Eigenvalue Problems, Part II

<u>Goal</u>: Find $\lambda \in \mathbb{C}$, $v \in \mathbb{C}^n$, $v \neq 0$, such that

$$Av = \lambda v$$

<u>Today</u>: Methods to find a single eig. value/vector.

- <u>Power iteration</u> (Find the dominate eig. val/vector)

  Suppose that A is diagonalizable,

  with eig. values $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n| \geq 0$

  eig. vectors $v_1, v_2, \cdots, v_n \in \mathbb{C}^n$, $\|v_i\| = 1$, $i = 1, \cdots, n$

  - Starting with an $x_0 \in \mathbb{C}^n$, keep multiplying it with A, what do we get?

  Since $\{v_1, \cdots, v_n\} \subseteq \mathbb{C}^n$ forms a basis in $\mathbb{C}^n$,

  we have $x_0 = a_1 v_1 + \cdots + a_n v_n$

$$A^k x_0 = a_1 \lambda_1^k v_1 + \cdots + a_n \lambda_n^k v_n$$

$$= \lambda_1^k \left[a_1 v_1 + a_2 \left(\frac{\lambda_2}{\lambda_1}\right)^k v_2 + \cdots + a_n \left(\frac{\lambda_n}{\lambda_1}\right)^k v_n \right]$$

if $\left|\frac{\lambda_i}{\lambda_1}\right| < 1$, $\forall i = 2, \cdots, n$, then

when $k \gg 1$, $A^k x_0 \sim \lambda_1^k a_1 v_1$

Now let $x_k = A^k x_0$, then $x_{k+1} \sim \lambda_1^{k+1} a_1 v_1 \sim \lambda_1 x_k$

so $x_{k+1}^{(i)} / x_k^{(i)} \sim \lambda_1$, and $x_k / \|x_k\| \sim v_1$

Implementation :

Given $x_0 \in \mathbb{C}^n$,

For $k = 1, 2, \dots, n, \cdots$

$$\hat{x}_k = A x_{k-1}$$

$$m_k = \max(\hat{x}_k)$$

$$x_k = \hat{x}_k / m_k$$

Define $\max(\cdot)$ so that $|\max(x)| = \|x\|_\infty$

Thm Suppose that $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n| \geq 0$

and $v_1^* x_0 \neq 0$ ← almost always possible due to rounding error

then $|m_k - \lambda_1| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$

$$\left\| x_k - \left(\pm \frac{v_1}{\max(v_1)}\right)\right\| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

Pf: $m_k = \max(\hat{x}_k) = \dfrac{\max(A\hat{x}_{k-1})}{\max(\hat{x}_{k-1})}$

$$= \frac{\max(A^2 \hat{x}_{k-2})}{\max(A\hat{x}_{k-2})} = \cdots = \frac{\max(A^k x_0)}{\max(A^{k-1} x_0)}$$

Now let $x_0 = a_1 v_1 + \cdots + a_n v_n$, then

$$m_k = \lambda_1 \frac{\max\left(a_1 v_1 + \sum_{i=2}^{n} \left(\frac{\lambda_i}{\lambda_1}\right)^k a_i v_i\right)}{\max\left(a_1 v_1 + \sum_{i=1}^{n} \left(\frac{\lambda_i}{\lambda_1}\right)^{k-1} a_i v_i\right)} = \lambda_1 \left(1 + O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)\right)$$

Note that x_k is in the same direction as $A^k x_0$

$\left(x_k = \dfrac{A x_{k-1}}{m_k} = \cdots = \dfrac{A^k x_0}{m_k \cdots m_1} \right)$

we have $x_k = \pm \dfrac{A^k x_0}{\max(A^k x_0)}$

$$= \pm \frac{a_1 v_1 + \sum_{i=2}^{n} \left(\frac{\lambda_i}{\lambda_1}\right)^k a_i v_i}{\max\left(a_1 v_1 + \sum_{i=1}^{n} \left(\frac{\lambda_i}{\lambda_1}\right)^k a_i v_i\right)}$$

$$= \pm \frac{v_1}{\max(v_1)} + O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right) \quad \blacksquare$$

Remark:

1) If there are a number of linearly independent eig. vectors corresponding to the dominant eig. value, we still get convergence

If $\lambda_1 = \lambda_2 = \cdots = \lambda_r$, $|\lambda_1| > |\lambda_{r+1}| \geq \cdots \geq |\lambda_n| \geq 0$

then $$A^k x_0 = \lambda_1^k \left[\sum_{i=1}^{r} a_i v_i + \sum_{i=r+1}^{n} \left(\frac{\lambda_i}{\lambda_1}\right)^k a_i v_i \right]$$

$$\sim \lambda_1^k \left[\sum_{i=1}^{r} a_i v_i + O\left(\left|\frac{\lambda_{r+1}}{\lambda_1}\right|^k\right) \right]$$

the limit of iteration lies in the subspace spanned by $v_1, \dots, v_r$ and depends on x_0.

2) If there are more than one eigenvalue with the same largest magnitude, the iterated vector does not converge. Instead, it will osillate. For example, when a real matrix has two conjugate dominate eigenvalues $(\lambda_1, \bar{\lambda}_1)$, starting with a real initial vector, all m_k's are real and it is impossible to converge to λ_1 or $\bar{\lambda}_1$. Actually, it will oscillate between some real numbers related to λ_1. Even though the outputs oscillate, it is still possible to extract the eigenvalues. (See Wilkinson. The algebraic eigenvalue problems, p.579)

- Variants of power iteration
  - Inverse iteration (Find the "smallest" eig. val / vector)

Suppose $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_{n-1}| > |\lambda_n| > 0$

$v_1, \quad v_2, \quad \cdots, \quad v_{n-1}, \quad v_n \in \mathbb{C}^n$

Apply power iteration to A^{-1} to compute λ_n^{-1} and v_n

Implementation:

Given $x_0 \in \mathbb{C}^n$,

For $k = 1, 2, \dots, n, \cdots$

$$\text{Solve } \hat{x}_k \text{ from } A\hat{x}_k = x_{k-1}$$

$$m_k = \max(\hat{x}_k)$$

$$x_k = \hat{x}_k / m_k$$

- Shifted inverse power iteration
(Find eig. val. / vector near μ)

Suppose $\dfrac{1}{|\lambda_i - \mu|} > \dfrac{1}{|\lambda_j - \mu|}$, $\forall j \neq i$ $\quad (\lambda_i \neq \mu)$

Apply inverse power iteration to $A - \mu I$

Remark: The convergence rate depends on how μ is close to λ_i. Shifted inverse power iteration can be used to find eigenvectors when we have a good approximation to some eigenvalues.

- Rayleigh quotient iteration

Power iteration is slow when $\left|\frac{\lambda_2}{\lambda_1}\right| \approx 1$.

Can we accelerate? When A is Hermitian, this is possible.

Need a better eig. val. estimator than $\max(Ax_k)$:

Def Given vector $x \in \mathbb{C}^n$, $R(x) = \dfrac{x^* A x}{x^* x}$ is called the Rayleigh quotient of A at x

If (λ, v) is an eigenpair, $R(v) = \lambda$.

Let $\tilde{v}$ be a perturbation to v, then Taylor expansion $R(\tilde{v})$

$$R(\tilde{v}) = \lambda + \underbrace{\nabla R(v)^* (\tilde{v} - v)}_{} + O(\|\tilde{v} - v\|_2^2)$$

when A is real symmetric

$$\nabla R(v) = \frac{v^T v (2Av) - v^T A v (2v)}{(v^T v)^2}$$

$$\overset{\|v\|_2 = 1}{=} \frac{2(Av - R(v)v)}{(v^T v)^2} = 0$$

We can use $R(x)$ as our eig. val. estimator in power iteration:

Implementation:

Given $x_0 \in \mathbb{C}^n$,

For $k = 1, 2, \dots, n, \dots$

$$\hat{x}_k = A x_{k-1} \qquad (\Delta)$$

$$x_k = \hat{x}_k / \|\hat{x}_k\|_2$$

$$m_k = R(x_k)$$

Thm For general $A \in \mathbb{C}^{n\times n}$. with $|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_n|$
$v_1, \quad v_2, \quad \ldots, \quad v_n$

the iteration (Δ) satisfies

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

$$\|x_k - \pm v_1\| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

Furthermore, when A is normal, we have

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

Pf: $$m_k = R(x_k) = \frac{(A^k x_0)^* A^{k+1} x_0}{(A^k x_0)^* A^k x_0}$$

$$= \frac{\left(\sum_{i=1}^n \lambda_i^k a_i v_i\right)^* \left(\sum_{i=1}^n \lambda_i^{k+1} a_i v_i\right)}{\left(\sum_{i=1}^n \lambda_i^k a_i v_i\right)^* \left(\sum_{i=1}^n \lambda_i^k a_i v_i\right)}$$

Assume $A^* = A$

when $A^* \neq A$ →

$$\overset{\text{orthonormality of } v_1,\ldots,v_n}{=} \frac{\sum_{i=1}^n |\lambda_i|^{2k} \lambda_i |a_i|^2}{\sum_{i=1}^n |\lambda_i|^{2k} |a_i|^2}$$

$$= \lambda_1 \left[1 + O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k}\right)\right]$$

☒

Note that in shifted inverse power iteration, the linear convergence rate is $\max_{i\neq j} \left|\frac{\lambda_j - \mu}{\lambda_i - \mu}\right|$. If we update μ whenever we get a better estimate of λ_j, the convergence factor will decrease during iteration. ← there is a hope for superlinear convergence

Method: Rayleigh Quotient Iteration

Given $x_0 \in \mathbb{C}^n$,

For $k = 1, 2, \dots, n, \dots$

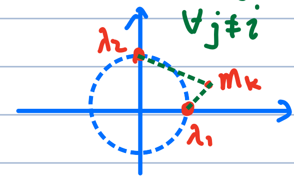
$m_k = R(x_{k-1})$ (RQI)

Solve $(A - m_k I)\hat{x}_k = x_{k-1}$

$x_k = \hat{x}_k / \|\hat{x}_k\|_2$

In practice, RQI doesn't suffer from eig. vals of the same magnitude b.c. the shifting $\rightarrow$

Pick a random m_k.
"Almost surely" that $\exists i$, s.t. $|\lambda_i - m_k| < |\lambda_j - m_k|$ $\forall j \neq i$



(RQI) almost always converges when it does (for good initial guess)

for general A, (RQI) converges quadratically

$|m_k - \lambda_j| = O(|m_{k-1} - \lambda_j|^2)$

$\|x_k - \pm v_j\| = O(\|x_{k-1} - \pm v_j\|^2)$

See Trefethen / Bau for an illustrative proof

for Hermitian A, (RQI) converges cubically

$|m_k - \lambda_j| = O(|m_{k-1} - \lambda_j|^3)$

$\|x_k - \pm v_j\| = O(\|x_{k-1} - \pm v_j\|^3)$

- Simultaneous Power Iteration

How to get all $\lambda_1, \dots, \lambda_n$, and $v_1, \dots, v_n$?

Idea: run power iteration on multiple vectors simultaneously

Given $Q_0 \in \mathbb{C}^{n \times n}$

For $k = 1, 2, \dots, n$

$X_k = A Q_{k-1}$ ← power iteration

QR fact. $X_k = Q_k R_k$ ← orthonormalize vectors

$T_k = Q_k^* A Q_k$ ← generalized Rayleigh Quotient

If the iteration "converges (e.g. $Q_k \to Q$ as $k \to +\infty$)"

then $T := Q^* A Q \approx Q_k^* A Q_{k-1} = Q_k^* X_k = R_k$ ← upper Δ

it is expected that T_k converges to the Schur form of A

This is guaranteed by the following theorem

Thm Suppose that $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$

and $Q^* A Q = T$ be Schur fact. of A

assume that Q_0 satisfies some non-deficiency conditions (the leading principal minors of $Q^* Q_0$ are all nonzero)

then $T_k \xrightarrow{k \to +\infty} T$

In particular, when A is normal, $T_k \to \text{diag}(\lambda_1, \cdots, \lambda_n)$

Let $\lambda_i^{(k)}$ be the i^{th} eig. val. of T_k. then

$$|\lambda_i^{(k)} - \lambda_i| \approx \left|\frac{\lambda_{i+1}}{\lambda_i}\right|^k$$

We can reformulate simultaneously power iteration

to get a clean form with T_k computed directly

Note that $T_{k-1} = Q_{k-1}^* A Q_{k-1} = Q_{k-1}^* (A Q_{k-1}) = \underline{(Q_{k-1}^* Q_k)} \underline{R_k}$

$$T_k = Q_k^* A Q_k = (Q_k^* A Q_{k-1})(Q_{k-1}^* Q_k)$$

$$= \underline{R_k} \underline{(Q_{k-1}^* Q_k)}$$

that is, T_k is obtained from T_{k-1} by computing the QR of T_{k-1} and multiplying the factors together in reverse order.

- QR iteration:

Given $A \in \mathbb{C}^{n\times n}$, unitary $Q \in \mathbb{C}^{n\times n}$

$T_0 = Q_0^* A Q_0$

for $k = 1, 2, \cdots$

QR fact. $T_{k-1} = Q_k R_k$

$T_k = R_k Q_k$

Output T_k

Remark: 1) A Single QR iteration cost $O(n^3)$ calculation for dense A

2) Convergence is linear (when it exists).

Pure QR is prohibitively expensive

3) If eigenvalues are not distinct, QR iteration converges to block upper triangular form, where each block corresponds to a group of eigenvalues sharing the same magnitude, with its size equal to the number of such eigenvalues.

$$|\lambda_1| = |\lambda_2| = |\lambda_3| > |\lambda_4| = |\lambda_5| > |\lambda_6|$$

$$T_k \approx \begin{bmatrix} A_1^{(k)} & & * \\ & A_2^{(k)} & \\ & & \lambda_6 \end{bmatrix} \quad \text{when } k \gg 1$$

where $A_1^{(k)} \in \mathbb{C}^{3\times 3}$, $A_2^{(k)} \in \mathbb{C}^{2\times 2}$

neither converges