1 Krylov subspace

The order-n Krylov subspace is defined as

$$\mathcal{K}_n(H, |v_0\rangle) = \text{span}\left\{|v_0\rangle, H|v_0\rangle, H^2|v_0\rangle, \ldots, H^{n-1}|v_0\rangle\right\} \tag{1}$$

By approximating H in this subspace, we can calculate eigenvalues and eigenvectors using Lanczos iteration. We can also calculate spectral functions and Green's functions using the kernel polymial method.

2 Power method

Let $|v_0\rangle$ be an arbitrary vector. We define the recurrence relation

$$|\tilde{v}_{n+1}\rangle = H|v_n\rangle \tag{2}$$

$$|v_{n+1}\rangle = \frac{|\tilde{v}_{n+1}\rangle}{\sqrt{\langle\tilde{v}_{n+1}|\tilde{v}_{n+1}\rangle}} \tag{3}$$

i.e., we multiply by H and normalize. If $|v_n\rangle$ converges to a vector $|v_\infty\rangle$, then we get

$$|v_\infty\rangle \propto H|v_\infty\rangle \tag{4}$$

Therefore, $|v_\infty\rangle$ is an eigenvector of H. This method usually converges on an eigenvector associated with the dominant (largest magnitude) eigenvalue since any non-zero component of the dominant eigenvector will get larger after each iteration.

3 Lanczos algorithm

Combining the power method with Gram-Schmidt orthonormalization, we can approximate H on the Krylov subspace $\mathcal{K}_{N+1}$ after N iterations. These notes are based on The Lanczos Method - Erik Koch.
Assume H is Hermitian. Let $|v_0\rangle$ be an arbitrary normalized vector, $\langle v_0|v_0\rangle = 1$. We multiply $|v_0\rangle$ by H and orthogonalize the new vector $H|v_0\rangle$ to $|v_0\rangle$.

$$|\tilde{v}_1\rangle = H|v_0\rangle - |v_0\rangle\langle v_0|H|v_0\rangle \tag{5}$$

Define

$$a_n = \langle v_n|H|v_n\rangle \tag{6}$$

$$b_n^2 = \langle\tilde{v}_n|\tilde{v}_n\rangle \tag{7}$$

Eq. (5) becomes

$$b_1|v_1\rangle = H|v_0\rangle - a_0|v_0\rangle \tag{8}$$

Rearranging gives

$$H|v_0\rangle = a_0|v_0\rangle + b_1|v_1\rangle \tag{9}$$

For the next iteration step, we multiply $|v_1\rangle$ by H and orthogonalize $H|v_1\rangle$ w.r.t. all previous vectors.

$$b_2|v_2\rangle = |\tilde{v}_2\rangle = H|v_1\rangle - \sum_{i=0}^{1}|v_i\rangle\langle v_i|H|v_1\rangle = H|v_1\rangle - a_1|v_1\rangle - b_1|v_0\rangle \tag{10}$$

Rearranging gives

$$H|v_1\rangle = b_1|v_0\rangle + a_1|v_1\rangle + b_2|v_2\rangle \tag{11}$$

Continuing the iteration, we get

$$b_3 |v_3\rangle = |\tilde{v}_3\rangle = H |v_2\rangle - \sum_{i=0}^{2} |v_i\rangle \langle v_i|H|v_2\rangle = H |v_2\rangle - a_2 |v_2\rangle - b_2 |v_1\rangle \tag{12}$$

Here, the term $|v_0\rangle \langle v_0|H|v_2\rangle$ vanishes. This can be seen from Eq. (9)

$$\langle v_2|H|v_0\rangle = a_0 \langle v_2|v_0\rangle + b_1 \langle v_2|v_1\rangle \tag{13}$$

The vectors are orthogonal by construction. Therefore, $\langle v_0|H|v_2\rangle = 0$. Rearranging gives

$$H |v_2\rangle = b_2 |v_1\rangle + a_2 |v_2\rangle + b_3 |v_3\rangle \tag{14}$$

We can repeat the process to get

$$H |v_n\rangle = b_n |v_{n-1}\rangle + a_n |v_n\rangle + b_{n+1} |v_{n+1}\rangle \tag{15}$$

This process is called tridiagonalization. After N iterations, the Hamiltonian on the $N+1$-dimensional Krylov subspace is

$$H_{\mathcal{K}_N(|v_0\rangle)} = \begin{pmatrix} \langle v_0|H|v_0\rangle & \dots & \langle v_0|H|v_N\rangle \\ \vdots & \ddots & \vdots \\ \langle v_N|H|v_0\rangle & \dots & \langle v_N|H|v_N\rangle \end{pmatrix} = \begin{pmatrix} a_0 & b_1 & & & & \\ b_1 & a_1 & b_2 & & & \\ & b_2 & a_2 & b_3 & & \\ & & & \ddots & & \\ & & & b_{N-1} & a_{N-1} & b_N \\ & & & & b_N & a_N \end{pmatrix} \tag{16}$$

3.1 Eigensolution

Let V be the matrix with columns $|v_0\rangle, \dots, |v_N\rangle$ and T be the tridiagonal matrix. Then $H \approx VTV^\dagger$. If $T |x\rangle = \lambda |x\rangle$ ($|x\rangle$ is an eigenvector of T), then $V |x\rangle$ is the corresponding eigenvector to H with eigenvalue λ.

$$HV |x\rangle \approx VTV^\dagger V |x\rangle = VT |x\rangle = \lambda V |x\rangle \tag{17}$$

This is beneficial since T is of lower dimension than H and also, there are specialized algorithms for diagonalizing tridiagonal matrices. However, like the power method, this converges on dominant eigenvalues. To find eigenvalues near σ, we can use the shift-invert method. This method uses Lanczos iteration on the matrix $(H - \sigma I)^{-1}$. The dominant eigenvalues of this matrix are near σ and the eigenvectors for $(H - \sigma I)^{-1}$ are the same as H. Also, this method is numerically unstable since after many iterations, orthogonality is lost. To circumvent this, implementations will "restart" after a certain number of iterations. These methods are implemented in scipy as scipy.sparse.linalg.eigsh.

3.2 Green's function

Consider

$$G(z) = \langle \psi_0|(z - H)^{-1}|\psi_0\rangle \tag{18}$$

By initializing the Lanczos algorithm with the vector $|\psi_0\rangle$, we get the tridiagonalization

$$z - H \approx V(z - T)V^\dagger = V \begin{pmatrix} z - a_0 & -b_1 & & & & \\ -b_1 & z - a_1 & -b_2 & & & \\ & -b_2 & z - a_2 & -b_3 & & \\ & & & \ddots & & \\ & & & -b_{N-1} & z - a_{N-1} & -b_N \\ & & & & -b_N & z - a_N \end{pmatrix} V^\dagger \tag{19}$$

To get $G(z)$, we need to calculate $[(z-T)^{-1}]_{00}$. We can use block inversion to get the inverse

$$z - T = \begin{pmatrix} z - a_0 & -B^{(1)T} \\ -B^{(1)} & z - T^{(1)} \end{pmatrix} \tag{20}$$

$$B^{(1)} = \begin{pmatrix} b_1 \\ 0 \\ \vdots \end{pmatrix} \qquad z - T^{(1)} = \begin{pmatrix} z - a_1 & -b_2 & & & \\ -b_2 & z - a_2 & -b_3 & & \\ & & \ddots & & \\ & & -b_{N-1} & z - a_{N-1} & -b_N \\ & & & -b_N & z - a_N \end{pmatrix} \tag{21}$$

$$[(z-T)^{-1}]_{00} = \left(z - a_0 - B^{(1)T}(z - T^{(1)})^{-1}B^{(1)}\right)^{-1} = \left(z - a_0 - b_1^2[(z - T^{(1)})^{-1}]_{00}\right)^{-1} \tag{22}$$

The inverse $(z - T^{(1)})^{-1}$ can similarly be inverted using block matrices. Repeating the inversion, we get the continued fraction

$$G(z) = \cfrac{1}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \dots}}} \tag{23}$$

which terminates with $-\frac{b_N^2}{z - a_N}$.

4 Kernel Polynomial Method

This section is based on Kernel Polynomial Method.

4.1 Chebyshev polynomials

The Chebyshev polynomials of the first kind are given by

$$\{T_n(x) = \cos(n \arccos(x)) : n = 0, 1, 2, 3, \dots\}$$

which are orthogonal under the inner product

$$\langle f, g \rangle = \int_{-1}^{1} \frac{f(x)g(x)}{\pi\sqrt{1 - x^2}} dx$$

with the orthogonality relation

$$\langle T_m, T_n \rangle = \begin{cases} 0 & m \neq n \\ 1 & m = n = 0 \\ 1/2 & m = n \neq 0 \end{cases}$$

A useful property of the Chebyshev polynomials is that they can be generated using the recurrence relation

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

The Chebyshev expansion for a function f defined on the domain $[-1, 1]$ is

$$f(x) = \sum_{n=0}^{\infty} \frac{\langle f, T_n \rangle}{\langle T_n, T_n \rangle} T_n(x) = \alpha_0 + 2\sum_{n=1}^{\infty} \alpha_n T_n(x)$$

with coefficients

$$\alpha_n = \int_{-1}^{1} \frac{f(x)T_n(x)}{\pi\sqrt{1-x^2}}dx$$

The denominator in the integral is troublesome so we rearrange the expansion

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}}\left(\mu_0 + 2\sum_{n=1}^{\infty}\mu_n T_n(x)\right)$$

$$\mu_n = \int_{-1}^{1} f(x)T_n(x)dx$$

4.1.1 Proof of rearrangement

Define a new inner product

$$\langle f, g\rangle_1 = \int_{-1}^{1} \pi\sqrt{1-x^2}f(x)g(x)dx$$

and polynomials

$$\phi_n(x) = \frac{T_n(x)}{\pi\sqrt{1-x^2}}$$

These polynomials have the same orthogonality relations

$$\langle \phi_m, \phi_n\rangle_1 = \langle T_m, T_n\rangle = \begin{cases} 0 & m \neq n \\ 1 & m = n = 0 \\ 1/2 & m = n \neq 0 \end{cases}$$

The expansion becomes

$$f(x) = \sum_{n=0}^{\infty} \frac{\langle f, \phi_n\rangle_1}{\langle \phi_n, \phi_n\rangle_1}\phi_n(x) = \frac{1}{\pi\sqrt{1-x^2}}\left(\mu_0 + 2\sum_{n=1}^{\infty}\mu_n T_n(x)\right)$$

$$\mu_n = \langle f, \phi_n\rangle_1 = \int_{-1}^{1} f(x)T_n(x)dx$$

4.1.2 Rescaling

Expanding $f(x)$ with Chebyshev polynomials requires $x \in [-1, 1]$. We will expand functions of energy so the eigenvalues of the Hamiltonian should be in the interval $E_k \in [-1, 1]$. To fit the spectrum in the interval, we apply a linear transformation to the Hamiltonian and energies.

$$\begin{aligned} H' &= (H - b)/a \\ \omega' &= (\omega - b)/a \\ a &= (E_{max} - E_{min})/(2 - \epsilon) \\ b &= (E_{max} + E_{min})/2 \end{aligned}$$

ϵ is a small cut-off for numerical stablity. All H and ω used afterwards refer to the scaled Hamiltonian and energies.

4.2 Density of states

The first basic application of Chebyshev expansion is the calculation of the density of states

$$\rho(\omega) = \sum_k \delta(\omega - E_k)$$

where E_k are the eigenvalues of the Hamiltonian matrix. The moments can be calculated by

$$\begin{aligned}\mu_n =& \int_{-1}^{1} \rho(\omega) T_n(\omega) d\omega \\ =& \sum_k T_n(E_k) \\ =& \sum_k \langle k|T_n(H)|k\rangle \\ =& \mathrm{Tr}(T_n(H))\end{aligned}$$

4.3 Local density of states

The retarded Green's function in terms of eigenvectors is

$$G^R(\omega) = \lim_{\delta\to 0^+} \sum_k \frac{|k\rangle \langle k|}{\omega + i\delta - E_k}$$

The local density of states is

$$\begin{aligned}\rho_i(\omega) =& -\frac{1}{\pi}\mathrm{Im}G^R_{ii}(\omega) \\ =& \lim_{\delta\to 0^+} -\frac{1}{\pi}\sum_k \mathrm{Im}\frac{\langle i|k\rangle \langle k|i\rangle}{\omega + i\delta - E_k} \\ =& \lim_{\delta\to 0^+} \frac{1}{\pi}\sum_k |\langle i|k\rangle|^2 \frac{\delta}{(\omega - E_k)^2 + \delta^2} \\ =& \sum_k |\langle i|k\rangle|^2 \delta(\omega - E_k)\end{aligned}$$

The moments are

$$\begin{aligned}\mu_n =& \int_{-1}^{1} \rho_i(\omega) T_n(\omega) d\omega \\ =& \sum_k |\langle i|k\rangle|^2 T_n(E_k) \\ =& \sum_k \langle i|T_n(H)|k\rangle \langle k|i\rangle \\ =& \langle i|T_n(H)|i\rangle\end{aligned}$$

4.4 Spectral function

The spectral function is

$$\begin{aligned}A(\omega) =& -\frac{G^R(\omega) - G^A(\omega)}{2\pi i} \\ =& -\frac{1}{2\pi i}\lim_{\delta\to 0^+}\sum_k |k\rangle\langle k| \left(\frac{1}{\omega + i\delta - E_k} - \frac{1}{\omega - i\delta - E_k}\right) \\ =& \lim_{\delta\to 0^+}\sum_k |k\rangle\langle k| \frac{1}{\pi}\frac{\delta}{(\omega - E_k)^2 + \delta^2} \\ =& \sum_k |k\rangle\langle k| \delta(\omega - E_k)\end{aligned}$$

For a matrix element $A_{ij}(\omega)$, the moments are

$$\begin{aligned}\mu_n &= \int_{-1}^{1} A_{ij}(\omega) T_n(\omega) d\omega \\ &= \sum_k \langle i|k\rangle \langle k|j\rangle T_n(E_k) \\ &= \sum_k \langle i|T_n(H)|k\rangle \langle k|j\rangle \\ &= \langle i|T_n(H)|j\rangle\end{aligned}$$

4.5 Lesser Green's function

The lesser Green's function in thermal equilibrium is

$$G^<_{ij}(\omega) = 2\pi i n_F(\omega) A_{ij}(\omega)$$

4.5.1 Mean-field equation

The expectation value is an integral over energy of the lesser Green's function given by

$$\begin{aligned}\langle c_j^\dagger c_i\rangle &= \int_{-1}^{1} \frac{d\omega}{2\pi i} G^<_{ij}(\omega) \\ &= \int_{-1}^{1} d\omega n_F(\omega) A_{ij}(\omega)\end{aligned}$$

4.5.2 Current

The current is given by

$$\begin{aligned}I_{ij} =& \frac{-2e}{\hbar} \int \frac{d\omega}{2\pi} \mathrm{Re}[t_{ji} G^<_{ij}(\omega)] \\ =& \frac{2e}{\hbar} \int d\omega n_F(\omega) \mathrm{Im}[t_{ji} A_{ij}(\omega)]\end{aligned}$$

4.5.3 Superconducting order parameter

An example of solving the mean-field equation is for the the superconducting order parameter Δ_{ij}

$$\begin{aligned}\Delta_{ij} =& -V \langle c_i^\dagger c_j^\dagger\rangle = -V \int_{-1}^{1} \frac{d\omega}{2\pi i} F^<_{ij}(\omega) \\ =& -V \int_{-1}^{1} d\omega n_F(\omega) A^{12}_{ij}(\omega)\end{aligned}$$

where A^{12} is the spectral function of the Bogoliubov-de-Gennes Hamiltonian in the anamolous block.

4.6 Calculating moments

Usually, H is a sparse matrix. In general, $T_n(H)$ is not a sparse matrix, but $T_n(H)$ usually acts on a vector. Instead, we can store the vector $|\alpha_n\rangle = T_n(H)|\alpha\rangle$.

4.6.1 $\mu_n = \langle\beta|T_n(H)|\alpha\rangle$

Starting from the state $|\alpha\rangle$, we can iteratively construct states $|\alpha_n\rangle = T_n(H)\,|\alpha\rangle$ using the recurrence relations

$$\begin{aligned} |\alpha_0\rangle &= |\alpha\rangle \\ |\alpha_1\rangle &= H\,|\alpha\rangle \\ |\alpha_{n+1}\rangle &= 2H\,|\alpha_n\rangle - |\alpha_{n-1}\rangle \\ \mu_n &= \langle\beta|\alpha_n\rangle \end{aligned}$$

Note that for a single starting vector α, the expansion coefficients can be calculated for many different β.

4.6.2 $\mu_n = \mathbf{Tr}(AT_n(H))$

We can use a stochastic method to estimate the trace.

$$\mathrm{Tr}(AT_n(H)) \approx \frac{1}{R}\sum_{r=0}^{R-1} \langle r|AT_n(H)|r\rangle$$

where $|r\rangle$ is a random vector, R is the number of random vectors, and the relative error is of the order $O(1/\sqrt{RD})$. The i-th component $\langle i|r\rangle = \xi_i$ can be Gaussian distributed or have a uniform random phase.

$$\xi_i = x \quad \text{or} \quad \xi_i = e^{i\phi}$$

where $x \in \mathbb{R}$ is a gausian distributed random number and $\phi \in [0, 2\pi)$ is a uniformly distributed random number. Then, we use the procedure for $\mu_n = \langle\beta|T_n(H)|\alpha\rangle$ for each random vector $|r\rangle$

$$\begin{aligned} \langle\beta_r| &= \langle r|\,A \\ |\alpha_{rn}\rangle &= T_n(H)\,|r\rangle \\ \mu_n &= \frac{1}{R}\sum_{r=0}^{R-1} \langle\beta_r|\alpha_{rn}\rangle \end{aligned}$$

4.6.3 $|\beta\rangle = |\alpha\rangle$

The recurrence relation can be simplified even further to

$$\begin{aligned} \mu_{2n} &= 2\,\langle\alpha_n|\alpha_n\rangle - \mu_0 \\ \mu_{2n+1} &= 2\,\langle\alpha_{n+1}|\alpha_n\rangle - \mu_1 \end{aligned}$$

4.7 Kernel

The Chebyshev expansion is exact for an infinite number of moments. However, we must approximate the expansion given a finite number of N moments μ_n. Truncating the series leads to Gibbs oscillations near points where the function $f(x)$ is not continuously differentiable. To damp these oscillations, we modify the expansion coefficients $\bar{\mu}_n = g_n\mu_n$.

4.7.1 Jackson kernel

$$g_n = \frac{(N-n+1)\cos\frac{\pi n}{N+1} + \sin\frac{\pi n}{N+1}\cot\frac{\pi}{N+1}}{N+1}$$

which is related to a Gaussian

$$\delta(x) \approx \frac{1}{\sqrt{2\pi\sigma^2}}\exp(-\frac{x^2}{2\sigma^2})$$

4.7.2 Lorentz kernel

$$g_n = \frac{\sinh(\epsilon(N-n))}{\sinh(\epsilon N)}$$

which is related to a Lorentzian

$$\delta(x) \approx \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}$$

For both of these kernels, a strictly positive function remains positive and delta functions are approximated using a Gaussian or Lorentzian. For most applications, the Jackson kernel converges best, but for approximating Green's functions the Lorentz kernel is best.

4.8 Discrete cosine transform

For a set $\{x_m\}$ of M points, the Chebyshev expansion is

$$f(x_m) = \frac{1}{\pi\sqrt{1-x_m^2}}\left(\bar{\mu}_0 + 2\sum_{n=1}^{N-1}\bar{\mu}_n T_n(x_m)\right)$$

By making a special choice for our data points x_m,

$$x_m = \cos\frac{\pi(m+1/2)}{M} \quad \text{with} \quad m = 0,\ldots,M-1$$

we have $T_n(x_m) = \cos(n\arccos(x_m)) = \cos\frac{\pi n(m+1/2)}{M}$. We then obtain

$$\gamma_m = \pi\sqrt{1-x_m^2}f(x_m) = \bar{\mu}_0 + 2\sum_{n=1}^{N-1}\bar{\mu}_n\cos\frac{\pi n(m+1/2)}{M}$$

which can be efficiently calculated using a fast discrete cosine transform found in many FFT packages. After discrete cosine transform of the moments, the approximated function at the data points $\{x_m\}$ are

$$f(x_m) = \frac{\gamma_m}{\pi\sqrt{1-x_m^2}}$$

4.9 Chebyshev-Gauss quadrature

In numerical analysis, Chebyshev-Gauss quadrature is a method of approximating integrals as

$$\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx \approx \frac{\pi}{M}\sum_{m=0}^{M-1}f(x_m) \quad \text{with} \quad x_m = \cos\frac{\pi(m+1/2)}{M}$$

The special choice of data points $\{x_m\}$ from the discrete cosine transform corresponds to the abscissas of Chebyshev-Gauss quadrature. Hence, integrals of the form $\int_{-1}^{1}f(x)g(x)dx$ become simple averages.

$$\begin{aligned}\int_{-1}^{1}f(x)g(x)dx &= \int_{-1}^{1}\frac{\sqrt{1-x^2}f(x)g(x)}{\sqrt{1-x^2}}dx \\ &\approx \frac{\pi}{M}\sum_{m=0}^{M-1}\sqrt{1-x_m^2}f(x_m)g(x_m) \\ &= \frac{1}{M}\sum_{m=0}^{M-1}\gamma_m g(x_m)\end{aligned}$$