Dario A. Bini, Stefano Massei, Leonardo Robol

Exploiting rank structures in the Cyclic Reduction for QBD stochastic processes

University of Pisa

Scuola Normale Superiore

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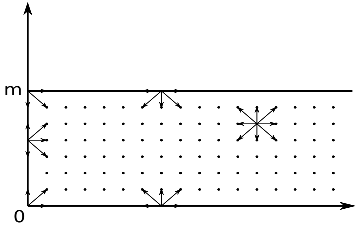
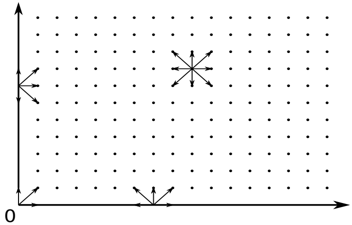
Quasi-birth-death processes

A QBD process, in discrete time, is a bidimensional Markov chain whose transition probability matrix has the tridiagonal block Töeplitz structure

$$P = \begin{pmatrix} B_0 & B_1 & & & 0 \\ A_{-1} & A_0 & A_1 & & \\ & A_{-1} & A_0 & A_1 & \\ & & A_{-1} & A_0 & \ddots \\ 0 & & & \ddots & \ddots \end{pmatrix},$$

with $A_i, B_i \in \mathbb{R}^{m \times m}$ $(m \in \mathbb{N} \cup \{+\infty\})$ non negative and P stochastic.





The main problem

Suppose $m < \infty$ and let the matrix P be irreducible and nonperiodic.
A problem of interest is to compute the stationary distribution of the QBD, i.e. an infinite vector $\boldsymbol{\pi}$ such that

$$\boldsymbol{\pi}^T P = \boldsymbol{\pi}^T, \quad \boldsymbol{\pi} \geq 0, \quad \text{and} \quad \| \boldsymbol{\pi} \|_1 = 1.$$

A crucial step, for computing $\boldsymbol{\pi}$, consists in finding the minimal non negative solution G of the quadratic matrix equation:

$$\boxed{X = A_{-1} + A_0 X + A_1 X^2, \quad X \in \mathbb{R}^{m \times m}.}$$

Many numerical methods have been proposed to address the problem and most of them are designed to deal with the general case where the block coefficients A_{-1},A_0 and A_1 have no particular structure.

Cyclic Reduction

The method on which we are going to focus is the Cyclic Reduction.
Its iterative scheme requires the computation of four sequences of matrices, $A_i^{(k)}$, $i = -1, 0, 1$ and $\hat{A}_0^{(k)}$, which follow the recurrence relations:

$$
\begin{aligned}
A_1^{(k+1)} &= A_1^{(k)} \, (I - A_0^{(k)})^{-1} \, A_1^{(k)}, \\
A_0^{(k+1)} &= A_0^{(k)} + A_1^{(k)} \, (I - A_0^{(k)})^{-1} \, A_{-1}^{(k)} \; + \; A_{-1}^{(k)} \, (I - A_0^{(k)})^{-1} \, A_1^{(k)}, \\
A_{-1}^{(k+1)} &= A_{-1}^{(k)} \, (I - A_0^{(k)})^{-1} \, A_{-1}^{(k)}, \\
\hat{A}_0^{(k+1)} &= \hat{A}_0^{(k)} + A_1^{(k)} \, (I - A_0^{(k)})^{-1} \, A_{-1}^{(k)}.
\end{aligned}
$$

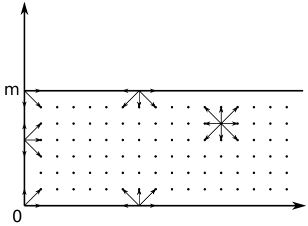
with $A_i^{(0)} = A_i$, $i = -1, 0, 1$ and $\hat{A}_0^{(0)} = A_0$.
After each step, an approximation of the matrix G is provided by

$$(I - \hat{A}_0^{(k)})^{-1} A_{-1}.$$

Under mild hypothesis applicability and quadratic convergence are guaranteed.
The cost of each iteration is $\mathcal{O}(m^3)$ because it involves four matrix multiplications and the resolution of $2m$ linear systems of size m.

Cyclic Reduction/ Tridiagonal blocks

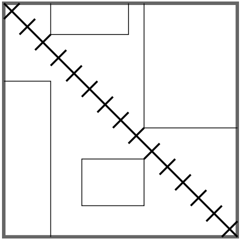
Let us consider the case in which A_i is tridiagonal for $i = -1, 0, 1$. This happen for example in a random walk on a strip where at each instant we can move at most of a unit horizontally and or vertically.

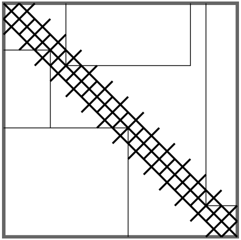


The band structure is lost immediately when applying CR due to the inversions in its iteration scheme. What we can hope to be maintained is the quasiseparable structure.

Definition

$A \in \mathbb{R}^{n\times n}$ has quasiseparable rank less or equal than k if any off diagonal submatrix of A has rank at most k.





Properties:

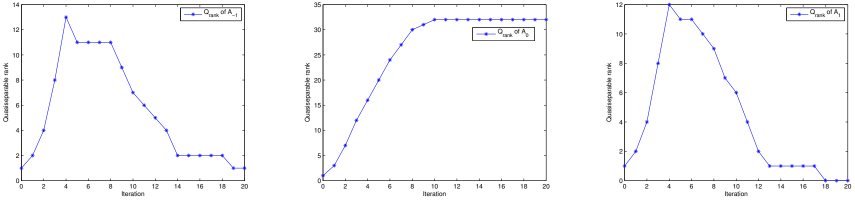
(i) $q_{rank}(A+B) \leq q_{rank}(A) + q_{rank}(B)$

(ii) $q_{rank}(A\cdot B) \leq q_{rank}(A) + q_{rank}(B)$

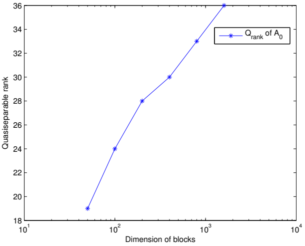
(iii) $q_{rank}(A) = q_{rank}(A^{-1})$

Cyclic Reduction/ Tridiagonal blocks

Performing 20 iterations of the algorithm on 500×500 random tridiagonal stochastic matrices provides encouraging results.



And this is the behavior of $q_{rank}(A_0)$ after 20 iterations as the size of the blocks grows exponentially.



Cyclic Reduction/ Functional interpretation

We associate at each step of the CR the matrix polynomial

$$\varphi^{(k)}(z) := -A_{-1}^{(k)} + z(I - A_0^{(k)}) - z^2 A_1^{(k)}$$

and the matrix function defined by recurrence

$$\begin{cases} \psi^{(0)}(z) := (z^{-1}\varphi^{(0)}(z))^{-1} \\ \psi^{(k+1)}(z^2) := \frac{1}{2}(\psi^{(k)}(z) + \psi^{(k)}(-z)) \end{cases}$$

Theorem (Bini,Meini)

Let $z \in \mathbb{C} \setminus \{0\}$ *be such that* $\det(\varphi^{(i)}(z))) \neq 0 \ \forall i = 0, \dots, k$ *and let* $\det(I - A_0^{(i)}) \neq 0 \ \forall i = 0, \dots, k-1$ *then*

$$\varphi^{(i)}(z) = z\psi^{(i)}(z)^{-1}, \qquad i = 0, \dots, k.$$

These tools have been introduced to address applicability and convergence issues.

Cyclic Reduction/ Functional interpretation

Let us concentrate on the recurrence relation satisfied by the sequence $\{\psi^{(k)}\}_{k\in\mathbb{N}}$:

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

$$\downarrow$$

$$\psi^{(k)}(z^4) = \frac{1}{4}\left(\psi^{(k-2)}(z) + \psi^{(k-2)}(-z) + \psi^{(k-2)}(i\cdot z) + \psi^{(k-2)}(-i\cdot z)\right)$$

$$\downarrow$$

$$\dots$$

$$\psi^{(k)}(z^{2^k}) = \frac{1}{2^k}\sum_{j=0}^{2^k-1}\psi^{(0)}(\zeta_j z), \qquad \zeta_j \ 2^k\text{-th root of the unit.}$$

This bring us to the key formula

$$\boxed{\varphi^{(k)}(z^{2^k}) = z^{2^k}\psi^{(k)}(z^{2^k})^{-1} = z^{2^k}\left(\frac{1}{2^k}\sum_{j=0}^{2^k-1}\psi^{(0)}(\zeta_j z)\right)^{-1}.} \qquad (1)$$

$$\varphi^{(k)}(z^{2^k}) = z^{2^k} \left(\frac{1}{2^k} \sum_{j=0}^{2^k-1} \psi^{(0)}(\zeta_j z) \right)^{-1}$$

When the A_i is tridiagonal for $i = -1, 0, 1$ the highlighted object is the inverse of a tridiagonal matrix, in particular is 1-quasiseparable. Therefore we can claim that $q_{rank}(\varphi^{(k)}(z)) \leq 2^k \ \forall z \in \mathbb{C} : \det(\varphi^{(k-h)}(\sqrt[2^h]{z})) \neq 0 \ h = 0, \dots, k$.
Combining this with the relations

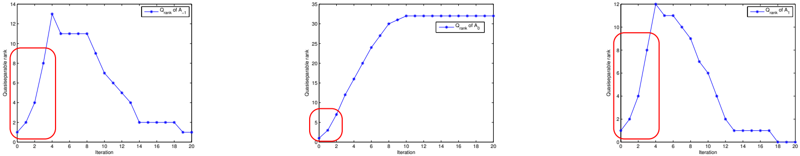
$$A_{-1}^{(k)} = -\lim_{z\to 0} \varphi^{(k)}(z),$$

$$A_1^{(k)} = -\lim_{z\to +\infty} \frac{\varphi^{(k)}(z)}{z^2},$$

$$I - A_0^{(k)} = \frac{1}{2}\left(\frac{\varphi^{(k)}(z)}{z} + \frac{\varphi^{(k)}(-z)}{-z} \right),$$

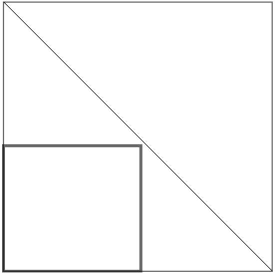
we get: $q_{rank}(A_{-1}^{(k)}), q_{rank}(A_1^{(k)}) \leq 2^k$ and $q_{rank}(A_0^{(k)}) \leq 2^{k+1}$.

The bounds obtained are not satifactory because they are exponential. Despite this we observe that the estimates are sharp for early iterations.

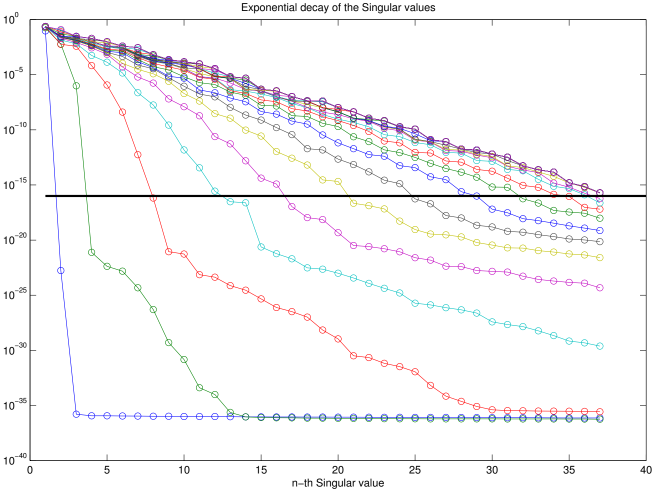


Motivated by this we turn our attention to bound the growth of the *numerical* rank.

If we plot the most significant singular values, over the iterations, of an offdiagonal sub-matrix in A_0 we see an important clue that an exponential decay property holds.



Exponential decay of the singular values



Exponential decay of the singular values

Goal: Prove that $\exists \gamma, \alpha > 0$ and $g_i : \mathbb{N} \to \mathbb{R}$ increasing function such that $\forall B_i^{(k)}$ offdiagonal submatrix of $A_i^{(k)}$ we have

$$\sigma_j(B_i^{(k)}) \leq \gamma \cdot e^{-\alpha \cdot g_i(j)}$$

Remark 1: The core issue is to prove the decay property for $A(z) := z^{-1}\varphi^{(k)}(z)$ for some points on the unit circle. Then we can retrieve the property on its coefficients $A_i^{(k)}$ performing an interpolation, i.e.

$$A_{-1}^{(k)} = \frac{1}{3}\left(\xi A(\xi) + \xi^5 A(\xi^5) - A(-1)\right)$$
$$I - A_0^{(k)} = \frac{1}{2}\left(A(z) + A(-z)\right)$$
$$A_1^{(k)} = \frac{1}{3}\left(\xi^5 A(\xi) + \xi A(\xi^5) - A(-1)\right)$$

with ξ primitive 6-th root of the unity.

Exponential decay of the singular values

Remark 2: The Inversion Lemma ensures that the exponential decay property is maintained when we move from $\psi^{(k)}$ to $\varphi^{(k)}$.

Lemma (Inversion Lemma)

Let

$$z^{-1}\varphi^{(k)}(z) = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad \psi^{(k)}(z) = \begin{pmatrix} \bar{A} & \bar{B} \\ \bar{C} & \bar{D} \end{pmatrix}$$

then

$$\sigma_k(C) \le \|D\|_2 \cdot \|S_D\|_2 \cdot \sigma_k(\bar{C})$$

$$\sigma_k(C) \le \|A\|_2 \cdot \|S_A\|_2 \cdot \sigma_k(\bar{C})$$

The property can be ruined if the diagonal blocks or their Schur complements are ill-conditioned. Fortunately this does not happen on $S^1 \setminus \{1\}$ because there $z^{-1}\varphi^{(k)}(z)$ is a diagonal dominant M-matrix and we manage to get the bound $\sigma_k(C) \le 4n \cdot \sigma_k(\bar{C})$.

Exponential decay of the singular values

Theorem

Let $\psi^{(0)}(z)$ be analytic and invertible for z in the annulus $r_{min} \leq |z| \leq r_{max}$ and quasiseparable of rank t on the unit circle. Then $\forall z \in S^1$ and for every off diagonal $(n \times n)$-submatrix $B(z)$ of $\psi^{(k)}(z)$, we have

$$\sigma_j(B(z)) \leq \frac{4M\sqrt{n}}{(1-e^{-\alpha})(1-e^{-\alpha N})} \cdot e^{-\alpha \lceil \frac{j-t}{2t} \rceil},$$

where $N = 2^k$, $M = \max_{|z|=\rho} \left\| \psi^{(0)}(z) \right\|_2$, $\alpha = \log(\rho)$ and $\rho \in [r_{min}, r_{max}]$.

Exponential decay of the singular values

Lemma (Bini,Meini)

There exist a rank 1 stochastic matrix Q such that the matrix polynomial $\tilde{\varphi}(z) = z^2\tilde{A}_1 + z\tilde{A}_0 + \tilde{A}_{-1}$ with

$$\tilde{A}_{-1} = A_{-1} - A_{-1}Q, \quad \tilde{A}_0 = A_0 + A_1 Q, \quad \tilde{A}_1 = A_1,$$

and $\varphi(z)$ share the same eigenvalues with the only exception of an eigenvalue 1 of $\varphi(z)$ that is moved to 0 in $\tilde{\varphi}(z)$. Moreover, Q is of the form eu^t where e is the vector of ones and $u > 0$ is such that $u^t e = 1$.

We can apply the CR on the shifted blocks $\tilde{A}_i$ and, at each step, obtain again an approximation for the solution of the original problem given by

$$(I - \hat{\tilde{A}}_0^{(k)})^{-1} A_{-1}.$$

Obviously one can also consider $\tilde{\psi}^{(k)}(z) := z \cdot \tilde{\varphi}^{(k)}(z)^{-1}$.

Exponential decay of the singular values

Summary of the proof:

$\tilde{\psi}^{(0)}(z)$ analytic in an annulus containing S^1

$\Downarrow$ Fourier expansion + key formula

$\tilde{\psi}^{(k)}(z)$ has the exponential decay property for $z \in S^1$

$\Downarrow$ Woodbury

$\psi^{(k)}(z)$ has the exponential decay property for $z \in S^1 \setminus \{1\}$

$\Downarrow$ Inversion Lemma

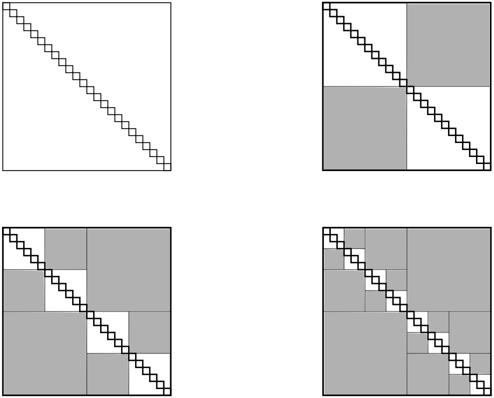
$\varphi^{(k)}(z)$ has the exponential decay property for $z \in S^1 \setminus \{1\}$

$\Downarrow$ Interpolation

$A_i^{(k)}$ has the exponential decay property $i = -1, 0, 1.$

How to exploit the rank structure

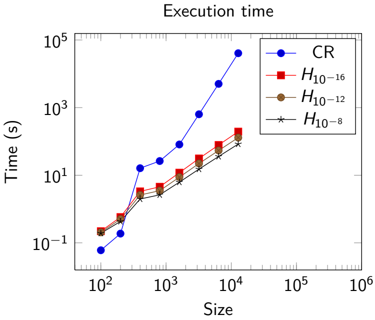
We have seen that numerically the submatrices of the blocks A_i during the CR execution mantain a low rank. In order to exploit this property we modify the original algorithm by implementing a *Hierarchical* representation.



Matrix operations:

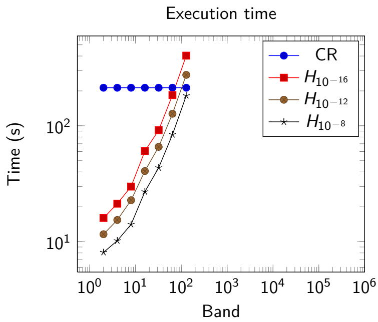
Addition	$\mathcal{O}(n\log(n))$
Multiplication	$\mathcal{O}(n\log(n)^2)$
Lin. System	$\mathcal{O}(n\log(n)^2)$

Numerical Results/ Tridiagonal: Size VS Execution Time



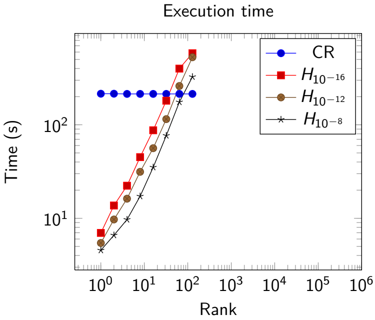
	CR		$H_{10^{-16}}$		$H_{10^{-12}}$		$H_{10^{-8}}$	
Size	Time (s)	Residue	Time (s)	Residue	Time (s)	Residue	Time (s)	Residue
100	$6.04e-02$	$1.91e-16$	$2.21e-01$	$1.79e-15$	$2.04e-01$	$8.26e-14$	$1.92e-01$	$7.40e-10$
200	$1.88e-01$	$2.51e-16$	$5.78e-01$	$1.39e-14$	$5.03e-01$	$1.01e-13$	$4.29e-01$	$2.29e-09$
400	$1.61e+01$	$2.09e-16$	$3.32e+00$	$1.41e-14$	$2.60e+00$	$1.33e-13$	$1.98e+00$	$1.99e-09$
800	$2.63e+01$	$2.74e-16$	$4.55e+00$	$1.94e-14$	$3.49e+00$	$2.71e-13$	$2.63e+00$	$2.69e-09$
1600	$8.12e+01$	$3.82e-12$	$1.18e+01$	$3.82e-12$	$8.78e+00$	$3.82e-12$	$6.24e+00$	$3.39e-09$
3200	$6.35e+02$	$5.46e-08$	$3.12e+01$	$5.46e-08$	$2.21e+01$	$5.46e-08$	$1.51e+01$	$5.43e-08$
6400	$5.03e+03$	$3.89e-08$	$7.83e+01$	$3.89e-08$	$5.38e+01$	$3.89e-08$	$3.58e+01$	$3.87e-08$
12800	$4.06e+04$	$1.99e-08$	$1.94e+02$	$1.99e-08$	$1.29e+02$	$1.99e-08$	$8.37e+01$	$1.97e-08$

Numerical Results/ Size=1600: Band VS Execution Time



	CR		$H_{10^{-16}}$		$H_{10^{-12}}$		$H_{10^{-8}}$	
Band	Time (s)	Residue	Time (s)	Residue	Time (s)	Residue	Time (s)	Residue
2	$2.13e+02$	$2.01e-16$	$1.60e+01$	$9.57e-15$	$1.16e+01$	$2.65e-13$	$8.09e+00$	$2.91e-09$
4	$2.13e+02$	$1.79e-16$	$2.13e+01$	$5.22e-15$	$1.54e+01$	$2.20e-13$	$1.02e+01$	$2.33e-09$
8	$2.13e+02$	$1.55e-16$	$2.99e+01$	$5.32e-15$	$2.28e+01$	$2.33e-13$	$1.41e+01$	$2.42e-09$
16	$2.13e+02$	$1.32e-16$	$6.05e+01$	$6.44e-15$	$4.07e+01$	$2.09e-13$	$2.70e+01$	$2.10e-09$
32	$2.13e+02$	$1.32e-16$	$9.16e+01$	$5.81e-15$	$6.58e+01$	$2.09e-13$	$4.35e+01$	$2.06e-09$
64	$2.13e+02$	$1.31e-16$	$1.84e+02$	$7.00e-15$	$1.27e+02$	$1.99e-13$	$8.40e+01$	$2.11e-09$
128	$2.13e+02$	$1.24e-16$	$4.03e+02$	$7.00e-15$	$2.75e+02$	$2.02e-13$	$1.82e+02$	$2.10e-09$

Numerical Results/ Size=1600: Q_{rank} VS Execution Time



	CR		$H_{10^{-16}}$		$H_{10^{-12}}$		$H_{10^{-8}}$	
Rank	Time (s)	Residue	Time (s)	Residue	Time (s)	Residue	Time (s)	Residue
1	$2.15e+02$	$1.33e-16$	$6.97e+00$	$1.86e-15$	$5.44e+00$	$2.23e-13$	$4.55e+00$	$2.49e-09$
2	$2.15e+02$	$1.31e-16$	$1.37e+01$	$5.74e-15$	$9.71e+00$	$3.88e-13$	$6.59e+00$	$1.46e-09$
4	$2.14e+02$	$1.28e-16$	$2.23e+01$	$4.68e-15$	$1.62e+01$	$2.17e-13$	$9.69e+00$	$1.24e-09$
8	$2.14e+02$	$1.27e-16$	$4.51e+01$	$4.33e-15$	$3.14e+01$	$2.40e-13$	$1.72e+01$	$4.13e-09$
16	$2.14e+02$	$1.22e-16$	$8.74e+01$	$2.58e-15$	$5.62e+01$	$4.03e-13$	$3.51e+01$	$3.78e-09$
32	$2.14e+02$	$1.25e-16$	$1.81e+02$	$8.61e-15$	$1.15e+02$	$1.83e-13$	$7.67e+01$	$2.88e-09$
64	$2.14e+02$	$1.22e-16$	$3.99e+02$	$1.08e-14$	$2.60e+02$	$1.34e-13$	$1.75e+02$	$1.26e-09$
128	$2.14e+02$	$1.22e-16$	$5.83e+02$	$1.24e-14$	$5.28e+02$	$2.14e-13$	$3.26e+02$	$2.44e-09$

Conclusions

- Numerical quasiseparable structures in the initial blocks are maintained during the execution of the CR.
- A property of exponential decay can be proved but the bound obtained is not sharp in pratice.
- Implementing a Hierarchical representation in the usual algorithm we can get an almost optimal complexity and a significant speed up.
- The performance is sensible to the accuracy at which the adaptive arithmetic is executed and to the dimension of the diagonal blocks.