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A Theorem on Maximum Variance

Wolfgang Textor

Institut für Theoretische Physik,
Johann Wolfgang Goethe-Universität, Frankfurt/Main, Germany

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The square variance function of a finite-dimensional Hamiltonian H obeys a maximum principle that leads to the determination of its maximum and minimum eigenvalues. A systematic algorithm is presented that generates a sequence of monotonically increasing values for the square variance. It is shown that the method converges to the exact two-dimensional eigenvalue problem determined by the lowest and highest eigenvalues. Preliminary numerical results are briefly outlined.

INTRODUCTION

A familiar result of elementary quantum mechanics states that the square variance of a finite-dimensional Hamiltonian attains its zeros for the eigenvectors of the problem. However, the usefulness of investigating the maximum of the square variance has not yet been recognized. The consideration of this question turns out to be a matter of interest in its own right; moreover it proves to be a practical tool for the numerical solution of eigenvalue problems.

With the aid of the maximum principle investigated in Section 1 of this paper, we can construct an iterative algorithm. As is demonstrated in Section 2, this algorithm yields the maximum (minimum) eigenvalue of the Hamiltonian. One need assume only that the trial vector contains nonvanishing components of the corresponding eigenvectors.

This paper is concerned mainly with the presentation of the basic theorems and their proofs. Detailed numerical results will be presented in a sequel, but a short review of preliminary computational data is included in this paper.

1. THE MAXIMUM PRINCIPLE

In what follows we will be concerned with the expectation value and square variance functions of a Hermitian operator $\mathbf{H}: \mathbb{R}^n \to \mathbb{R}^n$.

Introduce $V_n \subseteq \mathbb{R}^n$, the set of vectors whose norm is unity. Then we define the functions

$$\varphi_H: V_n \to \mathbb{R}$$

$$\psi_H: V_n \to \mathbb{R}$$

$$|x\rangle \mapsto \varphi_H(|x\rangle) := \langle x|\mathbf{H}x\rangle \equiv \langle \mathbf{H}\rangle_x$$

$$|x\rangle \mapsto \psi_H(|x\rangle) := \langle \mathbf{H}^2\rangle_x - \langle \mathbf{H}\rangle_x^{\,2}$$

As is well known from quantum mechanics, ψ_H is a nonnegative function, the zeros of ψ_H occurring for the eigenvectors of $\mathbf{H}$.

V_n is a compact set. Since ψ_H is continuous it must assume its maximum (minimum) on V_n. Our aim is to derive a theorem on the precise location of these points.

To simplify the demonstrations let us define the probability plane W_m as the set of points with cartesian coordinates $(w_1, \ldots, w_m)$ that satisfy

$$\sum_{\nu=1}^{m} w_\nu = 1, \qquad 0 \leqslant w_\nu \leqslant 1 \quad \forall \nu \tag{1.1}$$

The eigenvalues of $\mathbf{H}$ constitute a finite ordered set

$$E_1 < \cdots < E_m, \qquad m \leqslant n$$

$$E_1 = E_{\min}, \qquad E_m = E_{\max}$$

The respective eigenvectors are denoted as

$$|E_{1,1}\rangle, \ldots, |E_{1,k_1}\rangle, \ldots, |E_{m,k_m}\rangle$$

Here k_ν stands for the degeneracy of E_ν. Identifying w_ν with the quantum mechanical probability of finding E_ν in a measurement

$$w_\nu(|x\rangle) := \sum_{\lambda=1}^{k_\nu} |\langle E_{\nu,\lambda}|x\rangle|^2$$

φ_H and ψ_H can be defined as functions on W_m in a natural way.

$$\begin{aligned} \varphi_H(|x\rangle) &= \sum_{\lambda=1}^{m} w_\lambda(|x\rangle)\cdot E_\lambda \\ \psi_H(|x\rangle) &= \sum_{\lambda=1}^{m} w_\lambda(|x\rangle)\cdot E_\lambda^{\,2} - \left(\sum_{\lambda=1}^{m} w_\lambda(|x\rangle)\cdot E_\lambda\right)^2 \end{aligned} \tag{1.2}$$

To state the maximum principle for ψ_H, we must specify the notion of maximum. $\bar{w} \in W_m$ is called a maximum of ψ_H if it is a maximum with respect to a sufficiently small W_m-neighborhood of $\bar{w}$. An absolute maximum w_{abs}, however, fulfills the condition

$$\psi_H(w) \leqslant \psi_H(w_{\text{abs}}) \qquad \forall w \in W_m$$

Analogous definitions can be introduced for a minimum.

Theorem 1 (*Maximum Principle*).

(1.1) If $m > 1$, no inner point of W_m can be a minimum of ψ_H. The absolute minima are the zeros of ψ_H.

(1.2) If $m = 2$ there exists a unique maximum of ψ_H at $w_1 = w_2 = \frac{1}{2}$.

(1.3) If $m > 2$, no inner point of W_m can be a maximum of ψ_H. The absolute maximum is located on the boundary at $w_1 = w_m = \frac{1}{2}$.

(1.4) If $m > 2$, the only maximum of ψ_H on the boundary of W_m is the absolute maximum.

(1.5) The only minima of ψ_H on W_m ($m \geqslant 2$) are the zeros of ψ_H.

The maximum principle describes two fundamental properties of ψ_H. First, it can be applied as an error measure for determining eigenvectors of **H**. On the other hand, the problem of finding both the maximum and minimum eigenvalue is solved by determining the unique maximum of ψ_H.

Proof of Theorem 1. In the case $m = 2$ we have

$$\psi_H(w) = w_1 \cdot E_1^2 + w_2 \cdot E_2^2 - (w_1 \cdot E_1 + w_2 \cdot E_2)^2 \tag{1.3}$$

subject to the subsidiary condition

$$w_1 + w_2 = 1 \tag{1.4}$$

One then finds a maximum at $w_1 = w_2 = \frac{1}{2}$. The boundary points of W_2, namely $w_1 = 1$ and $w_2 = 1$, are the zeros of ψ_H. This proves statement (1.2) and statement (1.1) in case $m = 2$.

Let us now deduce item (1.3). We have to solve the problem

$$\sum w_\lambda \cdot E_\lambda^2 - \left(\sum w_\lambda \cdot E_\lambda\right)^2 = \text{extr} \tag{1.5}$$

$$\sum w_\lambda = 1 \tag{1.6}$$

This corresponds to the set of equations

$$\frac{\partial}{\partial w_\alpha}\left(\sum w_\lambda E_\lambda^2 - \left(\sum w_\lambda E_\lambda\right)^2 + k \cdot \sum w_\lambda\right) = 0; \qquad \alpha = 1, \ldots, m \tag{1.7}$$

$$E_\alpha^2 - 2 \cdot DE_\alpha + k = 0 \tag{1.8}$$

Here k denotes the Lagrange parameter, and the abbreviation $D = \sum w_\lambda E_\lambda$ was used. However, the system of m equations (1.8) leads to the apparent contradiction

$$D = \tfrac{1}{2}\cdot(E_\mu + E_\nu), \qquad \forall_{\mu,\nu;\mu\neq\nu}$$

So evidently no extrema can occur for the inner points of W_m. Since W_m is compact, ψ_H attains its absolute maximum, which from the preceding reasoning must be a boundary point. Recalling the definition of W_m, one sees that $w = (w_1, \ldots, w_m)$ is a boundary point if and only if $w_\lambda = 0$ for at least one λ. This means that $w_{\text{abs}} \in W_m$, the absolute maximum of ψ_H on W_m, can be regarded as an element of some properly chosen $(m - 1)$-dimensional probability plane.

If $m - 1 > 2$ the same argument again applies. Proceeding this way by induction, we arrive at a problem reduced to dimensionality two. From proposition (1.2) we can then deduce that w_{abs} must have two coordinates equal to $\frac{1}{2}$ and all others zero. If we call the two occurring eigenvalues E_+ and E_- ($E_+ > E_-$) and their respective probabilities w_+ and w_-, then straightforward computation yields

$$\psi_H(w_{\text{abs}}) = \tfrac{1}{4}\cdot(E_+ - E_-)^2$$

To achieve the absolute maximum we have to select $E_- = E_1$, $E_+ = E_m$. This proves our assertion. As inner points cannot be extrema on W_m, $m > 2$, statement (1.1) is trivially true.

The next point to be discussed is (1.4). Let us call the maximum in question $w_{\max}$. Repeating the induction procedure applied before, we find that $w_{\max}$ must have coordinates $w_+(w_{\max}) = w_-(w_{\max}) = \frac{1}{2}$.

Solving equation (1.6) for w_μ and inserting into equation (1.2) yields for $w \in W_m$:

$$\begin{aligned}\psi_H(w) = {}& \sum_{\lambda\neq\mu} w_\lambda\cdot E_\lambda^2 + \Big(1 - \sum_{\lambda\neq\mu} w_\lambda\Big)\cdot E_\mu^2 \\ & - \Big(\sum_{\lambda\neq\mu} w_\lambda E_\lambda + \Big(1 - \sum_{\lambda\neq\mu} w_\lambda\Big)\cdot E_\mu\Big)^2\end{aligned} \tag{1.9}$$

Identity (1.9) expresses ψ_H by a system of independent variables. The proof will now be given by contradiction.

Let $E_\mu = E_-$ and suppose $E_+ \neq E_m$, the maximal eigenvalue of **H**. Then

$$\left.\frac{\partial\psi_H}{\partial w_m}\right|_{w_{\max}} = (E_m - E_+)(E_m - E_-) > 0 \tag{1.10}$$

So in the direction of positive w_m the function increases locally on a W_m-neighbourhood of w_{max}. This contradiction leads to $E_+ = E_m$. By differentiating with respect to w_1, we can use similar reasoning to arrive at $E_- = E_1$.

The proof of proposition (1.5) is straightforward, since minima are not allowed in the interior of W_m.

Figure 1 illustrates the situation for W_3. One further remark on an orthogonality theorem is in order. Let $|\max\rangle \in V_n$ be a maximum vector of ψ_H. Then from the maximum principle we may write

$$\begin{aligned} |\max\rangle &= |E_1\rangle + |E_m\rangle \\ \mathbf{H}|\max\rangle &= E_1 \cdot |E_1\rangle + E_m \cdot |E_m\rangle \end{aligned} \tag{1.11}$$

A label of degeneracy has been suppressed for simplicity.

E_1 and E_m are functions of $\varphi_H(|\max\rangle)$ and $\psi_H(|\max\rangle)$:

$$\begin{aligned} E_m &= \varphi_H(|\max\rangle) + [\psi_H(|\max\rangle)]^{1/2} \\ E_1 &= \varphi_H(|\max\rangle) - [\psi_H(|\max\rangle)]^{1/2} \end{aligned} \tag{1.12}$$

of course

$$\langle E_1 | E_m \rangle = 0 \tag{1.13}$$

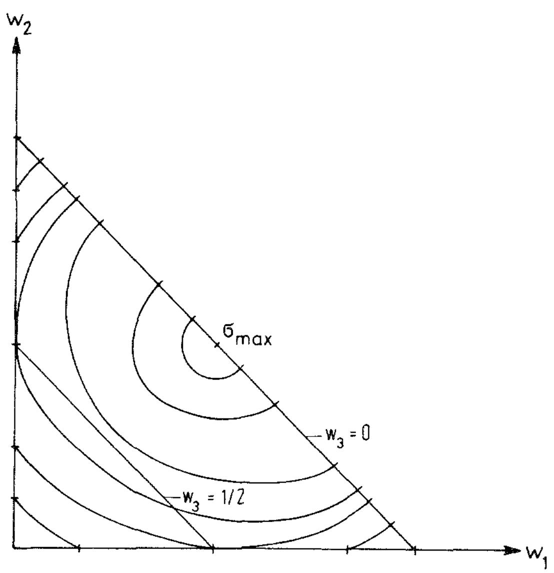

Fig. 1. The plane W_3. The lines of constant ψ_H are represented qualitatively. They visualize the assertions of the maximum principle.

Now replace $|\max\rangle$ by an arbitrary $|x\rangle \in V_n$ and define $|E_1\rangle$, E_1, $|E_m\rangle$, E_m by the expressions (1.11), (1.12). Then the orthogonality relation (1.13) still holds, as can be seen by direct calculation. (We have to convince ourselves that $|x\rangle$ is not an eigenvector of $\mathbf{H}$ so that system (1.11) can be uniquely solvable.)

2. A SYSTEMATIC ALGORITHM

The maximum principle leads us to the question of how to determine the maximum of ψ_H. A systematic algorithm is presented that provides a sequence of monotonically ascending ψ_H and, moreover, leads to the determination of the eigenvalues E_1 and E_m.

Consider an arbitrary $|x_0\rangle \in V_n$, which, however, must not be an eigenvector of $\mathbf{H}$. Given $|x_k\rangle \in V_n$ define

$$|x_{k+1}\rangle := (\psi_H(|x_k\rangle))^{-1/2} \cdot (\mathbf{H}|x_k\rangle - \varphi_H(|x_k\rangle) \cdot |x_k\rangle) \tag{2.1}$$

The two-dimensional subspace generated by $|x_k\rangle$ and $|x_{k+1}\rangle$ is denoted by Γ_k, and we introduce the orthogonal projection operator

$$\mathbf{P}_k := |x_k\rangle\langle x_k| + |x_{k+1}\rangle\langle x_{k+1}| \tag{2.2}$$

Next denote

$$\mathbf{h}_k := \Gamma_k \to \Gamma_k$$

$$\mathbf{h}_k := \mathbf{P}_k \mathbf{H} \mathbf{P}_k$$

with eigenvalues e_k^+ and e_k^- ($e_k^+ > e_k^-$), and the corresponding eigenvectors $|e_k^+\rangle$ and $|e_k^-\rangle$ respectively. Furthermore we write

$$\mathbf{H}|x_{k+1}\rangle = \mathbf{h}_k|x_{k+1}\rangle + |R_k\rangle \tag{2.3}$$

which defines the vector $|R_k\rangle$. Then the following theorem holds.

Theorem 2.

(2.1) $\psi_H(|x_0\rangle) \leqslant \psi_H(|x_1\rangle) \leqslant \cdots \leqslant \psi_H(|x_k\rangle) \leqslant \cdots \leqslant \lim_{k\to\infty} \psi_H(|x_k\rangle)$

(2.2) $\psi_H(|x_k\rangle) = \psi_H(|x_{k+1}\rangle)$ if and only if Γ_k is an invariant subspace under $\mathbf{H}$.

(2.3) Assume

$$w_1(|x_0\rangle) \neq 0, \qquad w_m(|x_0\rangle) \neq 0 \tag{2.4}$$

Then the following identities hold.

$$\lim_{k\to\infty} e_k^- = E_1, \qquad \lim_{k\to\infty} e_k^+ = E_m \tag{2.5}$$

Proof of Theorem 2. (2.1) On account of equation (2.3), we find

$$\psi_H(|x_{k+1}\rangle) = \psi_H(|x_k\rangle) + \langle R_k|R_k\rangle \tag{2.6}$$

which proves the inequality in question. So $(\psi_H(|x_k\rangle))$ is a monotonically ascending sequence, which converges since it is bounded. Its limit can be represented by the series

$$\psi := \lim_{k\to\infty} \psi_H(|x_k\rangle) = \psi_H(|x_0\rangle) + \sum_{k=0}^{\infty} \langle R_k|R_k\rangle \tag{2.7}$$

Item (2.2) is an obvious consequence of equation (2.6).
The proof of part (2.3) will be decomposed into several lemmas.

Lemma 1. The following sequences converge.

$$(\varphi_H(|x_k\rangle)), \qquad k \text{ even}$$

$$(\varphi_H(|x_k\rangle)), \qquad k \text{ odd}$$

We define the limits as

$$\varphi_e := \lim_{k\to\infty} \varphi_H(|x_k\rangle), \qquad k \text{ even}$$

$$\varphi_o := \lim_{k\to\infty} \varphi_H(|x_k\rangle), \qquad k \text{ odd}$$

Lemma 2. The following limits are eigenvalues of $\mathbf{H}$.

$$\begin{aligned} e^+ &:= \lim_{k\to\infty} e_k^+ = \tfrac{1}{2}\cdot(\varphi_e + \varphi_o) + [\psi + \tfrac{1}{4}(\varphi_e - \varphi_o)^2]^{1/2} \\ e^- &:= \lim_{k\to\infty} e_k^- = \tfrac{1}{2}\cdot(\varphi_e + \varphi_o) - [\psi + \tfrac{1}{4}(\varphi_e - \varphi_o)^2]^{1/2} \end{aligned} \tag{2.8}$$

Lemma 3. Unless $E_\lambda = e^+$ or $E_\lambda = e^-$, the following limit condition is satisfied.

$$\lim_{k\to\infty} w_\lambda(|x_k\rangle) = 0 \tag{2.9}$$

Lemma 4. The following limits of the sequences exist and are all different from zero.

$$(w_+(|x_k\rangle)), \qquad k \text{ even, odd}$$

$$(w_-(|x_k\rangle)) \qquad k \text{ even, odd}$$

Lemma 5. The following recursion formula holds.

$$w_\lambda(|x_{k+1}\rangle) = (\psi_H(|x_k\rangle))^{-1}\cdot w_\lambda(|x_k\rangle)\cdot(E_\lambda - \varphi_H(|x_k\rangle))^2 \tag{2.10}$$

The proof of Theorem 2, part (2.3), now proceeds as follows. An easy consequence of statements (2.4) and (2.10) is

$$\begin{aligned} w_m(|x_k\rangle) &\neq 0 \qquad \forall k \\ w_1(|x_k\rangle) &\neq 0 \qquad \forall k \end{aligned} \tag{2.11}$$

On account of Lemma 2, e^+ is an eigenvalue of $\mathbf{H}$. By contradiction let us assume $e^+ \neq E_m$. Then applying Lemmas 3 and 4, we arrive at

$$\lim_{k\to\infty} \frac{w_m(|x_k\rangle)}{w_+(|x_k\rangle)} = 0 \tag{2.12}$$

Select k_0 sufficiently large so that for all $k > k_0$

$$e^- < \varphi_H(|x_k\rangle) < e^+ \tag{2.13}$$

(see Lemma 3). Then (2.10), (2.11), and (2.13) yield

$$\frac{w_m(|x_{k+1}\rangle)}{w_+(|x_{k+1}\rangle)} = \frac{w_m(|x_k\rangle)}{w_+(|x_k\rangle)} \cdot \frac{(E_m - \varphi_H(|x_k\rangle))^2}{(e^+ - \varphi_H(|x_k\rangle))^2} > \frac{w_m(|x_k\rangle)}{w_+(|x_k\rangle)} \tag{2.14}$$

The sequence

$$\left(\frac{w_m(|x_k\rangle)}{w_+(|x_k\rangle)}\right)$$

is hence strictly positive and monotonically increasing a contradiction with respect to equation (2.12). Thus the assertion $e^+ = E_m$ has been proved. The proposition $e^- = E_1$ follows analogously.

3. PROOFS OF THE LEMMAS

Proof of Lemma 1. We prove that $(\varphi_H(|x_k\rangle))$, k even, is a Cauchy sequence. Going back to equations (2.1) and (2.3), we derive the relation

$$|x_{k+2}\rangle = \lambda \cdot |x_k\rangle + (\psi_H(|x_{k+1}\rangle))^{-1/2} \cdot |R_k\rangle \tag{3.1}$$

with the abbreviation

$$\lambda^2 = 1 - (\psi_H(|x_{k+1}\rangle))^{-1} \cdot \langle R_k | R_k \rangle$$

Consequently

$$\begin{aligned} |\varphi_H(|x_{k+2}\rangle) - \varphi_H(|x_k\rangle)| &= (\psi_H(|x_{k+1}\rangle))^{-1} \cdot |\langle R_k | \mathbf{H} R_k \rangle - \langle R_k | R_k \rangle \cdot \varphi_H(|x_k\rangle)| \\ &\leqslant (\psi_H(|x_0\rangle))^{-1} \cdot \langle R_k | R_k \rangle \cdot (E_m - E_1) \end{aligned}$$

For arbitrary even numbers k, k', we obtain

$$|\varphi_H(|x_{k'}\rangle) - \varphi_H(|x_k\rangle)| \leqslant (\psi_H(|x_0\rangle))^{-1}\cdot(E_m - E_1)\cdot \sum_{\lambda=k}^{k'} \langle R_\lambda|R_\lambda\rangle \quad (3.2)$$

The Cauchy property of $(\varphi_H(|x_k\rangle))$, k even, now readily follows from the convergence of series (2.7). A similar argument applies for the odd sequence.

Proof of Lemma 2. Remember the coordinate representation

$$w(|e_k{}^+\rangle) = (w_1(|e_k{}^+\rangle), \ldots, w_m(|e_k{}^+\rangle)) \in W_m$$

Since W_m is compact, the sequence $(w(|e_k{}^+\rangle))$ possesses a convergent subsequence $(w(|e^+_{\nu(k)}\rangle))$, say, whose limit point is denoted by $\bar{w}$. From continuity of φ_H it follows that

$$\varphi_H(\bar{w}) = e^+$$

On account of the inequality $\psi_H(|e_k{}^+\rangle) \leqslant \langle R_k|R_k\rangle$, which is evident from direct calculation, we deduce

$$\psi_H(\bar{w}) = 0,$$

which implies that e^+ is an eigenvalue of **H**. The same reasoning applies for e^-.

Proof of Lemma 3. It is evident that the sequence $(w(|e_k{}^+\rangle))$ converges to $\bar{w}$. For suppose it does not; then we can find a subsequence $(w(|e^+_{\mu(k)}\rangle)$ which remains outside an ϵ-neighbourhood of $\bar{w}$ which itself contains a convergent subsequence $(w(|e^+_{\lambda(k)}\rangle))$. According to the proof of Lemma 2, its limit would also be $\bar{w}$, an apparent contradiction. So the sequence $(w(|e_k{}^+\rangle))$ converges to $\bar{w}$. This means

$$\lim_{k\to\infty} w_\lambda(|e_k{}^+\rangle) = 0, \quad \text{for } E_\lambda \neq e^+$$

and correspondingly

$$\lim_{k\to\infty} w_\lambda(|e_k{}^-\rangle) = 0, \quad \text{for } E_\lambda \neq e^-$$

Let us write

$$|x_k\rangle = a_k\cdot|e_k{}^+\rangle + b_k\cdot|e_k{}^-\rangle$$

So, up to a phase convention

$$w_\lambda(|x_k\rangle) = (a_k\cdot[w_\lambda(|e_k{}^+\rangle)]^{1/2} + b_k\cdot[w_\lambda(|e_k{}^-\rangle)]^{1/2})^2 \quad (3.3)$$

Equation (3.3) leads in a straightforward manner to the desired result.

Proof of Lemma 4. The sequence $(w(|x_k\rangle))$, k even, contains a convergent subsequence $(w(|x_{\nu(k)}\rangle))$, k even, with the limit point $\hat{w}$, which, according to Lemmas 1 and 3, has coordinates that obey the set of linear equations

$$w_+(\hat{w})e^+ + w_-(\hat{w})e^- = \varphi_e$$
$$w_+(\hat{w}) + w_-(\hat{w}) = 1$$

Its solution is, of course, unique, and by an argument similar to the one applied in the last lemma it can be deduced that the sequence $(w(|x_k\rangle))$, k even, itself converges to $\hat{w}$. Since $\psi_H(\hat{w}) > 0$, obviously both coordinates $w_+(\hat{w})$ and $w_-(\hat{w})$ must be different from zero. This proves Lemma 4.

The proof of Lemma 5 is a matter of elementary calculus and is omitted for brevity.

4. NUMERICAL ASPECTS

The iteration scheme (2.1) can be exploited numerically. A preliminary calculation was performed with a 100 × 100 random matrix. On account of equation (2.7), one expects ψ_H to increase rapidly, especially during the initial iterations. The increment of ψ_H can be regarded as a measure of noninvariance of the subspace Γ_k under **H**. Figure 2 shows the plot of the number of iterations k versus $\psi_H(|x_k\rangle)$, $e_k{}^+$, and $e_k{}^-$.

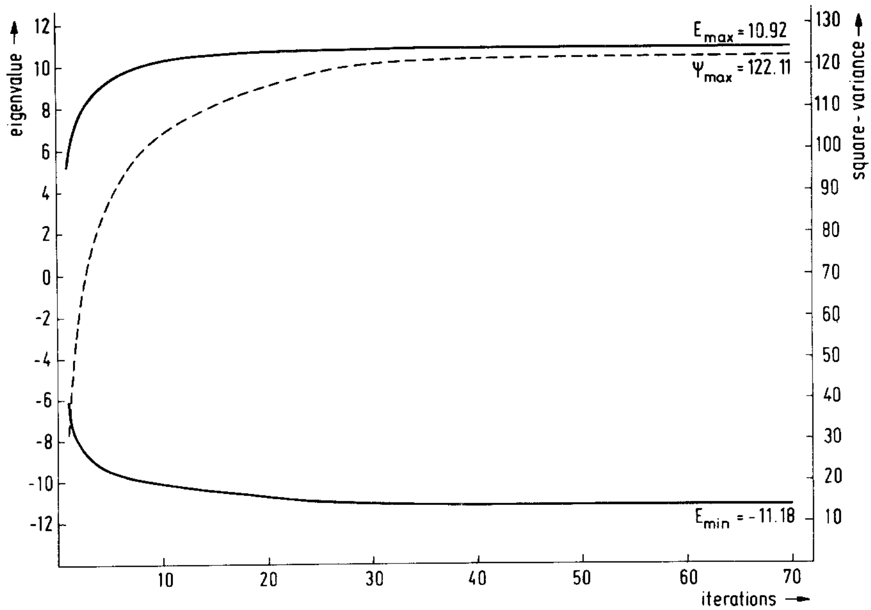

Fig. 2. Plot of the numerical example mentioned in the text.

The diagonalization of $\mathbf{h}_k$ after each iteration, however, is not necessary in applying the method. This is a major advantage as linear programming is applicable.

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