Computational aspects of complex orthogonal polynomials

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Computational complex analysis

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Orthogonal polynomials

Classical theory, after Szegő, Chihara, Ismail...:

Given a positive **weight function** $w(x)$ on $I \subset \mathbb{R}$, such that

$$\mu_k = \int_I x^k w(x) \mathrm{d}x < \infty, \qquad k = 0, 1, 2, \ldots,$$

con can construct a family of monic **orthogonal polynomials** $P_n(x)$ such that

$$\int_I P_n(x) x^k w(x) \mathrm{d}x = \begin{cases} 0, & k = 0, 1, \ldots, n-1, \\ h_n, & k = n, \end{cases}$$

- $P_n(x)$ exists uniquely, it has degree n.
- $P_n(x)$ can (in principle!) be computed using Gram–Schmidt.

Alternative (important!) formulation, in terms of the **Hankel determinant**

$$D_n = \det(\mu_{j+k})_{j,k=0,1,\ldots,n-1}, \qquad n \geq 1,$$

one can show that

$$P_n(x) = \frac{1}{D_n} \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_n & \mu_{n+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} & \mu_{2n-1} \\ 1 & x & \ldots & x^{n-1} & x^n \end{vmatrix} = x^n + \ldots$$

is the n-th (monic) orthogonal polynomial with respect to $w(x)$.

$P_n(x)$ is well defined provided that $D_n \neq 0$.

Orthogonal polynomials

Classical cases:

Family	Weight	Interval	Parameters
Hermite	$w(x) = \mathrm{e}^{-x^2}$	$\mathbb{R}$	-
Laguerre	$w(x) = x^{\alpha}\mathrm{e}^{-x}$	$(0, \infty)$	$\alpha > -1$
Jacobi	$w(x) = (1-x)^{\alpha}(1+x)^{\beta}$	$(-1, 1)$	$\alpha, \beta > -1$

Some deformations

- Basor, Chen & Ehrhardt (2009):

$$w(x,t) = (1-x)^{\alpha}(1+x)^{\beta}\mathrm{e}^{-tx}, \qquad \alpha,\beta > -1, \quad x \in (-1,1).$$

- Chen & Its (2010), Xu, Dai & Zhao 2014:

$$w(x,t) = x^{\alpha}\mathrm{e}^{-x-t/x}, \qquad \alpha > -1, \quad x \in (0,\infty).$$

- Van Assche, Filipuk & Zhang (2014), Clarkson, Loureiro, Van Assche (2015):

$$w(x,t) = \mathrm{e}^{-x^3+tx}, \qquad x \in \Gamma \subset \mathbb{C}.$$

- Boelen & Van Assche (2010), Clarkson & Jordaan (2014):

$$w(x,t) = x^{\lambda}\mathrm{e}^{-x^2+tx}, \qquad \lambda > -1, \quad x \in (0,\infty).$$

Some deformations

- Dai & Kuijlaars 2014, modified Laguerre weight:

$$w(x) = x^{-n+\nu} \mathrm{e}^{-Nx} (x-1)^{2b}, \qquad x > 0.$$

- Chen & Dai 2010 , Chen, Chen & Fang 2015, Pollaczek–Jacobi weight:

$$w(x;t,\alpha,\beta) = x^{\alpha}(1-x)^{\beta}\mathrm{e}^{-t/x}, \qquad x \in (0,1), \quad \alpha,\beta > -1, \quad t \geq 0.$$

- Dai & Zhang 2009, generalised Jacobi weight:

$$w(x) = (x-t)^{\gamma} x^{\alpha}(1-x)^{\beta}, \qquad x \in (0,1), \quad \alpha,\beta > 0, \ t < 0, \ \gamma \in \mathbb{R}.$$

Motivation 1: Complex OPs and numerical quadrature

In numerical analysis, construction of **Gaussian quadrature** rules: a quadrature rule

$$\int_a^b f(x)w(x)\mathrm{d}x \approx \sum_{j=1}^{n} \alpha_j f(x_j)$$

has maximum degree of exactness $2n-1$ if and only if the nodal polynomial $p_n(x) = \prod_{k=1}^{n}(x-x_k)$ satisfies

$$\int_a^b p_n(x)q(x)w(x)\mathrm{d}x = 0, \qquad q \in \mathbb{P}_{n-1}$$

where $w(x)$ is positive and has finite moments.

Motivation 1: Complex OPs and numerical quadrature

In the study of oscillatory integrals

$$I[f] = \int_a^b f(x) e^{i\omega g(x)} dx, \qquad \omega \gg 1,$$

direct Gaussian quadrature is not efficient or reliable (the number of sampling points scales with ω).

One alternative is to deform $[a,b]$ into the complex plane along paths of **steepest descent** and then integrate.

An interesting example: $g(x) = \frac{x^3}{3} - cx$, with $c \in (0,1)$.

Motivation 1: Complex OPs and numerical quadrature

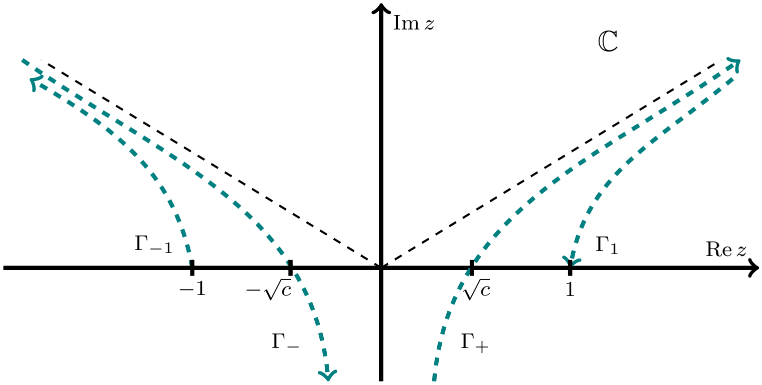
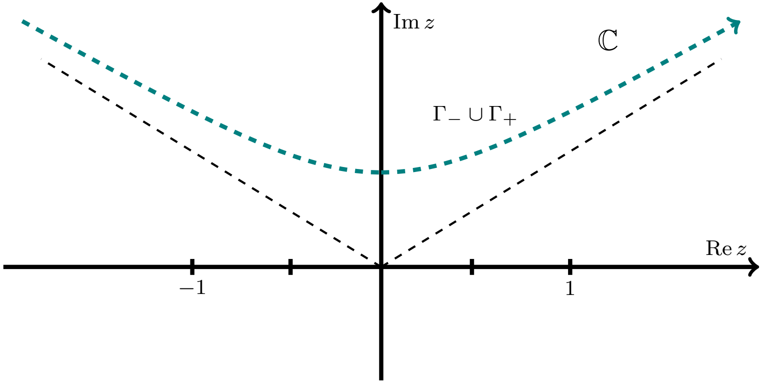


Figure: Steepest descent paths for the oscillator $g(x) = \frac{x^3}{3} - cx$.

Motivation 1: Complex OPs and numerical quadrature

- Standard approach: parametrize the paths, discretise and use Gauss–Laguerre or Gauss–Hermite quadrature.
- One not so standard approach: can we construct **one** quadrature rule for the path $\Gamma := \Gamma_+ \cup \Gamma_-$?



Motivation 1: Complex OPs and numerical quadrature

This leads to consider (formal, complex, non-Hermitian) OPs defined as

$$\int_\Gamma p_n^\delta(z) z^k \mathrm{e}^{\mathrm{i}(\frac{z^3}{3}-\delta z)} \mathrm{d}z = 0, \qquad z = 0, 1, \ldots, n-1,$$

with the scaled parameter $\delta = c\,\omega^{2/3}$.

Random matrix perspective (cubic log-gas model): Bleher, D. 2012, 2015, Bleher, D., Yattselev 2017.

Do $p_n^\delta(z)$ exist for any n and δ?

Motivation 1: Complex OPs and numerical quadrature

We can study the Hankel determinant

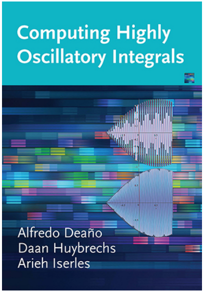
$$H_n(\delta) = \det\left(\mu_{j+k}(\delta)\right)_{j,k=0}^{n-1}, \qquad \mu_m(\delta) = \int_\Gamma z^m e^{i\left(\frac{z^3}{3} - \delta z\right)} dz,$$

and try to determine regimes for which $H_n(\delta) \neq 0$.

- D., Huybrechs & Kuijlaars 2010,
- Huybrechs, Kuijlaars & Lejon 2013, 2018.

A. DEAÑO, D. HUYBRECHS, A. ISERLES

Computing Highly Oscillatory Integrals
SIAM, 2018.



Motivation 2. SFS of Painlevé equations

Special function solutions of **Painlevé differential equations** can be written as Wronskian determinants:

$$\tau_n(z) = \det\left(\frac{\mathrm{D}^{j+k}}{\mathrm{D}z^{j+k}}\varphi(z)\right)_{j,k=0,1,\ldots n-1},$$

where $\varphi(z)$ is a **seed function**, a classical special function (Airy, Bessel, hypergeometric...).

For instance, for P_{II}

$$u''(z) = zu + 2u^3 + \alpha, \qquad \alpha \in \frac{1}{2}\mathbb{Z},$$

then special function solutions are generated by

$$\varphi(z) = C_1\,\mathrm{Ai}(-2^{-1/3}z) + C_2\,\mathrm{Bi}(-2^{-1/3}z).$$

Motivation 2. SFS of Painlevé equations

Information about these solutions, for finite n and as $n \to \infty$ and/or $z \to \infty$, can be obtained as follows:

- Match the seed function and its derivatives with the moments of a suitable weight function (in general complex!).
- Rewrite the Wronskian determinant as a Hankel determinant D_n for this new weight function.
- Use the machinery of asymptotics of OPs (Riemann–Hilbert or other) to obtain asymptotics for H_n.

Similar ideas for rational solutions have been used by Bertola, Bothner 2015, Balogh, Bertola, Bothner 2016, Buckingham 2017, Miller, Sheng 2017...

For special function solutions of P_{II}, D. 2018.

Motivation 3. Random matrix theory

For $n \geq 1$, the **Hankel determinant**

$$D_n = \det(\mu_{j+k})_{j,k=0,1,\ldots,n-1}, \qquad \mu_m = \int_a^b x^m w(x)\mathrm{d}x,$$

can be related, via Heine's formula,

$$D_n = \frac{1}{n!}\int_I \cdots \int_I \prod_{1\leq j<k\leq n} (x_k - x_j)^2 \prod_{j=1}^{n} w(x_j)\mathrm{d}x_j,$$

with the **partition function** of a **Hermitian random matrix ensemble**.

Non–Hermitian random matrix ensembles:
Hermitian, planar complex OPs $\rightarrow$ non-Hermitian, contour OPs!

D., Simm https://arxiv.org/abs/1909.06334

Orthogonal polynomials. Other applications

- Approximation theory: **Padé approximants**.
- Differential equations, in particular **spectral methods**.
- ...

OPs satisfy a **three-term recurrence relation**:

$$xp_n(x) = p_{n+1}(x) + \beta_n(x)p_n(x) + \gamma_n^2 p_{n-1}(x),$$

with initial values $p_{-1}(x) = 0$ and $p_0(x) = 1$. In matrix form,

$$x\mathbf{p}_n(x) = J_n\mathbf{p}_n(x) + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} p_n(x),$$

where $\mathbf{p}_n(x) = [p_0(x), p_1(x), \ldots, p_{n-1}(x)]^\top$, while

$$J_n = \operatorname{diag}(\gamma_k^2, \beta_k, 1)_{k=0,1,2,\ldots,n-1}$$

is a (tridiagonal) **Jacobi matrix**.

Computational ideas

In classical cases, use explicit formula or (fast) asymptotic methods as $n \to \infty$, Hale & Townsend, 2013, Townsend, Trogdon & Olver 2016, Gil & Segura 2018.

Non-classical cases: how to compute recurrence coefficients?

- Moment methods.
- Modified moment methods.
- Linear Algebra methods (Golub–Welsch): eigenvalues/eigenvectors of J_n.

General reference:
W. Gautschi. Orthogonal polynomials. Computation and Approximation. OUP, 2004.

Integrability properties

We write the TTRR and **ladder relations** (difference-differential equations) as follows:

$$\boldsymbol{p}_n(x) = \begin{pmatrix} P_n(x) \\ -2\pi \mathrm{i} h_{n-1}^{-1}(z) P_{n-1}(x) \end{pmatrix},$$

then

$$\boldsymbol{p}_{n+1}(x) = U_n(x)\boldsymbol{p}_n(x), \qquad \frac{\mathrm{d}}{\mathrm{d}x}\boldsymbol{p}_n(x) = V_n(x)\boldsymbol{p}_n(x),$$

where $U_n(x), V_n(x)$ are rational functions in x. More precisely,

$$U_n(x) = \begin{pmatrix} x - \beta_n & -\dfrac{h_{n-1}\gamma_n^2}{2\pi \mathrm{i}} \\ 1 & 0 \end{pmatrix}.$$

Compatibility says that

$$U_n'(x) + U_n(x)V_n(x) = V_{n+1}(x)U_n(x).$$

Integrability properties

Similarly, if $w(x,t)$ depends on extra parameter(s), then we write

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p}_n(x,t) = W_n(x,t)\boldsymbol{p}_n(x,t),$$

and impose compatibility between these three systems:

$$\boldsymbol{p}_{n+1}(x,t) = U_n(x,t)\boldsymbol{p}_n(x,t), \qquad \frac{\mathrm{d}}{\mathrm{d}x}\boldsymbol{p}_n(x,t) = V_n(x)\boldsymbol{p}_n(x,t),$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p}_n(x,t) = W_n(x)\boldsymbol{p}_n(x,t).$$

Rule of thumb:

$(x,n) \rightarrow$ string equations: discrete Painlevé.

$(t,n) \rightarrow$ evolution equations: Toda, Langmuir, Ablowitz–Ladik...

$(t,x) \rightarrow$ continuous Painlevé.

For example, if $w(x,t) = e^{i(\frac{z^3}{3} - \delta z)}$, then compatibility implies the following **string equations**:

$$\gamma_{n+1}^2 = \delta - \gamma_n^2 - \beta_n^2$$
$$\beta_{n+1} = \frac{i(n+1)}{\gamma_{n+1}^2} - \beta_n.$$

See Huybrechs, Kuijlaars & Lejon 2013, 2018. The initial values are

$$\beta_0(\delta) = -i\frac{\mathrm{Ai}'(-\delta)}{\mathrm{Ai}(-\delta)}, \qquad \gamma_0^2(\delta) = 0.$$

Eliminating γ_{n+1}^2 and writing $\beta_n = ib_n$, we get

$$\frac{n+1}{b_{n+1}+b_n} + \frac{n}{b_n + b_{n-1}} = b_n^2 + \delta$$

which is alternative discrete $\mathrm{P_I}$, Clarkson, Loureiro & Van Assche, 2018. They prove that there is a unique solution for which $b_n(\delta) > 0$ for all $n \geq 0$.

String equations

Can we use these nonlinear recursions?

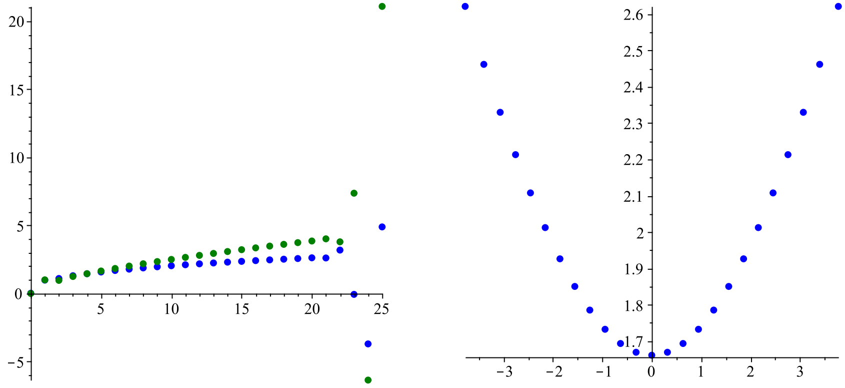
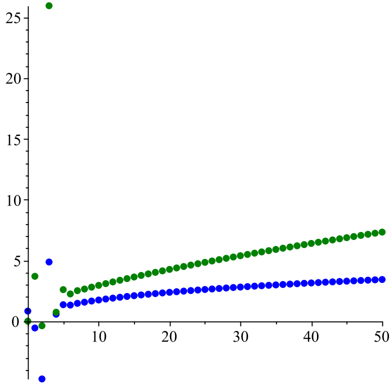


Figure: Recurrence coefficients $\mathrm{Im}\,\beta_n$ (left, blue) and γ_n^2 (left, green), computed from string equations with 20 digits, and location of the zeros of $P_n(z)$ for $\delta = 1$ (right).

String equations



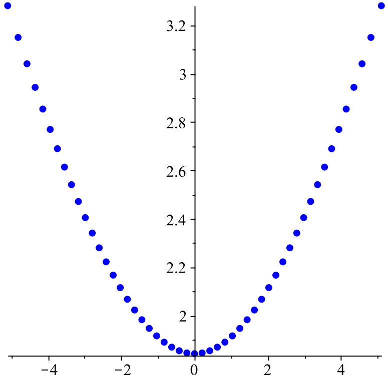


Figure: Recurrence coefficients $\operatorname{Im} \beta_n$ (left, blue) and γ_n^2 (left, green), computed from string equations with 60 digits, and location of tthe zeros of $P_n(z)$ for $\delta = 3$ (right).

Related problems

- Other examples shown in the book of W. Van Assche, 2018.
- More complicated cases given when parameters that appear as discontinuities of the weight function. For example

$$w(x; v, \alpha, s) = |x - v|^{\alpha} e^{-x^2} \begin{cases} s, & x < v, \\ 1, & x > v, \end{cases}$$

with $\alpha > -1$, $s > 0$ and $v \in \mathbb{R}$. Charlier, D. 2017.

Sometimes this leads to more general cases of special function solutions of Painlevé equations.

Related problems

- Instability related to the choice of special functions as initial values? Minimal solutions in the linear case?
- Boundary value problem (with asymptotic behaviour as $n \to \infty$) instead of initial value one for the string equations?
- Bleher & Its 2003 propose minimization of the Hamiltonian

$$H(\gamma, \beta) = n \, \mathrm{tr} V(J_n) - \sum_{k=1}^{\infty} k \ln \gamma_k^2,$$

where the weight function is $w(x) = \mathrm{e}^{-nV(x)}$. In particular,

$$w(x,t) = \mathrm{e}^{-n\left(\frac{g}{4}x^4 + \frac{t}{2}x^2\right)}, \qquad \in \mathbb{R}.$$

Is this a possibility for other weights?

- Fredholm determinant techniques? Bornemann 2010.
- Numerical solution of the corresponding RHP for orthogonal polynomials? Olver & Trogdon 2015...

That's all for now...

Thank you for your attention!