Superinterpolation in highly oscillatory quadrature

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SCIENTIFIC COMPUTING

Outline

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A first principle

Say a computable value Val has asymptotic behaviour for large values of a parameter ω:

$$Val(\omega) \sim \sum_{k=1}^{\infty} a_k\, \omega^{-b_k}, \qquad \omega \gg 1.$$

- Construct a numerical approximation such that

$$Approx(\omega) \sim \sum_{k=1}^{s} a_k\, \omega^{-b_k} + \mathcal{O}(\omega^{-b_{s+1}}), \qquad \omega \gg 1.$$

- Preserving asymptotic behaviour implies:

$$Val(\omega) - Approx(\omega) \sim \mathcal{O}(\omega^{-b_{s+1}}).$$

A second principle

Annoying observations

- asymptotic expansions do not converge
- we do not get to choose ω

Introduce a controllable parameter n (or h):

$$A(\omega, n) - V(\omega) \sim \; n^{-d}, e^{-\rho n}, \qquad\qquad n \to \infty.$$

What is the behaviour of:

$$err(\omega, n) := |A(\omega, n) - V(\omega)|$$

A few words about oscillatory integrals

The value of an oscillatory integral

$$I[f] := \int_a^b f(x) e^{i\omega g(x)} \mathrm{d}x$$

is determined by small regions near a, b and points where $g'(x) = 0$ (stationary point).

If

$$I[f] \sim \sum_{k=1}^{s} a_k \omega^{-b_k}, \qquad \omega \to \infty,$$

then, assuming one stationary point ξ:

$$\begin{array}{lcl} a_0[f] & \leftarrow & f(a), f(b), f(\xi) \\ a_1[f] & \leftarrow & f(a), f'(a), f(b), f'(b), f(\xi_1), f'(\xi_1) \\ a_k[f] & \leftarrow & f(a), f'(a), f''(a), \ldots, f^{(k-1)}(a), f(b), f'(b), \ldots \end{array}$$

Outline

1. Filon-type method (of Arieh and Syvert)

A standard approach:

- replace f by polynomial p using, e.g., interpolation
- integrate the result exactly:

$$I[f] \approx I[p] = \int_a^b p(x) e^{i\omega g(x)} \mathrm{d}x = \sum_{k=1}^{m} w_k f(x_k)$$

What is the asymptotic behaviour of $I[p]$?

- depends on $p(a)$, $p(b)$, $p'(a)$, ...
- conclusion: interpolate corresponding values of f!

1. Filon-type method (2)

Make sure that

$$p(a) = f(a), \quad p(b) = f(b), \quad p'(a) = f'(a), \quad p'(b) = f'(b)$$

- This leads to a quadrature rule using derivatives

$$I[p] = \int_a^b p(x) e^{i\omega g(x)} \mathrm{d}x = \sum_{k=1}^{m} \sum_{j=0}^{s-1} w_{jk} f^{(j)}(x_k)$$

- and the error $I[p] - I[f]$ behaves like $\omega^{-(s+1)}$ for a **fixed computational cost**
- in particular, the error $p - f$ may be very large on $[a, b]$!

2. Maximal order method

Can we maximize asymptotic order?

- **step 1**: localize the integral

$$\int_0^\infty f(x)e^{i\omega x}\mathrm{d}x \quad \left(= \int_\Gamma f(x)e^{i\omega x}\mathrm{d}x\right)$$

- **step 2**: extract data on which asymptotic expansion depends

$$\int_0^\infty f(x)e^{i\omega x}\mathrm{d}x = \int_0^\infty \sum_{j=0}^{d-1} \frac{f^{(j)}(0)}{j!} x^j e^{i\omega x}\mathrm{d}x + \int_0^\infty x^d f_{rem}(x)e^{i\omega x}\mathrm{d}x$$

2. Maximal order method (2)

Can we maximize asymptotic order?

- **step 3**: for clarity, set $t = \omega x$ or $x = t/\omega$

$$\int_0^\infty \sum_{j=0}^{d-1} a_j x^j e^{i\omega x} \mathrm{d}x + \int_0^\infty x^d f_{rem}(x) e^{i\omega x} \mathrm{d}x$$
$$= \frac{1}{\omega} \int_0^\infty \sum_{j=0}^{d-1} a_j \left(\frac{t}{\omega}\right)^j e^{it} \mathrm{d}t + \frac{1}{\omega^{d+1}} \int_0^\infty t^d f_{rem}(\tfrac{t}{\omega}) e^{it} \mathrm{d}t$$

- **step 4**: quadrature rule should be exact for the first integral

$$\int_0^\infty t^j e^{it} \mathrm{d}t = \sum_{j=1}^{s} w_j t_j^k, \qquad j = 0, 1, \ldots, d-1.$$

2. Maximal order method (3)

Can we maximize asymptotic order? Yes!

$$\int_0^\infty t^j e^{it} \mathrm{d}t = \sum_{j=1}^{s} w_j t_j^k, \qquad j = 0, 1, \ldots, d-1.$$

- **step 5**: Use Gaussian quadrature. In fact . . .

$$\int_0^\infty t^j e^{it} \mathrm{d}t = \int_\Gamma t^j e^{it} \mathrm{d}t = i \int_0^\infty (ip)^j e^{-p} \mathrm{d}p$$

- **step 6**: . . . use rescaled Gauss-Laguerre quadrature.

$$\int_0^\infty f(x) e^{i\omega x} \mathrm{d}x \approx \frac{1}{\omega} \sum_{j=1}^{s} w_j f\left(i \frac{x_k^{GL}}{\omega} \right)$$

2. Maximal order method (4)

Bringing it all together

$$I[f] = \int_a^b f(x) e^{i\omega x} \mathrm{d}x \quad \left(= \int_a^\infty \cdot - \int_\infty^b \cdot \right)$$

$$\approx Q[f] := \frac{1}{\omega} \sum_{j=1}^{s} w_j f\left(a + i \frac{x_k^{GL}}{\omega}\right) - \frac{1}{\omega} \sum_{j=1}^{s} w_j f\left(b + i \frac{x_k^{GL}}{\omega}\right)$$

And the error behaves as

$$I[f] - Q[f] \sim \omega^{-2s-1}.$$

(H. and Vandewalle, 2006), (Franklin and Friedman, 1957)

Outline

1. Design considerations
2. Two methods
3. Superinterpolation (with Olver)
4. Variations on a theme (with Deaño, Asheim)

Slightly worrying issues arise

More annoying observations:

- f is assumed to be analytic in an **infinitely large** region of the complex plane
- the method does not necessarily converge ...
- ...or it may converge to the wrong answer

Good news: failure of assumptions leads only to exponentially small errors (in ω)

A surprising observation

When $g(x) = x$ **then**

numerical steepest descent method = Filon-type method

Why is this so?

- because they are exact for (the same number of) polynomials

Another surprising observation

Complex Filon-type method

- asymptotic order doubles by interpolating at roots of Laguerre polynomials
- asymptotic order is **preserved when adding other points**

$$I[f] \approx \sum_{k=1}^{2s+n} w_k f(x_k)$$

with

$$\{x_k\} = \left\{a + i\frac{x_k^{GL}}{\omega}\right\}_{k=1}^{s} \cup \left\{b + i\frac{x_k^{GL}}{\omega}\right\}_{k=1}^{s} \cup \left\{x_k^{C}\right\}_{k=1}^{n}$$

Superinterpolation method

Complex Filon-type method

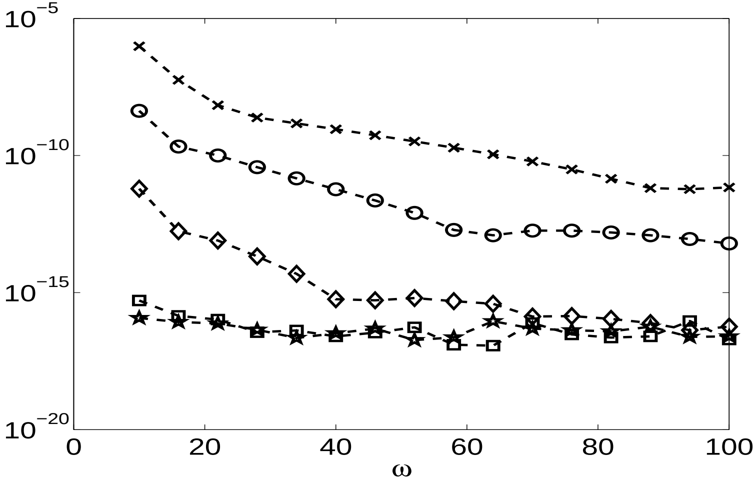
- using s quadrature points near a
- using s quadrature points near b
- using n (mapped) Chebyshev points on $[a, b]$

Error is

- for large ω: $\omega^{-2s-1} n^{2s-1} \rho^{-n}$
- for large m: $\omega^{-s} n^{-2} \rho^{-n}$

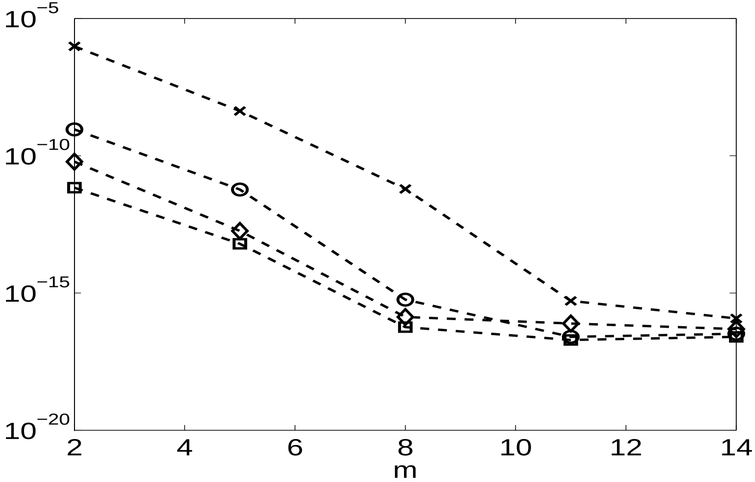
An example: $f(x) = \cos x + \sin x$

Error for increasing ω and various values of n



An example: $f(x) = \cos x + \sin x$

Error for increasing n and various values of ω



Outline

Other oscillators

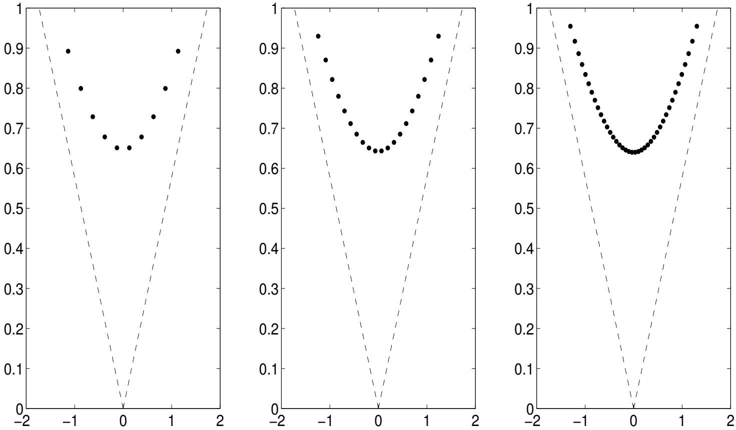
We are computing orthogonal polynomials with respect to the functional

$$F[f] = \int_\Gamma f(x)\, e^{i\omega g(x)}\, \mathrm{d}x$$

- $\Gamma = [0,\infty)$, $g(x) = x$: Laguerre
- $\Gamma = (-\infty,\infty)$, $g(x) = x^2$: Hermite
- $\Gamma = (-\infty,\infty)$, $g(x) = x^3$: non-classical

(Deaño and H., 2009), (Deaño, H. and Kuijlaars, 2011)

Example: $g(x) = x^3$



Other oscillators

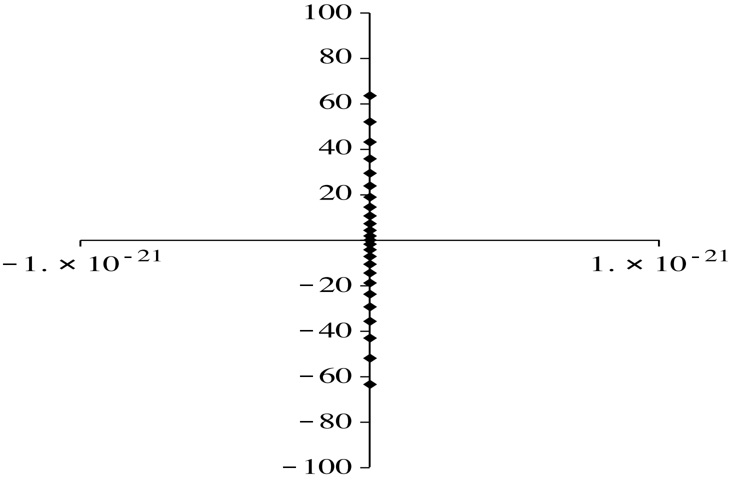
But we can consider more general oscillatory integrals

$$I[f] = \int_\Gamma f(x)\, w(\omega x)\, \mathrm{d}x$$

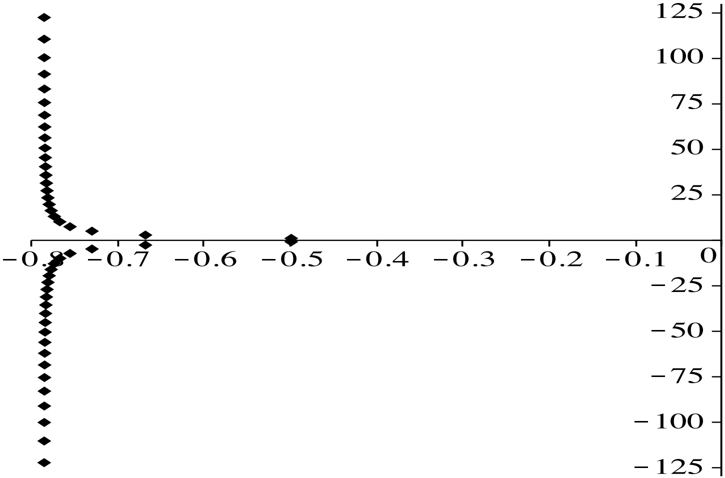
- extends work by R. Wong and W. Gautschi
- in each case for $w(\omega z)$ the error is ω^{-2n-1}

(Asheim and H., in preparation)

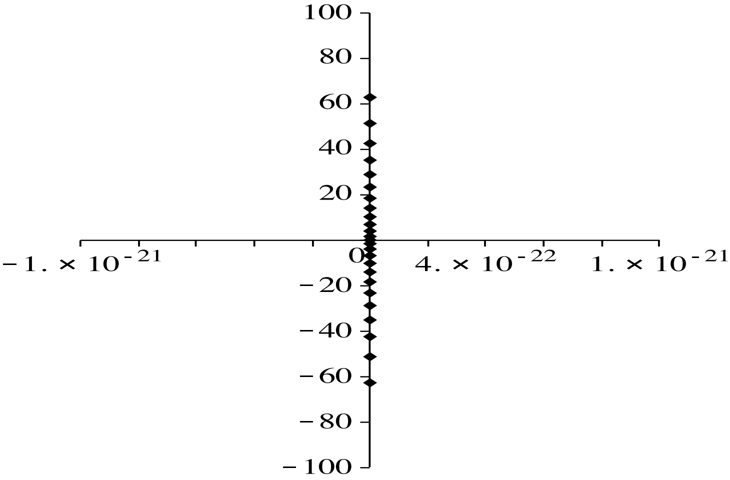
An example: $w(x) = \sin(x)$



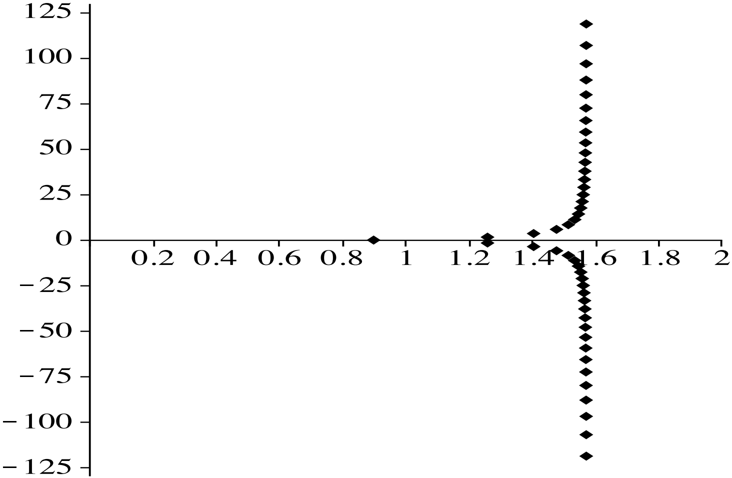
An example: $w(x) = \sin(x) + \cos(x)$



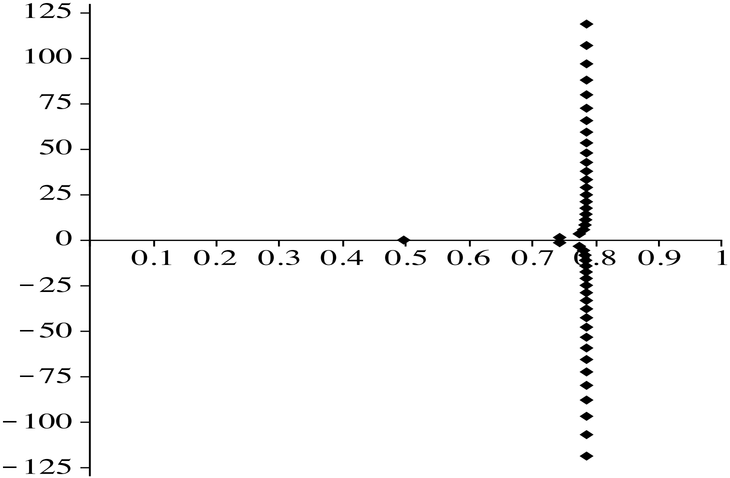
An example: $w(x) = J_0(x)$



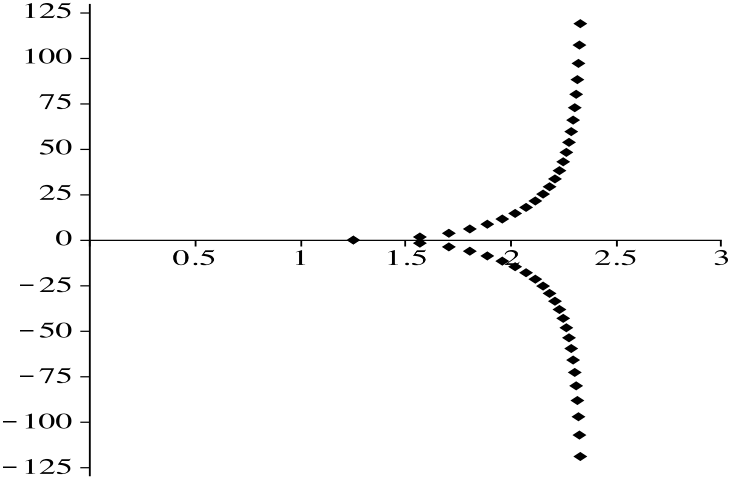
An example: $w(x) = J_1(x)$



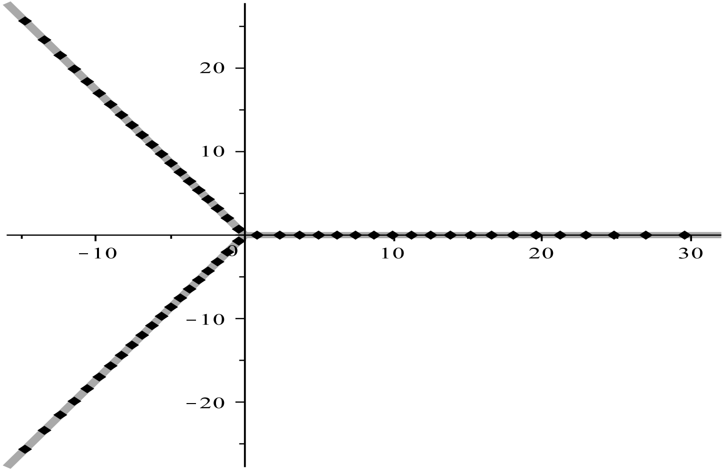
An example: $w(x) = J_{1/2}(x)$



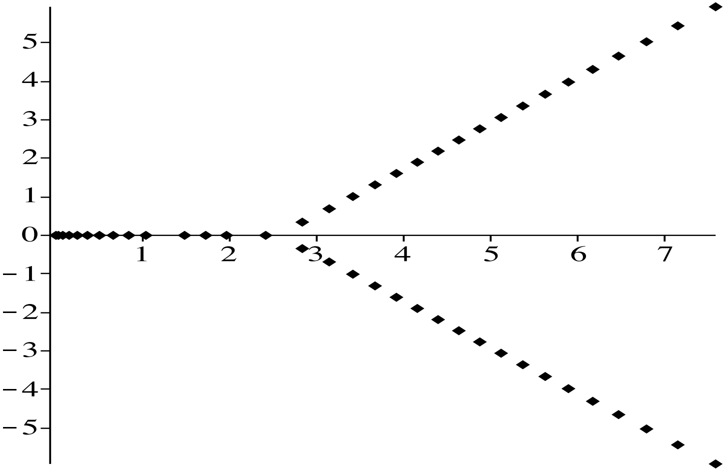
An example: $w(x) = J_{3/2}(x)$



An example: $w(x) = Ai(x)$



An example: $w(x) = \cos(x^2)$



The end

All pictures by Andreas Asheim.

Thanks!