singular values, the thin and compressed SVDs are the same and are obtained by $A = U_{3\times 2}\Sigma_{2\times 2}V_{2\times 2}^T$ where

$$\Sigma_{2\times 2} = \begin{bmatrix} \sqrt{7} & 0 \\ 0 & \sqrt{5} \end{bmatrix}, \quad V_{2\times 2} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}, \quad U_{3\times 2} = \begin{bmatrix} \frac{1}{\sqrt{14}} & \frac{3}{\sqrt{10}} \\ \frac{3}{\sqrt{14}} & -\frac{1}{\sqrt{10}} \\ \frac{2}{\sqrt{14}} & 0 \end{bmatrix}$$

Example: Computing the SVD

- For the full SVD, we need to find a vector $\mathbf{u}_3$ completing $\mathbf{u}_1$ and $\mathbf{u}_2$ to an orthonormal basis
- Recall that $\mathbf{u}_1 \times \mathbf{u}_2$ is orthogonal to both $\mathbf{u}_1$ and $\mathbf{u}_2$ thus $\mathbf{u}_3 = \sqrt{14}\mathbf{u}_1 \times \sqrt{10}\mathbf{u}_2 = [2, 6, -10]^T$ and normalizing by its norm $(\mathbf{u}_3 = \mathbf{u}_3/||\mathbf{u}_3||_2)$ we obtain $\mathbf{u}_3 = [2, 6, -10]^T/\sqrt{140}$
- Therefore, the full SVD is formed as $A = U_{3\times 3}\Sigma_{3\times 2}V_{2\times 2}^T$ where

$$\Sigma_{3\times 2} = \begin{bmatrix} \sqrt{7} & 0 \\ 0 & \sqrt{5} \\ 0 & 0 \end{bmatrix}, V_{2\times 2} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}, U_{3\times 3} = \begin{bmatrix} \frac{1}{\sqrt{14}} & \frac{3}{\sqrt{10}} & \frac{2}{\sqrt{140}} \\ \frac{3}{\sqrt{140}} & -\frac{1}{\sqrt{10}} & \frac{6}{\sqrt{140}} \\ \frac{2}{\sqrt{14}} & 0 & -\frac{10}{\sqrt{140}} \end{bmatrix}$$

The SVD and the Inverse

- If $A \in \mathbb{R}^{n\times n}$ and $\operatorname{rank}(A) = n$, then A is invertible and there exists a unique **inverse** $B = A^{-1} \in \mathbb{R}^{n\times n}$ such that $BA = AB = I_{n\times n}$
- If $A_{n\times n} = U_{n\times n}\Sigma_{n\times n}V^T_{n\times n}$, then
$$A^{-1} = V\Sigma^{-1}U^T$$
since $U^T_{n\times n}U_{n\times n} = I_{n\times n}$, $U^{-1} = U^T$, and similarly $(V^T)^{-1} = V$
- Combining these observations with the identity $(AB)^{-1} = B^{-1}A^{-1}$ we conclude that
$$\begin{aligned} A^{-1} &= (U_{n\times n}\Sigma_{n\times n}V^T_{n\times n})^{-1} \\ &= (V^T_{n\times n})^{-1}\Sigma^{-1}U^{-1} \\ &= V\Sigma^{-1}U^T \end{aligned}$$

The SVD and the Pseudoinverse

- If $A_{m\times n}$ with $m \geq n$ and $\text{rank}(A) = n$, then we define the **pseudoinverse** of A as the matrix $B = A^{\dagger}$ that satisifies

$$BA = I_{n\times n} \tag{9}$$

$$\text{and } AB \text{ is symmetric} \tag{10}$$

- If $m = n$, then the psuedoinverse coincides with the inverse

The SVD and the Pseudoinverse

- To show that the psuedoinverse is uniquely defined we start by multiplying (9) by A from the left to obtain

$$ABA = A \tag{11}$$

- Applying the transpose to both sides of (11) results in

$$A^T(AB)^T = A^T \tag{12}$$

The SVD and the Pseudoinverse

- It follows from (10) and (12) that

$$A^T AB = A^T \tag{13}$$

- Since A has full rank the matrix $A^T A$ is invertible and thus (13) implies that the pseudoinverse $B = A^\dagger$ is uniquely defined and can be computed as

$$A^\dagger = B = (A^T A)^{-1} A^T \tag{14}$$

The SVD and the Pseudoinverse

- We can also express the pseudoinverse in terms of the SVD of A
- If $A = U\Sigma V^T$, then plugging this into (14) yields

$$A^\dagger = V\Sigma^{-1}U^T \tag{15}$$

- Note that (15) implies that $AA^\dagger = UU^T$ (and that $A^\dagger A = I$), that is $AA^\dagger$ is the orthogonal projector onto the image of A (if $m = n$ then clearly this orthogonal projector is I)

The SVD and the Pseudoinverse

- It is worthy to note that the computation of the pseudoinverse by (15) is numerically more stable than that in (14)
- In particular, the multiplication $A^T A$ in (14) followed by matrix inversion accumulates significant numerical error

Review Question

Let

$$A = \begin{bmatrix} -3 & -4 \\ 0 & 0 \\ 0 & 0 \\ 0 & 5 \end{bmatrix}$$

- Find the thin SVD of A (use MATLAB to check your answer)

The Least Squares Problem

- Given $A \in \mathbb{R}^{m \times n}$ and $\mathbf{b} \in \mathbb{R}^m$, the **least squares problem** is to find an $\mathbf{x} \in \mathbb{R}^n$ that minimizes $||A\mathbf{x} - \mathbf{b}||_2$
- The minimizing vector $\mathbf{x}$ is called a **least squares solution** of $A\mathbf{x} = \mathbf{b}$

The Normal Equations

- A solution $\mathbf{x}$ of the least squares problem is a solution of the linear system

$$A^T A\mathbf{x} = A^T \mathbf{b}$$

  and the system is nonsingular iff A has linearly independent columns

- The linear system $A^T A\mathbf{x} = A^T \mathbf{b}$ is called the **normal equations**

Solving the Least Squares Problem using SVD

- Since $A^T A\mathbf{x} = A^T\mathbf{b}$ we obtain $\mathbf{x} = A^\dagger\mathbf{b}$ where $A^\dagger = (A^T A)^{-1}A^T$ is the pseudoinverse
- Using the SVD, we can compute the solution set as

$$\begin{aligned}\mathbf{x} &= A^\dagger\mathbf{b}\\ &= V\Sigma^{-1}U^T\mathbf{b}\end{aligned}$$

  and thus the pseudoinverse provides the optimal solution to the least squares problem

Review Question

Let

$$A = \begin{bmatrix} 1 & 3 & 1 \\ 6 & -1 & 2 \\ 9 & -4 & 3 \\ 7 & -2 & 1 \\ 3 & 8 & 4 \end{bmatrix}, \quad b = \begin{bmatrix} 2 \\ -1 \\ -3 \\ 7 \\ 9 \end{bmatrix}$$

- Using the MATLAB `svd` command, find a vector $\mathbf{x}$ that minimizes $||A\mathbf{x} - \mathbf{b}||_2$

Fitting a Line in $\mathbb{R}^2$

- Suppose $\{[x_i, y_i]^T\}_{i=1}^N \subseteq \mathbb{R}^2$ and for a line l in the plane define $t_i = t_i(x_i, y_i, l)$ as the vertical distance from a point $[x_i, y_i]^T$ to the line
- The goal is to minimize $\sum_{i=1}^N t_i^2$ among all possible lines l and if l is $f(x) = ax + b$ we want to minimize $\sum_{i=1}^N (f(x_i) - y_i)^2$
- Define the A, $\mathbf{x}$, and $\mathbf{b}$ by

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} a \\ b \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

and minimize $||A\mathbf{x} - \mathbf{b}||_2^2$ over all $\mathbf{x} = [a, b]^T \in \mathbb{R}^2$

Fitting a Line in $\mathbb{R}^{d+1}$

- In the more general case, let $\mathbf{x}_i = [x_{i,1}, \ldots, x_{i,d}, y_i]^T \in \mathbb{R}^{d+1}$
- We want to fit a linear function $f(x_i) = a_1 x_{i,1} + \cdots + a_d x_{i,d} + b$ which minimizes $\sum (f(x_i) - y_i)^2$
- Similar to the $\mathbb{R}^2$ case, define the A, $\mathbf{x}$, and $\mathbf{b}$ by

$$A = \begin{bmatrix} x_{1,1} & \cdots & x_{1,d} & 1 \\ \vdots & \vdots & \vdots & \vdots \\ x_{n,1} & \cdots & x_{n,d} & 1 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} a_1 \\ \vdots \\ a_d \\ b \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

and minimize $||A\mathbf{x} - \mathbf{b}||_2^2$ over all $\mathbf{x} \in \mathbb{R}^{d+1}$

Fitting a Quadratic Function

- If we need to fit a quadratic function rather than a linear function we can still use the same techniques
- Suppose $x_i, y_i \in \mathbb{R}$ and we want to fit a function $f(x_i) = ax_i^2 + bx_i + c$ that minimizes the sum of the squares of the vertical distances between the data points and $f(x)$
- Define A, $\mathbf{x}$, and $\mathbf{b}$ by

$$A = \begin{bmatrix} x_1^2 & x_1 & 1 \\ \vdots & \vdots & \vdots \\ x_n^2 & x_n & 1 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} a \\ b \\ c \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

and minimize $||A\mathbf{x} - \mathbf{b}||_2^2$ over all $\mathbf{x} \in \mathbb{R}^3$

Principal Component Analysis (PCA)

- In **principal component analysis** (PCA) we find the directions in the data with the most variation, i.e. the eigenvectors corresponding to the largest eigenvalues of the covariance matrix, and project the data onto these directions
- The motivation for doing this is that the most second order information is located along these directions

Finding the Best d-Dimensional Subspace

- Given the data points $\{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^D$ we want to find l, a d-dimensional subspace ($1 \leq d < D$) which minimizes $\sum_{i=1}^n \text{dist}(\mathbf{x}_i, l)$
- This is the orthogonal distance from the data points to the subspace among all d-dimensional subspaces l of $\mathbb{R}^d$

PCA via SVD

- The **PCA algorithm** for finding this d-dimensional subspace is as follows
- Step 1: Calculate

$$\mathbf{x}_{cm_i} = \frac{\sum_{j=1}^{n} x_{j,i}}{n}$$

  For example, to find the first coordinate of the center of mass $\mathbf{x}_{cm_i}$, sum the first coordiante of all data points and divide by n

- Step 2: Shift the data points so that the center of mass is at the origin, e.g. $\mathbf{x}_i = \mathbf{x}_i - \mathbf{x}_{cm}$

PCA via SVD

- Step 3: Form

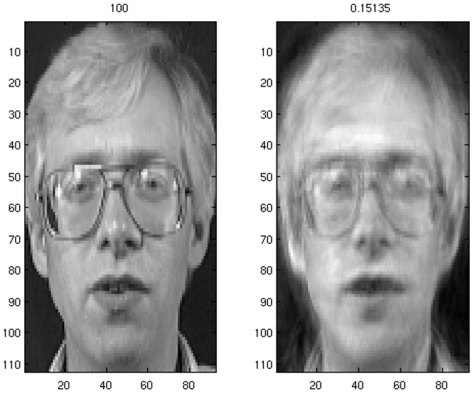
$$A = \begin{bmatrix} \mathbf{x}_i^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix}$$

  where the $\mathbf{x}_i$ are the new $\mathbf{x}_i$ formed in step 2

- Step 4: Calculate the right singular vectors $\mathbf{v}_1, \ldots, \mathbf{v}_d$ corresponding to the d largest singular values of A where the SVD of A is $A = U\Sigma V^T$ and the $\mathbf{v}_i$ are the columns of V (or the rows of V^T)

- Step 5: Output $l = \mathbf{x}_{cm} + \text{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_d\}$

Image Approximation using PCA



- The original image (left) compared to its approximating image using d principal components (right).

Summary

- The SVD allows us to obtain fundamental insights into the structure of a matrix
- Within the areas of image and data analysis, the SVD has numerous applications