Not tested on midterm exam #1

Math 6610: Analysis of Numerical Methods, I
The singular value decomposition and consequences

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Resources: Trefethen and Bau 1997, Lectures 4, 5
Salgado and Wise 2022, Chapter 2

Eigenvalue decompositions and "spectral" theorems

If $\mathbf{A} \in \mathbb{C}^{n \times n}$, then

- If $\mathbf{A}$ is not defective, it's diagonalizable

A not defective $\Longleftrightarrow$ A diagonalizable

- $\mathbf{A}$ is Hermitian iff it's unitarily real diagonalizable

Unitary diagonalizability, i.e., a "spectral theorem", is conceptually attractive: such matrices are diagonal under an appropriate rigid rotation/reflection of coordinates.

The spectral theorem

"The" spectral theorem on finite-dimensional spaces is an equivalence between the geometric notion of unitary diagonalizability and an algebraic characterization of matrices.

Definition

A matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ is a **normal matrix** if it commutes with its adjoint (conjugate transpose), i.e., $\mathbf{AA}^* = \mathbf{A}^*\mathbf{A}$.

NB: If $A = A^*$, then A is normal.

If $A = -A^*$, then A is normal.

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Now, here is the most general spectral theorem.

Theorem (The spectral theorem (for normal operators))

A square matrix is unitarily diagonalizable iff it is normal.

$$A = U \Lambda U^* \iff AA^* = A^*A$$

$$\lambda_j \in \mathbb{C}$$

Normal matrices

The definition of eigenvalues, $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$, suggests that the eigenvalues of a matrix are sufficient to quantitatively characterize its action. This is in many contexts false for *general* $\mathbf{A}$.

Normal matrices are the class of matrices for which eigenvalues *precisely* characterize the action of a matrix.

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If A is normal, ...

- then the induced 2-norm, spectral radius, and numerical radius $w(\mathbf{A}) \coloneqq \mathsf{max}_{z \in W(\mathbf{A})} |z|$ coincide
- then $\|\mathbf{A}\mathbf{x}\|_2 = \|\mathbf{A}^*\mathbf{x}\|_2$ for any vector $\mathbf{x}$
- then $\mathbf{A} = \mathbf{A}^*\mathbf{U}$ for some unitary $\mathbf{U}$

Actually, any of the above also implies that $\mathbf{A}$ is normal.

The Schur decomposition

One relatively simple proof of the spectral theorem exercises a general matrix decomposition.

Theorem (Schur factorization/decomposition)

Let $\mathbf{A} \in \mathbb{C}^{n \times n}$. Then there is a unitary matrix $\mathbf{U} \in \mathbb{C}^{n \times n}$ and an upper triangular matrix $\mathbf{T} \in \mathbb{C}^{n \times n}$ such that $\mathbf{A} = \mathbf{U}\mathbf{T}\mathbf{U}^*$.

(I.e.: all square matrices are unitarily triangularizable.)

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For now, the Schur factorization is essentially "just" a crutch for proving the spectral theorem.

But here's a preview for why it's useful more broadly: By the Schur factorization, every matrix $\mathbf{A}$ is *unitarily* similar to a triangular matrix $\mathbf{T}$.

A summary of similarity

Recall:

- All non-defective square matrices are diagonalizable (eigenvalue decomposition)
- All square matrices are bidiagonalizable (Jordan normal form)
- All square matrices are unitarily triangularizable (Schur decomposition)
- All *normal* matrices are exactly the set of unitarily diagonalizable square matrices (spectral theorem)

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What about rectangular matrices?

The singular value decomposition: Statement

Perhaps the most powerful matrix factorization is the following, which states that all matrices (even defective or rectangular ones) are *asymmetrically* unitarily diagonalizable, with non-negative diagonal.

Theorem (SVD: Singular Value Decomposition)

Any matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ can be written as the product,

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

where $\mathbf{U} \in \mathbb{C}^{m \times m}$ and $\mathbf{V} \in \mathbb{C}^{n \times n}$ are unitary.
The matrix $\mathbf{\Sigma} \in \mathbb{C}^{m \times n}$ is diagonal with non-negative entries.
By convention the diagonal elements of $\mathbf{\Sigma}$ are ordered in non-increasing order: $\Sigma_{i,i} \geq \Sigma_{i+1,i+1}$.
This decomposition is unique up to unitary transformations in subspaces with equal singular values.

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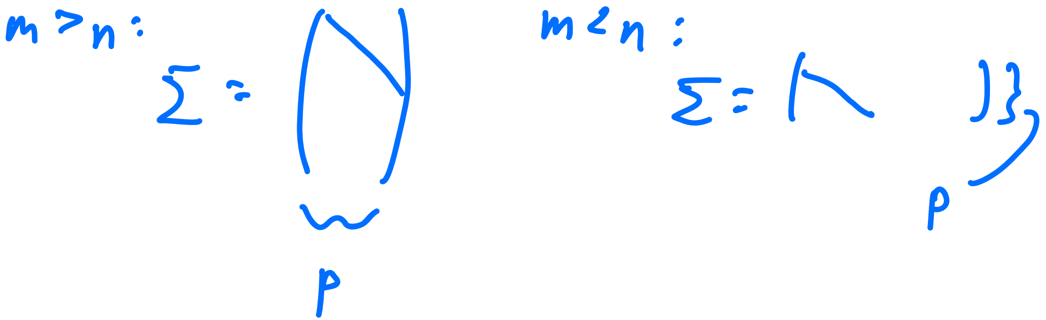
With $p = \mathsf{min}\{m, n\}$, notational convention:

- $\mathbf{\Sigma} = \mathsf{diag}(\sigma_1, \ldots, \sigma_p)$
- $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, the "singular values"
- $\mathbf{U} = [\mathbf{u}_1,\ \mathbf{u}_2,\ \ldots,\ \mathbf{u}_m]$, the "left singular vectors"
- $\mathbf{V} = [\mathbf{v}_1,\ \mathbf{v}_2,\ \ldots,\ \mathbf{v}_n]$, the "right singular vectors"



The singular value decomposition: Proof step 1

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Proof step 1: Assuming $m \geq n$, compute eigendecomposition of $\mathbf{A}^*\mathbf{A}$.

$A^*A \in \mathbb{C}^{n\times n}$, is Hermitian $\Longrightarrow A^*A = \underline{V}\,\underline{\Lambda}\,V^*$

<u>And</u>: $x \neq 0$, $R_{A^*A}(x) = \dfrac{\langle A^*Ax, x\rangle}{\|x\|^2}$

$= \dfrac{\|Ax\|^2}{\|x\|^2} \geq 0$

$R_{A^*A}(x) \geq 0 \implies A^*A$ is ~~spd~~.

positive semi-definite

$\Lambda = \text{diag}(\lambda_1 \ldots \lambda_n)$, $\lambda_j \geq 0$

Define $\sigma_j = \sqrt{\lambda_j}$, $j = 1 \ldots n$

Define $\underline{u}_j = \frac{1}{\sigma_j} \underline{\underline{A}}\, \underline{v}_j$ (if $\sigma_j > 0$)

$\underline{u}_j \in \mathbb{C}^m$

$$\langle \underline{u}_j, \underline{u}_k \rangle = \frac{1}{\sigma_j \sigma_k} \langle A v_j, A v_k \rangle$$

$$= \frac{1}{\sigma_j \sigma_k} \langle A^* A v_j, v_k \rangle$$

$$= \frac{\lambda_j}{\sigma_j \sigma_k} \langle v_j, v_k \rangle = \begin{cases} 0, & j \neq k \\ 1, & j = k \end{cases}$$

$\implies \{u_j\}_{j=1}^n$ are orthonormal (!!)

If $\sigma_j = 0$: define $\underline{u}_j$ as any vector orthonormal to the other $\underline{u}_k$ vectors.

$$\Longrightarrow \quad \underline{\underline{A}}\,\underline{v}_j = \sigma_j \underline{u}_j \qquad (1 \le j \le n)$$

$$\downarrow$$

$$\underline{\underline{A}} \begin{bmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{bmatrix} = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \begin{pmatrix} | & & | \\ u_1 & \cdots & u_n \\ | & & | \end{pmatrix}$$

$$= \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0_{(m-n)\times n} & \end{pmatrix} \begin{pmatrix} | & & | & | & & | \\ u_1 & \cdots & u_n & u_{n+1} & \cdots & u_m \\ | & & | & | & & | \end{pmatrix}$$

$$\underbrace{u_{n+1} \cdots u_m}_{\text{any orthonormal completion.}}$$

$$AV = \Sigma U$$

The singular value decomposition: Proof step 2

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Proof step 2: Define the positive σ_j, compute $\mathbf{u}_j = \frac{1}{\sigma_j}\mathbf{A}\mathbf{v}_j$ for $j \leq r = \mathsf{rank}(\mathbf{A})$, and show they are orthonormal.

The singular value decomposition: Proof step 3

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Proof step 3: Concatenate vector equalities, complete bases for $\mathbb{C}^m$, $\mathbb{C}^n$, solve for $\mathbf{A}$.

The SVD

The SVD is incredibly general and useful.

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^* = \sum_{j=1}^{p} \sigma_j \left(\mathbf{u}_j \mathbf{v}_j^*\right)$$

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$$\mathsf{rank}(\mathbf{A}) = r \quad \Longleftrightarrow \quad \sigma_r > 0, \text{ and } \sigma_j = 0, \quad j > r$$

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$\mathbf{A}$ has a *reduced* SVD:

$$\mathbf{A} = \sum_{j=1}^{r} \sigma_j \left(\mathbf{u}_j \mathbf{v}_j^*\right) = \widetilde{\mathbf{U}}\widetilde{\mathbf{\Sigma}}\widetilde{\mathbf{V}}^*, \qquad \widetilde{\mathbf{U}} = \left[\mathbf{u}_1, \ldots, \mathbf{u}_r\right], \qquad \widetilde{\mathbf{V}} = \left[\mathbf{v}_1, \ldots, \mathbf{v}_r\right]$$

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If $\mathbf{A}$ is square and invertible:

$$\mathbf{A}^{-1} = \mathbf{V}\boldsymbol{\Sigma}^{-1}\mathbf{U}^*$$

The four fundamental subspaces, redux

The SVD immediately reveals the 4 fundamental subspaces. Since,

$$\mathbf{A} = \widetilde{\mathbf{U}}\widetilde{\boldsymbol{\Sigma}}\widetilde{\mathbf{V}}^*,$$

then:

- $\mathsf{range}(\mathbf{A}) = \mathsf{span}\{\mathbf{u}_1, \ldots \mathbf{u}_r\}$
- $\mathsf{coker}(\mathbf{A}) = \mathsf{ker}(\mathbf{A}^*) = \mathsf{span}\{\mathbf{u}_{r+1}, \ldots \mathbf{u}_m\}$
- $\mathsf{ker}(\mathbf{A}) = \mathsf{span}\{\mathbf{v}_{r+1}, \ldots, \mathbf{v}_n\}$
- $\mathsf{corange}(\mathbf{A}) = \mathsf{range}(\mathbf{A}^*) = \mathsf{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_r\}$

I.e., the SVD (nearly) tells you *everything* about a matrix.

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- $\mathsf{ker}(\mathbf{A}) = \mathsf{span}\{\mathbf{v}_{r+1}, \ldots , \mathbf{v}_n\}$
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Q: Let $\mathbf{A}$ be a square matrix. How are the singular values σ_i of $\mathbf{A}$ related to its spectrum?
(Or maybe to the modulus of its spectrum?)

Low rank approximation

There are numerous (quite potent) uses of the SVD. Here's one of the more popular ones:

Suppose $\mathbf{A} \in \mathbb{C}^{m \times n}$ is a given matrix, and $r < \mathsf{min}\{m, n\}$. We wish to solve the optimization problem,

$$\underset{\mathbf{B} \in \mathbb{C}^{m \times n} \;\; \mathsf{rank}(\mathbf{B}) \leq r}{\mathsf{arg\,min}} \left\| \mathbf{A} - \mathbf{B} \right\|,$$

for some norm $\| \cdot \|$.

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Why?

- data compression
- simplification or denoising
- interpretable modeling

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Unsurprisingly, the choice of norm matters. There's a particular choice that is convenient to consider.

Definition

A norm $\|\cdot\|$ on $m \times n$ matrices is *unitarily invariant* if $\|\mathbf{A}\| = \|\mathbf{UAV}\|$ for any $\mathbf{A}$ and arbitrary unitary matrices $\mathbf{U}, \mathbf{V}$ of appropriate sizes. This implies the norm is a function of only the singular values. I.e., with $p = \min\{m, n\}$, $\|\cdot\|$ is a function $f : [0, \infty)^p \to [0, \infty)$ such that,

$$\|\mathbf{A}\| = f(\sigma_1, \ldots, \sigma_p).$$

Low rank approximation and the SVD

The main result is that an explicit solution to any unitarily invariant norm low-rank approximation problem is a truncated SVD.

Theorem (Schmidt-Eckart-Young-Mirsky)

Let $\mathbf{A} \in \mathbb{C}^{m \times n}$, and $k < \mathsf{rank}(\mathbf{A}) \leq \mathsf{min}\{m, n\}$. Suppose $\|\cdot\|$ is a unitarily invariant norm on $m \times n$ matrices. Then a solution $\mathbf{B}_k$ to,

$$\mathbf{B}_k \in \underset{\mathbf{B} \in \mathbb{C}^{m \times n} \;\; \mathsf{rank}(\mathbf{B}) \leq k}{\arg\min} \|\mathbf{A} - \mathbf{B}\|,$$

is

$$\mathbf{B}_k = \sum_{j=1}^{k} \sigma_j \mathbf{u}_j \mathbf{v}_j^*$$

The minimizer $\mathbf{B}_k$ is unique iff $\sigma_k > \sigma_{k+1}$.

(NB: $k \geq \mathsf{rank}(\mathbf{A})$ is fine, but the problem is then vacuous since one can choose $\mathbf{B} = \mathbf{A}$.)

Computing the SVD

It's kind of unclear how the SVD should be computed. However, the proof we've presented is actually constructive:

1. The Gram matrices $\mathbf{A}\mathbf{A}^* \in \mathbb{C}^{m\times m}$ and $\mathbf{A}^*\mathbf{A} \in \mathbb{C}^{n\times n}$ are Hermitian positive semidefinite. Their nonzero eigenvalues coincide, and if $r = \mathsf{rank}(\mathbf{A})$, then
   $\sigma_i^2(\mathbf{A}) = \lambda_i(\mathbf{A}\mathbf{A}^*) = \lambda_i(\mathbf{A}^*\mathbf{A})$ for $i \in [r]$.

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   By the spectral theorem, we can also compute (orthonormal!) eigenvectors $\mathbf{v}_i$ such that $\mathbf{A}^*\mathbf{A}\mathbf{v}_i = \sigma_i^2 \mathbf{v}_i$.

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3. As in the proof, set $\mathbf{u}_i = \mathbf{A}\mathbf{v}_i/\sigma_i$ only for $i \in [r]$. We now have $\sigma_i, \mathbf{u}_i, \mathbf{v}_i$ for $i \in [r]$.

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3. As in the proof, set $\mathbf{u}_i = \mathbf{A}\mathbf{v}_i/\sigma_i$ only for $i \in [r]$. We now have $\sigma_i, \mathbf{u}_i, \mathbf{v}_i$ for $i \in [r]$.

4. To compute the remaining columns $\mathbf{u}_{r+1}, \ldots, \mathbf{u}_m$, choose any $\mathbb{C}^m$-orthonormal completion of $\mathbf{u}_1, \ldots, \mathbf{u}_r$.

There are some minor details to iron out before this is actually implementable, e.g., we really only compute $\mathbf{u}_i$ for $i \leq \mathsf{rank}(\mathbf{A})$, and the rest we identify through orthogonal completion.

Back to eigenvalues

Hence, we arrive at the conclusion that the SVD is quite directly computable through an eigenvalue decomposition of Hermitian positive-semidefinite matrices!

So if we can compute eigenpairs of Hermitian matrices, the rest is “easy”.

Pro tip: computing eigenpairs of matrices of size $\gtrsim 10$ using roots of characteristic polynomials is an unattractive idea.

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In summary: eigenvalues are important to compute!
Most tasks we discussed rely on computing eigenvalues, at least of Hermitian matrices. How is this done?

For the next few weeks, we'll talk about how to compute eigenvalues. However, there's a lot of buildup we'll need before arriving there:

- What makes a good computational algorithm?
- How do we solve linear systems?
- How do we orthogonalize vectors?

References

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