

Mamba: Linear-Time Sequence Modeling with Selective State Spaces

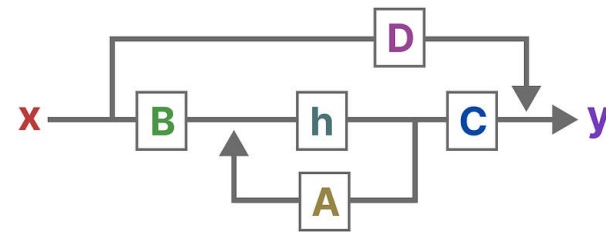
S4 (hard mode)



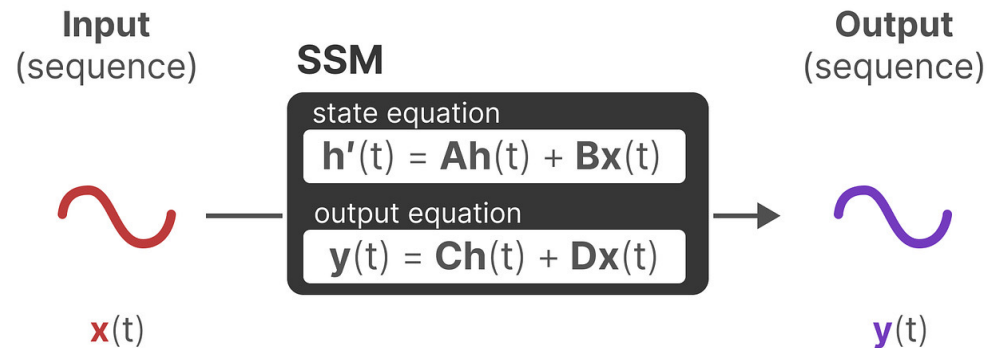
Chapter

- 1. Review Easy Mode
- 2. SSM Truncated Generation Functions
- 3. Diagonal Cases and DPLR
- 4. Code Explanation for S4

Review S4 (Contributions)



State Space Model

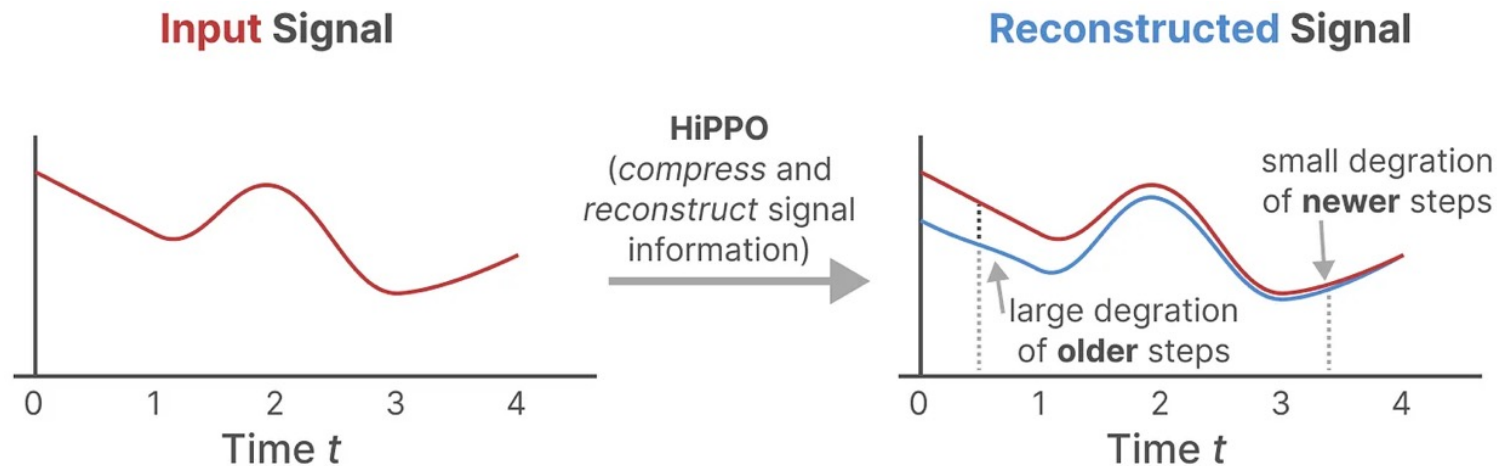


Train: (A, B, C, D)

(1) Cannot Remember Long Info

(2) Not Parallel (not efficient)

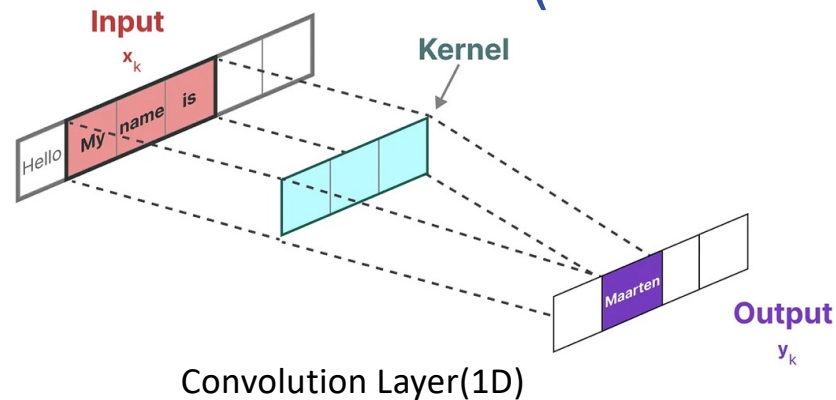
Review S4 (Cannot Remember Long Info)



(HiPPO Matrix)
$$\mathbf{A}_{nk} = - \begin{cases} (2n+1)^{1/2}(2k+1)^{1/2} & \text{if } n > k \\ n+1 & \text{if } n = k \\ 0 & \text{if } n < k \end{cases}$$

Mathematically, it does so by tracking the coefficients of a Legendre polynomial which allows it to approximate all of the previous history.

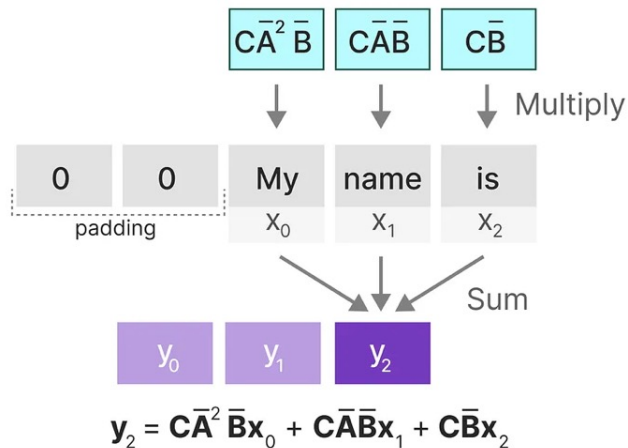
Review S4 (Not Parallel)



Kernel

Input
(x_k)

Output
(y_k)



$$y = \bar{K} * u$$

Convolutional Representation

time	hidden	prediction
0	$\bar{B}x_0$	$C\bar{B}x_0$
1	$\bar{A}h_0 + \bar{B}x_1$	$C\bar{A}\bar{B}x_0 + C\bar{B}x_1$
2	$\bar{A}(\bar{A}h_0 + \bar{B}x_1) + \bar{B}x_2$	$C\bar{A}^2\bar{B}x_0 + C\bar{A}\bar{B}x_1 + C\bar{B}x_2$
...

If conv size is fixed, like conv size = 3,

Conv kernel should be: $\bar{K} = (C\bar{A}^{L-1}\bar{B}, \dots, C\bar{A}^2\bar{B}, C\bar{A}\bar{B}, C\bar{B})$

Difficulties: **L times** for computing $y = \bar{K} * x$

Solve: truncated generating function (convert the power of matrix to the inverse of matrix, like

$$y = fun_1(A) * fun_2(A^{-1}) * x$$

Supplement (Convolution and FFT)

$$y = \bar{K} * u \quad \text{Time domain}$$



(FFT)

$$y = \text{FFT}(\bar{K})\text{FFT}(\bar{u}) \quad \text{Freq domain}$$



(IFFT)

$$y = \bar{K} * u \quad \text{Time domain}$$

```
def causal_convolution(u, K, nofft=False):
    if nofft:
        # 不使用FFT
        return np.dot(K[::-1], np.transpose(u))
    else:
        # 使用FFT
        assert K.shape[0] == u.shape[0]
        ud = np.fft.rfft(np.pad(u, (0, K.shape[0])))
        Kd = np.fft.rfft(np.pad(K, (0, u.shape[0])))
        out = ud * Kd
        return np.fft.irfft(out)[u.shape[0] - 1]
```

Computational Challenge of S4:

$$x_0 = \bar{B}u_0 \quad x_1 = \bar{A}\bar{B}u_0 + \bar{B}u_1 \quad x_2 = \bar{A}^2\bar{B}u_0 + \bar{A}\bar{B}u_1 + \bar{B}u_2 \quad \dots$$

$$y_0 = \bar{C}\bar{B}u_0 \quad y_1 = \bar{C}\bar{A}\bar{B}u_0 + \bar{C}\bar{B}u_1 \quad y_2 = \bar{C}\bar{A}^2\bar{B}u_0 + \bar{C}\bar{A}\bar{B}u_1 + \bar{C}\bar{B}u_2 \quad \dots$$

$$y_k = \bar{C}\bar{A}^k\bar{B}u_0 + \bar{C}\bar{A}^{k-1}\bar{B}u_1 + \dots + \bar{C}\bar{A}\bar{B}u_{k-1} + \bar{C}\bar{B}u_k \quad (\text{Naïve and Unstable})$$

Pipeline for Computational Challenge

Define:

- (1) Normal Plus Low Rank (NPLR): Matrix A (Hippo) can be separated a Normal Matrix Plus low rank matrix.
- (2) Diagonal Plus Low Rank (DPLR): Matrix A (Hippo) can be separated a Diagonal Matrix Plus low rank matrix.
- (3) Unitarily Equivalent: $SSM(A, B, C) \sim SSM(\Lambda - PQ^*, B, C)$
- (4) Cauchy Kernel : <https://baike.baidu.com/item/柯西核/22933987>

Pipeline :

- (1) Use **Truncated Generation Function** for calculating Kernel
- (2) the diagonal matrix case is equivalent to the computation of a **Cauchy Kernel**
- (3) Employ **DPLR** and **Woodbury Identity** to correct the result

SSM Generating Functions

Generation function: $f(x) = \sum a_i k_i(x)$; Specifically, in S4,

$$f(x) = \sum a_i x^i, i \geq 0 \quad (\text{Similiar to Z-transform})$$



$$K(x) = \sum \bar{C} \bar{A}^i \bar{B} x^{L-i}$$

Origin version:

Use **FFT** to get $y_1(x_0)y_2(x_0)$ quickly.

E.g., we have two polynomial function $y_1(x)$ and $y_2(x)$, and we want to get $y_1(x_0)y_2(x_0)$

Naïve method:

Step 1, calculate $y_1(x) * y_2(x)$

Step 2, get $x = x_0$, and calculate $y_1(x_0) * y_2(x_0)$

Time complexity: $O(n^2)$

SSM Generating Functions

FFT method:

$$Y = y_1(x) * y_2(x) = a_0 + a_1x + a_2x^2 + \cdots + a_{2n}x^{2n}$$

$$\begin{bmatrix} Y[0] \\ Y[1] \\ \cdot \\ \cdot \\ Y[2n] \end{bmatrix} = M(x) \begin{bmatrix} a_0 \\ a_1 \\ \cdot \\ \cdot \\ a_{2n} \end{bmatrix}$$

How to Choose M(x)

Intuition 1: (From FFT)

$$X_k = \sum_{n=0}^{N-1} x_n e^{-i\frac{2\pi}{N}kn}$$

Similar to

$$Y_k = \sum_{n=0}^{N-1} a_n e^{-i\frac{2\pi}{N}kn}$$

Also, $e^{-i\frac{2\pi}{N}k}$ ($k \leq 0$) is the root of a unit circle in complex domain. [这里也可以看成是一个负数边上的z-transform]

Intuition 2: **Cooley-Tukey** 算法

SSM Generating Functions

According to FFT, we can get:

$$\begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ \vdots \\ X_{N-1} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \alpha & \alpha^2 & \cdots & \alpha^{N-1} \\ 1 & \alpha^2 & \alpha^4 & \cdots & \alpha^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha^{N-1} & \alpha^{2(N-1)} & \cdots & \alpha^{(N-1)(N-1)} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_{N-1} \end{bmatrix}$$

X means value Y and x means coefficient a.

Obviously, the Matrix M here is a **Vandermonde matrix**.

In Generating Functions problems, we should have

$$\begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ \vdots \\ X_{N-1} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \alpha & \alpha^2 & \cdots & \alpha^{N-1} \\ 1 & \alpha^2 & \alpha^4 & \cdots & \alpha^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha^{N-1} & \alpha^{2(N-1)} & \cdots & \alpha^{(N-1)(N-1)} \end{bmatrix}$$

$$\text{Like } Y = MX \rightarrow M^{-1}Y = X$$

SSM Generating Functions

This problem equalt to two subproblem:

(1) How to get Y

$$\hat{\mathcal{K}}_L(z) = \sum_{i=0}^{L-1} \overline{\mathbf{C}} \overline{\mathbf{A}}^i \overline{\mathbf{B}} z^i = \overline{\mathbf{C}} (\mathbf{I} - \overline{\mathbf{A}}^L z^L) (\mathbf{I} - \overline{\mathbf{A}} z)^{-1} \overline{\mathbf{B}} = \widetilde{\mathbf{C}} (\mathbf{I} - \overline{\mathbf{A}} z)^{-1} \overline{\mathbf{B}}$$

Where $z^L = 1$ because z is a root of a unit circle.

(2) How to calculate the inverse of a **Vandermonde matrix**.

$$M^{-1} = \frac{M^*}{L}$$

Reference: <https://www.cnblogs.com/gzy-cjoier/p/9741950.html>

Have A Rest

What we have already known:

$$\hat{\mathcal{K}}_L(z) = \sum_{i=0}^{L-1} \overline{\mathbf{C}} \overline{\mathbf{A}}^i \overline{\mathbf{B}} z^i = \overline{\mathbf{C}} (\mathbf{I} - \overline{\mathbf{A}}^L z^L) (\mathbf{I} - \overline{\mathbf{A}} z)^{-1} \overline{\mathbf{B}} = \widetilde{\mathbf{C}} (\mathbf{I} - \overline{\mathbf{A}} z)^{-1} \overline{\mathbf{B}}$$

However, we can still simplify the inverse process:

$$(\mathbf{I} - \overline{\mathbf{A}} z)^{-1}$$

For the next two steps, we will simplify

$$\overline{\mathbf{A}} = \mathbf{\Lambda} + \mathbf{P} \mathbf{Q}^*$$

Then, we can employ Woodbury identity:

$$(\mathbf{\Lambda} + \mathbf{P} \mathbf{Q}^*)^{-1} = \mathbf{\Lambda}^{-1} - \mathbf{\Lambda}^{-1} \mathbf{P} (1 + \mathbf{Q}^* \mathbf{\Lambda}^{-1} \mathbf{P})^{-1} \mathbf{Q}^* \mathbf{\Lambda}^{-1}$$

to make this calculation easier and efficient.

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Definition Explanation (Unitarily Equivalent)

Unitarily Equivalent :

(Lemma 3.1 in S4 Paper): conjugation is an equivalence relation on

$$SSMs(A, B, C) \sim (V^{-1}AV, V^{-1}B, CV)$$

Write out the two SSMs with state denoted by x and \tilde{x} respectively:

$$\begin{cases} x' = Ax + Bu \\ y = Cx' \end{cases} \qquad \begin{cases} \tilde{x}' = V^{-1}AV\tilde{x} + V^{-1}Bu \\ y = CV\tilde{x}' \end{cases}$$

If we set $x = V\tilde{x}$ and after multiplying the right side SSM by V , the two SSMs can become identical. Therefore these compute the exact same operator $u \rightarrow y$, but with a change of basis by V in the state x

Explanation

$$\begin{aligned} y &= Cx' \\ &= C(Ax + Bu) \\ &= CVV^{-1}(AV\tilde{x} + Bu) \\ &= CV(V^{-1}AV\tilde{x} + V^{-1}Bu) \end{aligned} \quad \longrightarrow \quad \begin{cases} \tilde{x}' = V^{-1}AV\tilde{x} + V^{-1}Bu \\ y = CV\tilde{x}' \end{cases}$$

Definition Explanation (NPLR)

Normal Plus Low Rank:

For a Hippo Matrix A (Hippo-LegS):

$$A_{nk} = \begin{cases} (2n+1)^{1/2}(2k+1)^{1/2} & \text{if } n > k \\ n+1 & \text{if } n = k, \\ 0 & \text{if } n < k \end{cases}, \quad B_n = (2n+1)^{\frac{1}{2}}$$

Normal Matrix (Complex):

For a normal matrix A, it satisfies

$$AA^* = A^*A,$$

where A^* is the conjugate transpose of A.

Why Normal Matrix:

A normal matrix A satisfy:

$$A = U\Lambda U^*,$$

Where Λ is a diagonal matrix.

Definition Explanation (NPLR)

Convert Matrix A (Hippo-LegS) to NPLR matrix

$$A_{nk} = - \begin{cases} (2n+1)^{1/2}(2k+1)^{1/2} & \text{if } n > k \\ n+1 & \text{if } n = k \\ 0 & \text{if } n < k \end{cases}.$$

(1) Let A plus $\frac{1}{2}(2n+1)^{1/2}(2k+1)^{1/2}$ (we define it as M_{nk}) and we can get B =

$$- \begin{cases} \frac{1}{2}(2n+1)^{1/2}(2k+1)^{1/2} & \text{if } n > k \\ \frac{1}{2} & \text{if } n = k \\ -\frac{1}{2}(2n+1)^{1/2}(2k+1)^{1/2} & \text{if } n < k \end{cases}$$

Definition Explanation (NPLR -> DPLR)

(2) Let $B = -\frac{1}{2}I + S$, where S is a **skew - symmetric matrix**

$$S = \begin{cases} \frac{1}{2}(2n+1)^{\frac{1}{2}}(2k+1)^{\frac{1}{2}} & \text{if } n > k \\ 0, & \text{if } n = k \\ -\frac{1}{2}(2n+1)^{\frac{1}{2}}(2k+1)^{\frac{1}{2}}, & \text{if } n < k \end{cases}$$

An example of a skew-symmetric matrix

$$\begin{bmatrix} 0 & 1 & -2 \\ -1 & 0 & -4 \\ 2 & 4 & 0 \end{bmatrix}$$

(3) Summary and Conclusion:

Step 1: $A_{nk} + M_{nk} = -\frac{1}{2}I + S$ (tips 1: A Normal Matrix plus c Identity Matrix is still a Normal Matrix)

Step 2: $A_{nk} = M_{nk} + \text{Normal}$

Step 3: $A_{nk} = -PQ^T + \text{Normal}$

Where $P = -(2n+1)^{\frac{1}{2}}, Q = (2k+1)^{\frac{1}{2}}; n, k \in [1, N]$

Step 4: $\text{Normal} = V\Lambda V^*$

Step 5: $A_{nk} = V\Lambda V^* - PQ^T$

Step 6: $A_{nk} = V(\Lambda - (V^*P)(V^*Q)^*)V^* \sim \Lambda - (V^*P)(V^*Q)^*$

$$SSMs(A, B, C) \sim (V^{-1}AV, V^{-1}B, CV)$$

Diagonal Cases (Conclusion)

$$\hat{K}(z) = \frac{2}{1+z} \left[\tilde{C}^* R(z) B - \tilde{C}^* R(z) P (1 + Q^* R(z) P)^{-1} Q^* R(z) B \right]$$

$$\tilde{C} = (I - \bar{A}^L)^* C$$

$$R(z; \Lambda) = \left(\frac{2}{\Delta} \frac{1-z}{1+z} - \Lambda \right)^{-1}.$$

Woodbury Identity

$$(\Lambda + PQ^*)^{-1} = \Lambda^{-1} - \Lambda^{-1} P (1 + Q^* \Lambda^{-1} P)^{-1} Q^* \Lambda^{-1}$$

$$\begin{aligned} \tilde{C}^* (I - \bar{A}z)^{-1} \bar{B} &= \frac{2}{1+z} \tilde{C}^* \left(\frac{2}{\Delta} \frac{1-z}{1+z} - A \right)^{-1} B \\ &= \frac{2}{1+z} \tilde{C}^* \left(\frac{2}{\Delta} \frac{1-z}{1+z} - \Lambda + PQ^* \right)^{-1} B \\ &= \frac{2}{1+z} \left[\tilde{C}^* R(z) B - \tilde{C}^* R(z) P (1 + Q^* R(z) P)^{-1} Q^* R(z) B \right]. \end{aligned}$$

Diagonal Cases

Cachy-Kernel:

$$K_R(\tilde{C}, B) = \sum_i \frac{\tilde{C}_i^* B_i}{R(z; \Lambda)}$$

$$R(z; \Lambda) = \left(\frac{2}{\Delta} \frac{1-z}{1+z} - \Lambda \right)^{-1}.$$

$$\begin{aligned} \tilde{C}^* (I - \bar{A}z)^{-1} \bar{B} &= \frac{2}{1+z} \tilde{C}^* \left(\frac{2}{\Delta} \frac{1-z}{1+z} - A \right)^{-1} B \\ &= \frac{2}{1+z} \tilde{C}^* \left(\frac{2}{\Delta} \frac{1-z}{1+z} - \Lambda + PQ^* \right)^{-1} B \\ &= \frac{2}{1+z} \left[\underbrace{\tilde{C}^* R(z) B}_{K_R(\tilde{C}, B)} - \underbrace{\tilde{C}^* R(z) P}_{K_R(\tilde{C}, P)} (1 + \underbrace{Q^* R(z) P}_{K_R(Q^*, P)})^{-1} \underbrace{Q^* R(z) B}_{K_R(Q^*, B)} \right]. \end{aligned}$$

Pipeline of S4

Algorithm 1 S4 CONVOLUTION KERNEL (SKETCH)

Input: S4 parameters $\mathbf{\Lambda}, \mathbf{P}, \mathbf{Q}, \mathbf{B}, \mathbf{C} \in \mathbb{C}^N$ and step size Δ

Output: SSM convolution kernel $\overline{\mathbf{K}} = \mathcal{K}_L(\overline{\mathbf{A}}, \overline{\mathbf{B}}, \overline{\mathbf{C}})$ for $\mathbf{A} = \mathbf{\Lambda} - \mathbf{P}\mathbf{Q}^*$ (equation (5))

- 1: $\tilde{\mathbf{C}} \leftarrow (\mathbf{I} - \overline{\mathbf{A}}^L)^* \overline{\mathbf{C}}$ ▷ Truncate SSM generating function (SSMGF) to length L
 - 2: $\begin{bmatrix} k_{00}(\omega) & k_{01}(\omega) \\ k_{10}(\omega) & k_{11}(\omega) \end{bmatrix} \leftarrow [\tilde{\mathbf{C}} \mathbf{Q}]^* \left(\frac{2}{\Delta} \frac{1-\omega}{1+\omega} - \mathbf{\Lambda} \right)^{-1} [\mathbf{B} \mathbf{P}]$ ▷ Black-box Cauchy kernel
 - 3: $\hat{\mathbf{K}}(\omega) \leftarrow \frac{2}{1+\omega} [k_{00}(\omega) - k_{01}(\omega)(1 + k_{11}(\omega))^{-1}k_{10}(\omega)]$ ▷ Woodbury Identity
 - 4: $\hat{\mathbf{K}} = \{\hat{\mathbf{K}}(\omega) : \omega = \exp(2\pi i \frac{k}{L})\}$ ▷ Evaluate SSMGF at all roots of unity $\omega \in \Omega_L$
 - 5: $\overline{\mathbf{K}} \leftarrow \text{iFFT}(\hat{\mathbf{K}})$ ▷ Inverse Fourier Transform
-

$$\begin{aligned}
 \tilde{\mathbf{C}}^* (\mathbf{I} - \overline{\mathbf{A}}z)^{-1} \overline{\mathbf{B}} &= \frac{2}{1+z} \tilde{\mathbf{C}}^* \left(\frac{2}{\Delta} \frac{1-z}{1+z} - \mathbf{A} \right)^{-1} \mathbf{B} \\
 &= \frac{2}{1+z} \tilde{\mathbf{C}}^* \left(\frac{2}{\Delta} \frac{1-z}{1+z} - \mathbf{\Lambda} + \mathbf{P}\mathbf{Q}^* \right)^{-1} \mathbf{B} \\
 &= \frac{2}{1+z} \left[\underbrace{\tilde{\mathbf{C}}^* \mathbf{R}(z) \mathbf{B}}_{K_R(\tilde{\mathbf{C}}, \mathbf{B})} - \underbrace{\tilde{\mathbf{C}}^* \mathbf{R}(z) \mathbf{P}}_{K_R(\tilde{\mathbf{C}}, \mathbf{P})} (1 + \underbrace{\mathbf{Q}^* \mathbf{R}(z) \mathbf{P}}_{K_R(\mathbf{Q}^*, \mathbf{P})})^{-1} \underbrace{\mathbf{Q}^* \mathbf{R}(z) \mathbf{B}}_{K_R(\mathbf{Q}^*, \mathbf{B})} \right].
 \end{aligned}$$

Code and Experiment

1. $\bar{A} = \Lambda + PQ^* \rightarrow \Lambda - PP^* (P = Q)$
- 2.

$$A = - \begin{bmatrix} \frac{1}{2} + \beta & & & & \dots \\ & \frac{1}{2} + \beta & & & \\ & & \frac{1}{2} + \beta & & \\ & & & \frac{1}{2} + \beta & \\ \vdots & & & & \ddots \end{bmatrix} = -\beta I - \begin{bmatrix} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \dots \\ \frac{1}{2} & & -\frac{1}{2} & -\frac{1}{2} & \\ \frac{1}{2} & \frac{1}{2} & & -\frac{1}{2} & \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & & \\ \vdots & & & & \ddots \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & 1 & \\ 1 & 1 & 1 & 1 & \\ 1 & 1 & 1 & 1 & \\ \vdots & & & & \ddots \end{bmatrix}.$$

The first term is skew-symmetric, which is unitarily similar to a (complex) **diagonal** matrix with pure imaginary eigenvalues (i.e., real part 0). The second matrix can be factored as pp^* for $p = 2^{-1/2} [1 \ \dots \ 1]^*$. Thus the whole matrix A is unitarily similar to a matrix $\Lambda - pp^*$ where the eigenvalues of Λ have real part between $-\frac{1}{2}$ and 0.

Ref: <https://arxiv.org/abs/2202.09729>

Code and Experiment

3. Hermitian Matrix: $A = A^*$

(1) $A = V^{-1}\Lambda V$, for V , it composes a set of orthogonal basis

Ref: https://en.wikipedia.org/wiki/Hermitian_matrix

Lemma: for a Hermitian matrix A , if it satisfy:

$$\begin{cases} A = (B + kI) \\ A = V^{-1}\Lambda V \end{cases} \rightarrow B = V^{-1}\Lambda'V$$

Proof:

$$\begin{aligned} V(B + kI)V^{-1} &= VB V^{-1} + kI = \Lambda \\ VB V^{-1} &= \Lambda' \rightarrow B = V^{-1}\Lambda'V \end{aligned}$$

Where

$$\Lambda' = \Lambda - kI$$