Eigenvalue Problems, Part II

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

$$Av = \lambda v$$

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

- **Power iteration** (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 $x_0 = a_1 v_1 + \dots + a_n v_n$, 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 $A^k x_0$

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

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

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

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

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

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

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

  Implementation:

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

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

  Solve $\hat{x}_k$ 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 $\dfrac{1}{|\lambda_i - \mu|} > \dfrac{1}{|\lambda_j - \mu|}, \ \forall j \neq i \qquad (\lambda_i \neq \mu)$

    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 Hermittian, this is possible.

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

Def Given vector $x \in \mathbb{C}^n$, $R(x) = \frac{x^* A x}{x^* x}$ 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 $|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_n|$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad v_1, \quad v_2, \quad \dots, v_n$

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

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

Assume $A^* = A$

when $A^* \neq A$ → orthonormality of $v_1, \dots, v_n$

$$= \frac{\sum_{i=1}^n |\lambda_i|^{2k} \lambda_i |a_i|^2}{\sum_{i=1}^n |\lambda_i|^{2k} |a_i|^2}$$

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

$\blacksquare$

Note that in shifted inverse power iteration, the linear convergence rate is $\max_{i \neq j} \left|\dfrac{\lambda_j - \mu}{\lambda_i - \mu}\right|$. 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 $k = 1, 2, \cdots, n, \cdots$

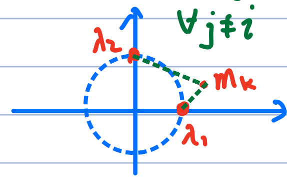
$$m_k = R(x_{k-1}) \qquad \text{(RQI)}$$

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

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 locally 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 globally, and locally 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 $\lambda_1, \cdots, \lambda_n$, and $v_1, \cdots, v_n$?

Idea: run power iteration on multiple vectors simultaneously

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

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

$X_k = A Q_{k-1}$ ← 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

<u>Thm</u> 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, $T_k \to \mathrm{diag}(\lambda_1, \cdots, \lambda_n)$

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

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

See Golub-Van Loan Matrix computations Section 7.3.3 for a proof

lower Δ entries → $$|(T_k)_{ij}| \approx \frac{|\lambda_{j+1}|}{|\lambda_j|}, \forall i > j$$

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 $k = 1, 2, \dots$

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

Pure QR is prohibitively expensive

2) Convergence is linear (when it exists).

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