

Large-scale eigenvalue problems



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Outline

- Power method
- Lanczos algorithm

Eigendecomposition

Consider a *symmetric* matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, where n is large

How to compute the eigenvalues and eigenvectors of \mathbf{A} efficiently?

- hopefully accomplished via a few matrix-vector products

Power method

Power iteration

$$\mathbf{q}_t = \frac{1}{\underbrace{\|\mathbf{A}\mathbf{q}_{t-1}\|_2}_{\text{re-normalization}}} \mathbf{A}\mathbf{q}_{t-1}, \quad t = 1, 2, \dots$$

- each iteration consists of a matrix-vector product
- equivalently,

$$\mathbf{q}_t = \frac{1}{\|\mathbf{A}^t \mathbf{q}_0\|_2} \mathbf{A}^t \mathbf{q}_0$$

Example

Consider $\mathbf{A} = \begin{bmatrix} 2 & \\ & 1 \end{bmatrix}$ and $\mathbf{q}_0 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, then

$$\mathbf{A}^t \mathbf{q}_0 = \begin{bmatrix} 2^t \\ 1 \end{bmatrix}$$

$$\implies \mathbf{q}_t = \frac{1}{\|\mathbf{A}^t \mathbf{q}_0\|_2} \mathbf{A}^t \mathbf{q}_0 = \begin{bmatrix} \frac{2^t}{\sqrt{2^{2t}+1}} \\ \frac{1}{\sqrt{2^{2t}+1}} \end{bmatrix} \rightarrow \underbrace{\begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{\text{leading eigenvector of } \mathbf{A}} \quad \text{as } t \rightarrow \infty$$

Power method

Algorithm 4.1 Power method

1: **initialize** $q_0 \leftarrow$ random unit vector

2: **for** $t = 1, 2, \dots$ **do**

3: $q_t = \frac{1}{\|Aq_{t-1}\|_2} Aq_{t-1}$

(power iteration)

4: $\hat{\lambda}_1^{(t)} = q_t^\top Aq_t$

- q_t : estimate of the leading eigenvector of A
- $\hat{\lambda}_1^{(t)}$: estimate of the leading eigenvalue of A

Convergence of power method

- $\mathbf{A} \in \mathbb{R}^{n \times n}$: eigenvalues $\lambda_1 > \lambda_2 \geq \dots \geq \lambda_n$; eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_n$

Theorem 4.1 (Convergence of power method)

If $\lambda_1 > \lambda_2 \geq |\lambda_n|$ and set $\nu_1 = \mathbf{q}_0^\top \mathbf{u}_1$, then

$$|\hat{\lambda}_1^{(t)} - \lambda_1| \leq (\lambda_1 - \lambda_n) \frac{1 - \nu_1^2}{\nu_1^2} \left(\frac{\lambda_2}{\lambda_1} \right)^{2t}$$

Proof of Theorem 4.1

Write $\mathbf{q}_0 = \sum_{i=1}^n \nu_i \mathbf{u}_i$, then

$$\mathbf{A}^t \mathbf{q}_0 = \sum_{i=1}^n \lambda_i^t \mathbf{u}_i \mathbf{u}_i^\top \mathbf{q}_0 = \sum_{i=1}^n \lambda_i^t \nu_i \mathbf{u}_i$$

$$\implies \|\mathbf{A}^t \mathbf{q}_0\|_2 = \left\| \sum_{i=1}^n \lambda_i^t \nu_i \mathbf{u}_i \right\|_2 = \sqrt{\sum_{i=1}^n \lambda_i^{2t} \nu_i^2}$$

Since $\mathbf{q}_t = \frac{1}{\|\mathbf{A}^t \mathbf{q}_0\|_2} \mathbf{A}^t \mathbf{q}_0$ and \mathbf{A} is symmetric, we get

$$\begin{aligned} \hat{\lambda}_1^{(t)} &= \mathbf{q}_t^\top \mathbf{A} \mathbf{q}_t = \frac{1}{\|\mathbf{A}^t \mathbf{q}_0\|_2^2} \mathbf{q}_0^\top \mathbf{A}^{2t+1} \mathbf{q}_0 \\ &= \frac{1}{\sum_{i=1}^n \lambda_i^{2t} \nu_i^2} \mathbf{q}_0^\top \left(\sum_{i=1}^n \lambda_i^{2t+1} \mathbf{u}_i \mathbf{u}_i^\top \right) \mathbf{q}_0 \\ &= \frac{1}{\sum_{i=1}^n \lambda_i^{2t} \nu_i^2} \sum_{i=1}^n \lambda_i^{2t+1} \nu_i^2 \end{aligned}$$

Proof of Theorem 4.1 (cont.)

As a consequence,

$$\begin{aligned} |\hat{\lambda}_1^{(t)} - \lambda_1| &= \frac{1}{\sum_{i=1}^n \lambda_i^{2t} \nu_i^2} \left| \sum_{i=1}^n \lambda_i^{2t+1} \nu_i^2 - \sum_{i=1}^n \lambda_1 \lambda_i^{2t} \nu_i^2 \right| \\ &= \frac{1}{\sum_{i=1}^n \lambda_i^{2t} \nu_i^2} \left| \sum_{i=2}^n \lambda_i^{2t} (\lambda_1 - \lambda_i) \nu_i^2 \right| \\ &\leq \frac{\lambda_1 - \lambda_n}{\lambda_1^{2t} \nu_1^2} \sum_{i=2}^n \lambda_i^{2t} \nu_i^2 && \text{(since } \lambda_1 - \lambda_i \leq \lambda_1 - \lambda_n \text{)} \\ &\leq \frac{\lambda_1 - \lambda_n}{\lambda_1^{2t} \nu_1^2} \lambda_2^{2t} \sum_{i=2}^n \nu_i^2 \\ &= \frac{\lambda_1 - \lambda_n}{\lambda_1^{2t} \nu_1^2} \lambda_2^{2t} (1 - \nu_1^2) && \text{(since } \sum_i \nu_i^2 = 1 \text{ (as } \|\mathbf{q}_0\|_2 = 1 \text{))} \end{aligned}$$

as claimed

Block power method

Computing the top- r eigen-subspace:

Algorithm 4.2 Power method

- 1: **initialize** $\mathbf{Q}_0 \in \mathbb{R}^{n \times r} \leftarrow$ random orthonormal matrix
 - 2: **for** $t = 1, 2, \dots$ **do**
 - 3: $\mathbf{Z}_t = \mathbf{A}\mathbf{Q}_{t-1}$
 - 4: compute QR decomposition $\mathbf{Z}_t = \mathbf{Q}_t\mathbf{R}_t$, where $\mathbf{Q}_t \in \mathbb{R}^{n \times r}$ has orthonormal columns and $\mathbf{R}_t \in \mathbb{R}^{r \times r}$ is upper-triangular
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- use QR decomposition to reorthogonalize power iterates

Lanczos algorithm

Key idea 1: reduction to a tridiagonal form

Intermediate step

$$\underbrace{\begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \end{bmatrix}}_A \quad \xrightarrow{\text{find orthonormal } Q} \quad \underbrace{\begin{bmatrix} \bullet & \bullet & & & \\ \bullet & \bullet & \bullet & & \\ & \bullet & \bullet & \bullet & \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \end{bmatrix}}_{T=Q^T A Q \text{ (tridiagonal)}}$$

- **motivation:** eigendecomposition of a tridiagonal matrix can be performed efficiently (via a number of specialized algorithms), due to its special structure

Key idea 2: tridiagonalization and Krylov subspaces

One way to tridiagonalize A is to compute an orthonormal basis of certain subspaces, defined as follows

- **Krylov subspaces** generated by $A \in \mathbb{R}^{n \times n}$ and $\mathbf{b} \in \mathbb{R}^n$ are defined as

$$\mathcal{K}_t := \text{span}\{\mathbf{b}, A\mathbf{b}, \dots, A^{t-1}\mathbf{b}\}, \quad t = 1, \dots, n$$

- **Krylov matrices**

$$K_t := [\mathbf{b}, A\mathbf{b}, \dots, A^{t-1}\mathbf{b}] \in \mathbb{R}^{n \times t}, \quad t = 1, \dots, n$$

Key idea 2: tridiagonalization and Krylov subspaces

Lemma 4.2

If $\mathbf{Q}_t := [\mathbf{q}_1, \dots, \mathbf{q}_t] \in \mathbb{R}^{n \times t}$ forms an orthonormal basis of \mathcal{K}_t for all $1 \leq t \leq n$. Then

$$\mathbf{T}_t := \mathbf{Q}_t^\top \mathbf{A} \mathbf{Q}_t \text{ is tridiagonal, } 1 \leq t \leq n$$

- tridiagonalization can be carried out by successively computing the orthonormal basis of Krylov subspaces $\{\mathcal{K}_t\}_{t=1,2,\dots}$

Proof of Lemma 4.2

For any $i > j + 1$,

$$(\mathbf{T}_t)_{i,j} = \langle \mathbf{q}_i, \mathbf{A}\mathbf{q}_j \rangle$$

Since \mathbf{Q}_j is orthonormal basis of $\text{span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \dots, \mathbf{A}^{j-1}\mathbf{b}\}$, we have

$$\mathbf{q}_j \in \text{span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \dots, \mathbf{A}^{j-1}\mathbf{b}\}$$

$$\implies \mathbf{A}\mathbf{q}_j \in \text{span}\{\mathbf{A}\mathbf{b}, \dots, \mathbf{A}^j\mathbf{b}\} \subset \text{span}\{\mathbf{q}_1, \dots, \mathbf{q}_{j+1}\}$$

Since $i > j + 1$, one has $\mathbf{q}_i \perp \{\mathbf{q}_1, \dots, \mathbf{q}_{j+1}\}$ and hence

$$(\mathbf{T}_t)_{i,j} = \langle \mathbf{q}_i, \mathbf{A}\mathbf{q}_j \rangle = 0$$

Similarly, $(\mathbf{T}_t)_{i,j} = 0$ if $j > i + 1$. This completes the proof

A simple formula: 3-term recurrence

Denote

$$T = Q_n^\top A Q_n = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \ddots & & \\ & \ddots & \ddots & & \\ & & & \beta_{n-1} & \\ & & & & \alpha_n \end{bmatrix} \quad \text{or} \quad \underbrace{A Q_n = Q_n T}_{\text{since } Q_n \in \mathbb{R}^{n \times n} \text{ is orthonormal}}$$

Exploiting the tridiagonal structure yields

$$\underbrace{A}_{Q_t} [\underbrace{q_1, \dots, q_t}_{Q_t}] = [\underbrace{q_1, \dots, q_{t+1}}_{Q_{t+1}}] \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \ddots & & \\ & \ddots & \ddots & & \\ & & & \beta_{t-1} & \\ & & & & \alpha_t \\ & & & & & \beta_t \end{bmatrix}$$
$$\implies A q_t = \beta_{t-1} q_{t-1} + \alpha_t q_t + \beta_t q_{t+1}$$

Lanczos iterations

$$\mathbf{A}\mathbf{q}_t = \beta_{t-1}\mathbf{q}_{t-1} + \alpha_t\mathbf{q}_t + \beta_t\mathbf{q}_{t+1}$$

This 3-term recurrence says $\mathbf{A}\mathbf{q}_t \in \text{span}\{\mathbf{q}_{t-1}, \mathbf{q}_t, \mathbf{q}_{t+1}\}$

- this means $\alpha_t = \underbrace{\mathbf{q}_t^\top \mathbf{A}\mathbf{q}_t}$, since $\{\mathbf{q}_{t-1}, \mathbf{q}_t, \mathbf{q}_{t+1}\}$ are orthonormal
projection of $\mathbf{A}\mathbf{q}_t$ onto $\text{span}(\mathbf{q}_t)$

Since \mathbf{q}_{t+1} needs to have unit norm, one has

- $\mathbf{q}_{t+1} \leftarrow \text{normalize}(\mathbf{A}\mathbf{q}_t - \beta_{t-1}\mathbf{q}_{t-1} - \alpha_t\mathbf{q}_t)$ (direction of residual)
- $\beta_t = \|\mathbf{A}\mathbf{q}_t - \beta_{t-1}\mathbf{q}_{t-1} - \alpha_t\mathbf{q}_t\|_2$ (size of residual)

Lanczos algorithm

Algorithm 4.3 Lanczos algorithm

- 1: **initialize** $\beta_0 = 0$, $\mathbf{q}_0 = \mathbf{0}$, $\mathbf{q}_1 \leftarrow$ random unit vector
 - 2: **for** $t = 1, 2, \dots$ **do**
 - 3: $\alpha_t = \mathbf{q}_t^\top \mathbf{A} \mathbf{q}_t$
 - 4: $\beta_t = \|\mathbf{A} \mathbf{q}_t - \beta_{t-1} \mathbf{q}_{t-1} - \alpha_t \mathbf{q}_t\|_2$
 - 5: $\mathbf{q}_{t+1} = \frac{1}{\beta_t} (\mathbf{A} \mathbf{q}_t - \beta_{t-1} \mathbf{q}_{t-1} - \alpha_t \mathbf{q}_t)$
-

- each iteration only requires a matrix-vector product
- systematic construction of the orthonormal bases for successive Krylov subspaces

Convergence of the Lanczos algorithm

- $A \in \mathbb{R}^{n \times n}$: eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$, eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_n$

- $T_t = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \beta_{t-1} & \alpha_t \end{bmatrix}$: eigenvalues $\theta_1 \geq \dots \geq \theta_t$

Theorem 4.3 (Kaniel-Paige convergence theory)

Let $\nu_1 = \mathbf{q}_1^\top \mathbf{u}_1$, $\rho = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$, and $C_{t-1}(x)$ be the Chebyshev polynomial of degree $t - 1$. Then

$$\lambda_1 \geq \theta_1 \geq \lambda_1 - (\lambda_1 - \lambda_n) \frac{1 - \nu_1^2}{\nu_1^2} \frac{1}{(C_{t-1}(1 + 2\rho))^2}$$

Convergence of the Lanczos algorithm

Corollary 4.4

Let $R = 1 + 2\rho + 2\sqrt{\rho^2 + \rho}$ with $\rho = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$. We have

$$|\lambda_1 - \theta_1| \leq \underbrace{\frac{4(1 - \nu_1^2)}{\nu_1^2} (\lambda_1 - \lambda_n)}_{\text{prefactor}} \underbrace{R^{-2(t-1)}}_{\text{convergence rate}}$$

- this follows immediately from the following fact

$$\underbrace{C_{t-1}^2(1 + 2\rho)}_{\text{properties of Chebyshev polynomials}} = \frac{(R^{t-1} + R^{-(t-1)})^2}{4} \geq \frac{R^{2(t-1)}}{4}$$

Power method vs. Lanczos algorithm

Consider a case where $\lambda_2 = -\lambda_n$. Recall that $\rho = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n} = \frac{\lambda_1 - \lambda_2}{2\lambda_2}$

- **power method:** convergence rate

$$\left(\frac{\lambda_2}{\lambda_1}\right)^{2t} = \frac{1}{(1 + 2\rho)^{2t}}$$

- **Lanczos algorithm:** convergence rate

$$\frac{1}{(1 + 2\rho + 2\sqrt{\rho^2 + \rho})^{2t}}$$

- if $\rho \gg 1$, then $1 + 2\rho + 2\sqrt{\rho^2 + \rho} \approx 1 + 4\rho \approx 2(1 + 2\rho)$
- if $\rho \ll 1$, then $1 + 2\rho + 2\sqrt{\rho^2 + \rho} \approx 1 + 2\sqrt{\rho} > 1 + 2\rho$
- outperforms the power method

Proof of Theorem 4.3

It suffices to prove the 2nd inequality. Recalling that $\mathbf{T}_t = \mathbf{Q}_t^\top \mathbf{A} \mathbf{Q}_t$, we have

$$\theta_1 = \max_{\mathbf{v}: \mathbf{v} \neq \mathbf{0}} \frac{\mathbf{v}^\top \mathbf{T}_t \mathbf{v}}{\mathbf{v}^\top \mathbf{v}} = \max_{\mathbf{v}: \mathbf{v} \neq \mathbf{0}} \frac{(\mathbf{Q}_t \mathbf{v})^\top \mathbf{A} (\mathbf{Q}_t \mathbf{v})}{(\mathbf{Q}_t \mathbf{v})^\top (\mathbf{Q}_t \mathbf{v})} = \max_{\mathbf{w} \in \mathcal{K}_t: \mathbf{w} \neq \mathbf{0}} \frac{\mathbf{w}^\top \mathbf{A} \mathbf{w}}{\mathbf{w}^\top \mathbf{w}}$$

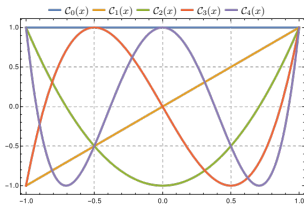
For any $\mathbf{w} \in \mathcal{K}_t := \{\mathbf{q}_1, \mathbf{A} \mathbf{q}_1, \dots, \mathbf{A}^{t-1} \mathbf{q}_1\}$, one can write it as $\mathcal{P}(\mathbf{A}) \mathbf{q}_1$ for some polynomial $\mathcal{P}(\cdot)$ of degree $t-1$. This means

$$\theta_1 = \max_{\mathcal{P}(\cdot) \in \mathcal{P}_{t-1}} \frac{(\mathcal{P}(\mathbf{A}) \mathbf{q}_1)^\top \mathbf{A} (\mathcal{P}(\mathbf{A}) \mathbf{q}_1)}{(\mathcal{P}(\mathbf{A}) \mathbf{q}_1)^\top (\mathcal{P}(\mathbf{A}) \mathbf{q}_1)}$$

where \mathcal{P}_{t-1} is set of polynomials of degree $t-1$. If $\mathbf{q}_1 = \sum_{i=1}^n \nu_i \mathbf{u}_i$, then

$$\begin{aligned} \frac{(\mathcal{P}(\mathbf{A}) \mathbf{q}_1)^\top \mathbf{A} (\mathcal{P}(\mathbf{A}) \mathbf{q}_1)}{(\mathcal{P}(\mathbf{A}) \mathbf{q}_1)^\top (\mathcal{P}(\mathbf{A}) \mathbf{q}_1)} &= \frac{\sum_{i=1}^n \nu_i^2 \mathcal{P}^2(\lambda_i) \lambda_i}{\sum_{i=1}^n \nu_i^2 \mathcal{P}^2(\lambda_i)} && \text{(check)} \\ &= \lambda_1 - \frac{\sum_{i=2}^n \nu_i^2 (\lambda_1 - \lambda_i) \mathcal{P}^2(\lambda_i)}{\nu_1^2 \mathcal{P}^2(\lambda_1) + \sum_{i=2}^n \nu_i^2 \mathcal{P}^2(\lambda_i)} \\ &\geq \lambda_1 - (\lambda_1 - \lambda_n) \frac{\sum_{i=2}^n \nu_i^2 \mathcal{P}^2(\lambda_i)}{\nu_1^2 \mathcal{P}^2(\lambda_1) + \sum_{i=2}^n \nu_i^2 \mathcal{P}^2(\lambda_i)} \end{aligned}$$

Proof of Theorem 4.3 (cont.)



Pick a polynomial $\mathcal{P}(x)$ that is large at $x = \lambda_1$. One choice is

$$\mathcal{P}(x) = C_{t-1} \left(\frac{2x - \lambda_2 - \lambda_n}{\lambda_2 - \lambda_n} \right)$$

where $C_{t-1}(\cdot)$ is the $(t-1)$ -th Chebyshev polynomial generated by

$$C_t(x) = 2xC_{t-1}(x) - C_{t-2}(x), \quad C_0(x) = 1, \quad C_1(x) = x$$

These polynomials are bounded by 1 on $[-1, 1]$, but grow rapidly outside

Proof of Theorem 4.3 (cont.)

Using boundedness of Chebyshev polynomial in $[-1, 1]$, we have

$$\begin{aligned}(\lambda_1 - \lambda_n) \frac{\sum_{i=2}^n \nu_i^2 \mathcal{P}^2(\lambda_i)}{\nu_1^2 \mathcal{P}^2(\lambda_1) + \sum_{i=2}^n \nu_i^2 \mathcal{P}^2(\lambda_i)} &\leq (\lambda_1 - \lambda_n) \frac{\sum_{i=2}^n \nu_i^2}{\nu_1^2 \mathcal{P}^2(\lambda_1)} \\ &= (\lambda_1 - \lambda_n) \frac{1 - \nu_1^2}{\nu_1^2 \mathcal{P}^2(\lambda_1)}\end{aligned}$$

where the last identity follows since $\sum_i \nu_i^2 = 1$ (given $\|\mathbf{q}_1\|_2 = 1$). This yields

$$\theta_1 \geq \lambda_1 - (\lambda_1 - \lambda_n) \frac{1 - \nu_1^2}{\nu_1^2} \frac{1}{\mathcal{C}_{t-1}^2(1 + 2\rho)}$$

as claimed

Warning: numerical instability

The vanilla Lanczos algorithm (which is efficient with exact arithmetic) is very sensitive to round-off issues

- orthogonality of $\{\mathbf{q}_1, \dots, \mathbf{q}_t\}$ might be lost quickly
- eigenvalues might be duplicated

Many variations have been proposed to prevent loss of orthogonality, and to remove spurious eigenvalues

Reference

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