A homotopy method for finding eigenvalues and eigenvectors

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ABSTRACT

Suppose we want to find the eigenvalues and eigenvectors for the linear operator L, and suppose that we have solved this problem for some other "nearby" operator K. In this paper we show how to represent the eigenvalues and eigenvectors of L in terms of the corresponding properties of K.

INTRODUCTION

Suppose we want to find the eigenvalues and eigenvectors for the linear operator L over some Hilbert space with inner product $\langle \cdot, \cdot \rangle$. That is, we want to find the vectors x and the scalars λ satisfying $Lx = \lambda x$. Also suppose that we have solved this problem for some other linear operator K. Is it possible to represent the eigenvalues and eigenvectors of L in terms of the corresponding properties of K? In this paper we address this question.

APPROACH

We use a homotopy technique. We form a convex combination $\theta L + (1-\theta)K$ of the operators K and L with parameter θ . As the parameter ranges from 0 to 1, the operator $\theta L + (1-\theta)K$ ranges from K to L. More precisely, at each value of θ the corresponding operator is given by $(\theta L + (1-\theta)K)x = \theta Lx + (1-\theta)Kx$ Next, we envision, for each choice of θ , a set of eigenvectors $\{x_i(\theta)\}_{i=1}^{\infty}$ and eigenvalues $\{\lambda_i(\theta)\}_{i=1}^{\infty}$ for the corresponding operator $\theta L + (1-\theta)K$, satisfying $\lambda_i(\theta)x_i(\theta) = \theta Lx_i(\theta) + (1-\theta)Kx_i(\theta)$. Then $x_i(0) = e_i$, where $\{e_i\}_{i=1}^{\infty}$ are eigenvectors of K, and $\{\lambda_i(0)\}_{i=1}^{\infty}$ are the corresponding eigenvalues.

Our strategy is to develop power series representations of $\{x_i(\theta)\}_{i=1}^{\infty}$ and $\{\lambda_i(\theta)\}_{i=1}^{\infty}$, and then, if possible, to evaluate them at the value $\theta = 1$. If the power series representations converge absolutely there, we may expect to find that $\{x_i(1)\}_{i=1}^{\infty}$ and $\{\lambda_i(1)\}_{i=1}^{\infty}$ are eigenvectors and eigenvalues of the operator L.

DERIVATION

We stipulated earlier that $\{e_i\}_{i=1}^{\infty}$ are eigenvectors of K, whence $x_i(0) = e_i$. We also assume that they are orthonormal: $\langle e_m, e_n \rangle = \delta_m^n$. Let $\{\lambda_i(0)\}_{i=1}^{\infty}$ represent their corresponding eigenvalues, so that $\lambda_i(0)e_i = Ke_i = Kx_i(0)$. We immediately $\det \langle Ke_i, e_j \rangle = \delta_i^j \lambda_i(0)$. In case i = j we get

$$\lambda_i(0) = \langle Ke_i, e_i \rangle$$

Next, we define $\{\varphi_{i,j}(\theta)\}_{i,j=1}^{\infty}$ as $\varphi_{i,j}(\theta) = \langle x_i(\theta), e_j \rangle$. We then have that

$$x_i(\theta) = \sum_{j=1}^{\infty} \varphi_{i,j}(\theta) e_j$$
. In particular $\varphi_{i,j}(0) = \langle x_i(0), e_j \rangle = \langle e_i, e_j \rangle = \delta_i^j$, whence

$$\varphi_{i,j}(0) = \delta_j^i$$

Making the appropriate substitutions into $\lambda_i(\theta)x_i(\theta) = (\theta L + (1-\theta)K)x_i(\theta)$ yields

$$\lambda_{i}(\theta)\sum_{i=1}^{\infty}\varphi_{i,j}(\theta)e_{j} = (\theta L + (1-\theta)K)\sum_{i=1}^{\infty}\varphi_{i,j}(\theta)e_{j}.$$

After rearrangement we get $\lambda_i(\theta)\sum_{j=1}^{\infty}\varphi_{i,j}(\theta)e_j = \theta\sum_{j=1}^{\infty}\varphi_{i,j}(\theta)Le_j + (1-\theta)\sum_{j=1}^{\infty}\varphi_{i,j}(\theta)Ke_j$

from which there results the equation

$$\lambda_{i}\left(\theta\right)\sum_{j=1}^{\infty}\varphi_{i,j}\left(\theta\right)\left\langle e_{j},e_{k}\right\rangle =\theta\sum_{j=1}^{\infty}\varphi_{i,j}\left(\theta\right)\left\langle Le_{j},e_{k}\right\rangle +\left(1-\theta\right)\sum_{j=1}^{\infty}\varphi_{i,j}\left(\theta\right)\left\langle Ke_{j},e_{k}\right\rangle$$

Recalling $\langle e_i, e_j \rangle = \delta_i^j$ and defining

 $X_{m,n} \equiv \langle Le_m, e_n \rangle$ leads, after substitution, to the equation

$$\lambda_{i}\left(\theta\right)\sum_{j=1}^{\infty}\varphi_{i,j}\left(\theta\right)\delta_{j}^{k}=\theta\sum_{j=1}^{\infty}\varphi_{i,j}\left(\theta\right)X_{j,k}+\left(1-\theta\right)\sum_{j=1}^{\infty}\varphi_{i,j}\left(\theta\right)\delta_{j}^{k}\lambda_{j}\left(0\right)$$

Simplifying yields

$$\lambda_{i}(\theta)\varphi_{i,k}(\theta) = \theta \sum_{j=1}^{\infty} \varphi_{i,j}(\theta)X_{j,k} + (1-\theta)\varphi_{i,k}(\theta)\lambda_{k}(0)$$

The approach from this point is to calculate about $\theta=0$ the Maclaurin series expansions of the functions $\left\{x_i\left(\theta\right)\right\}_{i=1}^{\infty}$ and $\left\{\lambda_i\left(\theta\right)\right\}_{i=1}^{\infty}$. To do this our procedure is to solve for the coefficients of power series which formally solve the above equation. That is, we assume the forms $\lambda_i\left(\theta\right)=\sum_{n=0}^{\infty}a_{i,n}\theta^n$ and $\varphi_{i,j}\left(\theta\right)=\sum_{r=0}^{\infty}b_{i,j,r}\theta^r$ and substitute them in that equation, then solve for the coefficients $\left\{a_{i,n}\right\}$ and $\left\{b_{i,j,r}\right\}$.

After performing the substitution, we get

$$\sum_{n=0}^{\infty} a_{i,n} \theta^n \sum_{m=0}^{\infty} b_{i,k,m} \theta^m = \theta \sum_{j=1}^{\infty} \sum_{r=0}^{\infty} b_{i,j,r} \theta^r X_{j,k} + \left(1-\theta\right) \sum_{r=0}^{\infty} b_{i,k,r} \theta^r \lambda_k \left(0\right).$$
 Upon rearranging, there

results
$$\sum_{s=0}^{\infty} \theta^{s} \sum_{m=0}^{s} a_{i,s-m} b_{i,k,m} = \sum_{r=1}^{\infty} \theta^{r} \sum_{j=1}^{\infty} X_{j,k} b_{i,j,r-1} + \sum_{r=0}^{\infty} \lambda_{k} \left(0\right) b_{i,k,r} \theta^{r} + \sum_{r=1}^{\infty} -\lambda_{k} \left(0\right) b_{i,k,r-1} \theta^{r}$$
. We

first set equal the coefficients of the constant terms to get $\sum_{m=0}^{0} a_{i,0-m}b_{i,k,m} = \lambda_k(0)b_{i,k,0}$,

which when simplified becomes $(a_{i,0} - \lambda_k(0))b_{i,k,0} = 0$. Since $\lambda_i(\theta) = \sum_{n=0}^{\infty} a_{i,n}\theta^n$, we must

have the equation $a_{i,0}=\lambda_i\left(0\right)$. Since $\varphi_{i,j}\left(\theta\right)=\sum_{r=0}^{\infty}b_{i,j,r}\theta^r$, we must have the equation

 $b_{i,j,0} = \varphi_{i,j}\left(0\right) = \delta_{j}^{i}$, and these two equations indeed satisfy $\left(a_{i,0} - \lambda_{k}\left(0\right)\right)b_{i,k,0} = 0$. Next,

for r > 0 we set equal the coefficients of the θ^r terms to get

$$\sum_{m=0}^{r} a_{i,r-m} b_{i,k,m} = \sum_{j=1}^{\infty} X_{j,k} b_{i,j,r-1} + \lambda_{k}(0) b_{i,k,r} - \lambda_{k}(0) b_{i,k,r-1}. \text{ Upon substituting } b_{i,k,0} = \delta_{i}^{k} \text{ we}$$

get
$$a_{i,r}\delta_{i}^{k} + \sum_{m=1}^{r} a_{i,r-m}b_{i,k,m} = \sum_{j=1}^{\infty} X_{j,k}b_{i,j,r-1} + \lambda_{k}(0)b_{i,k,r} - \lambda_{k}(0)b_{i,k,r-1}$$
. The examination of

this equation splits naturally into the two cases i = k and $i \neq k$. Considering the case

$$i = k$$
 first, we get $a_{i,r} = \sum_{j=1}^{\infty} X_{j,i} b_{i,j,r-1} + \lambda_i(0) b_{i,i,r} - \lambda_i(0) b_{i,i,r-1} - \sum_{m=1}^{r} a_{i,r-m} b_{i,i,m}$. In case

$$i \neq k$$
, we get $\sum_{m=1}^{r} a_{i,r-m} b_{i,k,m} = \sum_{j=1}^{\infty} X_{j,k} b_{i,j,r-1} + \lambda_k (0) b_{i,k,r} - \lambda_k (0) b_{i,k,r-1}$, which may be

rearranged as
$$a_{i,0}b_{i,k,r} = \sum_{j=1}^{\infty} X_{j,k}b_{i,j,r-1} + \lambda_k (0)(b_{i,k,r} - b_{i,k,r-1}) - \sum_{m=1}^{r-1} a_{i,r-m}b_{i,k,m}$$
. After

substituting $a_{i,0} = \lambda_i(0)$ and solving, we get

$$b_{i,k,r} = \frac{1 - \delta_i^k}{\lambda_i(0) - \lambda_k(0)} \left(\sum_{j=1}^{\infty} X_{j,k} b_{i,j,r-1} - \sum_{m=1}^{r-1} a_{i,r-m} b_{i,k,m} - \lambda_k(0) b_{i,k,r-1} \right)$$

We now perform this recursion to get some initial results. Using

$$a_{i,r} = \sum_{j=1}^{\infty} X_{j,i} b_{i,j,r-1} + \lambda_i(0) b_{i,i,r} - \lambda_i(0) b_{i,i,r-1} - \sum_{m=1}^{r} a_{i,r-m} b_{i,i,m}, \text{ we see that}$$

$$a_{i,1} = \sum_{j=1}^{\infty} X_{j,i} b_{i,j,0} + \lambda_i (0) b_{i,i,1} - \lambda_i (0) b_{i,i,0} - \sum_{m=1}^{1} a_{i,1-m} b_{i,i,m} \text{ hence}$$

$$a_{i,1} = \sum_{j=1}^{\infty} X_{j,i} \delta_i^j + \lambda_i(0) b_{i,i,1} - \lambda_i(0) \delta_i^i - \lambda_i(0) b_{i,i,1}$$
 and thus $a_{i,1} = X_{i,i} - \lambda_i(0)$. Using

$$b_{i,k,r} = \frac{1 - \delta_{i}^{k}}{\lambda_{i}\left(0\right) - \lambda_{k}\left(0\right)} \left(\sum_{j=1}^{\infty} X_{j,k} b_{i,j,r-1} - \sum_{m=1}^{r-1} a_{i,r-m} b_{i,k,m} - \lambda_{k}\left(0\right) b_{i,k,r-1}\right), \text{ we get that }$$

$$b_{i,k,1} = \frac{1 - \delta_i^k}{\lambda_i(0) - \lambda_k(0)} \left(\sum_{j=1}^{\infty} X_{j,k} b_{i,j,0} - \sum_{m=1}^{0} a_{i,r-m} b_{i,k,m} - \lambda_k(0) b_{i,k,0} \right) \text{ and thus}$$

$$b_{i,k,1} = \left(1 - \delta_i^k\right) \frac{X_{i,k}}{\lambda_i(0) - \lambda_k(0)}$$
. Similarly we use the recursion formula to produce

$$a_{i,2} = \sum_{j=1}^{\infty} X_{j,i} b_{i,j,1} + \lambda_i (0) (b_{i,i,2} - b_{i,i,1}) - \sum_{m=1}^{2} a_{i,2-m} b_{i,i,m}, \text{ which after substitution yields}$$

$$a_{i,2} = \sum_{j=1}^{\infty} X_{j,i} \left(1 - \delta_i^j \right) \frac{X_{i,j}}{\lambda_i \left(0 \right) - \lambda_j \left(0 \right)} = \sum_{\substack{j=1 \ j \neq i}}^{\infty} \frac{X_{i,j} X_{j,i}}{\lambda_i \left(0 \right) - \lambda_j \left(0 \right)}.$$
 Finally, we get

$$b_{i,k,2} = \frac{1 - \delta_{i}^{k}}{\lambda_{i}(0) - \lambda_{k}(0)} \left(\sum_{j=1}^{\infty} X_{j,k} b_{i,j,1} - \sum_{m=1}^{1} a_{i,2-m} b_{i,k,m} - \lambda_{k}(0) b_{i,k,1} \right)$$
 which after substitution

becomes
$$b_{i,k,2} = \frac{1 - \delta_i^k}{\lambda_i(0) - \lambda_k(0)} \left(\sum_{\substack{j=1 \ j \neq i}}^{\infty} X_{j,k} \frac{X_{i,j}}{\lambda_i(0) - \lambda_j(0)} + X_{i,k} \left(1 - \frac{X_{i,i}}{\lambda_i(0) - \lambda_k(0)} \right) \right)$$
. This

means that

$$\lambda_{i}(\theta) = \lambda_{i}(0) + (X_{i,i} - \lambda_{i}(0))\theta + \sum_{\substack{j=1\\j\neq i}}^{\infty} \frac{X_{i,j}X_{j,i}}{\lambda_{i}(0) - \lambda_{j}(0)}\theta^{2} + \cdots$$
 and

$$\begin{vmatrix} x_{i}(\theta) \\ = e_{i} + \sum_{\substack{j=1\\j\neq i}}^{\infty} \left(\frac{X_{i,j}}{\lambda_{i}(0) - \lambda_{j}(0)} \theta + \begin{pmatrix} \frac{1}{\lambda_{i}(0) - \lambda_{j}(0)} \sum_{\substack{k=1\\k\neq i}}^{\infty} \frac{X_{i,k} X_{k,j}}{\lambda_{i}(0) - \lambda_{k}(0)} \\ + \frac{X_{i,j}}{\lambda_{i}(0) - \lambda_{j}(0)} - \frac{X_{i,i} X_{i,j}}{(\lambda_{i}(0) - \lambda_{j}(0))^{2}} \end{pmatrix} \theta^{2} + \cdots \right) e_{j}$$

(at least formally). Now if it happens that these formal power series actually converge

absolutely at
$$\theta = 1$$
, we then have $\lambda_i(1) = X_{i,i} + \sum_{\substack{j=1 \ j \neq i}}^{\infty} \frac{X_{i,j} X_{j,i}}{\lambda_i(0) - \lambda_j(0)} + \cdots$ and

$$= e_{i} + \sum_{\substack{j=1\\j\neq i}}^{\infty} \left(\frac{X_{i,j}}{\lambda_{i}(0) - \lambda_{j}(0)} + \left(\frac{1}{\lambda_{i}(0) - \lambda_{j}(0)} \sum_{\substack{n=1\\n\neq i}}^{\infty} \frac{X_{i,n} X_{n,j}}{\lambda_{i}(0) - \lambda_{n}(0)} + \frac{X_{i,j}}{\lambda_{i}(0) - \lambda_{j}(0)} - \frac{X_{i,i} X_{i,j}}{(\lambda_{i}(0) - \lambda_{j}(0))^{2}} \right) + \cdots \right) e_{j}$$

These are eigenvalues and eigenvectors of the operator L, as desired.