## Bi7740: Scientific computing

## Eigenvalues and eigenvectors

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## Outline

(1) Eigenvalue problems

- Eigenvalue problems

2 Existence, uniqueness and conditioning
(3) Computation

- Special forms
- Power iteration
- Generalized eigenvalue problem


## Supplemental bibliography - online

## http:

//web.eecs.utk.edu/~dongarra/etemplates/book.html


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## Eigenvalue problems

## Standard eigenvalue problem

Given a square matrix $\mathbf{A} \in \mathcal{M}_{n \times n}(\mathbb{R})$, find a scalar $\lambda$ and a vector $\mathbf{x} \in \mathbb{R}^{n}, \mathbf{x} \neq \mathbf{0}$, such that

$$
\mathbf{A} \mathbf{x}=\lambda \mathbf{x}
$$

- $\lambda$ is called eigenvalue and $\mathbf{x}$ is called eigenvector
- a similar "left" eigenvector can be defined as $\mathbf{y}^{\top} \mathbf{A}=\lambda \mathbf{y}^{\top}$, but this would be equivalent to a "right" eigenvalue problem (as above) with $\mathbf{A}^{T}$ as matrix
- the definition can be extended to complex-valued matrices
- $\lambda$ can be complex, even if $\mathbf{A} \in \mathcal{M}_{n \times n}(\mathbb{R})$


## Characteristic polynomial

- previous eq. is equivalent to $(\mathbf{A}-\lambda \mathbf{I}) \mathbf{x}=0$ which admits nonzero solutions if and only if $(\mathbf{A}-\boldsymbol{\lambda})$ ) is singular, i.e.

$$
\operatorname{det}(\mathbf{A}-\lambda \mathbf{I})=0
$$

- $\operatorname{det}(\ldots)$ is the characteristic polynomial of matrix $\mathbf{A}$ and its roots $\lambda_{i}$ are the eigenvalues of $\mathbf{A}$
- (from Fundamental Theorem of Algebra) for an $n \times n$ matrix there are $n$ eigenvalues (may not all be real or distinct)
- reciprocal: a polynomial $p(\lambda)=c_{0}+c_{1} \lambda+c_{n-1} \lambda^{n-1}+\lambda^{n}$ has a companion matrix

$$
\left[\begin{array}{ccccc}
0 & 0 & \ldots & 0 & -c_{0} \\
1 & 0 & \ldots & 0 & -c_{1} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & 1 & -c_{n-1}
\end{array}\right]
$$

- the characteristic polynomial is not used in numerical computation, because:
- finding its roots may imply an infinite number of steps
- of the sensitivity of the coefficients
- too much work to compute the coefficients and find the roots


## Example

Let $\mathbf{A}=\left[\begin{array}{cc}0 & 1 \\ 0 & -1\end{array}\right]$. The characteristic equation is

$$
\begin{aligned}
\operatorname{det}(\mathbf{A}-\lambda \mathbf{I}) & =0 \Leftrightarrow \\
\lambda^{2}+\lambda & =0
\end{aligned}
$$

with solutions $\lambda_{1}=0$ and $\lambda_{2}=-1$. For eigenvectors $\mathbf{v}_{1}, \mathbf{v}_{2}$ (non-null!):

$$
\left(\mathbf{A}-\lambda_{1} \mathbf{I}\right) \mathbf{v}_{1}=\left[\begin{array}{cc}
0 & 1 \\
0 & -1
\end{array}\right]\left[\begin{array}{l}
v_{11} \\
v_{21}
\end{array}\right]=\left[\begin{array}{c}
v_{21} \\
-v_{21}
\end{array}\right]:=\left[\begin{array}{l}
0 \\
0
\end{array}\right]
$$

so $v_{21}=0$. We choose $v_{11}$ such that $\left\|\mathbf{v}_{1}\right\|=1$, so $v_{11}=1$.
Similarly, for $\lambda_{2}=-1$ we get $\mathbf{v}_{2}=\left[\begin{array}{c}1 / \sqrt{2} \\ -1 / \sqrt{2}\end{array}\right]$.

## Example - in Matlab

```
1 >> A = [l0 1; 0 -1];
2 >> [V, L] = eig(A) % V: eigenvectors, L: eigenvalues
3 V =
4 1.0000 -0.7071
5 0 0.7071
L =
7 rrr
9 >> eig(A) % only eigenvalues
10
11 >> roots(poly(A)) % not the way to go normally
```


## Sensitivity of the characteristic polynomial

- let $\mathbf{A}=\left[\begin{array}{ll}1 & \epsilon \\ \epsilon & 1\end{array}\right]$ with $\epsilon>0$ and slightly smaller than $\epsilon_{\text {mach }}$
- the exact eigenvalues are $1+\epsilon$ and $1-\epsilon$
- in floating-point arithmetic,

$$
\operatorname{det}(\mathbf{A}-\lambda \mathbf{I})=\lambda^{2}-2 \lambda+\left(1-\epsilon^{2}\right)=\lambda^{2}-2 \lambda+1
$$

with the solution 1 (double root)

- a simple eigenvalue is a simple solution of the characteristic polynomial (multiplicity of the root is 1 )
- a defective matrix has eigenvalues with multiplicity larger than 1, meaning less than $n$ independent eigenvectors
- a nondefective matrix has exactly $n$ linearly independent eigenvectors and can be diagonalized

$$
\mathbf{Q}^{-1} \mathbf{A} \mathbf{Q}=\Lambda
$$

where $\mathbf{Q}$ is a nonsingular matrix of eigenvectors
Matlab: Adiag $=\operatorname{inv}(Q) * A * Q$

## Eigen-decomposition

- it follows that if $\mathbf{A}$ admits $n$ independent eigenvectors, it can be decomposed (factorized) as

$$
\mathbf{A}=\mathbf{Q} \wedge \mathbf{Q}^{-1}
$$

with $\mathbf{Q}$ having the eigenvectors of $\mathbf{A}$ as columns, and $\wedge \mathrm{a}$ diagonal matrix with eigenvalues on the diagonal

- theoretically, $\mathbf{A}^{-1}=\mathbf{Q} \wedge^{-1} \mathbf{Q}^{-1}$ (if $\lambda_{i} \neq 0$ and all eigenvalues are distinct)
- if $\mathbf{A}$ is normal $\left(\mathbf{A}^{H} \mathbf{A}=\mathbf{A}^{H} \mathbf{A}\right)$ then $\mathbf{Q}$ becomes unitary
- if $\mathbf{A}$ is real symmetric, then $\mathbf{Q}$ is orthogonal


## Eigenvectors

- the eigenvectors can be arbitrarily scaled
- usually, the eigenvectors are normalized, $\|\mathbf{x}\|=1$
- the eigenspace is $\mathcal{S}_{\lambda}=\{\mathbf{x} \mid \mathbf{A} \mathbf{x}=\lambda \mathbf{x}\}$
- a subspace $\mathcal{S} \subset \mathbb{R}^{n}$ is invariant if $\mathbf{A} \mathcal{S} \subseteq \mathcal{S}$
- for $\mathbf{x}_{i}$ eigenvectors, $\operatorname{span}\left(\left\{\mathbf{x}_{i}\right\}\right)$ is an invariant subspace


## Some useful properties

- $\operatorname{det}(\mathbf{A})=\prod_{i=1}^{N} \lambda_{i}^{n_{i}}$, where $n_{i}$ is the multiplicity of eigenvalue $\lambda_{i}$
- $\operatorname{tr}(\mathbf{A})=\sum_{i=1}^{N} n_{i} \lambda_{i}$
- the eigenvalues of $\mathbf{A}^{-1}$ are $\lambda_{i}^{-1}$ (for $\lambda_{i} \neq 0$ )
- the eigenvectors of $\mathbf{A}^{-1}$ are the same as those of $\mathbf{A}$
- A admits an eigen-decomposition if all eigenvalues are distinct
- if $\mathbf{A}$ is invertible it does not imply that it can be eigen-decomposed; reciprocally, if $\mathbf{A}$ admits an eigen-decomposition, it does not imply it can be inverted
- A can be inverted if and only if $\lambda_{i} \neq 0, \forall i$


## Before solving an eigenvalue problem...

- do I need all the eigenvalues?
- do I need the eigenvectors as well?
- is A real or complex?
- is A small, dense or large and sparse?
- is there anything special about A? e.g.: symmetric, diagonal, orthogonal, Hermitian, etc etc
- conditioning of EV problem is different than conditioning of linear systems for the same matrix
- sensitivity is "not uniform" among eigenvectors/eigenvalues
- for a simple eigenvalue $\lambda$, the condition is $1 / \| \mathbf{y}^{H} \mathbf{x} \mid$, where $\mathbf{x}$ and $\mathbf{y}$ are the corresponding right and left normalized eigenvectors (and $\mathbf{y}^{H}$ is the conjugate transpose)
- so the condition is $1 / \cos (\widehat{\mathbf{x}, \mathbf{y}})$
- a perturbation of order $\epsilon$ in A may perturb the eigenvalue $\lambda$ by as much as $\epsilon / \cos (\widehat{\mathbf{x}, \mathbf{y}})$
- for special cases of $\mathbf{A}$, special forms of conditioning can be derived


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## Computation - general ideas

- a matrix $\mathbf{B}$ is similar to $\mathbf{A}$ if there exists a nonsingular matrix $\mathbf{T}$ such that $\mathbf{B}=\mathbf{T}^{-1} \mathbf{A} \mathbf{T}$
- if $\mathbf{y}$ is an eigenvector of $\mathbf{B}$ then $\mathbf{x}=\mathbf{T y}$ is an eigenvector of $\mathbf{A}$ and
HOMEWORK: prove that A and B have the same eigenvalues
- transformations:
- shift: $\mathbf{A} \leftarrow \mathbf{A}-\sigma \mathbf{I}$
- inversion: $\mathbf{A} \leftarrow \mathbf{A}^{-1}$ (if $\mathbf{A}$ is nonsingular)
- power: $\mathbf{A} \leftarrow \mathbf{A}^{k}$
- polynomial: let $p$ be a polynomial, then $\mathbf{A} \leftarrow p(\mathbf{A})$


## Forms attainable by similarity

For a matrix $\mathbf{A}$ with given property, the matrices $\mathbf{T}$ and $\mathbf{B}$ exist such that $\mathbf{B}=\mathbf{T}^{-1} \mathbf{A} \mathbf{T}$ has the desired property:

| A | T | B |
| :---: | :---: | :---: |
| distinct eigenvalues | nonsingular | diagonal |
| real symmetric | orthogonal | real diagonal |
| complex Hermitian | unitary | real diagonal |
| normal | unitary | diagonal |
| arbitrary real | orthogonal | real block triangular (Schur) |
| arbitrary | unitary | upper triangular (Schur) |
| arbitrary | nonsingular | almost diagonal |
|  |  |  |

If $\mathbf{A}$ is diagonal...

- the eigenvalues are the diagonal entries
- the eigenvectors are the columns of the identity matrix

If a matrix is not diagonalizable, one can obtain a Jordan form:


If $\mathbf{A}$ is triangular (Schur form, in general)...

- eigenvalues are the elements on the diagonal
- eigenvectors are obtained as follows: If

$$
\mathbf{A}-\lambda \mathbf{I}=\left[\begin{array}{ccc}
\mathbf{U}_{11} & \mathbf{u} & \mathbf{U}_{13} \\
\mathbf{0} & 0 & \mathbf{v}^{\top} \\
\mathbf{0} & \mathbf{0} & \mathbf{U}_{33}
\end{array}\right]
$$

is triangular, then $\mathbf{U}_{11} \mathbf{y}=\mathbf{u}$ can be solved for $\mathbf{y}$, so that

$$
\mathbf{x}=\left[\begin{array}{c}
\mathbf{y} \\
-1 \\
\mathbf{0}
\end{array}\right]
$$

is the corresponding eigenvector

## Symmetric matrices - Jacobi method

- idea: start with a symetric matrix $\mathbf{A}_{0}$ and iteratively form $\mathbf{A}_{k+1}=\mathbf{J}_{k}^{T} \mathbf{A}_{k} \mathbf{J}_{k}$, where $\mathbf{J}_{k}$ is a plane rotation chose to annihilate a symmetric pair of entries in $\mathbf{A}_{k}$ with the goal of diagonalizing A
- a rotation matrix has the form

$$
\left[\begin{array}{cc}
\cos \theta & \sin \theta \\
-\sin \theta & \cos \theta
\end{array}\right]
$$

- the problem is to find $\theta$
- for $\mathbf{A}=\left[\begin{array}{ll}a & b \\ b & c\end{array}\right]$ and requiring that $\mathbf{J}^{\top} \mathbf{A} \mathbf{J}$ is diagonal, we obtain

$$
1+\tan \theta \frac{a-c}{b}-\tan ^{2} \theta=0
$$

from which we use the root with the smallest magnitude

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## Power iterations

- is the simplest metod to compute one eigenvalue-eigenvector pair
- the matrix is repeatedly multiplied by an intial starting vector
- let $\lambda_{1}$ be the absolute largest eigenvalue of $\mathbf{A}$, with the corresponding eigenvector $\mathbf{v}_{1}$
- start with $\mathbf{x}_{0} \neq \mathbf{0}$ and iterate:

$$
\mathbf{x}_{k}=\mathbf{A} \mathbf{x}_{k-1} \quad k=1,2, \ldots
$$

- the process converges to a scaled version of $\mathbf{v}_{1}$ corresponding to the eigenvalue $\lambda_{1}$


## Power iterations - geometrical interpretation



## Power iterations - convergence

Let $\mathbf{v}_{1}, \ldots, \mathbf{v}_{n}$ be the eigenvectors of $\mathbf{A}$. Then, any vector $\mathbf{x}_{0}$ can be written as

$$
\mathbf{x}_{0}=\sum_{i=1}^{n} \alpha_{i} \mathbf{v}_{i}
$$

Then

$$
\begin{aligned}
\mathbf{x}_{k} & =\mathbf{A} \mathbf{x}_{k-1}=\cdots=\mathbf{A}^{k} \mathbf{x}_{0}=\sum_{i=1}^{n} \lambda_{i}^{k} \alpha_{i} \mathbf{v}_{i} \\
& =\lambda_{1}^{k}\left(\alpha_{1} \mathbf{v}_{1}+\sum_{i=2}^{n}\left(\lambda_{i} / \lambda_{1}\right)^{k} \alpha_{i} \mathbf{v}_{i}\right)
\end{aligned}
$$

and $\lim _{k \rightarrow \infty}\left(\lambda_{i} / \lambda_{1}\right)^{k} \rightarrow 0$ since $\left|\lambda_{i} / \lambda_{1}\right|<1$.

## Power iterations, cont'd

- theoretically, it can happen that $\mathbf{x}_{0}$ has no component in $\mathbf{v}_{1}$ (i.e. $\alpha_{1}=0$ )
- the iterations cannot converge to a complex solution
- there might be several equally large and maximal eigenvalues, so the iterations converge to a linear combination of the corresponding eigenvectors
- the values of $\mathbf{x}_{k}$ grow geometrically with $k$ and this can lead to over-/under-flow $\rightarrow$ use normalization: at each step normalize $\mathbf{x}_{k}$ by $\left\|\mathbf{x}_{k}\right\|_{\infty}$
- the rate of convergence depends on $\left|\lambda_{2} / \lambda_{1}\right|$ : smaller the ratio, faster the convergence $\rightarrow$ it might be possible to find a shift by $\sigma$ such that $\left|\left(\lambda_{2}-\sigma\right) /\left(\lambda_{1}-\sigma\right)\right|<\left|\lambda_{2} / \lambda_{1}\right|$ which accelerates convergence


## Power iterations: Exercise

Implement the following procedure in Matlab, to find the largest eigenvalue and the corresponding eignvector for a matrix $\mathbf{A}$ :

- start with an initial vector $\mathbf{x}_{0} \neq \mathbf{0}, \lambda_{0}=0$
- for $k=1,2, \ldots$ compute the new approximation of the
- eigenvector: $\mathbf{x}_{k}=\frac{\mathbf{A} \mathbf{x}_{k-1}}{\| \mathbf{x}_{k-1}} \|_{\infty}$
- eigenvalue: $\lambda_{k}=\max \left\{x_{1 k}, \ldots, x_{n k}\right\}$
- stop iterating if a maximum number of iterations has been attained or if the changes between two consecutive iterations is below a threshold: $\left\|x_{k}-x_{k-1}\right\|<\epsilon$ and $\left|\lambda_{k}-\lambda_{k-1}\right|<\epsilon$
- scale the final approximation such that $\left\|\mathbf{x}_{K}\right\|=1$

Scaling at each iteration prevents over-/under-flow and ensures that the largest component of $\mathbf{x}_{k}$ is $\lambda_{k}$.

## Inverse iteration

- if the smallest eigenvalue is needed: the eigenvalues of $\mathbf{A}$ are the reciprocals of the eigenvalues of $\mathbf{A}^{-1}$. Try:

$$
[v, 1]=\text { eig_power(inv(A)); l = 1/l; }
$$

- inverse iteration scheme:

$$
\begin{aligned}
\mathbf{A} \mathbf{y}_{k} & =\mathbf{x}_{k-1} \\
\mathbf{x}_{k} & =\mathbf{y}_{k} /\left\|\mathbf{y}_{k}\right\|_{\infty}
\end{aligned}
$$

- this is equivalent to power iterations applied to $\mathbf{A}$
- $\mathbf{A}^{-1}$ is not computed explicitly
- factorization of $\mathbf{A}$ is used to solve the system of linear eqs.
- converges to the eigenvector corresponding to the smallest eigenvalue
- the shifting strategy can also be applied


## Shifted inverse power iterations

- if one wants eigenvalues close to a certain value $s$ (not equal to any eigenvalue): transform the problem:

$$
\mathbf{A} \mathbf{v}=\lambda \mathbf{v} \longrightarrow(\mathbf{A}-\boldsymbol{s} \mathbf{I}) \mathbf{v}=(\lambda-\boldsymbol{s}) \mathbf{v}
$$

- the eigenvalue sought is

$$
\lambda_{s}=\frac{1}{\text { largest eigenvalue of }(\mathbf{A}-s \mathbf{I})^{-1}}+s
$$

- this method works only if there is a single eigenvalue $\lambda_{s}$
- try: [v,l] = eig_power(inv(A - ...
s*eye(size(A)))); l = 1/l+s;


## Rayleigh quotient

- let $\mathbf{A}$ be a real matrix with $\mathbf{x}$ an approximate eigenvector
- to find the corresponding eigenvalue $\lambda$ one can solve the system

$$
\mathbf{A x} \approx \lambda \mathbf{x}
$$

for $\lambda$ unknown ( $n \times 1$ least squares approx. problem)

- form normal eqs.: $\mathbf{x}^{\top} \mathbf{A} \mathbf{x}=\lambda \mathbf{x}^{\top} \mathbf{x}$ and obtain the LS solution

$$
\lambda=\frac{\mathbf{x}^{\top} \mathbf{A} \mathbf{x}}{\mathbf{x}^{\top} \mathbf{x}}
$$

- this is the Rayleigh quotient


## Rayleigh q., cont'd

- R.q. gives a good estimate of the eigenvalue corresponding to an eigenvector
- R.q. can be used as a shift to speed up convergence of the inverse iteration
- Rayleigh quotient iteration: for some $\mathbf{x}_{0} \neq \mathbf{0}$,

$$
\begin{aligned}
\sigma_{k} & =\frac{\mathbf{x}_{k}^{T} \mathbf{A} \mathbf{x}_{k}}{\mathbf{x}_{k}^{T} \mathbf{x}_{k}} \\
\text { solve }\left(\mathbf{A}-\sigma_{k} \mathbf{I}\right) \mathbf{y}_{k+1} & =\mathbf{x}_{k} \\
\mathbf{x}_{k+1} & =\mathbf{y}_{k+1} /\left\|\mathbf{y}_{k+1}\right\|_{\infty}
\end{aligned}
$$

- usually 2-3 iterations are enough


## Rayleigh q., cont'd

- R.q. iteration is very efficient for symmetric matrices
- solving a different system (different shift) at each iteration introduces some overhead, depending on the form of the matrix
- the method can be extended to complex matrices using the conjugate transpose
- the R.q. has values between the minimum and maximum eigenvalues of $\mathbf{A}$ - this is sometimes called numerical range (or field of values) of the matrix $\mathbf{A}$


## Deflation

- computes sequentially each of the (eigenvalue, eigenvector) pairs
- if $\lambda_{1}$ and $\mathbf{x}_{1}$ are already computed, then transform the matrix to remove them and proceed to compute $\lambda_{2}$ and $\mathbf{x}_{2}$; iterate
- this process is known as deflation
- let $\mathbf{H}$ be a nonsingular matrix such as $\mathbf{H} \mathbf{x}_{1}=\alpha_{1} \mathbf{e}_{1}$ (e.g. a Householder transformation)
- apply this transformation to $\mathbf{A}$ :

$$
\mathbf{H A H}^{-1}=\left[\begin{array}{cc}
\lambda_{1} & \mathbf{b}^{T} \\
\mathbf{0} & \mathbf{B}
\end{array}\right]
$$

where $\mathbf{B}$ is a matrix of order $n-1$ with eigenvalues $\lambda_{2}, \ldots, \lambda_{n}$

## Deflation, cont'd

- then, use $\mathbf{B}$ to compute $\lambda_{2}$
- eigenvectors and eigenvalues of $\mathbf{B}$ are linked to those of $\mathbf{A}$ as follows:
- if $\mathbf{y}_{2}$ is an eigenvector of $\mathbf{B}$ corresponding to $\lambda_{2}$, then

$$
\mathbf{x}_{2}=\mathbf{H}^{-1}\left[\begin{array}{c}
\alpha \\
\mathbf{y}_{2}
\end{array}\right]
$$

where

$$
\alpha=\frac{\mathbf{b}^{T} \mathbf{y}_{2}}{\lambda_{2}-\lambda_{1}}
$$

provided that $\lambda_{1} \neq \lambda_{2}$.

- ...and repeat...


## Alternative deflation

- let $\mathbf{u}_{1}$ be a vector such that $\mathbf{u}_{1}^{T} \mathbf{x}_{1}=\lambda_{1}$
- it follows that $\mathbf{A}-\mathbf{x}_{1} \mathbf{u}_{1}^{T}$ has the eigenvalues $0, \lambda_{2}, \ldots, \lambda_{n}$
- examples of $\mathbf{u}$ vectors:
- $\mathbf{u}_{1}=\lambda_{1} \mathbf{x}_{1}$ if $\mathbf{A}$ is symmetric and $\left\|\mathbf{x}_{1}\right\|_{2}=1$
- $\mathbf{u}_{1}=\lambda_{1} \mathbf{y}_{1}$ where $\mathbf{y}_{1}$ is the left eigenvector normalized such that $\mathbf{y}_{1}^{\top} \mathbf{x}_{1}=1$
- $\mathbf{u}_{1}=\mathbf{A}^{\top} \mathbf{e}_{k}$, is $\mathbf{x}_{1}$ is normalized such that $\left\|\mathbf{x}_{1}\right\|_{\infty}=1$ and the $k$-th component of $\mathbf{x}_{1}$ is 1 .


## Simultaneous iteration

- in power iteration method, $\mathbf{x}_{k}=\mathbf{A} \mathbf{x}_{k-1}$ converged to an eigevector
- why not using a matrix, such that $\mathbf{X}_{k}=\mathbf{A} \mathbf{X}_{k-1}$ would converge simultaneously to several eigenvectors?
- start with a $n \times p$ matrix $\mathbf{X}_{0}$ of rank $p$ and iterate

$$
\mathbf{X}_{k}=\mathbf{A} \mathbf{X}_{k-1}
$$

- span $\left(b X_{k}\right)$ converges to an invariant space determined by the $p$ largest eigenvalues of $\mathbf{A}$, provided that $\left|\lambda_{p}\right|>\left|\lambda_{p+1}\right|$
- the method is called simultaneous iteration of subspace iteration


## Simultaneous iteration, cont'd

- to avoid over-/under-flow and bad conditioning with increasing $k$, the columns of $\mathbf{X}_{k}$ need to be normalized
- using the reduced $Q R$ decomposition avoids these problems:

$$
\begin{aligned}
\mathbf{Q}_{k} \mathbf{R}_{k} & =\mathbf{X}_{k-1} \quad \text { QR decomposition of previous } \mathbf{X} \\
\mathbf{X}_{k} & =\mathbf{A} \mathbf{Q}_{k}
\end{aligned}
$$

- this is the orthogonal iteration scheme
- if the eigenvalues are distinct in modulus, the process converges to a block trinagular form
- if $p=n$ and $\mathbf{X}_{0}=\mathbf{I}$, the series of matrices

$$
\mathbf{A}_{k}=\mathbf{Q}_{k}^{H} \mathbf{A} \mathbf{Q}_{k}
$$

converges to (block) triangular form yielding all the eigenvalues of $\mathbf{A}$

## Simultaneous iteration, cont'd

- alternative: QR iteration: compute $\mathbf{A}_{k}$ without forming the product explicitly
- start with $\mathbf{A}_{0}=\mathbf{A}$ and at step $k$ :

$$
\begin{aligned}
\mathbf{Q}_{k} \mathbf{R}_{k} & =\mathbf{A}_{k-1} \quad \text { compute the QR decomposition } \\
\mathbf{A}_{k} & =\mathbf{R}_{k} \mathbf{Q}_{k} \quad \text { form the inverse product }
\end{aligned}
$$

- diagonal entries (or eigenvalues of diagonal blocks) converge to eigenvalues of $\mathbf{A}$
- the product of orthogonal matrices $\mathbf{Q}_{k}$ converges to the matrix of corresponding eigenvectors
- if $\mathbf{A}$ is symmetric, $\mathbf{A}_{k}$ converges to a diagonal matrix
- special forms of $\mathbf{A}$ lead to faster convergence $\rightarrow$ use some pretransformations of the matrix to speed up
- cost of QR iteration method:
- for symmetric matrices: $\sim \frac{4}{3} n^{3}$ for eigenvalues only and $\sim 9 n^{3}$ for both eigenvalues and eigenvectors
- for general matrices: $\sim 10 n^{3}$ for eigenvalues only and $\sim 25 n^{3}$ for both eigenvalues and eigenvectors
- other methods:
- Krylov subspace methods: reduce A to a tridiagonal matrix and find eigen-values/-vectors by QR
- Lanczos method for symmetric matrices
- spectrum-slicing: for real symmetric matrices, it can find how many eigenvalues are below a given $\sigma \in \mathbb{R} \rightarrow$ by "slicing" the space, the eigenvalues can be isolated; see also the Sturm sequence


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## The generalized eigenvalue problem

- it has the form

$$
\mathbf{A} \mathbf{x}=\lambda \mathbf{B} \mathbf{x}
$$

where $\mathbf{A}$ and $\mathbf{B}$ are $n \times n$ matrices

- if any of $\mathbf{A}$ or $\mathbf{B}$ is nonsingular, the problem can be transformed in a standard eigenvalue problem
- this is not recommended because loss of accuracy (roundoff errors) and loss of symmetry (if one of $\mathbf{A}$ or $\mathbf{B}$ is symmetric
- better: use the QZ algorithm


## QZ algorithm

- if $\mathbf{A}$ and $\mathbf{B}$ are triangular, the eigenvalues are $\lambda_{i}=a_{i i} / b_{i i}$, for $b_{i i} \neq 0$
- the QZ algorithm reduces A and B simultaneously to upper triangular matrices by orthogonal transformations


## Singular Value Decomposition - again

- we saw that SVD of a $m \times n$ matrix $\mathbf{A}$ has the form

$$
\mathbf{A}=\mathbf{U} \Sigma \mathbf{V}^{\top}
$$

where $\mathbf{U}$ is $m \times m$ orthogonal matrix and $\mathbf{V}$ is $n \times n$ orthogonal matrix and $\Sigma$ is $m \times n$ diagonal matrix with non-negative elements on the diagonal

- this is a eigenvalue-like problem
- the columns of $\mathbf{U}$ and $\mathbf{V}$ are the left and right singular vectors, respectively and $\sigma_{i i}$ are the singular values


## The relation between SVD and the eigen-decomposition

- SVD can be applied to any $m \times n$ matrix, while the eigen-decomposition is applied only to square matrices
- the singular values are non-negative while the eigenvalues can be negative
- let $\mathbf{A}=\mathbf{U} \Sigma \mathbf{V}^{\top}$ be SVD of $\mathbf{A} \Rightarrow$ $\mathbf{A}^{T} \mathbf{A}=\left(\mathbf{V} \Sigma^{\top} \mathbf{U}^{T}\right)\left(\mathbf{U} \Sigma \mathbf{V}^{T}\right)=\mathbf{V} \Sigma^{\top} \Sigma \mathbf{V}^{T}$
- also, $\mathbf{A}^{\top} \mathbf{A}$ is symmetric real matrix, so it has a eigendecomposition $\mathbf{A}^{\top} \mathbf{A}=\mathbf{Q} \wedge \mathbf{Q}^{\top}$, with $\mathbf{Q}$ orthogonal. By unicity of decompositions, it follows that

$$
\begin{aligned}
\Sigma^{T} \Sigma & =\Lambda \\
\mathbf{V} & =\mathbf{Q}
\end{aligned}
$$

- so $\sigma_{i}=\sqrt{\lambda_{i}}$

