A GENERALIZATION OF THE FRANK MATRIX

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Abstract

In this paper, we give a generalization of the well-known Frank matrix and show how to compute its eigensystem accurately. As well, we attempt to explain the ill-condition of its eigenvalues by treating it as a perturbation of a defective matrix.

1. Introduction

Over twenty-five years ago, Frank (1958) introduced two matrix examples as tests for an eigenvalue routine. The first, with

$$a_{i,j} = n+1 - max(i,j),$$

was the discrete Green's function matrix arising from the standard three-point difference approximation to $\frac{d^2y}{dx^2}$. The inverse of this matrix is tridiagonal and its eigenvalues are known explicitly, so the computed eigenvalues could be checked.

Frank had little trouble getting good approximations to the eigenvalues, so he tried a variant of this matrix by truncating it to upper Hessenberg form, producing

$$F_n = \begin{pmatrix} n & n-1 & n-2 & \cdots & 1 \\ n-1 & n-1 & n-2 & \cdots & 1 \\ 0 & n-2 & n-2 & \cdots & 1 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 1 \end{pmatrix}$$

He had much more difficulty with this matrix (with $n=12$), and in the years since, this matrix has come to be recognized as a good test case for eigenvalue routines: the eigenvalues are real and positive, are extremely ill-conditioned for moderate values of n, yet can be calculated accurately by other means. For example, F_{12} has eigenvalues ranging from 32.2 down to 0.031 (approximately) with condition numbers $\frac{1}{|s(\lambda)|}$ increasing to more than 10^{+7} for the smallest few eigenvalues. Here we define, for a real distinct eigenvalue λ with left and

right eigenvectors $\underline{w}$ and $\underline{z}$, the sensitivity

$$s(\lambda) = \frac{\underline{w}^T \underline{z}}{\|\underline{w}\|_2 \|\underline{z}\|_2}.$$

As is well known (see e.g. Wilkinson (1965), pg. 68), $\frac{1}{s(\lambda)}$ is effectively the first order perturbation coefficient in the expansion of the eigenvalue $\lambda(\epsilon)$ in a power series in ϵ, when the original matrix A is subjected to a perturbation $A + \epsilon B$. Thus $|s(\lambda)| < 10^{-7}$ means that a change in an element of F_{12} of order 10^{-7} can result in a change in the eigenvalue λ of order 1.

In this paper, we shall give a generalization of this matrix, show how to accurately compute its eigenvalues and eigenvectors, estimate the condition numbers of its eigenvalues, and attempt to explain the seemingly pathological ill-condition which ensues. We feel it is important to fully understand this matrix, as it illuminates the difficulties inherent in computing the eigenstructure, or invariant subspace structure, of general unsymmetric matrices.

2. The Generalization

Start with the symmetric tridiagonal matrix

$$S = \begin{pmatrix} 0 & b_1 & & & \\ b_1 & 0 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & & b_{n-1} & \\ & & b_{n-1} & 0 & \end{pmatrix} \tag{2.1}$$

with $b_i > 0$. Then S has real eigenvalues $\mu_1 \geq \cdots \geq \mu_n$ with $\mu_{n+1-i} = -\mu_i$, and these are all well-conditioned. Let the corresponding

eigenvectors be $\underline{x}^{(i)}$.

First from $T = \bar{D}^{-1} S \bar{D}$, with

$$\bar{D} = diag\,(1, \frac{1}{b_1}, \frac{1}{b_1 b_2}, \ldots, \frac{1}{b_1 b_2 \cdots b_{n-1}}).$$

This gives

$$T = \begin{pmatrix} 0 & 1 & & & \\ b_1^2 & 0 & 1 & & \\ & b_2^2 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & b_{n-1}^2 & 0 \end{pmatrix}. \tag{2.2}$$

Now consider $T - \mu I$ for each μ, and relate μ and $\lambda \geq 0$ by

$$\mu = \frac{\lambda - a}{\sqrt{\lambda}} \tag{2.3}$$

for $a \geq 0$. Then $\lambda - \mu\sqrt{\lambda} - a = 0$ and hence

$$\lambda(\mu) = \left(\frac{\mu}{2} \pm \sqrt{(\frac{\mu}{2})^2 + a} \right)^2 \tag{2.4}$$

Each μ thus gives two λ's, say $\lambda_+(\mu)$, $\lambda_-(\mu)$. However since $(-\mu)$ generates the same pair of λ's, we can make the identification for positive μ, of $+\mu$ with $\lambda_+(\mu)$ and $-\mu$ with $\lambda_-(\mu)$. Now form $G(\lambda) = \sqrt{\lambda} D^{-1}(T - \mu I)D$, where $D = diag\,(1, \lambda^{1/2}, \lambda, \lambda^{3/2}, \ldots)$. Then

$$G(\lambda) = \begin{pmatrix} a - \lambda & \lambda & & \\ b_1^2 & a - \lambda & \lambda & \\ & \ddots & \ddots & \ddots \end{pmatrix}$$

and hence $L^{-1} G = F - \lambda I$, with

$$L = \begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & \ddots & \ddots & \\ & & & -1 & \\ & & & 1 & \end{bmatrix} \quad \text{and} \quad F = \begin{bmatrix} a+b_1^2 & a+b_2^2 & \cdots & a+b_{n-1}^2 & a \\ b_1^2 & a+b_2^2 & \ddots & & \\ & b_2^2 & \ddots & & \\ & & & a+b_{n-1}^2 & a \\ & & & b_{n-1}^2 & a \end{bmatrix} \tag{2.5}$$

Since $F-\lambda I = \sqrt{\lambda} L D^{-1}(T-\mu I)D$, then (except possibly at $\lambda = 0$) the eigenvalues $\{\lambda_i\}$ of F and $\{\mu_i\}$ of S are related as λ and μ are related above. Thus if $sx = \mu x$, then

$$Fz = \lambda z, \qquad z = D^{-1}\bar{D}^{-1}x$$

$$w^T F = \lambda w^T, \qquad w^T = x^T \bar{D} D L.$$

Thus given a matrix F as above, with any a, $\{b_i\}$, we can find its eigenvalues (λ_i) and eigenvectors $(\underline{z}^{(i)}, \underline{w}^{(i)})$ using the above technique. The $\{\lambda_i\}$ will be accurate, and so will the vectors as long as the $\{\mu_i\}$ are well-separated. Notice that for $a > 0$, we get all $\lambda_i > 0$ and in pairs $(\lambda_+, a^2/\lambda_+)$, with an extra root $\lambda = a$ $(\mu = 0)$ for n odd. And for $a = 0$, we get pairs $\lambda_- = 0$, $\lambda_+ = \mu^2$, with an extra root $\lambda = 0$ $(\mu = 0)$ for n odd. In this latter case, the formulas above for z and w don't hold for $\lambda = 0$. The following special cases are of particular interest:

1. $b_i = \sqrt{n-i}$, $a = 1$, giving $F = F_n$ (the Frank matrix).

In this case, the matrix

$$S = \begin{bmatrix} 0 & \sqrt{n-1} & & & \\ \sqrt{n-1} & 0 & \sqrt{n-2} & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 1 & 0 \end{bmatrix}$$

which is (apart from a constant factor $\sqrt{2}$) the tridiagonal matrix arising using the recurrence relations for the Hermite polynomials $H_n(x)$. Thus the eigenvalues $\{\mu_i\}$ of S are $\sqrt{2}$ times the roots of $H_n(x)$.

2. $b_i = \sqrt{n}$, $a = 1$.

This gives S with eigenvalues $\mu_j = 2\sqrt{n}\ \cos(\frac{j\pi}{n+1})$, and

$$F \equiv \tilde{F}_n = \begin{bmatrix} n+1 & n+1 & \cdots & n+1 & 1 \\ n & n+1 & \cdots & n+1 & 1 \\ & n & \ddots & | & | \\ & & & n+1 & 1 \\ & & & n & 1 \end{bmatrix}. \tag{2.6}$$

3. Estimating $s(\lambda)$

Given a matrix F as in (2.5), and corresponding tridiagonal matrix S with eigenvalues $\{\mu_i\}$, we can find F's eigenvalues $\{\lambda_i\}$ using (2.4), and for each λ the corresponding eigenvectors $\underline{z}$ and $\underline{w}$ by forming $\mu = \frac{\lambda - a}{\sqrt{\lambda}}$ and the corresponding eigenvector $\underline{x}$ of S. Then

$$z_i = \frac{x_i \left(\prod_1^{i-1} b_j \right)}{\lambda^{\frac{i-1}{2}}}, \qquad w_i = \frac{x_i \lambda^{\frac{i-1}{2}}}{\prod_1^{i-1} b_j} - \frac{x_{i-1} \lambda^{\frac{i-2}{2}}}{\prod_1^{i-2} b_j}.$$

We are interested here in the sensitivity $s(\lambda) = \frac{w^T z}{\|w\|_2 \|z\|_2}$, for the smaller

eigenvalues λ. First, $w^T z = x^T \bar{D} D L D^{-1} \bar{D}^{-1} x = x^T \tilde{L} x$, where

$$\tilde{L} = \begin{bmatrix} 1 & -b_1/\sqrt{\lambda} & & \\ & 1 & -b_2/\sqrt{\lambda} & \\ & & \ddots & \ddots \\ & & & 1 \end{bmatrix}.$$

Thus $w^T z = x^T \left(\frac{\tilde{L}+\tilde{L}^T}{2}\right) x$, and since $\tilde{L}+\tilde{L}^T = 2I - \frac{S}{\sqrt{\lambda}}$,

$$w^T z = x^T x - \frac{x^T S x}{2\sqrt{\lambda}} = 1 - \frac{\mu}{2\sqrt{\lambda}}.$$

Also, $\|z\|_2 \geq |z_n| = \dfrac{|x_n| \left(\prod_1^{n-1} b_i\right)}{\lambda^{\frac{n-1}{2}}}$ and $\|w\|_2 \geq |w_1| = |x_1|$.

Note: for $\lambda \ll 1$, z_n is by far the largest component of z, so the above bound is quite sharp; however the bound for $\|w\|_2$ is off by a factor $\sqrt{2}$ in this case. This gives

$$|s(\lambda)| \leq \frac{|1-\frac{\mu}{2\sqrt{\lambda}}| \lambda^{\frac{n-1}{2}}}{|x_1| \, |x_n| \left(\prod_1^{n-1} b_i\right)} \leq \frac{\mu \lambda^{\frac{n}{2}-1}}{2|x_1| \, |x_n| \left(\prod_1^{n-1} b_i\right)}. \tag{3.1}$$

For the Frank matrix F_{12}, this bound gives $|s(\lambda)| \leq 1.2 \times 10^{-7}$ for the smallest λ. For the matrix $\tilde{F}_{12}$ (with $a=1$ and $b_i = \sqrt{12}$), this gives $|s(\lambda)| \leq 2 \times 10^{-12}$ for the smallest λ. In fact, the smallest few eigenvalues of F_{12} and $\tilde{F}_{12}$ are as follows:

$\lambda(F_{12})$	$s(\lambda)$	$\lambda(\tilde{F}_{12})$	$s(\lambda)$
.08122...	3.8×10^{-8}	.03465...	1.6×10^{-12}
.04950...	2.6×10^{-8}	.02524...	7.8×10^{-13}
.03102...	5.5×10^{-8}	.02117...	1.3×10^{-12}

4. Understanding the Poor Condition

To see why these matrices F have such poorly conditioned (small) eigenvalues, one can consider F as the sum of two matrices:

$$F = H + aT, \tag{4.1}$$

$$H = \begin{bmatrix} b_1^2 & b_2^2 & & & b_{n-1}^2 & 0 \\ b_1^2 & b_2^2 & & & b_{n-1}^2 & 0 \\ & b_2^2 & \ddots & & \vdots & \vdots \\ & & & & b_{n-1}^2 & 0 \end{bmatrix}, \quad T = \begin{bmatrix} 1 & 1 & & & 1 \\ & 1 & & & 1 \\ & & \ddots & & \vdots \\ & & & & 1 \end{bmatrix},$$

and treat "a" as a small parameter. Note: in the examples used, $a=1$ doesn't appear to be small, but both F_n and $\tilde{F}_n$ can be scaled by $1/n$ so the elements are $O(1)$ rather than $O(n)$, and the eigenvalues will be scaled by the same amount. This is equivalent to using, for F_n, $b_i = \sqrt{\frac{n-i}{n}}$, $a = \frac{1}{n}$, and for $\tilde{F}_n$, $b_i = 1$, $a = \frac{1}{n}$.

With a as a small parameter, F can be viewed as a *special* perturbation of H, and H has a well-defined eigenstructure: if we assume n is even, then H has $\frac{n}{2}$ eigenvalues at $\lambda = 0$, corresponding to one Jordan block of order $\frac{n}{2}$, and the other $\frac{n}{2}$ eigenvalues at $\lambda = \mu_i^2$, where $\{\mu_i\}$ are the eigenvalues of S (recall

these are in (+,-) pairs).

Notice that F is a very special perturbation of H; the eigenvalues remain real, and look asymptotically as follows, using the formula (2.4) for $\lambda(\mu)$:

$$\lambda_+(\mu_i) = \mu_i^2 + 2a + O(a^2) \quad (\textit{perturbed from } \mu_i^2)$$

$$\lambda_-(\mu_i) = a^2/\mu_i^2 + O(a^3) \quad (\textit{perturbed from zero}).$$

An arbitrary perturbation of H of order a, would result in generally complex eigenvalues, with $\lambda = O(a^{2/n})$ perturbation from zero, whereas these are $O(a^2)$. However, the sensitivities $|s(\lambda)|$ are still very small for these λ's: $s(\lambda) = O(a^{n-1})$ again using the formulas given earlier.

For the special examples, $a = \frac{1}{n}$ implies $s(\lambda) = O(\frac{1}{n^n})$, and this is independent of any constant scaling. These very small values for $s(\lambda)$ can be seen in the smaller eigenvalues of $\tilde{F}_{12}$; for the larger eigenvalues, and for F_{12}, the other constants involved serve to increase the actual values obtained.

We feel this matrix F serves as a very instructive example in connection with the general computational problem of resolving eigenspaces, or more generally invariant subspaces, of unsymmetric matrices. Although all the eigenvalues of F are distinct, as long as $a > 0$, the smaller ones are remarkably ill-conditioned, and the corresponding eigenvectors are not well-determined. Thus one should treat F as a matrix with an invariant subspace of order $\frac{n}{2}$, corresponding to the $\frac{n}{2}$ eigenvalues perturbed from zero in H. However it is not

easy to discern this, given only F, since the amount of the perturbation (a) from H is much larger than the machine precision η. Indeed, all those matrices which differ from F by $O(\eta)$ look much like F, and the canonical matrix H which is strongly influencing F, is a much greater distance away.

5. A Note on Computing Eigenvectors

In the course of checking the eigenvectors of these matrices, the author had occasion to return to the standard "inverse iteration" algorithm for computing eigenvectors. Even with a matrix like F, with poorly conditioned eigenvalues and thus poorly determined eigenvectors, we should at least expect each computed eigenvectors $\underline{\bar{z}}$ (corresponding to computed eigenvector $\bar{\lambda}$ to give a small residual: $||F\underline{\bar{z}} - \bar{\lambda}\underline{\bar{z}}|| = O(\eta)$. This in fact occurred using the EISPACK routines, which however do not use inverse iteration explicitly, but instead perform a back-substitution, using the triangularized form of the matrix.

If inverse iteration is used (normally with the Hessenberg form) for F and computed eigenvalue $\bar{\lambda}$, one solves $(F - \bar{\lambda}I)\underline{y} = \underline{v}$ for some vector $\underline{v}$. Almost always, using a reasonably clever choice of $\underline{v}$, $||y|| \cong 1/\eta_1$ so that the normalized vector $\bar{z} = y/||y||$ gives a small residual. However it can happen that $||y||$ is not "large enough", and one is tempted to do another inverse iteration, solving $(F - \bar{\lambda}I)\underline{z} = \underline{y}$. For badly conditioned eigenvalues, this is *not* a good idea: the computed $\underline{z}$ vector will not give a small residual, because the vector $\underline{y}$ is not a good choice of "initial" vector for the inverse iteration.

Because of this phenomenon, it is much safer (although a little more expensive) to iterate with the matrix $(F-\bar{\lambda}I)^T(F-\bar{\lambda}I)$ (with transpose replaced by conjugate transpose in the complex case), as suggested by Wilkinson (1979). The enforced symmetry avoids the possible embarrassment of large residuals when more iterations are used, essentially because we are now dealing with the *orthogonal* singular vectors not the eigenvectors of F. The algorithm is:

1. decompose $F-\bar{\lambda}I = PLU$.

   If F is upper Hessenberg, $||L||$ and $||L^{-1}||$ are not large, so the near-singularity of $(F-\bar{\lambda}I)$ is reflected in U; so

2. perform a (double) inverse iteration: solve $U^T U\underline{z} = \underline{y}$, for $\underline{y}$ your favorite initial vector; in the very unlikely case that $||z||/||\underline{r}|| \ll \eta^{-1}$, do another iteration.

3. get the left-hand eigenvector $\underline{w}^T$ as well: solve $UU^T\underline{y} = \underline{y}$ (and again if necessary as in 2.) with finially $\underline{w}^T(PL) = \underline{y}^T$.

4. finally, compute $s(\lambda)$ using the computed $\underline{w}^T$ and $\underline{z}$.

We cannot emphasize the last step enough; most eigenvalue routines do not compute $s(\lambda)$, and it really is a reliable estimate of the accuracy of the computed eigenvalue.

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