The computation of highly oscillatory integrals

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Oscillatory integrals

V. LEDOUX AND M. VAN DAELE, *Gauss-type quadrature rules for highly-oscillatory integrals*
submitted for publication in SINUM

$$I[f] = \int_0^h f(x) e^{i\omega x} dx$$

Gaussian quadrature rules

How to obtain

$$\int_0^h f(x)dx \approx h \sum_{j=1}^{\nu} b_j f(c_j h) \text{ ?}$$

By replacing $f(x)$ by the interpolating polynomial

$$\bar{f}(x) = \sum_{j=1}^{\nu} \ell_j(h) f(c_j\, h).$$

- nodes $c_1, \ldots, c_\nu \in [0, 1]$: $c_i = 2\hat{c}_i - 1$ with $P_\nu(\hat{c}_i) = 0$

- weights $b_1, \ldots, b_\nu$: $b_j = \int_0^1 \ell_j(t)dt$

- order $= 2\nu$: the Gauss rule is exact if the integrand $f(x)$ is a polynomial of degree $2\nu - 1$.

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Gaussian quadrature rules applied to $I[f]$

$$I[f] = \int_0^h f(x)e^{i\omega x}dx$$

$$I[f] \approx Q_\nu^G[f] = h\sum_{l=1}^{\nu} b_l f(c_l h)e^{i\omega c_l h}$$

If the integrand oscillates rapidly, and unless we use a huge number of function evaluations, the polynomial interpolation underlying the classical Gauss rule is useless.

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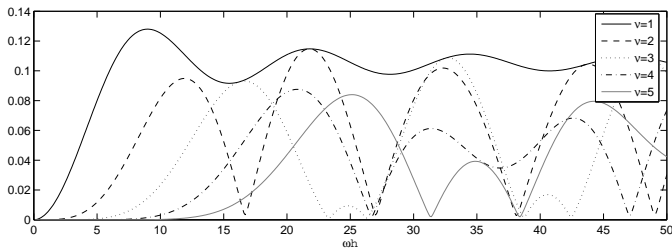
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Gauss rule applied to oscillatory integrands

Example : $f(x) = exp(x)$ and $h = 1/10$

$$\int_0^h e^x e^{i\omega x} dx = \frac{-1 + e^{h(1+i\omega)}}{1 + i\omega}$$

The absolute error in Gauss-Legendre quadrature for different values of the characteristic frequency $\psi = \omega\,h$.

Asymptotic expansion

$$
\begin{aligned}
I[f] &= \int_a^b f(x) e^{i\omega x} dx \\
&= \frac{1}{i\omega} \left(f(b)\, e^{i\omega b} - f(a)\, e^{i\omega a} \right) - \frac{1}{i\omega} I[f'] \\
&= \frac{1}{i\omega} \left(f(b)\, e^{i\omega b} - f(a)\, e^{i\omega a} \right) \\
&\quad - \frac{1}{(i\omega)^2} \left(f'(b)\, e^{i\omega b} - f'(a)\, e^{i\omega a} \right) + \frac{1}{(i\omega)^2} I[f'']
\end{aligned}
$$

$$
I[f] = -\sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[e^{i\omega b} f^{(m)}(b) - e^{i\omega a} f^{(m)}(a) \right]
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Introduction
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Asymptotic expansions
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Exponentially fitted rules
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Rules of Filon-type
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Adaptive Filon rules
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Conclusions

Asymptotic expansion

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$$Q_s^A[f] - I[f] \sim O(\omega^{-s-1}) \quad \omega \to +\infty$$

This asymptotic method is of asymptotic order $s+1$.
The asymptotic order gives us the rate at which the error
decreases with increasing ω.

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Exponential fitting

M. VAN DAELE, G. VANDEN BERGHE AND H. VANDE VYVER,
Exponentially fitted quadrature rules of Gauss type for oscillatory integrands, Appl. Numer. Math., 53 (2005), pp. 509–526.

How to compute

$$\int_{-1}^{1} F(t)dt$$

whereby $F(x)$ has an oscillatory behaviour with frequency μ?

$$I[f] = \int_0^h f(x)e^{i\omega x}dx = \frac{h}{2}e^{i\mu}\int_{-1}^{1} f(h(t+1)/2)e^{i\mu t}dt \quad \mu = \frac{\omega h}{2}$$

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$$\mathcal{L}[F; x; h; \mathbf{a}] = \int_{x-h}^{x+h} F(z)dz - h\sum_{k=1}^{\nu} w_k F(x + \hat{c}_k h), \quad \hat{c}_k \in [-\mathbf{1}, \mathbf{1}]$$

(put $x = \mathbf{0}$ and $h = \mathbf{1}$ to obtain $\int_{-\mathbf{1}}^{\mathbf{1}} F(t)dt$)

$\mathcal{L}[F; x; h; \mathbf{a}] = \mathbf{0}$ for a reference set of $K + \mathbf{2}(P + \mathbf{1}) + \mathbf{1} = \mathbf{2}\nu$ functions

$$\mathbf{1}, t, t^{\mathbf{2}}, ... t^{K},$$

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In this talk we only consider the case $P = \nu - \mathbf{1}$.

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1-node EF rule

$$\int_{-1}^{1} F(x)dx \approx w_1\, F(\hat{c}_1)$$

$$\int_{-1}^{1} \exp(\pm i\mu x)dx - w_1 \exp(\pm i\,\hat{c}_1\,\mu) = 0$$

$$w_1 = 2\sin(\mu)/\mu \qquad \hat{c}_1 = 0$$

$$I[f] = \int_0^h F(x)dx = \int_0^h f(x)\exp(i\omega x)dx$$

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2-node EF rule

$$\int_{-1}^{1} F x) dx \approx w_1\, F(\hat{c}_1) + w_2\, F(\hat{c}_2)$$

$$\begin{cases} \displaystyle\int_{-1}^{1} \exp(\pm \mathrm{i}\mu x) dx - w_1 \exp(\pm \mathrm{i}\,\hat{c}_1\,\mu) - w_2 \exp(\pm \mathrm{i}\,\hat{c}_2\,\mu) = 0 \\ \displaystyle\int_{-1}^{1} x\, \exp(\pm \mathrm{i}\mu x) dx - w_1\, \hat{c}_1 \exp(\pm \mathrm{i}\,\hat{c}_1\,\mu) - w_2 \hat{c}_2 \exp(\pm \mathrm{i}\,\hat{c}_2\,\mu) = 0 \end{cases}$$

Assuming $w_1 = w_2$ and $\hat{c}_1 = -\hat{c}_2$:

$$\iff \begin{cases} w_2\mu \cos(\mu\hat{c}_2) - \sin(\mu) = 0 \\ w_2\hat{c}_2\mu^2 \sin(\mu\hat{c}_2) - \sin(\mu) + \mu \cos(\mu) = 0 \end{cases}$$

$$Q_2^{EF}[f] = \frac{h}{2} w_2 \left[F\left(\frac{h(1+\hat{c}_2)}{2}\right) + F\left(\frac{h(1-\hat{c}_2)}{2}\right) \right] \qquad \mu = \frac{\omega h}{2}$$

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If $\cos(\mu\hat{c}_2) \neq 0$ then $w_2 = \sin\mu/(\mu\cos(\mu\hat{c}_2))$

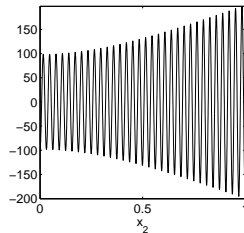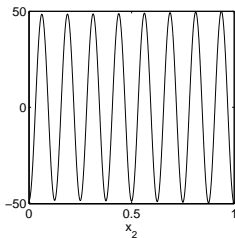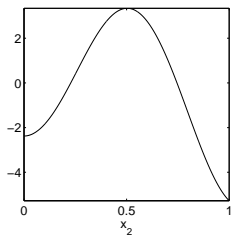$G(\hat{c}_2) := (\sin\mu - \mu\cos\mu)\cos(\mu\hat{c}_2) - \mu\hat{c}_2\sin\mu\sin(\mu\hat{c}_2) = 0$

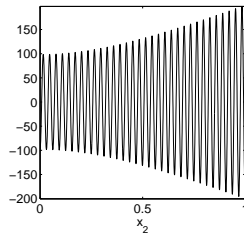Figure: $G(x_2)$ for $\mu = 5$, $\mu = 50$ and $\mu = 200$.

2-node EF rule

$$\begin{cases} w_2\mu\cos(\mu\hat{c}_2) - \sin(\mu) = 0 \\ w_2\hat{c}_2\mu^2\sin(\mu\hat{c}_2) - \sin(\mu) + \mu\cos(\mu) = 0 \end{cases}$$

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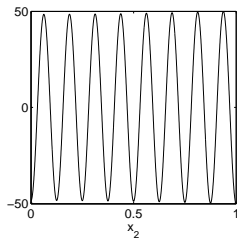$$G(\hat{c}_2) := (\sin\mu - \mu\cos\mu)\cos(\mu\hat{c}_2) - \mu\hat{c}_2\sin\mu\sin(\mu\hat{c}_2) = 0$$
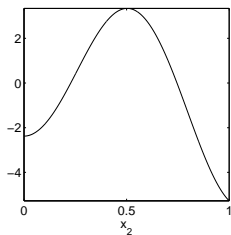

Figure: $G(x_2)$ for $\mu = 5$, $\mu = 50$ and $\mu = 200$.
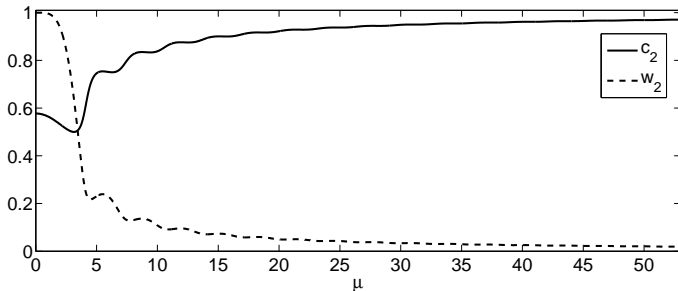
2-node EF rule

Figure: The $\hat{c}_2(\mu)$ and $w_2(\mu)$ curve for the EF method with $\nu = 2$.

3-node EF rule

$$\hat{c}_1 = 1 - \hat{c}_3 \qquad \hat{c}_2 = 0 \qquad w_1 = w_3$$
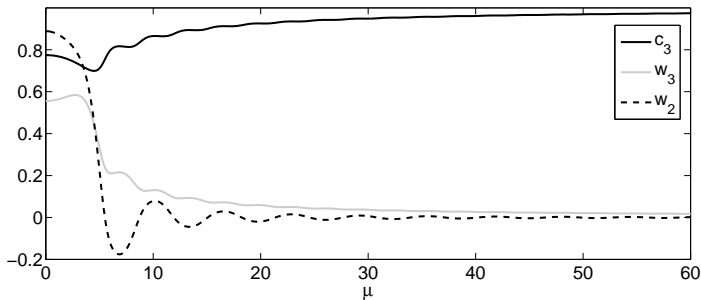

Figure: The $\hat{c}_3(\mu)$, $w_1(\mu) = w_3(\mu)$ and $w_2(\mu)$ curves for the $\nu = 3$ EF rule

4-node EF rule

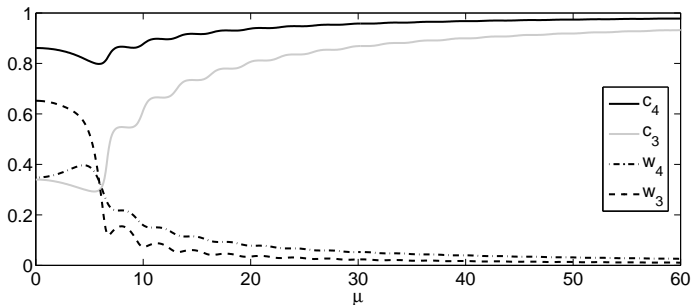$$\hat{c}_1 = 1 - \hat{c}_4 \qquad \hat{c}_2 = 1 - \hat{c}_3 \qquad w_1 = w_4 \qquad w_2 = w_3$$

Figure: Nodes and weights of the EF rule with $\nu = 4$ quadrature nodes.

Accuracy of EF rules

All EF rules reduce to the classical ν-point Gauss(-Legendre) method in the limiting case $\mu = 0$.

Thus for small μ : $O(h^{2\nu+1})$

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$$\int_{-1}^{1} F(t)dt \approx \int_{-1}^{1} \bar{F}(t)dt$$

$$\bar{F}(t) \in \text{span}\{\exp(\pm i\mu t), t\exp(\pm i\mu t), t^2\exp(\pm i\mu t), \ldots, t^P\exp(\pm i\mu t)\}$$

$$I[f] = \int_0^h f(x)e^{i\omega x}dx = \frac{h}{2}e^{i\frac{\omega h}{2}}\int_{-1}^{1} f(\frac{h}{2}(t+1))e^{i\frac{\omega h}{2}t}dt$$

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Suppose ν is even

$$a < c_1 < c_2 < \ldots < c_\nu < b$$

$$c_j = a + \lambda_j/\omega \qquad c_{\nu-j+1} = b - \lambda_j/\omega \quad j = 1, \ldots, \nu/2$$

$$v(x) = s(x) \prod_{i=1}^{\nu/2} (x - b + \lambda_i/\omega) \qquad s(x) = \frac{f^\nu(\xi(x))}{\nu!} \prod_{j=1}^{\nu/2} (x - a - \lambda_j/\omega)$$

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$$v(b) = O(\omega^{-\nu/2}) \qquad\qquad v'(b) = O(\omega^{-\nu/2+1})$$

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Filon-type

L. N. G FILON, *On a quadrature formula for trigonometric integrals*, Proc. Royal Soc. Edinburgh, 49 (1928), pp. 38–47.

Interpolate only the function $f(x)$ at $c_1 h, \ldots, c_\nu h$ by a polynomial $\bar{f}(x)$

$$I[f] \approx Q_\nu^F[f] = \int_0^h \bar{f}(x) e^{i\omega x} dx = h \sum_{l=1}^{\nu} b_l(i h \omega) f(c_l h)$$

$$b_l(i h \omega) = \int_0^1 \ell_l(x) e^{i h \omega x} dx$$

ℓ_l is the *l*th cardinal polynomial of Lagrangian interpolation.

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                                         oooooo   ooo

1-node Filon-type rule

$$I[f] = \int_0^h F(x)dx = \int_0^h f(x)\exp(\mathrm{i}\omega x)dx$$

$$Q_1^F[f] = \frac{\exp(\mathrm{i}h\omega) - 1}{\mathrm{i}\omega} f(c_1\, h)$$

$$Q_1^{EF}[F] = f(h/2)\frac{e^{\mathrm{i}h\omega} - 1}{\mathrm{i}\omega}$$

$$Q_1^F[f] = Q_1^{EF}[F] \text{ iff } c_1 = \frac{1}{2}$$

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2-node Filon-type rule

$$I[f] = \int_0^h F(x)dx = \int_0^h f(x)\exp(\mathrm{i}\omega x)dx$$

If f is interpolated at $c_1\,h$ and $c_2\,h$, then

$$
\begin{aligned}
Q_2^F[f] \;=\; & h\left[\left(\frac{i\left(\left(e^{i\psi}-1\right)c_2 - e^{i\psi}\right)}{(c_1-c_2)\psi} + \frac{e^{i\psi}-1}{(c_1-c_2)\psi^2}\right)f(c_1\,h)\right.\\
& \left. + \left(\frac{i\left(\left(e^{i\psi}-1\right)c_1 - e^{i\psi}\right)}{(c_2-c_1)\psi} + \frac{e^{i\psi}-1}{(c_2-c_1)\psi^2}\right)f(c_2\,h)\right]
\end{aligned}
$$

$Q_2^F[f] = Q_2^{EF}[F]$ iff the same nodes are used

2-node Filon-type rule

$$I[f] = \int_0^h F(x)dx = \int_0^h f(x)\exp(i\omega x)dx$$

If f is interpolated at $c_1\,h$ and $c_2\,h$, then

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\begin{aligned}
Q_2^F[f] &= h\left[\left(\frac{i\left((e^{i\psi}-1)\,c_2 - e^{i\psi}\right)}{(c_1-c_2)\psi} + \frac{e^{i\psi}-1}{(c_1-c_2)\psi^2}\right)f(c_1\,h)\right.\\
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Accuracy of Filon-type rules

A. ISERLES, *On the numerical quadrature of highly-oscillating integrals. I. Fourier transforms*, IMA J. Numer. Anal., 24 (2004), pp. 365–391.

For small ω, a Filon-type quadrature method has an order as if $\omega = 0$.

Legendre nodes : order 2ν Lobatto nodes : order $2\nu - 2$
For large ω :

$$Q_\nu^F[f] - I[f] \sim \begin{cases} O(\omega^{-1}) & c_1 > 0 \text{ or } c_\nu < 1 \\ O(\omega^{-2}) & c_1 = 0, c_\nu = 1 \end{cases}$$

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$$Q_\nu^F[f] - I[f] \sim \begin{cases} O(\omega^{-1}) & c_1 > 0 \text{ or } c_\nu < 1 \\ O(\omega^{-2}) & c_1 = 0, c_\nu = 1 \end{cases}$$

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Accuracy of Filon-type rules

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$$Q_\nu^F[f] - I[f] = I[\bar{f}] - I[f] = I[v]$$
$$= -\sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[e^{i\omega h} v^{(m)}(h) - v^{(m)}(0) \right]$$

If $(c_1, c_\nu) = (0, 1)$ then $v(h) = v(0) = 0$

$\implies Q_\nu^F[f] - I[f] = O(\omega^{-2}).$

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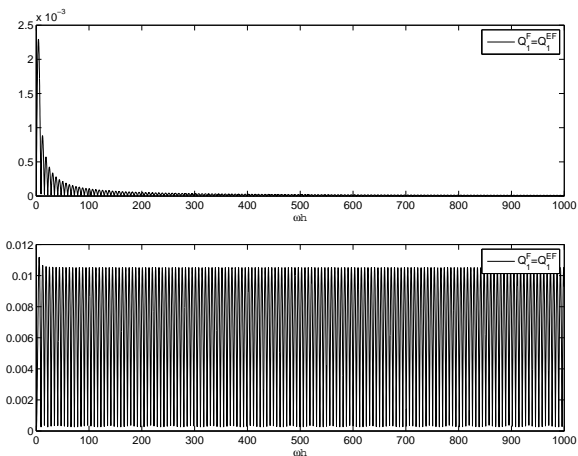
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$Q_1^F[f] = Q_1^{EF}[F]$ illustrated

Figure: The errors in $Q_1^F[f] = Q_1^{EF}[F]$ for $f(x) = e^x$, $h = 1/10$ as a function of $\psi = \omega h$. The top graph shows the absolute error E, the bottom graph shows the normalised error $(\omega h)E$.

$Q_2^F[f]$ and $Q_2^{EF}[F]$ illustrated
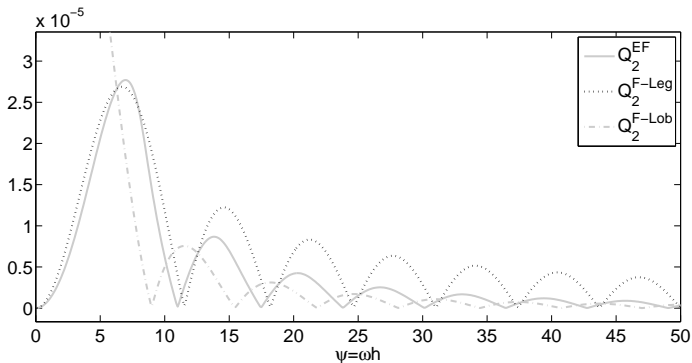
Figure: The absolute error in some $\nu = 2$ Filon-type schemes for $f(x) = e^x$, $h = 1/10$ and different values of ωh.

How to improve the accuracy of Filon-rules ?

- by using Hermite interpolation : asymptotic order $p + 1$ can be reached where p is the number of derivatives at the endpoints:

$$\overline{f}^{(l)}(h) = f^{(l)}(h), \overline{f}^{(l)}(0) = f^{(l)}(0), l = 0, \ldots, p - 1$$

$$Q^F_\nu[f] - I[f] = O(\omega^{-p-1})$$

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Method of steepest descent

D. HUYBRECHS AND S. VANDEWALLE, *On the evaluation of highly oscillatory integrals by analytic continuation*, SIAM J. Numer. Anal., 44 (2002) pp 1026–1048.

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Method of steepest descent

$$\int_a^b f(x) e^{i\omega x} dx$$

$$= e^{i\omega a} \int_0^\infty f(a + ip) e^{-\omega p} dp - e^{i\omega b} \int_0^\infty f(b + ip) e^{-\omega p} dp$$

$$= \frac{e^{i\omega a}}{\omega} \int_0^\infty f(a + i\frac{q}{\omega}) e^{-q} dq - \frac{e^{i\omega b}}{\omega} \int_0^\infty f(b + i\frac{q}{\omega}) e^{-q} dq$$

This leads to the numerical evaluation of the two resulting integrals with classical Gauss-Laguerre quadrature.

High asymptotic order is obtained : using ν points for each integral, the error behaves as $O(\omega^{-2\nu-1})$.

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One ends up evaluating f at the points

$$a+i\frac{x_{nj}}{\omega}, \text{ and } b+i\frac{x_{nj}}{\omega}, \ j=1,...,n,$$

where x_{nj} are the n roots of the Laguerre polynomial of degree n.

This approach is equivalent to using a Filon rule with the same interpolation points.

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Adaptive Filon-type rules

Idea : combine best properties of EF and Filon quadrature

- EF
    - + accurate for small ωh since the method reduces to Gauss-Legendre quadrature
    - + good results for large ωh since the nodes tend to the endpoints (at a rate proportional to ω^{-1})
    - - but : difficult to determine the nodes and weights for a given ωh (iteration needed and ill-conditioned)

- Filon
    - + any set of nodes can be used
    - - there is no optimal set of nodes for all ωh
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Adaptive Filon-type methods

$$S(\psi; r; n) = \frac{1 - \frac{\psi^n - r^n}{1 + |\psi^n - r^n|}}{1 + \frac{r^n}{1 + r^n}}$$

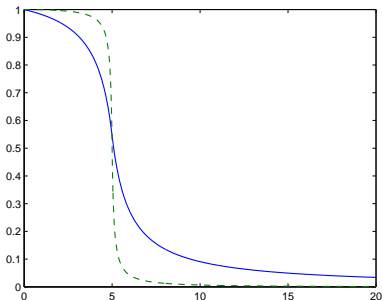Figure: $S(x, r, 1)$ and $S(x, r, 2)$ (dashed) for $r = 5$ in $[0, 20]$

Adaptive Filon-type methods

- $\nu = 2 : c_1(\psi) = \dfrac{3 - \sqrt{3}}{6} S(\psi; 2\pi; 1); c_2(\psi) = 1 - c_1(\psi)$

- $\nu = 3 : c_1(\psi) = \dfrac{10 - \sqrt{15}}{5} S(\psi; 3\pi; 1); c_3(\psi) = 1 - c_1(\psi)$
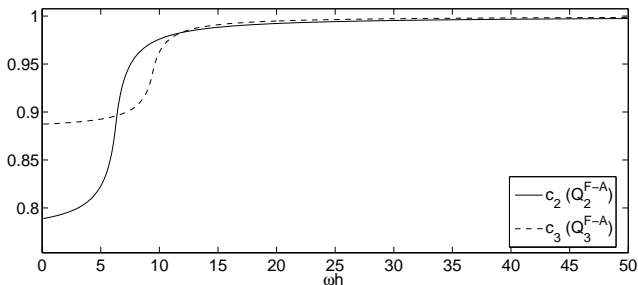
Figure: $c_2(\psi)$ of the adaptive Filon method $Q_2^{F\text{-}A}$ and $c_3(\psi)$ of the adaptive Filon method $Q_3^{F\text{-}A}$.

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Asymptotic analysis for $Q_2^{F\text{-}A}$

$\tilde{c}_1 = c_1 h = \sigma_1(\omega)$ and $\tilde{c}_2 = c_2 h = h + \sigma_2(\omega)$ with $\sigma_{1,2}(\omega) \sim \omega^{-1}$

$$v(x) = s_h(x)(x - h - \sigma_2) \qquad s_h(x) = \frac{f''(\xi_h(x))}{2}(x - \sigma_1)$$

$$
\begin{aligned}
v'(x) &= s_h(x) + s_h'(x)(x - h - \sigma_2) \\
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\end{aligned}
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Similar results for the other endpoint.

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$$Q_2^{F-A}[f] - I[f] = I[v] \sim \sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[e^{i\omega h} v^{(m)}(h) - v^{(m)}(0) \right]$$

Reordering for $s_h(h) = f''(\xi_h(x))$, $s_h'(h) = f^{(iii)}(\xi_h(x))$, ...

$$
\begin{aligned}
I[v] \quad &\sim \quad s_h(h)e^{i\psi} \left[\frac{\sigma_2}{i\omega} - \frac{1}{\omega^2} \right] + s_h'(h)e^{i\psi} \left[\frac{\sigma_2}{\omega^2} + \frac{2}{i\omega^3} \right] + \dots \\
&+ \quad s_0(0) \left[\frac{\sigma_1}{i\omega} - \frac{1}{\omega^2} \right] + s_0'(0) \left[\frac{\sigma_1}{\omega^2} + \frac{2}{i\omega^3} \right] + \dots
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$\sigma_2 = -\sigma_1$ with $\sigma_{1,2}(\omega) \sim \psi^{-1} \iff Q_2^{F-A}[f] - I[f] \sim O(\psi^{-2})$

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$\sigma_2 = -\sigma_1$ with $\sigma_{1,2}(\omega) \sim \psi^{-1} \iff Q_2^{F-A}[f] - I[f] \sim O(\psi^{-2})$

A complex adaptive Filon-rule : $Q_2^{F\text{-}C}$

Are there better options than choosing $\sigma_2 = -\sigma_1$?

$$I[v] \sim s_h(h)e^{i\psi}\left[\frac{\sigma_2}{i\omega} - \frac{1}{\omega^2}\right] + s'_h(h)e^{i\psi}\left[\frac{\sigma_2}{\omega^2} + \frac{2}{i\omega^3}\right] + \dots$$
$$+ s_0(0)\left[\frac{\sigma_1}{i\omega} - \frac{1}{\omega^2}\right] + s'_0(0)\left[\frac{\sigma_1}{\omega^2} + \frac{2}{i\omega^3}\right] + \dots$$

Yes : Suppose $\sigma_1 = \sigma_2 = i/\omega \implies Q_2^{F-C}[f] - I[f] \sim O(\psi^{-3})$.

$$Q_2^{F\text{-}C} = \frac{ih\left[f(ih/\psi) - e^{i\psi}f\left((i + \psi)h/\psi\right)\right]}{\psi}, \quad \psi = \omega h$$

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Yes : Suppose $\sigma_1 = \sigma_2 = i/\omega \Longrightarrow Q_2^{F-C}[f] - I[f] \sim O(\psi^{-3})$.

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Q_2^{F\text{-}C} = \frac{ih\left[f(ih/\psi) - e^{i\psi}f\left((i+\psi)h/\psi\right)\right]}{\psi}, \quad \psi = \omega h
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A complex adaptive Filon-rule : $Q_2^{F\text{-}C}$

Are there better options than choosing $\sigma_2 = -\sigma_1$?

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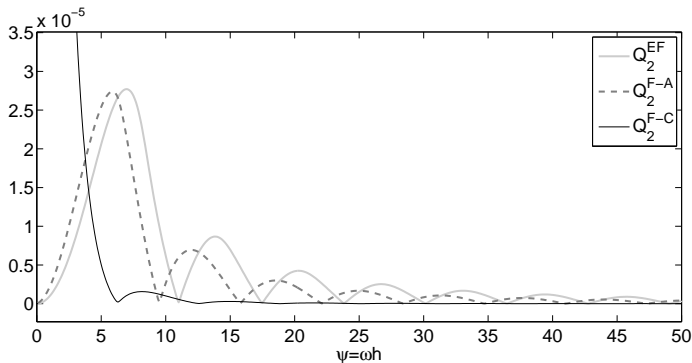$$

Illustration

Figure: The errors in some $\nu = 2$ Filon-type schemes for $f(x) = e^x$, $h = 1/10$ and different values of ω.
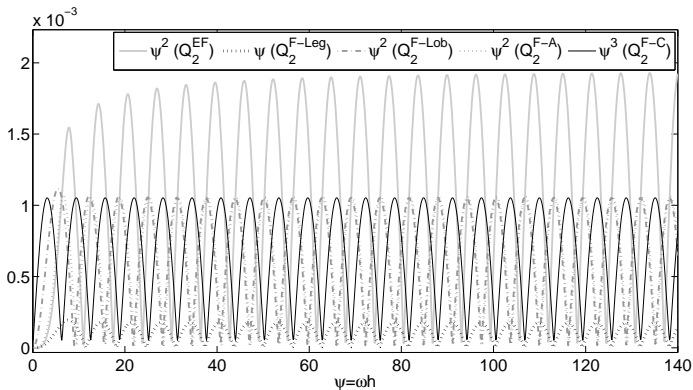
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Figure: The normalised errors in some $\nu = 2$ Filon-type schemes for $f(x) = e^x$, $h = 1/10$ and different values of ω.

Error control for $Q_2^{F\text{-}C}$

$$Q_2^{F\text{-}C} = \frac{\mathrm{i}h\left[f(\mathrm{i}h/\psi) - e^{\mathrm{i}\psi}f\left((\mathrm{i}+\psi)h/\psi\right)\right]}{\psi}, \quad \psi = \omega h.$$

Obtained by replacing f by interpolating polynomial $\bar{f}$ in nodes $\mathrm{i}\,h/\omega$ and $h + \mathrm{i}\,h/\omega$ (for large ψ : $\sim \psi^{-3}$)

Similarly : $Q_3^{F\text{-}C}$ by replacing f by interpolating polynomial $\tilde{f}$ in nodes $\mathrm{i}\,h/\omega$, $h/2$ and $h + \mathrm{i}\,h/\omega$ (for large ψ : also $\sim \psi^{-3}$ but about 100 times more accurate)

$$I[\tilde{f}] - I[\bar{f}] = \frac{(1 - e^{\mathrm{i}\psi})2h}{\psi^2(4 + \psi^2)} \times$$
$$\left((2 - \mathrm{i}\psi)f(\frac{\mathrm{i}}{\omega}) - (2 + \mathrm{i}\psi)f(h + \frac{\mathrm{i}}{\omega}) + (2\mathrm{i}\psi)f(\frac{h}{2})\right)$$

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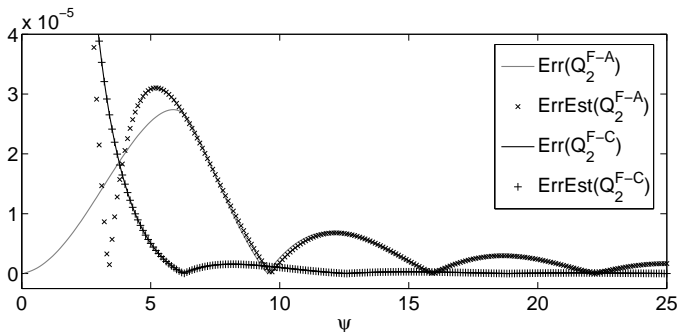
Illustration

Figure: Error estimations for the $Q_2^{F\text{-}A}$ and $Q_2^{F\text{-}C}$ method applied on the problem with $f(x) = e^x, h = 2$.
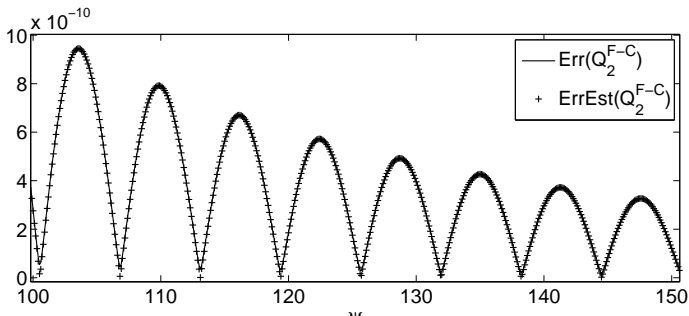
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Conclusions

- Filon rules, EF rules, and steepest descent rules are built up starting from different points op view, the basic underlying idea is the same : $f(x)$ is interpolated by a polynomial.

- Different choices can be made for the interpolation nodes.

- A choice of the (complex) interpolation nodes can improve the asymptotic behaviour of the quadrature rule.

- Even better asymptotic behaviour is obtained if the nodes are frequency dependent.

- Cheap error estimation is possible.

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