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A Schur–Padé Algorithm for Fractional Powers of a Matrix

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Joint work with Lijing Lin

Dynamical Systems, Control and Optimization
Paul Van Dooren 60
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MATLAB: Exponentiation

```
>> A = [1 2; 1 1];

>> 2.^A
ans =
       2       4
       2       2

>> 2^A
ans =
   3.0404e+000   3.2384e+000
   1.6192e+000   3.0404e+000

>> expm( log(2)*A )
ans =
   3.0404e+000   3.2384e+000
   1.6192e+000   3.0404e+000
```

MATLAB: Fractional Powers

```
>> A = [1 1e-8; 0 1]
A =
   1.0000e+000   1.0000e-008
             0   1.0000e+000

>> A^0.1
ans =
      1     0
      0     1

>> expm(0.1*logm(A))
ans =
   1.0000e+000   1.0000e-009
             0   1.0000e+000
```

MATLAB: Integer Powers

```
>> e = 1e-1; A = [1 1+e; 1-e 1]
A =
    1.0000    1.1000
    0.9000    1.0000

>> X = A^(-3); Y = inv(A)^3;

>> Z = double(vpa(A)^(-3));
>> norm(X-Z,1)/norm(Z,1), norm(Y-Z,1)/norm(Z,1)
ans =
  1.2412e-009
ans =
  6.6849e-016
```

Arbitrary Power

Definition

For $A \in \mathbb{C}^{n\times n}$ with no eigenvalues on $\mathbb{R}^-$ and $p \in \mathbb{R}$, $A^p = e^{p \log A}$, where $\log A$ is the principal logarithm.

$$A^p = \frac{\sin(p\pi)}{p\pi} A \int_0^\infty (t^{1/p} I + A)^{-1} \, dt, \qquad p \in (0,1).$$

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Applications:

- Pricing American options (Berridge & Schumacher, 2004).
- Finite element discretizations of fractional Sobolev spaces (Arioli & Loghin, 2009).
- Computation of geodesic-midpoints in neural networks (Fiori, 2008).

Email from a Power Company

The problem has arisen through proposed methodology on which the company will incur charges for use of an electricity network.

$\vdots$

I have the use of a computer and Microsoft Excel.

$\vdots$

I have an Excel spreadsheet containing the transition matrix of how a company's [Standard & Poor's] credit rating changes from one year to the next. I'd like to be working in eighths of a year, so the aim is to find the ***eighth root of the matrix****.*

HIV to Aids Transition

- Estimated 6-month transition matrix.
- Four AIDS-free states and 1 AIDS state.
- 2077 observations (Charitos et al., 2008).

$$P = \begin{bmatrix} 0.8149 & 0.0738 & 0.0586 & 0.0407 & 0.0120 \\ 0.5622 & 0.1752 & 0.1314 & 0.1169 & 0.0143 \\ 0.3606 & 0.1860 & 0.1521 & 0.2198 & 0.0815 \\ 0.1676 & 0.0636 & 0.1444 & 0.4652 & 0.1592 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Want to estimate the **1-month transition matrix**.

$$\Lambda(P) = \{1, 0.9644, 0.4980, 0.1493, -0.0043\}.$$

N. J. Higham and L. Lin.
On *p*th roots of stochastic matrices, LAA, 2010.

Basic Idea

Assume $p \in (-1, 1)$, A has no nonpositive real ei'vals.

- For suitable p, write

$$\boxed{A^p = (A^{1/2^k})^{p \cdot 2^k}} \equiv (I - X)^{p \cdot 2^k}.$$

- Choose suitable Padé approximant $r_m(x)$ to $(1 - x)^p$.
- Compute $r_m(X)^{2^k}$.

Questions:

- Existence of r_m.
- Choice of k and m.
- How to evaluate r_m.
- How to handle general $p \in \mathbb{R}$ $(A^{3.4} = A^3 A^{0.4} = A^4 A^{-0.6})$.

Evaluating r_m

$$r_m(x) = 1 + \cfrac{c_1 x}{1 + \cfrac{c_2 x}{1 + \cfrac{c_3 x}{\cdots \cfrac{}{1 + \cfrac{c_{2m-1} x}{1 + c_{2m} x}}}}},$$

$$c_1 = -p, \quad c_{2j} = \frac{-j+p}{2(2j-1)}, \quad c_{2j+1} = \frac{-j-p}{2(2j+1)}, \quad j = 1, 2, \ldots .$$

Bottom-up evaluation:

$Y_{2m} = c_{2m} X$
for $j = 2m-1\colon -1\colon 1$
    Solve $(I + Y_{j+1}) Y_j = c_j X$ for Y_j
end
$r_m = I + Y_1$

Choice of m

Variation of result of Kenney & Laub (1989).

Theorem (H & Lin, 2010)

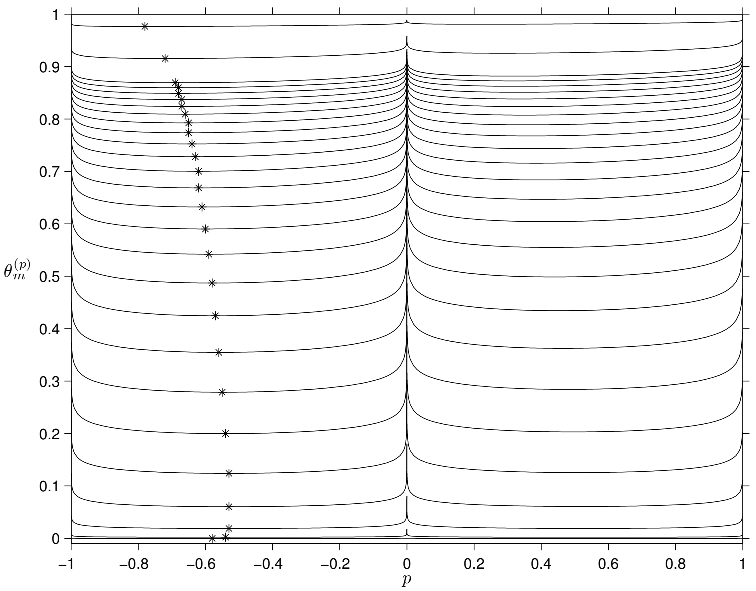
For $p \in (-1,1)$ and $\|X\| < 1$,

$$\|(I-X)^p - r_m(X)\| \le |(I - \|X\|)^p - r_m(\|X\|)|.$$

Let

$$\theta_m^{(p)} := \max\{\, \|X\| : |(I - \|X\|)^p - r_m(\|X\|)| \le u \,\}.$$

$\theta_m^{(p)}$ for $p \in (-1, 1)$, $m \in [1, 64]$



Strategy

- Initial Schur decomposition.
- Keep taking square roots until $\|I - T^{1/2^k}\| \le \theta_7 = 0.279$.

  Logic based on

  $$\|I - T^{1/2}\| = \|(I + T^{1/2})^{-1}(I - T)\| \approx \tfrac{1}{2}\|I - T\|.$$

- Squaring phase forms $r_m(T^{1/2^k})^{2^j} \approx (I - T^{1/2^k})^{p/2^{k-j}}$, $j = 1\colon k$.
  - Compute diagonal and first superdiagonal **exactly!**

Diag and Superdiag

$$F = \begin{bmatrix} \lambda_1 & t_{12} \\ 0 & \lambda_2 \end{bmatrix}^p = \begin{bmatrix} \lambda_1^p & t_{12}(\lambda_2^p - \lambda_1^p)/(\lambda_2 - \lambda_1) \\ 0 & \lambda_2^p \end{bmatrix}.$$

Diag and Superdiag

$$F = \begin{bmatrix} \lambda_1 & t_{12} \\ 0 & \lambda_2 \end{bmatrix}^p = \begin{bmatrix} \lambda_1^p & t_{12}(\lambda_2^p - \lambda_1^p)/(\lambda_2 - \lambda_1) \\ 0 & \lambda_2^p \end{bmatrix}.$$

$$f_{12} = t_{12} \exp\left(\tfrac{p}{2}\left(\log\lambda_2 + \log\lambda_1\right)\right) \times \frac{2\sinh\left(p\left(\operatorname{atanh}(z) + \pi i\,\mathcal{U}(\log\lambda_2 - \log\lambda_1)\right)\right)}{\lambda_2 - \lambda_1},$$

where $z = (\lambda_2 - \lambda_1)/(\lambda_2 + \lambda_1)$,
$\mathcal{U}(z)$ is the **unwinding number** of $z \in \mathbb{C}$,

$$\mathcal{U}(z) := \frac{z - \log(e^z)}{2\pi i} = \left\lceil \frac{\operatorname{Im} z - \pi}{2\pi} \right\rceil \in \mathbb{Z}.$$

General $p \in \mathbb{R}$

$$\begin{aligned} p &= \lfloor p \rfloor + p_1, \qquad & p_1 > 0, \\ p &= \lceil p \rceil + p_2, \qquad & p_2 < 0. \end{aligned}$$

If A is Hermitian positive definite then

$$\kappa_{x^p}(A) \gtrsim \begin{cases} |p|\kappa_2(A)^{1-p}, & p \ge 0, \\ |p|\kappa_2(A), & p \le 0, \end{cases}$$

where $\kappa_2(A) = \|A\|_2\|A^{-1}\|_2 = \lambda_1/\lambda_n$.

- Choose p_1 if $\kappa_2(A) \ge \exp(p_1^{-1}\log\bigl(p_1/(1-p_1)\bigr))$.
- For general A, use $\kappa_2(A) \ge \max_i |t_{ii}|/\min_i |t_{ii}|$.

A^p for $p = -k \in \mathbb{Z}^-$

Power then invert.

$Y = A^k$ by binary powering
$X = Y^{-1}$ via GEPP

Invert then power.

$Y = A^{-1}$ via GEPP
$X = Y^k$ by binary powering

Repeated triangular solves.

Compute a factorization $PA = LU$ by GEPP.
$X_0 = I$
for $i = 0\colon k-1$
    Solve $LX_{i+1/2} = PX_i$
    Solve $UX_{i+1} = X_{i+1/2}$
end
$X = X_k$

Numerical Experiments

`powerm` essentially

```
[V,D] = eig(A);
X = V*diag(diag(D).^p)/V;
```

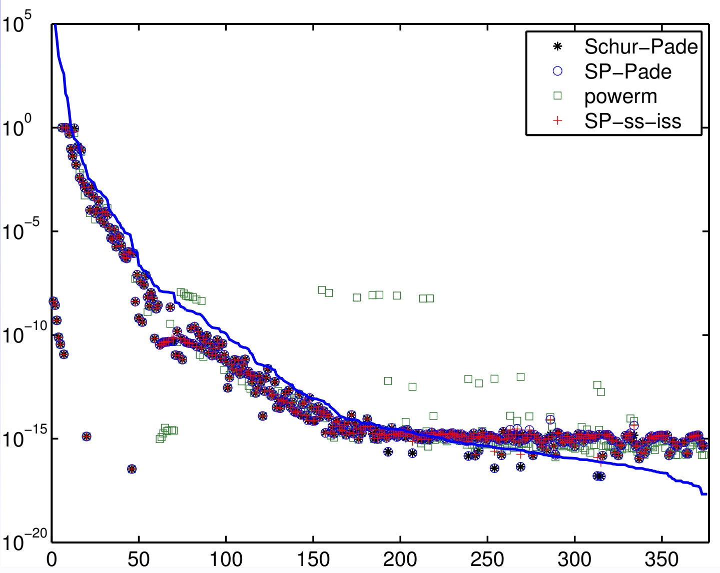
`Schur-Pade` New algorithm.

`SP-Pade:` Mod. of `funm` using `Schur-Pade` on the diagonal blocks.

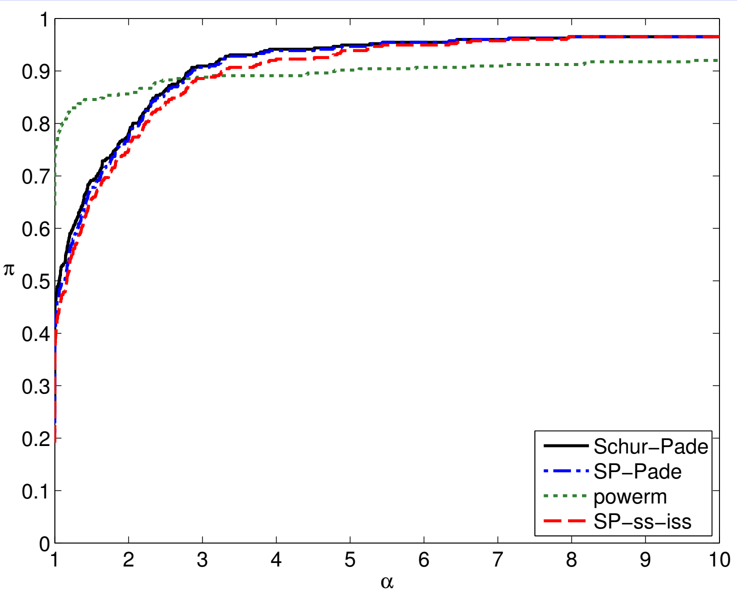
`SP-ss-iss` Mod. of `funm` with evaluation of $\exp(p \log(T_{ii}))$ by ISS for log and SS for exp.

Experiment 1: Relative Errors

195 10×10 matrices, $p \in \{1/52,\ 1/12,\ 1/3,\ 1/2\}$.

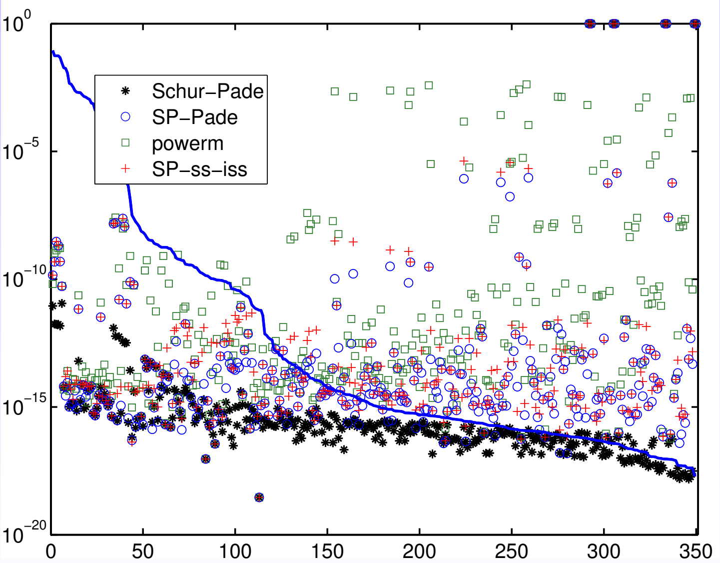


Performance Profile

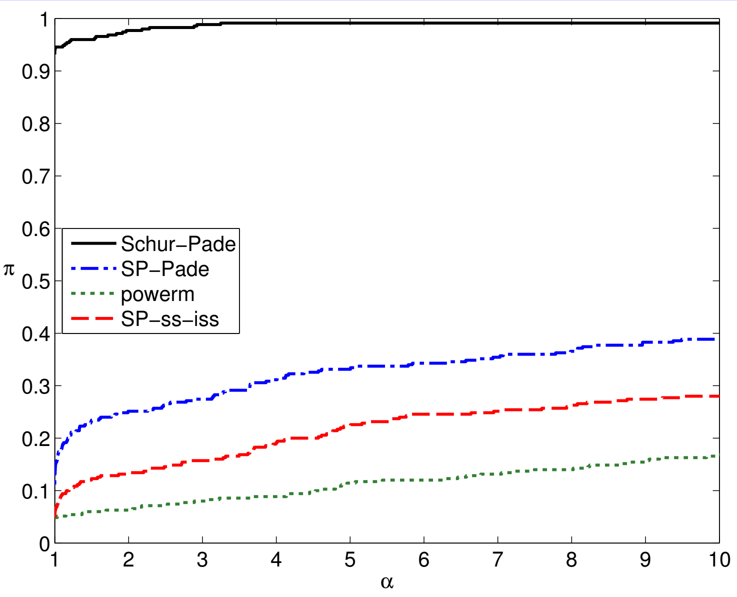


Experiment 2: Relative Errors

Triangular QR factors of previous test set, $r_{ii} \leftarrow |r_{ii}|$.

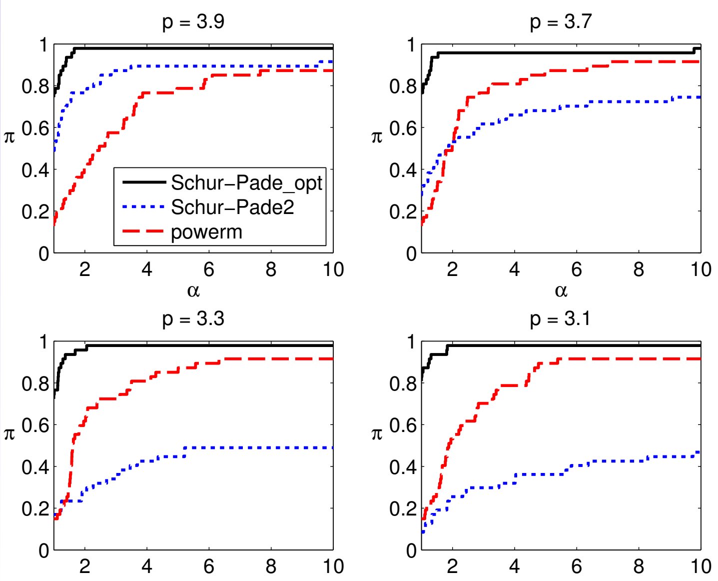


Performance Profile



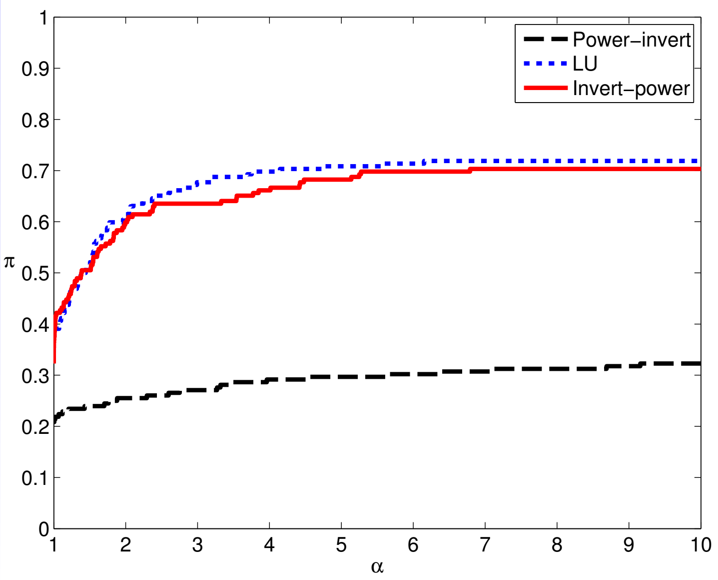
Experiment 3: $p \notin (-1, 1)$

Same matrices; $p = 3.9, 3.7, 3.3, 3.1$.



Experiment 4: Negative Integer *p*

Same matrices; $p = -3, -5, -7, -9$.



Conclusions

- MATLAB `A^p` is unreliable
  - for fractional p due to use of eigendecomposition,
  - for negative integer p due to “power then invert”.
- New Schur–Padé alg works for any $p \in \mathbb{R}$.
  - Schur decomposition,
  - square roots and Padé approximant,
  - choice of parameters balancing speed & accuracy,
  - exact computation of diag and superdiag,
  - superior to direct use of $\exp(p \log(A))$.
- Various alternative methods available when $p^{-1} \in \mathbb{Z}$.

N. J. Higham and L. Lin.
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