An introduction to fractional calculus

Fundamental ideas and numerics

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The curse of dimensionality

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  - reformulation as *matrix equations*,
  - reformulation as *tensor problems*.

Matrix equation reformulations

The simplest way of introducing this reformulation is to go back to the 1D problem (now with a *source term*):

$$\begin{cases} \frac{\partial W}{\partial t} = \theta \, {}^{RL}D^{\alpha}_{[0,x]} W(x,t) + (1-\theta)\, {}^{RL}D^{\alpha}_{[x,1]} W(x,t) + f(x,t), \qquad \theta \in [0,1], \\ W(0,t) = W(1,t) = 0, \qquad W(x,t) = W_0(x). \end{cases}$$

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To solve everything we have to solve the **sequence of linear systems**

$$\frac{1}{\Delta t}\left(\mathbf{W}^{(m+1)} - \mathbf{W}^{(m)}\right) = \frac{1}{h^{\alpha}}\left(\theta G_N + (1-\theta) G_N^T\right) \mathbf{W}^{(m+1))} + \mathbf{f}^{(m+1)}, \; m = 0, \ldots, M-1.$$

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Do we really have to solve this sequentially?

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Following (Breiten, Simoncini, and Stoll 2016), we can **collect the time steps altogether**:

$$\left(B_M \otimes I_N - \frac{\Delta t}{h^\alpha} I_M \otimes T_N \right) \hat{\mathbf{W}} = \mathbf{F},$$

since

$$\begin{bmatrix} I_N - \frac{\Delta t}{h^\alpha} T_N & & & \\ -I_N & I_N - \frac{\Delta t}{h^\alpha} T_N & & \\ & \ddots & \ddots & \\ & & -I_N & I_N - \frac{\Delta t}{h^\alpha} T_N \end{bmatrix} \begin{bmatrix} \mathbf{W}^{(1)} \\ \mathbf{W}^{(2)} \\ \vdots \\ \mathbf{W}^{(M-1)} \end{bmatrix} = \begin{bmatrix} \mathbf{W}^{(0)} + \Delta t \mathbf{f}^{(1)} \\ \Delta t \mathbf{f}^{(2)} \\ \vdots \\ \Delta t \mathbf{f}^{(M)}, \end{bmatrix}$$

for $T_N = \left(\theta G_N + (1-\theta) G_N^T\right)$, $B_M = T_M(1 - e^{i\theta})$.

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This is now a **coupled system** of size $MN \times MN$, that is larger and uglier than before...

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Let's call $W = [\mathbf{W}^{(1)}|\cdots|\mathbf{W}^{(M)}]_{N\times M}$, $F = [\mathbf{W}^{(0)} + \Delta t\mathbf{f}^{(1)}|\cdots|\Delta t\mathbf{f}^{M}]_{N\times M}$, and rewrite our problem as

Compute $W \in \mathbb{R}^{N\times M}$ s.t. $A_N W + W B_M^T = F$.

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- ❓ Did we gain anything? Back to this in a few moment...
- ❓ Since we are accumulating all the time steps in one step, is it appropriate to simply use one of the methods we already know (e.g. Euler, BDFs, Adams', etc.) or can we do better? Next lecture!

What about the 2D problem?

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By the usual procedure

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$$+ \mathbf{f}^{(m+1)}, \quad m = 0, \ldots, M-1.$$

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- We now have a **sequence of Sylvester equations** for $m = 0, \ldots, M-1$.
- The matrix coefficients are related to *rescaled* 1D problems.

Solving Sylvester equations (Simoncini 2016)

This rewriting effort will be worth it only if we can **efficiently solve** Sylvester equations:

$$AX + XB = C, \quad A \in \mathbb{R}^{N\times N},\ B \in \mathbb{R}^{M\times M}, \quad C \in \mathbb{R}^{N\times M}.$$

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The solution can be expressed in **closed form** in a number of ways, e.g., as *integrals of resolvents*

$$X = -\frac{1}{4\pi^2}\int_{\Gamma_1}\int_{\Gamma_2} \frac{(\gamma I_N - A)^{-1} C (\mu I_M - B)^{-1}}{\lambda + \mu}\,\mathrm{d}\mu\mathrm{d}\lambda,$$

for Γ_1, Γ_2 contours containing and sufficiently close to the spectra of A and B, respectively.

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The solution can be expressed in **closed form** in a number of ways, e.g., as *integrals of exponentials*

$$X = -\int_0^{+\infty} e^{At} C e^{Bt}\, \mathrm{d}t,$$

for A and B with a spectra separated by a vertical line.

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The solution can be expressed in **closed form** in a number of ways, e.g., in the *diagonalizable case*, by means of *similarity transformations*

$$U^{-1}AU = \mathrm{diag}(\lambda_1, \dots, \lambda_N), \qquad V^{-1}BV = \mathrm{diag}(\mu_1, \dots, \mu_M),$$

then

$$X = U\tilde{X}V, \quad \tilde{x}_{i,j} = \frac{1}{\lambda_i + \mu_j}(U^{-1}CV)_{i,j}.$$

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Numerical mehtods

These formulations can exploited to devise numerical methods, to avoid a very long detour, we are going to just mention a couple of them; read (Simoncini 2016) for the full story.

The Bartels and Stewart 1972 algorithm

Input: A, B, C
Compute Schur factorizations
$URU^H = A^H$ and $B = VSV^H$;
Solve $R^H Y + YS = U^H CV$ for Y;
Compute $X = UYV^H$;

The Bartels and Stewart 1972 algorithm

- The first step costs $O(N^3)$ and $O(M^3)$ operations by **QR algorithm** for general A and B,

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$$R^H Y + YS = U^H CV$$

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$(Y)_{1,1}$ element is readily obtained by solving: $(\spadesuit + \clubsuit)(Y)_{11} = \bigstar$.

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$\Rightarrow$ The **leading cost** is the Schur factorization $O(N^3 + M^3)$! only **small matrices**.
We may gain something if A and B are in **upper Hessenberg form**...

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☺ But our cases are not small. . .

If only we knew a way to from a large matrix setting, to a small one made of Hessenberg matrices. . . wait a second, we may know a trick or two for this! ☺

When in doubt: project!

When we have to solve **linear systems** with a **large matrix**, we have seen that a good solution is represented by the Krylov projection methods.

❓ Can we do something similar for this problem too?

Theorem (Simoncini 2016, Theorem 4)

Let A and B be stable[1] and real symmetric, with spectra contained in $[a, b]$ and $[c, d]$, respectively. Define $\eta = 2(b-a)(d-c)/((a+c)(b+d))$. Assume C is of **rank** p. Then the singular values $\sigma_1 \geq \cdots \geq \sigma_{\min\{M,N\}}$ of the solution X to the Sylvester equation satisfy

$$\frac{\sigma_{pr+1}}{\sigma_1} \leq \left(\frac{1-\sqrt{k_r'}}{1+\sqrt{k_r'}}\right)^2, \; 1 \leq pr < n, \; k_r' = \frac{1}{1+\eta+\sqrt{\eta(\eta+2)}}.$$

[1] A matrix is called stable (or sometimes *Hurwitz*) if every eigenvalue has strictly negative real part.

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Call $\tilde{\mathbf{x}} = \operatorname{vec}(\tilde{X}) = (W_j \otimes V_k)\operatorname{vec}(Y)$, then we want V_k and W_k to be selected as

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$$V_k^H A V_k Y + Y W_j^H B W_j = V_k^H C_1 (W_j^H C_2)^H.$$

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Existence of the solution

If $V_k^H A V_k$ and $-W_j^H B W_j$ have **disjoint spectra** we can solve

$$V_k^H A V_k Y + Y W_j^H B W_j = V_k^H C_1 (W_j^H C_2)^H \qquad \forall\, C = C_1 C_2^H.$$

To enforce it, is sufficient to have A and $-B$ with disjoint field of values.

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The cost of **one iteration** for $m > n$ and $p = \mathrm{rank}(C)$ is then given by

Input: A, B, C_1 and C_2
Orthogonalize columns of C_1 to get $\mathbf{v}_1 = V_1$;
Orthogonalize columns of C_2 to get $\mathbf{v}_2 = W_1$;
for $k = 1, 2, \ldots,$ **do**
  Compute Y_k solution to
  $V_k^H A V_k Y + Y W_k^H B W_k - V_k^H C_1 (W_k^H C_2)^H = 0$;
  if *converged* **then**
    Return V_k, Y_k and W_k such that
    $X_k = V_k Y_k W_k^*$ and **stop**.
  end
  `/* Compute next bases blocks */`
  Compute $\tilde{v}$ and $\hat{w}$ from the **approximate space**;
  Make $\hat{v}$ orthogonal w.r.t. $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$;
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- $O((kp)^3)$ flops for the solution of the projected problem,

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- $O((kp)^3)$ flops for the solution of the projected problem,
- Orthogonalization of the new basis vectors with respect to the older vectors: $O(mkp^2)$,

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  Orthogonalize col.s of $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$ for $\mathbf{v}_{k+1}$ and $\mathbf{w}_{k+1}$;
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Projection methods for low-rank right-hand sides

The cost of **one iteration** for $m > n$ and $p = \mathrm{rank}(C)$ is then given by

- $O((kp)^3)$ flops for the solution of the projected problem,
- Orthogonalization of the new basis vectors with respect to the older vectors: $O(mkp^2)$,
- Orthogonalization of the new block: $O(mp^2)$.

Input: A, B, C_1 and C_2
Orthogonalize columns of C_1 to get $\mathbf{v}_1 = V_1$;
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for $k = 1, 2, \ldots,$ **do**
  Compute Y_k solution to
  $V_k^H A V_k Y + Y W_k^H B W_k - V_k^H C_1 (W_k^H C_2)^H = 0$;
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  `/* Compute next bases blocks */`
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If the generated basis experiences loss of rank, deflation procedures can be applied to remove redundant columns.

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Selection of $\mathcal{V}$ and $\mathcal{W}$

How do we select the approximation spaces $\mathcal{V}$ and $\mathcal{W}$?

Standard **block** Krylov subspace

$$\mathcal{V} = \mathrm{range}\{[C_1, AC_1, A^2 C_2, \dots]\}, \quad \mathcal{W} = \mathrm{range}\{[C_2, B^H C_1, (B^H)^2 C_2, \dots]\},$$

Rational **block** Krylov subspace

$$\begin{aligned} \mathcal{V} &= \mathrm{range}\{[(A + \sigma_1 I)^{-1} C_1, (A + \sigma_2 I)^{-1}(A + \sigma_1 I)^{-1} C_1, \dots]\}, \\ \mathcal{W} &= \mathrm{range}\{[(B^H + \eta_1 I)^{-1} C_2, (B^H + \eta_2 I)^{-1}(B^H + \eta_1 I)^{-1} C_2, \dots]\}, \end{aligned}$$

Global Krylov subspace:

$$\mathcal{V} = \left\{ \sum_{i \geq 0} A^i C_i \gamma_i, \quad \gamma_i \in \mathbb{R} \right\} = \mathrm{span}\{C_1, AC_1, A^2 C_2, \dots\}$$

where the linear combination is performed blockwise, and analogously for $\mathcal{W}$.

Stopping criterions

To change the "**if** *converged*" in the algorithm we have to monitor the residual, e.g.,

$$\|R\|_2 = \|A\tilde{X} + \tilde{X}B - C_1C_2^*\|_2 \text{ or } \|R\|_F = \|A\tilde{X} + \tilde{X}B - C_1C_2^*\|_F.$$

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  with $[V_k, \hat{v}_k]$ and $[W_j, \hat{w}_j]$ having orthonormal columns.
- If $\exists\, C_1^{(k)}$ and $C_2^{(j)}$ s.t. $C_1 = [V_k, \hat{v}_k]C_1^{(k)}$ and $C_2 = [W_j, \hat{w}_j]C_2^{(j)}$

$$\begin{aligned}
\|R\|_F &= \|AV_kYW_j^H + V_kYW_j^HB - \hat{V}_kC_1^{(k)}(\hat{W}_jC_2^{(j)})^H\|_F \\
&= \left\|[V_k\hat{v}_k]\left(\underline{H}_kY[I,0] + [I;0]Y\underline{K}_j^H - C_1^{(k)}(C_2^{(j)})^H\right)[W_j,\hat{w}_j]^H\right\|_F \\
&= \|\underline{H}_kY[I,0] + [I;0]Y\underline{K}_j^H - C_1^{(k)}(C_2^{(j)})^H\|_F.
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$$\|R\|_F = \|\underline{H}_k Y[I, 0] + [I; 0]Y\underline{K}_j^H - C_1^{(k)}(C_2^{(j)})^H\|_F.$$

- The matrix in the last norm is small **if** k and j are small, if we are under the conditions on the spaces we can **monitor the residual along the way**.

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Where were we?

For the two equations we wanted to solve we have then the following questions:

- Is our C low-rank?
- What type of Krylov subspace should we select?
- Does any of this stuff converge at all?

Low-rank, regularity and separability

For the 1D+1D case we have to solve

$$A_N W + W B_M^T = F, \text{ with } F = [\mathbf{W}^{(0)} + \Delta t \mathbf{f}^{(1)} | \cdots | \Delta t \mathbf{f}^{M}]_{N \times M},$$

with $(\mathbf{f}^{(m)})_i = f(x_i, t_m)$.

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For the 1D+2D case we have to solve for $m = 0, \ldots, M-1$

$$\left(\frac{1}{2} I_{N_x} - \Delta t \tilde{G}_{N_x}\right) \tilde{W}^{(m+1)} + \tilde{W}^{(m+1)} \left(\frac{1}{2} I^{N_y} - \Delta t \tilde{G}_{N_y}\right)^T = \tilde{W}^{(m)} + \Delta t F^{(m+1)},$$

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Low-Rank

When is it that these matrices have a fixed, size-independent "small" rank?

Low-rank, regularity and separability

- If a function $f(x, y) = f_1(x) f_2(y)$ then

$$\begin{bmatrix} f(x_1, y_1) & f(x_1, y_2) & \cdots & f(x_1, y_n) \\ f(x_2, y_1) & f(x_2, y_2) & \cdots & f(x_2, y_n) \\ \vdots & \vdots & \ddots & \vdots \\ f(x_n, y_1) & f(x_n, y_2) & \cdots & f(x_n, y_n) \end{bmatrix}$$

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To have a simple example:

```
n = 10;
f1 = @(x) exp(-2*x); f2 = @(y) sin(2*pi*y); f = @(x,y) f1(x).*f2(y);
x = linspace(0,1,n); y = linspace(0,1,n);
[X,Y] = meshgrid(x,y);
A = f(X.',Y.'); a1 = f1(x); a2 = f2(y);
norm(A-a1.'*a2)
```

that answers us `>> ans = 0`.

Low-rank, regularity and separability

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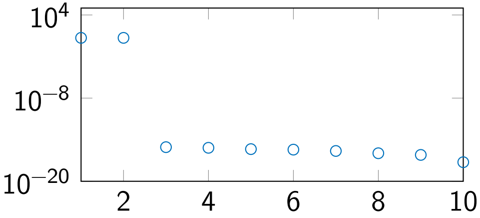
What happens if $f(x,y)$ is not separable? E.g., if $f(x,y) = \sin(\pi(x+y))$?

```
n = 10;
f = @(x,y) sin(pi*(x+y));
x = linspace(0,1,n);
y = linspace(0,1,n);
[X,Y] = meshgrid(x,y); A = f(X.',Y.');
sv = svd(A);
```



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$$\sin(\pi(x+y)) = \sin(\pi x)\cos(\pi y) + \cos(\pi x)\sin(\pi y)$$

is the **sum of** two **separable functions**, i.e., we get a matrix that has rank equal to 2.

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We can try to **generalize** this **decomposition idea** to more general functions!

Low-rank, regularity and separability

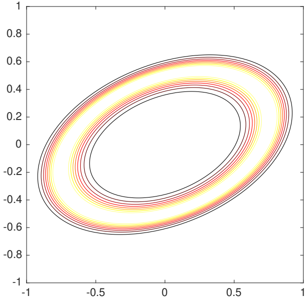
We can approximate a function of two variables as the sum of separable functions

$$f(x,y) = \sum_{k=1}^{K} f_k T_k(x) T_k(y), \quad \{T_k(\cdot)\}_k \text{ Čebyšëv polynomials.}$$

Example (Using Chebfun (Driscoll, Hale, and Trefethen 2014))

Consider $f(x,y) = \exp(-40(x^2 - xy + 2y^2 - 1/2)^2)$.

```
cheb.xy
ff=@(x,y)exp(-40*(x.^2-x.*y+2*y.^2-1/2).^2);
f=chebfun2(ff);
levels = 0.1:0.1:0.9;
contour(f,levels);
axis([-1 1 -1 1]);
axis square
```



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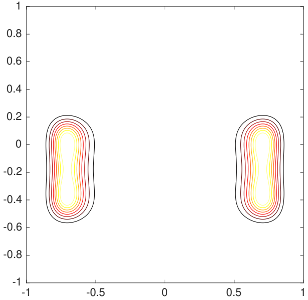
Forcing a rank K approximation

```
levels = 0.1:0.1:0.9;
for K = 1:9
 contour(chebfun2(ff,K),levels)
 xlim([-1 1]), axis equal
end
```



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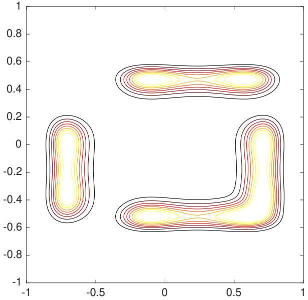

Low-rank, regularity and separability

We can approximate a function of two variables as the sum of separable functions

$$f(x, y) = \sum_{k=1}^{K} f_k T_k(x) T_k(y), \quad \{T_k(\cdot)\}_k \text{ Čebyšëv polynomials.}$$

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Consider $f(x, y) = \exp(-40(x^2 - xy + 2y^2 - 1/2)^2)$.

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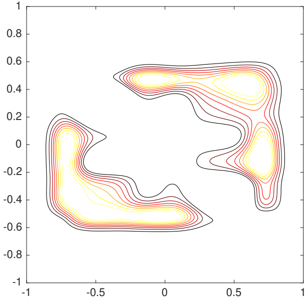

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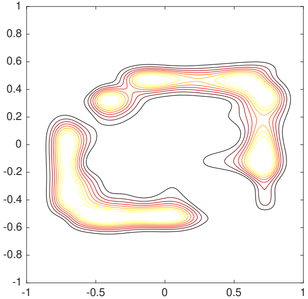

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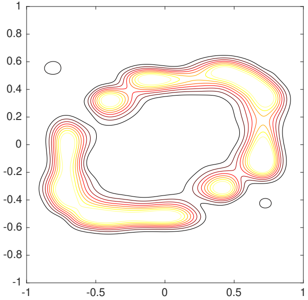

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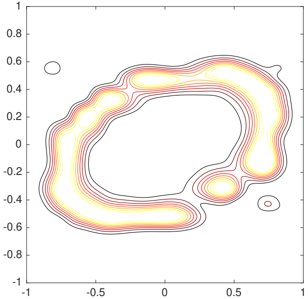

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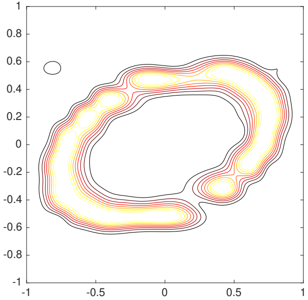

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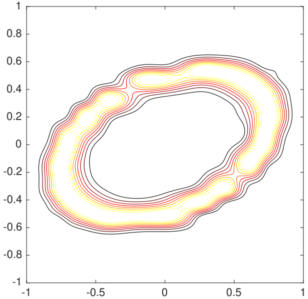

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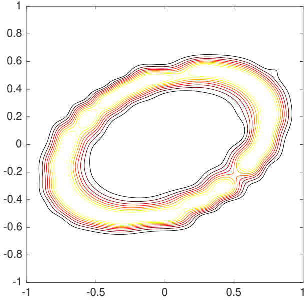

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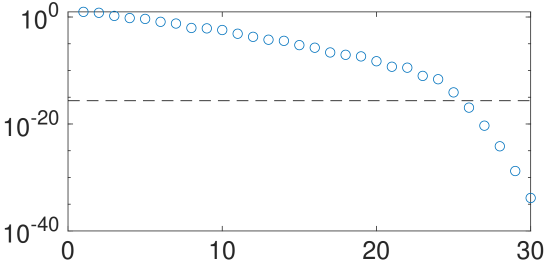

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Approximating approximating we could get where we wanted...

Let us remember that the approximation of the low-rank term must be done together with the approximation induced by the FDE solution method. We may not need to go as far as machine precision.

Selecting the Krylov subspace

If we are now in the case of a **low rank** right-hand side, we have to select Krylov subspaces for the spaces $\mathcal{V}$ and $\mathcal{W}$.

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- Rational (block) Krylov subspace can therefore be a good choice!

$$\mathcal{V} = \operatorname{range}\{[(A + \sigma_1 I)^{-1} C_1, (A + \sigma_2 I)^{-1}(A + \sigma_1 I)^{-1} C_1, \ldots]\},$$
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- ... but how do we **select the poles**?
- This is not an easy problem in general! A maybe lazy (but surprisingly well behaving) choice is to set $\{\sigma_i, \eta_i\} \in \{0, \infty\} \Rightarrow$ if we choose the two values alternately, then we get the Extended Krylov Subspace.

The Extended Krylov Subspace approach

If $B = A^T$ and $C = C_1 C_2^T$ with $C_1 = C_2$, we can generate the space:

$$\mathbb{EK}(A, C_1) = \mathrm{range}([C_1, A^{-1}C_1, AC_1, A^{-2}C_1, A^2C_1, \ldots]) = \mathcal{V} = \mathcal{W}.$$

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For our two problems, we have to solve systems and do mat-vec with matrices

$$\text{1D: } A = \frac{-\Delta t}{h_N^\alpha}(\theta G_N + (1-\theta)G_N^T) \qquad B = T_M(1 - e^{i\theta})$$

$$\text{2D: } A = \frac{1}{2}I_{N_x} - \frac{\Delta t}{h_{N_x}^\alpha}(\theta G_{N_x} + (1-\theta)G_{N_x}^T) \qquad B = \frac{1}{2}I_{N_y} - \frac{\Delta t}{h_{N_y}^\alpha}(\theta G_{N_y} + (1-\theta)G_{N_y}^T)$$

A couple of examples - I

Let us start from the 1D+1D case

$$\begin{cases} \frac{\partial W}{\partial t} = \Gamma(3-\alpha)x^{\alpha}\,{}^{RL}D^{\alpha}_{[0,x]}W + \Gamma(3-\alpha)(2-x)^{\alpha}\,{}^{RL}D^{\alpha}_{[x,2]}W - x(x-2)e^{-t}, \\ W(0,t) = W(1,t) = 0, \quad W(x,0) = 5x(2-x); \end{cases}$$

We can **discretize it** in the usual way:

```
w0 = @(x) 5*x.*(2-x);
hN = 2/(N-1); x = 0:hN:2;
dt = hN; t = 0:dt:1; M = length(t);
dplus=@(x,t)gamma(3-alpha).*x.^alpha;
dmin=@(x,t)gamma(3-alpha).*(2-x).^alpha;
f= @(x,t) -x.*(x-2).*exp(-t);
G = glmatrix(N,alpha);
Gr = G; Grt = G.';
Dplus = diag(dplus(x,0));
Dminus = diag(dmin(x,0));
I = eye(N,N); e = ones(N,1);
```

```
A = -dt*(Dplus*Gr +
↪  Dminus*Grt)/hN^alpha;
B = spdiags([-e,e],-1:0,M,M);
[X,T] = meshgrid(x,t);
C = dt*f(X,T);
C(1,:) = w0(x) + C(1,:);
C = -C';
[U,S,V] = svd(C);
C1 = U(:,1:2)*sqrt(S(1:2,1:2));
C2 = (sqrt(S(1:2,1:2))*
↪  V(:,1:2).').';
```

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And then use the `kpik_sylv` solver from V. Simoncini's software:

```
m = 100;
tol = 1e-9;
[LA,UA] = lu(A); % Direct solutions!
[LB,UB] = lu(B);
[X1,X2,res]=kpik_sylv(A,LA,UA,
↪  B,LB,UB,C1,C2,m,tol);
SOL = X1*X2'; % Not clever al all!
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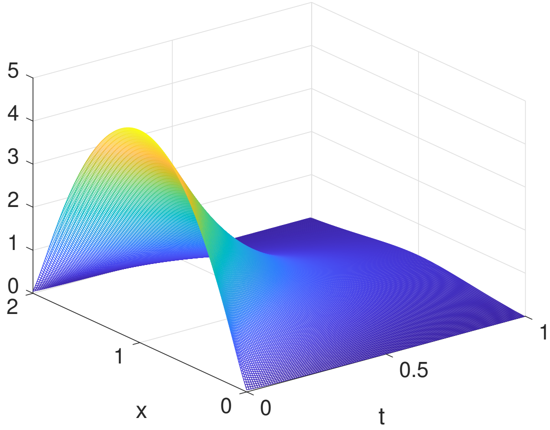

$N = 2^8, \ M = 2^7, \ \alpha = 1.5$

- We are using LU-factorization and direct solutions;
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α	$N = 2M$	IT	Rel. Residual
1.2	2^5	7	4.982093e-10
	2^6	11	7.629176e-11
	2^7	15	3.721767e-10
	2^8	21	2.406077e-10
	2^9	28	4.726518e-10
	2^{10}	37	8.250742e-10
	2^{11}	50	5.928325e-10

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α	$N = 2M$	IT	Rel. Residual
1.3	2^5	8	7.473189e-41
	2^6	10	3.324155e-10
	2^7	14	1.876221e-10
	2^8	18	6.104754e-10
	2^9	24	4.098504e-10
	2^{10}	31	5.142375e-10
	2^{11}	40	6.702602e-10

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1.4	2^5	7	4.900654e-10
	2^6	10	4.402728e-11
	2^7	13	1.970841e-10
	2^8	17	2.024635e-10
	2^9	22	5.120085e-10
	2^{10}	28	8.263324e-10
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1.5	2^5	7	1.235969e-10
	2^6	9	2.799035e-10
	2^7	13	1.007848e-10
	2^8	16	6.145733e-10
	2^9	21	7.639171e-10
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α	$N = 2M$	IT	Rel. Residual
1.6	2^5	7	2.480357e-11
	2^6	9	8.683894e-11
	2^7	13	7.692141e-11
	2^8	16	3.792143e-10
	2^9	21	3.991222e-10
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1.7	2^5	7	5.588528e-12
	2^6	8	6.692127e-10
	2^7	12	8.189936e-10
	2^8	16	3.403250e-10
	2^9	20	9.093120e-10
	2^{10}	26	3.550244e-10
	2^{11}	32	7.478792e-10

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1.8	2^5	6	6.097527e-10
	2^6	8	9.737670e-11
	2^7	13	6.202872e-11
	2^8	16	2.193864e-10
	2^9	20	7.469866e-10
	2^{10}	25	8.191797e-10
	2^{11}	32	5.086938e-10

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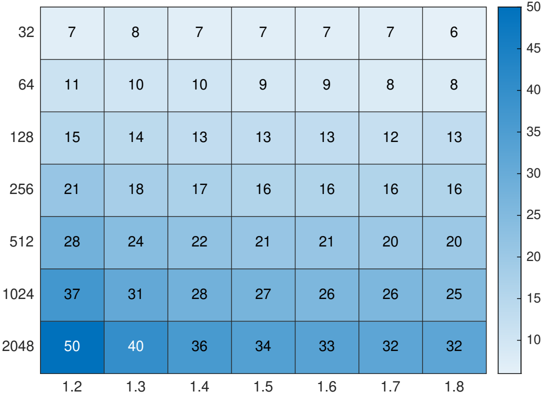
SOL = X1*X2'; % Not clever al all!
```



- ⚠ We are using LU-factorization and direct solutions;
- ⚠ We are reassembling the solution!

A couple of examples - II

We can then try the 1D+2D case

$$\begin{cases} \frac{\partial W}{\partial t} = \Gamma(3-\alpha)x^{\alpha}\, {}^{RL}D^{\alpha}_{[0,x]} W + \Gamma(3-\alpha)(2-x)^{\alpha}\, {}^{RL}D^{\alpha}_{[x,2]} W \\ \qquad + \Gamma(3-\alpha)y^{\alpha}\, {}^{RL}D^{\alpha}_{[0,y]} W + \Gamma(3-\alpha)(2-y)^{\alpha}\, {}^{RL}D^{\alpha}_{[y,2]} W \\ \qquad + \sin(\pi x)\sin(\pi y)e^{-t}, \\ W(x,y,t) = 0, & (x,y) \in \partial[0,2]^2, \\ W(x,y,0) = 5x(2-x)y(2-y), \end{cases}$$

for which the discretization proceeds along the usual lines, i.e,

```
hN = 2/(N-1); x = 0:hN:2; y = 0:hN:2; [X,Y] = meshgrid(x,y);
dt = hN; t = 0:dt:1; M = length(t);
w0 = @(x,y) 5*x.*(2-x).*y.*(2-y);
dplus = @(x,t) gamma(3-alpha).*x.^alpha;
dminus = @(x,t) gamma(3-alpha).*(2-x).^alpha;
f = @(x,y,t) sin(pi*x).*sin(pi*y).*exp(-t);
```

A couple of examples - II

We can then try the 1D+2D case

$$
\begin{cases}
\frac{\partial W}{\partial t} = \Gamma(3-\alpha)x^{\alpha}\, {}^{RL}D^{\alpha}_{[0,x]} W + \Gamma(3-\alpha)(2-x)^{\alpha}\, {}^{RL}D^{\alpha}_{[x,2]} W \\
\qquad + \Gamma(3-\alpha)y^{\alpha}\, {}^{RL}D^{\alpha}_{[0,y]} W + \Gamma(3-\alpha)(2-y)^{\alpha}\, {}^{RL}D^{\alpha}_{[y,2]} W \\
\qquad + \sin(\pi x)\sin(\pi y)e^{-t}, \\
W(x,y,t) = 0, & (x,y) \in \partial[0,2]^2, \\
W(x,y,0) = 5x(2-x)y(2-y),
\end{cases}
$$

for which the discretization proceeds along the usual lines, i.e,

```
G = glmatrix(N,alpha); Gr = G; Grt = G.';
Dplus = diag(dplus(x,0)); Dminus = diag(dminus(x,0));
I = eye(N,N); e = ones(N,1);
A = 0.5*I -dt*(Dplus*Gr + Dminus*Grt)/hN^alpha; % Left-hand side
B = (0.5*I -dt*(Dplus*Gr + Dminus*Grt)/hN^alpha).';
C = w0(X,Y) + dt*f(X,Y,t(1)); C = -C'; [U,S,V] = svd(C);  % Right-hand side
C1 = U(:,1:2)*sqrt(S(1:2,1:2)); C2 = (sqrt(S(1:2,1:2))*V(:,1:2).').';
```

A couple of examples - II

And then use the kpik_sylv solver from V. Simoncini's software:

```
m = 100;
tol = 1e-9;
[LA,UA] = lu(A); % Direct solutions!
[LB,UB] = lu(B);
[X1,X2,res]=kpik_sylv(A,LA,UA,
↪  B,LB,UB,C1,C2,m,tol);
SOL = X1*X2'; % Not clever al all!
```

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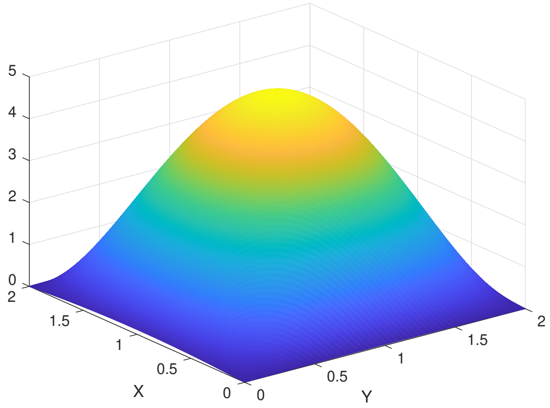

$N = 2^8,\ M = 2^8,\ \alpha = 1.5$

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SOL = X1*X2'; % Not clever al all!
```

α	$N = M$	IT	Rel. Residual
1.2	2^5	7	8.572314e-12
	2^6	9	1.035235e-10
	2^7	10	6.376925e-10
	2^8	11	4.294848e-10
	2^9	11	4.831316e-10
	2^{10}	11	3.340377e-10
	2^{11}	10	8.493637e-10

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α	$N = M$	IT	Rel. Residual
1.3	2^5	7	7.117681e-11
	2^6	9	7.410001e-11
	2^7	10	6.311608e-10
	2^8	11	6.629092e-10
	2^9	11	7.935697e-10
	2^{10}	11	5.256769e-10
	2^{11}	11	3.021361e-10

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```

α	$N = M$	IT	Rel. Residual
1.4	2^5	7	6.199844e-11
	2^6	9	5.440959e-11
	2^7	10	6.223106e-10
	2^8	12	2.743756e-10
	2^9	12	6.270319e-10
	2^{10}	12	4.310692e-10
	2^{11}	11	4.849822e-10

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```

α	$N = M$	IT	Rel. Residual
1.5	2^5	7	5.108938e-11
	2^6	8	7.696608e-10
	2^7	10	5.554438e-10
	2^8	12	3.501633e-10
	2^9	13	4.696907e-10
	2^{10}	13	5.839644e-10
	2^{11}	12	6.172378e-10

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A couple of examples - II

And then use the `kpik_sylv` solver from V. Simoncini's software:

```
m = 100;
tol = 1e-9;
[LA,UA] = lu(A); % Direct solutions!
[LB,UB] = lu(B);
[X1,X2,res]=kpik_sylv(A,LA,UA,
↪  B,LB,UB,C1,C2,m,tol);
SOL = X1*X2'; % Not clever al all!
```

α	$N = M$	IT	Rel. Residual
1.6	2^5	7	4.147318e-11
	2^6	9	1.120891e-10
	2^7	10	4.652358e-10
	2^8	12	3.624143e-10
	2^9	13	6.835564e-10
	2^{10}	14	5.920602e-10
	2^{11}	13	8.882506e-10

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α	$N = M$	IT	Rel. Residual
1.7	2^5	7	3.321348e-11
	2^6	9	9.437180e-11
	2^7	10	7.551800e-10
	2^8	12	3.268160e-10
	2^9	13	7.715645e-10
	2^{10}	14	8.954668e-10
	2^{11}	15	5.806398e-10

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SOL = X1*X2'; % Not clever al all!
```

- We are using LU-factorization and direct solutions;
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α	$N = M$	IT	Rel. Residual
1.8	2^5	7	2.639521e-11
	2^6	9	7.654578e-11
	2^7	10	6.909946e-10
	2^8	12	4.424195e-10
	2^9	13	7.255110e-10
	2^{10}	15	4.728355e-10
	2^{11}	15	8.400505e-10

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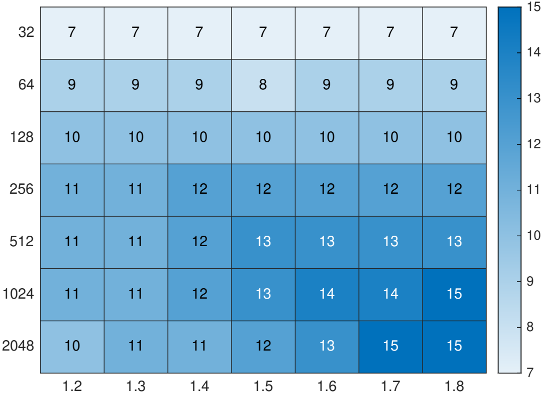

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Convergence

❓ What can we say about the convergence?

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If A is symmetric and positive definite, and $B = A^T$, i.e., we are solving a Lyapunov equation, and using **polynomial Krylov subspace**:

Theorem (Simoncini and Druskin 2009, Proposition 3.1)

Let A be symmetric and positive definite, and let $\lambda_{\min}$ be the smallest eigenvalue of A. Let $\hat{\lambda}_{\min}$, $\hat{\lambda}_{\max}$ be the extreme eigenvalue of $A + \lambda_{\min} I$ and $\hat{\kappa} = \hat{\lambda}_{\max}/\hat{\lambda}_{\min}$. Then

$$\|X - X_m\| \leq 4 \frac{\sqrt{\hat{\kappa}} + 1}{\hat{\lambda}_{\min}\sqrt{\hat{\kappa}}} \left(\frac{\sqrt{\hat{\kappa}} - 1}{\sqrt{\hat{\kappa}} + 1} \right)^m .$$

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⚠ If $B = A^T$ but A is **no longer symmetric**, one then needs again bounds related to the Field-of-Values of A, see (Simoncini and Druskin 2009).

Convergence

If we have $B \neq A^T$ things are more involved and due to (Beckermann 2011), and we need preliminary work.

- First of all, we need a more manageable expression of the rational Krylov subspace, let us re-brand the poles in the extended complex plane $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$ as

$$z_{A,1}, \dots, z_{A,m} \in \overline{\mathbb{C}} \setminus \Lambda(A), \qquad z_{B,1}, \dots, z_{B,n} \in \overline{\mathbb{C}} \setminus \Lambda(B),$$

  and introduce the polynomials

$$Q_A(z) = \prod_{\substack{j=1 \\ z_{A,j} \neq \infty}}^{m} (z - z_{A,j}) \text{ and } Q_B(z) = \prod_{\substack{j=1 \\ z_{B,j} \neq \infty}}^{n} (z - z_{A,j}).$$

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- The two rational spaces can then be written as

$$\mathcal{V} = \{R_A(A)C_1 \,:\, R_A \in \mathbb{P}_{m-1}/Q_A\}, \qquad \mathcal{W} = \{R_B(B)^H C_2 \,:\, R_B \in \mathbb{P}_{n-1}/Q_B\}.$$

Convergence

Consider the **rational functions** for the projected matrices A_m and B_n on $\mathcal{V}$ and $\mathcal{W}$

$$R_A^G(z) = \frac{\det(zI - A)}{Q_A(z)} \in \mathbb{P}_m / Q_A, \qquad R_B^G(z) = \frac{\det(zI - B_n)}{Q_B(z)} \in \mathbb{P}_n / Q_B$$

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Theorem (Beckermann 2011, Theorem 2.1)

Let $\operatorname{rank}(C) = 1$. The rational Galerkin residual ρ can be decomposed into the sum

$$\rho = \rho_{1,2} + \rho_{2,1} + \rho_{2,2}, \qquad \|\rho\|_F^2 = \|\rho_{1,2}\|_F^2 + \|\rho_{2,1}\|_F^2 + \|\rho_{2,2}\|_F^2,$$

with, $C_{1,m} = U^H C_1$, $C_{2,n} = V^H C_2$, and

$$\rho_{1,2} U \frac{1}{R_B^G}(A_m) C_{1,m} C_2^H R_B^G(B), \;\; \rho_{2,1} = R_A^G(A) C_1 C_{2,n}^H \frac{1}{R_A^G}(B_n) V^H,$$

$$\rho_{2,2} = \frac{R_A^G(A) C_1 C_2^H R_B^G(B)}{R_A^G(\infty) R_B^G(\infty)}.$$

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with, $C_{1,m} = U^H C_1$, $C_{2,n} = V^H C_2$, and

$$\|\rho_{2,2}\|_F = \inf_{\substack{R_A \in \mathbb{P}_m/Q_A \\ R_B \in \mathbb{P}_n/Q_B}} \left\| \frac{R_A(A) C_1 C_2^H R_B(B)}{R_A(\infty) R_B(\infty)} \right\|_F = \|(I - UU^H) C_1 C_2^H (I - VV^H)\|_F,$$

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with, $C_{1,m} = U^H C_1$, $C_{2,n} = V^H C_2$, and

$$\|\rho_{1,2}\|_F = \min_{R_B \in \mathbb{P}_m/Q_B} \left[\|R_B(A_m) C_{1,m} C_2^H R_B(B)\|_F + c_0 \|\frac{1}{R_B}(A_m) C_{1,m} C_{2,n}^H R_B(B_n)\|_F \right],$$

for $c_0 = 2\operatorname{diam}(W(A), W(B))/\operatorname{dist}(W(A), W(B))$.

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$$\|\rho_{2,1}\|_F = \min_{R_A \in \mathbb{P}_m/Q_A} \left[\|R_A(A) C_1 C_{2,n}^H \frac{1}{R_A}(B_n)\|_F + c_0 \|R_A(A_m) C_{1,m} C_{2,n}^H \frac{1}{R_A}(B_n)\|_F \right],$$

for $c_0 = 2 \operatorname{diam}(W(A), W(B)) / \operatorname{dist}(W(A), W(B))$.

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- Now we have a **representation of the residual** in the **orthogonal bases** associated to the given Krylov subspaces, and furthermore we know that $\rho_{2,2} = 0$ if at least one of the $z_{A,j}$ or $z_{B,j}$ is ∞, i.e., if either of the initial vectors are in the subspace.

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- The bounds are then obtained by having upper-bounds of the quantities

$$E_m(\spadesuit, Q_\spadesuit, z) = \min_{p \in \mathbb{P}_\heartsuit} \frac{\left\| \frac{P}{Q_\spadesuit}(\spadesuit) \right\|}{\left| \frac{P}{Q_\spadesuit}(z) \right|}, \text{ for } \spadesuit = \{A, B\},\ \heartsuit = \{m, n\}.$$

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$\Rightarrow$ This can be faced by using the upper bound given by Crouziex upper-bound for matrix-functions.

Convergence: potential theory

In order to obtain the bounds and the rate of convergence, we need to work with the **Green functions** of $\overline{\mathbb{C}} \setminus W(A)$ and $\overline{\mathbb{C}} \setminus W(B)$ with poles at $\zeta \in \mathbb{C}$ called $g_A(\cdot, \zeta)$ and $g_B(\cdot, \zeta)$ respectively; (Saff and Totik 1997).

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With this **potential functions** the bound can then be expressed in terms of the functions

$$u_{A,m}(z) = \exp\left(-\sum_{j=1}^{m} g_A(z, z_{A,j})\right), \text{ and } u_{B,n}(z) = \exp\left(-\sum_{j=1}^{n} g_B(z, z_{B,j})\right).$$

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A mad research idea

Given the case we are interested in, can we find **optimal poles**, i.e., the one minimizing the bounds and have both α robustness, and M and N independence?

Let's blow up the bridges

What do we do if the **space coefficients** are **not separable**?

Let's blow up the bridges

What do we do if the **space coefficients** are **not separable**?

We decompose

$$d^{\pm}(x,y) = \sum_{k=1}^{K} t_k^{\pm} T_k(x) T_k(y)$$

and substitute in our equation obtaining

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- How do we select $\mathcal{V}$ and $\mathcal{W}$? How do we generate nested subspace? How do we solve the reduced multiterm equation? $\Rightarrow$ many more questions than answers... ☹.

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$$(P^{-1}AP)P^{-1}XP^{-H} + P^{-1}XP^{-H}(P^{H}BP^{-H}) = P^{-1}CP^{-H},$$

that is of no use since $P^{-1}AP \sim A$ and $P^{-1}BP \sim B$.

Can we use the **Kronecker structure** to put together **1D+2D** case as a **single matrix equation** or, more generally, **1D+dD equations** as a **single matrix equation**?

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This is a whole *different can of worms* and it's called *tensor equations*.

What if the **right-hand side** is **not low rank**?

We can use some **approximation strategy**, solve the matrix-equation **incompletely** and use it as a **preconditioner** inside a FGMRES method, or *turn to other structures*...

Rank-structured matrices

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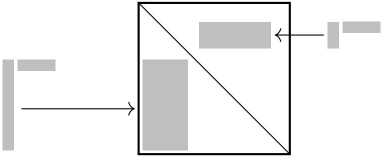
Quasiseparable matrix

A matrix A is *quasiseparable* of order k if the maximum of the ranks of all its submatrices contained in the strictly upper or lower part is less or equal than k.



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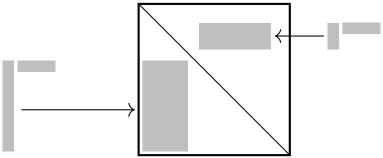
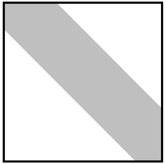


Example: k-banded matrices

A banded matrix with bandwidth k is quasiseparable of order (at most) k. In particular, diagonal matrices are quasiseparable of order 0, tridiagonal matrices are quasiseparable of order 1, *etc.*



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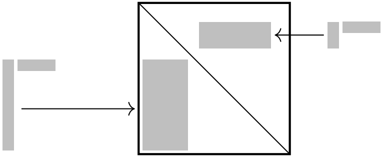

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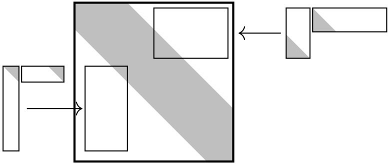

Rank-structured matrices

Theorem (Massei, Palitta, and Robol 2018, Theorem 2.7)

Let A and B be **symmetric positive definite** matrices of **quasiseparable** rank k_A and k_B, respectively, and suppose that the spectra of A and B are both contained in the interval $[a, b]$. Then, if X solves the Sylvester equation $AX + XB = C$, with C of **quasiseparable** rank k_C, a generic off-diagonal block Y of X satisfies

$$\frac{\sigma_{1+k\ell}(Y)}{\sigma_1(Y)} \leq 4\rho^{-2\ell},$$

where $k \triangleq k_A + k_B + k_C$, $\rho = \exp\left(\frac{\pi^2}{2\mu(\frac{b}{a})}\right)$ and $\mu(\cdot)$ the Grötzsch ring function

$$\mu(\lambda) \triangleq \frac{\pi}{2}\frac{K(\sqrt{1-\lambda^2})}{K(\lambda)}, \qquad K(\lambda) \triangleq \int_0^1 \frac{1}{(1-t^2)(1-\lambda^2 t^2)}\,\mathrm{d}t.$$

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⚠ As usual, the **non-symmetric case** requires using the field-of-values!

Rank-structured matrices

Theorem (Massei, Palitta, and Robol 2018, Theorem 2.12)

Let A, B be matrices of quasiseparable rank k_A and k_B respectively and such that $W(A) \subseteq E$ and $W(-B) \subseteq F$. Consider the Sylvester equation $AX + XB = C$, with C of quasiseparable rank k_C. Then a generic off-diagonal block Y of the solution X satisfies

$$\frac{\sigma_{1+k\ell}(Y)}{\sigma_1(Y)} \leq \mathcal{C}^2 \cdot Z_\ell(E, F), \qquad k := k_A + k_B + k_C.$$

Where $Z_\ell(E, F)$ is the solution of the **Zolotarev problem**

$$Z_\ell(E, F) \triangleq \inf_{r(x) \in \mathcal{R}_{\ell,\ell}} \frac{\max_{x \in E} |r(x)|}{\min_{y \in F} |r(y)|}, \qquad \ell \geq 1,$$

for $\mathcal{R}_{\ell,\ell}$ is the set of rational functions of degree at most (ℓ, ℓ), and $\mathcal{C}$ is the Crouzeix universal constant.

The Zolotarev 3rd Problem

Zolotarev's **third problem** is exactly the computation of

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Example: two equal intervals

One can prove that for $E = [-b, -1]$ and $F = [1, b]$ the solution is

$$\sup_{x\in[-b,1]\cup[1,b]} |R(x) - \mathrm{sgn}(x)| = \frac{\sqrt{Z_\ell(E,F)}}{1 + Z_\ell(E,F)}$$

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The Zolotarev 4^{th} Problem

A closed form solution, involving Jacobi elliptic functions, is available in the RKToolbox

```
b = 3; % E = [-b,-1] and F = [1,b]
k = 8; % Degree of rational approximant to sign.
% Solution to Z's fourth problem:
r = rkfun.gallery('sign', k/2, b);
% Plot the computed rational function:
x = linspace(-5, 5, 1000);
y1 = linspace(-3, -1, 1000);
y2 = linspace(1, 3, 1000);
fill([-b -1 -1 -b -b], 1.5*[-1 -1 1 1 -1], .9*[1 1
↪  1] ),
hold on
fill([b 1 1 b b],1.5*[-1 -1 1 1 -1],.9*[1 1 1] )
[~,l1,l2] = plotyy(x,r(x),[y1 0 y2],[(1-abs(r(y1)))
↪  NaN (1-abs(r(y2)))]);
l1.LineWidth = 2; l2.LineWidth = 2;
hold off
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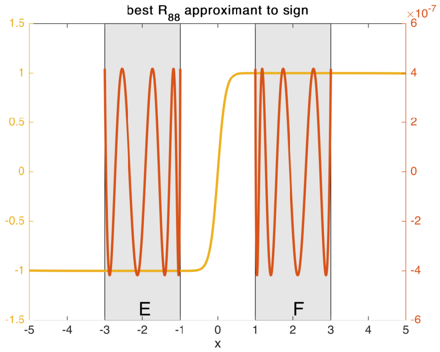

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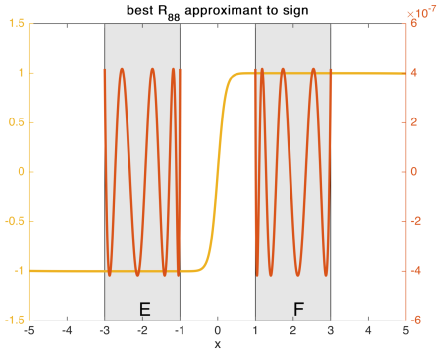


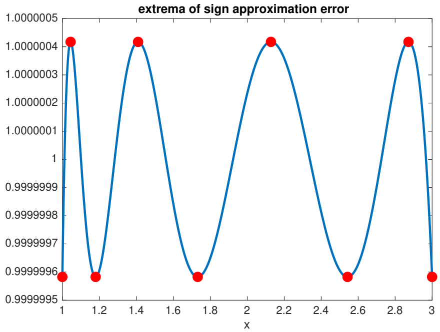
$\Rightarrow$ Zolotarev problem is then solved by solving for $Z_\ell(E, F)$.

The Zolotarev 3rd Problem

$$\text{Solve for } Z_\ell(E,F) \text{ s.t. } \sup_{x\in[-b,1]\cup[1,b]} |R(x) - \mathrm{sgn}(x)| = \frac{\sqrt{Z_\ell(E,F)}}{1+Z_\ell(E,F)}$$

```
% Extrema for [-1,-1/b]\cup [1/b,1]:
K = ellipke(1-1/b^2);
[sn, cn, dn] = ellipj((0:k)*K/k, 1-1/b^2);
% Transplant to [-b,-1]\cup [1,b]:
extrema = b*dn;
vals = 1-r(extrema);
c = mean( vals(1:2:end) );
e = eig( [ 2-4/c^2 1 ; 1 0 ] );
Zk = min(abs(e))
```

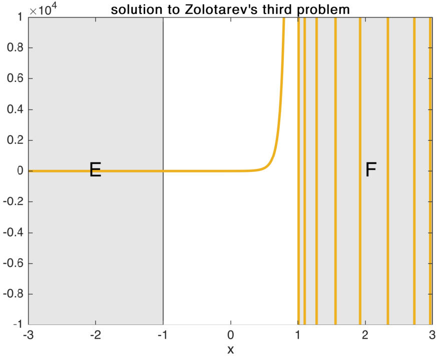
From which we obtain `Zk = 4.3542e-14`.



The Zolotarev 3rd Problem

To visualize the function realizing the extrema, one can use a Mobius transform to convert the best rational approximation to the sgn function that solves the 4th problem $r(x)$ to the extremal rational function $R_{\ell,\ell}(x)$ solving the 3rd:

$$R_{\ell,\ell}(x) = \frac{\frac{1+Z_\ell(E,F)}{(1-Z_\ell(E,F))r(x)}}{\left(1 - \frac{1+Z_\ell(E,F)}{1-Z_\ell(E,F)} r(x)\right)}$$



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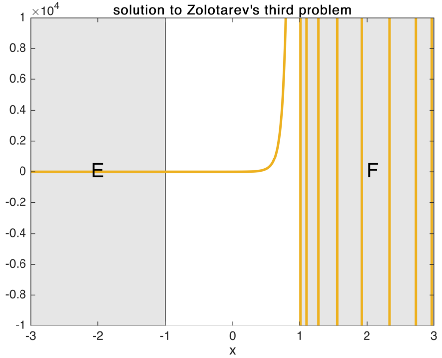

- There are **other cases** for which one can solve the 3rd problem, e.g., *unsymmetrical intervals*, or *rectangles* (Istace and Thiran 1995).

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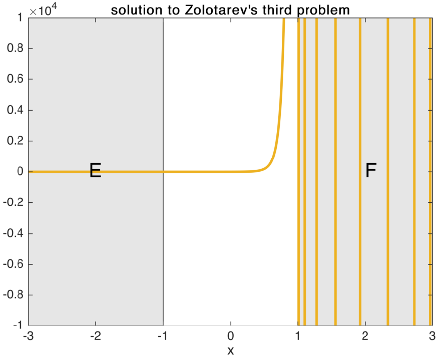

- There are **other cases** for which one can solve the 3rd problem, e.g., *unsymmetrical intervals*, or *rectangles* (Istace and Thiran 1995).
- If we are satisfied by the quasi-separability rank of the solution we can then attempt it!

Conclusion and summary

- ✅ We have reformulated several of our problems in terms of matrix equations,
- ✅ We have discussed projection methods for the solution of Sylvester equations,
- ✅ We have seen some limitations of the approach and shown a possible extension.

Next up

- 📋 More on rank-structured matrices and related solution strategies,
- 📋 All-at-once in time: using different methods to march in time than the standard ones,
- 📋 Still some other approaches with structured preconditioners.

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