Computation of matrix functions with fully automatic Schur-Parlett and Rational Krylov methods.

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Matrix Functions

$\mathrm{sqrt}(A), \exp(A), f(A)$ ... where A is a square matrix.

Useful generalization of scalar function $f: \mathbb{C} \to \mathbb{C}$

Applications:

› Stiff differential equations;

› Nuclear magnetic resonance;

› Control theory.

Matrix Functions – examples

- Matrix polynomials:
  $$p(x) = x^3 + 4x - 7, \qquad p(A) = A^3 + 4A - 7I$$
- Taylor series definition: $\exp(A) = \sum_{k=0}^{\infty} A^k/k!$
- Matrix square root: $\mathrm{sqrt}(A)^2 = A$

The mathematical definition of the generic $f(A)$ involves the values of f and its derivatives on the spectrum of A.

Computation of Matrix Functions

There are specialized methods (scaling and squaring for `expm` and `logm`, Björk-Hammarling for `sqrtm`).

We want an algorithm that is both:

- **Generic** – working for any function f and matrix A;
- **Automatic** – requiring no other information from the user (such as derivatives of f or other data structures).

Automatic Differentiation

Dual numbers can be used to compute derivatives in an automatic, efficient and stable manner:

$\boldsymbol{x} + \boldsymbol{y\varepsilon}$ with $\varepsilon \neq 0,\ \varepsilon^2 = 0$

$$f(x + y\varepsilon) = f(x) + f'(x)y\varepsilon \quad \Rightarrow \quad f'(x) = \mathrm{Eps}(f(x + \varepsilon))$$

We use the Julia language (a “new Matlab”), whose type-system allows for pain-free use of dual numbers on user-defined functions.

Dual numbers can be generalized for higher-order derivatives (TaylorSeries.jl).

Automatic Differentiation – example

$f(x) = (x-3)^8$

```
function f(x)
      x -= 3
      for i = 1:3
            x *= x
      end
      return x
end
```

We can compute $f'(5)$ with

$f(5+\varepsilon)$:

$(5+\varepsilon)-3 = 2+\varepsilon$

$(2+\varepsilon)(2+\varepsilon) = 4+4\varepsilon$

$(4+4\varepsilon)(4+4\varepsilon) = 16+32\varepsilon$

$(16+32\varepsilon)(16+32\varepsilon) = 256+1024\varepsilon$

The result $f(5+\varepsilon) = 256+1024\varepsilon$ means

$f(5) = 256$ and $f'(5) = 1024$

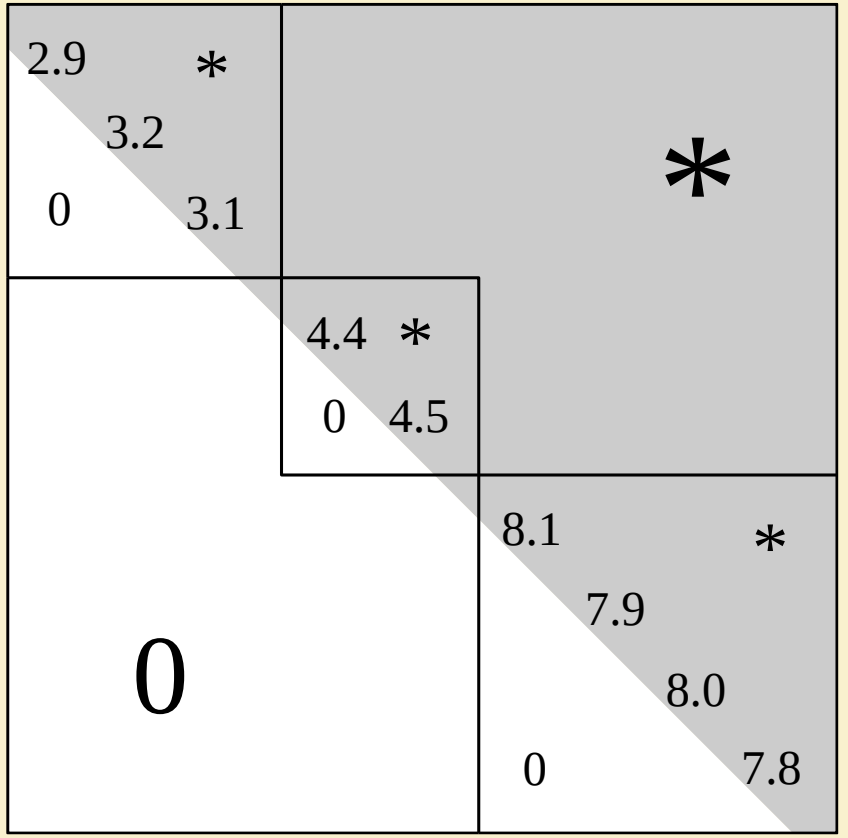
Schur-Parlett – dense matrix functions

Proposed by Higham and Davies in 2003.

$A = QTQ^* \Rightarrow$
$f(A) = f(QTQ^*) = Qf(T)Q^*$

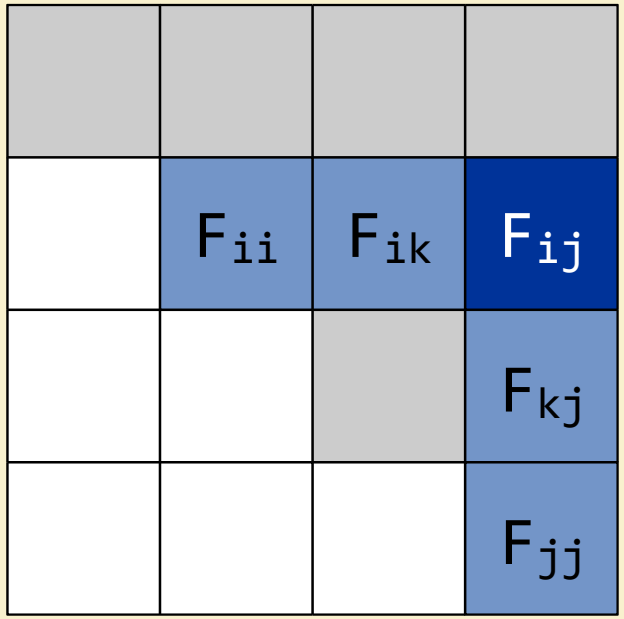
Need to compute $F = f(T)$:

1. Group eigenvalues in blocks by proximity;
2. Compute $f(T_{ii})$ of diagonal blocks with Taylor;
3. Use the Parlett recurrence to reconstruct the upper part.

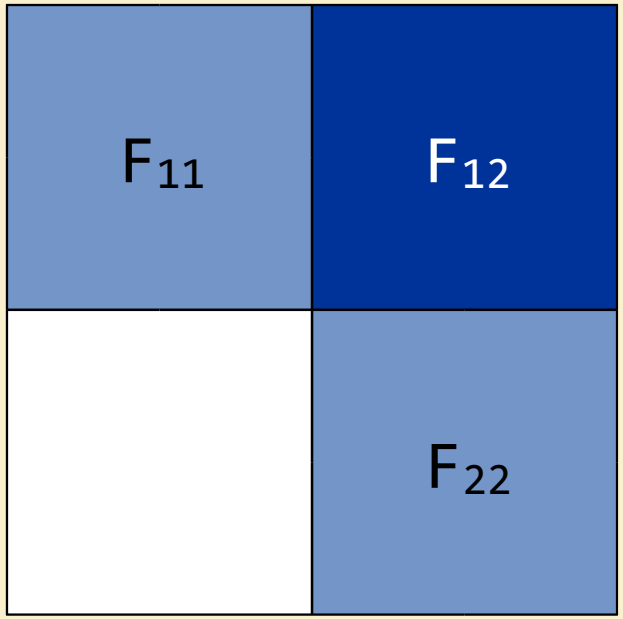


Schur-Parlett – Parlett recurrence

Parlett recurrence made recursive and cache-oblivious.



$\Rightarrow$



$$T_{ii}F_{ij} - F_{ij}T_{jj} = F_{ii}T_{ij} - T_{ij}F_{jj} + \sum_{k=i+1}^{j-1}(F_{ik}T_{kj} - T_{ik}F_{kj})$$

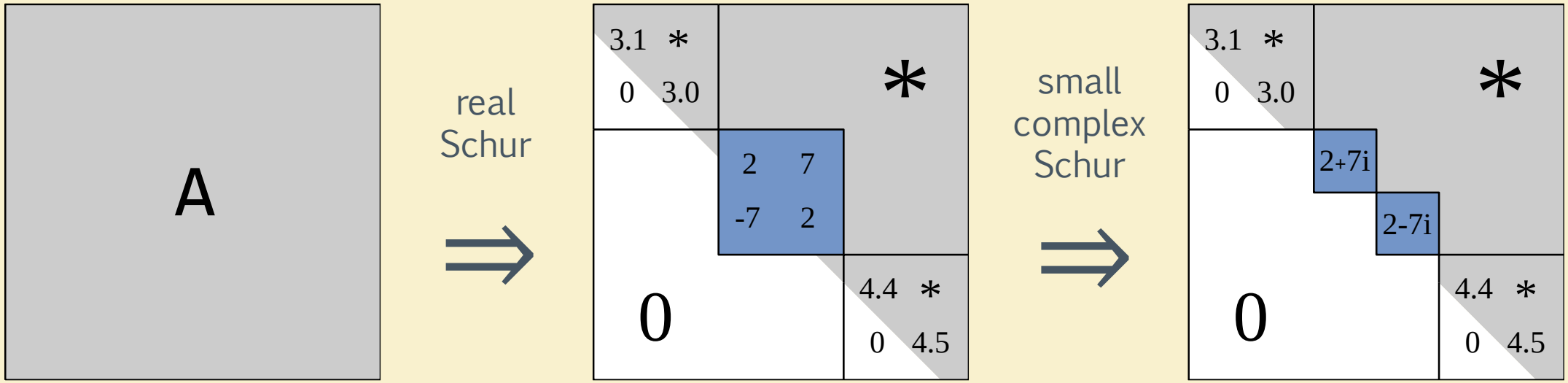
$$T_{11}F_{12} - F_{12}T_{22} = F_{11}T_{12} - T_{12}F_{22}$$

~3x speedup for n = 2500

Problem: conjugated eigenvalues with big imaginary part must go in different blocks, even with real A.

Original solution: do everything in complex arithmetic.

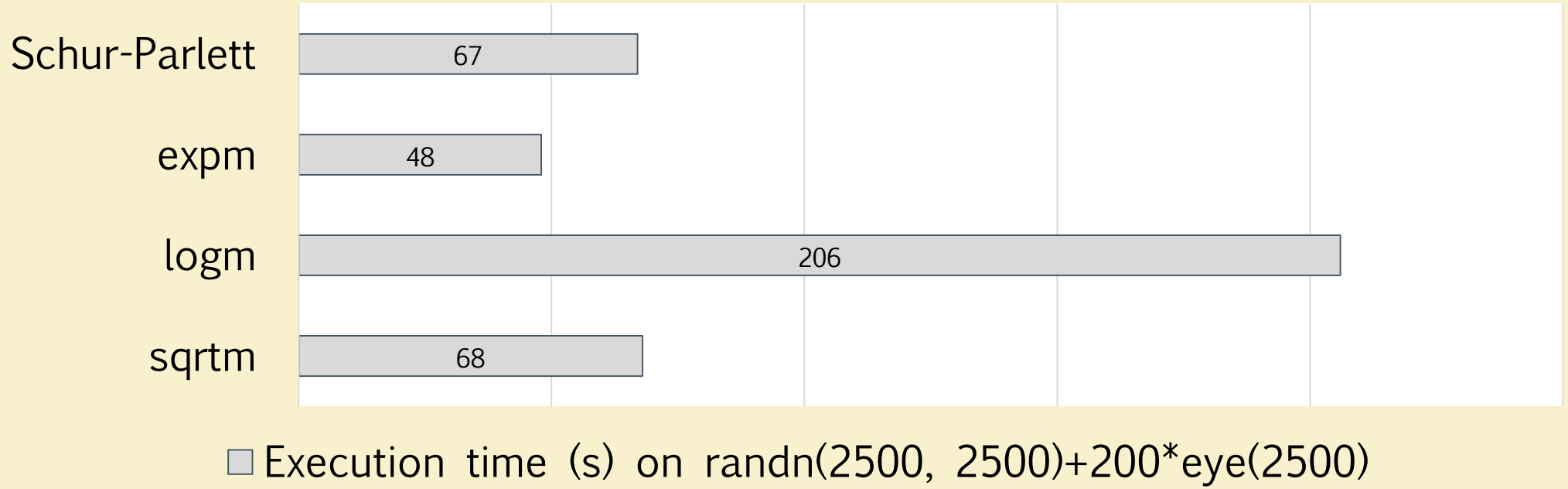
Our solution: complex Schur factorization can be “delayed” and done on small blocks:



Also allows for Parlett recurrence in real arithmetic, ~2x speedup for n = 2500 on whole Schur-Parlett.

Schur-Parlett – performance results

The whole procedure typically spends ~2/3 of the time doing A's Schur decomposition (varies depending on the eigenvalues' distribution).



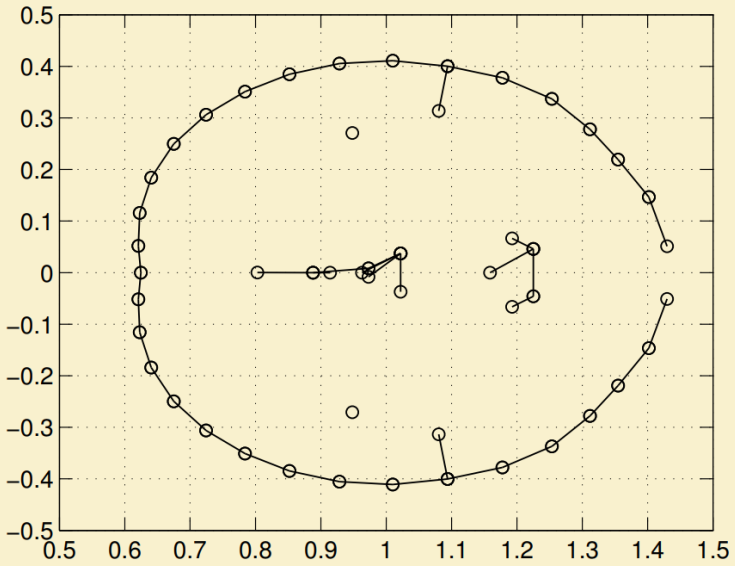
Schur-Parlett – numerical accuracy

	Specialized method	Schur-Parlett
exp	1.0e-14	1.5e-13
log	4.0e-14	4.1e-14
sqrt	4.3e-14	4.5e-14

Relative error versus Matlab's Symbolic Toolbox (on 50x50 random matrix).

Boils down to how well the eigenvalues can be clustered.

Can behave badly (7e-4) with "snake" eigenvalues (as shown in original paper, experiment 4)



Code comparison for the matrix cube root $A^{1/3}$

Matlab

```
function r = cuberoot(x, k)
      c = 1.0;
      for i = 0:k-1
            c = c*(1/3 – i);
      end
      r = c*x^(1/3 - k);
end

funm(A, @cuberoot)
```

Our Julia implementation

```
schurparlett((x)->x^(1/3), A)
```

Rational Krylov – sparse matrix functions

(as described by Güttel in 2013)

Goal: compute $f(A)b$ for a sparse A.

Approximate $f(A)b$ with a rational function $r_m(A)b$
$(r_m = p_{m-1}/q_{m-1})$

The method finds an orthonormal basis V for the rational Krylov space with the rational Arnoldi algorithm.

Then $r_m(A)b$ is computed by projecting A into the Krylov space:
$A_m = V^*AV$ (dense but small), $r_m(A)b = Vf(A_m)V^*b$

Downside: poles of r_m must be provided by the user.

Rational Krylov – approximation accuracy

Depends on two factors:

- How well f can be approximated on A's spectrum by a rational function, hopefully with low degree (ill-posed problem);
- How well we choose the poles.

We use the AAA algorithm for rational approximation to find good poles automatically.

AAA algorithm for rational approximation

Proposed by Nakatsukasa, Sète, Trefethen in 2017.

Input: function samples (real or complex).
Output: rational barycentric function of type $(m-1, m-1)$:

$$r(z) = \frac{n(z)}{d(z)} = \sum_{j=1}^{m} \frac{w_j f_j}{z - z_j} \Bigg/ \sum_{j=1}^{m} \frac{w_j}{z - z_j}$$

$r(z_j) = \infty/\infty$ but $\lim_{z \to z_j} r(z) = f_j$

Support/interpolation points (z_j) are chosen incrementally from samples in a greedy way, to avoid instabilities:

next z_j is chosen where $|f(z_j) - r(z_j)|$ is maximized.

After a new support point is found, weights are recomputed to minimize the approximation error:

$$f(z) \approx \frac{n(z)}{d(z)} \rightarrow minimize||f(z)d(z) - n(z)||, \qquad z \in Z^{(m)}$$

Is a least squares problem solvable with SVD:

$$minimize||Aw||, \qquad ||w|| = 1$$

When approximation error is small, we are done.

Poles can be then retrieved by solving a generalized eigenvalue problem, with accuracy up to machine precision.

Rational Krylov + AAA

1. Sample f on the 0-centered disk of radius $\mathrm{norm}(A)$;
2. Find the poles of f with AAA;
3. Use the poles for the rational Arnoldi approximation.

Computational costs:

Rational Krylov: m times sparse linear system;

AAA: m times SVD.

Number of samples for AAA is chosen to balance costs.

Rational Krylov + AAA, Experiment 1

Matrices are from the SuiteSparse Matrix Collection.

$\exp(A)b$ with Krylov is compared with dense expm:

Problem type	name	cond(A)	cond (exp, A)	# poles	error	# poles	error
2D/3D problem	jagmesh3	1168	7.0e0	9	1.5e-6	15	6.0e-14
Fluid dynamics	sherman4	2178	1.2e2	11	6.6e-6	19	6.7e-10
Structural problem	can_1072	2.0e34	3.4e1	11	7.3e-6	23	1.7e-14
Directed graph	SmaGri	Inf	7.8e1	9	2.6e-7	21	7.3e-13

Rational Krylov + AAA, Experiment 2

$\mathrm{sqrt}(A)b$ (positive definite A) against dense sqrtm:

Problem type	name	min eig(A)	norm(A)	# poles	error	# poles	error
Circuit simulatio	rajat19	1.7e-1	3.9e1	20	5.8e-6	45	3.7e-14
Structural problem	nos3	1.8e-2	7.7e2	50	8.8e-4	100	5.2e-9
Power network	685_bus	6.2e-2	2.6e4	50	1.5e-3	95	8.0e-5
Electro magnetic	mhd 1280b	1.5e-11	8.0e1	50	2.5e-2	50	8.8e-3

Custom sampling for AAA, more dense near 0, brings error from 10^{-3} to 10^{-12} (matrix “685_bus”).

Future Work

Different algorithms could be used for the evaluation of the diagonal blocks in Schur-Parlett (replacing Taylor).

An AAA solution could solve some of Schur-Parlett's instability issues and lift the dependency on automatic differentiation, bringing the automatic algorithm to other languages such as Matlab and C (more research needed).

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Questions?