Efficient numerical solution of large scale matrix equations arising in LQR/LQG design for parabolic PDEs

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Department of Mathematics
CHEMNITZ UNIVERSITY OF TECHNOLOGY

Outline

Origin of the Matrix Equations

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LQR for linear parabolic PDEs

semi discrete parabolic PDE

$$\dot{x}(t) = Ax(t) + Bu(t) \quad x(0) = x_0 \in \mathcal{X}. \qquad \text{(Cauchy)}$$

output equation

$$y(t) = Cx(t) \qquad \text{(output)}$$

cost function

$$\mathcal{J}(u) = \frac{1}{2}\int_0^{T_f} < y, y > + < u, u > dt \qquad \text{(cost)}$$

and the linear quadratic regulator problem is

LQR problem

Minimize the **quadratic** (cost) with respect to the **linear** constraints (Cauchy),(output).

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LQR for linear parabolic PDEs

In the open literature[1] it is well understood that the

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is given as

$$u = -B^T X_\infty x,$$

where in case $T_f = \infty$, X_∞ is the minimal, positive semidefinite, selfadjoint solution of the

algebraic Riccati equation (ARE)

$$0 = \mathcal{R}(X) := C^T C + A^T X + XA - XBB^T X.$$

[1] e.g. [Lions '71; Lasiecka/Triggiani '00; Bensoussan et al. '92; Pritchard/Salamon '87; Curtain/Zwart '95]

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MPC/LQG design for Nonlinear Optimal Control Problems

nonlinear parabolic PDE with noise

$$\begin{aligned} \dot{x}(t) &= f(x(t)) + B\,u(t) + F\,v(t) \quad \text{for } t > 0, \quad x(0) = x_0 + \eta_0, \\ y(t) &= C\,x(t) + w(t). \end{aligned}$$

Here,

- $v(t)$ is the input noise
- $w(t)$ is the output noise
- η_0 is the noise in the initial condition.

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Strategy [Benner, Hein (geb. Görner) 2006] (based on [Ito, Kunisch 2006])

1. Linearize the nonlinear state equation on sub-intervals (Model Predictive Control (MPC) or Receding Horizon Control (RHC)).
2. Find estimates of the states (Linear Quadratic Gaussian Design (LQG)) on the sub-intervals.

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Needs the additional solution of the Filter Algebraic Riccati Equation (FARE)

$$0 = A\Sigma + \Sigma A^T - \Sigma C^T W^{-1} C \Sigma + FVF^T.$$

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$$0 = A\Sigma + \Sigma A^T - \Sigma C^T W^{-1} C \Sigma + FVF^T.$$

- Here V, W are the symmetric and positive definite covariance matrices.
- Σ is used to compute the best approximation to the state for the feedback loop

Origin of the Matrix Equations

Exponential Stabilization of Navier-Stokes and Oseen Equations

SPP 1253 Project Benner/Bänsch (Researcher: A. Heubner)

[Raymond 2006]

Navier Stokes equation exponentially stabilizable by boundary feedback control for sufficiently small initial conditions.

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- LQR design for the Cauchy equation

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origin of saddle-point formulation

- Problem: Test space of divergence free functions not directly FE discretizable.
- Strategies:
  1. Matrix assembly after Helmholtz projection of the basis functions (expensive for reasonable grids)
  2. projections on matrix level after standard Galerkin discretization following [Heinkenschloss,Sorenson,Sun 2007]

Numerical methods for DRE

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Matrix versions of the ODE solvers

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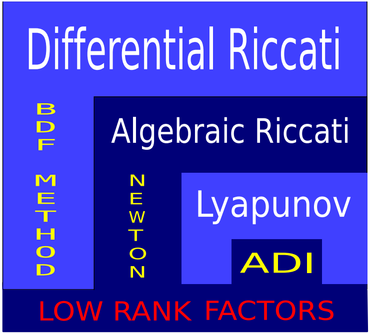

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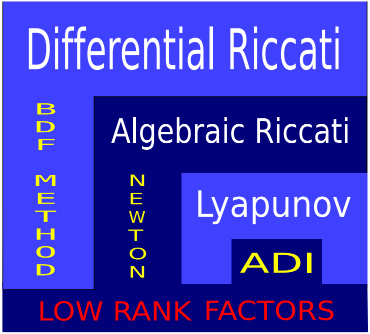


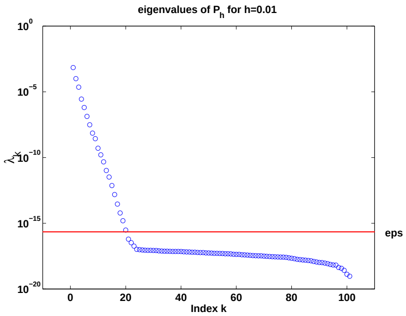
Low Rank Approximation guarantees efficiency in terms of computational effort and memory usage

Motivation of the low rank approximation

The spectrum of an AREs solution

Motivating example

- Linear 1D heat equation with point control.
- $\Omega = [0, 1]$.
- FEM discretization using linear B-splines.
- h=0.01.



$$X = X^T \geq 0 \Longrightarrow X = ZZ^T = \sum_{k=1}^{n} \lambda_k z_k z_k^T \approx \sum_{k=1}^{r} \lambda_k z_k z_k^T = Z_{(r)} Z_{(r)}^T.$$

LRCF Newton Method for the ARE

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Large Scale Riccati and Lyapunov Equations

We are interested in solving

algebraic Riccati equations

$$0 = A^T X + XA - XBB^T X + C^T C =: \mathfrak{R}(X). \qquad \text{(ARE)}$$

where

- $A \in \mathbb{R}^{n \times n}$ sparse, $n \in \mathbb{N}$ "large"
- $B \in \mathbb{R}^{n \times m}$ and $m \in \mathbb{N}$ with $m \ll n$
- $C \in \mathbb{R}^{p \times n}$ and $p \in \mathbb{N}$ with $p \ll n$

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and

Lyapunov equations

$$F^T X + XF = -GG^T. \qquad \text{(LE)}$$

with

- $F \in \mathbb{R}^{n\times n}$ sparse or sparse + low rank update, $n \in \mathbb{N}$ "large"
- $G \in \mathbb{R}^{n\times m}$ and $m \in \mathbb{N}$ with $m \ll n$

LRCF Newton Method for the ARE

Newton's method for solving the ARE

Newton's iteration for the ARE

$$\mathfrak{R}'|_X(N_l) = -\mathfrak{R}(X_l), \qquad X_{l+1} = X_l + N_l,$$

where the Frechét derivative of $\mathfrak{R}$ at X is the Lyapunov operator

$$\mathfrak{R}'|_X : \quad Q \mapsto (A - BB^T X)^T Q + Q(A - BB^T X),$$

can be rewritten as

one iteration step

$$(A - BB^T X_l)^T X_{l+1} + X_{l+1}(A - BB^T X_l) = -C^T C - X_l BB^T X_l$$

i.e. in every Newton step we have to solve a Lyapunov equation of the form (LE)

LRCF Newton Method for the ARE

Cholesky factor ADI for Lyapunov equations

Recall **Peaceman Rachford ADI**[2]**:**
Consider $Au = s$ where $A \in \mathbb{R}^{n\times n}$ spd, $s \in \mathbb{R}^n$. ADI Iteration Idea:
Decompose $A = H + V$ with $H, V \in \mathbb{R}^{n\times n}$ such that

$$(H + pI)v = r$$
$$(V + pI)w = t$$

can be solved easily/efficiently.

[2] [Peaceman & Rachford 1954], see also [Wachspress 1966]

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ADI Iteration

If H, V spd $\Rightarrow \exists p_j,\ j = 1, 2, \ldots J$ such that

$$\begin{aligned} u_0 &= 0\\ (H + p_j I)u_{j-\frac{1}{2}} &= (p_j I - V)u_{j-1} + s\\ (V + p_j I)u_j &= (p_j I - H)u_{j-\frac{1}{2}} + s \end{aligned} \qquad \text{(PR-ADI)}$$

converges to $u \in \mathbb{R}^n$ solving $Au = s$.

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The Lyapunov operator

$$\mathcal{L}: \quad X \quad \mapsto \quad F^T X + XF$$

can be decomposed into the linear operators

$$\mathcal{L}_H : X \mapsto F^T X \qquad \mathcal{L}_V : X \mapsto XF.$$

Such that in analogy to (PR-ADI) we find the

ADI iteration for the Lyapunov equation (LE)

$$\begin{array}{rcl} X_0 & = & 0 \\ (F^T + p_j I)X_{j-\frac{1}{2}} & = & -GG^T - X_{j-1}(F - p_j I) \\ (F^T + p_j I)X_j^T & = & -GG^T - X_{j-\frac{1}{2}}^T(F - p_j I) \end{array} \qquad \text{(LE-ADI)}$$

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Remarks:

- If F is sparse or sparse + low rank update, i.e. $F = A + VU^T$ then $F^T + p_j I$ can be written as $\tilde{A} + UV^T$, where $\tilde{A} = A^T + p_j I$ and its inverse can be expressed as

$$(F^T + p_j I)^{-1} = (\tilde{A} + UV^T)^{-1} = \tilde{A}^{-1} - \tilde{A}^{-1}U(I + V^T\tilde{A}^{-1}U)^{-1}V^T\tilde{A}^{-1}$$

  by the Sherman-Morrison-Woodbury formula.

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  Note: We only need to be able to multiply with A, solve systems with A and solve shifted systems with $A^T + p_j I$

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- (LE-ADI) can be rewritten to iterate on the low rank Cholesky factors Z_j of X_j to exploit $\mathrm{rk}(X_j) \ll n$. [Li & White 2002; Penzl 1999; Benner, Li, Penzl 2000]

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- When solving (ARE) to compute the feedback in an LQR-problem for a semidiscretized parabolic PDE, the LRCF-Newton-ADI can directly iterate on the feedback matrix $K \in \mathbb{R}^{n \times p}$ to save even more memory. [Penzl 1999; Benner, Li, Penzl 2000]

Recent Improvements in the Software

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Reordering Strategies

Use sparse direct solvers ⇒ Store LU or Cholesky factors frequently used (e.g. for M or $A + p_j I$ in case of cyclically used shifts).

⇒ Save storage by reordering

Upcoming LyaPack 2.0 let's you choose between:

- symmetric reverse Cuthill-McKee (RCM[3]) reordering
- approximate minimum degree (AMD[4]) reordering
- symmetric AMD[4]

[3] [A. George and J. W.-H. Liu 1981]
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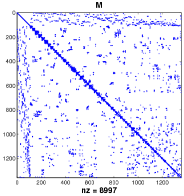
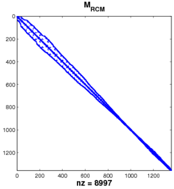
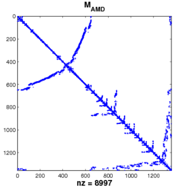
Motivating example: Mass matrix M from a FEM semidiscretization of a 2d heat equation. Dimension of the discrete system: 1357







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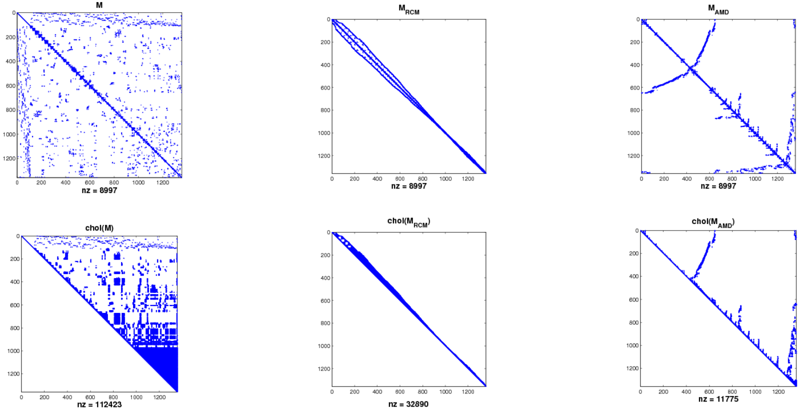

Recent Improvements in the Software

ADI Shift Parameters

Optimal ADI parameters solve the

min-max-problem

$$\min_{\{p_j | j=1,\ldots,J\} \subset \mathbb{R}} \quad \max_{\gamma \in \sigma(F)} \left| \prod_{j=1}^{J} \frac{(p_j - \lambda)}{(p_j + \lambda)} \right| .$$

Remark

- Also known as rational Zolotarev problem since he solved it first on real intervals enclosing the spectra in 1877.
- Another solution for the real case was presented by Wachspress/Jordan in 1963.

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Remark

- Wachspress and Starke presented different strategies to compute suboptimal shifts for the complex case around 1990.
- Wachspress: elliptic Integral evaluation based shifts
- Starke: Leja Point based shifts (see also [Sabino 2006])

Recent Improvements in the Software

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ADI shift parameter choices in upcoming MESS 1.0

1. heuristic parameters [Penzl 1999]
   - use selected Ritz values as shifts
   - suboptimal ⇒ convergence might be slow
   - in general complex for complex spectra
2. approximate Wachspress parameters [Benner, Mena, S. 2006]
   - optimal for real spectra
   - parameters real if imaginary parts are "small"
   - good approximation of the "outer" spectrum of F needed
     ⇒ possibly expensive computation
3. only real heuristic parameters
   - avoids complex computation and storage requirements
   - can be slow if many Ritz values are complex
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Recent Improvements in the Software

ADI Shift Parameters

Test example

Centered finite difference discretized 2d convection diffusion equation:

$$\dot{\mathbf{x}} = \Delta\mathbf{x} - 10\mathbf{x}_x - 100\mathbf{x}_y + \mathbf{b}(x,y)\mathbf{u}(t)$$

on the unit square with Dirichlet boundary conditions. (`demo_l1.m`)

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grid size: $75 \times 75 \Rightarrow \#\text{states} = 5625 \Rightarrow \#\text{unknowns in } X = 5625^2 \approx 32 \cdot 10^6$

Computations carried out on Intel Core2 Duo @2.13GHz Cache: 2048kB RAM: 2GB

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heuristic parameters time: 44s residual norm: 1.0461e-11

heuristic real parts time: 13s residual norm: 9.0846e-12

appr. Wachspress time: 16s residual norm: 5.3196e-12

Remark

- heuristic parameters are complex
- problem size exceeds memory limitations in complex case

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Recent Improvements in the Software

Column Compression for the low rank factors

Problem

- Low rank factors Z of the solutions X grow rapidly, since a constant number of columns is added in every ADI step.
- If many ADI steps are used, at some point $\#\text{columns in } Z > \text{rk}(Z)$.

Recent Improvements in the Software

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Idea: Column compression using rank revealing QR factorization (RRQR)

Consider $X = ZZ^T$ and $\text{rk}(Z) = r$. Compute the RRQR[5] of Z

$$Z^T = QR\Pi \quad \text{where} \quad R = \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \quad \text{and } R_{11} \in \mathbb{R}^{r \times r}$$

now set $\tilde{Z}^T = [R_{11} R_{12}]\,\Pi^T$ then $\tilde{Z}\tilde{Z}^T =: \tilde{X} = X$.

[5] [Bischof & Quintana-Ortí 1998]

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Test example

Centered finite difference discretized 2d convection diffusion equation:

$$\dot{\mathbf{x}} = \Delta \mathbf{x} - 10\mathbf{x}_x - 100\mathbf{x}_y + \mathbf{b}(x,y)\mathbf{u}(t)$$

on the unit square with Dirichlet boundary conditions. (`demo_l1.m`)

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grid size: $75 \times 75 \Rightarrow \#\text{states} = 5625 \Rightarrow \#\text{unknowns in } X = 5625^2 \approx 32 \cdot 10^6$

truncation TOL	# col. in LRCF	time	res. norm
–	47	13s	9.0846e-12
eps	46	14s	1.9516e-11
$\sqrt{\text{eps}}$	28	13s	1.9924e-11

Computations carried out on Intel Core2 Duo @2.13GHz Cache: 2048kB RAM: 2GB

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Observation

[Benner & Quintana-Ortí 2005] showed that truncation tolerance $\sqrt{eps}$ in the low rank factor Z is sufficient to achieve an error eps in the solution X.

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Recent Improvements in the Software

Generalized Systems

Current Method

Transform

$$\begin{aligned} M\dot{x} &= Ax + Bu \\ y &= Cx \end{aligned}$$

to

$$\begin{aligned} \dot{\tilde{x}} &= \tilde{A}\tilde{x} + \tilde{B}u \\ y &= \tilde{C}\tilde{x} \end{aligned}$$

where $M = M_L M_U$ and $\tilde{x} = M_U x$, $\tilde{A} = M_L^{-1} A M_U^{-1}$, $\tilde{B} = M_L^{-1} B$, $\tilde{C} = C M_U^{-1}$.

- 2 additional sparse triangular solves in every multiplication with A
- 2 additional sparse matrix vector multiplies in solution of $\tilde{A}x = b$ and $(\tilde{A} + p_j I)x = b$
- $\tilde{B}$ and $\tilde{C}$ are dense even if B and C are sparse.

\+ preserves symmetry if M, A are symmetric.

Recent Improvements in the Software

Generalized Systems

Alternative Method

Transform

$$\begin{aligned} M\dot{x} &= Ax + Bu \\ y &= Cx \end{aligned}$$

to

$$\begin{aligned} \dot{x} &= \tilde{A}x + \tilde{B}u \\ y &= Cx \end{aligned}$$

where $\tilde{A} = M^{-1}A$ and $\tilde{B} = M^{-1}B$

- \+ state variable untouched $\Rightarrow$ solution to (ARE), (LE) not transformed
- \+ exploiting pencil structure in $(\tilde{A} + p_j I) = M^{-1}(A + p_j M)$ reduces overhead
- \- current user supplied function structure inefficient here
  $\Rightarrow$ rewrite of LyaPack kernel routines needed (work in progress)

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- Column compression via RRQR also drastically reduces storage requirements. Especially helpful in differential Riccati equation solvers where 1 ARE (BDF) or 1 Lyapunov (Rosenbrock) solution needs to be stored in every step.
- Optimized treatment of generalized systems is work in progress

Conclusions and Outlook

Outlook

Theoretical Outlook

- Improve stopping Criteria for the ADI process.
  e.g. inside the LRCF-Newton method by interpretation as inexact Newton method following the ideas of Sachs et al.
- Optimize truncation tolerances for the RRQR
  Investigate dependence of residual errors in X on the truncation tolerance
- Stabilizing initial feedback computation
  Investigate whether the method in [GALLIVAN, RAO, VAN DOOREN 2006] can be implemented exploiting sparse matrix arithmetics.

Conclusions and Outlook

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Implementation TODOs

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- Introduce solvers for DREs
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- Improve the current Arnoldi implementation inside the heuristic ADI Parameter computation
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Thank you for your attention!