Calculating numerically eigenvalues by cascading power method iterations

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(I reinvented a method that is called deflation. See Izaac, Joshua, et al. "The eigenvalue problem." Computational Quantum Mechanics (2018): 265-307.)

Let $M(d,\mathbb{F})$ be the space of $d\times d$ matrices with coefficients in number field $\mathbb{F}$. A pair (λ,v) of eigenvalue λ and eigenvector v satisfies

$$Mv=\lambda v$$

One can find the eigenvalues by solving the characteristic polynomial:

$$|M-\lambda I|=0.$$

The fundamental theorem of algebra yields the following polynomial factorization:

$$|M-\lambda I|=\prod_{i=1}^{d}(\lambda-\lambda_i).$$

Let $\lambda_1^{\downarrow},\ldots,\lambda_d^{\downarrow}$ denote the d eigenvalues sorted in decreasing order. The algebraic multiplicity of an eigenvalue $m_a(\lambda_i)$ is the multiplicity as a root of the characteristic polynomial:

$$|M-\lambda I|=\prod_{i=1}^{l}(\lambda-\lambda_i)^{m_a(\lambda_i)},$$

where $l\leq d$ is the number of distinct eigenvalues.

Eigenvalues of symmetric real matrices are always real, but some eigenvalues of real non-symmetric matrices may be complex.

A matrix $M\in M(d,\mathbb{C})$ is Hermitian iff $\bar{M}^\top=M$ where $\bar{z}$ is the complex conjugation and $M^\top$ the transpose matrix operation. Eigenvalues of positive definite Hermitian matrices are always real (includes the real symmetric positive definite matrices).

The spectral decomposition theorem of a symmetric positive definite matrix P states that

$$P=\sum_{i=1}^{d}\lambda_i e_i e_i^\top=E\mathrm{diag}(\lambda_1,\ldots,\lambda_d)E^\top,$$

where $E[=e_1,\ldots,e_d]$. Let λ_i denote the i-th dominant eigenvalue so that

$$|\lambda_1|\geq\ldots\geq|\lambda_d|.$$

1 Cascading power method iterations to numerically calculate the matrix spectrum

The power method [5] (1929) is a simple method to calculate the maximum absolute eigenvalue of a real symmetric invertible matrix: the spectral radius $\rho(M)=\max_i|\lambda_i(M)|$. Start with a random vector v_0 and iteratively repeat:

$$v_{t+1} = \frac{Mv_t}{\|Mv_t\|}$$

After T iterations, we have

$$\rho(M) \approx \frac{v_T^\top M v_T}{v_T^\top v_T}.$$

We normalize v_T such that $\|v_T\| = 1$ is an approximation of the eigenvector.

The convergence is geometric with ratio $\left|\frac{\lambda_2}{\lambda_1}\right|$, where λ_2 is the second dominant eigenvalue.

Eigenspace, rank and geometric multiplicity.

2 A simple algorithm for calculating numerically the matrix spectrum

Power method [4], p. 259-261.

Algorithm PowerSpectrum($M, n_1, \ldots, n_d$):

1. Initialization: Let $t \leftarrow 1$ and $M_t = M$.
2. Compute $\lambda_t = \mathrm{PowerMethod}(M_t, n_t)$ using the power method with n_t iterations
3. Let $M_{t+1} = M_t - \lambda_t e_t e_t^\top$. If $t \leq d$ goto Step 2.

The PM converges to the spectral radius of the matrix but the eigenvector may jump at iterations [4].

shifted inverse PM, deflation

When $E[= e_1, \ldots, e_d]$ is not an orthonormal basis (up to prescribed ϵ), we adjust n_t according to the current estimate $\left|\frac{\lambda_t}{\lambda_{t+1}}\right|$, and restart until we get an orthonormal basis.

If e_i is orthonormal to e_j for $j < i$, Then λ_i is, the ith dominant eigenvalue, is the dominant eigenvalue of M_i.

For example,

$$\lambda_2 = \lambda_1(M - \lambda_1 e_1 e_1^\top)$$

$$(M - \lambda_1 e_1 e_1^\top)e_2 = \lambda_2 e_2$$

yields

$$Me_2 = \lambda_2 e_2$$

since

$$-\lambda_1 e_1 e_1^\top e_2 = 0$$

because $e_1^\top e_2 = 0$ (orthonormal bases).

Thus at stage t, we can test that $|e_j^\top e_t| \leq \epsilon$ for all $j < t$ in order to determine n_t.

Books [6, 2]

References

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