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Mini-Workshop: Multivariate Orthogonal Polynomials: New synergies with Numerical Analysis

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Abstract. Multivariate polynomials and, in particular, multivariate orthogonal polynomials (MOPs) are research areas within the fields of special functions, Lie groups, quantum groups, computer algebra to name only some of them. However, there are many important areas in the field of numerical analysis where multivariate polynomials (of high order) play a crucial role: approximation by spectral methods and finite elements, discrete calculus, polynomial trace liftings, exact sequence properties, sparsity, efficient and stable recursions, analysis of the geometry of the zeros. The miniworkshop brought together experts from the fields of MOPs and numerical analysis of partial differential equations.

Mathematics Subject Classification (2020): 33-XX, 31-XX, 41-XX, 65-XX.

Introduction by the Organizers

The Oberwolfach miniworkshop on "Multivariate Orthogonal Polynomials: New synergies with Numerical Analysis" took place 24.9.-29.9. 2023 with 16 onsite and 2 online participants. The broad topic of the workshop covered different fields in mathematics such as approximation theory, numerical analysis, multivariate polynomials, and the theory of special functions with the aim to foster new collaborations between these different fields. Although orthogonal polynomials (OPs) have always been an important tool in the analysis of high-order numerical discretization methods, new applications now require the development of new theories and techniques in the field of OPs and conversely new developments in OPs open up possibilities for new algorithms for partial differential equations.

Discrete calculus or, more generally, structure-awareness is an important paradigm in discretizations of PDEs. One requires polynomial interpolation operators with certain properties ("Fortin interpolation"), the construction of right-inverse of operators in suitable pairs of polynomial spaces, and the investigation of the exact sequence and commuting diagram properties of discrete de Rham and more general complexes. For the Stokes problem and non-conforming high order discretizations based on Crouzeix-Raviart elements, these aspects were discussed by Stefan Sauter. High order interpolation operator with the commuting diagram property for the classical de Rham complex involving $H(\mathrm{curl})$ and $H(\mathrm{div})$ was presented by Jens Markus Melenk with applications to a wave-number explicit analysis for Maxwell's equations. The classical de Rham complex can be embedded into a much larger complex that includes matrix-valued spaces, which turns out to be the suitable framework for many problems in computational mechanics and physics. A detailed discussion with many new results in this active field was given by Joachim Schöberl. Francesci Rapetti presented recent result on choosing polynomial basis functions on triangles with an emphasis on suitable choices for $H(\mathrm{curl})$.

The topic of orthogonal polynomials was addressed by various talks. Tom Koornwinder gave a survey presentation; in particular the Askey scheme for OPs which are eigenfunctions of second order operators was a highlight. Yuan Xu presented new families of orthogonal polynomials on domains of revolution such as hyperboloids, cones, and higher dimensional analogues. Bivariate extensions of Bernstein-Szegő measures along families of orthonormal polynomials were considered in the talk by Plamen Iliev and a characterization of these classes was given. Miguel Piñar presented families of polynomials which are orthogonal with respect to certain weighted Sobolev inner products. Tomas Sauer developped abstract connections between orthogonal polynomials, quadrature, and continued fractions.

Topics in approximation theory and its application were covered by Dietrich Braess, Annie Cuyt, Wolfgang Hackbusch, and Gerlind Plonka. Annie Cuyt started her talk from an algebraic setting of the problem and showed how to derive concrete approximation results (quadrature, exponential analysis, Padé approximation) within this setting. Dietrich Braess presented recent results on the best approximation by exponentials and rational functions. Such approximations have many applications including the construction of separable approximations of kernel functions and fractional diffusion problems. Gerlind Plonka studied the reconstruction of signals from data using exponential functions. Wolfgang Hackbusch presented new Remez-based algorithms for the numerical construction of best approximation by exponentials or rational functions.

High order discretizations of (time-)fractional equations were presented by Jie Shen. The recently developed "log-polynomials", i.e., functions $t \mapsto \pi(\log t)$ with polynomial π were presented, which have the remarkable feature to be able to resolve typical singularities at $t = 0$ at exponential (in the polynomial degree) rates without requiring explicitly knowledge of the singularity.

Two presentations by Sheehan Olver and Tim Haubold focused on optimal complexity algorithms for setting up stiffness matrices and solving PDEs using very high polynomial degrees. Key to these results are efficient and new recurrence relations for orthogonal polynomials and matrix entries. Sheehan Olver presented such constructions for new orthogonal polynomial arising when discretizing differential operators on domains bounded by algebraic curves. Tim Haubold considered classical geometries such as simplices but delveloped new recurrence relations discovered by an interaction with symbolic algebra tools.

Mini-Workshop: Multivariate Orthogonal Polynomials: New synergies with Numerical Analysis

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Abstracts

Orthogonal polynomials on domains of revolution

Yuan Xu

We report new families of orthogonal polynomials (OPs) on domains of revolution, such as cones and hyperboloids, as well as several of their varieties in the high-dimensional Euclidean space. In the multivariate setting, the structure of orthogonal polynomials (OPs) is much more complex than that in one variable. In order to use OPs as a tool for analysis, we need to understand their intrinsic properties and structures, which require the domain and the weight function that define orthogonality to be regular and possess certain symmetry.

Let Ω be a domain in $\mathbb{R}^d$ and let w be a nonnegative weight function defined on Ω, so that the inner product

$$\langle f, g\rangle = \int_\Omega f(x)g(x)w(x)dx$$

is well-defined for all polynomials restricted on Ω. Let $\mathcal{V}_n$ be the space of OPs of (total) degree n for this inner product. A quintessential example of OPs on the regular domains is spherical harmonics, which are orthogonal on the unit sphere $\Omega = \mathbb{S}^{d-1}$ with respect to the surface measure $w(x)dx = d\sigma(x)$. Not only an orthogonal basis of spherical harmonics can be written explicitly in terms of the product of Jacobi polynomials, but it also possesses two distinguished properties:

- Spherical harmonics are eigenfunctions of the Laplace-Beltrami operator.
- The reproducing kernel of $\mathcal{V}_n^d$ satisfies an addition formula.

More specifically, let Δ_0 be the Laplace-Beltrami operator, which is the restriction of the Laplace operator on the unit sphere; then

$$\Delta_0 Y = -n(n+d-2)Y, \qquad \forall Y \in \mathcal{V}_n, \quad n = 0, 1, 2, \ldots.$$

Moreover, if $\{Y_\nu^n : 1 \le \nu \le \dim \mathcal{V}_n\}$ is an orthonormal basis of spherical harmonics, then the addition formula of the reproducing kernel $P_n(\cdot,\cdot)$ of $\mathcal{V}_n$ means

$$P_n(\xi,\eta) = \sum_{1\le\nu\le\dim\mathcal{V}_n} Y_\nu^n(\xi)Y_\nu^n(\eta) = Z_n^{\frac{d-2}{2}}(\langle \xi,\eta\rangle),$$

where $Z_n^\lambda(t) = \frac{n+\lambda}{\lambda}C_n^\lambda(t)$ in terms of the Gegenbauer polynomial C_n^λ. Together, these two properties play essential roles in a substantial portion of analysis on the unit sphere.

We are interested in other OPs that are eigenfunctions of a second-order differential operator, which we shall call *spectral operator*, and have a closed-form formula for the reproducing kernel of $\mathcal{V}_n$, which we retain the name *addition formula*. It should be mentioned that these are special properties that one cannot expect to exist in general, but they provide powerful tools for analysis when they do exist; see, for example, [6] and the references therein. It is known that OPs on the unit ball $\mathbb{B}^d$, with weigh function $(1-\|x\|^2)^\mu$, and the simplex $\triangle^d$, with weight function $x_1^{\alpha_1} \cdots x_d^{\alpha_d}(1 - x_1 - \cdots - x_d)^{\alpha_{d+1}}$, have these two properties (cf. [1]), both have been studied and utilized extensively in the literature.

Recently, we initiated the study of OPs in domains of revolution [2, 3, 4]. There are two types of such domains. Let ϕ be either a linear polynomial or the square root of a polynomial of degree at most 2, non-negative on its domain of definition. The first type is quadratic surfaces , denoted by $\mathbb{V}_0^{d+1}$ and defined by

$$\mathbb{V}_0^{d+1} = \{(x,t) : \|x\| = \phi(t),\, x \in \mathbb{R}^d,\, t \in \mathbb{R}_+\}$$

and the second type is the solid domain bounded by $\mathbb{V}_0^{d+1}$ and hyperplanes if t is restricted to a finite interval,

$$\mathbb{V}^{d+1} = \{(x,t) : \|x\| \le \phi(t),\, x \in \mathbb{R}^d,\, t \in \mathbb{R}_+\}.$$

On $\mathbb{V}_0^{d+1}$, we consider OPs for weight function $w(t)$ that depends only on t, whereas on $\mathbb{V}^{d+1}$ we consider OPs for wright function $W(x,t) = w(t)(t^2 - \|x\|^2)^\mu$, for example. For $\phi(t) = 1$, the domain is a cylinder. For $\phi(t) = t$, the domain becomes the unit sphere and the unit ball. Up to an affine change of variables, below is a list of other domains:

- Conic surface and cone: $\phi(t) = t$, $0 \le t \le b \le +\infty$.
- Double conic surface and double cone: $\phi(t) = t$, $0 \le |t| \le b \le +\infty$.
- Hyperbolic surface and hyperboloid of two sheets: $\phi(t) = \sqrt{t^2 - \rho^2}$, $0 < |\rho| \le |t|$.
- Hyperbolic surface and hyperboloid: $\phi(t) = \sqrt{t^2 + \rho^2}$, $0 < |\rho| \le |t|$.
- Paraboloid: $\phi(t) = \sqrt{t}$, $0 \le t \le b \le +\infty$,

where b can be infinity, so that the domain could either be compact or infinite. For a family of weight functions, OPs on each of these domains can be given in terms of spherical harmonics and OPs of one variable that are semi-classical and, more importantly, classical for some domains [2]. Of particular interest are several domains on which there are OPs that possess the two desired properties: spectral operator and addition formula. Without getting into details, we mention a couple of domains and weight functions for the latter, as well as references.

1. Conic domains

(1) Laguerre polynomials on the infinite conic surface with $w(t) = t^{-1}e^{-t}$ and Jacobi polynomials on finite cone surfaces with $w(t) = t^{-1}(1-t)^\gamma$. Spectral operator: [3, Theorems 7.2 & 7.3]. Addition formula: [5, Theorems 3.7] and [3, Corollary 8.3].

(2) Laguerre polynomials on infinite cone with $w(x,t) = t^{-1}e^{-t}(t^2 - \|x\|^2)^\mu$ and Jacobi polynomials on the cone with $w(x,t) = t^{-1}(1-t)^\gamma(t^2 - \|x\|^2)^\mu$. Spectral operator: [3, Theorems 3.2 & 3.4]. Addition formula: [5, Theorem 5.4] and [3, Theorem 4.3].

2. Double conic and hyperbolic domains of two sheets. The double conic domains can be considered as the special case of $\rho = 0$ of the hyperbolic domains of two sheets. Hence, we shall only state the results for the latter.

In this case, we assume the weight function $w(t)$ to be an even function, so that the space $\mathcal{V}_n(\Omega)$ can be decomposed as a union of two subspaces:

$$\mathcal{V}_n(\Omega) = \mathcal{V}_n^E(\Omega) \bigcup \mathcal{V}_n^O(\Omega), \qquad \Omega = \mathbb{V}_0^{d+1} \text{ or } \mathbb{V}^{d+1},$$

where $\mathcal{V}_n^E(\Omega)$ (or $\mathcal{V}_n^O(\Omega)$) consists of OPs of degree n that are even (or odd) in the t variable. The spectral operator and the addition formula hold either for $\mathcal{V}_n^E(\Omega)$ or for $\mathcal{V}_n^E(\Omega)$ but for different weight functions. The two properties, however, can still be utilized to study functions that are assumed to be even, or odd, in the t variable [4, 7]. Below we list only properties for $\mathcal{V}_n^E(\Omega)$.

(1) Hermite polynomials on the infinite hyperbolic surface with the weight $w(t) = |t|(t^2-\rho^2)^{-\frac{1}{2}} e^{-t^2}$ and Gegenbauer polynomials on the finite hyperbolic surface with $w(t) = |t|(t^2-\rho^2)^{-\frac{1}{2}}(1-t^2)^\gamma$. Spectral operator: [3, Theorems 7.5 & 4.4]. Poisson kernel: [3, Theorems 7.6 & 7.13]

(2) Hermite polynomials on the infinite hyperboloid with the weight $w(x,t) = |t|e^{-t^2}(t^2-\rho^2-\|x\|^2)^{\mu-\frac{1}{2}}$ and Gegenbauer polynomials on the hyperboloid with $w(x,t) = |t|(\rho^2+1-t^2)^\gamma(t^2-\rho^2-\|x\|)^{\mu-\frac{1}{2}}$. Spectral operator: [3, Theorems 7.12 & 4.8]. Poisson kernel: [3, Theorems 7.13 & Theorem 5.6 and (5.16)]

3. Other double domains In an ongoing work [8], we regard a domain of revolution as rotating a domain on $\mathbb{R}_+^2$ around the t axis, which allows us to go beyond quadratic domains. It leads to several families of OPs on domains that can be mapped from the hyperboloid. For example, we can consider the intersections of two touching ellipsoids, which is defined by, for $0 \le \mathfrak{b} < \mathfrak{a}$,

$$\mathbb{V}^{d+1} = \left\{ (x,t) : \sqrt{1-\frac{t^2}{\mathfrak{b}}} \le \|x\| \le \sqrt{1-\frac{t^2}{\mathfrak{a}}},\ |t| \le \mathfrak{a} \right\}.$$

For each of such domains, analog results like the Gegenbauer polynomials on hyperboloid hold for a family of weight functions.

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On orthogonality, rational approximation, quadrature and exponential analysis, in one and more variables

Annie Cuyt

We establish connections between the concept of orthogonal polynomials and several numerical techniques from rational approximation, Gaussian quadrature and exponential analysis, both in one as well as in several variables.

1. Univariate case

For a linear functional $L : \mathbb{C}[t] \to \mathbb{C} : t^i \to e_i$, a sequence of orthogonal polynomials $\{V_m(z)\}_{m\in\mathbb{N}}$ can be defined by

$$L\left(t^i V_m(t)\right) = 0, \qquad i = 0, \ldots, m-1.$$

In [7] these formally orthogonal polynomials are called Hadamard polynomials.

With the $V_m(z)$ we can define associated polynomials

$$W_{m-1}(z) = L\left(\frac{V_m(z) - V_m(t)}{z-t}\right)$$

and reverse polynomials

$$\tilde{V}_m(z) = z^m V_m(1/z).$$

The Padé approximant $[m-1/m]_F$ of degree $m-1$ in the numerator and degree m in the denominator to the formal power series

$$F(z) = \sum_{i=0}^{\infty} e_i z^i$$

precisely equals $\tilde{W}_{m-1}(z)/\tilde{V}_m(z)$. Hence the denominator of this Padé approximant is closely related to the orthogonal polynomial $V_m(z)$.

When the e_i are so-called moments, for instance

$$e_i = \int_{-1}^{1} w(t) t^i \, dt, \qquad 0 < \int_{-1}^{1} w(t)\, dt,$$

then

$$F(z) = \int_{-1}^{1} w(t) \frac{1}{1-tz}\, dt$$

and the m-point Gaussian quadrature rule

$$\int_{-1}^{1} w(t) \frac{1}{1-tz}\, dt \approx \sum_{i=1}^{m} A_i^{(m)} \frac{1}{1 - z_i^{(m)} z},$$

approximating $F(z)$, equals the $[m-1/m]_F$ Padé approximant. The Gaussian nodes $z_i^{(m)}$ are the zeroes of $V_m(z)$ and the weights $A_i^{(m)}$ are given by

$$A_i^{(m)} = \frac{W_{m-1}(z_i^{(m)})}{V_m'(z_i^{(m)})}, \qquad i = 1, \ldots, m.$$

Since this Gaussian quadrature rule exactly integrates polynomials of degree $2m-1$, we also have

$$e_j = \sum_{i=1}^{m} A_i^{(m)} \left(z_i^{(m)}\right)^j, \qquad j = 0, \ldots, 2m-1.$$

Hence the nodes and weights can be obtained as the solution of the exponential analysis or Prony problem [6]

$$e_j = \sum_{i=1}^{m} A_i^{(m)} \exp(j\phi_i^{(m)}), \qquad z_i^{(m)} = \exp(\phi_i^{(m)}), \quad j = 0, \ldots, 2m-1,$$

where only m and the e_j are given. The $z_i^{(m)}$ are the generalized eigenvalues of a Hankel structured generalized eigenvalue problem and the $A_i^{(m)}$ are the solution of a Vandermonde structured linear system [8].

2. Multivariate case

The concept of the formally orthogonal polynomial $V_m(z)$ is generalized in [4], for different radial weight functions, to so-called spherical orthogonal polynomials. The latter differ from several other definitions of multivariate orthogonal polynomials, in that they preserve the connections laid out above.

Homogeneous multivariate Padé approximants, as defined in [2, 3], can also be obtained from the spherical orthogonal polynomials in a similar way as described here. The homogeneous definition satisfies a very strong projection property, in the sense that this multivariate Padé approximant reduces to the univariate Padé approximant on every one-dimensional subspace.

A whole lot of Gaussian cubature rules on the disk can be united in a single approach [1] when developing the existing rules from these spherical orthogonal polynomials. What's more, the nodes and weights of such Gaussian cubature rules on the disk can be obtained as the solution of a multivariate Prony-like system of interpolation conditions [1]. And this brings us to the next connection.

Prony's result that an m-term exponential analysis problem can be solved uniquely from $2m$ samples e_i, is a one-dimensional result. In [5] this result is proven, more than 200 years later, to hold for higher dimensions $d > 1$: a multivariate linear combination of m exponential terms with unknown inner product exponents can, under mild conditions, be fitted using only $(d+1)m$ data.

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Wavenumber-explicit regularity theory for the time-harmonic Maxwell equations in piecewise smooth media

Markus Melenk
(joint work with David Wörgötter)

We consider the time-harmonic Maxwell equations with piecewise smooth permeability and permittivity tensors in a bounded, smooth and simply connected domain $\Omega \subseteq \mathbb{R}^3$. At the boundary Γ of Ω we impose natural and impedance boundary conditions. More precisely, we assume that there exists a decomposition $\Gamma = \Gamma_{\mathrm{N}} \cup \Gamma_{\mathrm{Im}}$, where Γ_{N} and Γ_{Im} are disjoint, $|\Gamma_{\mathrm{Im}}| > 0$, and both Γ_{N} and Γ_{Im} can be written as a union of finitely many compact and simply connected smooth surfaces.[1]

In addition, we suppose that on $\overline{\Omega}$ we have real-valued, symmetric and uniformly positive definite tensor fields μ^{-1} and ε given, and we assume that these tensor fields are piecewise smooth and discontinuous only across certain smooth and mutually disjoint surfaces Γ_{int} inside of Ω.

We consider the following problem: For a given wavenumber $k \in \mathbb{R}$ with $|k| \geq 1$ find a solution $\mathbf{u}$ of

$$\begin{aligned} \operatorname{curl} \mu^{-1} \operatorname{curl} \mathbf{u} - k^2 \varepsilon \mathbf{u} &= \mathbf{f} && \text{in } \Omega, \\ \mu^{-1} \operatorname{curl} \mathbf{u} \times \mathbf{n} &= \mathbf{g}_{\mathrm{N}} && \text{on } \Gamma_{\mathrm{N}}, \\ \mu^{-1} \operatorname{curl} \mathbf{u} \times \mathbf{n} - ik\mathbf{u}_T &= \mathbf{g}_{\mathrm{I}} && \text{on } \Gamma_{\mathrm{Im}}. \end{aligned} \tag{1}$$

Here, $\mathbf{f}$, $\mathbf{g}_{\mathrm{N}}$ and $\mathbf{g}_{\mathrm{I}}$ are given data, i is the imaginary unit, $\mathbf{n}$ is the outer unit normal vector field to Γ, and $\mathbf{u}_T := \mathbf{n} \times (\mathbf{u}|_{\Gamma_{\mathrm{Im}}} \times \mathbf{n})$.

We define

$$\mathbf{H}_{\mathrm{imp}}(\Omega) := \left\{ \mathbf{v} \in \mathbf{H}(\operatorname{curl}, \Omega) \;\middle|\; \mathbf{v}_T \in (\mathrm{L}^2(\Gamma_{\mathrm{Im}}))^3 \right\},$$

and with this, the weak formulation of (1) reads as follows: Find $\mathbf{u} \in \mathbf{H}_{\mathrm{imp}}(\Omega)$ such that for all $\mathbf{v} \in \mathbf{H}_{\mathrm{imp}}(\Omega)$ there holds

$$A_k(\mathbf{u}, \mathbf{v}) = (\mathbf{f}, \mathbf{v})_{\mathrm{L}^2(\Omega)} + (\mathbf{g}_{\mathrm{N}}, \mathbf{v}_T)_{\mathrm{L}^2(\Gamma_{\mathrm{N}})} + (\mathbf{g}_{\mathrm{I}}, \mathbf{v}_T)_{\mathrm{L}^2(\Gamma_{\mathrm{Im}})}, \tag{2}$$

where

$$A_k(\mathbf{u}, \mathbf{v}) := \left(\mu^{-1} \operatorname{curl} \mathbf{u}, \operatorname{curl} \mathbf{v}\right)_{\mathrm{L}^2(\Omega)} - k^2 \left(\varepsilon \mathbf{u}, \mathbf{v}\right)_{\mathrm{L}^2(\Omega)} - ik \left(\mathbf{u}_T, \mathbf{v}_T\right)_{\mathrm{L}^2(\Gamma_{\mathrm{Im}})}.$$

[1] We require $|\Gamma_{\mathrm{Im}}| > 0$ in order to suppress possible resonance frequencies and assert unique solvability of the weak form (2) below. Note that we have no such restriction on Γ_{N}, i.e., $\Gamma_{\mathrm{N}} = \emptyset$ is admissible.

If $\mathbf{f}$ is square integrable and the boundary data $\mathbf{g}_{\mathrm{N}}$ and $\mathbf{g}_{\mathrm{I}}$ are square integrable tangent fields on Γ_{N} and Γ_{Im}, respectively, the weak formulation (2) is uniquely solvable and the solution depends continuously on the data; more precisely there holds

$$\|\mathbf{u}\|_{\mathbf{H}_{\mathrm{imp}}(\Omega),k} \leq C_k \left(\|\mathbf{f}\|_{\mathrm{L}^2(\Omega)} + \|\mathbf{g}_{\mathrm{N}}\|_{\mathrm{L}^2(\Gamma_{\mathrm{N}})} + \|\mathbf{g}_{\mathrm{I}}\|_{\mathrm{L}^2(\Gamma_{\mathrm{Im}})} \right), \tag{3}$$

where the constant $C_k > 0$ depends only on Ω, μ^{-1}, ε and k, and

$$\|\mathbf{u}\|^2_{\mathbf{H}_{\mathrm{imp}}(\Omega),k} := \|\operatorname{curl} \mathbf{u}\|^2_{\mathrm{L}^2(\Omega)} + k^2 \|\mathbf{u}\|^2_{\mathrm{L}^2(\Omega)} + |k| \, \|\mathbf{u}_T\|^2_{\mathrm{L}^2(\Gamma_{\mathrm{Im}})} .$$

This existence and uniqueness result is not obvious but can be shown similarly as [5, Theorem 4.17] by Fredholm theory and a uniqueness result provided by [1, 6].

One main focus of our work is regularity theory for Maxwell's equation (1). We start with the definition of piecewise regular vector fields: For $\ell \in \mathbb{N}_0$, let $\mathbf{PH}^\ell(\Omega)$ denote the space of all vector fields on Ω which are piecewise in $\mathbf{H}^\ell$ and (possibly) discontinuous at the surfaces Γ_{int} of discontinuity of μ^{-1} and ε. The following theorem provides a regularity shift result for solutions $\mathbf{u}$ of (1). For essential boundary conditions (that is, $\mathbf{u} \times \mathbf{n} = 0$ on Γ) a similar result is proved in [8] by a difference quotient method; our proof is less technical and is based on the theory of elliptic transmission problems and a result from [2].

Theorem 1. *Let $\ell \in \mathbb{N}_0$ be given, and suppose $\mathbf{f} \in \mathbf{H}(\operatorname{div}, \Omega) \cap \mathbf{PH}^\ell(\Omega)$ with $\operatorname{div} \mathbf{f} \in \mathbf{PH}^\ell(\Omega)$ and $\mathbf{f} \cdot \mathbf{n} \in \mathrm{H}^{\ell+1/2}(\Gamma_{\mathrm{N}})$. Moreover, assume that $\mathbf{g}_{\mathrm{N}}$ and $\mathbf{g}_{\mathrm{I}}$ are tangential fields on Γ_{N} and Γ_{Im}, respectively, with $\mathbf{g}_{\mathrm{N}} \in \mathbf{H}^{\ell+1/2}(\Gamma_{\mathrm{N}})$, as well as $\operatorname{div}_{\Gamma_{\mathrm{N}}} \mathbf{g}_{\mathrm{N}} \in \mathrm{H}^{\ell+1/2}(\Gamma_{\mathrm{N}})$ and $\mathbf{g}_{\mathrm{I}} \in \mathbf{H}^{\ell+1/2}(\Gamma_{\mathrm{Im}})$.*

Then, there holds $\mathbf{u} \in \mathbf{PH}^{\ell+1}(\Omega)$ and $\operatorname{curl} \mathbf{u} \in \mathbf{PH}^{\ell+1}(\Omega)$ with

$$\|\mathbf{u}\|_{\mathbf{PH}^{\ell+1}(\Omega)} + \|\operatorname{curl} \mathbf{u}\|_{\mathbf{PH}^{\ell+1}(\Omega)} \leq C_{\ell,k} \left(\mathbf{F} + \mathbf{G} \right),$$

where

$$\mathbf{F} := \|\mathbf{f}\|_{\mathbf{PH}^\ell(\Omega)} + \|\operatorname{div} \mathbf{f}\|_{\mathbf{PH}^\ell(\Omega)} + \|\mathbf{f} \cdot \mathbf{n}\|_{\mathbf{H}^{\ell+\frac{1}{2}}(\Gamma_{\mathrm{N}})},$$

$$\mathbf{G} := \|\mathbf{g}_{\mathrm{N}}\|_{\mathbf{H}^{\ell+\frac{1}{2}}(\Gamma_{\mathrm{N}})} + \|\operatorname{div}_{\Gamma_{\mathrm{N}}} \mathbf{g}_{\mathrm{N}}\|_{\mathbf{H}^{\ell+\frac{1}{2}}(\Gamma_{\mathrm{N}})} + \|\mathbf{g}_{\mathrm{I}}\|_{\mathbf{H}^{\ell+\frac{1}{2}}(\Gamma_{\mathrm{Im}})},$$

and $C_{\ell,k} > 0$ depends only on $\ell, k, \Omega, \mu^{-1}$ and ε.

In combination with the Sobolev embedding theorem, the above result ensures piecewise smoothness of $\mathbf{u}$ if the given data is (piecewise) smooth.

Under certain additional assumptions we can improve the previous result. Henceforth, we assume that, in addition to being smooth and simply connected, Ω is analytic, i.e., Γ can be locally parametrized by analytic charts. Under this assumption we can establish (almost) k-explicit piecewise analyticity of $\mathbf{u}$, as long as the given coefficients and data are (piecewise) analytic with analytic discontinuity surfaces Γ_{int}.

The main idea is to use the nested ball technique employed, e.g., also in [7]. One key feature of our proof is that we do not rewrite the time-harmonic Maxwell equation as an elliptic system, but apply the nested ball technique directly to the non-elliptic system (1).

Theorem 2. *Let Ω be a simply connected, analytic domain and assume that the tensor fields μ^{-1} and ε are piecewise analytic on $\overline{\Omega}$. Moreover, suppose that the surfaces of discontinuity Γ_{int} of μ^{-1} and ε are analytic and that $\mathbf{f} \in \mathbf{H}(\text{div}, \Omega)$ is piecewise analytic on $\overline{\Omega}$ and (possibly) discontinuous only across Γ_{int}. If $\mathbf{g}_{\text{N}}$ and $\mathbf{g}_{\text{I}}$ are analytic on Γ_{N}, Γ_{Im}, respectively, the solution $\mathbf{u}$ of (1) is piecewise analytic on $\overline{\Omega}$ and satisfies the estimate*

$$\|\mathbf{u}\|_{\mathbf{PH}^{\ell}(\Omega)} \leq C_k M^{\ell+1}(\ell + |k|)^{\ell}$$

for all $\ell \in \mathbb{N}_0$, where $M > 0$ depends only on Ω, μ^{-1}, ε, $\mathbf{f}$, $\mathbf{g}_{\text{N}}$ and $\mathbf{g}_{\text{I}}$. $C_k > 0$ is the stability constant from (3).

Note that the constant C_k still depends in an unknown way on k, therefore this theorem is only "almost" k-explicit. Analyzing the dependence of C_k on k, however, is a challenging task. At least if μ^{-1} and ε are chosen to be the identity tensors (matrices) and some further assumptions are made on Ω, wavenumber-explicit estimates on C_k are available [4].

For the purposes of numerical analysis, one has to assume $C_k \leq C|k|^{\theta}$ for constants $C > 0$ and $\theta \in \mathbb{R}$ that depend only on Ω. Under this assumption, Theorem 2 indeed proves k-explicit analytic regularity of $\mathbf{u}$.

Having established the above two regularity results for solutions $\mathbf{u}$ of (1), we follow the arguments from, e.g., [4] to decompose $\mathbf{u}$ into a part with finite Sobolev regularity, which is controlled uniformly in k, and an analytic part with explicit k-dependence. For the sake of simplicity we state the next theorem only for homogeneous boundary data and solenoidal right-hand sides $\mathbf{f}$.

Theorem 3. *Let Ω be a simply connected, analytic domain and assume that the tensor fields μ^{-1} and ε are piecewise analytic on $\overline{\Omega}$ and discontinuous only across certain analytic and mutually disjoint surfaces Γ_{int}. We suppose that the stability constant C_k satisfies the assumption $C_k \leq C|k|^{\theta}$.*

Furthermore, let $\mathbf{g}_{\text{N}} = 0$, $\mathbf{g}_{\text{I}} = 0$, and let a right-hand side $\mathbf{f} \in \mathbf{PH}^1(\Omega)$ with $\text{div}\,\mathbf{f} = 0$ in Ω and $\mathbf{f} \cdot \mathbf{n} = 0$ on Γ_{N} be given. Then, the solution $\mathbf{u}$ of (1) can be decomposed as $\mathbf{u} = \mathbf{u}_{\mathbf{H}^2} + \mathbf{u}_{\mathcal{A}}$ with

$$\|\mathbf{u}_{\mathbf{H}^2}\|_{\mathbf{PH}^2(\Omega)} \leq C'|k|^{-1}\,\|\mathbf{f}\|_{\mathbf{PH}^1(\Omega)} \text{ and } \|\mathbf{u}_{\mathcal{A}}\|_{\mathbf{PH}^{\ell}(\Omega)} \leq |k|^{\lambda} M^{\ell+1}(\ell + |k|)^{\ell}$$

for all $\ell \in \mathbb{N}_0$, where $C' > 0$ depends only on Ω, μ^{-1} and ε; the constant $\lambda \in \mathbb{R}$ depends only on θ; and $M > 0$ is only dependent of Ω, C, μ^{-1}, ε and $\mathbf{f}$.

Theorem 3 can be used for the analysis of Galerkin discretizations of (1) based on Nédélec elements of order p with mesh width h. The analysis then follows [4] and proves a quasi-optimal approximation property of such a Galerkin discretization under the scale resolution condition that $h|k|/p$ is sufficiently small and $p/\ln|k|$ is bounded from below.

The proof of this quasi-optimality result is based on a modified duality argument as in [4], [5, Sec. 7.2] in that the dual problem is split into two parts. The first part involves a classical duality argument and hinges on the k-explicit regularity theory developed in Theorem 3. The second part is treated with the

p-version projection-based interpolation operator of [3], which features p-optimal approximation properties and a commuting diagram property.

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Critical entities in finite element meshes for the Stokes equation in d dimensions

Stefan Sauter

1. Introduction

The development of finite elements for linear, stationary flow problems is usually based on the paradigm of the Stokes equation. Although the continuous problem is well posed, the numerical discretization by the most natural finite elements: continuous, vector valued polynomials of degree k on a simplicial mesh for the velocity and discontinuous polynomials of degree $k-1$ for the pressure can lead to a discrete problem which is singular. These situations are rare and we describe here some of them in general spatial dimension d.

2. Setting

Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz polytope with boundary $\partial\Omega$. Let $L^2(\Omega)$ and $H^1(\Omega)$ be the usual Lebesgue and Sobolev space with vector valued analogon denoted by $\mathbf{L}^2(\Omega)$ and $\mathbf{H}^1(\Omega)$. The subspace of $\mathbf{H}^1(\Omega)$ with zero boundary traces is denoted by $\mathbf{H}_0^1(\Omega)$ and $L_0^2(\Omega) := \left\{q \in L^2(\Omega) \mid \int_\Omega q = 0\right\}$.

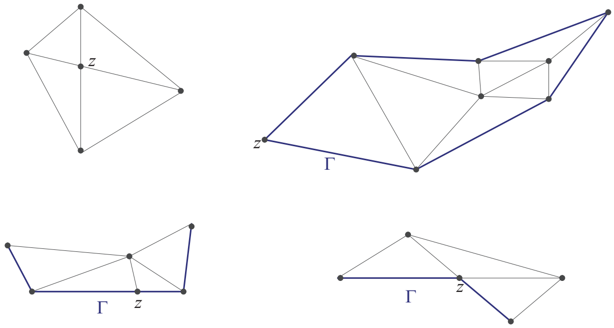

FIGURE 1. All four configurations of critical entities (vertices) in two dimensions.

Definition 1. *A pair* $(\mathbf{H}, M) \subset \mathbf{H}^1(\Omega) \times L^2(\Omega)$ *satisfies the inf-sup condition for the Stokes equation if there exists a constant* $c > 0$ *such that*

$$\inf_{q \in M \backslash \{0\}} \sup_{\mathbf{v} \in \mathbf{H} \backslash \{\mathbf{0}\}} \frac{(q, \operatorname{div} \mathbf{v})_{L^2(\Omega)}}{\|\mathbf{v}\|_{\mathbf{H}^1(\Omega)} \|q\|_{L^2(\Omega)}} \geq c > 0. \tag{1}$$

It is well known (see, e.g., [1]) that the pair $\left(\mathbf{H}_0^1(\Omega), L_0^2(\Omega)\right)$ satisfied the inf-sup condition so that the continuous Stokes problem is well posed.

Next, we introduce finite element spaces on a conforming finite element mesh $\mathcal{T}$ consisting of closed simplices. By $\mathbb{P}_k(K)$ we denote the space of polynomials on $K \in \mathcal{T}$ with degree $\leq k$ and set

$$\begin{aligned}
&\mathbb{P}_k(\mathcal{T}) := \left\{ q \in L^2(\Omega) \mid \forall K \in \mathcal{T} : q|_{\overset{\circ}{K}} \in \mathbb{P}_k\left(\overset{\circ}{K}\right) \right\}, \\
&\mathbb{P}_{k,0}(\mathcal{T}) := \left\{ q \in \mathbb{P}_k(\mathcal{T}) \mid \textstyle\int_\Omega q = 0 \right\} = \mathbb{P}_k(\mathcal{T}) \cap L_0^2(\Omega), \\
&\mathbf{S}_k(\mathcal{T}) := \left(\mathbb{P}_k(\mathcal{T}) \cap H^1(\Omega)\right)^d, \\
&\mathbf{S}_{k,0}(\mathcal{T}) := \mathbf{S}_k(\mathcal{T}) \cap \mathbf{H}_0^1(\Omega).
\end{aligned}$$

It is well known that the canonical pair $(\mathbf{S}_{k,0}(\mathcal{T}), \mathbb{P}_{k,0}(\mathcal{T}))$ can be instable for certain meshes and we will introduce the corresponding critical pressure functions. Let $\mathcal{V}(\mathcal{T})$ be the set of $(d-2)$-dimensional geometric entities in the mesh, i.e., for $d = 2$, $\mathcal{V}(\mathcal{T})$ is the set of triangle vertices and for $d = 3$, $\mathcal{V}(\mathcal{T})$ is the set of tetrahedron edges. For each $\mathbf{z} \in \mathcal{V}(\mathcal{T})$, we define the simplex patch $\mathcal{T}_\mathbf{z} := \{K \in \mathcal{T} \mid \mathbf{z} \subset K\}$ and number the elements in $\mathcal{T}_\mathbf{z}$ consecutively, i.e., $\mathcal{T}_\mathbf{z} = \{K_j : 1 \leq j \leq N_\mathbf{z}\}$ and K_j and K_{j+1} share a common $(d-1)$-dimensional surface simplex.

Definition 2. *A* $(d-2)$*-dimensional mesh entity* $\mathbf{z} \in \mathcal{V}(\mathcal{T})$ *is a* critical entity *if all* $(d-1)$*-dimensional surface simplices in the mesh which contain* $\mathbf{z}$ *fall on two (infinite)* $(d-1)$*-dimensional hyperplanes. The set of critical entities is* $\mathcal{C}(\mathcal{T}) := \{\mathbf{z} \in \mathcal{V}(\mathcal{T}) \mid \mathbf{z}$ *is a critical entity*$\}$.

Definition 3. *For a critical entity $\mathbf{z} \in \mathcal{C}(\mathcal{T})$ and any vertex*[1] $\mathbf{p}$ *of* $\mathbf{z}$, *the higher-dimensional analogue of critical pressure functions (cf.* [2, Def. 3.11], [3, Def. 5.4, 5.7]*) is defined by*

$$b_{\mathbf{z},\mathbf{p},k} := \sum_{j=1}^{N_{\mathbf{z}}} \frac{(-1)^j}{|K_j|} \chi_{K_j} P_k^{(0,d)} \left(1 - 2\lambda_{K_j,\mathbf{p}}\right),$$

where $\lambda_{K,\mathbf{p}}$ is the barycentric coordinate in K for the vertex $\mathbf{p}$, χ_K the characteristic function for K, and $P_k^{(\alpha,\beta)}$ denote the Jacobi polynomial.

Theorem 4. *If a mesh $\mathcal{T}$ contains critical entities, the pair $(\mathbf{S}_{k,0}(\mathcal{T}), \mathbb{P}_{k-1,0}(\mathcal{T}))$ is not inf-sup stable.*

Proof. Let $\mathbf{z} \in \mathcal{C}(\mathcal{T})$, We choose in (1) $q := b_{\mathbf{z},\mathbf{p},k}$. The relation

$$(q, \operatorname{div} \mathbf{v})_{L^2(\Omega)} = 0 \quad \forall \mathbf{v} \in \mathbf{S}_{k,0}(\mathcal{T})$$

follows as in [2, Proof of Lem. 3.12], [3, Proof of Prop. 5.6 and 5.8] and implies that the inf-sup constant is 0. □

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From Heron to high-dimensional integrals (Approximation of Laplace–Stieltjes and Cauchy–Stieltjes functions)

Dietrich Braess

(joint work with Wolfgang Hackbusch)

Two approximation problems have reccently got interest due to new applications. The approximation of the function $x^{-\alpha}, \alpha > 0$, by exponential sums helps to compute some high-dimensional integrals in quantum chemistry. The d-dimensional integrals have the form

$$\int \frac{g(x)}{\|x-y\|^{2\alpha}} dx, \text{ where } g(x) = g_1(x_1)g_2(x_2)\dots g_d(x_d)$$

and $\|\cdot\|$ refers to the Euklidean distance. Approximating the negative power $x^{-\alpha}$ by an exponential sum

$$u_n(x) = \sum_{\nu=1}^{n} c_\nu e^{-t_\nu x}, \text{ with } c_\nu \in \mathbb{R},\ t_\nu > 0,$$

[1] For $d = 2$, $\mathbf{p} = \mathbf{z}$; for $d = 3$, $\mathbf{p}$ is an element in the set of endpoints of a critical edge, for $d = 4$, $\mathbf{p}$ is a vertex of a critical facet $\mathbf{z}$ of a four-dimensional simplex.

we obtain a sum of separable integals avoiding the curse of dimension

$$\int c_\nu g(x) e^{-t_\nu \|x-y\|^2} dx = c_\nu \prod_{i=1}^{d} \int g(x_i) e^{-t_\nu (x_i - y_i)^2} dx_i \,.$$

In the study of differential equations with nonlocal differential operators, the equations with fractional elliptic differential operators have recently attracted interest. The fractional operators are defined via eigenvalues and eigenfunctions, but numerical computations via eigenfunctions are too expansive. The rational approximation of inverses of fractional powers changes the nonlocal differential equations into systems with local differential operators. They can be solved in a well-known manner.

Stieltjes functions

In both cases the given functions are associated Stieltjes functions. In the study of the approximation by exponential sums, a function $f : (0, \infty) \to \mathbb{R}$ is said to be a Laplace–Stieltjes function if

$$f(x) = \int_0^\infty e^{-tx} d\mu(t)$$

holds with some nonnegative measure $d\mu$ and the integral is absolutely convergent. The function $x^{-\alpha},\ 0 < \alpha \le 1$, belongs to this class since a representation with a nonnegative measure follws from the well-known definition of the Γ-function. In the study of rational approximation, a function $f : (0, \infty) \to \mathbb{R}$ is said to be a Cauchy–Stieltjes function if

$$f(x) = \int_0^\infty \frac{d\mu(t)}{1 + tx}$$

holds with some nonnegative measure $d\mu$ and the integral is absolutely convergent.The function $x^{-\alpha},\ 0 < \alpha < 1$, belongs to this class due to the Balakrishnan formula.

Weighted rational approximation of the square root function

A powerful tool for the analysis of the two approximation problems is a weighted rational approximation of the square root function. Results on the auxiliary approximation problem were already known to Zolotarev in 1877. We denote the sets of rational functions as usual as

$$R_{m,n} := \left\{ \frac{p_m}{q_n} : \text{degree}(p_m) \le m \text{ and degree}(q_n) \le n \right\}.$$

The point of departure is Heron's method for the computation of the square root of a positive real number. It coincides with the Newton method for determining the root of the associated quadratic equation. Let $v_j = p_m / q_{m-1} \in R_{m,m-1}$. The iteration step yields

$$v_{j+1} = \frac{1}{2}(v_j + \frac{x}{v_j}) = \frac{1}{2} \frac{p_m^2 + x\, q_{m-1}^2}{p_m q_{m-1}} \in R_{2m,2m-1}.$$

If $u_{m,m-1}$ is the best approximation of the square root function with respect to the weighted norm $\sup\{|f(x)/\sqrt{x}|,\ x \in [a,b]\}$, the Newton step combined with rescalings yields the best approximation $u_{2m,2m-1} \in R_{2m,2m-1}$ with the same weight.

Now, Gauss' arithmetic-geometric process enters into the analysis. Given $0 < a_0 \le b_0$, the process yields the double seqence $a_{j+1} = \sqrt{a_j b_j},\ b_{j+1} = \frac{1}{2}(a_j + b_j)$. The quotients $\lambda_j := b_j/a_j$ converges very fast to 1. The recursion relation $\lambda_{j+1} = \frac{1}{2}(\lambda^{1/2} + \lambda^{-1/2})$ is denoted as Landen transformation. The exponential decay of the degree of approximation can be obtained by a few steps of the inverse Landen transformation or it is expressed in terms of elliptic integrals.

Application of results for the square root function to the approximation by exponential sums

The main tool for treating the approximation of Laplace–Stieltjes functions is the following theorem.

Theorem 5. *Let $n \ge 1$, f be a Laplace–Stieltjes function and assume that*

$$\left|\frac{p_n(x)}{q_{n-1}(x)} - \sqrt{x}\right| \le \theta_n \sqrt{x} \quad \text{for } x \in [a^2, b^2]$$

with $\theta_n \le 1$. Then there exists an exponential sum v_n of order n such that

$$|f(x) - v_n(x)| \le 2\theta_n f(1/n) \quad \text{for } x \in [a,b].$$

Sketch of a proof. Put $x = z^2$ and set $P_{2n}(z) := p_n(z^2) - z q_{n-1}(z^2)$:

$$\left|\frac{P_{2n}(z)}{P_{2n}(-z)}\right| \le \theta \qquad \text{for} z \in [a,b].$$

Let v_n be the exponential sum that interpolates the given function f at the zeros of P_{2n} in $[a,b]$. Then $(f - v_n)P_{2n}(-x)/P_{2n}(x)$ is an analytic function in the right half-plane. The assertion of the theorem follows now from the maximum priciple.

Numerical computations show that the theorem yields the correct exponential decay of the approximation error for $x^{-\alpha}$, although there is no theoretical result on lower bounds of the error. We note that the convergence is slower than for the square root function, since the assumption in the theorem refers to the larger interval $[a^2, b^2]$.

Application of results for the square root function to the approximation of Cauchy–Stieltjes functions

Formally, Theorem 1 holds as well for the rational approximation of Cauchy–Stieltjes functions. Here the interpolation problem is solvable by rational functions without poles in the right half-plane. Numerical experiments, however, have shown that the exponential decay of the error is much faster. It is determined by the approximation of the square root function on the interval $[a,b]$ and not on the larger interval $[a^2, b^2]$. Indeed, let

$$\left|\frac{p_n(x)/q_{n-1} - \sqrt{x}}{\sqrt{x}}\right| \le \theta_n \text{ for } x \in [a,b].$$

The error depends only on the quotient b/a. Hence, the error is the same on the interval $[b^{-1}, a^{-1}]$. By setting $x = 1/z$ we obtain

$$\left| \frac{p_n(1/z)}{q_{n-1}(1/z)} - z^{-1/2} \right| \leq a^{-1/2}\theta_n \text{ for } x \in [a,b].$$

Multiplying the numerator and the denominator by z^n we obtain a rational function in $R_{n,n} \subset R_{n,n+1}$. The asymptotic behavior is therefore the same as for the approximation of the square root function on the interval $[a,b]$. The exponential decay of the approximation error is faster than in the situation with the approximation by exponential sums.

We conclude from the estimates with the Landen transformation that this result is also a lower bound for th asymptotic behavior up to a constant. The same exponential behavior is expected for all (non-degenerate) Cauchy–Stieltjes functions due to the results by Gončar and Ganelius. This behavior is confirmed by numerical computations for $x^{-\alpha},\ 0 < \alpha < 1$.

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Numerical computations of best-approximations of $1/x$ by exponential sums w.r.t. the maximum norm

Wolfgang Hackbusch

1. Exponential Sums

Exponential sums are of the form

$$E_n(x) = \sum\nolimits_{\nu=1}^{n} a_\nu \exp(-b_\nu x) \qquad (x \in [a,b] \text{ with } 0 < a < b \leq \infty).$$

Approximations $E_n(x) \approx 1/\sqrt{x}$ are interesting for Coulomb or Newton potentials $\iiint \frac{f(y)}{\|x-y\|}\mathrm{d}y$, since in the case of $f(y) = f_1(y_1)f_2(y_2)f_3(y_3)$ the replacement of $1/\|x-y\|$ by $E_n(\|x-y\|^2)$ yields a product of one-dimensional integrals.

A similar effect is used in the second-order Møller–Plesset theory (MP2) in quantum chemistry, where an expression of the form $\cdots/\sum_i e_i$ can be decoupled by using $E_n(x) \approx 1/x$ (cf. [12]). In [5] exponential sums are used for solving pdes with fractional time derivative. Another application of $E_n(x) \approx 1/x$ is the inversion of separable differential operators of the form $\mathbf{L} = L_1 \otimes I \otimes I + I \otimes L_2 \otimes I + I \otimes I \otimes L_3$, since $E_n(\mathbf{L}) \approx \mathbf{L}^{-1}$ is a sum of n Kronecker products (cf. [8]).

Here it is essential that the approximation error $1/x - E_n(x)$ can be estimated with respect to the maximum norm. This leads us to the Chebyshev problem

$$\text{minimise } \|1/x - E_n(x)\|_{\infty,[a,b]}$$

for a fixed interval $[a, b]$ with $0 < a < b \leq \infty$. The minimiser E_n is called the best-approximation. Its approximation error is denoted by $\eta_n([a, b])$. It is proved in [3, 4] that the asymptotic behaviour is $\|\eta_n([a, b])\|_\infty \sim \rho^n_{[a,b]}$ ($\rho_{[a,b]} < 1$) for finite intervals, while $\|\eta_n([a, \infty))\|_\infty \sim \rho_a^{\sqrt{n}}$ holds for a semi-infinite interval.

The best-approximations E_n in $[a, b]$ depend mainly on the ratio $R = b/a$, i.e., it suffices to consider the interval $[1, R]$. Approximations in $[\lambda, \lambda R]$ can be obtained by a simple scaling of the coefficients a_ν, b_ν.

2. Computation of Exponential Sums

Because of the interesting applications, the author computed the best-approximations of $1/x$ as well as $1/\sqrt{x}$ for various intervals $[a, b]$ and $1 \leq n \leq 56$ (see data collection in [6]). Later he became aware that in the literature the computation of optimal exponential sums is considered as rather difficult (see, e.g., [2], [10]).

The best-approximation is characterised by the equi-oscillation of the error $\eta_n(x) = 1/x - E_n(x)$ in $[a, b]$ with an alternant $(\alpha_0, \alpha_1, \ldots, \alpha_{2n})$ containing points in $[a, b]$ with $\eta_n(\alpha_j) = (-1)^j \|\eta_n\|_\infty$. In the case of polynomial approximation, the classical Remez algorithm converges to the best polynomial (cf. [11]). In the case of exponential sums one obtains $2n$ nonlinear equations $F_j(a_\nu, b_\nu) := \eta_n(\alpha_{j-1}) + \eta_n(\alpha_j) = 0$ $(1 \leq j \leq 2n)$ for the $2n$ coefficients (a_ν, b_ν) of E_n. Since F is analytic and $F = 0$ has a unique solution, Newton's method (together with a damping strategy) seem to be appropriate. However, this approach fails except for rather small n. The reason is the fact that all iterates must be admissible functions, i.e., the error $1/x - E_n(x)$ must oscillate with $n+1$ extrema defining an alternant. Note that for larger n the approximation error η_n is already very small and perturbations of the coefficient lead to an inadmissible exponential sum.

The remedy used by the author is the use of appropriate parameters. E_n is admissible if and only if η_n has $2n$ zeros ξ_j $(1 \leq j \leq 2n)$. The zeros of η_n are the interpolation points of E_n. It is known that for $1/x$ the interpolating exponential sum is uniquely determined. This formally allows us to consider E_n as a function of $\boldsymbol{\xi} = (\xi_j)_{1 \leq j \leq 2n}$. For all $\boldsymbol{\xi} \subset [a, b]$, $E_n(\boldsymbol{\xi})$ is an admissible function. Now, Newton's method can be applied to $E_n(\boldsymbol{\xi})$ yielding corrections of $\boldsymbol{\xi}$. The functional matrix F' can be determined by divided differences. However, a drawback is the fact that — different from the polynomial case — there is no explicit representation of E_n belonging to $\boldsymbol{\xi}$. For this purpose, a secondary Newton method can be used to compute the coefficients (a_ν, b_ν) of $E_n(x) = \sum_{\nu=1}^{n} a_\nu \exp(-b_\nu x)$ interpolating at $\boldsymbol{\xi}$. Note that this iteration does not require admissible iterates. The result are coefficients $a_\nu(\boldsymbol{\xi})$ and $b_\nu(\boldsymbol{\xi})$, so that $E_n(\boldsymbol{\xi}) = E_n(a_\nu(\boldsymbol{\xi}), b_\nu(\boldsymbol{\xi}))$.

A critical point is always the start of Newton's iteration because of the local convergence. The strategy is as follows. Computations for $n = 1$ are easy. If one has a best-approximation in some interval $[1, R]$, this is a good starting value for the computation in $[1, R']$ with R' sufficiently close to R. More delicate is the continuation from n to $n+1$. To obtain an admissible E_{n+1} one adds two further interpolation points larger than the previous ones. To obtain a starting value for the Newton process solving the interpolation problem, one adds two small coefficients a_0, b_0 which one can obtain by extrapolation of the previous a_ν, b_ν. Having solved the interpolation problem, one has an admissible E_{n+1} and can start Newton's iteration for $F = 0$ (cf. [9]).

3. Best Rational Approximation

The same approach can be used to the computation of the optimal rational approximation of a Cauchy-Stieltjes function like, e.g., x^{-s}. The appropriate set of rational functions is $R_{n,n-1}$, i.e., of functions $r = p_n/q_{n-1}$ with polynomial degrees $\deg(p_n) \leq n$ and $\deg(q_{n-1}) \leq n-1$. It is known that for Cauchy-Stieltjes functions a unique best-approximation $r \in R_{n,n-1}$ exists and is of the form

$$r(x) = \sum\nolimits_{\nu=1}^{n} \frac{a_\nu}{x + b_\nu} \qquad \text{with } a_\nu, b_\nu > 0.$$

Again, formally, the rational function is considered as a function of the interpolations points $\boldsymbol{\xi} = (\xi_j)_{1 \leq j \leq 2n}$. As before, given $\boldsymbol{\xi}$, a secondary Newton process is used to determine the coefficients $a_\nu(\boldsymbol{\xi})$ and $b_\nu(\boldsymbol{\xi})$ of the interpolant.

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Reconstruction and approximation with short exponential sums

Gerlind Plonka
(joint work with Nadiia Derevianko)

Consider the weighted space $L_2(\mathbb{R}, \rho)$ with the norm

$$\|f\|^2_{L_2(\mathbb{R},\rho)} := \int_{-\infty}^{\infty} |f(t)|^2 \, \mathrm{e}^{-t^2/2\rho} \, \mathrm{d}t \tag{1}$$

for some given $\rho > 0$. Our goal is to find an exponential sum $y_N(t) = \sum_{j=1}^{N} \gamma_j \, \mathrm{e}^{\lambda_j t}$ with γ_j, $\lambda_j \in \mathbb{C}$ that optimally approximates the Gaussian $\mathrm{e}^{-t^2/2\sigma}$ with fixed positive σ on $\mathbb{R}$ with regard to the weighted norm (1). This leads to the non-linear and non-convex minimization problem

$$\min_{\boldsymbol{\lambda}\in\mathbb{C}^N, \boldsymbol{\gamma}\in\mathbb{C}^N} \|\mathrm{e}^{-\cdot^2/2\sigma} - \sum_{j=1}^{N} \gamma_j \, \mathrm{e}^{\lambda_j \cdot}\|_{L_2(\mathbb{R},\rho)}.$$

Therefore, we use a suboptimal approximation method as in [2]. This method is based on the following observation. For every exponential sum $y_N(t) = \sum_{j=1}^{N} \gamma_j \, \mathrm{e}^{\lambda_j t}$, there exists a differential operator D_N given by

$$D_N f(t) := \frac{d^N}{dt^N} f(t) + b_{N-1} \frac{d^{N-1}}{dt^{N-1}} f(t) + \ldots + b_0 f(t), \qquad f \in C^N(\mathbb{R}), \tag{2}$$

with constant coefficients $b_0, \ldots, b_{N-1} \in \mathbb{C}$ such that $D_N y(t) = 0$. This differential operator is determined by the coefficients of the monomial representation of the (characteristic) polynomial

$$P_N(\lambda) = \prod_{j=1}^{N} (\lambda - \lambda_j) = \lambda^N + \sum_{k=0}^{N-1} b_k \, \lambda^k. \tag{3}$$

Therefore, if a function f can be well approximated by a short exponential sum, it should be possible to find a differential operator D_N such that $D_N f$ is small. Consequently, we apply the following strategy to approximate $f(t) = \mathrm{e}^{-t^2/2\sigma}$ by an exponential sum $y_N(t)$. In a first step, we determine a polynomial $P_N(\lambda)$ of the form (3), i.e., we determine the vector $\mathbf{b} = (b_0, \ldots, b_{N-1})^T$ of coefficients of $P_N(\lambda)$ by solving

$$\operatorname*{argmin}_{\mathbf{b}\in\mathbb{C}^N} \|D_N f\|_{L^2(\mathbb{R},\rho)}. \tag{4}$$

Then the zeros λ_j of the characteristic polynomial $P_N(\lambda)$ in (3) are taken as the frequencies of the exponential sum to approximate f. In a second step, we compute the vector $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_N)^T$ of coefficients of the exponential sum by solving

$$\operatorname*{argmin}_{\boldsymbol{\gamma}\in\mathbb{C}^N} \|f - \sum_{j=1}^{N} \gamma_j \, \mathrm{e}^{\lambda_j \cdot}\|_{L^2(\mathbb{R},\rho)}. \tag{5}$$

The minimization problem (4) can be solved analytically for $f(t) = \mathrm{e}^{-t^2/2\sigma}$. Moreover, the corresponding characteristic polynomial $P(\lambda)$ in (3) is a normalized scaled Hermite polynomial of degree N, such that the zeros λ_j can be simply precomputed with high accuracy. The second minimization problem (5) leads to an equation system of size $N \times N$, where the coefficient matrix is positive definite. Since N is small, the obtained algorithm requires only a small computational effort. The resulting exponential sum to approximate the Gaussian is a cosine sum of length $\lfloor (N+1)/2 \rfloor$. We can show that the proposed method leads to an approximation error

$$\Big\| \mathrm{e}^{-\cdot^2/2\sigma} - \sum_{j=1}^{\lfloor (N+1)/2 \rfloor} \tilde{\gamma}_j \cos(|\lambda_j| \cdot) \Big\|_{L_2(\mathbb{R},\rho)} < \Big(\frac{r}{\sqrt{2(2r+1)}} \Big)^N N^{3/4},$$

where $r := \frac{\rho}{\sigma}$. For example, for $r = \frac{1}{2}$, we therefore obtain the error decay rate $4^{-N} N^{3/4}$. The proof of this error estimate is heavily based on the fact that the Gauss-Hermite quadrature rule leads to exponential decay rates for Gaussian functions. Since the Gaussian $\mathrm{e}^{-t^2/2\sigma}$ itself decays exponentially, we further derive an error estimate in the $L_2(\mathbb{R})$ norm of the form

$$\int_{-\infty}^{\infty} \Big| \mathrm{e}^{-t^2/2\sigma} - \chi_{[-T,T]}(t) \sum_{k=1}^{\lfloor (N+1)/2 \rfloor} \tilde{\gamma}_k \cos(|\lambda_k| t) \Big|^2 \mathrm{d}t \le \frac{\tilde{c}}{16^{N/2}} N^{3/2},$$

using a truncated cosine sum, where $T := \sqrt{2\sigma N \ln(2)}$.

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Orthogonal Polynomials, Quadrature and Continued Fractions

Tomas Sauer
(joint work with Yuan Xu)

Continued fractions and orthogonal polynomials have a long joint history, even Gauss' original paper [2] is actually based on continued fractions. One of these fundamental relationships is that numerator p_n and denominator q_n of the *convergents*

$$\frac{p_n(x)}{q_n(x)} = \frac{1|}{|r_1(x)} + \cdots + \frac{1|}{|r_n(x)}, \qquad r_j(x) = \alpha_j x + \beta_j,$$

satisfy a *three-term recurrence*

$$p_n(x) = (\alpha_n x + \beta_n)\, p_{n-1}(x) + p_{n-2}(x), \qquad q_n(x) = (\alpha_n x + \beta_n)\, q_{n-1}(x) + q_{n-2}(x),$$

distinguished only by the initial values for p_{-1}, p_0 and q_{-1}, q_0. A classical result from continued fractions states that a formal Laurent series of the form

$$\lambda(x) = \sum_{j=0}^{\infty} \lambda_j x^{-j}, \qquad \lambda_j \in \mathbb{R},$$

has an *associated continued fractions*, i.e., a sequence of coefficients r_j, such that

$$\lambda(x) - \frac{1|}{|r_1(x)} + \cdots + \frac{1|}{|r_n(x)} = O(x^{-2n-1}), \qquad n \in \mathbb{N}$$

if and only if $\lambda_0 = 0$ and

$$\det \begin{pmatrix} \lambda_1 & \dots & \lambda_n \\ \vdots & \ddots & \vdots \\ \lambda_n & \dots & \lambda_{2n-1} \end{pmatrix} \neq 0, \qquad n \in \mathbb{N}.$$

Now, let $\mu : \mathbb{N}_0 \to \mathbb{R}$ be a (moment) sequence such that for $n \in \mathbb{N}_0$

$$\det M_n \neq 0, \qquad M_n := \begin{pmatrix} \mu_0 & \dots & \mu_n \\ \vdots & \ddots & \vdots \\ \mu_n & \dots & \mu_{2n} \end{pmatrix},$$

i.e., a sequence such that the Laurent series $\mu(x)$ has an associated continued fraction. The sequence defines a definite signed inner product $(p, q) = p^T M_n q$, $p, q \in \Pi_n$, where we identify polynomials with their coefficient vector. The monic orthogonal polynomial q_n, defined by $q_n(x) = x^n + q_{n-1}x^{n-1} + \cdots + q_0$ and $(\Pi_{n-1}, q_n) = 0$ can be obtained as

$$0 = \begin{pmatrix} M_{n-1} & \begin{pmatrix} \mu_n \\ \vdots \\ \mu_{2n} \end{pmatrix} \\ \begin{pmatrix} \mu_n & \dots & \mu_{2n} \end{pmatrix} & t \end{pmatrix} q_n, \qquad t := \begin{pmatrix} \mu_n & \dots & \mu_{2n} \end{pmatrix} M_{n-1}^{-1} \begin{pmatrix} \mu_n \\ \vdots \\ \mu_{2n} \end{pmatrix},$$

i.e., as the unique monic kernel polynomial of the *flat extension* of the initial segment M_{n-1} of the infinite Hankel operator defined by μ. If we factor $q_n(x) = (x - \zeta_1) \cdots (x - \zeta_n)$, $\zeta_j \in \mathbb{C}$, then q is the *Prony polynomial* for the exponential sum

$$f(x) = \sum_{k=1}^{n} f_k \, \zeta_k^x,$$

at least provided all the zeros are simple; multiple zeros have to be dealt according to their multiplicity and lead to exponential polynomials, cf. [6]. If we now sample the function f into $\hat{\mu}_k = f(k)$, then

(1) $\mu_j = \hat{\mu}_j$, $j = 0, \dots, 2n-1$,
(2) $\hat{\mu}(x) = \frac{p_n(x)}{q_n(x)}$ for some polynomial p_n,
(3) the infinite Hankel operator with respect to $\hat{\mu}$ has rank $n-1$.

The equivalence of the last two statements is well-known as Kronecker's Theorem. cf. [3].

This "detour to quadrature" has the advantage that in principle it can be extended to d variables where the starting point is now a multiindexed moment sequence μ_α, $\alpha \in \mathbb{N}_0^d$ and we consider

$$M_n := \left(\mu_{\alpha+\beta} : \begin{array}{c} |\alpha| \le n \\ |\beta| \le n \end{array} \right) \quad \text{and} \quad M_{n,n+1} := \left(\mu_{\alpha+\beta} : \begin{array}{c} |\alpha| \le n \\ |\beta| = n+1 \end{array} \right).$$

The rank preserving extension of M_{n-1} is

$$\begin{pmatrix} M_{n-1} & M_{n-1,n} \\ M_{n-1,n}^T & M_{n-1,n}^T M_{n-1}^{-1} M_{n-1,n} \end{pmatrix}$$

and its kernel defines a *vector* P_n of orthogonal polynomials of degree n. These polynomials satisfy a three-term recurrence

$$x_j P_{n-1}(x) = A_{n,j} P_n(x) + B_{n,j} P_n(x) + C_{n,j} P_{n-1}(x), \qquad j = 1, \ldots, d,$$

and the fact that these matrices represent the behavior of multiplication relative to the functional L that defines μ via $\mu_\alpha = L\left((\cdot)^\alpha\right)$, $\alpha \in \mathbb{N}_0^d$, implies commuting relations among them, cf. [1]. It turns out that the existence of a associated continued fraction or, equivalently, a Gaussian cubature formula is equivalent to the orthogonal polynomials being an H-basis which leads to a complete characterization of all these properties. In addition, it turns to be equivalent to the fact that the completing matrix $M_{n-1,n}^T M_{n-1}^{-1} M_{n-1,n}$, determined by the Schur complement in the flat extension, has Hankel structure, i.e., that the naive Linear Algebra extension of the truncated Hankel operator is structure preserving.

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Classical orthogonal polynomials of two and more variables, a survey

Tom H. Koornwinder

For general literature see [5] and the forthcoming Chapter 37 in [12] by the author and Yuan Xu on *Orthogonal polynomials of several variables.*

For μ a positive measure on $\mathbb{R}^d$ with all moments finite let $\mathcal{P}_n$ be the space of all polynomials of degree $\le n$ such that $\int_{\mathbb{R}^d} p(x)\, q(x)\, \mathrm{d}\mu(x) = 0$ for all polynomials q of degree $< n$. Then $\{\mathcal{P}_n\}_{n=0,1,2,\ldots}$ is called a *system of orthogonal polynomials (OPs)* with respect to μ. Such a system is called *classical* if there is a second order partial differential operator (PDO) L such that $L\,p = \lambda_n\,p \quad (p \in \mathcal{P}_n)$. For $d = 2$ and with $\mathrm{d}\mu(x, y) = w(x, y)\,\mathrm{d}x\,\mathrm{d}y$ on an open set U in $\mathbb{R}^2$ and otherwise 0, there are essentially the following classical cases $(w(x, y), U)$ [10], [11] $(\alpha, \beta, \gamma > -1)$: (i) $(\mathrm{e}^{-x^2-y^2}, \mathbb{R}^2)$; (ii) $(x^\alpha y^\beta \mathrm{e}^{-x-y}, (0, \infty)^2)$; (iii) $(y^\beta \mathrm{e}^{-x^2-y}, \mathbb{R} \times (0, \infty))$; (iv) $(x^\alpha y^\beta (1 - x - y)^\gamma,\ x, y, 1 - x - y > 0)$; (v) $((1 - x^2 - y^2)^\alpha,\ x^2 + y^2 < 1)$.

Analogues for general d of these five cases are easily suspected (for (iv) on the simplex and for (v) on the ball), but there is no classification result for $d > 2$. For classical OPs of d variables we can get an orthogonal basis for $\mathcal{P}_n$ as the eigenbasis of L and $d - 1$ further PDOs, mutually commuting and self-adjoint with respect to μ. For the triangle case (iv) $(d = 2)$ one thus considers OPs [13, 8]

$$P^{\alpha,\beta,\gamma}_{n,k}(x, y) = P^{(\alpha,\beta+\gamma+2k+1)}_{n-k}(1 - 2x)\,(1 - x)^k\, P^{(\beta,\gamma)}_k\left(1 - \frac{2y}{1 - x}\right), \tag{1}$$

where $P^{(\alpha,\beta)}_n(x)$ is a *Jacobi polynomial* [12, §18.3]. These OPs are much used in numerical analysis [3, 7, 1, 9].

More general OPs on the triangle for weight function $w(x, y) = w_1(x)\, w_2\big(\frac{y}{1-x}\big)$ are $p_{n,k}(x, y) = p^k_{n-k}(x)(1 - x)^k q_k\big(\frac{y}{1-x}\big)$, where $p^k_n(x)$ are OPs for weight function $w_1(x)(1 - x)^{2k+1}$ on $(0, 1)$ and $q_n(x)$ are OPs for weight function $w_2(x)$ on $(0, 1)$. Such $p_{n,k}(x, y)$ only contain monomials $x^{m-j}y^j$ with $m \le n$ and $j \le k$, and the recurrence relations for $xp_{n,k}$ and $yp_{n,k}$ only contain 3 respectively 9 terms. Compare this with the recurrence relations for general OPs of 2 variables, where the number of terms grows with n. Still this seems to be numerically doable [2].

The *Askey scheme* [12, Figure 18.21.1] extends the notion of classical OPs in one variable (i.e., Jacobi, Lagurre, Hermite being eigenfunctions of a second order differential operator) to OPs which are eigenfunctions of a second order difference operator. All these OPs are hypergeometric functions (${}_4F_3$ on the four-parameter top level of Wilson and Racah polynomials). The other families in the scheme are special or limit cases of the top level polynomials. A wider notion of classical OPs of d variables considers eigenfunctions of a partial difference operator instead of a PDO. In particular, there are such OPs similar to (1) but built from one-variable OPs on a higher level in the Askey scheme [15, 16]. For instance, from *Hahn polynomials* $Q_n(x; \alpha, \beta, N) = {}_3F_2(-n, n+\alpha+\beta+1, -x; \alpha+1, -N; 1)$ $(n = 0, 1, \ldots, N)$, orthogonal for $x = 0, 1, \ldots, N$ with respect to weights $\frac{(\alpha+1)_x}{x!}\,\frac{(\beta+1)_{N-x}}{(N-x)!}$, one can build OPs $Q_{n,k}(x, y; \alpha, \beta, \gamma, N) = Q_{n-k}(x; \alpha, \beta+\gamma+2k+1, N-k)(-N+x)_k\, Q_k(y; \beta, \gamma, N-x)$ [6] with weights $\frac{(\alpha+1)_x}{x!}\,\frac{(\beta+1)_y}{y!}\,\frac{(\gamma+1)_{N-x-y}}{(N-x-y)!}$, $x, y = 0, \ldots, N$, $x+y \le N$. For $N \to \infty$ the OPS $Q_{n,k}(Nx, Ny; \alpha, \beta, \gamma, N)$, orthogonal on an increasingly denser uniform triangular grid, tend to the OPs (1) (up to a constant factor). Compare this with the non-uniform triangular grid obtained by the Duffy transform [4] from the uniform 1D grids for handling the Jacobi polynomial factors in (1).

Disk polynomials $R^\alpha_{m,n}(z)$ $(z \in \mathbb{C},\ m, n \in \mathbb{Z}_{\ge 0},\ \alpha > -1)$ are given by

$$R^\alpha_{m,n}(r\mathrm{e}^{\mathrm{i}\theta}) = \text{const.}\, P^{(\alpha,|m-n|)}_{\min(m,n)}(2r^2 - 1)\, r^{|m-n|}\, \mathrm{e}^{\mathrm{i}(m-n)\theta}. \tag{2}$$

The polynomials $R^{\alpha}_{k,n-k}(x+\mathrm{i}y)$ $(k=0,\ldots,n)$ form a complex orthogonal basis of $\mathcal{P}_n$ in case (v) of the 2D classical OPs. A real orthogonal basis can be formed as well by taking the real and imaginary parts of the disk polynomials. For $\alpha=0$ these real OPs are the *Zernike polynomials* [18], introduced for usage in optics, and they are still much used there, notably in chip machine design at ASML and Zeiss. In (2) we may replace $P_n^{(\alpha,k)}(x)$ by $p_n^{(k)}(x)$, being an OP for weight functioon $x^k w(x)$ on $(0,\infty)$. Then the resulting 2D polynomials are OPs for weight function $w(x^2+y^2)$ on $\mathbb{R}^2$. In the most recent EUV technology at ASML OPs on an annulus (disk with small central hole) instead of a disk are needed [17]: the *Tatian polynomials* [14] coming from OPs on $(\delta,1)$ orthogonal with respect to weight function x^k. These are *semiclassical* OPs.

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Vector and Matrix-valued High Order Finite Elements

Joachim Schöberl

Legendre polynomials provide an L_2 orthogonal basis on the interval. By tensorization, it is straight forward to obtain an orthogonal basis on higher dimensional intervals. Based on Duffy's transformation, Dubiner's basis

$$P_i\left(\frac{x}{1-y}\right)(1-y)^i\,P_j^{(2i+1,0)}(2y-1)$$

is an orthogonal basis on triangles, and similar on simplices in higher dimensions. To build finite element sub-spaces of the Sobolev space H^1, we have to construct piecewise polynomials on a mesh, which are continuous across element interfaces. For this, the basis is split into subsets associated with mesh nodes, for example vertices, edges, faces, and cells for the 3D case.

Function spaces $H(\mathrm{curl})$ and $H(\mathrm{div})$ consist of functions with continuous tangential and normale traces, respectively. These spaces fit into the de Rham sequence

$$H^1 \xrightarrow{\mathrm{grad}} H(\mathrm{curl}) \xrightarrow{\mathrm{curl}} H(\mathrm{div}) \xrightarrow{\mathrm{div}} L_2.$$

In [1, 2], high order finite element spaces built on similar tensor product constructions were built for for $H(\mathrm{curl})$ and $H(\mathrm{div})$. The basis functions associated with mesh nodes satisfy a local version of the de Rham sequence, what allow to vary the polynomial order for every node. This constructions has been used successfully for solving problems in electromagnetics as well as fluid dynamics.

In recent years, the construction has been extended for matrix-valued function spaces with certain continuity. In [9, 8] for matrix valued spaces with normal-normal continuity used in solid and structural mechanics, in [4, 3] for spaces with normal-tangential continuity with applications in fluid dynamics, and in [5, 6, 7] for spaces with tangential-tangential continuity with applications in curvature computation and numerical relativity.

All these finite element spaces together with canonical differential operators are available in the open source finite element software NGSolve (www.ngsolve.org).

Current active research is to connect these matrix-valued spaces within a complex similar to the de Rham complex.

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Bivariate Bernstein-Szegő polynomials

Plamen Iliev
(joint work with Jeffrey S. Geronimo)

The Bernstein-Szegő measures and polynomials on the real line play an important role in probability, numerical analysis and approximation theory. In this talk, I will define bivariate extensions of these measures and associated spaces of polynomials, and discuss their spectral and characteristic properties. The talk is based on the work [4].

Bernstein-Szegő measures on $\mathbb{R}$. An important class of measures on $\mathbb{R}$ introduced by Bernstein and Szegő are the measures of the form

$$d\mu = \frac{2}{\pi}\frac{\sqrt{1-x^2}}{Q(x)}\chi_{(-1,1)}(x)\,dx, \tag{1}$$

where $Q(x)$ is a polynomial nonvanishing on $(-1,1)$, with at most simple zeros at $x=\pm1$ and χ_J denotes the characteristic function of a set J. Recall that if $\{p_k(x)\}_{k=0}^{\infty}$ are orthonormal polynomials with respect to a measure μ on the real line, then the multiplication by x can be represented by a three-term operator

$$a_{k+1}p_{k+1}(x) + b_k p_k(x) + a_k p_{k-1}(x) = xp_k(x).$$

Suppose that $Q(x)$ is a polynomial of degree at most $2n$ for some positive integer n, and let $q(z)$ denote the stable Fejér-Riesz factor of $Q(x)$, i.e. $q(z)$ is the unique polynomial with real coefficients and no zeros in the closed unit disk, except possibly for simple zeros at $z=\pm1$, such that

$$Q(x) = q(z)q(1/z), \qquad \text{where} \qquad x = \frac{1}{2}\left(z+\frac{1}{z}\right),$$

normalized so that $q(0)>0$. We can define orthonormal polynomials with respect to μ in (1) by

$$p_k(x) = \frac{z^{k+1}q(1/z) - z^{-k-1}q(z)}{z-1/z} \quad \text{for } k\geq n. \tag{2}$$

The last equation implies that

$$a_{k+1} = \frac{1}{2} \quad \text{and} \quad b_k = 0 \qquad \text{for } k \geq n. \tag{3}$$

Conversely, if (3) holds then (1) holds for some polynomial $Q(x)$ of degree at most $2n$ if and only if

$$q(z) = z^n \left(p_n(x) - 2za_n p_{n-1}(x)\right) \neq 0 \qquad \text{for} \qquad z \in (-1,1),$$

see [1, 2] and the references therein.

Bivariate extension. Let $\mathbb{R}[x,y]$ denote the space of all polynomials of x and y with real coefficients, and for $k,l \in \mathbb{N}_0$, let $\mathbb{R}_k[x] = \text{span}_{\mathbb{R}}\{x^i : 0 \leq i \leq k\}$, $\mathbb{R}_l[y] = \text{span}_{\mathbb{R}}\{y^i : 0 \leq i \leq l\}$, $\mathbb{R}_{k,l}[x,y] = \text{span}_{\mathbb{R}}\{x^i y^j : 0 \leq i \leq k, 0 \leq j \leq l\}$. For a measure μ on $\mathbb{R}^2$ we set

$$\mathsf{P}_{k,l;\mu}[x,y] = \mathbb{R}_{k,l}[x,y] \ominus \mathbb{R}_{k-1,l}[x,y] \text{ and } \tilde{\mathsf{P}}_{k,l;\mu}[x,y] = \mathbb{R}_{k,l}[x,y] \ominus \mathbb{R}_{k,l-1}[x,y].$$

We can construct an orthonormal basis $\{p^j_{k,l}(x,y) : 0 \leq j \leq l\}$ of the space $\mathsf{P}_{k,l;\mu}[x,y]$ using lexicographical order of the monomials and we set $P_{k,l}(x,y) = [p^0_{k,l}(x,y), p^1_{k,l}(x,y), \ldots, p^l_{k,l}(x,y)]^t$. Similarly, we use reverse lexicographical order of the monomials to construct a basis $\{\tilde{p}^j_{k,l}(x,y) : 0 \leq j \leq k\}$ for $\tilde{\mathsf{P}}_{k,l;\mu}[x,y]$, and we set $\tilde{P}_{k,l}(x,y) = [\tilde{p}^0_{k,l}(x,y), \tilde{p}^1_{k,l}(x,y), \ldots, \tilde{p}^k_{k,l}(x,y)]^t$. These vector polynomials satisfy the following recurrence relations

$$xP_{k,l}(x,y) = A_{k+1,l}P_{k+1,l}(x,y) + B_{k,l}P_{k,l}(x,y) + A^t_{k,l}P_{k-1,l}(x,y),$$
$$y\tilde{P}_{k,l}(x,y) = \tilde{A}_{k,l+1}\tilde{P}_{k,l+1}(x,y) + \tilde{B}_{k,l}\tilde{P}_{k,l}(x,y) + \tilde{A}^t_{k,l}\tilde{P}_{k,l-1}(x,y),$$

where $A_{k,l}, B_{k,l}$ are $(l+1)\times(l+1)$ matrices and $\tilde{A}_{k,l}, \tilde{B}_{k,l}$ are $(k+1)\times(k+1)$ matrices. Suppose that $x = \frac{1}{2}\left(z + \frac{1}{z}\right)$, $y = \frac{1}{2}\left(w + \frac{1}{w}\right)$ and

- $\omega(z,w) \in \mathbb{R}_{n_0,m_0}[z,w]$ is nonzero for $|z| \leq 1$, $|w| \leq 1$;
- $q_1(x) \in \mathbb{R}_{2n_1}[x]$ is positive for $x \in (-1,1)$, having at most simple zeros at ± 1;
- $q_2(y) \in \mathbb{R}_{2m_1}[y]$ is positive for $y \in (-1,1)$, having at most simple zeros at ± 1.

Then the recurrence coefficients of the measure

$$d\mu(x,y) = \frac{4}{\pi^2} \frac{\chi_{(-1,1)^2}(x,y)\sqrt{1-x^2}\sqrt{1-y^2}}{q_1(x)q_2(y)\omega(z,w)\omega(1/z,w)\omega(z,1/w)\omega(1/z,1/w)}\, dx\, dy, \tag{4}$$

satisfy

$$A_{k+1,l} = \frac{1}{2}I_{l+1}, \qquad B_{k,l} = 0, \qquad \text{for all } k \geq n, \quad l \geq m, \tag{5a}$$

$$\tilde{A}_{k,l+1} = \frac{1}{2}I_{k+1}, \qquad \tilde{B}_{k,l} = 0, \qquad \text{for all k} \geq n, \quad l \geq m, \tag{5b}$$

where $n = n_0 + n_1$, $m = m_0 + m_1$. In view of the spectral properties (5), we can regard the measures (4) as bivariate extensions of the Bernstein-Szegő measures. Note that (5) are invariant if we replace $P_{k,l}(x,y)$ by $O_l P_{k,l}(x,y)$ and $\tilde{P}_{k,l}(x,y)$ by $\tilde{O}_k \tilde{P}_{k,l}(x,y)$, where O_l and $\tilde{O}_k$ are orthogonal matrices depending only on l and k, respectively. We use this freedom to define explicit bases of the spaces $\mathsf{P}_{k,l;\mu}[x,y]$, $\tilde{\mathsf{P}}_{k,l;\mu}[x,y]$ for $k \geq n$ and $l \geq m$ which provide a bivariate extension of the Szegő mapping (2). Let $\tilde{q}_1(z)$ and $\tilde{q}_2(w)$ be the stable Fejér-Riesz factors of $q_1(x)$ and $q_2(y)$, respectively. If $\{U_j^{q_2}(y)\}$ denote the orthonormal polynomials with respect to $\frac{2}{\pi}\frac{\sqrt{1-y^2}}{q_2(y)}\chi_{(-1,1)}(y)dy$ on the real line, and if we set

$$\hat{p}(z,y) = \tilde{q}_1(z)\omega(z,w)\omega(z,1/w) \text{ and } \hat{p}_k(x;y) = \frac{z^{k+1}\hat{p}(1/z,y) - z^{-k-1}\hat{p}(z,y)}{z-1/z},$$

then the one-dimensional Bernstein-Szegő theory implies that $\{\hat{p}_k(x;y)U_j^{q_2}(y)\}_{j=0}^{l-m_0}$ are orthonormal elements in $\mathsf{P}_{k,l;\mu}[x,y]$. Note that we have already used the stable Fejér-Riesz factor of the inverse of the weight, and we need m_0 new quantities for a basis of the complement. It turns out that the elements in the space $\mathsf{P}_{n_0,m_0-1;\mu_\omega}[z,w] = \mathbb{R}_{n_0,m_0-1}[z,w] \ominus \mathbb{R}_{n_0-1,m_0-1}[z,w]$ for the Bernstein-Szegő measure $d\mu_\omega = \frac{1}{(2\pi)^2}\frac{|dz|\,|dw|}{|\omega(z,w)|^2}$ on the torus $\mathbb{T}^2 = \{(z,w) \in \mathbb{C}^2 : |z| = |w| = 1\}$ can be used to build the necessary m_0 orthonormal elements in the complement. On the space of Laurent polynomials $\mathbb{R}[z^{\pm 1}, w^{\pm 1}]$ we define the involution $\mathcal{R}_w^{n_0}$ by $\mathcal{R}_z^{n_0}(g(z,w)) = z^{n_0}g(1/z,w)$, and for $f(z,w) \in \mathbb{R}[z,w]$ we denote by $\mathcal{M}_{f(z,w)}$ the multiplication by $f(z,w)$, i.e. $\mathcal{M}_{f(z,w)}(g(z,w)) = f(z,w)g(z,w)$. Finally, let $S_{z,k}$ and $S_{w,l}$ denote the mappings $S_{z,k}(f(z)) = \frac{z^{k+1}f(1/z)-z^{-k-1}f(z)}{z-1/z}$, $S_{w,l}(g(w)) = \frac{w^{l+1}g(1/w)-w^{-l-1}g(w)}{w-1/w}$, and $\mathcal{S}_{k,l} = S_{z,k} \circ S_{w,l} : \mathbb{R}[z,w] \to \mathbb{R}[x,y]$. With these notations, we define $\mathcal{T}_{k,l} = \mathcal{S}_{k,l} \circ \mathcal{M}_{\tilde{q}_1(z)\tilde{q}_2(w)\omega(z,w)} \circ \mathcal{R}_z^{n_0}$.
Then $\mathcal{T}_{k,l} : \mathsf{P}_{n_0,m_0-1;\mu_\omega}[z,w] \to \mathsf{P}_{k,l;\mu}[x,y]$ is an isometry and

$$\mathsf{P}_{k,l;\mu}[x,y] = \mathcal{T}_{k,l}(\mathsf{P}_{n_0,m_0-1;\mu_\omega}[z,w]) \bigoplus_{j=0}^{l-m_0} \operatorname{span}_{\mathbb{R}}\{\hat{p}_k(x;y)U_j^{q_2}(y)\}.$$

Note that the space $\mathsf{P}_{n_0,m_0-1;\mu_\omega}[z,w]$ in the last formula is independent of k and l. Therefore, if we fix an orthonormal basis of this space, the multiplications by x and y on its image in $\mathsf{P}_{k,l;\mu}[x,y]$ will be represented by Chebyshev relations. An analogous decomposition holds for $\tilde{\mathsf{P}}_{k,l;\mu}[x,y]$ and can be obtained by exchanging the roles of x and y.

Detailed proofs, examples, different extensions of the above constructions and connections to the theory of matrix-valued orthogonal polynomials can be found in [4]. In particular, an interesting new phenomenon in the bivariate case is that the characterization of the Bernstein-Szegő measures in terms of finitely many moments requires new polynomial identities which connect the Fejér-Riesz factorizations of the weight (4) to canonical polynomials depending on three variables associated with a measure on $\mathbb{R}^2$. A challenging open question is to give a complete characterization of the Bernstein-Szegő measures in terms of appropriate recurrence coefficients for the orthogonal spaces similarly to the spectral characterization of the Bernstein-Szegő measures on the torus $\mathbb{T}^2$ in [3]. Another interesting direction is to explore applications of the bivariate Bernstein-Szegő polynomials in numerical analysis, approximation theory and probability.

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Sobolev orthogonal polynomials and spectral methods in boundary value problems

Miguel A. Piñar
(joint work with Lidia Fernández, Francisco Marcellán, and Teresa E. Pérez)

The solution of the boundary value problem (BVP, in short) for the ordinary linear differential equation associated with a stationary Schrödinger equation with potential $V(x) = x^{2k}$,

$$\begin{aligned} -u'' + \lambda\, x^{2k}\, u &= f(x), \\ u(-1) = u(1) &= 0, \end{aligned} \tag{1}$$

where $\lambda > 0$, can be studied from a variational perspective according to the fact you can associate a Sobolev inner product

$$\langle u, v\rangle_\lambda = \lambda \int_{-1}^{1} u(x)\, v(x)\, x^{2k}\, dx + \int_{-1}^{1} u'(x)\, v'(x)\, dx, \tag{2}$$

appearing in the variational formulation of (1). This problem, when $k = 1$, has been considered in [5].

Orthogonal polynomials with respect to Sobolev inner products

$$\langle f, g\rangle_S = \int f(x)g(x)d\mu_0(x) + \int f'(x)g'(x)d\mu_0(x), \tag{3}$$

defined by a pair of positive measures (μ_0, μ_1) supported on the real line have attracted the interest of many researchers (see [8], [9], and references therein). They are interesting from several points of view. In approximation theory they constitute a basic tool in smooth approximations by polynomials in the framework of least square problems (see the seminal paper [7]). On the other hand, some authors have considered Fourier expansions in terms of those polynomials as an alternative to the standard ones (see [6]). In numerical analysis, for spectral methods for boundary value problems for ordinary differential equations the Sobolev orthogonal polynomials play an efficient role with respect to the classical ones (see [2], [3], [4]). Indeed, they have been recently studied in the framework of the so called diagonalized spectral methods for boundary value problems for some elliptic differential operators, see [1], [10].

As it is well known, the multiplication by x is not a symmetric operator with respect to the Sobolev inner product (3) and, as a consequence, the three term recurrence relation that standard orthogonal polynomials satisfy does not hold any more. Therefore, aside from the classical Gram-Schmidt method, a key problem is the generation of sequences of Sobolev orthogonal polynomials. For some special cases, when the measures constitute a coherent pair ([6]), they can be explicitly given.

In this work, monic Sobolev orthogonal polynomials with respect to the pair of measures $(x^{2k}dx, dx)$ supported on the interval $[-1,1]$ are introduced. Let $\{\phi_n^{(k)}\}_{n\geq 0}$ be the MOPS associated with (2) that we will call *k-Sobolev MOPS*. From the definition, we deduce the first monic k-Sobolev polynomials:

$$\phi_0^{(k)}(x) = 1, \qquad \phi_1^{(k)}(x) = x, \qquad \phi_2^{(k)}(x) = x^2 - \frac{2k+1}{2k+3},$$

Next, we obtain a short connectio formula with monic generalized Gegenbauer polynomials $P_n^{(-1/2)}(x)$ in terms of the k-Sobolev MOPS. For $n \geq 2$, we have

$$P_n^{(-1/2)}(x) = \phi_n^{(k)}(x) + \sum_{i=1}^{k+1} a_{2i}^{(n,k)}\, \phi_{n-2i}^{(k)}(x),$$

where the coeficients $a_{2i}^{(n,k)}$ can be recursively computed with the aid of the coefficients in the three term recurrence relation of generalized Gegenbauer polynomial $P_n^{(-1/2)}(x)$. From this connection formula, estimates for the Sobolev norms as well as outer relative asymptotics with respect to the Legendre polynomials can be deduced, in fact we have

$$\lim_{n\to+\infty} \frac{\phi_n^{(k)}(x)}{P_n(x)} = \frac{1}{\Phi'(x)},$$

uniformly on compact subsets of $\mathbb{C} \setminus [-1,1]$, where $\Phi(x) = \dfrac{x+\sqrt{x^2-1}}{2}$.

To construct spectral methods for the solution of the BVP (1) we have to choose our test functions from a basis in $(x^2-1)\,\mathbb{P}$ of polynomials vanishing at the ends of the interval $[-1,1]$ and orthogonal with respect to the Sobolev inner product (2). Let us denote this basis by $\{(x^2-1)\psi_n\}_{n\geq 0}$. It can be shown that they are orthogonal with respect to the Sobolev inner product

$$\begin{aligned} \langle p,q\rangle_S = &\int_{-1}^{1} p(x)q(x)(\lambda x^{2k}(1-x^2)+2)(1-x^2)dx \\ &+ \int_{-1}^{1} p'(x)q'(x)(1-x^2)^2 dx, \end{aligned} \tag{4}$$

and they satisfy again a short connection formula with classical Gegenbauer polynomials.

Finally, we consider the Fourier expansion of the solution $u = (x^2 - 1)v$ of the BVP (1) in terms of the orthogonal sequence $\{(x^2 - 1)\psi_n(x)\}_{n\geq 0}$

$$\sum_{n=0}^{+\infty} \widehat{u}_n (x^2 - 1)\psi_n(x),$$

where, using (4), we get

$$\widehat{u}_n = \frac{\langle u, (x^2-1)\psi_n\rangle_\lambda}{\|(x^2-1)\psi_n\|_\lambda^2} = \frac{\langle (x^2-1)v, (x^2-1)\psi_n\rangle_\lambda}{\|(x^2-1)\psi_n\|_\lambda^2} = \frac{\langle v, \psi_n\rangle_S}{\|\psi_n\|_S^2} = \widehat{v}_n,$$

whith $\widehat{v}_n$ being the nth coefficient of the Fourier expansion of v in terms of the Sobolev orthogonal basis $\{\psi_n(x)\}_{n\geq 0}$,.

On the other hand,

$$\begin{aligned}\widehat{u}_n \|\psi_n\|_S^2 =& \langle u, (x^2-1)\psi_n\rangle_\lambda = \int_{-1}^{1} [-u''(x) + \lambda x^{2k} u(x)](x^2-1)\psi_n(x)dx \\ =& \int_{-1}^{1} f(x)(x^2-1)\psi_n(x)dx =: \widetilde{f}(n).\end{aligned}$$

and therefore, the Fourier coefficients of the solution $u = (x^2 - 1)v$ of the BVP (1) in terms of the orthogonal sequence $\{(x^2 - 1)\psi_n(x)\}_{n\geq 0}$ can be easily computed from f and the sequence itself. From the short connection formula with classical Gegenbauer polynomials, we will be able to obtain a recursive algorithm to compute the coefficients $\widetilde{f}(n)$.

A consistent study of the error, the reliability and accuracy of the Sobolev spectral method, and the extension to PDE are still some of our open problems.

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Efficient and accurate space-time numerical methods for solving time-fractional PDEs

Jie Shen

We present efficient and accurate space-time methods for solving a class of linear and nonlinear time fractional PDEs. The method is based on a spectral method with generalized Jacobi functions for the time variable and a generic spatial discretization. With suitable generalized Jacobi functions, the nonlocal time fractional derivative becomes a simple local operator in the frequency space, making the method very efficient. We also present special techniques, that can achieve exponential convergence in time, to resolve the singularity at the initial time associated with the time fractional derivatives. While the method leads to a coupled systems in space and time, we show that for linear problems, it can be reduced to a sequence of spatial discretization problems, and for nonlinear problems, one can use a Jacobean-free Newton Krylov iteration with a suitable linear solver as the preconditioner. The outline of this talk is as follows:

(1) Introduction and a general space-time framework
(2) Space-time Petrov-Galerkin method using generalized Jacobi functions (GJFs)
(3) Accelerating the convergence rate with enrichment
(4) Space-time Galerkin method using generalized log orthogonal functions (GLOFs)
(5) Extension to nonlinear problems
(6) concluding remarks

Basics on high order polynomial interpolation of physical fields on simplices

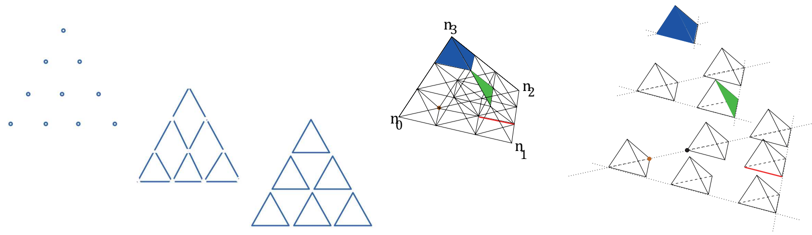
Francesca Rapetti
(joint work with Ana Maria Alonso Rodríguez)

Polynomial interpolation is a key aspect in numerical analysis, used in very classical settings such as reconstructing a physical field from measures or replacing a field expression by a simpler one, defining quadrature formulas to compute integrals. In engineering and science, one often has a number N_s of real data $\{\alpha_i\}$, obtained by sampling or experimentation, which refer to a physical field ω for a limited number of values $\{s_i\}$ of the independent variable. Let us denote by $\langle w, s\rangle$ the sampling or result of the experimentation on the field ω for the value s of the variable. Interpolation stands for generating a new value, say α^*, for the field ω at an intermediate value, say s^*, of the variable, by using a reconstruction ω_δ of ω, i.e., $\alpha^* = \langle \omega_\delta, s^*\rangle$. In polynomial interpolation, the field ω_δ is expressed on a selected basis of polynomials $\{\psi_i\}$, i.e., $\omega_\delta = \sum_i \beta_i \, \psi_i$ with the real coefficients β_i determined in order to have $\langle \omega_\delta, s_i\rangle = \alpha_i$. If the polynomials ψ_i are the *cardinal functions*, they verify the condition $\langle \psi_i, s_\ell\rangle = \delta_{\ell,i}$, with $\delta_{\cdot,\cdot}$ the Kronecker's symbol, and then $\beta_i = \alpha_i$, for any i. Note that the sampling type has to be physically meaningful for the field ω.

In electromagnetism, fields are invisible and forces act without contact. A field ω can thus be detected only because it perturbes the surrounding. Indeed, if the trajectory of a protron moving in the empty space is pertubed, either a gravity or a magnetic field is acting on it, through the Newton or the Lorentz force, respectively. This fact is at the origin of the term "field" itself, introduced by Michael Faraday in 1849. Perturbations are observed via quantities, which correspond with line integrals (circulations), surface integrals (fluxes), etc., other than simply pointwise evaluations. As explained in [5], the mathematical way to encode all this is to identify the entity of physical significance ω with a *p-form*, a *mapping* from geometrical objects of dimension p, the *probes* $\{s_i\}$, to real numbers, the *measures* $\{\alpha_i\}$. The order p of the form depends on the type of field we are considering. A datum α_i results from an evaluation of the p-form ω on a p-object s_i, namely $\langle \omega, s_i \rangle = \int_{s_i} \omega$, which is the *weight* of ω on s_i. In a simplicial mesh τ_h with tetrahedra of maximal diameter h, elementary probes for polynomial p-forms of degree $r = 1$ are facets f_k of dimension p. Any generic probe s of dimension p is represented in τ_h by a p-chain $s \approx \sum_k c_k^s f_k$ with real coeficients c_k^s (a formal linear combination of mesh facets f_k of dimension p). We have $\langle \omega, s \rangle = \sum_k c_k^s \langle \omega, f_k \rangle$. For $p = 0$, the f_k are mesh points and $\langle \omega, f_k \rangle$ stands for the value $\omega(f_k)$.

In [15], with regard to proving the de Rham theorem, Whitney introduced particular polynomial p-forms w_j of degree $r = 1$ associated with the p-facets f_k of a mesh. In three dimensions, on a simplicial mesh τ_h, the w_j turn out to be the piece-wise linear polynomial forms which allow for interpolating a smooth p-form ω from its weights on p-facets f_j, that means $\omega_\delta = \sum_j \langle \omega, f_j \rangle \, w_j$ with indeed $\langle w_j, f_k \rangle = \delta_{k,j}$. To generalize this geometrical point of view, if we aim at enhancing the accuracy of the interpolation with respect to r, without refining the mesh, we need to enrich the sampling set at the interior of each facet f_j or volume T. The *small p-simplices* (shown in the figure, left side, for $p = 0, 1, 2$ in a triangle, and right side, for $p = 0, 1, 2, 3$ in a tetrahedron) have been proposed in [14] as new positions for probes to compute more weights inside each mesh facet f_j or element T for the interpolation of polynomial p-forms of degree $r > 1$. Weights on the small p-simplices are a sound alternative to high order moments, a set of degrees of freedom (DoFs) classically used in finite element spaces, *e.g.*, [6, 11], which fit in a discrete de-Rham complex [4]. These new DoFs, namely the weights on the small p-simplices, are integrals of the field, intended as a differential p-form, on some small facets of dimension p. Small 0-simplices are the nodes defining the principal lattice of degree r in a simplex [7] where are located the DoFs for the reconstruction of 0-forms in Lagrange finite elements. For $p > 0$, small p-simplices extend the geometrical localization of DoFs to edge, face or volume finite elements, while keeping a clear physical interpretation, such as circulations along curves, fluxes across surfaces, densities in volumes, depending on the value of p.

In this contribution, we have explained how the weights on the small p-simplices make it possible to generalize for $p > 0$ the definition of Vandermonde matrix and



Lebesgue constant [1]. The Lebesgue constant pops up naturally to measure the stability of the interpolation and the Runge phenomenon may appear in case of instability [3]. In the case $p = 0$, the distributions of Fekete, symmetrized Lobatto or warp & blend points [9] in a simplex (which keep low the Lebesgue's constant value when r increases), together with the use of orthogonal polynomials [10, 8] (which keep low the condition number of the Vandermonde matrix that has to be inverted to compute the cardinal functions for high order polynomial degrees), have yielded optimal interpolations even for stiff scalar fields [12, 13]. Similarly to the case $p = 0$, the interpolation on uniform distributions of the supports of the weights for $p > 0$ is not stable on the polynomial degree r and the problem increases with the dimension of the space [2]. Clearly, for any $p \geq 0$, the distribution of the supports that minimises the Lebesgue constant is not uniform. However, for $p > 0$, the optimal distribution of small p-simplices in a simplex T is not known.

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Orthogonal Polynomials on Algebraic Curves/Surfaces via Cholesky, QR and QL

Sheehan Olver

In this talk we overviewed several different interlinking research results related to orthogonal polynomials (OPs) on algebraic curves/surfaces:

(1) Multivariate orthogonal polynomials on annuli and their usage in the solution of partial differential equations. These are defined in terms of semi-classical Jacobi polynomials.
(2) Computing univariate orthogonal polynomials via infinite-dimensional matrix factorisations, including the case of semiclassical Jacobi polynomials. We can use this to determine Jacobi and differentiation matrices via the aforementioned matrix factorisation methods in optimal complexity.
(3) Construction of orthogonal polynomials on a certain class of algebraic curves.

1. Multivariate OPs on disk and annuli

Consider orthogonal polynomials (in x/y) on the unit disk with respect to a Jacobi-like inner-product:

$$\iint_{\text{Disk}} f(x,y)g(x,y)(1-r^2)^{\alpha}\mathrm{d}x\mathrm{d}y$$

where $r = x^2 + y^2$. A convenient basis for these OPs are the *Generalised Zernike Polynomials*

$$Z_{m,k}^{(\alpha)}(x,y) := r^m \mathrm{e}^{\mathrm{i}m\theta} P_{(k-m)/2}^{(m,\alpha)}(1-2r^2)$$

Using this basis to discretise PDEs leads to very sparse matrices [12] with optimal complexity solves.

This extends to an annulus with inner radius ρ and outer radius 1 with inner product

$$\iint_{\text{Annulus}} f(x,y)g(x,y)(1-r^2)^{\beta}(r^2-\rho^2)^{\alpha}\mathrm{d}x\mathrm{d}y$$

via the orthogonal polynomials

$$Z_{m,k}^{\rho,(\alpha,\beta)}(x,y) := r^m \mathrm{e}^{\mathrm{i}m\theta} Q_{(k-m)/2}^{t,(\alpha,\beta,m)}((1-r^2)/(1-\rho^2))$$

where $t = 1/(1-\rho^2)$ and $Q_n^{t,(a,b,c)}(x)$ are *semiclassical Jacobi polynomials* with respect to

$$\int_0^1 f(x)g(x)x^a(1-x)^b(t-x)^c.$$

During the seminar Tom Koornwinder pointed out that these polynomials were introduced by Tatian [11] and Mahajan [5].

We are left with the question of how to compute $Q_n^{t,(a,b,c)}$ and its derivatives, which we need for discretising PDEs. This also applies to solving PDEs on disk slices [10] and spherical caps [9].

2. OPs and infinite-dimensional matrix factorisations

We review the results of [4] that look at rational modifications of known OPs, ie if we know the OPs $p_n(x)$ associated with μ we want the OPs $q_n(x)$ associated with

$$\int f(x)g(x)\frac{u(x)}{v(x)}\mathrm{d}\mu(x).$$

Semiclassical Jacobi polynomials are special case of this. In particular we want to compute the connection matrix

$$\underbrace{[p_0|p_1|\cdots]}_{\mathbf{P}} = \underbrace{[q_0|q_1|\cdots]}_{\mathbf{Q}} R$$

where R is upper triangular. Denoting the Jacobi matrix associated with $p_n(x)$ as X_P and suppose $v(x) = 1$, ie its a polynomial modification. As in [3] we can reduce this problem to a Cholesky factorisation

$$u(X_P) = R^\top R$$

and further $u(x)\mathbf{Q} = \mathbf{P}R^\top$. but we can go a step further: if u is a polynomial squared then we have

$$\sqrt{u}(X_P) = QR$$

where $\sqrt{u}\mathbf{Q} = \mathbf{P}Q$. For inverse polynomials, ie $u(x) = 1$ and $v(x)$ a polynomial, we have

$$v(X_P) = L^\top L$$

ie a *reverse Cholesky* (starting at the bottom right which can be approximated with finite sections), where $R^{-1} = L^\top$. further we can do $\sqrt{v}(X_P) = QL$, and other factorisations to compute connection matrices for general rational modifications.

We can use these to determine Jacobi and differentiation matrices via the aforementioned matrix factorisation methods in optimal complexity. For example we can construct the Jacobi matrix associated with q_n as

$$X_Q = RX_PR^{-1}$$

and the differentiation matrix associated with semiclassical Jacobi polynomials satisfies a similar hierarchical construction.

3. Algebraic curves

We switch tracks and consider another application of modifications of polynomials, describing recent work on orthogonal polynomials on algebraic curves, which extends a recent stream of results on quadratic [6] and cubic [2]. Consider algebraic curves of the form

$$y^2 = \underbrace{\phi(x)}_{\text{polynomial}}$$

and an inner product defined on a subset of the curve as

$$\int_a^b [f(x, \sqrt{\phi(x)})g(x, \sqrt{\phi(x)}) + f(x, -\sqrt{\phi(x)})g(x, -\sqrt{\phi(x)})]w\mathrm{d}x$$

We can construct an orthogonal basis of polynomials as

$$P_{n,0}(x, y) := p_n(w; x), P_{n,1}(x, y) := yp_{n-1}(\phi w; x)$$

where $p_n(w; x)$ denotes OPs wrt to a weight w and therefore $p_{n-1}(\phi w; x)$ is a polynomial modification.

However these polynomials are not graded. The connection matrix between these and the true (graded) OPs $Y_{n,k}$ are an orthogonal and banded matrix whose entries can be computed in optimal complexity via a Gram–Schmidt procedure, described in [1].

This extends to domains of revolution a la [7].

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Applications of Special Functions in High Order Finite Element Methods

Tim Haubold

(joint work with Sven Beuchler, Veronika Pillwein, Joachim Schöberl)

It is well known that high order finite element methods achieve better convergence rates per DOF compared to low order finite element methods. One of the drawbacks are the high numerical costs, i.e. the higher number of flops. In this talk, we tackle two different algorithmic optimizations which reduce the number of flops. The first one achieves optimal complexity in the assembly of the local finite element matrices on simplices. Here, we apply the symbolic software `Guess` to derive efficient recursive relations between the entries of the matrices. This recursive relations are proven by thorough analysis using multivariate hypergeometric series.

The second optimization, which we will present, are fast interpolation operators not only in $H^1(\Omega)$ but also in $H(\mathrm{Curl})$. Those interpolations operators are derived by duality arguments.

Fast assembly of element matrices. Consider the following model problem in weak form: Find $u \in H_0^1(\Omega)$, such that

$$a(u,v) := \int_\Omega (A\nabla u)\cdot\nabla v + uv\,\mathrm{d}\vec{x} = \int_\Omega fv\,\mathrm{d}\vec{x} =: F(v) \quad \forall v \in H_0^1(\Omega), \tag{1}$$

where $A \in \mathbb{R}^{2\times 2}$ is constant.

On the triangle $\triangle$ with vertices $(-1,-1), (1,-1)$ and $(0,1)$, high order interior basis functions for $H^1(\Omega)$ are given by

$$u_{ij}(x,y) = \hat{P}_i^0\left(\frac{2x}{1-y}\right)\left(\frac{1-y}{2}\right)^i \hat{P}_j^{2i}(y),$$

where $\hat{P}_n^\alpha = \int_{-1}^x P_{n-1}^{(\alpha,0)}(t)\mathrm{d}t$ and $P_n^{(\alpha,\beta)}(x)$ is a n-th degree Jacobi polynomial, see [1, 2]. Let

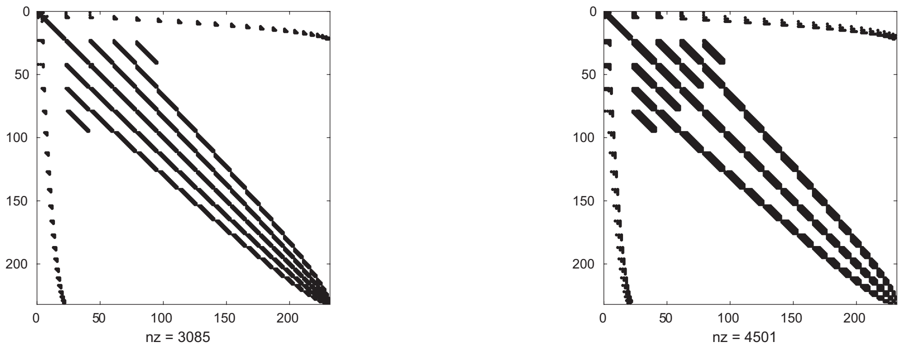
$$M_{ij;kl} = \int_\triangle u_{ij}(x,y)u_{kl}(x,y)\mathrm{d}\vec{x}$$

be an entry of the local element mass matrix. It has been shown in [2] that those matrices only have $\mathcal{O}(p^2)$ entries, where p is the maximal polynomial order. The resulting sparsity pattern can be seen in figure 1.

By application of the symbolic software `Guess`[6], we see that one entry of the mass matrix can be computed by

$$\begin{aligned}(i+j+k+l+2)M_{ij,kl} = \\ &(i+j-k-l-3)M_{i(j-1);kl} + (k+l-i-j-3)M_{ij;k(l-1)} \\ &+ (i+j+k+l)M_{i(j-1);k(l-1)}.\end{aligned} \tag{2}$$

Since (2) only has a constant number of degrees of freedom, all $\mathcal{O}(p^2)$ entries can be computed in optimal complexity. These results can be extended to the stiffness matrix, to $3D$ and also to the spaces $H(\mathrm{Curl})$ and $H(\mathrm{Div})$. Similar relations have



(A) Mass matrix, $p = 20$ (B) Stiffness matrix, $p = 20$

FIGURE 1. Sparsity pattern of local triangular element matrix

been found for the constraints of hanging nodes, see [3].
The proof of (2) can be found in [4] and is based on contiguous relations between multivariate hypergeometric series.

Dual functions. We apply dual functions in closed form to derive fast interpolation operator or transfer operators. An example would be the interpolation of starting values for time dependent problems onto the mesh. Let $\mathbb{V}_{hp} \subset H^1(\Omega)$ be a finite dimensional approximation. The interpolation problem in $2D$ reads as follows:

Problem 1. *Find $u_{hp} \in \mathbb{V}_{hp}$ such that*

$$\begin{aligned} u_{hp}(\lambda) &= u(\lambda) && \forall \text{ vertices } \lambda, \\ \int_E u_{hp} v &= \int_E uv && \forall v \in \mathcal{P}^{p-2} \text{ or } \mathcal{Q}^{p-2} \quad \forall \text{ edges } E, \\ \int_T u_{hp} v &= \int_T uv && \forall v \in \mathcal{P}^{p-3} \text{ or } \mathcal{Q}^{p-3} \quad \forall \text{ elements } T. \end{aligned}$$

For ease of presentation we will only consider the interior basis functions. We search for dual functions $B_{kl}(x,y) = b_k\left(\frac{2x}{1-y}\right) b_{kl}(y)$, such that

$$\int_\triangle u_{ij}(x,y) B_{kl}(x,y) \mathrm{d}(x,y) = c_{ij}\delta_{ik}\delta_{kl}.$$

By using the relations

$$\hat{L}_i(x) = \frac{(x^2-1)}{2(i-1)} P_{i-2}^{(1,1)}(x) \quad \text{and} \quad \hat{P}_i^\alpha(x) = \frac{(1+x)}{n} P_{i-1}^{(\alpha-1,1)}(x),$$

and the transformation $\chi = \frac{2x}{1-y}$ we can write the problem down as follows

$$\int_{-1}^1 \frac{\chi^2-1}{2} P_{i-2}^{(1,1)}(\chi) b_k(\chi) \mathrm{d}x \int_{-1}^1 \left(\frac{1-y}{2}\right)^{i+1} \left(\frac{1+y}{2}\right) P_{j-1}^{(2i-1,1)}(y) b_{kl}(y) \mathrm{d}y = c\delta_{ik}\delta_{kl}.$$

The solution to this problem is the choice

$$b_k\left(\frac{2x}{1-y}\right) = P_{k-2}^{(1,1)}\left(\frac{2x}{1-y}\right)$$

and

$$b_{kl}(y) = \left(\frac{1-y}{2}\right)^{k-2} P_{l-1}^{(2k-1,1)}.$$

These results can be extended to basis functions in

$$H(\mathrm{Curl},\Omega) = \{\vec{u} \in (L^2(\Omega))^d : \mathrm{Curl}(\vec{u}) \in \left(L^2(\Omega)\right)^{2d-3}\},$$

where $\Omega \in \mathbb{R}^d, d = 2, 3$.
In $2D$, the resulting basis functions are given by

$$\begin{aligned} v_{ij}^{\triangle,I}(x,y) &= \nabla(u_{ij}^{\triangle}(x,y)) = \nabla(f_i(x,y))g_{ij}(y) + f_i(x,y)\nabla(g_{ij}(y)) \\ v_{ij}^{\triangle,II}(x,y) &= \nabla(f_i(x,y))g_{ij}(y) - f_i(x,y)\nabla(g_{ij}(y)) \\ v_{1j}^{\triangle,III}(x,y) &= \nabla(f_1(x,y))\hat{P}_j^3(y), \end{aligned} \tag{3}$$

where $f_i(x,y) = \hat{L}_i(\frac{2x}{1-y})\left(\frac{1-y}{2}\right)^i$ and $g_{ij}(y) = \hat{P}_j^{2i}(y)$.
Our dual problem now reads: For $i, j, k, l \geq 2$ find $B_{kl}^{\omega_2}(x,y)$, s.t.

$$\int_{\triangle} v_{ij}^{\triangle,\omega_1}(x,y) B_{kl}^{\omega_2}(x,y)\mathrm{d}(x,y) = c\delta_{ik}\delta_{jl}\delta_{\omega_1,\omega_2},$$

for $\omega_{1/2} \in \{I, II, III\}$. Now, the main problem is that $v_{ij}^{\square,\omega_1}$ is vector valued, a linear combination of two auxiliary functions, and also appears in different types. This problem has been solved in [5] for the quadrilateral, triangular, hexahedral and tetrahedral case. We will present some of those results.

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