Cucheb: A GPU implementation of the Filtered Lanczos procedure

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The filtered Lanczos procedure

Many applications require the computation of all eigenvalues and associated eigenvectors lying inside a real interval $[\alpha, \beta]$ of a large and sparse symmetric matrix $A \in \mathbb{R}^{n \times n}$.

The Lanczos method is an efficient approach when $[\alpha, \beta]$ lies on the periphery of the spectrum, and engages A only through Matrix- Vector products. Lanczos is based on a three-term recurrence:

$$Aq_i = \beta_{i-1}q_{i-1} + \alpha_i q_i + \beta_i q_{i+1}, \; (q_0 = 0, \; \beta_1 = 0).$$

In theory, $\{q_1, \ldots, q_{i+1}\}$ form an orthonormal basis. In practice, orthonormality must be explicitly enforced.

The eigenvalues of A are approximated by those of

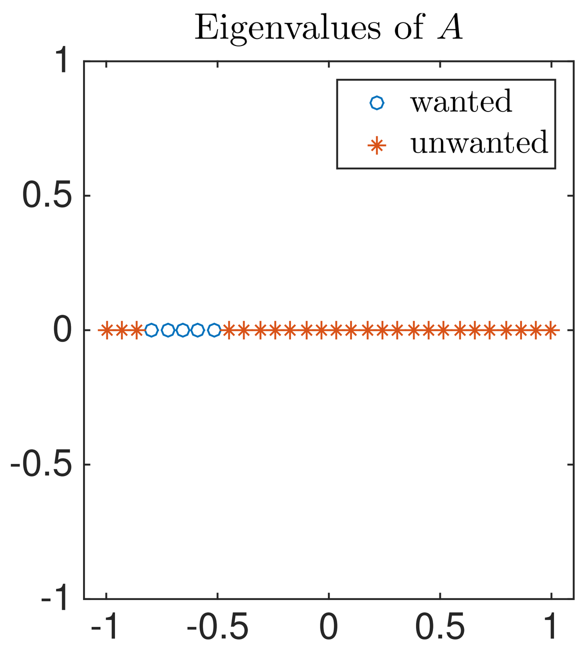
$$T_i = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & \alpha_{i-1} & \beta_{i-1} \\ & & & \beta_{i-1} & \alpha_i \end{pmatrix},$$

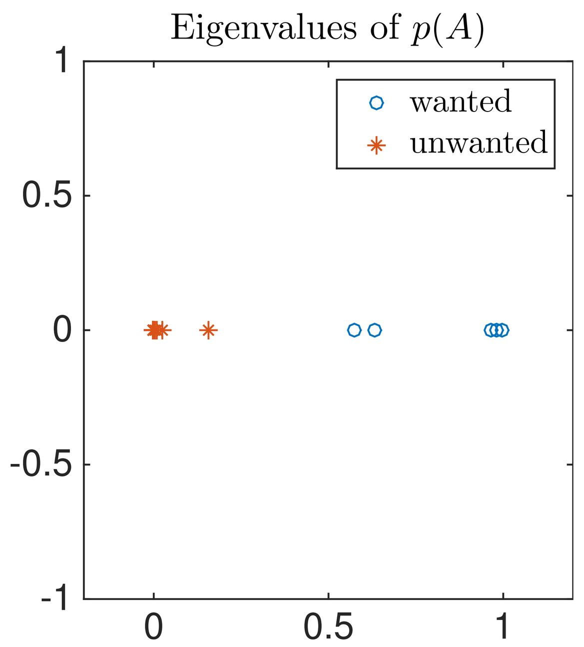
where the peripheral eigenvalues of A converge first and the convergence rate is affected by the relative separation.

What if $[\alpha, \beta]$ lies in the interior of the spectrum and/or includes a large number of eigenvalues $\rightarrow$ Lanczos will perform a large number of steps, increasing memory usage and orthogonalization costs.

The filtered Lanczos procedure applies Lanczos on a carefully chosen polynomial transformation $\rho(.)$ of A (see [2] for details). The goals of $\rho(.)$ are:

1. Eigenvalues of A located inside $[\alpha, \beta]$ are mapped to the top eigenvalues of $\rho(A)$.
2. Construction of $\rho(.)$ requires minimal knowledge of $\Lambda(A)$.
3. Multiplying $\rho(A)$ by a vector is practical.





Chebyshev polynomial filtering

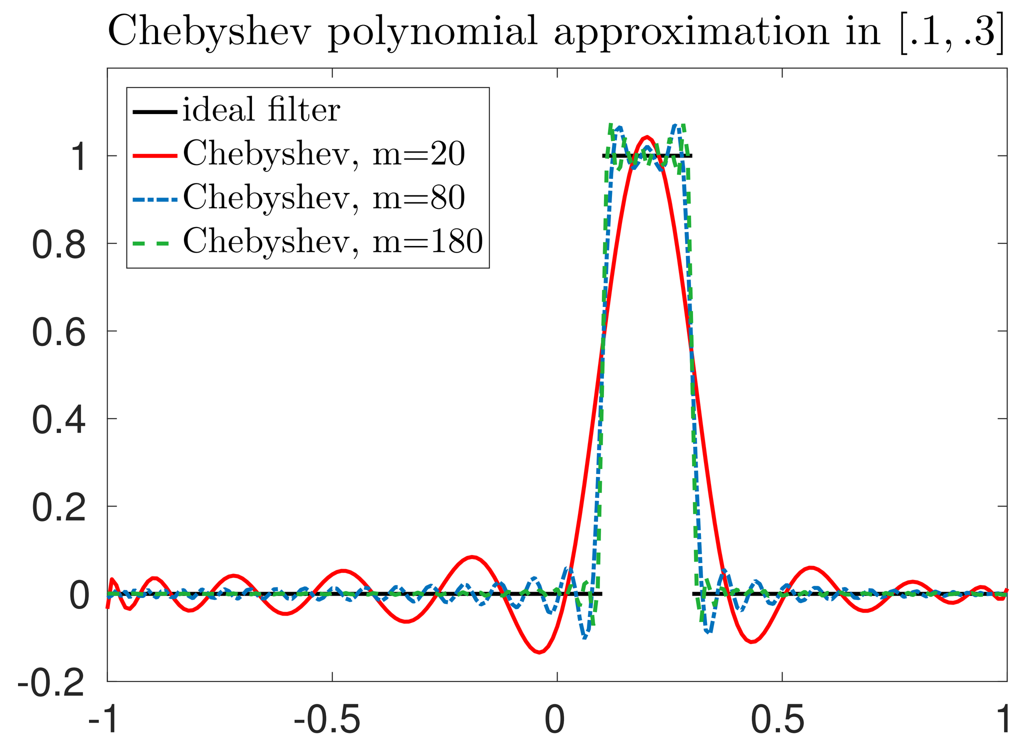
A simple and efficient approach for constructing $\rho(.)$ is to fix a degree m and approximate the step function $I_{[\alpha,\beta]}$ by

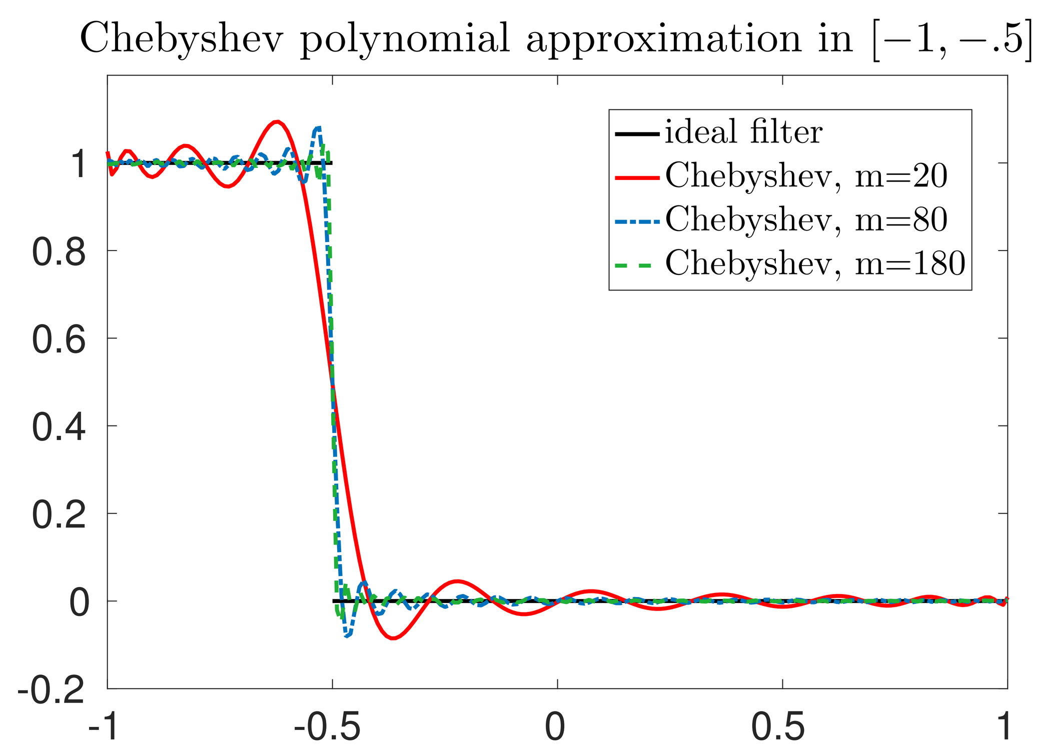
$$\rho_m(z) = \sum_{j=0}^{m} b_j T_j(z),$$

where T_j denotes the j'th degree Chebyshev polynomial of the first kind.

For a given α and β the $\{b_j\}$ are known analytically,

$$b_j = \begin{cases} (\arccos(\alpha) - \arccos(\beta))/\pi, & j = 0, \\ 2(\sin(j\arccos(\alpha)) - \sin(j\arccos(\beta)))/j\pi, & j > 0. \end{cases}$$





References

[1] Jared L. Aurentz, Vassilis Kalantzis, and Yousef Saad. *Cucheb: A GPU implementation of the filtered Lanczos procedure.* Submitted.

[2] Haw-Ren Fang, and Yousef Saad. *A Filtered Lanczos Procedure for Extreme and Interior Eigenvalue Problems.* SIAM J. Sci. Comput., **34**, A2220-A2246 (2012).

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GPU implementation

Image courtesy of *www.pny.com*

Cucheb is written in CUDA and as of now targets NVIDIA Graphic Processing Units:

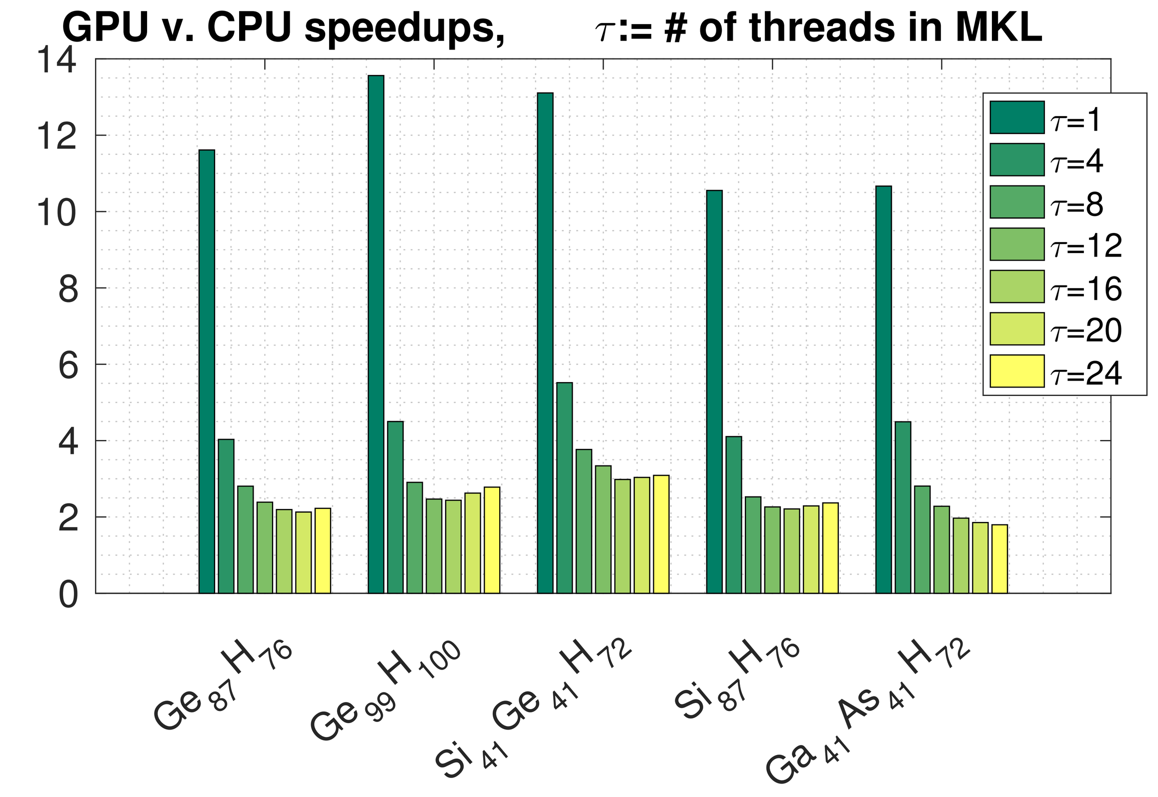
⇒ Cucheb implements a non-restarted, filtered block Lanczos procedure using full orthogonalization.

⇒ Matrices are loaded and handled using the CSR format. Sparse (dense) linear algebra is performed by cuSPARSE (cuBLAS).

⇒ The user need provide only the matrix and the interval of interest $[\alpha, \beta]$.

https://github.com/jaurentz/cucheb

Performance of Cucheb using a block variant of Lanczos



Matrix	n	nnz/n
Ge87H76	112,985	69.9
Ge99H100	112,985	74.8
Si41Ge41H72	185,639	80.9
Si87H76	240,369	44.4
Ga41As41H72	268,096	69.0

Test matrices: We tested Cucheb on a few Hamiltonians generated using the PARSEC package.

Hardware: K40m GPU with 11 GB of RAM and 2880 CUDA cores. The host CPU was a Haswell Xeon E5-2680 processor.

Matrix	interval	eigs	m	iters	MV	time
			50	210	31,500	31
			100	180	54,000	40
Ge87H76	$[-0.645, -0.0053]$	212	150	150	67,500	44
			50	210	31,500	32
			100	180	54,000	41
Ge99H100	$[-0.650, -0.0096]$	250	150	180	81,000	56
			50	210	31,500	56
			100	180	54,000	73
Si41Ge41H72	$[-0.640, -0.0028]$	218	150	180	81,000	99
			50	150	22,500	38
			100	90	27,000	35
Si87H76	$[-0.660, -0.3300]$	107	150	120	54,000	63
			200	180	144,000	225
			300	180	162,000	236
Ga41As41H72	$[-0.640, 0.0000]$	201	400	180	216,000	306