Intermediate report

Diagonalizing Spin Hamiltonians with the Lanczos Algorithm

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This report demonstrates the application of an efficient method for approximately diagonalizing sparse hermitian matrices—the *Lanczos method*. An espacially suitable usecase for this method is the application to spin Hamiltonians with only local interactions. Here, an Ising model coupled to a monochromatic cavity field—the Dicke-Ising model— is being considered and the time evolution of the expected number of photons in the cavity gets approximated using the Lanczos method. This method itself is being discussed in detail and is implemented in the programming language `julia`.

1 Introduction

- motivation and background for spin systems
  - study of matter and light-matter interaction
  - look into QFTCM for justification of the Hubbard model
- motivation and background for the Lanczos method
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The time evolution for a duration $t \in \mathbb{R}$ of a quantum system modeled by a time-independent self-adjoint operator H, the *Hamiltonian*, acting on some Hilbert space $\mathcal{H}$ is given by the unitary operator[1] $U(t) = e^{-\mathrm{i}tH}$.

The Lanczos method is a numerical method to approximate spectral properties of hermitian matrices. Given such a matrix $H \in \mathbb{C}^{N\times N}$, the method provides iteratively a d-dimensional approximation of H that is tri-diagonal after $d-1$ iterations and which can easily be diagonalized in $\mathcal{O}(N)$ time. The only necessary information specific to H is an oracle for the matrix-vector product $H \cdot v$. If the matrix is sparse, i.e. if the ratio of the number of non-zero and zero entries is constant in N and small, the matrix-vector product can be evaluated in $\mathcal{O}(N)$ time and storing such matrices takes $\mathcal{O}(N)$ memory. Due to fast convergence of the method with respect to a

[1] Here, and in the following we work in natural units where $\hbar = 1$.

growing number of iterations, approximating the lowest eigenvalue takes $\mathcal{O}(1)$ iterations and therefore $\mathcal{O}(N)$ memory and time [1]. In addition, eigenvectors and matrix-exponential may also be approximated using this method.

The idea of the Lanczos algorithm is to find an orthonormal basis $\{v_i\}_{0\leq i\leq K}$ for the *Krylov space*

$$\mathcal{K}_H^{(K)}(v) = \operatorname{span}\big(\{v, Hv, H^2v, H^3v, \dots, H^Kv\}\big) \tag{1}$$

of order $K \leq N-1$ such that $(\langle v_i,\ Hv_j\rangle)_{0\leq i,j\leq K}$ is a tri-diagonal matrix. Then when extending this basis to a basis $(\tilde{v}_i)_{0\leq i\leq N}$ of C^N, the non-trivial part of the projection

$$P_{K+1}HP_{K+1} = H_{\mathcal{K}_H^{(K)}(v)} \oplus 0_{(\mathcal{K}_H^{(K)}(v))^\perp}, \quad P_n v \coloneqq \sum_{i=1}^{n} \langle v_i,\ v\rangle v_i \tag{2}$$

onto the first $K+1$ basis elements of $(\tilde{v}_i)_{0\leq i\leq N}$ is tri-diagonal. This projection is known as the *Galerkin approximation* of H and converges to H when $K \to N-1$.

The algorithm computes this orthonormal basis for $\mathcal{K}_H^{(K)}(v)$ is computed very similar to *Gram-Schmidt orthogonalization* but of an iteratively defined set of vectors. Set $v_0 = v/\|v\|$, for some arbitrary vector $v \in \mathbb{C}^N$. The next vector v_1 is the normalized Gram-Schmidt orthogonalization of Hv_0 with respect to v_0:

$$b_1 v_1 = \tilde{v}_1 = Hv_0 - \langle v_0,\ Hv_0\rangle v_0, \tag{3}$$

where we introduced the notation $b_n = \|\tilde{v}_n\|$. In general, v_{n+1} is defined as

$$b_{n+1}v_{n+1} = \tilde{v}_{n+1} = Hv_n - \sum_{i=0}^{n} \langle v_i,\ Hv_i\rangle v_i. \tag{4}$$

With this definition the desired property of $(\langle v_i,\ Hv_j\rangle)_{0\leq i,j\leq K}$ follows due to H being hermitian.

Lemma 1. *Let $H \in \mathbb{C}^{N\times N}$ for $N \in \mathbb{N}$ be a hermitian matrix, $v_0 = v/\|v\|$, and $K \leq N-1$. Define v_n recursively for $1 \leq n \leq K$ by*

$$b_{n+1}v_{n+1} = \tilde{v}_{n+1} = Hv_n - \sum_{i=0}^{n} \langle v_i,\ Hv_i\rangle v_i, \tag{5}$$

with $b_n = \|\tilde{v}_n\|$. Then

$$b_{n+1}v_{n+1} = Hv_n - a_n v_n - b_n v_{n-1} \tag{6}$$

for $n \leq K$ with $a_n = \langle v_n,\ Hv_n\rangle$, the set $(v_n)_{0\leq n\leq K}$ is a orthonormal basis for $\mathcal{K}_H^{(K)}(v)$, and its matrix representation

$$(\langle v_i,\ Hv_j\rangle)_{0\leq i,j\leq K} = \begin{pmatrix} a_0 & b_1 & & & \\ b_1 & a_1 & b_2 & & 0 \\ & b_2 & a_3 & \ddots & \\ & & \ddots & \ddots & \ddots \\ & 0 & & \ddots & a_{K-1} & b_K \\ & & & & b_K & a_K \end{pmatrix} \tag{7}$$

is tri-diagonal.

References

[1] Koch, Erik, 'The Lanczos Method', in *Many-body physics: from Kondo to Hubbard: lecture notes of the Autumn School on Correlated Electrons 2015: at Forschungszentrum Jülich, 21-25 September 2015*, edited by Pavarini, Eva, Koch, Erik, Coleman, Piers, Institute for Advanced Simulation and German Research School for Simulation Sciences, Schriften Des Forschungszentrums Jülich. Reihe Modeling and Simulation Band 5 (Forschungszentrum Jülich, Jülich, 2015), ISBN: 978-3-95806-074-6.