

# Gauss-Radau and Christoffel-Darboux formulas for rational functions via structured matrices

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Cortona, Sept. 18, 2008



# Introduction: ORFs with real poles

Given the real numbers  $a_1, \dots, a_n$  all different from each other, consider the basis functions

$$f_0(x) = 1, \quad f_i(x) = (x - a_i)^{-1}, \quad i = 1, \dots, n, \quad f_{n+1}(x) = x.$$

Let  $\mathbf{f}(x) = (f_0(x), \dots, f_n(x))^T$ . Observe that

$$x\mathbf{f}(x) = \begin{pmatrix} 0 & & & \\ 1 & a_1 & & \\ \vdots & & \ddots & \\ 1 & & & a_n \end{pmatrix} \mathbf{f}(x) + f_{n+1}(x) \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = K\mathbf{f}(x) + f_{n+1}(x)\mathbf{e}_0.$$

Let  $d\mu(x)$  be a nonnegative measure on  $\mathbb{R}$  such that all integrals

$$\langle f_i, f_j \rangle = I(f_i f_j) = \int_{\mathbb{R}} f_i(x) f_j(x) d\mu(x), \quad i, j = 0, \dots, n+1,$$

exist and are finite, with  $\int f_i(x)^2 d\mu(x) > 0$ .



# Introduction: ORFs with real poles

Hence, the inner product  $\langle f, g \rangle = \int f(x)g(x) d\mu(x)$   
is positive definite on  $\text{Span}\{f_0, \dots, f_{n+1}\}$ .

$\Rightarrow$  the Gram matrix  $A \equiv (\langle f_i, f_j \rangle)$  is PD.

Orthogonalize  $f_0, \dots, f_n, f_{n+1} \rightarrow$  a set of ORFs  $\phi_0, \dots, \phi_n, \phi_{n+1}$ ,  
 $\langle \phi_i, \phi_j \rangle = \delta_{i,j}$ ,

$$\phi_i(x) = \frac{p_i(x)}{\prod_{k=1}^i (x - a_k)}, \quad \phi_{n+1}(x) = \frac{p_{n+1}(x)}{\prod_{k=1}^n (x - a_k)}, \quad \deg(p_i) = i.$$

With  $\phi(x) = (\phi_0(x), \dots, \phi_n(x))^T$  we have

$$\underbrace{\begin{pmatrix} L \\ \mathbf{v}^T & \alpha \end{pmatrix}}_{\hat{L}} \begin{pmatrix} \phi(x) \\ \phi_{n+1}(x) \end{pmatrix} = \begin{pmatrix} \mathbf{f}(x) \\ f_{n+1}(x) \end{pmatrix}, \quad A^{-1} = \hat{L} \hat{L}^T.$$



# ORFs and DPSS matrices

From  $x\mathbf{f}(x) = K\mathbf{f}(x) + f_{n+1}(x)\mathbf{e}_0$  we obtain:

$$\begin{aligned} x\phi(x) = xL^{-1}\mathbf{f}(x) &= [L^{-1}K \mid L^{-1}\mathbf{e}_0] \begin{pmatrix} \mathbf{f}(x) \\ f_{n+1}(x) \end{pmatrix} \\ &= [L^{-1}K \mid L^{-1}\mathbf{e}_0] \begin{pmatrix} L \\ \mathbf{v}^T \end{pmatrix} \begin{pmatrix} \phi(x) \\ \phi_{n+1}(x) \end{pmatrix} \\ &= \underbrace{[L^{-1}KL + L^{-1}\mathbf{e}_0\mathbf{v}^T]}_G \phi(x) + \phi_{n+1}(x) \underbrace{\alpha L^{-1}\mathbf{e}_0}_{\ell}. \end{aligned}$$

## Theorem

It holds  $x\phi(x) = G\phi(x) + \phi_{n+1}(x)\ell$ . The matrix  $G$  is a symmetric, diagonal-plus-semiseparable matrix,  $G = \text{Diag}(0, a_1, \dots, a_n) + S$ , and the vector  $\ell$  is parallel to the last column of  $S$ :  $\ell = \gamma_n S \mathbf{e}_n$ .



# ORFs and DPSS matrices

- Integral formula:

$$\int_{\mathbb{R}} x \phi(x) \phi(x)^T d\mu(x) = \int_{\mathbb{R}} [G \phi(x) + \phi_{n+1}(x) \ell] \phi(x)^T d\mu(x) = G.$$

- $G$  is diagonal-plus-semiseparable (DPSS):

$$\begin{aligned} G &= L^{-1} K L + \underbrace{L^{-1} \mathbf{e}_0}_{\mathbf{u}} \mathbf{v}^T = \begin{pmatrix} 0 & & & \\ * & a_1 & & \\ \vdots & \ddots & \ddots & \\ * & \dots & * & a_n \end{pmatrix} + \mathbf{u} \mathbf{v}^T \\ &= \text{Diag}(0, a_1, \dots, a_n) + \begin{pmatrix} u_0 v_0 & u_0 v_1 & \dots & u_0 v_n \\ u_0 v_1 & u_1 v_1 & \dots & u_1 v_n \\ \vdots & \vdots & \ddots & \vdots \\ u_0 v_n & u_1 v_n & \dots & u_n v_n \end{pmatrix}. \end{aligned}$$



# The Gauss quadrature formula

The numerator of  $\phi_{n+1}(x) = p_{n+1}(x)/\prod_{k=1}^n(x - a_k)$  is a multiple of  $\det(G - xl)$ .

$$\phi_{n+1}(\bar{x}) = 0 \implies G\phi(\bar{x}) = \bar{x}\phi(\bar{x}), \quad \bar{x} \in \mathbb{R}.$$

Moreover, the function  $\phi_{n+1}(x)$  has distinct zeros,  $x_0, \dots, x_n$ . Hence,

$$w_0\phi(x_0), \dots, w_n\phi(x_n), \quad w_j = \pm 1/\|\phi(x_j)\|$$

are orthonormal vectors;  $U \equiv (w_j\phi_i(x_j)) \Rightarrow G = U\text{Diag}(x_0, \dots, x_n)U^T$ .

Moreover,

$$UU^T = I \implies \sum_{k=0}^n w_k^2 \phi_i(x_k) \phi_j(x_k) = \delta_{i,j}, \quad i, j = 0, \dots, n.$$



# The Gauss quadrature formula

Consider the quadrature formula

$$I_{n+1}(f) = \sum_{k=0}^n w_k^2 f(x_k) \quad \sim \quad I(f) = \int_{\mathbb{R}} f(x) d\mu(x).$$

For  $i, j = 0, \dots, n$  we have

$$I_{n+1}(\phi_i \phi_j) = \delta_{i,j} = I(\phi_i \phi_j), \quad I_{n+1}(\phi_i \phi_{n+1}) = 0 = I(\phi_i \phi_{n+1}).$$

## Theorem

$f \in \mathcal{S}_{n,G} \implies I_{n+1}(f) = I(f)$ , where

$$\begin{aligned} \mathcal{S}_{n,G} &= \text{Span}\{\phi_i(x)\phi_j(x), 0 \leq i \leq n+1, 0 \leq j \leq n\} \\ &= \left\{ \frac{p(x)}{\prod_{i=1}^n (x - a_i)^2}, \quad p(x) \in \mathcal{P}_{2n+1} \right\}. \end{aligned}$$

## Earlier and related works

- Initial works: Van Assche and Vanherwegen [Math. Comp. '93], López and Illán ('87)
- Gautschi [1993–2001]. The approach: properly **modify the weights** of a classical (i.e., polynomial) Gauss formula in order to get the sought exactness for given spaces of rational functions.

**Collocating poles in the integrand gives much better results.**

- On the interplay between ORFs, rational quadrature, and numerical linear algebra, see Bultheel and coauthors [1999–2005] (Padé approx., rational moment pbs.), Zhedanov [1999–2001] (tridiag. pencils).
- Computational aspects of ORFs and rational Gauss-type quadrature formulas (with semiseparable matrices): F., Gemignani [2002–03], Van Barel, F. Gemignani, Mastronardi [2005].



# Motivations (from NLA)

Functionals  $u^T f(A)u$  can be recast as  $I(f) = \int f(x)d\mu(x)$ ,  
that can be approximated via Gauss rules,  
see Golub, Meurant; *Matrices, moments, and quadrature (I, II)*

Whenever  $f^{(k)}(x)$  has constant sign, Gauss, Gauss-Radau and  
Gauss-Lobatto rules provide **bracketings** for  $I(f)$ .

Classical (polynomial) case: construction via tridiagonals  $T_k$   
obtained from Lanczos process:  $u^T f(A)u \approx \mathbf{e}_1^T f(T_k) \mathbf{e}_1$ .

Recent approach: use **rational variants** (Ruhe's rational Lanczos).

DPSS matrices replace tridiagonals.

Bracketing properties for G, GR, GL, are the same; see  
López Lagomasino, Reichel, Wunderlich. *Matrices, moments, and rational  
quadrature* (2008).



# Motivations (from ORF theory)

Recurrence relations of ORFs are described in terms of tridiagonal pencils  
(see Bultheel and others; Zhedanov)

Borwein, Erdélyi, Zhang [J. London Math. Soc. 1994]  
give explicit forms for Chebyshev-type ORFs with arb. real poles

The construction of associated DPSS matrix  $G$  is immediate.



# Gauss-Radau formulas

**Goal:** a quadrature formula

$$I_{n+1}^R(f) = \sum_{k=0}^n \tilde{w}_k^2 f(\tilde{x}_k),$$

such that  $\tilde{x}_0 = a$  is **prescribed**, and  $I_{n+1}^R(f) = I(f)$  whenever  $f \in \mathcal{S}_{n,R}$ ,

$$\mathcal{S}_{n,R} = \left\{ \frac{p(x)}{\prod_{i=1}^n (x - a_i)^2}, \deg(p(x)) \leq 2n \right\} = \text{Span} \left\{ \phi_i \phi_j, 0 \leq i, j \leq n \right\}.$$

Equivalently, we look for a discrete inner product,

$$\langle f, g \rangle_R = I_{n+1}^R(fg) = \sum_{k=0}^n \tilde{w}_k^2 f(\tilde{x}_k)g(\tilde{x}_k),$$

with the property  $\langle \phi_i, \phi_j \rangle_R = \langle \phi_i, \phi_j \rangle$ , for  $i, j = 0, \dots, n$ .

**Remark.** If we orthogonalize  $f_0, \dots, f_n$  with respect to  $\langle \cdot, \cdot \rangle_R$ , we end up with  $\phi_0, \dots, \phi_n$ .



# Gauss-Radau formulas

Let

$$\mathcal{J}_R = \{(i, j) : 0 \leq i, j \leq n\} \setminus \{(0, 0)\}.$$

Remark that

$$(i, j) \in \mathcal{J}_R \iff I_{n+1}^R(x\phi_i(x)\phi_j(x)) = I(x\phi_i(x)\phi_j(x)).$$

Define

$$G_R \equiv (I_{n+1}^R(x\phi_i(x)\phi_j(x))).$$

Hence,  $G_R$  is a DPSS matrix such that  $G_R(\mathcal{J}_R) = G(\mathcal{J}_R)$ :

$$G = \begin{pmatrix} u_0 v_0 & u_0 \hat{\mathbf{v}}^T \\ u_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix} \implies G_R = \begin{pmatrix} \textcolor{blue}{u_0 \tilde{v}_0} & u_0 \hat{\mathbf{v}}^T \\ u_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix}, \quad \hat{\mathbf{v}}^T = (v_1, \dots, v_n).$$

We have to impose  $a \in \lambda(G_R)$ :  $G_R \phi(a) = a \phi(a)$ .



# Gauss-Radau formulas

Consider the eigenvalue-eigenvector equation  $G_R \phi(a) = a\phi(a)$ :

$$\underbrace{\begin{pmatrix} g_{0,0} & u_0 \hat{\mathbf{v}}^T \\ u_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix}}_{G_R} \underbrace{\begin{pmatrix} \phi_0 \\ \hat{\phi} \end{pmatrix}}_{\phi(a)} = \begin{pmatrix} g_{0,0}\phi_0 + u_0 \hat{\mathbf{v}}^T \hat{\phi} \\ u_0 \phi_0 \hat{\mathbf{v}} + \hat{G} \hat{\phi} \end{pmatrix} = \underbrace{\begin{pmatrix} a\phi_0 \\ a\hat{\phi} \end{pmatrix}}_{a\phi(a)}.$$

Here  $g_{0,0} = u_0 \tilde{v}_0$ . We obtain:

$$(\hat{G} - aI)\hat{\phi} = -u_0 \phi_0 \hat{\mathbf{v}}, \quad g_{0,0}\phi_0 = a\phi_0 - u_0 \hat{\mathbf{v}}^T \hat{\phi}.$$

Introduce the auxiliary vector  $\xi = -\hat{\phi}/\phi_0$ . Hence,

$$(\hat{G} - aI)\xi = u_0 \hat{\mathbf{v}}, \quad g_{0,0} = a + u_0 \hat{\mathbf{v}}^T \xi.$$



# Gauss-Lobatto formulas

**Goal:** a quadrature formula

$$I_{n+1}^L(f) = \sum_{k=0}^n \bar{w}_k^2 f(\bar{x}_k),$$

with  $\bar{x}_0 = a$  and  $\bar{x}_n = b$  **prescribed**, and  $I_{n+1}^L(f) = I(f)$  whenever  $f \in \mathcal{S}_{n,L}$ ,

$$\begin{aligned}\mathcal{S}_{n,L} &= \left\{ p(x) / \prod_{i=1}^n (x - a_i)^2, \deg(p(x)) \leq 2n - 1 \right\} \\ &= \text{Span} \{ \phi_i \phi_j, 0 \leq i \leq n, 1 \leq j \leq n \}.\end{aligned}$$

In other words, we look for a discrete inner product,

$$\langle f, g \rangle_L = I_{n+1}^L(fg) = \sum_{k=0}^n \bar{w}_k^2 f(\bar{x}_k)g(\bar{x}_k),$$

such that  $\langle \phi_i, \phi_j \rangle_L = \langle \phi_i, \phi_j \rangle$  for  $0 \leq i \leq n$  and  $1 \leq j \leq n$ .



# Gauss-Lobatto formulas

**Remark:** If we orthogonalize  $f_0, \dots, f_n$  with respect to  $\langle \cdot, \cdot \rangle_L$  then we obtain functions  $\varphi_0, \dots, \varphi_n$  such that  $\varphi_i(x) = \phi_i(x)$ , for  $1 \leq i \leq n$ , while in general  $\varphi_0 \neq \phi_0$ .

Let

$$\mathcal{J}_L = \{(i, j) : 1 \leq i, j \leq n\}.$$

Remark that

$$(i, j) \in \mathcal{J}_L \iff I_{n+1}^L(x\varphi_i(x)\varphi_j(x)) = I(x\phi_i(x)\phi_j(x)).$$

Now let

$$G_L \equiv (I_{n+1}^L(x\varphi_i(x)\varphi_j(x))).$$

Hence,  $G_L$  is a DPSS matrix such that  $G_L(\mathcal{J}_L) = G(\mathcal{J}_L)$ :

$$G = \begin{pmatrix} u_0 v_0 & u_0 \hat{\mathbf{v}}^T \\ u_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix} \implies G_L = \begin{pmatrix} \bar{u}_0 \bar{v}_0 & \bar{u}_0 \hat{\mathbf{v}}^T \\ \bar{u}_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix}.$$



# Gauss-Lobatto formulas

In other words, the problem of devising the Gauss-Lobatto formula reduces to scale the first row and column of  $G$  (i.e., determine  $\bar{u}_0, \bar{v}_0$ ) so that  $a, b \in \lambda(G_L)$ :

$$G_L \varphi(a) = a\varphi(a), \quad G_L \varphi(b) = b\varphi(b).$$

**Remark:** If  $(\bar{u}_0, \bar{v}_0)$  is a solution of this problem, then also  $(-\bar{u}_0, -\bar{v}_0)$  is a solution, since

$$\begin{pmatrix} \bar{u}_0 \bar{v}_0 & \bar{u}_0 \hat{\mathbf{v}}^T \\ \bar{u}_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix} = \begin{pmatrix} -1 & \\ & I \end{pmatrix} \begin{pmatrix} \bar{u}_0 \bar{v}_0 & -\bar{u}_0 \hat{\mathbf{v}}^T \\ -\bar{u}_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix} \begin{pmatrix} -1 & \\ & I \end{pmatrix}.$$



# Gauss-Lobatto formulas

Denote  $\varphi(x) = (\varphi_0(x), \dots, \varphi_n(x))^T$ .

Consider the eigenvalue-eigenvector equations  $G_L \varphi(a) = a\varphi(a)$ :

$$\underbrace{\begin{pmatrix} a\varphi_0 \\ a\hat{\varphi}_a \end{pmatrix}}_{a\varphi(a)} = \underbrace{\begin{pmatrix} \bar{u}_0 \bar{v}_0 & \bar{u}_0 \hat{\mathbf{v}}^T \\ \bar{u}_0 \hat{\mathbf{v}} & \hat{G} \end{pmatrix}}_{G_L} \underbrace{\begin{pmatrix} \varphi_0 \\ \hat{\varphi}_a \end{pmatrix}}_{\varphi(a)} = \begin{pmatrix} \bar{u}_0 \bar{v}_0 \varphi_0 + \bar{u}_0 \hat{\mathbf{v}}^T \hat{\varphi}_a \\ \bar{u}_0 \varphi_0 \hat{\mathbf{v}} + \hat{G} \hat{\varphi}_a \end{pmatrix}.$$

We obtain

$$(\hat{G} - aI)\hat{\varphi}_a = -\bar{u}_0 \varphi_0 \hat{\mathbf{v}}, \quad \bar{u}_0 \bar{v}_0 \varphi_0 = a\varphi_0 - \bar{u}_0 \hat{\mathbf{v}}^T \hat{\varphi}_a.$$

Introduce the auxiliary notations  $\xi_a = -\hat{\varphi}_a / (\bar{u}_0 \varphi_0)$ . We have:

$$(\hat{G} - aI)\xi_a = \hat{\mathbf{v}}, \quad \bar{u}_0 \bar{v}_0 = a + \bar{u}_0^2 \hat{\mathbf{v}}^T \xi_a.$$



# Gauss-Lobatto formulas

Consider analogously  $G_L \varphi(a) = a\varphi(a)$ . Eventually,

$$(\widehat{G} - bl)\xi_b = (\widehat{G} - al)\xi_a = \hat{v}, \quad \bar{u}_0\bar{v}_0 = a + \bar{u}_0^2 \hat{v}^T \xi_a = b + \bar{u}_0^2 \hat{v}^T \xi_b.$$

From the equations  $\bar{v}_0 = a/\bar{u}_0 + \bar{u}_0 \hat{v}^T \xi_a = b/\bar{u}_0 + \bar{u}_0 \hat{v}^T \xi_b$ ,  
we have

$$\frac{\hat{v}^T (\xi_a - \xi_b)}{b - a} = \frac{1}{\bar{u}_0^2}.$$

The resulting algorithm:

- Solve  $(\widehat{G} - al)\xi_a = \hat{v}$  and  $(\widehat{G} - bl)\xi_b = \hat{v}$ .
- Compute  $\bar{u}_0 = [\hat{v}^T (\xi_a - \xi_b)/(b - a)]^{-1/2}$ .
- Compute  $\bar{v}_0$  as either  $\bar{u}_0(a/\bar{u}_0^2 + \hat{v}^T \xi_a)$  or  $\bar{u}_0(b/\bar{u}_0^2 + \hat{v}^T \xi_b)$ .



# Gauss-Lobatto formulas

**Question:** Is the expression for  $\bar{u}^2 > 0$ ?

**Answer:** Suppose that  $a < (\text{the other nodes}) < b$ .

Hence,  $\hat{G} - al$  is positive definite, while  $\hat{G} - bl$  is negative definite.

As a consequence,  $\hat{\mathbf{v}}^T \xi_a = \xi_a^T (\hat{G} - al) \xi_a > 0$  and  
 $\hat{\mathbf{v}}^T \xi_b = \xi_b^T (\hat{G} - bl) \xi_b < 0$ , whence

$$\hat{\mathbf{v}}^T (\xi_a - \xi_b) > 0 \implies \bar{u}_0^2 = \frac{b-a}{\hat{\mathbf{v}}^T (\xi_a - \xi_b)} > 0.$$



# Christoffel-Darboux formula

## The CD identity for classical OPs

Let  $p_0(x), \dots, p_{n+1}(x)$  be a sequence of classical OPs. Then,

$$(x - y) \sum_{k=0}^n p_k(x)p_k(y) = \beta_{n+1}[p_{n+1}(x)p_n(y) - p_n(x)p_{n+1}(y)].$$

## Theorem

Let  $\phi_0(x), \dots, \phi_{n+1}(x)$  be as in the previous discussion. Then,

$$(x - y) \sum_{k=0}^n \phi_k(x)\phi_k(y) = \gamma_n[\phi_{n+1}(y)\phi_n(x)(x - a_n) - \phi_{n+1}(x)\phi_n(y)(y - a_n)].$$



## CD formula: proof

Start from  $G\phi(x) = x\phi(x) + \phi_{n+1}(x)\ell$ .

Multiply on the left by  $\phi(y)^T$  and interchange variables, to obtain

$$\begin{aligned} G\phi(x)\phi(y)^T &= x\phi(x)\phi(y)^T + \phi_{n+1}(x)\ell\phi(y)^T \\ G\phi(y)\phi(x)^T &= y\phi(y)\phi(x)^T + \phi_{n+1}(y)\ell\phi(x)^T. \end{aligned}$$

Transpose, and subtract. Since  $G = G^T$ ,

$$\begin{aligned} (x - y)\phi(x)\phi(y)^T &= G\phi(x)\phi(y)^T - \phi(x)\phi(y)^T G \\ &\quad + \phi_{n+1}(y)\phi(x)\ell^T - \phi_{n+1}(x)\ell\phi(y)^T. \end{aligned}$$

Take traces in both sides. Recall  $\text{tr}(AB) = \text{tr}(BA)$ . Hence

$$(x - y) \sum_{k=0}^n \phi_k(x)\phi_k(y) = \phi_{n+1}(y)\text{tr}(\phi(x)\ell^T) - \phi_{n+1}(x)\text{tr}(\ell\phi(y)^T).$$



# CD formula: proof

## Claim:

$$\text{tr}(\phi(x)\ell^T) = \gamma_n[(x - a_n)\phi_n(x) + \ell_n\phi_{n+1}(x)].$$

Using this claim, the proof is easily completed.

## Proof of the claim:

Recall that  $\ell = \gamma_n S \mathbf{e}_n$ . From  $(S + D)\phi(x) = x\phi(x) + \phi_{n+1}(x)\ell$  we have:

$$S\phi(x) = [xI - D]\phi(x) + \phi_{n+1}(x)\ell.$$

With simple arguments,

$$\begin{aligned}\text{tr}(\phi(x)\ell^T) &= \gamma_n \text{tr}(S\phi(x)\mathbf{e}_n^T) \\ &= \gamma_n \text{tr}([xI - D]\phi(x)\mathbf{e}_n^T) + \gamma_n \phi_{n+1}(x) \text{tr}(\ell \mathbf{e}_n^T) \\ &= \gamma_n(x - a_n)\phi_n(x) + \gamma_n \ell_n \phi_{n+1}(x),\end{aligned}$$

and we have the claim.

