

## Polynomials of matrices

Another **different** way to make polynomials and matrices interact: take a scalar polynomial, and apply a (**square**) matrix to it, e.g.,

$$p(x) = 1 + 3\underline{x} - 5\underline{x}^2 \implies \underbrace{p(A)} = \underbrace{I + 3A - 5A^2}.$$

### Lemma

If  $A = \underline{S} \text{blkdiag}(J_1, J_2, \dots, J_s) \underline{S}^{-1}$  is a Jordan form, then  $p(A) = \underline{S} \text{blkdiag}(\underline{p(J_1)}, p(J_2), \dots, p(J_s)) \underline{S}^{-1}$ , and

$$\rightarrow p(J_i) = \begin{bmatrix} p(\lambda_i) & p'(\lambda_i) & \dots & \frac{1}{k!} p^{(k)}(\lambda_i) \\ & p(\lambda_i) & \ddots & \vdots \\ & & \ddots & p'(\lambda_i) \\ & & & p(\lambda_i) \end{bmatrix}.$$

(Proof: Taylor expansion of  $p$  around  $\lambda$ .)

Valutare polinomio scalare in un blocco di Jordan:

$$J = \lambda I + N \quad N = \begin{bmatrix} 0 & & & \\ & \ddots & & \\ & & \ddots & \\ & & & 0 \end{bmatrix}$$

$$p(x) = p(\lambda) + p'(\lambda)(x-\lambda) + \dots + \frac{1}{d!} p^{(d)}(\lambda)(x-\lambda)^d$$

$$p(J) = p(\lambda)I + p'(\lambda)(J - \lambda I) + \dots + \frac{1}{d!} p^{(d)}(\lambda)(J - \lambda I)^d =$$

$$= p(\lambda)I + p'(\lambda)N + \frac{1}{2} p''(\lambda)N^2 + \dots + \frac{1}{d!} p^{(d)}(\lambda)N^d =$$

$$= \begin{bmatrix} p(\lambda) & p'(\lambda) & & \\ & \ddots & & \\ & & \ddots & \\ & & & p(\lambda) \end{bmatrix}$$



## Functions of matrices [Higham book, '08]

We can extend the same definition to arbitrary scalar functions:

Given a function  $f : U \subseteq \mathbb{C} \rightarrow \mathbb{C}$ , we say that  $f$  is **defined on  $A$**  if  $f$  is defined and differentiable at least  $\underline{m_g(\lambda_i)} - 1$  times on each eigenvalue  $\lambda_i$  of  $A$ .

### Definition

If  $A = \underline{S} \text{blkdiag}(J_1, J_2, \dots, J_s) \underline{S}^{-1}$  is a Jordan form, then  $f(A) = \underline{S} \text{blkdiag}(f(J_1), f(J_2), \dots, f(J_s)) \underline{S}^{-1}$ , where

$$f(J_i) = \begin{bmatrix} f(\lambda_i) & f'(\lambda_i) & \dots & \frac{1}{k!} f^{(k)}(\lambda_i) \\ & f(\lambda_i) & \ddots & \vdots \\ & & \ddots & f'(\lambda_i) \\ & & & f(\lambda_i) \end{bmatrix}$$



(Reasonable doubt: is it independent of the choice of  $S$ ?)

Def: Hermite interpolating polynomial:

Dati nodi  $\lambda_1, \lambda_2, \dots, \lambda_k$ , molteplicità

$1 \leq m_i$  per  $i=1, 2, \dots, k$ , e una funzione derivabile  $m_i-1$  volte in  $\lambda_i$ , esiste un (unico) polinomio di grado  $(\sum m_i) - 1$  tale che  $P^{(j)}(\lambda_i) = f^{(j)}(\lambda_i)$

per ogni  $i=1, 2, \dots, k$ ,  $j=1, 2, \dots, m_i$

ES: trovare un polinomio tale che

$$P(0) = 1 \quad P(1) = e$$

$$\rightarrow P'(0) = 1 \quad P'(1) = e$$

$$\rightarrow P''(0) = 1 \quad P''(1) = e$$

(coincide con  $\exp(x)$   
in 0 e 1, con  
due derivate uguali)

$$(deg = 5)$$

$$\begin{array}{l}
 x_1 \\
 x_2 \\
 x_3 \\
 x_4
 \end{array}
 \left( \begin{array}{l}
 f(x_1) \\
 f(x_2) \\
 f(x_3) \\
 f(x_4)
 \end{array} \right)
 \begin{array}{l}
 f[x_1, x_2] \\
 f[x_2, x_3] \\
 f[x_3, x_4]
 \end{array}
 \begin{array}{l}
 f[x_1, x_2, x_3] \\
 f[x_2, x_3, x_4]
 \end{array}
 f[x_1, x_2, x_3, x_4]$$

(forma di Newton)

$$f[x_i, x_{i+1}] = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \quad \leftarrow$$

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}$$

⋮

## Alternate definition: via Hermite interpolation

### Definition

$f(A) = p(A)$ , where  $p$  is a polynomial such that  $f(\lambda_i) = p(\lambda_i)$ ,  $f'(\lambda_i) = p'(\lambda_i), \dots, f^{(m_g(\lambda_i)-1)}(\lambda_i) = p^{(m_g(\lambda_i)-1)}(\lambda_i)$  for each  $i$ .

We may use this as a definition of  $f(A)$  (and it does not depend on  $S$ ).

Obvious from the definitions that it coincides with the previous one.

**Remark:** if  $A \in \mathbb{C}^{m \times m}$  has multiple Jordan blocks with the same eigenvalue, these may be fewer than  $m$  conditions.

**Remark:** be careful when you say “all matrix functions are polynomials”, because  $p$  depends on  $A$ .

Se  $f$  è un polinomio, allora  $f(A)$  definita in questo modo coincide con il valore  $f(x)$  in  $A$ :

$$A = SJS^{-1}$$

valore  $f(x)$  in  $A$  produce  $S \cdot \text{blkdiag}(f(J_1), \dots, f(J_k)) \cdot S^{-1}$

dove  $f(J_i) = \begin{bmatrix} f(\lambda_i) & f'(\lambda_i) & \dots & \frac{1}{(m_i-1)!} f^{(m_i-1)}(\lambda_i) \\ & \ddots & \ddots & \vdots \\ & & f(\lambda_i) & \\ & & & f(\lambda_i) \end{bmatrix}$

che coincide con  $\mathcal{P}(J_i)$  se  $\mathcal{P}(x)$  è il polinomio di interpolazione.

Quindi  $f$



## Some properties

- ▶ If the eigenvalues of  $A$  are  $\lambda_1, \dots, \lambda_s$ , the eigenvalues of  $f(A)$  are  $f(\lambda_1), \dots, f(\lambda_s)$ . (Remark: geometric multiplicities may drop)
- ▶  $f(A)g(A) = g(A)f(A) = (fg)(A)$  (since they are all polynomials in  $A$ ).
- ▶ If  $f_n \rightarrow f$  together with 'enough derivatives' (for instance because they are analytic and the convergence is uniform), then  $f_n(A) \rightarrow f(A)$ .
- ▶ If a sequence of matrix  $A_n \rightarrow A$ , then  $f(A_n) \rightarrow f(A)$ .  
Proof: let  $p_n$  be the (Hermite) interpolating polynomial on the eigenvalues of  $A_n$ . Interpolating polynomials are continuous in the nodes, so  $p_n \rightarrow p$  (coefficient by coefficient). Then  $\|p_n(A_n) - p(A)\| \leq \|p_n(A_n) - p_n(A)\| + \|p_n(A) - p(A)\| \leq \dots$

## Examples

- ▶  $\exp(A) = I + A + \frac{1}{2}A^2 + \frac{1}{3!}A^3 + \dots$ . The identity holds also for non-diagonalizable matrices (by continuity).
- ▶  $\operatorname{sgn}(A)$  from

$$\operatorname{sgn}(x) = \begin{cases} -1 & \operatorname{Re} x < 0, \\ 1 & \operatorname{Re} x > 0, \\ \text{undefined} & \operatorname{Re} x = 0. \end{cases}$$

- ▶  $A^{1/2}$  from  $f(x) = \sqrt{x}$ . Note that we can choose signs (branch) independently on each eigenvalue. All the various ways satisfy  $(A^{1/2})^2 = A$ .

## Nonprimary matrix functions

If a matrix  $A$  has multiple eigenvalues, one could also define a 'square root' by choosing different signs on Jordan blocks with the same eigenvalue: for instance,  $\begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$  as a square root of  $I_2$  (or also  $V \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} V^{-1}$  for any invertible  $V \dots$ ).

These are called **nonprimary** matrix functions (and they are **not** matrix functions with our definition).

(They all satisfy  $f(A)^2 = A$ .)

(They are **not** polynomials in  $A$ .)

## Cauchy integrals

If  $f$  is analytic on and inside a contour  $\Gamma$  that encloses the eigenvalues of  $A$ ,

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

Generalizes the analogous scalar formula.

**Proof** If  $A = V\Lambda V^{-1} \in \mathbb{C}^{m \times m}$  is diagonalizable, the integral equals

$$V \begin{bmatrix} \frac{1}{2\pi i} \int_{\Gamma} \frac{f(z)}{z-\lambda_1} dz & & \\ & \ddots & \\ & & \frac{1}{2\pi i} \int_{\Gamma} \frac{f(z)}{z-\lambda_m} dz \end{bmatrix} V^{-1} = V \begin{bmatrix} f(\lambda_1) & & \\ & \ddots & \\ & & f(\lambda_m) \end{bmatrix} V^{-1}.$$

By continuity, the equality holds also for non-diagonalizable  $A$ .

## Methods

Matrix functions arise in several areas: solving ODEs (e.g.  $\exp A$ ), matrix analysis (square roots), physics, ...

Main methods to compute them:

- ▶ Factorizations (eigendecompositions, Schur...),
- ▶ Matrix versions of scalar iterations (e.g., Newton on  $x^2 = a$ ),
- ▶ Interpolation / approximation,
- ▶ Complex integrals.