MAY 24, 2021

COMPUTATIONAL METHODS FOR LINEAR MATRIX EQUATIONS

$Ax = c$

OUTLINE:

- linear systems w/ multiple rhs $\quad AX = C = \left(\,|\,|\,|\,|\,\right)$
- Shifted systems $\quad (A + \sigma I)X = C \quad \sigma \in \mathbb{C}$
- Diagonal addend $\quad AX + XD = C \quad D = \begin{pmatrix} \delta_1 & & \\ & \delta_2 & \\ & & \ddots & \\ & & & \delta_s \end{pmatrix}$
- General matrix equations (linear):

$$AX + XB = C \quad \leftarrow \text{Sylvester eqn.}$$

$$\to \quad A_1 X B_1 + A_2 X B_2 = C \quad \text{Generalized Sylvester equation}$$

$$\sum_{i=1}^{\ell} A_i X B_i = C$$

- Algebraic Riccati eqn.

MULTIPLE RHS LINEAR SYSTEMS

$$AX = C, \qquad C = [c_1, c_2, \dots, c_s] \in \mathbb{R}^{n \times s}$$

C full rank $\qquad s \ll n$

NOTE: if C is not full rank, $C = C_1 C_2^T$

C_1 full rank $\qquad k \ll s$

$$AX = C_1 C_2^T$$

$$X = \underbrace{A^{-1} C_1}\, C_2^T \qquad AY = C_1$$

$$= Y C_2^T$$

1) Naive way: $\quad x_i = \underbrace{A^{-1} c_i}_{\varepsilon} \quad \leftarrow$

2) Direct methods: dense case: $\quad A = LU$ once!

$$X = U^{-1}(L^{-1}C)$$

sparse case: "\" uses only one reordering of the entries towards the actual Gaussian Elimination

$$AX = C$$

3) Iterative methods : . Information sharing (seed methods)
. Block methods $\rightarrow$ Projection methods

$$K_m^{\square}(A, C) = \text{Range}\left([C, AC, \dots, A^{m-1}C] \right)$$

block Krylov subspace

$$\dim(K_m^{\square}) \le m \cdot s \qquad C \in \mathbb{R}^{n \times s}$$

Note: loss of rank is not unlikely:

$$C = [c, Ac] \qquad [C, AC] = [c, Ac, Ac, A^2c]$$

$n \times 2$

Orthogonality: $V_i, V_j \in \mathbb{R}^{n \times s}$, $i \ne j$

$$V_i^T V_j = 0 \quad s \times s$$

Normalization: $V_i = QR$ skinny $\Rightarrow Q$ orthogonalization of V_i

$[V_1, V_2, \dots, V_m]$ orthonormal basis

$\hat{V}_{m+1} = A V_m$

block Gram-Schmidt

block Arnoldi method

$$A X = \underline{C}$$

$$\mathcal{V}_m = [V_1, V_2, \dots, V_m] \qquad \mathcal{V}_m^T \mathcal{V}_m = I_{ms}$$

$$X \approx X_m = \mathcal{V}_m Y_m \qquad\qquad x \approx x_m = V_m \underline{y}$$

- Galerkin condition: (for A sym pos. def this is CG)

$$R_m = C - A X_m \perp \mathcal{K}_m^{\square}$$

$\mathcal{V}_m$ orth basis, $\qquad \mathcal{V}_m^T R_m = 0$

$$\mathcal{V}_m^T (C - A \mathcal{V}_m Y_m) = 0$$

$$\underbrace{\mathcal{V}_m^T A \mathcal{V}_m}_{} \underline{Y_m} = \underbrace{\mathcal{V}_m^T C}_{} \qquad \text{reduced pb.}$$

$\mathcal{H}_m$ $\quad ms \times ms$ $\qquad\qquad m \cdot s \ll n$

A spd $\Rightarrow$ $\mathcal{H}_m$ spd $\Rightarrow$ block tridiag

$$\mathcal{H}_m = \begin{pmatrix} \square & \square & \square & \cdots & \square \\ \square & \square & \square & \cdots & \square \\ 0 & \square & \square & \cdots & \square \\ \vdots & & \ddots & & \\ 0 & 0 & \cdots & \square & \square \end{pmatrix} \qquad \text{upper Hessenberg}$$

A spd $(n \times n)$ $\qquad \mathcal{H}_w = \begin{pmatrix} \boxed{} & & \\ & \boxed{} & \\ & & \boxed{} \end{pmatrix}$

~~block~~ CG

$$\alpha_k = \frac{p_k^T A p_k}{r_k^T r_k}$$

$$A[x_1 \dots x_s] = [c_1 \dots c_s]$$

Minimization of the A-norm of the error. More precisely,

$E \in \mathbb{R}^{m \times s}$, $\|E\|_F^2 = \text{trace}(E^T E)$

$$\|E\|_{F,A}^2 = \text{trace}(E^T A E) \qquad A \text{ spd}$$
$$= \langle E, E \rangle_A$$

CG : $\displaystyle\min_{X_m \in K_m^{\square}} \langle X^* - X_m, X^* - X_m \rangle_A$

X^* = exact soln.

Notation : $\|X\|_F^2 = \|vec(X)\|_2^2$

$$\underset{m \times s}{X} = [x_1, \dots x_s] \Rightarrow vec(X) = \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \vdots \\ x_s \end{pmatrix} \in \mathbb{R}^{ms \times 1}$$

Galerkin $\rightarrow$ $x_m = V_m Y$, $\quad R_m \perp V_m$

- PETROV - GALERKIN CONDITION :

$$A K_m^{\square} \perp R_m \qquad V_m \text{ orth basis for } K_m^{\square}$$

$$(AV_m)^T R_m = 0$$

$$(AV_m)^T (C - AV_m Y_m) = 0$$

$$\underbrace{(AV_m)^T AV_m}\, Y_m = \underbrace{(AV_m)^T C} \quad \leftarrow \text{normal eqn.}$$

$$\min_{Y_m} \| C - (AV_m) Y_m \|_F = \min_{Y_m} \| R_m \|_F$$

$\uparrow$ block GMRES

$$\| R_m \|_F^2 = \| r_{1,m} \|^2 + \| r_{2,m} \|^2 + \dots + \| r_{s,m} \|^2 \quad R_m = [r_{1,m} \dots r_{s,m}]$$

Let us solve the least squares pb without normal eqn.

From the Arnoldi iteration, we get the Arnoldi relation:

$$A V_m = V_{m+1} \underline{H}_m$$

$$= [V_m, V_{m+1}] \begin{bmatrix} H_m \\ 0 \dots 0 \; \underbrace{h_{m+1,m}}_{s \times s} \end{bmatrix}$$

$$\| C - \underline{\underline{AV_m}} Y_m \| = \| C - V_{m+1} \underline{H}_m Y_m \|$$

$$\| C - \mathcal{V}_{m+1} \underline{H}_m Y \|_F = \| \mathcal{V}_{m+1} (C_m - \underline{H}_m Y) \|_F$$

$$C = \mathcal{V}_{m+1} C_m \qquad = \| C_m - \underline{H}_m Y \|_F$$

$\Uparrow$

$K_m^{\square}$

$$\left(\ \right) - \left(\underbrace{\left[\ \right]}_{(m+1)s \times ms} \right) \left(\ \right) \quad \mathcal{V}_{m+1}^T \mathcal{V}_{m+1} = I$$

$s \times s$

Computational issues:

- At each iteration, s new vectors to handle

SHIFTED SYSTEMS: $(A + \sigma_j I) X = C \quad \sigma_j \in \mathbb{C}$

$j = 1 \dots \ell$

For direct methods, this is a problem, you have to solve each system separately.

For iterative methods, cheaper alternatives are current:

PROP: For a given $v \in \mathbb{R}^n$, $K_m(A, v) = K_m(A + \sigma I, v)$ $\quad \sigma \in \mathbb{R}$

(shift invariance of Krylov spaces)

Dim: $\text{Range}([v, Av])$

$\text{Range}([v, (A + \sigma I) v]) = \text{Range}[v, Av + \sigma v]$ #

NOTE: $\sigma \in \mathbb{C}$ $\qquad \mathcal{V}_m \in \mathbb{R}^{n \times ms} \qquad \mathcal{V}_m y, \ y \in \mathbb{C}^{ms}$

In the Arnoldi relation:

$$A V_m = V_{m+1} \underline{H}_m \qquad (+\sigma I) V_m$$

$$(A+\sigma I) V_m = V_{m+1} \underline{H}_m + \sigma V_{m+1} \begin{bmatrix} I \\ 0 \end{bmatrix}$$

$$= V_{m+1} \left(\underline{H}_m + \sigma \underbrace{\begin{pmatrix} I \\ 0 \end{pmatrix}}_{\underline{I}} \right)$$

$$= V_{m+1} \left(\underline{H}_m + \sigma \underline{I} \right)$$

For Galerkin $\quad AX = C \Rightarrow \quad H_m Y = V_m^T C$

$$(A+\sigma I) X = C \underset{(*)}{\Rightarrow} (H_m + \sigma I) Y = V_m^T C$$

$\in \mathbb{C}^{m_{s+1}}$

$$\Rightarrow \quad X_m = V_m Y_m$$

real $\quad$ complex

For multiple σ_j, $j = 1..l$, $\quad Y = Y(\sigma_j)$

l different systems $(*)$

$n \gg 500$

n large

NOTE: $\quad A$ spd $\quad A = Q \Lambda Q^T$

$$A + \sigma I = Q(\Lambda + \sigma I) Q^T$$

Q: $\quad C = C(\sigma) = C_1 + \sigma C_2 = \left([C_1 \; C_2] \right) \begin{bmatrix} I \\ \sigma I \end{bmatrix}$

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Multiple rhs + diagonal matrix

$D = \text{diag}(\delta_1, \delta_2, \dots, \delta_s)$ $\qquad AX + XD = C$

Setting $X = [x_1 \dots x_s]$, $C = [c_1 \dots c_s]$ $\qquad s \ll m$

$$AX + XD = C$$

$$\big(\quad\big)\big(||||\big) + \big(||||\big)\underbrace{\big(\diagdown\big)}_{s\times s} = \big(||||\big)$$

j-th colm

$$Ax_j + x_j\delta_j = c_j \iff (A + \underline{\delta_j} I)x_j = \underline{c_j}$$

shifted linear systems

Direct methods $\Rightarrow$ One solve for each j

Iterative methods: $\quad K_m^{\square}(A, C)$ $\qquad V_m$ orthonormal basis

does not depend on D

$X \approx X_m = V_m Y$

$R_m = C - AX_m - X_m D$

Galerkin condition: $\quad V_m^T R_m = 0$

$$V_m^T C - \underbrace{V_m^T A V_m}_{H_m} Y - \underbrace{V_m^T V_m}_{= I} Y D = 0$$

Reduced eqn: $\qquad Y \in \mathbb{R}^{ms \times s}$

$$H_m Y + \underline{\underline{YD}} = V_m^T C \qquad ms \times ms$$

NOTE: $(A+\delta_j I)x_j = c_j$ iterative method!

LINEAR MATRIX EQUATION (in general):

$$AX + XB = C \qquad B \text{ not diag}$$

Sylvester equation $\quad A \in \mathbb{R}^{m_1 \times m_1},\ B \in \mathbb{R}^{m_2 \times m_2}$

$$C \in \mathbb{R}^{m_1 \times m_2}$$

$m_2 << m_1$:
$$\begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix}\begin{pmatrix} X \end{pmatrix} + \begin{pmatrix} X \end{pmatrix}\begin{pmatrix} B \end{pmatrix} = \begin{pmatrix} C \end{pmatrix}$$

If B is diagonalizable, $B = Q \Lambda Q^{-1}$

$$AX + XQ\Lambda Q^{-1} = C$$

$$A\underbrace{XQ}_{\hat{X}} + \underbrace{XQ}_{\hat{X}}\Lambda = \underbrace{CQ}_{\hat{C}} \iff A\hat{X} + \hat{X}\Lambda = \hat{C}$$

same as earlier, with $\Lambda \equiv D$

after that, $X = \hat{X} Q^{-1}$

$\Rightarrow$ Good idea as long as Q is not too ill-conditioned otherwise procedure is unstable

As a stable alternative, let us use the Schur decomposition:

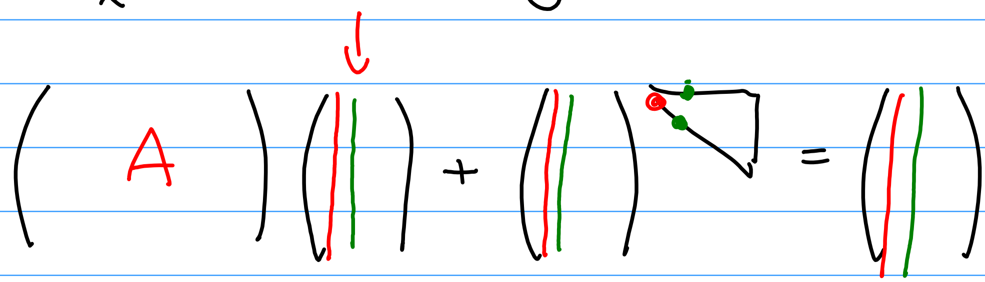
$$B = QRQ^* \qquad Q \text{ unitary } Q^*Q = I$$

$r_{ii} = \lambda_i(B) \in \mathbb{C} \qquad R = \nabla$ complex

$$B = QRQ^* \qquad R =$$

$$AX + XQRQ^* = C$$

$$A\underbrace{XQ}_{\hat{X}} + \underbrace{XQ}_{\hat{X}}R = \underbrace{CQ}_{\hat{C}} \iff A\hat{X} + \hat{X}R = \hat{C}$$



$$A\hat{x}_1 + \hat{x}_1 R_{11} = \hat{c}_1 \qquad (A + R_{11} I)\hat{x}_1 = \hat{c}_1$$

$$A\hat{x}_2 + \begin{bmatrix} \hat{x}_1 & \hat{x}_2 \end{bmatrix} \begin{bmatrix} R_{12} \\ R_{22} \end{bmatrix} = \hat{c}_2$$

$$A\hat{x}_2 + \hat{x}_2 R_{22} = \hat{c}_2 - \hat{x}_1 R_{12} \qquad \hat{x}_2 = \dots$$

$$\vdots$$

$$A\hat{x}_j + \hat{x}_j R_{jj} = \hat{c}_j - \sum_{k=1}^{j-1} \hat{x}_k R_{kj} \equiv \tilde{c}_j$$

$$(A + R_{jj} I)\hat{x}_j = \tilde{c}_j$$

Properties of Sylvester equations:

$\exists$ PROP (ROTH): $AX + XB = C$ admits a solution if and only if the two matrices

$\begin{pmatrix} A & -C \\ 0 & -B \end{pmatrix}$ and $\begin{pmatrix} A & 0 \\ 0 & -B \end{pmatrix}$ are similar. The similarity transformation is

$\begin{pmatrix} I & X \\ 0 & I \end{pmatrix}$ X solution to Sylv. equation

For discussing uniqueness, we need to introduce some tools and properties:

i) Kronecker operator: $A \in \mathbb{C}^{m_1 \times m_1}$, $B \in \mathbb{C}^{m_2 \times m_2}$

$$B \otimes A = \begin{pmatrix} b_{11} A & b_{12} A & \cdots & b_{1m_2} A \\ b_{21} A & b_{22} A & \cdots & b_{2m_2} A \\ \vdots & & \ddots & \\ b_{m_2 1} A & & \cdots & b_{m_2 m_2} A \end{pmatrix} \in \mathbb{C}^{m_1 m_2 \times m_1 m_2}$$

$B = (b_{ij})$

ex. $I \otimes A = \begin{pmatrix} A & & & \\ & A & & \\ & & \ddots & \\ & & & A \end{pmatrix}$, $A \otimes I = \begin{pmatrix} a_{11} I & a_{12} I & \cdots \\ & & \end{pmatrix}$

ii) $\text{vec}(\underbrace{[x_1 \dots x_m]}_{X \in \mathbb{C}^{m \times m}}) = \begin{pmatrix} \underline{x}_1 \\ \vdots \\ \vdots \\ \underline{x}_m \end{pmatrix}$ and $\text{vec}(AXB) = (B^T \otimes A)\,\text{vec}(X)$

↑ transposition

iii) $\lambda \in \text{spec}(A)$, $\mu \in \text{spec}(B) \Rightarrow$ • $\lambda \cdot \mu \in \text{spec}(A \otimes B)$

• $\lambda + \mu \in \text{spec}(I \otimes A + B \otimes I)$

$I \otimes A + B \otimes I$ is called Kronecker sum

PROP: thanks to the previous properties, solution X to $AX + XB = C$ is <u>unique</u> if and if $\lambda + \mu \neq 0$ for any $\lambda \in \text{spec}(A)$ and $\mu \in \text{spec}(B)$.

Proof: $\quad AX + XB = C \iff$

$$\underbrace{(I \otimes A + B^T \otimes I)}_{\mu+\lambda}\, x = c = \mathrm{vec}(C)$$

$\mathcal{A}\, x = c \qquad \mathcal{A}$ Kronecker form

$\#$

NOTE: the previous procedure used the complex Schur form, with $R \in \mathbb{C}^{s \times s}$

real form: $\quad B = Q R Q^T \qquad B \in \mathbb{R}^{s \times s}$

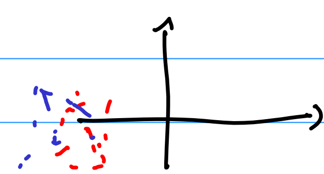
$$\begin{pmatrix} \square & \square & \square & & \\ & \square & \square & & \\ & & \square & & \\ & & & \ddots & \\ & & & & \square \end{pmatrix} \equiv R \text{ real !}$$

2x2 or 1x1

$\uparrow \mu, \bar{\mu}$

SOME CLOSED FORMS FOR THE SOLUTION MATRIX:

$$AX + XB = C$$



. Integral of exponents:

$$X = -\int_0^\infty e^{At}\, C\, e^{Bt}\, dt$$

. Finite power sum: Writing $C = C_1 C_2^T$, we have

$$X = \sum_{i=0}^{k_1-1} \sum_{j=0}^{k_2-1} \gamma_{ij} A^i C B^j$$

where k_1 is the degree of the minimal polynomial of A wrto C_1

k_2 is the degree of " " " of B wrto C_2

$$\varphi_A(A)C_1 = 0 \qquad \varphi_B(B)C_2 = 0$$

- Similarity transformations:

$$A = U\Lambda_A U^{-1}, \quad B = V\Lambda_B V^{-1} \Rightarrow X = U\hat{X}V^{-1}$$

λ_i $\qquad\qquad\qquad$ μ_j

where
$$\hat{x}_{ij} = \frac{(\underline{U^{-1}C}V)_{ij}}{\lambda_i + \mu_j}$$

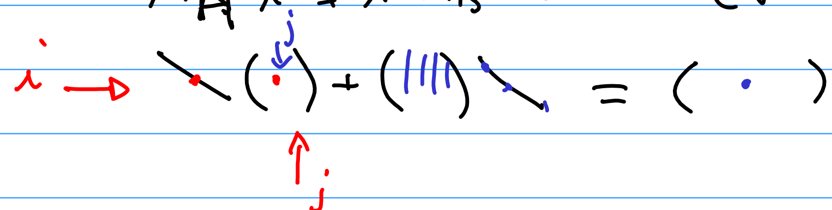
Indeed:

$$AX + XB = C$$

$$U\Lambda_A U^{-1}X + XV\Lambda_B V^{-1} = C$$

$$\Lambda_A \underbrace{U^{-1}XV}_{\hat{X}} + \underbrace{U^{-1}XV}_{\hat{X}}\Lambda_B = \underline{U^{-1}CV}$$

$$\Lambda_A\hat{X} + \hat{X}\Lambda_B = U^{-1}CV$$



$$\lambda_i \hat{x}_{ij} + \mu_j \hat{x}_{ij} = (U^{-1}CV)_{ij} \qquad \#$$

REMARK: Sylv. eqn equivalent to

$$(I \otimes A + B^T \otimes I)\, x = c \qquad \mathcal{A}\, x = c$$

A, B $m \times m$ $\qquad\qquad$ $m^2 \times m^2$

$m = 100$ $\qquad\qquad$ $m^2 = 10000$

(*) $AX + XA^T = C \implies \mathcal{A}\, x = c \implies \mathrm{vec}(X) = x$

↑ Lyapunov equation ($B = A^T$)

If C is symmetric $\implies$ X is symmetric in (*)

Indeed: transpose the eqn: $(AX)^T + (XA^T)^T = C^T$

$$X^T A^T + A \underbrace{X^T} = C$$

but solution is unique $\implies X^T = X$ $\qquad$ *

$$\mathcal{L} : X \longmapsto AX + XA^T \quad \text{symmetric}$$

If $C \geq 0$ and $A < 0$ (stable, $Re(\lambda_i(A)) < 0$)

$\implies X \geq 0$

REMARK: If $AX + XB = C$ $\qquad$ A, B large, sparse

If C is low rank, then X may be approximated by a low rank matrix.

$\mathrm{rank}(C) = p \ll m$ $\qquad\qquad$ $X \approx X_1 X_2^T = \left(\quad \right)\left(\qquad \right)$

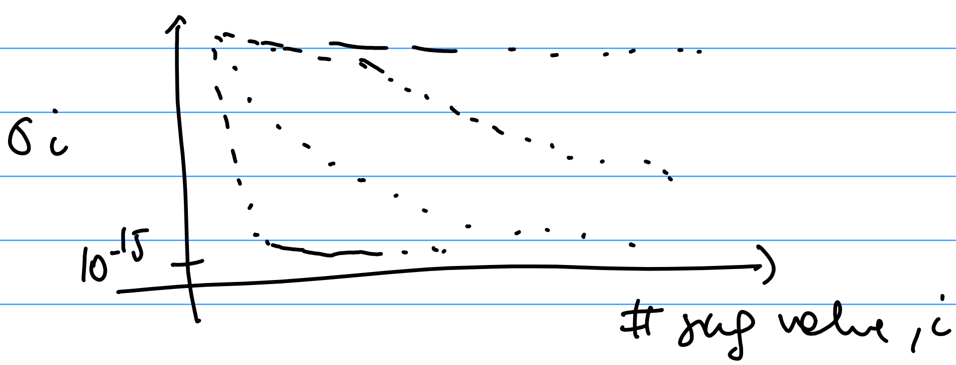
PROP: ~~For~~ A sym and $B = A$ and rank$(C) = p$, then

$$\frac{\sigma_{pr+1}}{\sigma_1} \lesssim 4 \exp\left(\frac{-\pi^2 r}{\log(4\kappa(A))} \right) \qquad 1 \le p \cdot r < n$$

$\kappa(A)$ condition number, $\kappa(A) = \frac{|\lambda_{max}|}{|\lambda_{min}|}$ and

σ_i are the singular values of X, solution to

$$AX + XA = C$$



$$X = U \Sigma V^T = U \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \sigma_3 & \\ & & & \ddots \end{pmatrix} V^T$$

10^{-15}

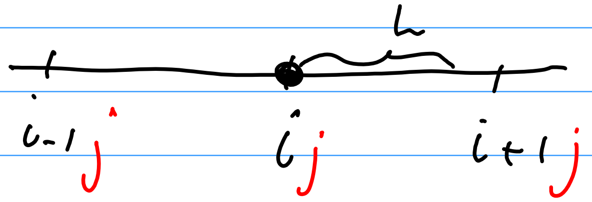
$$\approx [u_1, u_2] \begin{bmatrix} \sigma_1 & \\ & \sigma_2 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix}$$

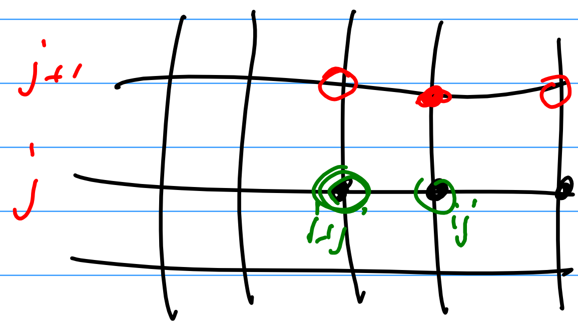
$\kappa(A) = \frac{\lambda_n}{\lambda_1}$ $\qquad \lambda_1 = 10^0 \longrightarrow \lambda_n = 10^{\text{condit}}$

May 26, 2021

$$AX + XB = C$$

See slides for the lecture





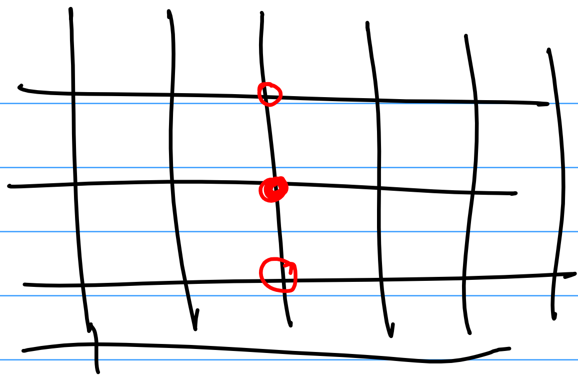
$$\begin{pmatrix} 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} u_{i-2,j} \\ u_{i-1,j} \\ u_{i,j} \\ u_{i+1,j} \end{pmatrix}$$

$$\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \end{pmatrix} \underbrace{\begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1m} \\ u_{21} & u_{22} & & u_{2m} \\ u_{31} & u_{32} & & \vdots \\ \vdots & \vdots & & \vdots \\ u_{n1} & \vdots & & \end{pmatrix}}_{U}$$

$$U \approx u(x_i, y_j)$$

$$T \cdot U$$

lexicographic ordering $\longrightarrow$ vec(U)



$$U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ u_{21} & & & \\ \vdots & & & \\ u_{n1} & & \cdots & u_{nn} \end{pmatrix}$$

$$u_{ij} \approx u(x_i, y_j)$$

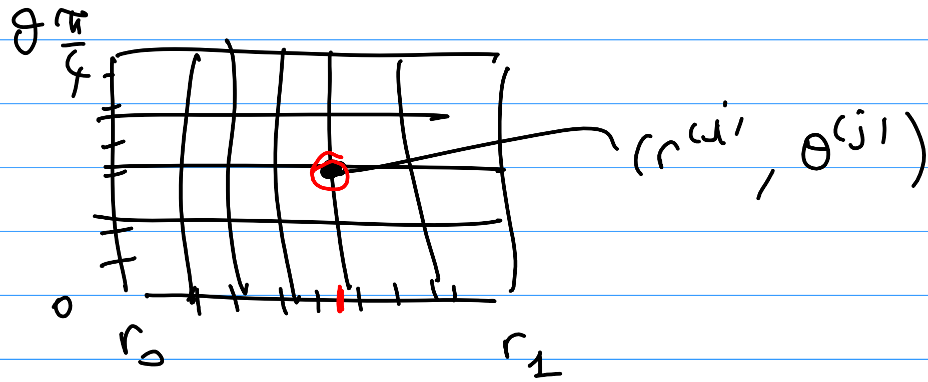
$$U \cdot \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & \ddots & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

$$100 \times 100 \quad \underbrace{T_1}_{x} U + U \underbrace{T_1^T}_{y} = F$$

$$\underbrace{(T_1 \otimes I + I \otimes T_1)\, u = \underline{f}}_{Au = f} = \mathrm{vec}(F)$$

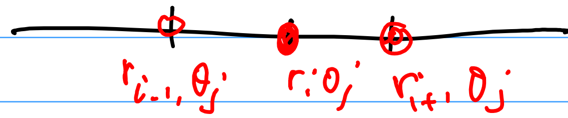
10 000

$r \longrightarrow \quad r^{(1)}, r^{(2)} \dots \quad r^{(m)}$



$$r^2 \tilde{u}_{rr} \rightsquigarrow \underbrace{\begin{pmatrix} r^{(1)} & & & \\ & r^{(2)} & & \\ & & \ddots & \\ & & & r^{(m)} \end{pmatrix}^2}_{\Phi^2} \underline{T \cdot \tilde{U}}$$

$$\Phi^2 T \tilde{U}$$



B

$$u_{r_i} \approx \frac{u_{r_{i+1}\theta_j} - u_{r_{i-1}\theta_j}}{2h} \approx \begin{pmatrix} 0 & 1 & & \\ -1 & 0 & 1 & \\ & -1 & 0 & 1 \end{pmatrix} \cdot U$$

if $u(x,y)$ sym

$\Longrightarrow$ U sym

$$\begin{vmatrix} -1 \\ 0 \\ +1 \end{vmatrix}$$

$$\frac{dy}{dt} = u' = u_{xx}$$

$$\underset{(x,y)}{A}X + X\underset{(t)}{B} = C$$

"All-at-once"

$$I - h_t A = h_t \underbrace{\left(\frac{1}{h_t} I - A \right)}_{\text{shifted linear system}}$$

$A \quad 10'000 \times 10'000$

$T \quad 100 \times 100$

$$e^{A+B} \neq e^{A} e^{B}$$

$$e^{T_2^T \otimes I + I \otimes T_1} = e^{T_2^T} \otimes e^{T_1}$$

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$$AX + XB = C$$

<u>DENSE APPROACH</u>: BARTELS-STEWART METHOD

$A = URU^*$, $B^* = VSV^*$ — R, S upper triang; U, V unitary

Schur decomp

$$U^*\left(URU^*X + XVS^*V^* = C \right)V$$

$$R\underbrace{U^*XV}_{\hat{X}} + \underbrace{U^*XV}_{\hat{X}}S^* = \underbrace{U^*CV}_{\hat{C}}$$

$$\to R\hat{X} + \hat{X}S^* = \hat{C} \qquad \hat{X} = [\hat{x}_1 \dots \hat{x}_n]$$

S_{nn}

$$R\hat{x}_n + S_{nn}\hat{x}_n = \hat{c}_n$$

$$(R + S_{nn}I)\hat{x}_n = \hat{c}_n$$

$$R\hat{x}_{n-1} + S_{n-1,n-1}\hat{x}_{n-1} + S_{n-1,n}\hat{x}_n = \hat{c}_{n-1}$$

$$(R + S_{n-1,n-1}I)\hat{x}_{n-1} = \dots$$

$$X = U\hat{X}V^* \to \text{real}$$

We used complex Schur decomposition

$\Rightarrow$ real Schur form $R = \begin{pmatrix} \square_{2\times 2} & & & & \\ & \square_{1\times 1} & & & \\ & & \square & & \\ & & & \square & \\ & & & & \square \ \ddots \end{pmatrix}$

S_{mm} 2×2

$$R\,[\hat{x}_{n-1}, \hat{x}_n] + [\hat{x}_{n-1}\ \hat{x}_n]\, \overset{2\times 2}{S_{n,n}} = \hat{C}_{n-1:n}$$

REMARK : $B = A^T$ $\quad AX + XA^T = C$ Lyapunov equ.

$A = URU^*$ cheaper than Sylvester

Matlab function lyap

REMARK : $\begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} X + X B = C = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$ $X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$

$$A_{11} X_1 + A_{12} X_2 + X_1 B = C_1 \leftarrow$$

$$A_{22} X_2 + X_2 B = C_2 \leftarrow \qquad \text{size}(A) \geq 2\,\text{size}(B)$$

$$\uparrow$$

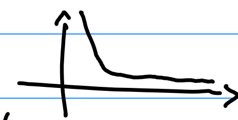
$$\begin{pmatrix} A_{33} & A_{34} \\ & A_{44} \end{pmatrix} \begin{pmatrix} x \\ x \end{pmatrix}$$

$$AX + XB = C \qquad A, B \text{ large and sparse}$$

We focus on the case C low rank $\quad \underline{\underline{C = C_1 C_2^T}}$

Even if A, B are sparse, $\Rightarrow X$ dense $\rightsquigarrow X \approx X_1 X_2^T$

PROJECTION METHODS :



C low rank $\Rightarrow$ X is "almost" low rank

Assume we have V_m, W_m with orth. columns, and we seek an approx x

$$X \approx X_m = V_m Y_m W_m^T$$

- m is not necessarily the dimension of Range (V_m) $\quad \leq m \cdot s$
- dim (V_m) is not necessarily the same as dim (W_m) $\quad W_k$

To determine Y_m, we impose a Galerkin condition :

$$R_m = C - AX_m - X_m B \rightsquigarrow r_m = c - (B^T \otimes I + I \otimes A) x_m$$

$$X_m = V_m Y W_m^T \rightsquigarrow x_m = \underbrace{(W_m \otimes V_m)}_{\text{basis}} y \qquad y = vec(Y)$$

Therefore, $\quad r_m = c - (B^T \otimes I + I \otimes A) \underline{(W_m \otimes V_m)} y$

$$r_m \perp \text{Range}(W_m \otimes V_m)$$

$$r_m \perp \underline{\text{Range}\,(W_m \otimes V_m)} \iff (W_m \otimes V_m)^T r_m = 0$$

$$\iff \underbrace{V_m^T R_m W_m = 0}$$

↑ Galerkin condition in matrix terms !

$$V_m^T \left(C - A V_m Y W_m^T - V_m Y W_m^T B \right) W_m = 0$$

$$\underbrace{(V_m^T A V_m)}_{H_{A,m}} Y + Y \underbrace{(W_m^T B W_m)}_{H_{B,m}} = \underbrace{V_m^T C W_m}_{C_m} \quad \leftarrow \text{REDUCED Pb.}$$

Solve with Bartels-Stewart method $\Rightarrow Y_m$

$$X_m = V_m Y_m W_m^T$$

$$(\;)(\;)(\;\;\;)$$

REMARK: $H_{A,m}$ and $-H_{B,m}$ have disjoint spectra to obtain a unique sol^n.

REMARK: $(B^T \otimes I + A \otimes I)\, x = c$ $\qquad$ A $n \times n$ $\quad B$ $m \times m$

$x_m \in \text{Range}(V_m) \subseteq \mathbb{R}^{n^2}$ $\qquad$ $n \gg 1000$, $n^2 \gg 10^6$

$$r_m = c - (B^T \otimes I + A \otimes I)\, x_m \qquad \underline{\underline{V_m^T r_m = 0}}$$

Galerkin: $r_m \perp \text{Range}(V_m)$

$$\overbrace{(B^T \otimes I + I \otimes A)}^{\mathcal{A}} x = \mathcal{C}$$

Preconditioning ! $\to K_m(P^{-1}\mathcal{A}, P^{-1}c)$

No preconditioning in $AX + XB = C$

$$P^{-1}AX + \underline{\underline{P^{-1}XB}} = P^{-1}C$$

$$P^{-1}AP\underbrace{P^{-1}X}_{\hat{X}} + P^{-1}XB = P^{-1}C$$

I How to choose the approximation spaces :

$C = C_1 C_2^T = (\,|\,)(\quad)$

We focus on the V_m space :

1990 (Y. Saad) $\quad K_m^{\square}(A, C_1) = \text{Range}([C_1, AC_1, \dots, A^{m-1}C_1])$

V_m spans this space $\quad W_m \to K_m^{\square}(B^T, C_2)$

$\Rightarrow$ Requires a large m to obtain good approx

Rational block Krylov subspaces:

$$K_m^R(A, C_1, \sigma) = \text{Range}\Big(\big[C_1, \underbrace{(A - \sigma_1 I)^{-1} C_1}, \dots, \prod_{j=1}^{m-1} (A - \sigma_j I)^{-1} C_1\big]\Big)$$

$\sigma = (\sigma_1, \sigma_2, \dots, \sigma_{m-1})$

2011

- I assumed $A < 0$ ($\text{eig}(A) \subset \mathbb{C}^-$), $\sigma_i \in \mathbb{C}^+$
- Cost of solving
- Choice of parameters $\{\sigma_j\}$

1. Fix σ_j's. Extended Krylov space

$$K_m^E(A, C) = \text{Range}\big([C_1, AC_1, A^{-1}C_1, A^2C_1, A^{-2}C_1 \dots]\big)$$

$$\underline{K_m^\square(A, C_1)} + K_m^\square(A^{-1}, A^{-1}C_1)$$

2007

this corresponds to K_m^R with $\sigma_1 = 0$, $\underline{\sigma_2 = +\infty}$

2. Fix $\sigma_j \equiv \sigma$, $\sigma = \lambda_{min}(A)$, $\sigma = -\sqrt{\lambda_{min}(A)\lambda_{max}(A)}$

3. In the case of A sym, $A < 0$, Lyapunov pb. the optimal shifts are obtained by solving the pb

$$\min_{\sigma_i \in \mathbb{C}^+} \max_{\lambda \in \text{spec}(A)} \prod_{j=1}^{m-1} \frac{|\lambda + \sigma_j|}{|\lambda - \sigma_j|}$$

Zolotaryov pb. it was solved by Zolotaryov for $\lambda \in [\lambda_{min}, \lambda_{max}]$

For complex spectrum

As an alternative, use a dynamic procedure to determine the next shift:

Assume $(A - sI)x = c$ $\qquad r_m = c - (A - sI)x_m$

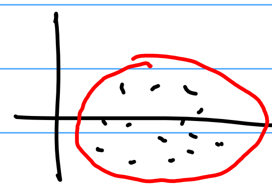
$$x_m \in K_m^R(A,c) \Rightarrow r_m(s) = \boxed{\frac{\varphi_m(A)c}{\varphi_m(s)}}$$

where $\varphi_m(z) = \prod_{j=1}^{m} \frac{z-\theta_j}{z-\sigma_j}$

$\{\theta_j\}$ are Ritz values $\quad$ eig$(V_m^T A V_m)$ $= H_m$

then

$$\sigma_m = \arg\left(\max_{\sigma \in \partial S_m} \frac{1}{|r_m(\sigma)|}\right)$$

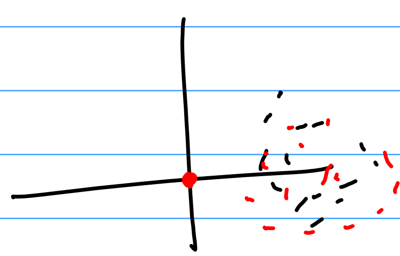


S_m is a region containing the eigs of A

REMARK $\qquad AX + XA^T = C \qquad A<0$

$$\underbrace{-A}_{>0}X + X(-A)^T = -C$$

REMARK



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May 28, 2021

$AX + XB = C$ large scale

$\uparrow$ x-dir $\uparrow$ y-dir C low rank

ADI (Alternating Direction Implicit iteration).

For simplicity, $C = C_1 C_1^T$, $B = A^T$ real arith

iteration $X_0 = 0$

$$\to \quad (A + \sigma_j I) X_{j-1/2} = -C_1 C_1^T - X_{j-1} (A^* - \sigma_j I)$$

$$\to \quad (A + \sigma_j I) X_j = -C_1 C_1^T - (X_{j-1/2})^T (A^* - \sigma_j I)$$

Originally proposed by Peaceman and Rachford

$Ax = c \iff (H + V)x = c$ $\quad H = I \otimes A$

$\uparrow$ x-dir $\uparrow$ y-dir $\quad V = A^T \otimes I$

(next step was Smith's method)

PROP: ADI with optimal parameters coincides with Galerkin method on rational Krylov space.

To be used for large problems, $X_j = Z_j Z_j^*$ so that the iteration becomes:

$$Z_1 = \sqrt{-2\sigma_1}\,(A^* + \sigma_1 I)^{-1} C_1 ; \qquad s = \text{rank}(C)$$

$$Z_{j+1} = [(A^* - \sigma_j I)(A^* + \sigma_j I)^{-1} Z_j, \underbrace{\sqrt{-2\sigma_j}(A^* + \sigma_j I)^{-1} C_1}_{s \text{ columns}}]$$

For ADI choice of shifts is more problematic

- Quasi-optimal shifts a-priori (Penzl)
- Hybrid procedure

Ellsner-Wachspress SINUM '91

CONVERGENCE : A sym, $A < 0$ ($\mathrm{eig}(A) < 0$)
Lyapunov eqn.

$\mathcal{A} x = c$ vs $AX + XA = C$

- CG for Kronecker form

$$\boxed{\|x^* - x_m\|_{\mathcal{A}} \le 2 \underbrace{\left(\frac{\sqrt{k}-1}{\sqrt{k}+1}\right)}^{m} \|x^* - x_0\|_{\mathcal{A}}}$$

x^* exact soln, $k = \mathrm{cond.}\#$ of $\mathcal{A}$ $\quad \|v\|_{\mathcal{A}}^2 = v^T \mathcal{A} v$

$\lambda_{\min}(\mathcal{A}) = \lambda_{\min} + \lambda_{\min} = 2\lambda_{\min}$ $\quad \lambda_{\max}(\mathcal{A}) = \lambda_{\max} + \lambda_{\max} = 2\lambda_{\max}$
$\lambda_{\min} = \lambda_{\min}(A)$, $\lambda_{\max} = \lambda_{\max}(A)$

$$\Rightarrow \quad k = \frac{2\lambda_{\max}}{2\lambda_{\min}} = \frac{\lambda_{\max}}{\lambda_{\min}} = \mathrm{Cond}(A)$$

- Matrix Galerkin ~~on~~ standard (polyn) Krylov :

$$\boxed{\|X^* - X_m\|_2 \le c \underbrace{\left(\frac{\sqrt{k_1}-1}{\sqrt{k_1}+1}\right)}^{m} \|X^* - X_0\|_2}$$

$k_1 = \mathrm{cond}\#$ of $A + \lambda_{\min} I$

- Matrix Galerkin with Extended Krylov space

$$\mathcal{K}(A, C_1) + \mathcal{K}(A^{-1}, A^{-1}C_1)$$

$$\|X^* - X_m\|_2 \lesssim c \cdot \left(\frac{\sqrt[4]{k}-1}{\sqrt[4]{k}+1}\right)^{2m} \qquad k = \mathrm{cond}(A)$$

- Matrix Galerkin with Rational Krylov space:

  A sym $\quad \mathrm{spec}(A) \subseteq \mathrm{disc}(c, 1)$

$$\overline{\lim_{m \to +\infty}} \|X^* - X_m\|^{\frac{1}{m}} \le \frac{2c^2 + c - 1 - (2c+1)\sqrt{c^2-1}}{c+1+\sqrt{c^2-1}}$$

REMARK: On approximate soln. rank:

$$X \approx X_m = V_m \underline{\underline{Y_m}} W_m^T \qquad \mathrm{rank}(V_m) = m \cdot s$$

$$\mathrm{rank}(X_m) \le ms$$

rank(Y_m) ?

If rank$(Y_m) \ll ms \Rightarrow$ you could represent the approx soln in a much smaller basis.

$$Y_m = U \Sigma V^T = (\ )(\ )(\ )$$

$$X_m = (V_m U) \Sigma (V^T W_m^T) \sim X$$

$$(\ )(\ )(\ )$$

$$A_1 X B_1 + A_2 X B_2 + \cdots + A_\ell X B_\ell = C \qquad \ell \geq 2$$

- CLASSICAL SOLN STRATEGY:

$$(B_1^T \otimes A_1 + B_2^T \otimes A_2 + \cdots + B_\ell^T \otimes A_\ell)\, x = c$$

$$\mathcal{A} x = c$$

- Special cases if the matrices have special structure:

$$\underbrace{AX + XA^T}_{} + NN^T X NN^T = C \qquad \ell = 3$$

N tall matrix

For instance, (P. Benner and co authors)

$$K(A, [C, N]), \quad K(A + NN^T, C)$$

Exploit the low rank by using Sherman-Morrison formula

$$NN^T X NN^T \rightsquigarrow (\underbrace{NN^T \otimes NN^T}_{\text{low rank}})\, x$$

$$[N \otimes N][N \otimes N]^T$$

(see my webpage)

- TRUNCATED CG IN MATRIX SETTING

Assume $\mathcal{A}$ is sym pos. def $\rightsquigarrow \mathcal{A}x = c$ CG

A_i $m\times m$ $\quad B_i$ $m\times m$

CG on $\mathcal{A}x = c$

$m \times m$

$$x_{k+1} = x_k + \alpha_k p_k \rightsquigarrow X_{k+1} = X_k + P_k \alpha_k$$

$$r_{k+1} = c - \mathcal{A} x_{k+1}$$

$$w_k = \mathcal{A} p_k \rightsquigarrow W_k = \sum_{i=1}^{\ell} A_i P_k B_i = \mathcal{L}(P_k)$$

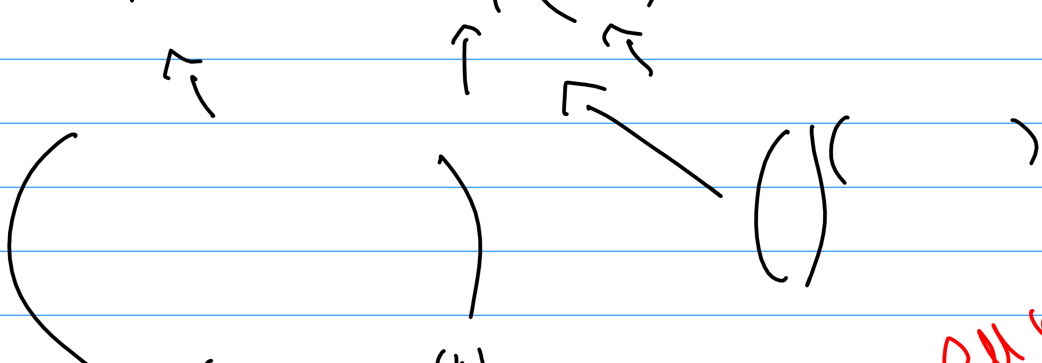
$$w_k = \cancel{\mathrm{vec}}(W_k)$$

SEE SLIDES:

$$\langle U, V\rangle = \underbrace{\mathrm{vec}(U)^T \mathrm{vec}(V)}_{?} = \mathrm{trace}(U^T V)$$

if C is low rank $\rightsquigarrow$ X low rank or well approx by low rank matrix

$$P^{(k)} \longrightarrow P_1^{(k)} (P_2^{(k)})^T$$



$$X^{(k+1)} = X^{(k)} + \omega_k P^{(k)}$$

$$= X_1^{(k)} (X_2^{(k)})^T + \omega_k P_1^{(k)} (P_2^{(k)})^T$$

$$= \left[X_1^{(k)}, P_1^{(k)} \right] \begin{bmatrix} I & \\ & \omega_k I \end{bmatrix} \begin{bmatrix} (X_2^{(k)})^T \\ (P_2^{(k)})^T \end{bmatrix}$$

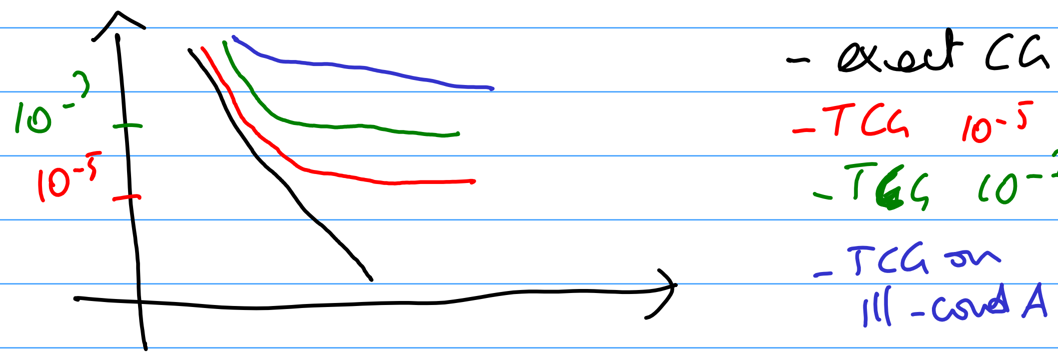
full rank?

$$X_1^{(k+1)} \cdot \left(X_2^{(k+1)}\right)^T \leftarrow \underbrace{\begin{bmatrix} X_1^{(k)}, & P_1^{(k)} \end{bmatrix}}_{\downarrow \text{ lower the rank}} \underbrace{\begin{bmatrix} I & \\ & \omega I \end{bmatrix} \begin{bmatrix} X_2^{(k)T} \\ P_2^{(k)T} \end{bmatrix}}_{\downarrow}$$

truncate $\downarrow$ $X_1^{(k+1)}$

truncate $\downarrow$ $X_2^{(k+1)}$

CAVEAT : After all these truncations, (convergence) properties of CG no longer hold



- PROJECTION METHODS : Apply Sylv. eqn. machinery to this case

$$X \sim X_m = V_m Y_m W_m^T$$

V_m: takes care of $\{A_i\}$; W_m^T: $\{B_i\}$

Galerkin condition : $R_m = C - \sum_{i=1}^{\ell} A_i X_m B_i$

$\iff V_m^T R_m W_m = 0$

$\iff \sum_{i=1}^{\ell} (\underline{V_m^T A_i V_m}) Y_m (W_m^T B_i W_m) = V_m^T C W_m$

TH: Galerkin still minimizes the error

$\Rightarrow$ How to choose V_m, W_m ???

1) $\{A_i\} \longrightarrow \{\hat{A}_i\}$: $\mathrm{spec}(\hat{A}_i) \subset I \quad \forall i$

V_m : $K_m(\hat{A}_1, C_1)$ Powell Silvester, VS

2) $AX + XA^T + MXM^T = C_1 C_1^T$ $\quad C_1$ vector

$$\mathrm{span}\{C_1, AC_1, MC_1, A^2C_1, MAC_1, AMC_1, M^2C_1, A^3C_1, MA^2C_1, \dots\}$$

$$\neq K(A, C_1) + K(M, C_1)$$

$$\mathcal{L}(X) \mapsto AX + XB$$

K. Meerbergen – H. Elman