Multiterm linear matrix equations and the numerical solution of (S)PDEs

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Some matrix equations

- Sylvester matrix equation

$$A\mathbf{X} + \mathbf{X}B + D = 0$$

Eigenvalue pbs and tracking, Control, MOR, Assignment pbs, Riccati eqn

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$$A\mathbf{X} + \mathbf{X}A^\top + D = 0, \qquad D = D^\top$$

Stability analysis in Control and Dynamical systems, Signal processing, eigenvalue computations

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Control, (Stochastic) PDEs, ...

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Focus: All or some of the matrices are large (and possibly sparse)

Solving the Lyapunov equation. The problem

Approximate $\mathbf{X}$ in:

$$A\mathbf{X} + \mathbf{X}A^\top + BB^\top = 0$$

$A \in \mathbb{R}^{n\times n}$ neg.real $\qquad B \in \mathbb{R}^{n\times p}, \qquad 1 \leq p \ll n$

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Time-invariant linear system:

$$\mathbf{x}'(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \qquad \mathbf{x}(0) = x_0$$

Closed form solution:

$$\mathbf{X} = \int_0^\infty e^{-tA} BB^\top e^{-tA^\top} dt$$

$\Rightarrow \qquad \mathbf{X}$ symmetric semidef.

see, e.g., Antoulas '05, Benner '06

Linear systems vs linear matrix equations

Large linear systems:

$$Ax = b, \quad A \in \mathbb{R}^{n\times n}$$

- Krylov subspace methods (CG, MINRES, GMRES, BiCGSTAB, etc.)
- Preconditioners: find P such that

$$AP^{-1}\widetilde{x} = b \qquad x = P^{-1}\widetilde{x}$$

is easier and fast to solve

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Large linear matrix equations:

$$A\mathbf{X} + \mathbf{X}A^\top + BB^\top = 0$$

- No preconditioning - to preserve symmetry
- $\mathbf{X}$ is a large, dense matrix $\Rightarrow$ low rank approximation

$$\mathbf{X} \approx \widetilde{X} = ZZ^\top, \quad Z \text{ tall}$$

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Large linear matrix equations:

$$A\mathbf{X} + \mathbf{X}A^\top + BB^\top = 0$$

Kronecker formulation:

$$(A \otimes I + I \otimes A)x = b \qquad x = \mathrm{vec}(\mathbf{X})$$

Projection-type methods

Given an approximation space $\mathcal{K}$,

$$\mathbf{X} \approx X_m \qquad \mathrm{col}(X_m) \in \mathcal{K}$$

Galerkin condition: $\quad R := AX_m + X_m A^\top + BB^\top \quad \perp \quad \mathcal{K}$

$$V_m^\top R V_m = 0 \qquad\qquad \mathcal{K} = \mathrm{Range}(V_m)$$

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Assume $V_m^\top V_m = I_m$ and let $X_m := V_m Y_m V_m^\top$.

Projected Lyapunov equation:

$$V_m^\top (A V_m Y_m V_m^\top + V_m Y_m V_m^\top A^\top + BB^\top) V_m \quad = \quad 0$$

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$$\begin{aligned} V_m^\top (A V_m Y_m V_m^\top + V_m Y_m V_m^\top A^\top + BB^\top) V_m &= 0 \\ (V_m^\top A V_m) Y_m + Y_m (V_m^\top A^\top V_m) + V_m^\top B B^\top V_m &= 0 \end{aligned}$$

Early contributions: Saad '90, Jaimoukha & Kasenally '94, for
$\mathcal{K} = \mathcal{K}_m(A, B) = \mathrm{Range}([B, AB, \ldots, A^{m-1}B])$

More recent options as approximation space

Enrich space to decrease space dimension

- Extended Krylov subspace

$$\mathcal{K} = \mathcal{K}_m(A, B) + \mathcal{K}_m(A^{-1}, A^{-1}B),$$

that is, $\mathcal{K} = \mathrm{Range}([B, A^{-1}B, AB, A^{-2}B, A^2B, A^{-3}B, \ldots,])$

(Druskin & Knizhnerman '98, Simoncini '07)

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- Rational Krylov subspace

$$\mathcal{K} = \mathbb{K} := \mathrm{Range}([B, (A - s_1 I)^{-1}B, \ldots, (A - s_m I)^{-1}B])$$

usually, $\{s_1, \ldots, s_m\} \subset \mathbb{C}^+$ chosen a-priori

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In both cases, for Range$(V_m) = \mathcal{K}$, projected Lyapunov equation:

$$(V_m^\top A V_m) Y_m + Y_m (V_m^\top A^\top V_m) + V_m^\top B B^\top V_m = 0$$

$X_m = V_m Y_m V_m^\top$

Multiterm linear matrix equation

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Applications:

- Matrix least squares
- Control
- (Stochastic) PDEs
- ...

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Main device: Kronecker formulation

$$\left(B_1^\top \otimes A_1 + \ldots + B_\ell^\top \otimes A_\ell\right) x = c$$

Iterative methods: matrix-matrix multiplications and rank truncation

(Benner, Breiten, Bouhamidi, Chehab, Damm, Grasedyck, Jbilou, Kressner, Matthies, Onwunta, Raydan, Stoll, Tobler, Zander, and **many** others...)

Matrix equations in PDEs

The Poisson equation - revisited

$$-u_{xx} - u_{yy} = f, \quad \text{in} \quad \Omega = (0,1)^2$$

$+$ Dirichlet b.c. (zero b.c. for simplicity)

Usual discretization $\Rightarrow$ $\quad Au = b \quad$ (with $A = T \otimes I + I \otimes T$, $b = \text{vec}(F)$)

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Discretization: $U_{i,j} \approx u_{x_i, y_j}$, with (x_i, y_j) interior nodes, so that

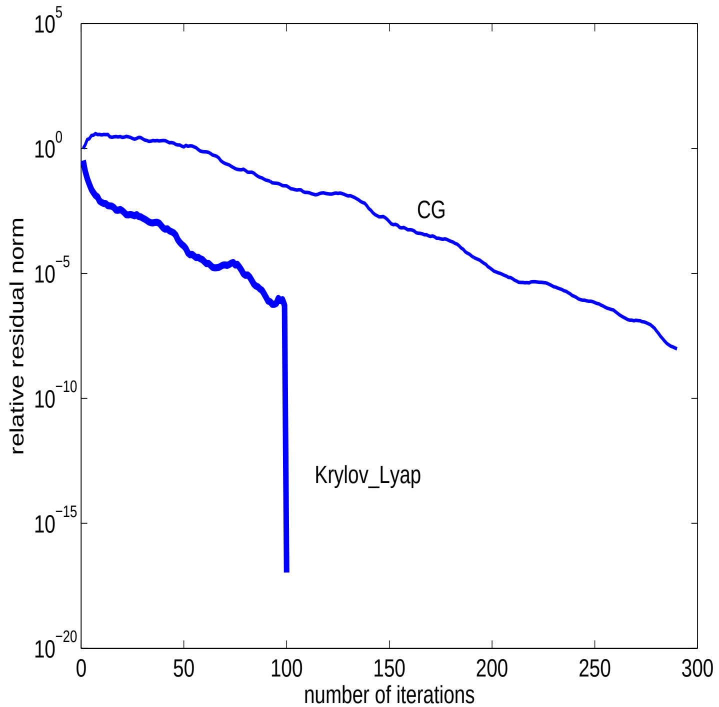
$$u_{xx}(x_i, y_j) \approx \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2} = \frac{1}{h^2}[1, -2, 1] \begin{bmatrix} U_{i-1,j} \\ U_{i,j} \\ U_{i+1,j} \end{bmatrix}$$

$$u_{yy}(x_i, y_j) \approx \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2} = \frac{1}{h^2}[U_{i,j-1}, U_{i,j}, U_{i,j+1}] \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

h: meshsize

$\color{red}{\text{CG for } Ax = b}$ vs $\color{blue}{\text{Iterative solver for } TU + UT = F}$

$T \in \mathbb{R}^{n\times n}$, $A \in \mathbb{R}^{n^2\times n^2}$, $n = 100$



For `tol` $= 10^{-6}$, Elapsed time: CG≈ 0.8, Krylov ≈ 0.4

```
>> tic;lyap(T,F);toc
Elapsed time is 0.019335 seconds.
>> tic;A\b;toc
Elapsed time is 0.030765 seconds.
```

$$-\Delta u = 1, \quad \Omega = (0,1)^3 \quad \Rightarrow \quad A = (T \otimes I \otimes I + I \otimes T \otimes I + I \otimes I \otimes T)$$

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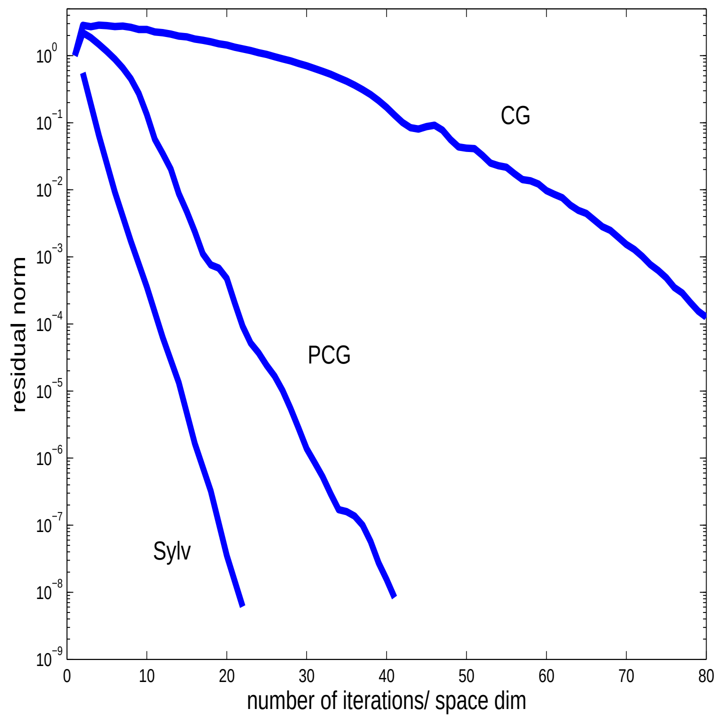
CG for $Ax = b$ vs Iterative solver for $(I \otimes T + T \otimes I)\mathbf{U} + \mathbf{U}T = F$

$T \in \mathbb{R}^{n \times n}$, $A \in \mathbb{R}^{n^3 \times n^3}$, $\qquad n = 50$



	CG	PCG	Matrix Eqn solver
Elapsed Time	2.91	0.56	0.08

A 3D convection-diffusion equation

$-\epsilon\Delta u + \mathbf{w}\cdot\nabla u = 1$, in $\Omega = (0,1)^3$, with convection term

$$\mathbf{w} = (x\sin x, y\cos y, e^{z^2-1})$$

Sylvester equation:

$$[I\otimes(T_1+\Phi_1 B_1) + (T_2+\Psi_2 B_2)^T \otimes I]\ \mathbf{U} + \mathbf{U}\ (T_3 + B_3\Upsilon_3) = \mathbf{1}\mathbf{1}^T$$

ϵ	n_x	FGMRES+AGMG CPU time (# its)	GMRES+MI20 CPU time (# its)	Sylv Solver CPU time (# its)
0.0050	100	8.0207 (15)	9.7207 (7)	0.5677 (22)
0.0010	100	7.6815 (14)	9.4935 (7)	0.5446 (22)
0.0005	100	7.3914 (14)	9.6274 (7)	0.5927 (24)

- Also for more general, separable coeff., operators on uniform grids
- If not separable coeff., use as preconditioner

(Palitta & Simoncini (tr 2014))

... A classical approach

Matrix formulation is not new...

- Bickley & McNamee, 1960: Early literature on difference equations
- Wachspress, 1963: Model problem for ADI algorithm
- Ellner & Wachspress (1980's): interplay between the matrix and vector formulations (via preconditioning)

Novel solvers for matrix equations allow faster convergence

PDEs with random inputs

Stochastic steady-state diffusion eqn: *Find* $u : D \times \Omega \to \mathbb{R}$ *s.t.* $\mathbb{P}$-*a.s.*,

$$\begin{cases} -\nabla \cdot (a(\mathbf{x},\omega)\nabla u(\mathbf{x},\omega)) = & f(\mathbf{x}) \quad in \;\; D \\ u(\mathbf{x},\omega) = & 0 \qquad on \;\; \partial D \end{cases}$$

f: deterministic;

a: f. of finite no. of real-valued random variables $\xi_r : \Omega \to \Gamma_r \subset \mathbb{R}$

Common choice: truncated Karhunen–Loève (KL) expansion,

$$a(\mathbf{x},\omega) = \mu(\mathbf{x}) + \sigma \sum_{r=1}^{m} \sqrt{\lambda_r}\phi_r(\mathbf{x})\xi_r(\omega),$$

$\mu(\mathbf{x})$: expected value of diffusion coef. σ: std dev.

$(\lambda_r, \phi_r(\mathbf{x}))$ eigs of the integral operator $\mathcal{V}$ wrto $V(\mathbf{x},\mathbf{x}') = \frac{1}{\sigma^2}C(\mathbf{x},\mathbf{x}')$

($\lambda_r \searrow$ $C : D \times D \to \mathbb{R}$ covariance fun.)

Discretization by stochastic Galerkin

Approx with space in tensor product form[a] $\mathcal{X}_h \times S_p$

$$\mathcal{A}\mathbf{x} = \mathbf{b}, \qquad \mathcal{A} = G_0 \otimes K_0 + \sum_{r=1}^{m} G_r \otimes K_r, \quad \mathbf{b} = \mathbf{g}_0 \otimes \mathbf{f}_0,$$

$\mathbf{x}$: expansion coef. of approx to u in the tensor product basis $\{\varphi_i \psi_k\}$

$K_r \in \mathbb{R}^{n_x \times n_x}$, FE matrices (sym)

$G_r \in \mathbb{R}^{n_\xi \times n_\xi}$, $r = 0, 1, \ldots, m$ Galerkin matrices associated w/ S_p (sym.)

$\mathbf{g}_0$: first column of G_0

$\mathbf{f}_0$: FE rhs of deterministic PDE

$n_\xi = \dim(S_p) = \frac{(m+p)!}{m!p!}$

---

[a] S_p set of multivariate polyn of total degree $\leq p$

The matrix equation formulation

$$(G_0 \otimes K_0 + G_1 \otimes K_1 + \ldots + G_m \otimes K_m)\,\mathbf{x} = \mathbf{g}_0 \otimes \mathbf{f}_0$$

transforms into

$$K_0 \mathbf{X} G_0 + K_1 \mathbf{X} G_1 + \ldots + K_m \mathbf{X} G_m = F, \qquad F = \mathbf{f}_0 \mathbf{g}_0^\top$$

$(G_0 = I)$

Solution strategy. Conjecture:

- $\{K_r\}$ from trunc'd Karhunen–Loève (KL) expansion

$$\Downarrow$$

Seek low rank $\widetilde{X} \approx \mathbf{X}$

(Possibly extending results of Gradesyk, 2004)

Matrix Galerkin approximation of the deterministic part. 1

Approximation space $\mathcal{K}_k$ and basis matrix V_k: $\qquad \mathbf{X} \approx X_k = V_k Y$

$$V_k^\top R_k = 0, \qquad R_k := K_0 X_k + K_1 X_k G_1 + \ldots + K_m X_k G_m - \mathbf{f}_0 \mathbf{g}_0^T$$

Computational challenges:

- Generation of $\mathcal{K}_k$ involved $m+1$ different matrices $\{K_r\}$!
- Matrices K_r have different spectral properties
- n_x, n_ξ so large that X_k, R_k should not be formed !

Ongoing joint project with Catherine Powell, David Silvester, Univ. Manchester

Matrix Galerkin approximation of the deterministic part. 2

Approximation space $\mathcal{K}_k$ and basis matrix V_k: $\quad \mathbf{X} \approx X_k = V_k Y$

$$V_k^\top R_k = 0, \qquad R_k := K_0 X_k + K_1 X_k G_1 + \ldots + K_m X_k G_m - \mathbf{f}_0 \mathbf{g}_0^T$$

- "Divide" by K_0 (stiffness matrix)

$$\widehat{\mathbf{X}} + \widehat{K}_1 \widehat{\mathbf{X}} G_1 + \ldots + \widehat{K}_m \widehat{\mathbf{X}} G_m = \widehat{\mathbf{f}}_0 \mathbf{g}_0^T$$

- Shift matrices by α_r, $r = 1, \ldots, m$ to get similar spectral interval

$$\widehat{\mathbf{X}} \left(I - \sum_{r=1}^{m} \alpha_r G_r \right) + (\widehat{K}_1 + \alpha_1 I) \widehat{\mathbf{X}} G_1 + \ldots + (\widehat{K}_r + \alpha_m I) \widehat{\mathbf{X}} G_m = \widehat{\mathbf{f}}_0 \mathbf{g}_0^T$$

- Generate $\mathcal{K}_k = \bigcup_r \mathbb{K}_k(\widehat{K}_r + \alpha_r I, \widehat{\mathbf{f}}_0)$

- Solve projected (reduced) problem by matrix-oriented CG

Example 1. SIFISS 1.0, Q1 Finite Elements

$$-\nabla \cdot (a \nabla u) = 1, \quad D = (0,1)^2, \quad u|_{\partial D} = 0, \text{ (fast decay)}$$ [a]

$n_x = 65{,}025$ tol$=10^{-5}$ (relative soln change)

[a] Eigel Gittelson Schwab Zander, CMAME 2014

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$n_x = 65,025$ tol$=10^{-5}$ (relative soln change)

	$m+1$	p	n_ξ	dim($\mathcal{K}_k$)	avr # inner	Elapsed Time
	9	3	165	139	14.60	184.19
	9	4	495	171	16.83	220.60
	9	5	1287	171	17.50	228.67
	11	3	286	168	14.60	232.48
	11	4	1001	168	15.80	232.94
	11	5	3003	213	18.00	295.10
	16	3	816	165	13.25	281.85
CG	9	5	1287		20	1229.3

(Direct solves for generating each rational space $\mathbb{K}_k$)

Dell PowerEdge R620 w/ 32 procs Intel(R) Xeon(R) CPU E5-2640 v2 @ 2.00GHz

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	9	3	165	138	14.20	51.91
	9	4	495	167	16.83	62.19
	9	5	1287	167	17.50	63.73
	11	3	286	166	14.60	58.84
	11	4	1001	166	15.40	65.49
	11	5	3003	210	17.83	83.00
	16	3	816	166	13.25	80.31
CG	9	5	1287		20	1229.3

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Conclusions

Multiterm (Kron) linear equations is the new challenge

- Great advances in solving really large linear matrix equations
- Second order (matrix) challenges rely on strength and maturity of linear system solvers
- Low-rank tensor formats is the new generation of approximations

Reference for linear matrix equations:

⋆ V. S., *Computational methods for linear matrix equations*,
March 2013, Submitted
available at `www.dm.unibo.it/~simoncin`