A Nonlinear QR Algorithm for Banded Nonlinear Eigenvalue Problems

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Nonlinear Eigenvalue Problem

Nonlinear Eigenvalue Problem

Find nonzero vectors x and y and scalar μ such that

$$H(\mu)x = 0, \qquad y^* H(\mu) = 0$$

$H(\lambda)$	$n \times n$ matrix-valued function (real or complex)
μ	eigenvalue
x	right eigenvector
y	left eigenvector

Linear eigenvalue problem: $H(\lambda) = A - \lambda I$

Finding an eigenvalue

1. Start with a guess λ_0
2. Use QR decomposition with column pivoting

$$H(\lambda_0)\Pi(\lambda_0) = Q(\lambda_0)R(\lambda_0)$$

   (Goal: use pivoting to make $R_{nn}(\lambda) \approx \sigma_{\min}$)
3. Solve $R_{nn}(\lambda) = 0$ by Newton iterations

$$\lambda_1 = \lambda_0 - \frac{R_{nn}(\lambda_0)}{R'_{nn}(\lambda_0)}$$

Kublanovskaya Method

$$R'_{nn} = (Qe_n)^* H' \Pi \begin{bmatrix} -R_{11}^{-1} R_{1n} \\ 1 \end{bmatrix} \qquad R = \begin{array}{c c} & \begin{array}{cc} n-1 & 1 \end{array} \\ \begin{array}{c} n-1 \\ 1 \end{array} & \begin{bmatrix} R_{11} & R_{1n} \\ 0 & R_{nn} \end{bmatrix} \end{array}$$

Check for convergence

$$|R_{nn}(\lambda_j)| / ||H(\lambda_j)||_F < \text{tolerance}$$

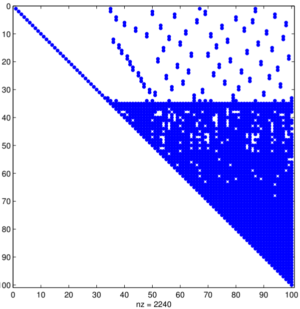
Once converged, the eigenvectors are

$$x = \Pi \begin{bmatrix} -R_{11}^{-1} R_{1n} \\ 1 \end{bmatrix} \qquad y = Qe_n$$

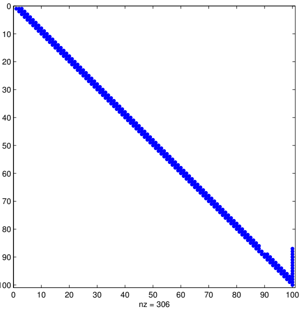
Banded Problem – Standard Lapack

If H is banded, need to be careful about use of Π

Ex: $H(\lambda) = (A - \lambda B + e^{-\lambda} D)$ with A, B, D tridiagonal



R from standard Lapack QR with column pivoting



R using new pivoting

Banded Problem – QR Overview

Lapack requires $O(n^3)$ flops
New method requires $O(n)$ flops

Three Steps

(QR)	$H = Q_1 R_1$
(Pivot)	$H\Pi = Q_1 R_1 \Pi$
(QR Again)	$H\Pi = Q_1(R_1\Pi) = Q_1(Q_2 R) = QR$

Banded Problem – Step 1 (QR)

Do a QR decomposition of H using Householder transformations
Only $O(b^2 n)$ flops for small bandwidth

$$\begin{pmatrix} x & x & 0 & 0 & 0 & 0 & 0 & 0 \\ x & x & x & 0 & 0 & 0 & 0 & 0 \\ 0 & x & x & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & x & x & 0 & 0 & 0 \\ 0 & 0 & 0 & x & x & x & 0 & 0 \\ 0 & 0 & 0 & 0 & x & x & x & 0 \\ 0 & 0 & 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & 0 & 0 & 0 & x & x \end{pmatrix}$$

Banded Problem – Step 1 (QR)

Do a QR decomposition of H using Householder transformations
Only $O(b^2 n)$ flops for small bandwidth

$$\begin{pmatrix} x & x & \mathbf{x} & 0 & 0 & 0 & 0 & 0 \\ \mathbf{0} & x & x & 0 & 0 & 0 & 0 & 0 \\ 0 & x & x & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & x & x & 0 & 0 & 0 \\ 0 & 0 & 0 & x & x & x & 0 & 0 \\ 0 & 0 & 0 & 0 & x & x & x & 0 \\ 0 & 0 & 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & 0 & 0 & 0 & x & x \end{pmatrix}$$

Banded Problem – Step 1 (QR)

Do a QR decomposition of H using Householder transformations
Only $O(b^2 n)$ flops for small bandwidth

$$\begin{pmatrix}
x & x & x & 0 & 0 & 0 & 0 & 0 \\
0 & x & x & \mathbf{x} & 0 & 0 & 0 & 0 \\
0 & \mathbf{0} & x & x & 0 & 0 & 0 & 0 \\
0 & 0 & x & x & x & 0 & 0 & 0 \\
0 & 0 & 0 & x & x & x & 0 & 0 \\
0 & 0 & 0 & 0 & x & x & x & 0 \\
0 & 0 & 0 & 0 & 0 & x & x & x \\
0 & 0 & 0 & 0 & 0 & 0 & x & x
\end{pmatrix}$$

Banded Problem – Step 1 (QR)

Do a QR decomposition of H using Householder transformations
Only $O(b^2 n)$ flops for small bandwidth

$$R_1 = \begin{pmatrix} x & x & \mathbf{x} & 0 & 0 & 0 & 0 & 0 \\ \mathbf{0} & x & x & \mathbf{x} & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & x & x & \mathbf{x} & 0 & 0 & 0 \\ 0 & 0 & \mathbf{0} & x & x & \mathbf{x} & 0 & 0 \\ 0 & 0 & 0 & \mathbf{0} & x & x & \mathbf{x} & 0 \\ 0 & 0 & 0 & 0 & \mathbf{0} & x & x & \mathbf{x} \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} & x & x \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{0} & x \end{pmatrix}$$

Store Q_1 as $n-1$ Householder vectors

Banded Problem – Step 2 (Pivot)

Theorem (Previously Known)

Let $A \in \mathbb{C}^{n\times n}$, $x \in \mathbb{C}^n$, $||x||_2 = 1$

$$k = \mathrm{argmax}_i |x_i|.$$

Let $\Pi \in \mathbb{R}^{n\times n}$ *be a permutation matrix such that* $\Pi e_n = e_k$*, and* $A\Pi = QR$*. If* $||Ax||_2 = \epsilon$*, then* $|R_{nn}| \leq \sqrt{n}\epsilon$*.*

1. Solve $||R_1 x|| \approx \sigma_{min}$ (inverse iteration on $R_1^* R_1$)
2. $k = \mathrm{argmax}_i |x_i|$
3. Pick $\Pi = (e_1, \dots, e_{k-1}, e_{k+1}, \dots, e_n, e_k)$

Banded Problem – Step 2 (Pivot)

Suppose we want to pivot 3rd column to last ($k = 3$)

$$\begin{pmatrix} x & x & \mathbf{x} & 0 & 0 & 0 & 0 & 0 \\ 0 & x & \mathbf{x} & x & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{x} & x & x & 0 & 0 & 0 \\ 0 & 0 & \mathbf{0} & x & x & x & 0 & 0 \\ 0 & 0 & \mathbf{0} & 0 & x & x & x & 0 \\ 0 & 0 & \mathbf{0} & 0 & 0 & x & x & x \\ 0 & 0 & \mathbf{0} & 0 & 0 & 0 & x & x \\ 0 & 0 & \mathbf{0} & 0 & 0 & 0 & 0 & x \end{pmatrix}$$

Banded Problem – Step 2 (Pivot)

Suppose we want to pivot 3rd column to last ($k = 3$)

$$\begin{pmatrix} x & x & 0 & 0 & 0 & 0 & 0 & \mathbf{x} \\ 0 & x & x & 0 & 0 & 0 & 0 & \mathbf{x} \\ 0 & 0 & x & x & 0 & 0 & 0 & \mathbf{x} \\ 0 & 0 & x & x & x & 0 & 0 & \mathbf{0} \\ 0 & 0 & 0 & x & x & x & 0 & \mathbf{0} \\ 0 & 0 & 0 & 0 & x & x & x & \mathbf{0} \\ 0 & 0 & 0 & 0 & 0 & x & x & \mathbf{0} \\ 0 & 0 & 0 & 0 & 0 & 0 & x & \mathbf{0} \end{pmatrix}$$

Banded Problem – Step 3 (QR Again)

Only one sub diagonal needs to be zeroed
Do this with givens rotations

$$\begin{pmatrix} x & x & 0 & 0 & 0 & 0 & 0 & x \\ 0 & x & x & 0 & 0 & 0 & 0 & x \\ 0 & 0 & x & x & 0 & 0 & 0 & x \\ 0 & 0 & \mathbf{x} & x & x & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{x} & x & x & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{x} & x & x & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{x} & x & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{x} & 0 \end{pmatrix}$$

Banded Problem – Step 3 (QR Again)

Only one sub diagonal needs to be zeroed
Do this with givens rotations: $O(n)$ flops

$$R = \begin{pmatrix} x & x & 0 & 0 & 0 & 0 & 0 & x \\ 0 & x & x & 0 & 0 & 0 & 0 & x \\ 0 & 0 & x & x & \mathbf{x} & 0 & 0 & x \\ 0 & 0 & 0 & x & x & \mathbf{x} & 0 & \mathbf{x} \\ 0 & 0 & 0 & 0 & x & x & \mathbf{x} & \mathbf{x} \\ 0 & 0 & 0 & 0 & 0 & x & x & \mathbf{x} \\ 0 & 0 & 0 & 0 & 0 & 0 & x & \mathbf{x} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{x} \end{pmatrix}$$

R has small bandwidth except for $R_{:n}$

Unstructurally Banded Problem

Some problems have varying size bandwidth
It is possible to take advantage of this

Characterize nonzeros of H by

$$\begin{array}{ll} B_U = \{\ell_1^U, \ell_2^U, \ldots, \ell_n^U\} & \text{(upper column boundaries)} \\ B_L = \{\ell_1^L, \ell_2^L, \ldots, \ell_n^L\} & \text{(lower column boundaries)} \\ B_R = \{\ell_1^R, \ell_2^R, \ldots, \ell_n^R\} & \text{(right row boundaries)} \end{array}$$

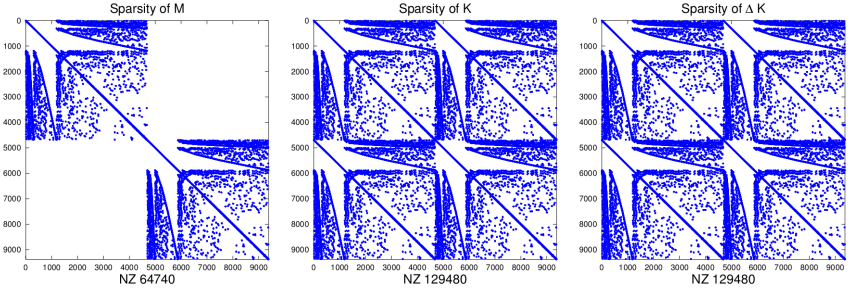
B_R is redundant, but useful

Numerical Example

From finite element model of a vibrating structure with nonproportional damping

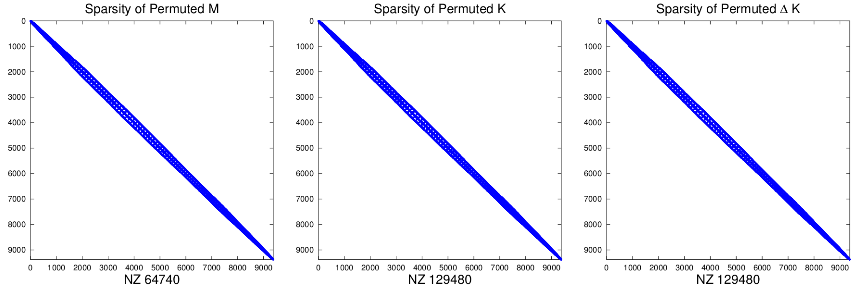
$$H(\lambda) = \lambda^2 M + K - \frac{1}{1+\beta\lambda}\Delta K$$

Matrix sizes: 9376 by 9376



Numerical Example

Use `symrcm` Octave command on $|M| + |K| + |\Delta K|$ to make banded



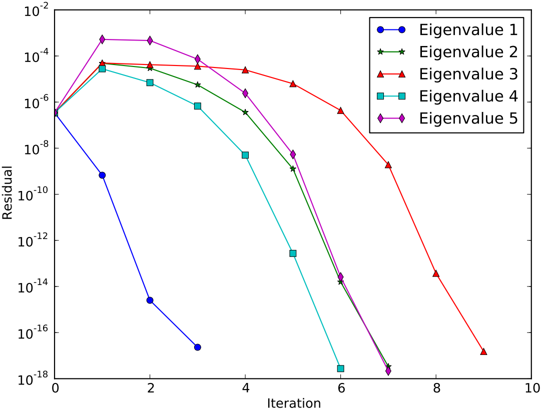
Numerical Example

Convergence Data

iteration	k	residual	eigenvalue
0	7	1.1e-05	-1.000000e0 - i1.000000e1
1	2455	8.9e-05	-1.578073e3 - i2.145839e4
2	2787	2.4e-05	-1.374332e3 - i2.143317e4
3	2787	2.1e-05	-1.410348e3 - i2.153883e4
4	2787	1.5e-06	-1.405421e3 - i2.149456e4
5	2787	1.4e-08	-1.408698e3 - i2.149333e4
6	2787	1.0e-12	-1.408685e3 - i2.149336e4
7	2787	1.5e-17	-1.408685e3 - i2.149336e4

Numerical Example

Can also solve for many eigenvalues
Initial condition: 1408 - 21493i



Questions?