Analytical insight is obtained by considering the SVD $\boldsymbol{S}=\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$, and $\boldsymbol{A}=\boldsymbol{S}^T\boldsymbol{S}=\boldsymbol{V}\boldsymbol{\Sigma}^2\boldsymbol{V}^T$ from which it results that singular values σ of $\boldsymbol{S}$ are square roots of the eigenvalues of $\boldsymbol{A}$. The eigenvalues of a symmetric matrix are real-valued.

Recall (see L14) that eigenvalues of

$$\boldsymbol{D}=\frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \\ & & & 1 & -2 \end{bmatrix}$$

can be obtained by the correspondence between continuum and discrete operators. The matrix $\boldsymbol{D}$ is a discrete version of the second-order differentiation operator ∂_t^2 obtained by centered finite differences

$$\partial_t^2\, u(t)=\frac{\partial^2 u}{\partial t^2}(t)\cong\frac{u(t-h)-2u(t)+u(t+h)}{h^2}.$$

In the continuum case, the derivative at a point requires knowledge of values within a neighborhood, e.g., $u'(t)=\lim_{h\to 0}(u(t+h)-u(t-h)/(2h))$. The corresponding feature of the discrete case is that the differentiation operator is not square. Consider the vector $\hat{\boldsymbol{u}}\in\mathbb{R}^{m+2}$ obtained by sampling $u(t)$ at nodes $t_k=kh$, $h=\pi/(m+1)$, for $k=0,\ldots,m+1$, and the extended matrix

$$\hat{\boldsymbol{D}}=\frac{1}{h^2}\begin{bmatrix} 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & 1 & -2 & 1 & & \\ & & & \ddots & \ddots & & \\ & & & & 1 & -2 & 1 \end{bmatrix}\in\mathbb{R}^{m\times(m+2)}.$$

The finite difference approximation of the second derivative at m interior points $u''(t_k), k=1,\ldots,m$ requires knowledge of $m+2$ function values, expressed in matrix form as

$$\boldsymbol{u}''=\hat{\boldsymbol{D}}\,\hat{\boldsymbol{u}}.$$

The eigensystem of the square matrix $\boldsymbol{D}\in\mathbb{R}^{m\times m}$ can however be obtained by noting that:

i. Eigenfunctions $\varphi(t)$ of ∂_t^2 are solutions of the ordinary differential equation $\partial_t^2\, u=\lambda u$, for $u{:}\,[0,\pi]\to\mathbb{R}$.

ii. Choosing boundary conditions on u to recover the desired matrix $\boldsymbol{D}$.

iii. Positing that eigenvectors of $\boldsymbol{D}$ are obtaining by evaluating $\varphi(t)$ at t_k, $\boldsymbol{z}=[\ \varphi(t_1)\ \ \ldots\ \ \varphi(t_m)\ ]$.

iv. Verifying that $\boldsymbol{D}\boldsymbol{z}=\mu\boldsymbol{z}$ is indeed verified with no dependence of μ on the component index k.

For the matrix $\boldsymbol{D}$, the appropriate boundary conditions are $u_0=u(t_0)=u(0)=0$ and $u_{m+1}=u(t_{m+1})=u(1)=0$, such that

$$\boldsymbol{u}''=\hat{\boldsymbol{D}}\,\hat{\boldsymbol{u}}=\boldsymbol{D}\boldsymbol{u}.$$

At the interval endpoints

$$\frac{\partial^2 u}{\partial t^2}(t_1)=\frac{\partial^2 u}{\partial t^2}(h)\cong\frac{u(0)-2u(h)+u(2h)}{h^2}=\frac{-2u(h)+u(2h)}{h^2},$$

$$\frac{\partial^2 u}{\partial t^2}(t_m)=\frac{\partial^2 u}{\partial t^2}(1-h)\cong\frac{u(1-2h)-2u(1-h)+u(1)}{h^2}=\frac{u(1-2h)-2u(1-h)}{h^2}.$$

Since the boundary value problem

$$u'' = \lambda u, u(0) = u(\pi) = 0,$$

has eigenfunctions $\sin(\xi t)$, $\xi \in \mathbb{Z}$, posit that the eigenvectors $\boldsymbol{z}$ of the $\boldsymbol{D}$ matrix have components $z_k = \sin(\xi t_k) = \sin(\xi k h)$. Verify that $\boldsymbol{z}$ is indeed an eigenvector by computing the k^{th} component of $\boldsymbol{D}\boldsymbol{z}$

$$(\boldsymbol{D}\boldsymbol{z})_k = \frac{1}{h^2}(\sin[\xi(k-1)h] - 2\sin[\xi k h] + \sin[\xi(k+1)h]) = \frac{2}{h^2}[\cos(\xi h) - 1]\sin(\xi k h) = \lambda \sin(\xi k h).$$

In the above calculation

$$\lambda = \frac{2}{h^2}[\cos(\xi h) - 1] = -\left[\frac{2}{h}\sin\left(\frac{\xi h}{2}\right)\right]^2,$$

does not depend on the component index k, hence indeed it is an eigenvalue since $\boldsymbol{D}\boldsymbol{z} = \lambda \boldsymbol{z}$ is satisfied. Verify numerically:

```
∴ function D(m)
    spdiagm(0 => -2*ones(m), -1 => ones(m-1) , 1 => ones(m-1))
  end;
∴ m=10; num=eigen(collect(D(m))).values;
∴ h=pi/(m+1); csi=m:-1:1; an=-(2*sin.(csi*h/2)).^2;
∴ [num an]
```

$$\left[\begin{array}{cc} -3.9189859472289936 & -3.9189859472289945 \\ -3.682507065662361 & -3.682507065662362 \\ -3.309721467890569 & -3.30972146789057 \\ -2.830830026003772 & -2.830830026003773 \\ -2.284629676546571 & -2.28462967654657 \\ -1.715370323453428 & -1.7153703234534299 \\ -1.1691699739962265 & -1.1691699739962276 \\ -0.6902785321094298 & -0.6902785321094301 \\ -0.31749293433763814 & -0.3174929343376377 \\ -0.08101405277100523 & -0.08101405277100529 \end{array}\right] \quad (1)$$

∴

From the above, the eigenvalues of $\boldsymbol{B} = h^2 \boldsymbol{D} + 4\boldsymbol{I}$ can readily be found as

$$\mu = 4\left[1 - \sin^2\left(\frac{\xi h}{2}\right)\right] = 4\cos^2\left(\frac{\xi h}{2}\right).$$

∴

The fact that the matrix $\boldsymbol{A} = \boldsymbol{S}^T \boldsymbol{S}$ differs from $\boldsymbol{B}$ just through a rank-one update at the right endpoint,

$$\boldsymbol{A} = \left[\begin{array}{cccccc} 2 & 1 & & & & \\ 1 & 2 & 1 & & & \\ & 1 & 2 & 1 & & \\ & & \ddots & \ddots & & \\ & & & 1 & 2 & 1 \\ & & & & 1 & 1 \end{array}\right] = \left[\begin{array}{cccccc} 2 & 1 & & & & \\ 1 & 2 & 1 & & & \\ & 1 & 2 & 1 & & \\ & & \ddots & \ddots & & \\ & & & 1 & 2 & 1 \\ & & & & 1 & 2 \end{array}\right] - \left[\begin{array}{cccccc} 0 & 0 & & & & \\ 0 & 0 & 0 & & & \\ & 0 & 0 & 0 & & \\ & & \ddots & \ddots & & \\ & & & 0 & 0 & 0 \\ & & & & 0 & 1 \end{array}\right] = \boldsymbol{B} - \boldsymbol{e}_m \boldsymbol{e}_m^T,$$

suggests one of two approaches:

i. Define different boundary conditions for the ordinary differential equation $\partial_t^2 u = \lambda u$.

ii. Find the effect of a rank-one perturbation upon the eigenvalues of $\boldsymbol{B}$.

Consider the first approach, and require

$$\boldsymbol{u}''=\hat{\boldsymbol{D}}\,\hat{\boldsymbol{u}}=\frac{1}{h^2}\begin{bmatrix} 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & 1 & -2 & 1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & 1 & -2 & 1 \end{bmatrix}\begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_m \\ u_{m+1} \end{bmatrix}=\frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \\ & & & 1 & -3 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{m-1} \\ u_m \end{bmatrix}=\boldsymbol{C}\boldsymbol{u}.$$

The left end-condition remains the same $u_0-2u_1+u_2=-2u_1+u_2\Rightarrow u_0=0$. At the right obtain

$$u_{m-1}-2u_m+u_{m+1}=u_{m-1}-3u_m\Rightarrow u_{m+1}=-u_m.$$

In the continuum case the above is satisfied when

$$u(t_m+h)+u(t_m)=0.$$

Carrying out a Taylor series expansion and truncating at first order gives the Robin boundary condition

$$2u(t_m)+h\,u'(t_m)=0.$$

This leads to consideration of the Sturm-Liouville problem

$$u''=\lambda u, u(0)=0, 2u(\pi)+h\,u'(\pi)=0.$$

Let $\lambda=\xi^2$ and obtain that a nontrivial solution $u(t)=\sin(\xi t)$ is obtained for ξ that satisfies the right end-condition

$$2\sin(\xi\pi)+\xi h\cos(\xi\pi)=0\Rightarrow\xi=-\frac{2}{h}\tan(\xi\pi)=-\frac{2(m+1)}{\pi}\tan(\xi\pi).$$

A numerical root-finding procedure determines solutions $\{\xi_1,\ldots,\xi_m\}$ of the above equation.

```
∴ using Roots
∴ f(x,m)=x+2*(m+1)*tan(x*pi)/pi; f10(x)=f(x,10);
∴ csi=find_zero.(f10,1:10);
∴ function C(m)
    d = -2*ones(m); d[m]=-3; h=pi/(m+1); s=1/h^2
    spdiagm(0 => s*d, -1 => s*ones(m-1) , 1 => s*ones(m-1))
  end;
∴ num=eigen(collect(C(10))).values
```

$$\begin{bmatrix} -48.76558779735465 \\ -46.61123661467208 \\ -42.4939578061028 \\ -36.7795896621686 \\ -29.97587886954959 \\ -22.687364989762944 \\ -15.561664466144167 \\ -9.231927060838379 \\ -4.260577719902124 \\ -1.0893426486848086 \end{bmatrix} \qquad (2)$$

∴ `collect(C(10))`

[−24.51972644144574, 12.25986322072287, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0; 12.25986322072287, −24.519\
72644144574, 12.25986322072287, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0; 0.0, 12.25986322072287, −24.5197264414\
4574, 12.25986322072287, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0; 0.0, 0.0, 12.25986322072287, −24.51972644144574,
12.25986322072287, 0.0, 0.0, 0.0, 0.0, 0.0; 0.0, 0.0, 0.0, 12.25986322072287, −24.51972644144574, 12.25986\
322072287, 0.0, 0.0, 0.0, 0.0; 0.0, 0.0, 0.0, 0.0, 12.25986322072287, −24.51972644144574, 12.2598632207\
2287, 0.0, 0.0, 0.0; 0.0, 0.0, 0.0, 0.0, 0.0, 12.25986322072287, −24.51972644144574, 12.25986322072287, 0.0,
0.0; 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 12.25986322072287, −24.51972644144574, 12.25986322072287, 0.0; 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.0, 12.25986322072287, −24.51972644144574, 12.25986322072287; 0.0, 0.0, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 12.25986322072287, −36.77958966216861] (3)

∴

Verify whether $\boldsymbol{u} = [\sin(\xi t_j)]$ is indeed an eigenvector of $\boldsymbol{C}$.

∴

```
∴ m=10; num=eigen(collect(D(m))).values;
∴ h=pi/(m+1); csi=m:-1:1; an=-(2*sin.(csi*h/2)).^2;
∴ [num an]
```

$$\begin{bmatrix} -3.9189859472289936 & -3.9189859472289945 \\ -3.682507065662361 & -3.682507065662362 \\ -3.309721467890569 & -3.30972146789057 \\ -2.830830026003772 & -2.830830026003773 \\ -2.284629676546571 & -2.28462967654657 \\ -1.715370323453428 & -1.7153703234534299 \\ -1.1691699739962265 & -1.1691699739962276 \\ -0.6902785321094298 & -0.6902785321094301 \\ -0.31749293433763814 & -0.3174929343376377 \\ -0.08101405277100523 & -0.08101405277100529 \end{bmatrix} \quad (4)$$

∴

```
∴ C10=collect(C(10))
```

$$\begin{bmatrix} -2.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & -2.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & -2.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & -2.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & -2.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & -2.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & -2.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & -2.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & -2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & -3.0 \end{bmatrix} \quad (5)$$

∴

For $m = 10$,

$$\{0.956778, 1.91503, 2.87596, 3.84033, 4.80847, 5.78035, 6.75572, 7.73422, 8.71545, 9.69905\}$$

are the roots. Since $\boldsymbol{A}=h^2\boldsymbol{C}+4\boldsymbol{I}$ the smallest and largest eigenvalues of $\boldsymbol{A}$ are

$$h^2\xi_1+4, h^2\xi_m+4$$

and the smallest, largest singular values of $\boldsymbol{S}$ are

$$\sigma_1=\left[\left(\frac{\pi}{m+1}\right)^2\xi_1+4\right]^{1/2}, \sigma_m=\left[\left(\frac{\pi}{m+1}\right)^2\xi_m+4\right]^{1/2}.$$

For $m=10,20,\ldots,100$ the root-finding procedure gives

m	10	20	30	40	50	60	70	80	90	100
ξ_1	0.956778	0.976784	0.98414	0.987957	0.990294	0.991872	0.993008	0.993866	0.994536	0.995074
ξ_m	9.69905	19.6899	29.6868	39.6852	49.6842	59.6836	69.6832	79.6828	89.6826	99.6824

The extremal singular values are

However the matrix $\boldsymbol{A}$ is a rank-one perturbation of $\boldsymbol{B}=\boldsymbol{Q}\Psi\boldsymbol{Q}^T$, $\boldsymbol{A}=\boldsymbol{Q}\Psi\boldsymbol{Q}^T-\boldsymbol{e}_m\boldsymbol{e}_m^T$, $\Psi=\operatorname{diag}(\mu_1,\ldots,\mu_m)$. Numerical experimentation shows that eigenvalues of $\boldsymbol{B}$

From here there are two ways to proceed:

1) Eigenvalues of $\boldsymbol{A}$ are roots of the characteristic polynomial

$$p(\alpha)=\det(\alpha\boldsymbol{I}-\boldsymbol{A})=\det(\alpha\boldsymbol{Q}\boldsymbol{Q}^T-\boldsymbol{Q}\Psi\boldsymbol{Q}^T+\boldsymbol{e}_m\boldsymbol{e}_m^T).$$

Use the factorization

$$\alpha\boldsymbol{Q}\boldsymbol{Q}^T-\boldsymbol{Q}\Psi\boldsymbol{Q}^T+\boldsymbol{e}_m\boldsymbol{e}_m^T=\boldsymbol{Q}(\alpha\boldsymbol{I}-\Psi+\boldsymbol{Q}^T\boldsymbol{e}_m\boldsymbol{e}_m^T\boldsymbol{Q})\boldsymbol{Q}^T,$$

and $\det(\boldsymbol{Q})=1$, $\det(\boldsymbol{F}\boldsymbol{G})=\det(\boldsymbol{F})\det(\boldsymbol{G})$, to obtain

$$p(\alpha)=\det$$

From the SVD $\boldsymbol{S}=\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$, $\boldsymbol{A}=\boldsymbol{S}^T\boldsymbol{S}=\boldsymbol{V}\boldsymbol{\Sigma}^2\boldsymbol{V}^T$ deduce that singular values σ of $\boldsymbol{S}$ are square roots of the eigenvalues of $\boldsymbol{A}$

$$\sigma=2\cos\left(\frac{\xi h}{2}\right)=2\cos\left[\frac{\xi\pi}{2(m+1)}\right].$$

The largest, smallest singular values σ_1, σ_m are obtained for $\xi=1$, $\xi=m$, respectively. This leads to

$$\kappa(\boldsymbol{S})=\|\boldsymbol{S}\|\,\|\boldsymbol{S}^{-1}\|=\frac{\sigma_1}{\sigma_m}=\cos\left[\frac{\pi}{2(m+1)}\right]/\cos\left[\frac{m\pi}{2(m+1)}\right].$$

Verify the above numerical experiment.

```
∴ kappa(m)=cos(pi/2/(m+1))/cos(m*pi/2/(m+1));
∴ r=250:250:1000; num=cond.(Matrix.(S.(r))) ./ r; an=kappa.(r) ./ r; [num an]
```

$$\left[\begin{array}{cc} 1.2757630315067137 & 1.2783158144633153 \\ 1.2745070304499295 & 1.2757818433925137 \\ 1.274085812988015 & 1.2749353382552424 \\ 1.273874725330594 & 1.2745117381282753 \end{array}\right] \qquad (6)$$