#### Matrix structures in queuing models

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# Exploiting Hidden Structure in Matrix Computations. Algorithms and Applications



- Structures
- Markov chains and queuing models
- 2 Fundamentals on structured matrices
  - Toeplitz matrices
  - Rank structured matrices
- 8 Algorithms for structured Markov chains: the finite case
  - Block tridiagonal matrices
  - Block Hessenberg matrices
  - A functional interpretation
  - Some special cases
  - 4 Algorithms for structured Markov Chains: the infinite case
    - Wiener-Hopf factorization
    - Solving matrix equations
    - Shifting techniques
    - Tree-like processes
    - Vector equations
    - Exponential of a block triangular block Toeplitz matrix

## 1- Introduction

Structures

#### Markov chains and queuing models

- Markov chains
- random walk
- bidimensional random walk
- shortest queue model
- M/G/1, G/M/1, QBD processes
- other structures
- computational problems

#### About structures

Structure analysis in mathematics is important not only for algorithm design and applications but also for the variety, richness and beauty of the mathematical tools that are involved in the research.

Alexander Grothendieck, who received the Fields medal in 1966, said:

"If there is one thing in mathematics that fascinates me more than anything else (and doubtless always has), it is neither number nor size, but always form. And among the thousand-and-one faces whereby form chooses to reveal itself to us, the one that fascinates me more than any other and continues to fascinate me, is the structure hidden in mathematical things."

In linear algebra, structures reveal themselves in terms of matrix properties

Their analysis and exploitation is not just a challenge but it is also a mandatory step which is needed to design highly effective *ad hoc* algorithms for solving large scale problems from applications

The structure of a matrix reflects the peculiarity of the mathematical model that the matrix describes

Often, structures reveal themselves in a clear form. Very often they are hidden and hard to discover.

Here are some examples of structures, with the properties of the physical model that they represent, the associated algorithms and their complexities

## Clear structures: Toeplitz matrices

Definition:  $A = (a_{i,j}), a_{i,j} = \alpha_{j-i}$ 

Original property: shift invariance (polynomials and power series, convolutions, derivatives, PSF, correlations, time-series, etc.)

Multidimensional problems lead to block Toeplitz matrices with Toeplitz blocks

Algorithms: based on FFT

- Multiplying an  $n \times n$  matrix and a vector costs  $O(n \log n)$
- Solving a Toeplitz system costs  $O(n^2)$  (Trench-Zohar-Levinson-Schur)  $O(n \log^2 n)$  Bitmead-Anderson, Musicus, Ammar-Gregg
- Preconditioned Conjugate Gradient:  $O(n \log n)$

### Clear structures: band matrices

Band matrices: 2k + 1-diagonal matrices

Definition:  $A = (a_{i,j})$ ,  $a_{i,j} = 0$  for |i - j| > k

Original property: Locality of some operators (PSF, finite difference approximation of derivatives)

Multidimensional problems lead to block band matrices with banded blocks

#### Algorithms:

- A  $n \times n \rightarrow$  LU and QR in  $O(nk^2)$  ops
- Solving linear systems  $O(nk^2)$
- QR iteration for symmetric tridiagonal matrices costs O(n) per step

#### Hidden structures: Toeplitz-like

Toeplitz like matrices:

20	15	10	5]
4	23	17	11
8	10	27	19
4	11	12	28

The inverse of a Toeplitz matrix is not generally Toeplitz. It maintains a structure of the form  $L_1U_1 + L_2U_2$  where  $L_i$ ,  $U_i^T$  are lower triangular Toeplitz, for i = 1, 2

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 $A - ZAZ^T$  and ZA - AZ have rank at most 2k for z =

Displacement operators, displacement rank

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

#### Hidden structures: rank-structured matrices

	11	T	3	4	2
	1 2 6 8	8	4		
Quasiseparable matrices:	6	12	-3	-4	-2
-	4	8	-2	6	3
	L2	4	$^{-1}$	3	8 _

The inverse of a tridiagonal matrix A is not generally banded

However, if A is nonsingular, the submatrices of  $A^{-1}$  contained in the upper (or lower) triangular part have rank at most 1. If A is also irreducible then

$$A^{-1} = \operatorname{tril}(uv^T) + \operatorname{triu}(wz^T), \quad u, v, w, z \in \mathbb{R}^n$$

Rank-structured matrices (quasi-separable, semi-separable) share this property, the submatrices contained in the upper/lower triangular part have rank bounded by k << n

This structure is hardly detectable

A wide literature exists in this regard

Markov chains and queuing models

### Markov chains and queuing models

A research area where structured matrices play an important role is Markov Chains and Queuing Models.

Just few words about Markov chains and then some important examples.

Stochastic process: Family  $\{X_t \in E : t \in T\}$ 

- X<sub>t</sub>: random variables
- E: state space (denumerable)  $E = \mathbb{N}$
- T: time space (denumerable)  $T = \mathbb{N}$

Example:  $X_t$  number of customers in the line at time t

Notation:  $\mathcal{P}(X = a | Y = b)$  conditional probability that X = a given that Y = b.

Markov chain: Stochastic process  $\{X_n\}_{n \in T}$  such that

$$\mathcal{P}(X_{n+1} = j | X_0 = i_0, X_1 = i_1, \dots, X_n = i_n) =$$
  
 $\mathcal{P}(X_{n+1} = j | X_n = i_n)$ 

The state  $X_{n+1}$  of the system at time n+1 depends only on the state  $X_n$  at time n. It does not depend on the past history of the system

Homogeneity assumption:  $\mathcal{P}(X_{n+1} = j | X_n = i) = \mathcal{P}(X_1 = j | X_0 = i) \quad \forall n$ 

Transition matrix of the Markov chain:

$$P = (p_{i,j})_{i,j\in T}, \qquad p_{i,j} = \mathcal{P}(X_1 = j | X_0 = i).$$

*P* is row-stochastic:  $p_{i,j} \ge 0$ ,  $\sum_{j \in T} p_{i,j} = 1$ . Equivalently: Pe = e,  $e = (1, 1, ..., 1)^T$ . Properties: If  $x^{(k)} = (x^{(k)})_i$  is the probability (row) vector of the Markov chain at time k, that is,  $x_i^{(k)} = \mathcal{P}(X_k = i)$ , then

$$x^{(k+1)} = x^{(k)}P, \quad k \ge 0$$

If the limit  $\pi = \lim_k x^{(k)}$  exists, then by continuity

$$\pi = \pi P$$

 $\pi$  is said the stationary probability vector

If P is finite then the Perron-Frobenius theorem provides the answers to all the questions

Define the spectral radius of an  $n \times n$  matrix A as

$$\rho(A) = \max_{i} |\lambda_i(A)|, \quad \lambda_i(A) \text{ eigenvalue of } A$$

**Theorem** [Perron-Frobenius] Let  $A = (a_{i,j})$  be an  $n \times n$  matrix such that  $a_{i,j} \ge 0$ , let A be irreducible then

- the spectral radius  $\rho(A)$  is a positive simple eigenvalue
- the corresponding right and left eigenvectors are positive
- if  $B \ge A$  and  $B \ne A$  then  $\rho(B) > \rho(A)$

In the case of P, if any other eigenvalue of P has modulus less than 1, then  $\lim P^k = e\pi$  and for any  $x^{(0)} \ge 0$  such that  $x^{(0)}e = 1$  it holds

$$\lim_{k} x^{(k)} = \pi, \quad \pi^{T} P = \pi^{T}, \quad \pi \mathbf{e} = 1$$

In the case where A is infinite, the situation is more complicated. Assume  $A = (a_{i,j})_{i,j \in \mathbb{N}}$  stochastic and irreducible. The existence of  $\pi > 0$  such that  $\pi \mathbf{e} = 1$  is not guaranteed

Examples:

$$\begin{bmatrix} 0 & 1 & & \\ 3/4 & 0 & 1/4 & & \\ & 3/4 & 0 & 1/4 & & \\ & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}, \qquad \begin{aligned} \pi &= \begin{bmatrix} \frac{1}{2}, \frac{2}{3}, \frac{2}{9}, \frac{2}{27}, \dots \end{bmatrix} \in \ell^{1} \\ \text{positive recurrent} \\ \begin{bmatrix} 0 & 1 & & & \\ 1/4 & 0 & 3/4 & & \\ & 1/4 & 0 & 3/4 & & \\ & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}, \qquad \begin{aligned} \pi &= \begin{bmatrix} 1, 4, 12, 16, \dots \end{bmatrix} \notin \ell^{\infty} \\ \text{negative recurrent} \\ \begin{bmatrix} 0 & 1 & & & \\ 1/2 & 0 & 1/2 & & \\ & & 1/2 & 0 & 1/2 & & \\ & & & \ddots & \ddots & \ddots & \end{bmatrix}, \qquad \begin{aligned} \pi &= \begin{bmatrix} 1/2, 1, 1, \dots \end{bmatrix} \notin \ell^{1} \\ \text{null recurrent} \end{aligned}$$

Intuitively, positive recurrence means that the global probability that the state changes into a "forward" state is less than the global probability of a change into a backward state

In this way, the probabilities  $\pi_i$  of the stationary probability vector get smaller and smaller as long as *i* grows

Negative recurrence means that it is more likely to move forward Null recurrence means that the probabilities to move forward/backward are equal

Positive recurrence plus additional properties guarantee that even in the infinite case  $\lim x^{(k)}=\pi$ 

Positive/negative/null recurrence can be detected by means of the drift

An important computational problem is: designing efficient algorithms for computing  $\pi_1, \pi_2, \ldots \pi_k$  for any given integer k

We present some examples of Markov chains which show how matrix structures reflect specific properties of the physical model

#### Some examples: Random walk

Random walk: At each instant a point Q moves along a line of a unit step

- to the right with probability p
- to the left with probability q

Clearly, the position of Q at time n + 1 depends only on the position of Q at time n.



- $E = \mathbb{Z}$ : coordinates of Q
- $T = \mathbb{N}$ : units of time
- $X_n$ : coordinate of Q at time n

$$X_{n+1} = \begin{cases} X_n + 1 & \text{with probability } p \\ X_n - 1 & \text{with probability } q \\ X_n & \text{with probability } 1 - p - q \end{cases}$$

$$\mathcal{P}(X_{n+1} = j | X_n = i) = \begin{cases} p & \text{if } j = i+1 \\ q & \text{if } j = i-1 \\ 1-p-q & \text{if } j = i \\ 0 & \text{otherwise} \end{cases}$$



#### bi-infinite tridiagonal Toeplitz matrix

Case where  $E = \mathbb{Z}^+$ 



$$P = \begin{bmatrix} 1 - p & p & & \\ q & 1 - q - p & p & \\ & q & 1 - q - p & p & \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

Semi-infinite tridiagonal almost Toeplitz matrix

Case where  $E = \{1, 2, ..., n\}$ 



$$P = \begin{bmatrix} 1-p & p & & & & \\ q & 1-q-p & p & & & \\ & q & 1-q-p & p & & \\ & & \ddots & \ddots & \ddots & \\ & & & & q & 1-q-p & p \\ & & & & & q & 1-q-p & p \\ & & & & & & q & 1-q \end{bmatrix}$$

Finite tridiagonal almost Toeplitz matrix

Some examples: A more general random walk

At each instant a point Q moves along a line

- to the right of k unit steps with probability  $p_k$ ,  $k \in \mathbb{N}$
- to the left with probability  $p_{-1}$

Semi-infinite case

$$P = \begin{bmatrix} \hat{p}_0 & p_1 & p_2 & p_3 & p_4 & \dots \\ p_{-1} & p_0 & p_1 & p_2 & p_3 & \ddots \\ p_{-1} & p_0 & p_1 & p_2 & \ddots \\ & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

Almost Toeplitz matrix in Hessenberg form M/G/1 Markov chain

#### Some examples: Bidimensional random walk

The particle can move in the plane: at each instant it can move right, left, up, down, up-right, up-left, down-right, down-left, with assigned probabilities  $a_i^{(j)}$ , i, j = -1, 0, 1.



Ordering the coordinates row-wise as

 $(0,0), (1,0), (2,0), \dots, (0,1), (1,1), (2,1), \dots, (0,2), (1,2), (2,2), \dots$ 

one finds that the matrix P has a block structure

#### For $E = \mathbb{Z} \times \mathbb{Z}$

$$P = \begin{bmatrix} \ddots & \ddots & \ddots & & \\ & A_{-1} & A_0 & A_1 & & \\ & & A_{-1} & A_0 & A_1 & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \text{ where } A_i = \begin{bmatrix} \ddots & \ddots & \ddots & \ddots & & \\ & p_{-1}^{(i)} & p_0^{(i)} & p_1^{(i)} & & \\ & & p_{-1}^{(i)} & p_0^{(i)} & p_1^{(i)} & \\ & & & p_{-1}^{(i)} & p_0^{(i)} & p_1^{(i)} & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix}$$

block tridiagonal block Toeplitz with tridiagonal Toeplitz blocks

- Blocks can be finite, semi-infinite or bi-infinite
- The block matrix can be finite semi-infinite or bi-infinite

Example: if  $E = \{0, 1, 2, ..., n\} \times \mathbb{N}$  then the blocks  $A_i$  are finite

$$P = \begin{bmatrix} \widehat{A}_{0} & A_{1} & & & \\ A_{-1} & A_{0} & A_{1} & & \\ & \ddots & \ddots & \ddots & \\ & & A_{-1} & A_{0} & A_{1} \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \text{ where } A_{i} = \begin{bmatrix} \widehat{p}_{0}^{(i)} & p_{1}^{(i)} & & \\ p_{-1}^{(i)} & p_{0}^{(i)} & p_{1}^{(i)} & \\ & \ddots & \ddots & \ddots & \\ & & p_{-1}^{(i)} & p_{0}^{(i)} & p_{1}^{(i)} \\ & & & p_{-1}^{(i)} & p_{0}^{(i)} & p_{1}^{(i)} \end{bmatrix}$$

For  $E = \mathbb{Z}^d$  one obtains a *multilevel structure with d levels*, that is, block Toeplitz, block tridiagonal matrices where the blocks have a multilevel structure with d - 1 levels

Some examples: The shortest queue model

Shortest queue model

- *m* servers with *m* queues
- at each time unit each server serves one customer
- at each time unit,  $\alpha$  new customers arrive with probability  $q_{\alpha}$
- each customer joins the shortest queue
- $X_n$ : total number of customers in the lines



$$X_{n+1} = \begin{cases} X_n + \alpha - m & \text{if } X_n + \alpha - m \ge 0\\ 0 & \text{if } X_n + \alpha - m < 0 \end{cases}$$

$$p_{i,j} = \begin{cases} q_0 + q_1 + \dots + q_{m-i} & \text{if } j = 0, \ 0 \le i \le m-1 \\ q_{j-i+m} & \text{if } j-i+m \ge 0 \\ 0 & \text{if } j-i+m < 0 \end{cases}$$

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if i < m then transition  $i \rightarrow 0$  occurs if the number of arrivals is at most m - i

$$X_{n+1} = \begin{cases} X_n + \alpha - m & \text{if } X_n + \alpha - m \ge 0\\ 0 & \text{if } X_n + \alpha - m < 0 \end{cases}$$
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transition  $i \rightarrow j$  if there are  $j - i + m \ge 0$  arrivals

$$X_{n+1} = \begin{cases} X_n + \alpha - m & \text{if } X_n + \alpha - m \ge 0\\ 0 & \text{if } X_n + \alpha - m < 0 \end{cases}$$
$$p_{i,j} = \begin{cases} q_0 + q_1 + \dots + q_{m-i} & \text{if } j = 0, \ 0 \le i \le m - 1\\ q_{j-i+m} & \text{if } j - i + m \ge 0\\ 0 & \text{if } j - i + m < 0 \end{cases}$$

transition  $i \rightarrow j$  impossible if j < i - m (at most *m* customers are served in a unit of time)

$$P_{i,j} = \begin{cases} q_0 + q_1 + \dots + q_{m-i} & \text{if } j = 0, \ 0 \le j \le m-1 \\ q_{j-i+m} & \text{if } j-i+m \ge 0 \\ 0 & \text{if } j-i+m < 0 \end{cases}$$

$$P = \begin{bmatrix} b_0 & q_{m+1} & q_{m+2} & q_{m+3} & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ b_{m-1} & q_2 & q_3 & q_4 & \dots & \dots \\ q_0 & q_1 & q_2 & q_3 & \dots & \dots \\ q_0 & q_1 & q_2 & q_3 & \ddots & \dots \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

 $b_i = q_0 + q_1 + \cdots + q_{m-i}, \ 0 \le i \le m-1$ 

Almost Toeplitz, generalized Hessenberg

Case m = 2 (for simplicity)

Г	<i>b</i> 0	$q_3$	94	$q_5$	<i>q</i> <sub>6</sub>	$q_7$	$q_8$	$q_9$	· · · ·	1				
	<i>b</i> <sub>1</sub>	$q_2$	<i>q</i> <sub>3</sub>	$q_4$	$q_5$	$q_6$	<b>q</b> 7	$q_8$						
	$q_0$	$q_1$	<i>q</i> <sub>2</sub>	<b>q</b> 3	<i>q</i> 4	$q_5$	$q_6$	$q_7$						
l									· .		$\widehat{Q}_1$	$Q_2$	$Q_3$	
I.		<b>q</b> 0	$q_1$	<b>q</b> 2	<i>q</i> <sub>3</sub>	$q_4$	$q_5$	<b>q</b> 6						
				-			-	_	·.		$Q_0$	$Q_1$	$Q_2$	· · .
			90	$q_1$	92	<i>q</i> 3	94	<i>q</i> 5		=				
				~		~	~	~	÷.			$Q_0$	$Q_1$	·.
1				40	$q_1$	4 <u>2</u>	43	44						
											L		· ·	· · .
					<i>q</i> 0	$q_1$	<i>q</i> <sub>2</sub>	<i>q</i> 3	q4 ·					
L						÷.,	·	÷.,	· · · ·					

Generalized Hessenberg  $\rightarrow$  Block Hessenberg (Almost) Toeplitz  $\rightarrow$  (Almost) Block Toeplitz

## M/G/1-Type Markov chains

Set of states: 
$$E = \mathbb{N} \times \{1, 2, ..., m\}$$
  
 $X_n = (\psi_n, \varphi_n) \in E, \quad \psi_n$ : level,  $\varphi_n$ : phase  
 $\mathcal{P}(X_{n+1} = (i', j') | X_n = (i, j)) = (A_{i'-i})_{j,j'}$ , for  $i' - i \ge -1$ ,  $1 \le j, j' \le m$   
 $\mathcal{P}(X_{n+1} = (i', j') | X_n = (0, j)) = (B_{i'})_{j,j'}$ , for  $i' - i \ge -1$ 

The probability to switch from level *i* to level *i'* depends on i' - i

$$P = \begin{bmatrix} B_0 & B_1 & B_2 & B_3 & \dots & \\ A_{-1} & A_0 & A_1 & A_2 & A_3 & \dots & \\ & A_{-1} & A_0 & A_1 & A_2 & A_3 & \ddots \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

Almost block Toeplitz, block Hessenberg

## G/M/1-Type Markov chains

Set of states: 
$$E = \mathbb{N} \times \{1, 2, ..., m\}$$
  
 $X_n = (\psi_n, \varphi_n) \in E, \quad \psi_n$ : level,  $\varphi_n$ : phase  
 $\mathcal{P}(X_{n+1} = (i', j') | X_n = (i, j)) = (A_{i'-i})_{j,j'}, \text{ for } i' - i \leq -1, \ 1 \leq j, j' \leq m$   
 $\mathcal{P}(X_{n+1} = (0, j') | X_n = (i, j)) = (B_{i'})_{j,j'}, \text{ for } i' - i \geq -1$ 

The probability to switch from level *i* to level *i'* depends on i' - i

$$P = \begin{bmatrix} B_0 & A_1 & & \\ B_{-1} & A_0 & A_1 & \\ B_{-2} & A_{-1} & A_0 & A_1 & \\ B_{-3} & A_{-2} & A_{-1} & A_0 & A_1 \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix}$$

Almost block Toeplitz, block lower Hessenberg
# Quasi-Birth-Death models

The level can move up or down only by one step

The phase can move anywhere





death

### The Tandem Jackson model



customers arrive at the first queue according to a Poisson process with rate  $\boldsymbol{\lambda}$ 

customers are served with an exponential service time with parameter  $\mu_1$ on leaving the first queue, customers enter the second queue and are served with an exponential service time with parameter  $\mu_2$  The model is described by a Markov chains where the set of states are the pairs  $(\alpha, \beta)$ , where  $\alpha$  is the number of customer in the first queue,  $\beta$  is the number of customer in the second queue

The transition matrix is

$$\begin{bmatrix} \widetilde{A}_0 & A_1 & & \\ A_{-1} & A_0 & A_1 & \\ & \ddots & \ddots & \ddots \end{bmatrix}$$

where

$$A_{-1} = \begin{bmatrix} 0 & & \\ \mu_1 & 0 & \\ & \mu_1 & 0 \\ & & \ddots & \ddots \end{bmatrix}, A_0 = \begin{bmatrix} 1 - \lambda - \mu_2 & \lambda & & \\ & 1 - \lambda - \mu_1 - \mu_2 & \lambda \\ & & \ddots & \ddots \end{bmatrix},$$
$$A_1 = \mu_2 I, \quad \widetilde{A}_0 = \begin{bmatrix} 1 - \lambda & \lambda & & \\ & 1 - \lambda - \mu_1 & \lambda \\ & & \ddots & \ddots \end{bmatrix}$$

# Non-Skip-Free models

In certain models, the transition to lower levels is limited by a positive constant N. That is the Toeplitz part of the matrix P has the generalized block Hessenberg form

Reblocking the above matrix into  $N \times N$  blocks yields a block Toeplitz matrix in block Hessenberg form where the blocks are block Toeplitz matrices

# Models from the real world

Queuing and communication systems IEEE 801.10 wireless protocol:

 $\begin{bmatrix} \hat{A}_{0} & \hat{A}_{1} & \dots & \dots & \hat{A}_{n-1} & \hat{A}_{n} \\ A_{-1} & A_{0} & A_{1} & \dots & A_{n-2} & \tilde{A}_{n-1} \\ & A_{-1} & A_{0} & A_{1} & \vdots & \vdots \\ & & \ddots & \ddots & \vdots & \vdots \\ & & & A_{-1} & A_{0} & \tilde{A}_{1} \\ & & & & & A_{-1} & \tilde{A}_{0} \end{bmatrix}$ 

Risk and insurance problems

State-dependent susceptible-infected-susceptible epidemic models

Inventory systems

J. Artalejo, A. Gomez-Corral, SORT 34  $\left(2\right)$  2010

In some cases, the blocks  $A_i$  in the QBD, M/G/1 or G/M/1 processes, have a tensor structure,

in other cases, the blocks  $A_i$  for  $i \neq 0$  have low rank

### Recursive structures

Tree-like stochastic processes are bivariate Markov chains over a d-ary tree

States:  $(j_1,\ldots,j_\ell;i)$ ,  $1\leq j_1,\ldots,j_\ell\leq d$ ,  $1\leq i\leq m$ 

The  $\ell$ -tuple  $(j_1,\ldots,j_\ell)$  denotes the generic node at the level  $\ell$  of the tree



Allowed transitions

- within a node  $(J; i) \rightarrow (J; i')$  with probability  $(B_j)_{i,i'}$
- within the root node  $i \rightarrow i'$  with probability  $(B_0)_{i,i'}$
- between a node and one of its children  $(J; i) \rightarrow ([J, k]; i')$  with probability  $(A_k)_{i,i'}$
- between a node and its parent  $([J, k]; i) \rightarrow (J; i')$  with probability  $(D_k)_{i,i'}$

Over an infinite tree, with a lexicographical ordering of the states according to the leftmost integer of the node J, the Markov chain is governed by

$$P = \begin{bmatrix} C_0 & \Lambda_1 & \Lambda_2 & \dots & \Lambda_d \\ V_1 & W & 0 & \dots & 0 \\ V_2 & 0 & W & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ V_d & 0 & \dots & 0 & W \end{bmatrix}$$

where  $C_0 = B_0 - I$ ,  $\Lambda_i = [A_i \ 0 \ 0 \ \dots]$ ,  $V_i^T = [D_i^T \ 0 \ 0 \ \dots]$ , we assume  $B_1 = \dots = B_d =: B$ , C = I - B and the matrix W is recursively defined by

$$W = \begin{bmatrix} C & \Lambda_1 & \Lambda_2 & \dots & \Lambda_d \\ V_1 & W & 0 & \dots & 0 \\ V_2 & 0 & W & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ V_d & 0 & \dots & 0 & W \end{bmatrix}$$

They model single server queues with LIFO service discipline, medium access control protocol with an underlying stack structure [LATOUCHE, RAMASWAMI 99]

### Computational problems

In all these problems the most important computational task is to compute a usually large number of components of the vector  $\pi$  such that

$$\pi P = \pi$$

where the stochastic matrix P is block upper (lower) Hessenberg, or generalized Hessenberg, almost block Toeplitz, with finite or with infinite size, with blocks that are either finite or infinite

In the infinite case, this problem can be reduced to solving the following matrix equation

$$\sum_{i=-1}^{\infty} A_i X^{i+1} = X$$

where X is an  $n \times n$  matrix, where the solution of interest is nonnegative and among all the solutions is the minimal one w.r.t. the component-wise ordering

# Markovian binary trees and vector equations

Markovian binary trees, a particular family of branching processes used to model the growth of populations and networking systems, are characterized by the following laws

- At each instant, a finite number of entities, called "individuals", exist.
- Each individual can be in any one of N different states (say, age classes or difference features in a population).
- Each individual evolves independently from the others. Depending on its state *i*, it has a fixed probability b<sub>i,j,k</sub> of being replaced by two new individuals ("children") in states *j* and *k* respectively, and a fixed probability a<sub>i</sub> of dying without producing any offspring.

The MBT is characterized by the vector  $a = (a_i) \in \mathbb{R}^N_+$  and by the tensor  $B = (b_{i,j,k}) \in \mathbb{R}^{N \times N \times N}_+$ 

One important issue related to MBTs is the computation of the extinction probability of the population, given by the minimal nonnegative solution  $x \in \mathbb{R}^N$  of the quadratic vector equation [N.G. BEAN, N. KONTOLEON, P.G. TAYLOR 2008]

$$x_k = a_k + x^T B_k x, \quad B_k = (b_{i,j,k})$$

 $x_k$  is the probability that a colony starting from a single individual in state k becomes extinct in a finite time

Compatibility condition:  $e = a + B(e \otimes e)$ 

the probabilities of all the possible events that may happen to an individual in state  $i\ {\rm sum}\ {\rm to}\ 1$ 

The equation can be rewritten as

$$x = a + \mathcal{B}(x \otimes x), \quad \mathcal{B} = \mathsf{Diag}(\mathsf{vec}(B_1^{\mathsf{T}})^{\mathsf{T}}, \dots, \mathsf{vec}(B_N^{\mathsf{T}})^{\mathsf{T}})$$

# A related problem: the Poisson problem

Given a stochastic matrix P, irreducible, non-periodic, positive recurrent; given a vector d, determine all the solutions  $x = (x_1, x_2, ...)$ , z of the following system

$$(I - P)x = d - ze, \quad e = (1, 1...)^T$$

Found in many places: Markov reward processes, Central limit theorem for M.C., perturbation analysis, heavy-traffic limit theory, variance constant analysis, asymptotic variance of single-birth process (ASMUSSEN, BLADT 1994)

Finite case:

for  $\pi$  such that  $\pi(I - P) = 0$  one finds that  $z = \pi d$  so that it remains to solve (I - P)x = c with c = d - ze

Infinite case: More complicated situation Example: (MAKOWSKI AND SHWARTZ, 2002)

$$P = egin{bmatrix} q & p & & & \ q & 0 & p & & \ & q & 0 & p & \ & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

with p + q = 1, p, q > 0. Take any d. For any real z, there exists a solution x

What happens for QBDs?

Computational problem: system of vector difference equations of the kind

$$\begin{bmatrix} B & A_1 & & \\ A_{-1} & A_0 & A_1 & \\ & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \end{bmatrix}$$

## Another problem in Markov chains

In the framework of continuous time Markov chains, the following problem is encountered:

Compute

$$\exp(A) = \sum_{i=0}^{\infty} \frac{1}{i!} A^i$$

where A is an  $n \times n$  block triangular block Toeplitz matrix with  $m \times m$  blocks; A is a generator, i.e.,  $Ae \leq 0$ ,  $a_{i,i} \leq 0$ ,  $a_{i,j} \geq 0$  for  $i \neq j$ 

Erlangian approximation of Markovian fluid queues

- S. ASMUSSEN, F. AVRAM, M. USÁBEL 2002
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# 2- Fundamentals on structured matrices

- Toeplitz matrices
  - Toeplitz matrices, polynomials and power series
  - Trigonometric matrix algebras and FFT
  - Displacement operators
  - Algorithms for Toeplitz inversion
  - Asymptotic spectral properties and preconditioning
- Rank structures

# Toeplitz matrices [OTTO TOEPLITZ 1881-1940] Let $\mathbb{F}$ be a field ( $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ )

Given a bi-infinite sequence  $\{a_i\}_{i \in \mathbb{Z}} \in \mathbb{F}^{\mathbb{Z}}$  and an integer *n*, the  $n \times n$  matrix  $T_n = (t_{i,j})_{i,j=1,n}$  such that  $t_{i,j} = a_{j-i}$  is called *Toeplitz matrix* 

$$T_5 = \begin{bmatrix} a_0 & a_1 & a_2 & a_3 & a_4 \\ a_{-1} & a_0 & a_1 & a_2 & a_3 \\ a_{-2} & a_{-1} & a_0 & a_1 & a_2 \\ a_{-3} & a_{-2} & a_{-1} & a_0 & a_1 \\ a_{-4} & a_{-3} & a_{-2} & a_{-1} & a_0 \end{bmatrix}$$

 $T_n$  is a leading principal submatrix of the (semi) infinite Toeplitz matrix  $T_{\infty} = (t_{i,j})_{i,j \in \mathbb{N}}, t_{i,j} = a_{j-i}$ 

$$T_{\infty} = \begin{bmatrix} a_0 & a_1 & a_2 & \dots \\ a_{-1} & a_0 & a_1 & \ddots \\ a_{-2} & a_{-1} & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{bmatrix}$$

**Theorem** [OTTO TOEPLITZ] The matrix  $T_{\infty}$  defines a bounded linear operator in  $\ell^2(\mathbb{N})$ ,  $x \to y = T_{\infty}x$ ,  $y_i = \sum_{j=0}^{+\infty} a_{j-i}x_j$  if and only if  $a_i$  are the Fourier coefficients of a function  $a(z) \in L^{\infty}(\mathbb{T})$ ,  $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$ 

$$a(z) = \sum_{n=-\infty}^{+\infty} a_n z^n, \quad a_n = rac{1}{2\pi} \int_0^{2\pi} a(e^{\mathbf{i}\theta}) e^{-\mathbf{i}n\theta} d\theta, \quad \mathbf{i}^2 = -1$$

In this case

$$||T|| = \operatorname{ess sup}_{z \in \mathbb{T}} |a(z)|, \text{ where } ||T|| := \sup_{||x||_2 = 1} ||Tx||_2$$

The function a(z) is called *symbol* associated with  $T_{\infty}$ 

Example If  $a(z) = \sum_{i=-k}^{k} a_i z^i$  is a Laurent polynomial, then  $T_{\infty}$  is a banded Toeplitz matrix which defines a bounded linear operator

### Block Toeplitz matrices

Let  $\mathbb{F}$  be a field  $(\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\})$ 

Given a bi-infinite sequence  $\{A_i\}_{i\in\mathbb{Z}}$ ,  $A_i \in \mathbb{F}^{m\times m}$  and an integer *n*, the  $mn \times mn$  matrix  $T_n = (t_{i,j})_{i,j=1,n}$  such that  $t_{i,j} = A_{j-i}$  is called *block Toeplitz* matrix

$$T_5 = \begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 \\ A_{-1} & A_0 & A_1 & A_2 & A_3 \\ A_{-2} & A_{-1} & A_0 & A_1 & A_2 \\ A_{-3} & A_{-2} & A_{-1} & A_0 & A_1 \\ A_{-4} & A_{-3} & A_{-2} & A_{-1} & A_0 \end{bmatrix}$$

 $T_n$  is a leading principal submatrix of the (semi) infinite block Toeplitz matrix  $T_{\infty} = (t_{i,j})_{i,j \in \mathbb{N}}$ ,  $t_{i,j} = A_{j-i}$ 

$$T_{\infty} = \begin{bmatrix} A_0 & A_1 & A_2 & \dots \\ A_{-1} & A_0 & A_1 & \ddots \\ A_{-2} & A_{-1} & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{bmatrix}$$

## Block Toeplitz matrices with Toeplitz blocks

**Theorem** The infinite block Toeplitz matrix  $T_{\infty}$  defines a bounded linear operator in  $\ell^2(\mathbb{N})$  iff the blocks  $A_k = (a_{i,j}^{(k)})$  are the Fourier coefficients of a matrix-valued function  $A(z) : \mathbb{T} \to \mathbb{C}^{m \times m}$ ,  $A(z) = \sum_{k=-\infty}^{+\infty} z^k A_k = (a_{i,j}(z))_{i,j=1,m}$  such that  $a_{i,j}(z) \in L^{\infty}(\mathbb{T})$ 

If the blocks  $A_i$  are Toeplitz themselves we have a block Toeplitz matrix with Toeplitz blocks

A function  $a(z, w) : \mathbb{T} \times \mathbb{T} \to \mathbb{C}$  having the Fourier series  $a(z, w) = \sum_{i,j=-\infty}^{+\infty} a_{i,j} z^i w^j$  defines an infinite block Toeplitz matrix  $T_{\infty} = (A_{j-i})$  with infinite Toeplitz blocks  $A_k = (a_{k,j-i})$ .  $T_{\infty}$  defines a bounded operator iff  $a(z, w) \in L_{\infty}$ 

For any pair of integers n, m we may construct an  $n \times n$  Toeplitz matrix  $T_{m,n} = (A_{j-i})_{i,j=1,n}$  with  $m \times m$  Toeplitz blocks  $A_{j-i} = (a_{k,j-i})_{i,j=1,m}$ 

### Multilevel Toeplitz matrices

A function  $a: \mathbb{T}^d \to \mathbb{C}$  having the Fourier expansion

$$a(z_1, z_2, \ldots, z_d) = \sum_{i_1, \ldots, i_d = -\infty}^{+\infty} a_{i_1, i_2, \ldots, i_d} z_{i_1}^{i_1} z_{i_2}^{i_2} \cdots z_{i_d}^{i_d}$$

defines a *d-multilevel Toeplitz* matrix: that is a block Toeplitz matrix with blocks that are themselves (d - 1)-multilevel Toeplitz matrices

# Generalization: Toeplitz-like matrices

Let  $L_i$  and  $U_i$  be lower triangular and upper triangular  $n \times n$  Toeplitz matrices, respectively, where i = 1, ..., k and k is independent of n

$$A = \sum_{i=1}^{k} L_i U_i$$

is called a *Toeplitz-like* matrix

If k = 2,  $L_1 = U_2 = I$  then  $A = U_1 + L_2$  is a Toeplitz matrix.

If A is an invertible Toeplitz matrix then there exist  $L_i$ ,  $U_i$ , i = 1, 2 such that

$$A^{-1} = L_1 U_1 + L_2 U_2$$

that is,  $A^{-1}$  is Toeplitz-like

Toeplitz matrices, polynomials and power series

## Toeplitz matrices, polynomials and power series Polynomial multiplication

$$a(x) = \sum_{i=0}^{n} a_{i}x^{i}, \quad b(x) = \sum_{i=0}^{m} b_{i}x^{i},$$
  

$$c(x) := a(x)b(x), \quad c(x) = \sum_{i=0}^{m+n} c_{i}x^{i},$$
  

$$c_{0} = a_{0}b_{0},$$
  

$$c_{1} = a_{0}b_{1} + a_{1}b_{0},$$
  
...

$$\begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ \vdots \\ \vdots \\ c_{m+n} \end{bmatrix} = \begin{bmatrix} a_0 & & & \\ a_1 & a_0 & & \\ \vdots & \ddots & \ddots & \\ a_n & \ddots & \ddots & a_0 \\ & \ddots & \ddots & a_1 \\ & & \ddots & \vdots \\ & & & a_n \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_m \end{bmatrix}$$

Let A be an  $n \times n$  Toeplitz matrix and b an n-vector, consider the matrix-vector product

c = Ab

rewrite it in the following form



Deduce that the Toeplitz-vector product can be viewed as part of the product of a polynomial of degree  $\leq 2n - 1$  and a polynomial of degree  $\leq n - 1$ .

Observe that the result is a polynomial of degree at most 3n - 2 whose coefficients can be computed by means of an evaluation-interpolation scheme at 3n - 1 points.

### **Polynomial product**

• Choose 
$$N \geq 3n-1$$
 different numbers  $x_1, \ldots, x_N$ 

(a) evaluate 
$$\alpha_i = a(x_i)$$
 and  $\beta_i = b(x_i)$ , for  $i = 1, ..., N$ 

$${f 3}\,$$
 compute  $\gamma_i=lpha_ieta_i,\ i=1,\ldots,N$ 

• interpolate  $c(x_i) = \gamma_i$  and compute the coefficients of c(x)

If the knots  $x_1, \ldots, x_N$  are *N*-th roots of 1 then the evaluation and the interpolation steps can be executed by means of FFT in time  $O(N \log N)$ 

Polynomial division

$$\begin{aligned} a(x) &= \sum_{i=0}^{n} a_i x^i, \ b(x) &= \sum_{i=0}^{m} b_i x^i, \ b_m \neq 0\\ a(x) &= b(x)q(x) + r(x), \quad \text{deg } r(x) < m\\ q(x) \text{ quotient, } r(x) \text{ remainder of the division of } a(x) \text{ by } b(x) \end{aligned}$$



The last n - m + 1 equations form a triangular Toeplitz system

Polynomial division

$$egin{aligned} a(x) &= \sum_{i=0}^n a_i x^i, \ b(x) &= \sum_{i=0}^m b_i x^i, \ b_m 
eq 0 \ a(x) &= b(x)q(x) + r(x), \quad \deg r(x) < m \ q(x) \ ext{quotient}, \ r(x) \ ext{remainder of the division of } a(x) \ ext{by } b(x) \end{aligned}$$



The last n - m + 1 equations form a triangular Toeplitz system

Polynomial division (in the picture n - m = m - 1)

$$\begin{bmatrix} b_m & b_{m-1} & \dots & b_{2m-n} \\ & b_m & \ddots & \vdots \\ & & \ddots & b_{m-1} \\ & & & & b_m \end{bmatrix} \begin{bmatrix} q_0 \\ q_1 \\ \vdots \\ q_{n-m} \end{bmatrix} = \begin{bmatrix} a_m \\ a_{m+1} \\ \vdots \\ a_n \end{bmatrix}$$

Its solution provides the coefficients of the quotient. The remainder can be computed as a difference.

$$\begin{bmatrix} r_0 \\ \vdots \\ r_{m-1} \end{bmatrix} = \begin{bmatrix} a_0 \\ \vdots \\ a_{m-1} \end{bmatrix} - \begin{bmatrix} b_0 & & \\ \vdots & \ddots & \\ b_{m-1} & \cdots & b_0 \end{bmatrix} \begin{bmatrix} q_0 \\ \vdots \\ q_{n-m} \end{bmatrix}$$

Polynomial gcd

If g(x) = gcd(a(x), b(x)), deg(g(x)) = k, deg(a(x)) = n, deg(b(x)) = m. Then there exist polynomials r(x), s(x) of degree at most m - k - 1, n - k - 1, respectively, such that (Bézout identity)

$$g(x) = a(x)r(x) + b(x)s(x)$$

In matrix form one has the  $(m + n - k) \times (m + n - 2k)$  system



Sylvester matrix

Polynomial gcd

The last m + n - 2k equations provide a linear system of the kind

$$S\begin{bmatrix}r\\s\end{bmatrix} = \begin{bmatrix}g_k\\0\\\vdots\\0\end{bmatrix}$$

where S is the  $(m + n - 2k) \times (m + n - 2k)$  submatrix of the Sylvester matrix in the previous slide formed by two Toeplitz matrices.

# Infinite Toeplitz matrices and power series

Let a(x), b(x) be polynomials of degree n, m with coefficients  $a_i, b_j$ , define the Laurent polynomial

$$c(x) = a(x)b(x^{-1}) = \sum_{i=-m}^{n} c_i x^i$$

Then the following infinite UL factorization holds



If the zeros of a(x) and b(x) lie outside the unit disk, this factorization is called Wiener-Hopf factorization. This factorization is encountered in many applications.

Remark about the condition  $a(x), b(x) \neq 0$  for  $|x| \leq 1$ 

Observe that if  $|\gamma| > 1$  and  $a(x) = x - \gamma$  then

$$\frac{1}{a(x)} = \frac{1}{x - \gamma} = -\frac{1}{\gamma} \frac{1}{1 - \frac{x}{\gamma}} = -\frac{1}{\gamma} \sum_{i=0}^{\infty} \left(\frac{x}{\gamma}\right)^{i}$$

the series  $\sum_{i=0}^\infty 1/|\gamma|^i$  is convergent since  $1/|\gamma|<1.$  This is not true if  $|\gamma|\leq 1$ 

Moreover, in matrix form

$$\begin{bmatrix} -\gamma & 1 & 0 & \dots \\ & -\gamma & 1 & 0 & \dots \\ & & \ddots & \ddots & \ddots \end{bmatrix}^{-1} = -\gamma^{-1} \begin{bmatrix} 1 & \gamma^{-1} & \gamma^{-2} & \dots \\ & 1 & \gamma^{-1} & \gamma^{-2} & \ddots \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

A similar property holds if all the zeros of a(x) have modulus > 1

A similar remark applies to the factor b(z)

The Wiener-Hopf factorization can be defined for matrix-valued functions  $C(x) = \sum_{i=-\infty}^{+\infty} C_i x^i$ ,  $C_i \in \mathbb{C}^{m \times m}$ , in the Wiener class  $\mathcal{W}_m$ , i.e, such that  $\sum_{i=-\infty}^{+\infty} ||C_i|| < \infty$ . It exists provided that det  $C(x) \neq 0$  for |x| = 1.

In this case, the Wiener-Hopf factorization takes the form

$$C(x) = A(x) \operatorname{diag}(x^{k_1}, \dots, x^{k_m}) B(x^{-1}), \quad A(x) = \sum_{i=0}^{\infty} x^i A_i, \ B(x) = \sum_{i=0}^{\infty} B_i x^i$$

where  $A(x), B(x) \in W_m$  and det A(x) and det B(x) are nonzero in the open unit disk BÖTTCHER, SILBERMANN.

If the partial indices  $k_i \in \mathbb{Z}$  are zero, the factorization takes the form  $C(x) = A(x)B(x^{-1})$  and is said canonical factorization

Its matrix representation provides a block UL factorization of the infinite block Toeplitz matrix  $(C_{j-i})$ 

#### Matrix form of the canonical factorization

Moreover, the condition det A(z), det  $B(z) \neq 0$  for  $|z| \leq 1$  make  $A(z)^{-1}$ ,  $B(z)^{-1}$  exist in  $\mathcal{W}_m$ . Consequently, the two infinite matrices have a block Toeplitz inverse which has bounded infinity norm

We will see that the Wiener-Hopf factorization is fundamental for computing the vector  $\pi$  for many Markov chains encountered in queuing models
Trigonometric matrix algebras and FFT

Let  $\omega_n = \cos \frac{2\pi}{n} + \mathbf{i} \sin \frac{2\pi}{n}$  be a primitive *n*th root of 1, that is, such that  $\omega_n^n = 1$  and  $\{1, \omega_n, \dots, \omega_n^{n-1}\}$  has cardinality *n*.

Define the  $n \times n$  matrix  $\Omega_n = (\omega_n^{ij})_{i,j=0,n-1}$ ,  $F_n = \frac{1}{\sqrt{n}}\Omega_n$ .

One can easily verify that  $F_n^*F_n = I$  that is,  $F_n$  is a unitary matrix. For  $x \in \mathbb{C}^n$  define

y = DFT(x) = <sup>1</sup>/<sub>n</sub>Ω<sup>\*</sup><sub>n</sub>x the Discrete Fourier Transform (DFT) of x
 x = IDFT(y) = Ω<sub>n</sub>y the Inverse DFT (IDFT) of y

Remark: cond<sub>2</sub>( $F_n$ ) =  $||F_n||_2 ||F_n^{-1}||_2 = 1$ , cond<sub>2</sub>( $\Omega_n$ ) = 1

This shows that the DFT and IDFT are numerically well conditioned when the perturbation errors are measured in the 2-norm. If *n* is an integer power of 2 then the IDFT of a vector can be computed with the cost of  $\frac{3}{2}n \log_2 n$  arithmetic operations by means of FFT

FFT is numerically stable in the 2-norm. That is, if  $\tilde{x}$  is the value computed in floating point arithmetic with precision  $\mu$  in place of x = IDFT(y) then

$$\|x - \widetilde{x}\|_2 \le \mu \gamma \|x\|_2 \log_2 n$$

for a moderate constant  $\gamma$ 

norm-wise well conditioning of DFT and the norm-wise stability of FFT make this tool very effective for **most numerical computations**.

Unfortunately, the norm-wise stability of FFT does not imply the component-wise stability. That is, the inequality

 $|x_i - \widetilde{x}_i| \le \mu \gamma |x_i| \log_2 n$ 

is **not generally true** for all the components  $x_i$ .

# Warning: be aware that FFT is not point-wise stable, otherwise unpleasant things may happen

Here is an example

## Warning: the example of Graeffe iteration Let $p(x) = \sum_{i=0}^{n} p_i x^i$ be a polynomial of degree *n* having zeros $|x_1| < \cdots < |x_m| < 1 < |x_{m+1}| < \cdots < |x_n|$

With  $p_0(x) := p(x)$ , define the sequence (Graeffe iteration)

$$q(x^2) = p_k(x)p_k(-x), \quad p_{k+1}(x) = q(x)/q_m, \quad \text{for } k = 0, 1, 2, \dots$$

The zeros of  $p_k(x)$  are  $x_i^{2^k}$ , so that  $\lim_{k\to\infty} p_k(x) = x^m$ 

If  $p_k(x) = \sum_{i=0}^n p_i^{(k)} x^i$  then

$$\lim_{k \to \infty} |p_{n-1}^{(k)}/p_n^{(k)}|^{1/2^k} = |x_n|$$

moreover, convergence is very fast. Similar equations hold for  $|x_i|$ 

$$\lim_{k \to \infty} |p_{n-1}^{(k)}/p_n^{(k)}|^{1/2^k} = |x_n|$$

On the other hand (if m < n - 1)

$$\lim_{k\to\infty}|p_{n-1}^{(k)}|=\lim_{k\to\infty}|p_n^{(k)}|=0$$

with double exponential convergence

Computing  $p_k(x)$  given  $p_{k-1}(x)$  by using FFT (evaluation interpolation at the roots of unity) costs  $O(n \log n)$  ops.

But as soon as  $|p_n^{(k)}|$  and  $|p_{n-1}^{(k)}|$  are below the machine precision the relative error in these two coefficients is greater than 1. That is, **no digit** is correct in the computed estimate of  $|x_n|$ .



Figure : The values of  $\log_{10} |p_i^{(6)}|$  for i = 0, ..., n for the polynomial obtained after 6 Graeffe steps starting from a random polynomial of degree 100. In red the case where the coefficients are computed with FFT, in blue the coefficients computed with the customary algorithm

step	custom	FFT
1	1.40235695	1.40235695
2	2.07798429	2.07798429
3	2.01615072	2.01615072
4	2.01971626	2.01857621
5	2.01971854	1.00375471
6	2.01971854	0.99877589

# End of warning

Trigonometric matrix algebras: Circulant matrices Given the row vector  $[a_0, a_1, \dots, a_{n-1}]$ , the  $n \times n$  matrix

$$A = (a_{j-i \mod n})_{i,j=1,n} = \begin{bmatrix} a_0 & a_1 & \dots & a_{n-1} \\ a_{n-1} & a_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_1 \\ a_1 & \dots & a_{n-1} & a_0 \end{bmatrix}$$

is called the *circulant* matrix associated with  $[a_0, a_1, \ldots, a_{n-1}]$  and is denoted by Circ $(a_0, a_1, \ldots, a_{n-1})$ .

If  $a_i = A_i$  are  $m \times m$  matrices we have a block circulant matrix

Any circulant matrix A can be viewed as a polynomial with coefficients  $a_i$  in the unit circulant matrix S defined by its first row (0, 1, 0, ..., 0)

$$A = \sum_{i=0}^{n-1} a_i S^i, \quad S = \begin{bmatrix} 0 & 1 & & \\ \vdots & \ddots & \ddots & \\ 0 & & \ddots & 1 \\ 1 & 0 & \cdots & 0 \end{bmatrix}$$

Clearly,  $S^n - I = 0$  so that circulant matrices form a matrix algebra isomorphic to the algebra of polynomials with the product modulo  $x^n - 1$ 

If A is a circulant matrix with first row  $\mathbf{r}^{T}$  and first column  $\mathbf{c}$ , then

$$A = \frac{1}{n} \Omega_n^* \text{Diag}(\mathbf{w}) \Omega_n = F^* \text{Diag}(\mathbf{w}) F$$

where  $\mathbf{w} = \Omega_n \mathbf{c} = \Omega_n^* \mathbf{r}$ .

Consequences

$$A\mathbf{x} = \mathsf{DFT}_n(\mathsf{IDFT}_n(\mathbf{c}) \odot \mathsf{IDFT}_n(\mathbf{x}))$$

where " $\odot$ " denotes the Hadamard, or component-wise product of vectors.

The product  $A\mathbf{x}$  of an  $n \times n$  circulant matrix A and a vector  $\mathbf{x}$ , as well as the product of two circulant matrices can be computed by means of two IDFTs and a DFT of length n in  $O(n \log n)$  ops

The inverse of a circulant matrix can be computed in  $O(n \log n)$  ops

$$A^{-1} = \frac{1}{n} \Omega_n^* \operatorname{Diag}(\mathbf{w}^{-1}) \Omega_n \qquad \Rightarrow \qquad A^{-1} \mathbf{e}_1 = \frac{1}{n} \Omega_n^* \mathbf{w}^{-1}$$

The definition of circulant matrix is naturally extended to block matrices where  $a_i = A_i$  are  $m \times m$  matrices.

The inverse of a block circulant matrix can be computed by means of  $2m^2$  IDFTs of length *n* and *n* inversions of  $m \times m$  matrices for the cost of  $O(m^2 n \log n + nm^3)$ 

The product of two block circulant matrices can be computed by means of  $2m^2$  IDFTs,  $m^2$  DFT of length *n* and *n* multiplications of  $m \times m$  matrices for the cost of  $O(m^2 n \log n + nm^3)$ .

#### z-circulant matrices

A generalization of circulant matrices is provided by the class of *z*-circulant matrices.

Given a scalar  $z \neq 0$  and the row vector  $[a_0, a_1, \ldots, a_{n-1}]$ , the  $n \times n$  matrix

$$A = \begin{bmatrix} a_0 & a_1 & \dots & a_{n-1} \\ za_{n-1} & a_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_1 \\ za_1 & \dots & za_{n-1} & a_0 \end{bmatrix}$$

is called the *z*-circulant matrix associated with  $[a_0, a_1, \ldots, a_{n-1}]$ .

Denote by  $S_z$  the z-circulant matrix whose first row is [0, 1, 0, ..., 0], i.e.,

$$S_{z} = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & 0 & 1 \\ z & 0 & \dots & 0 & 0 \end{bmatrix},$$

• Any z-circulant matrix can be viewed as a polynomial in  $S_z$ .

$$A=\sum_{i=0}^{n-1}a_iS_z^i.$$

- $S_{z^n} = zD_zSD_z^{-1}$ ,  $D_z = \text{Diag}(1, z, z^2, \dots, z^{n-1})$ , where S is the unit circulant matrix.
- If A is the z<sup>n</sup>-circulant matrix with first row r<sup>T</sup> and first column c then

$$A = \frac{1}{n} D_z \Omega_n^* \text{Diag}(\mathbf{w}) \Omega_n D_z^{-1},$$

with  $\mathbf{w} = \Omega_n^* D_z \mathbf{r} = \Omega_n D_z^{-1} \mathbf{c}$ .

- Multiplication of z-circulants costs 2 IDFTs, 1 DFT and a scaling
- Inversion of a z-circulant costs 1 IDFT, 1 DFT, n inversions and a scaling
- The extension to block matrices trivially applies to z-circulant matrices.

#### Embedding Toeplitz matrices into circulants

An  $n \times n$  Toeplitz matrix  $A = (t_{i,j})$ ,  $t_{i,j} = a_{j-i}$ , can be embedded into the  $2n \times 2n$  circulant matrix B whose first row is

 $[a_0, a_1, \ldots, a_{n-1}, *, a_{-n+1}, \ldots, a_{-1}]$ , where \* denotes any number.

B =	$a_0$	$a_1$	a <sub>2</sub>	*	$a_{-2}$	$a_{-1}$
	$a_{-1}$	$a_0$	$a_1$	a <sub>2</sub>	*	a_2
	<i>a</i> _2	$a_{-1}$	$a_0$	$a_1$	<i>a</i> <sub>2</sub>	*
	*	a_2	$a_{-1}$	$a_0$	$a_1$	<i>a</i> <sub>2</sub>
	<i>a</i> <sub>2</sub>	*	$a_{-2}$	$a_{-1}$	$a_0$	$a_1$
	$a_1$	$a_2$	*	a_2	$a_{-1}$	$a_0$

More generally, an  $n \times n$  Toeplitz matrix can be embedded into a  $q \times q$  circulant matrix for any  $q \ge 2n - 1$ .

Consequence: the product y = Ax of an  $n \times n$  Toeplitz matrix A and a vector x can be computed in  $O(n \log n)$  ops.

y = Ax,

$$\begin{bmatrix} y \\ w \end{bmatrix} = B \begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} A & H \\ H & A \end{bmatrix} \begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} Ax \\ Hx \end{bmatrix}$$

- embed the Toeplitz matrix A into the circulant matrix  $B = \begin{bmatrix} A & H \\ H & A \end{bmatrix}$
- embed the vector x into the vector  $v = \begin{bmatrix} x \\ 0 \end{bmatrix}$
- compute the product u = Bv
- set  $y = (u_1, ..., u_n)^T$

Cost: 3 FFTs of order 2n, that is  $O(n \log n)$  ops

Similarly, the product y = Ax of an  $n \times n$  block Toeplitz matrix with  $m \times m$  blocks and a vector  $x \in \mathbb{C}^{mn}$  can be computed in  $O(m^2 n \log n + m^3 n)$  ops.

Triangular Toeplitz matrices Let  $Z = (z_{i,j})_{i,j=1,n}$  be the  $n \times n$  matrix

$$Z = \left[ egin{array}{cccc} 0 & & 0 \ 1 & \ddots & & \ & \ddots & \ddots & \ 0 & & 1 & 0 \end{array} 
ight],$$

Clearly  $Z^n = 0$ , moreover, given the polynomial  $a(x) = \sum_{i=0}^{n-1} a_i x^i$ , the matrix  $a(Z) = \sum_{i=0}^{n-1} a_i Z^i$  is a lower triangular Toeplitz matrix defined by its first column  $(a_0, a_1, \dots, a_{n-1})^T$ 

$$a(Z) = \begin{bmatrix} a_0 & & 0 \\ a_1 & a_0 & & \\ \vdots & \ddots & \ddots & \\ a_{n-1} & \dots & a_1 & a_0 \end{bmatrix}$$

The set of lower triangular Toeplitz matrices forms an algebra isomorphic to the algebra of polynomials with the product modulo  $x^n$ .

#### Inverting a triangular Toeplitz matrix

The inverse matrix  $T_n^{-1}$  is still a lower triangular Toeplitz matrix defined by its first column  $v_n$ . It can be computed by solving the system  $T_n v_n = e_1$ 

Let n = 2h, h a positive integer, and partition  $T_n$  into  $h \times h$  blocks

$$T_n = \begin{bmatrix} T_h & 0 \\ W_h & T_h \end{bmatrix},$$

where  $T_h$ ,  $W_h$  are  $h \times h$  Toeplitz matrices and  $T_h$  is lower triangular.

$$T_n^{-1} = \begin{bmatrix} T_h^{-1} & 0 \\ \hline -T_h^{-1} W_h T_h^{-1} & T_h^{-1} \end{bmatrix}$$

The first column  $\mathbf{v}_n$  of  $T_n^{-1}$  is given by

$$\mathbf{v}_n = \mathcal{T}_n^{-1} \mathbf{e}_1 = \begin{bmatrix} \mathbf{v}_h \\ -\mathcal{T}_h^{-1} \mathcal{W}_h \mathbf{v}_h \end{bmatrix} = \begin{bmatrix} \mathbf{v}_h \\ -L(\mathbf{v}_h) \mathcal{W}_h \mathbf{v}_h \end{bmatrix},$$

where  $L(\mathbf{v}_h) = T_h^{-1}$  is the lower triangular Toeplitz matrix whose first column is  $\mathbf{v}_h$ .

The same relation holds if  $T_n$  is block triangular Toeplitz. In this case, the elements  $a_0, \ldots, a_{n-1}$  are replaced with the  $m \times m$  blocks  $A_0, \ldots, A_{n-1}$  and  $\mathbf{v}_n$  denotes the first block column of  $T_n^{-1}$ .

Recursive algorithm for computing  $v_n$  (block case)

INPUT: 
$$n = 2^k, A_0, ..., A_{n-1}$$

OUTPUT:  $v_n$ 

#### COMPUTATION:

Set v<sub>1</sub> = A<sub>0</sub><sup>-1</sup>
For i = 0, ..., k - 1, given v<sub>h</sub>, h = 2<sup>i</sup>:
Compute the block Toeplitz matrix-vector products w = W<sub>h</sub>v<sub>h</sub> and u = -L(v<sub>h</sub>)w.
Set
v<sub>2h</sub> = v<sub>2h</sub> = v<sub>1</sub> .

Cost:  $O(n \log n)$  ops

### z-circulant and triangular Toeplitz matrices

If  $\epsilon = |z|$  is "small" then a z-circulant approximates a triangular Toeplitz

$$\begin{bmatrix} a_0 & a_1 & \dots & a_{n-1} \\ za_{n-1} & a_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_1 \\ za_1 & \dots & za_{n-1} & a_0 \end{bmatrix} \approx \begin{bmatrix} a_0 & a_1 & \dots & a_{n-1} \\ a_0 & \ddots & \vdots \\ & \ddots & a_1 \\ & & & a_0 \end{bmatrix}$$

Inverting a z-circulant is less expensive than inverting a triangular Toeplitz (roughly by a factor of 10/3)

The advantage is appreciated in a parallel model of computation, over multithreading architectures

Numerical algorithms for approximating the inverse of (block) triangular Toeplitz matrices. Main features:

- Total error=approximation error + rounding errors
- Rounding errors grow as  $\mu\epsilon^{-1},$  approximation errors are polynomials in z
- $\bullet$  the smaller  $\epsilon$  the better the approximation, but the larger the rounding errors
- good compromise: choose ε such that ε = με<sup>-1</sup>. This implies that the total error is O(μ<sup>1/2</sup>): half digits are lost

Different strategies have been designed to overcome this drawback

Assume to work over  ${\mathbb R}$ 

- (interpolation) The approximation error is a polynomial in z. Approximating twice the inverse with, say z = ε and z = -ε and taking the arithmetic mean of the results the approximation error becomes a polynomial in ε<sup>2</sup>.
   ⇒ total error= O(μ<sup>2/3</sup>)

Remark: for k = n the approximation error is zero

- (Higham trick) Choose z = iε then the approximation error affecting the real part of the computed approximation is O(ε<sup>2</sup>).
   ⇒ total error= O(μ<sup>2/3</sup>), i.e., only 1/3 of digits are lost
- (combination) Choose  $z_1 = \epsilon(1 + \mathbf{i})/\sqrt{2}$  and  $z_2 = -z_1$ ; apply the algorithm with  $z = z_1$  and  $z = z_2$ ; take the arithmetic mean of the results. The approximation error on the real part turns out to be  $O(\epsilon^4)$ . The total error is  $O(\mu^{4/5})$ . Only 1/5 of digits are lost.
- (replicating the computation) In general choosing as z<sub>j</sub> the kth roots of i and performing k inversions the error becomes O(μ<sup>2k/(2k+1)</sup>), i.e., only 1/2k of digits are lost

#### Other matrix algebras

Matrices diagonalized by

- the Hartley transform  $H = (h_{i,j})$ ,  $h_{i,j} = \cos \frac{2\pi}{n} i j + \sin \frac{2pi}{n} i j$  [B., FAVATI]
- the sine transform  $S = \sqrt{\frac{2}{n+1}} (\sin \frac{\pi}{n+1} ij)$  (class  $\tau$ ) [B., CAPOVANI]
- the sine transform of other kind
- the cosine transform of kind k [KAILATH, OLSHEVSKY]

Displacement operators

#### **Displacement operators**

Recall that 
$$S_z = \begin{bmatrix} 0 & 1 \\ \ddots & \ddots \\ & \ddots & \\ & \ddots & 1 \\ z & & 0 \end{bmatrix}$$
 and let  $T = \begin{bmatrix} a & b & c & d \\ e & a & b & c \\ f & e & a & b \\ g & f & e & a \end{bmatrix}$   
Then

$$S_{z_1}T - TS_{z_2} = \begin{bmatrix} \uparrow \\ \uparrow \end{bmatrix} - \begin{bmatrix} \rightarrow \\ - \end{bmatrix}$$
$$= \begin{bmatrix} e & a & b & c \\ f & e & a & b \\ g & f & e & a \\ z_1a & z_1b & z_1c & z_1d \end{bmatrix} - \begin{bmatrix} z_2d & a & b & c \\ z_2c & e & a & b \\ z_2b & f & e & a \\ z_2a & g & f & e \end{bmatrix}$$
$$= \begin{bmatrix} * \\ \vdots \\ 0 \\ \hline * \\ \vdots \\ \cdots \\ * \end{bmatrix} = e_nu^T + ve_1^T \quad (\text{rank at most } 2)$$

\_

 $T \rightarrow S_{z_1}T - TS_{z_2}$  displacement operator of Sylvester type  $T \rightarrow T - S_{z_1}TS_{z_2}^T$  displacement operator of Stein type

If the eigenvalues of  $S_{z_1}$  are disjoint from those of  $S_{z_2}$  then the operator of Sylvester type is invertible. This holds if  $z_1 \neq z_2$ 

If the eigenvalues of  $S_{z_1}$  are different from the reciprocal of those of  $S_{z_2}$  then the operator of Stein type is invertible. This holds if  $z_1z_2 \neq 1$ 

For simplicity, here we consider  $Z := S_0^T = \begin{bmatrix} 0 & & \\ 1 & \ddots & \\ & \ddots & \ddots & \\ & & & 1 & 0 \end{bmatrix}$ 

If A is Toeplitz then  $\Delta(A) = AZ - ZA$  is such that

$$\Delta(A) = \begin{bmatrix} & \leftarrow & \\ & - & \\ & & \end{bmatrix} - \begin{bmatrix} & \downarrow & \\ & \downarrow & \end{bmatrix} = \begin{bmatrix} a_1 & a_2 & \dots & a_{n-1} & 0 \\ & & & & \\ & & & & \\ 0 & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

Any pair  $V, W \in \mathbb{F}^{n \times k}$  such that  $\Delta(A) = VW^T$  is called *displacement* generator of rank k.

Proposition.

If  $A \in \mathbb{F}^{n \times n}$  has first column *a* and  $\Delta(A) = VW^T$ ,  $V, W \in \mathbb{F}^{n \times k}$  then

$$A = L(a) + \sum_{i=1}^{k} L(v_i) L^{T}(Zw_i), \quad L(a) = \begin{bmatrix} a_1 \\ \vdots \\ a_n \\ \dots \\ a_n \end{bmatrix}$$

Outline of the proof.

Consider the case where k = 1. Rewrite the system  $AZ - ZA = vw^T$  in vec form as

$$(Z^T \otimes I - I \otimes Z)$$
vec $(A) = w \otimes v$ 

where vec(A) is the  $n^2$ -vector obtained by stacking the columns of ASolve the block triangular system by substitution

Equivalent representations can be given for Stein-type operators

#### Proposition.

For  $\Delta(A) = AZ - ZA$  it holds that  $\Delta(AB) = A\Delta(B) + \Delta(A)B$  and

$$\Delta(A^{-1}) = -A^{-1}\Delta(A)A^{-1}$$

Therefore

$$A^{-1} = L(A^{-1}e_1) - \sum_{i=1}^{k} L(A^{-1}v_i)L^{T}(ZA^{-T}w_i)$$

If  $A = (a_{j-i})$  is Toeplitz then  $\Delta(A) = VW^T$  where  $V = \begin{bmatrix} 1 & 0 \\ 0 & a_{n-1} \\ \vdots & \vdots \\ 0 & a_1 \end{bmatrix}, \quad W = \begin{bmatrix} a_1 & 0 \\ \vdots & \vdots \\ a_{n-1} & 0 \\ 0 & -1 \end{bmatrix}$ 

Therefore, the inverse of a Toeplitz matrix is Toeplitz-like

$$A^{-1} = L(A^{-1}e_1) - L(A^{-1}e_1)L^T(ZA^{-1}w_1) + L(A^{-1}v_2)L^T(ZA^{-1}e_n)$$
  
=  $L(A^{-1}e_1)L^T(e_1 - ZA^{-1}w_1) + L(A^{-1}v_2)L^T(ZA^{-1}e_n)$ 

The Gohberg-Semencul-Trench formula

$$T^{-1} = \frac{1}{x_1} \left( L(x) L^T (Jy) - L(Zy) L^T (ZJx) \right),$$
  
$$x = T^{-1} e_1, \quad y = T^{-1} e_n, \quad J = \begin{bmatrix} & & 1 \\ & & \end{bmatrix}$$

- The first and the last column of the inverse define all the entries
- Multiplying a vector by the inverse costs  $O(n \log n)$

#### Generalization of displacement operators

Given matrices X, Y define the operator

$$F_{X,Y}(A) = XA - AY$$

Assume rank(X - Y) = 1. Let A = BC where  $B = \sum_i b_i X^i$ ,  $C = \sum_i c_i Y^i$ . Then

$$XA - AY = XBC - BCY = BXC - BYC = B(X - Y)C$$

Thus,  $A = \sum_{j=1}^{k} B_j C_j$ , where  $B_j$  and  $C_j$  are polynomials in X and Y, respectively, implies rank  $F_{X,Y}(A) \le k$ .

If the spectra of X and Y are disjoint then  $F_{X,Y}(\cdot)$  is invertible and rank  $F_{X,Y}(A) = k \Rightarrow A = \sum_{j=1}^{k} B_j C_j$ 

Examples: X unit circulant, Y lower shift matrix X unit -1-circulant, Y unit circulant provide representations of Toeplitz matrices and their inverses

If A is invertible then  $F_{Y,X}(A^{-1}) = -A^{-1}F_{X,Y}(A)A^{-1}$  so that rank  $F_{Y,X}(A^{-1}) = \operatorname{rank} F_{X,Y}(A)$ 

#### Other operators: Cauchy-like matrices

Define 
$$\Delta(X) = D_1 X - X D_2$$
,  $D_1 = \text{diag}(d_1^{(1)}, \dots, d_n^{(1)})$ ,  
 $D_2 = \text{diag}(d_1^{(2)}, \dots, d_n^{(2)})$ , where  $d_i^{(1)} \neq d_j^{(2)}$  for  $i \neq j$ .

It holds that

$$\Delta(A) = uv^T \quad \Leftrightarrow \quad a_{i,j} = \frac{u_i v_j}{d_i^{(1)} - d_j^{(2)}}$$

Similarly, given  $n \times k$  matrices U, V, one finds that

$$\Delta(B) = UV^T \quad \Leftrightarrow \quad b_{i,j} = \frac{\sum_{r=1}^k u_{i,r} v_{j,r}}{d_i^{(1)} - d_j^{(2)}}$$

A is said Cauchy matrix, B is said Cauchy-like matrix

A nice feature of Cauchy-like matrices is that their Schur complement is still a Cauchy-like matrix

Consider the case k = 1: partition the Cauchy-like matrix C as

$$C = \begin{bmatrix} \frac{u_1 v_1}{d_1^{(1)} - d_1^{(2)}} & \frac{u_1 v_2}{d_1^{(1)} - d_2^{(2)}} & \cdots & \frac{u_1 v_n}{d_1^{(1)} - d_n^{(2)}} \\ \vdots & & & \\ \frac{u_2 v_1}{d_2^{(1)} - d_1^{(2)}} & & & \\ \vdots & & & \hat{C} \\ \frac{u_n v_1}{d_n^{(1)} - d_1^{(2)}} & & & & \\ \end{bmatrix}$$

where  $\widehat{C}$  is still a Cauchy-like matrix. The Schur complement is given by

$$\widehat{C} - \begin{bmatrix} \frac{u_2 v_1}{d_2^{(1)} - d_1^{(2)}} \\ \vdots \\ \frac{u_n v_1}{d_n^{(1)} - d_1^{(2)}} \end{bmatrix} \frac{d_1^{(1)} - d_1^{(2)}}{u_1 v_1} \begin{bmatrix} \frac{u_1 v_2}{d_1^{(1)} - d_2^{(2)}} & \cdots & \frac{u_1 v_n}{d_1^{(1)} - d_n^{(2)}} \end{bmatrix}$$

The entries of the Schur complement can be written in the form

$$\frac{\widehat{u}_i \widehat{v}_j}{d_i^{(1)} - d_j^{(2)}}, \quad \widehat{u}_i = u_i \frac{d_1^{(1)} - d_i^{(1)}}{d_i^{(1)} - d_1^{(2)}}, \quad \widehat{v}_j = v_j \frac{d_j^{(2)} - d_1^{(2)}}{d_1^{(1)} - d_j^{(2)}}.$$

The values  $\hat{u}_i$  and  $\hat{v}_j$  can be computed in O(n) ops.

The computation can be repeated until the LU decomposition of C is obtained

The algorithm is known as Gohberg-Kailath-Olshevsky (GKO) algorithm

Its overall cost is  $O(n^2)$  ops

There are variants which allow pivoting

## Algorithms for Toeplitz inversion

### Algorithms for Toeplitz inversion

Consider  $\Delta(A) = S_1A - AS_{-1}$  where  $S_1$  is the unit circulant matrix and  $S_{-1}$  is the unit (-1)-circulant matrix.

We have observed that the matrix  $\Delta(A)$  has rank at most 2

Now, recall that  $S_1 = F^*D_1F$ ,  $S_{-1} = DF^*D_{-1}FD^{-1}$ , where  $D_1 = \text{Diag}(1, \bar{\omega}, \bar{\omega}^2, \dots, \bar{\omega}^{n-1})$ ,  $D_{-1} = \delta D_1$ ,  $D = \text{Diag}(1, \delta, \delta^2, \dots, \delta^{n-1})$ ,  $\delta = \omega_n^{1/2} = \omega_{2n}$  so that

$$\Delta(A) = F^* D_1 F A - A D F^* D_{-1} F D^{-1}$$

multiply to the left by F, and to the right by  $DF^*$  and discover that

 $D_1B - BD_{-1}$  has rank at most 2, where  $B = FADF^*$ 

That is, B is Cauchy like of rank at most 2.

To eplitz systems can be solved in  $O(n^2)$  ops by means of the GKO algorithm

Software by G. Rodriguez and A. Arico: bugs.unica.it/~gppe/soft/#smt
### Super fast Toeplitz solvers

The term "fast Toeplitz solvers" denotes algorithms for solving  $n \times n$ Toeplitz systems in  $O(n^2)$  ops.

The term "super-fast Toeplitz solvers" denotes algorithms for solving  $n \times n$  Toeplitz systems in  $O(n \log^2 n)$  ops.

Idea of the Bitmead-Anderson superfast solver

Operator 
$$F(A) = A - ZAZ^T = \begin{bmatrix} & \\ & \end{bmatrix} - \begin{bmatrix} & \\ & \searrow \end{bmatrix} = \begin{bmatrix} * & \dots & * \\ \vdots & & \\ * & & \end{bmatrix}$$

Partition the matrix as

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix}$$

$$A = \begin{bmatrix} I & 0 \\ A_{2,1}A_{1,1}^{-1} & I \end{bmatrix} \begin{bmatrix} A_{1,1} & A_{1,2} \\ 0 & B \end{bmatrix}, \quad B = A_{2,2} - A_{2,1}A_{1,1}^{-1}A_{1,2}$$

#### Fundamental property

The Schur complement B is such that  $\operatorname{rank} F(A) = \operatorname{rank} F(B)$ ; the other blocks of the LU factorization have almost the same displacement rank of the matrix A

Solving two systems with the matrix A (for computing the displacement representation of  $A^{-1}$ ) is reduced to solving two systems with the matrix  $A_{1,1}$  for computing  $A_{1,1}^{-1}$  and two systems with the matrix B which has displacement rank 2, plus performing some Toeplitz-vector products

Cost: 
$$C(n) = 2C(n/2) + O(n \log n) \Rightarrow C(n) = O(n \log^2 n)$$

Asymptotic spectral properties and preconditioning

Definition: Let  $f(x) : [0, 2\pi] \to \mathbb{R}$  be a Lebesgue integrable function. A sequence  $\{\lambda_i^{(n)}\}_{i=1,n}, n \in \mathbb{N}, \lambda_i^{(n)} \in \mathbb{R}$  is distributed as f(x) if

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} F(\lambda_i^{(n)}) = \frac{1}{2\pi} \int_0^{2\pi} F(f(x)) dx$$

for any continuous F(x) with bounded support.

Example  $\lambda_i^{(n)} = f(2i\pi/n)$ , i = 1, ..., n,  $n \in \mathbb{N}$  is distributed as f(x).

With abuse of notation, given  $a(z) : \mathbb{T} \to \mathbb{R}$  we write  $a(\theta)$  in place of  $a(z(\theta)), z(\theta) = \cos \theta + \mathbf{i} \sin \theta \in \mathbb{T}$ 

Assume that

- the symbol  $a(\theta) : [0 : 2\pi] \to \mathbb{R}$  is a real valued function so that  $a(\theta) = a_0 + 2\sum_{k=1}^{\infty} a_k \cos k\theta$
- $T_n$  is the sequence of Toeplitz matrices associated with  $a(\theta)$ , i.e.,  $T_n = (a_{|j-i|})_{i,j=1,n}$ ; observe that  $T_n$  is symmetric
- m<sub>a</sub> = ess inf<sub>θ∈[0,2π]</sub>a(θ), M<sub>a</sub> = ess sup<sub>θ∈[0,2π]</sub>a(θ) are the essential infimum and the essential supremum
- $\lambda_1^{(n)} \leq \lambda_2^{(n)} \leq \cdots \leq \lambda_n^{(n)}$  are the eigenvalues of  $T_n$  sorted in nondecreasing order (observe that  $T_n$  is real symmetric).

Then

- if  $m_a < M_a$  then  $\lambda_i^{(n)} \in (m_a, M_a)$  for any n and i = 1, ..., n; if  $m_a = M_a$  then  $a(\theta)$  is constant and  $T_n(a) = m_a I_n$ ;
- $im_{n\to\infty} \lambda_1^{(n)} = m_a, \ \lim_{n\to\infty} \lambda_n^{(n)} = M_a;$
- **③** the eigenvalues sequence  $\{\lambda_1^{(n)}, \ldots, \lambda_n^{(n)}\}$  are distributed as  $a(\theta)$

Moreover

- if a(x) > 0 the condition number  $\mu^{(n)} = ||T_n||_2 ||T_n^{-1}||_2$  of  $T_n$  is such that  $\lim_{n\to\infty} \mu^{(n)} = M_a/m_a$
- $a(\theta) > 0$  implies that  $T_n$  is uniformly well conditioned
- $a(\theta) = 0$  for some  $\theta$  implies that  $\lim_{n \to \infty} \mu_n = \infty$



In red: eigenvalues of the Toeplitz matrix  $T_n$  associated with the symbol  $f(\theta) = 2 - 2\cos\theta - \frac{1}{2}\cos(2\theta)$  for n = 10, n = 20In blue: graph of the symbol. As n grows, the values  $\lambda_i^{(n)}$  for  $i = 1, \ldots, n$  tend to be shaped as the graph of the symbol

The same asymptotic property holds true for

- block Toeplitz matrices generated by a matrix valued symbol A(x)
- block Toeplitz matrices with Toeplitz blocks generated by a bivariate symbol a(x, y)
- multilevel block Toeplitz matrices generated by a multivariate symbol  $a(x_1, x_2, \ldots, x_d)$
- singular values of any of the above matrix classes

The same results hold for the product  $P_n^{-1}T_n$  where  $T_n$  and  $P_n$  are associated with symbols  $a(\theta)$ ,  $p(\theta)$ , respectively

- eigenvalues are distributed as  $a(\theta)/p(\theta)$
- (preconditioning) given  $a(\theta) \ge 0$  such that  $a(\theta_0) = 0$  for some  $\theta_0$ ; if there exists a trigonometric polynomial  $p(\theta) = \sum_{i=-k}^{k} p_k \cos(k\theta)$  such that  $p(\theta_0) = 0$ ,  $\lim_{\theta \to \theta_0} a(\theta)/p(\theta) \ne 0$  then  $P_n^{-1}T_n$  has condition number uniformly bounded by a constant

### Trigonometric matrix algebras and preconditioning

The solution of a positive definite  $n \times n$  Toeplitz system  $A_n x = b$  can be approximated with the Preconditioned Conjugate Gradient (PCG) method

Some features of the Conjugate Gradient (CG) iteration:

- it applies to positive definite systems Ax = b
- CG generates a sequence of vectors {x<sub>k</sub>}<sub>k=0,1,2,...</sub> converging to the solution in n steps
- each step requires a matrix-vector product plus some scalar products. Cost for Toeplitz systems O(n log n)
- residual error:  $||Ax_k b|| \le \gamma \theta^k$ , where  $\theta = (\sqrt{\mu} 1)/(\sqrt{\mu} + 1)$ ,  $\mu = \lambda_{\max}/\lambda_{\min}$  is the condition number of A
- convergence is fast for well-conditioned systems, slow otherwise. However:
- (Axelsson-Lindskog) Informal statement: if A has all the eigenvalues in the interval  $[\alpha, \beta]$  where  $0 < \alpha < 1 < \beta$  except for q outliers which stay outside, then the residual error is bounded by  $\gamma_1 \theta_1^{k-q}$  for  $\theta_1 = (\sqrt{\mu_1} 1)/(\sqrt{\mu_1} + 1)$ , where  $\mu_1 = \beta/\alpha$ .

Features of the Preconditioned Conjugate Gradient (PCG) iteration:

- it consists of the Conjugate Gradient method applied to the system  $P^{-1}A_n x = P^{-1}b$ , the matrix P is the preconditioner
- The preconditioner *P* must be chosen so that:
  - solving the system with matrix P is cheap
  - P mimics the matrix A so that P<sup>-1</sup>A has either condition number close to 1, or has eigenvalues in a narrow interval [α, β] containing 1, except for few outliers

For Toeplitz matrices, P can be chosen in a trigonometric algebra. In this case

- each step of PCG costs  $O(n \log n)$
- the spectrum of  $P^{-1}A$  is clustered around 1

### Example of preconditioners

If  $A_n$  is associated with the symbol  $a(\theta) = a_0 + 2\sum_{i=1}^{\infty} a_i$  and  $a(\theta) \ge 0$ , then  $\mu(A_n) \to \max a(\theta) / \min a(\theta)$ 

Choosing  $P_n = C_n$ , where  $C_n$  is the symmetric circulant which minimizes the Frobenius norm  $||A_n - C_n||_F$ , then the eigenvalues of  $B_n = P_n^{-1}C_n$  are clustered around 1. That is, for any  $\epsilon$  there exists  $n_0$  such that for any  $n \ge n_0$  the eigenvalues of  $P_n^{-1}A$  belong to  $[1 - \epsilon, 1 + \epsilon]$  except for a few outliers.

Effective preconditioners can be found in the  $\tau$  and in the Hartley algebras, as well as in the class of banded Toeplitz matrices

### Example of preconditioners

Consider the  $n \times n$  matrix A associated with the symbol  $a(\theta) = 6 + 2(-4\cos(\theta) + \cos(2\theta))$ , that is

Its eigenvalues are distributed as the symbol  $a(\theta)$  and its cond is  $O(n^4)$ 



The eigenvalues of the preconditioned matrix  $P^{-1}A$ , where P is circulant, are clustered around 1 with very few outliers.

### Example of preconditioners

The following figure reports the log of the eigenvalues of A (in red) and of the log of the eigenvalues of  $P^{-1}A$  in blue



Figure : Log of the eigenvalues of A (in red) and of  $P^{-1}A$  in blue

### Rank structured matrices

## Rank structured (quasiseparable) matrices

#### Definition

An  $n \times n$  matrix A is rank structured with rank k if all its submatrices contained in the upper triangular part or in the lower triangular part have rank at most k



A wide literature exists: Gantmacher, Kreĭn, Asplund, Capovani, Rózsa, Van Barel, Vandebril, Mastronardi, Eidelman, Gohberg, Romani, Gemignani, Boito, Chandrasekaran, Gu, ...

Books by Van Barel, Vandebril, Mastronardi, and by Eidelman

#### Some examples:

- The sum of a diagonal matrix and a matrix of rank k
- A tridiagonal matrix (k = 1)
- The inverse of an irreducible tridiagonal matrix (k = 1)
- Any orthogonal matrix in Hessenberg form (k = 1)
- A Frobenius companion matrix (k = 1)
- A block Frobenius companion matrix with  $m \times m$  blocks (k = m)

#### Definition

A rank structured matrix A of rank k has a generator if there exist matrices B, C of rank k such that triu(A) = triu(B), tril(A) = tril(C).

#### Remarks:

- An irreducible tridiagonal matrix has no generator,
- A (block) companion matrix has a generator defining the upper triangular part but no generator for the lower triangular part

### Some properties of rank-structured matrices

Nice properties have been proved concerning rank-structured matrices For a k-rank-structured matrix A

- The inverse of A is k rank structured
- The LU factors of A are k-rank structured
- The QR factors of A are rank-structured with rank k and 2k
- Solving an  $n \times n$  system with a k-rank structured matrix costs  $O(nk^2)$  ops
- the Hessenberg form H of A is (2k 1)-rank structured
- if A is the sum of a **real diagonal** matrix plus a matrix of rank k then the QR iteration generates a sequence A<sub>i</sub> of rank-structured matrices
- computing H costs  $O(nk^2)$  ops
- computing det *H* costs *O*(*nk*) ops

A nice representation, with an implementation of specific algorithms is given by Börm, Grasedyck and Hackbusch and relies on the hierarchical representation

It relies on splitting the matrix into blocks and in representing blocks non-intersecting the diagonal by means of low rank matrices



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# 3– Algorithms for structured Markov chains

### Finite case: block tridiagonal matrices

Let us consider the finite case and start with a QBD problem In this case we have to solve a homogeneous linear system where the matrix  $\mathcal{A}$  is  $n \times n$  block-tridiagonal almost block-Toeplitz with  $m \times m$ blocks. We assume  $\mathcal{A}$  irreducible

$$\begin{bmatrix} \pi_1 & \pi_2 & \dots & \pi_n \end{bmatrix} \begin{bmatrix} I - \widehat{A}_0 & -A_1 & & & \\ -A_{-1} & I - A_0 & -A_1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & -A_{-1} & I - A_0 & -A_1 \\ & & & -A_{-1} & I - \widetilde{A}_0 \end{bmatrix} = 0$$

The matrix is singular, the vector  $\mathbf{e} = (1, ..., 1)^T$  is in the right null space. By the Perron-Frobenius theorem aplied to trid $(A_{-1}, A_0, A_1)$ , the null space has dimension 1

**Remark.** If A = I - S, with S stochastic and irreducible, then all the proper principal submatrices of A are nonsingular.

Proof. Assume by contraddiction that a principal submatrix  $\widehat{\mathcal{A}}$  of  $\mathcal{A}$  is singular. Then the corresponding submatrix  $\widehat{\mathcal{S}}$  of  $\mathcal{S}$  has the eigenvalue 1. This contraddicts Lemma 2.6 [R. VARGA] which says that  $\rho(\widehat{\mathcal{S}}) < \rho(\mathcal{S})$ 

In particular, since the proper leading principal submatrices are invertible, there exists unique the LU factorization where only the last diagonal entry of U is zero.

The most immediate possibility to solve this system is to compute the LU factorization  $\mathcal{A} = \mathcal{LU}$  and solve the system

$$\pi \mathcal{L} = (0, \ldots, 0, 1)$$

since the vector  $[0, \ldots, 0, 1]U = 0$ 

This method is numerically stable (no cancellation is encountered), its cost is  $O(nm^3)$ , but it is not the most efficient method. Moreover, the structure is only partially exploited

A more efficient algorithm relies on the Cyclic Reduction (CR) technique introduced by Gene H. Golub in 1970

For the sake of notational simplicity denote

$$\begin{split} B_{-1} &= -A_1, \quad , B_0 = I - A_0, \quad B_1 = -A_1, \\ \widehat{B}_0 &= I - \widehat{A}_0, \quad \widetilde{B}_0 = I - \widetilde{A}_0 \end{split}$$

Thus, our problem becomes

$$[\pi_1, \pi_2, \dots, \pi_n] \begin{bmatrix} \hat{B}_0 & B_1 & & & \\ B_{-1} & B_0 & B_1 & & & \\ & B_{-1} & B_0 & B_1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & B_{-1} & B_0 & B_1 \\ & & & & & B_{-1} & \tilde{B}_0 \end{bmatrix} = 0$$

Outline of CR

Suppose for simplicity  $n = 2^q$ , apply an even-odd permutation to the block unknowns and block equation of the system and get



where

$$\begin{bmatrix} \pi_{\text{even}} & \pi_{\text{odd}} \end{bmatrix} = \begin{bmatrix} \pi_2 & \pi_4 & \dots & \pi_{\frac{n}{2}} \end{bmatrix} \pi_1 & \pi_3 & \dots & \pi_{\frac{n-2}{2}} \end{bmatrix}$$

[X	Х	•	•	•	•	•	.]
x	X	X	•	•	•	•	
.	X	X	X				
.		X	X	X			
.			X	X	X		
.				х	х	х	
.	•				х	х	x
L.						X	x

(1,1) block



(2,2) block



(1,2) block



(2,1) block



Denote by



the matrix obtained after the permutation

Compute its block LU factorization and get

$$\mathcal{A}' = \begin{bmatrix} I & 0 \\ WD_2^{-1} & I \end{bmatrix} \begin{bmatrix} D_1 & V \\ 0 & S \end{bmatrix}$$

where the Schur complement S, given by

$$S = D_2 - W D_1^{-1} V$$

is singular

The original problem is reduced to

$$\begin{bmatrix} \pi_{\text{even}} & \pi_{\text{odd}} \end{bmatrix} \begin{bmatrix} I & 0\\ WD_2^{-1} & I \end{bmatrix} \begin{bmatrix} D_1 & V\\ 0 & S \end{bmatrix} = \begin{bmatrix} 0 & 0 \end{bmatrix}$$

that is

$$\pi_{\rm odd} S = 0$$
  
$$\pi_{\rm even} = -\pi_{\rm odd} W D_2^{-1}$$

Computing  $\pi$  is reduced to computing  $\pi_{odd}$ From size *n* to size *n*/2 Examine the structure of the Schur complement S



A direct inspection shows that

$$S = \begin{bmatrix} \hat{B}'_{0} & B'_{1} & & \\ B'_{-1} & B'_{0} & B'_{1} & \\ & \ddots & \ddots & \ddots \\ & & B'_{-1} & B'_{0} & B'_{1} \\ & & & & B'_{-1} & \widetilde{B}'_{0} \end{bmatrix}$$

where, for  $C = B_0^{-1}$ ,

$$B'_{0} = B_{0} - B_{-1}CB_{1} - B_{1}CB_{-1}$$

$$B'_{1} = -B_{1}CB_{1}$$

$$B'_{-1} = -B_{-1}CB_{-1}$$

$$\widehat{B}'_{0} = \widehat{B}_{0} - B_{-1}\widehat{B}_{0}^{-1}B_{1}$$

$$\widetilde{B}'_{0} = \widetilde{B}_{0} - B_{1}CB_{-1}$$

(1)

Cost of computing S:  $O(m^3)$
The odd-even reduction can be cyclically applied to the new block tridiagonal matrix until we arrive at a Schur complement of size  $2 \times 2$ 

### Algorithm

- **(**) if n = 2 compute  $\pi$  such that  $\pi A = 0$  by using LU decomposition
- 2) otherwise compute the Schur complement S by means of (1)
- § compute  $\pi_{\mathrm{odd}}$  such that  $\pi_{\mathrm{odd}}S=0$  by using this algorithm

$${ extsf{0}}$$
 compute  $\pi_{ extsf{even}} = -(\pi_{ extsf{odd}} W) D_2^{-1}$ 

• output  $\pi$ 

Computational cost with size n (asymptotic estimate):  $C_n$ 

$$C_n = C_{n/2} + O(m^3) + O(nm^2), \quad C_2 = O(m^3)$$

Overall cost:

Schur complementation  $O(m^3 \log_2 n)$ 

Back substitution:  $O(m^2n + m^2\frac{n}{2} + m^2\frac{n}{4} + \dots + m^2) = O(m^2n)$ 

Total:  $O(m^3 \log n + m^2 n)$  vs.  $O(m^3 n)$  of the standard LU

**Remark** If n is odd, then after the even-odd permutation one obtains the matrix



The Schur complement is still block tridiagonal, block Toeplitz except for the first and last diagonal entry.

The inversion of only one block is required

Choosing  $n = 2^q + 1$ , after one step the size becomes  $2^{q-1} + 1$  so that CR can be cyclically applied

The finite case: block Hessenberg matrices

### Finite case: block Hessenberg

This procedure can be applied to the block Hessenberg case

For simplicity let us write  $B_0 = I - A_0$  and  $B_j = -A_j$  so that the problem is

$$\pi \begin{bmatrix} \hat{B}_{0} & \hat{B}_{1} & \hat{B}_{2} & \dots & \hat{B}_{n-2} & \hat{B}_{n-1} \\ B_{-1} & B_{0} & B_{1} & \ddots & B_{n-3} & \tilde{B}_{n-2} \\ & B_{-1} & \ddots & \ddots & \ddots & \vdots \\ & & \ddots & \ddots & B_{1} \\ & & & B_{-1} & B_{0} & \tilde{B}_{1} \\ & & & & B_{-1} & \tilde{B}_{0} \end{bmatrix} = 0$$

Assume n = 2m + 1, apply an even-odd block permutation to block-rows and block-columns and get

X	X	X	X	X	X	X	X	x
x	x	x	X	X	X	X	X	x
.	X	X	X	X	X	X	X	x
•	•	X	X	X	X	X	X	x
•	•	•	X	X	X	X	X	x
•	•	•	•	Х	Х	X	Х	x
•	•	•	•	•	Х	X	Х	x
	•	•	•	•	•	X	X	x
Ŀ	•	•	•	•	•	•	х	x





(2,2) block



$$(1,2)$$
 block







$$\begin{bmatrix} \pi_{\text{even}} & \pi_{\text{odd}} \end{bmatrix} \begin{bmatrix} D_1 & V \\ \hline W & D_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 \end{bmatrix}$$

where

$$D_{1} = \begin{bmatrix} B_{0} & B_{2} & \dots & B_{2m-4} \\ & B_{0} & \ddots & \vdots \\ & & \ddots & B_{2} \\ & & & & B_{0} \end{bmatrix}, \quad D_{2} = \begin{bmatrix} \widehat{B}_{0} & \widehat{B}_{2} & \widehat{B}_{4} & \dots & \widehat{B}_{2m-4} & \widehat{B}_{2m-2} \\ & B_{0} & B_{2} & \dots & B_{2m-6} & \widetilde{B}_{2m-4} \\ & & \ddots & \ddots & \vdots & \vdots \\ & & & B_{0} & B_{2} & \widetilde{B}_{4} \\ & & & & & B_{0} & \widetilde{B}_{2} \\ & & & & & & & B_{0} \end{bmatrix}$$

$$W = \begin{bmatrix} \widehat{B}_{1} & \widehat{B}_{3} & \dots & \widehat{B}_{2m-3} \\ B_{-1} & B_{1} & \dots & B_{2m-5} \\ & \ddots & \ddots & \vdots \\ & & B_{-1} & B_{1} \\ & & & & B_{-1} \end{bmatrix} \quad V = \begin{bmatrix} B_{-1} & B_{1} & \dots & B_{2m-5} & \widetilde{B}_{2m-3} \\ B_{-1} & \ddots & \vdots & \vdots \\ & & \ddots & B_{1} & \widetilde{B}_{3} \\ & & & & B_{-1} & \widetilde{B}_{1} \end{bmatrix}$$

Computing the LU factorization of  $\begin{bmatrix} D_1 & V \\ W & D_2 \end{bmatrix}$  yields

$$\begin{bmatrix} \pi_{\text{even}} & \pi_{\text{odd}} \end{bmatrix} \begin{bmatrix} I & 0 \\ WD_1^{-1} & I \end{bmatrix} \begin{bmatrix} D_1 & V \\ 0 & S \end{bmatrix} = 0$$

where the Schur complement, given by

$$S = D_2 - W D_1^{-1} V$$

is singular

The problem is reduced to computing

$$\pi_{
m odd} S = 0$$
  
 $\pi_{
m even} = -\pi_{
m odd} W D_1^{-1}$ 

Structure analysis of the Schur complement: assume  $n = 2^q + 1$ 



The structure is preserved under the Schur complementation

The size is reduced from  $2^q + 1$  to  $2^{q-1} + 1$ 

The process can be repeated recursively until a  $3\times 3$  block matrix is obtained

#### Algorithm

- **(**) if n = 3 compute  $\pi$  such that  $\pi A = 0$  by using LU decomposition
- @ otherwise compute the Schur complement S above
- ${f 0}$  compute  $\pi_{
  m odd}$  such that  $\pi_{
  m odd}S={f 0}$  by using this algorithm
- compute  $\pi_{\mathrm{even}} = -(\pi_{\mathrm{odd}} W) D_1^{-1}$
- ullet output  $\pi$

Cost analysis, Schur complementation:

- Inverting a block triangular block Toeplitz matrix costs  $O(m^3n + m^2n \log n)$
- Multiplying block triangular block Toeplitz matrices costs  $O(m^3n + m^2n \log n)$

Thus, Schur complementation costs  $O(m^3n + m^2n \log n)$ 

Computing  $\pi_{\text{even}}$ , given  $\pi_{\text{odd}}$  amounts to computing the product of a block Triangular Toeplitz matrix and a vector for the cost of  $O(m^2n + m^2n \log n)$ 

Overall cost:  $C_n$  is such that

$$C_n = C_{\frac{n+1}{2}} + O(m^3 n + m^2 n \log n), \quad C_3 = O(m^3)$$

The overall computational cost to carry out the computation is  $O(m^3n + m^2n \log n)$  vs.  $O(m^3n^2)$  of standard LU factorization

# Applicability of CR and functional interpretation

# Applicability of CR

In order to be applied, cyclic reduction requires the nonsingularity of certain matrices at all the steps of the iteration

Consider the first step where we are given  $\mathcal{A} = \operatorname{trid}_n(B_{-1}, B_0, B_1)$ 

Here, we need the nonsingularity of  $B_0$ , that is a principal submatrix of  $\mathcal A$ 

After the first step we have  $\mathcal{A}' = \operatorname{trid}_n(B'_{-1},B'_0,B'_1)$  where

$$B_0' = B_0 - B_{-1}CB_1 - B_1CB_{-1}, \quad C = B_0^{-1}$$

Observe that  $B'_0$  is the Schur complement of  $B_0$  in

$$\begin{bmatrix} B_0 & 0 & B_1 \\ 0 & B_0 & B_{-1} \\ B_{-1} & B_1 & B_0 \end{bmatrix}$$

which is similar by permutation to  $trid_3(B_{-1}, B_0, B_1)$ 

By the properties of the Schur complement we have  $\det \operatorname{trid}_3(B_{-1}, B_0, B_1) = \det B_0 \det B'_0$  Inductively, we can prove that

det trid<sub>2<sup>i</sup>-1</sub>(
$$B_{-1}, B_0, B_1$$
)  $\neq 0, i = 1, 2, ..., k$ 

if and only if CR can be applied for the first k steps with no breakdown

Recall that, since A = I - S, with S stochastic and irreducible, then all the principal submatrices of A are nonsingular.

Thus, in the block tridiagonal case, CR can be applied with no breakdown

A similar argument can be used to prove the applicability of CR in the block Hessenberg case

## More on applicability

CR can be applied also in case of breakdown where singular or ill-conditioned matrices are encountered

Denote  $B_{-1}^{(k)}, B_0^{(k)}, B_1^{(k)}$  the matrices generated by CR at step k

Assume det trid<sub>2<sup>k</sup>-1</sub>( $B_{-1}, B_0, B_1$ )  $\neq 0$ , set  $R^{(k)} = \text{trid}_{2^k-1}(B_{-1}, B_0, B_1)^{-1}$ ,  $R^{(k)} = (R_{i,j}^{(k)})$ . Then, playing with Schur complements one finds that

$$B_{-1}^{(k)} = -B_{-1}R_{n,1}^{(k)}B_{-1}$$
  

$$B_0^{(k)} = B_0 - B_{-1}R_{n,n}^{(k)}B_1 - B_1R_{1,1}^{(k)}B_{-1}$$
  

$$B_1^{(k)} = -B_1R_{1,n}^{(k)}B_1$$

Matrices  $B_i^{(k)}$  are well defined if det  $\operatorname{trid}_{2^k-1}(B_{-1}, B_0, B_1) \neq 0$ , no matter if det  $\operatorname{trid}_{2^h-1}(B_{-1}, B_0, B_1) = 0$ , for some h < k, i.e., if CR encounters breakdown

# More on CR: Functional interpretation

Cyclic reduction has a nice functional interpretation which relates it to the Graeffe-Lobachevsky-Dandelin iteration [OSTROWSKY]

This interpretation enables us to apply CR to infinite matrices and to solve QBD and M/G/1 Markov chains as well

Let us recall the Graeffe-iteration:

Let p(z) be a polynomial of degree *n* having *q* zeros of modulus less than 1 and n - q zeros of modulus greater than 1

Observe that in the product p(z)p(-z) the odd powers of z cancel out

This way,  $p(z)p(-z) = p_1(z^2)$  is a polynomial of degree *n* in  $z^2$ 

The zeros of  $p_1(z)$  are the squares of the zeros of p(z)

The sequence defined by

$$p_0(z) = p(z),$$
  
 $p_{k+1}(z^2) = p_k(z)p_k(-z), \quad k = 0, 1, \dots$ 

is such that the zeros of  $p_k(z)$  are the  $2^k$  powers of the zeros of  $p_0(z) = p(z)$ 

Thus, the zeros of  $p_k(z)$  inside the unit disk converge quadratically to zero, the zeros outside the unit disk converge quadratically to infinity.



Whence, the sequence  $p_k(z)/||p_k||_{\infty}$ obtained by normalizing  $p_k(z)$  with the coefficient of largest modulus converges to  $z^q$  Can we do something similar with matrix polynomials or with Laurent polynomials?

For simplicity, we consider the block tridiagonal case

Let  $B_{-1}, B_0, B_1$  be  $m \times m$  matrices,  $B_0$  nonsingular, and define the Laurent matrix polynomial

$$\varphi(z) = B_{-1}z^{-1} + B_0 + B_1z$$

Consider  $\varphi(z)B_0^{-1}\varphi(-z)$  and discover that the odd powers of z cancel out

$$arphi_1(z^2) = arphi(z) B_0^{-1} arphi(-z), \quad arphi_1(z) = B_{-1}^{(1)} z^{-1} + B_0^{(1)} + B_1^{(1)} z^{-1}$$

Moreover, the coefficients of  $\varphi_1(z) = B_{-1}^{(1)} z^{-1} + B_0^{(1)} + B_1^{(1)} z$  are such that

$$B_0^{(1)} = B_0 - B_{-1}CB_1 - B_1CB_{-1}, \qquad C = B_0^{-1}$$
$$B_1^{(1)} = -B_1CB_1$$
$$B_{-1}^{(1)} = B_{-1}CB_{-1}$$

#### These are the same equations which define cyclic reduction!

Cyclic reduction applied to a block tridiagonal Toeplitz matrix generates the coefficients of the Graeffe iteration applied to a matrix Laurent polynomial

Can we deduce nice asymptotic properties from this observation?

With  $\varphi_0(z) = \varphi(z)$  define the sequence

$$\varphi_{k+1}(z^2) = \varphi_k(z)(B_0^{(k)})^{-1}\varphi_k(-z), \quad k = 0, 1, \dots,$$

where we assume that det  $B_0^{(k)} \neq 0$ 

Define

$$\psi_k(z) = \varphi_k(z)^{-1}$$

Observe that  $B_0^{(k)} = rac{1}{2}(arphi_k(-z) + arphi_k(z))$  so that

$$\varphi_{k+1}(z^2) = \varphi_k(z) 2(\varphi_k(-z) + \varphi_k(z))^{-1} \varphi_k(-z)$$
  
= 2(\varphi\_k(z)^{-1} + \varphi\_k(-z)^{-1})^{-1}

Whence

$$\psi_{k+1}(z^2) = \frac{1}{2}(\psi_k(z) + \psi_k(-z))$$

 $\psi_1(z)$  is the even part of  $\psi_0(z)$  $\psi_2(z)$  is the even part of  $\psi_1(z)$ ....

If  $\psi(z)$  is analytic in the annulus  $\mathbb{A} = \{z \in \mathbb{C}: \ r < |z| < R\}$ 



For the analyticity of  $\psi$  in  $\mathbb{A}$  one has  $\forall \epsilon > 0 \exists \theta > 0$  such that

$$\begin{cases} ||H_i|| \le \theta(r+\epsilon)^i, & i > 0\\ ||H_i|| \le \theta(R-\epsilon)^i, & i < 0 \end{cases}$$

[Henrici 1988]

$$\begin{split} \psi_0(z) &= \dots + H_{-2}z^{-2} + H_{-1}z^{-1} + H_0 + H_1z^1 + H_2z^2 + \dots \\ \psi_1(z) &= \dots + H_{-4}z^{-2} + H_{-2}z^{-1} + H_0 + H_2z^1 + H_4z^2 + \dots \\ \psi_2(z) &= \dots + H_{-3}z^{-2} + H_{-4}z^{-1} + H_0 + H_4z^1 + H_8z^2 + \dots \\ \dots \\ \psi_k(z) &= \dots + H_{-3\cdot 2^k}z^3 + H_{-2\cdot 2^k}z^{-2} + H_{-2^k}z^{-1} + H_0 + H_{2^k}z^1 + H_{2\cdot 2^k}z^2 + H_{3\cdot 2^k}z^3 + \dots \end{split}$$

That is, if  $\psi(z)$  is analytic on  $\mathbb{A}$  then the sequence  $\psi_k(z)$  converges to  $H_0$ double exponentially for any z in a compact set contained in  $\mathbb{A}$ 

Consequently, if det  $H_0 \neq 0$  the sequence  $\varphi_k(z)$  converges to  $H_0^{-1}$  double exponentially for any z in any compact set contained in A

Practically, the sequence of block tridiagonal matrices generated by CR converges very quickly to a block diagonal matrix. The speed of convergence is faster the larger is the width of the annulus  $\mathbb A$ 

## Some computational consequences

This convergence property makes it easier to solve block tridiagonal block Toeplitz systems

It is not needed to perform  $\log_2 n$  iteration steps. It is enough to iterate until the Schur complement is numerically block diagonal

Moreover, convergence of CR enables us to compute any number of components of the solution of an infinite block tridiagonal block Toeplitz system:

Iteration is continued until a numerical block diagonal matrix is obtained; a finite number of block components is computed by solving the truncated block diagonal system; back substitution is applied We can provide a functional interpretation of CR also in the block Hessenberg case. But for this goal we have to carry out the analysis in the framework of infinite matrices

Therefore we postpone this analysis

### Questions about analyticity

Is the function  $\psi(z)$  analytic over some annulus A?

Recall that  $\psi(z) = \varphi(z)^{-1}$ , and that  $\varphi(z)$  is a Laurent polynomial

Thus, if det  $\varphi(z) \neq 0$  for  $z \in \mathbb{A}$  then  $\psi(z)$  is analytic in  $\mathbb{A}$ 

The equation det $(B_{-1} + zB_0 + z^2B_1) = 0$  plays an important role

Denote  $\xi_1, \ldots, \xi_{2m}$  the roots of the polynomial  $a(z) = \det(B_{-1} + zB_0 + z^2B_1)$ , ordered so that  $|\xi_i| \le |\xi_{i+1}|$ , where we have added  $2n - \deg a(z)$  roots at the infinity if  $\deg a(z) < 2n$ 

Assume that for some integer q

$$|\xi_q| < 1 < |\xi_{q+1}|$$

then  $\psi(z)$  is analytic on the annulus  $\mathbb{A}$  of radii  $r = |\xi_q|$  and  $R = |\xi_{q+1}|$ 

In the case of Markov chains the following scenario is encountered:

- Positive recurrent:  $\xi_m = 1 < \xi_{m+1}$
- Transient:  $\xi_m < 1 = \xi_{m+1}$
- Null recurrent:  $\xi_m = 1 = \xi_{m+1}$



In yellow the domain of analyticity of  $\psi(z)$ 

## Dealing with $\xi_m = 1$

In principle, CR can be still applied

A simple trick enables us to reduce the problem to the case where the inner part of the annulus  $\mathbb A$  contains the unit circle

Consider  $\widetilde{\varphi}(z) := \varphi(\alpha z)$  so that the roots of det  $\widetilde{\varphi}(z)$  are  $\xi_i \alpha^{-1}$ 

Choose  $\alpha$  so that  $\xi_m < \alpha < \xi_{m+1}$ , this way the function  $\widetilde{\psi}(z) = \widetilde{\varphi}(z)^{-1}$  is analytic in the annulus  $\widetilde{\mathbb{A}} = \{z \in \mathbb{C} : \xi_m \alpha^{-1} < |z| < \xi_{m+1} \alpha^{-1}\}$  which contains the unit circle

With the scaling of the variable one can prove that

- in the positive recurrent case where the analyticity annulus has radii  $\xi_m = 1$ ,  $\xi_{m+1} > 1$ , the blocks  $B_{-1}^{(k)}$  converge to zero with rate  $1/\xi_{m+1}^{2^k}$ , the blocks  $B_1^{(k)}$  have a finite nonzero limit
- in the transient case where the analyticity annulus has radii  $\xi_m < 1$ ,  $\xi_{m+1} = 1$ , the blocks  $B_1^{(k)}$  converge to zero with rate  $\xi_m^{2^k}$ , the blocks  $B_{-1}^{(k)}$  have a finite nonzero limit

However, this trick does not work in the null recurrent case where  $\xi_m = \xi_{m+1} = 1$ . In this situation, convergence of CR turns to linear with factor 1/2.

In order to restore the quadratic convergence we have to use a more sophisticated technique which will be described next

### Some general convergence results

**Theorem.** Assume we are given a function  $\varphi(z) = z^{-1}B_1 + B_0 + zB_1$  and positive numbers r < 1 < R such that

- $\bullet \ \ \, \text{for any } z\in \mathbb{A}(r,R) \text{ the matrix } \varphi(z) \text{ is analytic and nonsingular}$
- The function  $\psi(z) = \varphi(z)^{-1}$ , analytic in A(r, R), is such that det H<sub>0</sub> ≠ 0 where  $\psi(z) = \sum_{i=-\infty}^{+\infty} z^i H_i$

Then

- the sequence  $\varphi^{(k)}(z)$  converges uniformly to  $H_0^{-1}$  over any compact set in  $\mathbb{A}(r, R)$
- **2** for any  $\epsilon$  and for any norm there exist constants  $c_i > 0$  such that

$$\begin{split} \|B_{-1}^{(k)}\| &\leq c_{-1}(r+\epsilon)^{2^{k}} \\ \|B_{1}^{(k)}\| &\leq c_{1}(R-\epsilon)^{-2^{k}} \\ \|B_{0}^{(k)} - H_{0}^{-1}\| &\leq c_{0}\left(\frac{r+\epsilon}{R-\epsilon}\right)^{2^{k}} \end{split}$$

**Theorem.** Given  $\varphi(z) = z^{-1}A_{-1} + A_0 + zA_1$ . If the two matrix equations

$$B_{-1} + B_0 X + B_1 X^2 = 0$$
$$B_{-1} Y^2 + B_0 Y + B_1 = 0$$

have solutions X and Y such that  $\rho(X) < 1$  and  $\rho(Y) < 1$  then det  $H_0 \neq 0$ , the roots  $\xi_i$ , i = 1, ..., 2m of det  $\varphi(z)$  are such that  $|\xi_m| < 1 < |\xi_{m+1}|$ , moreover  $\rho(X) = |\xi_m|$ ,  $\rho(Y) = 1/|\xi_{m+1}|$ . Moreover,  $\psi(z) = \varphi(z)^{-1}$  is analytic in  $\mathbb{A}(\rho(X), 1/\rho(Y))$ 

$$\psi(z) = \sum_{i=-\infty}^{+\infty} z^i H_i, \qquad H_i = \left\{ egin{array}{cc} X^{-i} H_0, & i < 0 \ H_0 \ H_0 \ H_0 Y^i, & i > 0 \end{array} 
ight.$$

**Theorem.** Consider the case where  $\varphi(z) = \sum_{i=-1}^{+\infty} z^i B_i$  is analytic over  $\mathbb{A}(r, R)$  and has the following factorizations valid for |z| = 1

$$\varphi(z) = \left(\sum_{j=0}^{+\infty} z^j U_j\right) \left(I - z^{-1}G\right)$$
$$\varphi(z^{-1}) = \left(I - zV\right) \left(\sum_{j=0}^{+\infty} z^{-j} W_j\right)$$

where the matrix functions  $\sum_{j=0}^{+\infty} z^j U_j$  and  $\sum_{j=0}^{+\infty} z^{-j} W_j$  are nonsingular for |z| < 1 and  $\rho(G), \rho(V) < 1$ , then det  $H_0 \neq 0$ 

## Convergence in the critical case $\xi_m = \xi_{m+1}$

**Theorem** [GUO ET AL. 2008] Let  $\varphi(z) = z^{-1}B_{-1} + B_0 + zB_1$  be the function associated with a null recurrent QBD so that its roots  $\xi_i$  satisfy the condition  $\xi_m = 1 = \xi_{m+1}$ .

Then cyclic reduction can be applied and there exists a constant  $\gamma$  such that

$$||B_{-1}^{(k)}|| \le \gamma 2^{-k}$$
  
$$||B_0^{(k)} - H_0^{-1}|| \le \gamma 2^{-k}$$
  
$$||B_1^{(k)}|| \le \gamma 2^{-k}$$

# Some special cases

Block tridiagonal derived by a banded Toeplitz matrix

This case is handled by the functional form of CR

Assume we are given an  $n \times n$  banded Toeplitz matrix, up to some boundary corrections, having 2m + 1 diagonals. Say, with m = 2,

$$\begin{bmatrix} \widehat{b}_0 & b_1 & b_2 & & & \\ \widehat{b}_{-1} & b_0 & b_1 & b_2 & & \\ b_{-2} & b_{-1} & b_0 & b_1 & b_2 & & \\ & b_{-2} & b_{-1} & b_0 & b_1 & b_2 & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & b_{-2} & b_{-1} & b_0 & b_1 & b_2 \\ & & & b_{-2} & b_{-1} & b_0 & \widetilde{b}_1 \\ & & & & b_{-2} & b_{-1} & \widetilde{b}_0 \end{bmatrix}$$

Reblock it into  $m \times m$  blocks....
....and get a block tridiagonal matrix with  $m \times m$  blocks. The matrix is almost block Toeplitz as well the blocks.

Γ	$\widehat{b}_0$	$b_1$	<i>b</i> <sub>2</sub>						
.	$b_{-1}$	<i>b</i> <sub>0</sub>	$b_1$	<i>b</i> <sub>2</sub>					
	$b_{-2}$	$b_{-1}$	<i>b</i> 0	$b_1$	•••				
		$b_{-2}$	$b_{-1}$	<i>b</i> 0	·	·			
			•	·	·	·	·		
				·.	•.	<i>b</i> 0	$b_1$	b <sub>2</sub>	
						$b_{-1}$	<i>b</i> 0	$b_1$	<i>b</i> <sub>2</sub>
						$b_{-2}$	$b_{-1}$	$b_0$	$\widetilde{b}_1$
L							$b_{-2}$	$b_{-1}$	$\widetilde{b}_0$

Fundamental property 1: It holds that the Laurent polynomial  $\varphi(z) = B_{-1}z^{-1} + B_0 + B_1z$  obtained this way is a z-circulant matrix.

For m = 4,

$$B(z) = \begin{bmatrix} b_0 & b_1 & b_2 & b_3 \\ b_{-1} & b_0 & b_1 & b_2 \\ b_{-2} & b_{-1} & b_0 & b_1 \\ b_{-3} & b_{-2} & b_{-1} & b_0 \end{bmatrix} + z \begin{bmatrix} b_4 & & & \\ b_3 & b_4 & & \\ b_2 & b_3 & b_4 & \\ b_1 & b_2 & b_3 & b_4 \end{bmatrix} + z^{-1} \begin{bmatrix} b_{-4} & b_{-3} & b_{-2} & b_{-1} \\ & b_{-4} & b_{-3} & b_{-2} \\ & & b_{-4} & b_{-3} \\ & & & b_{-4} \end{bmatrix}$$

In fact, multiplying the upper triangular part by z we get a circulant matrix

Fundamental property 2: *z*-circulant matrices form a matrix algebra, i.e., they are a linear space closed under multiplication and inversion

Therefore  $\psi(z) = \varphi(z)^{-1}$  is z-circulant, in particular is Toeplitz

Toeplitz matrices form a vector space therefore

 $\psi_1(z^2) = \frac{1}{2}(\psi(z) + \psi(-z))$  is Toeplitz as well as  $\psi_2(z), \psi_3(z), \ldots$ 

Recall that the inverse of a Toeplitz matrix is Toeplitz-like in view of the Gohberg-Semencul formula, or in view of the properties of the displacement operator

Therefore  $\varphi_k(z) = \psi_k(z)^{-1}$  is Toeplitz like

The coefficients of  $\varphi_k(z)$  are Toeplitz-like

The relation between the matrix coefficients  $B_{-1}$ ,  $B_0$ ,  $B_1$  at two subsequent steps of CR can be rewritten in terms of the displacement generators

We have just to play with the properties of the displacement operators

More precisely, by using displacement operators we can prove that

$$\Delta(\varphi^{(k)}(z)) = -z^{-1}\varphi^{(k)}(z) \left( e_n e_n^T \psi^{(k)}(z) Z^T - Z^T \psi^{(k)}(z) e_1 e_1^T \right) \varphi^{(k)}(z)$$

where 
$$\Delta(X) = XZ^T - Z^TX$$
,  $Z = \begin{bmatrix} 0 \\ 1 & \ddots \\ \ddots & \ddots \\ 1 & 0 \end{bmatrix}$ 

This property implies that

$$\begin{split} \Delta(B_{-1}^{(k)}) &= a_{-1}^{(k)} u_{-1}^{(k)T} - v_{-1}^{(k)} c_{-1}^{(k)T} \\ \Delta(B_{0}^{(k)}) &= a_{-1}^{(k)} u_{0}^{(k)T} + a_{0}^{(k)} u_{-1}^{(k)T} - v_{-1}^{(k)} c_{0}^{(k)T} - v_{0}^{(k)} c_{-1}^{(k)T} \\ \Delta(B_{1}^{(k)}) &= r_{1}^{(k)} u_{0}^{(k)T} - v_{0}^{(k)} \widehat{c}^{(k)T} \end{split}$$

where the vectors  $a_{-1}^{(k)}$ ,  $a_0^{(k)}$ ,  $u_0^{(k)}$ ,  $u_{-1}^{(k)}$ ,  $c_0^{(k)}$ ,  $c_{-1}^{(k)}$ ,  $\hat{c}^{(k)}$ ,  $\hat{c}^{(k)}$  can be updated by suitable formulas

Moreover, the matrices  $B_{-1}^{(k)}$ ,  $B_0^{(k)}$ ,  $B_1^{(k)}$  can be represented as Toeplitz-like matrices through their displacement generator

The computation of the Schur complement has the asymptotic costs

 $t(m) + m \log m$ 

where t(m) is the cost of solving an  $m \times m$  Toeplitz-like system, and  $m \log m$  is the cost of multiplying a Toeplitz-like matrix and a vector

One step of back substitution stage can be performed in  $O(nm \log m)$  ops, that is, O(n) multiplications of  $m \times m$  Toeplitz-like matrices and vectors

The overall asymptotic cost C(n, m) of this computation is given by

$$C(m,n) = t(m)\log n + nm\log m$$

Recall that, according to the algorithm used,  $t(m) \in \{m^2, m \log^2 m, m \log m\}$ 

The same algorithm applies to solving an  $n \times n$  banded Toeplitz system with 2m + 1 diagonals. The cost is  $m \log^2 m \log(n/m)$  for the LU factorization and  $O(n \log m)$  for the back substitution

## Block tridiagonal with tridiagonal blocks

A challenging problem is to solve a block tridiagonal block Toeplitz system where the blocks are tridiagonal or, more generally banded matrices, not necessarily Toeplitz

CR can be applied once again but the initial band structure of the blocks apparently is destroyed in the CR iterations

This computational problem is encountered, say, in the analysis of bidimensional random walks, and in the tandem Jackson model

The analysis is still work in place. The results obtained so far are very promising

We give just an outline of the main properties

We are given  $\mathcal{B} = \text{trid}_n(B_{-1}, B_0, B_1)$  where  $B_i = \text{trid}_m(b_{-1}^{(i)}, b_0^{(i)}, b_1^{(i)})$ .

Denote  $\mathcal{B}^{(k)} = \operatorname{trid}_{\frac{n}{2^k}}(B_{-1}^{(k)}, B_0^{(k)}, B_1^{(k)})$  the matrix obtained after k steps of cyclic reduction

Recall that, denoting  $C^{(k)} = (B_0^{(k)})^{-1}$ , we have

$$B_0^{(k+1)} = B_0^{(k)} - B_{-1}^{(k)} C^{(k)} B_1^{(k)} - B_1^{(k)} C^{(k)} B_{-1}^{(k)}$$
  
$$B_1^{(k+1)} = -B_1^{(k)} C^{(k)} B_1^{(k)}, \quad B_{-1}^{(k+1)} = -B_{-1}^{(k)} C^{(k)} B_{-1}^{(k)}$$

The tridiagonal structure of  $B_{-1}$ ,  $B_0$ ,  $B_1$  is lost, and unfortunately the more general quasiseparable structure is not preserved. In fact the rank of the off-diagonal submatrices of  $B_i^{(k)}$  grows as  $2^k$  up to saturation

However, from the numerical experiments we discover that the "numerical rank" does not grow much

Given 0 < r < 1 < R, and  $\gamma > 0$  consider the class  $\mathcal{F}(r, R, \gamma)$  of matrix functions  $\varphi(z) = z^{-1}B_{-1} + B_0 + zB_1$ , such that

- $B_{-1}, B_0, B_1$  are  $m \times m$  irreducible tridiagonal matrices,
- $\varphi(z)$  is nonsingular in the annulus  $\mathbb{A} = \{z \in \mathbb{C}: r \le |z| \le R\}$
- $\|\varphi(z)^{-1}\| \leq \gamma$  for  $z \in \mathbb{A}$

We can prove the following

**Theorem.** There exists a constant  $\theta$  depending on  $r, R, \gamma$  such that for any function  $\varphi(z) \in \mathcal{F}(r, R, \gamma)$  the *i*th singular value of the off-diagonal submatrices of  $B_{-1}^{(k)}, B_0^{(k)}, B_1^{(k)}$  is bounded by  $\theta \sigma_1 \sqrt{n} \left(\frac{r}{R}\right)^i$ 

In other words, the singular values have an exponential decay depending on the width of the analyticity domain of  $\varphi(z)$ 

Let  $\sigma_1, \ldots, \sigma_m$  be the singular values of an  $m \times m$  matrix A. For a given  $\epsilon > 0$ , define the  $\epsilon$ -rank of A as

$$\max\{\sigma_i: \quad \sigma_i \ge \epsilon \sigma_1\}$$

Similarly define the  $\epsilon$ -quasiseparability rank of A as the maximum  $\epsilon$ -rank of the off-diagonal submatrices of A

**Corollary.** For any  $\epsilon > 0$  there exist h > 0 such that for any matrix function  $\varphi(z) \in \mathcal{F}(r, R, \gamma)$ , the  $\epsilon$ -quasiseparability rank of the matrices  $B_i^{(k)}$  generated by CR is bounded by h

## Implementation

CR has been implemented by using the package of  $[{\rm B\ddot{O}RM},~{\rm GRASEDYCK}$  and  ${\rm Hackbusch}]$  on hierarchical matrices





#### Residual errors

Size	CR	$H_{10^{-16}}$	$H_{10^{-12}}$	$H_{10^{-8}}$	
100	1.91 <i>e</i> — 16	1.79 <i>e</i> – 15	8.26 <i>e</i> - 14	7.40 <i>e</i> - 10	
200	2.51 <i>e</i> — 16	1.39 <i>e</i> – 14	1.01 <i>e</i> – 13	2.29 <i>e</i> - 09	
400	2.09 <i>e</i> — 16	1.41e - 14	1.33 <i>e</i> – 13	1.99 <i>e</i> – 09	
800	2.74 <i>e</i> — 16	1.94 <i>e</i> — 14	2.71 <i>e</i> — 13	2.69 <i>e</i> - 09	
1600	3.82 <i>e</i> – 12	3.82 <i>e</i> – 12	3.82 <i>e</i> – 12	3.39 <i>e</i> – 09	
3200	5.46 <i>e</i> – 08	5.46 <i>e</i> – 08	5.46 <i>e</i> – 08	5.43 <i>e</i> - 08	
6400	3.89 <i>e</i> – 08	3.89 <i>e</i> – 08	3.89 <i>e</i> – 08	3.87 <i>e</i> – 08	
12800	1.99 <i>e</i> – 08	1.99 <i>e</i> – 08	1.99 <i>e</i> – 08	1.97e - 08	

# 4– The infinite case: Wiener-Hopf factorization

## The infinite case

Compute the infinite invariant probability vector  $\pi = [\pi_0, \pi_1, \ldots]$ ,  $\pi_i = [\pi_1^{(i)}, \ldots, \pi_m^{(i)}]$  such that  $\pi \ge 0$ ,  $\pi e = 1$ ,  $e = [1, 1, \ldots]^T$  and  $\pi(P-I) = 0$ , where  $P \ge 0$ , Pe = e,  $e = [1, 1, \ldots]^T$ 

Three cases of interest:

$$M/G/1: \qquad P = \begin{bmatrix} \widehat{A}_{0} & \widehat{A}_{1} & \widehat{A}_{2} & \dots & \dots \\ A_{-1} & A_{0} & A_{1} & A_{2} & \dots \\ & A_{-1} & A_{0} & A_{1} & \ddots \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad A_{i}, \widehat{A}_{i} \ge 0, \quad \sum_{i=-1}^{\infty} A_{i} \text{ stoch.}$$

$$G/M/1: \qquad P = \begin{bmatrix} A_0 & A_1 \\ \widehat{A}_{-1} & A_0 & A_1 \\ \widehat{A}_{-2} & A_{-1} & A_0 & A_1 \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix}, \quad A_i, \widehat{A}_i \ge 0, \quad \sum_{i=-1}^{\infty} A_{-i} \text{ stoch.}$$

Quasi-Birth-Death Markov chains

$$P = \begin{bmatrix} \hat{A}_{0} & \hat{A}_{1} & & \\ \hat{A}_{-1} & A_{0} & A_{1} & \\ & A_{-1} & A_{0} & A_{1} \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

where Pe = e,  $A_i, \widehat{A}_i \ge 0$ ,  $A_{-1} + A_0 + A_1$  stochastic and irreducible

Other cases like Non-Skip-free Markov chains can be reduced to the previous classes by means of reblocking as in the shortest queue model

	$\widehat{A}_0$	$\widehat{A}_1$	$\widehat{A}_2$	$\widehat{A}_3$	$\widehat{A}_4$	$A_5$						
	$\widehat{A}_{-1}$	A <sub>0</sub>	$A_1$	$A_2$	A <sub>3</sub>	$A_4$	$A_5$	·	•	·	•	·
	$\widehat{A}_{-2}$	$A_{-1}$	A <sub>0</sub>	$A_1$	$A_2$	A <sub>3</sub>	$A_4$	$A_5$	·	·.	·	·
P =		$A_{-2}$	$A_{-1}$	A <sub>0</sub>	$A_1$	$A_2$	A <sub>3</sub>	$A_4$	$A_5$	·		·
			A_2	$A_{-1}$	A <sub>0</sub>	$A_1$	$A_2$	A <sub>3</sub>	$A_4$	$A_5$	·	·
				$A_{-2}$	$A_{-1}$	$A_0$	$A_1$	$A_2$	A <sub>3</sub>	$A_4$	$A_5$	· · .
	_				·	·	·	·	·	·	·	·

In this context, a fundamental role is played by the UL factorization (if it exists) of an infinite block Hessenberg block Toeplitz matrix  ${\cal H}$ 

For notational simplicity denote  $B_0 = I - A_0$ ,  $B_i = -A_i$ ,

where det  $U_0$ , det  $L_0 \neq 0$ ,  $\rho(G), \rho(R) \leq 1$ 

In the case of a QBD, the M/G/1 and G/M/1 structures can be combined together yielding

$$\begin{bmatrix} B_{0} & B_{1} & & \\ B_{-1} & B_{0} & B_{1} & \\ & B_{-1} & B_{0} & B_{1} \\ & & \ddots & \ddots & \ddots \end{bmatrix} = \begin{bmatrix} I & -R & & \\ & I & -R & \\ & & \ddots & \ddots & \end{bmatrix} D \begin{bmatrix} I & & \\ -G & I & \\ & G & I \\ & & \ddots & \ddots \end{bmatrix}$$

where

$$D = \begin{bmatrix} U_0 & & & \\ & U_0 & & \\ & & U_0 & \\ & & & \ddots \end{bmatrix}$$

The infinite case: M/G/1

$$[\pi_0, \pi_1, \ldots] \begin{bmatrix} \widehat{B}_0 & \widehat{B}_1 & \widehat{B}_2 & \ldots & \ldots \\ B_{-1} & B_0 & B_1 & B_2 & \ddots \\ & B_{-1} & B_0 & B_1 & \ddots \\ & & \ddots & \ddots & \ddots \end{bmatrix} = 0$$

The above equation splits into

$$\pi_{0}\widehat{B}_{0} + \pi_{1}B_{-1} = 0$$

$$[\pi_{1}, \pi_{2}, \ldots] \begin{bmatrix} B_{0} & B_{1} & B_{2} & \ldots \\ B_{-1} & B_{0} & B_{1} & \ddots \\ & \ddots & \ddots & \ddots \end{bmatrix} = -\pi_{0}[\widehat{B}_{0}, \widehat{B}_{1}, \ldots]$$

Unfortunately,  $B_{-1}$  is not generally invertible so that substitution cannot be applied (given  $\pi_0$  compute  $\pi_1$ ,...)

### Assumptions

Assume that  $\pi_0$  is known so that it is enough to solve the infinite block Hessenberg block Toeplitz system

$$[\pi_1, \pi_2, \ldots] H = -\pi_0[\widehat{B}_0, \widehat{B}_1, \ldots], \quad H = \begin{bmatrix} B_0 & B_1 & B_2 & \ldots \\ B_{-1} & B_0 & B_1 & \ddots \\ & & B_{-1} & B_0 & B_1 & \ddots \\ & & & \ddots & \ddots & \ddots \end{bmatrix}$$

Assume that there exists the UL factorization of H

$$H = \begin{bmatrix} U_0 & U_1 & U_2 & \dots & \\ & U_0 & U_1 & U_2 & \ddots \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} I & & & & \\ -G & I & & & \\ & -G & I & & \\ & & \ddots & \ddots & \end{bmatrix} = UL$$

where det  $U_0 \neq 0$  and  $G^k$  is bounded for  $k \in \mathbb{N}$ . Then the system turns into

$$[\pi_1, \pi_2, \ldots] UL = -\pi_0[\widehat{B}_0, \widehat{B}_1, \ldots]$$

which formally reduces to

$$[\pi_1, \pi_2, \ldots] U = -\pi_0[\widehat{B}_0, \widehat{B}_1, \ldots] L^{-1}, \quad L^{-1} = \begin{bmatrix} I & & & \\ G & I & & \\ G^2 & G & I & \\ \vdots & \ddots & \ddots & \ddots \end{bmatrix}$$

Thus, if the UL factorization of *H* exists the problem of computing  $\pi_0, \ldots, \pi_k$  is reduced to computing

- the UL factorization of H
- π0
- the first k block components of  $b = -\pi_0 [\hat{B}_0, \hat{B}_1, \ldots] L^{-1}$
- the solution of the block triangular block Toeplitz system  $[\pi_1, \ldots, \pi_k]U_k = b_k$

**Remark:** The boundedness of  $\sum_{i=0}^{\infty} |\widehat{B}_i|$  and of  $G^k$  imply the boundedness of b

The vector  $\pi_0$  can be computed as follows. The condition

$$[\pi_0, \pi_1, \ldots] \begin{bmatrix} \frac{\widehat{B}_0}{B_1} & \widehat{B}_1 & \widehat{B}_2 & \cdots & \cdots \\ B_{-1} & B_0 & B_1 & B_2 & \ddots \\ & & B_{-1} & B_0 & B_1 & \ddots \\ & & \ddots & \ddots & \ddots \end{bmatrix} = 0$$

is rewritten as

$$[\pi_0, \pi_1, \pi_2, \ldots] \left[ \begin{array}{c|c} \widehat{B}_0 & [\widehat{B}_1, \widehat{B}_2, \ldots] \\ \hline \widetilde{B}_{-1} & UL \end{array} \right] = 0$$

Multiply on the right by  $diag(I, L^{-1})$  and get

$$[\pi_0, \pi_1, \pi_2, \ldots] \left[ \begin{array}{c|c} \widehat{B}_0 & [\widehat{B}_1, \widehat{B}_2, \ldots] L^{-1} \\ \hline \widetilde{B}_{-1} & U \end{array} \right] = 0$$

$$[\pi_0, \pi_1, \pi_2, \ldots] \left[ \begin{array}{c|c} \widehat{B}_0 & [\widehat{B}_1, \widehat{B}_2, \ldots] L^{-1} \\ \hline \widetilde{B}_{-1} & U \end{array} \right] = 0$$

that is

$$[\pi_0, \pi_1, \pi_2, \ldots] \begin{bmatrix} \frac{\widehat{B}_0}{B_{-1}} & [\widehat{B}_1 \ \widehat{B}_2 \ \ldots] L^{-1} \\ \hline B_{-1} & U_0 \ U_1 \ U_2 \ \ldots \\ 0 & U_0 \ U_1 \ \ddots \\ \vdots & \ddots \ \ddots \ \ddots \end{bmatrix} = 0$$

Thus the first two equations of the latter system yield

$$[\pi_0, \pi_1] \begin{bmatrix} \widehat{B}_0 & B_1^* \\ B_{-1} & U_0 \end{bmatrix} = 0, \qquad B_1^* = \sum_{i=0}^{\infty} \widehat{B}_{i+1} G^i$$

which provide  $\pi_0$ 

**Remark:** The boundedness of  $\sum_{i=0}^{\infty} |\widehat{B}_i|$  and the boundedness of  $G^k$  imply the convergence of the series  $B_1^*$ 

## Complexity analysis

- the UL factorization of H: we will see this next
- $\pi_0$ :  $m^3 d$ , where d is such that  $\sum_{i=d}^{\infty} \|\widehat{B}_i\| < \epsilon$
- the vector  $b = -\pi_0[\hat{B}_0, \hat{B}_1, \ldots]L^{-1}$ :  $m^3d$
- the solution of the block triangular Toeplitz system  $[\pi_1, \ldots, \pi_k]U = b$ :  $m^3k + m^2k \log k$

Overall cost: computing the UL factorization plus  $m^{3}(k+d) + m^{2}k \log k$ 

The infinite case: G/M/1

$$[\pi_0, \pi_1, \ldots] P = 0, \qquad P = \begin{bmatrix} \hat{B}_0 & B_1 & & \\ \hat{B}_{-1} & B_0 & B_1 & \\ \hat{B}_{-2} & B_{-1} & B_0 & B_1 & \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix}$$

Consider the UL factorization of H

$$H = \begin{bmatrix} B_0 & B_1 & & \\ B_{-1} & B_0 & B_1 & & \\ B_{-2} & B_{-1} & B_0 & B_1 & \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix} = \begin{bmatrix} I & -R & & \\ I & -R & & \\ & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} L_0 & & \\ L_1 & L_0 & & \\ L_2 & L_1 & L_0 & \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

multiply to the left by  $[R, R^2, R^3, \ldots]$  and find that

 $[R, R^2, R^3, \ldots]H = [RL_0, 0, 0, \ldots] = [-B_1, 0, \ldots]$ 

Now, multiply P to the left by  $[I, R, R^2, ...]$  and get

$$[I, R, R^{2}, \ldots] \begin{bmatrix} \widehat{B}_{0} & B_{1} & & \\ \widehat{B}_{-1} & B_{0} & B_{1} & \\ \widehat{B}_{-2} & B_{-1} & B_{0} & B_{1} \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix} = [\sum_{i=0}^{\infty} R^{i} \widehat{B}_{-i}, 0, 0, \ldots]$$

Observe that, since Pe = 0 then  $[I, R, R^2, \ldots] Pe = 0$ , that is,  $\sum_{i=0}^{\infty} R^i \widehat{B}_{-i}[1, 1, \ldots, 1]^T = 0$ , i.e.  $\sum_{i=0}^{\infty} R^i \widehat{B}_{-i}$  is singular and there exists  $\pi_0$  such that  $\pi_0 \sum_{i=0}^{\infty} R^i \widehat{B}_{-i} = 0$ 

We deduce that

$$\pi_0[I,R,R^2,R^3,\ldots]P=0$$

that is

$$\pi_i = \pi_0 R^i$$

One can prove that if  $\pi_0(I-R)^{-1}[1,\ldots,1]^T=1$  then  $\|\pi\|_1=1$ 

In the  ${\rm G}/{\rm M}/{\rm 1}$  case the computation of any number of components of  $\pi$  is reduced to

- computing the matrix R in the UL factorization of H
- computing the matrix  $\sum_{i=0}^{\infty} R^i \widehat{B}_{-i}$
- solving the m imes m sytem  $\pi_0(\sum_{i=0}^\infty R^i \widehat{B}_{-i}) = 0$
- computing  $\pi_i = \pi_0 R^i$ ,  $i = 1, \ldots, k$

Overall cost: computing the UL factorization plus  $dm^3 + m^2k$ , where d is such that  $\|\sum_{i=d}^{\infty} \widehat{B}_i\| \le \epsilon$ 

The largest computational cost is the one of computing the UL factorization of the block lower Hessenberg block Toeplitz matrix H, or equivalently, of the block upper Hessenberg block Toeplitz matrix  $H^T$ 

Our next efforts are addressed to investigate this kind of factorization of block Hessenberg block Toeplitz matrices

Our next goals:

- prove that there exists the factorization H = UL
- more generally, find conditions under which this factorization exists
- design an algorithm for its computation
- prove that  $G^k$  and  $R^k$  are bounded
- extend the approach to more general situations

#### The infinite case: the Wiener-Hopf factorization

Let us examine first the case where the block Hessenberg matrix H is banded.

$$H = \begin{bmatrix} B_0 & B_1 & \dots & B_k & & \\ B_{-1} & B_0 & B_1 & \ddots & B_k & \\ & B_{-1} & B_0 & B_1 & \ddots & B_k & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} = UL$$
$$= \begin{bmatrix} U_0 & U_1 & \dots & U_k & & \\ & U_0 & U_1 & \ddots & U_k & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} I & & & \\ -G & I & & \\ & -G & I & \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

The equations of this system are equivalent to

$$[B_{-1} B_0 \dots B_k] = [U_0 \ U_1 \dots U_k] \begin{bmatrix} -G & I & & \\ & \ddots & \ddots & \\ & & -G & I \\ & & & -G \end{bmatrix}$$

that is, in polynomial form

$$\sum_{i=-1}^{k} B_{i} z^{k} = \left(\sum_{i=0}^{k} U_{i} z^{i}\right) (I - z^{-1} G)$$

That is a factorization of the Laurent matrix polynomial  $\sum_{i=-1}^{k} B_i z^k$ where we require that  $\rho(G) \leq 1$ 

This is a necessary condition in order that  $G^k$  is bounded

More in general, the block UL factorization of an infinite block Hessenberg block Toeplitz matrix  $H = (B_{i-j})$  can be formally rewritten in matrix power series form as

$$\sum_{i=-1}^{\infty} B_i z^i = \left(\sum_{i=0}^{\infty} U_i z^i\right) \left(I - z^{-1} G\right)$$

## Wiener-Hopf factorization

**Definition** Wiener algebra  $\mathcal{W}_m$ : set of  $m \times m$  matrix Laurent series  $A(z) = \sum_{i=-\infty}^{+\infty} A_i z^i$ , such that  $\sum_{i=-\infty}^{+\infty} |A_i|$  is finite, where  $|A| = (|a_{i,j}|)$ 

**Definition** A Wiener-Hopf factorization of  $a(z) \in W_1$  is

$$\begin{aligned} &a(z) = u(z)z^k \ell(z), \quad |z| = 1, \\ &u(z) = \sum_{i=0}^{\infty} u_i z^i, \ \ell(z) = \sum_{i=0}^{\infty} \ell_i z^{-i} \in \mathcal{W}_1 \\ &u(z) \neq 0 \text{ for } |z| \le 1, \quad \ell(z) \neq 0 \text{ for } 1 \le |z| \le \infty \end{aligned}$$

Example, if a(z) is a polynomial, then u(z) is the factor of a(z) with zeros outside the unit disk,  $z^k \ell(z)$  is the polynomial with zeros inside the unit disk

It is well known that if  $a(z) \in W_1$  and  $a(z) \neq 0$  for |z| = 1 then the W-H factorization exists [BÖTTCHER, SILBERMANN]

**Definition** A Wiener-Hopf factorization of  $A(z) \in W_m$  is

$$\begin{split} \mathsf{A}(z) &= U(z) \mathsf{diag}(z^{k_1}, \dots, z^{k_m}) \mathsf{L}(z), \quad |z| = 1, \quad k_1, \dots, k_m \in \mathbb{Z} \\ U(z) &= \sum_{i=0}^{\infty} U_i z^i, \ \mathsf{L}(z) = \sum_{i=0}^{\infty} \mathsf{L}_i z^{-i} \in \mathcal{W}_m \\ \det U(z) &\neq 0 \text{ for } |z| \leq 1, \quad \det \mathsf{L}(z) \neq 0 \text{ for } 1 \leq |z| \leq \infty \end{split}$$

If  $k_1 = k_2 = \ldots = k_m = 0$  the factorization is said canonical

It is well known that if  $A(z) \in W_m$  and det  $A(z) \neq 0$  for |z| = 1 then the W-H factorization exists [BÖTTCHER, SILBERMANN]

**Definition** If the conditions det  $U(z) \neq 0$  for  $|z| \leq 1$ , det  $L(z) \neq 0$  for  $1 \leq |z| \leq \infty$  are replaced with det  $U(z) \neq 0$  for |z| < 1, det  $L(z) \neq 0$  for  $1 < |z| \leq \infty$  then the factorization is called weak **Remark.** Let  $\xi$  be a zero of det B(z), that is assume that det $(\xi) = 0$ . Taking determinants on both sides of the canonical factorization

$$B(z) = U(z)L(z)$$

yields det  $B(z) = \det U(z) \det L(z)$  so that, either det  $L(\xi) = 0$  or det  $U(\xi) = 0$ .

Since U(z) is nonsingular for  $|z| \le 1$  and L(z) is nonsingular for  $|z| \ge 1$  then,  $\xi$  is a zero of det L(z) if  $|\xi| < 1$ , while  $\xi$  is zero of det U(z) if  $|\xi| > 1$ .

In the case of an M/G/1 Markov chains, where  $L(z) = I - z^{-1}G$ , the zeros of det L(z) are the zeros of det(zI - G), that is the eigenvalues of G.

Therefore a necessary condition for the existence of a canonical factorization in the M/G/1 case is that det B(z) has exactly *m* zeros of modulus  $\leq 1$ 

In the framework of Markov chains the  $m \times m$  matrix function B(z) = I - A(z), of which we are looking for the weak canonical W-H factorization, is in the Wiener class since  $A(z) = \sum_{i=-1}^{\infty} A_i z^i$ ,  $A_i \ge 0$  and  $\sum_{i=-1}^{\infty} A_i$  exists finite (stochastic)

Moreover, it can be proved that  $\det(I - A(z))$  has zeros  $\xi_1, \xi_2, \ldots$ , ordered such that  $|\xi_i| \leq |\xi_{i+1}|$ , where

- positive recurrent:  $\xi_m = 1 < \xi_{m+1}$
- negative recurrent:  $\xi_m < \xi_{m+1} = 1$
- null recurrent:  $\xi_m = \xi_{m+1} = 1$

Thus we are looking for the weak canonical W-H factorization

$$B(z) = U(z)(I - z^{-1}G)$$

where

- positive or null recurrent:  $\rho(G) = 1$ ,  $\xi_m$  simple eigenvalue
- negative recurrent: ho(G) < 1

### W-H factorization and matrix equations

Assume that there exists the UL factorization of H:

$$H = \begin{bmatrix} U_0 & U_1 & U_2 & \dots & \\ & U_0 & U_1 & U_2 & \ddots \\ & & \ddots & \ddots & \\ & & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} I & & & & \\ -G & I & & \\ & -G & I & \\ & & & \ddots & \ddots \end{bmatrix} = UL$$

multiply to the right by  $L^{-1}$  and get

$$\begin{bmatrix} B_0 & B_1 & \dots & \\ B_{-1} & B_0 & B_1 & \ddots & \\ & B_{-1} & B_0 & B_1 & \ddots \end{bmatrix} \begin{bmatrix} I & & & \\ G & I & & \\ G^2 & G & I & \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} = \begin{bmatrix} U_0 & U_1 & U_2 & \dots & \\ & U_0 & U_1 & U_2 & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

Reading this equation in the second block-row yields

$$\sum_{i=0}^{\infty} B_{i-1}G^{i} = 0, \qquad U_{k} = \sum_{i=0}^{\infty} B_{i+k}G^{i}, \quad k = 0, 1, 2, \dots$$

$$\sum_{i=0}^{\infty} B_{i-1}G^{i} = 0, \qquad U_{k} = \sum_{i=0}^{\infty} B_{i+k}G^{i}, \quad k = 0, 1, 2, \dots$$

That is,

- computing the matrix G is reduced to solving a matrix equation
- computing the blocks U<sub>k</sub> is reduced to computing infinite summations of matrices

The existence of the canonical factorization, implies the existence of the solution G of minimal spectral radius  $\rho(G) < 1$  of the matrix equation

$$\sum_{i=0}^{\infty} B_{i-1} X^i = 0$$

Conversely, if G solves the above equation where  $\rho(G) < 1$ , if det B(z) has exactly m roots of modulus less than 1 and no roots of modulus 1, then there exists a canonical factorization  $B(z) = U(z)(I - z^{-1}G)$
## General existence conditions of the W-H factorization

More generally, for a function  $B(z) = \sum_{i=-1}^{\infty} z^i B_i \in \mathcal{W}_m$  we can prove that

If there exists a weak canonical factorization  $B(z) = U(z)(I - z^{-1}G)$  then G solves the above matrix equation,  $\|G^k\|$  is uniformly bounded from above and is the solution with minimal spectral radius  $\rho(G) \leq 1$ 

Conversely, if

• 
$$\sum_{i=0}^{\infty}(i+1)|B_i| < \infty$$

- there exists a solution G of the matrix equation such that  $\rho(G) \leq 1$ ,  $\|G^k\|$  is uniformly bounded from above
- all the zeros of det B(z) of modulus less than 1 are eigenvalues of G

then there exists a canonical factorization  $B(z) = U(z)(I - z^{-1}G)$ 

## The QBD case

For a QBD process where  $B(z) = z^{-1}B_{-1} + B_0 + zB_1$  one has

$$B(z) = (zI - R)U_0(I - z^{-1}G), \qquad B(z^{-1}) = (zI - \widehat{R})\widehat{U}_0(I - z^{-1}\widehat{G})$$

moreover, the roots  $\xi_i$ , i = 1, ..., 2m of the polynomial det zB(z) are such that

$$|\xi_1| \leq \cdots \leq |\xi_m| = \xi_m \leq 1 \leq \xi_{m+1} = |\xi_{m+1}| \leq \cdots |\xi_{2m}|$$

where

- $\xi_m = 1 < \xi_{m+1}$ : positive recurrent
- $\xi_m < 1 = \xi_{m+1}$ : transient
- $\xi_m = 1 = \xi m + 1$ : null recurrent

The matrices  $G, R, \widehat{G}, \widehat{R}$  solve the equations

$$B_{-1} + B_0 G + B_1 G^2 = 0$$
  

$$R^2 B_{-1} + R B_0 + B_1 = 0$$
  

$$B_{-1} \widehat{G}^2 + B_0 \widehat{G} + B_1 = 0$$
  

$$B_{-1} + \widehat{R} B_0 + \widehat{R}^2 B_1 = 0$$

For a general function  $B(z) = z^{-1}B_{-1} + B_0 + zB_1$  we have

Theorem (About the existence)

If  $|\xi_n| < 1 < |\xi_{n+1}|$  and there exists a solution G with  $\rho(G) = |\xi_n|$  then

• the matrix  $K = B_0 + B_1G$  is invertible, there exists the solution  $R = -B_1K^{-1}$ , and B(z) has the canonical factorization

$$B(z) = (I - zR)K(I - z^{-1}G)$$

2 B(z) is invertible in the annulus  $\mathbb{A} = \{z \in \mathbb{C} : |\xi_n| < z < |\xi_{n+1}|\}$  and  $H(z) = B(z)^{-1} = \sum_{i=-\infty}^{+\infty} z^i H_i$  is convergent for  $z \in \mathbb{A}$ , where

$$H_i = \begin{cases} G^{-i}H_0, & i < 0, \\ \sum_{j=0}^{+\infty} G^j K^{-1} R^j, & i = 0, \\ H_0 R^i, & i > 0. \end{cases}$$

If  $H_0$  is nonsingular, then there exist the solutions  $\hat{G} = H_0 R H_0^{-1}$ ,  $\hat{R} = H_0^{-1} G H_0$  and  $\hat{B}(z) = B(z^{-1})$  has the canonical factorization

$$\widehat{B}(z) = (I - z\widehat{R})\widehat{K}(I - z^{-1}\widehat{G}), \qquad \widehat{K} = B_0 + B_{-1}\widehat{G} = B_0 + \widehat{R}B_1$$

#### Theorem (About the existence)

Let  $|\xi_n| \le 1 \le |\xi_{n+1}|$ . Assume that there exist solutions G and  $\widehat{G}$ . Then **1** B(z) has the (weak) canonical factorization

$$B(z) = (I - zR)K(I - z^{-1}G),$$

2  $\widehat{B}(z)$  has the (weak) canonical factorization

$$\widehat{B}(z) = (I - z\widehat{R})\widehat{K}(I - z^{-1}\widehat{G}),$$

3 if  $|\xi_n| < |\xi_{n+1}|$ , then the series

$$W = \sum_{i=0}^{\infty} G^i K^{-1} R^i, \qquad (W = H_0)$$

is convergent, W is the unique solution of the equation

$$X - GXR = K^{-1},$$

W is nonsingular and  $\widehat{G} = WRW^{-1}$ ,  $\widehat{R} = W^{-1}GW$ .

#### Solving matrix equations

Computing the W-H factorization is equivalent to solve a matrix equation

Here we examine some algorithms for solving matrix equations of the kind

 $X = A_{-1} + A_0 X + A_1 X^2$ , equivalently  $B_{-1} + B_0 X + B_1 = 0$ 

or, more generally, of the kind

$$X = \sum_{i=-1}^{\infty} A_i X^{i+1}$$
, equivalently  $\sum_{i=-1}^{\infty} B_i X^{i+1} = 0$ 

Most natural approach: fixed point iterations

$$X_{k+1} = \sum_{i=-1}^{\infty} A_i X_k^{i+1}$$
$$X_{k+1} = (I - A_0)^{-1} \sum_{i=-1, i \neq 0}^{\infty} A_i X_k^{i}$$

Properties:

- linear convergence if  $X_0 = 0$  or  $X_0 = I$
- monotonic convergence for  $X_0 = 0$
- slow convergence, sublinear in the null recurrent case
- easy to implement, QBD case: few matrix multiplications per step

Newton's iteration has a faster convergence but at each step it requires to solve a linear matrix equation

Cyclic reduction can combine a low cost and quadratic convergence

Solving matrix equations by means of CR Consider for simplicity a quadratic matrix equation

$$B_{-1} + B_0 X + B_1 X^2 = 0$$

rewrite it in matrix form as

$$\begin{bmatrix} B_0 & B_1 & & \\ B_{-1} & B_0 & B_1 & \\ & B_{-1} & B_0 & B_1 & \\ & & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} X \\ X^2 \\ X^3 \\ \vdots \end{bmatrix} = \begin{bmatrix} -B_{-1} \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

Apply one step of cyclic reduction and get

$$\begin{bmatrix} \widehat{B}_{0}^{(1)} & B_{1}^{(1)} & & \\ B_{-1}^{(1)} & B_{0}^{(1)} & B_{1}^{(1)} & \\ & B_{-1}^{(1)} & B_{0}^{(1)} & B_{1}^{(1)} \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} X \\ X^{3} \\ X^{5} \\ \vdots \end{bmatrix} = \begin{bmatrix} -B_{-1} \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

Cyclically repeating the same reduction yields

$$\begin{bmatrix} \widehat{B}_{0}^{(k)} & B_{1}^{(k)} & & \\ B_{-1}^{(k)} & B_{0}^{(k)} & B_{1}^{(k)} & & \\ & B_{-1}^{(k)} & B_{0}^{(k)} & B_{1}^{(k)} & \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} X \\ X^{2^{k}-1} \\ X^{2\cdot2^{k}-1} \\ \vdots \end{bmatrix} = \begin{bmatrix} -B_{-1} \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

where

$$B_{-1}^{(k+1)} = -B_{-1}^{(k)}S^{(k)}B_{-1}^{(k)}, \quad S^{(k)} = (B_0^{(k)})^{-1}$$
  

$$B_1^{(k+1)} = -B_1^{(k)}S^{(k)}B_1^{(k)}$$
  

$$B_0^{(k+1)} = B_0^{(k)} - B_1^{(k)}S^{(k)}B_{-1}^{(k)} - B_{-1}^{(k)}S^{(k)}B_1^{(k)}$$
  

$$\widehat{B}_0^{(k+1)} = B_0^{(k)} - B_1^{(k)}S^{(k)}B_{-1}^{(k)}$$

Observe that  $X = (\hat{B}_0^{(k)})^{-1}(-B_{-1} - B_1^{(k)}X^{2^k-1})$ , moreover  $||B_1^{(k)}|| = O((\frac{r}{R})^{2^k})$ ,  $\hat{B}_0^{(k)}$  is nonsingular with bounded inverse,  $||X^{2^k-1}|| = O(r^{2^k})$ 

## CR for infinite block Hessenberg matrices

Even-odd permutation applied to block rows and block columns of

$$H = \begin{bmatrix} \widehat{B}_{0} & \widehat{B}_{1} & \widehat{B}_{2} & \widehat{B}_{3} & \dots & \dots \\ B_{-1} & B_{0} & B_{1} & B_{2} & B_{3} & \ddots & \ddots \\ & B_{-1} & B_{0} & B_{1} & B_{2} & B_{3} & \ddots \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

leads to the following structure



# CR for infinite block Hessenberg matrices

Computing the Schur complements yields



Computational analysis

- inverting an infinite block-triangular block-Toeplitz matrix can be performed with the doubling algorithm until the (far enough) off-diagonal entries are sufficiently small. For the esponential decay, the stop condition is verified in few iterations
- multiplication of block-triangular block-Toeplitz matrices can be performed with FFT

Computational cost:  $O(Nm^2 \log m + Nm^3)$  where N is the number of the non-negligible blocks

#### Functional interpretation

Associate the block Hessenberg block Toeplitz matrix  $H = (B_{i-j})$  with the matrix function  $\varphi(z) = \sum_{i=-1}^{\infty} z^i B_i$ 

Using the interplay between infinite Toeplitz matrices and power series, the Schur complement can be written as

$$\varphi^{(k+1)}(z) = \varphi^{(k)}_{\text{even}}(z) - z\varphi^{(k)}_{\text{odd}}(z) \left(\varphi^{(k)}_{\text{even}}(z)\right)^{-1} \varphi^{(k)}_{\text{odd}}(z)$$
$$\widehat{\varphi}^{(k+1)}(z) = \widehat{\varphi}^{(k)}_{\text{even}}(z) - z\widehat{\varphi}^{(k)}_{\text{odd}}(z) \left(\varphi^{(k)}_{\text{even}}(z)\right)^{-1} \varphi^{(k)}_{\text{odd}}(z)$$

where for a matrix function F(z) we denote

$$F_{\text{even}}(z^2) = rac{1}{2}(F(z) + F(-z))$$
  
 $F_{\text{odd}}(z^2) = rac{1}{2}(F(z) - F(-z))$ 

#### Functional interpretation

By means of formal manipulation, relying on the identity

$$a-z^2ba^{-1}b=(a+zb)a^{-1}(a-zb)$$

we find that

$$\begin{split} \varphi^{(k+1)}(z^2) &= \varphi^{(k)}_{\text{even}}(z^2) - z^2 \varphi^{(k)}_{\text{odd}}(z^2) \varphi^{(k)}_{\text{even}}(z^2)^{-1} \varphi^{(k)}_{\text{odd}}(z^2) \\ &= (\varphi^{(k)}_{\text{even}}(z^2) + \varphi^{(k)}_{\text{odd}}(z^2)) \varphi^{(k)}_{\text{even}}(z^2)^{-1} (\varphi^{(k)}_{\text{even}}(z^2) - z \varphi^{(k)}_{\text{odd}}(z^2)) \end{split}$$

On the other hand, for a function  $\varphi(z)$  one has

$$arphi_{ ext{even}}(z^2)+zarphi_{ ext{odd}}(z^2)=arphi(z),\qquad arphi_{ ext{even}}(z^2)-zarphi_{ ext{odd}}(z^2)=arphi(-z)$$

so that

$$\varphi^{(k+1)}(z^2) = \varphi^{(k)}(z)\varphi^{(k)}_{even}(z)^{-1}\varphi^{(k)}(-z)$$

which extends the Graeffe iteration to matrix power series

#### Functional interpretation

Thus, the functional iteration for  $\varphi^{(k)}(z)$  can be rewritten in simpler form as

$$\varphi^{(k+1)}(z^2) = \varphi^{(k)}(z) \left(\frac{1}{2}(\varphi^{(k)}(z) + \varphi^{(k)}(-z))\right)^{-1} \varphi^{(k)}(-z)$$

Define  $\psi^{(k)}(z) = \varphi^{(k)}(z)^{-1}$  and find that

$$\psi^{(k+1)}(z^2) = \frac{1}{2}(\psi^{(k)}(z) + \psi^{(k)}(-z))$$

This property enables us to prove the following convergence result

# Convergence

#### Theorem.

Assume we are given a function  $\varphi(z) = \sum_{i=-1}^{+\infty} z^i A_i$  and positive numbers r < 1 < R such that

- **(**) for any  $z \in \mathbb{A}(r, R)$  the matrix  $\varphi(z)$  is analytic and nonsingular
- ② the function  $\psi(z) = \varphi(z)^{-1}$ , analytic in  $\mathbb{A}(r, R)$ , is such that det  $H_0 \neq 0$  where  $\psi(z) = \sum_{i=-\infty}^{+\infty} z^i H_i$

Then

- the sequence φ<sup>(k)</sup>(z) converges uniformly to H<sub>0</sub><sup>-1</sup> over any compact set in A(r, R)
- 2) for any  $\epsilon$  and for any norm there exist constants  $c_i > 0$  such that

$$\begin{split} \|A_{-1}^{(k)}\| &\leq c_{-1}(r+\epsilon)^{2^{k}} \\ \|A_{i}^{(k)}\| &\leq c_{i}(R-\epsilon)^{-i2^{k}}, \quad \text{for } i \geq 1 \\ \|A_{0}^{(k)} - H_{0}^{-1}\| &\leq c_{0} \left(\frac{r+\epsilon}{R-\epsilon}\right)^{2^{k}} \end{split}$$

# Convergence for $\xi_m = 1$

Theorem.

Assume we are given a function  $\varphi(z) = \sum_{i=-1}^{+\infty} z^i A_i$  and positive numbers r = 1 < R such that

- **(**) for any  $z \in \mathbb{A}(r, R)$  the matrix  $\varphi(z)$  is analytic and nonsingular
- The function  $\psi(z) = \varphi(z)^{-1}$ , analytic in A(r, R), is such that det  $H_0 \neq 0$  where  $\psi(z) = \sum_{i=-\infty}^{+\infty} z^i H_i$

Then

- the sequence φ<sup>(k)</sup>(z) converges uniformly to H<sub>0</sub><sup>-1</sup> over any compact set in A(r, R)
- 2 for any  $\epsilon$  and for any norm there exist constants  $c_i > 0$  such that

$$\begin{split} \lim_{k} A_{-1}^{(k)} &= A_{-1}^{(\infty)} \\ \|A_{i}^{(k)}\| \leq c_{i}(R-\epsilon)^{-i2^{k}}, \quad \text{for } i \geq 2 \\ \|A_{0}^{(k)} - H_{0}^{-1}\| \leq c_{0} \left(\frac{r+\epsilon}{R-\epsilon}\right)^{2^{k}} \end{split}$$

#### Remark

In principle, Cyclic Reduction in functional form can be applied to any function having a Laurent series of the kind

$$\varphi(z) = \sum_{i=-\infty}^{\infty} z^i B_i$$

provided it is analytic over an annulus including the unit circle.

In the matrix framework, CR can be applied to the associated block Toeplitz matrix, no matter if it is not Hessenberg

The computational difficulty for a non-Hessenberg matrix is that the block corresponding to  $\varphi_{even}(z)$  is not triangular. Therefore its inversion, required by CR is not cheap

Solution of the matrix equation

Consider the matrix equation

$$\sum_{i=-1}^{\infty} B_i X^{i+1} = 0$$

rewrite it in matrix form as

$$\begin{bmatrix} B_0 & B_1 & B_2 & B_3 & B_4 & \dots \\ B_{-1} & B_0 & B_1 & B_2 & B_3 & \ddots & \ddots \\ & B_{-1} & B_0 & B_1 & B_2 & \ddots & \ddots \\ & & \ddots & \ddots & \ddots & & & \end{bmatrix} \begin{bmatrix} X \\ X^2 \\ X^3 \\ \vdots \end{bmatrix} = \begin{bmatrix} -B_{-1} \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

Apply cyclic reduction and get

where  $B_i^{(k)}$  and  $\widehat{B}_i^{(k)}$  are defined in functional form by

$$\varphi^{(k+1)}(z) = \varphi^{(k)}_{\text{even}}(z) - z\varphi^{(k)}_{\text{odd}}(z) \left(\varphi^{(k)}_{\text{even}}\right)^{-1} \varphi^{(k)}_{\text{odd}}(z)$$
$$\widehat{\varphi}^{(k+1)}(z) = \widehat{\varphi}^{(k)}_{\text{even}}(z) - z\widehat{\varphi}^{(k)}_{\text{odd}}(z) \left(\varphi^{(k)}_{\text{even}}\right)^{-1} \varphi^{(k)}_{\text{odd}}(z)$$

where

$$\varphi^{(k)}(z) = \sum_{i=-1}^{\infty} B_i^{(k)} z^i, \quad \widehat{\varphi}^{(k)}(z) = \sum_{i=-1}^{\infty} \widehat{B}_i^{(k)}$$

From the first equation we have

$$X = (\widehat{B}_0^{(k)})^{-1} (-B_{-1} - \sum_{i=1}^{\infty} \widehat{B}_i^{(k)} X^{i \cdot 2^k - 1})$$
$$= -(\widehat{B}_0^{(k)})^{-1} B_{-1} - (\widehat{B}_0^{(k)})^{-1} \sum_{i=1}^{\infty} \widehat{B}_i^{(k)} X^{i \cdot 2^k - 1}$$

Properties:

 $(\widehat{B}_0^{(k)})^{-1}$  is bounded from above  $B_i^{(k)}$  converges to zero as  $k o \infty$ 

convergence is double exponential for positive recurrent or transient Markov chains

convergence is linear with factor 1/2 for null recurrent Markov chains

### Evaluation interpolation

Question: how to implement cyclic reduction for infinite M/G/1 or G/M/1 Markov chains?

One has to compute the coefficients of the matrix Laurent series  $\varphi^{(k)}(z) = \sum_{i=-1}^{\infty} z^i B_i^{(k)}$  such that

$$\varphi^{(k+1)}(z) = \varphi^{(k)}(z) \left(\frac{\varphi^{(k)}(z) + \varphi^{(k)}(-z)}{2}\right)^{-1} \varphi^{(k)}(-z)$$

A first approach

- Interpret the computation in terms of infinite block Toeplitz matrices
- Truncate matrices to finite size N for a sufficiently large N
- apply the Toeplitz matrix technology to perform each single operation in the CR step

$$\varphi^{(k+1)}(z) = \varphi^{(k)}(z) \left(\frac{\varphi^{(k)}(z) + \varphi^{(k)}(-z)}{2}\right)^{-1} \varphi^{(k)}(-z)$$

A second approach:

Remain in the framework of analytic functions and implement the iteration point-wise

- **(**) choose the *N*th roots of the unity, for  $N = 2^k$ , as knots
- 2 apply CR point-wise at the current knots
- S check if the remainder in the power series is small enough
- if not, set k = 2k and return to step 2 (using the already computed quantities)
- If the remainder is small then exit the cycle

Some reductions: from banded M/G/1 to QBD Let *G* be the minimal nonnegative solution of

$$B_{-1} + B_0 X + B_1 X^2 + \dots + B_N X^N = 0$$

Rewrite the equation in matrix form

$$\begin{bmatrix} B_0 & B_1 & \dots & B_N & & \\ B_{-1} & B_0 & B_1 & \dots & B_N & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} G \\ G^2 \\ \vdots \end{bmatrix} = \begin{bmatrix} -B_{-1} \\ 0 \\ \vdots \end{bmatrix}$$

Reblock the system into  $N \times N$  blocks and get

$$\begin{bmatrix} \mathcal{B}_0 & \mathcal{B}_1 & & \\ \mathcal{B}_{-1} & \mathcal{B}_0 & \mathcal{B}_1 & \\ & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \mathcal{G} \\ \mathcal{G}^2 \\ \vdots \end{bmatrix} = \begin{bmatrix} \mathcal{B}_{-1} \\ \mathbf{0} \\ \vdots \end{bmatrix}$$

$$\mathcal{B}_{-1} = \begin{bmatrix} 0 & \dots & 0 & B_{-1} \\ 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 0 \end{bmatrix}, \mathcal{B}_{0} = \begin{bmatrix} B_{0} & B_{1} & \dots & B_{N-1} \\ B_{-1} & B_{0} & \ddots & \vdots \\ \vdots & \ddots & \ddots & B_{1} \\ B_{-1} & B_{0} \end{bmatrix}, \mathcal{B}_{1} = \begin{bmatrix} B_{N} & B_{N-1} & B_{N-1} \\ B_{N-1} & B_{N} & B_{N-1} \\ \vdots & \ddots & \vdots \\ B_{1} & \dots & B_{N-1} & B_{N} \end{bmatrix}$$

This suggests to consider the auxliary equation

$$\mathcal{B}_{-1} + \mathcal{B}_0 \mathcal{X} + \mathcal{B}_1 \mathcal{X}^2 = 0$$

It is a direct verification to show that

$$\mathcal{G} = \begin{bmatrix} 0 & \dots & 0 & G \\ \vdots & \dots & \vdots & G^2 \\ \vdots & \dots & \vdots & \vdots \\ 0 & \dots & 0 & G^N \end{bmatrix}$$

solves the auxiliary equation

Solving a banded M/G/1 is reduced to solve a QBD with larger blocks

This technique does not apply to a power series. However...

Some reductions: from M/G/1 to QBD Let *G* be the minimal nonnegative solution of

$$B_{-1} + B_0 X + B_1 X^2 + \dots = 0$$

Consider the auxiliary equation

$$\mathcal{B}_{-1} + \mathcal{B}_0 \mathcal{X} + \mathcal{B}_1 \mathcal{X}^2 = 0$$

where  $\mathcal{B}_{-1}, \mathcal{B}_0, \mathcal{B}_1$  are infinite matrices defined by

$$\mathcal{B}_{-1} = \operatorname{diag}(B_{-1}, 0, \ldots), \quad \mathcal{B}_{0} = egin{bmatrix} B_{0} & B_{1} & B_{2} & \ldots \ & -I & 0 & \ldots \ & & -I & \ & & & \ddots \end{bmatrix}, \quad \mathcal{B}_{1} = egin{bmatrix} 0 & & & \ I & 0 & & \ & I & 0 & \ & I & 0 & \ & & & \ddots & \ddots \end{pmatrix}$$

A solution of the auxiliary equation is given by

$$\mathcal{X} = \mathcal{G} = \begin{bmatrix} G & 0 & \dots \\ G^2 & 0 & \dots \\ G^3 & 0 & \dots \\ \vdots & \vdots & \vdots \end{bmatrix}$$

$$\mathcal{B}_{-1} + \mathcal{B}_0 \mathcal{X} + \mathcal{B}_1 \mathcal{X}^2 = 0$$

$$\begin{bmatrix} B_{-1} & 0 & \dots \\ 0 & 0 & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} + \begin{bmatrix} B_0 & B_1 & \dots \\ 0 & -I & \\ \vdots & \ddots & \end{bmatrix} \begin{bmatrix} G & 0 & \dots \\ G^2 & -I & \\ \vdots & \ddots & \end{bmatrix} + \begin{bmatrix} 0 & & & \\ I & 0 & & \\ & & \ddots & \ddots & \\ \vdots & 0 & \dots \end{bmatrix}^2 = 0$$

$$\begin{bmatrix} B_{-1} & 0 & \dots \\ 0 & 0 & \dots \\ \vdots & \vdots & \ddots \\ \vdots & \vdots & \ddots \end{bmatrix} + \begin{bmatrix} \sum_{i=0}^{\infty} B_i G^{i+1} & 0 & \dots \\ -G^2 & 0 & \dots \\ -G^3 & \vdots & \ddots \\ \vdots & \vdots & \vdots \end{bmatrix} + \begin{bmatrix} 0 & 0 & \dots \\ G^2 & 0 & \dots \\ G^3 & \vdots & \ddots \\ \vdots & \vdots & \vdots \end{bmatrix}$$

Computing G is reduced to computing the solution  ${\mathcal G}$  of a QBD with infinite blocks

# Shifting techniques

## Shifting techniques

We have seen that in the solution of QBD Markov chains one needs to compute the minimal nonnegative solution G of the  $m \times m$  matrix equation

$$A_{-1} + A_0 X + A_1 X^2 = X$$

Moreover the roots  $\xi_i$  of the polynomial det $(A_{-1} + (A_0 - I)z + A_1z^2)$  are such that

$$|\xi_1| \leq \cdots \leq \xi_m \leq 1 \leq \xi_{m+1} \leq \cdots \leq |\xi_{2m}|$$

In the null recurrent case where  $\xi_m = \xi_{m+1} = 1$  the convergence of algorithms for computing *G* deteriorates

Moreover, the problem of computing G is ill-conditioned

Here we provide a tool for getting rid of this drawback

The idea is an elaboration of a result introduced by [BRAUER 1952] and extended to matrix polynomials by [HE, MEINI, RHEE 2001]

It relies on transforming the polynomial  $A(z) = A_{-1} + zA_0 + z^2A_1$  into a new one  $\widetilde{A}(z) = \widetilde{A}_{-1} + z\widetilde{A}_0 + z^2\widetilde{A}_1$  in such a way that  $\widetilde{a}(z) = \det \widetilde{A}(z)$  has the same roots of  $a(z) = \det A(z)$  except for  $\xi_m = 1$  which is shifted to 0, and  $\xi_{m+1} = 1$  which is shifted to infinity

This way, the roots of  $\tilde{a}(z)$  are

$$0, \xi_1, \ldots, \xi_{m-1}, \xi_{m+2}, \ldots, \xi_{2m}, \infty$$

#### The Brauer idea

Let A be an  $n \times n$  matrix, let u be an eigenvector corresponding to the eigenvalue  $\lambda$ , that is  $Au = \lambda u$ , let v be any vector such that  $v^T u = 1$ 

Then  $B = A - \lambda u v^T$  has the same eigenvalues of A except for  $\lambda$  which is replaced by 0

Proof

$$Bu = Au - \lambda uv^{T} u = \lambda u - \lambda u = 0$$
  
If  $w^{T}A = \mu w^{T}$  then  $w^{T}B = w^{T}A - \lambda w^{T}uv^{T} = \mu w^{T}$ 

Can we extend the same argument to matrix polynomials and to the polynomial eigenvalue problem?

Our assumptions:

 $A(z) = A_{-1}z^{-1} + A_0 + zA_1$ ,  $A_{-1}, A_0, A_1$  are  $m \times m$  matrices  $A_{-1}, A_0, A_1 \ge 0$   $(A_{-1} + A_0 + A_1)e = e, e = (1, ..., 1)^T$   $A_{-1} + A_0 + A_1$  irreducible  $\xi_m = 1 = \xi_{m+1}, z = 1$  is zero of  $a(z) = \det(zA(z))$  of multiplicity 2 The following equations have solution where  $B_{-1} = A_{-1}, B_0 = A_0 - I$ ,  $B_1 = A_1$ 

$$B_{-1} + B_0 G + B_1 G^2 = 0, \quad \rho(G) = \xi_m$$
  

$$R^2 B_{-1} + R B_0 + B_1 = 0, \quad \rho(R) = \xi_{m+1}^{-1}$$
  

$$B_{-1} \widehat{G}^2 + B_0 \widehat{G} + B_1 = 0, \quad \rho(\widehat{G}) = \xi_{m+1}^{-1}$$
  

$$B_{-1} + \widehat{R} B_0 + \widehat{R}^2 B_1 = 0, \quad \rho(\widehat{R}) = \xi_m.$$

Recall that the existence of these 4 solutions is equivalent to the existence of the canonical factorizations of  $\varphi(z) = z^{-1}B(z)$  and of  $\varphi(z^{-1})$  where  $B(z) = B_{-1} + zB_0 + z^2B_1$ 

$$arphi(z)=(\mathit{I}-\mathit{zR})\mathit{K}(\mathit{I}-\mathit{z}^{-1}\mathit{G}), \hspace{1em} \mathit{R}, \mathit{K}, \mathit{G}\in \mathbb{R}^{m imes m}, \hspace{1em} ext{det} \mathit{K}
eq 0$$

$$arphi(z^{-1})=(I-z\widehat{R})\widehat{K}(I-z^{-1}\widehat{G}),\quad \widehat{R},\widehat{K},\widehat{G}\in\mathbb{R}^{m imes m},\quad \det\widehat{K}
eq 0$$

## Shift to the right

Here, we construct a new matrix polynomial  $\tilde{B}(z)$  having the same roots as B(z) except for the root  $\xi_n$  which is shifted to zero.

- Recall that G has eigenvalues  $\xi_1, \ldots, \xi_m$
- denote  $u_G$  an eigenvector of G such that  $Gu_G = \xi_m u_G$
- denote v any vector such that  $v^T u_G = 1$
- define

$$\widetilde{B}(z) = B(z)\left(I + \frac{\xi_m}{z - \xi_m}Q\right), \quad Q = u_G v^T$$

#### Theorem

The function  $\widetilde{B}(z)$  coincides with the quadratic matrix polynomial  $\widetilde{B}(z) = \widetilde{B}_{-1} + z\widetilde{B}_0 + z^2\widetilde{B}_1$  with matrix coefficients

$$\widetilde{B}_{-1}=B_{-1}(I-Q), \hspace{0.2cm} \widetilde{B}_{0}=B_{0}+\xi_{n}B_{1}Q, \hspace{0.2cm} \widetilde{B}_{1}=B_{1}.$$

Moreover, the roots of  $\widetilde{B}(z)$  are  $0, \xi_1, \ldots, \xi_{m-1}, \xi_{m+1}, \ldots, \xi_{2m}$ .

#### Outline of the proof

Since  $B(\xi_m)u_G = 0$ , and  $Q = u_G v^T$ , then  $B(\xi_m)Q = 0$  so that  $B_{-1}Q = -\xi_m B_0 Q - \xi_m^2 B_1 Q$ , and we have

$$B(z)Q = -\xi_m B_0 Q - \xi_m^2 B_1 Q + B_0 Q z + B_1 Q z^2$$
  
=  $(z^2 - \xi_m^2) B_1 Q + (z - \xi_m) B_0 Q.$ 

This way  $\frac{\xi_m}{z-\xi_m}B(z)Q = \xi_m(z+\xi_m)B_1Q + \xi_mB_0Q$ , therefore

$$\widetilde{B}(z) = B(z) + rac{\xi_m}{z - \xi_m} B(z) Q = \widetilde{B}_{-1} + \widetilde{B}_0 z + \widetilde{B}_1 z^2$$

so that

$$\widetilde{B}_{-1}=B_{-1}(I-Q),\ \ \widetilde{B}_0=B_0+\xi_mB_1Q,\ \ \widetilde{B}_1=B_1$$

Since det $(I + \frac{\xi_m}{z - \xi_m}Q) = \frac{z}{z - \xi_m}$  then from the definition of  $\widetilde{B}(z)$  we have det  $\widetilde{B}(z) = \frac{z}{z - \xi_m}$  det B(z). This means that the roots of the polynomial det  $\widetilde{B}(z)$  coincide with the roots of det B(z) except the root equal to  $\xi_m$  which is replaced with 0.

## Shift to the left

Here, we construct a new matrix polynomial  $\tilde{B}(z)$  having the same roots as B(z) except for the root  $\xi_m$  which is shifted to infinity.

- Recall that R has eigenvalues  $\xi_{m+1}^{-1}, \ldots, \xi_{2m}^{-1}$
- denote  $v_R$  a left eigenvector of R such that  $v_R^T R = \xi_{m+1}^{-1} v_R^T$
- denote w any vector such that  $w^T v_R = 1$
- define

$$\widetilde{B}(z) = \left(I - \frac{z}{z - \xi_{n+1}}S\right)B(z), \quad S = wv_R^T$$

#### Theorem

The function  $\widetilde{B}(z)$  coincides with the quadratic matrix polynomial  $\widetilde{B}(z) = \widetilde{B}_{-1} + z\widetilde{B}_0 + z^2\widetilde{B}_1$  with matrix coefficients

$$\widetilde{B}_{-1} = B_{-1}, \quad \widetilde{B}_0 = B_0 + \xi_{m+1}^{-1} S B_{-1}, \quad \widetilde{B}_1 = (I - S) B_1.$$

Moreover, the roots of  $\widetilde{B}(z)$  are  $\xi_1, \ldots, \xi_m, \xi_{m+2}, \ldots, \xi_{2m}, \infty$ .

# Double shift

The right and left shifts can be combined together yielding a new quadratic matrix polynomial  $\tilde{B}(z)$  with the same roots of B(z), except for  $\xi_n$  and  $\xi_{n+1}$ , which are shifted to 0 and to infinity, respectively

Define the matrix function

$$\widetilde{B}(z) = \left(I - \frac{z}{z - \xi_{m+1}}S\right)B(z)\left(I + \frac{\xi_m}{z - \xi_m}Q\right),$$
  
and find that  $\widetilde{B}(z) = \widetilde{B}_{-1} + z\widetilde{B}_0 + z^2\widetilde{B}_1$ , with matrix coefficients  
 $\widetilde{B}_{-1} = B_{-1}(I - Q),$   
 $\widetilde{B}_0 = B_0 + \xi_m B_1 Q + \xi_{m+1}^{-1} SB_{-1} - \xi_{m+1}^{-1} SB_{-1} Q =$   
 $B_0 + \xi_m B_1 Q + \xi_{m+1}^{-1} SB_{-1} - \xi_m SB_1 Q$   
 $\widetilde{B}_1 = (I - S)B_1.$ 

The matrix polynomial  $\widetilde{B}(z)$  has roots  $0, \xi_1, \ldots, \xi_{m-1}, \xi_{m+2}, \ldots, \xi_{2m}, \infty$ . In particular,  $\widetilde{B}(z)$  is nonsingular on the unit circle and on the annulus  $|\xi_{m-1}| < |z| < |\xi_{m+2}|$ .

# Shifts and canonical factorizations

We are able to shift eigenvalues of matrix polynomials. What about eigenvalues? What about solutions to the 4 matrix equations?

We provide an answer to the following question

Under which conditions both the functions  $\tilde{\varphi}(z)$  and  $\tilde{\varphi}(z^{-1})$  obtained after applying the shift have a (weak) canonical factorization?

In different words:

Under which conditions there exist the four minimal solutions to the equations obtained after applying the shift where the matrices  $A_i$  are replaced by  $\tilde{A}_i$ , i = -1, 0, 1?

These matrix solutions will be denoted by  $\tilde{G}, \tilde{R}, \tilde{\widehat{G}}, \tilde{\widehat{R}}$ They are the analogous of the solutions  $G, R, \hat{G}, \hat{R}$  to the original equations

We examine the case of the shift to the right. The shift to the left can be treated similarly
Independently of the recurrent or transient case, the canonical factorization of  $\widetilde{\varphi}(z)$  always exists

We have the following theorem concerning  $\widetilde{B}(z) = B(z)(I + \frac{\xi_n}{z - \xi_n}Q)$ ,  $Q = u_G v^T$ 

### Theorem

• The function  $\widetilde{\varphi}(z) = z^{-1}\widetilde{B}(z)$ , has the following factorization

$$\widetilde{\varphi}(z) = (I - zR)K(I - z^{-1}\widetilde{G}), \quad \widetilde{G} = G - \xi_n Q$$

This factorization is canonical in the positive recurrent case, and weak canonical otherwise.

- The eigenvalues of  $\widetilde{G}$  are those of G, except for the eigenvalue  $\xi_n$  which is replaced by zero
- $X = \widetilde{G}$  and Y = R are the solutions with minimal spectral radius of the equations

$$\widetilde{B}_{-1} + \widetilde{B}_0 X + \widetilde{B}_1 X^2 = 0, \quad Y^2 \widetilde{B}_{-1} + Y \widetilde{B}_0 + \widetilde{B}_1 = 0$$

# The case of $\widetilde{\varphi}(z^{-1})$

In the positive recurrent case, the matrix polynomial  $\widetilde{B}(z)$  is nonsingular on the unit circle, so that the function  $\widetilde{\varphi}(z^{-1})$  has a canonical factorization

### Theorem (Positive recurrent)

If  $\xi_n = 1 < \xi_{n+1}$  then the Laurent matrix polynomial  $\tilde{\varphi}(z^{-1}) = z \tilde{B}(z^{-1})$ , has the canonical factorization

$$\widetilde{\varphi}(z^{-1}) = (I - z\widetilde{\widehat{R}})(\widetilde{\widehat{U}} - I)(I - z^{-1}\widetilde{\widehat{G}})$$

with  $\widetilde{\widehat{R}} = \widetilde{W}^{-1}\widetilde{G}\widetilde{W}$ ,  $\widetilde{G} = G - Q$ ,  $\widetilde{\widehat{G}} = \widetilde{W}R\widetilde{W}^{-1}$ ,  $\widetilde{\widehat{U}} = \widetilde{B}_0 + \widetilde{B}_{-1}\widetilde{\widehat{G}} = \widetilde{B}_0 + \widetilde{\widehat{R}}B_1$ , where  $\widetilde{W} = W - QWR$ . Moreover,  $X = \widetilde{\widehat{G}}$ and  $Y = \widetilde{\widehat{R}}$  are the solutions with minimal spectral radius of the matrix equations

$$\widetilde{B}_{-1}X^2 + \widetilde{B}_0X + \widetilde{B}_1 = 0, \quad \widetilde{B}_{-1} + X\widetilde{B}_0 + X^2\widetilde{B}_1 = 0,$$

## Null recurrent case: double shift

Consider the matrix polynomial obtained with the double shift

$$\widetilde{B}(z) = (I - \frac{z}{z - \xi_{n+1}}S)B(z)(I + \frac{\xi_n}{z - \xi_n}Q), \quad Q = u_G v^T, \ S = wv_R^T$$

#### Theorem

The function  $\widetilde{\varphi}(z) = z^{-1}\widetilde{B}(z)$  has the canonical factorization

$$\widetilde{\varphi}(z) = (I - z\widetilde{R})K(I - z^{-1}\widetilde{G}), \quad \widetilde{R} = R - \xi_{n+1}S, \ \widetilde{G} = G - \xi_nQ$$

The matrices  $\tilde{G}$  and  $\tilde{R}$  are the solutions with minimal spectral radius of the equations  $\tilde{A}_{-1} + (\tilde{A}_0 - I)X + \tilde{A}_1X^2 = 0$  and  $X^2\tilde{A}_{-1} + X(\tilde{A}_0 - I) + \tilde{A}_1 = 0$ , respectively

## Null recurrent case: double shift

### Theorem

Let 
$$Q = u_G v_{\hat{G}}^T$$
 and  $S = u_{\hat{R}} v_R^T$ , with  $u_G^T v_{\hat{G}} = 1$  and  $v_R^T u_{\hat{R}} = 1$ . Then  
 $\widetilde{\varphi}(z^{-1}) = (I - z^{-1}\widetilde{\hat{R}})\widetilde{\hat{K}}(I - z\widetilde{\hat{G}})$ 

### where

$$\begin{split} &\widetilde{\widehat{R}} = \widehat{R} - \gamma u_{\widehat{R}} v_{\widehat{G}}^T \widehat{K}^{-1}, \quad \widetilde{\widehat{G}} = \widehat{G} - \gamma \widehat{K}^{-1} u_{\widehat{R}} v_{\widehat{G}}^T, \\ &\gamma = 1/(v_{\widehat{G}}^T \widehat{K}^{-1} u_{\widehat{R}}) \\ &\widetilde{K} = A_{-1} \widehat{G} + A_0 - I, \quad \widetilde{\widehat{K}} = \widetilde{A}_{-1} \widetilde{\widehat{G}} + \widetilde{A}_0 - I \end{split}$$

## Applications

The Poisson problem for a QBD consists in solving the equation

$$(I-P)x = q + ze, \quad e = (1,1\ldots)^T$$

where q is an infinite vector, x and z are the unknowns and

$$P = \begin{bmatrix} A_0 + A_1 - I & A_1 & & \\ A_{-1} & A_0 - I & A_1 & \\ & A_{-1} & A_0 - I & A_1 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

where  $A_{-1}$ ,  $A_0$ ,  $A_1$  are nonnegative and  $A_{-1}$  +  $A_0$  +  $A_1$  is stochastic

If  $\xi_n < 1 < \xi_{n+1}$  then the general solution of this equation can be explicitly expressed in terms of the solutions of a suitable matrix difference equations

The shift technique provides a way o represent the solution by means of the solution of a suitable matrix difference equation even in the case of null recurrent models

# Generalizations

The shift technique explained in the previous sections can be generalized in order to shift to zero or to infinity a set of selected eigenvalues, leaving unchanged the remaining eigenvalues.

This generalization is particularly useful when one has to move a pair of conjugate complex eigenvalues to zero or to infinity still maintaining real arithmetic.

Potential application:

Deflation of already approximated roots within a polynomial rootfinder

Potential use in MPSolve http://numpi.dm.unipi.it/mpsolve a package for high precision computation of roots of polynomials of large degree

Let Y be a full rank  $n \times k$  matrix such that  $GY = Y\Lambda$ , where  $\Lambda$  is a  $k \times k$  matrix. The eigenvalues of  $\Lambda$  are a subset of the eigenvalues of G.

Let V be an  $n \times k$  matrix such that  $V^T Y = I_k$ . Define

$$\widetilde{B}(z) = B(z) \left( I + Y \Lambda (zI_k - \Lambda)^{-1} V^T \right).$$

We have the following

#### Theorem

The function  $\widetilde{B}(z)$  coincides with the quadratic matrix polynomial  $\widetilde{B}(z) = \widetilde{B}_{-1} + z\widetilde{B}_0 + z^2\widetilde{B}_1$  with matrix coefficients

$$\widetilde{B}_{-1} = B_{-1}(I - YV^T), \quad \widetilde{B}_0 = B_0 + B_1Y\Lambda V^T, \quad \widetilde{B}_1 = B_1.$$

Moreover, the roots B(z) are the same as those of B(z) except for the eigenvalues of  $\Lambda$  which are replaced by 0.

Concerning the canonical factorization of the function  $\tilde{\varphi}(z) = z^{-1}\tilde{B}(z)$  we have the following result

#### Theorem

The function  $\tilde{\varphi}(z) = z^{-1}\tilde{B}(z)$ , with  $\tilde{B}(z)$  has the following (weak) canonical factorization

$$\widetilde{\varphi}(z) = (I - zR)K(I - z^{-1}\widetilde{G})$$

where  $\tilde{G} = G - Y\Lambda V^T$ . Moreover, the eigenvalues of  $\tilde{G}$  are those of G, except for the eigenvalues of  $\Lambda$  which are replaced by zero; the matrices  $\tilde{G}$  and R are solutions with minimal spectral radius of the equations  $\tilde{B}_{-1} + \tilde{B}_0 X + \tilde{B}_1 X^2 = 0$  and  $X^2 \tilde{B}_{-1} + X \tilde{B}_0 + \tilde{B}_1 = 0$ , respectively.

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# Available software

There exists a matlab package and a Fortran 95 package, with a GUI, where the fast algorithms for solving structured Markov chains have been implemented

SMCSolver: A MATLAB Toolbox for solving M/G/1, GI/M/1, QBD, and Non-Skip-Free type Markov chains http://win.ua.ac.be/~vanhoudt/tools/

Fortran 95 version at http://bezout.dm.unipi.it:SMCSolver

## Tree-like processes

$$P = \begin{bmatrix} C_0 & \Lambda_1 & \Lambda_2 & \dots & \Lambda_d \\ V_1 & W & 0 & \dots & 0 \\ V_2 & 0 & W & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ V_d & 0 & \dots & 0 & W \end{bmatrix}$$

where  $C_0$  is  $m \times m$ ,  $\Lambda_i = [A_i \ 0 \ 0 \ ...]$ ,  $V_i^T = [D_i^T \ 0 \ 0 \ ...]$  and the matrix W is recursively defined by

$$W = \begin{bmatrix} C & \Lambda_1 & \Lambda_2 & \dots & \Lambda_d \\ V_1 & W & 0 & \dots & 0 \\ V_2 & 0 & W & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ V_d & 0 & \dots & 0 & W \end{bmatrix}$$

The matrix W can be factorized as W = UL where

$$U = \begin{bmatrix} S & \Lambda_1 & \Lambda_2 & \dots & \Lambda_d \\ 0 & U & 0 & \dots & 0 \\ 0 & 0 & U & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \dots & o & U \end{bmatrix}, \quad L = \begin{bmatrix} I & 0 & 0 & \dots & 0 \\ Y_1 & L & 0 & \dots & 0 \\ Y_2 & 0 & L & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ Y_d & 0 & \dots & o & L \end{bmatrix}$$

where S is the minimal solution of

$$X + \sum_{i=1}^d A_i X^{-1} D_i = C$$

Once the matrix S is known, the vector  $\pi$  can be computed by using the UL factorization of W

# Solving the equation

Multiply

$$X + \sum_{i=1}^d A_i X^{-1} D_i = C$$

to the right by  $X^{-1}D_i$  for  $i = 1, \ldots, d$  and get

$$D_i + (C + \sum_{j=1, j \neq i}^d A_j X^{-1} D_j) X^{-1} D_i + A_i (X^{-1} D_i)^2 = 0$$

that is,  $X_i := X^{-1}D_i$  solves

$$D_i + (C + \sum_{j=1, j \neq i}^d A_j X_j) X_i + A_i X_i^2 = 0$$

We can prove that  $X_i$  is the minimal solution

# Algorithm: fixed point

Set 
$$X_{i,0} = 0$$
,  $i = 1, ..., d$   
For  $k = 0, 1, 2, ...$ 

$$S_k = C + \sum_{i=1}^d A_i X_{i,k}$$
$$X_{i,k+1} = -S_k^{-1} D_i, \quad i = 1, \dots, d$$

The sequences  $\{S_k\}_k$  and  $\{X_{i,k}\}_k$  converge monotonically to S and to  $X_i$ , respectively [LATOUCHE, RAMASWAMI 99]

# Algorithm: CR + fixed point

Set 
$$X_{i,0} = 0$$
,  $i = 1, \ldots, d$ 

- For k = 0, 1, 2, ...
  - For i = 1, ..., d
  - set  $F_{i,k} = C + \sum_{j=1}^{i-1} A_j X_{j,k} + \sum_{j=i+1}^{d} A_j X_{j,k-1}$
  - compute by means of CR the minimal solution  $X_{i,k}$  to

$$D_i + F_{i,k}X + A_iX^2 = 0$$

The sequence  $\{X_{i,k}\}_k$  converges monotonically to  $X_i$  for i = 1, ..., d

# Newton's iteration

- Set  $S_0 = C$
- For k = 0, 1, 2, ...
  - compute  $L_k = S_k C + \sum_{i=1}^d A_i S_k^{-1} D_i$
  - compute the solution  $Y_k$  of

$$X - \sum_{i=1}^{d} A_i S_k^{-1} X S_k^{-1} D_i = L_k$$

• set  $S_{k+1} = S_k - Y_k$ 

The sequence  $\{S_k\}_k$  converges quadratically to S

Open issue: efficient solution of the above matrix equation



## Vector equations

The extinction probability vector in a Markovian binary tree is given by the minimal nonnegative solution  $x^*$  of the vector equation

$$x = a + b(x, x)$$

where  $a = (a_i)$  is a probability vector, and w = b(u, v) is a bilinear form defined by  $w_k = \sum_{i=1}^n \sum_{j=1}^n u_i v_j b_{i,j,k}$ 

Besides the minimal nonnegative solution  $x^*$ , this equation has the vector e = (1, ..., 1) as solution.

Some algorithms [BEAN, KONTOLEON, TAYLOR, 2008], [HAUTPHENNE, LATOUCHE, REMICHE 2008]

Converegnce turns to sublinear/linear when the problem is critical, i.e., if

## An optimistic approach [MEINI, POLONI 2011]

Define y = e - x the vector of survival probability. Then the vector equation becomes

$$y = b(y, e) + b(e, y) - b(y, y)$$

we are interested in the solution  $y^*$  such that  $0 \le y^* \le x^*$ 

The equation can be rewritten as

$$y = H_h y$$
,  $H_h = b(\cdot, e) + b(e, \cdot) - b(y, \cdot)$ 

Property: for  $0 \le y < e$ ,  $H_h$  is a nonnegative irreducible matrix. The Perron-Frobenius theorem insures that exists a positive eigenvector

A new iteration

$$Y_{k+1} = \operatorname{PerronVector}(H_{y_k})$$

Property: local convergence can be proved. Convergence is linear in the noncritical case and superlinear in the critical case



# Exponential of a block triangular block Toeplitz

In the Erlangian approximation of Markovian fluid queues, one has to compute

$$Y = e^X = \sum_{i=0}^{\infty} \frac{1}{i!} X^i$$

where

$$X = \begin{bmatrix} X_0 & X_1 & \dots & X_\ell \\ & \ddots & \ddots & \vdots \\ & & X_0 & X_1 \\ & & & & X_0 \end{bmatrix}, \quad m \times m \text{ blocks } X_0, \dots, X_\ell,$$

 $\boldsymbol{X}$  has negative diagonal entries, nonnegative off-diagonal entries, the sum of the entries in each row is nonpositive

Clearly, since block triangular Toeplitz matrices form a matrix algebra then Y is still block triangular Toeplitz

What is the most convenient way to compute Y in terms of CPU time and error?

Embed X into an infinite block triangular block Toeplitz matrix  $X_{\infty}$  obtained by completing the sequence  $X_0, X_1, \ldots, X_{\ell}$  with zeros

Denote  $Y_0, Y_1, \ldots$  the blocks defining  $Y_{\infty} = e^{X_{\infty}}$ 

Then Y is the  $(\ell+1) imes (\ell+1)$  principal submatrix of  $Y_\infty$ 

We can prove the following decay property

$$\|Y_i\|_{\infty} \leq e^{\alpha(\sigma^{\ell-1}-1)}\sigma^{-i}, \quad \forall \sigma > 1$$

where  $\alpha = \max_{j}(-(X_0)_{j,j}).$ 

This property is fundamental to prove error bounds of the following different algorithms

#### Using $\epsilon$ -circulant matrices

Approximate X with an  $\epsilon$ -circulant matrix  $X^{(\epsilon)}$  and approximate Y with  $Y^{(\epsilon)} = e^{X^{(\epsilon)}}$ . We can prove that if,  $\beta = \|[X_1, \ldots, X_\ell]\|_{\infty}$  then

$$\|Y - Y^{(\epsilon)}\|_{\infty} \leq e^{|\epsilon|eta} - 1 = |\epsilon|eta + O(|\epsilon|^2)$$

and, if  $\epsilon$  is purely imaginary then

$$\|Y - Y^{(\epsilon)}\|_{\infty} \leq e^{|\epsilon|^2 \beta} - 1 = |\epsilon|^2 \beta + O(|\epsilon|^4)$$

#### Using circulant matrices

Embed X into a  $K \times K$  block circulant matrix  $X^{(K)}$  for  $K > \ell$  large, and approximate Y with the  $(\ell + 1) \times (\ell + 1)$  submatrix  $Y^{(K)}$  of  $e^{X^{(K)}}$ . We can prove the following bound

$$\| [Y_0 - Y_0^{(\mathcal{K})}, \dots, Y_\ell - Y_\ell^{(\mathcal{K})}] \|_\infty \le (e^eta - 1) e^{lpha (\sigma^{\ell-1} - 1)} rac{\sigma^{-\mathcal{K} + \ell}}{1 - \sigma^{-1}}, \quad \sigma > 1$$

### Method based on Taylor expansion

The matrix Y is approximated by truncating the series expansion to r terms

$$Y^{(r)} = \sum_{i=0}^r \frac{1}{i!} X^i$$

In all the three aproaches, the computation remains inside a matrix algebra, more specifically:

block  $\epsilon\text{-circulant}$  matrices of fixed size  $\ell$ 

block circulant matrices of variable size  $K > \ell$ 

block triangular Toeplitz of fixed size  $\ell$ 



Figure : Norm-wise error, component-wise relative and absolute errors for the solution obtained with the algorithm based on  $\epsilon$ -circulant matrices with  $\epsilon = i\theta$ .



Figure : Norm-wise error, component-wise relative and absolute errors for the solution obtained with the algorithm based on circulant embedding for different values of the embedding size K.



Figure : CPU time of the Matlab function expm, and of the algorithms based on  $\epsilon$ -circulant, circulant embedding, power series expansion.

### Open issues

Can we prove that the exponential of a general block Toeplitz matrix does not differ much from a block Toeplitz matrix? Numerical experiments confirm this fact but a proof is missing.

Can we design effective ad hoc algorithms for the case of general block Toeplitz matrices?

Can we apply the decay properties of BENZI, BOITO 2014 ?





Figure : Graph of a Toeplitz matrix subgenerator, and of its matrix exponential

# Conclusions

- Matrix structures are the matrix counterpart of specific features of the model
- Their detection and exploitation is fundamental to design efficient algorithms
- Markov chains and queuing model offer a wide variety of structures
- Toeplitz, Hessenberg, Toeplitz-like, multilevel, quasiseparable are the main structures encountered
- the interplay between matrices, polynomials and power series, together with FFT and analytic function theory provide powerful tools for algorithm design
- these algorithms are the fastest currently available
- the computational tools designed in this framework, together with the methodologies on which they rely, have more general applications and can be used in different contexts