Matrix functions and network analysis

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Linear boundary-value problems

Linear BVPs

$\begin{bmatrix} x \\ y \end{bmatrix} : [0, \infty] \to \mathbb{R}^{n+m}$;

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} x(t) \\ y(t) \end{bmatrix},$$

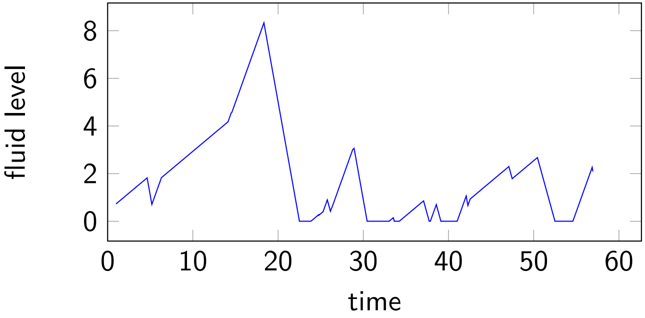
$$x(0) = x_0 \in \mathbb{R}^n, \quad \begin{bmatrix} x(t) \\ y(t) \end{bmatrix} \text{ bounded for } t \to \infty.$$

Linear, constant-coefficient ODE + ‘partial’ boundary conditions at 0 and ∞.

Application: fluid queues

Ingredients:

- $(n+m)$-state continuous-time Markov chain with rate matrix $Q \in \mathbb{R}^{(n+m)\times(n+m)}$.
  I.e., state transitions $i \to j$ may 'trigger' independently;
  $P[i \to j$ hasn't triggered yet after time $t] = \exp(-q_{ij}t)$.
- fluid that flows in/out of an infinite buffer at rate r_i in each state i.



Application: fluid queues [Rogers,'94]

Stationary distribution:

$u_i(x) = P$[being in state i with fluid level $\leq x$] satisfies

$$\mathrm{diag}(r)\frac{\mathrm{d}}{\mathrm{d}x}u(x) = Q^T u(x),$$
$$u_i(0) = 0 \text{ if } r_i > 0,$$
$$u(x) \text{ bounded for } x \to \infty \text{ (must have sum 1).}$$

(Q here has diagonal elements chosen so that $Qe = 0$, where e is the vector of all ones.)

Application: optimal control

Ingredients:

- Dynamical system $\frac{\mathrm{d}}{\mathrm{d}t}x(t) = Ax(t) + Mu(t)$ with $x(t) \in \mathbb{R}^n$ and input $u(t) \in \mathbb{R}^n$.
- Problem: choose $u(t)$ to 'reduce energy cost $x(t)^T Qx(t)$', but 'keeping $u(t)$ small':

$$\min \int_0^\infty (x(t)^T Qx(t) + u(t)^T u(t))\mathrm{d}t.$$

Optimal solution $x(t)$ and its Lagrange multiplier $\mu(t)$ satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} x(t) \\ \mu(t) \end{bmatrix} = \begin{bmatrix} A & -MM^T \\ -Q & -A^T \end{bmatrix} \begin{bmatrix} x(t) \\ \mu(t) \end{bmatrix},$$

$$x(0) \text{ given},$$

$$x(t), \mu(t) \text{ bounded for } t \to \infty.$$

Analytic solution

$$\begin{aligned}
\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} &= \exp\left(t \begin{bmatrix} A & B \\ C & D \end{bmatrix} \right) \begin{bmatrix} x_0 \\ y_0 \end{bmatrix} \\
&= \exp\left(tS \begin{bmatrix} J_1 & & \\ & \ddots & \\ & & J_k \end{bmatrix} S^{-1} \right) \begin{bmatrix} x_0 \\ y_0 \end{bmatrix} \\
&= S \begin{bmatrix} \exp(tJ_1) & & \\ & \ddots & \\ & & \exp(tJ_k) \end{bmatrix} S^{-1} \begin{bmatrix} x_0 \\ y_0 \end{bmatrix}
\end{aligned}$$

Which of these are bounded at ∞?

All entries of $S^{-1} \begin{bmatrix} x_0 \\ y_0 \end{bmatrix}$ which correspond to Jordan blocks with positive eigenvalues must be 0.

Analytic solution

All entries of $S^{-1}\begin{bmatrix}x_0\\y_0\end{bmatrix}$ which correspond to Jordan blocks with eigenvalues in the right half-plane

$$RHP = \{\lambda \in \mathbb{C} : \mathrm{Re}(\lambda) > 0\}$$

must be 0.

I.e., $\begin{bmatrix}x_0\\y_0\end{bmatrix} \in \mathcal{U}$, where

$$\mathcal{U} = \text{span(Jordan chains with eigenvalues in LHP)}.$$

$\mathcal{U}$ is known as stable invariant subspace.

Analytic solution

Let U be a basis matrix for $\mathcal{U}$:

$$\begin{bmatrix} x_0 \\ y_0 \end{bmatrix} = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} v_0 \quad \text{for some vector } v_0.$$

Recall: x_0 given by initial conditions, y_0 not.

The vector v_0, and hence the solution, is uniquely determined iff U_1 is square invertible.

Consequence 1 For the problem to be well-posed, $\begin{bmatrix} A & B \\ C & D \end{bmatrix}$ must have the exactly n eigenvalues in the LHP.
Often, this holds automatically in our applications because of matrix structures.

Consequence 2 To solve the problem, it is sufficient to compute U, a basis matrix for the stable invariant subspace.

Invariant subspaces

$\mathcal{U}$ known as invariant subspace because it is invariant:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \mathcal{U} \subseteq \mathcal{U}.$$

If U is a basis matrix for $\mathcal{U}$, then

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} U = UK$$

for a certain matrix K, whose eigenvalues are the stable eigenvalues of $\begin{bmatrix} A & B \\ C & D \end{bmatrix}$.

Stable solutions of the differential equation

$$\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = U \exp(Kt) v_0,$$

$v_0 \in \mathbb{R}^n$ chosen to satisfy initial condition.

Algorithms for the stable invariant subspace

Various families of algorithms, based on

- Manipulations of the Schur form, or
- Matrix functions such as $\mathrm{sign}(X)$, or
- Reformulation as a matrix equation.

The sign iteration [Higham, chapter 5]

Lemma

Suppose that $x_0 \in \mathbb{C}$ is not on the imaginary axis. Then, the iteration

$$x_{k+1} = \frac{1}{2}(x_k + x_k^{-1})$$

converges to 1 if $x \in RHP$, and -1 if $x \in LHP$.

Proof Define $y_k := \frac{x_k+1}{x_k-1}$. Then,

$$y_{k+1} = \frac{x_{k+1}+1}{x_{k+1}-1} = \frac{x_k + x_k^{-1} + 2}{x_k + x_k^{-1} - 2} = \frac{(x_k+1)^2}{(x_k-1)^2} = y_k^2.$$

$x_0 \in LHP \implies |x_0 - 1| > |x_0 + 1| \implies |y_0| < 1 \implies \lim y_k = 0 \implies \lim x_k = -1.$

$x_0 \in RHP \implies |y_0| > 1 \implies \lim y_k = \infty \implies \lim x_k = +1.$

The matrix sign iteration

Lemma

Whenever X_0 has no purely imaginary eigenvalues, the matrix iteration

$$X_{k+1} = \frac{1}{2}(X_k + X_k^{-1})$$

converges to $\operatorname{sign}(X_0)$.

Not obvious — we need x_k to be 'smooth enough' (as a rational function in x_0), because matrix functions involve derivatives as well.

(Alternative: make an analogous argument for matrices, setting $Y_k = (X_k - S)(X_k + S)^{-1}$, $S = \operatorname{sign}(X_0)$).

Sign iteration — the algorithm

1. Run the sign iteration on $X_0 = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ until convergence, obtaining S.
2. Compute $\mathcal{U} = \ker(S + I)$.

Caveat:

- It's best to rescale X_0 such that $\|X_0\| \approx 1$, as the iteration is faster there. Otherwise, "it's just an expensive way to divide by 2" [Higham].
- Need some care in the Markov chain application, because X_0 there is always singular. Solution: either shift the eigenvalue zero away, or use a variant (see following).

Structure preservation

The sign iteration (and variants) work well on 'hard' problems because they preserve structures.

Example In the control theory application,

$$X_0 = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \text{ is such that } JX_0 \text{ is symmetric, where } J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

(and actually that is the reason why it has the right number of stable eigenvalues).

Lemma

If JX_0 is symmetric, then in the sign iteration JX_k is symmetric for each $k \geq 0$.

Proof follows from $J^{-1} = J^T = -J$.

Another view on the sign iteration

1. Compute $Y_0 = (1 + X_0)(1 - X_0)^{-1}$
2. Square a sufficiently large number k of times:
   $Y_1 = Y_0^2,\ Y_2 = Y_1^2,\ \dots,\ Y_k = Y_{k-1}^2$

It is sort of a scaling and squaring algorithm to compute $\exp(2^k X_0)$.

$$\lim_{k\to\infty} \exp(2^k x_0) = \begin{cases} \infty & x_0 \in RHP, \\ 0 & x_0 \in LHP, \end{cases}$$

Y_k has the same eigenvectors of X_0; the eigenvalues of X_0 in the RHP are mapped to very large eigenvalues, and those in the LHP to very small eigenvalues.

We cannot implement the iteration working with the Y_i for reasons of (numerical) stability: all these very large/small numbers are not a good idea.

Structured doubling algorithm

[Chu-Fan-Lin '05], [Bini-Iannazzo-Meini, Ch. 5]

Idea

Work with 'LU-like' factorizations

$$Y_k = \begin{bmatrix} I & G_k \\ 0 & F_k \end{bmatrix}^{-1} \begin{bmatrix} E_k & 0 \\ H_k & I \end{bmatrix}.$$

Can we compute the factorization of Y_{k+1} from that of Y_k? Yes!

$$\begin{aligned} E_{k+1} &= E_k(I - G_k H_k)^{-1} E_k, \\ F_{k+1} &= F_k(I - H_k G_k)^{-1} F_k, \\ G_{k+1} &= G_k + E_k(I - G_k H_k)^{-1} G_k F_k, \\ H_{k+1} &= H_k + F_k(I - H_k G_k)^{-1} H_k E_k. \end{aligned}$$

Convergence

It's a sort of orthogonal iteration (generalized power method):

$$Y_0^{-2^k} \begin{bmatrix} 0 \\ I \end{bmatrix} = Y_k^{-1} \begin{bmatrix} I \\ 0 \end{bmatrix} = \begin{bmatrix} I \\ -H_k \end{bmatrix} E_k^{-1},$$

so $\operatorname{Im} \begin{bmatrix} I \\ -H_k \end{bmatrix} E_k^{-1}$ "converges" to the invariant subspace $\operatorname{Im} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$, i.e., $-H_k \to U_2 U_1^{-1}$.

Analogously, $\begin{bmatrix} -G_k \\ I \end{bmatrix}$ converges to a basis of the anti-stable invariant subspace (eigenvalues in RHP).

Structure preservation

Again, this algorithm is great at preserving structures.

Lemma

If X_0 is scaled suitably, then all the required inverses exist, at least one among E_k and F_k tends to zero, and

- In the control-theory problem, $E = F^T$, $G = G^T$, $H = H^T$; moreover $0 \preceq G_0 \preceq G_1 \preceq \dots$ and $0 \succeq H_0 \succeq H_1 \succeq \dots$ (positive definite ordering).
- In the queuing theory problem, $E, F \geq 0$; moreover, $0 \geq G_0 \geq G_1 \geq \dots$ and $0 \geq H_0 \geq H_1 \geq \dots$ (componentwise ordering).

Proof based on algebraic manipulations; we won't see it in full.

Reformulation as matrix equation

Another class of algorithms: via reformulation as a matrix equation.

Recall: $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$ basis for the invariant subspace, and we are assuming that $U_1 \in \mathbb{R}^{n \times n}$ is square invertible.

Hence we can change basis to $\begin{bmatrix} U_1 \\ U_2 \end{bmatrix} U_1^{-1} = \begin{bmatrix} I \\ U_2 U_1^{-1} \end{bmatrix}$.

Set $X = U_2 U_1^{-1} \in \mathbb{R}^{m \times n}$. Then, $\mathcal{U}$ stable invariant subspace $\iff$

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} I \\ X \end{bmatrix} = \begin{bmatrix} I \\ X \end{bmatrix} K$$

for some K with eigenvalues in the LHP.

Algebraic Riccati equation

[Bini-Iannazzo-Meini book], [CH Guo '01]

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} I \\ X \end{bmatrix} = \begin{bmatrix} I \\ X \end{bmatrix} K$$

implies $A + BX = K$, and

$$C + DX - XA - XBX = 0. \qquad (*)$$

(21) is known as algebraic Riccati equation.

Meta-theorem

In our two applications, many 'natural' matrix iterations converge monotonically when started from $X_0 = 0$.

(monotonically = in the positive definite ordering, or in the componentwise ordering.)

Basic iteration

We can set up a fixed-point iteration to solve the ARE, e.g.,

$$C + DX_{k+1} - X_{k+1}A - X_k B X_k = 0.$$

X_{k+1} solves the Sylvester equation

$$DX_{k+1} - X_{k+1}A = X_k B X_k - C.$$

$$\mathrm{vec}(X_{k+1}) = (I \otimes D - A^T \otimes I)^{-1} \mathrm{vec}(X_k B X_k - C).$$

In the queuing theory application, we shall see that $B \geq 0, -C \geq 0$, and $(I \otimes D - A^T \otimes I)^{-1} \geq 0$.

Under these conditions, one can prove by induction that $X_{k+1} \geq X_k$.

$$\mathrm{vec}(X_{k+1} - X_k) = (I \otimes D - A^T \otimes I)^{-1} \mathrm{vec}(X_k B X_k - X_{k-1} B X_{k-1}).$$

Structure in the queuing theory application

Q is such that $q_{ij} > 0$ for all $i \neq j$. $R = \begin{bmatrix} R_{11} & 0 \\ 0 & R_{22} \end{bmatrix}$ is diagonal and such that $\operatorname{diag}(R_{11}) > 0, \operatorname{diag}(R_2) < 0$.

Q, a continuous-time Markov chain, has an invariant measure, i.e., a vector $\pi = \begin{bmatrix} \pi_1 \\ \pi_2 \end{bmatrix} > 0$ such that $Q^T \pi = 0$.

Because of these signs, in

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = R^{-1} Q^T$$

- $B \geq 0$, $C \leq 0$
- D has $d_{ij} < 0$ for $i \neq j$
- $C\pi_1 + D\pi_2 = 0 \implies D\pi_2 \geq 0$, so D is an M-matrix
- $-A$ is an M-matrix (similarly).

M-matrices

Lemma

Let $M \in \mathbb{R}^{n\times n}$ be a matrix such that $m_{ij} < 0$ when $i \neq j$. Suppose that there is a vector $v > 0$ such that $Mv \geq 0$ (and $\neq 0$).
Then, $M^{-1} \geq 0$.

Proof: write $M = sI - P$, with $P \geq 0$. By the Perron-Frobenius theorem, P the largest eigenvalue of P has a positive left eigenvector z^T. Then, $z^T Pv \leq z^T sv$, hence $s \geq \rho(P)$ and we can use the Neumann series

$$(sI - P)^{-1} = s^{-1}(I - \frac{1}{s}P)^{-1} = s^{-1}\sum_{i\geq 0} s^{-i}P^i \geq 0.$$

Matrices M that satisfy this lemma are called (nonsingular) M-matrices.

Boundedness

Since the iteration $(X_k)_{k=0,1,2,\dots}$ is monotonic, it is sufficient to prove boundedness to get convergence.

Lemma

$X_k \pi_1 \leq \pi_2$ for $k = 0, 1, 2, \dots$.

Proof Induction! Multiply the iteration by π_1:

$$DX_{k+1}\pi_1 - X_{k+1}A\pi_1 = X_k B X_k \pi_1 - C\pi_1.$$

Rearrange, use $X_{k+1} \geq X_k$ and the blocks of $\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \pi_1 \\ \pi_2 \end{bmatrix} = 0$:

$$DX_{k+1}\pi_1 \leq X_k B\pi_2 + D\pi_2 - X_{k+1}B\pi_2 \leq D\pi_2$$

then multiply by $D^{-1} \geq 0$.

Further results

From here it is easy to show that $-K = -A - BX$ is an M-matrix, hence K has all eigenvalues in the LHP.

A more performant iteration:

Newton's method

$X_{k+1} = X_k + H$, where the correction H is chosen to have

$$C + D(X_k + H) - (X_k + H)A - (X_k + H)B(X_k + H) = O(\|H\|^2).$$

The correction H can be obtained by solving a Sylvester equation

$$(D - X_k B)H + H(-A - BX_k) = -C - DX_k + X_k A + X_k BX_k.$$

Converges quadratically if the root is simple, and has the same monotonicity properties.