Let me emphasize main points of the power methods described in [1]. Of course, I will add some points of myself to make some concepts more clear.

1 Baisc power methods

After establishing $A^k x$ converges to the eigenvector of A corresponding to the largest eigenvalue, we need some stopping criterion, which is the main concern in numerical analysis because we cannot set max_eiter simply.

Since $x^{(m)}$ cannot be eigenvector identically, there is no real number a satisfying $Ax^{(m)} = ax^{(m)}$. But we can expect the number a which makes

$$\|Ax^{(m)} - ax\|$$

minimizes is a good approximation of the largest eigenvalue. Now we elaborate on how to solve this a.

Rayleigh Quotient. If one see $Av = av$ as an overdetermined equation system, technique about **least square** can be applied to get the solution a which is called Rayleigh quotient.

$$\Lambda_A(v) := \frac{v^* A v}{v^* v} \tag{1}$$

Geometrically, the solution of least square is just to find a scalar a such that $Av - av$ is orthogonal to v.

> **Rayleigh quotient**
>
> One can also deduce the same result (1) algebraically by solving the following optimization problem
>
> $$\min_x \|Av - av\|_2^2, \tag{2}$$
>
> then eq (2) (take real case as example) boils down to finding the critical point of
> $$f(a) = v^T v a^2 - v^T (A^T + A) v a + v^T A^T A v$$
> If $v^T A^T v$ is a real number, then $v^T A^T v = v^T A v$, one can use the derivative of $f(a)$ to determine the critical point and the result matches the Least Square. When we consider the complex number field, the expansion of $f(x) = \min_x \|Av - av\|_2^2$ is subtle, saying
>
> $$f(a) \neq v^* v a^2 - v^* (A^* + A) v a + v^* A^* A v$$
>
> especially when a is complex.

The theoretical support is given by Theorem 4.6 in [1].

Combined with $\|x^{(m)} - v\| \approx 0$ and $|\lambda^{(m)} - \lambda| \approx 0$ where $\lambda, v \in \text{eig}(A)$, we can see that

$$\|Ax^{(m)} - \lambda^{(m)} x^{(m)}\| \to 0$$

where each components can be computed explicitly in the process of iteration. So one option for stopping criterion is to set ϵ and stop the iteration when

$$\|Ax^{(m)} - \lambda^{(m)x^{(m)}}\| < \epsilon$$

2 Simultaneous Iteration

Suppose we want to find the first k eigenvectors of A, we can use the simultaneous iteration. We expect $V^{(m+1)} = A^m V$ where V is matrix consisting of k independent column vectors to converge to the eigenvectors of A corresponding to the largest k eigenvalues. Although we can prove that $V^{(m+1)}$ is injective but it's just theoretical! In practice, we need to consider the numerical stability of the algorithm. Let me give an example to show the problem

Consider the symmetric matrix:

$$A = \begin{bmatrix} 4 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

We will start with the matrix V with two columns in the initial step:

$$V^{(0)} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Iteration Without Orthogonalization

Each column of $V^{(m)}$ is updated via:

$$V^{(m+1)} = AV^{(m)}$$

Perform a few iterations to illustrate the convergence:

First Iteration:

$$V^{(1)} = AV^{(0)} = \begin{bmatrix} 4 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 4 & 1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix}$$

Second Iteration:

$$V^{(2)} = AV^{(1)} = \begin{bmatrix} 4 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 2 \end{bmatrix} \begin{bmatrix} 4 & 1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 18 & 8 \\ 8 & 11 \\ 7 & 6 \end{bmatrix}$$

... 10th Iteration:

$$V^{(10)} = AV^{(9)} = \begin{bmatrix} 8490718 & 5843148 \\ 5843148 & 4032371 \\ 4458347 & 3073546 \end{bmatrix}$$

Observation

As iterations continue, each column increasingly aligns with the dominant eigenvector $\mathbf{v}_1 = \begin{bmatrix} 0.7558 \\ 0.5207 \\ 0.3971 \end{bmatrix}$ corresponding to $\lambda_{\max} = 5.2143$. For large m, the columns of $V^{(m)}$ converge to:

$$V^{(m)} \approx \begin{bmatrix} 0.7558 & 0.5207 \\ 0.3971 & 0.7558 \\ 0.5207 & 0.3971 \end{bmatrix}$$

This convergence indicates numerical instability, as the columns lose linear independence and all vectors converge toward the dominant eigenvector's direction.

Apply QR into Simultaneous Iteration

Orthogonalize (using QR Factorization): Perform QR factorization when computing $V^{(2)} = AV^{(1)} = A$ where

$$V^{(1)} = \begin{bmatrix} 4 & 1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} = Q^{(1)}R^{(1)} = \begin{bmatrix} -0.9428 & 0.2851 \\ -0.2357 & -0.9366 \\ -0.2357 & -0.2036 \end{bmatrix} \begin{bmatrix} -4.2426 & -1.8856 \\ 0 & -2.7285 \end{bmatrix}$$

, then we compute the QR of $AQ^{(1)} = Q^2 \hat{R}^{(2)}$,

$$V^{(2)} = Q^{(2)} \hat{R}^{(2)} R^{(1)}$$

$$= \begin{bmatrix} -0.8611 & 0.4685 \\ -0.3827 & -0.8531 \\ -0.3349 & -0.2297 \end{bmatrix} \begin{bmatrix} 4.9272 & 1.3987 \\ 0 & 2.5708 \end{bmatrix} \begin{bmatrix} -4.2426 & -1.8856 \\ 0 & -2.7285 \end{bmatrix}$$

Update $V^{(m)}$ with orthogonal columns: After orthogonalization:

$$V^{(m)} = Q^{(m)} R^{(m)} = \begin{pmatrix} -0.7559 & 0.6316 \\ -0.5205 & -0.7395 \\ -0.3971 & -0.2330 \end{pmatrix} 1.0e + 07 \begin{pmatrix} -5.8556 & -4.0339 \\ 0 & -0.0024 \end{pmatrix}$$

with $m = 10$ as example. One can verify that the columns of $Q^{(10)}$ closely approximate the eigenvectors of A corresponding to its two largest eigenvalues (in magnitude).

4

This orthogonalization corrects the numerical errors that lead to loss of linear independence, thus ensuring each iteration step mainly jumps to the invariant subspace.

References

[1] Steffen Börm and Christian Mehl. *Numerical methods for eigenvalue problems*. Walter de Gruyter, 2012.