Collocation matrices representing inverse operators

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1 Introduction

Differentiation matrices are known to suffer from large round-off error, especially for high orders and fine discretization [**?**]. They give rise to ill-conditioned systems for solving differential equations numerically. To combat the conditioning of these systems one may precondition the problem through a number of means. One such preconditioner is the pseudospectral integration matrix (PSIM) (nb: cite Wang and myself), which performs integration on the differential equation being solved.

Taking the ideas of the PSIM one can construct a preconditioning matrix that acts as an inverse operator to the linear operator involved in the given differential equation. This is equivalent to finding an approximation to the inverse of the spectral collocation matrix representing said linear operator.

This paper will provide the equations to construct the inverse operator matrix (IOM) for a general linear ODE. Several simplifications for constant coefficient linear operators will then be made. The focus of this paper is on Chebyshev collocation methods. However, much of the theory is readily extendable to other spectral methods.

1.1 Chebyshev collocation system

We begin by defining the basics of Chebyshev collocation. This method is used to consider differential equations defined on the interval [-1,1]. To approximate the equation discretely, a partition is used to consider the equations on a finite number of points. This partition, defined here as X, is known as the Chebyshev nodes, Chebyshev points of the second kind, or Chebyshev-Gauss-Lobatto (CGL) points:

$$X = \left\{ x_k = \cos\left(\frac{k\pi}{N}\right) \right\}_{k=0}^{N}, \quad 1 = x_0 > x_1 > \cdots > x_N = -1. \tag{1}$$

Let the vector $\vec{U}$ represent the function $u(x)$ evaluated at the CGL points. Then the vector representing the derivative of $u(x)$ can be found by multiplying

$\vec{U}$ by the Chebyshev differentiation matrix D, defined element-wise by [?]:

$$\begin{aligned} D_{00} &= \frac{2N^2+1}{6} \\ D_{kk} &= -\frac{x_k}{2(1-x_k^2)}, \quad k \neq 0, N \\ D_{jk} &= \frac{c_j}{c_k}\frac{(-1)^{j+k}}{x_j - x_k}, \quad k \neq j \\ D_{NN} &= -D_{00}, \end{aligned} \tag{2}$$

where

$$c_k = \begin{cases} 2 & \text{if} \quad k = 0, N \\ 1 & \text{otherwise.} \end{cases} \tag{3}$$

Higher order differentiation matrices can be found by multiplying D together: $D^{(m)} = D^m$. To reduce round-off error in calculations, one can use the "negative sum trick" [?]:

$$D_{kk} = -\sum_{j \neq k} D_{kj}. \tag{4}$$

Chebyshev collocation implicitly decomposes functions into linear combinations of the Chebyshev polynomials, defined recursively by [?]:

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x), \tag{5}$$

or in closed form by:

$$T_k(x) = \cos(k \arccos(x)). \tag{6}$$

The N–th order Chebyshev polynomial has extrema at the CGL points (1) [?].

Consider the general m–th order linear differential operator:

$$\mathcal{L}u(x) = u^{(m)}(x) + \sum_{n=1}^{m} q_n(x) u^{(m-n)}(x). \tag{7}$$

Consider also m boundary conditions:

$$\begin{aligned} \sum_{n=1}^{m} a_n^k u^{(m-n)}(1) = \mathcal{B}_k u(1) = a_0^k, \qquad & k = 1, ..., k_0, \\ \sum_{n=1}^{m} a_n^k u^{(m-n)}(-1) = \mathcal{B}_k u(-1) = a_0^k, \quad & k = k_0+1, ..., m. \end{aligned} \tag{8}$$

The ordinary differential equation to solve is then:

$$\begin{cases} \mathcal{L}u(x) = f(x) \\ \{\mathcal{B}_k u(\pm 1) = a_0^k\}_{k=1}^{m} \end{cases} \tag{9}$$

where $f(x)$ is a continuous function.

Let the matrix $\bar{A}$ represent the Chebyshev collocation matrix for this operator:

$$\bar{A} = D^{(m)} + \sum_{n=1}^{m} Q_n D^{(m-n)}, \quad Q_n = \begin{bmatrix} q_n(x_0) & & \\ & \ddots & \\ & & q_n(x_N) \end{bmatrix}. \tag{10}$$

The rows for the boundary conditions can be represented in Chebyshev collocation by taking linear combinations of the first and last rows of the various differentiation matrices. Let $\hat{A}$ be the matrix formed by the resulting rows, such that the k–th condition is $\hat{A}_k$, the k–th row of $\hat{A}$:

$$\hat{A} = \begin{bmatrix} \sum_{n=1}^{m} a_n^1 D_0^{(m-n)} \\ \vdots \\ \sum_{n=1}^{m} a_n^{k_0} D_0^{(m-n)} \\ \sum_{n=1}^{m} a_n^{k_0+1} D_N^{(m-n)} \\ \vdots \\ \sum_{n=1}^{m} a_n^{m} D_N^{(m-n)} \end{bmatrix} \tag{11}$$

where $D_0^{(j)}$ is the first row of the j–th order differentiation matrix, and $D_N^{(j)}$ the last row of the same matrix.

The Chebyshev collocation system for this equation is:

$$\begin{bmatrix} \bar{A} \\ \hat{A} \end{bmatrix} \vec{U} = \begin{bmatrix} \vec{f} \\ a_0^1 \\ \vdots \\ a_0^m \end{bmatrix} \tag{12}$$

where the elements of $\vec{f}$ are the values $\{f(x_i)\}$.

The matrix $\bar{A}$ is singular: if the vector $\vec{P}$ represents any homogeneous solution to the operator $\mathcal{L}$ evaluated at the CGL points, then $\bar{A}\vec{P} = 0$. Given that an m–th order linear operator has m linearly independent homogeneous solutions, the null space of $\bar{A}$ has dimension m. As such, m rows from $\bar{A}$ can be removed and the remaining matrix will have the same rank.

Each row in $\bar{A}$ is associated with a CGL point. Specifically, the i–th row of $\bar{A}$ enforces the linear operator at the point $x_i \in X$. To avoid any counting errors, the rows of $\bar{A}$ are labelled from 0 to N. In this way, the first row, labelled $\bar{A}_0$, is associated with the point $x_0 = 1$ and the last row, labelled $\bar{A}_N$, with the point $x_N = -1$. Therefore, choosing rows to remove from $\bar{A}$ is equivalent to choosing m points out of the CGL points X.

The choice of row removal is arbitrary, and provides an additional parameter to adjust. To proceed with the construction, let m rows be removed by choosing m CGL points. Let these m points form the set $V = \{v_k\}_{k=1}^{m}$ such that $v_k =$

$x_j \in X$ for each k for some $j \in \{0, ..., N\}$. Then the j–th row of $\bar{A}$ will be replaced by the k–th row of $\hat{A}$.

Let the matrix A represent the square Chebyshev collocation matrix for this equation, defined by its rows:

$$A_i = \begin{cases} \bar{A}_i & x_i \notin V \\ \hat{A}_k & x_i = v_k \in V \end{cases}. \tag{13}$$

The right-hand side for this system is defined element-wise as:

$$F_i = \begin{cases} f(x_i) & x_i \notin V \\ a_0^k & x_i = v_k \in V \end{cases}. \tag{14}$$

The system to solve is then:

$$A\vec{U} = \vec{F}. \tag{15}$$

Note that it is not necessary to remove rows to make room for boundary conditions. Rows can be added to A, creating an overdetermined system, and the system solved by least squares. However, for matrices A with round-off error the boundary conditions will no longer be satisfied exactly.

2 Inverse operators

We now seek to invert the matrix A defined in Section 1. Let $\mathcal{L}$ be the linear differential operator defined by

$$\mathcal{L}u(x) = u^{(m)}(x) + \sum_{n=1}^{m} q_n(x) u^{(m-n)}(x). \tag{16}$$

This operator has a fundamental set of m solutions. That is, there exists a set $\{P_k(x)\}_{k=1}^m$ such that $\mathcal{L}P_k(x) = 0$.

As seen in Section 1 the matrix A requires m boundary conditions to construct an invertible matrix for the operator $\mathcal{L}$. Let these boundary conditions be represented by $\{\mathcal{B}_k\}_{k=1}^m$, where $\mathcal{B}_k$ is a linear operator of at most degree $m-1$. The boundary conditions may then be written as $\mathcal{B}_k u(\pm 1) = a_0^k$. The rows associated with the set $V = \{v_k\}_{k=1}^m$ have been removed to make room in the matrix A for the boundary conditions.

We represent the inverse of A by R. The j–th column of R is an N–th degree polynomial $R_j(x)$ evaluated at the Chebyshev points, such that the elements of R are $R_{i,j} = R_j(x_i)$.

Lemma 1. *$AR = I$, the identity matrix, if and only if $R_j(x)$ satisfy:*

$$\begin{aligned} \mathcal{L}R_j(x_i) &= \begin{cases} \delta_{ij} & x_j \notin V \\ 0 & x_j \in V \end{cases}, \quad x_i \notin V \\ \mathcal{B}_k R_j(\pm 1) &= \begin{cases} 0 & x_j \neq v_k \in V \\ 1 & x_j = v_k \in V \end{cases}. \end{aligned} \tag{17}$$

Proof. The matrix A acts exactly on N–th degree polynomials. The j–th column of the product AR is therefore the linear operator that A represents acted on $R_j(x)$. Recall from section 1 that the i–th row of A performs the operator at the point $x_i \in X$ for $x_i \notin V$, and the k–th boundary condition for $x_i = v_k \in V$. In this way, the matrix product AR can be represented element-wise by:

$$(AR)_{ij} = \begin{cases} \mathcal{L}R_j(x_i) & x_i \notin V, \\ \mathcal{B}_k R_j(\pm 1) & x_i = v_k \in V. \end{cases} \tag{18}$$

Therefore, $AR = I$ is equivalent to the conditions in equation (19). □

Theorem 1. *The function $R_j(x)$ may be written as*

$$R_j(x) = \sum_{k=1}^{m} \left(C_{k,j} + \beta_{k,j} G_{k,j}(x) \right) P_k(x) \tag{19}$$

where

$$\mathcal{L}P_k(x) = 0, \;\; P_k^{(l)}(v_k) = \begin{cases} 0 & l = 0, ..., m-2, \\ 1 & l = m-1, \end{cases} \tag{20}$$

$$G_{k,j}(x) = \sum_{n=0}^{N-1} \frac{2}{c_n c_j N} \left(T_n(x_j) - \frac{T_N(x_j)}{T_N(v_k)} T_n(v_k) \right) \partial_x^{-1} T_n(x), \tag{21}$$

$$\begin{bmatrix} P_1(x_j) & \dots & P_m(x_j) \\ \vdots & \ddots & \vdots \\ P_1^{(m-1)}(x_j) & \dots & P_m^{(m-1)}(x_j) \end{bmatrix} \begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}, \tag{22}$$

and

$$\sum_{l=1}^{m} C_{l,j} \mathcal{B}_n P_l(\pm 1) = -\sum_{k=1}^{m} \beta_{k,j} G_{k,j}(\pm 1) \mathcal{B}_n P_k(\pm 1) \quad \forall n = 1, \dots, m \tag{23}$$

for $x_j \notin V$ and

$$\sum_{l=1}^{m} C_{l,j} \mathcal{B}_n P_l(\pm 1) = \begin{cases} 0 & x_j \neq v_n, \\ 1 & x_j = v_n \end{cases} \tag{24}$$

for $x_j \in V$.

Proof. The functions $G_{k,j}(x)$ (28) are taken from Wang et al. (nb: cite) and McCoid and Trummer (nb: cite). They have the properties

$$G'_{k,j}(x_i) = \begin{cases} 1 & x_i = x_j, \\ 0 & x_i \neq x_j, v_k. \end{cases} \tag{25}$$

The functions $P_k(x)$ (30) are a particular set of homogeneous solutions to the linear operator. Based on equations (32) and (27) we have the following conditions:

$$\sum_{k=1}^{m} \beta_{k,j} G'_{k,j}(x_j) P_k^{(l)}(x_j) = \begin{cases} 1 & l = m-1, \\ 0 & l = 0, ..., m-2. \end{cases}$$

To ensure the function $R_j(x)$ defined in equation (**??**) satisfies the conditions of equation (19) we must apply $\mathcal{L}$ to it. For this, we need its derivatives evaluated at the Chebyshev points. We begin with the first derivative:

$$\begin{aligned} R'_j(x_i) &= \sum_{k=1}^{m} \beta_{k,j} G'_{k,j}(x_i) P_k(x_i) + \left(C_{k,j} + \beta_{k,j} G_{k,j}(x_i)\right) P'_k(x_i) \\ &= \sum_{k=1}^{m} \left(C_{k,j} + \beta_{k,j} G_{k,j}(x_i)\right) P'_k(x_i), \end{aligned}$$

since $G'_{k,j}(x_i) = 0$ for $i \neq j$, $P_k(v_k) = 0$ and $\sum_{k=1}^{m} \beta_{k,j} G'_{k,j}(x_j) P_k(x_j) = 0$. In fact, this is the case for the first $m-1$ derivatives of $R_j(x)$ evaluated on the Chebyshev points:

$$\begin{aligned} R_j^{(l)}(x_i) &= \sum_{k=1}^{m} \beta_{k,j} G'_{k,j}(x_i) P_k^{(l-1)}(x_i) + \left(C_{k,j} + \beta_{k,j} G_{k,j}(x_i)\right) P_k^{(l)}(x_i) \\ &= \sum_{k=1}^{m} \left(C_{k,j} + \beta_{k,j} G_{k,j}(x_i)\right) P_k^{(l)}(x_i), \quad l = 1, \ldots, m-1. \end{aligned}$$

Therefore, for $x_j \notin V$,

$$\begin{aligned} \mathcal{L} R_j(x_i) &= R_j^{(m)}(x_i) + \sum_{n=1}^{m} q_n(x_i) R_j^{(m-n)}(x_i) \\ &= \sum_{k=1}^{m} \beta_{k,j} G'_{k,j}(x_i) P_k^{(m-1)}(x_i) + \left(C_{k,j} + \beta_{k,j} G_{k,j}(x_i)\right) \mathcal{L} P_k(x_i) \\ &= \sum_{k=1}^{m} \beta_{k,j} G'_{k,j}(x_i) P_k^{(m-1)}(x_i) \\ &= \begin{cases} 0 & i \neq j, \\ 1 & i = j, \end{cases} \quad x_i \notin V. \end{aligned} \tag{26}$$

For $x_j \in V$ equations (28) and (32) guarantee that $\beta_{k,j} G_{k,j}(x) = 0$ and $\mathcal{L} R_j(x_i) = 0$ for all $x_i \notin V$. Thus, $R_j(x)$ satisfies the first half of equation (19).

Moreover,

$$\mathcal{B}_l R_j(\pm 1) = \sum_{k=1}^{m} \left(C_{k,j} + \beta_{k,j} G_{k,j}(\pm 1)\right) \mathcal{B}_l P_k(\pm 1). \tag{27}$$

Enforcing the second half of equation (19) gives immediately the two $m \times m$ systems described in equations (34) and (**??**). $\square$

While we now have a form for the function $R_j(x)$, it is not necessarily straightforward to construct the individual components. In particular, finding the specific homogeneous solutions that satisfy equation (30) may prove computationally intensive.

Suppose, instead, that we have a different set of homogeneous solutions, $\left\{\hat{P}_k(x) \,\middle|\, \mathcal{L}\hat{P}_k(x) = 0 \quad \forall k = 1, \ldots, m\right\}$. It is always possible to construct a particular set of homogeneous solutions from a given set: $P_k(x) = \sum_{n=1}^{m} \gamma_{k,n} \hat{P}_n(x)$. The value of $\gamma_{k,n}$ can be found by solving the system

$$\begin{bmatrix} \hat{P}_1(v_k) & \ldots & \hat{P}_m(v_k) \\ \vdots & \ddots & \vdots \\ \hat{P}_1^{(m-1)}(v_k) & \ldots & \hat{P}_m^{(m-1)}(v_k) \end{bmatrix} \begin{bmatrix} \gamma_{k,1} \\ \vdots \\ \gamma_{k,m} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}. \tag{28}$$

The matrix of this system is identical in form to that of equation (32). This form is called the fundamental matrix of a set of equations, and its inverse is well-known (nb: cite?). Using this knowledge we may write down the solutions to equations (32) and (**??**):

$$\beta_{k,j} = (-1)^{k+m} \frac{W\left(\{P_n\}_{n \neq k}; x_j\right)}{W\left(\{P_n\}; x_j\right)}, \tag{29}$$

$$\gamma_{k,n} = (-1)^{n+m} \frac{W\left(\left\{\hat{P}_j\right\}_{j \neq n}; v_k\right)}{W\left(\left\{\hat{P}_j\right\}; v_k\right)} \tag{30}$$

where $W\left(\{f_k\}; x\right)$ is the determinant of the fundamental matrix of the functions $\{f_k\}$ evaluated at the point x, called the Wronskian.

The Wronskians are themselves functions and are related to the linear operator for which the set $\{f_k\}$ is the fundamental solution set. Naturally, if the set is linearly dependent then the Wronskian is zero. Since we know the linear operator for which $\{P_k\}$ and $\left\{\hat{P}_n\right\}$ are fundamental solution sets, we can use Abel's identity (nb: cite) to write down a new expression for the Wronskians:

$$W\left(\{P_k\}; x\right) = W\left(\{P_k\}; 0\right) \exp\left(-\int_0^x q_1(s)ds\right),$$
$$W\left(\left\{\hat{P}\right\}; x\right) = W\left(\left\{\hat{P}_k\right\}; 0\right) \exp\left(-\int_0^x q_1(s)ds\right).$$

Sadly, in general the linear operator for the set $\{P_k\}_{k \neq j}$ is not self-evident and Abel's identity cannot be used.

Some simplification can be made to equation (32) if the values of $\gamma_{k,n}$ are known. Let Γ be the matrix with entries $\Gamma_{k,n} = \gamma_{k,n}$. Then

$$\begin{bmatrix} P_1(x_j) & \dots & P_m(x_j) \\ \vdots & \ddots & \vdots \\ P_1^{(m-1)}(x_j) & \dots & P_m^{(m-1)}(x_j) \end{bmatrix} \begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} =$$

$$\begin{bmatrix} \hat{P}_1(x_j) & \dots & \hat{P}_m(x_j) \\ \vdots & \ddots & \vdots \\ \hat{P}_1^{(m-1)}(x_j) & \dots & \hat{P}_m^{(m-1)}(x_j) \end{bmatrix} \Gamma \begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \implies$$

$$\Gamma \begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} = \frac{(-1)^m}{W\left(\left\{\hat{P}_n\right\}; x_j\right)} \begin{bmatrix} -W\left(\left\{\hat{P}_n\right\}_{n\neq 1}; x_j\right) \\ W\left(\left\{\hat{P}_n\right\}_{n\neq 2}; x_j\right) \\ \vdots \\ (-1)^m W\left(\left\{\hat{P}_n\right\}_{n\neq m}; x_j\right) \end{bmatrix}.$$

The values $\gamma_{k,n}$ are themselves evaluations of the Wronskians of $\left\{\hat{P}_n\right\}$ on the set V. Therefore, to find the values of $\beta_{k,j}$ one needs the value of the Wronskians of a given fundamental solution set on all the Chebyshev points and then solve an $m \times m$ system of equations. The Wronskians of the specific fundamental solution set are not required.

3 Constant coefficients

The inverse operator matrix (IOM) R constructed in the previous section requires a fundamental solution set to the linear operator $\mathcal{L}$. This precludes using the IOM as a black box preconditioner for a general problem. Instead, we focus on a narrower range of problems, where the coefficients of the linear operator are constant,

$$\mathcal{L}u(x) = u^{(m)}(x) + \sum_{j=1}^{m} a_j u^{(m-j)}(x).$$

There is a polynomial associated with this operator, $p(x) = x^m + \sum_{j=1}^m a_j x^{m-j}$. This polynomial has roots $\{\lambda_k\}_{k=1}^M$ and each root has multipliciity m_k, such that $\sum_{k=1}^M m_k = m$. The linear operator then has homogeneous solutions

$$E = \left\{ \frac{x^j}{j!} e^{\lambda_k x} \;\middle|\; 1 \leq k \leq M, \quad 0 \leq j < m_k \right\}.$$

It is useful at this stage to define the matrices Ω_k, Λ and $\Lambda_{k,j}$. The element in the i–th row and j–th column of Ω_k is equal to $\binom{i}{j-1}\lambda_k^{i-(j-1)}$, using the conventions $\binom{i}{j-1} = 0$ if $j-1 > i$ and $0^0 = 1$. The matrix Ω_k has m rows and m_k columns. This has the appearance of

$$\Omega_k = \begin{bmatrix} 1 & & \\ \lambda_k & \ddots & \\ \vdots & & 1 \\ \vdots & & \vdots \\ \lambda_k^n & \dots & \binom{n}{m_1-1}\lambda_k^{n-(m_k-1)} \\ \vdots & & \vdots \\ \lambda_k^m & \dots & \binom{m}{m_1-1}\lambda_k^{m-(m_k-1)} \end{bmatrix}. \tag{31}$$

Note that if $m_k = 1$ then Ω_k is a column vector, and that if $\lambda_k = 0$ then Ω_k is a diagonal matrix of 1's.

The matrix Λ is the concatenation of the matrices Ω_k, $\Lambda = \begin{bmatrix}\Omega_1 & \Omega_2 & \dots & \Omega_M\end{bmatrix}$. If $M = 1$ then Λ is a lower triangular matrix equal to Ω_1. If $M = m$ then Λ is full with columns Ω_k. Let $\Lambda_{k,j-1}$ be the submatrix of Λ formed by removing the last row and the j–th column of Ω_k.

Theorem 2 (Wronskians for constant coefficient operators)**.** *Let E be the set of homogeneous solutions to the linear operator $\mathcal{L}$ with constant coefficients. Let $E_{k,j}$ be the set $E \setminus \left\{\frac{x^j}{j!}e^{-\lambda_k x}\right\}$. Then*

$$\frac{W\left(E_{k,j};x\right)}{W(E;x)} = \frac{e^{-\lambda_k x}}{|\Lambda|}\sum_{n=0}^{m_k-1-j}\frac{x^n}{n!}\left|\Lambda_{k,n+j}\right|.$$

Proof. Take the portion of the determinant $W(E;x)$ that is associated with the root λ_k. This root has multiplicity m_k. We examine the first two columns of this portion:

$$\begin{vmatrix} \dots & e^{\lambda_k x} & xe^{\lambda_k x} & \dots \\ & \lambda_k e^{\lambda_k x} & x\lambda_k e^{\lambda_k x} + e^{\lambda_k x} & \\ & \vdots & \vdots & \vdots \\ \dots & \lambda_k^{m-1}e^{\lambda_k x} & x\lambda_k^{m-1}e^{\lambda_k x} + (m-1)\lambda_k^{m-2}e^{\lambda_k x} & \dots \end{vmatrix}.$$

First note that both columns are multiplied by $e^{\lambda_k x}$. This can be brought to the outside of the determinant:

$$e^{2\lambda_k x}\begin{vmatrix} \dots & 1 & x & \dots \\ & \lambda_k & x\lambda_k + 1 & \\ & \vdots & \vdots & \\ \dots & \lambda_k^{m-1} & x\lambda_k^{m-1} + (m-1)\lambda_k^{m-2} & \dots \end{vmatrix}.$$

The first column is exactly the first column of Ω_k. The second column is the sum of the first column of Ω_k times x and the second column of Ω_k. Represent the j–th column of Ω_k by $\omega_{k,j}$. Then the determinant may be written more compactly as

$$\begin{aligned}\left|\ldots \quad \omega_{k,1} \quad x\omega_{k,1}+\omega_{k,2} \quad \ldots\right| &= \\ \left|\ldots \quad \omega_{k,1} \quad x\omega_{k,1} \quad \ldots\right| &+ \left|\ldots \quad \omega_{k,1} \quad \omega_{k,2} \quad \ldots\right| \\ &= \left|\ldots \quad \omega_{k,1} \quad \omega_{k,2} \quad \ldots\right|.\end{aligned}$$

This procedure can be repeated to leave the determinant in the form of $|\Lambda|$. First, note that the l–th derivative of $\frac{x^j}{j!}e^{\lambda_k x}$ is

$$\left(\frac{x^j}{j!}e^{\lambda_k x}\right)^{(l)} = \sum_{n=0}^{j}\binom{l}{n}\lambda_k^{l-n}\frac{x^{j-n}}{(j-n)!}e^{\lambda_k x}.$$

The terms $\binom{l}{n}\lambda_k^{l-n}$ are exactly those appearing in $\omega_{k,n+1}$. Thus, the associated column of the fundamental matrix for a set that includes this function is equal to $e^{\lambda_k x}\sum_{n=0}^{j}\frac{x^{j-n}}{(j-n)!}\omega_{k,n+1}$.

The portion of the determinant $W(E;x)$ associated with λ_k may then be written as

$$\begin{aligned}& e^{m_k\lambda_k x}\left|\ldots \quad \omega_{k,1} \quad x\omega_{k,1}+\omega_{k,2}\ldots \quad \sum_{n=0}^{m_k-1}\frac{x^{m_k-1-n}}{(m_k-1-n)!}\omega_{k,n+1}\ldots\right| \\ &= e^{m_k\lambda_k x}\left|\ldots \quad \omega_{k,1} \quad \omega_{k,2}\ldots \quad \sum_{n=1}^{m_k-1}\frac{x^{m_k-1-n}}{(m_k-1-n)!}\omega_{k,n+1}\ldots\right| \\ &\quad\vdots \\ &= e^{m_k\lambda_k x}\left|\ldots \quad \omega_{k,1} \quad \omega_{k,2}\ldots \quad \omega_{k,m_k}\ldots\right| \\ &= e^{m_k\lambda_k x}\left|\ldots \quad \Omega_k \ldots\right|.\end{aligned}$$

This procedure was done for an arbitrary value of k. It may therefore be repeated for all values of k, so that $W(E;x) = \exp\left(x\sum_{k=1}^{M} m_k\lambda_k\right)|\Lambda|$.

As a corollary,

$$W\left(E_{k,m_k-1};x\right) = \exp\left(x\left(\sum_{i=1}^{M} m_i\lambda_i - \lambda_k\right)\right)\left|\Lambda_{k,m_k-1}\right|,$$

since the set E_{k,m_k-1} has all the same properties as E but with m and m_k reduced by 1. By dividing $W\left(E_{k,m_k-1};x\right)$ by $W(E;x)$ one proves the statement of the theorem for $j = m_k - 1$.

Consider, now, $W\left(E_{k,j};x\right)$; The portion of the determinant associated with the other roots, λ_i with $i \neq k$, are unchanged from the formulation presented above. We need only consider the effects on that portion pertaining to λ_k:

$$W\left(E_{k,j};x\right) = e^{x\left(\sum_{i=1}^{M} m_i\lambda_i - \lambda_k\right)}\left|\ldots \quad \Omega_{k-1} \quad \tilde{\Omega}_{k,j} \quad \Omega_{k+1} \quad \ldots\right|.$$

The columns found in $\tilde{\Omega}_{k,j}$ are

$$\tilde{\Omega}_{k,j} = \begin{bmatrix} \omega_{k,1} & x\omega_{k,1} + \omega_{k,2} & \dots \end{bmatrix}.$$

As before, remove those parts of subsequent columns that are parallel with $\omega_{k,1}$ and $\omega_{k,2}$ and so on up to $\omega_{k,j+1}$, so that

$$\left|\dots \tilde{\Omega}_{k,j} \dots\right| = \begin{vmatrix} \dots & \omega_{k,1} & \omega_{k,2} & \dots & \omega_{k,j} & x\omega_{k,j+1} + \omega_{k,j+2} & \dots \end{vmatrix},$$

since the column associated with $\frac{x^j}{j!}e^{\lambda_k x}$ is the $(j+1)$–th column of Ω_k, where $\omega_{k,j+1}$ first appears.

The next step is to split the determinant into two parts along the $(j+1)$–th column of $\tilde{\Omega}_{k,j}$:

$$\begin{aligned}
\left|\dots \tilde{\Omega}_{k,j} \dots\right| =& \begin{vmatrix} \dots & \omega_{k,j} & x\omega_{k,j+1} + \omega_{k,j+2} & \dots \end{vmatrix} \\
=& \begin{vmatrix} \dots & \omega_{k,j} & x\omega_{k,j+1} & x\omega_{k,j+2} + \omega_{k,j+3} & \dots \end{vmatrix} \\
&+ \begin{vmatrix} \dots & \omega_{k,j} & \omega_{k,j+2} & \frac{x^2}{2!}\omega_{k,j+1} + \omega_{k,j+3} & \dots \end{vmatrix} \\
=& x\left|\dots \tilde{\Omega}_{k,j+1} \dots\right| + \begin{vmatrix} \dots & \omega_{k,j} & \omega_{k,j+2} & \frac{x^2}{2!}\omega_{k,j+1} + \omega_{k,j+3} & \dots \end{vmatrix}.
\end{aligned}$$

The second determinant may be split again in the $(j+2)$–th column. This procedure may be repeated until all options have been exhausted. To see how, we perform an induction step.

Suppose the procedure is at step n, such that the determinant can be split into two at the $(j+n)$–th column. Then

$$\begin{aligned}
&\begin{vmatrix} \dots & \frac{x^n}{n!}\omega_{k,j+1} + \omega_{k,j+n+1} & \frac{x^{n+1}}{(n+1)!}\omega_{k,j+1} + x\omega_{k,j+n+1} + \omega_{k,j+n+2} & \dots \end{vmatrix} \\
=& \begin{vmatrix} \dots & \frac{x^n}{n!}\omega_{k,j+1} & x\omega_{k,j+n+1} + \omega_{k,j+n+2} & \dots \end{vmatrix} \\
&+ \begin{vmatrix} \dots & \omega_{k,j+n+1} & \frac{x^{n+1}}{(n+1)!}\omega_{k,j+1} + \omega_{k,j+n+2} & \dots \end{vmatrix} \\
=& (-1)^{n+1}\frac{x^n}{n!}\left|\dots \tilde{\Omega}_{k,j+n} \dots\right| + \begin{vmatrix} \dots & \omega_{k,j+n+1} & \frac{x^{n+1}}{(n+1)!}\omega_{k,j+1} + \omega_{k,j+n+2} & \dots \end{vmatrix},
\end{aligned}$$

where the term $(-1)^{n+1}$ indicates $n+1$ column interchanges so as to maintain a consistent form of $\tilde{\Omega}_{k,j+n}$.

The determinant can now be written out in full:

$$\left|\dots \tilde{\Omega}_{k,j} \dots\right| = \sum_{n=1}^{m_k-1-j} (-1)^{n+1}\frac{x^n}{n!}\left|\dots \tilde{\Omega}_{k,j+n} \dots\right| + \begin{vmatrix} \dots & \omega_{k,j} & \omega_{k,j+2} & \dots \end{vmatrix}.$$

This determinant can be used as part of the larger determinant $W(E_{k,j};x)$, as none of the work has precluded the presence of additional columns:

$$\begin{aligned}
W(E_{k,j};x) = \exp\left(x\left(\sum_{i=1}^{M} m_i\lambda_i - \lambda_k\right)\right)\left|\Lambda_{k,j}\right| \\
+ \sum_{n=1}^{m_k-1-j} (-1)^{n+1}\frac{x^n}{n!}W(E_{k,j+n};x).
\end{aligned}$$

Dividing by $W(E;x)$ one arrives at

$$\begin{aligned}&\frac{W\left(E_{k,j};x\right)}{W(E;x)} = \\ &e^{-\lambda_k x}\frac{\left|\Lambda_{k,j}\right|}{\left|\Lambda\right|} + \sum_{n=1}^{m_k-1-j}(-1)^{n+1}\frac{x^n}{n!}\frac{W\left(E_{k,j+n};x\right)}{W(E;x)}.\end{aligned} \tag{32}$$

We may then proceed by induction over the finite set $j = 0, \ldots, m_k - 1$.

The base case, $j = m_k - 1$, has already been proven. Suppose that the statement of the theorem is true for $l < j \leq m_k - 1$. That is, for $l < j \leq m_k - 1$,

$$\frac{W\left(E_{k,j};x\right)}{W(E;x)} = \frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\sum_{n=0}^{m_k-1-j}\frac{x^n}{n!}\left|\Lambda_{k,n+j}\right|.$$

We then prove the statement for $j = l$ using equation (**??**):

$$\begin{aligned}
&\frac{W\left(E_{k,l};x\right)}{W(E;x)} = \\
&e^{-\lambda_k x}\frac{\left|\Lambda_{k,l}\right|}{\left|\Lambda\right|} + \sum_{i=1}^{m_k-1-l}(-1)^{i+1}\frac{x^i}{i!}\frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\sum_{n=0}^{m_k-1-l-i}\frac{x^n}{n!}\left|\Lambda_{k,n+l+i}\right| \\
=&\frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\left[\left|\Lambda_{k,l}\right| + \sum_{i=1}^{m_k-1-l}\sum_{n=0}^{m_k-1-l-i}(-1)^{i+1}\frac{x^{i+n}}{(i+n)!}\binom{i+n}{i}\left|\Lambda_{k,n+l+i}\right|\right] \\
=&\frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\left[\left|\Lambda_{k,l}\right| + \sum_{i=1}^{m_k-1-l}\sum_{n=i}^{m_k-1-l}(-1)^{i+1}\frac{x^n}{n!}\binom{n}{i}\left|\Lambda_{k,n+l}\right|\right] \\
=&\frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\left[\left|\Lambda_{k,l}\right| + \sum_{n=1}^{m_k-1-l}\sum_{i=1}^{n}(-1)^{i+1}\frac{x^n}{n!}\binom{n}{i}\left|\Lambda_{k,n+l}\right|\right] \\
=&\frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\left[\left|\Lambda_{k,l}\right| + \sum_{n=1}^{m_k-1-l}\frac{x^n}{n!}\left|\Lambda_{k,n+l}\right|\sum_{i=1}^{n}(-1)^{i+1}\binom{n}{i}\right] \\
=&\frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\left[\left|\Lambda_{k,l}\right| + \sum_{n=1}^{m_k-1-l}\frac{x^n}{n!}\left|\Lambda_{k,n+l}\right|\right] = \frac{e^{-\lambda_k x}}{\left|\Lambda\right|}\sum_{n=0}^{m_k-1-l}\frac{x^n}{n!}\left|\Lambda_{k,n+l}\right|.
\end{aligned}$$

A detailled explanation of each step follows.

Continuing from equation (**??**), the index n there is replaced by i, j by l and the fraction of Wronskians by the induction hypothesis, using n as a counting variable to remain consistent with the statement of the theorem. The product of the polynomials, x^{i+n}, is made to adhere to the prescribed form by the introduction of the factorial $(i+n)!$. This factorial also simplifies the remaining factorials into binomial coefficients.

Next, the counting variable n is reduced by i ($n \to n - i$) to simplify the polynomial, binomial coefficient, limit of the summation and index of $\Lambda_{k,n+l+i}$.

The two summations are then exchanged. This allows those elements that do not contain reference to i to be removed from that summation.

The summation over i is now equal to 1 thanks to an identity of the binomial coefficients (nb: cite),

$$\sum_{i=0}^{n}(-1)^i\binom{n}{i} = 0 \implies \sum_{i=1}^{n}(-1)^i\binom{n}{i} = -(-1)^0\binom{n}{0} = -1.$$

Lastly, the term for $n = 0$ is simply $\frac{x^0}{0!}\left|\Lambda_{k,l+0}\right|$ and so $\left|\Lambda_{k,l}\right|$ is subsumed into the summation as the term for $n = 0$. Thus concludes the proof. $\square$

There are a number of special cases of this theorem, providing the Wronskians for polynomials, exponentials, and their products.

Corollary 1 (Special cases of Theorem (nb: ref))**.** *If $M = m$ then*

$$\frac{W\left(E \setminus \left\{e^{\lambda_k x}\right\}; x\right)}{W(E; x)} = e^{-\lambda_k x}\frac{\left|\Lambda_{k,0}\right|}{\left|\Lambda\right|}. \tag{33}$$

If $M = 1$ then

$$\frac{W\left(E \setminus \left\{\frac{x^j}{j!}e^{\lambda x}\right\}; x\right)}{W(E; x)} = e^{-\lambda x}\frac{x^{m-1-j}}{(m-1-j)!}. \tag{34}$$

This remains true for $\lambda = 0$.

Proof. If $M = m$ then $m_k = 1$ for all $k = 1, \ldots, M$. As such, the summation in Theorem (nb: ref) reduces to the first term.

For $M = 1$ the matrix Λ is a lower triangular matrix with 1's along the diagonal. Therefore, $\left|\Lambda\right| = 1$. Moreover, $\left|\Lambda_{1,k}\right| = \delta_{k,m-1}$. Thus, the sum in Theorem (nb: ref) reduces to the term for $n + j = m - 1$. $\square$

It is therefore possible to give exact formulae for the values of $\gamma_{k,n}$. In practice, however, these may prove cumbersome to calculate. Instead, the system found in equation (**??**) can be simplified for constant coefficients.

First, let $F_k(x)$ represent the fundamental matrix for the set of polynomials $\left\{\frac{x^j}{j!} \;\middle|\; 0 \le j \le m_k - 1\right\}$. That is,

$$F_k(x) = \begin{bmatrix} 1 & x & \cdots & \frac{x^{m_k-1}}{(m_k-1)!} \\ & 1 & & \frac{x^{m_k-2}}{(m_k-2)!} \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix} = \exp\left(x\begin{bmatrix} 0 & 1 & & \\ & & \ddots & \\ & & & 1 \\ & & & 0 \end{bmatrix}\right).$$

Thanks to the second form of this matrix, its inverse is trivial to write down:

$$F_k^{-1}(x) = \exp\left(-x\begin{bmatrix} 0 & 1 & & \\ & & \ddots & \\ & & & 1 \\ & & & 0 \end{bmatrix}\right) = \begin{bmatrix} 1 & -x & \cdots & (-1)^{m_k-1}\frac{x^{m_k-1}}{(m_k-1)!} \\ & 1 & & (-1)^{m_k-2}\frac{x^{m_k-2}}{(m_k-2)!} \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix}.$$

Based on the proof of Theorem (nb: ref) equation (**??**) can be written as

$$\Lambda \begin{bmatrix} e^{\lambda_1 v_k} F_1(v_k) & & & \\ & e^{\lambda_2 v_k} F_2(v_k) & & \\ & & \ddots & \\ & & & e^{\lambda_M v_k} F_M(v_k) \end{bmatrix} \begin{bmatrix} \gamma_{k,1} \\ \vdots \\ \gamma_{k,m} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}.$$

The vector of $\gamma_{k,n}$ can then be expressed as

$$\begin{bmatrix} \gamma_{k,1} \\ \vdots \\ \gamma_{k,m} \end{bmatrix} = \begin{bmatrix} e^{-\lambda_1 v_k} F_1^{-1}(v_k) & & & \\ & e^{-\lambda_2 v_k} F_2^{-1}(v_k) & & \\ & & \ddots & \\ & & & e^{-\lambda_M v_k} F_M^{-1}(v_k) \end{bmatrix} \Lambda^{-1} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}.$$

The inverses of $F_j(v_k)$ are known and are of size $m_j \times m_j$. Each $F_j^{-1}(v_k)$ is a principal submatrix of $F_i^{-1}(v_k)$ where $m_i = \max_{1 \le j \le M} m_j$. The only remaining unknown is Λ^{-1}. However, this is constant for all values of x and so need only be done once for a given problem. Moreover, only the last column of this inverse is needed, further reducing computational costs.

The vector of $\beta_{n,j}$ can likewise be expressed as

$$\begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} = \\ \Gamma^{-1} \begin{bmatrix} e^{-\lambda_1 x_j} F_1^{-1}(x_j) & & & \\ & e^{-\lambda_2 x_j} F_2^{-1}(x_j) & & \\ & & \ddots & \\ & & & e^{-\lambda_M x_j} F_M^{-1}(x_j) \end{bmatrix} \Lambda^{-1} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}.$$

Recall that Γ is the matrix whose entries are $\gamma_{k,n}$. Like Λ, the inverse of Γ is unknown but constant for all x.

4 Application and experiments

4.1 Example

To illustrate the application of this work we consider a problem with $m = 4$ and two roots, each with multiplicity two. This gives $E = \{e^{\lambda_1 x}, xe^{\lambda_1 x}, e^{\lambda_2 x}, xe^{\lambda_2 x}\}$. From Abel's identity and lemma 1 we know

$$W(E; x) = \begin{vmatrix} 1 & 0 & 1 & 0 \\ \lambda_1 & 1 & \lambda_2 & 1 \\ \lambda_1^2 & 2\lambda_1 & \lambda_2^2 & 2\lambda_2 \\ \lambda_1^3 & 3\lambda_1^2 & \lambda_2^3 & 3\lambda_2^2 \end{vmatrix} e^{(2\lambda_1 + 2\lambda_2)x}.$$

To calculate the IOM we need the functions $W\left(E \setminus E_{k,j}; x\right)$, of which there are four:

$$
\begin{aligned}
W\left(E \setminus E_{1,0}; x\right) e^{-(\lambda_1+2\lambda_2)x} &= \begin{vmatrix} 0 & 1 & 0 \\ 1 & \lambda_2 & 1 \\ 2\lambda_1 & \lambda_2^2 & 2\lambda_2 \end{vmatrix} + x \begin{vmatrix} 1 & 1 & 0 \\ \lambda_1 & \lambda_2 & 1 \\ \lambda_1^2 & \lambda_2^2 & 2\lambda_2 \end{vmatrix}, \\
W\left(E \setminus E_{1,1}; x\right) e^{-(\lambda_1+2\lambda_2)x} &= \begin{vmatrix} 1 & 1 & 0 \\ \lambda_1 & \lambda_2 & 1 \\ \lambda_1^2 & \lambda_2^2 & 2\lambda_2 \end{vmatrix}, \\
W\left(E \setminus E_{2,0}; x\right) e^{-(2\lambda_1+\lambda_2)x} &= \begin{vmatrix} 1 & 0 & 0 \\ \lambda_1 & 1 & 1 \\ \lambda_1^2 & \lambda_1 & \lambda_2 \end{vmatrix} + x \begin{vmatrix} 1 & 0 & 1 \\ \lambda_1 & 1 & \lambda_2 \\ \lambda_1^2 & 2\lambda_1 & \lambda_2^2 \end{vmatrix}, \\
W\left(E \setminus E_{2,1}; x\right) e^{-(2\lambda_1+\lambda_2)x} &= \begin{vmatrix} 1 & 0 & 1 \\ \lambda_1 & 1 & \lambda_2 \\ \lambda_1^2 & 2\lambda_1 & \lambda_2^2 \end{vmatrix}.
\end{aligned}
$$

Note that all of the 3×3 determinants could be calculated as part of calculating the 4×4 determinant of $W(E;x)$ if one expands along the bottom row. As such, calculating the other four Wronskians should be no more than $\mathcal{O}\left(m\right)$ additional operations.

4.2 Algorithm for IOM for constant coefficients

Step 1: Identify the roots and their multiplicities $\{\lambda_k; m_k\}_{k=1}^{M}$ of the polynomial associated with the linear operator. Order them such that m_1 is the largest of the m_k.

Step 2: Construct the matrix Ω. This may be done by constructing Pascal's triangle with m rows and a lower triangular $m \times m_k$ Toeplitz matrix with each diagonal corresponding to a power of λ_k. Take the Hadamard product of Pascal's triangle with each of the M matrices so constructed and concatenate these products.

Step 3: Form $F_1^{-1}(x)$ for all x. This is a $m_k \times m_k \times N+1$ size object, each page of which is an upper triangular Toeplitz matrix with each diagonal corresponding to $(-1)^j \frac{x^j}{j!}$. The polynomials may be calculated sequentially then used to construct the matrices.

Step 4: Calculate $\omega(x)$ for all x. This creates a $m \times N+1$ matrix. This is done by first solving $\Omega z = \begin{bmatrix} 0 & \dots & 0 & 1 \end{bmatrix}^\top$ then multiplying the first m_1 rows of z by $F_1^{-1}(x)e^{-\lambda_1 x}$. Next, multiply the next m_2 rows of z by the $m_2 \times m_2$ principal submatrix of $F_1^{-1}(x)e^{-\lambda_2 x}$. Continue in this fashion for $k = 1, ..., M$.

Step 5: Let Γ be the matrix formed by taking the columns of $\omega(x)$ corresponding to the points in V. Calculate the coefficients $\beta_{k,j}$ by solving the system

$\Gamma\beta = \omega(x)$, where β is the $m \times N + 1$ matrix containing the coefficients $\beta_{k,j}$.

Step 6: Form the fundamental solution set. The best solution here seems to be to use a Hadamard product of a matrix of the exponential functions layered with their multiplicities in mind with a matrix of the polynomials, the information for which may be extracted from $F_1^{-1}(x)$ calculated in step 3. Right multiply this Hadamard product by Γ.

Step 7: Form the Birkhoff interpolants $G_{k,j}(x)$. One must first form the Chebyshev polynomials and their integrals. Once this is done, they may be calculated with the formulas given in equation (28).

Step 8: Find C_{kj} and combine ingredients to form the IOM. The system for the C_{kj} requires storing the derivatives of the fundamental solution set at $x = 1$ and -1, done by multiplying Ω, $e^{\pm\lambda_k}$, $F_k(\pm 1)$ and Γ. The right hand side requires the same as well as $G_{k,j}(\pm 1)$.