0.1 Matrix Adapted Orthogonal Polynomials Method

In order to approximate the matrix function $f(\mathbf{A})\mathbf{b}$, we estimate the probability distribution of the eigenvalues of $\mathbf{A}$ as a discrete measure $d\lambda_N$, generate a set of orthogonal polynomials $\{\pi_k\}$ with respect to $d\lambda_N$, and represent f as a linear combination of $\{\pi_k\}$. Then, $f(\mathbf{A})\mathbf{b}$ can be approximated with a truncated series of polynomial expansion.

First, we use the Kernel Polynomial Method (KPM) to estimate the cumulative distribution F of the eigenvalues of $\mathbf{A}$, and convert it to a discrete measure. We take a set of $N-2$ evenly spaced points with the two endpoints as the initial grid on the interval $[\lambda_{\min}, \lambda_{\max}]$, where $\lambda_{\min}$ and $\lambda_{\max}$ are the smallest and largest eigenvalues of $\mathbf{A}$. Assume $\lambda_{\min} = t_1 < t_2 < \cdots < t_{N-1} < t_N = \lambda_{\max}$, we generate the weights for the grid points $\{t_i\}$ by taking the difference $F(t_i + \Delta t/2) - F(t_i - \Delta t/2)$ for $i = 2, 3, \cdots, N-1$, where $\Delta t = (\lambda_{\max} - \lambda_{\min})/(N-2)$. The weights at both endpoints are set to 1. Then, we normalize all the weights by dividing with the total number of eigenvalues.

Next, we generate a set of orthogonal polynomials $\{\pi_k\}$ with respect to the discrete measure with the method described in section **??**.

The function f can be approximated with its projection onto the subspace spanned by $\{\pi_0, \pi_1, \cdots, \pi_k\}$, i.e. the first $K+1$ terms in its polynomial expansion. We first take the inner product of f and π_k on the discrete measure $d\lambda_N$:

$$\langle f, \pi_k \rangle_{d\lambda_N} = \sum_{i=1}^{N} w_i f(t_i) \pi_k(t_i), \quad k = 0, 1, 2, \cdots. \tag{1}$$

For each grid point t_i, we have

$$f(t_i) = \sum_{k=0}^{N} \gamma_k \pi_k(t_i) \approx \sum_{k=0}^{K} \gamma_k \pi_k(t_i), \quad i = 1, 2, \cdots, N, \tag{2}$$

where

$$\gamma_k = \frac{\langle f, \pi_k \rangle_{d\lambda_N}}{\langle \pi_k, \pi_k \rangle_{d\lambda_N}}.$$

For an arbitrary matrix $\mathbf{A} \in \mathbb{C}^{N \times N}$ and vector $\mathbf{b} \in \mathbb{C}^N$, it follows from the three-term recurrence relationship in (**??**) that

$$\begin{gathered} \pi_{k+1}(\mathbf{A})\mathbf{b} = (\mathbf{A} - \alpha_k \mathbf{I})\pi_k(\mathbf{A})\mathbf{b} - \beta_k \pi_{k-1}(\mathbf{A})\mathbf{b}, \quad k = 0, 1, 2, \cdots, \\ \pi_{-1}(\mathbf{A})\mathbf{b} = \mathbf{0}, \ \pi_0(A)\mathbf{b} = \mathbf{b}. \end{gathered} \tag{3}$$

Therefore, the matrix function $f(\mathbf{A})\mathbf{b}$ can be approximated with a finite linear combination of $\{\pi_k(\mathbf{A})\mathbf{b}\}$, with $k \in \{0, \cdots, K\}$, as follows:

$$f(\mathbf{A})\mathbf{b} \approx p(\mathbf{A})\mathbf{b} = \sum_{k=0}^{N-1} \gamma_k \pi_k(\mathbf{A})\mathbf{b} \approx \sum_{k=0}^{K} \gamma_k \pi_k(\mathbf{A})\mathbf{b}. \tag{4}$$