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AN ITERATIVE METHOD FOR COMPUTING THE EIGENVALUES OF SECOND KIND FREDHOLM OPERATORS AND APPLICATIONS*

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Abstract. An inverse iteration method is used to approximate the eigenvalues of second kind Fredholm operators. Numerical examples are given.

Key words. Fredholm Integral equation, eigenvalues, inverse iteration method, Rayleigh-Ritz method.

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1. Introduction. Let $K(x,y) \in L^2(Q)$, $Q := I \times I$ ($I = [a,b]$), and consider the second kind homogeneous Fredholm integral equation

$$\phi(x) - \lambda \int_I K(x,y)\phi(y)dy = 0, \tag{1.1}$$

where $\lambda \in \mathbf{C}$ is a complex parameter.

By introducing the operator $\mathcal{K} : L^2(I) \to L^2(I)$, defined by

$$\mathcal{K}\phi = \int_I K(x,y)\phi(y)dy, \tag{1.2}$$

and the identity operator $\mathcal{I}$, (1.1) becomes

$$(\mathcal{I} - \lambda\mathcal{K})\phi = 0. \tag{1.3}$$

It is well known that (1.1) admits at most a denumerable set of nonvanishing characteristic values which do not accumulate to finite points. Writing (1.1)

$$(\mathcal{K} - \mu\mathcal{I})\phi = 0, \qquad (\mu = \lambda^{-1}), \tag{1.4}$$

or equivalently as

$$\mathcal{K}\phi = \mu\phi, \tag{1.5}$$

one can, therefore, order the eigenvalues of the operator $\mathcal{K}$ with respect to their modulus in a decreasing sequence:

$$0 \le \ldots \le |\mu_3| \le |\mu_2| \le |\mu_1|.$$

In the particular case of symmetric or Hermitian positive operators ($K(x,y) = K(y,x)$ or $K(x,y) = \overline{K(y,x)}$, $(\mathcal{K}\phi,\phi) > 0$ if $\phi \ne 0$ and $\phi \in L^2(0,1)$), the eigenvalues always

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exist, and in the last formula the modulus symbols can be avoided, since the eigenvalues are real and positive:

$$0 < \ldots \leq \mu_3 \leq \mu_2 \leq \mu_1. \tag{1.6}$$

We will limit ourselves to this last case, since this is the most important case in physical applications.

In this case it is well known that by using the Rayleigh-Ritz method (see, for example, [5]), for every $n \in \mathbf{N}$, we can find lower bound approximations for the eigenvalues (1.6). By using the *orthogonal invariants method*, due to G. Fichera, corresponding upper bounds for the same eigenvalues can always be computed. These two methods can be used in a general abstract framework, namely, they can be applied to any positive definite compact operator.

The orthogonal invariants method is sometimes computationally very expensive, so we developed simpler iterative method to approximate the eigenvalues when the Rayleigh-Ritz approximations have been computed.

This can be done by using the *inverse iteration method*, described in [1], which will be summarized in section 3. We note, however, that this method does not ensure monotone convergence of the iterations, while the method of Fichera produces monotone convergence, it is sometimes a cumbersome approach the eigenvalues approximation problem. In our opinion the inverse iteration method could be applied to more general situations, but for the sake of simplicity, we will limit ourselves to the above mentioned case of a second kind Fredholm operator.

In section 2 we will give, for completeness, a simple sketch of results of the Rayeigh-Ritz and Fichera theories.

In section 3 we will present the above-mentioned inverse iteration method. This method has been tested in different cases, and in particular in a very difficult one, connected with the computation of the eigenvalues of a kernel considered by A.M. Ostrowski (see [10], [6], [7], [9]).

A priori bounds for the absolute error are given using the Aronszajn Theorem.

2. The Rayleigh-Ritz and orthogonal invariants methods.

Let $\{v_k\}_{k\in\mathbf{N}}$ be a complete system of linearly independent vectors in a Hilbert space $\mathcal{H}$, put $\mathcal{V}_\nu := span\{v_1, v_2, \ldots, v_\nu\}$, denote by P_ν the orthogonal projector, $P_\nu : \mathcal{H} \to \mathcal{V}_\nu$, and consider a positive definite Hermitian operator $T : \mathcal{H} \to \mathcal{H}$ and the corresponding eigenvalue problem

$$T\phi = \mu\phi. \tag{2.1}$$

PROPOSITION 1. (Rayleigh-Ritz). *Consider the positive eigenvalues*

$$\mu_1^{(\nu)} \geq \mu_2^{(\nu)} \geq \ldots \geq \mu_\nu^{(\nu)} \tag{2.2}$$

of the operator $P_\nu T P_\nu$. Then the following hold:

1. *The positive eigenvalues (2.2) of $P_\nu T P_\nu$ are obtained by solving the equation:*

$$det\{(Tv_j, v_h) - \mu(v_j, v_h)\} = 0, \ j, h = 1, \ldots, \nu,$$

($\mu = 0$ is always an eigenvalue of $P_\nu T P_\nu$).

2. *For any fixed k and for any $\nu \geq k$ the following inequalities hold true*

$$\mu_k^{(\nu)} \leq \mu_k^{(\nu+1)} \leq \mu_k.$$

3. The limit condition is valid

$$\lim_{\nu\to\infty} \mu_k^{(\nu)} = \mu_k.$$

That is, the Rayleigh-Ritz method always gives lower bounds for the first ν eigenvalues of the operator T, and furthermore these lower bounds become closer and closer to the exact eigenvalues, when ν increases.

The method of the orthogonal invariants was introduced by G. Fichera [4] and [5], and provides upper bounds for these eigenvalues. In these papers G. Fichera defines a complete system of orthogonal invariants for a given operator T as a complete sequence of numbers which is invariant under the equivalence of operators and by means of which *all* the eigenvalues of T can be recovered (completeness).

Such a system must depend only on the eigenvalues of T which remain unchanged under unitary equivalence. Theoretically we could consider the system of numbers defined by

$$\mathcal{I}_s^n(T) := \sum_{k_1<k_2<\ldots<k_s} [\mu_{k_1}\mu_{k_2}\cdots\mu_{k_s}]^n,$$

for any fixed s (order of the invariant) and $n = 1, 2, 3, \ldots$ (degree of the invariant), *provided that all these numbers can be computed independently by the knowledge of the eigenvalues of* T. As a matter of fact G. Fichera proved (see the following Proposition 2) that the knowledge of the system $\mathcal{I}_s^n(T)$ (s fixed, $n = 1, 2, 3, \ldots$) permits to recover all the eigenvalues of T.

Let

$$v_1{}^{(\nu)}, v_2{}^{(\nu)}, \ldots, v_\nu{}^{(\nu)},$$

be normalized eigenvectors of $P_\nu T P_\nu$ corresponding to the eigenvalues (2.2) and set

$$\mathcal{V}_\nu^{(k)} := span\{v_1^{(\nu)}, \ldots, v_{k-1}^{(\nu)}, v_{k+1}^{(\nu)}, \ldots, v_\nu^{(\nu)}\}$$

and let $P_\nu^{(k)}$ be the orthogonal projector $P_\nu^{(k)} : \mathcal{H} \to \mathcal{V}_\nu^{(k)}$.

PROPOSITION 2. (Fichera) *If* $\mathcal{I}_s^n(T) < \infty$, *for any fixed* $n, s \in \mathbf{N}$ *and* $\forall k, k \le n$, *put*

$$\sigma_k^{(\nu)} := \left[\frac{\mathcal{I}_s^n(T) - \mathcal{I}_s^n(P_\nu T P_\nu)}{\mathcal{I}_{s-1}^n(P_\nu^{(k)} T P_\nu^{(k)})} + [\mu_k^{(\nu)}]^n\right]^{\frac{1}{n}}$$

Then

$$\sigma_k^{(\nu)} \ge \sigma_k^{(\nu+1)} \ge \mu_k,$$

and the limit condition

$$\lim_{\nu\to\infty} \sigma_k^{(\nu)} = \mu_k$$

holds.

In the particular case we considered in section 1, namely, the case of a Hilbert space $\mathcal{H} = L^2(I)$, it follows that

$$\begin{aligned} &\forall n, s \in \mathbf{N},\ \ \mathcal{I}_s^n(T) < \infty \ \text{ iff } \ T^n\varphi = \textstyle\int_I K(x,y)\varphi(y)dy, \\ &\text{where } \ K(x,y) = \textstyle\int_I H(x,z)H(z,y)dz, \ \ H(x,y) = \overline{H(y,x)} \in L^2[Q]. \end{aligned}$$

Then the orthogonal invariants can be expressed (see [4]) by the multiple integral

$$\mathcal{I}_s^n(T) = \frac{1}{s!}\int_I \cdots \int_I f(x_1, \ldots, x_s)dx_1 \cdots dx_s,$$

where $f(x_1, \cdots, x_s)$ denotes the Fredholm determinant

$$f(x_1, x_2, \cdots, x_s) := \begin{vmatrix} K(x_1,x_1) & K(x_1,x_2) & \ldots & K(x_1,x_s) \\ K(x_2,x_1) & K(x_2,x_2) & \ldots & K(x_2,x_s) \\ \ldots\ldots & \ldots\ldots & \ldots & \ldots\ldots \\ K(x_s,x_1) & K(x_s,x_2) & \ldots & K(x_s,x_s) \end{vmatrix}.$$

Note that, at least in this case, the values of $\mathcal{I}_s^n(T)$ are obtained independently of the eigenvalues of T, so that the method described in Proposition 2 (i.e. the orthogonal invariants method) can be applied.

In particular, for $s = 1$:

$$\mathcal{I}_1^n(T) = \int_I K(x,x)dx = \int\int_Q |H(x,y)|dxdy,$$

and, for $s = 2$:

$$\mathcal{I}_2^n(T) = \frac{1}{2}\int\int_Q [K(x,x)K(y,y) - |K(x,y)|]dxdy.$$

REMARK 2.1. *We insist that, in our opinion, the above mentioned methods give theoretically precise tools for approximating the eigenvalues of a positive definite compact operator in a Hilbert space $L^2(I)$, since they permit to control the error of the obtained approximation of the eigenvalue μ_k by evaluating the difference $\sigma_k^{(\nu)} - \mu_k^{(\nu)}$.*

However, the use of the orthogonal invariants method leads sometimes to very expensive compational procedures. In this case, we suggest the use of the iterative method described in section 3.

3. The inverse iteration method. It is well known that the eigenvalue of maximum modulus of the operator $\mathcal{K}$ can be computed by using the Kellog method (see [8]). For the subsequent eigenvalues the *inverse iteration method*, which we now introduce, is nothing else than an extension of a classical method for matrices which is known as the *Wielandt method*.

Suppose we know an initial approximation $\tilde{\mu}$ of the desired eigenvalue $\mu_j, j \geq 2$, such that

$$|\tilde{\mu} - \mu_j| < \frac{1}{2} \min_{\substack{\mu_k \neq \mu_j \\ k = 1, 2, \ldots, \nu}} |\mu_k - \mu_j|$$

for a suitable choice of the integer ν. In practice the desired eigenvalues will be replaced by their Raileigh-Ritz approximations, for sufficiently large ν:

$$|\tilde{\mu} - \mu_j^{(\nu)}| < \frac{1}{2} \min_{\substack{\mu_k^{(\nu)} \neq \mu_j^{(\nu)} \\ k=1,2,\ldots,\nu}} |\mu_k^{(\nu)} - \mu_j^{(\nu)}|. \tag{3.1}$$

¿From (1.5) we have

$$(\mathcal{K} - \tilde{\mu}\mathcal{I})\phi = (\mu - \tilde{\mu})\phi. \tag{3.2}$$

Consequently, if μ_j is an eigenvalue of $\mathcal{K}$ with eigenfunction ϕ_j, then $\mu_j - \tilde{\mu}$ is an eigenvalue of $\mathcal{K} - \tilde{\mu}\mathcal{I}$ with eigenfunction ϕ_j. By writing (3.2) in the form

$$(\mathcal{K} - \tilde{\mu}\mathcal{I})^{-1}\phi = (\mu - \tilde{\mu})^{-1}\phi, \tag{3.3}$$

it follows that $(\mu_j - \tilde{\mu})^{-1}$ is an eigenvalue of $(\mathcal{K} - \tilde{\mu}\mathcal{I})^{-1}$ with the same eigenfunction ϕ_j.

By using condition (3.1), for ν sufficiently large, the eigenvalue $(\mu_j - \tilde{\mu})^{-1}$ becomes the (unique) eigenvalue of maximum modulus for the operator $(\mathcal{K} - \tilde{\mu}\mathcal{I})^{-1}$. This leads to the possibility to apply the Kellog method in order to approximate $(\mu_j - \tilde{\mu})^{-1}$, and a corresponding eigenfunction. This can be done in the usual way, starting from an arbitrary function ω_0 (which theoretically should not be orthogonal to the eigenspace associated with $(\mu_j - \tilde{\mu})^{-1}$), and defining the sequence

$$\omega_{n+1} := (\mathcal{K} - \tilde{\mu}\mathcal{I})^{-1}\omega_n, \quad (n = 0, 1, 2, \ldots).$$

Then (see [8]):

$$lim_{n\to\infty} \frac{||\omega_{n+1}||_2}{||\omega_n||_2} = (\mu_j - \tilde{\mu})^{-1}, \tag{3.4}$$

$$lim_{n\to\infty} \frac{\omega_{2n}}{||\omega_{2n}||_2} = \pm\phi_j. \tag{3.5}$$

After computing the eigenvalue $\xi_j := (\mu_j - \tilde{\mu})^{-1}$ to the prescribed accuracy (see section 4), one finds

$$\mu_j = \frac{1}{\xi_j} + \tilde{\mu},$$

so that, by recalling $\mu = \lambda^{-1}(\tilde{\mu} =: \tilde{\lambda}^{-1})$, we obtain, for the characteristic values of the kernel, the expressions

$$\lambda_j = \frac{\tilde{\lambda}\xi_j}{\tilde{\lambda} + \xi_j}.$$

It is important to note that (as in the finite dimensional case) we can avoid the determination of the inverse operator $(\mathcal{K} - \tilde{\mu}\mathcal{I})^{-1}$, since the equation

$$\omega_{n+1} = (\mathcal{K} - \tilde{\mu}\mathcal{I})^{-1}\omega_n$$

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is equivalent to

$$(\mathcal{K} - \tilde{\mu}\mathcal{I})\omega_{n+1} = \omega_n. \tag{3.6}$$

However, this leads to the necessity to solve numerically, at each step, a Fredholm integral equation of the first kind. This can be done by using different methods (see [2],[3]), namely, we could use, for example, the Fast Galerkin method, or the Nyström method. The latter method was used in our calculations, since it turned out to be very simple and efficient both with respect to time and number of iterations. In applying the Nyström method we used the modified Gauss-Legendre quadrature formula with at most 60 nodes.

4. Error estimate and prescribed accuracy. The rate of convergence of the method is given by the formula:

$$\frac{||\omega_n||_2}{||\omega_0||_2} = \mathcal{O}\left[(\mu'(\mu_j - \tilde{\mu}))^n\right],$$

where $\mu' \neq (\mu_j - \tilde{\mu})^{-1}$ denotes a suitable eigenvalue of $(\mathcal{K} - \tilde{\mu}\mathcal{I})^{-1}$ (see [12]).

As a matter of fact, from the numerical point of view, the use of Nyström method in the solution of equation (3.6) is substantially equivalent to the substitution of the original kernel $K(x, y)$ by an approximating kernel $\tilde{K}(x, y)$ given by a suitably defined two-dimensional step function (that is, instead of the original operator, we consider an approximating finite dimensional operator given by a suitable matrix).

In order to define this finite dimensional operator, and to discuss the accuracy of our approximation we introduce some notations.

Let n be the number of nodes in the application of the Nyström method, and denote by $x_1, x_2, \ldots, x_n$ (or $y_1, y_2, \ldots, y_n$) the knots of the modified Gauss-Legendre quadrature formula on the x (or y) axis, and by $w_1, w_2, \ldots, w_n$ the corresponding Christoffel constants.

In the sequel we suppose that the kernel is sufficiently regular in $Q := [0, 1] \times [0, 1]$, and precisely such that the Peano-Jordan measure of the eventual singularities of K in Q is zero. These assumptions are natural when dealing with a compact operator.

Divide Q into the sub-squares $Q_{i,j}$ defined by

$$Q_{i,j} := \left\{(x, y)| \sum_{l=1}^{i-1} w_l \leq x < \sum_{l=1}^{i} w_l; \sum_{k=1}^{j-1} w_k \leq y < \sum_{k=1}^{j} w_k\right\},$$

assuming $\sum_{s=1}^{i-1} w_s := 0$, if $i = 1$, and recalling that $\sum_{s=1}^{n} w_s = 1$. Denote by $Q^*_{i,j}$ those particular sub-squares in which $K(x, y)$ is not bounded, then define

$$\tilde{K}(x, y) = \begin{cases} K(x_i, y_j), & \text{if} \quad (x, y) \in Q_{i,j} \\ K_{i,j}, & \text{if} \quad (x, y) \in Q^*_{i,j}, \end{cases}, \tag{4.1}$$

where $K_{i,j}$ are such constants that

$$||K(x, y) - \tilde{K}(x, y)||_{L^2(\cup_{i,j} Q^*_{i,j})} < \epsilon,$$

where ϵ denotes an acceptable error tolerance. This condition can always be satisfied provided that n is sufficiently large.

Then the numerical computation by using the inverse iteration method yields to approximate the exact eigenvalues $\tilde{\mu}_j$, $(j = 1, 2, \ldots, n)$ of the kernel $\tilde{K}(x, y)$.

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In addition, by using the well known Aronszajn Theorem (see e.g. [5]), it is possible to find an upper bound for the absolute error $|\mu_j - \tilde{\mu}_j|$, which is given simply, for every j, by the estimate

$$|\mu_j - \tilde{\mu}_j| \leq ||K(x,y) - \tilde{K}(x,y)||_{L^2(Q)}.$$

Then, in order to find an approximation $\tilde{\mu}_j$ which is exact, with respect to the corresponding μ_j, up to the p-th digit, it is sufficient to increase n (and eventually to use adaptive composite quadrature formulas, increasing the number of knots close to the singularities) in such a way that the further inequality $||K(x,y) - \tilde{K}(x,y)||_{L^2(Q)} < .5 \times 10^{-p}$ holds true.

This can always be done, and permits to control the error of our approximation, independently by the use of the orthogonal invariants method.

5. Computation of the first few eigenvalues of a kernel considered by A.M. Ostrowski. A.M. Ostrowski [10] considered the problem of finding the maximum value M of the functional, $\forall \phi \in L^2(0,1)$:

$$I(\phi) := \left[\int_0^1 \phi^2(t)dt\right]^{-1} \int_0^1 \int_0^1 \left[\frac{1}{x-y}\int_y^x \phi(t)dt\right]^2 dxdy. \tag{5.1}$$

As a consequence of a theorem by A. Garsia, cited in the same article of A.M. Ostrowski, the preceding problem can be reduced to the computation of the greatest eigenvalue μ_1 of the positive compact operator, defined in $L^2(0,1)$

$$\mathcal{K}\phi = \int_0^1 K(x,y)\phi(y)dy, \tag{5.2}$$

where

$$K(x,y) = \begin{cases} 2\log\frac{x(1-y)}{x-y}, & \text{if } 0 \leq y < x \leq 1 \\ \\ 2\log\frac{y(1-x)}{y-x}, & \text{if } 0 \leq x < y \leq 1. \end{cases} \tag{5.3}$$

This problem was solved by G. Fichera and M.A. Sneider in a paper [6]. By a very accurate computation they have established the inequalities

$$1.2029315225711 < M = \mu_1 < 1.202931525733.$$

They used the classical Rayleigh-Ritz method for the lower bounds, and the orthogonal invariants method to computing the upper bounds.

The computation of lower bounds for M was considerably simplified by A. Ghizzetti in [7] by using a basis of modified Legendre polynomials, instead of powers, in the application of the Rayleigh-Ritz method.

In the above mentioned paper [6] G. Fichera and M.A. Sneider deal with a more general framework with respect to the problem introduced by A.M. Ostrowski, considered also the problem of approximating the first few eigenvalues of the same operator (5.2) with kernel (5.3).

They have found these following results for the first five eigenvalues μ_k, $k = 1,2,3,4,5$:

1.202931525711	$< \mu_1 <$	1.202931525733
0.729012156602	$< \mu_2 <$	0.740766
0.52709392618	$< \mu_3 <$	0.54902
0.4135343103	$< \mu_4 <$	0.44775
0.3407196076	$< \mu_5 <$	0.38842

Table I

In a earlier paper (see [9]), we applied the above mentioned method to obtain the first few correct digits of the eigenvalues of Table I.

The numerical results for the first five eigenvalues of the kernel (5.3) considered by A.M. Ostrowski were obtained by using a Turbo C^{++} program written by S. Delle Monache.

Starting from the secular equations considered by A. Ghizzetti in section 3 of his paper [7], we found (for $n = 19$) an equation of order 20, whose first five roots, in decreasing order, are given by

$$\begin{aligned} \tilde{\mu_1} &= 1.20293152571347 \\ \tilde{\mu_2} &= 0.72901215660725 \\ \tilde{\mu_3} &= 0.52709392620653 \\ \tilde{\mu_4} &= 0.41353431036983 \\ \tilde{\mu_5} &= 0.34071960754549. \end{aligned}$$

These values improve the Rayleigh-Ritz (lower) approximations of Table I, and can be considered as initial approximations $\tilde{\mu}$ for the inverse iteration method.

Our results are contained in Table II.

1.20293152571347	$< \mu_1 <$	1.209
0.72901215660725	$< \mu_2 <$	0.739
0.52709392620653	$< \mu_3 <$	0.530
0.41353431036983	$< \mu_4 <$	0.414
0.34071960754549	$< \mu_5 <$	0.345

Table II

Since we used a simple personal computer for the computation, we chose $p = 2$, and consequently we found only the first two correct decimal figures of the eigenvalues $\mu_k, (k = 1, 2, 3, 4, 5)$ of the given kernel. We want to point out that the very good approximation for the first eigenvalue which appears in Table I was obtained by G. Fichera and M.A. Sneider by using an IBM mainframe and 100 digits multiple precision arithmetic for computations, and, moreover, using the orthogonal invariants method they were able to find only the first correct decimal figure for the subsequent four eigenvalues of the operator $\mathcal{K}$.

6. Conclusion and Remarks. The problem of computing the eigenvalues of second kind Fredholm operators is, in general, a very difficult subject. However, in case of a symmetric (or Hermitian) positive definite kernel (more generally for a positive definite compact operator) the problem can be treated by using the Rayleigh-Ritz method for the lower bound approximations, and Fichera's orthogonal invariants method for computing the upper bounds.

A computationally less expensive method which has been presented here, consists in using the information given by the Rayleigh-Ritz method for starting with an iterative convergent procedure for every fixed eigenvalue.

We want to remark that the application of the *inverse iteration method* leads to the problem of solving numerically integral equations of the first kind. Although this problem could be affected in general by severe ill-conditioning, in case of the symmetric kernels, we found that this can be done effectively using the classical Nyström method.

Examining the equations used is the application of the Nyström method, one finds that inverse iterations converge to the exact eigenvalues of an approximating finite dimensional kernel, which can be found by considering a suitable partition of the integration domain, defined in terms of the Christoffel constants of a Gaussian quadrature formula, and substituting the original kernel with a two dimensional step function determined by the values of $K(x, y)$ on the nodes of the quadrature.

REMARK 6.1. *Since discretization approximates a finite number of the eigenvalues of the kernel $\mathcal{K}$ by the corresponding eigenvalues of a symmetric (Hermitian) matrix, it is not necessary to use the Wielandt method for this computation: more modern and efficient method can be applied at this stage.*

REMARK 6.2. *Since an explicit uniform bound for the absolute error can be derived by using the Aronszajn theorem, it is possible to control the error by the beginning, whereas in the Fichera's method the computation of the error can be done only at the end of computation.*

The inverse iteration method, discussed above, will be applied in some forthcoming papers to the approximation of the eigenvalues of some Sturm-Liouville problems from the mathematical physics for which the transformation of the problem into a second kind Fredholm integral equation can be performed by constructing explicitly the Green function (see e.g. [5]).

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