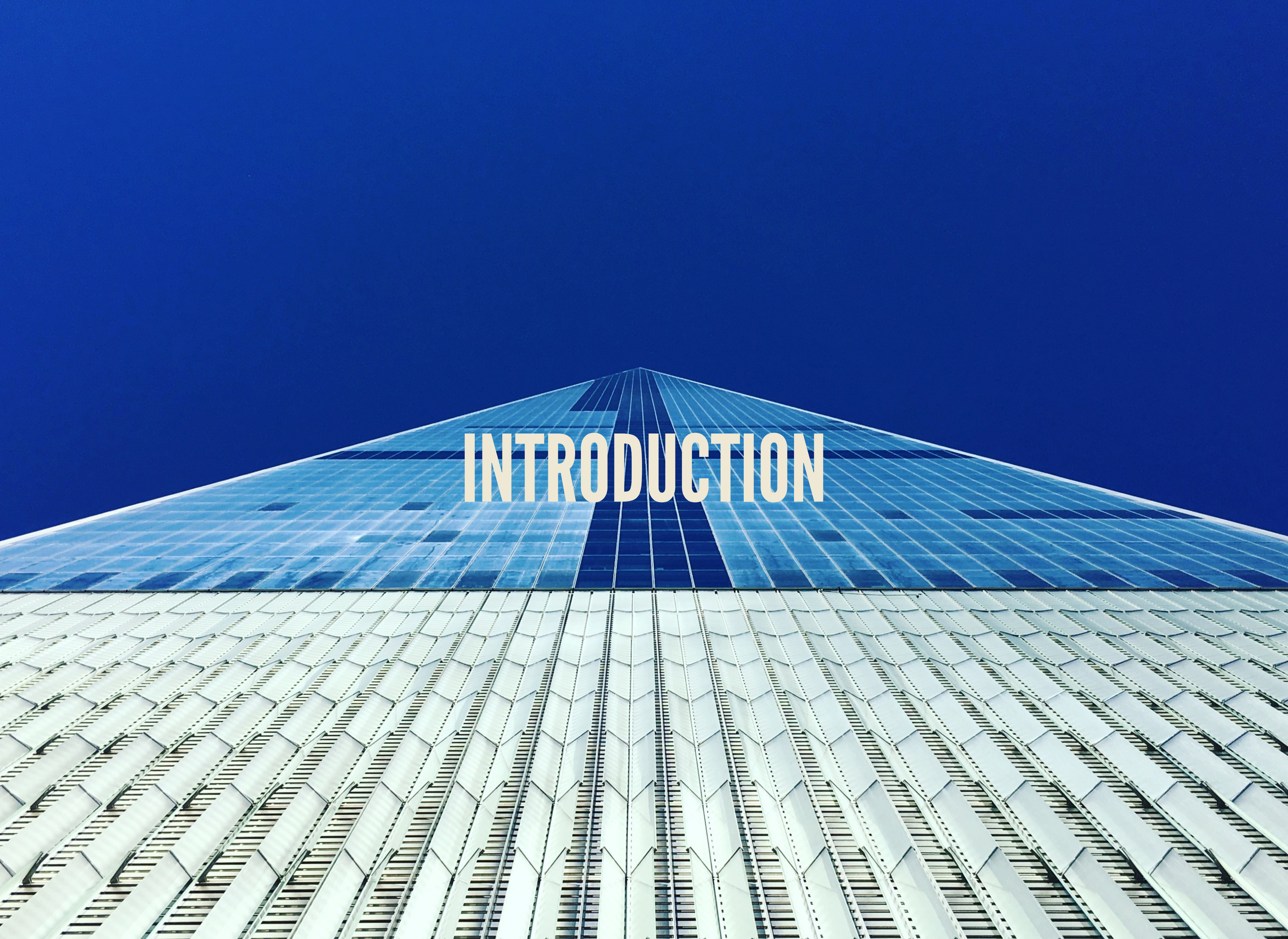
TOWARDS A COMPUTATIONAL EFFICIENT, IMPLICITLY RESTARTED RATIONAL KRYLOV METHOD

Daan Camps, Karl Meerbergen, Raf Vandebril

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 $v \in \mathbb{C}^N$:

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

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: $H_i\, y_j = \theta_j\, y_j$

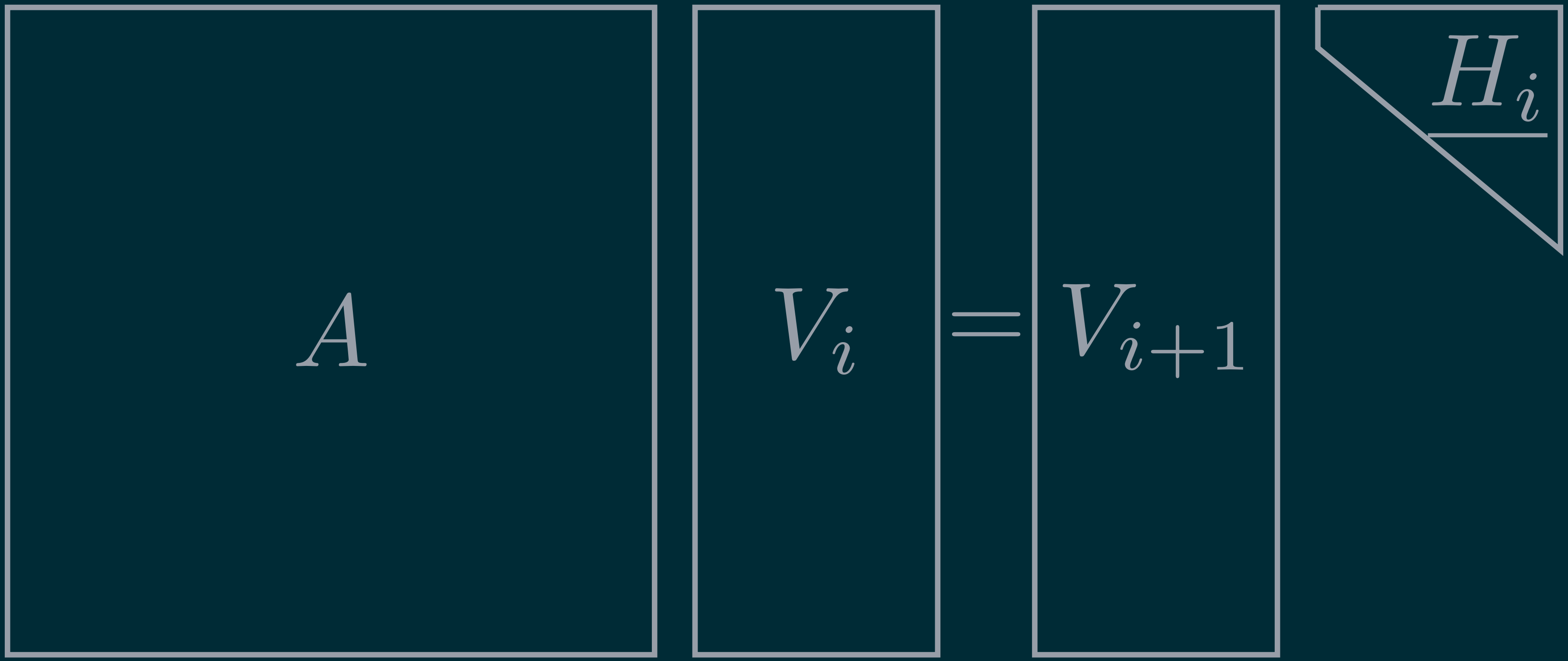
$$A\, V_i = V_i\, H_i + h_{i+1,i}\, v_{i+1}\, e_i^T$$

or

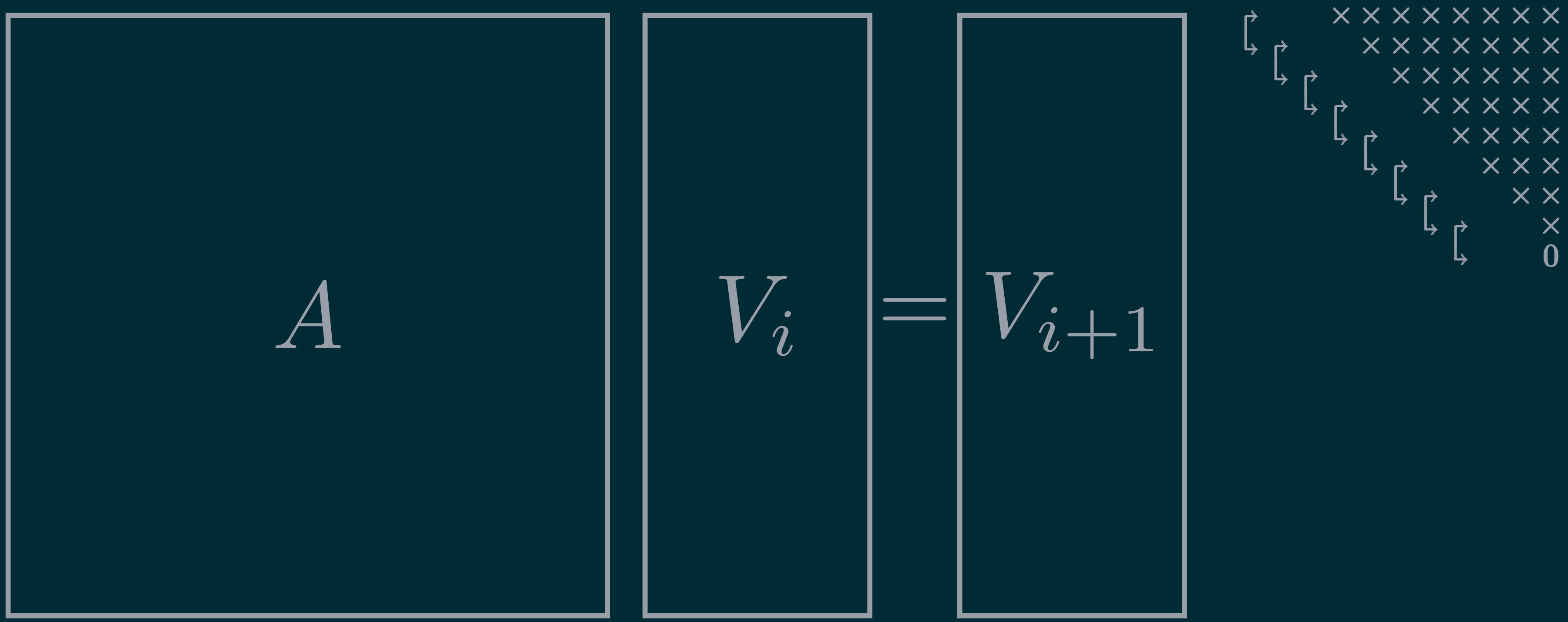
$$A\, V_i = V_{i+1}\, \underline{H}_{i+1,i}$$

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

Arnoldi Decomposition



Rotational Arnoldi Decomposition



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 $v \in \mathbb{C}^N$:

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

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

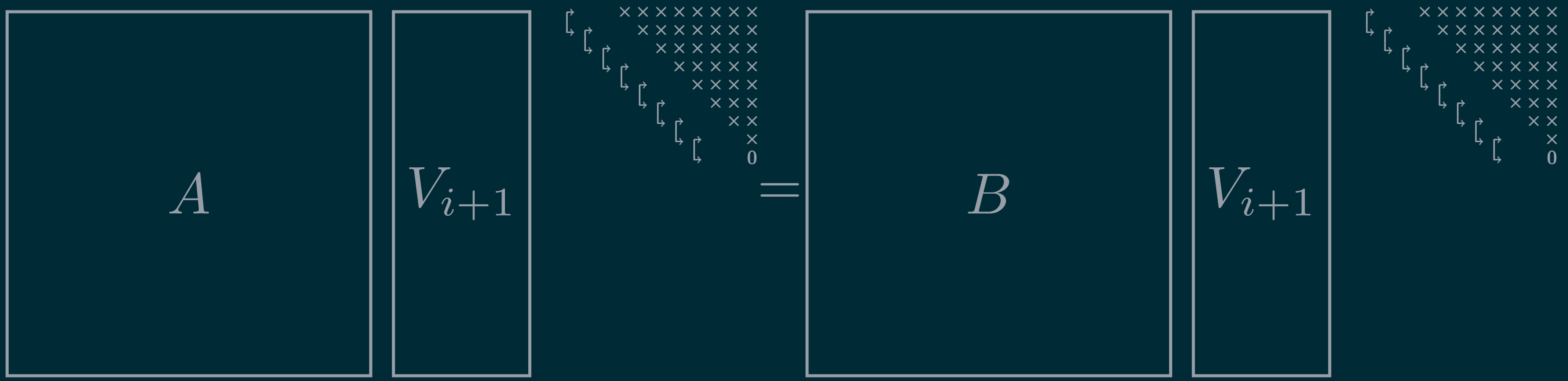
Extended Krylov:

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

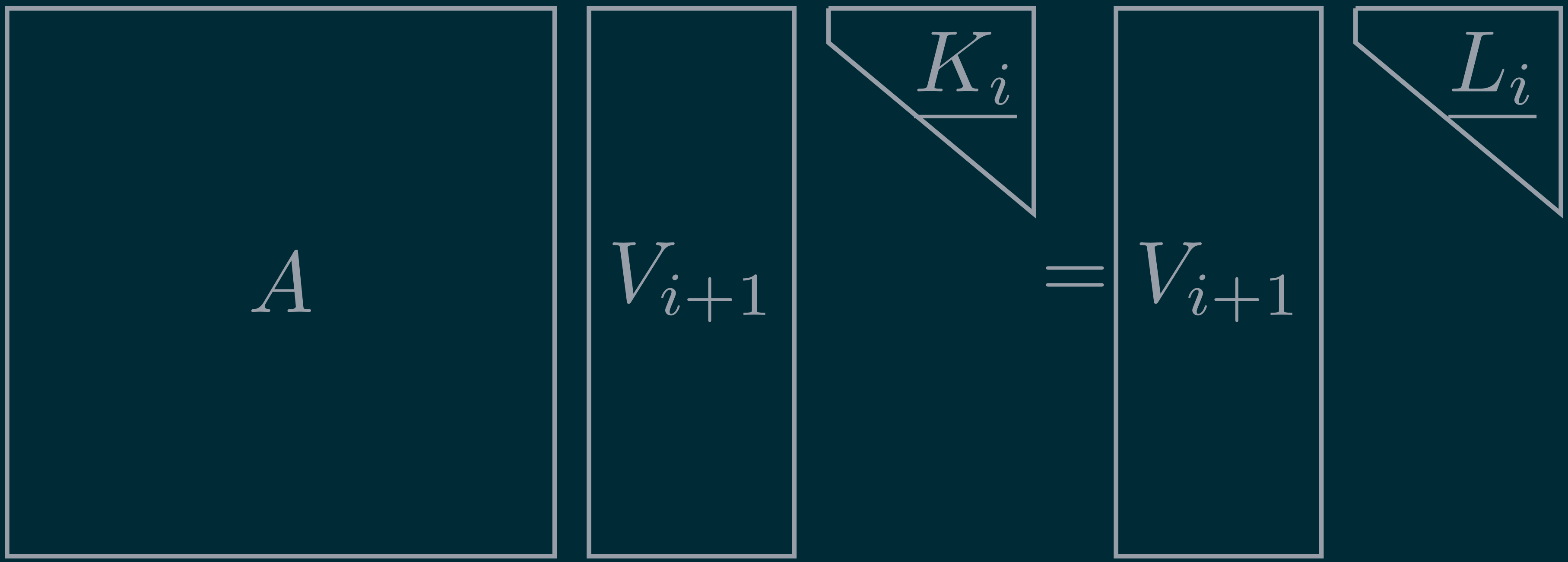
RKS Decomposition

$$A V_{i+1} \underline{K_i} = B V_{i+1} \underline{L_i}$$

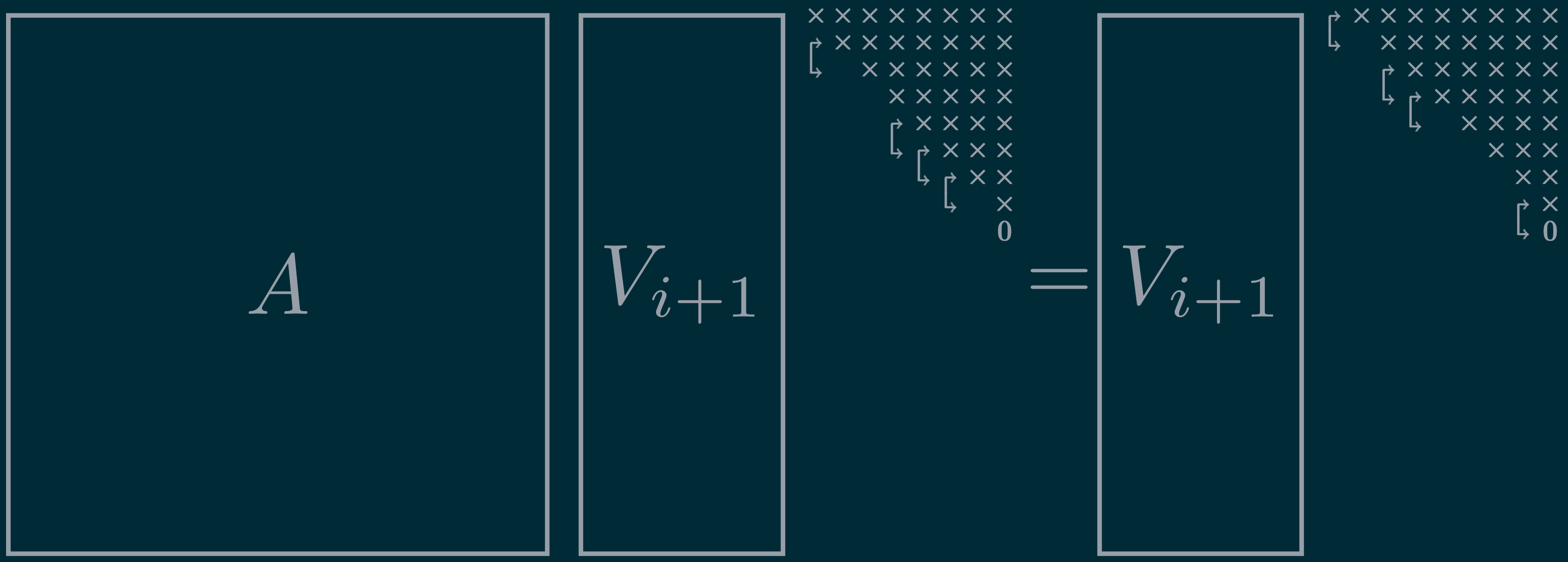
Rotational RKS Decomposition



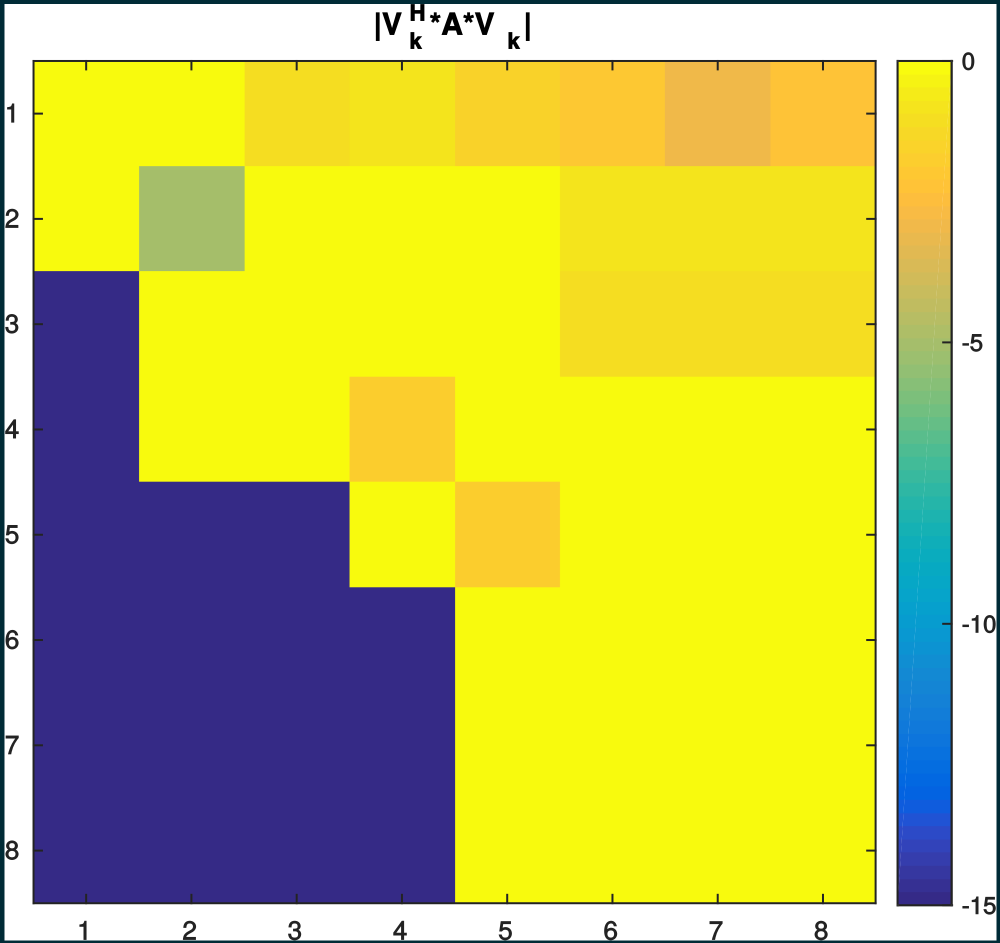
Special case: Extended Krylov Decomposition



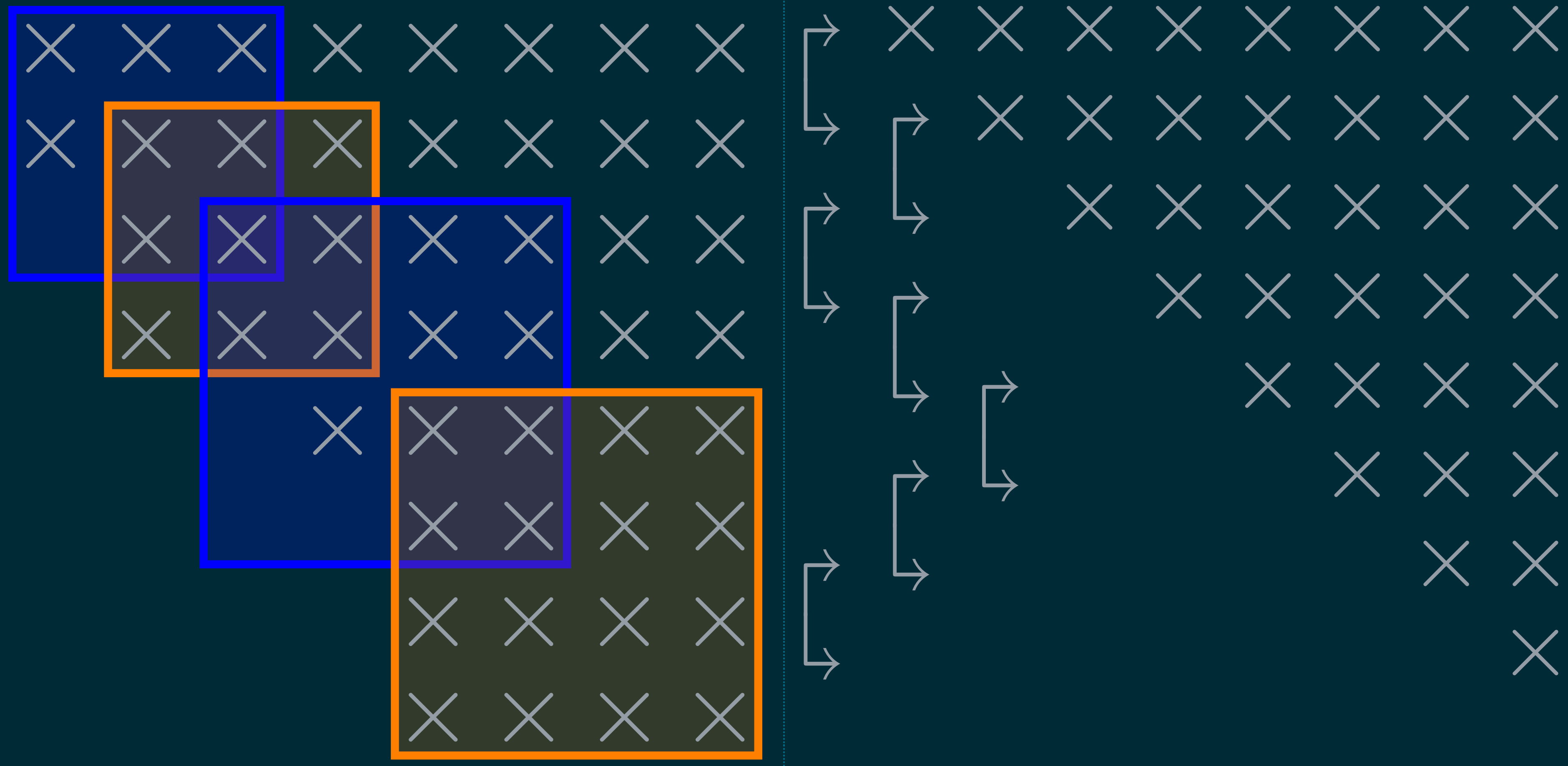
Rotational Extended Krylov Decomposition



Structure in projected counterpart



Structure in projected counterpart




IMPLICIT RESTART OF KRYLOV ITERATIONS

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:

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

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

$$V \leftarrow V Q$$

Improved solution

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

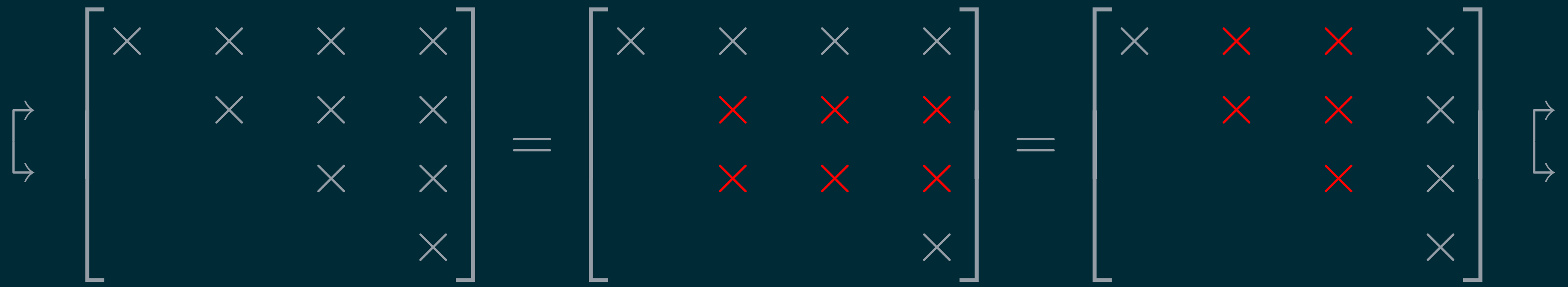
Advantages

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

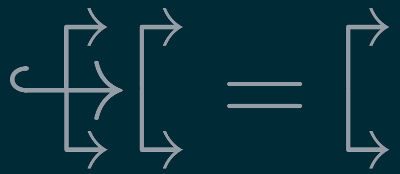
Ingredients

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

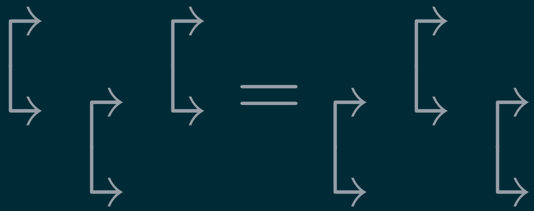
Bring a (pattern of) rotations through an upper triangular matrix



Fusion of two rotations



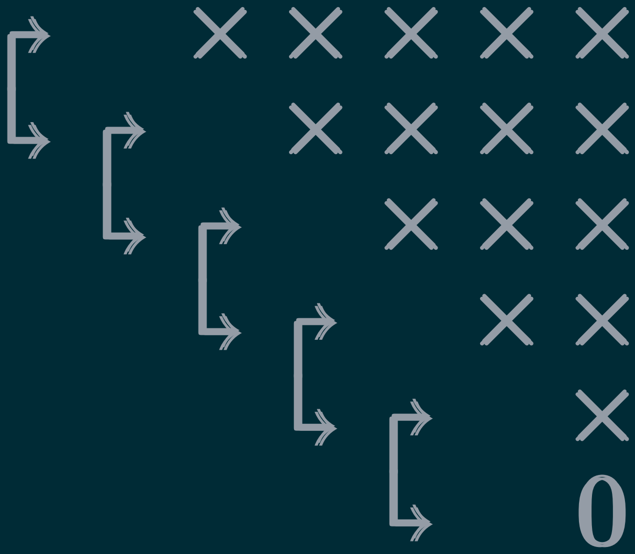
Shift-through of a pattern of 3 rotations



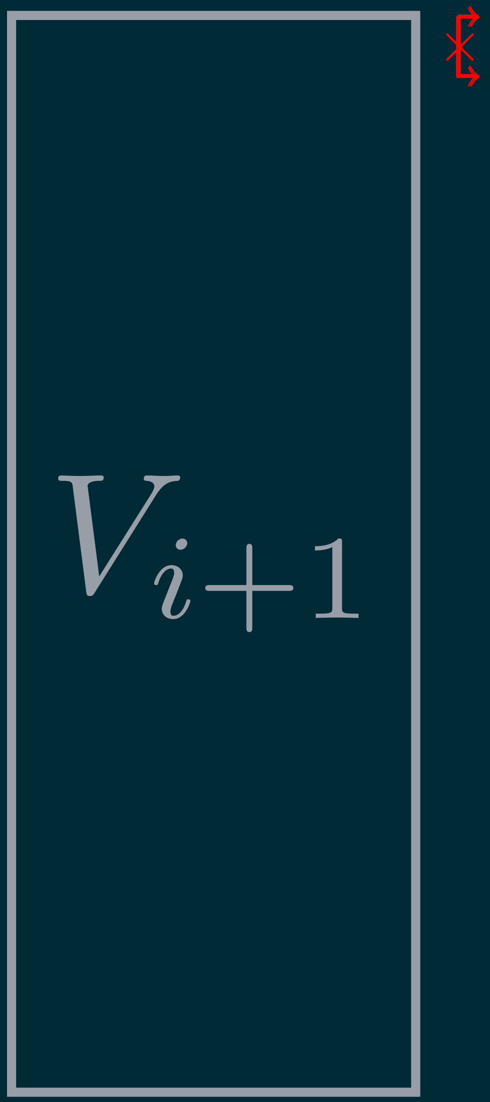
ROTATIONALLY IMPLICITLY RESTARTED ARNOLDI METHOD (RIRA)

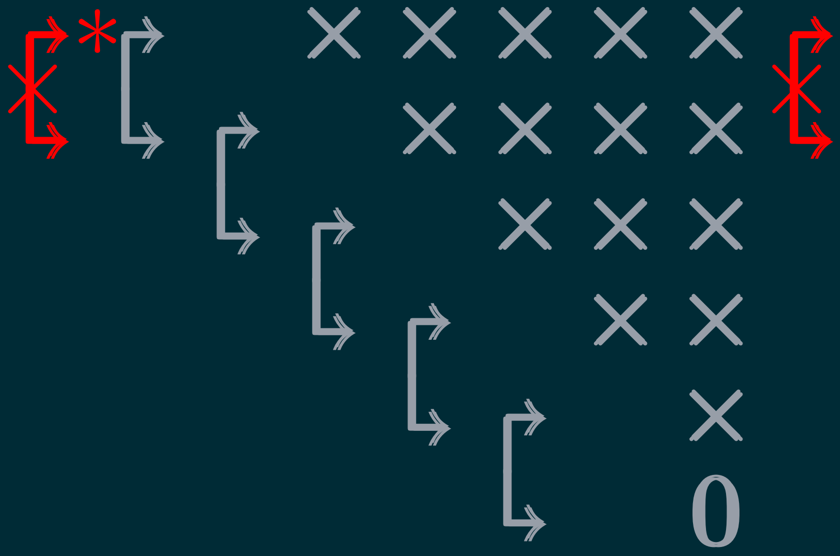
An example

Initial situation

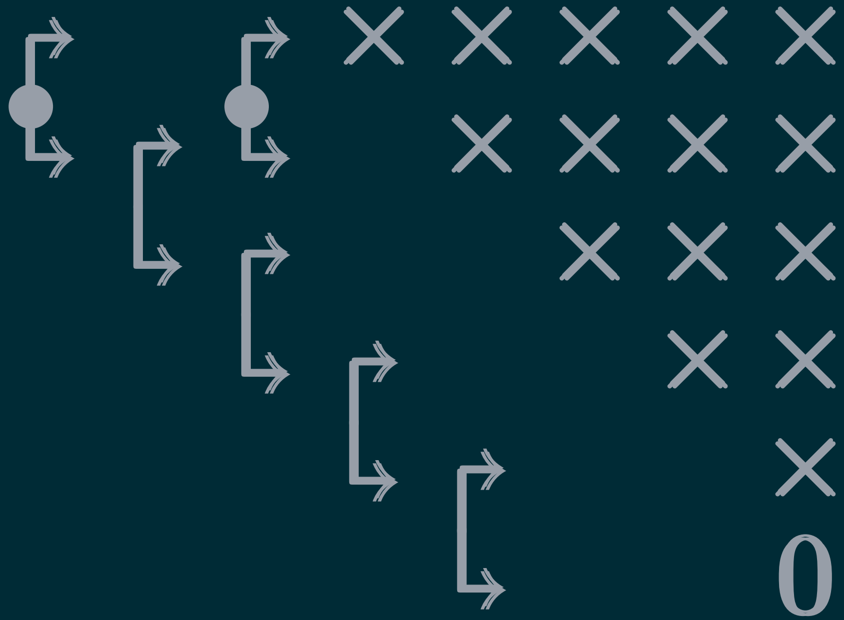


First similarity transformation

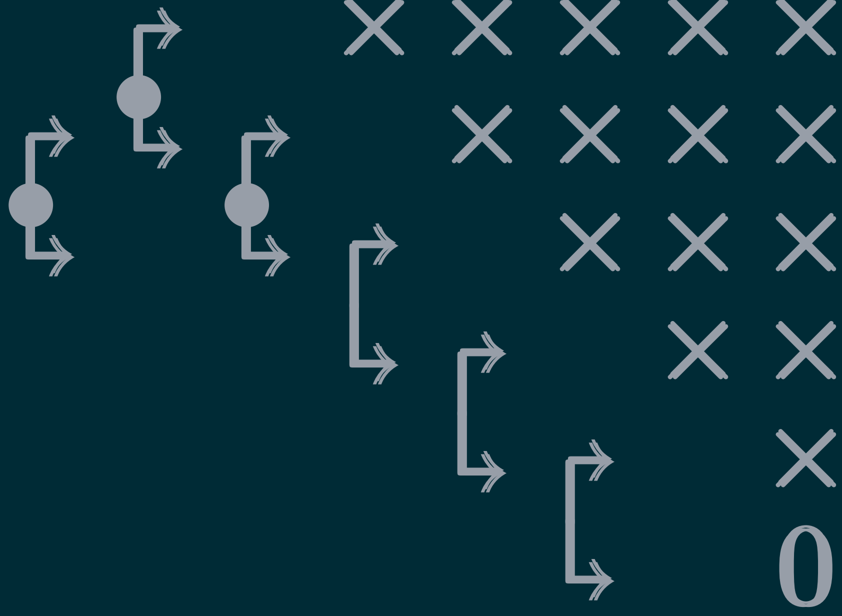




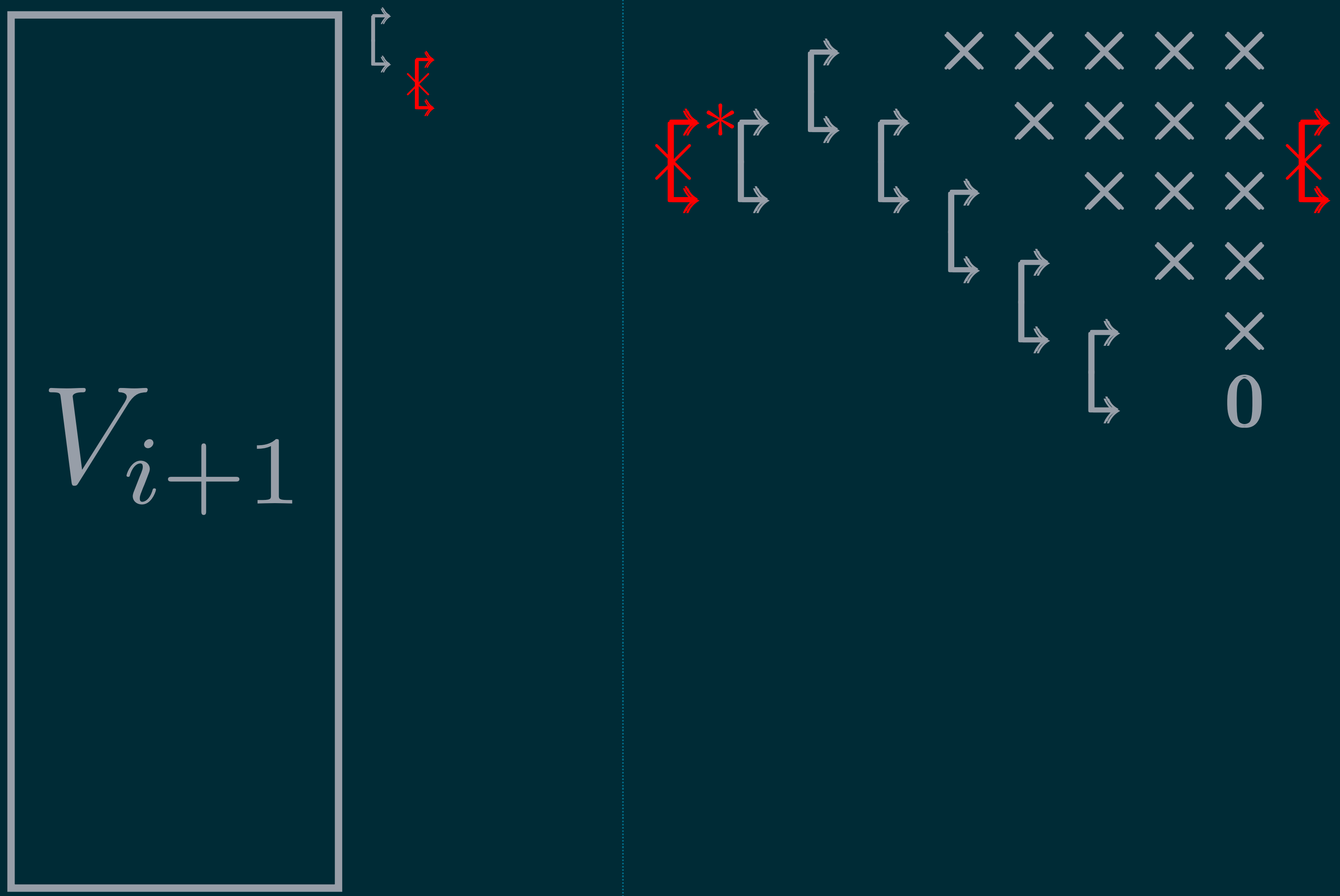
Fusion & right rotation through upper triangular



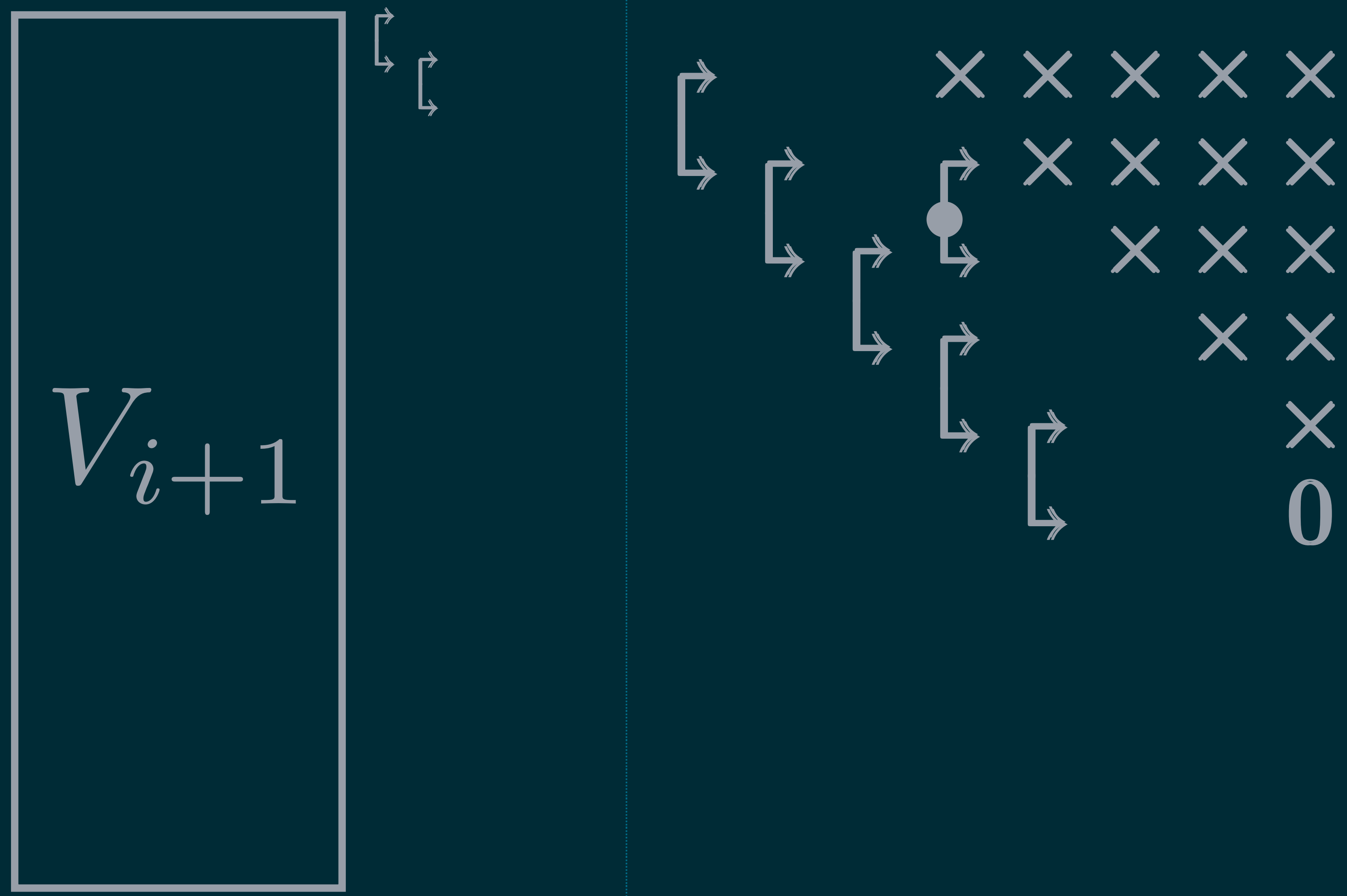
Shift-through



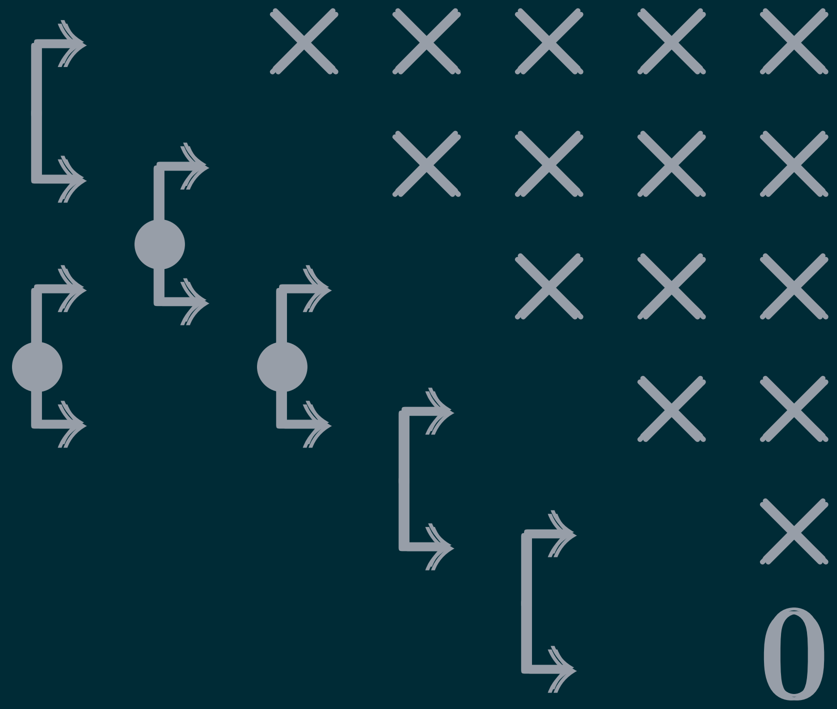
Second similarity transformation



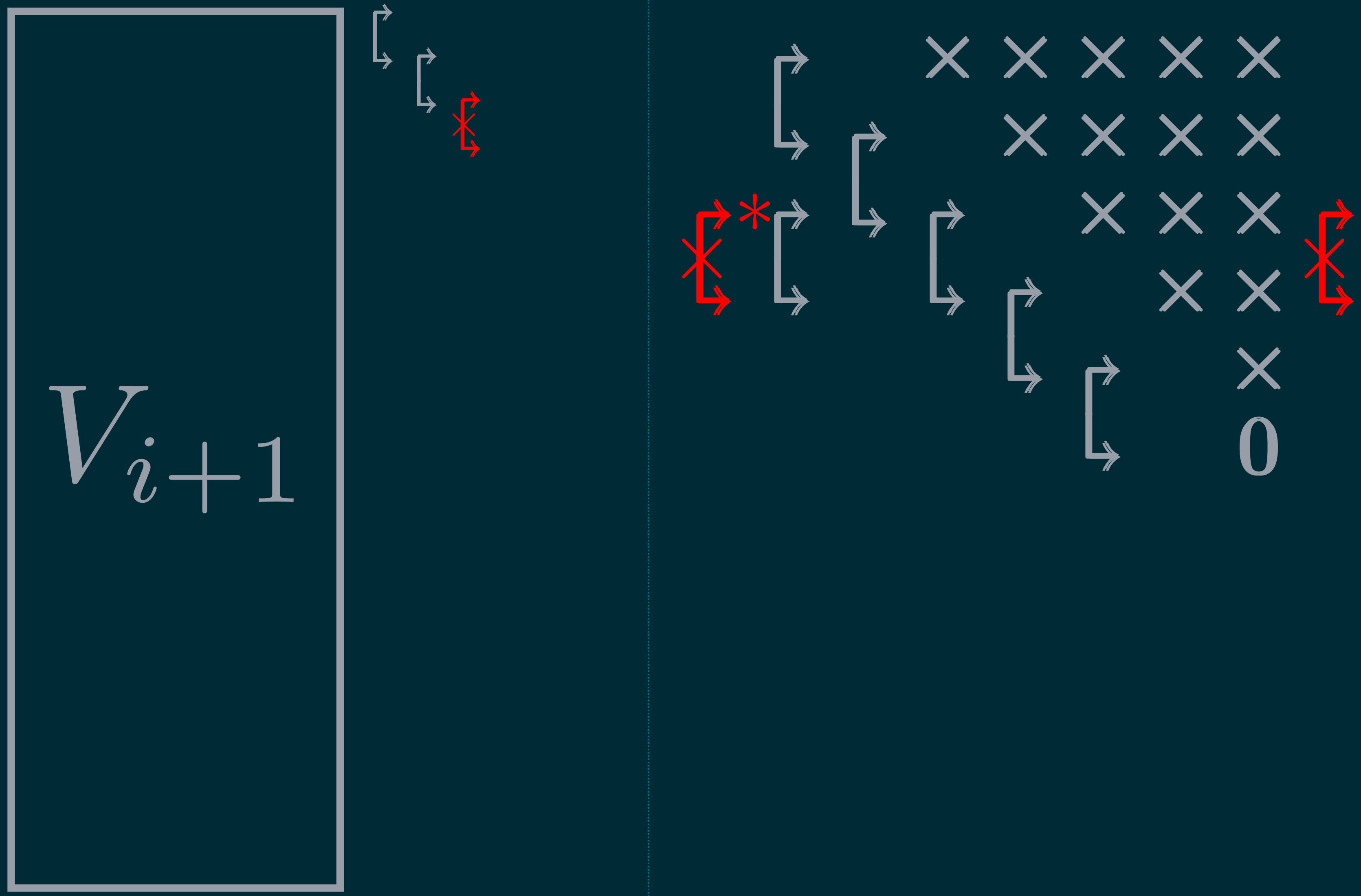
Fusion & right rotation through upper triangular



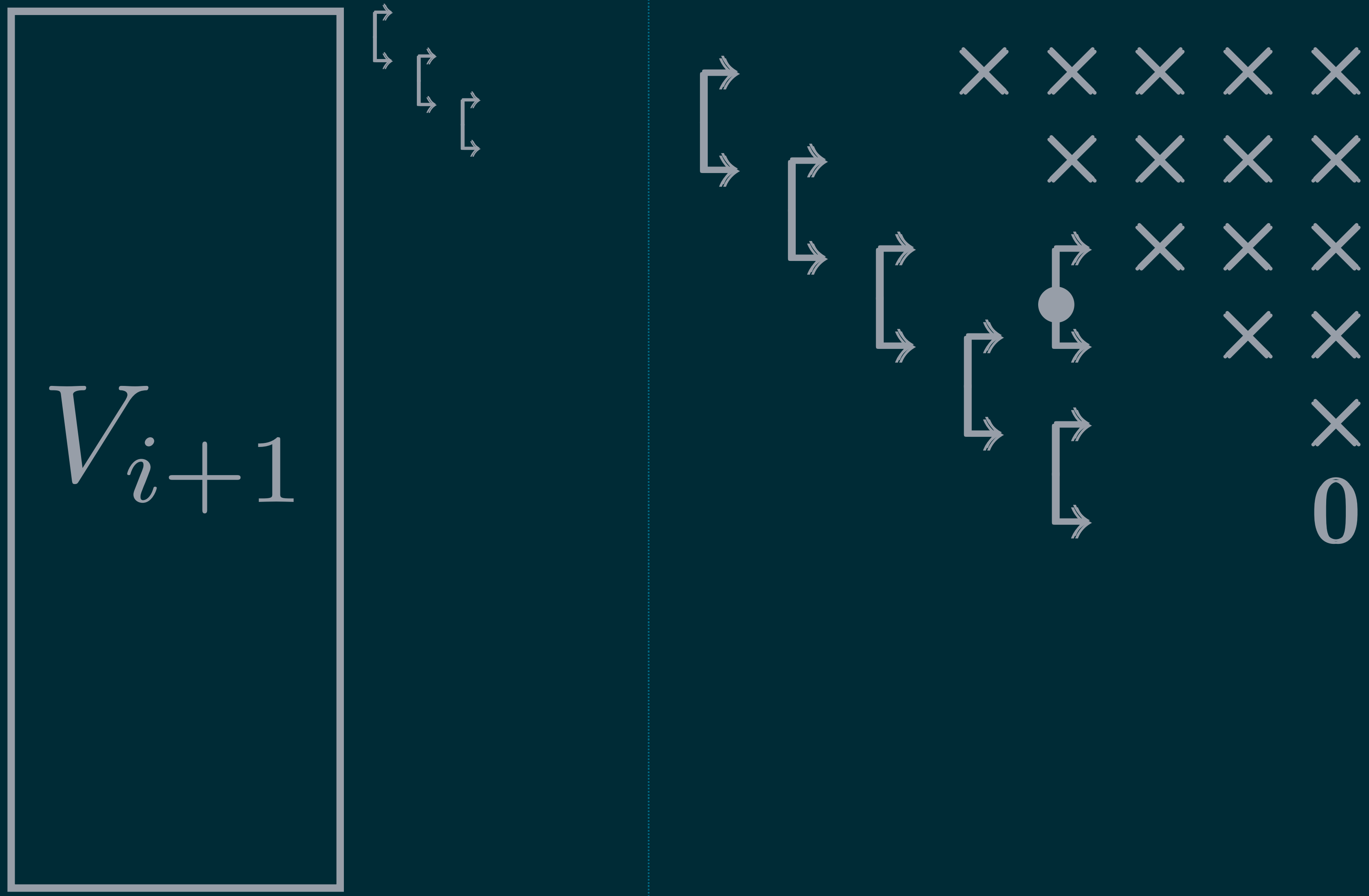
Shift-through



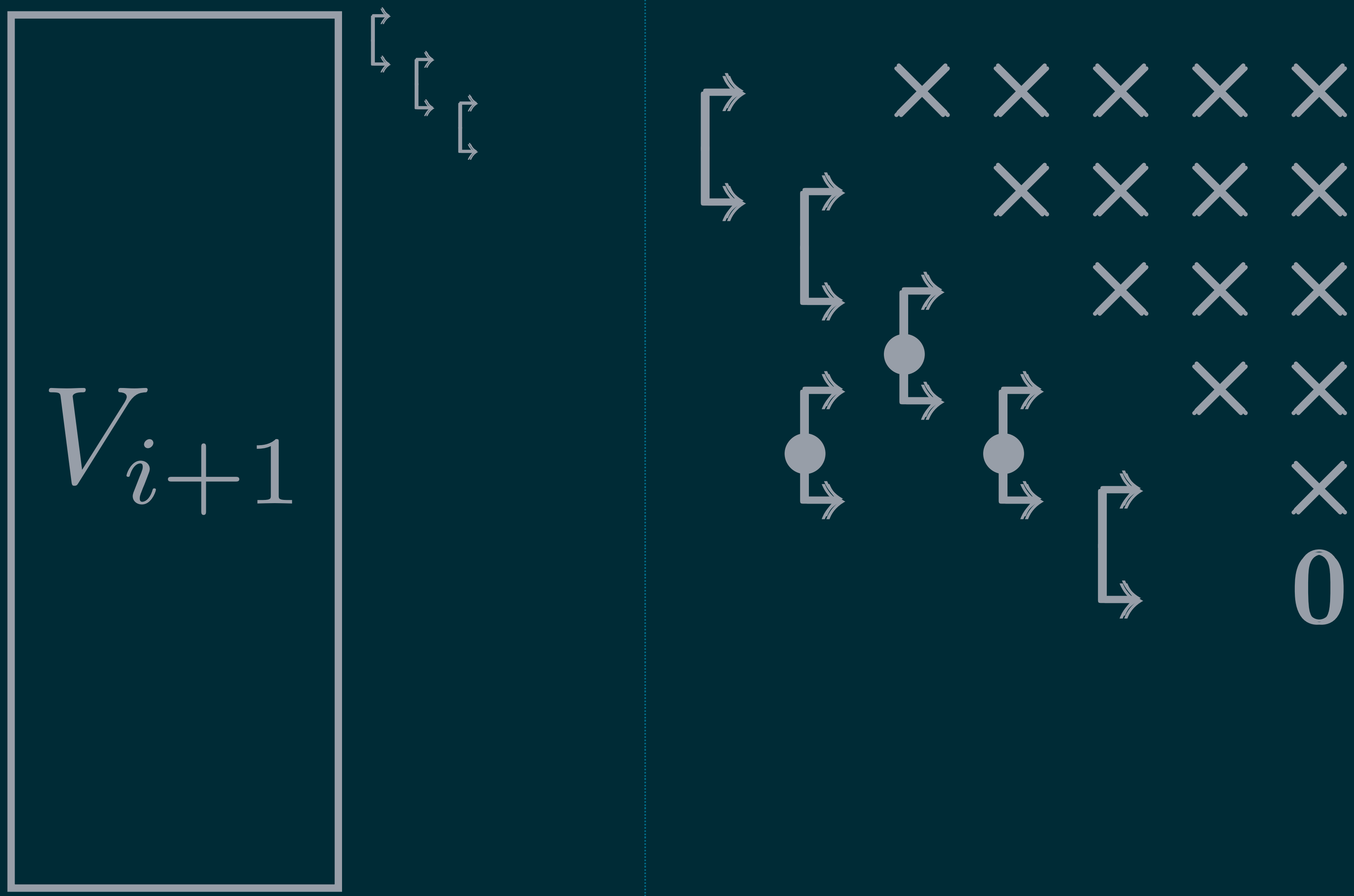
Third similarity transformation



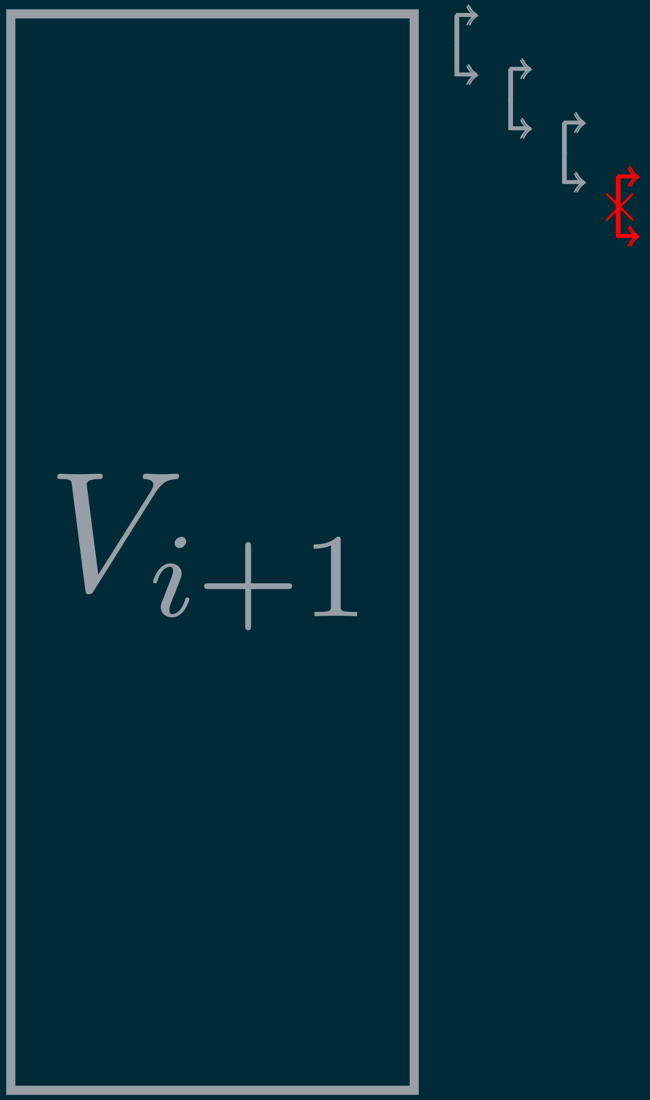
Fusion & right rotation through upper triangular



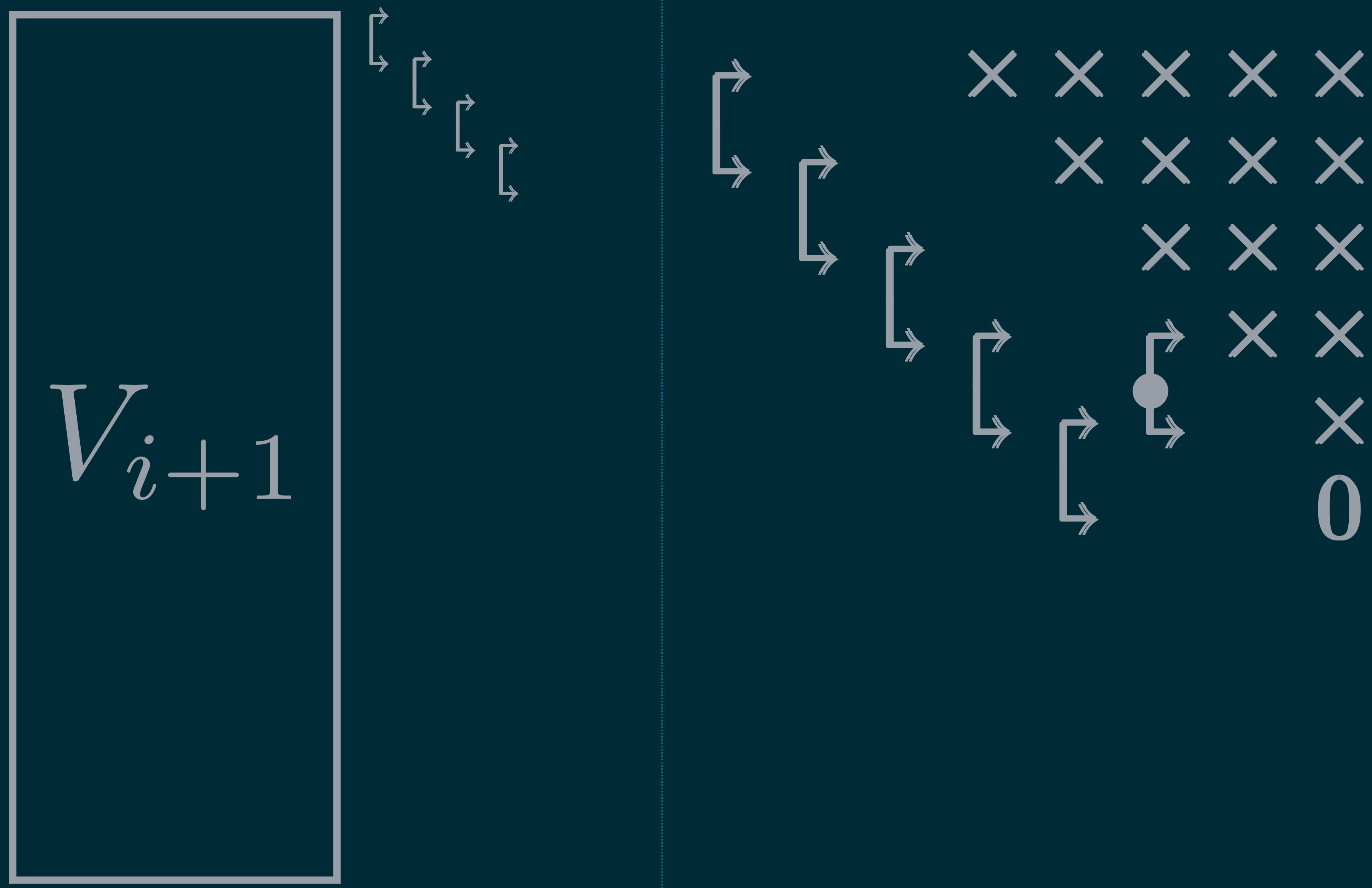
Shift-through



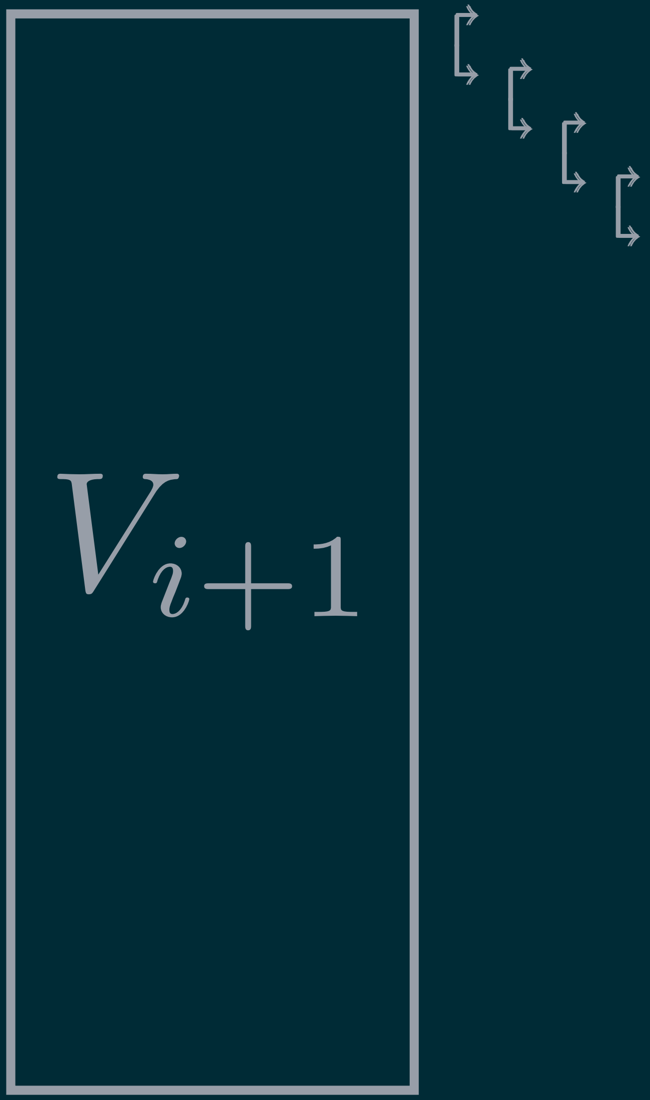
Fourth similarity transformation

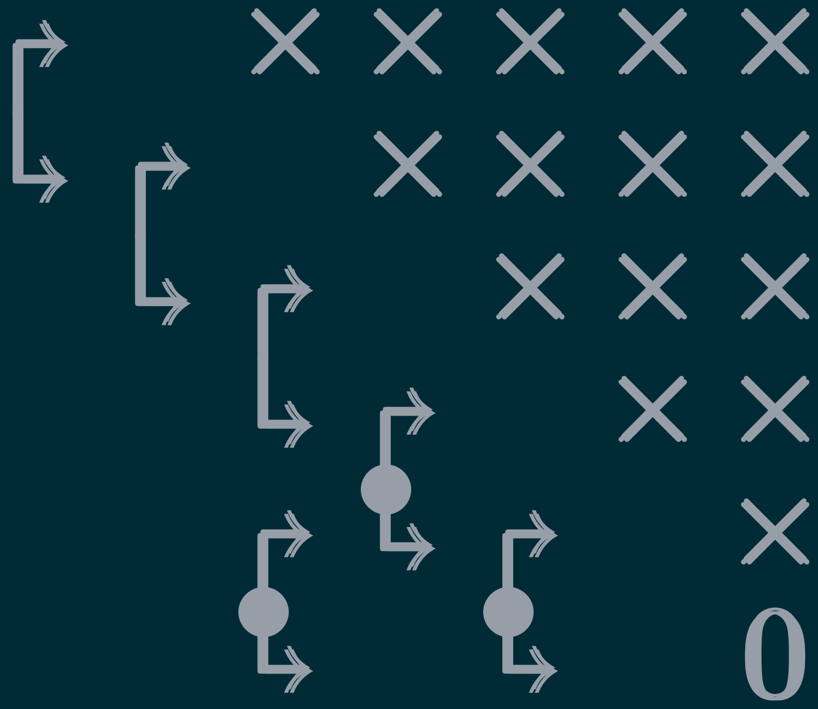


Fusion & right rotation through upper triangular

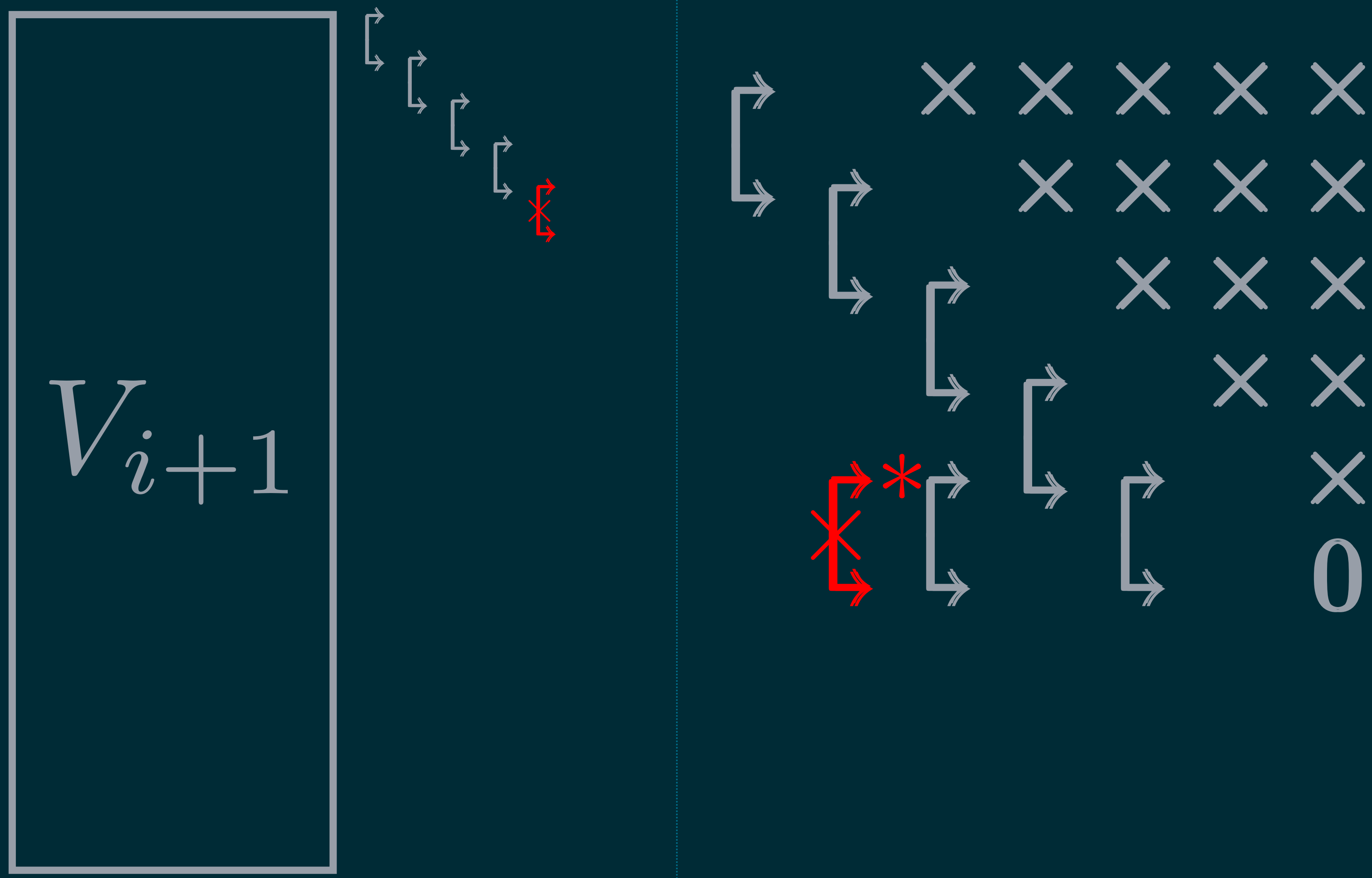


Shift-through

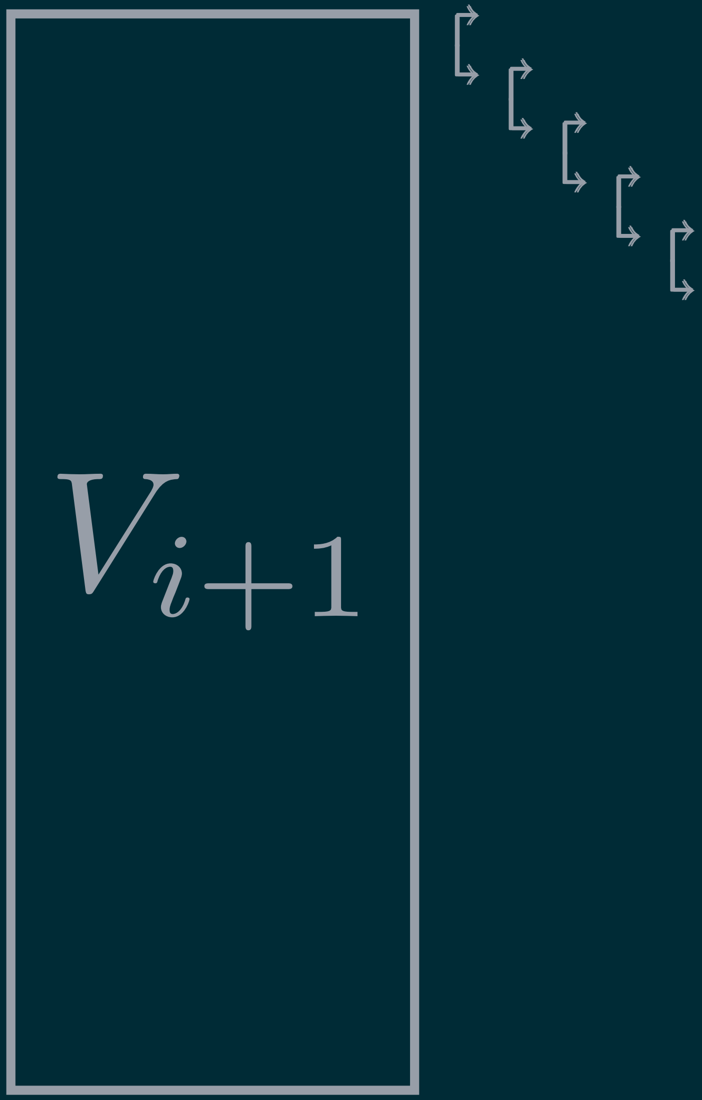


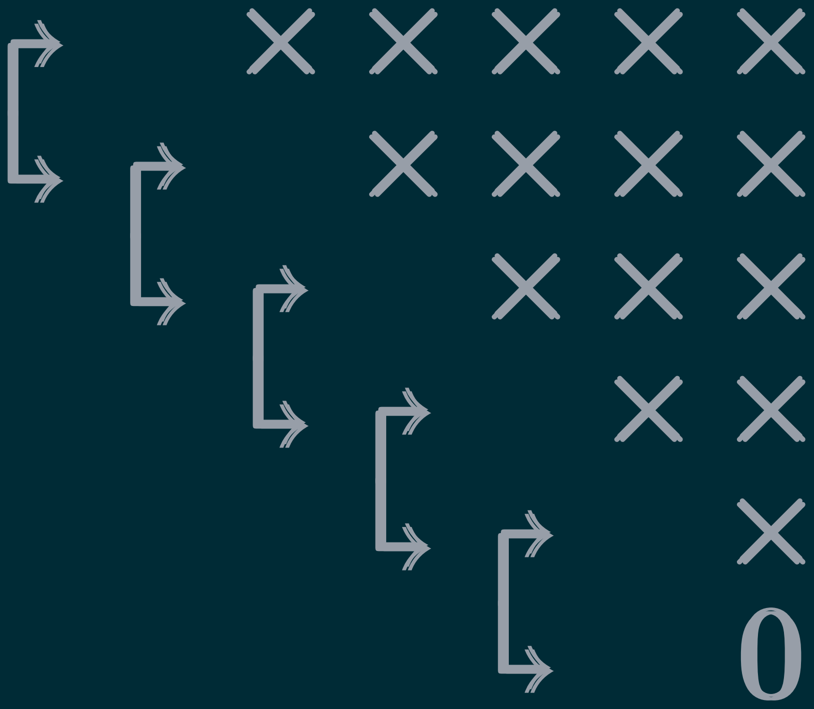


Fifth *similarity* transformation

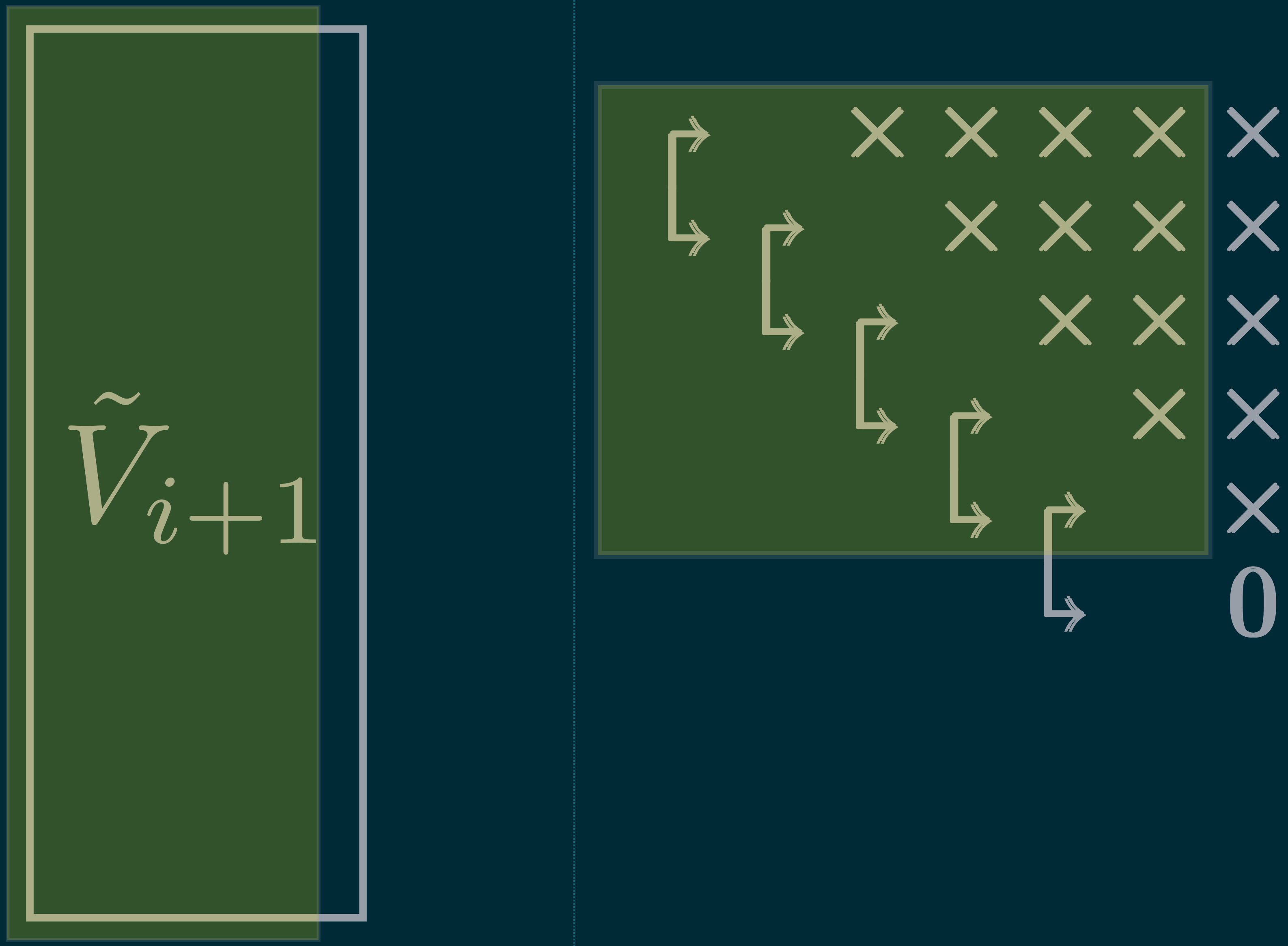


Final fusion





Extract reduced Arnoldi decomposition



ROTATIONALLY IMPLICITLY RESTARTED EXTENDED KRYLOV (RIREK)

An example for

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

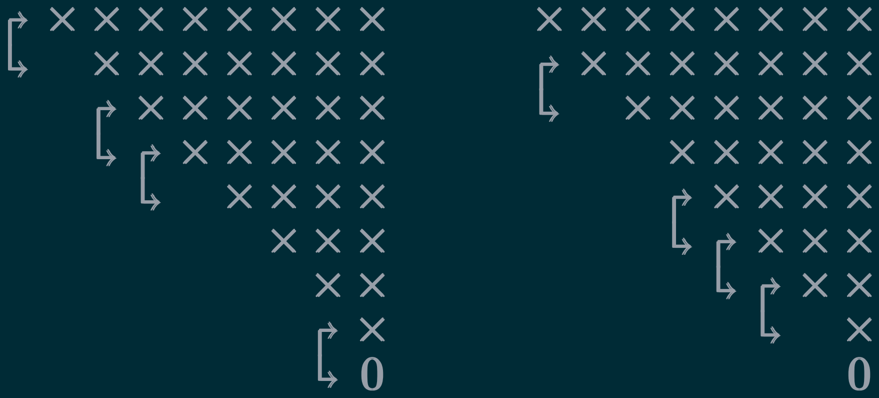
STEP 1: TRANSFORM THE PENCIL TO SUITABLE COMPRESSED FORMAT

Two options:

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

Option 1: left removal of K rotations

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



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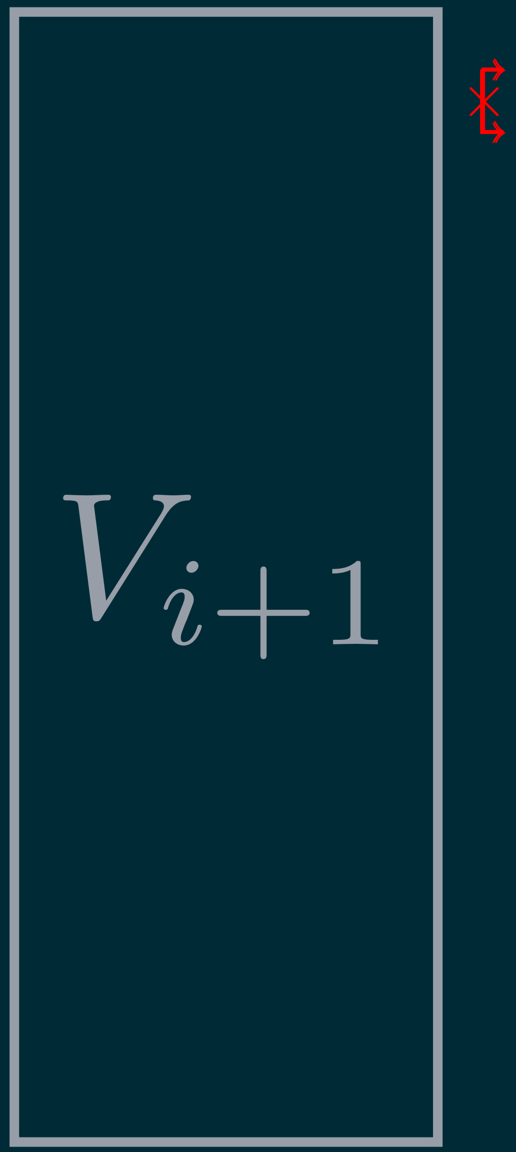

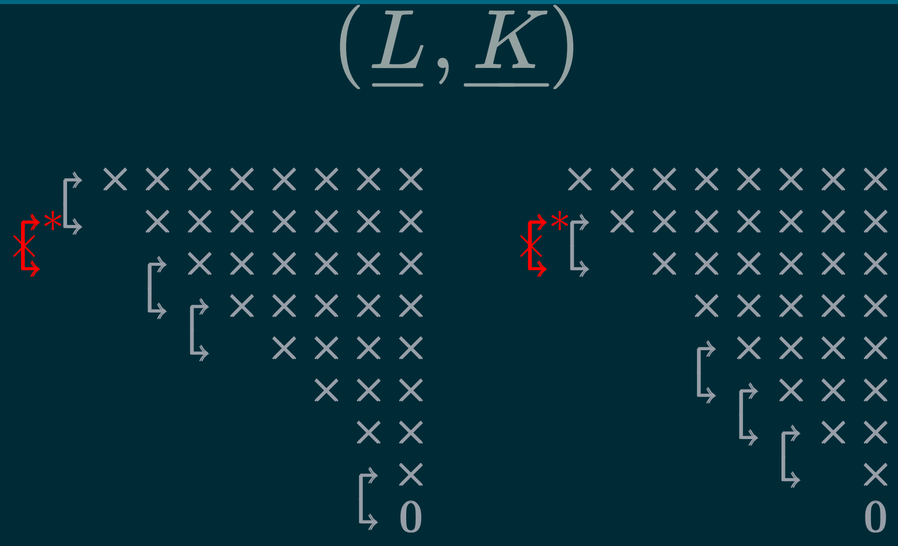

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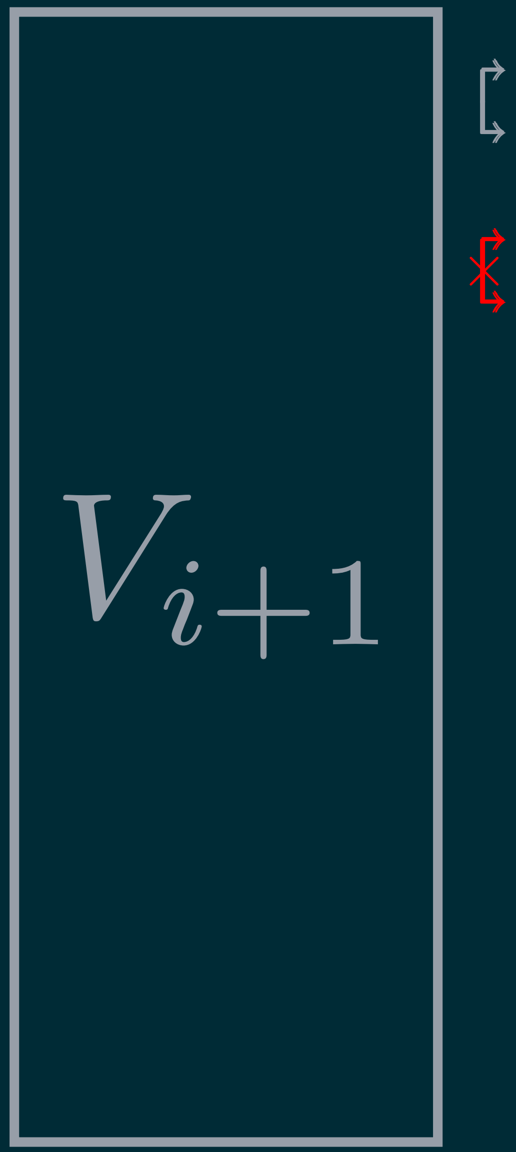

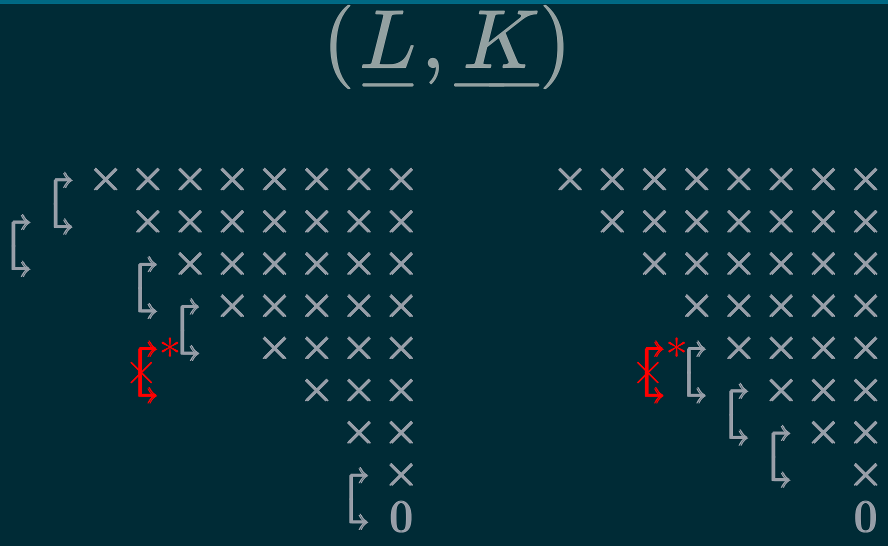

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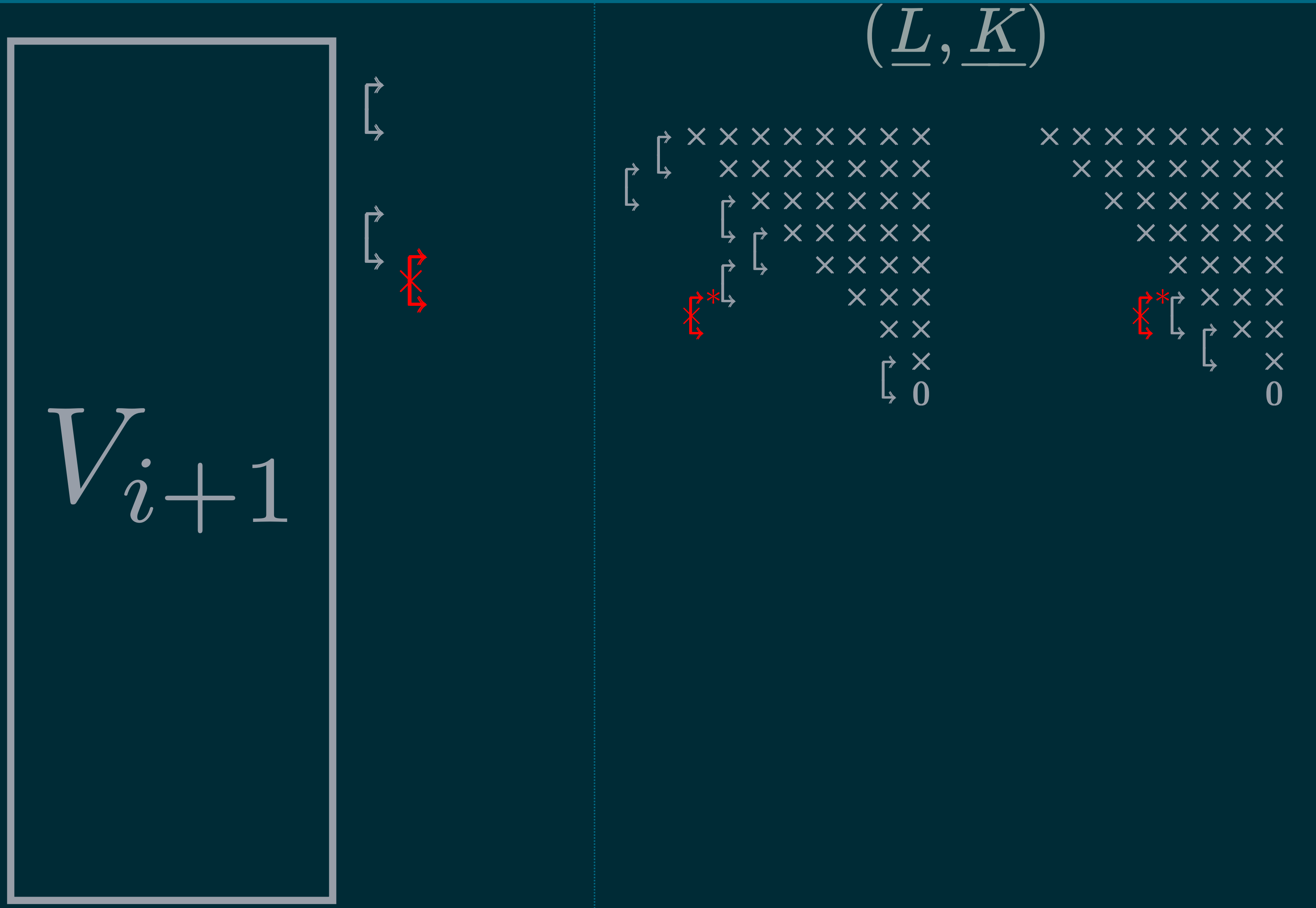

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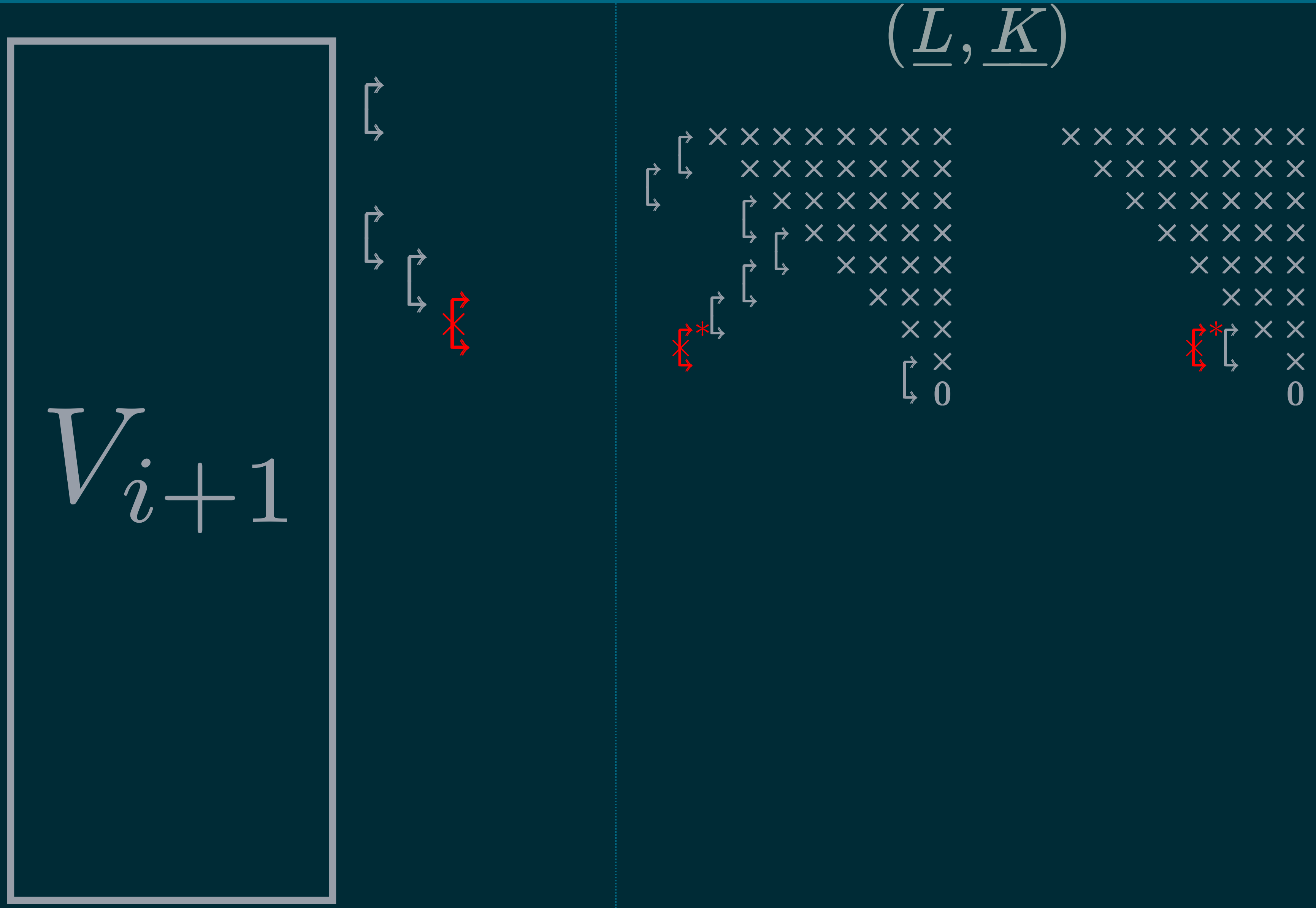

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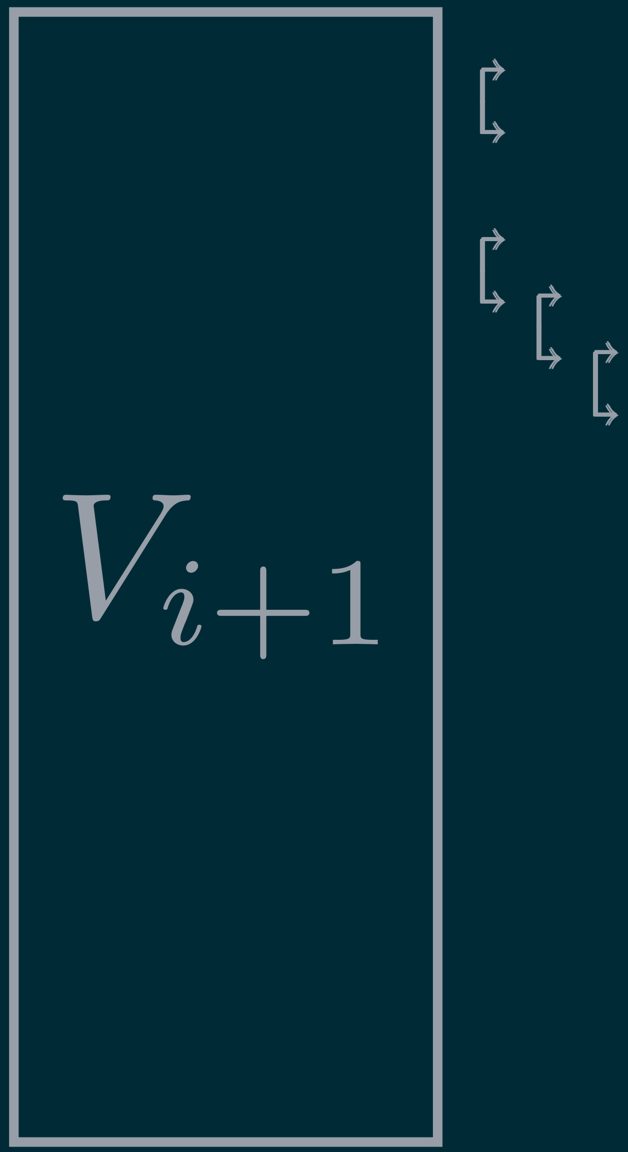
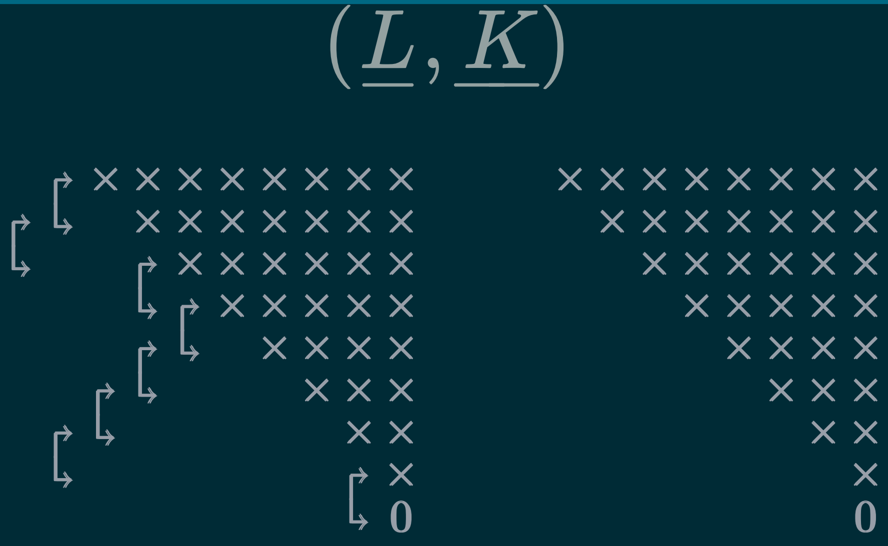
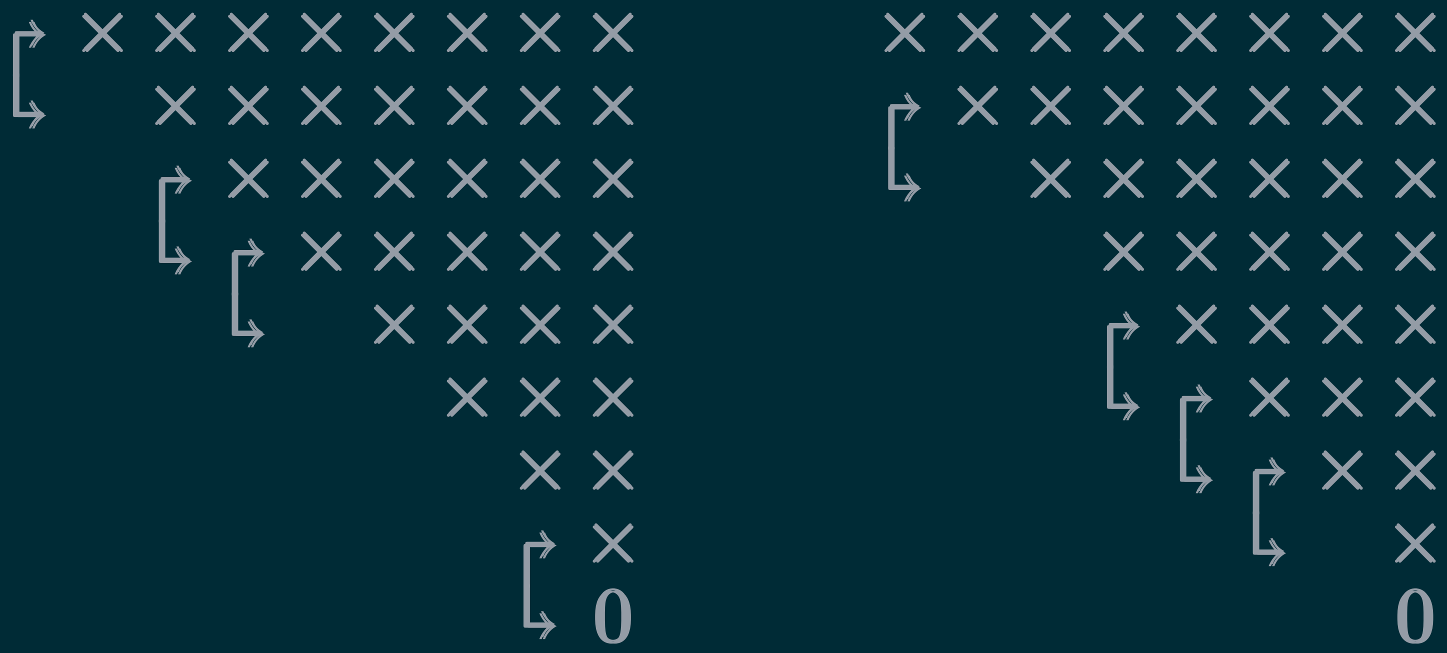




Option 2: right removal of K rotations

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



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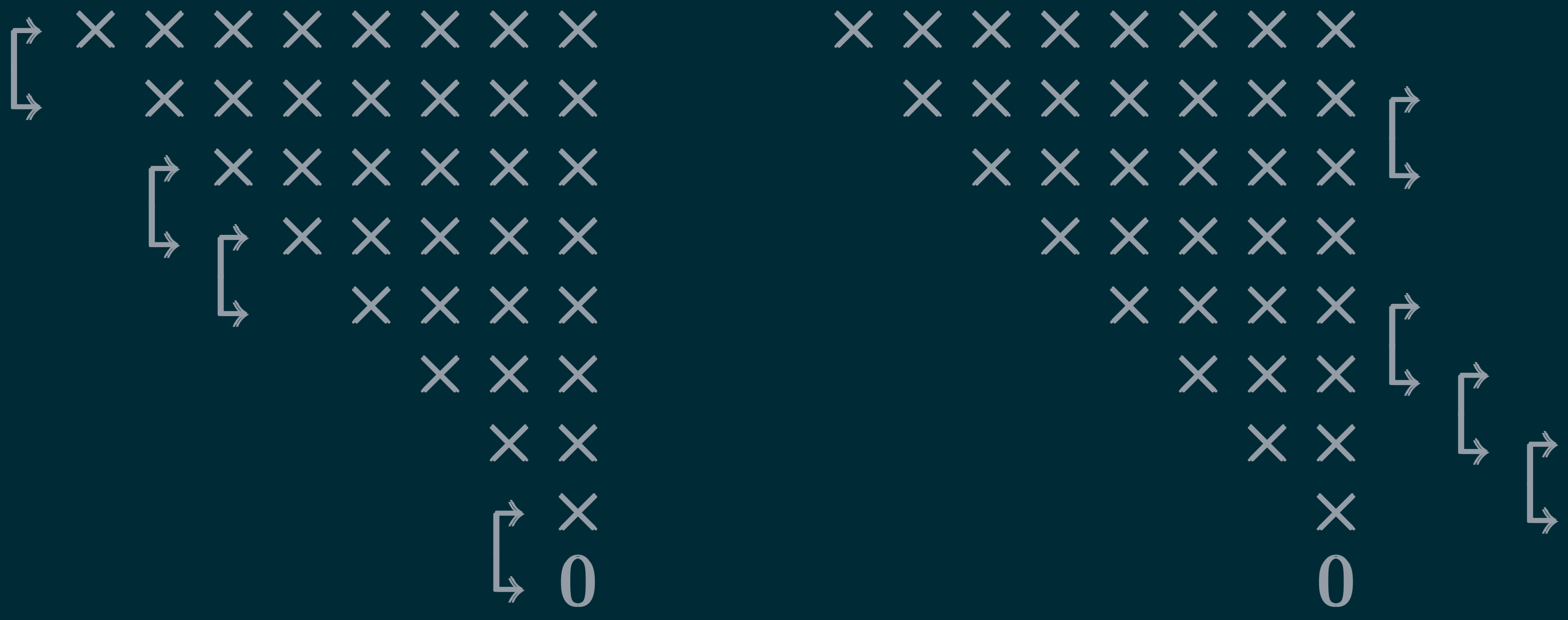

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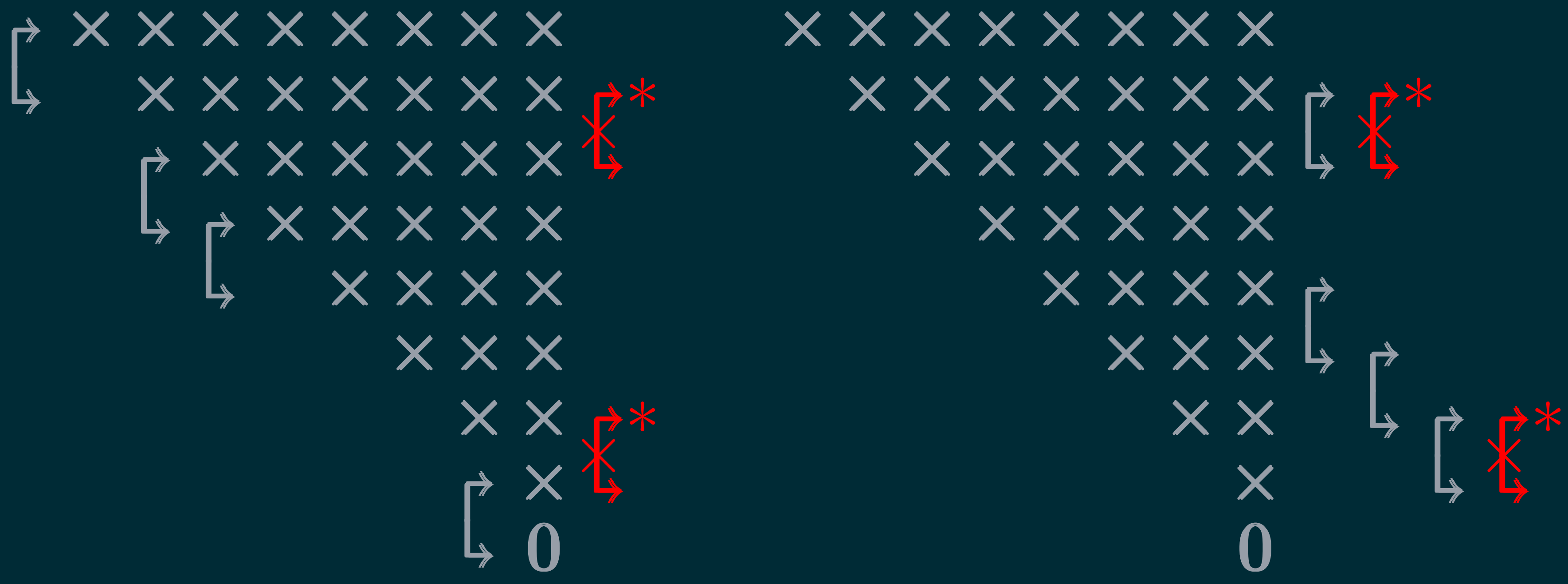

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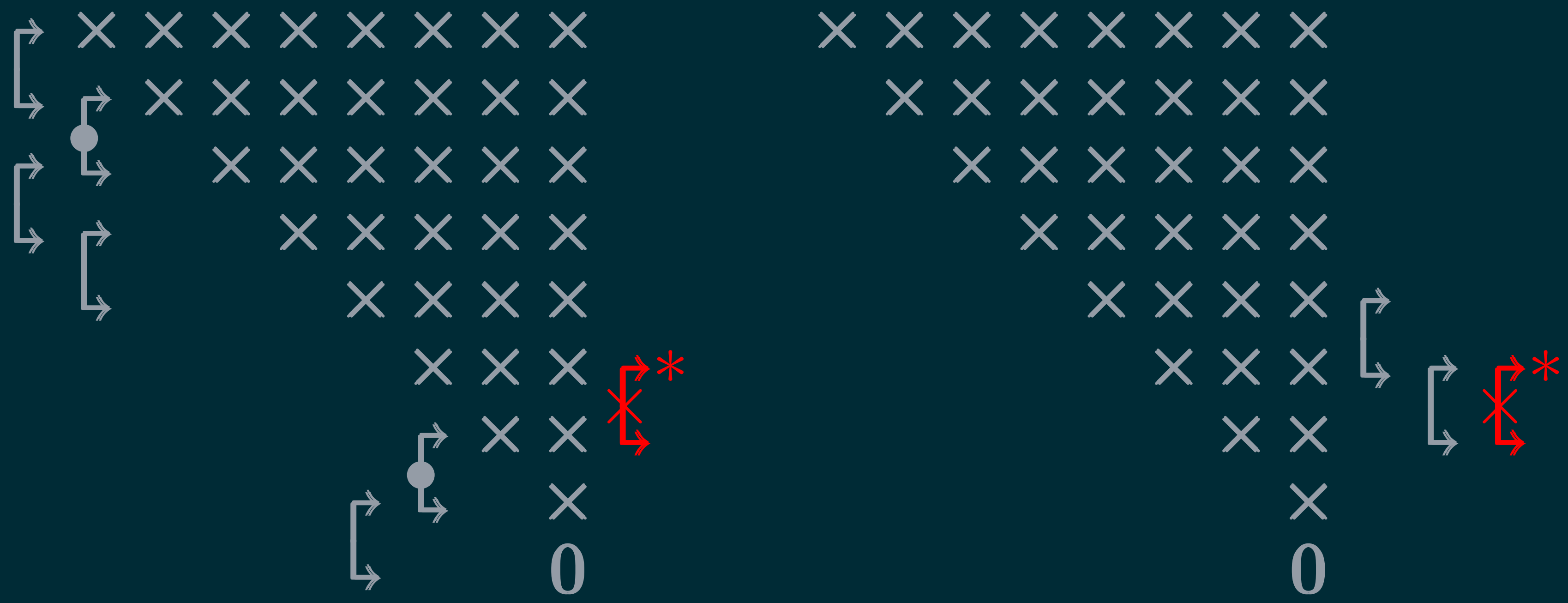

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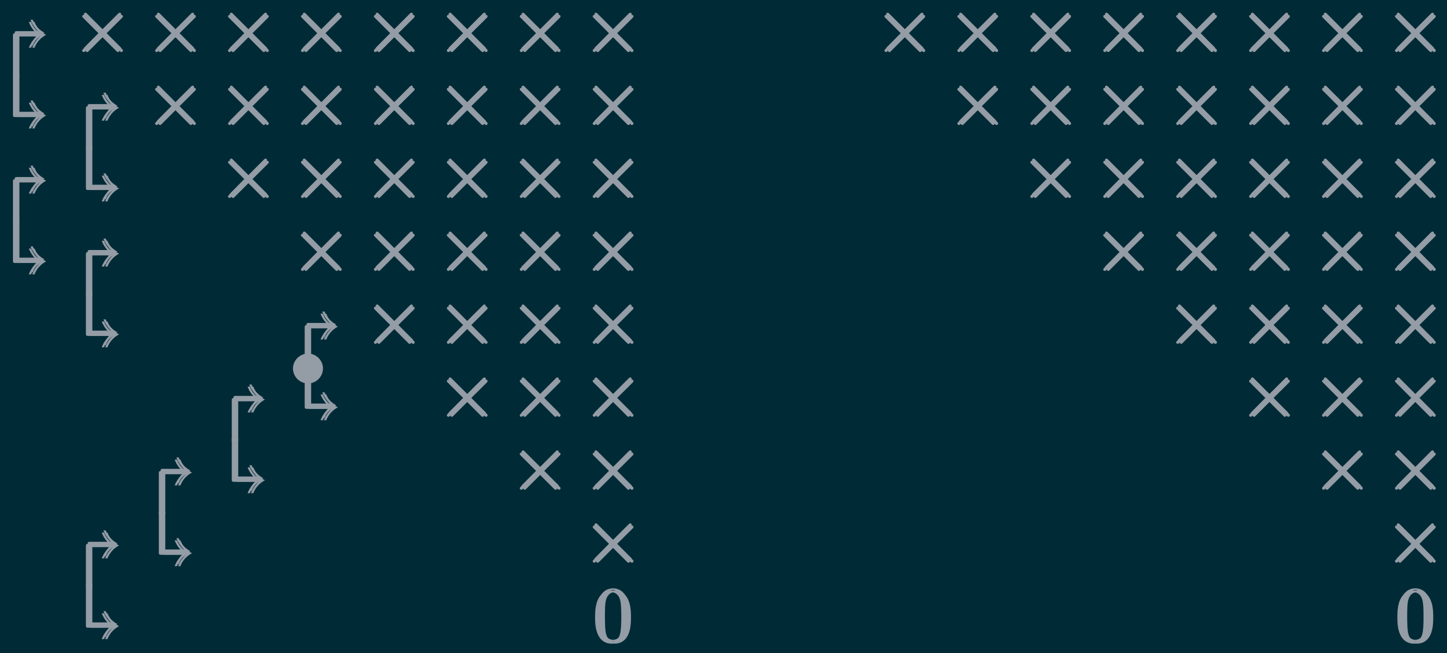
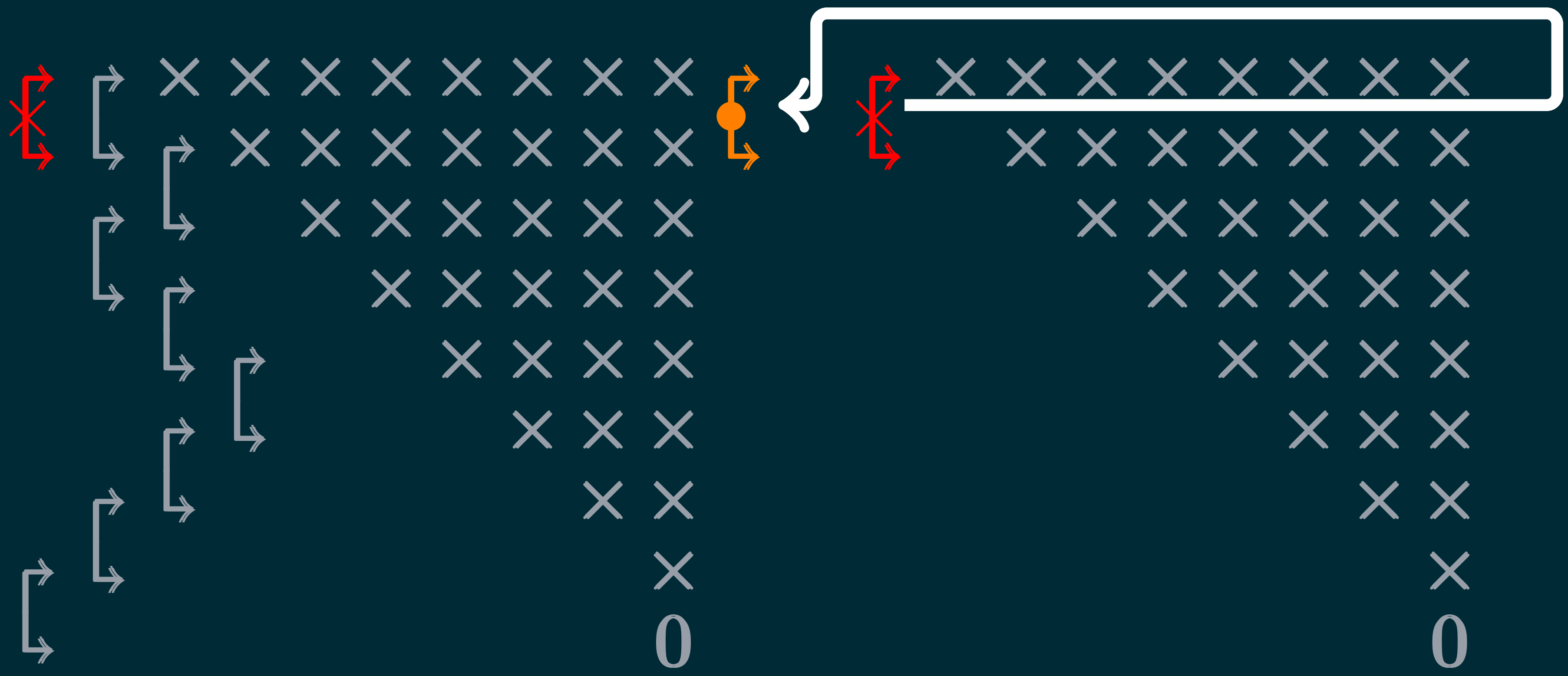


STEP 2: PERTURB THE PENCIL AND CHASE THE PERTURBATION DOWNWARDS

Chasing procedure

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



Chasing procedure

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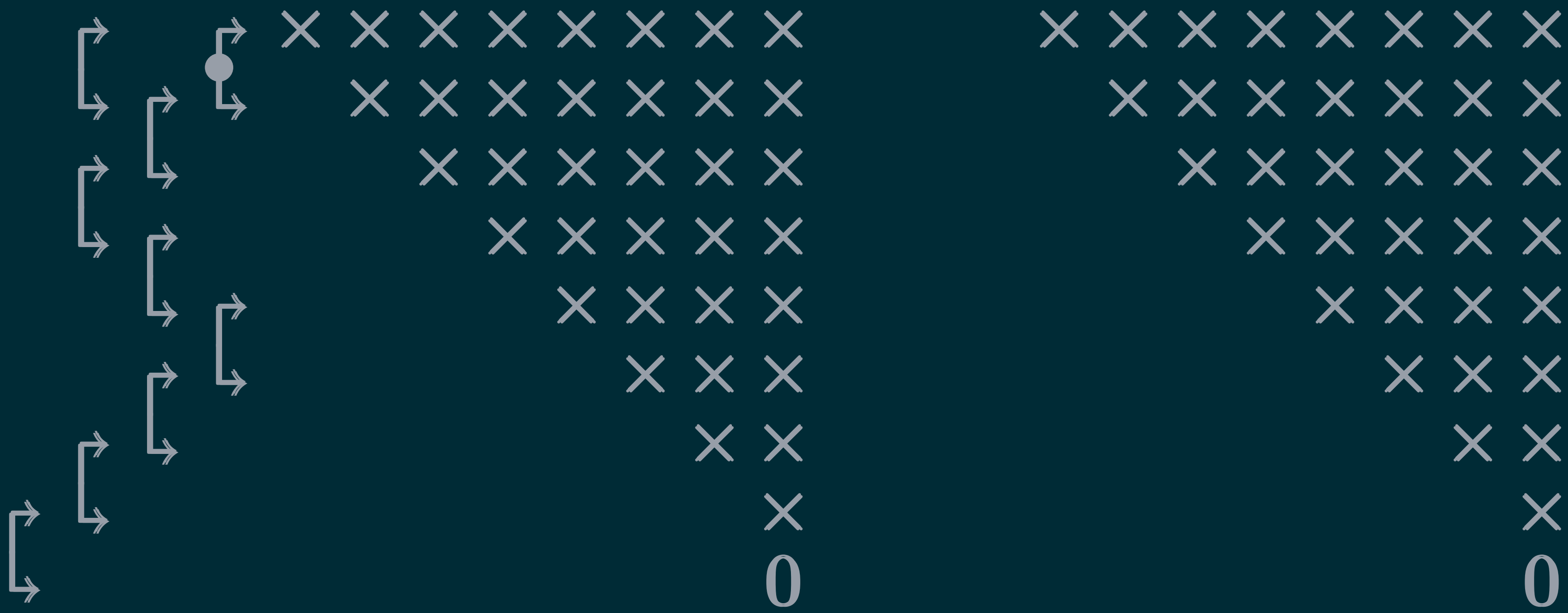

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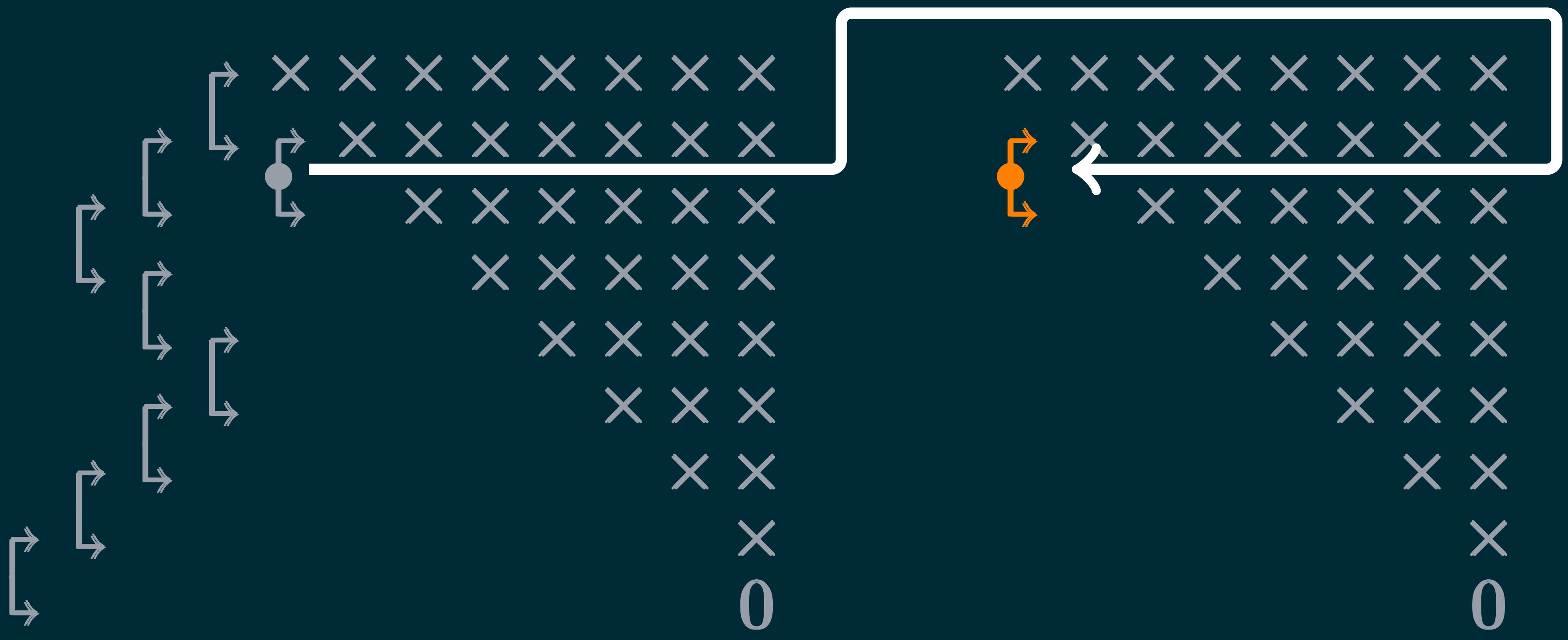

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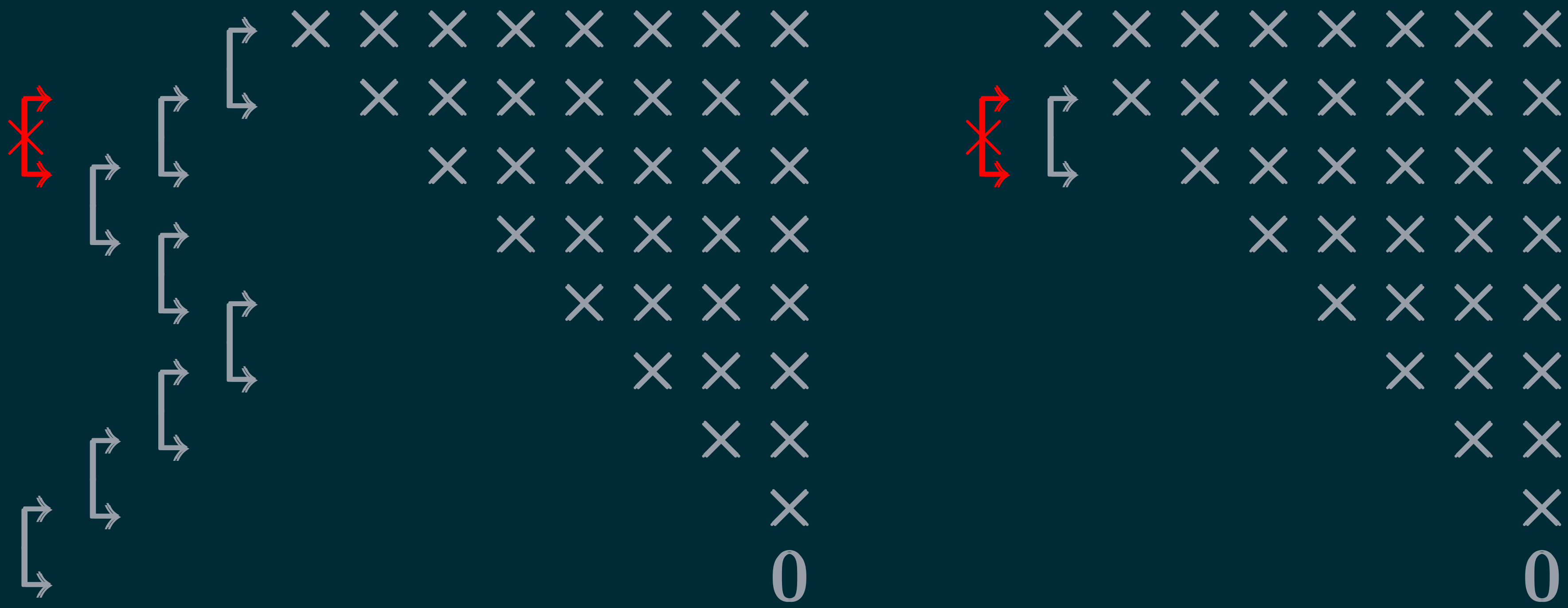

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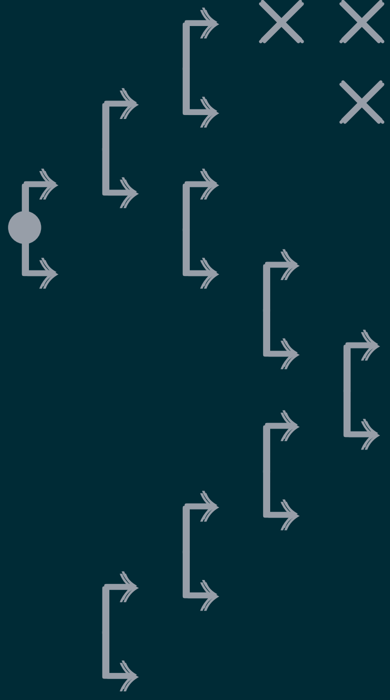

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Chasing procedure

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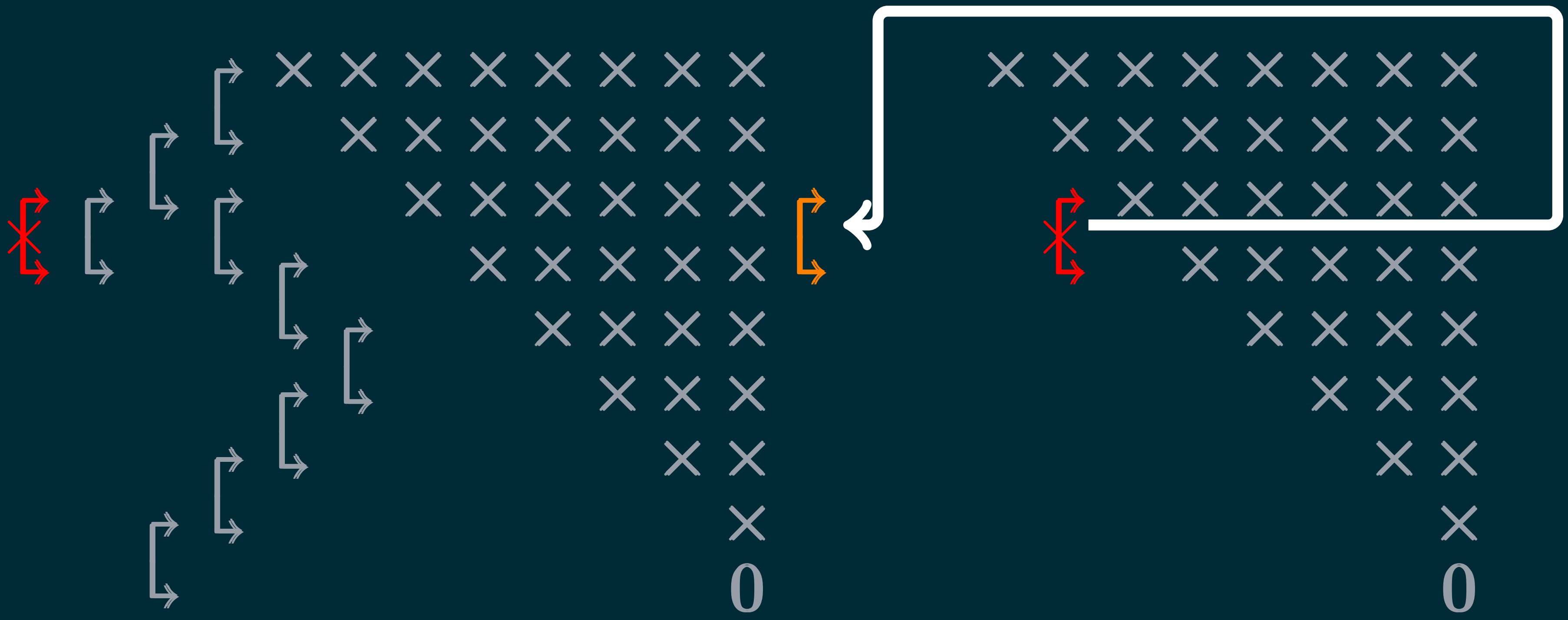

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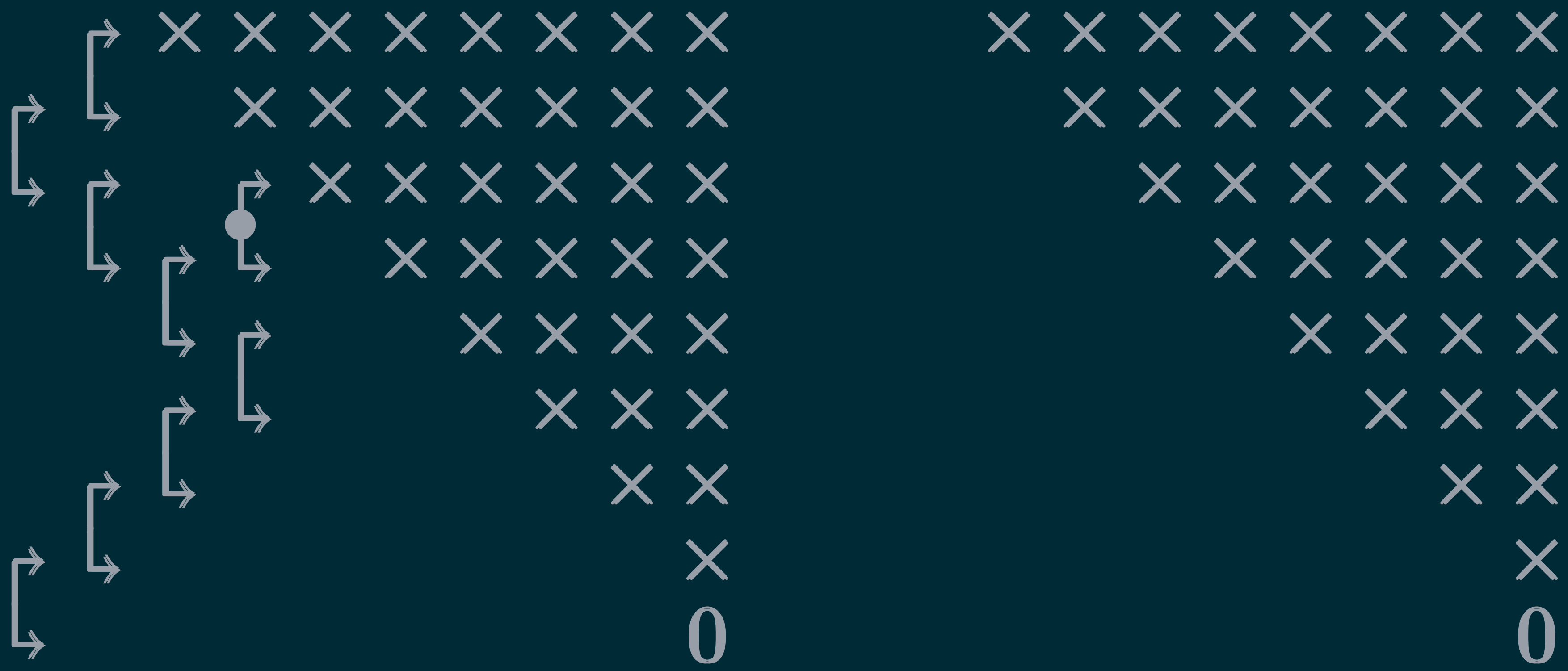

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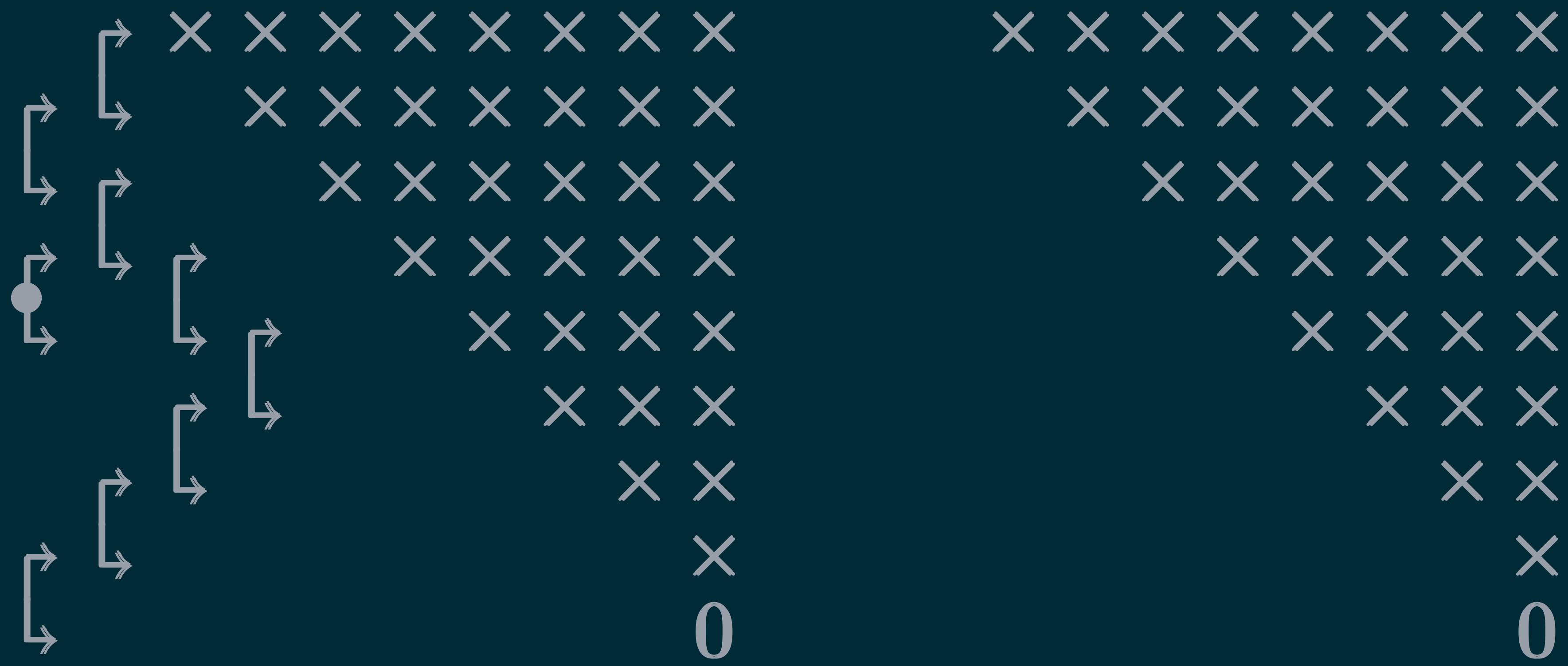
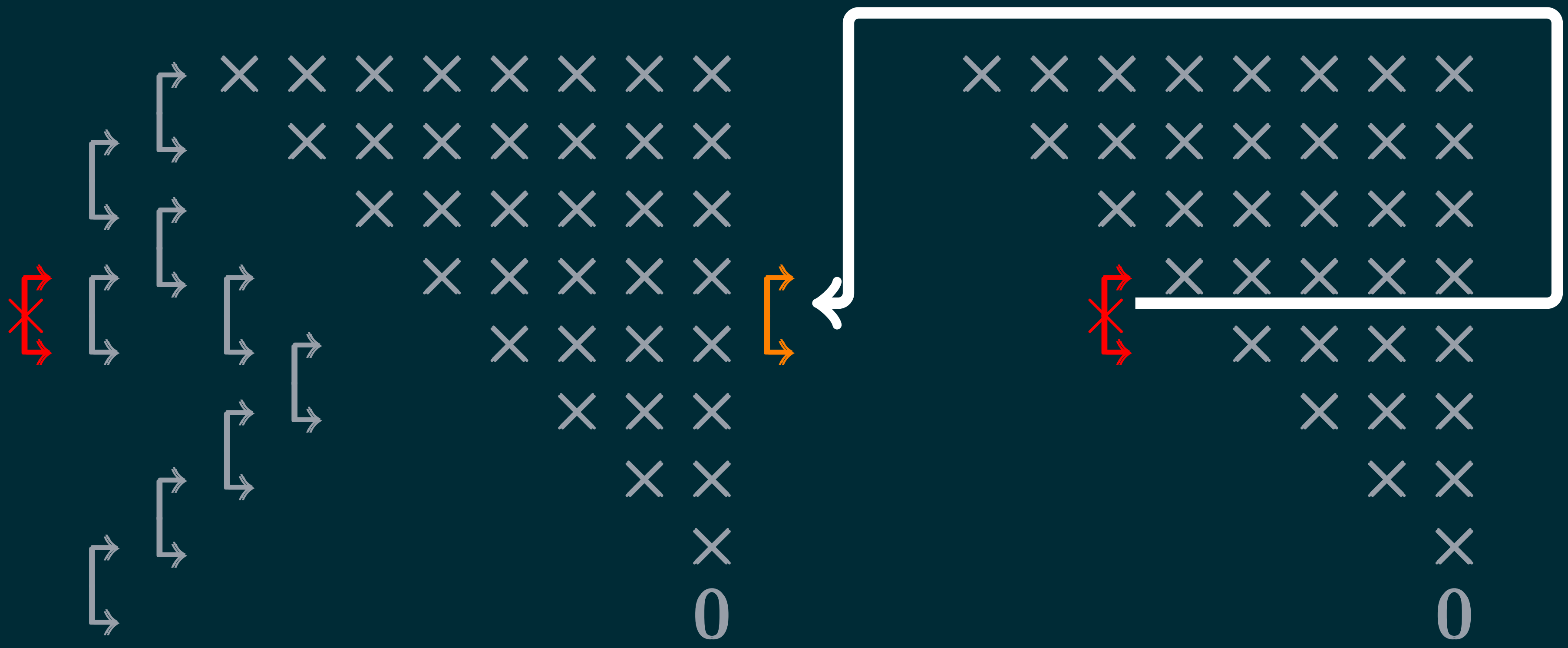


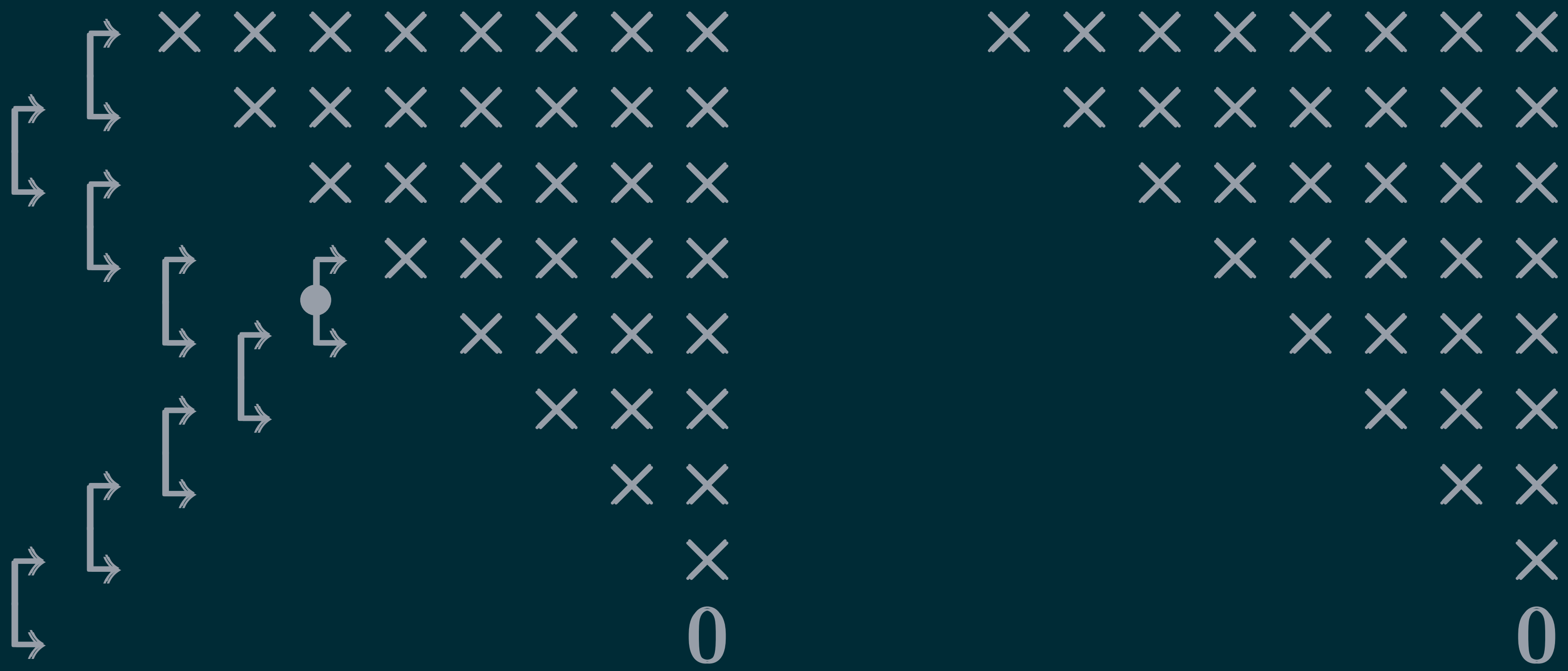
Chasing procedure

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



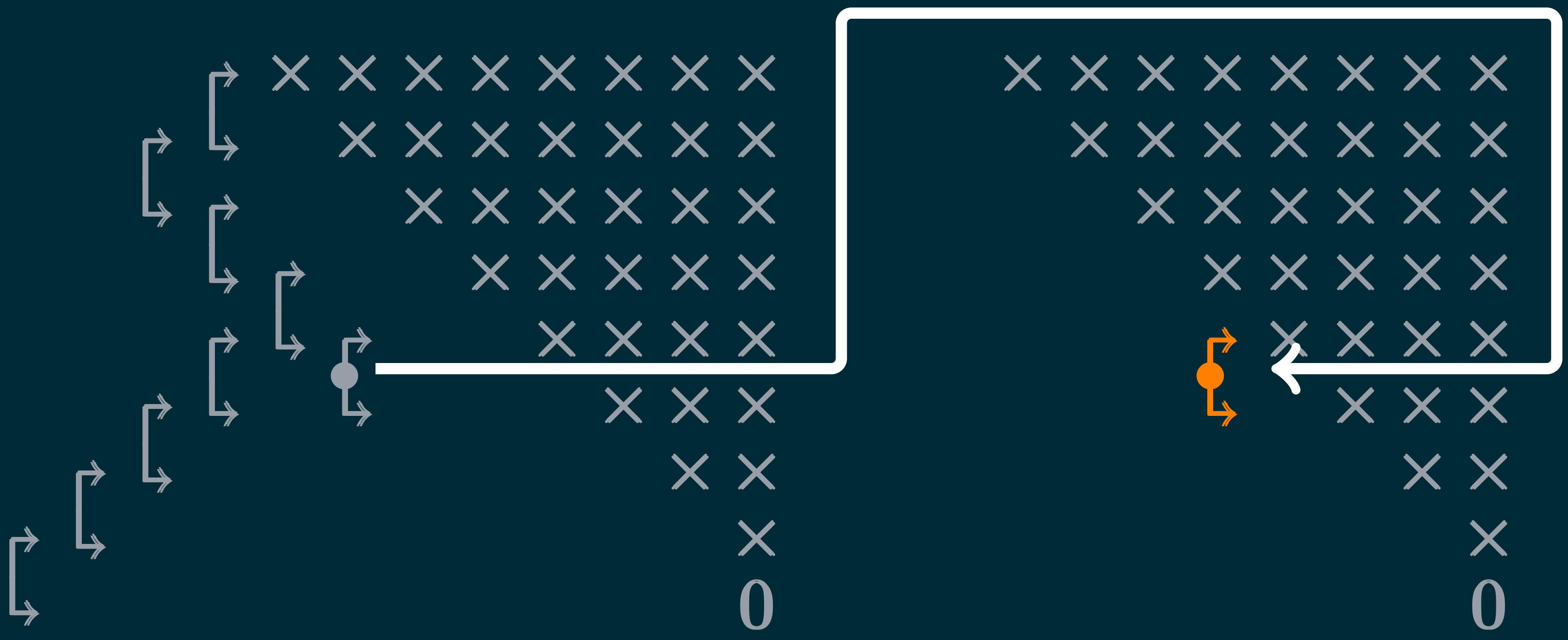
Chasing procedure

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



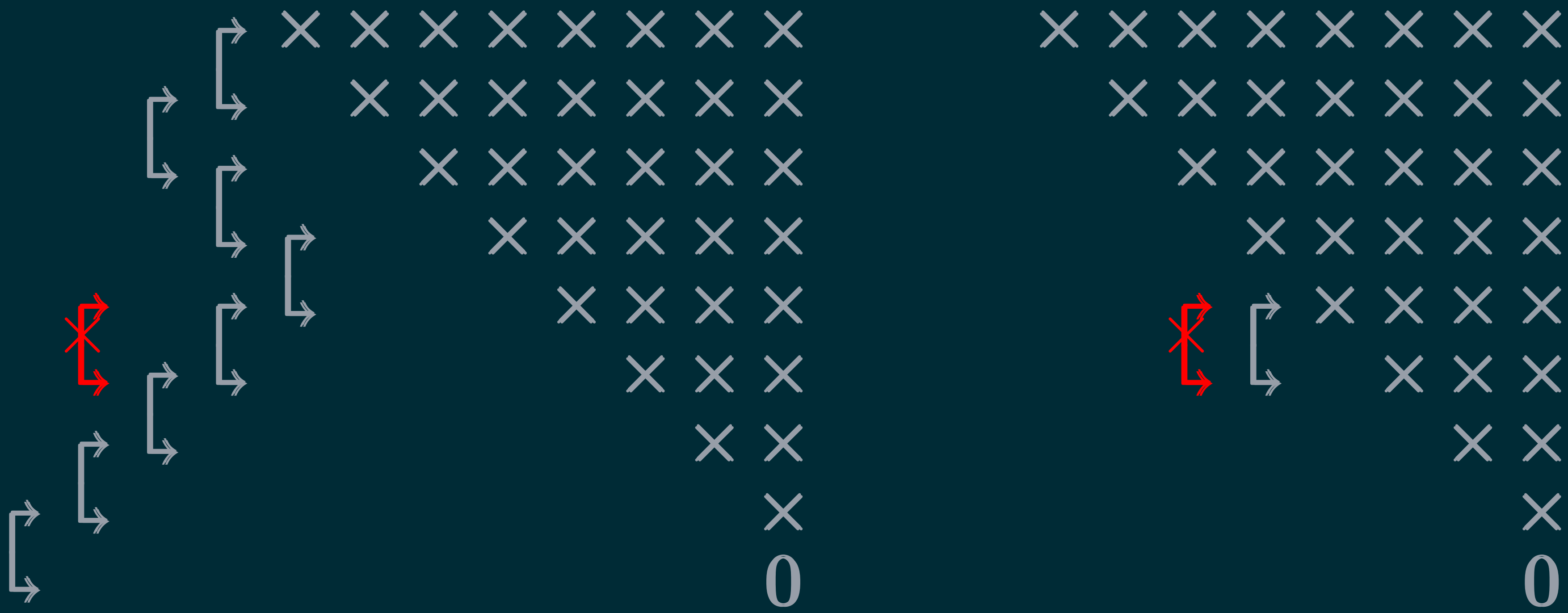
Chasing procedure

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



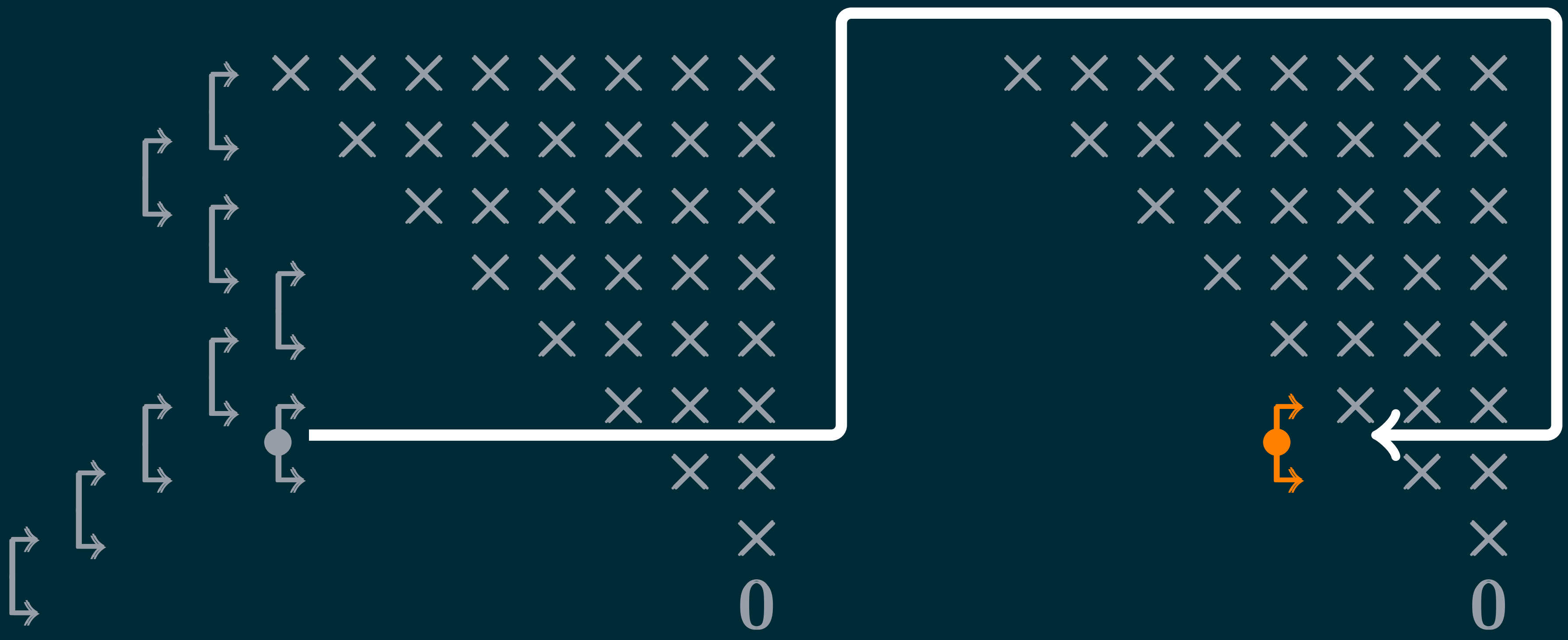
Chasing procedure

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



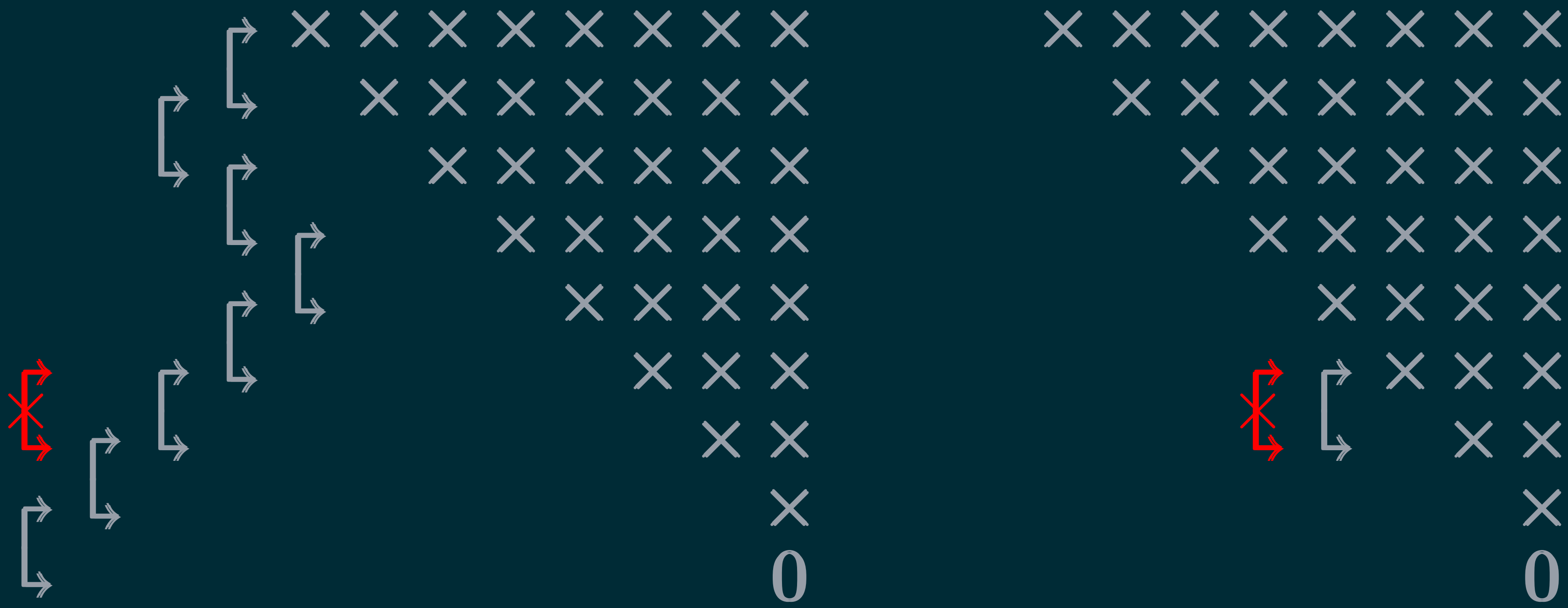
Chasing procedure

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



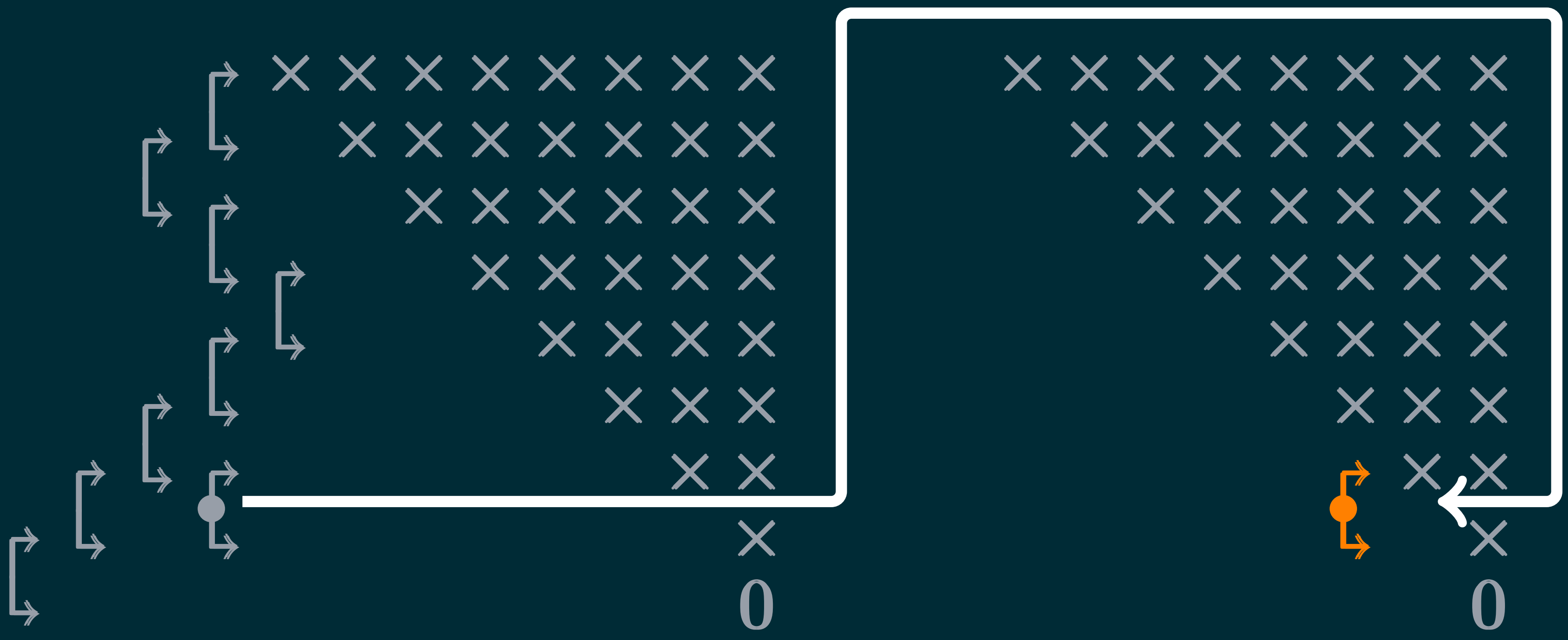
Chasing procedure

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



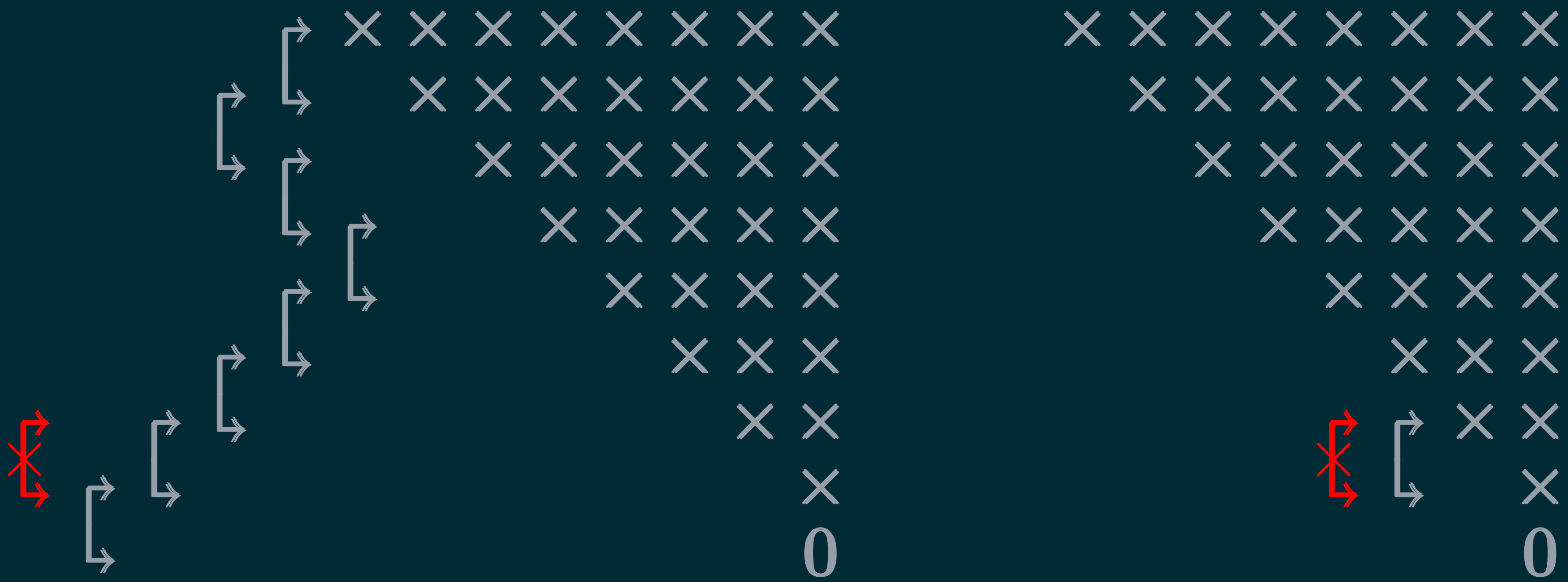
Chasing procedure

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



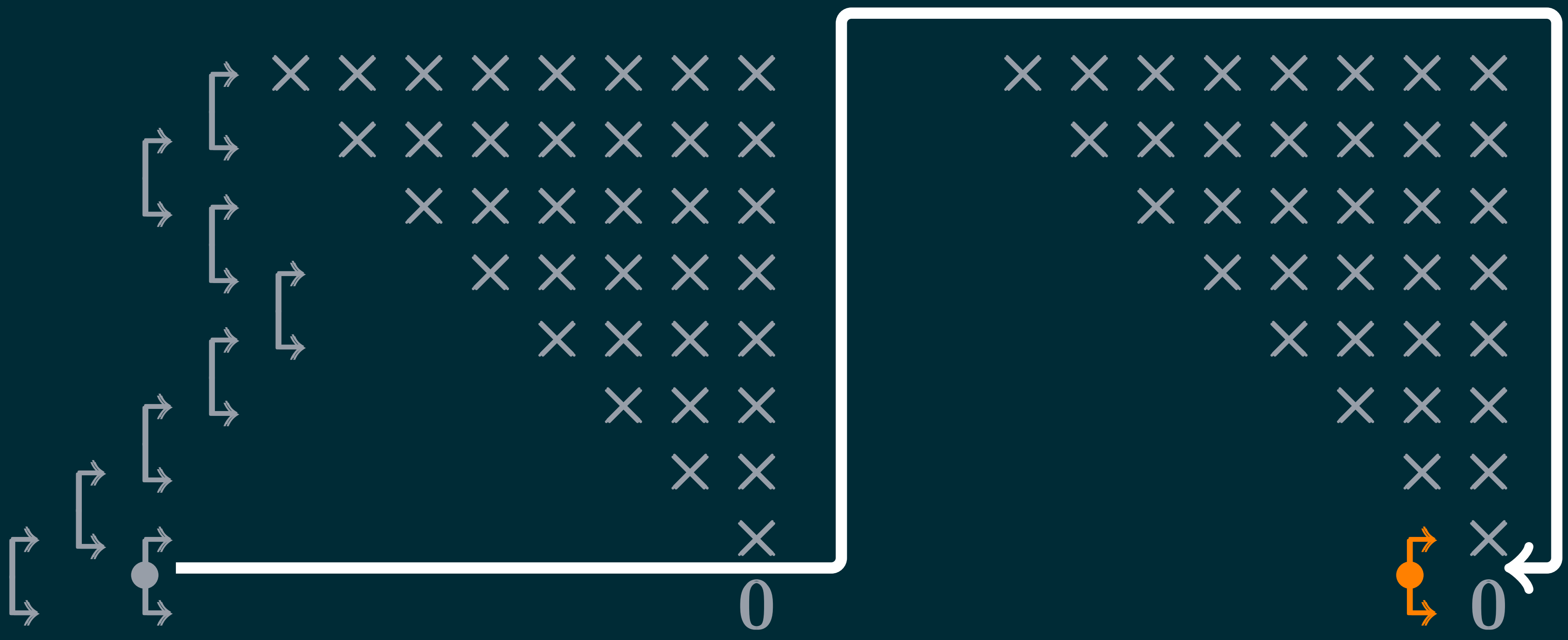
Chasing procedure

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



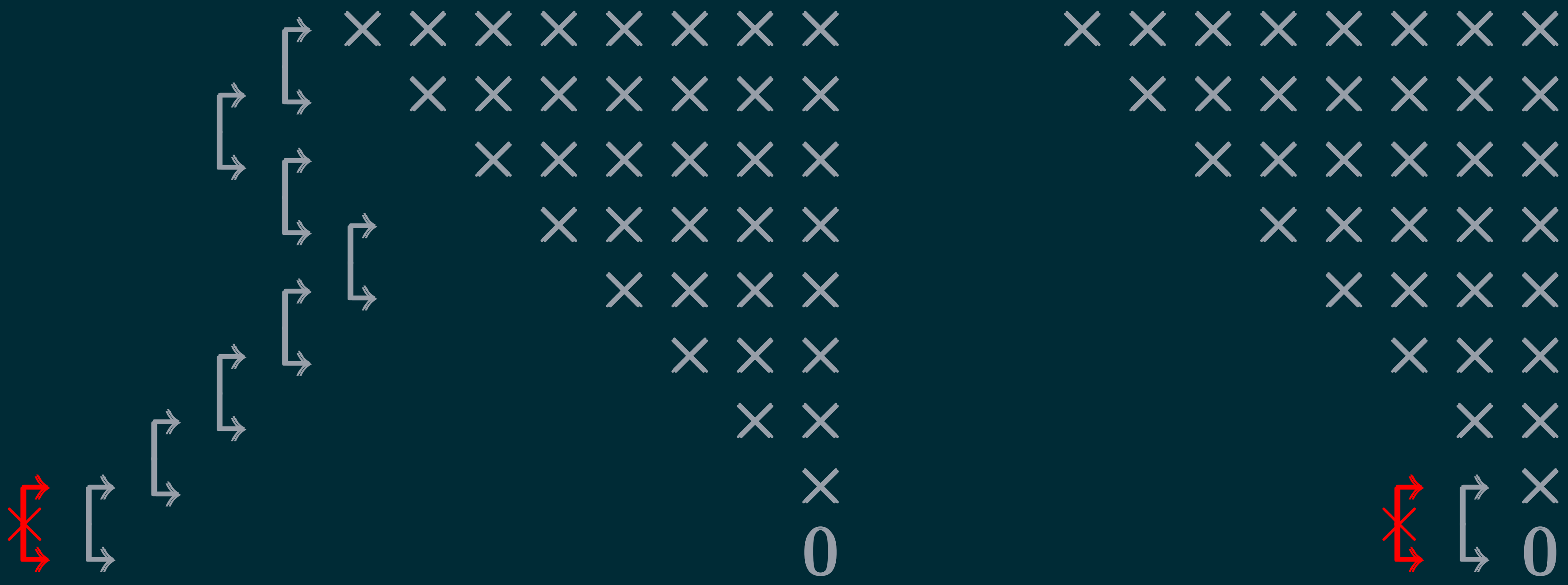
Chasing procedure

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



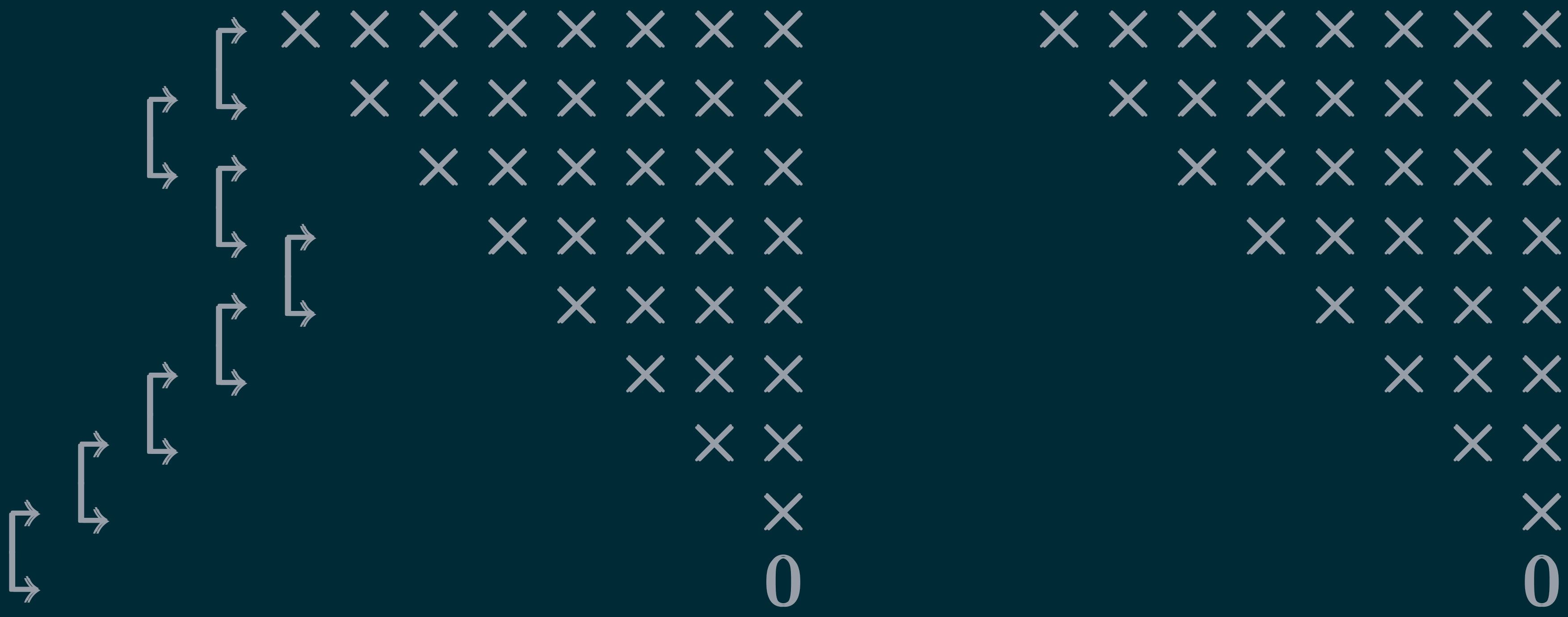
Chasing procedure

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



Chasing procedure

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




NUMERICAL EXAMPLE

BRUSSELATOR MODEL

[De Samblanx, 1997]

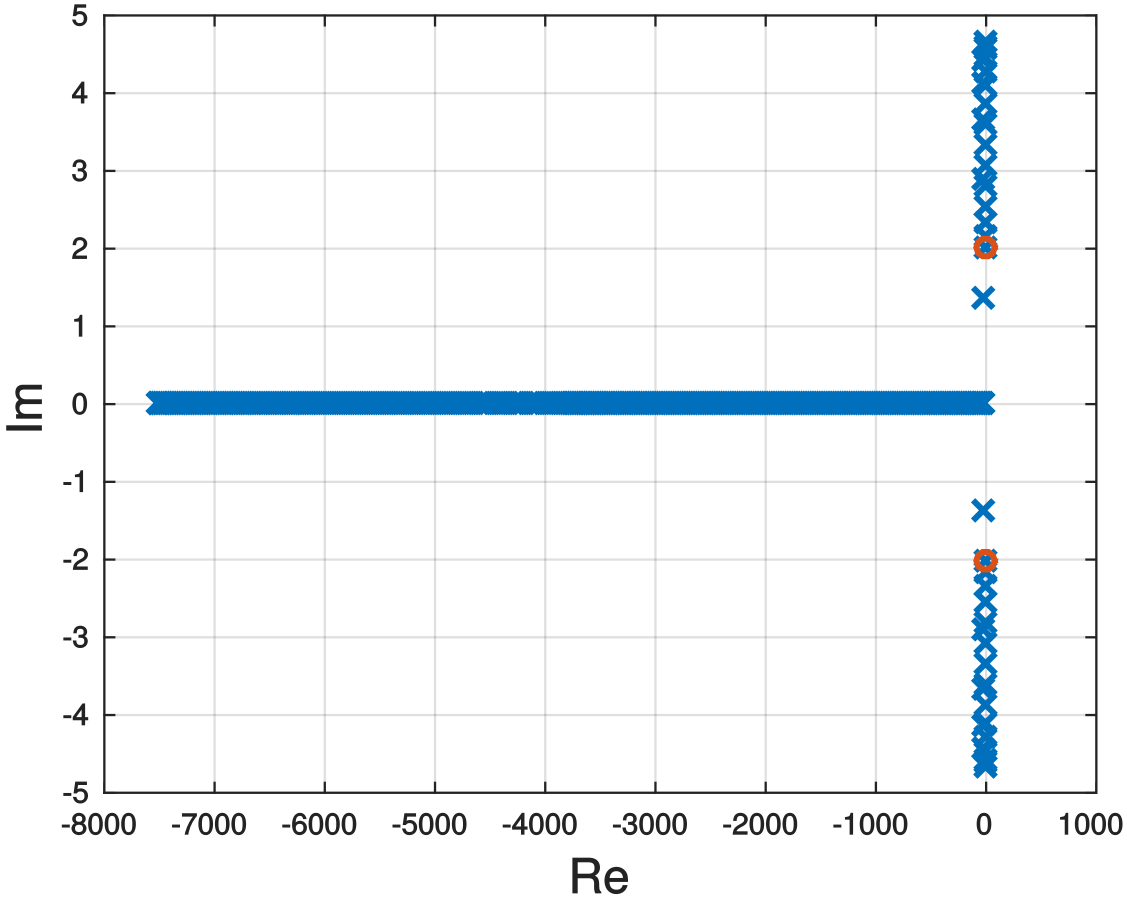
2D reaction-diffusion model

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

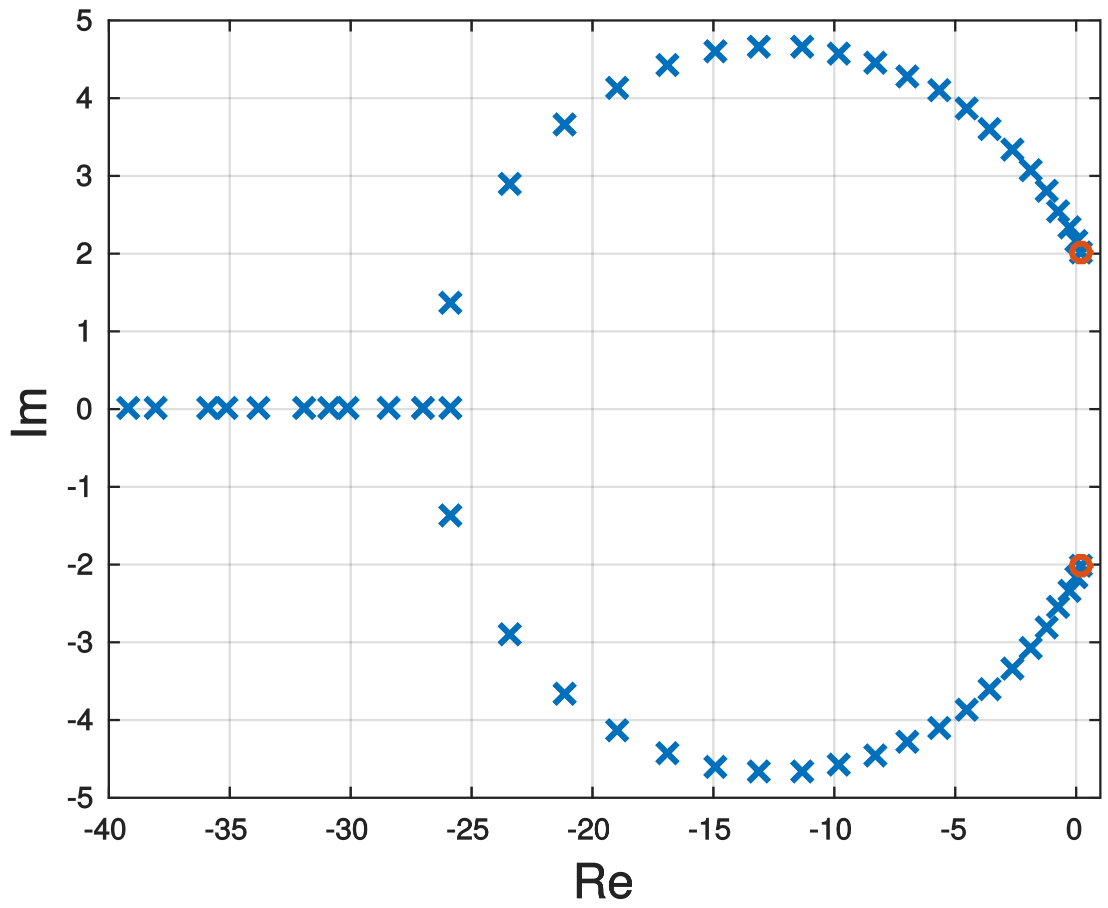
$$\frac{\partial v}{\partial t} = \frac{D_v}{L^2}\left[\frac{\partial^2 v}{\partial X^2} + \frac{\partial^2 v}{\partial Y^2}\right] - u^2 v + Bu$$

- 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 $L = 1$

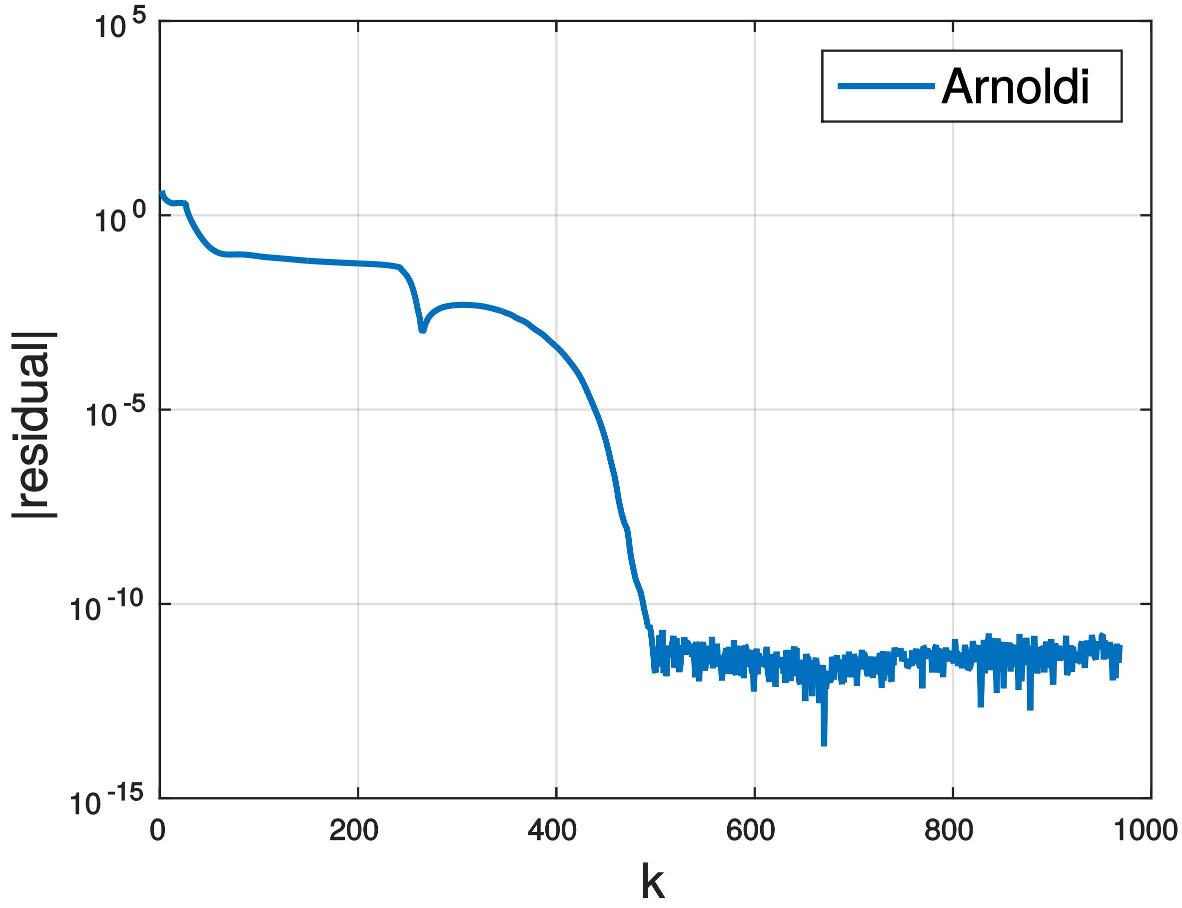
Matrix $A \in \mathbb{C}^{968\times968}$



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

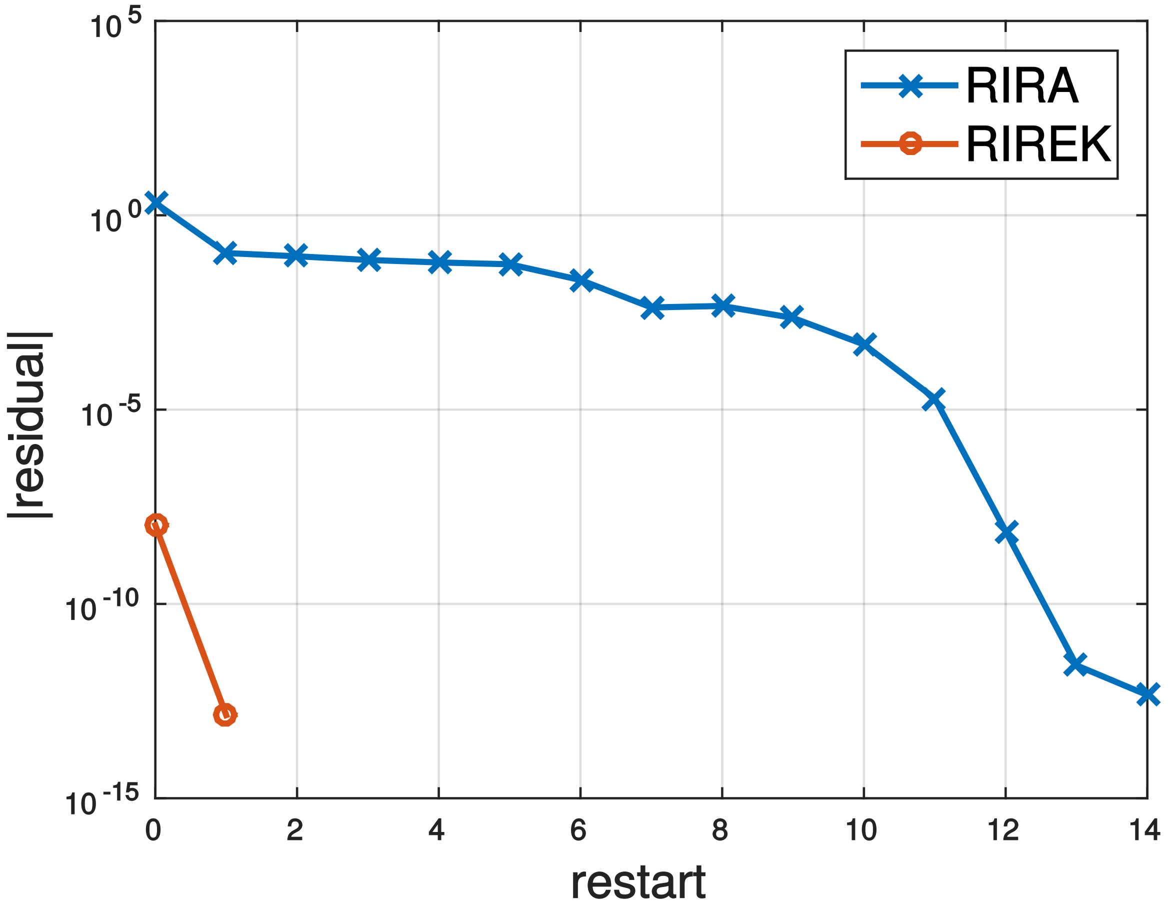


Arnoldi



Arnoldi
|residual|
10 5
10 0
10 -5
10 -10
10 -15
0
200
400
600
800
1000
k

RIRA & RIREK



10^5
10^0
10^-5
10^-10
10^-15
|residual|
0
2
4
6
8
10
12
14
restart
RIRA
RIREK

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