

# TOWARDS A COMPUTATIONAL EFFICIENT, IMPLICITLY RESTARTED RATIONAL KRYLOV METHOD

Daan Camps, Karl Meerbergen, Raf Vandebril

**KU LEUVEN**

*ILAS Conference, Leuven - July 12, 2016*





# INTRODUCTION

# OVERVIEW

1. Krylov methods: Arnoldi & RKS
2. Implicit restart of Krylov methods
3. Numerical example
4. Conclusion & outlook





# **KRYLOV METHODS: ARNOLDI & RKS**



## Definition Krylov subspace

Given a matrix  $A \in \mathbb{C}^{N \times N}$  and a non-zero vector  $v \in \mathbb{C}^N$ :

$$\mathcal{K}_m(A, v) = \text{span}\{v, Av, \dots, A^{m-1}v\}$$



# ARNOLDI'S METHOD

[ARNOLDI, 1951]



## Arnoldi's method

```
function [V,H] = Arnoldi(A,v,m)
    v = v/norm(v,2); V(:,1) = v;
    for i = 1:m
        V(:,i+1) = A*V(:,i);
        for j = 1:i
            H(j,i) = V(:,j)'*V(:,i+1);
            V(:,i+1) = V(:,i+1) - H(j,i)*V(:,j);
        end
        H(i+1,i) = norm(V(:,i+1),2);
        V(:,i+1) = V(:,i+1)/norm(V(:,i+1),2);
    end
end
```



## Arnoldi's method

- Orthonormal basis  $V_i$  of  $\mathcal{K}_i$
- Partial reduction to upper Hessenberg form
- Ritz values:  $H_i y_j = \theta_j y_j$

$$A V_i = V_i H_i + h_{i+1,i} v_{i+1} e_i^T$$

or

$$A V_i = V_{i+1} \underline{H}_{i+1,i}$$

$$\Rightarrow V_i^* A V_i = H_i$$



# Arnoldi Decomposition

 $A$  $V_i$  $=$  $V_{i+1}$  $H_i$



# Rotational Arnoldi Decomposition

 $A$  $V_i$  $=$  $V_{i+1}$ 



# RATIONAL KRYLOV SEQUENCES

[RUHE, 1984], [RUHE, 1994], [RUHE, 1998]

## Definition RKS

Given a matrix pencil  $(A, B) \in \mathbb{C}^{N \times N}$  and a non-zero vector  $v \in \mathbb{C}^N$ :

$$\text{span}\{v, S_1 v, S_1 S_2 v, \dots\} \text{ with}$$
$$S_i = (\alpha_i A + \beta_i B)^{-1} (\gamma_i A + \delta_i B)$$



## RKS method

```
function [V,K,L] = RKS(A,B,v,m)
    v = v/norm(v,2); V(:,1) = v;
    for i = 1:m
        [alpha,beta,gamma,delta] = choose_parameters();
        t = determine_cont_vec();
        w = (alpha*A + beta*B) \ (gamma*A + delta*B) * V(:,1:i-1) * t;
        [w, h] = orthogonalise(w,V(1:i-1));
        V(:,i+1) = V(:,i+1)/norm(V(:,i+1),2)
        K(1:i+1,i) = alpha * h - gamma * t;
        L(1:i+1,i) = -beta * h + delta * t;
    end
end
```

## RKS method

- Partial reduction to upper Hessenberg pencil  $(L, K)$
- Poles:  $-\beta_i / \alpha_i$

$$A V_{i+1} \underline{K}_i = B V_{i+1} \underline{L}_i$$

with

$$\underline{K}_i = \underline{H}_i D_{\alpha,i} - \underline{T}_i D_{\gamma,i}$$

$$\underline{L}_i = -\underline{H}_i D_{\beta,i} + \underline{T}_i D_{\delta,i}$$



## Special cases

### Arnoldi:

- $(\alpha, \beta, \gamma, \delta) = (0, 1, 1, 0)$
- $S_i = (0A + 1I)^{-1} (1A + 0I)$

## Special cases

### Shift-and-invert Arnoldi:

- $(\alpha, \beta, \gamma, \delta) = (1, \beta, 0, 1)$
- $S_i = (1A + \beta I)^{-1} (0A + 1I)$



## Special cases

### Extended Krylov:

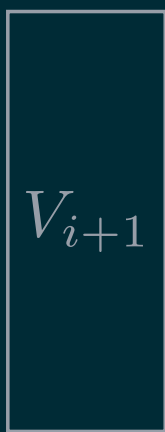
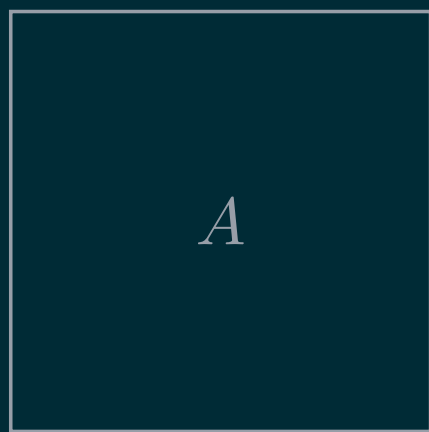
- $(\alpha, \beta, \gamma, \delta) = (0, 1, 1, 0)$  for  $A$
- $(\alpha, \beta, \gamma, \delta) = (1, 0, 0, 1)$  for  $A^{-1}$
- $S_i^+ = (0A + 1I)^{-1} (1A + 0I)$
- $S_i^- = (1A + 0I)^{-1} (0A + 1I)$

## RKS Decomposition

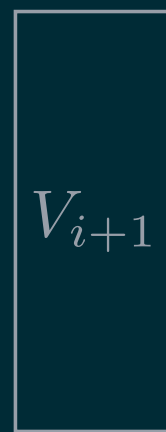
$$\begin{array}{|c|} \hline A \\ \hline \end{array} \begin{array}{|c|} \hline V_{i+1} \\ \hline \end{array} \begin{array}{|c|} \hline K_i \\ \hline \end{array} = \begin{array}{|c|} \hline B \\ \hline \end{array} \begin{array}{|c|} \hline V_{i+1} \\ \hline \end{array} \begin{array}{|c|} \hline L_i \\ \hline \end{array}$$



## Rotational RKS Decomposition



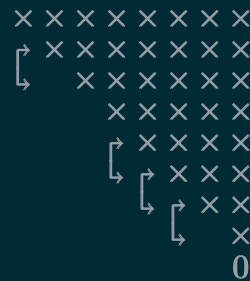
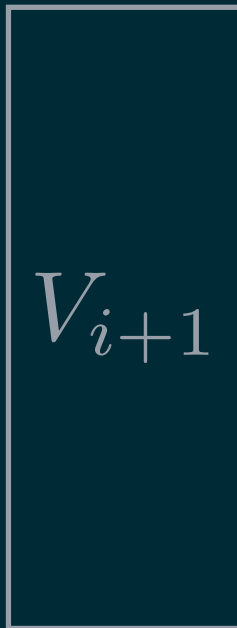
=



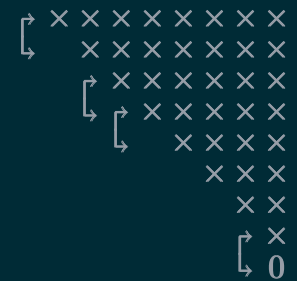
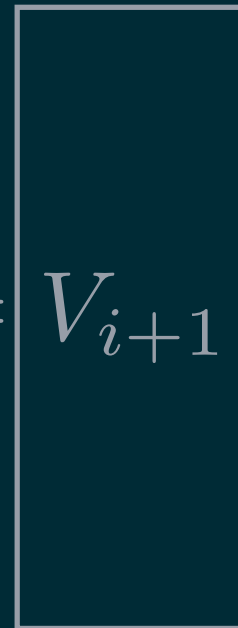
## Special case: Extended Krylov Decomposition

$$\boxed{A} \quad \boxed{V_{i+1}} \quad \boxed{\begin{array}{c} \underline{K_i} \end{array}} = \boxed{V_{i+1}} \quad \boxed{\begin{array}{c} \underline{L_i} \end{array}}$$

# Rotational Extended Krylov Decomposition

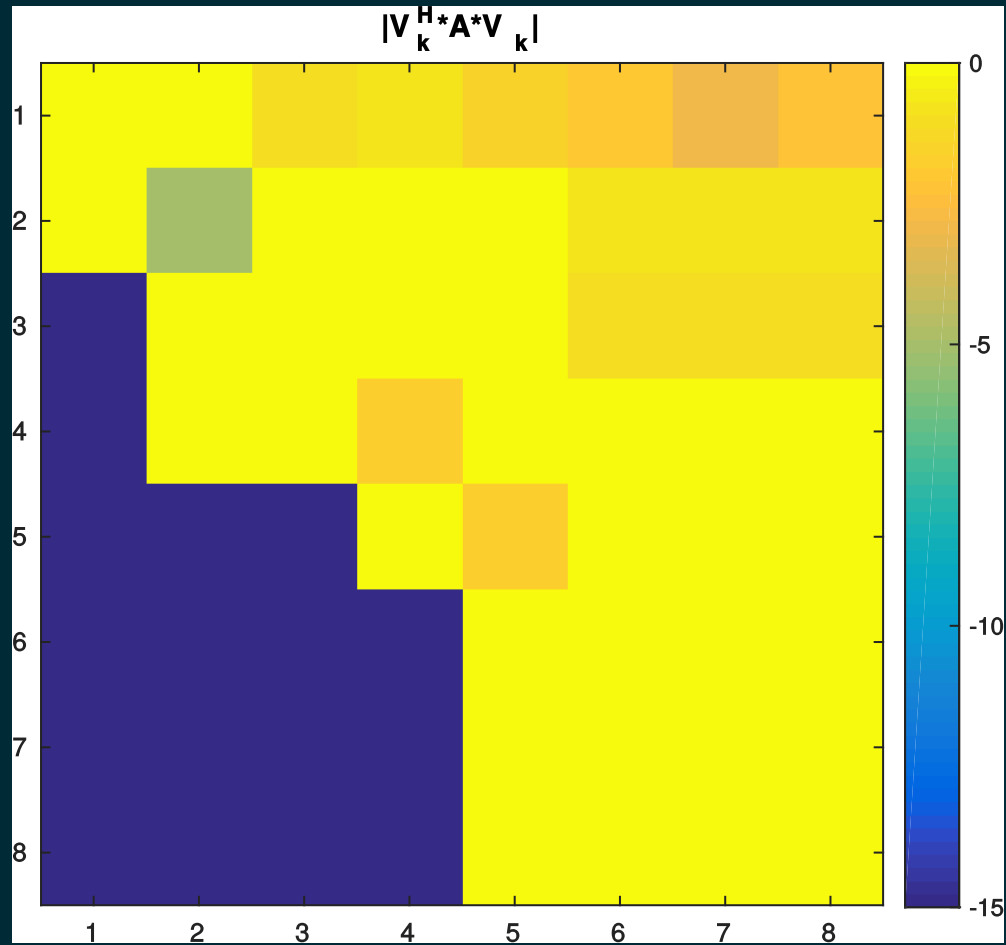


=





# Structure in projected counterpart







# IMPLICIT RESTART OF KRYLOV ITERATIONS

A long-exposure photograph of a starry night sky, showing a dense field of stars and their trails. The stars are concentrated in a central region, creating a circular pattern of light trails. In the foreground, the dark silhouette of a person is visible, looking up at the sky. The overall scene is dark, with the bright light of the stars providing the primary illumination.



# SORENSEN'S IMPLICITLY RESTARTED ARNOLDI METHOD (IRA)

[SORENSEN, 1992]

## Problem

As Arnoldi's method proceeds:

- cost of orthogonalisation increases
- new basis vector needs to be stored
- cost of computing Ritz values increases

## Solution

Implicit restart of the iteration:

$$\underline{H} - \mu I = [Q \quad q] \begin{bmatrix} R \\ 0 \end{bmatrix}$$

$$\underline{H} \leftarrow Q^* \underline{H} Q_{i,i-1}$$

$$V \leftarrow V Q$$

## Improved solution

Implicit QR step on the factorised Hessenberg matrix by chasing the rotations [VANDEBRIL, 2011]

## Advantages

- Optimal computational complexity
- Multiple shifts at once or tightly packed shifts
- ...



## Ingredients

- implicit Q-theorem [FRANCIS, 1961]
- elementary operations with Givens rotations

## Bring a (pattern of) rotations through an upper triangular matrix

$$\left[ \begin{array}{cccc} \times & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \\ & & & \times \end{array} \right] = \left[ \begin{array}{cccc} \times & \times & \times & \times \\ & \times & \times & \times \\ & \times & \times & \times \\ & & & \times \end{array} \right] = \left[ \begin{array}{cccc} \times & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \\ & & & \times \end{array} \right]$$

## Fusion of two rotations

$$\left[ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \right] \left[ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \right] = \left[ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \right]$$

## Shift-through of a pattern of 3 rotations

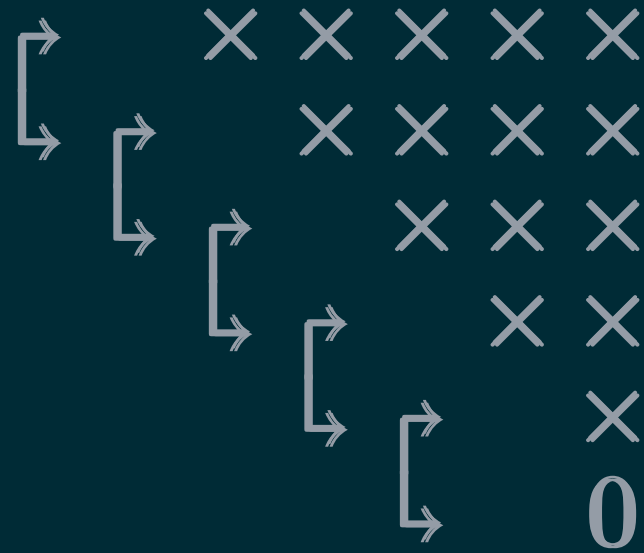
$$\left[ \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \right] \left[ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \right] \left[ \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \right] = \left[ \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \right] \left[ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \right] \left[ \begin{array}{c} \rightarrow \\ \rightarrow \end{array} \right]$$

# ROTATIONALLY IMPLICITLY RESTARTED ARNOLDI METHOD (RIRA)

*An example*



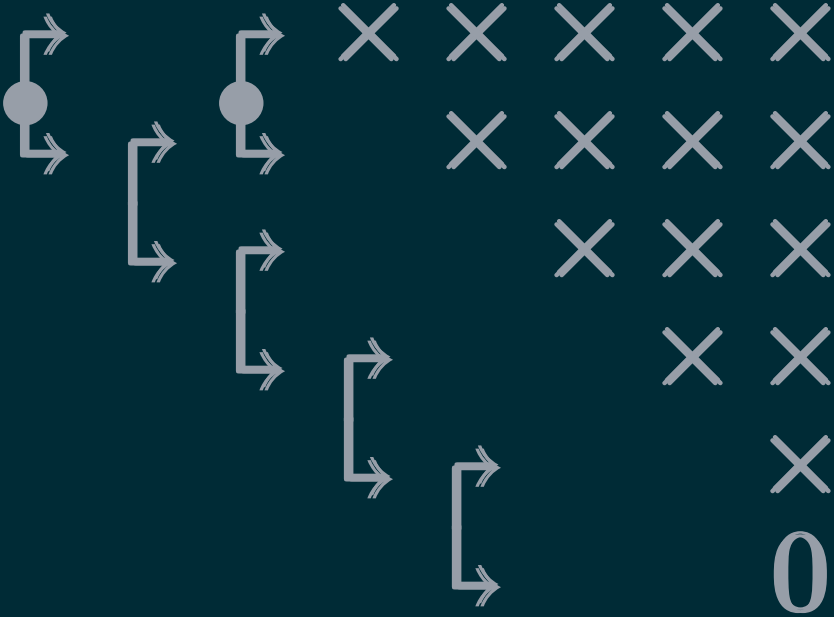
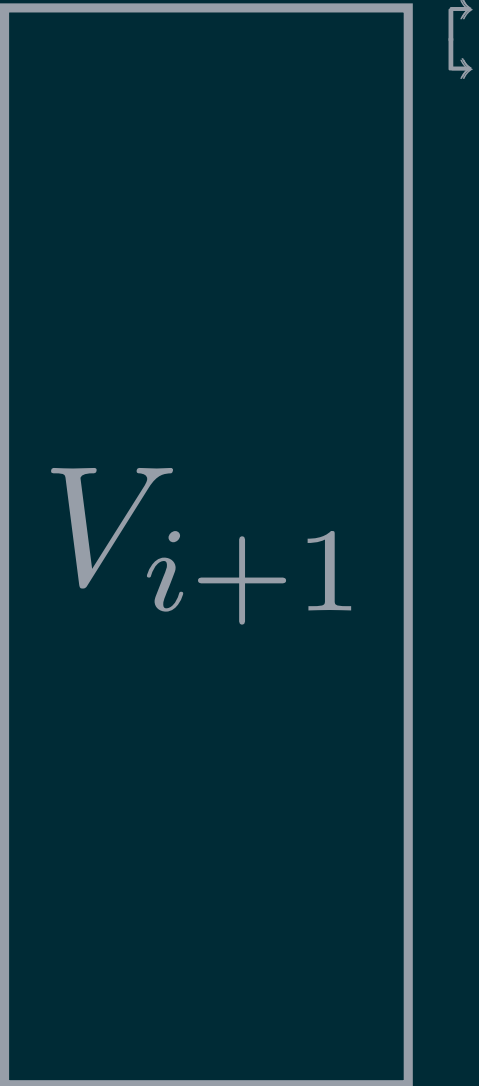
# Initial situation



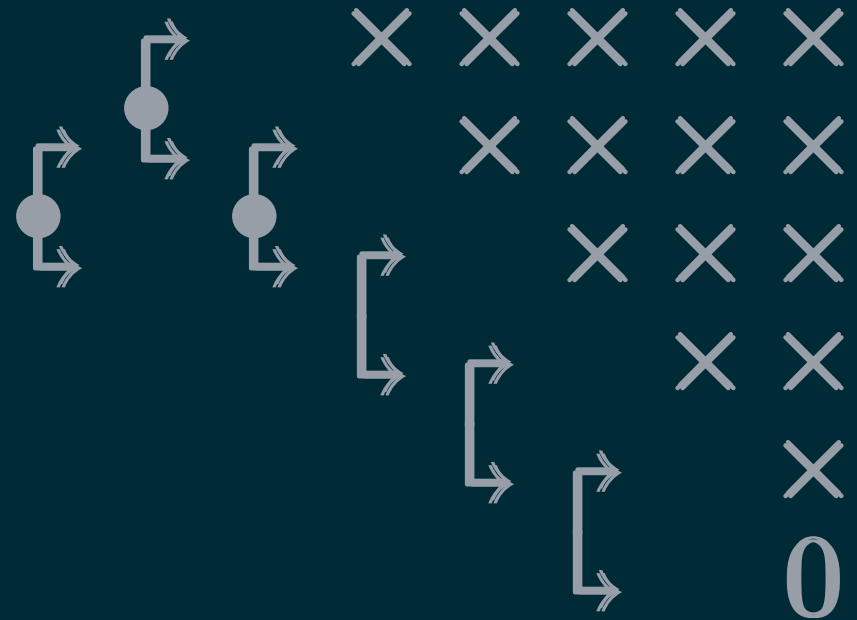
# First similarity transformation



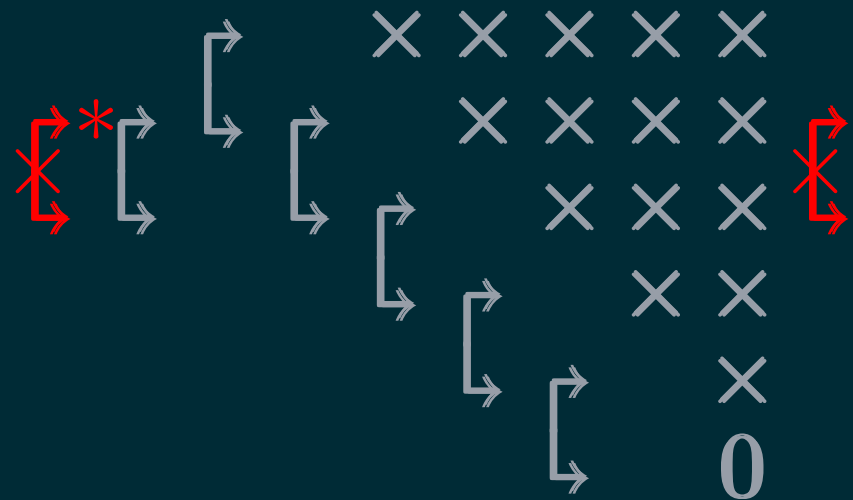
# Fusion & right rotation through upper triangular



# Shift-through

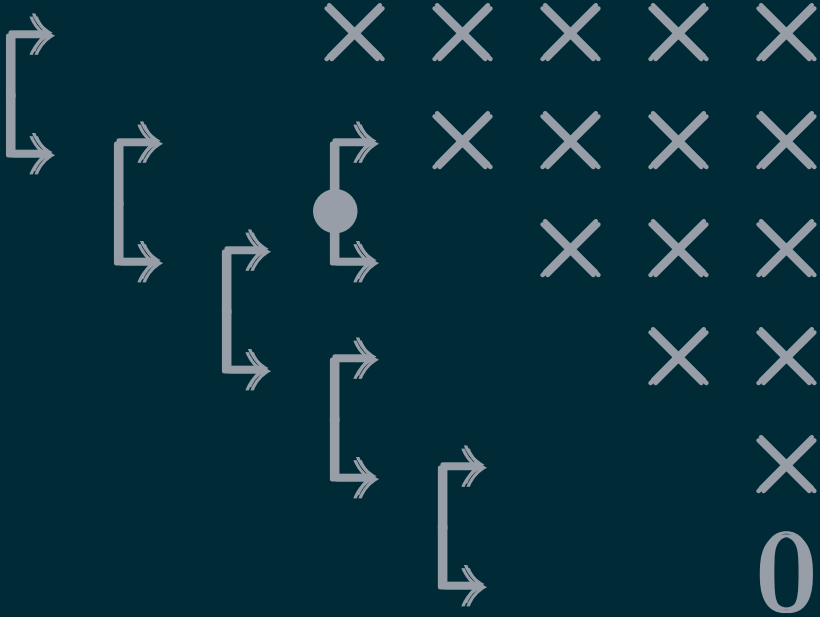


# Second similarity transformation

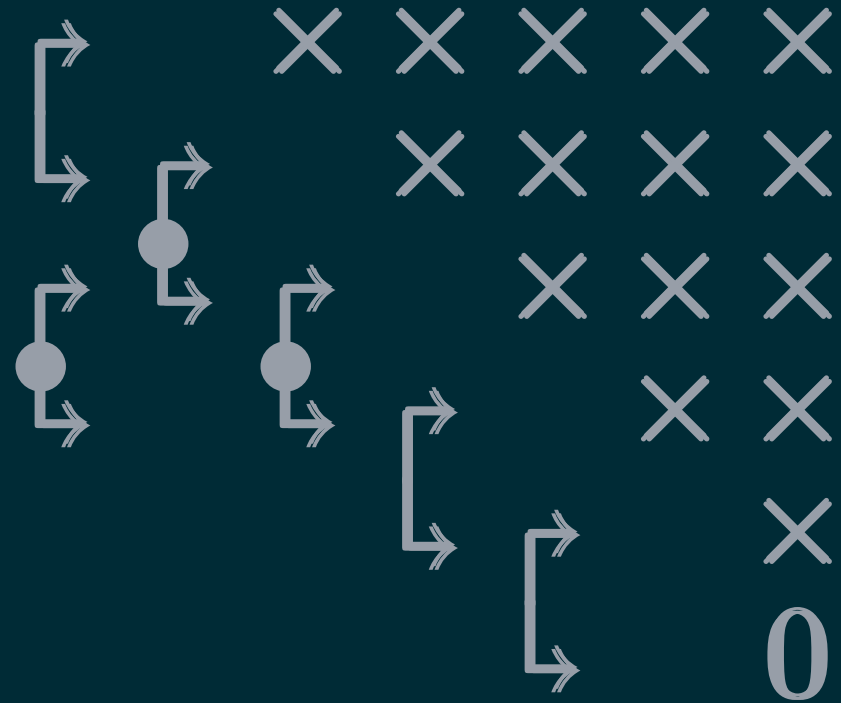




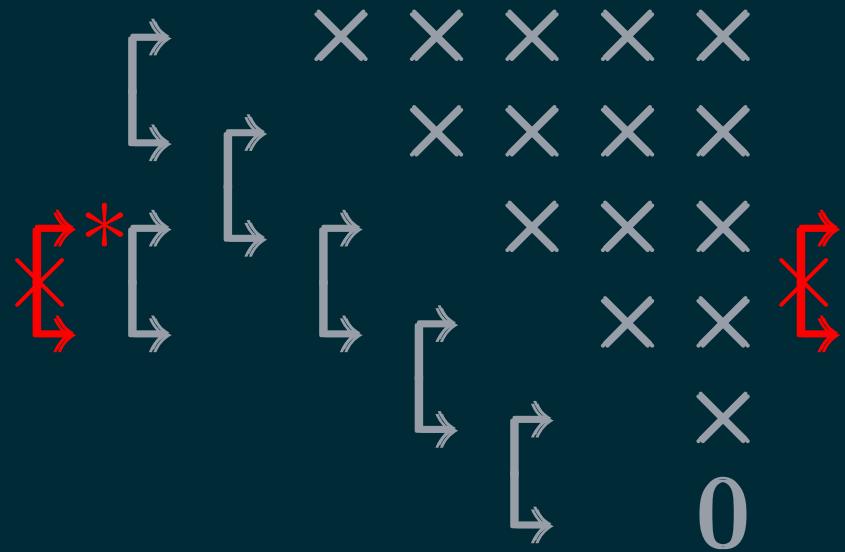
# Fusion & right rotation through upper triangular



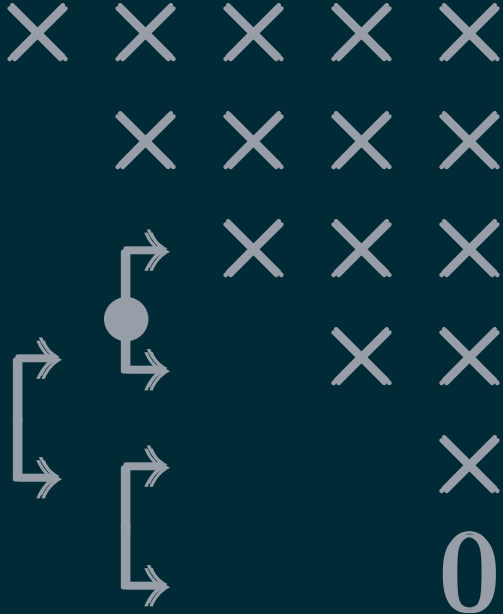
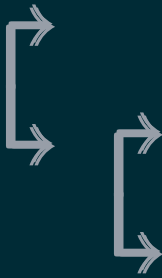
# Shift-through



# Third similarity transformation

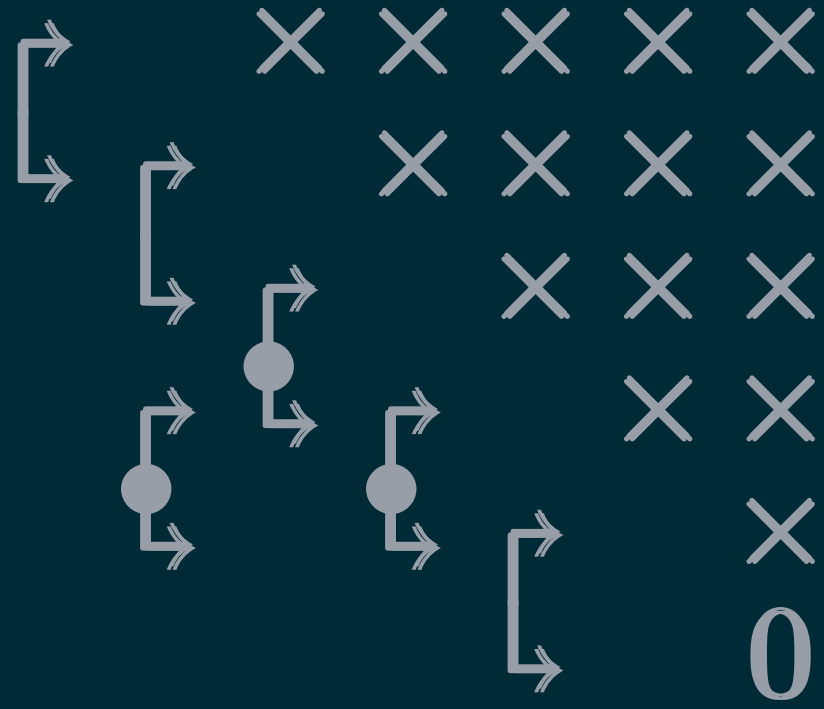


# Fusion & right rotation through upper triangular



0

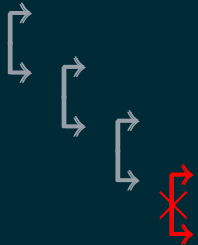
# Shift-through



# Fourth similarity transformation

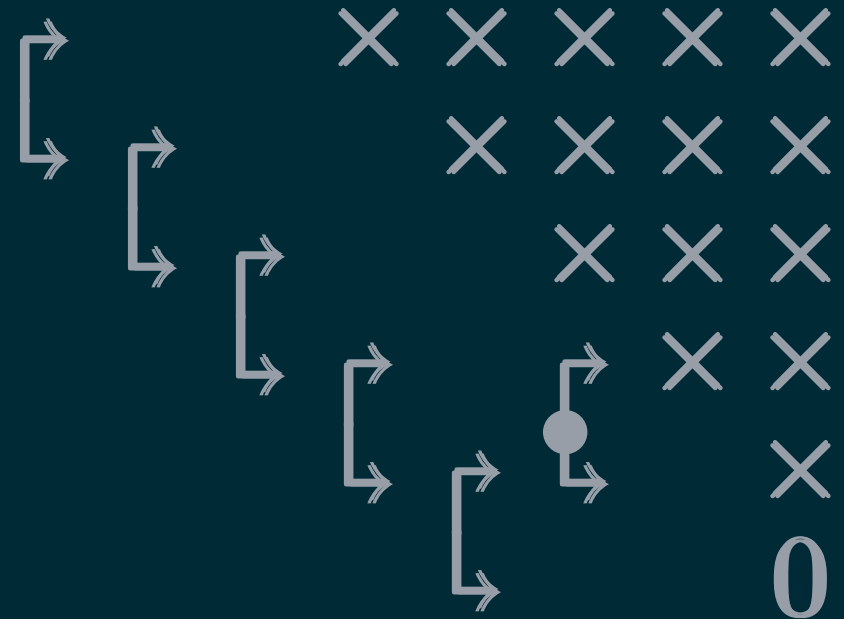
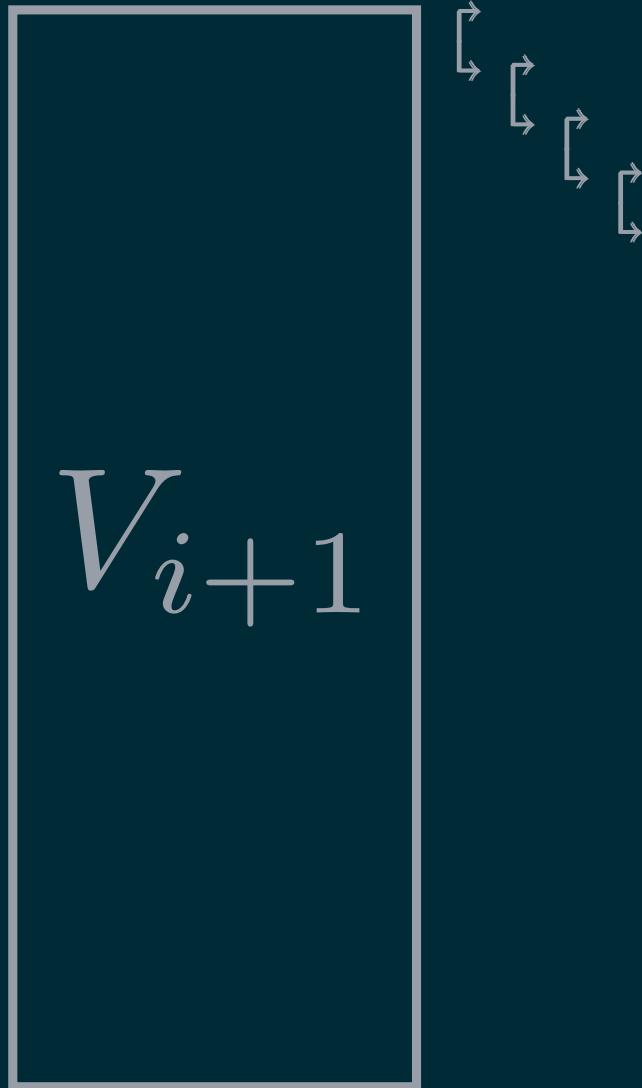


$$V_{i+1}$$

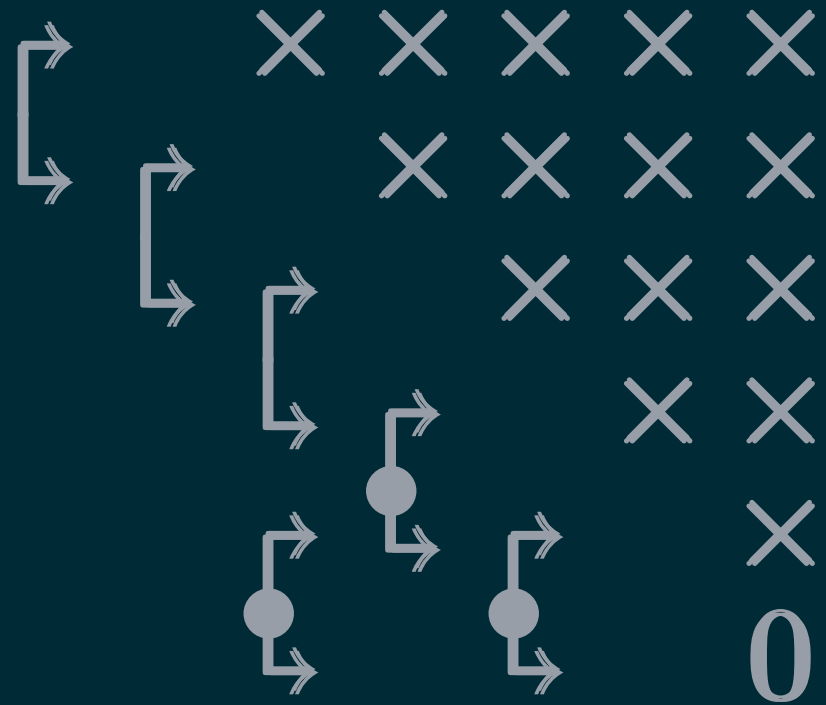
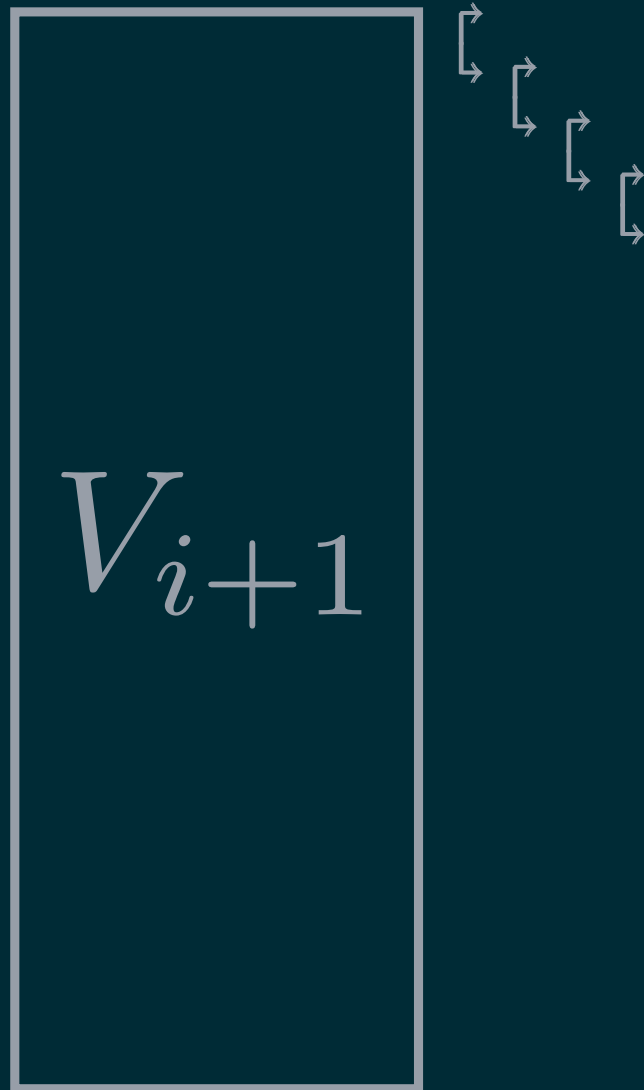




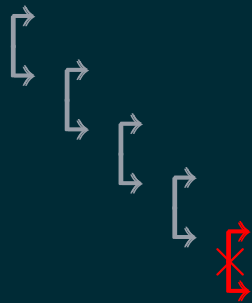
# Fusion & right rotation through upper triangular



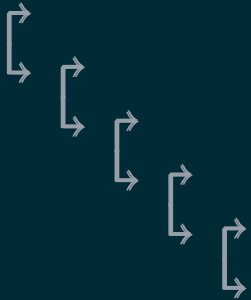
# Shift-through



# Fifth similarity transformation

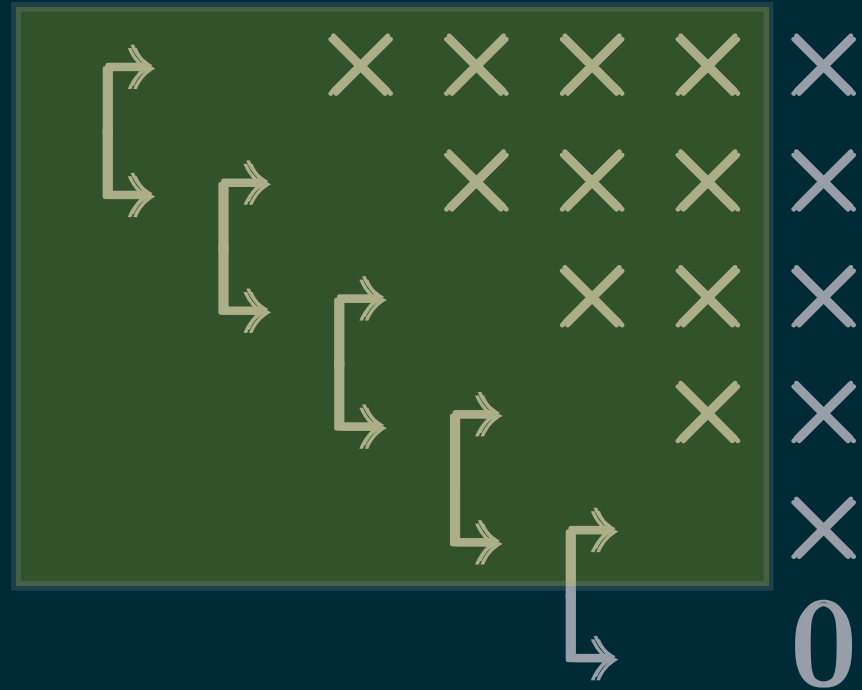


# Final fusion



# Extract reduced Arnoldi decomposition

$$\tilde{V}_{i+1}$$



# ROTATIONALLY IMPLICITLY RESTARTED EXTENDED KRYLOV (RIREK)

*An example for*

$\text{span}(v, A v, A^{-1} v, A^2 v, A^3 v A^{-2} v, A^{-3} v, A^{-4} v, A^4 v)$

## STEP 1: TRANSFORM THE PENCIL TO SUITABLE COMPRESSED FORMAT

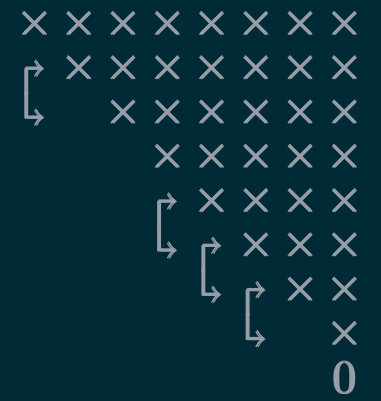
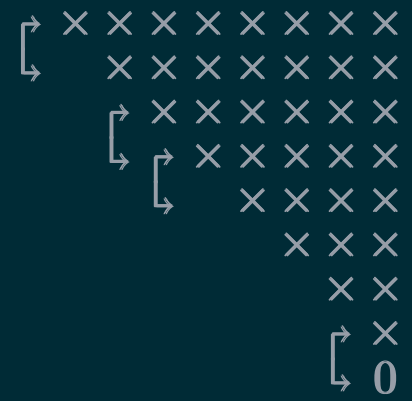
Two options:

- left removal of  $K$  rotations
- right removal of  $K$  rotations

# Option 1: left removal of $K$ rotations



$(\underline{L}, \underline{K})$

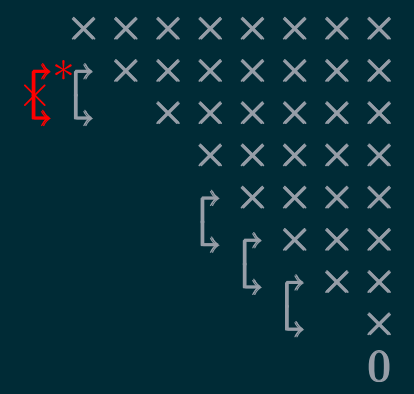
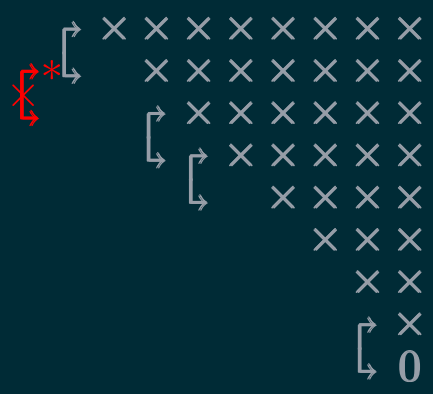




# Option 1: left removal of $K$ rotations



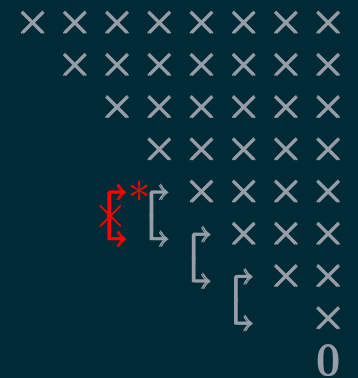
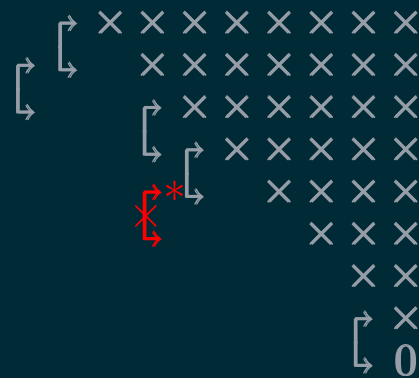
$(\underline{L}, \underline{K})$



# Option 1: left removal of $K$ rotations



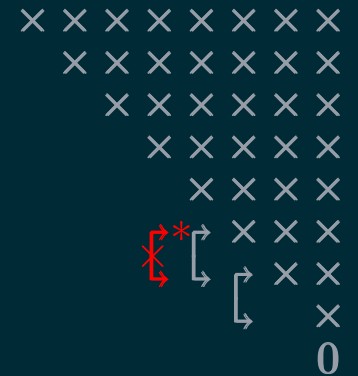
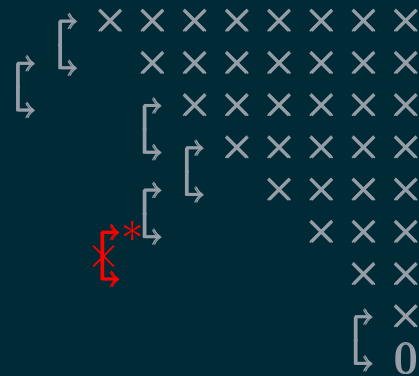
$(\underline{L}, \underline{K})$



# Option 1: left removal of $K$ rotations



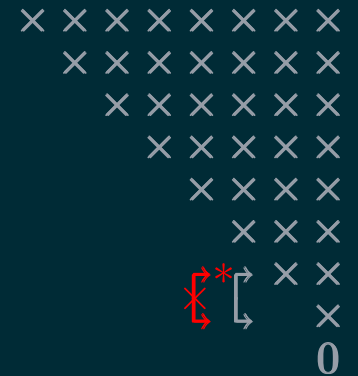
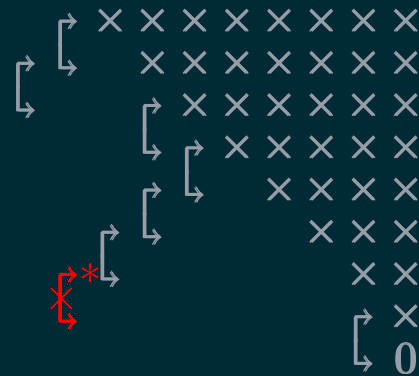
$(\underline{L}, \underline{K})$



# Option 1: left removal of $K$ rotations



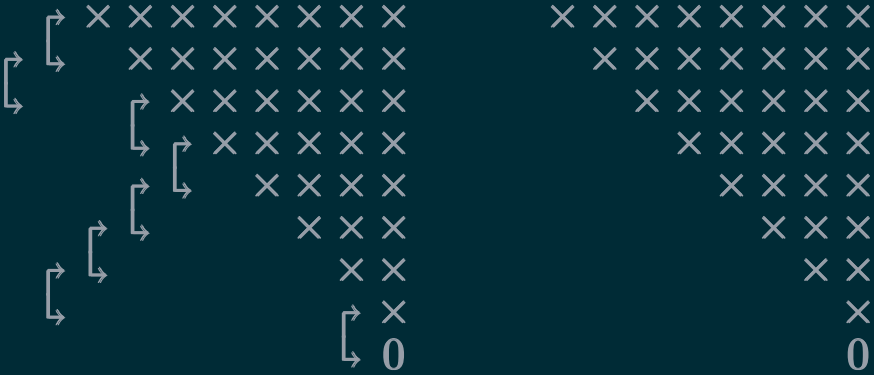
$(\underline{L}, \underline{K})$



# Option 1: left removal of $K$ rotations

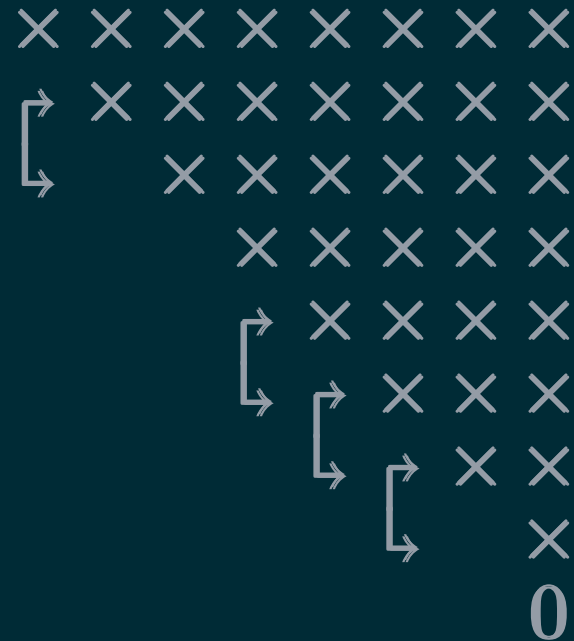
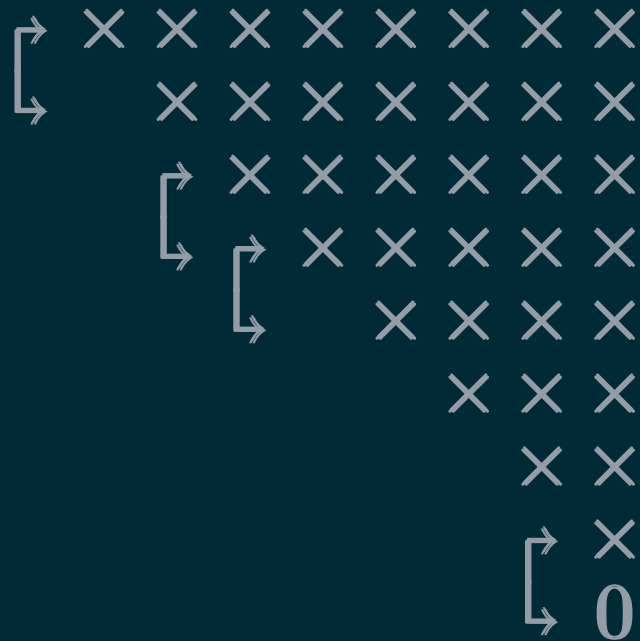


$(\underline{L}, \underline{K})$



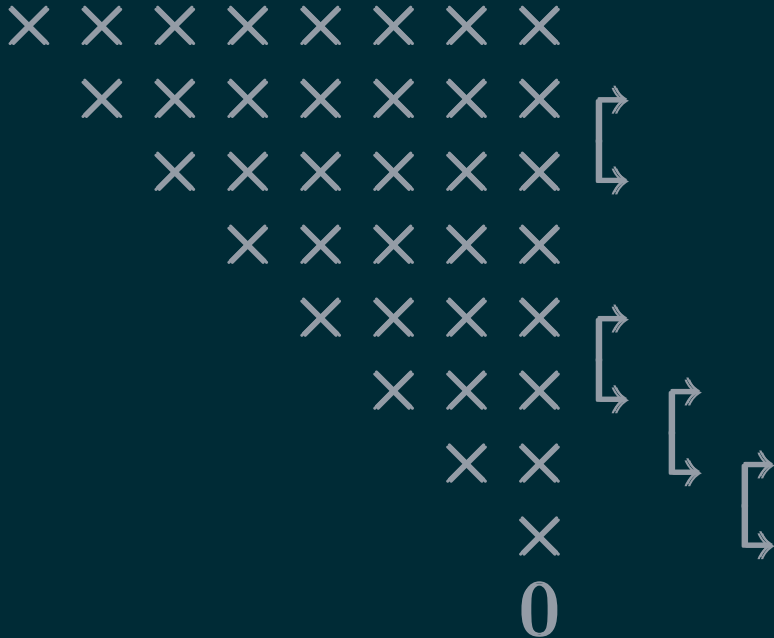
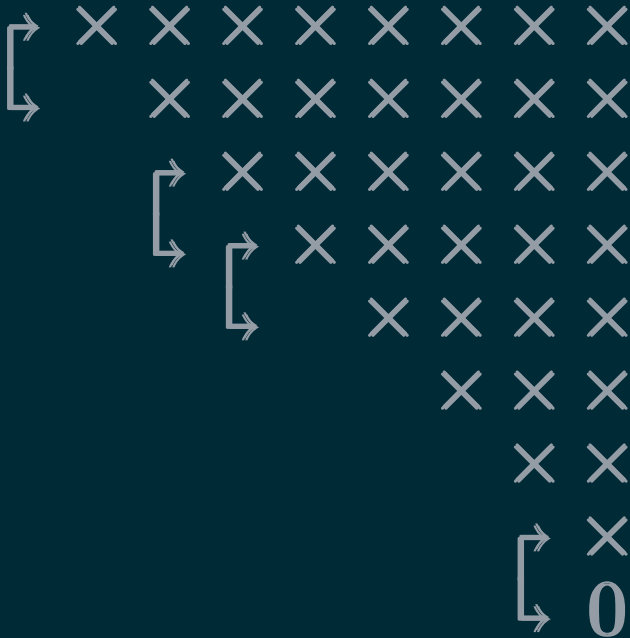
## Option 2: right removal of $K$ rotations

$(\underline{L}, \underline{K})$



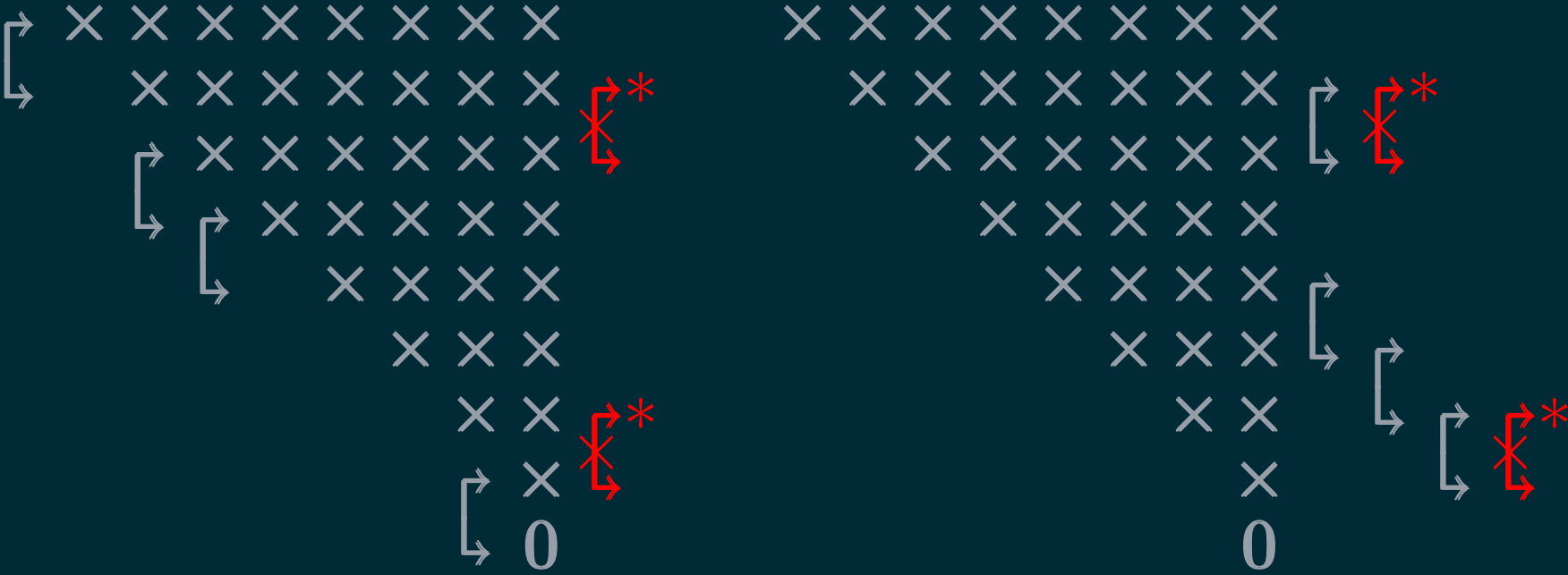
# Option 2: right removal of $K$ rotations

$$(\underline{L}, \underline{K})$$



# Option 2: right removal of $K$ rotations

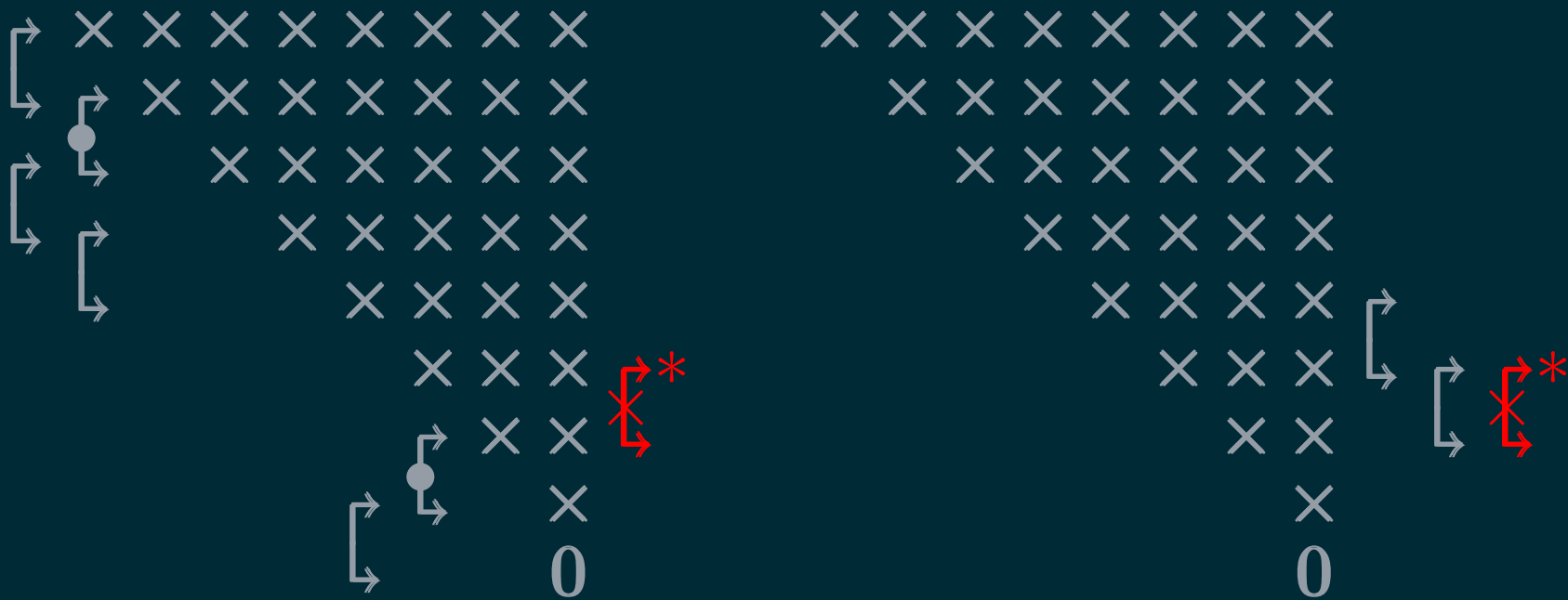
$$(\underline{L}, \underline{K})$$





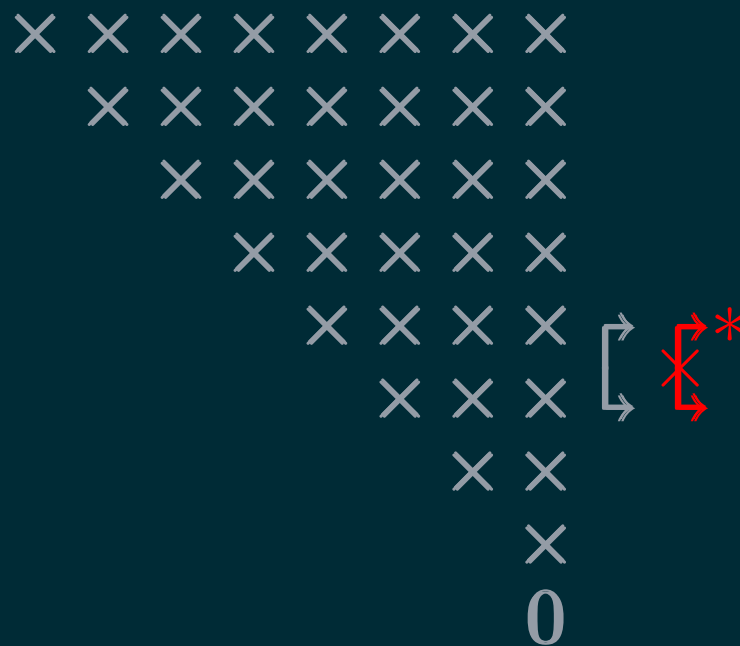
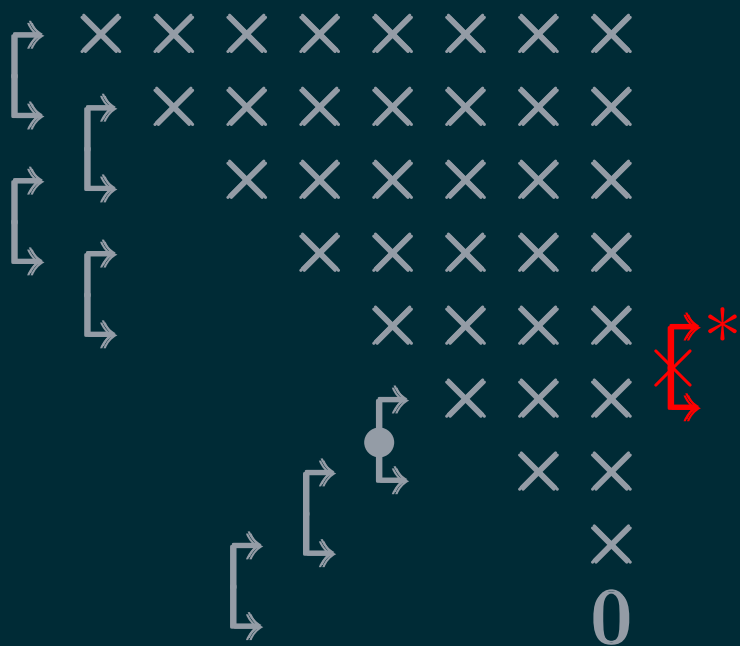
## Option 2: right removal of $K$ rotations

$(\underline{L}, \underline{K})$



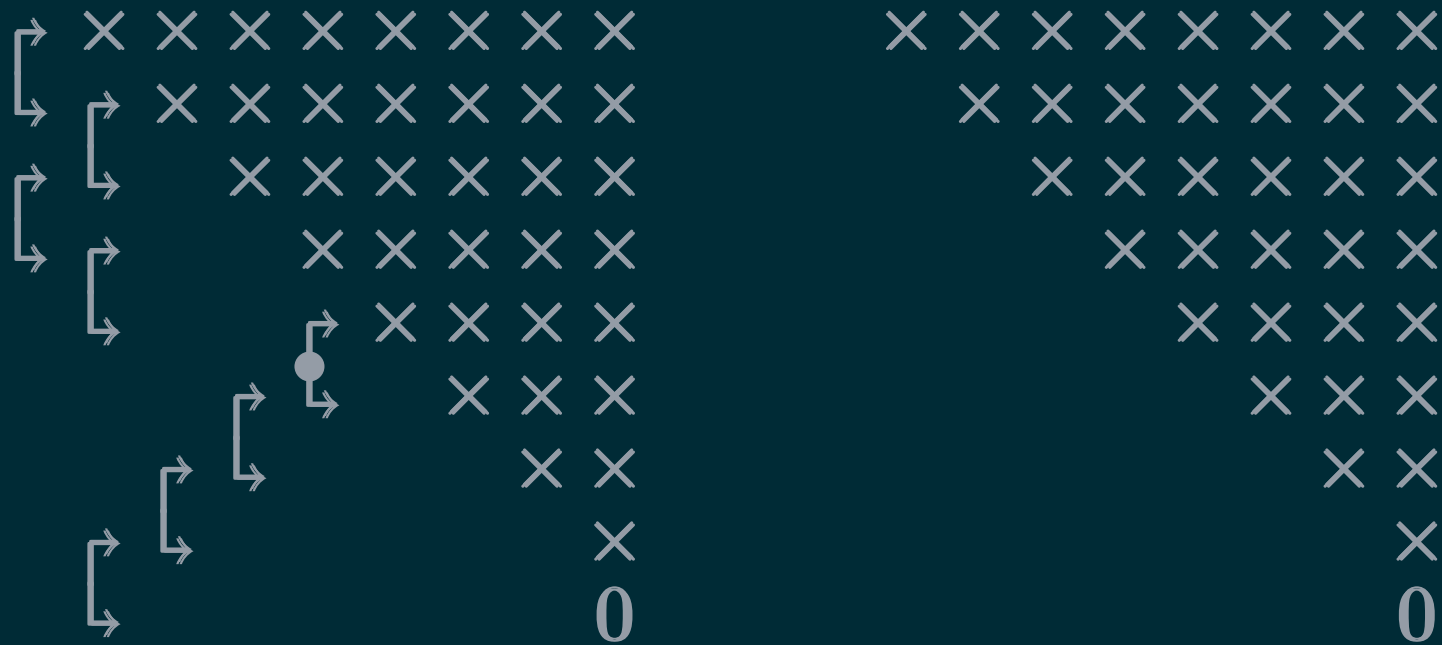
## Option 2: right removal of $K$ rotations

$(\underline{L}, \underline{K})$



## Option 2: right removal of $K$ rotations

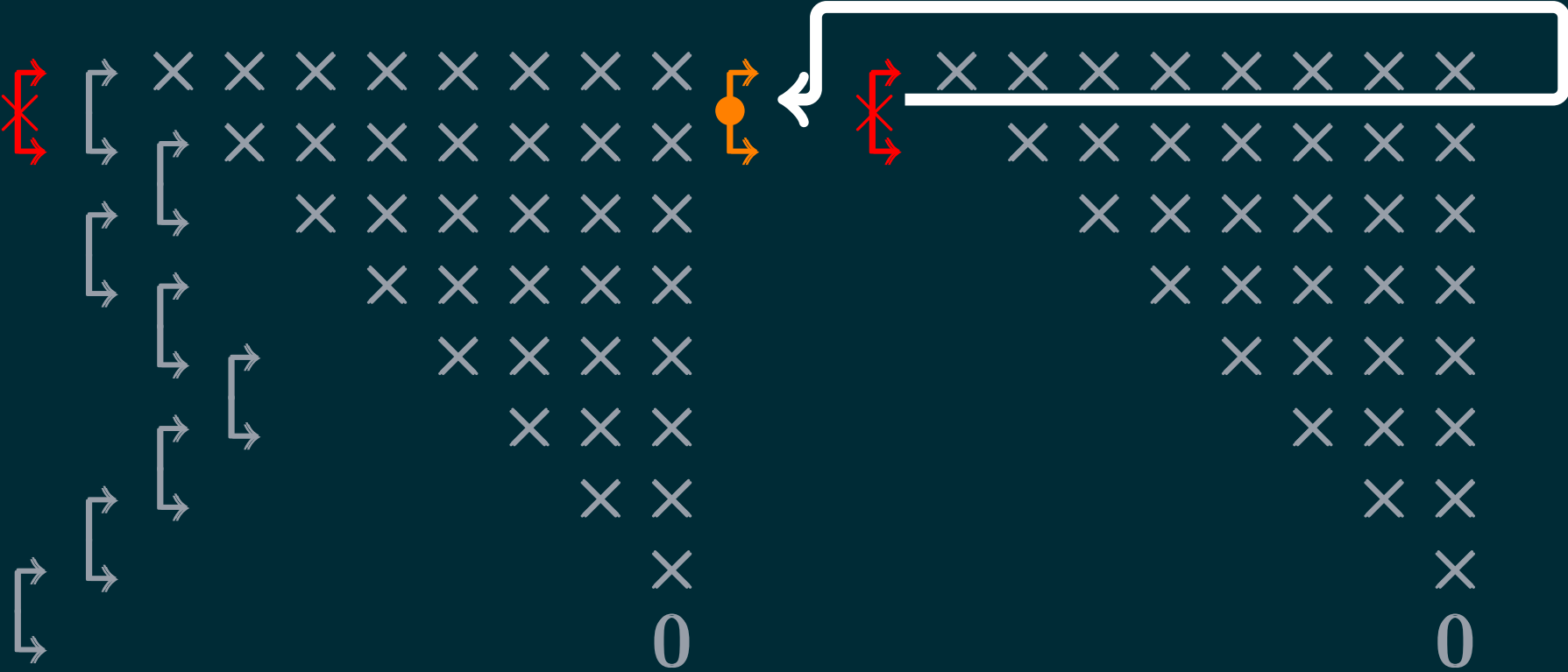
$(\underline{L}, \underline{K})$



**STEP 2: PERTURB THE PENCIL AND CHASE THE PERTURBATION DOWNWARDS**

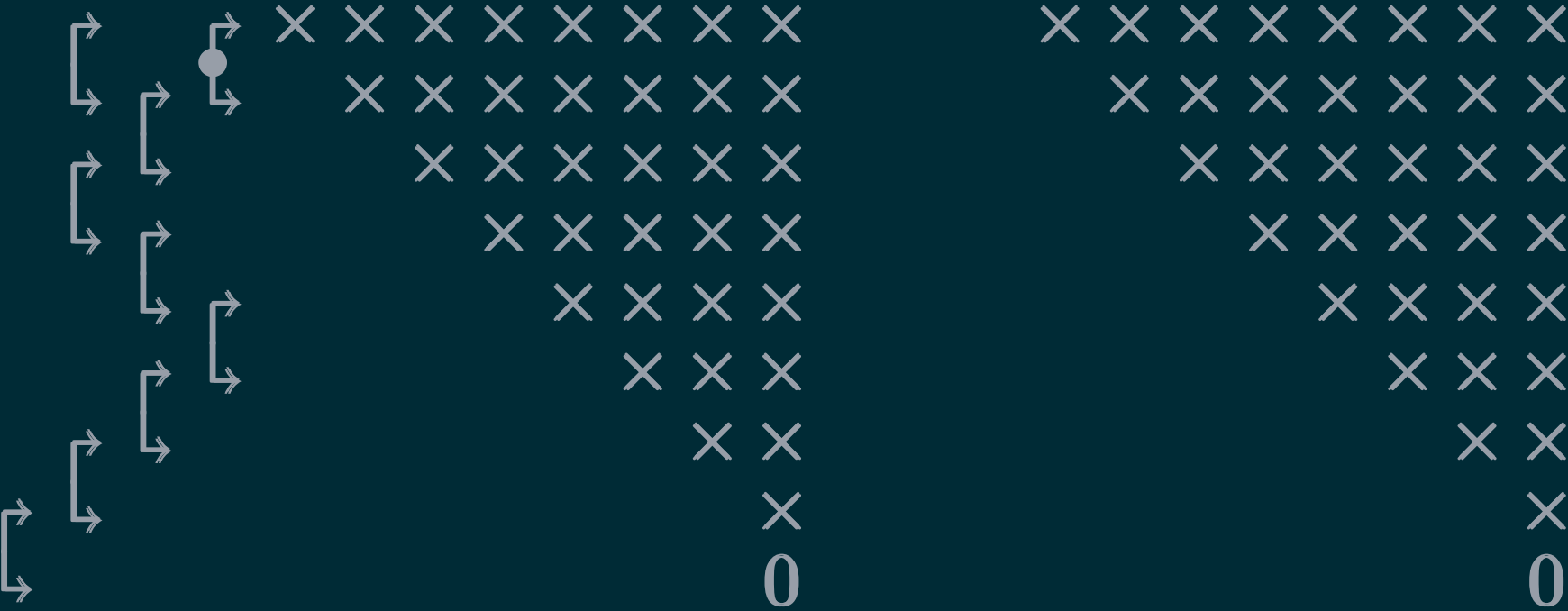
# Chasing procedure

$(\underline{L}, \underline{K})$



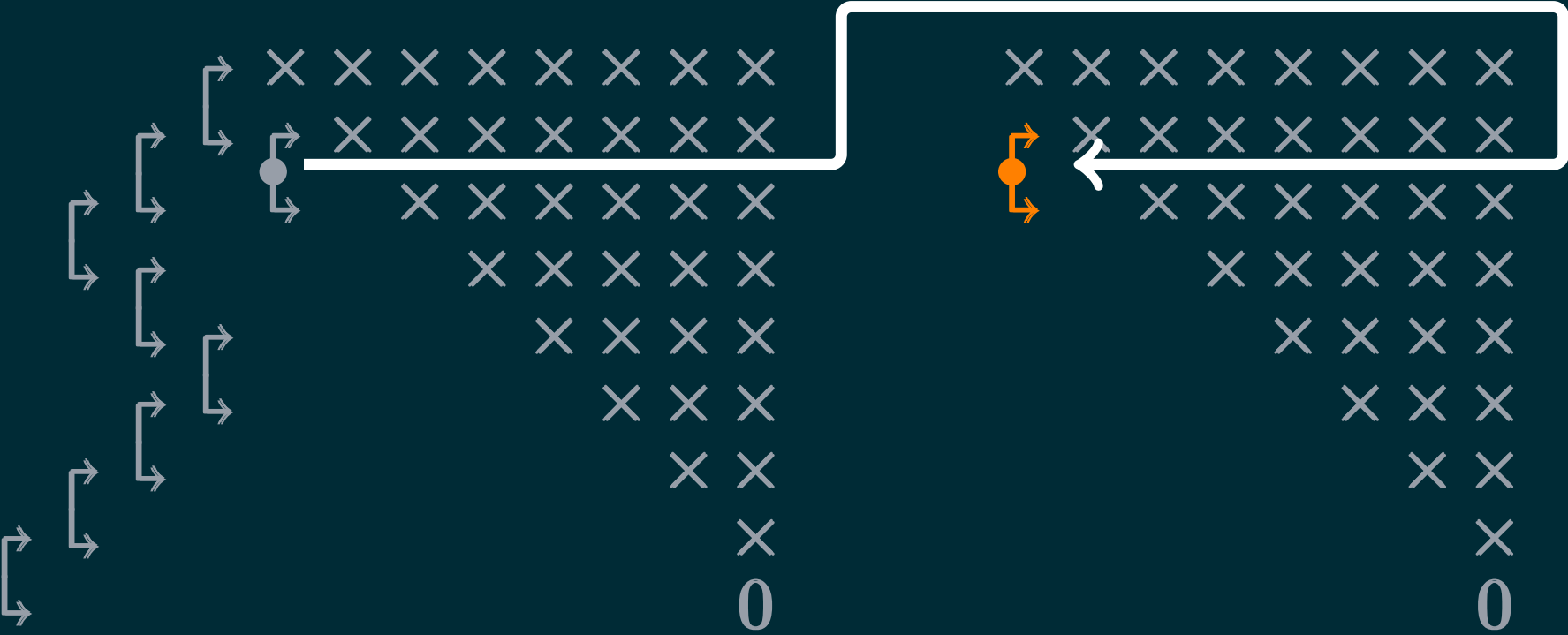
# Chasing procedure

$$(\underline{L}, \underline{K})$$



# Chasing procedure

$$(\underline{L}, \underline{K})$$

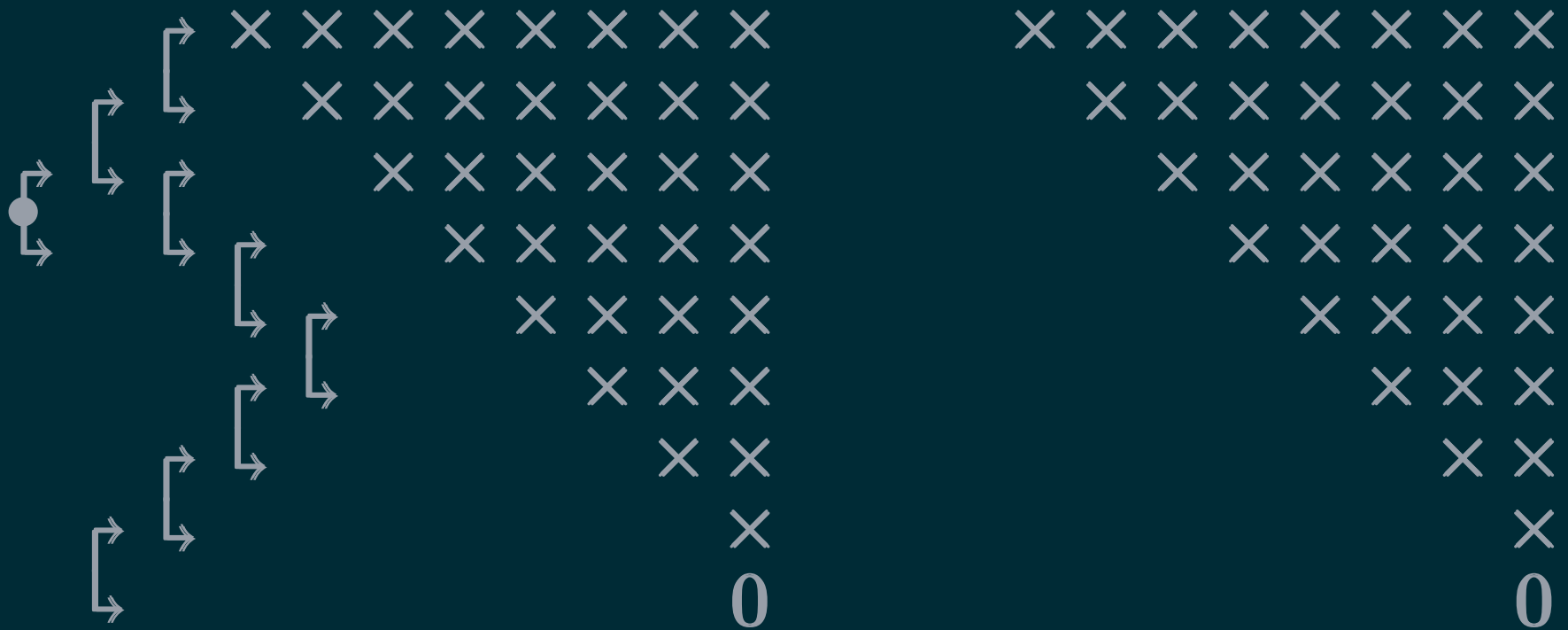






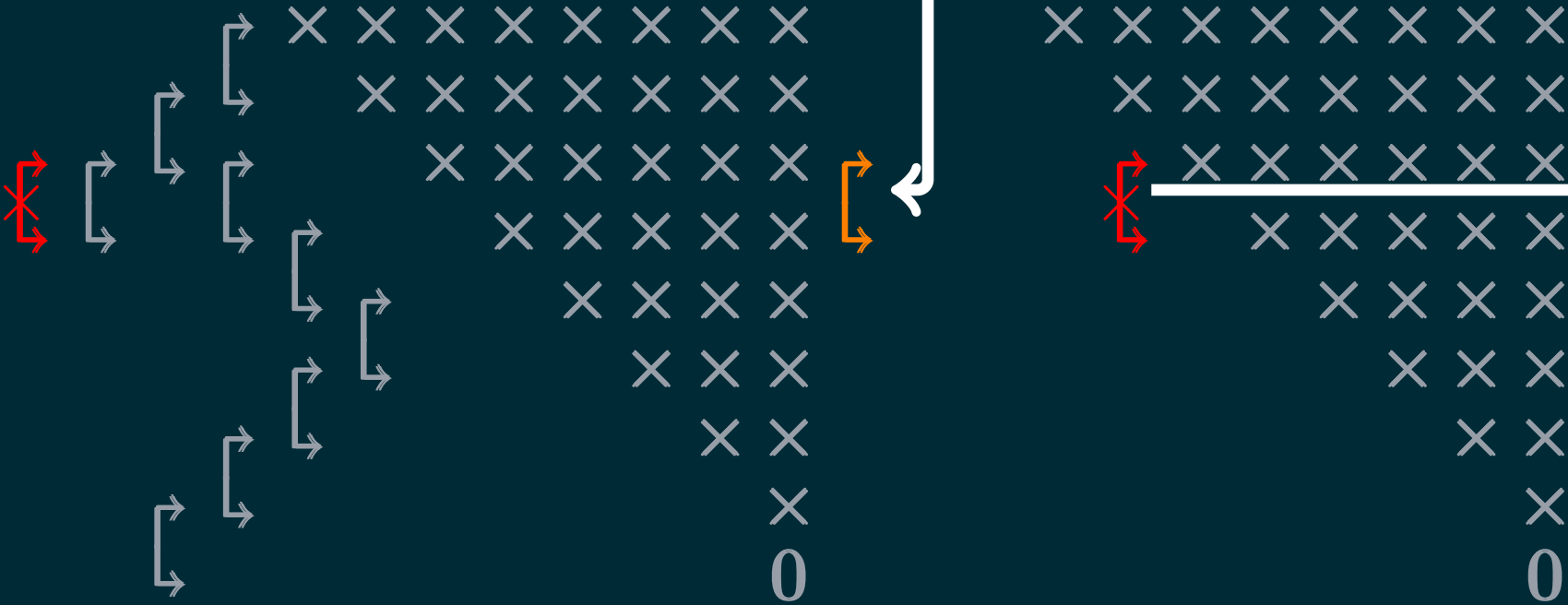
# Chasing procedure

$(\underline{L}, \underline{K})$



# Chasing procedure

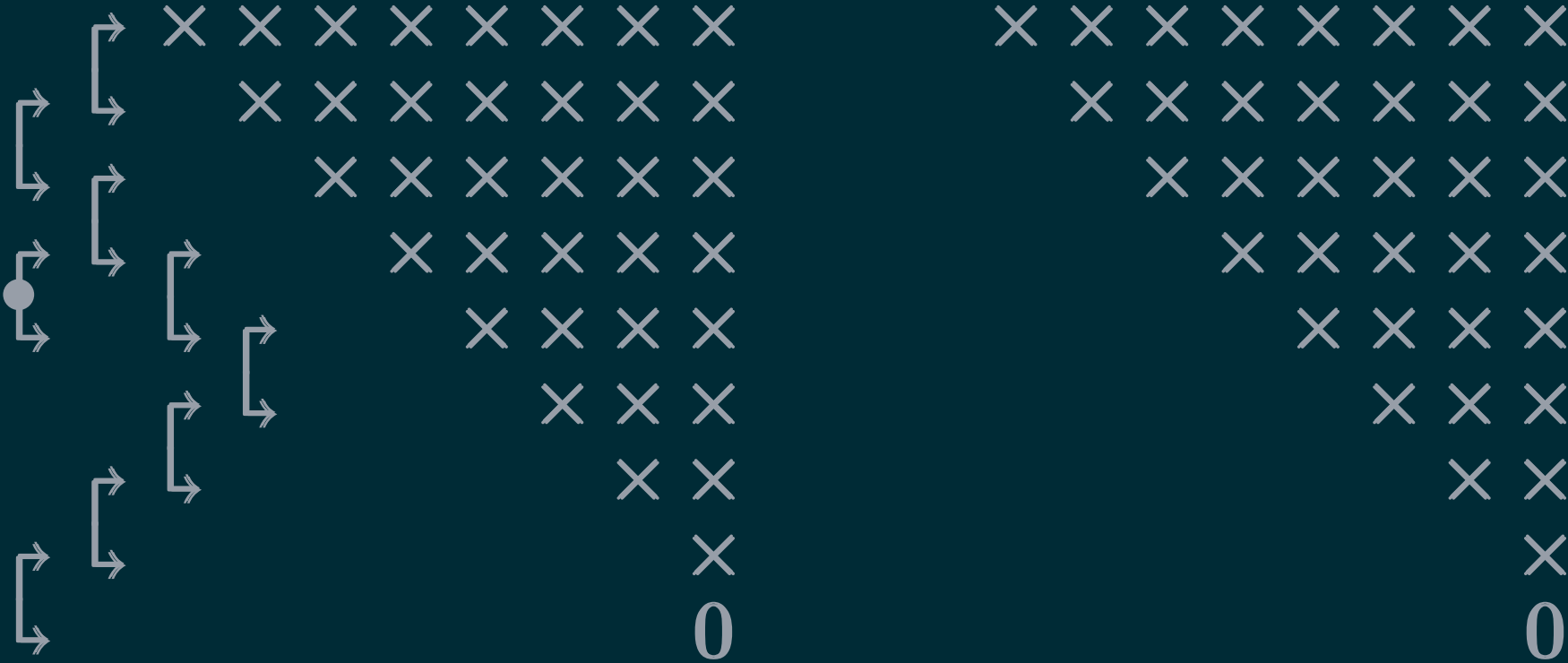
$(\underline{L}, \underline{K})$





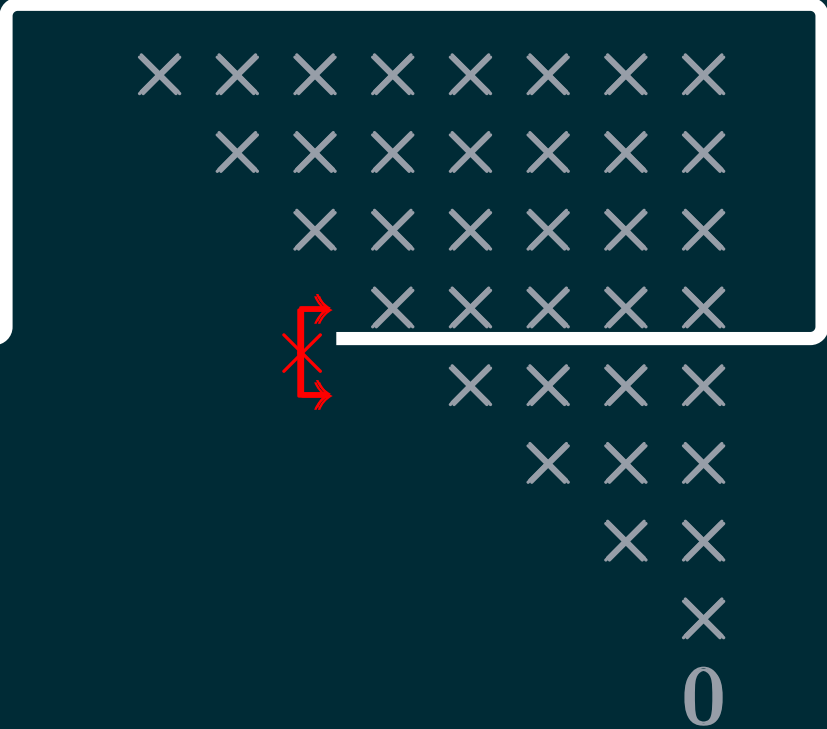
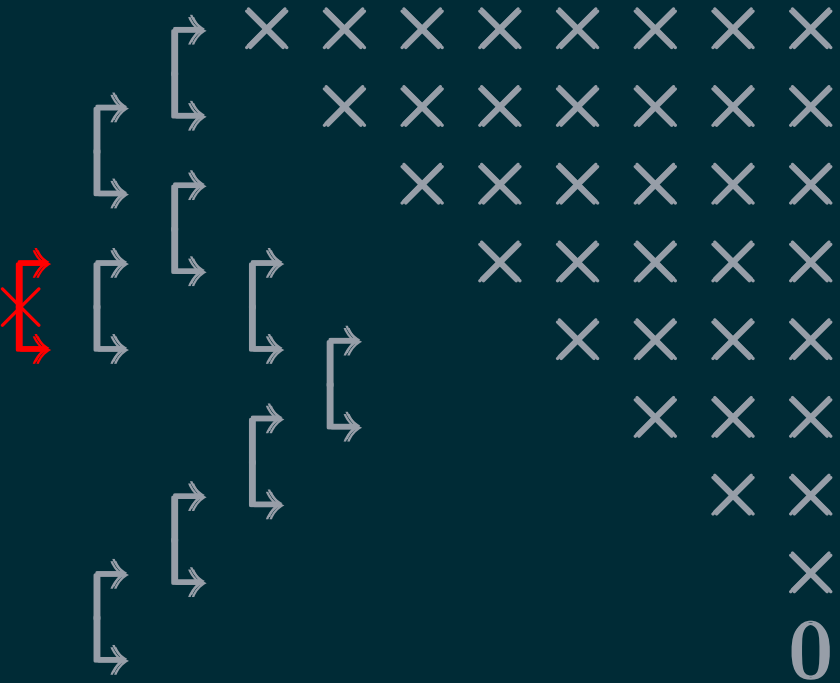
# Chasing procedure

$$(\underline{L}, \underline{K})$$



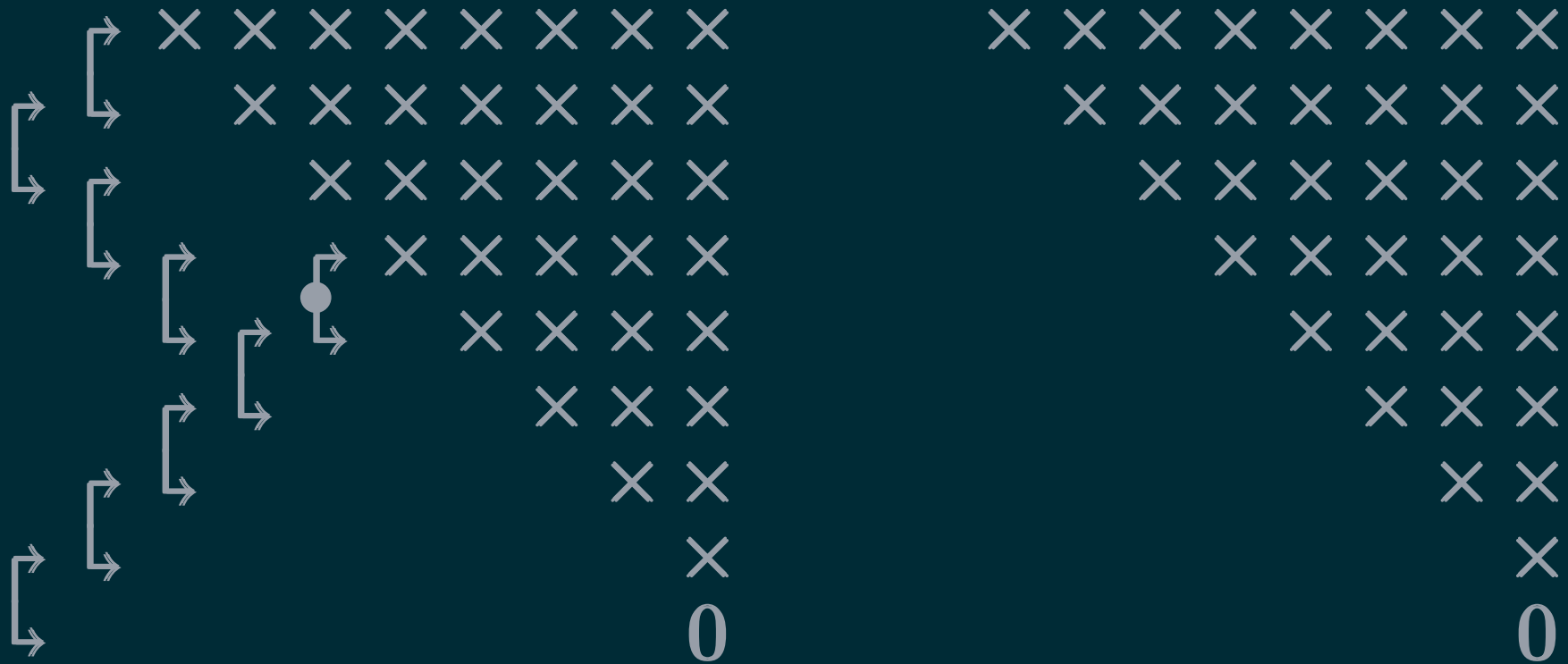
# Chasing procedure

$$(\underline{L}, \underline{K})$$



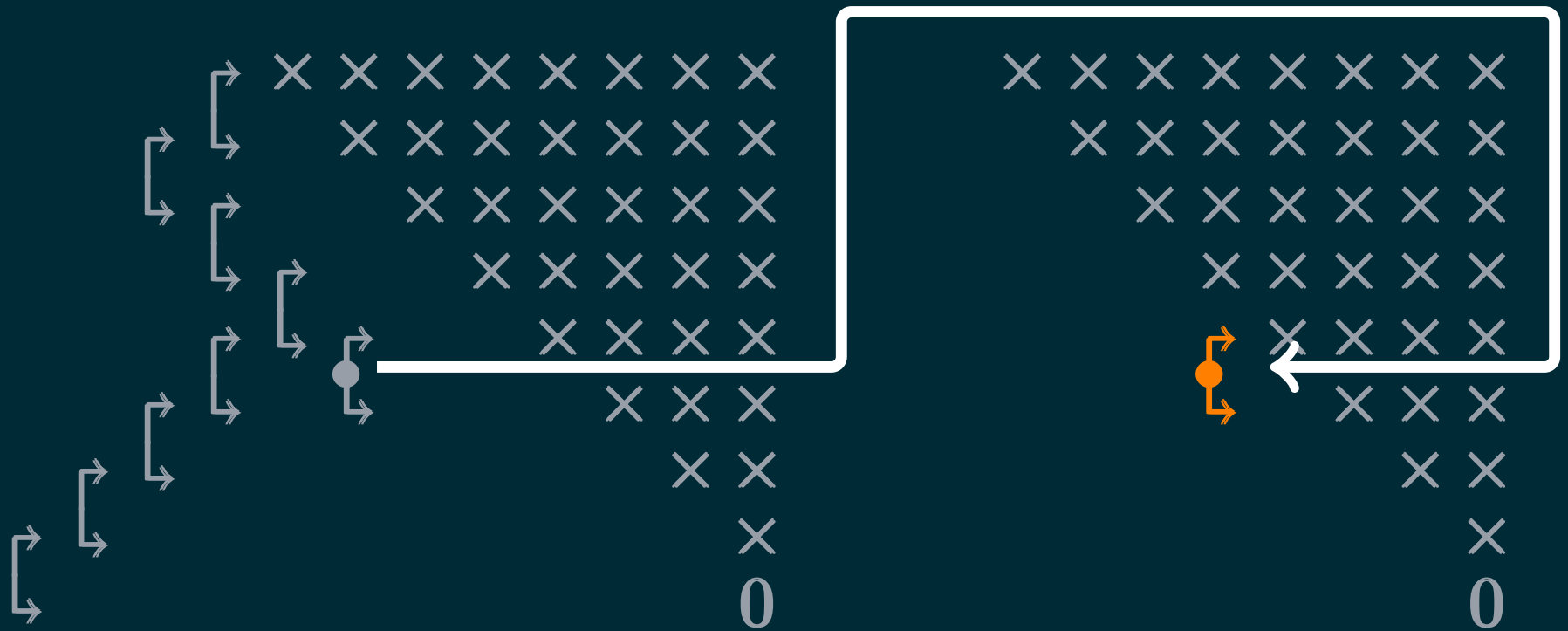
# Chasing procedure

$(\underline{L}, \underline{K})$



# Chasing procedure

$(\underline{L}, \underline{K})$

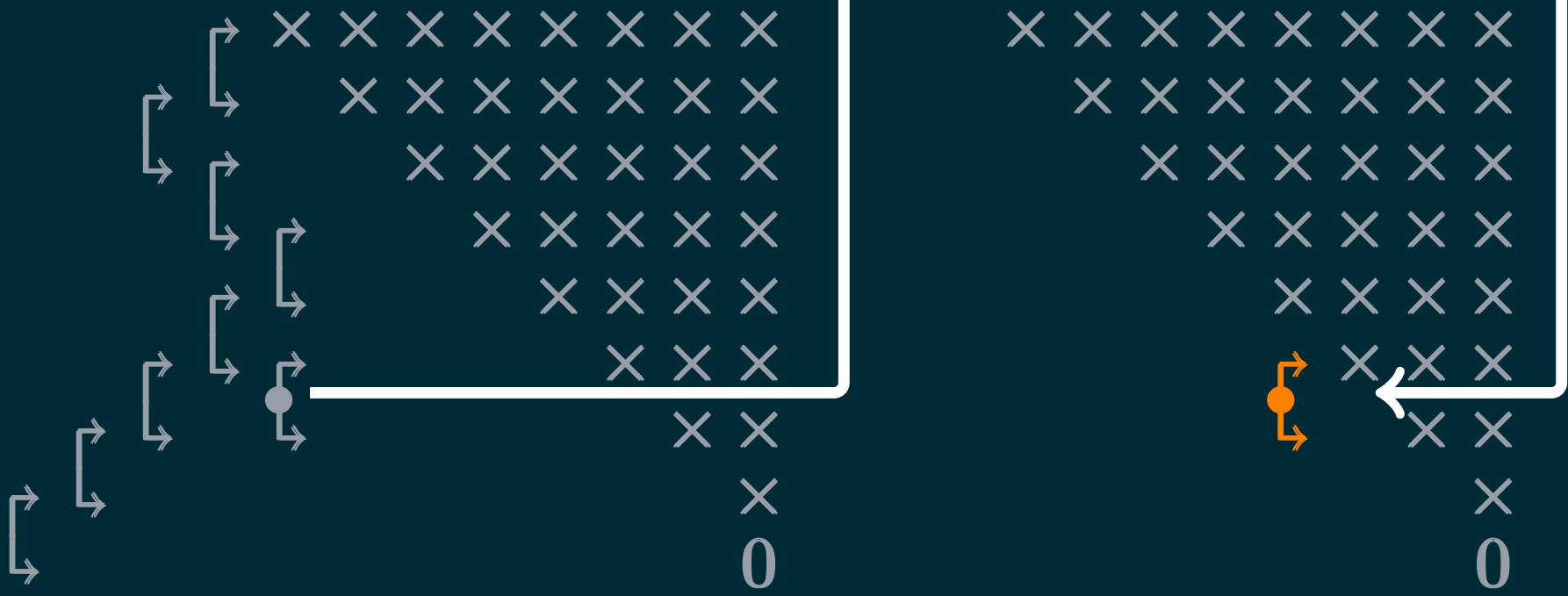






# Chasing procedure

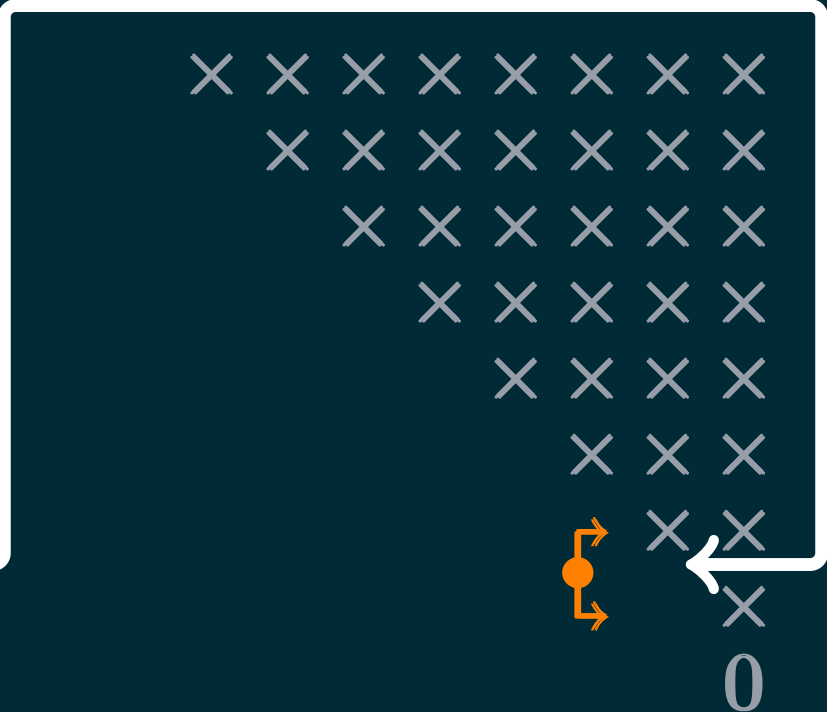
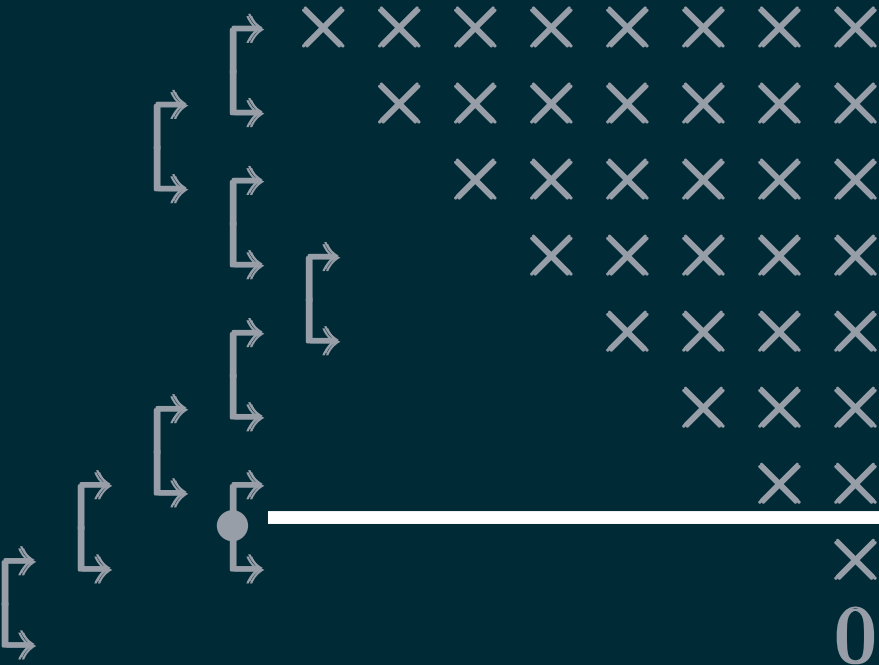
$(\underline{L}, \underline{K})$





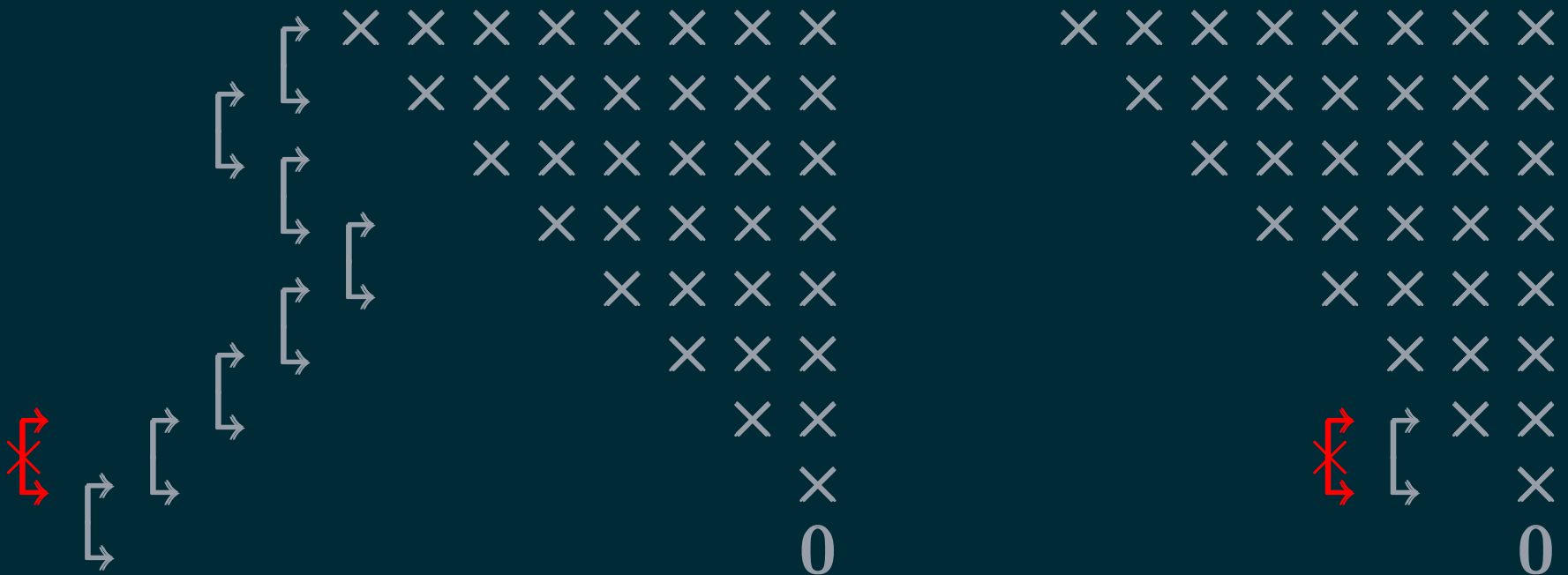
# Chasing procedure

$$(\underline{L}, \underline{K})$$



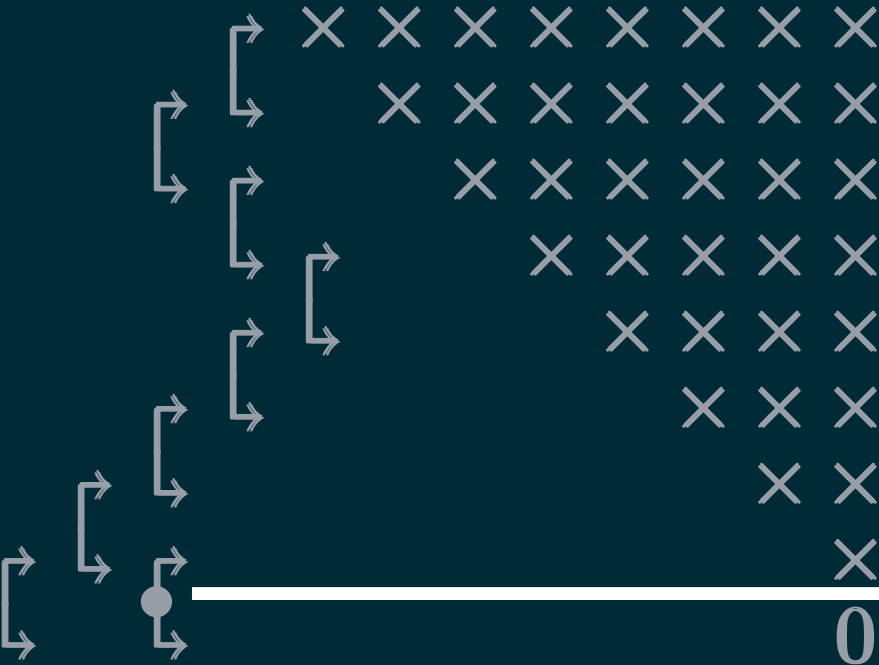
# Chasing procedure

$(\underline{L}, \underline{K})$



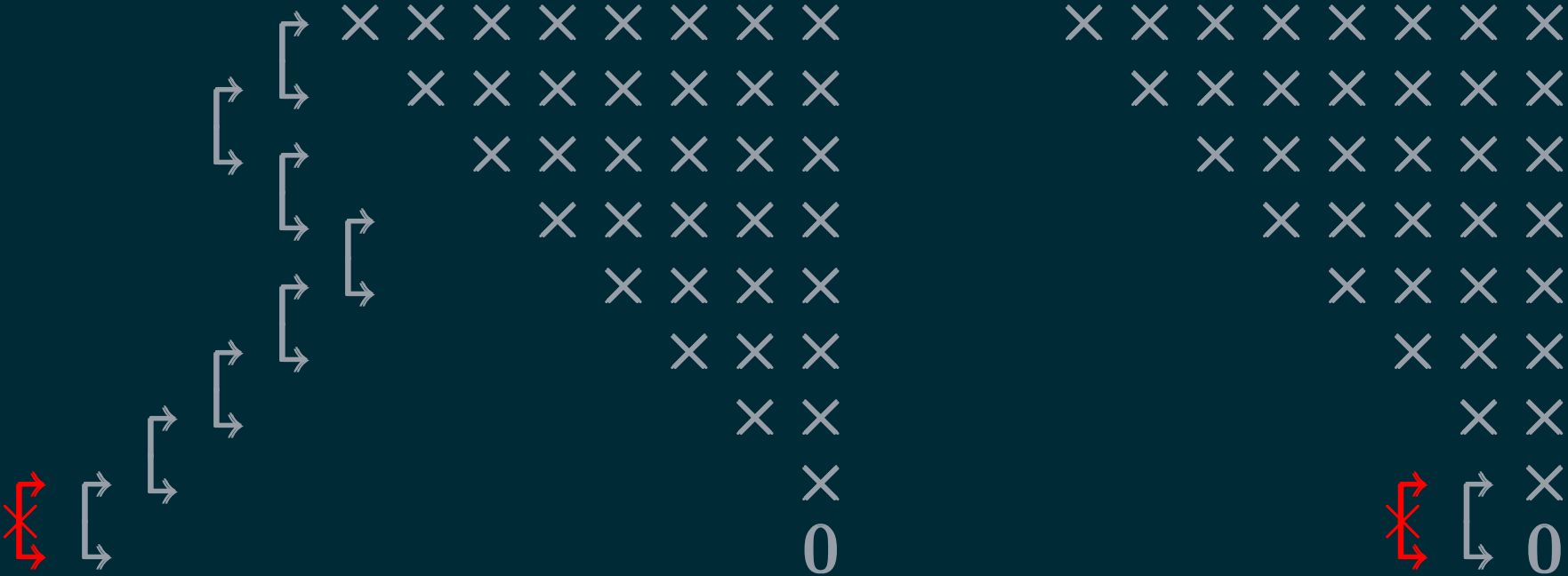
# Chasing procedure

$$(\underline{L}, \underline{K})$$



# Chasing procedure

$$(\underline{L}, \underline{K})$$







A low-angle, upward-looking photograph of a dark wooden structure, possibly a tower or a large gazebo, against a deep blue night sky. The sky is filled with numerous long, thin, golden-yellow light trails that radiate from the top of the structure, creating a starburst effect. The structure's beams and supports are silhouetted against the light trails.

# NUMERICAL EXAMPLE



# BRUSSELATOR MODEL

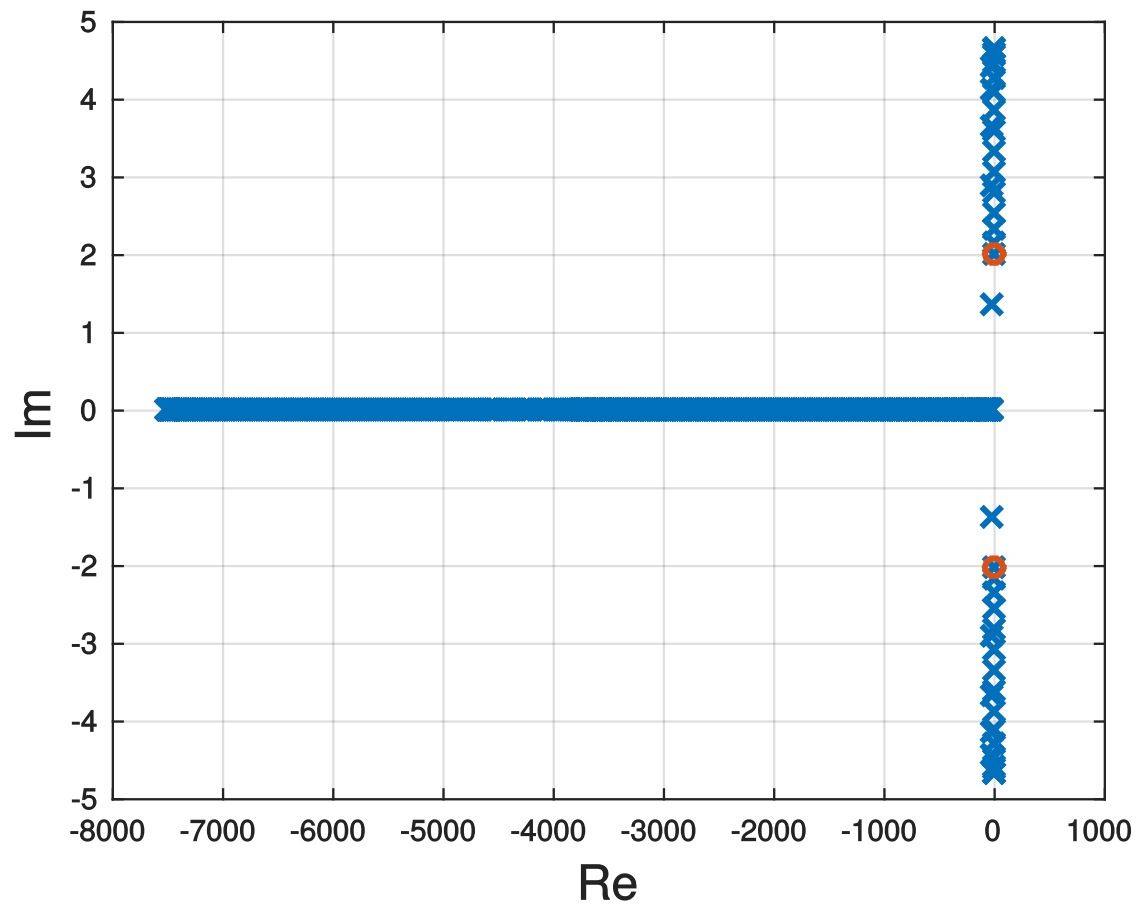
[DE SAMBLANX, 1997]

## 2D reaction-diffusion model

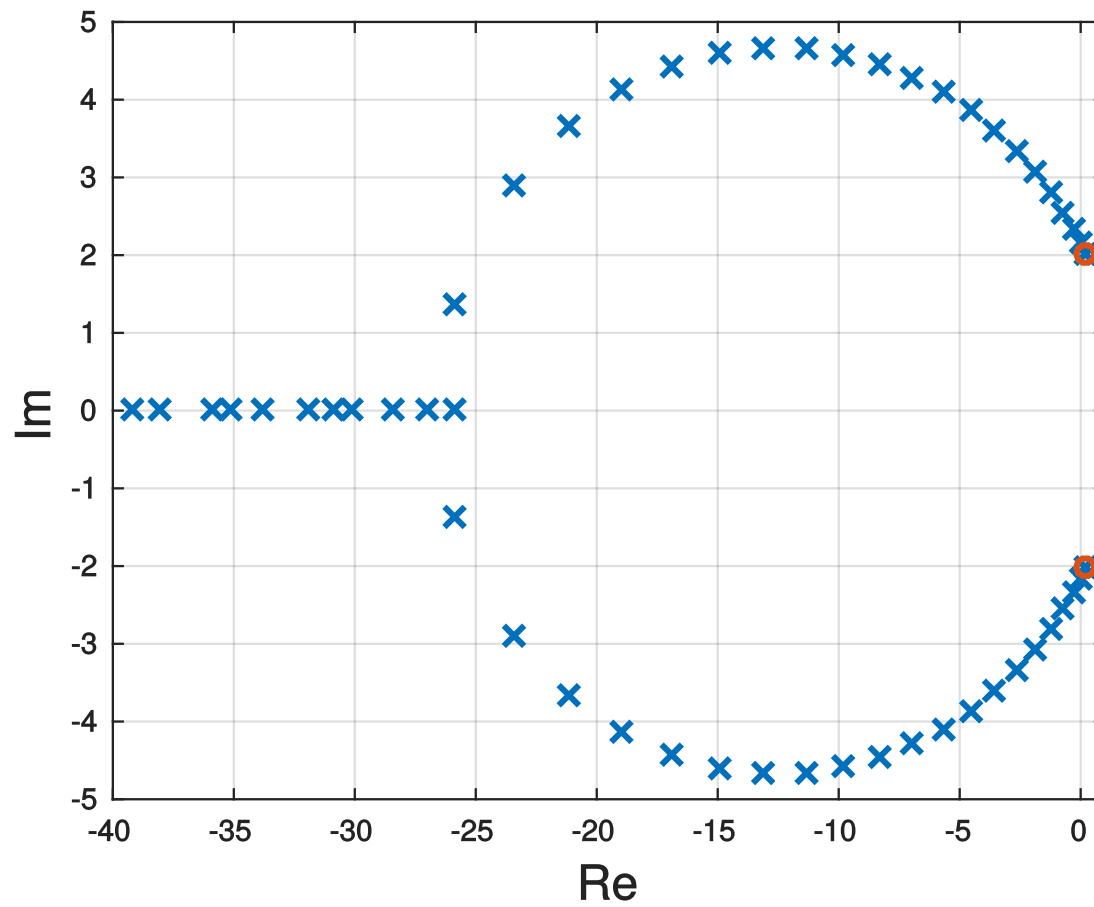
$$\frac{\partial u}{\partial t} = \frac{D_u}{L^2} \left[ \frac{\partial^2 u}{\partial X^2} + \frac{\partial^2 u}{\partial Y^2} \right] - (B + 1)u + u^2 v + C$$
$$\frac{\partial v}{\partial t} = \frac{D_v}{L^2} \left[ \frac{\partial^2 v}{\partial X^2} + \frac{\partial^2 v}{\partial Y^2} \right] - u^2 v + Bu$$

- $u, v$ : concentrations of two reactants
- homogeneous Dirichlet boundary conditions
- discretised with central differences
- parameters:  $B = 5.45, C = 2, D_u = 0.004, D_v = 0.008$  and  $L = 1$

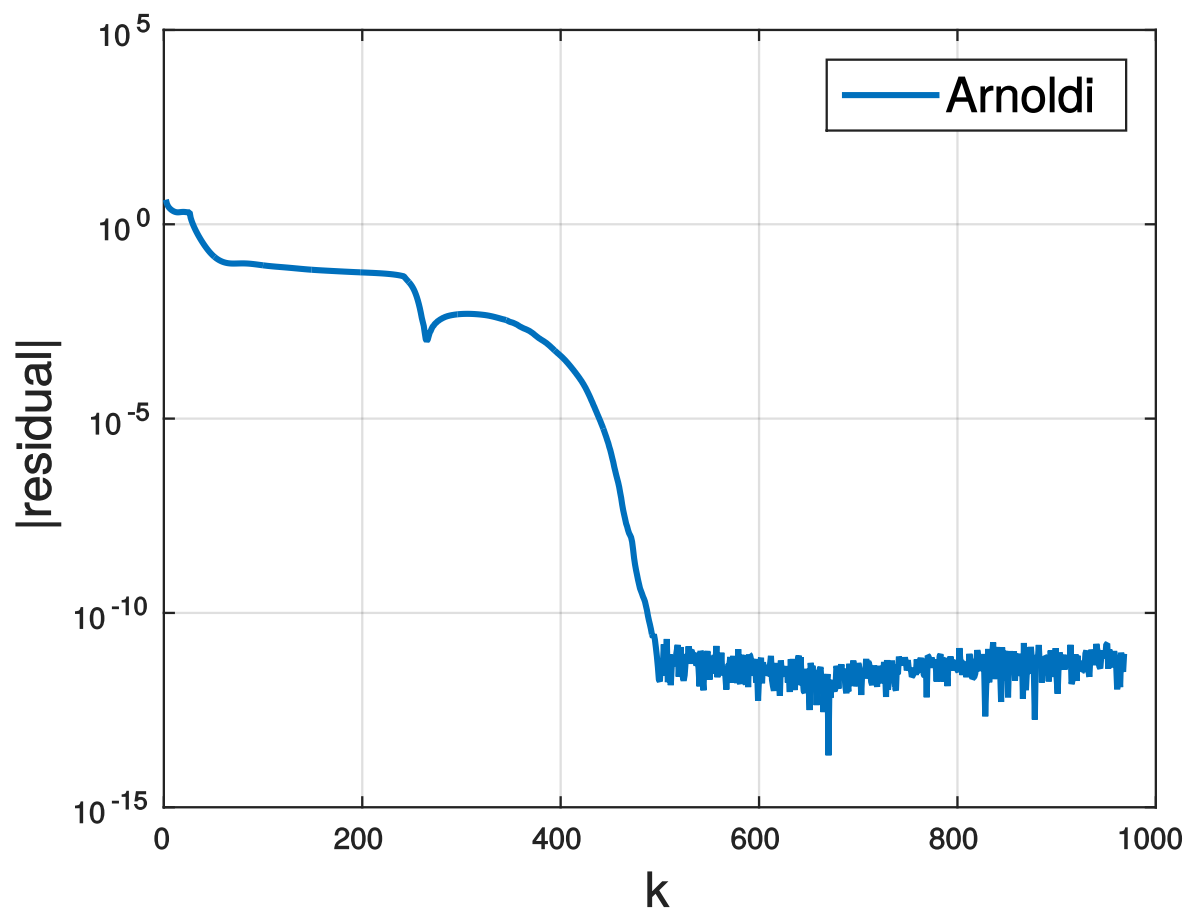
Matrix  $A \in \mathbb{C}^{968 \times 968}$



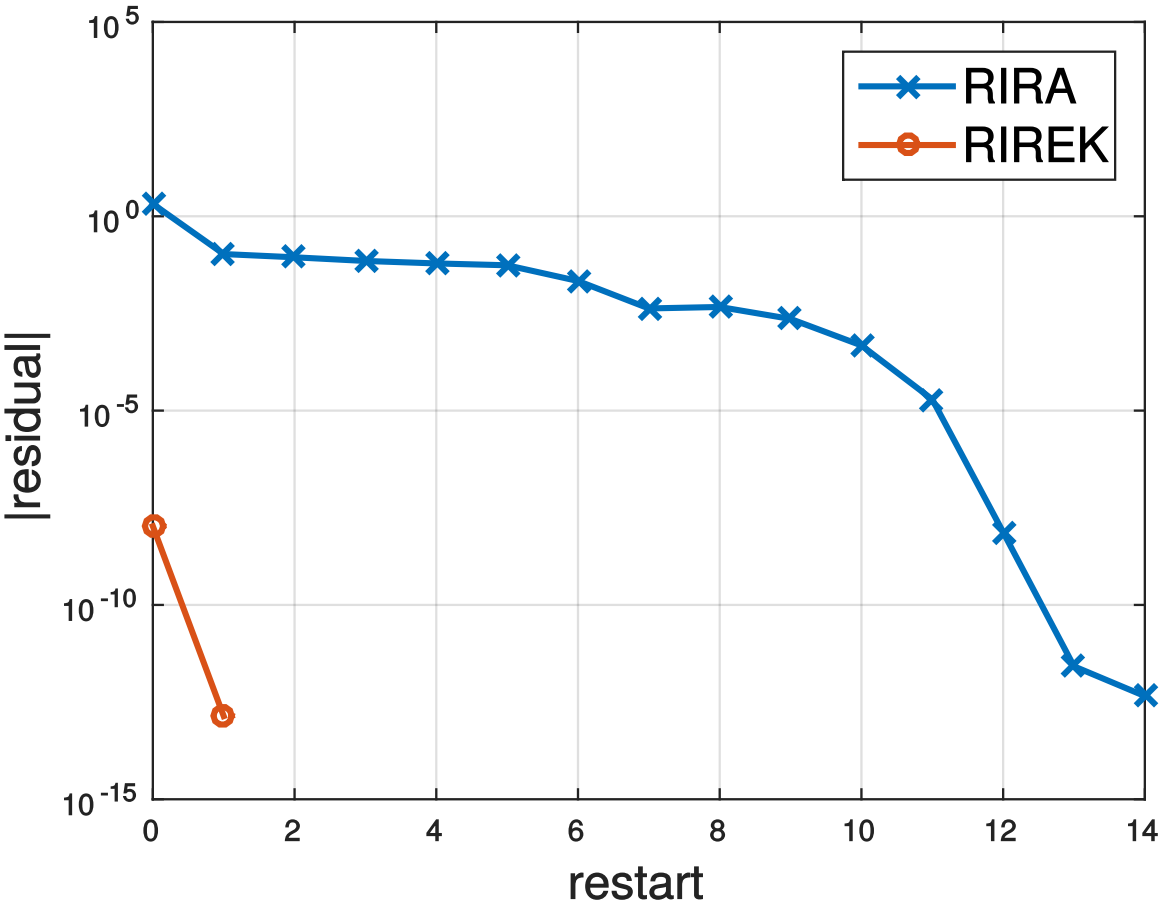
Matrix  $A \in \mathbb{C}^{968 \times 968}$



# Arnoldi



# RIRA & RIREK





An aerial photograph of a vast, snow-covered mountain range. The terrain is characterized by smooth, rounded peaks and deep, shadowed valleys. A line of approximately ten small figures, likely hikers or mountaineers, is visible at the bottom of the frame, standing on a ridge. The overall scene is serene and majestic, with a cool color palette dominated by whites and blues.

# CONCLUSION & OUTLOOK

## Conclusion

- Krylov methods: Arnoldi & RKS
- Implicit restart of Arnoldi & EK in an implicit manner:
  - optimal computational complexity
  - multi-shift
  - unitary operations

## Outlook

- Generalise to fully rational Krylov sequences
- Applications
- ...

## REFERENCES