Functions of Difference Matrices are Toeplitz plus Hankel

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Model problem

Heat equation with homogeneous Dirichlet boundary conditions

$$\begin{cases} \partial_t u &= \partial_{xx} u, & \text{on } (0,\infty) \times (0,1) \\ u(t,0) &= 0 & t \in [0,\infty) \\ u(t,1) &= 0 & t \in [0,\infty) \\ u(0,x) &= u_0(x), & x \in [0,1]. \end{cases}$$

Model problem

Heat equation with homogeneous Dirichlet boundary conditions

$$\begin{cases} \partial_t u &= \partial_{xx} u, \quad \text{on } (0,\infty)\times(0,1) \\ u(t,0) &= 0 \qquad t \in [0,\infty) \\ u(t,1) &= 0 \qquad t \in [0,\infty) \\ u(0,x) &= u_0(x), \quad x \in [0,1]. \end{cases}$$

Approach: Discretize in space and solve ODE in time.

- step size $h = \frac{1}{N+1}$
- grid points

$$x_0 = 0, x_1 = h, \ldots, x_N = Nh, x_{N+1} = 1$$

- intermediate points

$$x_{0.5} = h/2, x_{1.5} = (1.5)h, \ldots, x_{N.5} = (N.5)h$$

Discretization of the heat equation

- central differences for $i = 0, \dots, N$ yield

$$\partial_x u(t, x_{i.5}) = \frac{u(t, x_{i+1}) - u(t, x_i)}{h} + \mathcal{O}(h)$$

- and again central differences for $i = 1, \dots, N$ yield

$$\begin{aligned}\partial_{xx} u(t, x_i) &= \frac{\partial_x u(t, x_{i.5}) - \partial_x u(t, x_{(i-1).5})}{h} + \mathcal{O}(h) \\ &= \frac{u(t, x_{i+1}) - 2u(t, x_i) + u(t, x_{i-1})}{h^2} + \mathcal{O}(h^2),\end{aligned}$$

  together with the Dirichlet boundary conditions

$$u(t, x_0) = 0 = u(t, x_{N+1}).$$

Discretization of the heat equation

Semidiscrete approximation

Obtain the initial value problem

$$(1) \qquad \begin{cases} \mathbf{u}'(t) &= -\left(\frac{K}{h^2}\right)\mathbf{u}(t), \quad \text{for } t > 0 \\ \mathbf{u}(0) &= \mathbf{u}_0 \end{cases}$$

According to our discretization the $N \times N$ difference matrix K is given by

$$K = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

Solution of the Semidiscrete Approximation

Solution to (1)

The solution to the initial value problem (1) is given by

$$\mathbf{u}(t) = e^{-Kt/h^2}\mathbf{u}_0. \tag{2}$$

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- We already know that e^{-Kt/h^2} decays fast from the diagonal [Ise00].
- This presentation is about the structure of e^{-Kt/h^2}.

Functions of difference matrices are Toeplitz plus Hankel.

2nd model problem: wave equation

Wave equation with Dirichlet boundary conditions

$$\begin{cases} \partial_{tt} u &= \partial_{xx} u, \quad \text{on } (0,\infty)\times(0,1) \\ u(t,0) &= 0, \quad t\in[0,\infty) \\ u(t,1) &= 0, \quad t\in[0,\infty) \\ u(0,x) &= u_0(x), \quad x\in[0,1] \\ \partial_t u(0,x) &= v_0(x), \quad x\in[0,1]. \end{cases}$$

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Same steps lead to:

Semidiscrete approximation, initial value problem

$$(3) \qquad \begin{cases} \mathbf{u}''(t) & = \left(-\frac{K}{h^2}\right) \mathbf{u}(t), \quad \text{for } t > 0 \\ \mathbf{u}(0) & = \mathbf{u}_0 \\ \mathbf{u}'(0) & = \mathbf{v}_0. \end{cases}$$

Solution to semidiscrete wave equation

Solution to (3)

The solution to the initial value problem (3) is given by

$$\begin{aligned}\mathbf{u}(t) &= \cos(\sqrt{K}t/h)\mathbf{u}_0 + hK^{-1/2}\sin(\sqrt{K}t/h)\mathbf{v}_0 \\ &= \cos(\sqrt{K}t/h)\mathbf{u}_0 + t\,\mathrm{sinc}(\sqrt{K}t/h)\mathbf{v}_0.\end{aligned}$$

We are interested in the structure of

- $\sqrt{K}$
- e^{-tK/h^2}
- $\cos(\sqrt{K}t/h)$
- $\mathrm{sinc}(\sqrt{K}t/h)$

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Definition

Toeplitz, Hankel

A matrix $A = (a_{i,j}) \in \mathbb{C}^{N \times N}$ is called Toeplitz if

$$a_{i,j} = a_{i+1,j+1}$$

holds for all $i, j \in \{1, \ldots, N-1\}$.
A matrix $A = (a_{i,j}) \in \mathbb{C}^{N \times N}$ is called Hankel if

$$a_{i,j} = a_{i+1,j-1}$$

holds for all $i \in \{1, \ldots, N-1\}$ and $j \in \{2, \ldots, N\}$.

For more information about Toeplitz matrices see [Wid65].

Functions of K

Start with Eigenvectors of K. We have the following correspondence:

$$K \leftrightsquigarrow -\frac{d^2}{dx^2} \text{ with homogeneous boundary conditions}$$

The Eigenfunctions of the right side are sines:

$$-\frac{d^2}{dx^2}\sin(k\pi x) = k^2\pi^2\sin(k\pi x).$$

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Get the orthonormal Eigenvalues in the discrete case by sampling in the grid points:

$$\mathbf{v}_k = \sqrt{\frac{2}{N+1}}\left(\sin(k\pi h), \sin(2k\pi h), \dots, \sin(Nk\pi h)\right)^T.$$

Functions of K (cont.)

$$\mathbf{v}_k = \sqrt{\frac{2}{N+1}}\left(\sin(k\pi h), \sin(2k\pi h), \ldots, \sin(Nk\pi h)\right)^T,$$

with corresponding Eigenvalues

$$\lambda_k = 2 - 2\cos(k\pi h),\ k = 1, \ldots, N.$$

Functions of K (cont.)

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with corresponding Eigenvalues

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Write the difference matrix as

$$K = \sum_{k=1}^{N} \lambda_k \mathbf{v}_k \mathbf{v}_k^T.$$

For a function f (defined on the spectrum of K) the matrix function $f(K)$ is defined by

$$f(K)_{m,n} = \frac{2}{N+1} \sum_{k=1}^{N} f(\lambda_k) \sin(mk\pi h) \sin(nk\pi h).$$

Functions of K are Toeplitz and Hankel

The trigonometric identity

$$\sin(x)\sin(y) = \frac{1}{2}\left(\cos(x-y) - \cos(x+y)\right)$$

is essential for the following (see also [BBR13]).

Functions of K are Toeplitz and Hankel

The trigonometric identity

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is essential for the following (see also [BBR13]). For $\theta_k = k\pi h$ this implies

$$\begin{aligned} f(K)_{m,n} &= \frac{2}{N+1}\sum_{k=1}^{N} f(\lambda_k)\sin(m\theta_k)\sin(n\theta_k) \\ &= \frac{1}{N+1}\sum_{k=1}^{N} f(\lambda_k)\left(\underbrace{\cos((m-n)\theta_k)}_{\text{Toeplitz}} - \underbrace{\cos((m+n)\theta_k)}_{\text{Hankel}}\right). \end{aligned}$$

Approximate sum by integral

For $N \to \infty$ we get the following limit (see also [BBR13]).
Remember therefore $\theta_k = \frac{k\pi}{N+1}$ and $\lambda_k = 2 - 2\cos\left(\frac{k\pi}{N+1}\right)$:

$$f(K)_{m,n} = \frac{1}{N+1} \sum_{k=1}^{N} f(\lambda_k) \left(\cos((m-n)\theta_k) - \cos((m+n)\theta_k)\right)$$

$$\xrightarrow{N\to\infty} \frac{1}{\pi} \int_0^{\pi} f\left(2 - 2\cos(\theta)\right) \left(\cos((m-n)\theta) - \cos((m+n)\theta)\right) d\theta$$

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This are the Fourier cosine coefficients of $f(2-2\cos(\cdot))$ times $1/2$.

$\sqrt{K}$

For $f = \sqrt{\cdot}$ we obtain

$$f(2 - 2\cos(\theta)) = \sqrt{2 - 2\cos(\theta)} = 2\sin\left(\frac{\theta}{2}\right),$$

and so for $p = m - n$, respectively $p = m + n$, we get the Fourier cosine coefficients (times $1/2$) of the periodic, even function

$$\left|\sin\left(\frac{\theta}{2}\right)\right|, \text{ for } \theta \in (-\pi, \pi).$$

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With

$$a_p = \frac{4}{\pi(1 - 4p^2)},$$

we obtain

$$\left(\sqrt{K}\right)_{m,n} = a_{m-n} - a_{m+n}.$$

Aliasing

In the Hankel part

$$\frac{1}{N+1}\sum_{k=1}^{N} f(\lambda_k)\cos(pk\pi h)$$

of the exact $f(K)$ we observe the following aliasing effect

$$\begin{aligned}\cos(pk\pi h) &= \cos(2k\pi - pk\pi h)\\ &= \cos\left(\frac{(2N+2-p)k\pi}{N+1}\right) = \cos((2N+2-p)k\pi h).\end{aligned}$$

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This implies a reflection across the main antidiagonal. The integral is closer to a sum over the lower frequencies. Therefore choose the Hankel part as $a_{2N+2-m-n}$ if $(m+n) > N+1$.

e^{-tK}

The same steps lead to

$$(e^{-tK})_{m,n} = \frac{2}{N+1} \sum_{k=1}^{N} e^{2t\cos(\theta_k)-2t} \sin(m\theta_k)\sin(n\theta_k),$$

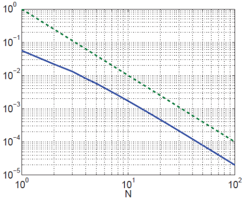
and for $p = m - n$ and $p = m + n$ the limits for $N \to \infty$ are

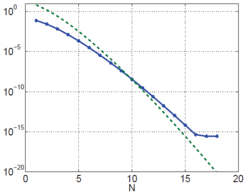
$$\begin{aligned} b_p &= \frac{e^{-2t}}{\pi} \int_0^{\pi} e^{2t\cos(\theta)} \cos(p\theta) d\theta \\ &= e^{-2t} I_p(2t), \end{aligned}$$

where I_p is the modified Bessel function of the first kind.

Remarks

- Note that the entries of $\sqrt{K}$ decay with $\mathcal{O}(p^{-2})$. This corresponds to the fact that the derivative of $f(\theta) = \left|\sin\left(\frac{\theta}{2}\right)\right|$ has a discontinuity in 0, which means $\mathcal{O}(p^{-2})$ in the 2nd Fourier coefficient [Wei02].
- Also, the convergence rate of the Riemann sum to the exact integral is only N^{-2} because f is not analytic. In contrary, this convergence is faster than exponential, if f is analytic [TW14].





Remarks (cont)

For a two dimensional problem, discretize the Laplacian

$$-\triangle = -\partial_{xx} - \partial_{yy}$$

(with homogeneous boundary conditions) via the Kronecker sum

$$\mathcal{K} = K \oplus K = (K \otimes I) + (I \otimes K).$$

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For a two dimensional problem, discretize the Laplacian

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(with homogeneous boundary conditions) via the Kronecker sum

$$\mathcal{K} = K \oplus K = (K \otimes I) + (I \otimes K).$$

The N^2 Eigenvectors of $\mathcal{K}$ are given by ([Hor86])

$$\mathbf{v}_k \otimes \mathbf{v}_l, \text{ for } k, l = 1, \ldots, N$$

with corresponding Eigenvalues

$$\lambda_{k,l} = \lambda_k + \lambda_l.$$

Similar steps as above lead to $\sqrt{\mathcal{K}}$. For $e^{-\mathcal{K}}$ observe

$$e^{-\mathcal{K}} = e^{-(K \oplus K)} = e^{-K} \otimes e^{-K}.$$

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The heat equation

Recall the semidiscrete approximation

$$\begin{cases} \mathbf{u}'(t) & = \left(-\frac{K}{h^2}\right)\mathbf{u}(t), \quad \text{for } t > 0 \\ \mathbf{u}(0) & = \mathbf{u}_0 \end{cases}$$

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$$\mathbf{u}(t) = e^{-Kt/h^2}\mathbf{u}_0.$$

As we just saw the centrosymmetric (aliasing!) e^{-Kt/h^2} is given by the entries

$$b_{m-n} - b_{m+n}, \text{ for } m + n \leq N + 1$$

with

$$b_p = e^{-2t/h^2} I_p(2t/h^2).$$

Shifts

Without boundary conditions a shift in the initial condition $\mathbf{u}_0$ produces the same shift in $\mathbf{u}(t)$ in all times. $\leftrightsquigarrow$ Toeplitz.

$$\begin{pmatrix} b & a & & \\ c & b & a & \\ & c & b & a \\ & & c & b \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} a & 0 \\ b & a \\ c & b \\ 0 & c \end{pmatrix}$$

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The Hankel produces a shift in the other directions.

$$\begin{pmatrix} & & a & b \\ & a & b & c \\ a & b & c & \\ b & c & & \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & a \\ a & b \\ b & c \\ c & 0 \end{pmatrix}$$

Why?

Method of images and shifts

Recall that the function

$$\Phi(t,x) = \frac{1}{\sqrt{4\pi t}} e^{-\frac{x^2}{4t}}, \text{ for } x \in \mathbb{R}, t > 0$$

is a fundamental solution of the 1D Heat equation.

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Suppose the initial condition is given by $u(0,x) = \delta_a(x)$ and suppose we have only the left boundary with homogeneous boundary conditions.

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Suppose the initial condition is given by $u(0,x) = \delta_a(x)$ and suppose we have only the left boundary with homogeneous boundary conditions.
Take an additional image source $-\delta_{-a}(x)$. By symmetry the solution is then given by

$$u(t,x) = (\Phi(t,\cdot) * (\delta_a - \delta_{-a}))(x) = \frac{1}{\sqrt{4\pi t}} \left(e^{-(x-a)^2/4t} - e^{-(x+a)^2/4t} \right).$$

Methods of images and shifts (cont.)

$$u(t,x) = \frac{1}{\sqrt{4\pi t}} \left(e^{-(x-a)^2/4t} - e^{-(x+a)^2/4t} \right)$$

Let the source at $x = a$ move to the right, then the second exponential from the image source moves to the left.

$\leftrightsquigarrow$ anti-shift-invariant, Hankel.

Methods of images and shifts (cont.)

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Let the source at $x = a$ move to the right, then the second exponential from the image source moves to the left.

$\leftrightsquigarrow$ anti-shift-invariant, Hankel.

For two boundary points do basically the same, but both, the source $\delta_a(x)$ and the image $-\delta_{-a}(x)$, have to be balanced also at $x = 1$ by $-\delta_{2-a}(x)$ and $\delta_{2+a}(x)$ ... This leads to

$$u(0,x) = \sum_{k=-\infty}^{\infty} \delta_{-2k+a}(x) - \sum_{k=-\infty}^{\infty} \delta_{2k-a}(x), \text{ for } x \in \mathbb{R}.$$

Both boundary conditions are then satisfied by symmetry and

$$\delta_a(x) \text{ moves to the right} \Rightarrow \delta_{2k-a}(x) \text{ moves to the left .}$$

The wave equation

Wave equation with Dirichlet boundary conditions

$$\begin{cases} \partial_{tt} u &= \partial_{xx} u, & \text{on } (0,\infty) \times (0,1) \\ u(t,0) &= 0 & t \in [0,\infty) \\ u(t,1) &= 0 & t \in [0,\infty) \\ u(0,x) &= u_0(x), & x \in [0,1] \\ \partial_t u(0,x) &= v_0(x), & x \in [0,1]. \end{cases}$$

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The wave equation (cont.)

Recall d'Alembert's formula for the solution:

$$u(t,x) = \frac{1}{2}\left(u_0(x+t) + u_0(x-t)\right) + \frac{1}{2}\int_{x-t}^{x+t} v_0(s)ds,$$

The wave equation (cont.)

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and compare it with the solution to the semidiscrete approximation

$$\begin{aligned}\mathbf{u}(t) &= \cos(\sqrt{K}t/h)\mathbf{u}_0 + hK^{-1/2}\sin(\sqrt{K}t/h)\mathbf{v}_0 \\ &= \cos(\sqrt{K}t/h)\mathbf{u}_0 + t\,\mathrm{sinc}(\sqrt{K}t/h)\mathbf{v}_0.\end{aligned}$$

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$\cos(\sqrt{K}t/h)$ and $\mathrm{sinc}(\sqrt{K}t/h)$ are both Toeplitz plus Hankel and the entries can be explicitly calculated via *Bessel function values.*

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Test for Toeplitz plus Hankel

Test

A matrix $M \in \mathbb{C}^{N\times N}$ is of the form Toeplitz plus Hankel iff it satisfies the $(N-2)^2$ conditions

$$M_{i-1,j} + M_{i+1,j} = M_{i,j-1} + M_{i,j+1}, \text{ for } 1 < i,j < N. \tag{4}$$

For a proof of this *cross-sum* relation, see [BBB95].

The four corner theorem

Consider the same K for a second difference, but with different corner entries $(1,1),(1,N),(N,1),(N,N)$. This corresponds to different boundary conditions:

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Consider the same K for a second difference, but with different corner entries $(1,1),(1,N),(N,1),(N,N)$. This corresponds to different boundary conditions:

$K_{1,1} = 1, K_{N,N} = 1$	Neumann boundary
$K_{1,N} = -1, K_{N,1} = -1$	Periodic boundary
$K_{1,1} = 1, K_{N,N} = 2$	mixed Neumann-Dirichlet
$K_{1,1} = 2, K_{N,N} = 1$	mixed Dirichlet-Nuemann

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It turns out, that independently of the entries in the four corners, every matrix function is of the form Toeplitz plus Hankel, as long as K is symmetric.

The four corner theorem (cont.)

The equation (4) is equivalent to

$$M_{i-1,j} - 2M_{i,j} + M_{i+1,j} = M_{i,j-1} - 2M_{i,j} + M_{i,j+1}, \text{ for } 1 < i, j < N.$$

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Consider now $M = \mathbf{v}\mathbf{v}^T$ for an Eigenvector $\mathbf{v}$ of K. Then this becomes

$$\mathbf{v}(j)\triangle^2\mathbf{v}(i) = \mathbf{v}(i)\triangle^2\mathbf{v}(j), \text{ for } 1 < i,j < N. \tag{5}$$

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Since $\mathbf{v}$ is an Eigenvector of the difference matrix, we know that $\triangle^2\mathbf{v}(i) = \lambda\mathbf{v}(i)$ for $1 < i < N$. Equation (5) is passed, since it becomes

$$\mathbf{v}(j)\lambda\mathbf{v}(i) = \mathbf{v}(i)\lambda\mathbf{v}(j), \text{ for } 1 < i,j < N.$$

The four corner theorem (cont.)

The equation (4) is equivalent to

$$M_{i-1,j} - 2M_{i,j} + M_{i+1,j} = M_{i,j-1} - 2M_{i,j} + M_{i,j+1}, \text{ for } 1 < i,j < N.$$

Consider now $M = \mathbf{v}\mathbf{v}^T$ for an Eigenvector $\mathbf{v}$ of K. Then this becomes

$$\mathbf{v}(j)\triangle^2\mathbf{v}(i) = \mathbf{v}(i)\triangle^2\mathbf{v}(j), \text{ for } 1 < i,j < N. \quad (5)$$

Since $\mathbf{v}$ is an Eigenvector of the difference matrix, we know that $\triangle^2\mathbf{v}(i) = \lambda\mathbf{v}(i)$ for $1 < i < N$. Equation (5) is passed, since it becomes

$$\mathbf{v}(j)\lambda\mathbf{v}(i) = \mathbf{v}(i)\lambda\mathbf{v}(j), \text{ for } 1 < i,j < N.$$

Every matrix function of K is Toeplitz plus Hankel.

Resolvents

Recall the definition of a matrix function by Cartan:

Equivalent characterizations for Toeplitz plus Hankel

Let f be analytic inside a closed simple contour Γ enclosing $\sigma(A)$. Then

$$f(A) = \frac{1}{2\pi i} \int_{\Gamma} f(z)(zI - A)^{-1} dz,$$

where the integral is taken entry-wise.

Furthermore, if the contour Γ_k encloses one simple Eigenvalue λ_k we get the projection

$$P_k = \mathbf{v}_k \mathbf{v}_k^T = \frac{1}{2\pi i} \int_{\Gamma_k} (zI - A)^{-1} dz.$$

Equivalent conditions for Toeplitz plus Hankel (cont.)

This gives us the following three equivalent conditions for a matrix function to be of the form Toeplitz plus Hankel:

- For all analytic functions f, the matrix function $f(A)$ is Toeplitz plus Hankel.
- The *Resolvent* $R(z) = (zI - A)^{-1}$ is Toeplitz plus Hankel for all $z \in \mathbb{C} \setminus \sigma(A)$.
- The projections onto all Eigenspaces of A are Toeplitz plus Hankel.

For a explicit form of the Resolvent $(zI - K)^{-1}$ via Bessel functions and the Laplace transform, see [SM14].

What to take home?

- Heat, wave equations in 1D and their semidiscrete approximations.
- Solutions of the approximations via Matrix functions in K.
- Discrete sines and cosines as Eigenvectors of the difference matrix K lead to the Toeplitz plus Hankel structure.
- Approximate the resulting sums via Riemann integrals and (often) find explicit expressions.
- Method of image sources connects the Hankel structure with boundary conditions.

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