Computation of functions of matrices and multivectors using generalised spectral basis

A. Acus* and A. Dargys**

*Vilnius University, Institute of theoretical physics and astronomy, Vilnius
**Center for Physical Sciences and Technology, Vilnius

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Matrix functions: examples and methods of computation

"...for I cannot believe that anything so ugly as the multiplication of matrices is an essential part of the scheme of nature."

sir Arthur Eddington

Examples of application

- Quantum mechanics: Hamilton evolution $\exp \mathrm{H}\, t$, here H operator is represented by finite dimensional matrix
- Linear system of equations: $y''(x) + \mathrm{A}y(x) = 0; y(0) = y_0, y'(0) = y_0'$. Solution: $y(t) = \cos(\sqrt{\mathrm{A}}t)y_0 + (\sqrt{\mathrm{A}})^{-1}\sin(\sqrt{\mathrm{A}}t)y_0'$
- Markov process: transition probability $\mathrm{P}(t)$ and intensity Q are related as $\mathrm{P}(t) = \exp(Qt)$.

Subject is well known. Is it possible to find something new?

Matrix functions: examples and methods of computation

Computation methods

- Taylor series:

$$f(\mathrm{A}) = f(0) + f'(0)\mathrm{A} + \frac{1}{2!}f''(0)\mathrm{A}^2 + \cdots + \frac{1}{k!}f^{(k)}(0)\mathrm{A}^k + \cdots$$

- Jordan decomposition: $\mathrm{J} = \begin{pmatrix} 3 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix}$, where $\mathrm{A} = \mathrm{T}\mathrm{J}\mathrm{T}^{-1}$.

- Integral formula (follows from residue theorem)

- Generalised spectral basis: based on matrix polynomials

Taylor expansion

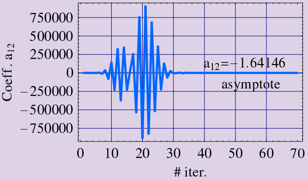
Taylor formula is incorrect!

Cayley-Hamilton theorem claims that matrix A is a solution of it's own characteristic equation

$$\sum_{k=0}^{d} \mathrm{A}^k C_{(d-k)}(\mathrm{A}) = \mathrm{A}^d C_{(0\ )}(\mathrm{A}) + \mathrm{A}^{d-1} C_{(1)}(\mathrm{A}) + \cdots + C_{(d)}(\mathrm{A}) = 0\,.$$

$C_{(k)}$ are the coefficients of characteristic polynomial. The correct expansion formula, therefore is $f(\mathrm{A}) =$
$\big(f(0)+\cdots\big) + \big(f'(0)+\cdots\big)\mathrm{A} + \cdots + \Big(\frac{1}{(d-1)!} f^{(d-1)}(0) + \cdots\Big)\mathrm{A}^{d-1}$.

Convergence of coefficient of exp(A)



Convergence is alternating

The graphics shows change of value of the coefficient of 8×8 matrix exp(A) by summing series terms. Summation of 20 terms yields value $a_{12} = 0.902645 \times 10^6$. A sum of 70 terms gives $a_{12} = -1.64146$ value. The coefficient of initial matrix A is $a_{12} = 5$.

The standard method

Jordan decomposition

Each matrix $\mathsf{A} \in \mathbb{C}(n \times n)$ can be decomposed into a block diagonal form $\mathsf{A} = \mathsf{T}\mathsf{J}\mathsf{T}^{-1}$, where

$$\mathsf{J} = \begin{pmatrix} J_{m_1}(\lambda_1) & & 0 \\ & \ddots & \\ 0 & & J_{m_\ell}(\lambda_\ell) \end{pmatrix} \text{ ir } \mathsf{J}_{\mathsf{m_j}} = \begin{pmatrix} \lambda_j & 1 & 0 & \cdots & 0 \\ 0 & \lambda_j & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & 1 \\ 0 & \cdots & \cdots & 0 & \lambda_j \end{pmatrix} = \lambda_j \mathsf{I} + S^0_{m_j} \in \mathbb{C}(m_j \times m_j).$$

The Jordan decomposition method

Function $f : \mathbb{C} \to \mathbb{C}$, $(m_j - 1)$-th times differentiable in the vicinity of eigenvalue λ_j of matrix A with spectrum $\mathrm{spec}(\mathsf{A}) = \lambda_1, \ldots, \lambda_\ell$ and Jordan decomposition $\mathsf{J} = \mathsf{T}^{-1}\mathsf{A}\mathsf{T} = \mathrm{diag}(\mathsf{J}_{m_1}(\lambda_1), \cdots, \mathsf{J}_{m_\ell}(\lambda_\ell))$ is computed as: $f(\mathsf{A}) = \mathsf{T}f(\mathsf{J})\mathsf{T}^{-1}$, where $f(\mathsf{J}) = \mathrm{diag}(f(\mathsf{J}_{m_1}(\lambda_1)), \cdots, f(\mathsf{J}_{m_\ell}(\lambda_\ell)))$, and

$$f(\mathsf{J}_{m_j}(\lambda_j)) = \sum_{\nu=0}^{m_j-1} \frac{1}{\nu!} f^{(\nu)}(\lambda_j) \cdot S^\nu_{m_j}; \quad S^\nu_{m_j} = (S^0_{m_j})^\nu; \quad f^{(\nu)}(\lambda_j) \text{ denotes}$$

derivatives.

Integral formula

From residue theorem, the resolvent

$$f(\mathsf{A}) = \frac{1}{2\pi \mathrm{i}} \oint_{\gamma} f(t)(t\mathsf{I} - \mathsf{A})^{-1} \mathrm{d}t$$

The function is assumed to be analytic in the region which covers the spectrum of matrix $\mathrm{spec}(\mathsf{A})$. Integration is around contour which encompasses the region in a positive direction. Requires symbolic matrix inverse. Integration is performed for each matrix element.

The generalised spectral basis: a definition

Matrix A $\rightarrow$ matrix polynomial $\mu(\mathsf{A}) = \mu(x) \rightarrow$
basis polynomials $p_i(x), q_i(x) \rightarrow$ matrix basis $p_i(\mathsf{A}), q_i(\mathsf{A})$

A very general basis [1]. Can be computed for arbitrary (finite dim) linear operator. First construct the basis for commutative variable x (not matrix). To this end we start form some matrix polynomial (characteristic $\chi(\mathsf{A})$ or minimal $\mu(\mathsf{A})$ polynomial, etc.). Then substituting the variable x by matrix A we obtain a generalised spectral basis.

Generalised spectral basis: $\mu(x) \rightarrow p_i(x), q_i(x)$

Start from matrix minimal polynomial $\mu(x)$. Root count list is $\{m_1, \ldots, m_r\}$. The polynomial has r different roots named as $\lambda_1, \ldots, \lambda_r$. Our goal is to construct a set of polynomials $p_j(x), q_k^s(x)$ with properties:

$$p_1 + \cdots + p_r = 1, \quad p_i p_j = \delta_{ij} p_i, \quad q_k p_k = q_k,$$
$$q_k^{m_k - 1} \neq 0, \quad \text{however} \quad q_k^{m_k} = 0.$$

Product of polynomials $\{p_j, q_k^t|,\ 1 \leq j \leq r,\ h+1 \leq k \leq r,\ 1 \leq t < m_k\}$ is understood as product modulus polynomial $\mu(x, \lambda)$. The index $h = 0$ characterises unique root (for non repeating root polynomials q_k are absent).

The generalised spectral basis: the algorithm

Traditionally the basis is obtained by expanding $\frac{1}{\mu(x)}$ in partial fractions. After expansion we find polynomials $p_i(x)$. Then polynomials $q_i(x)$ are computed $q_i(x) = p_i(x)(x-\lambda_i)$. Division polynomials in modulo $\mu(x)$! We propose the basis computation from the polynomial $q_i^{m_i-1}(x,\lambda)$, which is of "largest weight" (the basis definition imply $q_i^{m_i}(x,\lambda)=0$).

Main result

Recursive algorithm

Start computation from opposite end. We need a largest weight function $S^{(0)}$.

$$q_i^{m_i-1}(x,\lambda) = \frac{S^{(0)}(x,\lambda)}{\mu^{(m_i)}(\lambda)}$$

$$q_i^{m_i-2}(x,\lambda) = \frac{S^{(1)}(x,\lambda) - q_i^{m_i-1}(x,\lambda)\mu^{(m_i+1)}(\lambda)}{\mu^{(m_i)}(\lambda)}$$

$$q_i^{m_i-3}(x,\lambda) = \frac{S^{(2)}(x,\lambda) - q_i^{m_i-2}(x,\lambda)\mu^{(m_i+1)}(\lambda) - q_i^{m_i-1}(x,\lambda)\mu^{(m_i+2)}(\lambda)}{\mu^{(m_i)}(\lambda)}$$

$$\vdots$$

$$p_i(x,\lambda) = q_i^0(x,\lambda) = \frac{S^{(m_i-1)}(x,\lambda) - q_i^1(x,\lambda)\mu^{(m_i+1)}(\lambda) - q_i^2(x,\lambda)\mu^{(m_i+2)}(\lambda) - \cdots - q_i^{m_i-1}(x,\lambda)\mu^{(2m_i-1)}(\lambda)}{\mu^{(m_i)}(\lambda)}.$$

The generalised basis: the function of largest weight

Definition of largest weight function $S^{(0)}$

$$S^{(0)}(x,\lambda) = \sum_{k=0}^{r-1}\left(\sum_{s=0}^{r-k-1}\lambda^s C_{(r-s-k-1)}(x)\right)x^k,$$

$$S^{(k)}(x,\lambda) = \frac{1}{k!}\frac{\mathrm{d}^k S(x,\lambda)}{\mathrm{d}\lambda^k}; \qquad \mu^{(k)}(\lambda) = \frac{1}{k!}\frac{\mathrm{d}^k \mu(\lambda)}{\mathrm{d}\lambda^k}.$$

Expression of function of matrix in generalised spectral basis

A matrix function $f(x)$ computes as:

$$f(x) = \sum_j f(\lambda_j + q_j)p_j(x), \quad \text{where}$$

$$f(\lambda_j + q_j) = f(\lambda_j) + f'(\lambda_j)q_j(x) + \cdots + \frac{f^{(m_j-1)}(\lambda_j)}{(m_j-1)!}q_j^{(m_j-1)}(x)$$

The generalised basis: the characteristic polynomial $\chi(\mathsf{A})$

Matrix $\mathsf{A} \to$ matrix polynomial $\mu(\mathsf{A}) = \mu(x) \to$
basis polynomials $p_i(x), q_i(x) \to$ matrix basis $p_i(\mathsf{A}), q_i(\mathsf{A})$

The characteristic $\chi_{\mathsf{A}}(\lambda) = \sum_{k=0}^{d} C_{(d-k)}(\mathsf{A})\,\lambda^k$ and the minimal $\mu(\mathsf{A})$.
Arbitrary polynomial $g(\mathsf{A}) = 0$ is suitable for function computation.

Algorithm for characteristic polynomial (Faddeev-LeVerrier-Souriau)

Input is a matrix A. The output is polynomial $\chi_{\mathsf{A}}(x)$ of commutative variable.

$$
\begin{aligned}
\mathsf{A}_{(1)} = \mathsf{A} \quad &\to \quad C_{(1)}(\mathsf{A}) = \tfrac{1}{1}\operatorname{Tr}\left(\mathsf{A}_{(1)}\right),\\
\mathsf{A}_{(2)} = \mathsf{A}\big(\mathsf{A}_{(1)} - C_{(1)}(\mathsf{A})\mathsf{I}\big) \quad &\to \quad C_{(2)}(\mathsf{A}) = \tfrac{1}{2}\operatorname{Tr}\left(\mathsf{A}_{(2)}\right),\\
&\vdots\\
\mathsf{A}_{(d)} = \mathsf{A}\big(\mathsf{A}_{(d-1)} - C_{(d-1)}(\mathsf{A})\mathsf{I}\big) \quad &\to \quad C_{(d)}(\mathsf{A}) = \tfrac{1}{d}\operatorname{Tr}\left(\mathsf{A}_{(d)}\right).
\end{aligned}
$$

First step yields the matrix trace $C_{(1)}(\mathsf{A})$. Last step returns the determinant $-\operatorname{Det}(\mathsf{A}) = C_{(d)}(\mathsf{A}) = \frac{1}{d}\operatorname{Tr}\left(\mathsf{A}\big(\mathsf{A}_{(d-1)} - C_{(d-1)}(\mathsf{A})\mathsf{I}\big)\right)$. Attempt to extend by one more step $(d+1)$ gives zero, $\mathsf{A}_{(d+1)} = \mathsf{A}\big(\mathsf{A}_{(d)} - C_{(d)}(\mathsf{A})\mathsf{I}\big) = 0$.

Cayley-Hamilton theorem: the matrix satisfies it's own characteristic polynomial.

The generalised basis: the minimal polynomial $\mu(\mathsf{A})$

Physicists compute characteristic polynomial as $\det(\mathsf{A} - \lambda \mathsf{I})$.

Comparison of minimal $\mu(\mathsf{A})$ and characteristic $\chi(\mathsf{A})$ polynomials

$\mu(\mathsf{A})$ can be computed with "null space" algorithm (formula don't exists). The degree of minimal polynomial $\deg(\mu(\mathsf{A})) \leq \deg(\chi(\mathsf{A}))$. Minimal polynomial is more informative.

Jordan's block	$\left.\begin{matrix} \lambda_i & 0 & 0 & \cdots & 0 \\ 0 & \lambda_i & 0 & \cdots & 0 \\ & & & \vdots & \\ 0 & 0 & \cdots & \lambda_i & 0 \\ 0 & 0 & \cdots & 0 & \lambda_i \end{matrix}\right\} k$	$\left.\begin{matrix} \lambda_i & 1 & 0 & \cdots & 0 \\ 0 & \lambda_i & 1 & \cdots & 0 \\ & & & \vdots & \\ 0 & 0 & \cdots & \lambda_i & 1 \\ 0 & 0 & \cdots & 0 & \lambda_i \end{matrix}\right\} k$
$\mu_{\mathsf{A}(x)}$	$(x - \lambda_i)$	$(x - \lambda_i)^k$
$\chi_{\mathsf{A}(x)}$	$(x - \lambda_i)^k$	$(x - \lambda_i)^k$

When minimal polynomial has repeating root, a matrix is defective (non diagonalizible).

Results

Conclusion

- Simple and effective recursive procedure to compute generalised spectral basis of matrix/multivector is proposed.
- The procedure don't require polynomial division or computation of inverse.
- The algorithm is implemented and freely available from `https://resources.wolframcloud.com/FunctionRepository` (look for ComputeMatrixFunction).

Examples of application

is demonstrated in Mathematica :
https://resources.wolframcloud.com/FunctionRepository/resources/ComputeMatrixFunction/

Bibliography

Sobczyk G.
The Generalized Spectral Decomposition of a Linear Operator,
The College Mathematics Journal. 1997;28(1):27–38.

A. Acus, A. Dargys
Multivector (MV) Functions in Clifford Algebras of Arbitrary Dimension: Defective MV Case,
Mathematical Methods in the Applied Sciences, 2025; 48:11025–11036

Thank You