Affine Iterations and Wrapping Effect: an Approach Based on the SVD

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Linear IIR filters

Linear Infinite Impulse Response filter

Let's consider a system with inputs u_n and states x_n at (discrete) time steps n ($n \in \mathbb{N}$).
Each state x_n depends linearly on the last inputs u_{n-l}, with $1 \leq l \leq L-1$ and also on the K previous states.

$$x_n = \sum_{k=0}^{K-1} a_k * x_{n-k} + \sum_{l=1}^{L-1} c_l * u_{n-l}$$

The problematic example: linear IIR filter

Linear Infinite Impulse Response filter

$u_n \in \boldsymbol{x}$ are the inputs of the system and x_n the states at time steps n.

$$x_n = 1.8 * x_{n-1} - 0.9 * x_{n-2} + 4.7.10^{-2} * (u_{n-2} + u_{n-1} + u_n)$$

Question: if the interval $\boldsymbol{u}$ is given for the u_n, determine an interval $\boldsymbol{x}$ containing every state x_n, for any n.
Preferably a small $\boldsymbol{x}$...
Here: $\boldsymbol{u} = [9.95\,,\, 10.05]$.

The problematic example: divergence of the interval simulation

$x_n = 1.8 * x_{n-1} - 0.9 * x_{n-2} + 4.7.10^{-2} * (u_{n-2} + u_{n-1} + u_n)$
with $\boldsymbol{u} = 9.95 + [0, 0.1]$
gives larger and larger intervals.
Even if it is asymptotically stable (the moduli of the roots of the characteristic polynomial are < 0.95)...
One can even prove the interval simulation diverges
(well, it converges to $[-\infty, +\infty]$).

The troublesome property

$$w(\boldsymbol{a} \pm \boldsymbol{b}) = w(\boldsymbol{a}) + w(\boldsymbol{b})$$

$$\begin{array}{rcl} x_n & = & 1.8 * x_{n-1} - 0.9 * x_{n-2} \\ & & +4.7.10^{-2} * (u_{n-2} + u_{n-1} + u_n) \end{array}$$

Let's consider the width of the intervals:

$$\begin{array}{rcl} w(x_n) & = & 1.8 * w(x_{n-1}) + 0.9 * w(x_{n-2}) \\ & & +4.7.10^{-2} * (w(u_{n-2}) + w(u_{n-1}) + w(u_n)) \end{array}$$

The recurrence satisfied by the widths diverges (the moduli of the roots of the characteristic polynomial are $\simeq 0.4$ and $\simeq 2.2$).

Another formulation matrix powers

$x_n = 1.8 * x_{n-1} - 0.9 * x_{n-2} + 4.7.10^{-2} * (u_{n-2} + u_{n-1} + u_n)$
can also be written as

$$\begin{pmatrix} x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -0.9 & 1.8 \end{pmatrix} \times \begin{pmatrix} x_{n-2} \\ x_{n-1} \end{pmatrix} + \begin{pmatrix} 0 \\ 0.047 * 3 * \boldsymbol{u} \end{pmatrix}$$

A first solution

$\rho(A) \simeq 0.94$ whereas $\rho(|A|) \simeq 2.2$
$\rho(A^2) \simeq 0.90$ whereas $\rho(|A^2|) \simeq 3.5$
$\rho(A^3) \simeq 0.85$ whereas $\rho(|A^3|) \simeq 4.4$
$\rho(A^4) \simeq 0.81$ whereas $\rho(|A^4|) \simeq 4.8$
$\rho(A^5) \simeq 0.77$ whereas $\rho(|A^5|) \simeq 4.7$
$\rho(A^6) \simeq 0.73$ whereas $\rho(|A^6|) \simeq 4.2$
$\rho(A^7) \simeq 0.69$ whereas $\rho(|A^7|) \simeq 3.4$
$\rho(A^8) \simeq 0.66$ whereas $\rho(|A^8|) \simeq 2.3$
$\rho(A^9) \simeq 0.62$ whereas $\rho(|A^9|) \simeq 1.3$
$\rho(A^{10}) \simeq 0.59$ whereas $\rho(|A^{10}|) \simeq 0.78$
$\rho(A^{19}) \simeq 0.63$ whereas $\rho(|A^{19}|) \simeq 0.37$
and $\forall k \geq 19$, $\rho(|A^k|) < 1$.

Interpretation

Computing every 10 (or 19) time steps with A^{10} (or A^{19}) as the matrix of the recurrence can be simulated using interval arithmetic! In other words, the time step should be 10 (or 19) times larger.

Another formulation matrix powers

$x_{n+1} = \sum_{k=0}^{K-1} a_k * x_{n-k} + \sum_{l=0}^{L-1} c_l * u_{n-l}$ can also be written as

$$\begin{pmatrix} x_{n-K+2} \\ \vdots \\ x_{n+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \dots & \dots & 0 \\ 0 & 0 & 1 & 0 & & 0 \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & \dots & \dots & 0 & 1 \\ a_{K-1} & a_{K-2} & \dots & \dots & a_1 & a_0 \end{pmatrix} \times \begin{pmatrix} x_{n-K+1} \\ \vdots \\ x_n \end{pmatrix}$$

$$+ \begin{pmatrix} 0 \\ \vdots \\ 0 \\ c^t.\boldsymbol{u} \end{pmatrix}$$

State of the art
convergence of interval matrix powers

- **Formalism:** $\boldsymbol{x}_{n+1} = \boldsymbol{A}.\boldsymbol{x}_n + \boldsymbol{b}$.
- **Problem: convergence of A^k** where A is the matrix defining the recurrence.
- **Mayer and Warnke 2003, Guu and Pang 2004:** divergence when $\rho(|A|) > 1$, even when $\rho(A) < 1$: stable filter.

Solution: general case

Theorem

There exists a index k_0 such that, $\forall k \geq k_0$, A^k satisfies
$\rho(|A^k|) < 1$,
which ensures the convergence of the simulation using interval arithmetic.

Choice of k_0?

Current method:

compute A^k and $\rho(|A^k|)$ until it is < 1, then choose this k as the time step.

Problem:

there exists no formula to deduce k_0 from the coefficients of A.

Agenda

The considered problem: $x_{n+1} = Ax_n + b$

Let A be an $d \times d$ matrix, $x_0 \in \mathbb{R}^d$, $b \in \mathbb{R}^d$.
Problem: compute the iterates

$$x_{n+1} = Ax_n + b,\ x_0 \text{ given}$$

Variants:

- **let x_0 and b be known with uncertainties: $x_0 \in \boldsymbol{x}_0$, $b \in \boldsymbol{b}$, compute $\boldsymbol{x}_{n+1} = A\boldsymbol{x}_n + \boldsymbol{b}$,**
- account for roundoff errors,
- let A be known with uncertainties: $A \in \boldsymbol{A}$.

Ubiquity of the Wrapping Effect (after Lohner, 2001)

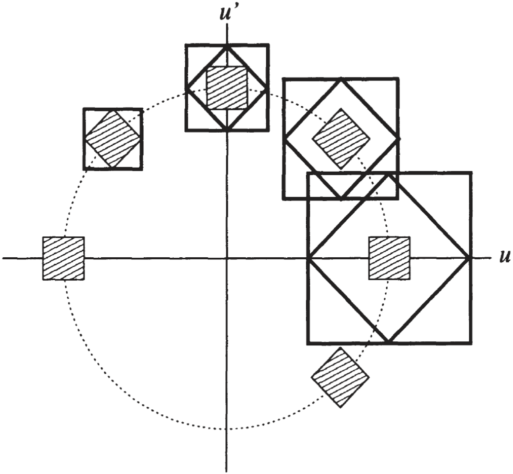


Figure 1: Wrapping effect for the harmonic oscillator.

Ubiquity of the Wrapping Effect (after Lohner, 2001)

Where does the Wrapping Effect appear?

- matrix-vector iterations: $\mathbf{x}_{n+1} = A_n \mathbf{x}_n + b_n,\ \mathbf{x}_0 \in I\!R^n$;
- discrete dynamical systems: $\mathbf{x}_{n+1} = f(\mathbf{x}_n)$, $\mathbf{x}_0$ given and f sufficiently smooth;
- continuous dynamical systems (ODEs): $x'(t) = g(t, x(t))$, $x(0) = x_0$, which is studied through a numerical one step method (or more) of the kind $\mathbf{x}_{n+1} = \mathbf{x}_n + h\Phi(\mathbf{x}_n, t_n) + \mathbf{z}_{n+1}$;
- difference equations: $a_0 \mathbf{z}_n + a_1 \mathbf{z}_{n+1} + \ldots + a_m \mathbf{z}_{n+m} = b_n$ with $\mathbf{z}_0, \ldots \mathbf{z}_m$ given;
- linear systems with (banded) triangular matrix;
- automatic differentiation.

The matrix-vector iteration is archetypal of the wrapping effect in all of these cases.

Agenda

Coordinate transformations

Well-known problem with the power method: $\boldsymbol{x}_n$ becomes aligned with the eigenvector corresponding to the largest eigenvalue (in module).

Principle: replace

$$\boldsymbol{x}_{n+1} = A\boldsymbol{x}_n + \boldsymbol{b}$$

by

$$\begin{array}{rcl} \boldsymbol{x}_{n+1} & = & B\boldsymbol{y}_{n+1} \\ \boldsymbol{y}_{n+1} & = & B^{-1}AB\boldsymbol{y}_n + B^{-1}\boldsymbol{b} \end{array}$$

Choice of B?

Discussion: better choose an orthogonal transformation.

QR-preconditioning

Principle: Factor A as $A = QR$ with Q orthogonal : $Q^{-1} = Q^T$,and R upper triangular.

In

$$x_{n+1} = Ax_n + b$$

replace x_n by

$$\begin{cases} x_n & = & Qy_n \\ \boldsymbol{y}_{n+1} & = & RQ\boldsymbol{y}_n + Q^T\boldsymbol{b} \end{cases} \Leftrightarrow y_n = Q^T x_n \text{ and thus } \boldsymbol{y}_n = Q^T \boldsymbol{x}_n$$

QR-preconditioning

Iteration:

$$\begin{cases} \mathbf{y}_n & = & Q^T \mathbf{x}_n \\ \mathbf{y}_{n+1} & = & RQ\mathbf{y}_n + Q^T \mathbf{b} \end{cases}$$

Theoretical results:

$$\begin{array}{rcl} w(\mathbf{y}_n) & \leq & \mathrm{cond}(Q^T P)^n \rho(A)^n w(\mathbf{y}_0) \\ & & + \frac{\mathrm{cond}(Q^T P)^{n-1} \rho(A)^{n-1} - 1}{\mathrm{cond}(Q^T P)\rho(A) - 1} w(\mathbf{b}) \\ & & + |Q^T| w(\mathbf{b}) \end{array}$$

where A diagonalizable: $A = P \Lambda P^{-1}$.

SVD-preconditioning

(idea also present in Beaumont, 2000)

Idea: choose B which is orthogonal and iterate with BA.

Principle: Factor A as $A = UDV^T$ with U and V orthogonal, and D diagonal.

In

$$x_{n+1} = Ax_n + b$$

replace x_n by

$$\left\{ \begin{array}{lcl} x_n & = & Uy_n \\ \boldsymbol{y}_{n+1} & = & U^T AU\boldsymbol{y}_n + U^T\boldsymbol{b} \end{array} \right. \Leftrightarrow y_n = U^T x_n \text{ and thus } \boldsymbol{y}_n = U^T \boldsymbol{x}_n$$

Similarly, *SVD*-preconditioning

Principle: U and V play similar roles, choose V:
Factor A as $A = UDV^T$ with U and V orthogonal, and D diagonal.

In

$$x_{n+1} = Ax_n + b$$

replace x_n by

$$\left\{ \begin{array}{lcl} x_n & = & Vy_n \\ \mathbf{y}_{n+1} & = & V^T A V \mathbf{y}_n + V^T \mathbf{b} \end{array} \right. \Leftrightarrow y_n = V^T x_n \text{ and thus } \mathbf{y}_n = V^T \mathbf{x}_n$$

SVD-preconditioning

Iteration:

$$\left\{ \begin{array}{lcl} x_n & = & U y_n \\ \boldsymbol{y}_{n+1} & = & DVU^T \boldsymbol{y}_n + U^T \boldsymbol{b} \end{array} \right. \Leftrightarrow y_n = U^T x_n \text{ and thus } \boldsymbol{y}_n = U^T \boldsymbol{x}_n$$

Theoretical results:

$$\begin{array}{rcl} w(\boldsymbol{y}_n) & \leq & (\mathrm{cond}(P) d \rho(A)))^n E w(\boldsymbol{y}_0) \\ & & + \frac{(\mathrm{cond}(P) d \rho(A))^{n-1} - 1}{\mathrm{cond}(P) d \rho(A) - 1} \| w(\boldsymbol{b}) \| e \\ & & + \| w(\boldsymbol{b}) \| e \end{array}$$

where A $d \times \boldsymbol{d}$ diagonalizable: $A = P \Lambda P^{-1}$,
E the matrix of 1s and e the vector of 1s.

Classical approach: Lohner's QR-preconditioning

(after Lohner, and Nedialkov&Jackson, 2001)

Principle: at each step, perform a QR factorization.

In

$$x_{n+1} = Ax_n + b$$

replace x_n by

$$\left\{ \text{with the factorization} \quad \begin{array}{lcl} x_n & = & Q_n y_n \qquad\qquad \Leftrightarrow y_n = Q_n^T x_n \\ B_n & = & Q_n R_n \\ B_{n+1} & = & R_n Q_n \\ \boldsymbol{y}_{n+1} & = & B_{n+1} \boldsymbol{y}_n + Q_n^T \boldsymbol{b} \end{array} \right.$$

with $Q_0 R_0 = A$.

Classical approach: Lohner's QR-preconditioning

(after Lohner, and Nedialkov&Jackson, 2001)

Iteration:

$$\left\{ \begin{array}{lrcl} \text{with the factorization} & B_n & = & Q_n R_n \\ & B_{n+1} & = & R_n Q_n \\ & \boldsymbol{y}_{n+1} & = & B_{n+1} \boldsymbol{y}_n + Q_n^T \boldsymbol{b} \end{array} \right.$$

Theoretical results:

$$\begin{array}{rcl} w(\boldsymbol{y}_n) & \leq & \mathrm{cond}(Q^T P) \rho(A)^n w(\boldsymbol{y}_0) \\ & & + \frac{\mathrm{cond}(Q^T P)\rho(A)^{n-1} - 1}{\mathrm{cond}(Q^T P)\rho(A) - 1} w(\boldsymbol{b}) \\ & & + |Q^T| w(\boldsymbol{b}) \end{array}$$

where A diagonalizable: $A = P \Lambda P^{-1}$.

Agenda

Iterations and Wrapping Effect
- Brief history

Two preconditionings
- QR
- SVD
- Lohner' QR

Experimental results

Conclusion
- Conclusion and future work
- References

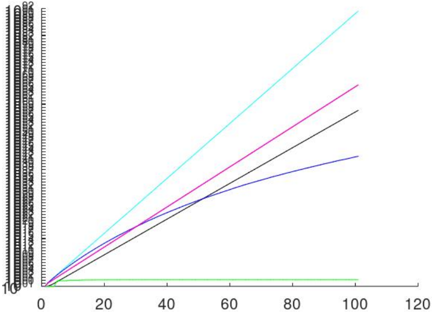
Experimental setup

Software: Octave with the interval package.
(Not shown here: similar results with Matlab and Rump's Intlab, even with affine arithmetic.)

Matrices:

- matrix with a prescribed condition number e^{κ}:
  `A=gallery("randsvd",d,exp(kappa));`
- unscaling: A is replaced by $D.A.D^{-1}$ where D is diagonal, with elements varying from 10 to 10^s (s is the scaling factor);
- usually such unscaling degrades the previously prescribed condition number.

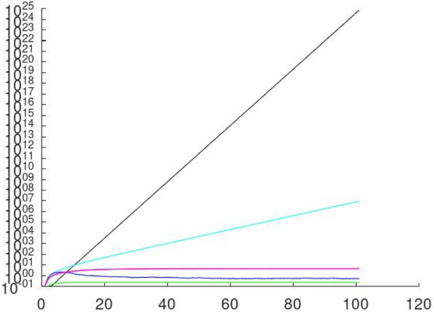
Well-conditioned and well-scaled matrix
A 100 × 100, 100 **iterates**, $kappa = 2$, $s = 2$



$\rho(A) \simeq 0.554$, $\rho(|A|) \simeq 3.955$, $\mathrm{cond}(A) \simeq 370$, $\mathrm{cond}(P) \simeq 350$.
In black: "bare" iterations, in green: k-power with $k = 4$, in cyan: QR, in blue: Lohner's QR, in red and magenta: SVD.

Ill-conditioned and well-scaled matrix

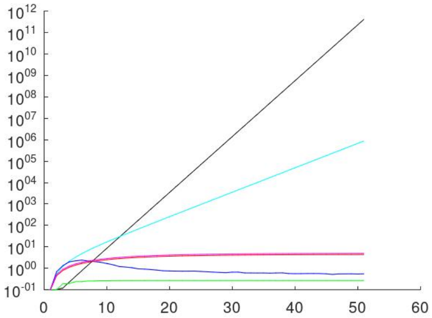
A 100×100, 100 **iterates**, *kappa* $= 10$, $s = 2$



$\rho(A) \simeq 0.208$, $\rho(|A|) \simeq 1.808$, $\mathrm{cond}(A) \simeq 6\,10^5$, $\mathrm{cond}(P) \simeq 10^3$.
In black: "bare" iterations, in green: k-power with $k = 2$, in cyan: QR, in blue: Lohner's QR, in red and magenta: SVD.

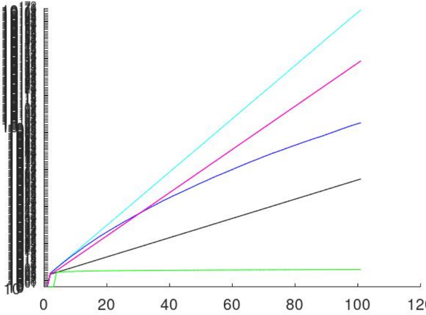
Ill-conditioned and well-scaled matrix

A 100×100, 50 **iterates**, $kappa = 10$, $s = 2$



$\rho(A) \simeq 0.208$, $\rho(|A|) \simeq 1.808$, $\mathrm{cond}(A) \simeq 6\ 10^5$, $\mathrm{cond}(P) \simeq 10^3$.
In black: "bare" iterations, in green: k-power with $k = 2$, in cyan: QR, in blue: Lohner's QR, in red and magenta: SVD.

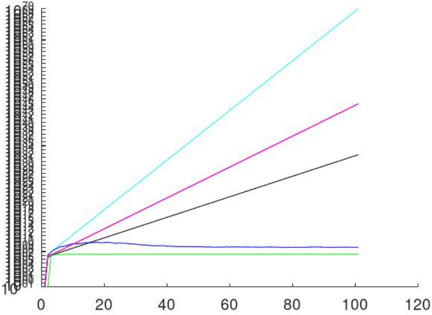
Well-conditioned and ill-scaled matrix
A 100×100, 100 **iterates**, $kappa = 2$, $s = 10$



$\rho(A) \simeq 0.527$, $\rho(|A|) \simeq 3.968$, $\mathrm{cond}(A) \simeq 6\ 10^{17}$, $\mathrm{cond}(P) \simeq 10^{10}$.
In black: "bare" iterations, in green: k-power with $k = 3$, in cyan: QR, in blue: Lohner's QR, in red and magenta: SVD.

Ill-conditioned and ill-scaled matrix

A 100 × 100, 100 **iterates**, $kappa = 10$, $s = 10$



$\rho(A) \simeq 0.223$, $\rho(|A|) \simeq 1.828$, $\mathrm{cond}(A) \simeq 2\,10^{21}$, $\mathrm{cond}(P) \simeq 10^{11}$.
In black: "bare" iterations, in green: k-power with $k = 2$, in cyan: QR, in blue: Lohner's QR, in red and magenta: SVD.

Comparison of the different methods large number of iterations ($n = 100$)

	well-scaled	**ill-scaled**
well-conditioned	LQR $\gg$ brut $>$ SVD $\gg$ QR	brut $>$ LQR $>$ SVD $>$ QR
ill-conditioned	LQR $>$ SVD $\gg$ QR $\gg$ brut	LQR $>$ brut $>$ SVD $>$ QR

brut = no preconditioning - LQR = Lohner's QR - SVD = one of the SVD preconditioning - QR = QR preconditioning

Comparison of the different methods small number of iterations ($10 \geq n \geq 20$)

	well-scaled	**ill-scaled**
well-conditioned	brut $>$ SVD $>$ LQR $>$ QR	brut $>$ SVD $>$ LQR $>$ QR
ill-conditioned	LQR $\simeq$ SVD $>$ QR $>$ brut	brut $>$ SVD $\simeq$ LQR $>$ QR

brut = no preconditioning - LQR = Lohner's QR - SVD = one of the SVD preconditioning - QR = QR preconditioning

Comparison of the different methods

- when the naïve method works best: use it, it is the cheapest one (well-conditioned matrices);
- when the matrix is ill-conditioned and well-scaled: Lohner's QR and SVD give the best results, however
  - each iteration of Lohner's QR requires $\mathcal{O}(d^3)$ operations $\Rightarrow \mathcal{O}(n.d^3)$ operations in total,
  - SVD requires one SVD factorization: $\mathcal{O}(d^3)$ operations, then each iteration needs $\mathcal{O}(d^2)$ operations only, thus $\Rightarrow \mathcal{O}(d^3 + n.d^2)$ operations in total;
- when the matrix is ill-conditioned and ill-scaled: Lohner's QR is the method of choice.

Agenda

Conclusion

Problem: matrix-vector iteration compute $x_{n+1} = Ax_n + b$ with uncertainty on $\boldsymbol{x}_n$ and $\boldsymbol{b}$.

Difficulty: wrapping effect.

Considered solutions:

- determine k such that A^k gives no difficulty with interval arithmetic: $\rho(|A^k|) < 1$;
- orthogonal coordinate transformation: using QR or SVD.

Experimental results:

- divergence except for the "k-power" method,
- when the matrix is well-conditioned: do not use anything sophisticated;
- when the matrix is ill-conditioned and well-scaled: Lohner's QR and SVD give the best results, SVD is cheaper;
- when the matrix is ill-conditioned and ill-scaled: Lohner's QR

Future work

- compare more thoroughly with affine arithmetic;
- investigate more properties of SVD decomposition, to get a nice theoretical bounds (as the one for Lohner's QR);
- expand the set of test matrices, use real-life ones:
  - taken from the integration of ODEs: $A = I + hB$ with h small,
  - taken from real-life control theory: A companion, take benefit from the zeros
- experiment with interval matrix A
- experiment with the numerical quality of the SVD, with certified SVD (van der Hoeven&Yakoubsohn, 2018)

References 1/3

Software: Octave and interval package from Oliver Heimlich.
Also used, but more anecdotically (for the time being): Intlab, the Matlab package by Siegfried Rump.

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