Matrix Decomposition

✓ LU

✓ QR

→ Spectral (square matrices)

SVD

$\underline{A}\,\underline{x} = \lambda \underline{x}$ ← Eigenvector $\underline{x}$ is scaled by λ when premultiplied by $\underline{A}$

$\underline{A}$ must be square (column & row space must be equal)

To solve analytically, find all λ, such that

$$|\underline{A} - \lambda \underline{I}| = 0$$

Determinant search

Issue: No closed form solutions for polynomials of size ≥ 5

One could do numerical root finding, but that is typically not stable, and one would still need the eigenvectors $\underline{x}$ ⇒ Need iterative solvers for the eigenproblem

Two classes of solvers:

* 1) Finding largest (or smallest) λ

2) Finding the entire spectrum (or a portion of it)

Largest Eigenvalue

Restrict to real, symmetric $\underline{A}$

Rayleigh Quotient

Let $\underline{x}$ be an eigenvector of $\underline{A}$, then

$$\underline{A}\,\underline{x} = \lambda \underline{x}$$

and

$$\underline{x}^T \underline{A}\,\underline{x} = \lambda \underline{x}^T \underline{x} \qquad \text{(scalar equation)}$$

$$\therefore \lambda = \frac{\underline{x}^T \underline{A}\,\underline{x}}{\underline{x}^T \underline{x}} \quad \leftarrow \text{Given } \underline{x} + \underline{A}, \text{ find } \lambda$$

Power Iteration

Let $\underline{v}_0$ be any vector such that

$\|\underline{v}_0\| = 1$ and $\underline{v}_0$ is not an eigenvector

Let $\underline{q}_1, \underline{q}_2, \ldots, \underline{q}_n$ be the orthonormal set of eigenvectors,

then

$$\underline{v}_0 = a_1 \underline{q}_1 + a_2 \underline{q}_2 + \ldots + a_n \underline{q}_n$$

Consider $\underline{A}\,\underline{v}_0$

$$\underline{A}\,\underline{v}_0 = \underline{A}\left(a_1 \underline{q}_1 + a_2 \underline{q}_2 + \ldots + a_n \underline{q}_n\right)$$

$$= a_1 \underline{A}\,\underline{q}_1 + a_2 \underline{A}\,\underline{q}_2 + \ldots + a_n \underline{A}\,\underline{q}_n$$

$$= a_1 \lambda_1 \underline{q}_1 + a_2 \lambda_2 \underline{q}_2 + \ldots + a_n \lambda_n \underline{q}_n$$

$$= \lambda_1 \left(a_1 \underline{q}_1 + a_2 \frac{\lambda_2}{\lambda_1} \underline{q}_2 + \ldots + a_n \frac{\lambda_n}{\lambda_1} \underline{q}_n\right)$$

$$\underline{A}^2 \underline{v}_0 = \underline{A}\left(\underline{A}\,\underline{v}_0\right) = \underline{A}\,\lambda_1 \left(a_1 \underline{q}_1 + \ldots + a_n \frac{\lambda_n}{\lambda_1} \underline{q}_n\right)$$

$$= \lambda_1 \left(a_1 \underline{A}\,\underline{q}_1 + a_2 \underline{A} \frac{\lambda_2}{\lambda_1} \underline{q}_2 + \ldots + a_n \frac{\lambda_n}{\lambda_1} \underline{A}\,\underline{q}_n\right)$$

$$= \lambda_1 \left(a_1 \lambda_1 \underline{q}_1 + a_2 \frac{\lambda_2^2}{\lambda_1} \underline{q}_2 + \ldots + a_n \frac{\lambda_n^2}{\lambda_1} \underline{q}_n\right)$$

$$= \lambda_1^2 \left(a_1 \underline{q}_1 + a_2 \left(\frac{\lambda_2}{\lambda_1}\right)^2 \underline{q}_2 + \ldots + a_n \left(\frac{\lambda_n}{\lambda_1}\right)^2 \underline{q}_n\right)$$

$$\underline{A}^p \underline{v}_0 = \lambda_1^p \left(a_1 \underline{q}_1 + a_2 \left(\frac{\lambda_2}{\lambda_1}\right)^p \underline{q}_2 + \dots + a_n \left(\frac{\lambda_n}{\lambda_1}\right)^p \underline{q}_n \right)$$

Let $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$ (order eigenvalues)

Then

$$\lim_{p\to\infty} \left(\frac{\lambda_j}{\lambda_1}\right)^p = 0 \quad \text{for } j \neq 1$$

$$\Rightarrow \lim_{p\to\infty} \frac{\underline{A}^p \underline{v}_0}{\lambda_1^p} = a_1 \underline{q}_1 \quad \text{with } a_1 = \underline{q}_1^T \underline{v}_0$$

Combine this result with the Rayleigh Quotient

Algorithm: Power Algorithm

$\underline{v}_0 \Rightarrow$ Some vector with $\|\underline{v}_0\| = 1$

for $k = 1, 2, \dots$

$$\underline{A}^k \underline{v}_0 = \underline{A}\,\underline{A}\,\overbrace{A \underbrace{(\underline{A}\,\underline{v}_0)}_{\underline{v}_1}}^{\underline{v}_2}$$

$\underline{w} = \underline{A}\,\underline{v}_{k-1}$

$\underline{v}_k = \underline{w} / \|\underline{w}\|$ $\rightarrow$ $\underline{v}_k^T \underline{v}_k = 1$

$\lambda_{(k)} = \underline{v}_k^T \underline{A}\,\underline{v}_k$ $\rightarrow$ Rayleigh quotient end

This converges at a rate of

$$\| \underline{v}_k - (\pm \underline{q}_1) \| = \mathcal{O}\left(\left| \frac{\lambda_2}{\lambda_1} \right|^k \right)$$

$$| \lambda_{(k)} - \lambda_1 | = \mathcal{O}\left(\left| \frac{\lambda_2}{\lambda_1} \right|^{2k} \right)$$

This causes an issue if $\lambda_1 \sim \lambda_2$

In this case, try an inverse iteration w/shift

Inverse Iteration with Shift

Let $\mu \in \mathbb{R}$, such that μ is not an eigenvalue of $\underline{A}$. Then, $(\underline{A} - \mu \underline{I})$ has the same eigenvectors as $\underline{A}$ with eigenvalues $\lambda_j - \mu = \hat{\lambda}_j$

Note: $[(\underline{A} - \mu \underline{I}) - \hat{\lambda} \underline{I}] \underline{q} = \underline{0} \Rightarrow \lambda = \mu + \hat{\lambda}$

Extension: Eigenvectors of $(\underline{A} - \mu \underline{I})^{-1}$ are the same as those for $\underline{A}$, and the eigenvalues for $(\underline{A}-\mu\underline{I})^{-1}$ are $(\lambda_j-\mu)^{-1}$

Let μ be close to λ_1, then $|\lambda_1-\mu|^{-1}$ will be

much larger than $|\lambda_j-\mu|^{-1}$ for $j>1$

Algorithm: Inverse iteration with shift

Let $\underline{v}_0$ be some vector with $\|\underline{v}_0\|=1$,

choose $\mu>0$

for $k=1,2,\ldots$

Solve $(\underline{A}-\mu\underline{I})\underline{w}=\underline{v}_{k-1}$ for $\underline{w}$

$\underline{v}_k=\underline{w}/\|\underline{w}\|$ Normalize $\underline{v}_k$

$\lambda_{(k)}=\underline{v}_k^T\underline{A}\,\underline{v}_k$ Rayleigh Quotient

end

Convergence order of

$$\|\underline{v}_k-(\pm\underline{q}_1)\|=\mathcal{O}\left(\left|\frac{\mu-\lambda_1}{\mu-\lambda_2}\right|^k\right)$$

$$|\lambda_{(k)}-\lambda_1|=\mathcal{O}\left(\left|\frac{\mu-\lambda_1}{\mu-\lambda_2}\right|^{2k}\right)$$

\\

Now combine above ideas

Algorithm: Rayleigh Quotient Iteration

$\underline{v}_0$ is some vector w/ $\|\underline{v}_0\| = 1$

$\lambda_{(0)} = \underline{v}_0^T \underline{A}\, \underline{v}_0$ Do not need to select a shift μ

for $k = 1, 2, \ldots$

Solve $(\underline{A} - \lambda_{(k-1)} \underline{I})\underline{w} = \underline{v}_{k-1}$ for $\underline{w}$

$\underline{v}_k = \underline{w} / \|\underline{w}\|$

$\lambda_{(k)} = \underline{v}_k^T \underline{A}\, \underline{v}_k$

end

This method has a convergence of

$$\|\underline{v}_{k+1} - (\pm \underline{q}_J)\| = O\left(\|\underline{v}_k - (\pm \underline{q}_J)\|^3\right)$$

$$|\lambda_{(k+1)} - \lambda_J| = O\left(|\lambda_{(k)} - \lambda_J|^3\right)$$

Cubic order convergence of the eigenvector $\underline{q}_J$ closest to $\underset{\sim}{v_0}$

See Lecture 27 of Trefethan & Bau

$\underline{A}\,\underline{x} = \lambda \underline{x}$ ← Eigenvector $\underline{x}$ is scaled by λ when premultiplied by $\underline{A}$

Two classes of solvers:

1) Finding largest (or smallest) λ

* 2) Finding the entire spectrum (or a portion of it)

Spectrum Calculations

Try to find all or a subset of the eigenvalue spectrum

Recall that any square matrix has the Schur Decomposition

$\underline{A} = \underline{Q}\,\underline{T}\,\underline{Q}^T$, where $\underline{T}$ is upper triangular

Eigenvalue computations can try the find this decomposition, in which A + $\underline{T}$ are similar this decomposition, in which $\underline{A}$ & $\underline{T}$ are similar

Recall, eigenvalues of $\underline{A}$ appear on the diagonal of $\underline{T}$

Note: If $\underline{A}$ is symmetric and real, then

$$\underline{A} = \underline{Q}\,\underline{T}\,\underline{Q}^T = \underline{S}\,\underset{\text{diagonal}}{\underline{\Lambda}}\,\underline{S}^{-1}$$

The above looks similar to QR decomposition, where $\underline{A} = \underline{Q}\,\underline{R}$ upper triangular

Recall Householder reflections

$$\underset{\underline{A}}{\begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix}} \xrightarrow{\underline{Q}_1^T} \underset{\underline{Q}_1^T\underline{A}}{\begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \end{bmatrix}}$$

For the eigenproblem, we need $\underline{Q}_1^T\,\underline{A}\,\underline{Q}_1$

Then

$$\underbrace{\underline{Q}_n^T \underline{Q}_{n-1}^T \cdots \underline{Q}_1^T}_{\underline{Q}^T} \, \underline{A} \, \underbrace{\underline{Q}_1 \underline{Q}_2 \cdots \underline{Q}_n}_{\underline{Q}} = \underline{T}$$

and then $\underline{A} = \underline{Q} \, \underline{T} \, \underline{Q}^T$

Consider $\underline{Q}_1^T \underline{A} \, \underline{Q}_1$

$$\underset{\underline{Q}_1^T \underline{A}}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}} \longrightarrow \underset{\underline{Q}_1^T \underline{A} \, \underline{Q}_1}{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}}$$

Fill-in of the zeros

$\therefore$ The original Householder approach will not work

$\Rightarrow$ Not possible to get a Schur Decomposition directly

Instead, two steps are needed:

1) Reduce to upper Hessenberg form, which is nearly upper triangular

2) Iterate until upper triangular is obtained

Details of these two steps:

1) Upper Hessenberg Matrix: A matrix with zeros below the first sub-diagonal

$$\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \end{bmatrix}$$

diagonal

first sub-diagonal

Let $\underline{Q}_1^T$ be a unitary matrix $(\underline{Q}_1^T \underline{Q}_1 = \underline{I})$ that zeros out values below the first subdiagonal of the first column, but does not touch the first row values

untouched

$$\begin{bmatrix} x & x & x & x \end{bmatrix} \qquad \begin{bmatrix} x & x & x & x \end{bmatrix} \qquad \begin{bmatrix} x & x & x & x \end{bmatrix}$$

$$\begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix} \rightarrow \begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix} \rightarrow \begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix}$$

$$\underline{A} \qquad\qquad \underline{Q}_1^T \underline{A} \qquad\qquad \underline{Q}_1^T \underline{A}\, \underline{Q}_1$$

Use a Householder reflector to assure ortho-normality

$$\underline{Q} = \begin{bmatrix} \underline{I} & \underline{0} \\ \underline{0} & \underline{F} \end{bmatrix}$$

Algorithm: Householder Reduction to Upper Hessenberg Form

for $k = 1$ to $m-2$ $\qquad$ with $\underline{A} \in \underline{M}_{mm}$

$\quad \underline{x} = \underline{A}(k+1:m, k)$

$\quad \underline{v}_k = \text{sign}(x_1)\|\underline{x}\|_2 \underline{e}_1 + \underline{x}$

$\quad \underline{A}(k+1:m, k:m) = \underline{A}(k+1:m, k:m)$ $\qquad \underline{Q}^T\underline{A}$

$$-2\underline{v}_k\left(\underline{v}_k^T\,\underline{A}(k+1:m,\,k:m)\right)$$

$$\underline{A}(1:m,\,k+1:m) = \underline{A}(1:m,\,k+1:m)$$

$$-2\left(\underline{A}(1:m,\,k+1:m)\,\underline{v}_k\right)\underline{v}_k^T$$

end

$$\leadsto \underline{Q}^T\underline{A}\,\underline{Q}$$

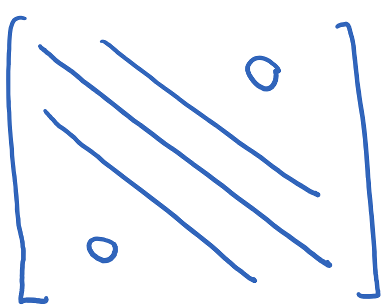
$\Rightarrow$ $\underline{A}$ then converts to upper Hessenberg

Note: $\underline{Q}$ is never formed

Cost: $\Theta\left(\frac{10}{3}m^3\right)$

If $\underline{A}$ is symmetric, then the cost reduces to $\Theta\left(\frac{4}{3}m^3\right)$

and the result is tri-diagonal



Why?

2) Iterate to Upper Triangular Form

Focus on real, symmetric matrices

Turn to $\underline{A} = \underline{Q}\,\underline{T}\,\underline{Q}^T$ (Schur decomposition)

$\underline{A}$ could be any matrix or the result of part 1) (i.e., upper Hessenberg)

$\underline{T} = \underline{Q}^T \underline{A}\,\underline{Q}$

Make this an iteration

Given $\underline{A}_k$, let $\underline{A}_{k+1} = \underline{Q}_k^T \underline{A}_k \underline{Q}_k$

Now, let $\underline{A}_k = \underline{Q}_k \underline{R}_k$ be the QR decomposition of $\underline{A}_k$

Then,

$$\underline{A}_{k+1} = \underline{Q}_k^T \underline{A}_k \underline{Q}_k = \underline{Q}_k^T(\underline{Q}_k \underline{R}_k)\underline{Q}_k$$
$$= \underline{I}\,\underline{R}_k \underline{Q}_k = \underline{R}_k \underline{Q}_k$$

Given $\underline{A}_k$, find $\underline{Q}_k \underline{R}_k$, then $\underline{A}_{k+1} = \underline{R}_k \underline{Q}_k$

$\Rightarrow$ This is the QR Algorithm for eigenproblems

Algorithm: QR for Eigenproblems

Let $\underline{A}_0 = \underline{A}$

for $k = 1, 2, \ldots$

$\underline{Q}_k \underline{R}_k = \underline{A}_{k-1}$ (QR of $\underline{A}_{k-1}$)

$\underline{A}_k = \underline{R}_k \underline{Q}_k$ Recombination in reverse

end

Converge to some tolerance, result will be upper triangular matrix $\underline{T}$

Eigensystem Solutions - Summary

12:30 PM

$\underline{A}\,\underline{x} = \lambda\,\underline{x}$ for square $\underline{A}$

λ: eigenvalue

$\underline{x}$: eigenvector

$(\underline{A} - \lambda \underline{\underline{I}})\underline{x} = \underline{0}$

For nontrivial solutions $\det(\underline{A} - \lambda \underline{I}) = 0$

Solution approaches:

- Characteristic equation $\rightarrow$ find roots λ
- Iteration methods

  Power iteration method (largest $|\lambda|$)

  Inverse power iteration method (smallest $|\lambda|$)

  Inverse iteration with shifts

Rayleigh quotient iteration

- Spectrum calculations

Schur decomposition

$\underline{A} = \underline{Q}\,\underline{T}\,\underline{Q}^T$ with T: Upper triangular

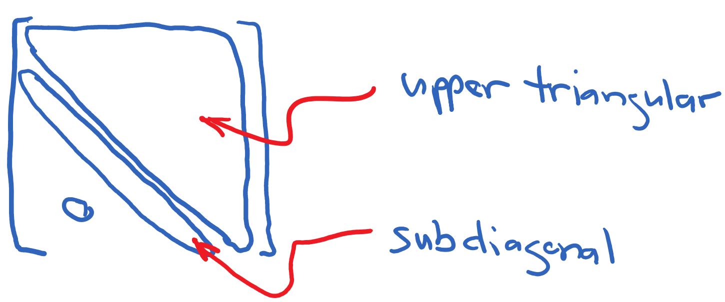
Q: Unitary $(\underline{Q}^T\underline{Q} = \underline{I})$

$\underline{A}$ & $\underline{T}$ are similar & consequently have same eigenvalues

Diagonals of $\underline{T}$ are its eigenvalues

Multi-step process to obtain eigenvalues:

① Compute upper Hessenberg form (upper triangle plus subdiagonal) by using Householder reflections $\rightarrow \underline{H} = \underline{Q}_1^T\,\underline{A}\,\underline{Q}_1$

$\underline{H} =$ 

② Iterate from upper Hessenberg form to

upper triangular $\underline{T} = \underline{Q}_2^T \underline{H} \underline{Q}_2$

③ Eigenvalues of $\underline{A}$ are on diagonal of $\underline{T}$

Other approaches (beyond current scope)

- Givens rotations replacing Householder reflections (both have unitary Q)
- Subspace iteration

$\left.\begin{array}{l}\text{Lanczos}\\ \\ \text{Arnoldi}\end{array}\right\}$ Krylov subspaces