Spectral decomposition of $H^1(\mu)$ and Poincaré inequality on a compact interval. Application to kernel quadrature.

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Part I

Sketch and highlights

Problem considered

We consider quadrature formula of the form

$$\int_a^b f(x)d\mu(x) = \sum_{i=1}^{n} w_i f(x_i), \tag{1}$$

where

- μ is a continuous probability distribution on $[a, b]$, with pdf $\rho > 0$.
- $x_1, \dots, x_n$ are quadrature nodes in $[a, b]$
- $w_1, \dots, w_n$ are quadrature weights, ≥ 0 and summing to 1
- $f \in H^1(\mu) = \{f \in L^2(\mu),\ s.t.\ f' \in L^2(\mu)\}$

Such integrals are present in uncertainty quantification of complex systems.

Kernel quadrature formulation

- We will show that $H^1(\mu)$ is a reproducing kernel Hilbert space (RKHS), which extends a known result for $H^1(a,b)$ [Duc-Jacquet, 1973]
  Its kernel is continuous, and has the "single-pair" form

$$K(x,y) = \psi(\min(x,y))\chi(\max(x,y))$$

- In a RKHS $\mathcal{H}$, the worst-case error of a quadrature (X, w)

$$\mathrm{wce}(X, w, \mathcal{H}) = \sup_{h \in \mathcal{H}, \|h\|_{\mathcal{H}} \leq 1} \left| \int h(x) d\mu(x) - \sum_{i=1}^{n} w_i h(x^i) \right|$$

  has an analytical expression.
- We then consider the *kernel quadrature* problem:

$$(P): \qquad \min_{X,w} \mathrm{wce}(X, w, H^1(\mu))$$

Spectral decomposition of $H^1(\mu)$, Poincaré inequality and T-systems

- Difficulty: (P) is in general intractable, as K has not an explicit form
- Fortunately, the spectral decomposition of K can be connected with Poincaré inequalities, through the formula

$$K(x, y) = \sum_{m=0}^{\infty} \frac{1}{1+\lambda_m} \varphi_m(x)\varphi_m(y) \qquad (x, y \in [a, b])$$

  where $(\lambda_m, \varphi_m)_{m\in\mathbb{N}}$ are the eigenvalues and eigenfunctions associated to Poincaré inequalities.
- One can compute numerically (λ_m, φ_m) with a finite element technique [Roustant et al., 2017].
- Furthermore, $(\varphi_m)_{m\in\mathbb{N}}$ forms a T-system (Tchebytchev system, see [Karlin and Studden, 1966]). T-systems extend orthogonal polynomials and have nice properties for quadrature.

Problem resolution in a finite-dimensional proxy space.

- We replace problem (P) by the tractable proxy problem

$$(P_M): \qquad \min_{X,w} \mathrm{wce}(X, w, \mathcal{H}_M)$$

  where $\mathcal{H}_M$ is the RKHS spanned by $\varphi_0, \varphi_1, \dots, \varphi_M$.

- As $(\varphi_m)_{m\in\mathbb{N}}$ is a T-system, we have a Gaussian quadrature: $\exists!(X, w)$, with $w > 0$ s.t. $\mathrm{wce}(X, w, \mathcal{H}_M) = 0$, where $M = 2n - 1$ is maximal. (the quadrature is exact for $\varphi_0, \dots, \varphi_{2n-1}$)

- This Gaussian quadrature will be called **Poincaré quadrature**. It can be computed efficiently by linear programming.

Part II

Spectral decomposition of $H^1(\mu)$

Reproducing kernel Hilbert space (RKHS) [Aronszajn, 1943, Berlinet and Thomas-Agnan, 2011]

For a given set T, let $\mathcal{H}$ be a Hilbert space of functions $T \to \mathbb{R}$.
$\mathcal{H}$ is a **RKHS** if $\forall x \in T$, the evaluations $h \in \mathcal{H} \mapsto h(x)$ are continuous

Equivalence RKHS $\Leftrightarrow$ kernel

- By Riesz theorem, $\exists! K_x \in \mathcal{H}$ s.t.

$$\forall h \in \mathcal{H}, \quad \langle h, K_x \rangle_{\mathcal{H}} = h(x) \qquad \text{(reproducing property)}$$

  Denote $K(x,y) = \langle K_x, K_y \rangle_{\mathcal{H}} = K_x(y) = K_y(x)$.
  Then K is a kernel, i.e. a positive definite function.

- Conversely, if K is a kernel on $T \times T$, then $\exists!$ RKHS with kernel K:

$$\mathcal{H}_K = \overline{\text{span}\{K(x,.), x \in T\}}, \qquad \langle K(x,.), K(y,.) \rangle_{\mathcal{H}_K} = K(x,y)$$

Worst-case in RKHS
see e.g. [Novak and Woźniakowski, 2008], chapter 10

- By Cauchy-Schwartz inequality, and reproducing property

$$\sup_{h \in \mathcal{H}_K, \|h\| \leq 1} |h(x)| = \sup_{h \in \mathcal{H}_K, \|h\| \leq 1} |\langle h, K(x,.)\rangle| = \|K(x,.)\| = \sqrt{K(x,x)}.$$

- Define the worst-case error of a quadrature (X, w) as

$$\mathrm{wce}(X, w, \mathcal{H}) = \sup_{h \in \mathcal{H}, \|h\| \leq 1} \left| \int h(x) d\mu(x) - \sum_{i=1}^{n} w_i h(x_i) \right|$$

If $\mathcal{H}$ is a RKHS with kernel K, then

$$\mathrm{wce}(X, w, \mathcal{H}_K)^2 = \left\| \int K(x,.) d\mu(x) - \sum_{i=1}^{n} w_i K(x_i,.) \right\|_{\mathcal{H}_K}^2$$

$$= \iint K(x,x') d\mu(x) d\mu(x') - 2 \sum_{i=1}^{n} w_i \int K(x_i, x) d\mu(x) + \sum_{i,j} w_i w_j K(x_i, x_j)$$

Poincaré inequalities

μ satisfies a **Poincaré inequality** if for all f in $L^2(\mu)$ such that $\int f(x)d\mu(x) = 0$, and $f' \in L^2(\mu)$:

$$\int f(x)^2 d\mu(x) \leq C(\mu) \int f'(x)^2 d\mu(x)$$

The smallest constant (still denoted $C(\mu)$) is the **Poincaré constant**.

An existence assumption (bounded perturbation of the uniform p.d.)

We consider the set $\mathcal{B}$ of continuous p.d. μ whith bounded support (a, b) and non-vanishing pdf $\rho = e^{-V}$, with V continuous and piecewise C^1 on $[a, b]$.

- In practice, one may need to truncate with high-order quantiles
- In theory, this implies that there exist m, M in $\mathbb{R}$ such that

$$\forall t \in [a, b], \qquad 0 < m \leq \rho(t) \leq M < +\infty.$$

Hence $L^2(\mu) = L^2(a, b)$ and $H^1(\mu) = H^1(a, b)$ with equivalent norms.

Spectral theorem (see e.g. [Bakry et al., 2014], [Roustant et al., 2017])

As for matricial problems, the minimum of the Rayleigh ratio (s.t. $\int f d\mu = 0$)

$$\frac{\int f'(x)^2 d\mu(x)}{\int f(x)^2 d\mu(x)} = \frac{\|f'\|^2}{\|f\|^2}$$

is given by the smallest (non-zero) eigenvalue of a spectral problem.

More precisely, if $\mu \in \mathcal{B}$, then finding $f \in H^1(\mu)$ and $\lambda > 0$ such that

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in H^1(\mu) \qquad (\star)$$

gives an orthonormal basis of eigenfunctions $(\varphi_n)_{n \geq 0}$ of $L^2(\mu)$ (**"Poincaré basis"**) and a sequence of eigenvalues $(\lambda_n)_{n \geq 0}$, with

$$0 = \lambda_0 < \lambda_1 = C(\mu)^{-1} < \lambda_2 < \cdots < \lambda_n < \cdots \to +\infty$$

The underlying operator is $L_P f = f'' - V' f'$, and solving $(\star)$ is equivalent to finding $f \in H^2(\mu)$ and $\lambda > 0$ such that

$$L_P f = -\lambda f, \qquad \text{with} \quad f'(a) = f'(b) = 0.$$

Main result

Proposition (Mercer's representation of $H^1(\mu)$ with the Poincaré basis)

Assume that $\mu \in \mathcal{B}$. Then,

1. *$H^1(\mu)$, with its usual Hilbert norm $\|f\|^2_{H^1(\mu)} = \|f\|^2 + \|f'\|^2$, is a RKHS. Its kernel K is continuous on $[a,b]^2$ and $\int_a^b K(x,y)d\mu(y) = 1$ $(x \in [a,b])$.*
2. *The Mercer decomposition of K is written, with unif. conv. on $[a,b]^2$,*

$$K(x,y) = \sum_{m=0}^{\infty} \frac{1}{1+\lambda_m} \varphi_m(x)\varphi_m(y) \qquad (x,y \in [a,b]) \tag{2}$$

3. *K has the single-pair form [Gantmakher and Krejn, 2002]*

$$K(x,y) = \frac{1}{C}\psi(\min(x,y))\chi(\max(x,y)). \qquad (x,y \in [a,b]) \tag{3}$$

Furthermore, ψ, χ are two linearly independent solutions of the homogeneous equation $f'' - f'V' - f = 0$ such that $\psi'(a) = 0$ and $\chi'(b) = 0$, and $C = \chi(b)\int_a^b \psi(x)d\mu(x) = \psi(a)\int_a^b \chi(y)d\mu(y)$ is a normalization constant.

Proof of the main result

1.
- $H^1(\mu)$ is a RKHS because $\mu \in \mathcal{B}$ and $H^1(a,b)$ is a RKHS, by
$$\begin{array}{ccccc} H^1(\mu) & \longrightarrow & H^1(a,b) & \longrightarrow & \mathbb{R} \\ \text{f} & \mapsto & \text{f} & \mapsto & \text{f(x)} \end{array}$$
- $\int K(x,y)d\mu(y) = 1$ because $1 \in H^1(\mu)$:
$$1 = 1(x) = \langle 1, K(x,.)\rangle_{H^1(\mu)} = \int_a^b K(x,y)d\mu(y).$$
- Continuity will be seen in point 3.

Proof of the main result

2. Equivalence between eigenproblems of Poincaré inequality and K

$$
\begin{array}{lccc}
 & \langle f', g' \rangle = \lambda \langle f, g \rangle & & \forall g \in H^1(\mu) \\
\Leftrightarrow & \langle f, g \rangle_{H^1(\mu)} = (1+\lambda)\langle f, g \rangle & & \forall g \in H^1(\mu) \\
\Leftrightarrow & \langle f, K(x,.) \rangle_{H^1(\mu)} = (1+\lambda)\langle f, K(x,.) \rangle & & \forall x \in [a,b] \\
\Leftrightarrow & f(x) = (1+\lambda) \int K(x,y) f(y) d\mu(y) & & \forall x \in [a,b] \\
\Leftrightarrow & \int K(x,y) f(y) d\mu(y) = \frac{1}{1+\lambda} f(x) & & \forall x \in [a,b]
\end{array}
$$

Anticipating the continuity of K, this gives the form of the Mercer representation of K and the uniform convergence on $[a,b]^2$.

Proof of the main result

3. Form of the kernel and link to Green functions
   - [Gantmakher and Krejn, 2002] derives the Green function G associated to the differential operator $Lf = f'' - V'f' - f = L_P f - f$,

$$LG(x,y) = \delta_x(y) \qquad (x, y, \in [a,b])$$

   - We have $G = K$, because, formally (with $K_x = K(x,.)$):

$$\begin{aligned} f(x) &= \langle f, K_x \rangle_{H^1(\mu)} = \int f K_x e^{-V} d\lambda + \int f' K_x' e^{-V} d\lambda \\ &= \int f K_x e^{-V} d\lambda + [f K_x' e^{-V}]_a^b - \int f [K_x'' - K_x' V'] e^{-V} d\lambda \\ &= [f K_x' e^{-V}]_a^b - \int f \underbrace{[K_x'' - K_x' V' - K_x]}_{LK_x} d\mu \end{aligned}$$

   leading to $K_x'(a) = K_x'(b) = 0$ and $LK_x(y) = \delta_x(y)$.

   - A rigourous computation of K_x can be done by considering each interval $[a, x]$ and $[x, b]$. The continuity of K is a consequence of its single-pair form.

Examples

- For the uniform case, we obtain, with $\omega = \pi/(b-a)$:

$$
\begin{aligned}
K(x,y) &= \frac{\pi/\omega}{\sinh(\pi/\omega)} \cosh[\min(x,y)-a]\,\cosh[b-\max(x,y)] \\
&= 1 + 2\sum_{n=1}^{+\infty} \frac{1}{1+n^2\omega^2} \underbrace{\cos[n\omega(x-a)]}_{\propto e_n(x)} \cos[n\omega(y-a)]
\end{aligned}
$$

- As a by-product, we can compute 'shifted' Riemann series. Using $x=y=a$ (resp. $x=a, y=b$) and $r = 1/\omega$, we get for all $r>0$:

$$
\sum_{n=1}^{+\infty} \frac{1}{n^2+r^2} = \frac{1}{2r^2}\left(\frac{\pi r}{\tanh(\pi r)} - 1\right), \qquad \sum_{n=1}^{+\infty} \frac{(-1)^{n-1}}{n^2+r^2} = \frac{1}{2r^2}\left(1 - \frac{\pi r}{\sinh(\pi r)}\right)
$$

- For the exponential distribution, truncated on $[a,b]$, everything is also explicit (but less convenient to write).

Link to literature

- The Mercer representation of Sobolev spaces seems unexplored for non-uniform probability distributions.
- For the uniform distribution,
  - By connecting RKHS to Green's functions, [Fasshauer, 2012] gives Mercer representations of various kernels associated to Sobolev spaces, such as $H^1_{\mathrm{anchored}}(0,1) = \{f \in H^1(0,1), f(0) = f(1) = 0\}$, with the usual norm.
  - [Dick et al., 2014] provides the Mercer representation of $H^1(0,1)$ for the norm given by $\|f\|^2 = (\int_0^1 f(x)dx)^2 + \int_0^1 f'(x)^2 dx$.
  - The case of $H^1(0,1)$, with its usual norm, can be found in [Novak and Woźniakowski, 2008, Appendix A.2.1].

Transition: a property of the Poincaré basis

The Poincaré basis function of 'degree' n has at most n zeros.
Actually this property is stable by linear combination $\rightarrow$ **T-system**.

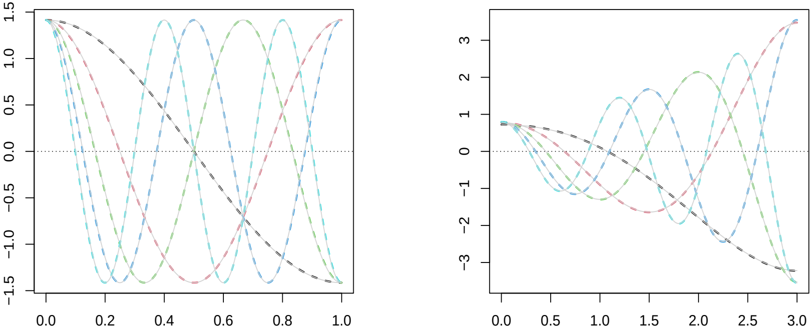


Figure: First Poincaré basis functions for $\mathcal{U}[0,1]$ and $\mathcal{E}(1)$ truncated on $[0,3]$. Solid line: analytic expression; Dotted curves: estimated by finite elements.

Part III

T-systems. Poincaré quadrature.

T-systems [Karlin and Studden, 1966]

Definition (T-systems)

Let $u_0, u_1, \ldots, u_n, \ldots$ be real-valued continuous functions on $[a, b] \subset \mathbb{R}$. Consider the generalized Vandermonde matrix

$$V(u_0, \ldots, u_{n-1}; t_1, \ldots, t_n) := \begin{pmatrix} u_0(t_1) & \ldots & u_0(t_n) \\ \vdots & \ddots & \vdots \\ u_{n-1}(t_1) & \ldots & u_{n-1}(t_n) \end{pmatrix}$$

We say that $(u_n)_{n \in \mathbb{N}}$ is a ***complete Tchebytchev system****, or* ***T-system****, if*

$$\forall n \in \mathbb{N}, \forall t_1 < \cdots < t_n \in [a, b] : \qquad \det[V(u_0, \ldots, u_{n-1}; t_1, \ldots, t_n)] > 0$$

$\Leftrightarrow$ *any nontrivial linear combination of $u_0, \ldots, u_{n-1}$ has at most $n - 1$ zeros*

$\Rightarrow$ if $\sum_{i=0}^{n-1} \beta_i u_i(t_j) = 0$ for $j = 1, \ldots, n$ then $\beta^\top V = 0$ hence $\beta = 0$.

Prototype: polynomials $u_\ell = t^\ell$ (up to a change sign)

T-systems and Newton-Cotes quadrature

If $(u_n)_{n\in\mathbb{N}}$ is a T-system, for any choice of n knots $t_1 < \dots t_n$ there exists a unique quadrature

$$\int_a^b f(t)d\mu(t) = \sum_{j=1}^{n} w_j f(t_j)$$

which is exact at order n, i.e. on $\text{span}(u_0, \dots, u_{n-1})$

Indeed, this gives the invertible linear system

$$V(u_0, \dots, u_{n-1}; t_1, \dots, t_n) \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} \int_a^b u_0 d\mu \\ \vdots \\ \int_a^b u_{n-1} d\mu \end{pmatrix}$$

Drawback: the weights can be < 0, the quadrature error may be unbounded (for the other u_ℓ's with $\ell \geq n$).

T-systems and Gaussian quadrature

Proposition ([Karlin and Studden, 1966])

Let $u = (u_n)_{n \in \mathbb{N}}$ be a T-system, and μ be a probability distribution in $\mathcal{B}$. Then,

1. *There exists a unique quadrature of n nodes (1) with positive weights which is exact at order $2n-1$, i.e. exact on span$(u_0, \dots, u_{2n-1})$. The nodes are in (a, b) and the weights sum to 1.*
2. *This quadrature is obtained by solving the minimization problem*

$$\min_{\sigma \in V_{2n-1}(c)} \int_a^b u_{2n}(t) d\sigma(t) \tag{4}$$

over the set $V_{2n-1}(c)$ of all probability distributions subject to moment conditions $\int_a^b u_i(t)d\sigma(t) = \int_a^b u_i(t)d\mu(t)$, for $i = 0, 1, \dots, 2n-1$.

T-systems and Gaussian quadrature

Comments.

- This generalizes the Gaussian quadrature for polynomials
  $\rightarrow$ we still call it (generalized) **Gaussian quadrature**

- Problem (4) provides a numerical method to compute the quadrature, by searching σ in a set of discrete measures with many support points
  $\rightarrow$ linear programming problem

- Replacing min by max in (4), gives the (generalized) **Lobatto quadrature**.

The Poincaré basis is a T-system. Poincaré quadrature

Proposition

If $\mu \in \mathcal{B}$, the Poincaré basis $(\varphi_m)_{m\in\mathbb{N}}$ is a T-system.
The associated Gaussian quadrature is called ***Poincaré quadrature****.*

This comes from a general result of **Sturm-Liouville operators** (here $Lf = f'' - V'f' - f$) proved in [Gantmakher and Krejn, 2002]. Main steps:

- Prove that K is an **oscillatory kernel**, i.e. every matrix $(K(x_i, s_j))_{1\leq i,j\leq n}$ with $x_1 < \cdots < x_n$ and $s_1 < \cdots < s_n$ is positive semidefinite.
  $\rightarrow$ This comes from the single-pair form of K.
- If K is an oscillatory kernel, then the solutions of the integral equation

$$\varphi(x) = \lambda \int_a^b K(x,s)\varphi(s)d\sigma(s) \tag{5}$$

  form a T-system.

Part IV

The Poincaré quadrature is the optimal kernel quadrature of $H^1(\mu)$

Generalities on kernel quadrature

Recall that for a RKHS $\mathcal{H}_K$ with kernel K, the worst-case error of (X, w)

$$\mathrm{wce}(X, w, K) = \sup_{h \in \mathcal{H}_K, \|h\| \leq 1} \left| \int h(x) d\mu(x) - \sum_{i=1}^{n} w_i h(x_i) \right|$$

is a quadratic form with respect to w,

$$\mathrm{wce}(X, w, K)^2 = w^\top K(X, X) w - 2\ell_K(X)^\top w + c_K$$

where

- $K(X, X) = (K(x_i, x_j))_{1 \leq i,j \leq n}$ is the Gram matrix
- $\ell_K(X) = (\int K(x_i, x) d\mu(x))_{1 \leq i \leq n}$ is a column vector

Assumption

(1) *If for all $i \neq j, x_i \neq x_j$ then the Gram matrix $K(X, X)$ is invertible.*

Under this assumption, $\mathrm{wce}(X, w, K)$ has a unique minimum w.r.t. w,

$$w^\star(X, K) = K(X, X)^{-1} \ell_K(X)$$

Equivalence between Poincaré and kernel quadratures in $H^1(\mu)$

(Settings)

Let K_M the finite dimensional approximation of the kernel K of $H^1(\mu)$:

$$K_M(x, y) = \sum_{m=0}^{M} \alpha_m \varphi_m(x) \varphi_m(y), \qquad (x, y \in [a, b])$$

By the T-system property of the Poincaré basis, we deduce:

Proposition (Kernel quadrature is well-defined for K and K_M)

Assumption 1 is verified for K for all set X composed of distinct knots.
Assumption 1 is verified for K_M when X contains at most $M + 1$ distinct points.

Equivalence between Poincaré and kernel quadratures in $H^1(\mu)$

Let (X_P, w_P) be the Poincaré quadrature with n nodes and order $M = 2n - 1$.

Proposition

(X_P, w_P) is an optimal kernel quadrature for $\mathcal{H}_{K_M}$, with positive weights, and

$$w_P = w^\star(X_P, K_M) = K_M(X_P, X_P)^{-1}\mathbb{1}.$$

Conversely, if (X, w) defines a kernel quadrature for $\mathcal{H}_{K_M}$ such that $\mathrm{wce}(X, w, K_M) = 0$ and the weights are positive, then $X = X_P$ and $w = w_P$.

Sketch of proof:

- As (X_P, w_P) is exact for $\varphi_0, \dots, \varphi_M$, we have $\mathrm{wce}(X_P, w_P, K_M) = 0$
- The $\mathbb{1}$ comes from the property $\int K(x,.)d\mu = \int K_M(x,.)d\mu = 1$.

Quadrature error: definitions

Radius of information

$$r(n) = \inf_{X,w} \mathrm{wce}(X, w, H^1(\mu)).$$

Worst-case error

If (X_P, w_P) denotes the Poincaré quadrature with n nodes,

$$\mathrm{wce}(n) = \mathrm{wce}(X_P, w_P, H^1(\mu)).$$

Recall that $(X_P, w_P) = \operatorname{argmin}_{X,w} \mathrm{wce}(X, w, \mathcal{H}_{K_M})$.

The worst-case error may be a good proxy of the radius of information for large n, and we always have

$$\mathrm{wce}(n) \geq r(n)$$

Quadrature error: formulas

Proposition

The worst-case error of the Poincaré quadrature with n nodes and order $M = 2n - 1$ can be expressed with the Mercer representation of $H^1(\mu)$, by:

$$\mathrm{wce}(n)^2 = \sum_{m \geq M+1} \alpha_m \left(\sum_{i=1}^{n} w_i \varphi_m(x_i) \right)^2,$$

or with formulas involving the kernel of $H^1(\mu)$:

$$\begin{aligned} \mathrm{wce}(n)^2 &= w_P^\top (K(X_P, X_P) - K_M(X_P, X_P)) w_P \\ &= \mathbb{1}^\top K_M(X_P, X_P)^{-1} (K(X_P, X_P) - K_M(X_P, X_P)) K_M(X_P, X_P)^{-1} \mathbb{1} \end{aligned}$$

Furthermore, we have, for all $n \in \mathbb{N}$,

$$\mathrm{wce}(n) \leq \sqrt{\|K - K_{2n-1}\|_\infty} \underset{n \to +\infty}{\longrightarrow} 0$$

Links with literature

- Quadrature problems on Sobolev spaces with a non-uniform probability is relatively small (exceptions for the Normal distribution)
- Our quadrature problem is not equivalent to the more standard problem

$$\int_a^b f(x)w(x)dx = \sum_{i=1}^n w_i f(x_i)$$

  where $f \in H^1(0,1)$, because the worst-case criterion is different.
- For $H^1(0,1)$ (unif. case),
  - [Zhang and Novak, 2019] provide expressions of the radius of information in function of the nodes, for the semi-norm $\int_0^1 f'(x)^2 dx$
  - [Duc-Jacquet, 1973] gives the optimal kernel quadrature for the usual norm
- The link between T-systems and kernel quadrature has been exploited in [Oettershagen, 2017]. There, K is explicit and the T-system is formed by a family of $K(x_i, .)$ with $x_1 < \cdots < x_n$.

Part V

The case of $H^1(0,1)$

(unif. case) Poincaré quadrature nodes = zeros of a basis function

Proposition

The nodes of the Poincaré quadrature of $H^1(0,1)$ with n nodes are equal to the zeros of the Poincaré basis function φ_n.

N.B. This is wrong for a general $\mu \in \mathcal{B}$.
Main reason: here the Poincaré basis is formed by trigonometric functions,

$$\varphi_m(x) = \sqrt{2}\cos(m\pi x)$$

and is thus stable by multiplication:

$$\varphi_n(x)\varphi_m(x) = \frac{1}{2}\left(\varphi_{n+m}(x) + \varphi_{n-m}(x)\right).$$

The proof then mimics the proof for orthogonal polynomials.

(unif. case) Poincaré quadrature = midpoint (rectangle) quadrature

Proposition

The Poincaré quadrature of $H^1(0,1)$ with n nodes corresponds to the midpoint (or rectangle) quadrature rule

$$\int_0^1 f(x)dx = \frac{1}{n}\sum_{i=1}^{n} f\left(\frac{2i-1}{2n}\right).$$

It is exact for all $\varphi_m \propto \cos(m\pi x)$ with $m \leq 2n-1$, for all φ_m such that m is not a multiple of $2n$, and for polynomials of order 1.

The nodes are the zeros of φ_n, thus equal to $x_i = \frac{2i-1}{2n}$.
The weights are then defined uniquely. One can check that the formula above is verified for all φ_m with $m \leq 2n-1$, using that, for $m \in \mathbb{Z}$ and $n \in \mathbb{N}^\star$,

$$\sum_{i=1}^{n} \cos\left(\frac{2i-1}{2}\frac{m\pi}{n}\right) = \begin{cases} 0 & \text{if } m \text{ is not a multiple of } 2n \\ n(-1)^p & \text{if } m = (2n)p, \text{ for all } p \in \mathbb{Z}. \end{cases}$$

(unif. case) Explicit formula for the worst-case error

Proposition (Quadrature error)

For $H^1(0,1)$, we have

$$\mathrm{wce}(n) = \left(\frac{\frac{1}{2n}}{\tanh\left(\frac{1}{2n}\right)} - 1 \right)^{1/2} \sim \frac{1}{\sqrt{12}} \frac{1}{n}$$

Using the previous result, and starting from

$$\mathrm{wce}(n)^2 = \sum_{m=2n}^{\infty} \alpha_m \frac{1}{n^2} \left(\sum_{i=1}^{n} \varphi_m(x_i) \right)^2$$

we obtain

$$\mathrm{wce}(n)^2 = 2 \sum_{p=1}^{\infty} \alpha_{2np} = 2 \sum_{p=1}^{\infty} \frac{1}{1 + p^2/r^2}$$

with $r = (2n\omega)^{-1}$. Multiplying by r^2, we obtain a shifted Riemann sum, whose expression has been derived previously.

(unif. case) Asymptotic optimality of the Poincaré quadrature

Proposition ([Duc-Jacquet, 1973])

The optimal kernel quadrature of $H^1(0,1)$ *is given explicitely by*

$$x_i^\star = \frac{2i-1}{2n}, \qquad w_i^\star = 2\tanh\left(\frac{1}{2n}\right) \sim \frac{1}{n}.$$

Furthermore,

$$r(n) = \left(1 - 2n\tanh\left(\frac{1}{2n}\right)\right)^{1/2} \sim \frac{1}{\sqrt{12}}\frac{1}{n}.$$

Consequently, we see that for large n, the Poincaré quadrature, i.e. the optimal kernel quadrature of K_{2n-1}, coincides with the optimal kernel quadrature of K, and $\frac{\mathrm{wce}(n)}{r(n)} \to 1$.

N.B. *This was derived with the expression of* K*, unknown for a general* μ*.*

Mapping the optimal quadrature on $H^1(0,1)$ to $H^1(\mu)$ is not a good idea

Let us define the *quantile quadrature on* $H^1(\mu)$,

$$w_i = w_i^\star, x_i = q_\mu(x_i^\star), \qquad (1 \leq i \leq n)$$

Proposition (The quantile quadrature is an optimal kernel quadrature)

Let $\mu \in \mathcal{B}$ *with pdf* ρ *and cdf* $R = (q_\mu)^{-1}$*. Let*

$$K_\rho : (x, x') \in [a,b]^2 \mapsto K(R(x), R(x'))$$

where K *is the kernel of* $H^1(0,1)$*.*
The quantile quadrature on $H^1(\mu)$ *is the optimal kernel quadrature on* $\mathcal{H}_{K_\rho}$*.*
The RKHS $\mathcal{H}_{K_\rho}$ *is the Hilbert space* $(H^1(\mu), \|\cdot\|_{K_\rho})$*, with*

$$\|f\|^2_{K_\rho} = \int_a^b f^2 d\mu + \int_a^b (f')^2 \frac{1}{\rho^2} d\mu. \tag{6}$$

$\rightarrow$ *Quantile quadrature* $\neq$ *Optimal kernel quadrature of the standard* $H^1(\mu)$*.*

Part VI

Numerical experiments

Uniform distribution

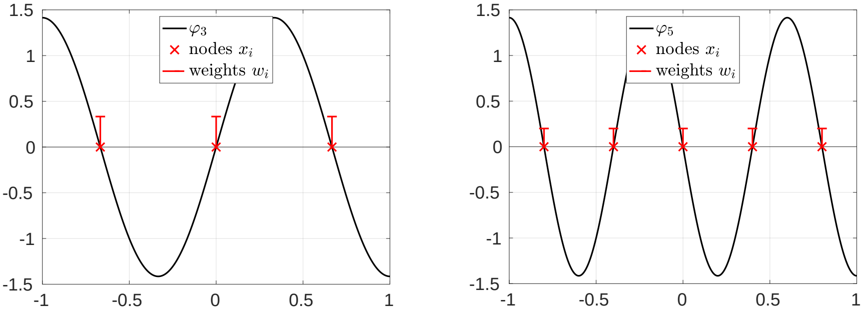
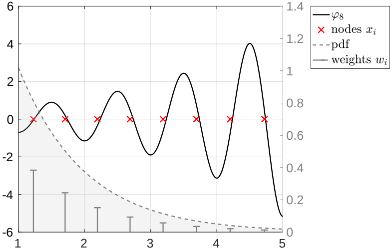
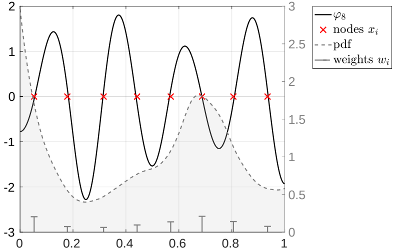


Figure: Poincaré quadrature for the uniform distribution on $(0, 1)$, with $n = 3$ nodes (left) and $n = 5$ nodes (right). The curve represents the Poincaré basis function with n roots, and the red crosses and lines the quadrature nodes and weights obtained by the numerical procedure.

Other distributions



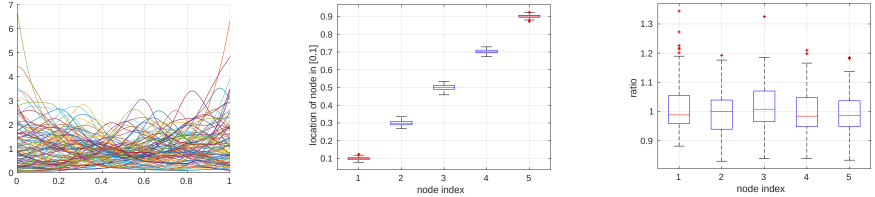
(a) Truncated exponential ($n = 8$)



(b) Nonparametric density ($n = 8$)

Figure: Poincaré nodes and weights for the truncated exponential distribution on $[1, 5]$ (left) and a nonparametric density (right).

Other distributions



(a) 100 random densities **(b)** Distribution of nodes **(c)** Ratio $\frac{n \times \text{weights}}{\text{pdf}}$

Figure: Left: 100 random pdfs. Middle: Location of nodes for the Poincaré quadratures associated to the same densities, with $n = 5$. Right: Ratio $\frac{n\, w_i}{\rho(x_i)}$.

Worst-case error

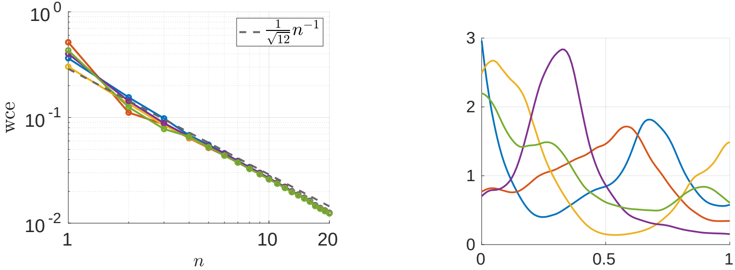


Figure: Worst-case error (left) for 5 random densities supported on [0, 1] (right). The worst-case error is computed using Equation (6) as $\mathrm{wce}(X_P, w_P, K_T)$ for $T = 100$.

Part VII

Conclusion and outlook

Summary of contributions

- Remarking that $H^1(\mu)$ is a RKHS, we made a connection between the spectral decomposition of its kernel, Poincaré inequality and T-systems.

- We used this connection to do optimal kernel quadrature in $H^1(\mu)$ with the Gaussian quadrature for the Poincaré basis (Poincaré quadrature).

- For the uniform case, we proved that
  - the Poincaré quadrature is equal to the midpoint quadrature, and asymptotically optimal.
  - transporting the optimal quadrature of $H^1(0, 1)$ to $H^1(\mu)$ is not a good idea

- We proposed an efficient numerical procedure for a general μ.
  We observed that asymptotically,
  - the nodes might be evenly spaced and close to the zeros of φ_n
  - the weights follow approximately the pdf
  - the worst-case error scales as $\frac{1}{\sqrt{12}} n^{-1}$, as for the uniform case

More details on the paper [Roustant et al., 2024].

Directions for future research

- Theoretically investigate the observed asymptotical properties
  $\rightarrow$ techniques from large covariance matrices?

- Extend the result to $H^2(\mu), H^3(\mu)$...
  $\rightarrow$ still using the Poincaré basis?

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