The Min-Max Theorem

Ken Shiozaki

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Let H be an $n \times n$ Hermitian matrix. For simplicity, first assume that the eigenvalues are nondegenerate. Order the eigenvalues of H as

$$E_1 < \cdots < E_n. \tag{1}$$

Clearly,

$$E_1 = \min_{v, ||v||=1} \langle v|H|v \rangle, \tag{2}$$

$$E_n = \max_{v, ||v||=1} \langle v|H|v \rangle. \tag{3}$$

The min-max theorem gives a similar variational characterization of the other eigenvalues.

Let V_1 be the eigenspace with eigenvalue $E = E_1$ (the ground state), and write $V_1^\perp$ for its orthogonal complement (the space of excited states). Similarly, write V_k for the eigenspace with eigenvalue $E = E_k$. For the second eigenvalue (the first excited state), one has

$$E_2 = \min_{v \in V_1^\perp, ||v||=1} \langle v|H|v \rangle. \tag{4}$$

This can be rewritten as a variational problem over $(n-1)$-dimensional subspaces. Expanding an arbitrary state $v \in V, ||v|| = 1$ as

$$v = \alpha v_1 + \beta v_\perp, \quad v_1 \in V_1, \quad v_\perp \in V_\perp, \quad ||v_1|| = ||v_\perp|| = 1, \tag{5}$$

one obtains

$$\langle v|H|v \rangle = |\alpha|^2 E_1 + \sqrt{1 - |\alpha|^2} \langle v_\perp|H|v_\perp \rangle. \tag{6}$$

If this is minimized without restriction, $v = v_1$ is selected. If instead the minimization is carried out on $v \in V_1^\perp$, one obtains E_2. Depending on the choice of subspace $V' \in V$, we have

$$\min_{v \in V', ||v||=1} \langle v|H|v \rangle = \begin{cases} E_1 & (V' \cap V_1 \neq \{0\}) \\ E_2 & (V' \cap V_1 = \{0\} \&\& V' \cap V_2 \neq \{0\}) \\ > E_2 & (V' \subset (V_1 \oplus V_2)^\perp) \end{cases} \tag{7}$$

The third possibility, $V' \subset (V_1 \oplus V_2)^\perp$, can be excluded if $\dim V' > n - 2$. Hence

$$\dim V' \geq n - 1 \quad \Rightarrow \quad \min_{v \in V', ||v||=1} \langle v|H|v \rangle \leq E_2. \tag{8}$$

For $V' = V_1^\perp$ with $\dim V_1^\perp = n - 1$, the equality condition is satisfied, and therefore

$$\max_{V' \subset V, \dim V' \geq n-1} \min_{v \in V', ||v||=1} \langle v|H|v \rangle = E_2. \tag{9}$$

Since equality is achieved with $\dim V' = n - 1$, it is enough to restrict the search to $\dim V' = n - 1$, giving

$$\max_{V' \subset V, \dim V' = n-1} \min_{v \in V', ||v||=1} \langle v|H|v \rangle = E_2. \tag{10}$$

Similarly, for the k-th eigenvalue E_k,

$$\min_{v \in V', ||v||=1} \langle v|H|v\rangle = \begin{cases} \leq E_k & (V' \cap (V_1 \oplus \cdots \oplus V_k) \neq \{0\}), \\ > E_k & (V' \subset (V_1 \oplus \cdots \oplus V_k)^\perp), \end{cases} \tag{11}$$

Note that

$$V' \cap (V_1 \oplus \cdots \oplus V_k) = \{0\} \quad \Leftrightarrow \quad V' \in (V_1 \oplus \cdots \oplus V_k)^\perp. \tag{12}$$

If $\dim V' > n-k$, then $V' \in (V_1 \oplus \cdots \oplus V_k)^\perp$ cannot hold, and hence

$$\max_{V' \subset V, \dim V' \geq n-k+1} \min_{v \in V', ||v||=1} \langle v|H|v\rangle = E_k. \tag{13}$$

Here equality is achieved for $V' = (V_1 \oplus \cdots \oplus V_{k-1})^\perp$. Since $\dim V' = \dim(V_1 \oplus \cdots \oplus V_{k-1})^\perp = n-k+1$, we may restrict to that dimension and obtain

$$\max_{V' \subset V, \dim V' = n-k+1} \min_{v \in V', ||v||=1} \langle v|H|v\rangle = E_k. \tag{14}$$

If eigenvalue degeneracies are present, it suffices to take into account the dimensions of the eigenspaces. Let

$$d_k = \dim V_k. \tag{15}$$

Equation (11) still holds. The condition excluding $V' \subset (V_1 \oplus \cdots \oplus V_k)^\perp$ is

$$\dim V' > n - \sum_{i=1}^{k} d_i. \tag{16}$$

Moreover, if

$$\dim V' > n - \sum_{i=1}^{k-1} d_i = \dim(V_1 \oplus \cdots \oplus V_{k-1})^\perp, \tag{17}$$

then necessarily $V' \cap (V_1 \oplus \cdots \oplus V_{k-1}) \neq \{0\}$, and hence $\min_{v \in V', ||v||=1} \langle v|H|v\rangle = E_{k-1} < E_k$. Thus we may assume

$$\dim V' \leq n - \sum_{i=1}^{k-1} d_i. \tag{18}$$

Therefore

$$\max_{V' \subset V, n - \sum_{i=1}^{k-1} d_i \geq \dim V' > n - \sum_{i=1}^{k} d_k} \min_{v \in V', ||v||=1} \langle v|H|v\rangle = E_k. \tag{19}$$

For the range

$$n - \sum_{i=1}^{k-1} d_i \geq \dim V' > n - \sum_{i=1}^{k} d_k, \tag{20}$$

one can find a subspace V' satisfying the equality condition

$$V' \cap V_k \neq \{0\} \tag{21}$$

for any fixed dimension in this range. Thus

$$\max_{V' \subset V, \dim V' = d} \min_{v \in V', ||v||=1} \langle v|H|v\rangle = E_k, \quad d = n - \sum_{i=1}^{k} d_k + 1, \ldots, n - \sum_{i=1}^{k-1} d_i. \tag{22}$$

Consequently, if eigenvalues are listed with multiplicity as

$$E_1 \le E_2 \le \cdots \le E_n, \tag{23}$$

then

$$\max_{V' \subset V, \dim V' = n-k+1} \min_{v \in V', ||v||=1} \langle v|H|v\rangle = E_k. \tag{24}$$

Applying the same argument to $-H$, and writing $E'_k = -E_{n-k+1}$, one obtains

$$\max_{V' \subset V, \dim V' = n-k+1} \min_{v \in V', ||v||=1} \langle v|H|v\rangle = E'_k, \tag{25}$$

that is,

$$\max_{V' \subset V, \dim V' = n-k+1} \min_{v \in V', ||v||=1} \langle v|H|v\rangle = -E_{n-k+1}. \tag{26}$$

Replacing k by $n-k+1$, we get

$$\min_{V' \subset V, \dim V' = k} \max_{v \in V', ||v||=1} \langle v|H|v\rangle = E_k. \tag{27}$$

Min-max theorem. Let the eigenvalues of an $n \times n$ Hermitian matrix H be ordered as

$$E_1 \le \cdots \le E_n. \tag{28}$$

Then

$$E_k = \max_{\dim V = n-k+1} \min_{v \in V} \frac{\langle v|H|v\rangle}{\langle v|v\rangle} \tag{29}$$

$$= \min_{\dim V = k} \max_{v \in V} \frac{\langle v|H|v\rangle}{\langle v|v\rangle}. \tag{30}$$

We also record the formulation in which the eigenvalues are ordered in the opposite direction.

Min-max theorem. Let the eigenvalues of an $n \times n$ Hermitian matrix H be ordered as

$$\lambda_1 \ge \cdots \ge \lambda_n. \tag{31}$$

Then

$$\lambda_k = \max_{\dim V = k} \min_{v \in V} \frac{\langle v|H|v\rangle}{\langle v|v\rangle} \tag{32}$$

$$= \min_{\dim V = n-k+1} \max_{v \in V} \frac{\langle v|H|v\rangle}{\langle v|v\rangle}. \tag{33}$$

An analogous variational formula can also be derived for singular values. Let the singular values of $A \in \mathrm{Mat}_{n,m}(\mathbb{C})$ be ordered decreasingly as

$$\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_{\min(m,n)}. \tag{34}$$

The squares of the singular values of A are precisely the eigenvalues of the Hermitian matrix $A^\dagger A$. Using the elementary equivalence

$$\sqrt{\langle v|A^\dagger A|v\rangle} \ge \sqrt{\langle v'|A^\dagger A|v'\rangle} \Leftrightarrow \langle v|A^\dagger A|v\rangle \ge \langle v'|A^\dagger A|v'\rangle\,, \tag{35}$$

we have

$$\sigma_k = \max_{\dim V = k} \min_{v \in V, ||v||=1} \sqrt{\langle v|A^\dagger A|v\rangle} = \max_{\dim V = k} \min_{v \in V, ||v||=1} ||Av||. \tag{36}$$

Min-max theorem for singular values. Let the singular values of an $n \times m$ matrix A be ordered as

$$\sigma_1 \geq \cdots \geq \sigma_{\min(m,n)}. \tag{37}$$

Then

$$\sigma_k = \max_{\dim V = k} \min_{v \in V, ||v||=1} ||Av|| \tag{38}$$

$$= \min_{\dim V = n-k+1} \max_{v \in V, ||v||=1} ||Av||. \tag{39}$$