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Chapter 8: Eigenvalues and Singular Values

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Slides for the book

A First Course in Numerical Methods (published by SIAM, 2011)

<http://www.ec-securehost.com/SIAM/CS07.html>

Goals of this chapter

- To find out how eigenvalues and singular values of a given matrix are computed;
- to find out how the largest (and smallest) few eigenvalues and singular values are computed;
- to see some interesting applications of eigenvalues and singular values.

Outline

- Algorithms for a few eigenvalues
- Uses of eigenvalues and eigenvectors
- Uses of SVD
- (A taste of) algorithms for all eigenvalues and SVD

Recall eigenvalues and singular values (Ch. 4)

- For a real, square $n \times n$ matrix A , an eigenvalue λ and corresponding eigenvector $\mathbf{x} \neq \mathbf{0}$ satisfy $A\mathbf{x} = \lambda\mathbf{x}$.
- There are n (possibly complex) eigenpairs $\lambda_1, \lambda_2, \dots, \lambda_n$ and eigenvectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ s.t. $A\mathbf{x}_i = \lambda_i\mathbf{x}_i$. For $\Lambda = \text{diag}(\lambda_i)$

$$AX = X\Lambda.$$

- If A is non-defective then the eigenvector matrix X is nonsingular:

$$X^{-1}AX = \Lambda.$$

- For a real, $m \times n$ matrix A , the singular value decomposition (SVD) is

$$A = U\Sigma V^T$$

where U $m \times m$ and V $n \times n$ are orthogonal matrices and Σ is “diagonal” consisting of zeros and singular values $\sigma_1 \geq \sigma_2, \dots \geq \sigma_r > 0$, $r \leq \min(m, n)$.

- Note: singular values are square roots of eigenvalues of $A^T A$.

Classes of methods for eigenvalue problem

- In general, **must iterate to find eigenvalues**. Nonetheless, methods for finding all eigenvalues for non-large matrices resemble properties of direct solvers; in particular, they are based on matrix decompositions.
- To find a few eigenvalues there are the basic **power** and **inverse power** methods, and their generalization to **orthogonal** iterations. Large and sparse eigenvalue solvers are based on Lanczos and Arnoldi iterations (will not be discussed). In MATLAB: **eigs**
- Methods for finding all eigenvalues are based on **orthogonal similarity transformations**. In MATLAB: **eig**
- In general, algorithms for finding SVD are related to those for finding eigenvalues. In MATLAB: **svd**

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Power method

- Given \mathbf{v}_0 , expand using eigenpairs

$$\mathbf{v}_0 = \sum_{j=1}^n \beta_j \mathbf{x}_j,$$

where $A\mathbf{x}_j = \lambda_j \mathbf{x}_j$, $j = 1, \dots, n$.

- Then

$$A\mathbf{v}_0 = \sum_{j=1}^n \beta_j A\mathbf{x}_j = \sum_{j=1}^n (\beta_j \lambda_j) \mathbf{x}_j.$$

- Multiplying by A $k-1$ times gives

$$A^k \mathbf{v}_0 = \sum_{j=1}^n \beta_j \lambda_j^{k-1} A\mathbf{x}_j = \sum_{j=1}^n (\beta_j \lambda_j^k) \mathbf{x}_j.$$

Power method (cont.)

Assuming:

- A non-defective
- $|\lambda_1| > |\lambda_j|, j = 2, \dots, n$
- $\beta_1 \neq 0$

Obtain

$$A^k \mathbf{v}_0 \rightarrow \mathbf{x}_1.$$

Given eigenvector, obtain eigenvalue from Rayleigh quotient

$$\lambda_1 = \frac{\mathbf{x}_1^T A \mathbf{x}_1}{\mathbf{x}_1^T \mathbf{x}_1}.$$

Power method (cont.)

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Power method algorithm and properties

- Algorithm:

For $k = 1, 2, \dots$ until termination

$$\tilde{\mathbf{v}} = A\mathbf{v}_{k-1}$$

$$\mathbf{v}_k = \tilde{\mathbf{v}} / \|\tilde{\mathbf{v}}\|_2$$

$$\lambda_1^{(k)} = \mathbf{v}_k^T A \mathbf{v}_k.$$

- Properties:

- Simple, basic, can be slow.
- Can be applied to large, sparse or implicit matrices.
- Limiting assumptions.
- Used as a building block for other, more robust algorithms.

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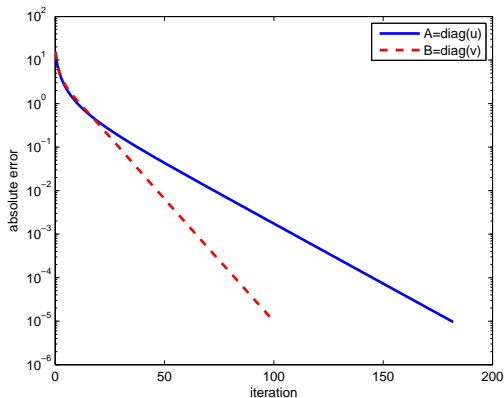
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Example: power method

```
u = [1:32]; v = [1:30, 30, 32];  
A = diag(u); B = diag(v);
```



Inverse power method

- Power method good only for a well-separated dominant eigenvalue. What about other eigenvalues? What about more general case of looking for a non-dominant eigenpair?
- If we know α that approximates well some simple eigenvalue λ_s then $|\lambda_s - \alpha| \ll |\lambda_i - \alpha|$, all $i \neq s$. Hence

$$|\lambda_s - \alpha|^{-1} \gg |\lambda_i - \alpha|^{-1}, \text{ all } i \neq s.$$

- These are the eigenvalues of $(A - \alpha I)^{-1}$ with the same eigenvectors!
- The parameter α is a **shift**.

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Inverse power method algorithm

- **Algorithm:** For $k = 1, 2, \dots$ until termination

Solve $(A - \alpha I)\tilde{\mathbf{v}} = \mathbf{v}_{k-1}$

$$\mathbf{v}_k = \tilde{\mathbf{v}} / \|\tilde{\mathbf{v}}\|$$

$$\lambda^{(k)} = \mathbf{v}_k^T A \mathbf{v}_k.$$

- **Properties:**

- Can apply to find different eigenvalues using different shifts.
- But must solve (possibly many) linear systems.
- If α is fixed then there is one matrix and many right hand sides: if a direct method can be applied then form LU decomposition of $A - \alpha I$ once. (See Chapter 5)
- Alternatively, can set $\alpha = \alpha_k$ and learn it as the iteration proceeds using λ_{k-1} . Now each iteration is more expensive, but the algorithm may converge much faster.

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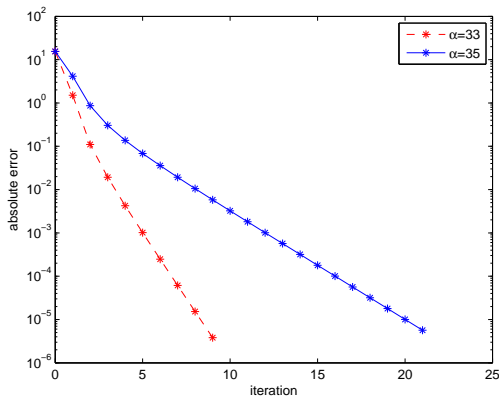
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Example: inverse power method

$u = [1:32]; A = \text{diag}(u);$



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Uses of eigenvalues and eigenvectors

- The famous **PageRank** algorithm for enabling quick www searching amounts to finding the dominant eigenvector, corresponding to the largest eigenvalue $\lambda = 1$ in a huge matrix A where relations among web pages are recorded.
- Often, the matrix A represents a discretization of a differential equation (such as those in Chapters 7 and 16). Correspondingly, A may be large and sparse. The eigenvector \mathbf{x} in the relation $A\mathbf{x} = \lambda\mathbf{x}$ then corresponds to a discretization of an **eigenfunction**.
- Eigenvalues are used for determining ℓ_2 condition numbers and naturally arise in many other analysis-related tasks.

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Singular value decomposition (SVD)

- Recall material from Chapter 4 (where there is also a PCA example):
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where U $m \times m$ and V $n \times n$ are orthogonal matrices and Σ is “diagonal” consisting of zeros and singular values $\sigma_1 \geq \sigma_2, \dots \geq \sigma_r > 0$, $r \leq \min(m, n)$.

- Singular values are square roots of eigenvalues of $A^T A$.
- If $r = n \leq m$ then

$$\kappa_2(A) = \frac{\sigma_1}{\sigma_n} = \sqrt{\kappa_2(A^T A)}.$$

- Note that, unlike for eigenvalues, A need not be square, the singular values are real and nonnegative, and the transformation to “diagonal” form is always well-conditioned.

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Solving the linear least squares problem using SVD

- $A = U\Sigma V^T$, so

$$\|\mathbf{b} - A\mathbf{x}\| = \|U^T\mathbf{b} - \Sigma\mathbf{y}\|, \quad \mathbf{x} = V\mathbf{y}.$$

- If $\kappa(A) = \sigma_1/\sigma_n$ is not too large then can proceed as with QR decomposition (Chapter 6).
- If $\kappa(A) = \sigma_1/\sigma_n$ is too large then proceed to determine an effective cutoff: going from n backward find r , $1 \leq r < n$, such that σ_1/σ_r is not too large and set $\sigma_{r+1} = \dots = \sigma_n = 0$, obtaining $\tilde{\Sigma}$. This changes the problem, from A to $\tilde{A} = U\tilde{\Sigma}V^T$, regularizing it!
- Precisely the same procedure can be also applied for problems $A\mathbf{x} = \mathbf{b}$ where A is square but too ill-conditioned (so the solution using GEPP may be meaningless).

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Regularization

Solve a nearby well-conditioned problem safely:

- 1 For $n, n-1 \dots$ until r found s.t. $\frac{\sigma_1}{\sigma_r}$ is tolerable in size. This is the condition number of the problem that we actually solve:

$$\min\{\|\mathbf{x}\| \ ; \ \mathbf{x} = \operatorname{argmin}\|\mathbf{b} - \tilde{A}\mathbf{x}\|\}$$

- 2 Let \mathbf{u}_i be i th column vector of U ; set $z_i = \mathbf{u}_i^T \mathbf{b}$, $i = 1, \dots, r$.
- 3 Set $y_i = \sigma_i^{-1} z_i$, $i = 1, 2, \dots, r$, $y_i = 0$, $i = r+1, \dots, n$.
- 4 Let \mathbf{v}_i be i th column vector of V ; set $\mathbf{x} = \sum_{i=1}^r y_i \mathbf{v}_i$.

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Example

- The least squares problem $\min_{\mathbf{x}} \|C\mathbf{x} - \mathbf{b}\|$ is easily solved for

$$C = \begin{pmatrix} 1 & 0 & 1 \\ 2 & 3 & 5 \\ 5 & 3 & -2 \\ 3 & 5 & 4 \\ -1 & 6 & 3 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 4 \\ -2 \\ 5 \\ -2 \\ 1 \end{pmatrix}.$$

Call the solution $\hat{\mathbf{x}}$.

- Next consider $\min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|$, where we add to C a column that is sum of the three previous ones:

$$A = \begin{pmatrix} 1 & 0 & 1 & 2 \\ 2 & 3 & 5 & 10 \\ 5 & 3 & -2 & 6 \\ 3 & 5 & 4 & 12 \\ -1 & 6 & 3 & 8 \end{pmatrix}.$$

- Note that A has $m = 5$, $n = 4$, $r = 3$: can't reliably solve this using normal equations or even QR.
- But the truncated SVD method works: if \mathbf{x} solves the problem with A , obtain $\|\mathbf{x}\| \approx \|\hat{\mathbf{x}}\|$, and $\|A\mathbf{x} - \mathbf{b}\| \approx \|C\hat{\mathbf{x}} - \mathbf{b}\|$.

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Truncated SVD and data compression

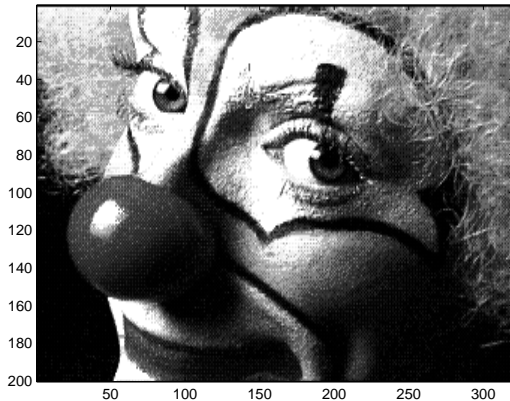
- Given an $m \times n$ matrix A , the best rank- r approximation of $A = U\Sigma V^T$ is the matrix

$$A_r = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T.$$

- This is another example of **truncated SVD (TSVD)**, so named because only the first r columns of U and V are utilized.
- It is a **model reduction** technique, which is a best approximation in the sense that $\|A - A_r\|_2$ is minimal over all possible rank- r matrices. The minimum residual norm is equal to σ_{r+1} .
- Note A_r uses only $r(m + n + 1)$ storage locations – significantly fewer than mn if $r \ll \min(m, n)$.

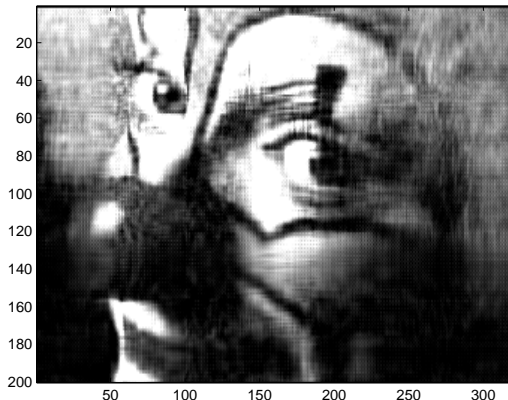
Example

Consider the following clown image, taken from MATLAB's image repository:



Compressed image of clown example

Here is what we get if we use $r = 20$.



Assessment

- The original image requires $200 \times 320 = 64000$ matrix entries to be stored; the compressed image requires merely $20 \cdot (200 + 320 + 1) \approx 10000$ storage locations.
- By storing less than 16% of the data, we get a reasonable image. It's not great, but all main the features of the clown are clearly shown.
- What are less clear in the compressed image are fine features (high frequency), such as the fine details of the clown's hair.
- Certainly, specific techniques such as [DCT](#) (Chapter 13) and [wavelet](#) are far superior to SVD for the task of image compression. Still, our example visually shows that most information is stored already in the leading singular vectors.

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Finding all eigenvalues

- Consider A real and square. Apply similarity orthogonal transformations

$$A_0 = A; \quad A_{k+1} = Q_k^T A_k Q_k, \quad k = 0, 1, 2, \dots,$$

so that $A_k \rightarrow$ upper triangular (diagonal for symmetric case) form.

- QR algorithm (distinct from QR decomposition!): two stages.

- Stage I

Given A , use Householder reflections (Chapter 6) to zero out elements in first diagonal: $Q^{(1)T} A = A^{(1)}$. However, to maintain similarity must multiply by $Q^{(1)}$ on the right, so

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QR algorithm: stages I-II

- Define

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But can only zero elements *below main subdiagonal*.

- Leads to an **upper Hessenberg** form. (Tridiagonal if A is symmetric.)
- **Stage II**

Let A_0 be the given matrix, transformed into upper Hessenberg form;
for $k = 0, 1, 2, \dots$ until termination

QR decomposition: $Q_k R_k = A_k - \alpha_k I;$

Construct next iterate: $A_{k+1} = R_k Q_k + \alpha_k I$

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