

Iterative methods

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1 Eigenvalue problem

We will consider symmetric matrix $A \in \mathbb{R}^{m \times m}$. We define the Rayleigh Quotient,

$$r(x) = \frac{x^t A x}{x^t x}. \quad (1)$$

Note that if x is an eigenvector of A , $r(x) = \lambda$ is its eigenvalue.

One way to understand this formula is: given x , what is the scale α which acts almost like an eigenvalue of x in the sense that $Ax - \alpha x$ is minimized? This is a least square problem, but x is the matrix α is the unknown vector, and Ax is the right-hand side b vector. We can see that $\alpha = r(x)$ if we consider the normal equation.

Take the derivative of $r(x)$ with respect to all component x_j of x , we can easily derive that,

$$\nabla r(x) = \frac{2}{x^t x} (Ax - r(x)x). \quad (2)$$

We can see that when x is the eigenvector, the gradient vanishes. Conversely, if the gradient is trivial with $x \neq 0$, x is an eigenvector with eigenvalue $r(x)$.

Theorem 1.1. Let q_j be an eigenvector of A , we have

$$r(x) - q_j = \mathcal{O}(\|x - q_j\|^2), \quad (3)$$

as $x \rightarrow q_j$.

The Power iteration is expected to return an eigenvector corresponding to the largest eigenvalues.

Algorithm 1: Power Iteration

- 1 Set v_0 with $\|v_0\| = 1$.
 - 2 **for** $k = 1$ to ... **do**
 - 3 $w = Av^k$
 - 4 $v^k = w/\|w\|$
 - 5 $\lambda^k = (v^k)^T Av^k$
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Theorem 1.2. Suppose $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_m| \geq 0$ and $q_1^T v^0 \neq 0$. Then the algorithm satisfies,

$$\|v^{(k)} - q_1\| = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right), \quad (4)$$

$$|\lambda^{(k)} - \lambda_1| = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k}\right), \quad (5)$$

as $k \rightarrow \infty$

Rayleigh quotient of $A \in \mathbb{R}^{m \times m}$

$$r(x) = \frac{x^T A x}{x^T x}, \quad x \in \mathbb{R}^m$$

i. Suppose (x, λ) is an eigen-pair of A , $Ax = \lambda x$,

$$r(x) = \frac{x^T \lambda x}{x^T x} = \lambda$$

ii.
$$\nabla r(x) = \begin{pmatrix} \frac{\partial r}{\partial x_1} \\ \dots \\ \frac{\partial r}{\partial x_m} \end{pmatrix} = \frac{2}{x^T x} (Ax - r(x)x)$$

when x is an eigenvector of A ,

$$\Rightarrow \nabla r(x) = 0$$

when $\nabla r(x) = 0$, $\Rightarrow x \neq 0$ is an eigenvector of A

Thm 1.1.

Let (ξ_j, λ_j) be an eigen-pair of A ,

$$r(x) - \lambda_j = \mathcal{O}(\|x - \xi_j\|^2), \quad \text{as } x \rightarrow \xi_j$$

→ Rayleigh quotient is quadratically accurate estimation of the eigenvalue.

→ Given the approximation to e-vector we have an approximation of the 2nd to the eigenvalue.

Power iteration.

set $v^{(0)}$, $\|v^{(0)}\| = 1$.

for $k = 1, \dots, \textcircled{1}$

$$w = A v^{(k-1)}$$

$$v^{(k)} = w / \|w\|$$

$$\lambda^{(k)} = \underbrace{(v^{(k)})^t A (v^{(k)})}_{\text{Rayleigh quotient of } A}$$

By thm 1.1, $\lambda^{(k)} \rightarrow \lambda_1$

① $k \rightarrow \infty$, we have the convergence, but to write the code, we need some terminate condition.

② $K_n(A)$ Krylov subspace

$$= [b, Ab, A^2b, \dots, A^{n-1}b]$$

Here $b = v^{(0)}$

Represent $v^{(k)}$ in $K_n(A)$

③ A is symmetric, \Rightarrow all eigenvalues of A are real, e.g., $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m$
& Power iteration can find (λ_1, v_1)

④ The convergence is linear, specifically, the algorithm will reduce the error by a factor $(\frac{\lambda_2}{\lambda_1})$ in each iteration.

⑤ When eigen-gap is small the algo converges slowly.

Inverse iteration.

Motivation, we want to design an algorithm which

can identify any eval & e.vectors of A .

Suppose μ is not an eigenvalue of A .

Suppose (v, α) is an eigen-pair of $(A - \mu I)^{-1}$

$$(A - \mu I)^{-1} v = \alpha v$$

$$v = \alpha (A - \mu I) v$$

$$v = \alpha A v - \alpha \mu v$$

$$\alpha A v = (1 + \alpha \mu) v \quad (\text{assume } \alpha \neq 0)$$

$$A v = (1 + \alpha \mu) / \alpha v$$

$\Rightarrow v$ is also an eigenvector of A .

Now let $A v_i = \lambda_i v_i$

$$\Rightarrow \alpha = \frac{1}{\lambda_i - \mu}$$

Here, if $\mu \rightarrow \lambda_i$, $\Rightarrow \alpha$ is large, α should be larger than the eigenvalues of $(A - \mu I)^{-1}$ (eigenvalue of $(A - \mu I)^{-1}$)

\Rightarrow We can use the power iteration to identify eigen-pair (α, v) of $(A - \mu I)^{-1}$.

\Rightarrow we can get the eigen-vector of A .

Rank, why is this called the inverse iteration?

approximation μ to $\lambda_i \longrightarrow$ eigenvectors of A .

Inverse iteration

$$v^{(0)}, \|v^{(0)}\| = 1$$

For $k = 1, \dots, \infty$

solve $(A - \mu I)w = v^{(k-1)}$ for w .

$$v^{(k)} = w / \|w\|$$

$$\lambda^{(k)} = (v^{(k)})^t A v^{(k)}$$

\uparrow

eigenval of A .

\longmapsto

A & $(A - \mu I)^{-1}$

share the eigenvectors.

Remark 1. Power iteration has some limitations.

1. It can only find the largest eigenvectors corresponding to the largest eigenvalues.
2. The convergence is linear, i.e., the algorithm reduces the error by a factor $|\frac{\lambda_2}{\lambda_1}|$ in every iteration.
3. The quality of the convergence depends on the quotient. If there is no huge eigen-gap, the convergence is slow.

1.1 Inverse Iteration

Let μ be a number which is not an eigenvalue of A , the eigenvectors of $(A - \mu I)^{-1}$ are the same as the eigenvectors of A , and the corresponding eigenvalues are $(\lambda_j - \mu)^{-1}$, where $\{\lambda_j\}$ are the eigenvalues of A .

This motivates us to design an algorithm to identify λ_j and the corresponding eigenvectors of A . Suppose we know any estimate of λ_j and denote it as μ . $(\mu - \lambda_j)^{-1}$ will be very large. According to the Remark, the power iteration can identify q_j , which are the eigenvectors of $(A - \mu I)^{-1}$ (also the eigenvectors of A). This idea is called the inverse iteration.

Algorithm 2: Inverse iteration

```
1  $v^0 =$  some vectors with norm 1
2 for  $k = 1$  to ... do
3   Solve  $(A - \mu I)w = v^{k-1}$  for  $w$ 
4    $v^k = w / \|w\|$ 
5    $\lambda^k = (v^k)^T A v^k$ .
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Rayleigh quotient is one method to estimate eigenvalues from an eigenvector estimation. Inverse iteration is an estimate of eigenvector from the eigenvalues.

Algorithm 3: RQ iteration

```
1  $v^0 =$  some vectors with norm 1
2  $\lambda^0 = v^0 A v^0 =$  corresponding Rayleigh quotient. for  $k = 1$  to ... do
3   Solve  $(A - \lambda^{k-1} I)w = v^{k-1}$  for  $w$ 
4    $v^k = w / \|w\|$ 
5    $\lambda^k = (v^k)^T A v^k$ .
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Without proof, the Rayleigh Quotient iteration has cubic convergence.

2 Iterative methods

In this section, let us consider matrix $A \in \mathbb{R}^{m \times m}$. Broadly speaking, the idea of iterative methods is to:

1. Gradually refine the solution iteratively.
2. Each iteration should be (a lot) cheaper than direct methods.