
Algorithm 2 CHEBYCHEV-PROPAGATOR Evaluate $\vec{w} = f(\pm \hat{A} dt) \vec{v}$,
with $f(\pm \hat{A} dt) = e^{\pm i \hat{A} dt}$.

Input: input vector $\vec{v} \in \mathbb{C}^N$; operator $\hat{A} \in \mathbb{C}^{N \times N}$; time step dt ;
Output: Approximation of propagated vector $\vec{w} = e^{-i \hat{A} dt} \vec{v} \in \mathbb{C}^N$

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1: procedure CHEBY( $\vec{v}$ ,  $\hat{A}$ ,  $dt$ )
2:    $\Delta =$  spectral radius of  $\hat{A}$ 
3:    $E_{\min} =$  minimum eigenvalue of  $\hat{A}$ 
4:    $[a_0 \dots a_n] = \text{EXPCHEBYCOEFFS}(\Delta, E_{\min}, dt)$ 
5:    $d = \frac{1}{2} \Delta$ ;  $\beta = d + E_{\min}$ 
6:    $\vec{v}_0 = \vec{v}$ 
7:    $\vec{w}^{(0)} = a_0 \vec{v}_0$ 
8:    $\vec{v}_1 = \pm \frac{i}{d} \left( \hat{A} \vec{v}_0 - \beta \vec{v}_0 \right)$ 
9:    $\vec{w}^{(1)} = \vec{w}^{(0)} + a_1 \vec{v}_1$ 
10:  for  $i = 2 : n$  do
11:     $\vec{v}_i = \pm \frac{2i}{d} \left( \hat{A} \vec{v}_{i-1} - \beta \vec{v}_{i-1} \right) + \vec{v}_{i-2}$ 
12:     $\vec{w}^{(i)} = \vec{w}^{(i-1)} + a_i \vec{v}_i$ 
13:  end for
14:  return  $e^{\pm i \beta dt} \vec{w}^{(n)}$ 
15: end procedure

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