Numerical computation of eigenspaces of spatio–spectral limiting on hypercubes

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***Abstract*—Hypercubes $\mathcal{B}_N$ are Cayley graphs of groups $\mathbb{Z}_2^N$. Spatio–spectral limiting on $\mathcal{B}_N$ refers to truncation to the path neighborhood of a vertex, followed by projection onto small eigenmodes of the graph Laplacian. We present a method to compute eigenspaces of spatio–spectral limiting on $\mathcal{B}_N$ leveraging recent work of the authors that provides a geometric identification of the eigenspaces.**

I. INTRODUCTION

This work outlines a method to compute eigen decompositions of spatio–spectral limiting on hypercubes. Spatio–spectral limiting on a graph refers to truncation to a neighborhood of a vertex followed by restriction to a subset of eigenvectors of an appropriate analogue of the Fourier transform. On the real line (and discrete–periodic settings) this is known as time and band limiting, e.g., [1]–[6], [7]–[11]. Extensions to other settings including spheres, e.g., Simons et al., [12], [13] and locally compact abelian groups, e.g., Zhu and Wakin [14] have been studied recently.

Fourier transforms and bandlimiting operators have been studied recently in the setting of graphs $G = (V, E)$ [15]–[17]; connections with sampling have been made [18]–[21] and some initial, general studies of spatio-spectral limiting on graphs have been done [22], [23]. The goal here is to study some computational aspects of spatio-spectral limiting on hypercubes $\mathcal{B}_N$, which are Cayley graphs of the groups $\mathbb{Z}_2^N$. The space-limiting and spectral-limiting operators are respectively sparse and full matrices in the standard basis. They do not commute, and computing the singular value decomposition of their composition (product) is infeasible except for small N, because of the size 2^N of the matrix and, potentially, because the eigenvectors may not be well separated: eigenvalues have large multiplicities; also, some approximate eigenvalues cannot be separated. An initial study was made in [24]. In [25], eigenvectors of spatio–spectral limiting on $\mathcal{B}_N$ were identified in a manner that, in principal, leads to computation of eigenvectors and eigenvalues for reasonably large N by representing eigenspaces in terms of ranges of certain $N \times N$ matrices that *represent* the spatio-spectral limiting operator. These matrices are not self-adjoint. A bigger problem is that they are poorly conditioned. Their eigen-decompositions cannot be computed accurately by standard methods even for N on the order of twenty. This does not necessarily prohibit accurate numerical computation of eigenvectors and eigenvalues: it just means that approximation methods need to be tailored to the specific form of the matrices.

Here we present technical apparatus to make numerical computation of eigenvectors and eigenvalues of spatio-spectral limiting on $\mathcal{B}_N$ feasible. First we review briefly the reduction of the spatio-spectral limiting operator on $\mathcal{B}_N$, which we denote by $BPQP$, on invariant subspaces to certain $N \times N$ matrices and outline briefly issues with computation of the matrices. Next we discuss a certain tridiagonal matrix reduction of a *Boolean difference operator* (3) analogue of the so-called prolate differential operator [11, p. 6] that arguably *almost commutes* with the spatio-spectral limiting operator on $\mathcal{B}_N$ (the prolate differential operator on $\mathbb{R}$ actually commutes with time and band limiting—denoted by PQP–on $\mathbb{R}$) and thereby provides effective means to compute the eigenvectors of $BPQP$. On $\mathcal{B}_N$, The eigenvectors of this tridiagonal matrix are simple to compute and provide effective *seed vectors* for a version of the power method to compute eigenvectors of a corresponding $N \times N$ representation of the Boolean analogue of the time and bandlimiting operator. For a self-adjoint matrix, one version of the power method effectively starts with random orthogonal seeds, and iteratively applies the matrix, followed by orthogonal projection onto prior eigenvectors, and renormalization, until a convergence criterion is satisfied. Preferably the seeds are, in a sense, close to the target vectors. We argue that eigenvectors of BDO are effective seeds for eigenvectors of BPQP. Since our matrices are not self-adjoint, their eigenvectors are not orthogonal and the power method has to be adapted accordingly. It turns out that, for different eigenvalues, the eigenvectors of the matrices corresponding to BDO and BPQP are orthogonal with respect to a certain weighted inner product, which allows for application of a simple variant of the power method. As indicated, computing the matrix corresponding to BPQP in floating point is problematic. This is because entries are represented through N-term products of matrices with entries ranging on orders from $1/N$ to N, and the product has entries ranging on order of N^{-N} to

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N^N. However, when the products are applied factor by factor to an approximate eigenvector, floating point errors appear not to be drastic. Examples are provided. The presentation is outlined as follows.

II. Definition of Boolean hypercubes $\mathcal{B}_N$, Hadamard–Fourier transform, and spatio–spectral limiting on $\mathcal{B}_N$

Given a group G with generating set S such that $S = S^{-1}$ and identity $e \notin S$, the Cayley graph $\Gamma(G,S)$ is the graph whose vertices are the elements of G and whose edges have the form (g, gs), that is, two vertices g_1, g_2 share an edge if $g_1 g_2^{-1} \in S$. $\mathcal{B}_N$ is the Cayley graph of the group $\mathbb{Z}_2^N \sim \{0,1\}^N$. Rather than indexing vertices directly by elements $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_N)$ of $\mathbb{Z}_2^N$, it is convenient to index by subsets $S \subset \{1, 2, \dots, N\}$ with $j \in S$ if $\epsilon_j = 1$. Two vertices v_R and v_S share an edge precisely if $R\Delta S$ is a singleton. We then write $R \sim S$. $v_\emptyset$ corresponds to the identity in $\mathbb{Z}_2^N$. The adjacency matrix A is indexed by vertex pairs. We write $A_{RS} = 1$ if $R \sim S$ and $A_{RS} = 0$ otherwise. The *Laplacian* of $\mathcal{B}_N$ is $L = NI - A$. Its eigenvectors H_S can also be indexed by subsets of $\{1, \dots, N\}$ with $H_S(R) = (-1)^{|R\cap S|}$ where $|S|$ is the cardinality of S, and $LH_S = 2|S|H_S$. The Fourier transform of $\mathcal{B}_N$ can be identified with the matrix H with entries $H_{RS} = H_S(R)$. The matrix $2^{-N/2}H_{RS}$ is unitary.

We denote by Σ_r the *Hamming sphere* $\Sigma_r = \{S : |S| = r\}$ of vertices having Hamming or path distance r from the identity $v_\emptyset$. We denote the closed Hamming ball $B_K = \{S : |S| \le K\}$. The space-limiting operater $Q = Q_K$ truncates to B_K and the bandlimiting operator P_K is defined by $2^{-N}HQ_KH$. We denote by $BPQP$ the operator $P_KQ_KP_K$ for fixed K. The analysis of $BPQP$ outlined below extends fairly readily to operators $P_{K_1}Q_{K_2}P_{K_1}$ when $K_1 \ne K_2$. Analysis for more general truncations, such as replacing Hamming balls by Hamming annuli, will be done in future work.

III. Outer and inner adjacency and their compositions on data on Hamming spheres

That each edge in $\mathcal{B}_N$ originating in Σ_r terminates in $\Sigma_{r\pm1}$ allows one to express the adjacency matrix as $A = A_+ + A_-$ where A_+ maps data on Σ_r to data on Σ_{r+1} and $A_- = A_+^T$ (see [25]). Define spaces $\mathcal{W}_r$ to consist of those vectors supported in Σ_r and in the kernel of A_-, and let $\mathcal{V}_r = \{V = \sum_{k=0}^{N-r} c_k A_+^k W : W \in \mathcal{W}_r,\, c_k \in \mathbb{R}\}$. In [25] we proved the following:

$$\begin{aligned} A_- A_+^{k+1} W &= m(r,k) A_+^k W, \quad W \in W_r \quad \text{where} \\ m(r,k) &= (k+1)(N-2r+k) \end{aligned} \tag{1}$$

when $0 \le k \le N - r - 1$. It follows that $\mathcal{V}_r$ is invariant under A for each $r = 0, \dots, N-1$. The representation $V = \sum_{k=0}^{N-r} c_k A_+^k W$ of generic $V \in \mathcal{V}_r$ means that $\mathcal{V}_r$ is isomorphic to $\mathcal{W}_r \times \mathbb{R}^{N-r+1}$. The space $\mathcal{W}_r$ has dimension $\binom{N}{r} - \binom{N}{r-1}$. Summation by parts gives $\sum_{r=0}^{N}(N+1-r)\left(\binom{N}{r} - \binom{N}{r-1}\right) = 2^N$ so these spaces provide a decomposition of real vectors defined on $\mathcal{B}_N$. For each r, A_+ acts as a shift on $\mathcal{V}_r$: $A_+\left(\sum_{k=0}^{N-r} c_k A_+^k W\right) = \sum_{k=1}^{N-r} c_{k-1} A_+^k W$ whereas $A_-\left(\sum_{k=0}^{N-r} c_k A_+^k W\right) = \sum_{k=0}^{N-r} c_{k+1} m(r,k) A_+^k W$. The action of A on $\mathcal{V}_r$ can be represented by a matrix $MA = MA_r$ of size $N+1$ with entries $MA(k, k-1) = 1$; $MA(k, k+1) = m(k, r)$ and zeros elsewhere.

The bandlimiting operator $P = P_K$ can also be represented by $p(A)$ where

$$p_k(x) = \prod_{j=0, j\ne k}^{N} \frac{x - (N-2j)}{2(j-k)}; \qquad p(x) = \sum_{k=0}^{K} p_k(x)\,. \tag{2}$$

Thus P also preserves $\mathcal{V}_r$ and its action can be represented as a coefficient matrix obtained by replacing A by MA and I_{2^N} by I_{N+1-r} in (2) when x is replaced by A.

Conjugating $BPQP$ by $2^{-N/2}H$ gives an operator that we denote by $BQPQ$. On $\mathcal{V}_r$, $BQPQ$ can be represented by truncation of the matrix MP to its $(K+1-r)$-principal minor. Computing the eigen-decomposition of the latter then again applying a Hadamard conjugation provides an eigendecomposition of $BPQP$.

Unfortunately, the matrices MP are ill conditioned, with condition numbers on the order of N^N. Even for moderate N, e.g., $N = 20$ the path just outlined to eigen-decompositions of $BPQP$ is barred by the simple inability to compute eigen-decompositions of MP in floating point using standard methods.

As an alternative, given an input coefficient vector $\boldsymbol{c} = [c_0, \dots, c_{N-r}]$ one can compute $(MP)(\boldsymbol{c})$ by computing each of the successive factors of MP in (2) and adding up terms. This suggests potential application of the power method, that is, iterative application of MP to an input, projection onto the orthogonal complement of prior identified eigenvectors, and renormalization. The orthogonal projection part is problematic because MP is not self-adjoint (P and Q themselves are).

Because of (1) (and $A_- = A_+^T$), if $W_1, W_2 \in \mathcal{W}_r$, one has

$$\begin{aligned} &\langle A_+^k W_1,\, A_+^k W_2\rangle \\ &\quad = m(r,k-1)m(r,k-2)\cdots m(r,0)\langle W_1, W_2\rangle \\ &\quad \equiv M(r,k)\langle W_1, W_2\rangle \end{aligned}$$

where $\langle\cdot,\cdot\rangle$ denotes the standard inner product on $\mathcal{B}_N$. It follows that

$$\Big\langle \sum_{k=0}^{N-r} c_k A_+^k W_1, \sum_{k=0}^{N-r} d_k A_+^k W_2 \Big\rangle = \langle W_1, W_2\rangle \sum_{k=0}^{N-r} c_k d_k M(r,k)\,.$$

In particular, if two vectors in $\mathcal{V}_r$ (with same $W \in \mathcal{W}_r$) are eigenvectors of $BQPQ$ for different eigenvalues, then their coefficient vectors are orthogonal with respect to the weighted inner product $\sum c_k d_k M(r,k)$.

IV. Matrices of HBDO and HBPQP

The power method with weighted inner product $M(r,k)$ can be applied to find eigenvectors of $BQPQ$ via coefficient eigenvectors of $MBQPQ$, the coefficient matrix of $BQPQ$. In principal the algorithm will work with random seeds. Convergence is faster if one can identify a complete, $M(r,k)$-orthogonal set of vectors in $\mathbb{R}^{N+1-r}$ that are in a sense close to the coefficient eigenvectors of $MBQPQ$.

The prolate differential operator $\mathcal{P}_c : \frac{\mathrm{d}}{\mathrm{d}t}(t^2-1)\frac{\mathrm{d}}{\mathrm{d}t} + c^2t^2$, $c > 0$ fixed, has the prolate spheroidal wave functions as eigenfunctions. On $\mathbb{R}$, $\mathcal{P}_c$ commutes with time and band limiting (for appropriate $c > 0$), and therefore the eigenfunctions of the latter are also the prolate functions. In [24] we identified a *Boolean difference operator* (BDO) analogous to the prolate differential operator. On $\mathbb{R}$, differentiation and multiplication by t are related through a multiple of conjugation by the Fourier transform. Let T be the diagonal matrix on $\mathcal{B}_N$ with entries $T_{RR} = \sqrt{2|R|}$ and $D = 2^{-N}HTH$, and define

$$\text{BDO}: \qquad D(\alpha I - T^2)D + \alpha T^2 \,. \tag{3}$$

Then BDO can be regarded as a Boolean analogue of the prolate differential operator. Unlike on $\mathbb{R}$, BDO does not commute with BPQP. However, BDO arguably *almost commutes* with BPQP. In [24] it was shown that when $\alpha = 2\sqrt{K(K+1)}$, P_K commutes with BDO (but $Q = Q_K$ does not commute). Formulas for their commutator (*loc. cit.*) and numerical estimates suggest that the commutator has relatively small norm compared to that of BDO (Fig. 1).

Just as with BQPQ, the spaces $\mathcal{V}_r$ are invariant under the conjugation of BDO by H and so $H\text{BDO}H$ can be represented by a coefficient matrix $M\text{HBDO}$ of size $N-r+1$. In fact, this matrix is tridiagonal [25]. Its eigen-decomposition is easily computed numerically. Figure 1 plots the coefficient-wise differences between the corresponding unit-norm eigenvectors of the coefficient matrices $M\text{HBDO}$ and $M\text{BQPQ}$ ($(N, K, r) = (20, 6, 1)$) when the former are used as seed vectors for a version of the power method outlined below. The norm differences between the corresponding (unit-norm) eigenvectors of these almost commuting matrices is on the order of 10^{-2}. Eigenvalues of $M\text{BQPQ}$, hence of BQPQ, are computed by comparing the input and output norms of the numerically computed eigenvectors of $M\text{BQPQ}$. Eigenvalues for $N = 20$ and $K = 6$ are listed in Tab. I.

V. Adapted power method

Here is an outline of the adapted power method used to compute the eigen-decomposition of BQPQ on $\mathcal{V}_r$ for each fixed $r = 0, \ldots, K$.

Inputs N, $K \in \{0, \ldots, N\}$, $r \in \{0, \ldots, K\}$

```
Compute coefficient matrix MHBDO of
2^{-N} HBDOH on V_r
Compute eigen-decomposition of MBQPQ
Sort eigenvectors c^k = [c^k_0, ..., c^k_{N-r}] satisfying
c^k_{K+1} = ... = c^k_{N-r} = 0
For k = 0 to K - r
  d^k = c^k
  While stopping criteria = False
    Apply MBQPQ factor-wise to d^k
    Project output onto weighted
    (span{d^0, ..., d^{k-1}})^⊥
    Update d^k = normalized projection
  end [when stopping criteria is satisfied]
end [loop over k]
```

Output: coefficient eigenvectors $\boldsymbol{d}^0$, ..., $\boldsymbol{d}^{K-r}$ of $M\text{BQPQ}$. Note: The application of $M\text{BQPQ}$ is accomplished by computing the coefficient matrix Mp_k corresponding to each term p_k in (2) applied to the vector then adding terms. The application of Mp_k is done by iteratively multiplying the vector by the successive factors in the product defining Mp_k.

TABLE I
Eigenvalues of $BPQP$ for $N = 20$ and $K = 6$

$r=0$	$r=1$	$r=2$	$r=3$	$r=4$	$r=5$	$r=6$
0.9996	0.9953	0.9604	0.7857	0.3971	8.6e-2	5.9e-3
0.9206	0.6612	0.2595	4.3e-2	2.8e-3	5.7e-5	
0.2056	3.3e-2	2.6e-3	8.9e-5	8.9e-7		
2.6e-3	1.3e-4	3.0e-6	1.9e-8			
5.9e-6	1.0e-7	4.3e-9				
3.6e-9	1.6e-10					
4.1e-10						

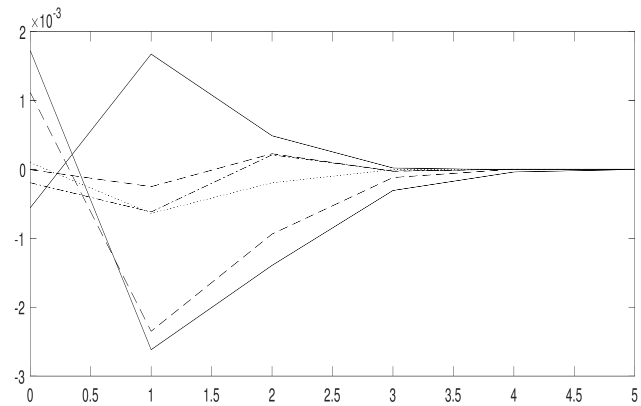

Fig. 1. Difference between seed eigenvectors of $M\text{HBDO}$ and computed eigenvectors of $MQPQ$, $(N, K, r) = (20, 6, 1)$.

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