Modification Algorithms in the Theory of Orthogonal Polynomials

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Orthogonal Polynomials

$\mathrm{d}\lambda$	(positive) measure on $[a,b]$, $-\infty \le a < b \le \infty$
$(\,\cdot\,,\,\cdot\,) = (\,\cdot\,,\,\cdot\,)_{\mathrm{d}\lambda}$	inner product $(u,v)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} u(t)v(t)\mathrm{d}\lambda(t)$
$\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\mathrm{d}\lambda)$	(monic) polynomial of degree k orthogonal relative to the measure $\mathrm{d}\lambda$
	$(\pi_k,\pi_\ell)_{\mathrm{d}\lambda} \begin{cases} = 0 & \text{if } k \neq \ell \\ > 0 & \text{if } k = \ell \end{cases}$
$\|\pi_k\|_{\mathrm{d}\lambda}$	norm $\sqrt{(\pi_k,\pi_k)_{\mathrm{d}\lambda}}$

Three-Term Recurrence Relation

$$\pi_{k+1}(z) = (z - \alpha_k)\pi_k(z) - \beta_k \pi_{k-1}(z), \quad k = 0, 1, 2, \ldots$$

$$\pi_{-1}(z) = 0, \quad \pi_0(z) = 1$$

where $\alpha_k = \alpha_k(\mathrm{d}\lambda) \in \mathbb{R}$, $\beta_k = \beta_k(\mathrm{d}\lambda) > 0$ (if $\mathrm{d}\lambda$ is positive)

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Darboux formulae

$$\alpha_k = \frac{(t\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}, \quad k = 0, 1, 2, \ldots$$
$$\beta_k = \frac{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_{k-1}, \pi_{k-1})_{\mathrm{d}\lambda}}, \quad k = 1, 2, \ldots$$

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convention: $\beta_0 = \int_{\mathbb{R}} \mathrm{d}\lambda(t)$

Jacobi matrix

of infinite order

$$\boldsymbol{J}_\infty = \boldsymbol{J}_\infty(\mathrm{d}\lambda) := \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} & \\ & & \ddots & \ddots & \ddots \\ \mathbf{0} & & & & \end{bmatrix}$$

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The n-point Gauss quadrature formula for $\mathrm{d}\lambda$ is computable from the eigenvalues and first components of the corresponding normalized eigenvectors of $\boldsymbol{J}_n$ (Golub and Welsch, 1969)

Cauchy integrals of orthogonal polynomials

$$\rho_n(z) = \rho_n(z; \mathrm{d}\lambda) = \int_{\mathbb{R}} \frac{\pi_n(t; \mathrm{d}\lambda)}{z - t}\, \mathrm{d}\lambda(t), \quad n \geq 0,\ z \in \mathbb{C}\backslash[a, b]$$

Theorem If the moment problem for $\mathrm{d}\lambda$ is determined, and $z \in \mathbb{C}\backslash[a, b]$, then the sequence $\rho_{-1}(z) = 1, \rho_0(z), \rho_1(z), \ldots$ is a minimal solution of the basic three-term recurrence relation, i.e.,

$$\lim_{n\to\infty} \frac{\rho_n(z)}{y_n} = 0$$

for any solution $\{y_n\}$ linearly independent of $\{\rho_n\}$. Moreover,

$$\frac{\rho_n(z)}{\rho_{n-1}(z)} = \frac{\beta_n}{z - \alpha_n -}\ \frac{\beta_{n+1}}{z - \alpha_{n+1} -}\ \frac{\beta_{n+2}}{z - \alpha_{n+2} -} \cdots, \quad n \geq 0$$

Continued Fraction Algorithm

Problem compute $\rho_n(z)$ for $z \in \mathbb{C} \backslash [a, b],\ n = 0, 1, 2, \dots N$

Solution define $r_n = \rho_{n+1}(z)/\rho_n(z)$ and let $\nu \geq N$

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in theory

$$r_{n-1} = \frac{\beta_n}{z - \alpha_n - r_n}, \quad n = \nu, \nu - 1, \dots, 0$$

$$\rho_{-1}(z) = 1,\ \rho_n(z) = r_{n-1}\rho_{n-1}(z), \quad n = 0, 1, \dots N$$

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in practice

$$r_\nu^{[\nu]} = 0,\ r_{n-1}^{[\nu]} = \frac{\beta_n}{z - \alpha_n - r_n^{[\nu]}}, \quad n = \nu, \nu - 1, \dots, 0$$

$$\rho_{-1}^{[\nu]} = 1,\ \rho_n^{[\nu]} = r_{n-1}^{[\nu]}\rho_{n-1}^{[\nu]},\ n = 0.1.\dots, N$$

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Fact under the assumptions of the Theorem,

$$\lim_{\nu\to\infty} \rho_n^{[\nu]} = \rho_n(z)$$

Modification algorithms

Problem: given the recurrence coefficients of $\mathrm{d}\lambda$, generate those of

$$\mathrm{d}\hat{\lambda}(t) = r(t)\mathrm{d}\lambda(t),\; r \geq 0 \text{ on } \mathrm{supp}(\mathrm{d}\lambda),\; \text{rational}$$

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Example: Galant, 1971

$$r(t) = s(t-c), \quad c \in \mathbb{R}\backslash\mathrm{supp}(\mathrm{d}\lambda), \quad s = \pm 1$$

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$$r(t) = s(t-c), \quad c \in \mathbb{R}\backslash\mathrm{supp}(\mathrm{d}\lambda), \quad s = \pm 1$$

one step of (symmetric, shifted) LR algorithm:

$$s[\boldsymbol{J}_{n+1}(\mathrm{d}\lambda) - c\boldsymbol{I}] = \boldsymbol{L}\boldsymbol{L}^T$$
$$\boldsymbol{J}_n(\mathrm{d}\hat{\lambda}) = \left(\boldsymbol{L}^T\boldsymbol{L} + c\boldsymbol{I}\right)_{[1:n,1:n]}$$

nonlinear recurrence algorithm

generalized Christoffel theorem (Uvarov, 1969)

$$d\hat{\lambda}(t) = \frac{u(t)}{v(t)}d\lambda(t),\ u(t) = \pm\prod_{\lambda=1}^{\ell}(t - u_\lambda),\ v(t) = \prod_{\mu=1}^{m}(t - v_\mu)$$

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Let $m \le n$. Then

$$u(t)\pi_n(t;\mathrm{d}\hat{\lambda}) = \text{const} \times \begin{vmatrix} \pi_{n-m}(t) & \cdots & \pi_{n-1}(t) & \pi_n(t) & \cdots & \pi_{n+\ell}(t) \\ \pi_{n-m}(u_1) & \cdots & \pi_{n-1}(u_1) & \pi_n(u_1) & \cdots & \pi_{n+\ell}(u_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \pi_{n-m}(u_\ell) & \cdots & \pi_{n-1}(u_\ell) & \pi_n(u_\ell) & \cdots & \pi_{n+\ell}(u_\ell) \\ \rho_{n-m}(v_1) & \cdots & \rho_{n-1}(v_1) & \rho_n(v_1) & \cdots & \rho_{n+\ell}(v_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \rho_{n-m}(v_m) & \cdots & \rho_{n-1}(v_m) & \rho_n(v_m) & \cdots & \rho_{n+\ell}(v_m) \end{vmatrix}$$

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Christoffel's theorem: $m = 0$

Theorem (Uvarov, 1969) **Let $m > n$. Then**

$$u(t)\pi_n(t;\mathrm{d}\hat{\lambda}) = \text{const} \times$$

$$\begin{vmatrix} 0 & 0 & \cdots & 0 & \pi_0(t) & \cdots & \pi_{n+\ell}(t) \\ 0 & 0 & \cdots & 0 & \pi_0(u_1) & \cdots & \pi_{n+\ell}(u_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & \pi_0(u_\ell) & \cdots & \pi_{n+\ell}(u_\ell) \\ 1 & v_1 & \cdots & v_1^{m-n-1} & \rho_0(v_1) & \cdots & \rho_{n+\ell}(v_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & v_m & \cdots & v_m^{m-n-1} & \rho_0(v_m) & \cdots & \rho_{n+\ell}(v_m) \end{vmatrix}$$

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The generalized Christoffel theorems remain valid for complex u_λ, v_μ if orthogonality is understood in the sense of formal orthogonality.

linear factor $\mathrm{d}\hat{\lambda}(t) = (t-z)\mathrm{d}\lambda(t),\ z \in \mathbb{C}\backslash[a,b]$

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$$(t-z)\hat{\pi}_n(t) = \frac{\begin{vmatrix} \pi_n(t) & \pi_{n+1}(t) \\ \pi_n(z) & \pi_{n+1}(z) \end{vmatrix}}{-\pi_n(z)} = \pi_{n+1}(t) - r_n\pi_n(t),\ r_n = \frac{\pi_{n+1}(z)}{\pi_n(z)}$$

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write $(t-z)t\hat{\pi}_k(t)$ in two ways (Verlinden, 1999)

$$(t-z)t\hat{\pi}_k(t) = t\pi_{k+1}(t) - r_k \cdot t\pi_k(t)$$

$$= \pi_{k+2}(t) + (\alpha_{k+1} - r_k)\pi_{k+1}(t) + (\beta_{k+1} - r_k\alpha_k)\pi_k(t) - r_k\beta_k\pi_{k-1}(t)$$

$$(t-z)t\hat{\pi}_k(t) = (t-z)[\hat{\pi}_{k+1} + \hat{\alpha}_k\hat{\pi}_k(t) + \hat{\beta}_k\hat{\pi}_{k-1}(t)]$$

$$= \pi_{k+2}(t) + (\hat{\alpha}_k - r_{k+1})\pi_{k+1}(t) + (\hat{\beta}_k - r_k\hat{\alpha}_k)\pi_k(t) - r_{k-1}\hat{\beta}_k\pi_{k-1}(t)$$

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comparison:

$$\hat{\alpha}_k - r_{k+1} = \alpha_{k+1} - r_k, \quad r_{k-1}\hat{\beta}_k = r_k\beta_k$$

Algorithm **modification by a linear factor $t - z$**

initialization:

$$r_0 = z - \alpha_0, \quad r_1 = z - \alpha_1 - \beta_1 / r_0,$$
$$\hat{\alpha}_0 = \alpha_1 + r_1 - r_0, \quad \hat{\beta}_0 = -r_0 \beta_0$$

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continuation (if $n > 1$): for $k = 1, 2, \ldots, n-1$ do

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Matlab

```
ab=chri1(N,ab0,z)
```

see:

`http://www.cs.purdue.edu/archives/2002/wxg/codes/`

Algorithm **quadratic factor** $(t-x)^2+y^2=(t-z)(t-\overline{z})$

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$$\hat{\beta}_k = \beta_k\frac{r_{k+1}''r_{k-1}''}{[r_k'']^2}\left|\frac{r_k}{r_{k-1}}\right|^2$$

Matlab `ab=chri2(N,ab0,x,y)`

special quadratic factor $\mathrm{d}\hat{\lambda}(t) = (t-x)^2 \mathrm{d}\lambda(t),\ x \in \mathbb{R}$

warning: x is often inside the support of $\mathrm{d}\lambda$

one step of the QR algorithm with shift x

$$\boldsymbol{J}_{n+2}(\mathrm{d}\lambda) - x\boldsymbol{I} = QR$$

$$\boldsymbol{J}_n(\mathrm{d}\lambda) = (RQ + x\boldsymbol{I})_{[1:n,1:n]}$$

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higher-order factors

$\mathrm{d}\hat{\lambda}(t) = (t-x)^{2m} \mathrm{d}\lambda(t)$

m applications of the shifted QR algorithm applied to $\boldsymbol{J}_{n+2m}(\mathrm{d}\lambda)$

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$\mathrm{d}\hat{\lambda}(t) = (t-x)^{2m+1} \mathrm{d}\lambda(t), \quad x \in \mathbb{R} \backslash [a,b]$

m applications of the shifted QR algorithm applied to $\boldsymbol{J}_{n+2m+1}(\mathrm{d}\lambda)$ followed by one step of the symmetric, shifted LR algorithm

linear divisor $\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{t-z}, \; z \in \mathbb{C}\backslash[a,b]$

generalized Christoffel:

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Algorithm modification by a linear divisor $t - z$

initialization:

$$\hat{\alpha}_0 = \alpha_0 + r_0, \quad \hat{\beta}_0 = -\rho_0(z)$$

continuation (if $n > 1$): for $k = 1, 2, \ldots, n-1$ do

$$\hat{\alpha}_k = \alpha_k + r_k - r_{k-1},$$

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computation of the r_k: continued fraction algorithm

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Matlab

```
[ab,nu]=chri4(N,ab0,z,eps0,nu0,numax,rho0,iopt)
```

quadratic divisor $\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{(t-x)^2+y^2}, \quad z = x + iy$

notations

$$r_n = \frac{\rho_{n+1}(z)}{\rho_n(z)} = r'_n + \mathrm{i}r''_n$$

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Algorithm

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Matlab

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[ab,nu]=chri5(N,ab0,z,eps0,nu0,numax,rho0,iopt)
```

Applications

constrained least squares approximation

Problem given a function f on $[a, b]$ and a discrete (positive) N-point measure $\mathrm{d}\lambda_N$ on $[a, b]$, find $p \in \mathbb{P}_n$, $n \ll N$, such that

$$\|f - p\|^2_{\mathrm{d}\lambda_N} = \min$$

subject to

$$p(s_j) = f_j, \quad j = 1, 2, \ldots, m;\ m \le n,$$

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simplifying assumption the s_j are different from the support points of $\mathrm{d}\lambda_N$

Solution reduction to an unconstrained problem: write $p(t) = p_m(f;t) + \sigma_m(t)q(t), \quad q \in \mathbb{P}_{n-m}$, where $\sigma_m(t) = \prod_{j=1}^{m}(t - s_j)$ and $p_m(f;\,\cdot\,) \in \mathbb{P}_{m-1}$ is the polynomial interpolating f at the s_j

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$$\|f^* - q\|_{\mathrm{d}\lambda_N^*} = \min, \quad q \in \mathbb{P}_{n-m}$$

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$\Longrightarrow$ multiplication of $\mathrm{d}\lambda_N$ by m quadratic factors $(t - s_j)^2$

Example Bessel function $f = J_0$ on $[0, j_{0,3}]$

$$s_1 = j_{0,1},\ \ s_2 = j_{0,2}\ \ s_3 = j_{0,3} \quad \Longrightarrow \quad p_3(f;\,\cdot\,) \equiv 0$$

$$f^*(t) = \frac{J_0(t)}{\sigma_3(t)}, \quad \sigma_3(t) = (t - j_{0,1})(t - j_{0,2})(t - j_{0,3})$$

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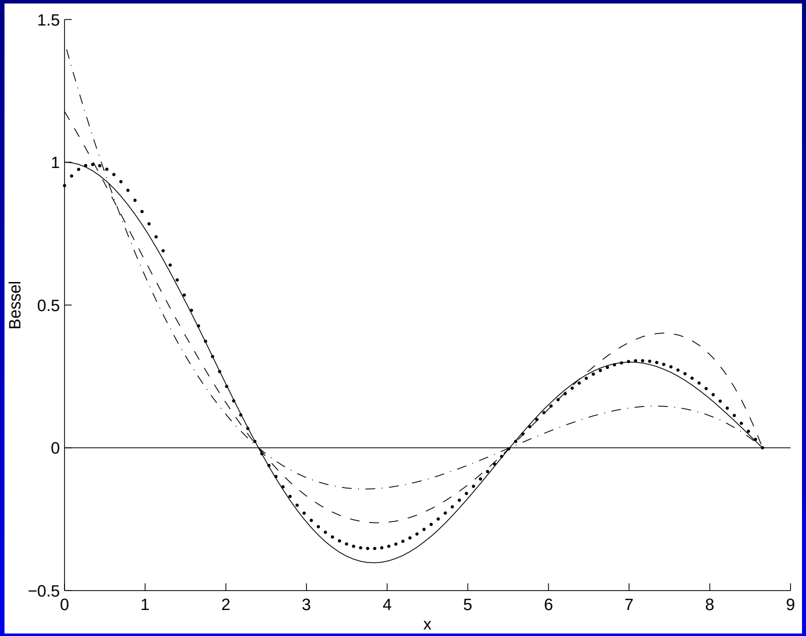
results for $n - m = 0, 1, 2$



Example (continued)

derivative constraints

$$p(0) = 1, \quad p'(0) = 0$$

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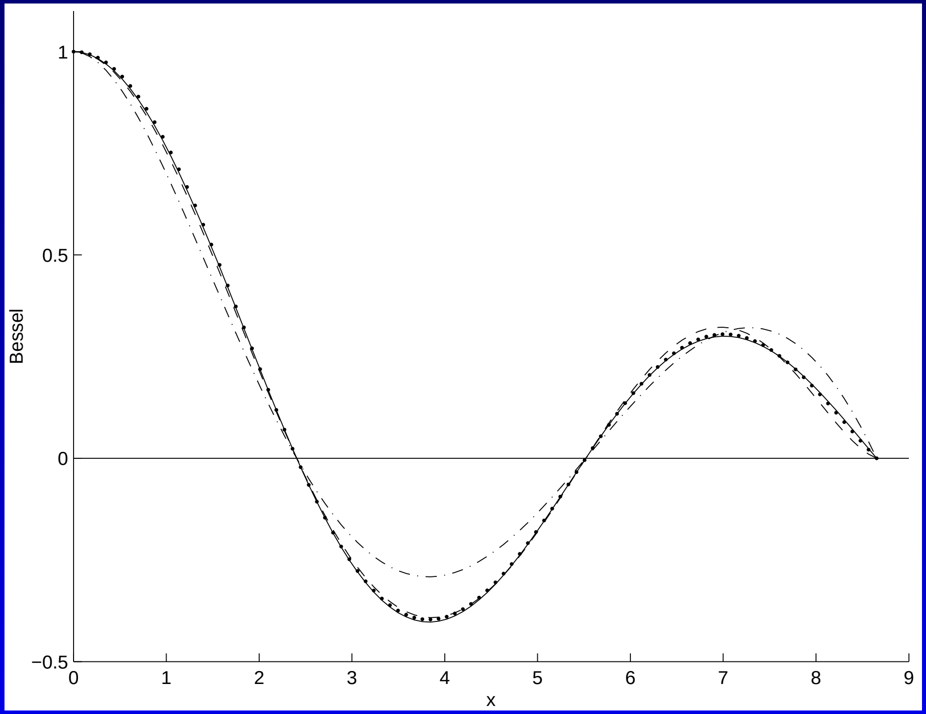

A quadrature problem

$$G(x,y;a) = \int_{-\infty}^{\infty} J_0(at)\frac{e^{-t^2}}{(t-x)^2+y^2}\,\mathrm{d}t$$

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modification of the Hermite weight by a quadratic divisor followed by the Golub/Welsch algorithm to generate Gaussian quadrature formulae for

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Example $x=0$, $y=0.1$, $a=7.5$

n	Modified Hermite	Hermite
5	22.7...	94.7...
10	19.7...	−0.6...
15	19.966...	55.4...
20	19.96350...	4.1...
25	19.96352269...	42.8...
30	19.9635226624...	7.3...
35	19.96352266263	36.5...
40	19.96352266263	9.6...