Computational methods for large-scale matrix equations and application to 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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$$A_1\mathbf{X}B_1 + A_2\mathbf{X}B_2 + \ldots + A_\ell\mathbf{X}B_\ell = C$$

Control, (Stochastic) PDEs, ...

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Survey article: V.Simoncini, SIAM Review 2016.

More matrix equations

- Systems of linear matrix equations:

$$\begin{aligned} A_2\mathbf{X} + \mathbf{X}A_1 + B^T\mathbf{P} &= F_1 \\ A_1\mathbf{Y} + \mathbf{Y}A_2 + \mathbf{P}B &= F_2 \\ B\mathbf{X} + \mathbf{Y}B^T &= F_3 \end{aligned}$$

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- Riccati equation: Find $\mathbf{X} \in \mathbb{R}^{n\times n}$ such that

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

workhorse in Control Theory

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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 $\qquad B \in \mathbb{R}^{n\times p}, \qquad 1 \le p \ll n$

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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

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

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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 a low dimensional 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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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

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

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

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

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

$X_m = V_m Y_m V_m^\top$

Bilinear systems of matrix equations

Find $\mathbf{X} \in \mathbb{R}^{n_1 \times n_2}$ and $\mathbf{P} \in \mathbb{R}^{m \times n_2}$ such that

$$
\begin{aligned}
A_1\mathbf{X} + \mathbf{X}A_2 + B^T\mathbf{P} &= F_1 \\
B\mathbf{X} &= F_2
\end{aligned}
$$

with $A_i \in \mathbb{R}^{n_i \times n_i}$, $B \in \mathbb{R}^{m \times n_1}$, $F_1 \in \mathbb{R}^{n_1 \times n_2}$, $F_2 \in \mathbb{R}^{m \times n_2}$, $m \leq n_1$

Emerging matrix formulation of different application problems

- Constraint control
- Mixed formulations of stochastic diffusion problems
- Discretized deterministic/stochastic (Navier-)Stokes equations
- ...

An example. Mixed FE formulation of stochastic Galerkin diffusion pb

$$\begin{aligned} c^{-1}\vec{u} - \nabla p &= 0, \\ -\nabla \cdot \vec{u} &= f, \end{aligned}$$

Assume that $c^{-1} = c_0 + \sum_{r=1}^{\ell} \sqrt{\lambda_r} c_r(\vec{x}) \xi_r(\omega)$ and that an appropriate class of finite elements is used for the discretization of the problem

(see, e.g., the derivation in Elman & Furnival & Powell, 2010)

After discretization the problem reads:

$$\begin{bmatrix} G_0 \otimes K_0 + \sum_{r=1}^{\ell} \sqrt{\lambda} G_r \otimes K_r & G_0^T \otimes B_0^T \\ G_0 \otimes B_0 & \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} 0 \\ f \end{bmatrix}$$

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For $\ell = 1$ we obtain

$$\begin{aligned} K_0 \mathbf{X} G_0 + K_1 \mathbf{X} G_1 + B_0^T \mathbf{P} G_0 &= 0, \\ B_0 \mathbf{X} G_0 &= F \end{aligned}$$

The bilinear case. Computational strategies

$$\begin{aligned} A_1\mathbf{X} + \mathbf{X}A_2 + B^T\mathbf{P} &= F_1 \\ B\mathbf{X} &= F_2 \end{aligned}$$

Kronecker formulation (monolithic):

$$\begin{bmatrix} \mathcal{A} & \mathcal{B}^T \\ \mathcal{B} & \mathcal{O} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \quad \mathcal{A} = I \otimes A_1 + A_2^T \otimes I, \quad \mathcal{B} = B \otimes I$$

with $\mathbf{x} = \mathrm{vec}(\mathbf{X})$, $\mathbf{p} = \mathrm{vec}(\mathbf{P})$, $f_1 = \mathrm{vec}(F_1)$ and $f_2 = \mathrm{vec}(F_2)$

Extremely rich literature from saddle point algebraic linear systems

Trouble: Coefficient matrix has size $(n_1n_2 + mn_2) \times (n_1n_2 + mn_2)$

The bilinear case. Computational strategies. Cont'd

$$\begin{aligned} A_1\mathbf{X} + \mathbf{X}A_2 + B^T\mathbf{P} &= F_1 \\ B\mathbf{X} &= F_2 \end{aligned}$$

⋆ Derive numerical strategies that directly work with the matrix equations:

- Small scale: Null space method
- Small and medium scale: Schur complement method
  (also directly applicable to trilinear case)
- Large scale: Iterative method for low rank F_i, $i = 1, 2$

"Small and medium scale" actually means "Large scale" for the Kronecker form!

Large scale problem. Iterative method. 1/3

$$\begin{aligned} A_1\mathbf{X} + \mathbf{X}A_2 + B^T\mathbf{P} &= F_1 \\ B\mathbf{X} &= F_2 \end{aligned}$$

Rewrite as

$$\begin{bmatrix} A_1 & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} + \begin{bmatrix} I_{n_1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} A_2 = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix}, \quad \Leftrightarrow \quad \mathcal{M}\mathbf{Z} + \mathcal{D}_0\mathbf{Z}A_2 = F$$

with

$\mathcal{M}, \mathcal{D}_0 \in \mathbb{R}^{(n_1+m)\times(n_1+m)}$

$A_2 \in \mathbb{R}^{n_2\times n_2}$ nonsingular

$\mathcal{D}_0$ highly singular

If F low rank, exploit projection-type strategies for Sylvester equations

Large scale problem. Iterative method. 2/3

$$\begin{bmatrix} A_1 & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} + \begin{bmatrix} I_{n_1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} A_2 = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} \quad \Leftrightarrow \quad \mathcal{M}\mathbf{Z} + \mathcal{D}_0 \mathbf{Z} A_2 = F$$

with F low rank. We rewrite the matrix equation as a Sylvester equation:

$$\boxed{\mathbf{Z} A_2^{-1} + \mathcal{M}^{-1} \mathcal{D}_0 \mathbf{Z} = \widehat{F}}$$

with $\widehat{F} = \mathcal{M}^{-1} F A_2^{-1}$ of low rank if F is of low rank, $\quad \widehat{F} = \widehat{F}_\ell \widehat{F}_r^T$

$$\Rightarrow \qquad \mathbf{Z} \approx \widetilde{\mathbf{Z}}_k = V_k \mathcal{Z}_k W_k^T$$

with $\mathrm{Range}(V_k), \mathrm{Range}(W_k)$ appropriate approximation spaces of small dimensions

Large scale problem. Iterative method. 3/3

Galerkin-Projection method

$$\mathbf{Z}A_2^{-1} + \mathcal{M}^{-1}\mathcal{D}_0\mathbf{Z} = \widehat{F}_l\widehat{F}_r^T \quad \Rightarrow \quad \mathbf{Z} \approx \widetilde{\mathbf{Z}}_k = V_k\mathcal{Z}_kW_k^T$$

Choice of V_k, W_k. A possible strategy:

- $W_k = \mathbb{E}\mathbb{K}_k(A_2^{-T}, \widehat{F}_r)$, Extended Krylov subspace
- $V_k = K_k(\mathcal{M}^{-1}\mathcal{D}_0, \widehat{F}_l) \cup K_k((\mathcal{M}^{-1}\mathcal{D}_0 + \sigma I)^{-1}, \widehat{F}_l)$
  Augmented Krylov subspace, $\sigma \in \mathbb{R}$
  (see, e.g., Shank & Simoncini, 2013)

Note: $\mathcal{M}$ has size $(n_1 + m) \times (n_1 + m)$

(Compare with $(n_1n_2 + mn_2) \times (n_1n_2 + mn_2)$ of the Kronecker form)

Numerical experiments

$$\begin{aligned} A_1\mathbf{X} - \mathbf{X}A_2 + B^T\mathbf{P} &= 0, \qquad \text{vs} \qquad \mathcal{A}\mathbf{z} = f \\ B\mathbf{X} &= F_2 \end{aligned}$$

$A_1 \to \mathcal{L}_1 = -u_{xx} - u_{yy}$, $\qquad F_2$ rank-1

$A_2 \to \mathcal{L}_2 = -(e^{-10xy}u_x)_x - (e^{10xy}u_y)_y + 10(x+y)u_x$

$B = \mathrm{bidiag}(-1, \underline{1}) \in \mathbb{R}^{(n_2-n_1)\times n_2}$, $\qquad$ params: tol$=10^{-6}$, $\sigma = 10^{-2}$

n_1	n_2	size($\mathcal{A}$)	Monolithic Elapsed Time	Matrix eqns Elapsed Time
400	100	79,000	6.9769e-02	3.1523e-02 (4)
900	225	401,625	3.4808e-01	5.0447e-02 (4)
1600	400	1272,000	1.1319e+00	7.8018e-02 (4)
2500	625	3109,375	3.1212e+00	1.5282e-01 (5)
3600	900	6453,000	1.0210e+01	2.8053e-01 (5)
4900	1225	11,962,125	3.7699e+01	1.4754e+00 (5)

Monolithic: direct solver (iterative not competitive)

Numerical experiments. 2D stochastic Stokes problem

$$\begin{bmatrix} \mathcal{H} & \mathcal{B}^T \\ \mathcal{B} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \qquad \begin{array}{l} \mathcal{H} = \mathrm{blkdiag}((\nu_0 \mathrm{G}_0 + \nu_1 \mathrm{G}_1) \otimes \mathrm{A}_\mathrm{x}, (\nu_0 \mathrm{G}_0 + \nu_1 \mathrm{G}_1) \otimes \mathrm{A}_\mathrm{y}) \\ \mathcal{B} = [G_0 \otimes B_x,\ G_0 \otimes B_y] \end{array}$$

$$\mathcal{M}\mathbf{Z} + \mathcal{D}_0 \mathbf{Z} G_1 = F \qquad \text{vs} \qquad \mathcal{A}\mathbf{z} = f$$

n_1	n_2	size($\mathcal{A}$)	Monolithic	Matrix eqns
2512	4	11,604	0.55	0.28 (2)
7052	4	32,168	3.73	1.26 (2)
19624	4	88,956	11.93	3.95 (2)

n_1	n_2	size($\mathcal{A}$)	Monolithic	Matrix eqns
2512	165	478 665	7.60	0.33 (2)
7052	165	1 326 930	34.08	1.08 (2)
19624	165	3 669 435	–	5.69 (3)

$\nu_0 = 1/10, \nu_1 = 3\nu_0/10$ Powell-Silvester (2012)

Multiterm linear matrix equation

$$A_1\mathbf{X}B_1 + A_2\mathbf{X}B_2 + \ldots + A_\ell\mathbf{X}B_\ell = C$$

Applications:

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

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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...)

Multiterm linear matrix equation

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Applications:

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Alternative approaches:

- Projection onto rich approximation space
- Compression to two-term matrix equation
- Splitting strategy towards two-term matrix equation
- ...

PDEs on uniform grids and separable coeffs

$$-\varepsilon\Delta u+\phi_1(x)\psi_1(y)u_x+\phi_2(x)\psi_2(y)u_y+\gamma_1(x)\gamma_2(y)u=f \quad (x,y)\in\Omega$$

ϕ_i, ψ_i, γ_i, $i=1,2$ sufficiently regular functions + b.c.

Problem discretization by means of a tensor basis

Multiterm linear equation:

$$-\varepsilon T_1\mathbf{U}-\varepsilon\mathbf{U}T_2+\Phi_1 B_1\mathbf{U}\Psi_1+\Phi_2\mathbf{U}B_2^\top\Psi_2+\Gamma_1\mathbf{U}\Gamma_2=F$$

Finite Diff.: $\mathbf{U}_{i,j}=\mathbf{U}(x_i,y_j)$ approximate solution at the nodes

PDEs with random inputs

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

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

f: deterministic;

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

Use 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.

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

$$n_\xi = \dim(S_p) = \frac{(m+p)!}{m!p!} \qquad \Rightarrow \boxed{n_x \cdot n_\xi} \text{ huge}$$

[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

$$\Downarrow$$

$\mathbf{X} \approx \widetilde{X}$ low rank, $\widetilde{X} = X_1 X_2^T$

(Possibly extending results of Grasedyck, 2004)

Matrix Galerkin approximation of the deterministic part. 1

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

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

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 !

(Powell & Silvester & Simoncini, SISC 2017)

Not discussed but in this category

- Sylvester-like linear matrix equations

$$AX + f(X)B = C$$

typically (but not only!): $f(X) = \bar{X},\ f(X) = X^\top$, or $f(X) = X^*$
(Bevis, Braden, Byers, Chiang, De Terán, Dopico, Duan, Feng, Gonzalez, Guillery, Hall, Hartwig, Ikramov, Kressner, Montealegre, Reyes, Schröder, Vorntsov, Watkins, Wu, ...)

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- Linear systems with complex tensor structure

  $$\mathcal{A}\mathbf{x} = b \quad \text{with} \quad \mathcal{A} = \sum_{j=1}^{k} I_{n_1} \otimes \cdots \otimes I_{n_{j-1}} \otimes A_j \otimes I_{n_{j+1}} \cdots \otimes I_{n_k}.$$

  Dolgov, Grasedyck, Khoromskij, Kressner, Oseledets, Tobler, Tyrtyshnikov, and many more...

Conclusions

Large-scale (Multiterm) linear equations are a new computational tool

- 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. Simoncini,

Computational methods for linear matrix equations,

SIAM Review, Sept. 2016.