Representation of ND PI Operators using Quadratic Kernels

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These notes consider the representation of univariate and multivariate PI operators, representing the kernels defining these operators in a quadratic format. We specifically focus on establishing composition rules for these operators in terms of the coefficients representing the operator in the quadratic format.

1 Preliminaries

1.1 Notation

For given parameters $\boldsymbol{P}_i$, we use $\Pi_{\{\boldsymbol{P}_i\}}$ to denote the associated PI operator, where the number of parameters determines the type of operator.

1.2 Kronecker Products and the Mixed Product Property

For $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{p\times q}$, define the Kronecker product $A \otimes B \in \mathbb{R}^{mp\times nq}$ in the standard manner

$$A \otimes B = \begin{bmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{bmatrix}$$

Note that the Kronecker product is bilinear, and associative, so that

$$A \otimes (B + C) = A \otimes B + A \otimes C, \qquad (kA) \otimes B = A \otimes (kB) = k(A \otimes B) \qquad (A \otimes B) \otimes C = A \otimes (B \otimes C).$$

Moreover, we have the *mixed product property* by which for any A, B, C, D such that the matrix products AC and BD are well-defined, we have

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD).$$

Note then that, for any $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{p\times q}$, $u \in \mathbb{R}^n$, and $v \in \mathbb{R}^q$, we also have $Au \otimes Bv = (A \otimes B)(u \otimes v)$. Moreover, we have

$$A \otimes B = (A \otimes I_p)(I_n \otimes B) = (I_m \otimes B)(A \otimes I_q),$$

so that also $(I_m \otimes B)A = (A \otimes I_p)(I_n \otimes B)$ if $q = 1$, or $B(A \otimes I_q) = (A \otimes I_p)(I_n \otimes B)$ if $m = 1$. Furthermore, the mixed product property also implies

$$I_m \otimes AB = I_m I_m \otimes AB = (I_m \otimes A)(I_m \otimes B), \qquad \text{and} \qquad AB \otimes I_q = AB \otimes I_q I_q = (A \otimes I_q)(B \otimes I_q).$$

In addition, for any $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{p\times q}$, we have

$$B \otimes A = P_{m,p}(A \otimes B)P_{n,q}^T,$$

where for $p, q \in \mathbb{N}$, $P_{p,q} \in \mathbb{R}^{pq\times pq}$ is the *commutation matrix*, defined by

$$P_{p,q} := \begin{bmatrix} I_{pq}(1 : q : pq, :) \\ I_{pq}(2 : q : pq, :) \\ \vdots \\ I_{pq}(p : q : pq, :) \end{bmatrix} = \begin{bmatrix} I_p \otimes \mathrm{e}_1^T \\ I_p \otimes \mathrm{e}_2^T \\ \vdots \\ I_p \otimes \mathrm{e}_q^T \end{bmatrix}, \quad \text{for } \mathrm{e}_i \in \mathbb{R}^q \text{ the } i\text{th canonical basis vector}$$

note here that $P_{1,q} = I_q$ and $P_{p,1} = I_p$.

2 Quadratic Representation of Semi-Separable Kernels

2.1 3-PI Operators

Consider first the class of 3-PI operators of the form

$$(\mathcal{R}\boldsymbol{x})(s) := (\Pi_{\{\boldsymbol{R}_0,\boldsymbol{R}_1,\boldsymbol{R}_2\}}\mathbf{x})(s) := \boldsymbol{R}_0(s)\mathbf{x}(s) + \int_a^s \boldsymbol{R}_1(s,\theta)\mathbf{x}(\theta)d\theta + \int_s^b \boldsymbol{R}_2(s,\theta)\mathbf{x}(\theta)d\theta,$$

for $\mathbf{x} \in L_2^n[a,b]$, and where we assume the parameters $\boldsymbol{R}_i$ to be separable as

$$\boldsymbol{R}_0(s) = (I_m \otimes \boldsymbol{Z}(s))^T C_0, \qquad \boldsymbol{R}_i(s,\theta) = (I_m \otimes \boldsymbol{Z}(s))^T C_i (I_m \otimes \boldsymbol{Z}(\theta)),\ i \in \{1,2\},$$

for some vector of basis functions $\boldsymbol{Z}$, and coefficient matrices $C_0 \in \mathbb{R}^{m(d+1)\times n}$ and $C_i \in \mathbb{R}^{m(d+1)\times n(d+1)}$. Throughout these notes, we will assume the basis $\boldsymbol{Z}(s)$ to be the vector of monomials of degree at most d in s, $\boldsymbol{Z}(s) = \boldsymbol{Z}_d(s) = \begin{bmatrix} 1 \\ \vdots \\ s^d \end{bmatrix}$, although another basis (e.g. Lengendre or Chebyshev polynomials) would also be possible. Then, we can numerically represent $\mathcal{R}$ by a Matlab structure `R` with fields

- `R.C`: 3×1 cell with each element a sparse matrix, representing the coefficient matrices C_i;
- `R.deg`: scalar value specifying the maximal degree d of the monomials;
- `R.dom`: 1×2 array specifying the interval $[a,b]$ on which the operator is defined;
- `R.dim`: (optional) 1×2 array specifying the dimensions $[m,n]$ of the matrix-valued operator (should also follow from the size of the coefficients, but is easier to store separately);
- `R.vars`: (optional) 1×2 `pvar` array representing the spatial variable s and dummy variable θ.

Rudimentary functions for converting from `opvar` format to this "coefficients-based" format and back have been implemented as `opvar2coeffs` and `coeffs2opvar`.

Of course, we could also allow for different maximal degrees d for the different kernels, or for the primary and dummy variables.

2.2 2D PI Operators

Consider now a class of 2D PI operator of the form

$$\begin{aligned}\Pi_{\{\boldsymbol{Q}_{ij}\}}\mathbf{x}(s_1,s_2) = &\int_{a_1}^{s_1}\int_{a_2}^{s_2} \boldsymbol{Q}_{11}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1 + \int_{a_1}^{s_1}\int_{s_2}^{b_2} \boldsymbol{Q}_{12}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1 \\ &+ \int_{s_1}^{b_1}\int_{a_2}^{s_2} \boldsymbol{Q}_{21}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1 + \int_{s_1}^{b_1}\int_{s_2}^{b_2} \boldsymbol{Q}_{22}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1,\end{aligned}$$

where

$$\boldsymbol{Q}_{ij}(s,\theta) = \boldsymbol{Z}_d(s) C_{ij} \boldsymbol{Z}(\theta) = (I_m \otimes \boldsymbol{Z}_d(s_1) \otimes \boldsymbol{Z}_d(s_2))^T C_{ij} (I_n \otimes \boldsymbol{Z}_d(\theta_1) \otimes \boldsymbol{Z}_d(\theta_2)), \quad i,j \in \{1,2\},$$

for $C_{ij} \in \mathbb{R}^{m(d+1)^2 \times n(d+1)^2}$. For simplicity, we consider no multiplier terms here, although those can be included in a similar manner as in the 1D case. Then, we can represent the operator $\mathcal{Q}$ by a Matlab structure `Q` with fields

- `Q.C`: 3×3 cell with each element a sparse matrix, representing the coefficient matrices C_{ij};
- `Q.deg`: scalar value specifying the maximal degree d of the monomials;
- `Q.dom`: 2×2 array specifying the intervals $[a_1,b_1]$ (first row) and $[a_2,b_2]$ (second row) on which the operator is defined;
- `Q.dim`: (optional) 1×2 array specifying the dimensions $[m,n]$ of the matrix-valued operator;
- `Q.vars`: (optional) 2×2 `pvar` array representing the spatial variables s_1, s_2 (first column) and dummy variables θ_1, θ_2 (second column).

For simplicity, we will use the same maximal monomial degree in all variables, though of course, we could also allow for different maximal monomial degrees for different variables. Rudimentary functions for converting from `opvar2d` format to this "coefficients-based" format and back have been implemented as `opvar2d2coeffs` and `coeffs2opvar2d`.

2.3 ND PI Operators

We parameterize a class of 2^N-PI operators by 2^N polynomials, $\boldsymbol{Q}_\alpha \in \mathbb{R}^{m\times n}[s,\theta]$ for $\alpha \in \{1,2\}^N$, as

$$(\mathcal{Q}\mathbf{x})(s) = \sum_{\alpha\in\{1,2\}^N} \int_a^b \mathbf{I}_\alpha(s,\theta)\boldsymbol{Q}_\alpha(s,\theta)\mathbf{x}(\theta)\, d\theta$$

for $\mathbf{x} \in L_2^n[[a_1 b,_1] \times \cdots \times [a_N, b_N]]$, and where

$$\mathbf{I}_\alpha(s,\theta) := \prod_{i=1}^N \mathbf{I}_{\alpha_i}(s_i,\theta_i), \qquad \mathbf{I}_j(x,y) := \begin{cases} \mathbf{1}(x-y), & j=1, \\ \mathbf{1}(y-x), & j=2, \end{cases}$$

where $\mathbf{1}$ is the indicator function,

$$\mathbf{1}(z) := \begin{cases} 1, & z \geq 0, \\ 0, & \text{else.} \end{cases}$$

Again, we consider parameters of the form

$$\boldsymbol{Q}_\alpha(s,\theta) = (I_n \otimes \boldsymbol{Z}_d(s))^T C_\alpha (I_m \otimes \boldsymbol{Z}_d(\theta)),$$

where $\alpha \in \{1,2\}^N$, and

$$\boldsymbol{Z}_d(s) = \boldsymbol{Z}_d(s_1) \otimes \boldsymbol{Z}_d(s_2) \otimes \cdots \otimes \boldsymbol{Z}_d(s_N).$$

Then, we can represent the operator $\mathcal{Q}$ by a structure `Q` with fields

- `Q.C`: $3 \times \cdots \times 3 = 3^N$ cell with each element a sparse matrix, representing the coefficient matrices C_α;
- `Q.deg`: scalar value specifying the maximal degree d of the monomials;
- `Q.dom`: $N \times 2$ array specifying the intervals $[a_i, b_i]$ on which the operator is defined;
- `Q.dim`: (optional) 1×2 array specifying the dimensions $[m, n]$ of the matrix-valued operator;
- `Q.vars`: (optional) $N \times 2$ `pvar` array representing the spatial variables s_i (first column) and dummy variables θ_i (second column).

Note that this format does not allow for maps from $L_2[a_i, b_i] \to L_2[a_j, b_j]$, so this is still quite limiting.

2.4 Decision Variable Operator

We parameterize a class of decision variable 2^N-PI operators by 2^N polynomials, $\boldsymbol{Q}_\alpha \in \mathbb{R}^{m\times n}[s,\theta]$ for $\alpha \in \{1,2\}^N$, as

$$(\mathcal{Q}\mathbf{x})(s) = \sum_{\alpha\in\{1,2\}^N} \int_a^b \mathbf{I}_\alpha(s,\theta)\boldsymbol{Q}_\alpha(s,\theta;\xi)\mathbf{x}(\theta)\, d\theta$$

for $\mathbf{x} \in L_2^n[[a_1 b,_1] \times \cdots \times [a_N, b_N]]$, and where now we consider parameters of the form

$$\boldsymbol{Q}_\alpha(s,\theta;\xi) = (I_n \otimes \boldsymbol{Z}_d(s))^T (I_{n(d+1)^N} \otimes [\begin{smallmatrix}1\\ \xi\end{smallmatrix}])^T C_\alpha (I_m \otimes \boldsymbol{Z}_d(\theta)),$$

where $C_\alpha \in \mathbb{R}^{n(q+1)(d+1)^N \times m(d+1)^N}$ for $\alpha \in \{1,2\}^N$, parameterized by decision variables $\xi \in \mathbb{R}^q$. Then, we can represent the operator $\mathcal{Q}$ by a structure `Q` with fields

- `Q.C`: 3^N cell with each element a sparse matrix, representing the coefficient matrices C_α;
  Alternatively: 3^N cell with each element a `dpvar` object, representing $(I_{n(d+1)^N} \otimes [\begin{smallmatrix}1\\ \xi\end{smallmatrix}])^T C_\alpha$;
- `Q.deg`: scalar value specifying the maximal degree d of the monomials;
- `Q.dom`: $N \times 2$ array specifying the intervals $[a_i, b_i]$ on which the operator is defined;
- `Q.dvars`: $q \times 1$ `cellstr` specifying the names of the decision variables $\xi \in \mathbb{R}^q$;
- `Q.dim`: (optional) 1×2 array specifying the dimensions $[m, n]$ of the matrix-valued operator;
- `Q.vars`: (optional) $N \times 2$ `pvar` array representing the spatial variables s_i (first column) and dummy variables θ_i (second column).

3 Composition Operation in Quadratic Representation

We now establish composition rules for 1D PI operators in terms of the coefficients C_i representing them in the quadratic representation. We also show how we can inductively use these composition rules to perform composition of multivariate PI operators.

3.1 Composition of Scalar-Valued 2-PI Operators

Consider the composition of two 2-PI operators, defined by parameters $\boldsymbol{Q}_i(s,\theta) = \boldsymbol{Z}_d(s)C_i\boldsymbol{Z}_d(\theta)$ and $\boldsymbol{R}_i(s,\theta) = \boldsymbol{Z}_d(s)D_i\boldsymbol{Z}_d(\theta)$, where $\boldsymbol{Z}_d(s) \in \mathbb{R}^{d+1}[s]$ is a basis for degree d polynomials. Then we know that $\Pi_{\{\boldsymbol{Q}_i\}} \circ \Pi_{\{\boldsymbol{R}_i\}} = \Pi_{\{\boldsymbol{P}_i\}}$, where

$$\begin{aligned}
\boldsymbol{P}_1(s,\theta) &= \int_a^\theta \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_2(\eta,\theta)\,d\eta + \int_\theta^s \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_1(\eta,\theta)\,d\eta + \int_s^b \boldsymbol{Q}_2(s,\eta)\boldsymbol{R}_1(\eta,\theta)\,d\eta \\
&= \boldsymbol{Z}_d(s)^T C_1 \left[\int_a^\theta \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T\,d\eta\right] D_2\boldsymbol{Z}(\theta) + \boldsymbol{Z}_d(s)^T C_1 \left[\int_\theta^s \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T\,d\eta\right] D_1\boldsymbol{Z}_d(\theta) \\
&\quad + \boldsymbol{Z}_d(s)^T C_2 \left[\int_s^b \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T\,d\eta\right] D_1\boldsymbol{Z}_d(\theta) \\
\boldsymbol{P}_2(s,\theta) &= \int_a^s \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_2(\eta,\theta)\,d\eta + \int_s^\theta \boldsymbol{Q}_2(s,\eta)\boldsymbol{R}_2(\eta,\theta)\,d\eta + \int_\theta^b \boldsymbol{Q}_2(s,\eta)\boldsymbol{R}_1(\eta,\theta)\,d\eta \\
&= \boldsymbol{Z}_d(s)^T C_1 \left[\int_a^s \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T\,d\eta\right] D_2\boldsymbol{Z}_d(\theta) + \boldsymbol{Z}_d(s)^T C_2 \left[\int_s^\theta \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T\,d\eta\right] D_2\boldsymbol{Z}_d(\theta) \\
&\quad + \boldsymbol{Z}_d(s)^T C_2 \left[\int_\theta^b \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T\,d\eta\right] D_1\boldsymbol{Z}_d(\theta)
\end{aligned}$$

To compute these parameters, we must first take the integral of the product $\boldsymbol{Z}_d(s)\boldsymbol{Z}_d(\eta)^T$. For this, we have the following result:

Lemma 1. *Let $\boldsymbol{Z}_d(s) \in \mathbb{R}^{d+1}[s]$ is the degree-d monomial basis. Then*

$$\int \boldsymbol{Z}_d(s)\boldsymbol{Z}_d(s)^T = S_d\big(I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(s)\big) = \big(I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(s)\big)^T S_d^T$$

where $\int \boldsymbol{F}(s)$ denotes the antiderivative of $\boldsymbol{F}(s)$, and where

$$S_d := \begin{bmatrix} \mathrm{e}_2^T & \frac{1}{2}\mathrm{e}_3^T & \cdots & \frac{1}{d+1}\mathrm{e}_{d+2}^T \\ \frac{1}{2}\mathrm{e}_3^T & \frac{1}{3}\mathrm{e}_4^T & \cdots & \frac{1}{d+2}\mathrm{e}_{d+3}^T \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{d+1}\mathrm{e}_{d+2}^T & \frac{1}{d+2}\mathrm{e}_{d+3}^T & \cdots & \frac{1}{2d+1}\mathrm{e}_{2d+2}^T \end{bmatrix}, \qquad \textit{for } \mathrm{e}_i \in \mathbb{R}^{2d+2} \textit{ the } i\textit{th canonical Euclidean basis vector.}$$

Proof. For $Z_d(s)$ the vector of monomials, we have

$$\int \boldsymbol{Z}_d(s)\boldsymbol{Z}_d(s)^T = \int \begin{bmatrix} 1 & s & \cdots & s^d \\ s & s^2 & \cdots & s^{d+1} \\ \vdots & \vdots & \ddots & \vdots \\ s^d & s^{d+1} & \cdots & s^{2d} \end{bmatrix} = \begin{bmatrix} s & \frac{1}{2}s^2 & \cdots & \frac{1}{d+1}s^{d+1} \\ \frac{1}{2}s^2 & \frac{1}{3}s^3 & \cdots & \frac{1}{d+2}s^{d+2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{d+1}s^{d+1} & \frac{1}{d+2}s^{d+2} & \cdots & \frac{1}{2d+1}s^{2d+1} \end{bmatrix}.$$

By definition of the matrix S_d, the result follows immediately. □

Applying Lem. 1, we find that e.g.

$$Z_d(s)^T C_1 \left[\int_\theta^s \boldsymbol{Z}(\eta)\boldsymbol{Z}(\eta)^T\,d\eta\right] D_1\boldsymbol{Z}_d(\theta) = Z_d(s)^T C_1 \Big[(I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(s))^T S_d^T - S_d(I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(\theta))\Big] D_1\boldsymbol{Z}_d(\theta)$$

To express this result in the form $Z_{d'}(s)^T G Z_{d'}(\theta)$ for some $d' \in \mathbb{N}$ and $G \in \mathbb{R}^{d'+1\times d'+1}$, we use the following result.

Lemma 2. *Let $m \in \mathbb{N}$ and $d_1, d_2 \in \mathbb{N}_0$, and let $C \in \mathbb{R}^{m \times d_2+1}$. Then*

$$(I_m \otimes \boldsymbol{Z}_{d_1+1}(s)) C \boldsymbol{Z}_{d_2}(s) = (C \otimes I_{d_1+1}) E_{d_1,d_2}\, \boldsymbol{Z}_{d_1+d_2}(s),$$

where

$$E_{d_1,d_2} := \begin{bmatrix} \begin{bmatrix} I_{d_1+1} & 0_{d_1+1\times d_2} \end{bmatrix} \\ \begin{bmatrix} 0_{d_1+1\times 1} & I_{d_1+1} & 0_{d_1+1\times d_2-1} \end{bmatrix} \\ \vdots \\ \begin{bmatrix} 0_{d_1+1\times d_2} & I_{d_1+1} \end{bmatrix} \end{bmatrix} \in \mathbb{R}^{(d_1+1)(d_2+1)\times(d_1+d_2+1)}$$

Proof. By the mixed product property, we have

$$(I_m \otimes \boldsymbol{Z}_{d_1+1}(s)) C \boldsymbol{Z}_{d_2}(s) = (C \otimes I_{d_1+1})(I_{d_2+1} \otimes \boldsymbol{Z}_{d_1}(s)) \boldsymbol{Z}_{d_2}(s) = (C \otimes I_{d_1+1})\big(\boldsymbol{Z}_{d_2}(s) \otimes \boldsymbol{Z}_{d_1}(s)\big).$$

Here, by definition of the matrix K_{d_1,d_2}, we have

$$\big(\boldsymbol{Z}_{d_2}(s) \otimes \boldsymbol{Z}_{d_1}(s)\big) = \begin{bmatrix} \boldsymbol{Z}_{d_1}(s) \\ s\boldsymbol{Z}_{d_1}(s) \\ \vdots \\ s^{d_2} \boldsymbol{Z}_{d_1}(s) \end{bmatrix} = E_{d_1,d_2}\, \boldsymbol{Z}_{d_1+d_2+1}(s).$$

Thus, the result follows. □

Finally,

Proposition 3. *For $[a,b] \subseteq \mathbb{R}$, $d \in \mathbb{N}$, and $C_1, C_2, D_1, D_2 \in \mathbb{R}^{d+1\times d+1}$, let $\boldsymbol{Q}_i(s,\theta) = \boldsymbol{Z}_d(s)^T C_i \boldsymbol{Z}_d(\theta)$ and $\boldsymbol{R}_i(s,\theta) = \boldsymbol{Z}_d(s)^T D_i \boldsymbol{Z}_d(\theta)$ for $i \in \{1,2\}$ and $s,\theta \in [a,b]$, and define*

$$A_d := \begin{bmatrix} a & \frac{1}{2}a^2 & \cdots & \frac{1}{d+1}a^{d+1} \\ \frac{1}{2}a^2 & \frac{1}{3}a^3 & \cdots & \frac{1}{d+2}a^{d+2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{d+1}a^{d+1} & \frac{1}{d+2}a^{d+2} & \cdots & \frac{1}{2d+1}a^{2d+1} \end{bmatrix}, \qquad B_d := \begin{bmatrix} b & \frac{1}{2}b^2 & \cdots & \frac{1}{d+1}b^{d+1} \\ \frac{1}{2}b^2 & \frac{1}{3}b^3 & \cdots & \frac{1}{d+2}b^{d+2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{d+1}b^{d+1} & \frac{1}{d+2}b^{d+2} & \cdots & \frac{1}{2d+1}b^{2d+1} \end{bmatrix}.$$

Then $\Pi_{\{\boldsymbol{Q}_i\}} \circ \Pi_{\{\boldsymbol{R}_i\}} = \Pi_{\{\boldsymbol{P}_i\}}$, where $\boldsymbol{P}_i(s,\theta) = \boldsymbol{Z}_d(s)^T G_i \boldsymbol{Z}_d(\theta)$ for

$$\begin{aligned} G_1 :=& \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix} \Big(C_2 B_d D_1 - C_1 A_d D_2 \Big) \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix} \\ &+ \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix} C_1 S_d\big([D_2 - D_1] \otimes I_{2d+2}\big) E_{2d+1,d} \\ &+ E_{2d+1,d}^T\big([C_1 - C_2] \otimes I_{2d+2}\big) S_d^T D_1 \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix} \\ G_2 :=& \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix} \Big(C_2 B_d D_1 - C_1 A_d D_2 \Big) \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix} \\ &+ \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix} C_2 S_d\big([D_2 - D_1] \otimes I_{2d+2}\big) E_{2d+1,d} \\ &+ E_{2d+1,d}^T\big([C_1 - C_2] \otimes I_{2d+2}\big) S_d^T D_2 \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix}, \end{aligned}$$

where S_d is as in Lem. 1 and $E_{2d+1,d}$ is as in Lem. 2.

Proof. By the composition rules of 2-PI operators, we know that $\Pi_{\{\boldsymbol{Q}_i\}} \circ \Pi_{\{\boldsymbol{R}_i\}} = \Pi_{\{\boldsymbol{P}_i\}}$, where

$$\boldsymbol{P}_1(s,\theta) = \int_a^\theta \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_2(\eta,\theta)\, d\eta + \int_\theta^s \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_1(\eta,\theta)\, d\eta + \int_s^b \boldsymbol{Q}_2(s,\eta)\boldsymbol{R}_1(\eta,\theta)\, d\eta.$$

Here, by Lem. 1 and Lem. 1, we have

$$\begin{aligned} \int_a^\theta \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_2(\eta,\theta)\, d\eta &= \boldsymbol{Z}_d(s)^T C_1 \left[\int_a^\theta \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T\, d\eta \right] D_2 \boldsymbol{Z}(\theta) \\ &= \boldsymbol{Z}_d(s)^T C_1 \left[\int \boldsymbol{Z}_d(\eta)\boldsymbol{Z}_d(\eta)^T \right]\Bigg|_{\eta=a}^{\theta} D_2 \boldsymbol{Z}(\theta) \\ &= \boldsymbol{Z}_d(s)^T C_1 \Big[S_d\big(I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(\theta)\big) - A_d \Big] D_2 \boldsymbol{Z}(\theta) \\ &= \boldsymbol{Z}_{3d+1}(s)^T \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix} C_1 \Big[S_d\big(D_2 \otimes I_{2d+2}\big) E_{2d+1,d} - A_d D_2 \Big] \boldsymbol{Z}_{3d+1}(\theta), \end{aligned}$$

where we remark that $\boldsymbol{Z}_d(s)^T = \boldsymbol{Z}_{3d+1}(s)^T \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}$. By similar reasoning, we find that

$$\begin{aligned}
&\int_\theta^s \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_1(\eta,\theta)\,d\eta \\
&= \boldsymbol{Z}_{3d+1}(s)^T \left[E_{2d+1,d}^T\big(C_1\otimes I_{2d+2}\big)S_d^T D_1 \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix} - \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix} C_1 S_d\big(D_1\otimes I_{2d+2}\big)E_{2d+1,d}\right]\boldsymbol{Z}_{3d+1}(\theta),
\end{aligned}$$

and

$$\begin{aligned}
&\int_a^\theta \boldsymbol{Q}_2(s,\eta)\boldsymbol{R}_1(\eta,\theta)\,d\eta \\
&\qquad = \boldsymbol{Z}_{3d+1}(s)^T\Big[C_2B_d - E_{2d+1,d}^T\big(C_2\otimes I_{2d+2}\big)S_d^T\Big]D_1 \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\boldsymbol{Z}_{3d+1}(\theta).
\end{aligned}$$

Adding these terms, we find that $\boldsymbol{P}_1(s,\theta) = \boldsymbol{Z}_{3d+1}(s)^T G_1 \boldsymbol{Z}_{3d+1}(\theta)$. By similar reasoning, we find that also $\boldsymbol{P}_2(s,\theta) = \boldsymbol{Z}_{3d+1}(s)^T G_2 \boldsymbol{Z}_{3d+1}(\theta)$. □

Note that S_d and $E_{d,d'}$ are sparse matrices. The matrices A_d and B_d are Hankel matrices, which we may be able to exploit.

3.2 Matrix-Valued Operators

Suppose now the parameters are matrix-valued, $\boldsymbol{Q} \in \mathbb{R}^{m\times q}[s]$ and $\boldsymbol{R}_i \in \mathbb{R}^{q\times n}[s,\theta]$, so that

$$\boldsymbol{Q}_i(s,\theta) = (I_m\otimes \boldsymbol{Z}_d(s))^T C_i (I_q \otimes \boldsymbol{Z}_d(\theta)) \qquad \text{and} \qquad \boldsymbol{R}_i(s,\theta) = (I_q\otimes \boldsymbol{Z}_d(s))^T D_i (I_n \otimes \boldsymbol{Z}_d(\theta)).$$

Proposition 4. *For $[a,b]\subseteq\mathbb{R}$, $m,n,q\in\mathbb{N}$, and $d\in\mathbb{N}_0$, let*

$$C_1, C_2 \in \mathbb{R}^{m(d+1)\times q(d+1)}, \qquad \text{and} \qquad D_1, D_2 \in \mathbb{R}^{q(d+1)\times n(d+1)},$$

and define

$$\boldsymbol{Q}_i(s,\theta) = (I_m\otimes \boldsymbol{Z}_d(s))^T C_i (I_q \otimes \boldsymbol{Z}_d(\theta)), \qquad \boldsymbol{R}_i(s,\theta) = (I_q\otimes \boldsymbol{Z}_d(s))^T D_i (I_n \otimes \boldsymbol{Z}_d(\theta)),$$

for $i\in\{1,2\}$ and $s,\theta\in[a,b]$. Then $\Pi_{\{\boldsymbol{Q}_i\}}\circ\Pi_{\{\boldsymbol{R}_i\}} = \Pi_{\{\boldsymbol{P}_i\}}$, where $\boldsymbol{P}_i(s,\theta) = (I_m\otimes \boldsymbol{Z}_d(s))^T G_i (I_n\otimes \boldsymbol{Z}_d(\theta))$ for

$$\begin{aligned}
G_1 := &\left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)\Big(C_2(I_q\otimes B_d)D_1 - C_1(I_q\otimes A_d)D_2\Big)\Big(I_n\otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big) \\
&+ \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)C_1(I_q\otimes S_d)\big([D_2 - D_1]\otimes I_{2d+2}\big)(I_n\otimes E_{2d+1,d}) \\
&\quad + (I_m\otimes E_{2d+1,d})^T\big([C_1 - C_2]\otimes I_{2d+2}\big)(I_q\otimes S_d)^T D_1\Big(I_n\otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big), \\
G_2 := &\left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)\Big(C_2(I_q\otimes B_d)D_1 - C_1(I_q\otimes A_d)D_2\Big)\Big(I_n\otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big) \\
&+ \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)C_2(I_q\otimes S_d)\big([D_2 - D_1]\otimes I_{2d+2}\big)(I_n\otimes E_{2d+1,d}) \\
&\quad + (I_m\otimes E_{2d+1,d})^T\big([C_1 - C_2]\otimes I_{2d+2}\big)(I_q\otimes S_d)^T D_2\Big(I_n\otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big).
\end{aligned}$$

where the various matrices S_d, $E_{2d+1,d}$, A_d and B_d are as in Prop. 3.

Proof. By the composition rules of 2-PI operators, we have $\Pi_{\{\boldsymbol{Q}_i\}}\circ\Pi_{\{\boldsymbol{R}_i\}} = \Pi_{\{\boldsymbol{P}_i\}}$, where

$$\begin{aligned}
\boldsymbol{P}_1(s,\theta) = &\int_a^\theta \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_2(\eta,\theta)\,d\eta + \int_\theta^s \boldsymbol{Q}_1(s,\eta)\boldsymbol{R}_1(\eta,\theta)\,d\eta + \int_s^b \boldsymbol{Q}_2(s,\eta)\boldsymbol{R}_1(\eta,\theta)\,d\eta \\
&= (I_m\otimes \boldsymbol{Z}_d(s))^T C_1\left[\int_a^\theta (I_q\otimes \boldsymbol{Z}_d(\eta))(I_q\otimes \boldsymbol{Z}_d(\eta))^T\,d\eta\right] D_2(I_n\otimes \boldsymbol{Z}(\theta)) \\
&\quad + (I_m\otimes \boldsymbol{Z}_d(s))^T C_1\left[\int_\theta^s (I_q\otimes \boldsymbol{Z}_d(\eta))(I_q\otimes \boldsymbol{Z}_d(\eta))^T\,d\eta\right] D_1(I_n\otimes \boldsymbol{Z}_d(\theta)) \\
&\quad\quad + (I_m\otimes \boldsymbol{Z}_d(s))^T C_2\left[\int_s^b (I_q\otimes \boldsymbol{Z}_d(\eta))(I_q\otimes \boldsymbol{Z}_d(\eta))^T\,d\eta\right] D_1(I_n\otimes \boldsymbol{Z}_d(\theta)).
\end{aligned}$$

Here, by Lem. 1, we have

$$\begin{aligned}\int (I_q \otimes \boldsymbol{Z}_d(s))(I_q \otimes \boldsymbol{Z}_d(s))^T &= I_q \otimes \int \boldsymbol{Z}_d(s)\boldsymbol{Z}_d(s)^T \\ &= I_q \otimes \left[S_d(I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(s))\right] \\ &= \big(I_q \otimes S_d\big)\big(I_q \otimes (I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(s))\big) = \big(I_q \otimes S_d\big)\big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(s)\big).\end{aligned}$$

and equivalently

$$\begin{aligned}\int (I_q \otimes \boldsymbol{Z}_d(s))(I_q \otimes \boldsymbol{Z}_d(s))^T &= I_q \otimes \int \boldsymbol{Z}_d(s)\boldsymbol{Z}_d(s)^T \\ &= I_q \otimes \left[(I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(s))^T S_d^T\right] \\ &= \big(I_q \otimes (I_{d+1} \otimes \boldsymbol{Z}_{2d+1}(s))^T\big)\big(I_q \otimes S_d^T\big) = \big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(s)\big)^T\big(I_q \otimes S_d\big)^T.\end{aligned}$$

It follows that e.g.

$$\begin{aligned}&(I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \left[\int_\theta^s (I_q \otimes \boldsymbol{Z}_d(\eta))(I_q \otimes \boldsymbol{Z}_d(\eta))^T \, d\eta\right] D_1(I_n \otimes \boldsymbol{Z}_d(\theta)) \\ &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \Big[\big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(s)\big)^T\big(I_q \otimes S_d\big)^T - \big(I_q \otimes S_d\big)\big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(\theta)\big)\Big] D_1(I_n \otimes \boldsymbol{Z}_d(\theta))\end{aligned}$$

Applying Lem. 2, we then find that

$$\begin{aligned}\big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(\theta)\big) D_1(I_n \otimes \boldsymbol{Z}_d(\theta)) &= \big(D_1 \otimes I_{2d+2}\big)\big(I_{n(d+1)} \otimes \boldsymbol{Z}_{2d+1}(\theta)\big)\big(I_n \otimes \boldsymbol{Z}_d(\theta)\big) \\ &= \big(D_1 \otimes I_{2d+2}\big)\big(I_n \otimes [(I_{d+1}\boldsymbol{Z}_{2d+1}(\theta))\boldsymbol{Z}_d(\theta)]\big) \\ &= \big(D_1 \otimes I_{2d+2}\big)\big(I_n \otimes [\boldsymbol{Z}_d(\theta) \otimes \boldsymbol{Z}_{2d+1}(\theta)]\big) \\ &= \big(D_1 \otimes I_{2d+2}\big)\big(I_n \otimes [E_{2d+1,d}\boldsymbol{Z}_{3d+1}(\theta)]\big) \\ &= \big(D_1 \otimes I_{2d+2}\big)\big(I_n \otimes E_{2d+1,d}\big)\big(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)\big).\end{aligned}$$

Similarly

$$\begin{aligned}&\big(I_m \otimes \boldsymbol{Z}_d(s)\big)^T C_1 \big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(s)\big)^T = \Big[\big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(s)\big) C_1^T \big(I_m \otimes \boldsymbol{Z}_d(s)\big)\Big]^T \\ &= \Big[\big(C_1^T \otimes I_{2d+2}\big)\big(I_m \otimes E_{2d+1,d}\big)\big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)\Big]^T = \big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)^T\big(I_m \otimes E_{2d+1,d}\big)^T\big(C_1 \otimes I_{2d+2}\big).\end{aligned}$$

Since, furthermore

$$\big(I_n \otimes \boldsymbol{Z}_d(\theta)\big) = \Big(I_n \otimes \begin{bmatrix}I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix} \boldsymbol{Z}_{3d+1}(\theta)\Big) = \Big(I_n \otimes \begin{bmatrix}I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big)\big(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)\big)$$

it follows that

$$\begin{aligned}&(I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \left[\int_\theta^s (I_q \otimes \boldsymbol{Z}_d(\eta))(I_q \otimes \boldsymbol{Z}_d(\eta))^T \, d\eta\right] D_1(I_n \otimes \boldsymbol{Z}_d(\theta)) \\ &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(s)\big)^T\big(I_q \otimes S_d\big)^T D_1(I_n \otimes \boldsymbol{Z}_d(\theta)) \\ &\qquad - (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \big(I_q \otimes S_d\big)\big(I_{q(d+1)} \otimes \boldsymbol{Z}_{2d+1}(\theta)\big) D_1(I_n \otimes \boldsymbol{Z}_d(\theta)) \\ &= \big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)^T\big(I_m \otimes E_{2d+1,d}\big)^T\big(C_1 \otimes I_{2d+2}\big)\big(I_q \otimes S_d\big)^T D_1\Big(I_n \otimes \begin{bmatrix}I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big)\big(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)\big) \\ &\qquad - (I_m \otimes \boldsymbol{Z}_{3d+1}(s))^T \left(I_m \otimes \begin{bmatrix}I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right) C_1\big(I_q \otimes S_d\big)\big(D_1 \otimes I_{2d+2}\big)\big(I_n \otimes E_{2d+1,d}\big)\big(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)\big)\end{aligned}$$

By similar reasoning, we find that

$$\begin{aligned}&\big(I_m \otimes Z_d(s)\big)^T C_1 \left[\int_a^\theta \boldsymbol{Z}(\eta)\boldsymbol{Z}(\eta)^T \, d\eta\right] D_2\big(I_n \otimes \boldsymbol{Z}_d(\theta)\big) \\ &\quad = \big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)^T \left(I_m \otimes \begin{bmatrix}I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right) C_1 \\ &\qquad \left[\big(I_q \otimes S_d\big)\big(D_2 \otimes I_{2d+2}\big)\big(I_n \otimes E_{2d+1,d}\big) - (I_q \otimes A_d) D_2\Big(I_n \otimes \begin{bmatrix}I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big)\right]\big(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)\big)\end{aligned}$$

and

$$\big(I_m \otimes Z_d(s)\big)^T C_2 \left[\int_s^b \boldsymbol{Z}(\eta)\boldsymbol{Z}(\eta)^T\, d\eta\right] D_1\big(I_n \otimes \boldsymbol{Z}_d(\theta)\big)$$
$$= \big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)^T \left[\left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right) C_2(I_q \otimes B_d) - \big(I_m \otimes E_{2d+1,d}\big)^T \big(C_2 \otimes I_{2d+2}\big)\big(I_q \otimes S_d\big)^T\right]$$
$$D_1\Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big)\big(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)\big)$$

Combining these results, it follows that $\boldsymbol{P}_1(s,\theta) = (I_m \otimes \boldsymbol{Z}_d(s))^T G_1(I_n \otimes \boldsymbol{Z}_d(\theta))$. By similar reasoning, we find that also $\boldsymbol{P}_2(s,\theta) = (I_m \otimes \boldsymbol{Z}_d(s))^T G_2(I_n \otimes \boldsymbol{Z}_d(\theta))$. □

3.3 3-PI Operators

Next, we add a multiplier term to the 2-PI operator, to get a 3-PI operator, taking the form

$$\big(\Pi_{\{\boldsymbol{P}_0,\boldsymbol{P}_1,\boldsymbol{P}_2\}}\mathbf{x}\big)(s) = \boldsymbol{P}_0(s)\mathbf{x}(s) + \int_a^1 \boldsymbol{P}_1(s,\theta)\mathbf{x}(\theta)d\theta + \int_s^b \boldsymbol{P}_2(s,\theta)\mathbf{x}(\theta)d\theta.$$

To establish composition rules of such 3-PI operators, we use the following identity.

Lemma 5. *For $d_1, d_2, d_3 \in \mathbb{N}_0$ such that $d_3 \geq d_1 + d_2$, define*

$$F_{d_1,d_2,d_3} := \begin{bmatrix} E_{d_2,d_1} & 0_{(d_1+1)(d_2+1)\times(d_3-d_1-d_2)}\end{bmatrix}.$$

Then, for any $C \in \mathbb{R}^{m\times n(d_2+1)}$ for $m, n \in \mathbb{N}$, we have

$$\big(I_m \otimes \boldsymbol{Z}_{d_1}(s)\big)^T C\big(I_n \otimes \boldsymbol{Z}_{d_2}(s)\big)^T = \big(I_m \otimes \boldsymbol{Z}_{d_3}(s)\big)^T \big(I_m \otimes F_{d_1,d_2,d_3}\big)^T (C \otimes I_{d_1+1}).$$

Proof. By the mixed product property, we note that

$$\begin{aligned}\big(I_m \otimes \boldsymbol{Z}_{d_1}(s)\big)^T C\big(I_n \otimes \boldsymbol{Z}_{d_2}(s)\big)^T &= \big(I_m \otimes \boldsymbol{Z}_{d_1}(s)\big)^T \big(I_{m(d_1+1)} \otimes \boldsymbol{Z}_{d_2}(s)\big)^T (C \otimes I_{d_2+1}) \\ &= \Big[I_m \otimes \big[\boldsymbol{Z}_{d_1}(s)^T \big(I_{d_1+1} \otimes \boldsymbol{Z}_{d_2}(s)\big)^T\big]\Big](C \otimes I_{d_1+1}).\end{aligned}$$

By Lem. 2, we have $(I_{d+1} \otimes \boldsymbol{Z}_{d_2}(s))\boldsymbol{Z}_{d_1}(s) = E_{d_2,d_1}\boldsymbol{Z}_{d_1+d_2}$, and thus

$$\begin{aligned}\big(I_m \otimes \boldsymbol{Z}_{d_1}(s)\big)^T C\big(I_n \otimes \boldsymbol{Z}_{d_2}(s)\big)^T &= \Big[I_m \otimes \big[\boldsymbol{Z}_{d_1}(s)^T \big(I_{d_1+1} \otimes \boldsymbol{Z}_{d_2}(s)\big)^T\big]\Big](C \otimes I_{d_1+1}) \\ &= \Big[I_m \otimes \big[\boldsymbol{Z}_{d_1+d_2}(s)^T E_{d_2,d_1}^T\big]\Big](C \otimes I_{d_1+1}) \\ &= \left[I_m \otimes \left(\boldsymbol{Z}_{d_3}(s)^T \begin{bmatrix} E_{d_2,d_1}^T \\ 0_{(d_3-d_1-d_2)\times(d_1+1)(d_2+1)}\end{bmatrix}\right)\right](C \otimes I_{d_1+1}) \\ &= \Big[I_m \otimes \big(\boldsymbol{Z}_{d_3}(s)^T F_{d_1,d_2,d_3}^T\big)\Big](C \otimes I_{d_1+1}) \\ &= \big(I_m \otimes \boldsymbol{Z}_{d_3}(s)\big)^T \big(I_m \otimes F_{d_1,d_2,d_3}\big)^T (C \otimes I_{d_1+1}).\end{aligned}$$

□

We will also make use of the following lemma

Lemma 6. *For $d_1, d_2, d_3 \in \mathbb{N}_0$ such that $d_3 \geq d_1 + d_2$, define $H_{d_1,d_2,d_3} \in \mathbb{R}^{d_1+1\times(d_2+1)(d_3+1)}$ by*

$$H_d := \Big[\begin{bmatrix} I_{d_1+1} & 0_{d_1+1\times d_3-d_1}\end{bmatrix} \quad \begin{bmatrix} 0_{d_1+1\times 1} & I_{d_1+1} & 0_{d_1+1\times d_3-d_1-1}\end{bmatrix} \quad \cdots \quad \begin{bmatrix} 0_{d_1+1\times d_2} & I_{d_1+1} & 0_{d_1+1\times d_3-d_1 d_2}\end{bmatrix}\Big].$$

Then

$$\boldsymbol{Z}_{d_1}(s)\boldsymbol{Z}_{d_2}(s)^T = \hat{H}_{d_1,d_2,d_3}\big(I_{d_2+1} \otimes \boldsymbol{Z}_{d_3}(s)\big).$$

Proof. First, we note that we can express

$$\boldsymbol{Z}_{d_1}(s)\boldsymbol{Z}_{d_2}(s)^T = \hat{H}_{d_1,d_2}\big(I_{d_2+1} \otimes (\boldsymbol{Z}_{d_2}(s) \otimes \boldsymbol{Z}_{d_1}(s))\big)$$

where

$$\hat{H}_{d_1,d_2} := \left[\begin{bmatrix} I_{d_1+1} & 0_{(d_1+1)\times d_2(d_1+1)} \end{bmatrix} \quad \begin{bmatrix} 0_{d_1+1} & I_{d_1+1} & 0_{(d_1+1)\times(d_2-1)(d_1+1)} \end{bmatrix} \quad \cdots \quad \begin{bmatrix} 0_{(d_1+1)\times d_2(d_1+1)} & I_{d_1+1} \end{bmatrix}\right].$$

Here, by the mixed product property,

$$\boldsymbol{Z}_{d_2}(s) \otimes \boldsymbol{Z}_{d_1}(s) = \big(I_{d_2+1} \otimes \boldsymbol{Z}_{d_1}(s)\big)\boldsymbol{Z}_{d_2}(s),$$

and thus, by Lem. 5,

$$\boldsymbol{Z}_{d_2}(s) \otimes \boldsymbol{Z}_{d_1}(s) = \Big[\boldsymbol{Z}_{d_2}(s)^T\big(I_{d_2+1} \otimes \boldsymbol{Z}_{d_1}(s)\big)^T\Big]^T = \Big[\boldsymbol{Z}_{d_3}(s)^T F_{d_2,d_1,d_3}^T\Big]^T = F_{d_2,d_1,d_3}\boldsymbol{Z}_{d_3}(s).$$

By definition of H_{d_1,d_2,d_3}, we have $H_{d_1,d_2,d_3} = \hat{H}_{d_1,d_2}\big(I_{d_2+1} \otimes F_{d_2,d_1,d_3}\big)$. It follows that

$$\begin{aligned}
\boldsymbol{Z}_{d_1}(s)\boldsymbol{Z}_{d_2}(s)^T &= \hat{H}_{d_1,d_2}\big(I_{d_2+1} \otimes (\boldsymbol{Z}_{d_2}(s) \otimes \boldsymbol{Z}_{d_1}(s))\big) \\
&= \hat{H}_{d_1,d_2}\Big[I_{d_2+1} \otimes \big(F_{d_2,d_1,d_3}\boldsymbol{Z}_{d_3}(s)\big)\Big] \\
&= \hat{H}_{d_1,d_2}\big(I_{d_2+1} \otimes F_{d_2,d_1,d_3}\big)\big(I_{d_2+1} \otimes \boldsymbol{Z}_{d_3}(s)\big) = \hat{H}_{d_1,d_2,d_3}\big(I_{d_2+1} \otimes \boldsymbol{Z}_{d_3}(s)\big).
\end{aligned}$$

□

Using these lemmas, we obtain the following result for composition of two 3-PI operators.

Proposition 7. *For $[a,b] \subseteq \mathbb{R}$, $m,n,q \in \mathbb{N}$, and $d \in \mathbb{N}_0$, let*

$$C_0 \in \mathbb{R}^{m(d+1)\times q}, \quad C_1, C_2 \in \mathbb{R}^{m(d+1)\times q(d+1)}, \qquad \text{and} \qquad D_0 \in \mathbb{R}^{q(d+1)\times n}, \quad D_1, D_2 \in \mathbb{R}^{q(d+1)\times n(d+1)},$$

and define

$$\begin{aligned}
\boldsymbol{Q}_0(s) &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_0, & \boldsymbol{Q}_i(s,\theta) &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_i (I_q \otimes \boldsymbol{Z}_d(\theta)), \\
\boldsymbol{R}_0(s) &= (I_q \otimes \boldsymbol{Z}_d(s))^T D_0, & \boldsymbol{R}_i(s,\theta) &= (I_q \otimes \boldsymbol{Z}_d(s))^T D_i (I_n \otimes \boldsymbol{Z}_d(\theta)),
\end{aligned}$$

for $i \in \{1,2\}$ and $s,\theta \in [a,b]$. Then $\Pi_{\{\boldsymbol{Q}_j\}} \circ \Pi_{\{\boldsymbol{R}_j\}} = \Pi_{\{\boldsymbol{P}_j\}}$, where $\boldsymbol{P}_0(s) = (I_m \otimes \boldsymbol{Z}_d(s))^T G_0$ and $\boldsymbol{P}_i(s,\theta) = (I_m \otimes \boldsymbol{Z}_d(s))^T G_i (I_n \otimes \boldsymbol{Z}_d(\theta))$ for

$$\begin{aligned}
G_0 &:= (I_m \otimes F_d)^T (C_0 \otimes I_{d+1}) D_0, \\
G_1 &:= (I_m \otimes F_d)^T (C_0 \otimes I_{d+1}) D_1 \Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix}\Big) + \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix}\right) C_1 \big(I_q \otimes H_d\big)(D_0 \otimes I_{3d+2}) \\
&\quad + \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix}\right)\Big(C_2(I_q \otimes B_d)D_1 - C_1(I_q \otimes A_d)D_2\Big)\Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix}\Big) \\
&\quad + \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix}\right) C_1 (I_q \otimes S_d)\big([D_2 - D_1] \otimes I_{2d+2}\big)(I_n \otimes E_{2d+1,d}) \\
&\quad + (I_m \otimes E_{2d+1,d})^T \big([C_1 - C_2] \otimes I_{2d+2}\big)(I_q \otimes S_d)^T D_1 \Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix}\Big) \\
G_2 &:= (I_m \otimes F_d)^T (C_0 \otimes I_{d+1}) D_2 \Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix}\Big) + \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix}\right) C_2 \big(I_q \otimes H_d\big)(D_0 \otimes I_{3d+2}) \\
&\quad + \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix}\right)\Big(C_2(I_q \otimes B_d)D_1 - C_1(I_q \otimes A_d)D_2\Big)\Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix}\Big) \\
&\quad + \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1} \end{bmatrix}\right) C_2 (I_q \otimes S_d)\big([D_2 - D_1] \otimes I_{2d+2}\big)(I_n \otimes E_{2d+1,d}) \\
&\quad + (I_m \otimes E_{2d+1,d})^T \big([C_1 - C_2] \otimes I_{2d+2}\big)(I_q \otimes S_d)^T D_2 \Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1} \end{bmatrix}\Big).
\end{aligned}$$

where the matrices S_d, $E_{2d+1,d}$, A_d and B_d are as in Prop. 3, and where $F_d = F_{d,d,3d+1} \in \mathbb{R}^{(d+1)^2\times 3d+2}$ and $H_d = H_{d,d,3d+1} \in \mathbb{R}^{(d+1)\times(d+1)(3d+2)}$ for F_{d_1,d_2,d_3} and H_{d_1,d_2,d_3} as in Lem. 5 and Lem. 6, respectively.

Proof. First, by definition of 3-PI operators, we note that

$$\begin{aligned}
\Pi_{\{\boldsymbol{Q}_i\}} \circ \Pi_{\{\boldsymbol{R}_i\}} = \Pi_{\{\boldsymbol{Q}_0,0,0\}} \circ \Pi_{\{\boldsymbol{R}_0,0,0\}} &+ \Pi_{\{\boldsymbol{Q}_0,0,0\}} \circ \Pi_{\{0,\boldsymbol{R}_1,\boldsymbol{R}_2\}} \\
&+ \Pi_{\{0,\boldsymbol{Q}_1,\boldsymbol{Q}_2\}} \circ \Pi_{\{\boldsymbol{R}_0,0,0\}} + \Pi_{\{0,\boldsymbol{Q}_1,\boldsymbol{Q}_2\}} \circ \Pi_{\{0,\boldsymbol{R}_1,\boldsymbol{R}_2\}}.
\end{aligned}$$

Here, an expression for the composition $\Pi_{\{0,\boldsymbol{Q}_1,\boldsymbol{Q}_2\}} \circ \Pi_{\{0,\boldsymbol{R}_1,\boldsymbol{R}_2\}}$ was already presented in Prop. 4. We derive expressions for the remaining three terms separately. Starting with the first term, we have $\Pi_{\{\boldsymbol{Q}_0,0,0\}} \circ \Pi_{\{\boldsymbol{R}_0,0,0\}} = \Pi_{\{\hat{\boldsymbol{P}}_0,0,0\}}$, where $\boldsymbol{P}_0(s) = \boldsymbol{Q}_0(s)\boldsymbol{R}_0(s)$. By Lem. 5, we find

$$\begin{aligned}\boldsymbol{P}_0(s) = \boldsymbol{Q}_0(s)\boldsymbol{R}_0(s) &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_0 (I_q \otimes \boldsymbol{Z}_d(s))^T D_0 \\ &= \big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)^T (I_m \otimes F_d)^T (C_0 \otimes I_{d+1}) D_0 = \boldsymbol{P}_0(s).\end{aligned}$$

Next, by the composition rules of 3-PI operators, we have $\Pi_{\{\boldsymbol{Q}_0,0,0\}} \circ \Pi_{\{0,\boldsymbol{R}_1,\boldsymbol{R}_2\}} = \Pi_{\{0,\hat{\boldsymbol{K}}_1,\hat{\boldsymbol{K}}_2\}}$, where $\boldsymbol{K}_i(s,\theta) = \boldsymbol{Q}_0(s)\boldsymbol{R}_i(s,\theta)$ for $i \in \{1,2\}$. Here, again applying Lem. 5, we find

$$\begin{aligned}\boldsymbol{Q}_0(s)\boldsymbol{R}_1(s,\theta) &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_0 (I_q \otimes \boldsymbol{Z}_d(s))^T D_1 (I_n \otimes \boldsymbol{Z}_d(\theta)) \\ &= \big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)^T (I_m \otimes F_d)^T (C_0 \otimes I_{d+1}) D_1 (I_n \otimes \boldsymbol{Z}_d(\theta)) \\ &= \big(I_m \otimes \boldsymbol{Z}_{3d+1}(s)\big)^T (I_m \otimes F_d)^T (C_0 \otimes I_{d+1}) D_1 \Big(I_n \otimes \big[I_{d+1} \quad 0_{d+1\times 2d+1}\big]\Big)(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)).\end{aligned}$$

Finally, we have $\Pi_{\{0,\boldsymbol{Q}_1,\boldsymbol{Q}_2\}} \circ \Pi_{\{\boldsymbol{R}_0,0,0\}} = \Pi_{\{0,\boldsymbol{N}_1,\boldsymbol{N}_2\}}$, where $\boldsymbol{N}_i(s,\theta) = \boldsymbol{Q}_i(s,\theta)\boldsymbol{R}_0(\theta)$ for $i \in \{1,2\}$. Here, applying Lem. 6, we find

$$\begin{aligned}\boldsymbol{Q}_1(s,\theta)\boldsymbol{R}_0(\theta) &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 (I_q \otimes \boldsymbol{Z}_d(\theta))(I_q \otimes \boldsymbol{Z}_d(\theta))^T D_0 \\ &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \Big[I_q \otimes \big(\boldsymbol{Z}_d(\theta)\boldsymbol{Z}_d(\theta)^T\big)\Big] D_0 \\ &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \Big[I_q \otimes \big[H_d\big(I_{d+1} \otimes \boldsymbol{Z}_{3d+1}(s)\big)\big]\Big] D_0 \\ &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \big(I_q \otimes H_d\big)\big(I_{q(d+1)} \otimes \boldsymbol{Z}_{3d+1}(s)\big) D_0 \\ &= (I_m \otimes \boldsymbol{Z}_d(s))^T C_1 \big(I_q \otimes H_d\big)(D_0 \otimes I_{3d+2})\big(I_n \otimes \boldsymbol{Z}_{3d+1}(s)\big)\end{aligned}$$

Combining these results, we find that $\Pi_{\{\boldsymbol{Q}_j\}} \circ \Pi_{\{\boldsymbol{R}_j\}} = \Pi_{\{\boldsymbol{P}_j\}}$, where $\boldsymbol{P}_0(s) = (I_m \otimes \boldsymbol{Z}_d(s))^T G_0$ and $\boldsymbol{P}_i(s,\theta) = (I_m \otimes \boldsymbol{Z}_d(s))^T G_i (I_n \otimes \boldsymbol{Z}_d(\theta))$. $\square$

3.4 Composition of Matrix and PI operator

Having established composition rules of 3-PI operators, note that a matrix is also a 3-PI operator, with just a multiplier term. However, since matrices do not involve monomials, we can derive slightly simpler composition rules for matrices with 3-PI operators. In particular, for the composition $C\Pi_{\{\boldsymbol{R}_i\}}$, note that

$$C\boldsymbol{R}_0(s) = C(I_q \otimes \boldsymbol{Z}_d(s))^T D_0 = (I_m \otimes \boldsymbol{Z}_d(s))^T (C \otimes I_{d+1}) D_0$$

and

$$C\boldsymbol{R}_i(s,\theta) = C(I_q \otimes \boldsymbol{Z}_d(s))^T D_i (I_n \otimes \boldsymbol{Z}_d(\theta)) = (I_m \otimes \boldsymbol{Z}_d(s))^T (C \otimes I_{d+1}) D_i (I_n \otimes \boldsymbol{Z}_d(\theta)).$$

Thus, $C\Pi_{\{\boldsymbol{R}_i\}}$ is defined by coefficients $(C \otimes I_{d+1})D_i$. Similarly, for the composition $\Pi_{\{\boldsymbol{Q}_i\}}D$, we have

$$\boldsymbol{Q}_0(s)D = (I_m \otimes \boldsymbol{Z}_d(s))^T C_0 D$$

and

$$\boldsymbol{Q}_i(s,\theta)D = (I_m \otimes \boldsymbol{Z}_d(s))^T C_i (I_q \otimes \boldsymbol{Z}_d(\theta)) D = (I_m \otimes \boldsymbol{Z}_d(s))^T C_i (D \otimes I_{d+1})(I_n \otimes \boldsymbol{Z}_d(\theta)),$$

so that $\Pi_{\{\boldsymbol{Q}_i\}}D$ is defined by coefficients $C_0 D$ and $C_i(D \otimes I_{d+1})$.

3.5 2D-PI Operators

Consider now a scalar-valued 2D PI operator, parameterized by four scalar kernel functions as

$$\begin{aligned}\Pi_{\{\boldsymbol{Q}_{ij}\}}\mathbf{x}(s_1,s_2) = &\int_{a_1}^{s_1}\int_{a_2}^{s_2} \boldsymbol{Q}_{11}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1 + \int_{a_1}^{s_1}\int_{s_2}^{b_2} \boldsymbol{Q}_{12}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1 \\ &+ \int_{s_1}^{b_1}\int_{a_2}^{s_2} \boldsymbol{Q}_{21}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1 + \int_{s_1}^{b_1}\int_{s_2}^{b_2} \boldsymbol{Q}_{22}(s_1,s_2,\theta_1,\theta_2)\mathbf{x}(\theta_1,\theta_2)\, d\theta_2 d\theta_1,\end{aligned}$$

where now

$$\boldsymbol{Q}_{ij}(s,\theta) = \boldsymbol{Z}_d(s) C_{ij} \boldsymbol{Z}(\theta) = (I_m \otimes \boldsymbol{Z}_d(s_1) \otimes \boldsymbol{Z}_d(s_2))^T C_{ij} (I_n \otimes \boldsymbol{Z}_d(\theta_1) \otimes \boldsymbol{Z}_d(\theta_2))$$

for $C_{ij} \in \mathbb{R}^{m(d+1)^2 \times n(d+1)^2}$. We can represent this operator numerically by the four coefficient matrices C_{ij}, and the maximal monomial degree d.

To establish composition rules of 2D-PI operators in terms of the coefficients C_{ij}, note first that $\boldsymbol{Z}_d(s_1) \otimes \boldsymbol{Z}_d(s_2) = (I_{d+1} \otimes \boldsymbol{Z}_d(s_2))\boldsymbol{Z}_d(s_1)$. As such, we can equivalently represent the parameters $\boldsymbol{Q}_{ij}$ as

$$\begin{aligned}
\boldsymbol{Q}_{ij}(s,\theta) &= (I_m \otimes \boldsymbol{Z}_d(s_1) \otimes \boldsymbol{Z}_d(s_2))^T C_{ij} (I_n \otimes \boldsymbol{Z}_d(\theta_1) \otimes \boldsymbol{Z}_d(\theta_2)) \\
&= \Big(I_m \otimes \big[(I_{d+1} \otimes \boldsymbol{Z}_d(s_2))\boldsymbol{Z}_d(s_1)\big]\Big)^T C_{ij} \Big(I_n \otimes \big[(I_{d+1} \otimes \boldsymbol{Z}_d(\theta_2))\boldsymbol{Z}_d(\theta_1)\big]\Big) \\
&= \big(I_m \otimes \boldsymbol{Z}_d(s_1)^T \hat{\boldsymbol{C}}_{ij}(s_2,\theta_2)\big(I_n \otimes \boldsymbol{Z}_d(\theta_1)\big)
\end{aligned}$$

where now $\hat{\boldsymbol{C}}_{ij} \in \mathbb{R}^{m(d+1) \times n(d+1)}$ are "polynomial-valued" coefficients,

$$\hat{\boldsymbol{C}}_{ij}(s_2,\theta_2) := (I_{m(d+1)} \otimes \boldsymbol{Z}_d(s_2))^T C_{ij} (I_{n(d+1)} \otimes \boldsymbol{Z}_d(\theta_2)).$$

Accordingly, we represent the 2D PI operator as a 1D operator along $s_1 \in [a_1, b_1]$,

$$\begin{aligned}
(\mathcal{Q}\mathbf{x})(s) = (\Pi_{\{\boldsymbol{Q}_{ij}\}}\mathbf{x})(s) = &\int_{a_1}^{s_1} (I_m \otimes \boldsymbol{Z}_d(s_1))^T \Big(\hat{\mathcal{C}}_1\big(I_n \otimes \boldsymbol{Z}_d(\theta_1)\big)\mathbf{x}(\theta_1,\cdot)\Big)(s_2)\, d\theta_1 \\
&+ \int_{s_1}^{b_1} \big(I_m \otimes \boldsymbol{Z}_d(s_1)\big)^T \Big(\hat{\mathcal{C}}_2\big(I_n \otimes \boldsymbol{Z}_d(\theta_1)\big)\mathbf{x}(\theta_1,\cdot)\Big)(s_2)\, d\theta_1
\end{aligned}$$

where now $\hat{\mathcal{C}}_1$ and $\hat{\mathcal{C}}_2$ are matrix-valued 1D PI operators along $s_2 \in [a_2, b_2]$,

$$(\hat{\mathcal{C}}_j\mathbf{y})(s_2) = \int_{a_2}^{s_2} \hat{\boldsymbol{C}}_{1j}(s_2,\theta_2)\mathbf{y}(\theta_2)\, d\theta_1 + \int_{s_2}^{b_2} \hat{\boldsymbol{C}}_{2j}(s_2,\theta_2)\mathbf{y}(\theta_2)\, d\theta_2,$$

for $\mathbf{y} \in L_2^{d+1}[a_2, b_2]$ and $j \in \{1, 2\}$. Given, then, a 2D-PI operator $\mathcal{R}$ of a similar form,

$$\begin{aligned}
(\mathcal{R}\mathbf{x})(s) = (\Pi_{\{\boldsymbol{R}_{ij}\}}\mathbf{x})(s) = &\int_{a_1}^{s_1} (I_m \otimes \boldsymbol{Z}_d(s_1))^T \Big(\hat{\mathcal{D}}_1\big(I_n \otimes \boldsymbol{Z}_d(\theta_1)\big)\mathbf{x}(\theta_1,\cdot)\Big)(s_2)\, d\theta_1 \\
&+ \int_{s_1}^{b_1} \big(I_m \otimes \boldsymbol{Z}_d(s_1)\big)^T \Big(\hat{\mathcal{D}}_2\big(I_n \otimes \boldsymbol{Z}_d(\theta_1)\big)\mathbf{x}(\theta_1,\cdot)\Big)(s_2)\, d\theta_1,
\end{aligned}$$

we find that $\mathcal{P} = \mathcal{Q} \circ \mathcal{R}$ takes the form

$$\begin{aligned}
(\mathcal{P}\mathbf{x})(s_1,s_2) = &\int_{a_1}^{s_1} (I_m \otimes \boldsymbol{Z}_d(s_1))^T \big(\hat{\mathcal{G}}_1(I_n \otimes \boldsymbol{Z}_d(\theta_1))\mathbf{x}(\theta_1,\cdot)\big)(s_2)\, d\theta_1 \\
&+ \int_{s_1}^{b_1} (I_m \otimes \boldsymbol{Z}_d(s_1))^T \big(\hat{\mathcal{G}}_2(I_n \otimes \boldsymbol{Z}_d(\theta_1))\mathbf{x}(\theta_1,\cdot)\big)(s_2)\, d\theta_1,
\end{aligned}$$

where

$$\begin{aligned}
\hat{\mathcal{G}}_1 :=& \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)\Big(\hat{\mathcal{C}}_2(I_q \otimes B_d)\hat{\mathcal{D}}_1 - \hat{\mathcal{C}}_1(I_q \otimes A_d)\hat{\mathcal{D}}_2\Big)\Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big) \\
&+ \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)\hat{\mathcal{C}}_1(I_q \otimes S_d)\big([\hat{\mathcal{D}}_2 - \hat{\mathcal{D}}_1] \otimes I_{2d+2}\big)(I_n \otimes E_{2d+1,d}) \\
&\quad + (I_m \otimes E_{2d+1,d})^T\big([\hat{\mathcal{C}}_1 - \hat{\mathcal{C}}_2] \otimes I_{2d+2}\big)(I_q \otimes S_d)^T\hat{\mathcal{D}}_1\Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big) \\
\hat{\mathcal{G}}_2 :=& \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)\Big(\hat{\mathcal{C}}_2(I_q \otimes B_d)\hat{\mathcal{D}}_1 - \hat{\mathcal{C}}_1(I_q \otimes A_d)\hat{\mathcal{D}}_2\Big)\Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big) \\
&+ \left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)\hat{\mathcal{C}}_2(I_q \otimes S_d)\big([\hat{\mathcal{D}}_2 - \hat{\mathcal{D}}_1] \otimes I_{2d+2}\big)(I_n \otimes E_{2d+1,d}) \\
&\quad + (I_m \otimes E_{2d+1,d})^T\big([\hat{\mathcal{C}}_1 - \hat{\mathcal{C}}_2] \otimes I_{2d+2}\big)(I_q \otimes S_d)^T\hat{\mathcal{D}}_2\Big(I_n \otimes \begin{bmatrix} I_{d+1} & 0_{d+1\times 2d+1}\end{bmatrix}\Big).
\end{aligned}$$

This approach would inductively extend to higher-dimensional operators as well. However, it requires taking compositions of the form $\hat{\mathcal{C}}_1 S_d\big(\hat{\mathcal{D}} \otimes I_{2d+2}\big)$. To compute such compositions, note that if $\hat{\mathcal{D}}$ is a 2-PI operator, $\mathcal{D} = \Pi_{\{\boldsymbol{D}_1,\boldsymbol{D}_2\}}$, then $\hat{\mathcal{D}} \otimes I_n = \Pi_{\{\boldsymbol{D}_1 \otimes I_n, \boldsymbol{D}_2 \otimes I_n\}}$. To define the Kronecker products $\boldsymbol{D}_i \otimes I_n$, we use the fact that

$$\boldsymbol{Z}_d(s_1)^T \otimes I_{2d+2} = (I_{2d+2} \otimes \boldsymbol{Z}_d(s_2))^T P_{2d+2,d+1}^T \qquad \text{and} \qquad \boldsymbol{Z}_d(\theta_2) \otimes I_{2d+2} = P_{2d+2,d+1}(I_{2d+2} \otimes \boldsymbol{Z}_d(s_2))$$

where $P_{2d+2,d+1} \in \mathbb{R}^{(2d+2)(d+1)\times(2d+2)(d+1)}$ is defined by

$$P_{2d+2,d+1} = \begin{bmatrix} I_{2d+2} \otimes \mathrm{e}_1 \\ I_{2d+2} \otimes \mathrm{e}_2 \\ \vdots \\ I_{2d+2} \otimes \mathrm{e}_{d+1} \end{bmatrix}, \quad \text{for } \mathrm{e}_i \in \mathbb{R}^{d+1} \text{ the } i\text{th canonical basis vector.}$$

Given these identities, we find that if $\boldsymbol{D}_1(s_1,\theta_1) = (I_m \otimes \boldsymbol{Z}_d(s_1))^T D_1(I_n \otimes \boldsymbol{Z}_d(\theta))$, then

$$\begin{aligned}
&\boldsymbol{D}_1(s_2,\theta_2) \otimes I_{2d+2} = \left[(I_{m(d+1)} \otimes \boldsymbol{Z}_d(s_2))^T D_1(I_{n(d+1)} \otimes \boldsymbol{Z}_d(\theta_2))\right] \otimes I_{2d+2} \\
&= \left[I_{m(d+1)} \otimes \boldsymbol{Z}_d(s_2)^T \otimes I_{2d+2}\right]\left[C_1 \otimes I_{2d+2}\right]\left[I_{n(d+1)} \otimes \boldsymbol{Z}_d(\theta_2) \otimes I_{2d+2}\right] \\
&= \left[I_{m(d+1)} \otimes \left((I_{2d+2} \otimes \boldsymbol{Z}_d(s_2))^T P^T_{2d+1,2d+1}\right)\right]\left[C_1 \otimes I_{2d+2}\right]\left[I_{n(d+1)} \otimes (P_{2d+2,d+1}(I_{2d+2} \otimes \boldsymbol{Z}_d(\theta_2))\right] \\
&= \left(I_{m(d+1)(2d+2)} \otimes \boldsymbol{Z}_d(s_2)\right)^T\left(I_{m(d+1)} \otimes P_{2d+2,d+1}\right)^T\left(D_1 \otimes I_{2d+2}\right)\left(I_{n(d+1)} \otimes P_{2d+2,d+1}\right)\left(I_{n(d+1)(2d+2)} \otimes \boldsymbol{Z}_d(\theta_2)\right)
\end{aligned}$$

It follows that, for $\hat{\mathcal{D}} = \Pi_{\{\hat{\boldsymbol{D}}_1,\hat{\boldsymbol{D}}_2\}}$ defined by coefficients D_1 and D_2 and monomial degree d, the operator $\hat{\mathcal{D}} \otimes I_{2d+2}$ is defined by coefficients $\left(I_{m(d+1)} \otimes P_{2d+2,d+1}\right)^T\left(D_1 \otimes I_{2d+2}\right)\left(I_{n(d+1)} \otimes P_{2d+2,d+1}\right)$ and $\big(I_{m(d+1)} \otimes P_{2d+2,d+1}\big)^T\left(D_2 \otimes I_{2d+2}\right)\left(I_{n(d+1)} \otimes P_{2d+2,d+1}\right)$, and monomial degree d. Using this result, we can compute the operators $\hat{\mathcal{G}}_1$ and $\hat{\mathcal{G}}_2$, and thus the composition of the 2D PI operators.

3.6 Composition of ND PI Operators

We parameterize a class of 2^N-PI operators by 2^N polynomials, $\boldsymbol{Q}_\alpha \in \mathbb{R}^{m\times n}[s,\theta]$ for $\alpha \in \{1,2\}^N$, as

$$(\mathcal{Q}\mathbf{x})(s) = \sum_{\alpha\in\{1,2\}^N} \int_a^b \mathbf{I}_\alpha(s,\theta)\boldsymbol{Q}_\alpha(s,\theta)\mathbf{x}(\theta)\, d\theta$$

for $\mathbf{x} \in L_2^n[[a_1 b,_1] \times \cdots \times [a_N, b_N]]$, and where

$$\mathbf{I}_\alpha(s,\theta) := \prod_{i=1}^N \mathbf{I}_{\alpha_i}(s_i,\theta_i), \qquad \mathbf{I}_j(x,y) := \begin{cases} \mathbf{1}(x-y), & j=1, \\ \mathbf{1}(y-x), & j=2, \end{cases}$$

where $\mathbf{1}$ is the indicator function,

$$\mathbf{1}(z) := \begin{cases} 1, & z \geq 0, \\ 0, & \text{else.} \end{cases}$$

Again, we consider parameters of the form

$$\boldsymbol{Q}_\alpha(s,\theta) = (I_n \otimes \boldsymbol{Z}_d(s))^T C_\alpha (I_m \otimes \boldsymbol{Z}_d(\theta)),$$

where $\alpha \in \{1,2\}^N$, and

$$\boldsymbol{Z}_d(s) = \boldsymbol{Z}_d(s_1) \otimes \boldsymbol{Z}_d(s_2) \otimes \cdots \otimes \boldsymbol{Z}_d(s_N).$$

Then, we remark that

$$\begin{aligned}
\boldsymbol{Z}_d(s) &= \boldsymbol{Z}_d(s_1) \otimes \boldsymbol{Z}_d(s_2) \otimes \cdots \otimes \boldsymbol{Z}_d(s_N) \\
&= \big(I_{d+1} \otimes \boldsymbol{Z}_d(s_2) \otimes \cdots \otimes \boldsymbol{Z}_d(s_N)\big)\boldsymbol{Z}_d(s_1) = \big(I_{d+1} \otimes \boldsymbol{Z}_d(s_2,\ldots,s_{N-1})\big)\boldsymbol{Z}_d(s_1)
\end{aligned}$$

and thus we can represent

$$\begin{aligned}
\boldsymbol{Q}_\alpha(s,\theta) &= \big(I_m \otimes \boldsymbol{Z}_d(s)\big)^T C_\alpha\big(I_n \otimes \boldsymbol{Z}_d(s)\big) \\
&= \big(I_m \otimes \boldsymbol{Z}_d(s_1)\big)^T\big(I_{m(d+1)} \otimes \boldsymbol{Z}_d(s_2,\ldots,s_{N-1})\big)^T C_\alpha\big(I_{n(d+1)} \otimes \boldsymbol{Z}_d(s_2,\ldots,s_{N-1})\big)\big(I_n \otimes \boldsymbol{Z}_d(s_1)\big) \\
&= \big(I_m \otimes \boldsymbol{Z}_d(s_1)\big)^T \hat{\boldsymbol{Q}}_\alpha(s_2,\ldots,s_N,\theta_2,\ldots,\theta_N)\big(I_n \otimes \boldsymbol{Z}_d(s_1)\big),
\end{aligned}$$

where

$$\hat{\boldsymbol{Q}}_\alpha(s_2,\ldots,s_N,\theta_2,\ldots,\theta_N) := \big(I_{m(d+1)}\otimes\boldsymbol{Z}_d(s_2,\ldots,s_{N-1})\big)^T C_\alpha\big(I_{n(d+1)}\otimes\boldsymbol{Z}_d(s_2,\ldots,s_{N-1})\big), \qquad \alpha \in \{1,2\}^N.$$

Defining then the 2^{N-1}-PI operators $\hat{\mathcal{Q}}_i$ for $i\in\{1,2\}$ by

$$\big(\mathcal{Q}_i\mathbf{y}\big)(\hat{s})=\sum_{\hat{\alpha}\in\{1,2\}^{N-1}}\int_a^b \mathbf{I}_\alpha(\hat{s},\hat{\theta})\hat{\boldsymbol{Q}}_{(i,\alpha)}(\hat{s},\hat{\theta})\mathbf{y}(\hat{\theta})\,d\hat{\theta},\qquad \hat{s}\in[a_2,b_2]\times\cdots\times[a_N,b_N],$$

for $\mathbf{y}\in L_2^{n(d+1)}[[a_2,b_2]\times\cdots\times[a_N,b_N]]$, we can represent

$$\begin{aligned}(\mathcal{Q}\mathbf{x})(s)=&\int_{a_1}^{s_1}(I_m\otimes\boldsymbol{Z}_d(s_1))^T\Big(\hat{\mathcal{Q}}_1[I_n\otimes\boldsymbol{Z}_d(s_1)]\mathbf{x}(\theta_1,\cdot)\Big)(s_2,\ldots,s_N)\,d\theta_1\\&+\int_{s_1}^{b_1}(I_m\otimes\boldsymbol{Z}_d(s_1))^T\Big(\hat{\mathcal{Q}}_2[I_n\otimes\boldsymbol{Z}_d(s_1)]\mathbf{x}(\theta_1,\cdot)\Big)(s_2,\ldots,s_N)\,d\theta_1\end{aligned}$$

Now, $\hat{\mathcal{Q}}_1$ and $\hat{\mathcal{Q}}_2$ are 2^{N-1}-PI operators, each of which we can represent in terms of two 2^{N-2}-PI operators. In this manner, we should be able to inductively apply the 1D composition rules to compute the composition of ND PI operators.

3.7 Composition with Decision Variable 3-PI Operator

We now consider composition of 3-PI operators with variable coefficients. In particular, suppose we have a 3-PI operator $\Pi_{\{\boldsymbol{Q}_i\}}$ with parameters $\boldsymbol{Q}_i$ defined by decision variables $\xi\in\mathbb{R}^p$ as

$$\boldsymbol{Q}_0(s):=(I_m\otimes\boldsymbol{Z}_d(s))^T(I_{m(d+1)}\otimes[\begin{smallmatrix}1\\\xi\end{smallmatrix}])^T\hat{C}_0,\quad \boldsymbol{Q}_i(s,\theta):=(I_m\otimes\boldsymbol{Z}_d(s))^T(I_{m(d+1)}\otimes[\begin{smallmatrix}1\\\xi\end{smallmatrix}])^T\hat{C}_i(I_q\otimes\boldsymbol{Z}_d(\theta)),$$

for $i\in\{1,2\}$. Note that this is equivalent to the representation of 3-PI operators in e.g. Prop. 7, setting $C_j=(I_{m(d+1)}\otimes[\begin{smallmatrix}1\\\xi\end{smallmatrix}])^T\hat{C}_j$ for $j\in\{0,1,2\}$. As such, we can also use the same result for computing the composition of $\Pi_{\{\boldsymbol{Q}_i\}}$ with some operator $\Pi_{\{\boldsymbol{R}_i\}}$ defined by coefficients D_j, find that $\Pi_{\{\boldsymbol{Q}_i\}}\circ\Pi_{\{\boldsymbol{R}_i\}}$ is then defined by coefficients G_i given by

$$\begin{aligned}G_0:=&(I_m\otimes F_d)^T(C_0\otimes I_{d+1})D_0,\\
G_1:=&(I_m\otimes F_d)^T(C_0\otimes I_{d+1})D_1\Big(I_n\otimes\begin{bmatrix}I_{d+1}&0_{d+1\times 2d+1}\end{bmatrix}\Big)+\left(I_m\otimes\begin{bmatrix}I_{d+1}\\0_{2d+1\times d+1}\end{bmatrix}\right)C_1\big(I_q\otimes H_d\big)(D_0\otimes I_{3d+2})\\
&+\left(I_m\otimes\begin{bmatrix}I_{d+1}\\0_{2d+1\times d+1}\end{bmatrix}\right)\Big(C_2(I_q\otimes B_d)D_1-C_1(I_q\otimes A_d)D_2\Big)\Big(I_n\otimes\begin{bmatrix}I_{d+1}&0_{d+1\times 2d+1}\end{bmatrix}\Big)\\
&+\left(I_m\otimes\begin{bmatrix}I_{d+1}\\0_{2d+1\times d+1}\end{bmatrix}\right)C_1(I_q\otimes S_d)\big([D_2-D_1]\otimes I_{2d+2}\big)(I_n\otimes E_{2d+1,d})\\
&+(I_m\otimes E_{2d+1,d})^T\big([C_1-C_2]\otimes I_{2d+2}\big)(I_q\otimes S_d)^TD_1\Big(I_n\otimes\begin{bmatrix}I_{d+1}&0_{d+1\times 2d+1}\end{bmatrix}\Big)\\
G_2:=&(I_m\otimes F_d)^T(C_0\otimes I_{d+1})D_2\Big(I_n\otimes\begin{bmatrix}I_{d+1}&0_{d+1\times 2d+1}\end{bmatrix}\Big)+\left(I_m\otimes\begin{bmatrix}I_{d+1}\\0_{2d+1\times d+1}\end{bmatrix}\right)C_2\big(I_q\otimes H_d\big)(D_0\otimes I_{3d+2})\\
&+\left(I_m\otimes\begin{bmatrix}I_{d+1}\\0_{2d+1\times d+1}\end{bmatrix}\right)\Big(C_2(I_q\otimes B_d)D_1-C_1(I_q\otimes A_d)D_2\Big)\Big(I_n\otimes\begin{bmatrix}I_{d+1}&0_{d+1\times 2d+1}\end{bmatrix}\Big)\\
&+\left(I_m\otimes\begin{bmatrix}I_{d+1}\\0_{2d+1\times d+1}\end{bmatrix}\right)C_2(I_q\otimes S_d)\big([D_2-D_1]\otimes I_{2d+2}\big)(I_n\otimes E_{2d+1,d})\\
&+(I_m\otimes E_{2d+1,d})^T\big([C_1-C_2]\otimes I_{2d+2}\big)(I_q\otimes S_d)^TD_2\Big(I_n\otimes\begin{bmatrix}I_{d+1}&0_{d+1\times 2d+1}\end{bmatrix}\Big).\end{aligned}$$

To get composition rules for the case with decision variables, we can simply substitute the expression $C_i=(I_r\otimes[\begin{smallmatrix}1\\\xi\end{smallmatrix}])^T\hat{C}_i$ into these relations. Note here that for each of the parameters G_i, we need to compute a product of the form $(I_m\otimes M)^TC$ or $(I_m\otimes M)(C_i\otimes I_n)$ for some matrix M and scalar n. To factor the decision variables out of these expressions, we have the following result.

Lemma 8. *For $M\in\mathbb{R}^{k\times q}$, $K\in\mathbb{R}^{mq\times rn}$, and $\xi\in\mathbb{R}^p$, we have*

$$(I_m\otimes M)K(I_r\otimes[\begin{smallmatrix}1\\\xi\end{smallmatrix}]^T\otimes I_n)=\big(I_{mk}\otimes[\begin{smallmatrix}1\\\xi\end{smallmatrix}]^T\big)P_{mk,p+1}^T\big(I_{m(p+1)}\otimes M\big)\big(I_{p+1}\otimes K\big)\big(P_{p+1,r}^T\otimes I_n\big).$$

Proof. Recall that, for any $A\in\mathbb{R}^{m\times n}$ and $B\in\mathbb{R}^{p\times q}$, we have

$$B\otimes A=P_{m,p}(A\otimes B)P_{n,q}^T,$$

where $P_{1,p}=I_p$ and $P_{m,1}=I_m$. Using this property, we find that

$$(I_r\otimes[\begin{smallmatrix}1\\\xi\end{smallmatrix}]^T\otimes I_n)=\big[([\begin{smallmatrix}1\\\xi\end{smallmatrix}]^T\otimes I_r)P_{p+1,r}^T\big]\otimes I_n=\big([\begin{smallmatrix}1\\\xi\end{smallmatrix}]^T\otimes I_{rn}\big)\big(P_{p+1,r}^T\otimes I_n\big).$$

and thus $K(I_r \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_n) = K\big(\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{rn}\big)\big(P_{p+1,r}^T \otimes I_n\big)$. Here, by the mixed product property,

$$K\big(\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{rn}\big) = \big(\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{mq}\big)\big(I_{p+1} \otimes K\big),$$

so that we get

$$(I_m \otimes M)K(I_r \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_n) = (I_m \otimes M)\big(\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{mq}\big)\big(I_{p+1} \otimes K\big)\big(P_{p+1,r}^T \otimes I_n\big).$$

Again applying the mixed product property (twice), we can here express

$$\begin{aligned}
(I_m \otimes M)\big(\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{mq}\big) &= (I_m \otimes M)\big(\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_m \otimes I_q\big) \\
&= (\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_m) \otimes M \\
&= (\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{mk})(I_{p+1} \otimes (I_m \otimes M)) = (\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{mk})(I_{m(p+1)} \otimes M)
\end{aligned}$$

Finally, using the commutation matrix, we find

$$(\left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_{mk}) = (I_{mk} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T)P_{mk,p+1}^T.$$

Combining these results, it follows that

$$(I_m \otimes M)K(I_r \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T \otimes I_n) = \big(I_{mk} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T\big)P_{mk,p+1}^T\big(I_{m(p+1)} \otimes M\big)\big(I_{p+1} \otimes K\big)\big(P_{p+1,r}^T \otimes I_n\big)$$

$\square$

Using this result, we obtain the following explicit formulae for the composition of a decision variable3-PI operator $\mathcal{Q}$ with a fixed 3-PI operator $\mathcal{R}$.

Proposition 9. *For $[a,b] \subseteq \mathbb{R}$, $m,n,q,p \in \mathbb{N}$, and $d \in \mathbb{N}_0$, let*

$$\hat{C}_0 \in \mathbb{R}^{mp(d+1)\times q}, \quad \hat{C}_1, \hat{C}_2 \in \mathbb{R}^{mp(d+1)\times q(d+1)}, \qquad \text{and} \qquad D_0 \in \mathbb{R}^{q(d+1)\times n}, \quad D_1, D_2 \in \mathbb{R}^{q(d+1)\times n(d+1)},$$

and define

$$\begin{aligned}
\boldsymbol{Q}_0(s) &:= (I_m \otimes \boldsymbol{Z}_d(s))^T(I_{m(d+1)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right])^T\hat{C}_0, & \boldsymbol{Q}_i(s,\theta) &:= (I_m \otimes \boldsymbol{Z}_d(s))^T(I_{m(d+1)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right])^T\hat{C}_i(I_q \otimes \boldsymbol{Z}_d(\theta)), \\
\boldsymbol{R}_0(s) &:= (I_q \otimes \boldsymbol{Z}_d(s))^T D_0, & \boldsymbol{R}_i(s,\theta) &:= (I_q \otimes \boldsymbol{Z}_d(s))^T D_i(I_n \otimes \boldsymbol{Z}_d(\theta)),
\end{aligned}$$

for $i \in \{1,2\}$ and $s,\theta \in [a,b]$. Then $\Pi_{\{\boldsymbol{Q}_j\}} \circ \Pi_{\{\boldsymbol{R}_j\}} = \Pi_{\{\boldsymbol{P}_j\}}$, where

$$\begin{aligned}
\boldsymbol{P}_0(s) &:= (I_m \otimes \boldsymbol{Z}_{3d+1}(s))^T(I_{m(3d+1)} \otimes \xi)^T\hat{G}_0, \\
\boldsymbol{P}_i(s,\theta) &:= (I_m \otimes \boldsymbol{Z}_{3d+1}(s))^T(I_{m(3d+1)} \otimes \xi)^T\hat{G}_i(I_n \otimes \boldsymbol{Z}_{3d+1}(\theta)),
\end{aligned}$$

for

$$\begin{aligned}
\hat{G}_0 :=\; & P_{m(3d+2),p+1}^T\big(I_{m(p+1)} \otimes F_d\big)^T\big(P_{p+1,m(d+1)}^T \otimes I_{d+1}\big)\big(\hat{C}_0 \otimes I_{d+1}\big)D_0, \\
\hat{G}_1 :=\; & P_{m(3d+2),p+1}^T\big(I_{m(p+1)} \otimes F_d\big)^T\big(P_{p+1,m(d+1)}^T \otimes I_{d+1}\big)\big(\hat{C}_0 \otimes I_{d+1}\big)D_1\Big(I_n \otimes \big[I_{d+1} \quad 0_{d+1\times 2d+1}\big]\Big) \\
& + P_{m(3d+2),p+1}^T\left(I_{m(p+1)} \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)P_{p+1,m(d+1)}^T\hat{C}_1\big(I_q \otimes H_d\big)(D_0 \otimes I_{3d+2}) \\
& + P_{m(3d+2),p+1}^T\left(I_{m(p+1)} \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)P_{p+1,m(d+1)}^T\Big(\hat{C}_2(I_q \otimes B_d)D_1 - \hat{C}_1(I_q \otimes A_d)D_2\Big)\Big(I_n \otimes \big[I_{d+1} \quad 0_{d+1\times 2d+1}\big] \\
& + P_{m(3d+2),p+1}^T\left(I_{m(p+1)} \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)P_{p+1,m(d+1)}^T\hat{C}_1(I_q \otimes S_d)\big([D_2 - D_1] \otimes I_{2d+2}\big)(I_n \otimes E_{2d+1,d}) \\
& + P_{m(3d+2),p+1}^T\big(I_{m(p+1)} \otimes E_{2d+1,d}\big)^T\big(P_{p+1,m(d+1)}^T \otimes I_{2d+2}\big)\big([\hat{C}_1 - \hat{C}_2] \otimes I_{2d+2}\big)(I_q \otimes S_d)^T D_1\Big(I_n \otimes \big[I_{d+1} \quad 0_{d+1} \\
\hat{G}_2 :=\; & P_{m(3d+2),p+1}^T\big(I_{m(p+1)} \otimes F_d\big)^T\big(P_{p+1,m(d+1)}^T \otimes I_{d+1}\big)\big(\hat{C}_0 \otimes I_{d+1}\big)D_2\Big(I_n \otimes \big[I_{d+1} \quad 0_{d+1\times 2d+1}\big]\Big) \\
& + P_{m(3d+2),p+1}^T\left(I_{m(p+1)} \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)P_{p+1,m(d+1)}^T\hat{C}_2\big(I_q \otimes H_d\big)(D_0 \otimes I_{3d+2}) \\
& + P_{m(3d+2),p+1}^T\left(I_{m(p+1)} \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)P_{p+1,m(d+1)}^T\Big(\hat{C}_2(I_q \otimes B_d)D_1 - \hat{C}_1(I_q \otimes A_d)D_2\Big)\Big(I_n \otimes \big[I_{d+1} \quad 0_{d+1\times 2d+1}\big] \\
& + P_{m(3d+2),p+1}^T\left(I_{m(p+1)} \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1\times d+1}\end{bmatrix}\right)P_{p+1,m(d+1)}^T\hat{C}_2(I_q \otimes S_d)\big([D_2 - D_1] \otimes I_{2d+2}\big)(I_n \otimes E_{2d+1,d}) \\
& + P_{m(3d+2),p+1}^T\big(I_{m(p+1)} \otimes E_{2d+1,d}\big)^T\big(P_{p+1,m(d+1)}^T \otimes I_{2d+2}\big)\big([\hat{C}_1 - \hat{C}_2] \otimes I_{2d+2}\big)(I_q \otimes S_d)^T D_2\Big(I_n \otimes \big[I_{d+1} \quad 0_{d+1}
\end{aligned}$$

where the matrices S_d, $E_{2d+1,d}$, A_d and B_d are as in Prop. 3, and where $F_d = F_{d,d,3d+1}$ and $H_d = H_{d,d,3d+1}$ for F_{d_1,d_2,d_3} and H_{d_1,d_2,d_3} as in Lem. 5 and Lem. 6, respectively.

Proof. Note first that

$$(C_0 \otimes I_{d+1}) = \Big(\big[(I_{m(d+1)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right])^T \hat{C}_0\big] \otimes I_n\Big) = \big(I_{m(d+1)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right] \otimes I_{d+1}\big)^T \big(\hat{C}_0 \otimes I_{d+1}\big)$$

and similarly

$$([C_1 - C_2] \otimes I_{2d+2}) = \big(I_{m(d+1)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right] \otimes I_{2d+2}\big)^T \big([\hat{C}_1 - \hat{C}_2] \otimes I_{d+1}\big).$$

Applying Lem. 8, it follows that

$$\begin{aligned}(I_m \otimes F_d)^T (C_0 \otimes I_{d+1}) &= (I_m \otimes F_d)^T \big(I_{m(d+1)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right] \otimes I_{d+1}\big)^T \big(\hat{C}_0 \otimes I_{d+1}\big) \\ &= \big(I_{m(3d+2)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T\big) P^T_{m(3d+2),p+1} \big(I_{m(p+1)} \otimes F_d\big)^T \big(P^T_{p+1,m(d+1)} \otimes I_{d+1}\big)\big(\hat{C}_0 \otimes I_{d+1}\big),\end{aligned}$$

and

$$\begin{aligned}\big(I_m \otimes E_{2d+1,d}\big)^T \big([C_1 - C_2] \otimes I_{2d+2}\big) &= \big(I_m \otimes E_{2d+1,d}\big)^T \big(I_{m(d+1)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right] \otimes I_{2d+2}\big)^T \big([\hat{C}_1 - \hat{C}_2] \otimes I_{d+1}\big) \\ &= \big(I_{m(3d+2)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T\big) P^T_{m(3d+2),p+1} \big(I_{m(p+1)} \otimes E_{2d+1,d}\big)^T \big(P^T_{p+1,m(d+1)} \otimes I_{2d+2}\big)\big([\hat{C}_1 - \hat{C}_2] \otimes I_{d+1}\big).\end{aligned}$$

Furthermore, we find that

$$\left(I_m \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1 \times d+1} \end{bmatrix}\right) C_i = \big(I_{m(3d+2)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right]^T\big) P^T_{m(3d+2),p+1} \left(I_{m(p+1)} \otimes \begin{bmatrix} I_{d+1} \\ 0_{2d+1 \times d+1} \end{bmatrix}\right) P^T_{p+1,m(d+1)} \hat{C}_i$$

for each $i \in \{1, 2\}$. Substituting these relations into the expressions for G_0, G_1, and G_2 in Prop. 7, we find that $G_i = (I_{m(3d+2)} \otimes \left[\begin{smallmatrix}1\\ \xi\end{smallmatrix}\right])^T \hat{G}_i$ for each $i \in \{0, 1, 2\}$. □