

## Matrix Functions

$$J = \begin{bmatrix} 0 & 1 & & 0 \\ 0 & 0 & \ddots & \\ & & \ddots & 1 \\ 0 & & & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$$J_2 = \begin{bmatrix} 0 & 0 & 1 & \\ & 0 & 0 & \ddots \\ & & \ddots & 0 & 1 \\ & & & 0 & 0 \end{bmatrix}$$

$$J_3 = \begin{bmatrix} 0 & 0 & 0 & 1 & \\ & 0 & 0 & 0 & \ddots \\ & & \ddots & 0 & 0 & 1 \\ & & & 0 & 0 & 0 \end{bmatrix}$$

$$J^{n-1} = \begin{bmatrix} 0 & & & 1 \\ & & & \\ & & & \\ & & & 0 \end{bmatrix}$$

$$J^n = 0$$

$$f(x) = p_0 + p_1 x + \dots + p_d x^d$$

$$f(J) = p_0 I + p_1 J + p_2 J^2 + \dots + p_d J^d =$$

$$= \begin{bmatrix} P_0 P_1 P_2 \dots P_{n-1} \\ P_0 \dots P_2 \dots P_{n-1} \\ \vdots \\ P_0 \end{bmatrix}$$

Trapezoidal (constant entries on diagonals)  
& upper triangular

$$J_A = \begin{bmatrix} \lambda & & & 0 \\ & \lambda & & \\ & & \ddots & \\ 0 & & & \lambda \end{bmatrix} \in \mathbb{R}^{n \times n}$$

Jordan block with eigenvalue  $\lambda$

$$J_A - \lambda I = \begin{bmatrix} 0 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix}$$

$$P(J_A) = ?$$

$$P(x) = P(\lambda) + P'(\lambda)(x-\lambda) + \frac{P''(\lambda)}{2!}(x-\lambda)^2 + \frac{P'''(\lambda)}{3!}(x-\lambda)^3 + \dots + \frac{P^{(d)}(\lambda)}{d!}(x-\lambda)^d$$

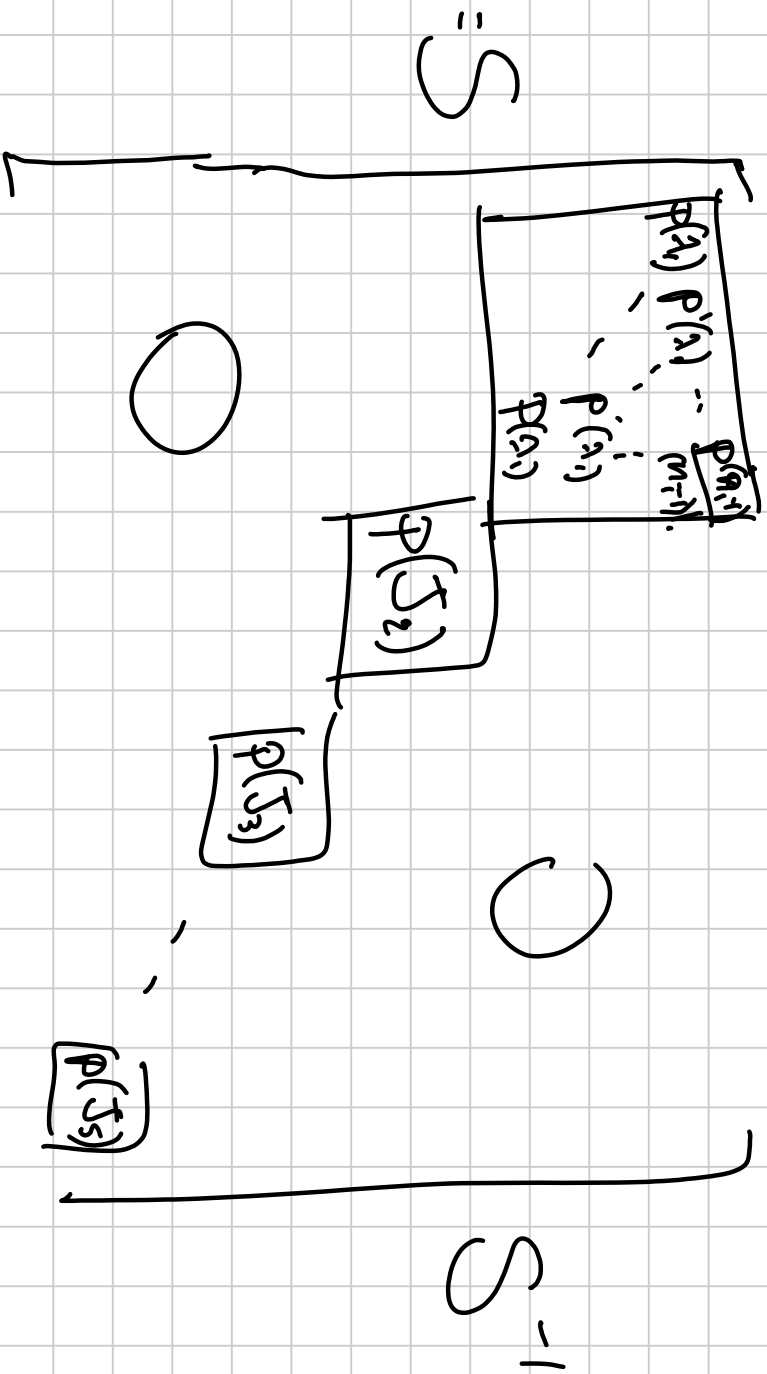
$$\begin{aligned}
P(J_\lambda) &= P(\lambda)I + P'(\lambda)(J_\lambda - \lambda I) + \frac{P''(\lambda)}{2}(J_\lambda - \lambda I)^2 + \dots + \frac{P^{(d)}(\lambda)}{d!}(J_\lambda - \lambda I)^d \\
&= P(\lambda)I + P'(\lambda)J_0 + \frac{P''(\lambda)}{2}J_0^2 + \dots + \frac{P^{(d)}(\lambda)}{d!}J_0^d \\
&= \begin{bmatrix} P(\lambda) & P'(\lambda) & \frac{P''(\lambda)}{2} & \dots & \frac{P^{(n-1)}(\lambda)}{(n-1)!} \\ & P(\lambda) & P'(\lambda) & \dots & \frac{P^{(n-2)}(\lambda)}{(n-2)!} \\ & & P(\lambda) & \dots & P'(\lambda) \\ & & & \dots & P(\lambda) \end{bmatrix}
\end{aligned}$$

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If  $A = SJS^{-1}$  is a Jordan form of  $A$ ,

with  $J = \begin{pmatrix} J_1 & & 0 \\ & \ddots & \\ 0 & & J_s \end{pmatrix}$

$$f(A) = f_0 I + f_1 A + \dots + f_d A^d = S \left( f_0 I + f_1 J + \dots + f_d J^d \right) S^{-1}$$



Idea: Let us use the same definition for an arbitrary function

Definition: Given  $f: U \subseteq \mathbb{C} \rightarrow \mathbb{C}$ , we say  $f$  is defined on  $A$  if  $f$  is defined and  $n_i = -1$  times differentiable on each eigenvalue  $\lambda_i$  of  $A$  (with maximum size of associated Jordan block  $n_i$ ).

Definition: <sup>(attempted)</sup> Given  $f: U \subseteq \mathbb{C} \rightarrow \mathbb{C}$  defined on  $A$ , and

A with Jordan form  $A = S \operatorname{diag}(J_1, J_2, \dots, J_s) S^{-1}$ ,

then  $f(A) := S \operatorname{diag}(f(J_1), \dots, f(J_s)) S^{-1}$ , where



(Interpolation conditions)

$$\left. \begin{aligned} \varphi(A_i) &= P(A_i) \\ \varphi'(A_i) &= P'(A_i) \\ &\vdots \\ \varphi^{(m_i-1)}(A_i) &= P^{(m_i-1)}(A_i) \end{aligned} \right\}$$

for each eigenvalue  $\lambda_i$  of  $A$  with maximum Jordan block size  $m_i$

(Is there one such polynomial?)

Then,  $P(A) := P(A) = P_0 I + P_1 A + \dots + P_d A^d$

1) This definition coincides with the previous one (we know what  $P(A)$  is, and it coincides with  $P(A)$ )

2) This definition does not depend of  $P$  (only the values of  $P(A_i), \dots, P^{(m_i-1)}(A_i)$  appear in it).

3) Does not depend on  $S$

Remark: if there are repeated eigenvalues, there are fewer than  $n$  conditions

Remark 2:  $P$  depends on  $A$ :

$$\exp(A) = P_A(A)$$

$$\exp(B) = P_B(B)$$

Ex:

$$A = \begin{pmatrix} 4 & 1 & 0 \\ 0 & 4 & 1 \\ 0 & 0 & 4 \end{pmatrix} \quad \begin{matrix} 0 \\ 0 \\ 0 \end{matrix}$$

$$f(x) = \sqrt{x}$$



$$f(A) = \sqrt{A} = ?$$

I want a polynomial with

$$P(0) = f(0) = 0 \quad P(4) = f(4) = 2 \quad P'(4) = f'(4) = \frac{1}{4} \quad P''(4) = f''(4) = -\frac{1}{32}$$

Then,

$$f(A) = P(A) =$$

$$\begin{bmatrix} P(4) & P'(4) & \frac{P''(4)}{2} \\ 0 & P(4) & P'(4) \\ 0 & 0 & P(4) \end{bmatrix} \begin{bmatrix} P(0) \\ P(4) & P'(4) \\ 0 & P(4) \end{bmatrix} = \begin{bmatrix} 2 & \frac{1}{4} & -\frac{1}{64} \\ 2 & 2 & \frac{1}{4} \\ 2 & 2 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 2 & \frac{1}{4} \\ 2 & 2 \end{bmatrix}$$

(Note that  $(P(A))^2 = A$ )

Also, note that  $f$  is defined in  $A$

(If we had  $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ , we'd have a problem, because  $f'(0)$  is not defined  $\left( f'(x) = \frac{1}{2} \frac{1}{\sqrt{x}} \right)$



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How do I compute  $\mathcal{P}$  explicitly?

I have 4 conditions, let us look for

$$\mathcal{P}(x) = a + bx + cx^2 + dx^3$$

$$\mathcal{P}'(x) = b + 2cx + 3dx^2$$

$$\mathcal{P}''(x) = 2c + 6dx$$

$$\mathcal{P}(0) = 0 \quad \mathcal{P}(4) = 2 \quad \mathcal{P}'(4) = \frac{1}{4} \quad \mathcal{P}''(4) = -\frac{1}{32}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 4 & 4^2 & 4^3 \\ 0 & 1 & 2 \cdot 4 & 3 \cdot 4^2 \\ 0 & 0 & 2 & 6 \cdot 4 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ 1/4 \\ -1/32 \end{bmatrix} \quad (*)$$

$$p(x) = \frac{3}{256}x^3 - \frac{5}{32}x^2 + \frac{15}{16}x.$$

$$p(A) = p(A) = \frac{3}{256}A^3 - \frac{5}{32}A^2 + \frac{15}{16}A = \left[ \begin{array}{c} \text{some matrix as} \\ \text{before} \end{array} \right]$$

## Hermite interpolation

and  $y_{i,0}, \dots, y_{i,m_i-1}, i=1, \dots, n$

Given points  $x_1, x_2, \dots, x_n$ , multiplies  $m_1, m_2, \dots, m_n$ ,

there exists a unique polynomial of degree

$$d < m_1 + m_2 + \dots + m_n =: m \quad \text{such that}$$

$$p(x_i) = y_{i,0}, \quad p'(x_i) = y_{i,1}, \quad \dots, \quad p^{(m_i-1)}(x_i) = y_{i,m_i-1} \quad i=1, 2, \dots, n$$

**Proof:** This is a linear system in the coefficients of the polynomial, like in (\*).

I just have to prove that the associated "generalized Vandermonde" matrix is invertible:

$$V = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{m-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{m-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^{m-1} \end{bmatrix}$$

$$z = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{bmatrix} \quad \sqrt{z=0}$$

Let us take z ∈ Ker V  $\sqrt{z=0}$  Define  $z(x) = z_1 + z_2x + \dots + z_mx^{m-1}$

$$\text{Tr Ker } V \sqrt{z=0} \Leftrightarrow z(x_1) = 0$$

$$z'(x_1) = 0$$

$$\vdots$$

$$z^{(m-1)}(x_1) = 0$$

$$z(x_2) = 0$$

$$\vdots$$

$$z^{(m-1)}(x_1) = 0$$

$$z(x_n) = 0$$

$$\vdots$$

$$z^{(m-1)}(x_n) = 0$$

$$\stackrel{=0}{z(x)} = (x-x_1)^{m_1} (x-x_2)^{m_2} \dots (x-x_n)^{m_n} \cdot q(x)$$

But  $\deg z(x) < m_1 + \dots + m_n$ , so  $z(x) \equiv 0 \Rightarrow \ker V = \{0\}$ .

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Methods:	$\text{sqrt}(A)$	elementwise	$\text{exp}(A)$
	$\text{sqrtm}(A)$	matrix function	$\text{expm}(A)$

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Example:

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \quad f(x) = \sqrt{x}$$

$f$  is not defined in  $A$ , because  $f'(0)$  does not exist.

Indeed, there is no matrix  $X$  s.t.  $X^2 = A$ .

if there were one, it would have to have two zero eigenvalues  
so Jordan form  $\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$  or  $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ , but in both

Cases  $X^2=0$ .

$$A = S \begin{pmatrix} -1 & & \\ & 0 & \\ & & 0 \end{pmatrix} S^{-1} \quad f(x) = \exp(x)$$

$$\exp(A) = I + A + \frac{1}{2}A^2 + \frac{1}{6}A^3 + \dots$$

we have not proved that  
if coincides with the  
Taylor series

$$\exp(A) = S$$

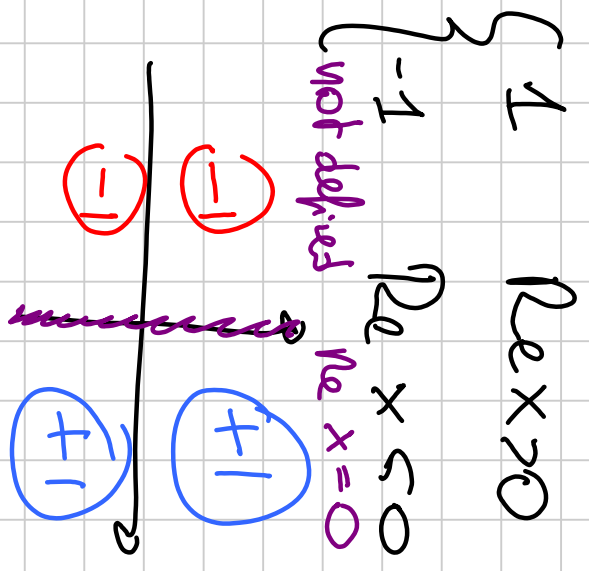
$$\exp(A) = S \begin{pmatrix} e^{-1} & & \\ & 1 & \\ & & 1 \end{pmatrix} S^{-1} \quad \begin{matrix} f''(1) \\ e \\ 0 \end{matrix}$$

$$A = S \begin{pmatrix} -3 & & \\ & -2 & \\ & & \begin{matrix} | & | \\ 0 & 1 \end{matrix} \end{pmatrix} S^{-1}$$

$$\text{sign}(A) = S \begin{pmatrix} -1 & & \\ & -1 & \\ & & \begin{matrix} | & | \\ 0 & 1 \end{matrix} \end{pmatrix} S^{-1}$$

$\text{sign}(A)$

$$f(x) = \text{sign}(x) = \begin{cases} 1 & \text{Re } x > 0 \\ -1 & \text{Re } x < 0 \\ \text{not defined} & \text{Re } x = 0 \end{cases}$$





$$\text{Ker}(\text{sign}(A) - I) = \text{Ker} \left( S \begin{pmatrix} -1 & & & \\ & -1 & & \\ & & 1 & \\ & & & 0 \end{pmatrix} - I \right) S^{-1} =$$

$$\text{Ker} \left( S \begin{pmatrix} -2 & & & \\ & -2 & & \\ & & 0 & \\ & & & 0 \end{pmatrix} S^{-1} \right) = \text{span}(S_3, S_4)$$

last two columns of  $S$

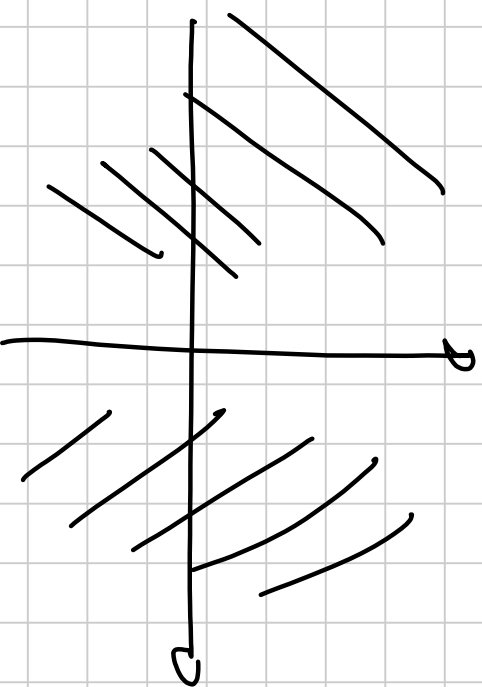
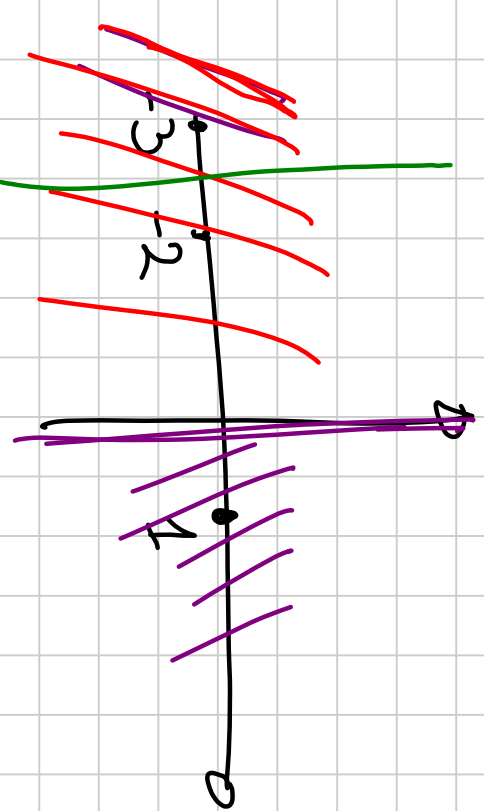
$$\text{Ker}(\text{sign}(A) + I) = \text{Ker} \left( S \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 2 & \\ & & & 2 \end{pmatrix} S^{-1} \right) = \text{span}(S_1, S_2)$$

first two columns of  $S$

$\ker(\text{sign}(A) - I) = \text{Span}(\text{Jordan chains associated to eigen values with } \text{Re}(\lambda) > 0)$

$\ker(\text{sign}(A) + I) = \text{Span}(\text{Jordan chains } \text{Re}(\lambda) < 0)$

(two invariant subspaces of  $A$ )



Example

$$A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$P(x) = \sqrt{x}$$

What is  $f(A)$ ?

It depends?

$$\text{eig}(A) = \{+i, -i\}$$

We need to choose branches

For each eigenvalue do  
have  $f(x)$  Rully defined

Usual choice: the root in the right

half-plane (Principal square root)

$$f(i) = \frac{1}{\sqrt{2}}(1+i)$$

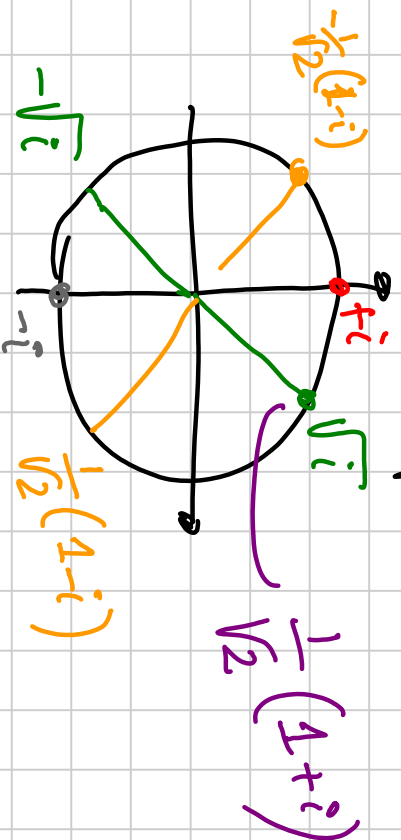
$$\varphi(i) = \frac{1}{\sqrt{2}}(1+i)$$

$$f(-i) = \frac{1}{\sqrt{2}}(1-i)$$

$$\varphi(-i) = \frac{1}{\sqrt{2}}(1-i)$$

↳ interp. polynomial:

$$\varphi(x) = \frac{1}{\sqrt{2}}(1+x)$$



$$f(A) = \varphi(A) = \frac{1}{\sqrt{2}} (I+A) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \quad \text{Principal square root of } A$$

Remark: with non-conjugated choices for  $\tilde{f}(i)$ ,  $\tilde{f}(-i)$

$$\tilde{f}(i) = \frac{1}{\sqrt{2}} (1+i)$$

Then  $f(A)$  is not real

$$\tilde{f}(-i) = -\frac{1}{\sqrt{2}} (1-i)$$

$$\varphi(x) = \frac{1}{\sqrt{2}} (i-ix)$$

$$\tilde{\varphi}(A) = \frac{1}{\sqrt{2}} i (I-A) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$\left[ \tilde{\varphi}(A) \right]^2 = A$$

$$\left[ \varphi(A) \right]^2 = A$$


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$$A = S \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} S^{-1} \quad f(x) = \sqrt{x}$$

Can I choose branches to obtain

NOT A MATRIX FUNCTION  
(with our definition)

$$f(A) = S \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} S^{-1}$$

$$[f(A)] = S \begin{bmatrix} 1 & \\ & 2 \end{bmatrix} S^{-1} = A$$

No! With our definition,  $f(A_i)$  has to be defined uniquely on all distinct  $\lambda_i$ 's "  $f(\lambda_i) = f(\lambda_i)$ " (In interp. poly nomials, I have to choose  $f(\lambda_i)$  uniquely)

These are sometimes called non-primary matrix functions

Given a multi-valued function  $f(x)$  (something with branches:  $\sqrt{x}$ ,  $\log(x)$ , ...)

a nonprimary function of  $A = SJS^{-1}$  is obtained by taking

$$f(A) = S \left[ \begin{array}{c} f(J_1) \\ f(J_2) \\ \vdots \\ f(J_s) \end{array} \right] S^{-1}, \text{ where each } f(J_i) \text{ is constructed taking possibly a different branch of } f.$$

This does depend on the choice of  $S$ .

Example:  $A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$  Jordan form:  $A = S \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \cdot S^{-1}$  with any invertible  $S$ . All matrices of the form

$B = S \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} S^{-1}$ , for all  $S$ , are nontrivial square roots

of  $A$ , They all satisfy  $B^2 = I$

They are not, in general, polynomials in  $A$  (because  $p(A)$  is a scalar multiple of  $I$  for each  $p$ )