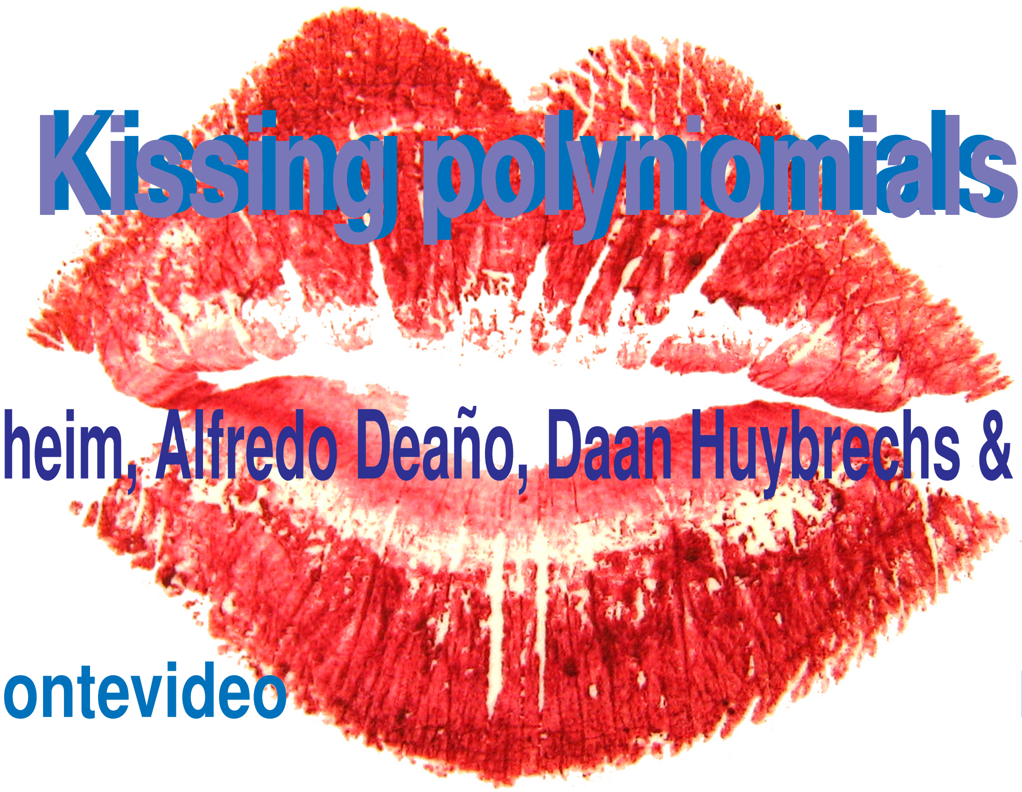
UNIVERSITY OF CAMBRIDGE

CENTRE FOR MATHEMATICAL SCIENCES

DEPARTMENT OF APPLIED MATHEMATICS
& THEORETICAL PHYSICS



Kissing polynomials

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The motivation: Highly oscillatory quadrature

Compute

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

★ Classical Gaussian quadrature requires $\mathcal{O}(\omega)$ points – useless!

★ Modern methods (Filon, Levin, numerical steepest descent), based on asymptotic expansions, are very effective and very high accuracy is attainable uniformly in ω – paradoxically, accuracy increases as ω grows.

But... why not consider complex-valued Gaussian quadrature?

Use the sesquilinear form

$$\langle p, q\rangle_\omega = \int_a^b p(x)q(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\,\mathrm{d}x, \qquad \omega \ge 0,$$

to define orthogonal polynomials – thus, we seek monic $p_n \in \mathbb{P}_n$ s.t.

$$\langle p_n, x^\ell\rangle_\omega = 0, \qquad \ell = 0, \ldots, n-1.$$

Provided that such a p_n exists, let its zeros be $c_k = c_k(\omega)$, $k = 1, \ldots, n$,

$$b_k = b_k(\omega) = \int_a^b \prod_{\substack{\ell=1\\ \ell\neq k}}^{n} \frac{x - c_\ell}{c_k - c_\ell}\mathrm{e}^{\mathrm{i}\omega g(x)}\,\mathrm{d}x, \qquad k = 1, \ldots, n$$

and set

$$Q[f] = \sum_{k=1}^{n} b_k f(c_k).$$

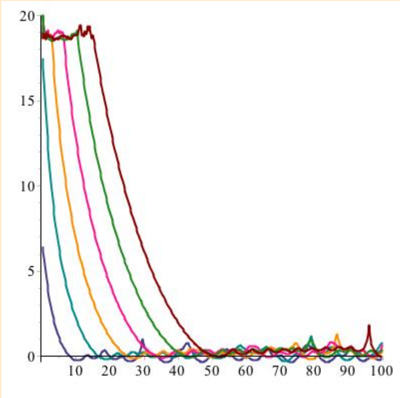
How good is $Q[f]$? Consider

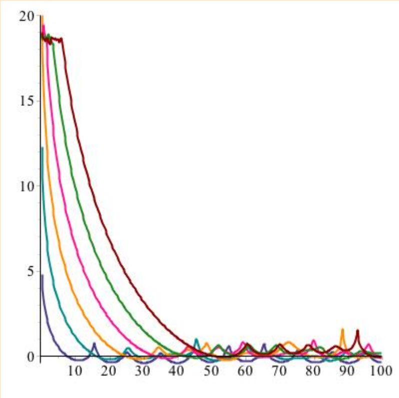
$$I[f] = \int_{-1}^{1} f(x) e^{i\omega x} \, dx \qquad \text{and} \qquad I[f] = \int_{-1}^{1} f(x) e^{i\omega x^2} \, dx$$

for $f(x) = e^x$.

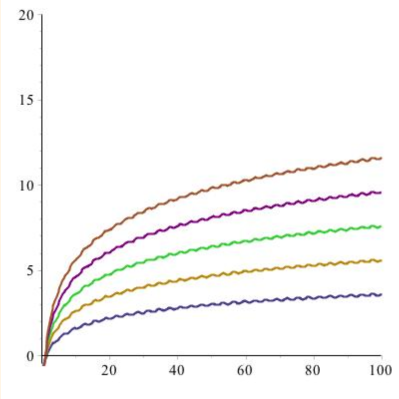
In all figures we display $-\log_{10}$ (i.e., the number of significant digits) of the error for $\omega \in [0, 100]$. For plain Gaussian quadrature we plot it for $n = 4, 8, \ldots, 24$, for asymptotic methods and for complex Gaussian quadrature for an increasing number of points.

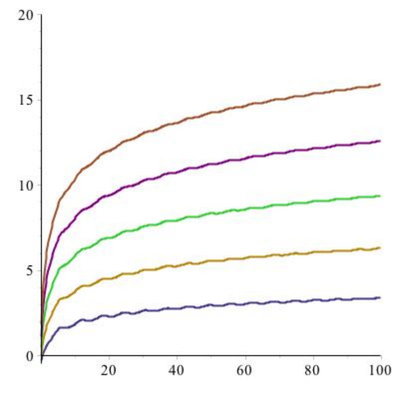
Gaussian quadrature



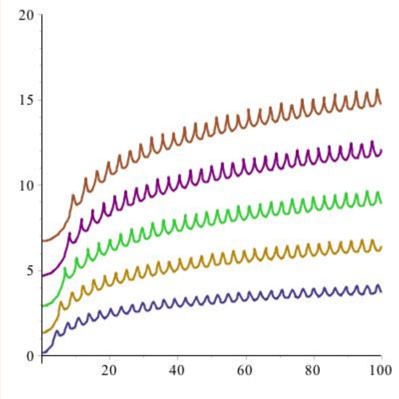


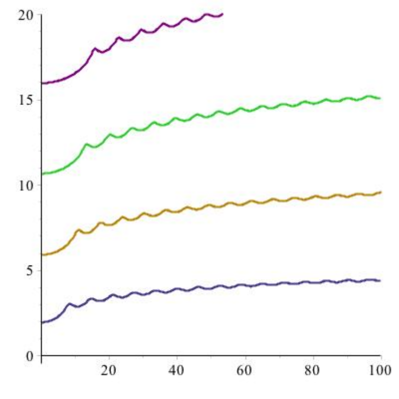
Asymptotic quadrature



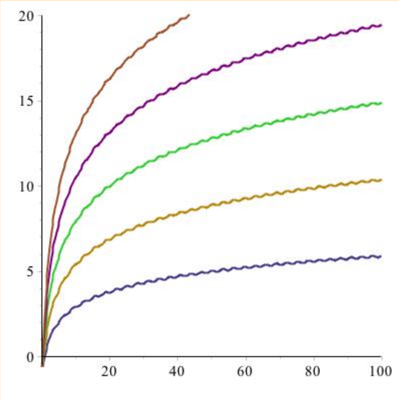


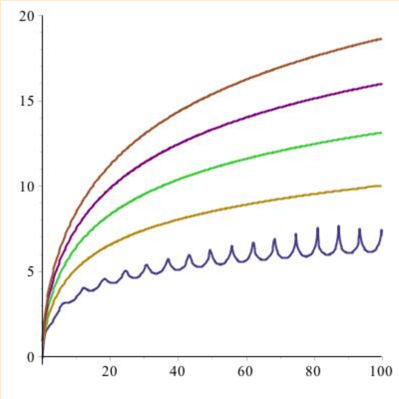
Filon-type quadrature



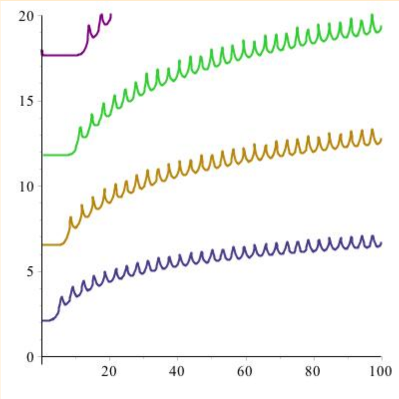


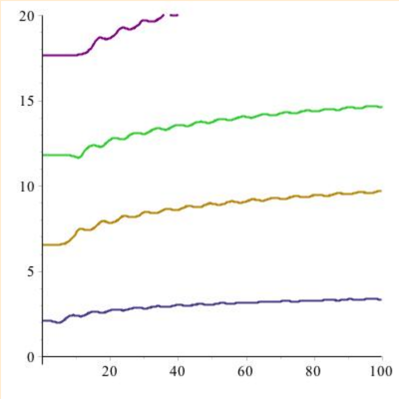
Numerical steepest descent





Complex-valued Gaussian quadrature





Asheim, Deaño, Huybrechs & Wang:

1. The error of complex Gaussian quadrature is $\mathcal{O}\left(\omega^{-2n-1}\right)$;

2. The quadrature seems to exist for all even n but fails for a countable number of values of ω for an odd n;

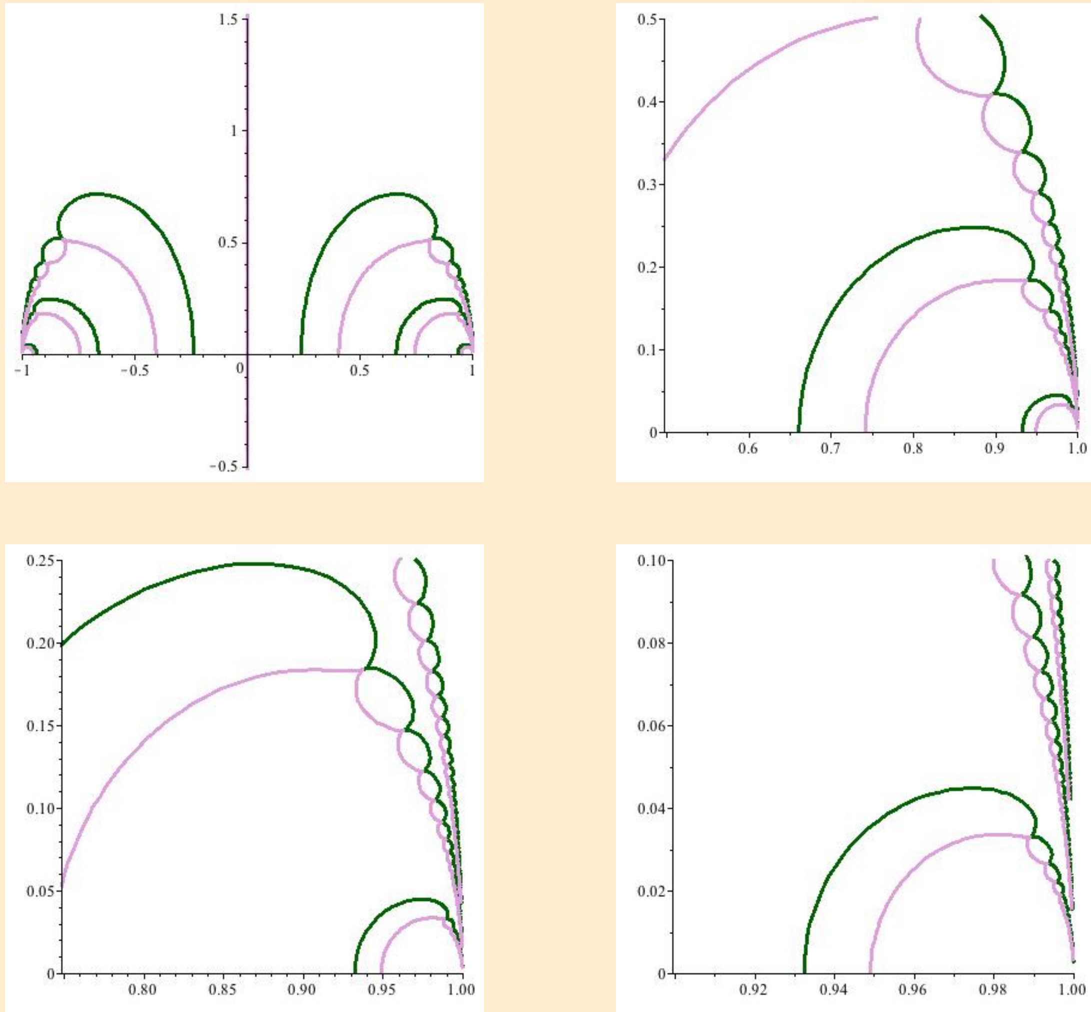
3. The zeros of $p_n(\,\cdot\,,\omega)$, the nth-degree orthogonal polynomial w.r.t. $\mathrm{d}\mu(x,\omega) = \mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x$, describe a strange pattern in the complex plane.

In this talk we explain this and much more, describing in great detail the **kissing polynomials**: the polynomials orthogonal w.r.t.

$$\langle p, q\rangle_\omega = \int_{-1}^{1} p(x)q(x)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x.$$

The zeros and beyond: An anatomy of a kiss

The zeros of p_6 (in green) and p_7 (in purple) as ω travels from 0 to $+\infty$



Moments and Hankel determinants Let

$$h_n(\omega) = \det \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & \vdots & & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n} \end{bmatrix}, \quad \text{where} \quad \mu_n = \int_{-1}^{1} x^n \mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x.$$

Then p_n exists iff $h_{n-1} \neq 0$ – indeed,

$$p_n(x,\omega) = \frac{1}{h_{n-1}} \det \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} & 1 \\ \mu_1 & \mu_2 & \cdots & \mu_n & x \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n-1} & x^n \end{bmatrix}.$$

Hankel determinants are often of minor importance in OP theory because $h_n > 0$ for all Borel measures – but in our case all we can say by this stage is that h_n is complex and, at least in principle, it might be zero.

The asymptotics of Hankel determinants

We commence from an old result of Heine,

$$h_{n-1} = \frac{1}{n!} \int_{-1}^{1} \cdots \int_{-1}^{1} \prod_{0 \le k < \ell \le n-1} (x_\ell - x_k)^2 \mathrm{e}^{\mathrm{i}\omega \mathbf{1}^\top \boldsymbol{x}} \,\mathrm{d}x_0 \cdots \,\mathrm{d}x_{n-1},$$

which we expand asymptotically in ω. Iterating

$$\int_{-1}^{1} f(x) \mathrm{e}^{\mathrm{i}\omega x} \,\mathrm{d}x \sim -\sum_{m=0}^{\infty} \frac{1}{(-\mathrm{i}\omega)^{m+1}} [\mathrm{e}^{\mathrm{i}\omega} f^{(m)}(1) - \mathrm{e}^{-\mathrm{i}\omega} f^{(m)}(-1)],$$

we have

$$\int_{-1}^{1} \cdots \int_{-1}^{1} f(\boldsymbol{x}) \mathrm{e}^{\mathrm{i}\omega \mathbf{1}^\top \boldsymbol{x}} \,\mathrm{d}\boldsymbol{x}$$
$$\sim (-1)^n \sum_{m=0}^{\infty} \frac{1}{(-\mathrm{i}\omega)^{m+n}} \sum_{|\boldsymbol{k}|=m} \sum_{\boldsymbol{v} \in \mathcal{V}_n} (-1)^{s(\boldsymbol{v})} \mathrm{e}^{\mathrm{i}\omega \mathbf{1}^\top \boldsymbol{v}} \partial_{\boldsymbol{x}}^{\boldsymbol{k}} f(\boldsymbol{v}),$$

where $\mathcal{V}_n$ are the vertices of $[-1, 1]^n$ and $s(\boldsymbol{v})$ is the number of (-1)s at the vertex $\boldsymbol{v}$.

We need to consider derivatives of

$$f(\boldsymbol{x}) = \prod_{k=0}^{n-2} \prod_{\ell=k+1}^{n-1} (x_\ell - x_k)^2$$

at a vertex $\boldsymbol{v} \in \mathcal{V}_n$. The problem is that many derivatives vanish!

Everything is symmetric, hence we can assume that for $s(\boldsymbol{v}) = r$ we have

$$\boldsymbol{v} = (\overbrace{-1, \ldots, -1}^{r \text{ times}}, \overbrace{+1, \ldots, +1}^{n-r \text{ times}}).$$

Let

$$\alpha_r(\boldsymbol{x}) = \prod_{0 \le k < \ell \le r-1} (x_\ell - x_k), \qquad \beta_{n,r}(\boldsymbol{x}) = \prod_{k=0}^{r-1} \prod_{\ell=r}^{n-1} (x_\ell - x_k),$$

then

$$f(\boldsymbol{x}) = \alpha_r^2(x_0, \ldots, x_{r-1}) \alpha_{n-r}^2(x_r, \ldots, x_{n-1}) \beta_{n,r}^2(x_0, \ldots, x_{n-1}).$$

To determine the leading expansion term, we note that $\beta_{n,r}(\boldsymbol{v}) = 2^{r(n-r)}$, therefore we need be concerned just with α_r at -1 and α_{n-r} at $+1$. Since $\alpha(\boldsymbol{x} + a\mathbf{1}) = \alpha(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^n$, $a \in \mathbb{R}$, it is sufficient to examine these expansions at $\boldsymbol{x} = \mathbf{0}$.

By the definition of a determinant,

$$\alpha_r(\boldsymbol{x}) = \mathsf{VDM}(x_0, \ldots, x_{r-1}) = \sum_{\boldsymbol{\pi} \in \Pi_r} (-1)^{\sigma(\boldsymbol{\pi})} x_0^{\pi_0} x_1^{\pi_1} \cdots x_{r-1}^{\pi_{r-1}},$$

where Π_r is the set of permutations of length r and $\sigma(\boldsymbol{\pi})$ is the sign of $\boldsymbol{\pi}$. We deduce that $\partial_{\boldsymbol{x}}^{\boldsymbol{k}} \alpha_r(\mathbf{0}) = 0$ unless $\boldsymbol{k} = \boldsymbol{\pi} \in \Pi_r$ – in the latter case

$$\partial_{\boldsymbol{x}}^{\boldsymbol{\pi}} \alpha_r(\mathbf{0}) = (-1)^{\sigma(\boldsymbol{\pi})} \prod_{j=0}^{r-1} \pi_j! = (-1)^{\sigma(\boldsymbol{\pi})} \mathsf{sf}(r-1),$$

where $\mathsf{sf}(m) = 0!1! \cdots m!$ is a super-factorial.

Consequently,

$$\partial_{\boldsymbol{x}}^{\boldsymbol{k}} \alpha_r^2(\boldsymbol{0}) = \begin{cases} (-1)^{\sigma(\boldsymbol{\pi}_1)+\sigma(\boldsymbol{\pi}_2)} \mathsf{sf}^2(r-1), & \boldsymbol{k} = \boldsymbol{\pi}_1 + \boldsymbol{\pi}_2, \\ 0, & \text{otherwise.} \end{cases}$$

We have for the multi-index $\boldsymbol{k} = [k_0, \ldots, k_{n-1}]$

$$\begin{aligned} \partial_{\boldsymbol{x}}^{\boldsymbol{k}} f(\boldsymbol{v}) &= \partial_{\boldsymbol{x}}^{\boldsymbol{k}} [\alpha_r^2(-\boldsymbol{1}) \alpha_{n-r}^2(+\boldsymbol{1})] \\ &= \sum_{\ell=0}^{k_0} \cdots \sum_{\ell_{n-1}=0}^{k_{n-1}} \prod_{j=0}^{n-1} \binom{k_j}{\ell_j} \partial_{\boldsymbol{x}}^{\boldsymbol{\ell}} \alpha_r^2(\boldsymbol{0}) \partial_{\boldsymbol{x}}^{\boldsymbol{k}-\boldsymbol{\ell}} \alpha_{n-r}^2(\boldsymbol{0}). \end{aligned}$$

A term is nonzero *only* for $\boldsymbol{\ell} = \boldsymbol{\pi}_1^{[1]} + \boldsymbol{\pi}_2^{[1]}$ and $\boldsymbol{k} - \boldsymbol{\ell} = \boldsymbol{\pi}_1^{[2]} + \boldsymbol{\pi}_2^{[2]}$, where $\boldsymbol{\pi}_i^{[1]} \in \Pi_r$ and $\boldsymbol{\pi}_i^{[2]} \in \Pi_{n-r}$.

Therefore, for $\boldsymbol{k} = \boldsymbol{\pi}_1^{[1]} + \boldsymbol{\pi}_2^{[1]} + \boldsymbol{\pi}_1^{[2]} + \boldsymbol{\pi}_2^{[2]}$,

$$\begin{aligned}
\partial_{\boldsymbol{x}}^{\boldsymbol{k}} f(v) =& \sum_{\boldsymbol{\pi}_1^{[1]}, \boldsymbol{\pi}_2^{[1]} \in \Pi_r} \prod_{i=0}^{r-1} \binom{\pi_{1,i}^{[1]} + \pi_{2,i}^{[1]}}{\pi_{1,i}^{[1]}} \partial_{\boldsymbol{x}}^{\boldsymbol{\pi}_1^{[1]}} \alpha_r(\boldsymbol{0}) \partial_{\boldsymbol{x}}^{\boldsymbol{\pi}_2^{[1]}} \alpha_r(\boldsymbol{0}) \\
& \times \sum_{\boldsymbol{\pi}_1^{[2]}, \boldsymbol{\pi}_2^{[2]} \in \Pi_{n-r}} \prod_{i=0}^{n-r-1} \binom{\pi_{1,i}^{[2]} + \pi_{2,i}^{[2]}}{\pi_{1,i}^{[2]}} \partial_{\boldsymbol{x}}^{\boldsymbol{\pi}_1^{[2]}} \alpha_{n-r}(\boldsymbol{0}) \partial_{\boldsymbol{x}}^{\boldsymbol{\pi}_2^{[2]}} \alpha_{n-r}(\boldsymbol{0}) \\
=& \,\mathsf{sf}^2(r-1)\mathsf{sf}^2(n-r-1) \\
& \times \sum_{\boldsymbol{\pi}_1 \in \Pi_r} (-1)^{\sigma(\boldsymbol{\pi}_1)} \sum_{\boldsymbol{\pi}_2 \in \Pi_r} (-1)^{\sigma(\boldsymbol{\pi}_2)} \prod_{i=0}^{r-1} \binom{\pi_{1,i} + \pi_{2,i}}{\pi_{1,i}} \\
& \times \sum_{\boldsymbol{\pi}_1 \in \Pi_{n-r}} (-1)^{\sigma(\boldsymbol{\pi}_1)} \sum_{\boldsymbol{\pi}_2 \in \Pi_{n-r}} (-1)^{\sigma(\boldsymbol{\pi}_2)} \prod_{i=0}^{n-r-1} \binom{\pi_{1,i} + \pi_{2,i}}{\pi_{1,i}}.
\end{aligned}$$

Identifying a sum with a determinant and permuting rows,

$$\sum_{\pi_2 \in \Pi_s} (-1)^{\sigma(\pi_2)} \prod_{i=0}^{s-1} \binom{\pi_{1,i} + \pi_{2,i}}{\pi_{1,i}} = \det(A^{[s]}_{\pi_{1,i},j})_{i,j=0,\dots,s-1}$$
$$= (-1)^{\sigma(\pi_1)} \det(A^{[s]}_{i,j})_{i,j=0,\dots,s-1},$$

where $A^{[s]}_{i,j} = \binom{i+j}{i}$, $i, j = 0, \dots, s-1$. Therefore,

$$\partial_{\boldsymbol{x}}^{\boldsymbol{k}} f(\boldsymbol{v}) = \mathsf{sf}(r-1)\mathsf{sf}(r)\mathsf{sf}(n-r-1)\mathsf{sf}(n-r) \det A^{[r]} \det A^{[n-r]}.$$

It is easy to see that $\det A^{[s]} \equiv 1$, consequently

$$\partial_{\boldsymbol{x}}^{\boldsymbol{k}} f(\boldsymbol{v}) = \mathsf{sf}(r-1)\mathsf{sf}(r)\mathsf{sf}(n-r-1)\mathsf{sf}(n-r)$$

and we are done.

For each $r = 0, \ldots, n$ we consider the contribution of the $\binom{n}{r}$ vertices with r (-1)s. The *least* non-zero derivative occurs when $|n-2r|$ is minimised and it follows that

Theorem *It is true for $\omega \gg 1$ that*

$$h_{2N-1}(\omega) \sim \frac{(-1)^N 4^{N^2} \mathsf{sf}^4(N-1)}{\omega^{2N^2}} + \mathcal{O}\left(\omega^{-2N^2-1}\right),$$
$$h_{2N}(\omega) \sim \frac{2(-1)^{N+1} 4^{N(N+1)} \mathsf{sf}^2(N-1)\mathsf{sf}^2(N)}{\omega^{2N(N+1)+1}} \sin\omega + \mathcal{O}\left(\omega^{-2(N^2+N+1)}\right).$$

Corollary *For $\omega \gg 1$ the polynomial $p_{2N}(\cdot,\omega)$ always exists, while $p_{2N+1}(\cdot,\omega)$ exists except for a countable number of points asymptotically spaced at distance π.*

Explaining a kiss Many features of classical orthogonal polynomials are lost but the three-term recurrence relation, being a purely algebraic artefact, remains true,

$$p_{n+1}(x,\omega) = (x-\alpha_n)p_n(x,\omega) - \frac{h_{n-2}h_n}{h_{n-1}^2}p_{n-1}(x,\omega),$$

where

$$\alpha_n = \frac{h_{n-1}}{h_n}\int_{-1}^{1} x p_n^2(x,\omega)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x.$$

Once $h_n(\omega^\star) = 0$, it follows that $p_{n+1}(\,\cdot\,,\omega^\star)$ blows up – more specifically, letting

$$\tilde{p}_n(x,\omega) = h_{n-1}(\omega)p_n(x,\omega) = \det\begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} & 1 \\ \mu_1 & \mu_2 & \cdots & \mu_n & x \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n-1} & x^n \end{bmatrix},$$

we deduce that $\tilde{p}_{n+1}(\,\cdot\,,\omega^\star) = \tilde{p}_n(\,\cdot\,,\omega^\star)$ – one zero of $\tilde{p}_{n+1}$ travels to ∞ and the remaining ones coincide with the zeros of $\tilde{p}_n$: **a kiss!**

We therefore deduce that (at least for $\omega \gg 1$) kisses occur between p_{2N} and p_{2N+1}.

Symmetric functions Let $w(\boldsymbol{x})$ be any symmetric function of $x_0, \ldots, x_{n-1}$. Then

$$\int_{-1}^{1} \cdots \int_{-1}^{1} w(\boldsymbol{x}) \prod_{0 \le k < \ell \le n-1} (x_\ell - x_k)^2 \mathrm{e}^{\mathrm{i}\omega \mathbf{1}^\top \boldsymbol{x}} \,\mathrm{d}\boldsymbol{x}$$

can be expanded in similar fashion. In particular, for $z \in \mathbb{C}$ s.t. $|z \pm 1| > \delta$

$$\begin{aligned} p_{2N}(x,\omega) &\sim (x^2-1)^N + \mathcal{O}\left(\omega^{-1}\right), \\ p_{2N+1}(x,\omega) &\sim (x^2-1)^N (x + \mathrm{i}\cot\omega) + \mathcal{O}\left(\omega^{-1}\right). \end{aligned}$$

Moreover,

$$\begin{aligned} p_{2N}(1,\omega) &\sim \frac{2^N N!}{(\mathrm{i}\omega)^N} + \mathcal{O}\left(\omega^{-N-1}\right), \\ p_{2N+1}(1,\omega) &\sim \frac{2^N N!}{(\mathrm{i}\omega)^N}(1 + \mathrm{i}\cot\omega) + \mathcal{O}\left(\omega^{-N-1}\right). \end{aligned}$$

Finally, expanding zeros of p_n near $+1$,

$$p_{2N}\left(1+\frac{c}{-\mathrm{i}\omega}\right) \sim \frac{2^N N!}{\omega^N}\mathsf{L}_N(c) + \mathcal{O}\left(\omega^{-N-1}\right),$$
$$p_{2N+1}\left(1+\frac{c}{-\mathrm{i}\omega}\right) \sim \frac{2^N N!}{\omega^N}\mathsf{L}_N(c) + \mathcal{O}\left(\omega^{-N-1}\right),$$

where $\mathsf{L}_n = \mathsf{L}_n^{(0)}$ is the Laguerre polynomial.

Theorem *For $\omega \gg 1$ the zeros of p_n (except for the one zero on $\mathrm{i}\mathbb{R}$ for odd n) are of the form $\pm[1+c/(-\mathrm{i}\omega)] + \mathcal{O}\left(\omega^{-2}\right)$, where $\mathsf{L}_{\lfloor n/2 \rfloor}(c) = 0$.*

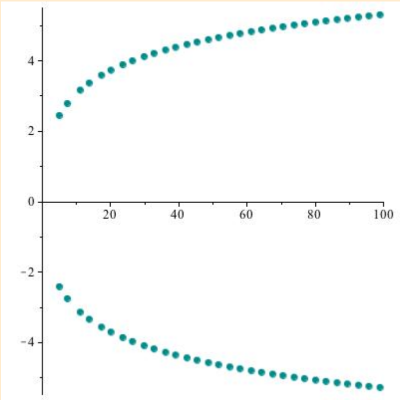
Recall that the zeros of p_n are the quadrature points of our scheme.

This creates a bridge between complex Gaussian quadrature and other highly oscillatory quadrature methods, which tend – for perfectly valid reasons of asymptotics – to aggregate near the endpoints. For example, numerical steepest descent uses *exactly* the points $\pm[1+c/(-\mathrm{i}\omega)]$ where c is as above.

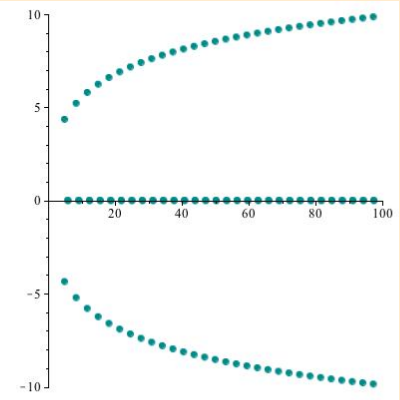
Further developments An aftermath of a kiss

Zeros of h_{n-1} They can be again analysed using asymptotic expansions, whereby they become expressible using the Lambert W function.

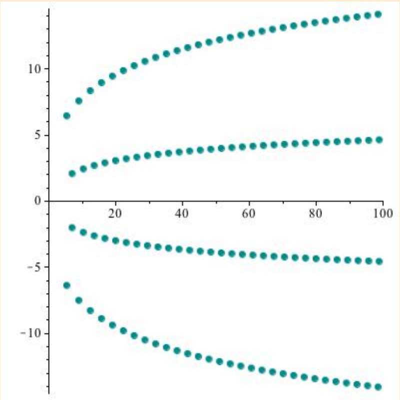
h_1

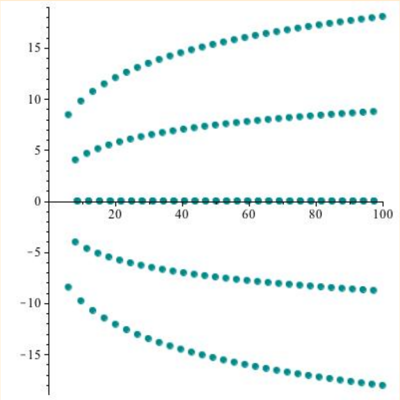


h_2

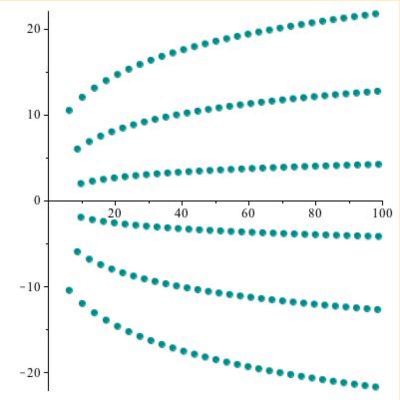


h_3

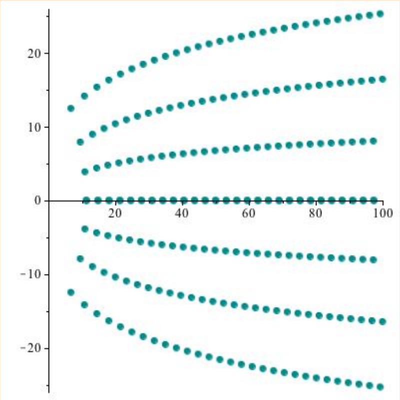




h_4



h_5



h_6

Existence – or otherwise – of p_{2N} for all $\omega \geq 0$

The method of proof is a homotopy from $\omega \gg 1$ (where we know that $h_{2N-1}(\omega) \neq 0$) to all $\omega \geq 0$. An important role is played by σ_n such that $p_n(x) = x^n - \sigma_n x^{n-1} + \cdots$ – e.g. in the recurrence relation

$$p_{n+1}(x) = (x - \sigma_{n+1} + \sigma_n)p_n(x) - \frac{h_{n-2}h_n}{h_{n-1}^2} p_{n-1}.$$

It is possible to prove that

$$h'_{n-1}(\omega) = \mathrm{i}\sigma_n(\omega)h_{n-1}(\omega)$$

and this gives us a handle on h'_{n-1}.

Theorem *The Hankel determinant h_{2N-1} is nonzero for all $\omega \geq 0$.*

Suppose that this isn't true and let $\omega^\star$ be the *largest* value of ω for which a zero occurs. Then $h_{n-1}(\omega^\star) = h'_{n-1}(\omega^\star) = 0$, but we can prove that this is impossible.

Other complex measures Sky is the limit! So far, we have analysed the sesquilinear form

$$\langle p, q\rangle_\omega = \int_{-1}^{1} p(x)q(x)\mathrm{e}^{\mathrm{i}\omega x^2}\,\mathrm{d}x$$

and we can say a great deal about the underlying polynomials. Their behaviour (and the proofs) is *much* more complicated but, at least asymptotically, all h_{n-1}s are nonzero. The zeros don't kiss but they display a wide range of other fascinating behaviour.

But this belongs to another talk...

You must remember this,

A kiss is just a kiss,

A ψ is just a ψ.

The fundamental things apply

As $t \gg 1$.