RKFUNctions

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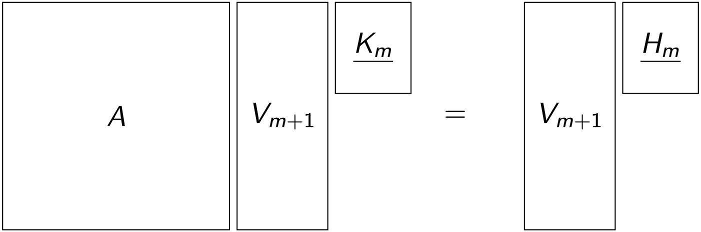
What is an RKFUNction?

An RKFUNction is a representation of a rational function based on a *rational Arnoldi decomposition* (RAD)

$$AV_{m+1}\underline{K_m} = V_{m+1}\underline{H_m}$$

for the space $\mathcal{Q}_{m+1}(A, b, q_m) = q_m^{-1}(A)\mathcal{K}_{m+1}(A, b)$. The upper Hessenberg matrices $\underline{H_m}$ and $\underline{K_m}$ form an unreduced pencil $(\underline{H_m}, \underline{K_m})$.



What is an RKFUNction?

The RAD encodes a basis of rational functions $\{r_j\}_{j=0}^{m}$ of type at most $[m, m]$ with fixed denominator q_m. A rational function can then be specified as a linear combination of these basis functions.

- Scalar coefficients $\implies$ RKFUN

$$r(z) = \sum_{j=0}^{m} c_j r_j(z), \text{ where } c_j \in \mathbb{C} \text{ for } j = 0, 1, \ldots, m.$$

- Matrix coefficients $\implies$ RKFUNM

$$R(z) = \sum_{j=0}^{m} r_j(z) C_j, \text{ where } C_j \in \mathbb{C}^{n_1 \times n_2} \text{ for } j = 0, 1, \ldots, m.$$

And so $r \equiv (\underline{H_m}, \underline{K_m}, \texttt{coeffs})$.

RKFUN basis functions

An RKFUN can be evaluated at a scalar $z \in \mathbb{C}$ ($q_m(z) \neq 0$). When evaluating at a scalar, the basis functions must satisfy the RAD,

$$z[r_0(z), r_1(z), \ldots, r_m(z)]\underline{K_m} = [r_0(z), r_1(z), \ldots, r_m(z)]\underline{H_m}.$$

Reading the decomposition columnwise, assuming $r_0(z) \equiv 1$, gives:

$$\begin{gathered} zk_{11} + zr_1(z)k_{21} = h_{11} + r_1(z)h_{21} \\ zk_{12} + zr_1(z)k_{22} + zr_2(z)k_{32} = h_{12} + r_1(z)h_{22} + r_2(z)h_{32} \\ \vdots \end{gathered}$$

The basis functions are

$$r_j(z) = \frac{p_j(z)}{q_j(z)},$$

where $p_j(z) = \det(zK_j - H_j)$ and $q_j(z) = \prod_{i=1}^{j}(h_{i+1,i} - k_{i+1,i}z)$.

Creating an RKFUN

- Using MATLABs symbolic toolbox:

```
r = rkfun('(x+1)*(x-2)/(x-3)^2')
```

- Specifying the roots and poles of the rational function:

```
r = rkfun.nodes2rkfun([-1, 2], [3, 3])
```

- Converting from barycentric representation using the function

```
util_bary2rkfun
```

rkfun.nodes2rkfun

Split into type [0, 1], [1, 0] or [1, 1] rational functions, convert to RKFUNs then multiply together.

- $\frac{1}{z-\xi} \equiv \left(\begin{pmatrix} 1 \\ \xi \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, [0, 1] \right)$
- $z - \zeta \equiv \left(\begin{pmatrix} \zeta \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, [0, 1] \right)$
- $\frac{z-\zeta}{z-\xi} \equiv \left(\begin{pmatrix} -\zeta \\ \xi \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \end{pmatrix}, [0, 1] \right)$

So `r = rkfun.nodes2rkfun([-1, 2], [3, 3])` gives

$$\underline{H_2} = \begin{pmatrix} 1 & 0 \\ 3 & -2 \\ 0 & 3 \end{pmatrix}, \quad \underline{K_2} = \begin{pmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{pmatrix},$$

and

$$c = [0, 0, 1].$$

Barycentric representation

Rational barycentric representation is given by:

$$r(z) = \frac{n(z)}{d(z)} = \sum_{j=0}^{m} \frac{w_j f_j}{z - z_j} \Big/ \sum_{j=0}^{m} \frac{w_j}{z - z_j}$$

$$= \sum_{j=0}^{m} f_j \left(\frac{\frac{w_j}{z-z_j}}{\sum_{i=0}^{m} \frac{w_i}{z-z_i}} \right) = \sum_{j=0}^{m} f_j r_j(z),$$

- $z_0, z_1, \ldots, z_m$ - distinct 'support points',
- $f_0, f_1, \ldots, f_m$ - 'data values',
- $w_0, w_1, \ldots, w_m$ - 'weights'.

Interpolation property: $\lim_{z \to z_j} r(z) = f_j$.

Type of barycentric representation

Node polynomial $\ell(z)$ associated to $z_0, z_1, \cdots, z_m$ is

$$\ell(z) = \prod_{j=1}^{m} (z - z_j).$$

Define $p(z) = \ell(z)n(z)$ and $q(z) = \ell(z)d(z)$.

Then

$$r(z) = \frac{p(z)/\ell(z)}{q(z)/\ell(z)} = \frac{p(z)}{q(z)}$$

is a type $[m, m]$ rational function.

util_bary2rkfun

The barycentric form basis funcions r_j can be written as a recursion by

$$z(w_{j-1}r_j(z) - w_j r_{j-1}(z)) = w_{j-1}z_j r_j(z) - w_j z_{j-1} r_{j-1}(z),$$

which forms a RAD

$$z[r_0(z)\ r_1(z)\ \cdots\ r_m(z)]\underline{W_m} = [r_0(z)\ r_1(z)\ \cdots\ r_m(z)]Z_m\underline{W_m},$$

with

$$Z_m = \begin{bmatrix} z_0 & & & & \\ & z_1 & & & \\ & & \ddots & & \\ & & & z_{m-1} & \\ & & & & z_m \end{bmatrix}, \quad \underline{W_m} = \begin{bmatrix} -w_1 & & & \\ w_0 & -w_2 & & \\ & \ddots & \ddots & \\ & & w_{m-2} & -w_m \\ & & & w_{m-1} \end{bmatrix}.$$

So $r \equiv (Z_m\underline{W_m}, \underline{W_m}, f)$. See [Elsworth & Güttel, 2017].

RKFUNctions from BRADs?

Consider a *block rational Arnoldi decomposition* (BRAD)

$$A\mathbf{V}_{m+1}\underline{\mathbf{K}_m} = \mathbf{V}_{m+1}\underline{\mathbf{H}_m}$$

for the space $\mathcal{Q}^{\square}_{m+1}(A, \mathbf{b}, q_m) = q_m(A)^{-1}\mathcal{K}^{\square}_{m+1}(A, \mathbf{b})$. The block upper-Hessenberg matrices $\underline{\mathbf{H}_m}$ and $\underline{\mathbf{K}_m}$ form an unreduced pencil $(\underline{\mathbf{H}_m}, \underline{\mathbf{K}_m})$.

$$A \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 \end{bmatrix} \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \\ & K_{32} \end{bmatrix} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 \end{bmatrix} \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \\ & H_{32} \end{bmatrix}$$

Unreduced means: $\nu_j H_{j+1,j} = \mu_j K_{j+1,j}$ with at least one of $H_{j+1,j}$ and $K_{j+1,j}$ invertible.

Basis functions

The BRAD encodes a set of matrix-valued basis functions $\{R_j\}_{j=0}^{m}$ of type at most $[m, m]$. The functions can be evaluated at a scalar $z \in \mathbb{C}$ $(q_m(z) \neq 0)$. When evaluating at a scalar, the basis functions evaluated at the scalar satisfy the BRAD,

$$z[R_0(z), R_1(z), \ldots, R_m(z)]\underline{\mathbf{K}_m} = [R_0(z), R_1(z), \ldots, R_m(z)]\underline{\mathbf{H}_m}.$$

Reading the decomposition columnwise, assuming $R_0(z) \equiv I$ gives:

$$\begin{gathered} zK_{11} + zR_1(z)K_{21} = H_{11} + R_1(z)H_{21} \\ zK_{12} + zR_1(z)K_{22} + zR_2(z)K_{32} = H_{12} + R_1(z)H_{22} + R_2(z)H_{32} \\ \vdots \end{gathered}$$

Basis functions are RKFUNMs

Now

$$zK_{11} + zR_1(z)K_{21} = H_{11} + R_1(z)H_{21}$$

can be written as

$$(\mu_1 - \nu_1 z)R_1(z) = (z\tilde{K}_{11} - \tilde{H}_{11}),$$

so

$$R_1(z) = (\mu_1 - \nu_1 z)^{-1}(z\tilde{K}_{11} - \tilde{H}_{11}).$$

Furthermore

$$(\mu_1 - \nu_1 z)(\mu_2 - \nu_2 z)R_2(z) = (z\tilde{K}_{11} - \tilde{H}_{11})(z\tilde{K}_{22} - \tilde{H}_{22}) - (\nu_1 z - \mu_1)(z\tilde{K}_{12} - \tilde{H}_{12}).$$

Overview

- RKFUN:
  - $r(z) : \mathbb{C} \to \mathbb{C}$
  - $r(A)b : (\mathbb{C}^{N \times N}, \mathbb{C}^N) \to \mathbb{C}^N$
- RKFUNM (from RAD):
  - $r(z) : \mathbb{C} \to \mathbb{C}^{n_1 \times n_2}$
- BRAD basis functions are RKFUNMs, rerunning provides efficient evaluation.
- Implementation of RKFUNMs in RKToolbox v2.6.
- As of RKToolbox v2.7, can use this in combination with AAA algorithm [Nakatsukasa et al., 2016] to sample and evaluate matrix-valued rational functions. See `http://guettel.com/rktoolbox/examples/html/example_aaa.html`.