Spectral Differentiation Matrices for the Numerical Solution of Schrödinger's Equation

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"I have no satisfaction in formulas
unless I feel their numerical magnitude"

Lord Kelvin

Overview of talk:

1. Quick Introduction
2. Software (DMSUITE)
3. Solving Schrödinger's Equation

1. Quick Introduction

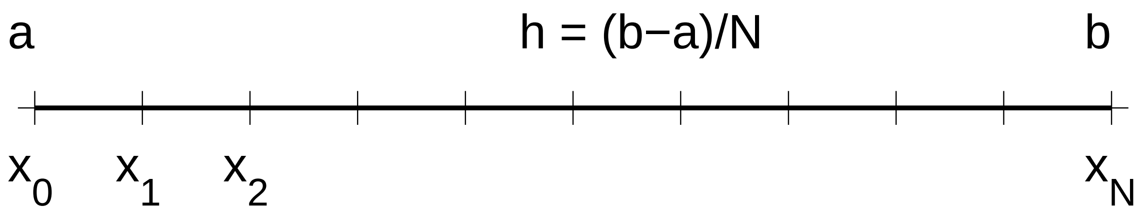
Consider toy problem

$$y''(x) = \lambda\, y(x), \qquad -1 \le x \le 1,$$

subject to boundary conditions

$$y(-1) = y(+1) = 0.$$

Discretize by Method of Finite Differences



Denote

$$y_j \approx y(x_j)$$

Approximate second derivative by central differences

$$y''(x) = \lambda\, y(x)$$

$$\Longrightarrow \qquad \frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} = \lambda\, y_j, \qquad j = 1, \ldots, N-1$$

$$\Longrightarrow \qquad D_2 \mathbf{y} = \lambda\, \mathbf{y}$$

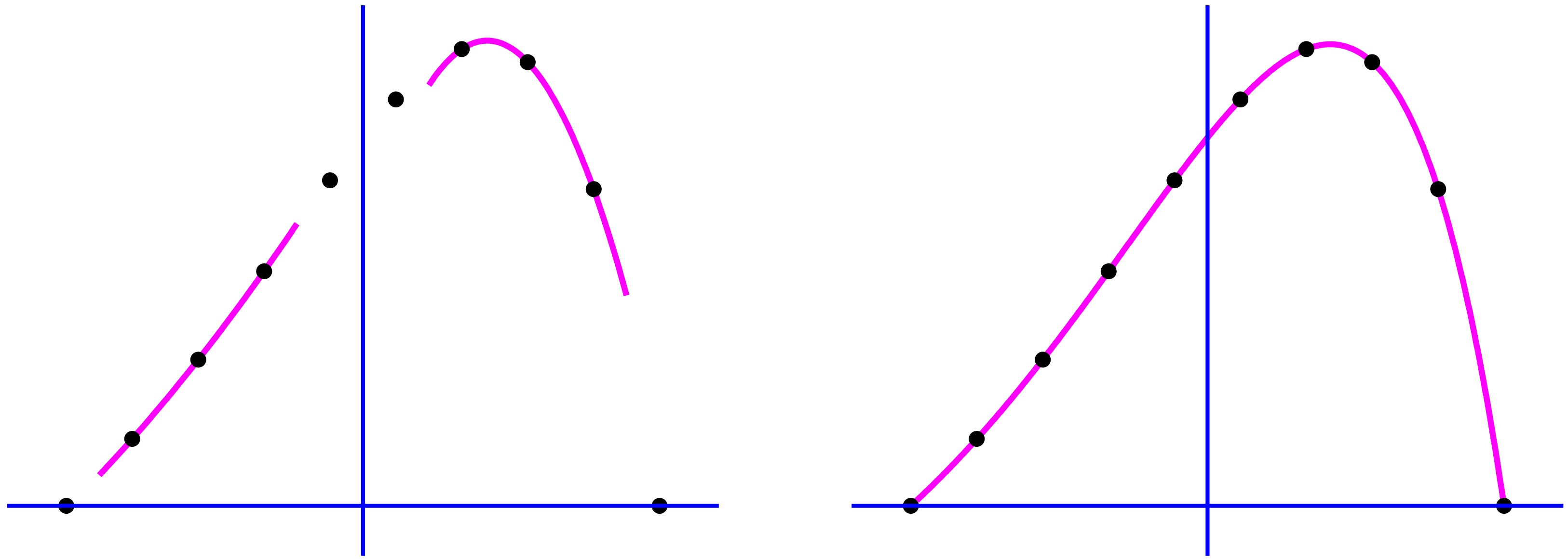
Here

$$D_2 = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}, \qquad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \end{pmatrix}$$

Differentiation matrix: $D_2 =$ matrix representation of $\frac{d^2}{dx^2}$ + BCs

Basic idea of Spectral Collocation a.k.a. Pseudospectral Method:
Do not use local interpolants, use a single global interpolant instead

Finite Differences   Spectral Collocation



Lagrange form of polynomial interpolant

$$p_N(x) = L_0(x)\,u_0 + L_1(x)\,u_1 + \ldots + L_N(x)\,u_N$$

where

$$L_k(x) = \text{pol. degree } N, \qquad L_k(x_j) = \begin{cases} 1 & k = j \\ 0 & k \neq j \end{cases}$$

Differentiate twice and evaluate at $x = x_j$

$$p_N''(x_j) = L_0''(x_j)\,u_0 + L_1''(x_j)\,u_1 + \ldots + L_N''(x_j)\,u_N$$

Substitute into

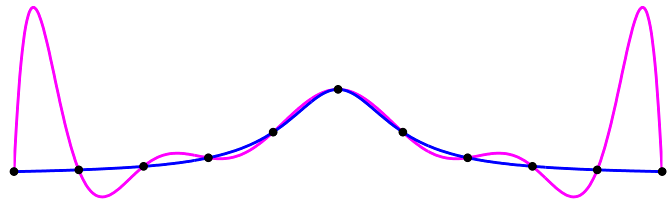
$$p_N''(x_j) = \lambda\, y(x_j)$$

$\Longrightarrow$

$$\begin{pmatrix} L_1''(x_1) & L_2''(x_1) & \ldots & L_{N-1}''(x_1) \\ L_1''(x_2) & L_2''(x_2) & \ldots & L_{N-1}''(x_2) \\ \vdots & \vdots & & \vdots \\ L_1''(x_{N-1}) & L_2''(x_{N-1}) & \ldots & L_{N-1}''(x_{N-1}) \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{pmatrix}$$

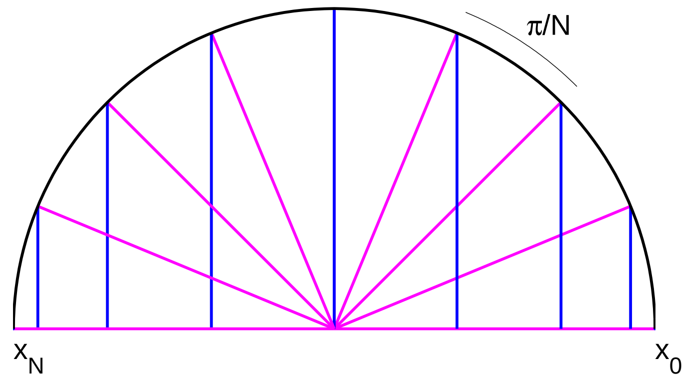
Defines spectral differentiation matrix D_2.

Important: Do not use equidistant points: they lead to ill-conditioning & Runge phenomenon $\longrightarrow$



Rather use Chebyshev points of the second kind, defined by

$$x_k = \cos\left(\frac{k\pi}{N}\right), \qquad k = 0, \ldots, N$$



References:

L.N. Trefethen, *Spectral Methods in* MATLAB, SIAM, 2000

B. Fornberg, *A Practical Guide to Pseudospectral Methods*, CUP, 1996

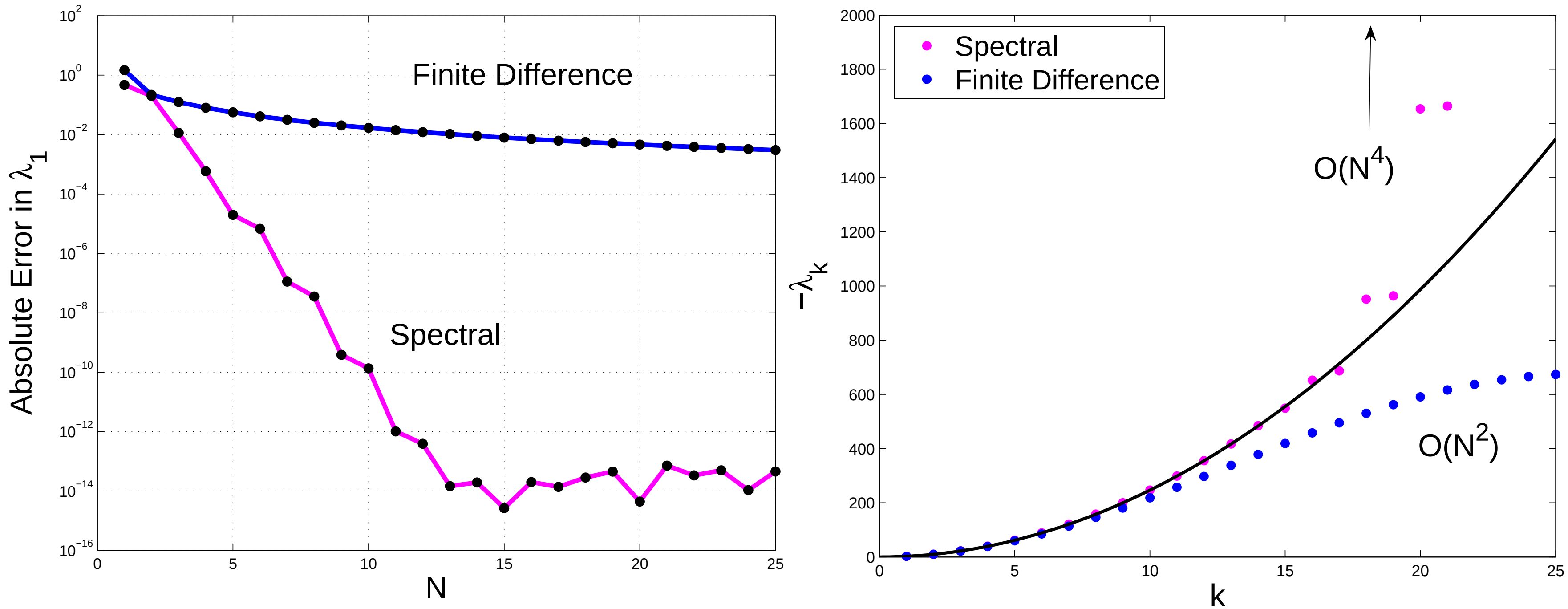
Solve Toy Example as test problem

$$y''(x) = \lambda\, y(x) \qquad \Longrightarrow \qquad D_2 \mathbf{y} = \lambda\, \mathbf{y}$$

On [-1,1] exact eigenvalues/functions are given by

$$\lambda_k = -\frac{k^2\pi^2}{4}, \qquad y_k(x) = \begin{cases} \cos\left(\frac{1}{2}k\pi x\right) & k \text{ odd} \\ \sin\left(\frac{1}{2}k\pi x\right) & k \text{ even.} \end{cases}$$

Solve algebraic eigenvalue problem $D_2 \mathbf{y} = \lambda\, \mathbf{y}$ numerically
and plot absolute errors in $k = 1$ eigenvalues as functions of N:



Absolute Error in λ_1
N
Finite Difference
Spectral
$-\lambda_k$
k
Spectral
Finite Difference
$O(N^4)$
$O(N^2)$

Variations on the Theme

Weighted Polynomial Methods:

$$p_N(x) = w(x)\Big(L_0(x)\,u_0 + L_1(x)\,u_1 + \ldots + L_N(x)\,u_N\Big)$$

⋆ Hermite weight:

$$w(x) = e^{-x^2/2}, \quad x \in (-\infty, \infty), \quad x_k = \text{zeros of } H_{N+1}(x)$$

⋆ Laguerre weight:

$$w(x) = e^{-x}, \quad x \in [0, \infty), \quad x_k = \text{zeros of } L_{N+1}(x)$$

Non-Polynomial Methods:

⋆ Trigonometric (Fourier)

⋆ Sinc (cardinal)

2. SOFTWARE

DMSUITE $=$ MATLAB package developed by JACW and SC Reddy

- ⋆ It computes pseudospectral D matrices corresponding to
  - Chebyshev
  - Hermite
  - Laguerre
  - Fourier
  - Sinc
- ⋆ plus utilities for BCs.

Attention to:

- ⋆ efficient MATLAB coding (i.e., vectorization)
- ⋆ numerical stability

Paper in ACM Trans Math Software, Vol. 26, pp. 465–519 (2000)

Software is free and may be downloaded from

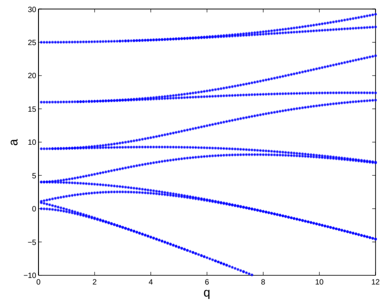
www.mathworks.com   http://dip.sun.ac.za/ weideman

Tutorial-style Applications:

- ⋆ Schrödinger $\quad -y''(x) + y(x) = \lambda\, q(x)\, y(x), \qquad x \in [0, \infty)$
- ⋆ Error Function $\quad y(x) = e^{x^2}\mathrm{erfc}(x), \qquad x \in [0, \infty)$
- ⋆ Mathieu Equation

$$y''(x) + (a - 2\,q\,\cos 2x)y = 0$$

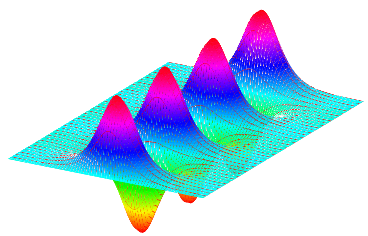
$$x \in [0, 2\pi)$$



- ⋆ Sine-Gordon

$$u_{tt} = u_{xx} - \sin u,$$

$$x \in (-\infty, \infty)$$



- ⋆ Orr-Sommerfeld $R^{-1}\,(y'''' - 2y'' + y) - 2\,i\,y - i\,(1 - x^2)\,(y'' - y) = c\,(y - y'')$

3. Application

Schrödinger's equation on $-\infty < x < \infty$

$$-y''(x) + p(x)\, y(x) = \lambda\, y(x)$$

Approximate by

$$-D_2 \mathbf{y} + \text{diag}\big(p(x_k)\big)\, \mathbf{y} = \lambda\, \mathbf{y}$$

Numerically compute the eigenvalues of

$$A = -D_2 + \text{diag}\big(p(x_k)\big)$$

For D_2, we use Hermite differentiation matrix. I.e., $D_2\mathbf{y}$ provides exact second derivatives whenever $\mathbf{y}$ is sampled from a function of the form

$$y(x) = e^{-x^2/2} \times \Big(\text{Polyn. degree} < N\Big)$$

Quadratic oscillator

$$-y''(x) + x^2 y(x) = \lambda\, y(x)$$

Eigenvalues/functions $k = 0, 1, 2, \dots,$

$$\lambda_k = 2k + 1, \qquad y_k(x) = e^{-x^2/2} H_k(x)$$

Expect numerical method based on $N \times N$ Hermite differentiation matrix to produce exact eigenvalues/functions, for $k = 0, \dots, N-1$.

```
[x, DM] = herdif(N, 2, b)
     D2 = DM(:,:,2)
     A  = -D2+diag(x.^2)
 lambda = sort(eig(A))
```

Test quartic oscillator against WKB formula (Bender & Orszag, p. 523)

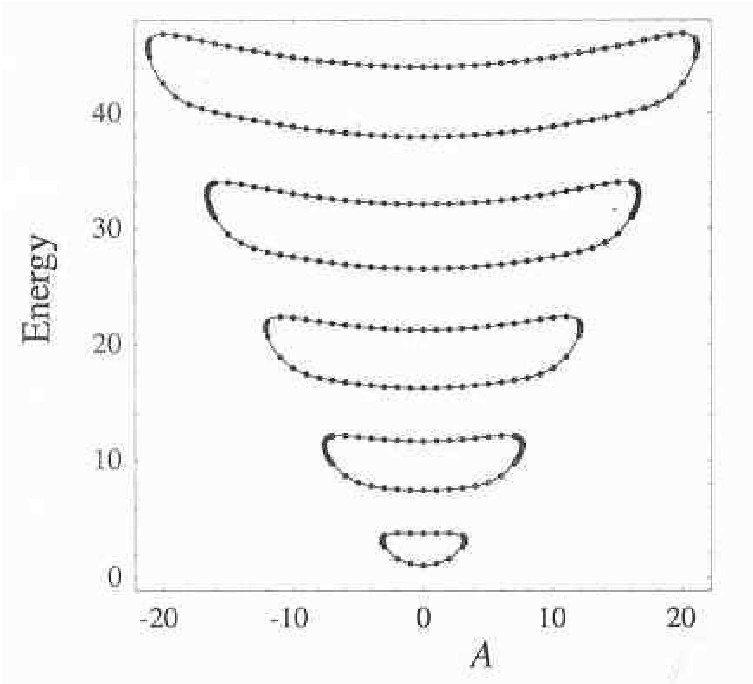
$$\lambda_k \sim \left[\frac{3\sqrt{\pi}\,\Gamma\left(\frac{3}{4}\right)\left(k+\frac{1}{2}\right)}{\Gamma\left(\frac{1}{4}\right)}\right]^{4/3}, \qquad k \to \infty.$$

Numerical	WKB
1.0604	0.8671
3.7997	3.7519
7.4557	7.4140
11.6447	11.6115
16.2618	16.2336
21.2384	21.2137
26.5285	26.5063
32.0986	32.0785
37.9230	37.9045
43.9812	43.9639

Now change problem to

$$-y''(x) + \left(x^4 + iax\right) y(x) = \lambda\, y(x)$$

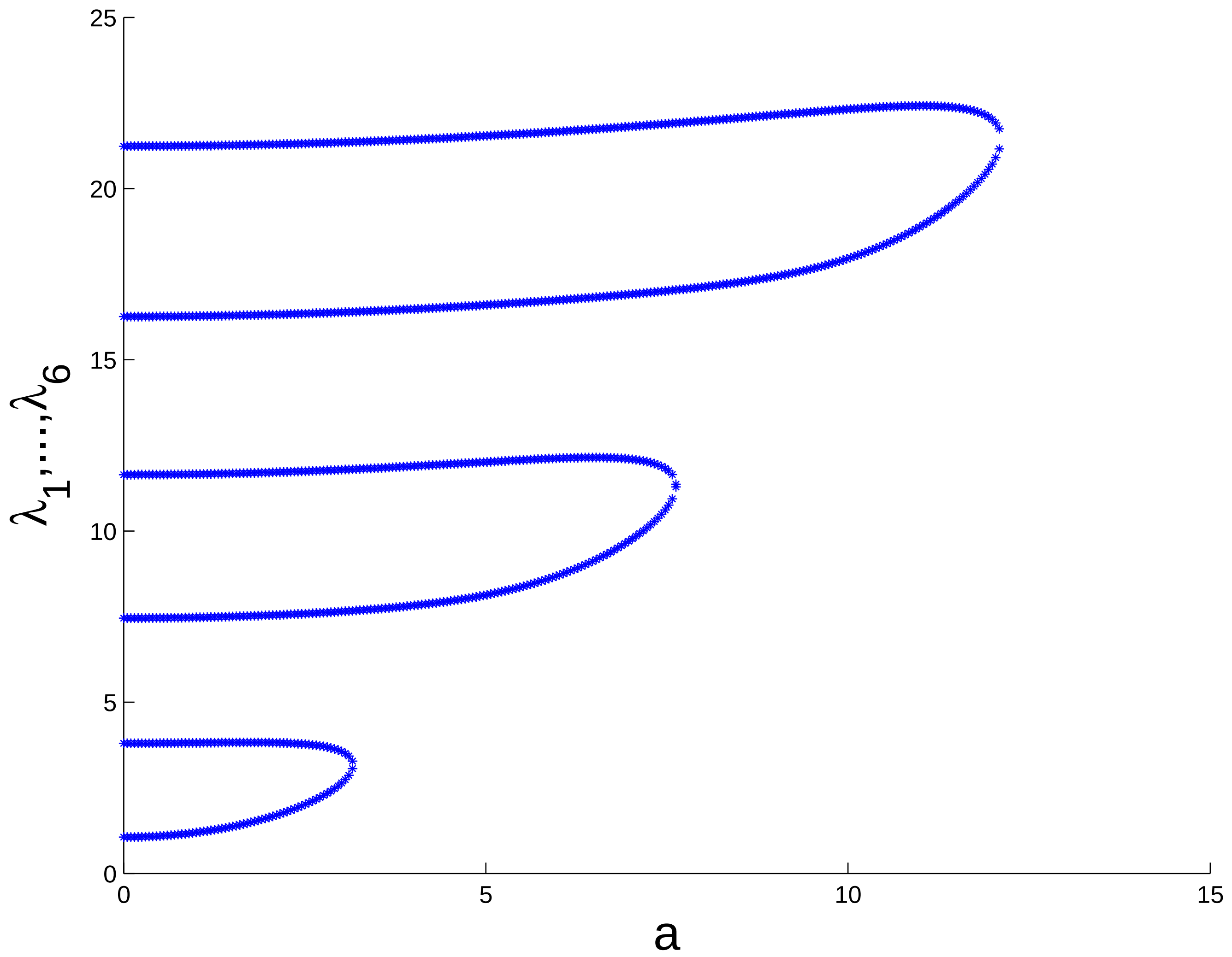
CM Bender, M Berry, et. al., "Complex WKB Analysis of energy-level degeneracies of non-Hermitian Hamiltonians", J. Phys. A: Math. Gen. Vol. 34 (2001) L31-L36.



With D_2 defined as above the complete code is

```
figure(1); axis([0 15 0 25]); hold on;

for   a = linspace(0,15,300);
    A   = -D2+diag(x.^4+i*a*x);
lambda = sort(eig(A));
lambda = lambda(1:6);
   ell = find(abs(imag(lambda)) < sqrt(eps));
lambda = lambda(ell);
plot(a*ones(size(lambda)),lambda,'*','MarkerSize',4);
drawnow
end;
```



$\lambda_1,\ldots,\lambda_6$
a
0
5
10
15
20
25
0
5
10
15

DMSUITE combines well with EigTool (Trefethen, Wright)

For example, compute pseudospectrum of matrix

$$A = -D_2 + \mathrm{diag}\left(x_k^4 + i\,a\,x_k\right), \qquad a = 3.169$$

Plots show values of $F(z) = \|(A - zI)^{-1}\|$