The Singular Value Decomposition (SVD)

Objectives

- Define singular value decomposition (SVD)
- Express skinny SVD
- Write SVD as sum of outer products
- Use SVD to find best low-rank approximation
- Interpret matrix as an operator

SVD

- matrix decomposition that leads to good low-rank approximations
- vast range of applications

Definition:

Any $N \times M$ matrix $\underline{A}$ can be written as

$$\underline{A} = \underline{U}\,\underline{\Sigma}\,\underline{V}^T$$

- $\underline{U}$: $N \times N$, orthonormal columns
- $\underline{V}$: $M \times M$, orthonormal columns
- $\underline{\Sigma}$: $N \times M$, diagonal, $\underline{\Sigma}_{ii} \geq 0$

$N > M$

$$\begin{bmatrix} \sigma_1 & & \underline{0} \\ & \sigma_2 \ddots & \\ \underline{0} & & \sigma_M \\ & \underline{0} & \end{bmatrix}$$

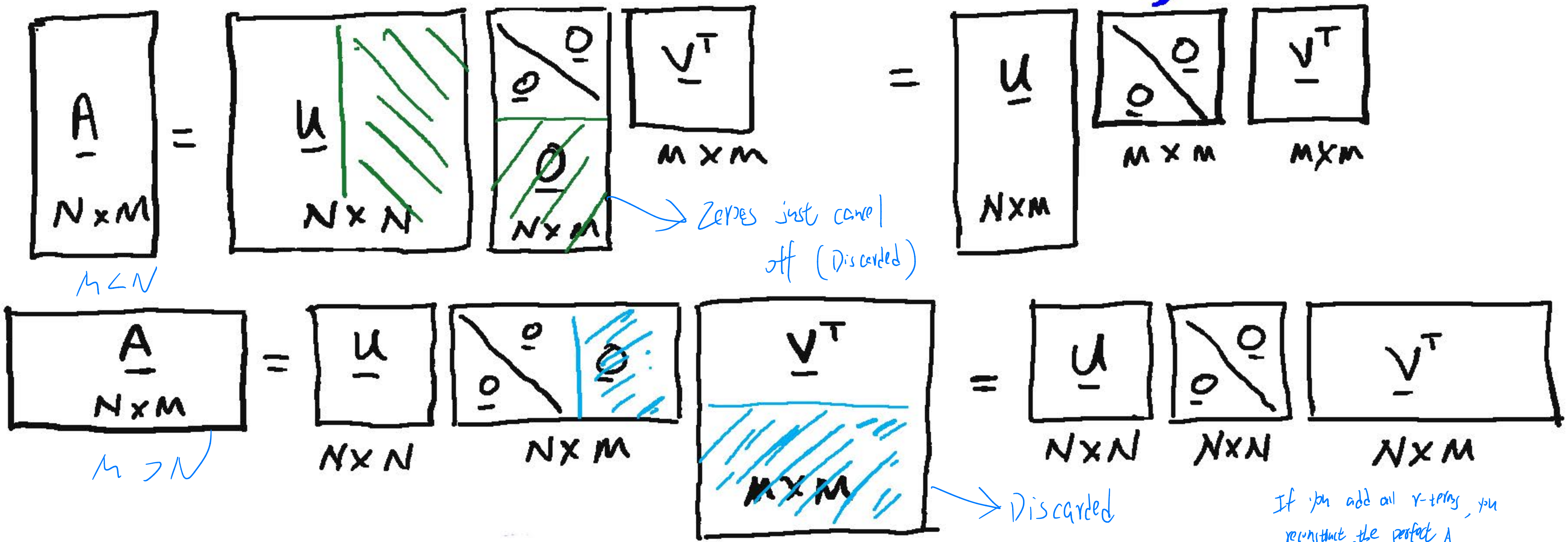
$M > N$

$$\begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & \underline{0} & \underline{0} \\ \underline{0} & & \ddots & \\ & & & \sigma_N \end{bmatrix}$$

$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{N/M} \geq 0$

SVD Dimensions

Skinny SVD



If you add all r-terms, you reconstruct the perfect A

"rank 1"

Sum of Outer Products Form:

$$\underline{A} = \begin{bmatrix} | & | & & | \\ \underline{u}_1 & \underline{u}_2 & \cdots & \underline{u}_M \\ | & | & & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_M \end{bmatrix} \begin{bmatrix} - & \underline{v}_1^T & - \\ - & \underline{v}_2^T & - \\ & \vdots & \\ - & \underline{v}_M^T & - \end{bmatrix} = \sum_{i=1}^{M} \sigma_i \underline{u}_i \underline{v}_i^T = \sum_{i=1}^{M} \underbrace{\boxed{\sigma_i \underline{u}_i \underline{v}_i^T}}_{N\times M}$$

SVD gives the "best" low-rank approximation

Frobenius norm $\|\underline{A}\|_F^2 = \sum_{i=1}^{N} \sum_{j=1}^{M} \left([\underline{A}]_{i,j}\right)^2 = \|\mathrm{vec}(\underline{A})\|_2^2$

(Sum of squares of all the elements in A)

Eckart-Young Theorem (1936) Let $\mathrm{rank}(\underline{A}) = r$ and $k < r$: $\min_{\mathrm{rank}(\underline{B}) \le k} \|\underline{A} - \underline{B}\|_F^2 = \sum_{i=k+1}^{r} \sigma_i^2$ for $\underline{B} = \sum_{i=1}^{k} \sigma_i \underline{u}_i \underline{v}_i^T$

where $\underline{A} = \underline{U}\,\underline{\Sigma}\,\underline{V}^T$ is the SVD.

(The theorem that shows the SVD is the best for low-rank decomposition)

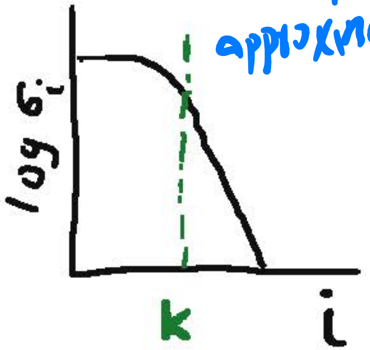
cols: scaled $\underline{u}_i$

rows: scaled $\underline{v}_i^T$

k-rank approximation

$$\underline{A} \approx \sigma_1 \underline{u}_1 \underline{v}_1^T + \sigma_2 \underline{u}_2 \underline{v}_2^T + \cdots + \sigma_k \underline{u}_k \underline{v}_k^T$$

patterns: most important, 2nd most, ..., kth most



σ_i provide ordered ranking of components

SVD describes matrix as an operator

$\underline{A}: N \times M$, $\underline{x}: M \times 1$, $\underline{y}: N \times 1$

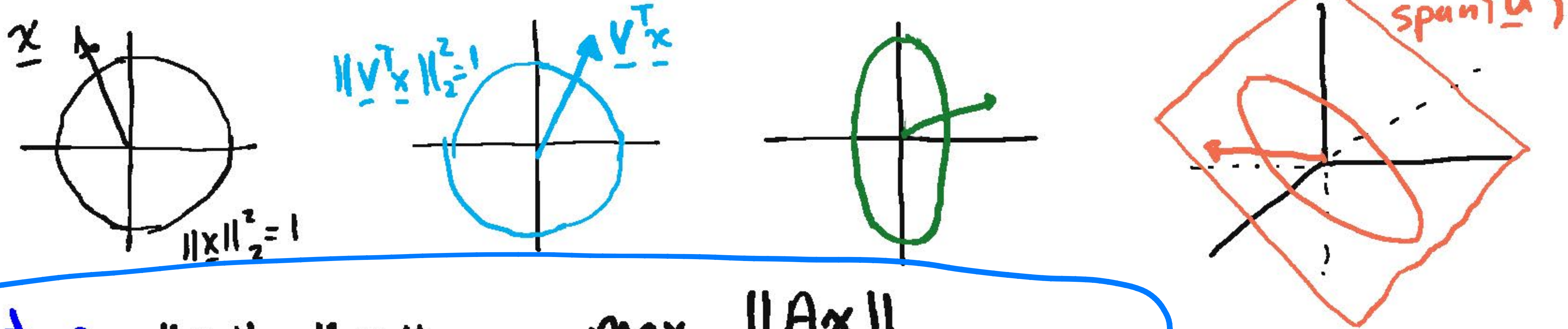
$$\underline{y} = \underline{A}\,\underline{x} = \underline{U}\,\underline{\Sigma}\,\underline{V}^T \underline{x} = \underline{U}\left[\underline{\Sigma}\left(\underline{V}^T \underline{x}\right)\right]$$

$$x : \mathbb{R}_M \xrightarrow[\text{rotate}]{\underline{V}^T} \underline{V}^T\underline{x} : \mathbb{R}_M \xrightarrow[\underline{\Sigma}]{\text{scale}} \underline{\Sigma}\,\underline{V}^T\underline{x} : \mathbb{R}_M \xrightarrow[\text{rotate (up dim)}]{\underline{U}} \underline{y} : \mathbb{R}_N$$

Note: $\|\underline{V}^T\underline{x}\|_2^2 = \underline{x}^T\underbrace{\underline{V}\,\underline{V}^T}_{\text{o/n}}\underline{x} = \underline{x}^T\underline{x} = \|\underline{x}\|_2^2$

$N = 3$

$M = 2$



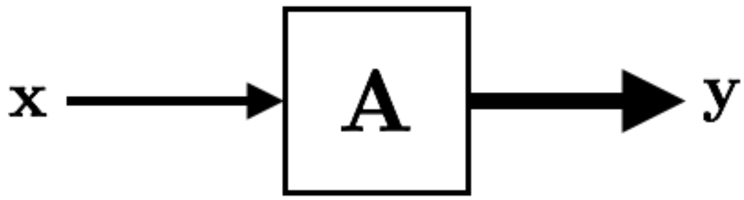
Operator Norm

$$\|\underline{A}\|_2 = \|\underline{A}\|_{op} := \max_{\underline{x} \neq 0} \frac{\|\underline{A}\underline{x}\|_2}{\|\underline{x}\|_2} = \sigma_1$$

(proof: notes)

Singular Value Decomposition
Proof: Operator Norm is the Largest Singular Value

A matrix $\boldsymbol{A}$ may be viewed as an "operator" that acts on a vector $\boldsymbol{x}$ to produce a new vector $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ as shown below.



The operator or two norm of a matrix measures the largest possible amplification a given matrix $\boldsymbol{A}$ applies to any vector $\boldsymbol{x}$. That is, the operator norm is the maximum of the ratio $||\boldsymbol{y}||_2/||\boldsymbol{x}||_2$. This is written formally as

$$||\boldsymbol{A}||_2 = ||\boldsymbol{A}||_{op} = \max_{\boldsymbol{x}\neq\boldsymbol{0}} \frac{||\boldsymbol{A}\boldsymbol{x}||_2}{||\boldsymbol{x}||_2}$$

We use the fact that $||c\boldsymbol{x}||_2 = c||\boldsymbol{x}||_2$ to rewrite the operator norm in the more convenient form

$$||\boldsymbol{A}||_2 = ||\boldsymbol{A}||_{op} = \max_{||\boldsymbol{x}||_2=1} ||\boldsymbol{A}\boldsymbol{x}||_2$$

Theorem: $||\boldsymbol{A}||_{op} = \sigma_1$ where σ_1 is the largest singular value of the matrix $\boldsymbol{A}$.

Proof: Substitute the singular value decomposition for $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$ where $\boldsymbol{U}$ and $\boldsymbol{V}$ are square matrices (the non-economy or non-skinny SVD) to write

$$||\boldsymbol{A}||_2 = ||\boldsymbol{A}||_{op} = \max_{||\boldsymbol{x}||_2=1} ||\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T\boldsymbol{x}||_2$$

Now let $\boldsymbol{z} = \boldsymbol{V}^T\boldsymbol{x}$ and note that $||\boldsymbol{z}||_2^2 = \boldsymbol{x}^T\boldsymbol{V}\boldsymbol{V}^T\boldsymbol{x} = \boldsymbol{x}^T\boldsymbol{x} = ||\boldsymbol{x}||_2^2$ because the right singular vectors in $\boldsymbol{V}$ are orthonormal. That is, $\boldsymbol{V}\boldsymbol{V}^T = \boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}$. Hence we may write

$$||\boldsymbol{A}||_2 = ||\boldsymbol{A}||_{op} = \max_{||\boldsymbol{z}||_2=1} ||\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{z}||_2$$

We may use the properties of the left singular vectors in $\boldsymbol{U}$ to eliminate the dependence on $\boldsymbol{U}$. We have $||\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{z}||_2^2 = \boldsymbol{z}^T\boldsymbol{\Sigma}^T\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{z} = \boldsymbol{z}^T\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\boldsymbol{z} = ||\boldsymbol{\Sigma}\boldsymbol{z}||_2^2$ since the left singular vectors are also orthonormal, that is, $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$. This results in

$$||\boldsymbol{A}||_2^2 = ||\boldsymbol{A}||_{op}^2 = \max_{||\boldsymbol{z}||_2=1} ||\boldsymbol{\Sigma}\boldsymbol{z}||_2^2$$

Let $\boldsymbol{A}$ have rank p so there are p nonzero singular values in the diagonal matrix $\boldsymbol{\Sigma}$. We thus may write

$$||\boldsymbol{\Sigma z}||_2^2 = \sum_{i=1}^{p} \sigma_i^2 z_i^2$$

where σ_i are the singular values and z_i is the i^{th} element of $\boldsymbol{z}$. We may rewrite the squared norm as

$$||\boldsymbol{A}||_2^2 = ||\boldsymbol{A}||_{op}^2 = \max_{z_1^2+z_2^2+\cdots+z_M^2=1} \sum_{i=1}^{p} \sigma_i^2 z_i^2$$

The unit norm constraint on $\boldsymbol{z}$ implies that an increase in the magnitude of any one element z_k must be offset by a decrease in the magnitudes of the other elements of $\boldsymbol{z}$. Clearly we should set $z_{p+1} = \cdots = z_M = 0$ since these elements do not contribute to the cost function. Since $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p > 0$, the best element to allocate the unit energy in $\boldsymbol{z}$ is z_1. To see this, consider the case where $p = M = 2$ and $\sigma_1 > \sigma_2$. In this case we require $z_2^2 = 1 - z_1^2$ and

$$\sum_{i=1}^{p} \sigma_i^2 z_i^2 = \sigma_1^2 z_1^2 + \sigma_2^2(1 - z_1^2) = z_1^2(\sigma_1^2 - \sigma_2^2) + \sigma_2^2$$

Since $\sigma_1^2 - \sigma_2^2 > 0$, this quantity is maximized by choosing z_1^2 to be as large or possible, that is, $z_1^2 = 1$. Any energy allocated to z_2 is multiplied by σ_2^2, which results in a lower value than had that same energy been allocated to z_1 because $\sigma_1 > \sigma_2$. A similar argument applies to the case $p > 2$. The strategy that maximizes $\sum_{i=1}^{p} \sigma_i^2 z_i^2$ allocates all of the unit energy in $\boldsymbol{z}$ to z_1, since σ_1 is the largest singular value.

Thus, we've shown that

$$||\boldsymbol{A}||_2 = ||\boldsymbol{A}||_{op} = \max_{||\boldsymbol{x}||_2=1} ||\boldsymbol{Ax}||_2 = \sigma_1$$

and this maximum value is obtained when $\boldsymbol{x} = \boldsymbol{Vz} = \boldsymbol{v}_1$ where $\boldsymbol{v}_1$ is the right singular vector corresponding to the largest singular value.