MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

The Hamiltonian Extended Krylov Subspace Method (HEKS)

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Given a function $f : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$, we are interested in approximating

$$f(A)v$$

for a large and sparse matrix A and a vector v (where we assume that f is sufficiently regular so that $f(A)$ is well defined).

Typical approach for large-scale computations:
find a matrix $V \in \mathbb{R}^{n\times k}$ with orthogonal columns so that

$$f(A)v \approx V f(V^T AV)V^T v.$$

- As $A_k = V^T AV \in \mathbb{R}^{k\times k}$, the evaluation of $V f(A_k)V^T v$ should be much faster than that of $f(A)v$.
- **Note:** The problem of approximating the action of $f(A)$ to a vector is significantly different from that of approximating $f(A)$ (see seminal Higham book).

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$$f(A)x \approx Vf(V^TAV)V^Tv. \tag{1}$$

Use, e.g., Arnoldi method to compute V as an orthogonal basis of Krylov subspace

$$\mathcal{K}_k(A, v) = \operatorname{span}\{v, Av, A^2v, \ldots, A^{k-1}v\}.$$

As $Ve_1 = v/\|v\|_2$, (1) simplifies to

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[Druskin/Knizhnerman 1998] suggest to use orthogonal basis of the extended Krylov subspace

$$\mathcal{K}_k(A, v) + \mathcal{K}_k(A^{-1}, A^{-1}v) = \operatorname{span}\{A^{-k}v, \ldots, A^{-2}v, A^{-1}v, v, Av, A^2v, \ldots, A^{k-1}v\}.$$

Given v, A, set $\mathbf{V}_1 = \mathtt{gram\_sh}([v, A^{-1}v])$, $\mathcal{V}_0 = \emptyset$.
For $m = 1, 2, \dots,$
1. $\mathcal{V}_m = [\mathcal{V}_{m-1}, \mathbf{V}_m]$
2. Set $\mathcal{T}_m = \mathcal{V}_m^T A \mathcal{V}_m$
3. Compute $y_m = f(\mathcal{T}_m)e_1$
4. If converged then $u_m = \mathcal{V}_m y_m$ and stop
5. $\mathbf{V}'_{m+1} = [A\mathbf{V}_m e_1, A^{-1}\mathbf{V}_m e_2]$
6. $\widehat{\mathbf{V}}_{m+1} \leftarrow$ orthogonalize $\mathbf{V}'_{m+1}$ w.r.to $\mathcal{V}_m$
7. $\mathbf{V}_{m+1} = \mathtt{gram\_sh}(\widehat{\mathbf{V}}_{m+1})$

- At each iteration, two new vectors are added to the space.
- Unless breakdown occurs, at the mth iteration the method has constructed an orthonormal basis of dimension $2m$, given by $\mathcal{V}_m = [V_1, V_2, \dots, V_m]$, $V_i \in \mathbb{R}^{n\times 2}$.
- The orthogonalization is performed first with respect to the previous basis vectors, and then within the new block of 2 vectors.
- Arnoldi-like recurrence

$$A\mathcal{V}_m = \mathcal{V}_m \mathcal{T}_m + V_{m+1}\tau_{m+1,1}E_m^T$$

holds, where $E_m = [e_{2m-1} e_{2m}] \in \mathbb{R}^{2m\times 2}$ and $\tau_{m+1,1} = V_{m+1}^T A V_m$.

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- $H \in \mathbb{R}^{2n\times 2n}$ is *Hamiltonian* matrix iff
  - $J_nH = (J_nH)^T$, where $J_n = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix} \in \mathbb{R}^{2n\times 2n}$ and I_n is the $n\times n$ identity matrix, or, equivalently,
  - there exist matrices E, $B = B^T$, $C = C^T \in \mathbb{R}^{n\times n}$ such that $H = \begin{bmatrix} E & B \\ C & -E^T \end{bmatrix}$.

  In case H is nonsingular, H^{-1} is Hamiltonian as well.
- J_n is orthogonal and skew-symmetric, $J_n^T = J_n^{-1} = -J_n$.
- Let $V \in \mathbb{R}^{2n\times 2m}$ have orthogonal columns and $H \in \mathbb{R}^{2n\times 2n}$ Hamiltonian. Then $V^THV \in \mathbb{R}^{2m\times 2m}$ is (in general) not Hamiltonian.
- A matrix $S \in \mathbb{R}^{2n\times 2n}$ is called *symplectic* if $S^TJ_nS = J_n$. Its columns are *J-orthogonal*.
- A symplectic matrix S is nonsingular with $S^{-1} = J_n^TS^TJ_n$.
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- Let $S \in \mathbb{R}^{2n\times 2m}, m \leq n$, have J-orthogonal columns, $S^TJ_nS = J_m$.
  Let $H \in \mathbb{R}^{2n\times 2n}$ be Hamiltonian.
  1. The matrix $J_m^TS^TJ_n$ is the left inverse of S, $J_m^TS^TJ_nS = I_{2m}$.
  2. The matrix $(J_m^TS^TJ_n)HS$ is Hamiltonian.

Hamiltonian Lanczos Method [B./Faßbender 1997, Ferng et al 1997]

- J-orthogonal basis of Krylov subspace $\mathcal{K}_{2r}(H, u_1) = \mathrm{span}\{u_1, Hu_1, \ldots, H^{2r-1}u_1\}$.
- Generates $S = [U_r \;\; V_r]$ with $U_r, V_r \in \mathbb{R}^{2n\times r}$ with J-orthogonal columns such that

$$H[U_r \; V_r] = [U_r \; V_r] \begin{bmatrix} G^{(r)} & T^{(r)} \\ D^{(r)} & -G^{(r)} \end{bmatrix} + u_{r+1}t_{r+1,r}e_{2r}^T$$

  where $G^{(r)}, D^{(r)} \in \mathbb{R}^{r\times r}$ are diagonal and $T^{(r)} \in \mathbb{R}^{r\times r}$ is tridiagonal.
- Short recurrence to compute the next vectors u_{r+1} and v_{r+1} of the basis involving only the three preceding vectors v_r, u_r, u_{r-1}.
- Requires $2r$ matrix-vector products and $3r$ inner products.
- Arnoldi method requires $2r$ matrix-vector products and r^2 inner products.
- $f(H)u_1 \approx \|u_1\|_2 Sf(J_r^T S^T J_n HS)e_1$ as $J_r^T(S^T(J_n u_1)) = \|u_1\|_2 e_1$.

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Hamiltonian Extended Krylov Subspace (HEKS) Method

Let a Hamiltonian matrix $H \in \mathbb{R}^{2n\times 2n}$ and a vector $u_1 \in \mathbb{R}^{2n}$ be given.

Construct $S_{r+s} \in \mathbb{R}^{2n\times 2(r+s)}$ with J-orthonormal columns such that the columns of S_{r+s} span the same subspace as $\mathcal{K}_{2r}(H, u_1) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u_1)$.

Assume that dim $\mathcal{K}_{2r}(H, u_1) = 2r$ and dim $\mathcal{K}_{2s}(H^{-1}, H^{-1}u_1) = 2s$.

In [Meister 2011], it is suggested to construct S_{r+s} in the following way:

- Step 1: Start with the two vectors in $\mathcal{K}_2(H, u_1)$ and construct

$$S_1 = [u_1 \mid v_1] \in \mathbb{R}^{2n\times 2}$$

  with $S_1^T J_n S_1 = J_1$ and span$\{S_1\} = \mathcal{K}_2(H, u_1)$. $(r = 1, s = 0)$

- Step 2: Take the two vectors in $\mathcal{K}_2(H^{-1}, H^{-1}u_1)$ and construct

$$S_2 = [y_1 \quad u_1 \mid x_1 \quad v_1] = [Y_1 \quad U_1 \mid X_1 \quad V_1] \in \mathbb{R}^{2n\times 4}$$

  with $S_2^T J_n S_2 = J_2$ and span$\{S_2\} = \mathcal{K}_2(H, u_1) + \mathcal{K}_2(H^{-1}, H^{-1}u_1)$. $(r = s = 1)$

Proceed in this fashion by alternating between $\mathcal{K}_{2r}(H, u_1)$ and $\mathcal{K}_{2s}(H^{-1}, H^{-1}u_1)$.

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Assume that

$$S_{2k} = \begin{bmatrix} Y_k & U_k \mid X_k & V_k \end{bmatrix} \in \mathbb{R}^{2n \times 4k}, \qquad Y_k, U_k, X_k, V_k \in \mathbb{R}^{2n \times k}$$

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Repeat the following steps until done:

- Construct u_{k+1} and v_{k+1} and set

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  such that $S_{2k+1}^T J_n S_{2k+1} = J_{2k+1}$ and

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with J-orthonormal columns has been constructed such that its columns span the same space as $\mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$.

Repeat the following steps until done:

- Construct u_{k+1} and v_{k+1} and set

$$\begin{aligned} S_{2k+1} &= \begin{bmatrix} Y_k & U_k & u_{k+1} \mid X_k & V_k & v_{k+1} \end{bmatrix} \\ &= \begin{bmatrix} Y_k & U_{k+1} \mid X_k & V_{k+1} \end{bmatrix} \in \mathbb{R}^{2n\times 4k+2} \end{aligned}$$

  such that $S_{2k+1}^T J_n S_{2k+1} = J_{2k+1}$ and

$$\operatorname{span}\{S_{2k+1}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1).$$

- Construct y_{k+1} and x_{k+1} and set

$$\begin{aligned} S_{2k+2} &= \begin{bmatrix} y_{k+1} & Y_k & U_{k+1} \mid x_{k+1} & X_k & V_{k+1} \end{bmatrix} \\ &= \begin{bmatrix} Y_{k+1} & U_{k+1} \mid X_{k+1} & V_{k+1} \end{bmatrix} \in \mathbb{R}^{2n\times 4k+4} \end{aligned}$$

  such that $S_{2k+2}^T J_n S_{2k+2} = J_{2k+2}$ and

$$\operatorname{span}\{S_{2k+2}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k+2}(H^{-1}, H^{-1}u_1).$$

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$$S_{2k} = \begin{bmatrix} Y_k & U_k \mid X_k & V_k \end{bmatrix} \in \mathbb{R}^{2n \times 4k}, \qquad Y_k, U_k, X_k, V_k \in \mathbb{R}^{2n \times k}$$

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$$\operatorname{span}\{S_{2k+2}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k+2}(H^{-1}, H^{-1}u_1).$$

Observation: In case $r = s = k$, $H_{2k} = J_{2k} S_{2k}^T J_n H S_{2k} \in \mathbb{R}^{4k \times 4k}$ has the form (Hamiltonian)

$$
\left[\begin{array}{cccc|cccc||cccc|cccc}
0 & & & & & & & & \lambda_k & & & & & & & \gamma_k \\
& \ddots & & & & & & & & \ddots & & & & & \iddots & \mu_k \\
& & \ddots & & & & & & & & \ddots & & & \iddots & \iddots & \\
& & & 0 & & & & & & & & \lambda_1 & \gamma_1 & \mu_2 & & \\
\hline
& & & & 0 & & & & & & & \gamma_1 & \alpha_1 & \beta_2 & & \\
& & & & & \ddots & & & & & \iddots & \mu_2 & \beta_2 & \ddots & \ddots & \\
& & & & & & \ddots & & & \iddots & \iddots & & & \ddots & \ddots & \beta_k \\
& & & & & & & 0 & \gamma_k & \mu_k & & & & & \beta_k & \alpha_k \\
\hline\hline
\delta_k & & & & & & & & 0 & & & & & & & \\
& \ddots & & & & & & & & \ddots & & & & & & \\
& & \ddots & & & & & & & & \ddots & & & & & \\
& & & \delta_1 & & & & & & & & 0 & & & & \\
\hline
& & & & \vartheta_1 & & & & & & & & 0 & & & \\
& & & & & \ddots & & & & & & & & \ddots & & \\
& & & & & & \ddots & & & & & & & & \ddots & \\
& & & & & & & \vartheta_k & & & & & & & & 0
\end{array}\right]
$$

Observation: In case $r = s + 1 = k + 1$ the special form of the Hamiltonian matrix $H_{2k+1} = J_{2k+1} S_{2k+1}^T J_n H S_{2k+1}$ is given by

$$
\left[\begin{array}{c|c||c|c}
\begin{matrix} 0 & & & \\ & \ddots & & \\ & & \ddots & \\ & & & 0 \end{matrix} & &
\begin{matrix} \lambda_k & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \lambda_1 \end{matrix} &
\begin{matrix} & & & \gamma_k & \mu_{k+1} \\ & & \iddots & \mu_k & \\ & \iddots & \iddots & & \\ \gamma_1 & \mu_2 & & & \end{matrix} \\
\hline
& \begin{matrix} 0 & & & & \\ & \ddots & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & 0 \end{matrix} &
\begin{matrix} & & & \gamma_1 \\ & & \iddots & \mu_2 \\ & \iddots & \iddots & \\ \gamma_k & \mu_k & & \\ \mu_{k+1} & & & \end{matrix} &
\begin{matrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \ddots & \beta_k & \\ & & \ddots & \ddots & \beta_{k+1} \\ & & & \beta_{k+1} & \alpha_{k+1} \end{matrix} \\
\hline\hline
\begin{matrix} \delta_k & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \delta_1 \end{matrix} & &
\begin{matrix} 0 & & & \\ & \ddots & & \\ & & \ddots & \\ & & & 0 \end{matrix} & \\
\hline
& \begin{matrix} \vartheta_1 & & & & \\ & \ddots & & & \\ & & \ddots & & \\ & & & \vartheta_k & \\ & & & & \vartheta_{k+1} \end{matrix} & &
\begin{matrix} 0 & & & & \\ & \ddots & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & 0 \end{matrix}
\end{array}\right]
$$

Inductive proof:
Assume that we have constructed

$$S_{2k} = [y_k \ \cdots \ y_1 \ u_1 \ \cdots \ u_k \mid x_k \ \cdots \ x_1 \ v_1 \ \cdots \ v_k] = [Y_k \ U_k \mid X_k \ V_k] \in \mathbb{R}^{2n \times 4k}$$

such that $S_{2k}^T JnS_{2k} = J_{2k}$,

$$\begin{aligned} H_{2k} &= J_{2k}^T S_{2k}^T J_n H S_{2k} \\ &= \begin{bmatrix} -X_k^T J_n HY_k & -X_k^T J_n HU_k & -X_k^T J_n HX_k & -X_k^T J_n HV_k \\ -V_k^T J_n HY_k & -V_k^T J_n HU_k & -V_k^T J_n HX_k & -V_k^T J_n HV_k \\ Y_k^T J_n HY_k & Y_k^T J_n HU_k & Y_k^T J_n HX_k & Y_k^T J_n HV_k \\ U_k^T J_n HY_k & U_k^T J_n HU_k & U_k^T J_n HX_k & U_k^T J_n HV_k \end{bmatrix} \\ &= \begin{bmatrix} 0 & 0 & \Lambda_k & B_{kk} \\ 0 & 0 & B_{kk}^T & T_k \\ \Delta_k & 0 & 0 & 0 \\ 0 & \Theta_k & 0 & 0 \end{bmatrix} \end{aligned}$$

and

$$\mathrm{span}\{S_{2k}\} = \mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1).$$

The next two vectors $H^{2k}u_1$ and $H^{2k+1}u_1$ from $\mathcal{K}_{2k+2}(H,u_1)$ are added as u_{k+1} and v_{k+1}

$$\begin{aligned} S_{2k+1} &= [y_k \ \cdots \ y_1 \ u_1 \ \cdots \ u_{k+1} \mid x_k \ \cdots \ x_1 \ v_1 \ \cdots \ v_{k+1}] \\ &= [Y_k \ U_{k+1} \mid X_k \ V_{k+1}] \in \mathbb{R}^{2n \times 4k+2}. \end{aligned}$$

Then by construction

$$S_{2k+1}^T J_n S_{2k+1} = J_{2k+1}$$

and

$$\mathrm{span}\{S_{2k+1}\} = \mathcal{K}_{2k+2}(H,u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1).$$

It remains to prove the special form of $H_{2k+1} = J_{2k+1}^T S_{2k+1}^T J_n H S_{2k+1}$.

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\begin{aligned}
S_{2k+1} &= [y_k \ \cdots \ y_1 \ u_1 \ \cdots \ u_{k+1} \mid x_k \ \cdots \ x_1 \ v_1 \ \cdots \ v_{k+1}] \\
&= [Y_k \ U_{k+1} \mid X_k \ V_{k+1}] \in \mathbb{R}^{2n \times 4k+2}.
\end{aligned}
$$

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$$S_{2k+1}^T J_n S_{2k+1} = J_{2k+1}$$

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$$H_{2k+1} = J_{2k+1}^T S_{2k+1}^T J_n H S_{2k+1} =$$

$$\left[\begin{array}{c|c|c||c|c|c}
0 & 0 & -X_k^T J_n H u_{k+1} & \Lambda_k & B_{kk} & -X_k^T J_n H v_{k+1} \\ \hline
0 & 0 & -V_k^T J_n H u_{k+1} & {B_{kk}}^T & T_k & -V_k^T J_n H v_{k+1} \\
-v_{k+1}^T J_n H Y_k & -v_{k+1}^T J_n H U_k & -v_{k+1}^T J_n H u_{k+1} & -v_{k+1}^T J_n H X_k & -v_{k+1}^T J_n H V_k & -v_{k+1}^T J_n H v_{k+1} \\ \hline\hline
\Delta_k & 0 & Y_k^T J_n H u_{k+1} & 0 & 0 & Y_k^T J_n H v_{k+1} \\ \hline
0 & \Theta_k & U_k^T J_n H u_{k+1} & 0 & 0 & U_k^T J_n H v_{k+1} \\
u_{k+1}^T J_n H Y_k & u_{k+1}^T J_n H U_k & u_{k+1}^T J_n H u_{k+1} & u_{k+1}^T J_n H X_k & u_{k+1}^T J_n H V_k & u_{k+1}^T J_n H v_{k+1}
\end{array}\right]$$

$$= \left[\begin{array}{c|cc||c|c|c}
0 & 0 & 0 & \Lambda_k & B_{kk} & \begin{smallmatrix}\mu_k \\ 0 \\ \vdots \\ 0\end{smallmatrix} \\ \hline
0 & 0 & 0 & {B_{kk}}^T & T_k & \begin{smallmatrix}0 \\ \vdots \\ 0 \\ \beta_{k+1}\end{smallmatrix} \\
0 & 0 & 0 & \mu_k \; 0 \cdots 0 & 0 \cdots 0 \; \beta_{k+1} & \alpha_{k+1} \\ \hline\hline
\Delta_k & 0 & 0 & 0 & 0 & 0 \\ \hline
0 & \Theta_k & 0 & 0 & 0 & 0 \\
0 & 0 & \vartheta_{k+1} & 0 & 0 & 0
\end{array}\right]$$

Yields algorithm with short recurrences, about 1 page long.

Efficient implementation requires

- 4 matrix-vector-multiplications with H,
- 3 linear solves with H,
- 14 scalar products.

Theorem

Let $H \in \mathbb{R}^{2n \times 2n}$ be a Hamiltonian matrix. Let $r + s = n$ and either $r = s + 1$ or $r = s$. Then in case the procedure sketched does not break down for $u_1 \in \mathbb{R}^{2n}$ with $\|u_1\|_2 = 1$, there exists a symplectic matrix $S \in \mathbb{R}^{2n \times 2n}$ such that $Se_{s+1} = u_1$,

$$\operatorname{span}\{S\} = \mathcal{K}_{2r}(H, u_1) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u_1),$$

and

$$S^{-1}HS = H_{r+s}.$$

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Hamiltonian Extended Krylov Subspace (HEKS) Method

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- HEKS-recursion for $r = s = k$

$$HS_{2k} = S_{2k}H_{2k} + u_{k+1}(\mu_{k+1}e_{2k+1}^T + \beta_{k+1}e_{4k}^T).$$

In case $\mu_{k+1} = \beta_{k+1} = 0$ or $u_{k+1} = 0$, we have a lucky breakdown as

$$\text{span}\{S_{2k}\} = \mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$$

is H-invariant.

- HEKS-recursion for $r = s + 1 = k + 1$

$$HS_{2k+1} = S_{2k+1}H_{2k+1} + (\gamma_{k+1}y_{k+1} + \beta_{k+2}u_{k+2})e_{4k+2}^T.$$

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Note that $y_{k+1} \neq 0$ as it is a column of S_{2k+1}!

- Serious breakdown is possible.

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$$H = \begin{bmatrix} A & 0 \\ 0 & -A^T \end{bmatrix},$$

for `A = diag(logspace(-1,0,500));`
(500 logarithmically equally spaced points between 10^{-1} and 10^{0}).

Consider

- exp(H)v
- cos(H)v
- sign(H)v

for random vector $v = x$ or all-ones-vector $v = e$.

Numerical Experiment 1

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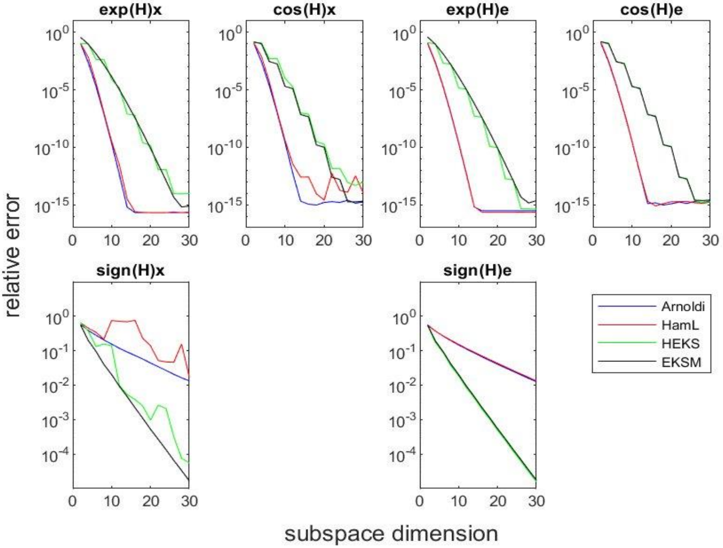
exp(H)x
cos(H)x
exp(H)e
cos(H)e
sign(H)x
sign(H)e
relative error
subspace dimension
Arnoldi
HamL
HEKS
EKSM

$$H = \begin{bmatrix} A & -G \\ -Q & -A^T \end{bmatrix} \in \mathbb{R}^{1998 \times 1998},$$

with $N = 500$ and

$$G = \mathrm{diag}(1, 0, 1, 0, \ldots 1, 0, 1) \in \mathbb{R}^{2N-1 \times 2N-1},$$

$$Q = \mathrm{diag}(0, 10, 0, 10, \ldots 0, 10, 0) \in \mathbb{R}^{2N-1 \times 2N-1},$$

$$A = \begin{bmatrix} A_{11} & A_{12} & 0 & \cdots & \cdots & 0 \\ 0 & A_{22} & A_{23} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots & \\ 0 & \cdots & 0 & A_{N-2,N-2} & A_{N-2,N-1} & 0 \\ 0 & \cdots & 0 & 0 & A_{N-1,N-1} & \begin{bmatrix} 0 \\ -1 \end{bmatrix} \\ 0 & \cdots & 0 & 0 & \begin{bmatrix} 0 & 0 \end{bmatrix} & -1 \end{bmatrix} \in \mathbb{R}^{2N-1 \times 2N-1}$$

with

$$A_{kk} = \begin{bmatrix} -1 & 0 \\ 1 & 0 \end{bmatrix}, \qquad A_{k,k+1} = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix}.$$

Numerical Experiment 2