

Adaptive Filon methods for the computation of highly oscillatory integrals

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Oscillatory integrals

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

We focus on the particular case

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

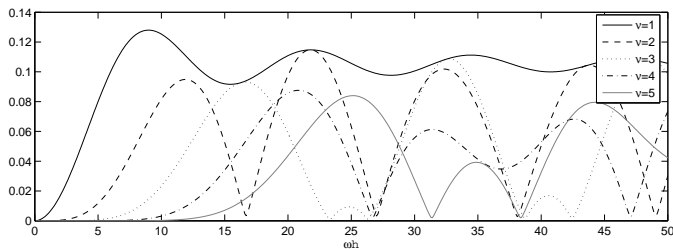
If the integrand oscillates rapidly, and unless we use a huge number of function evaluations, the classical ν -point Gauss rule is useless.



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

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

$$I[f] = - \sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[e^{i\omega b} f^{(m)}(b) - e^{i\omega a} f^{(m)}(a) \right]$$

Asymptotic rules

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

$$I[f] = - \sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[e^{i\omega b} f^{(m)}(b) - e^{i\omega a} f^{(m)}(a) \right]$$

$$Q_s^A[f] = - \sum_{m=0}^{s-1} \frac{1}{(-i\omega)^{m+1}} \left[e^{i\omega b} f^{(m)}(b) - e^{i\omega a} f^{(m)}(a) \right]$$

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

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

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 ?

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

Exponential fitting

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

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

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

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

$$\exp(\pm i\mu t), t \exp(\pm i\mu t), t^2 \exp(\pm i\mu t), \dots, t^P \exp(\pm i\mu t)$$

In this talk we only consider the case $K = -1, P = \nu - 1$.

1-node EF rule

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

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

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

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

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

2-node EF rule

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

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

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

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

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

2-node EF rule

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

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

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

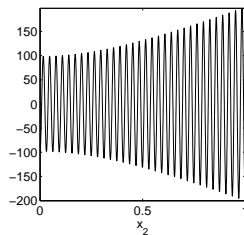
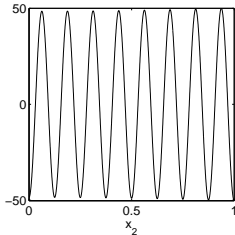
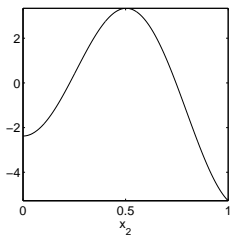


Figure: $G(x_2)$ for $\mu = 5$, $\mu = 50$ and $\mu = 200$.

2-node EF rule

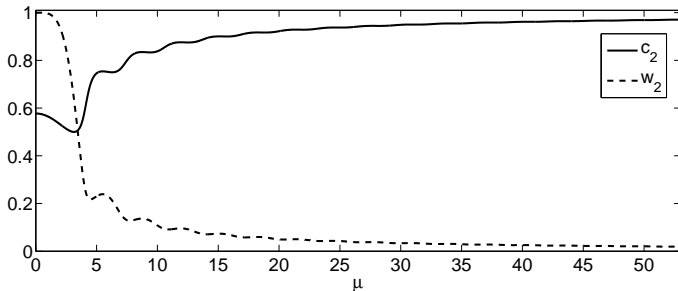


Figure: The $\hat{c}_2(\mu)$ and $w_2(\mu)$ curve for the EF method with $\nu = 2$.

3-node EF rule

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

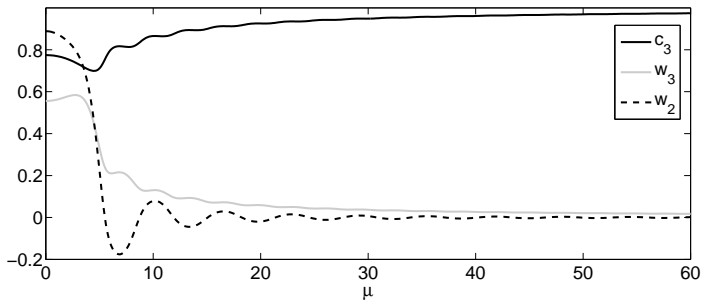


Figure: The $\hat{c}_3(\mu)$, $w_1(\mu) = w_3(\mu)$ and $w_2(\mu)$ curves for the $\nu = 3$ EF rule

4-node EF rule

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

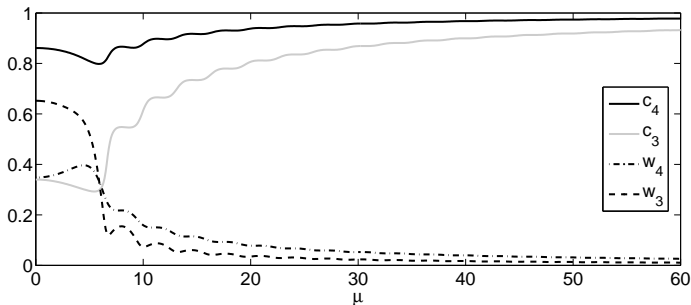


Figure: Nodes and weights of the EF rule with $\nu = 4$ quadrature nodes.

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 : $O(h^{2\nu+1})$

What about the accuracy for larger values of $\mu = \omega h/2$?

J. P. COLEMAN AND L. GR. IXARU, *Truncation errors in exponential fitting for oscillatory problems*, SIAM. J. Numer. Anal., 44 (2006), pp. 1441–1465.

for large μ : $O(\mu^{\bar{\nu}-\nu})$ with $\bar{\nu} = \lfloor(\nu - 1)/2\rfloor$

$$\nu = 1 : O(\omega^{-1})$$

$$\nu = 2, 3 : O(\omega^{-2})$$

$$\nu = 4, 5 : O(\omega^{-3})$$

Proof

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

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

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

$$\text{If } \frac{\omega h}{2} = \mu \text{ then } I[f] \approx I[\bar{f}] \text{ with } \bar{f}(x) \in \text{span}\{1, x, x^2, \dots, x^{\nu-1}\}$$

$$Q_{\nu}^{EF}[f] - I[f] = I[\bar{f}] - I[f] = I[v] \quad v(x) := \bar{f}(x) - f(x)$$

Proof

Suppose ν is even and $a < c_1 < c_2 < \dots < c_\nu < b$

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

$$v(x) = \frac{f^{(\nu)}(\xi(x))}{\nu!} \prod_{i=1}^{\nu} (x - c_i)$$

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

$$v(b) = s(b) \prod_{i=1}^{\nu/2} (\lambda_i/\omega) = O(\omega^{-\nu/2})$$

$$v'(b) = s(b)\omega^{-\nu/2+1} \sum_{k=1}^{\nu/2} \prod_{i \neq k} \lambda_i + O(\omega^{-\nu/2}) = O(\omega^{-\nu/2+1})$$

Proof

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

$$v^{(n)}(b) = O(\omega^{-\nu/2+n}), \quad n = 0, 1, \dots, \nu/2 - 1$$

$$v^{(n)}(a) = O(\omega^{-\nu/2+n}), \quad n = 0, 1, \dots, \nu/2 - 1$$

$$\begin{aligned} Q_\nu^{EF}[f] - I[f] &= I[v] \\ &= - \sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[e^{i\omega b} v^{(m)}(b) - e^{i\omega a} v^{(m)}(a) \right] \\ &= - \sum_{m=0}^{\nu/2-1} \frac{1}{(-i\omega)^{m+1}} O(\omega^{-\nu/2+m}) + O(\omega^{-\nu/2-1}) \\ &= O(\omega^{-\nu/2-1}) = O(\omega^{\lfloor(\nu-1)/2\rfloor-\nu}) \end{aligned}$$

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 $c_1 h, \dots, c_\nu h$ by a polynomial $\bar{f}(x)$

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

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

ℓ_l is the l th cardinal polynomial of Lagrangian interpolation.

1-node Filon-type rule

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

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

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

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

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

$$Q_2^F[f] = h \left[\left(\frac{i((e^{i\psi} - 1)c_2 - e^{i\psi})}{(c_1 - c_2)\psi} + \frac{e^{i\psi} - 1}{(c_1 - c_2)\psi^2} \right) f(c_1 h) + \left(\frac{i((e^{i\psi} - 1)c_1 - e^{i\psi})}{(c_2 - c_1)\psi} + \frac{e^{i\psi} - 1}{(c_2 - c_1)\psi^2} \right) f(c_2 h) \right]$$

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

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 :

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

Accuracy of Filon-type rules

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

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

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

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

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:

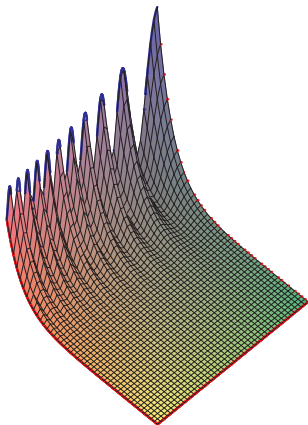
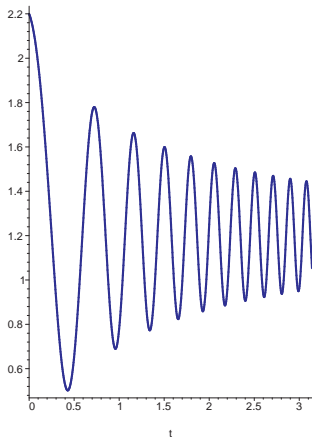
$$\bar{f}^{(l)}(h) = f^{(l)}(h), \bar{f}^{(l)}(0) = f^{(l)}(0), l = 0, \dots, p - 1$$

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

- by using **adaptive Filon-type methods** : allowing the interpolation points to depend on ω (is discussed later)
- by using **nodes in the complex plane** (=method of steepest descent)

Method of steepest descent

D. HUYBRECHS AND S. VANDEWALLE, *On the evaluation of highly oscillatory integrals by analytic continuation*, SIAM J. Numer. Anal., 44 (2007) pp 1026–1048.



Method of steepest descent

$$\begin{aligned} & \int_a^b f(x) e^{i\omega x} dx \\ &= e^{i\omega a} \int_0^\infty f(a + ip) e^{-\omega p} dp - e^{i\omega b} \int_0^\infty f(b + ip) e^{-\omega p} dp \\ &= \frac{e^{i\omega a}}{\omega} \int_0^\infty f\left(a + i\frac{q}{\omega}\right) e^{-q} dq - \frac{e^{i\omega b}}{\omega} \int_0^\infty f\left(b + i\frac{q}{\omega}\right) e^{-q} dq \end{aligned}$$

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 $O(\omega^{-2\nu-1})$.

Method of steepest descent

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

One ends up evaluating f at the points

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

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.

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
 - most accurate for small ωh if the method is built on Legendre nodes
 - most accurate for large ωh if the endpoints are included in the set of nodes

Adaptive Filon-type rules

Idea : create quadrature rules with ω -dependent nodes that

- reduce to Legendre-nodes for small ω
- reduce to Lobatto-nodes for large ω
- for given value of ω are easy to compute

To do so, we introduce S-shaped functions.

Adaptive Filon-type methods

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

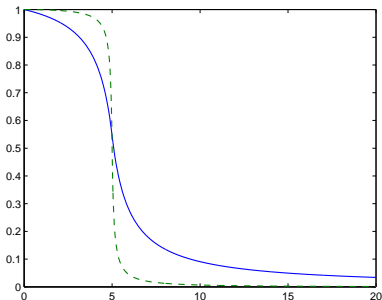


Figure: $S(x, r, 1)$ and $S(x, r, 2)$ (dashed) for $r = 5$ in $[0, 20]$

Adaptive Filon-type methods

- $\nu = 2$: $c_1(\psi) = \frac{3 - \sqrt{3}}{6} S(\psi; 2\pi; 1)$; $c_2(\psi) = 1 - c_1(\psi)$
- $\nu = 3$: $c_1(\psi) = \frac{10 - \sqrt{15}}{5} S(\psi; 3\pi; 1)$; $c_3(\psi) = 1 - c_1(\psi)$

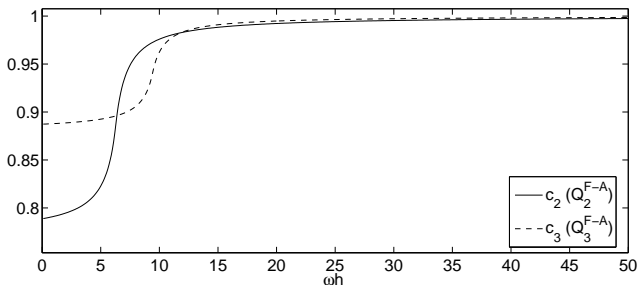


Figure: $c_2(\psi)$ of the adaptive Filon method Q_2^{F-A} and $c_3(\psi)$ of the adaptive Filon method Q_3^{F-A} .

Asymptotic analysis for Q_2^{F-A}

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

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

$$v'(x) = s_h(x) + s'_h(x)(x - h - \sigma_2)$$

$$v''(x) = 2s'_h(x) + s''_h(x)(x - h - \sigma_2)$$

$$\vdots$$

$$v(h) = -s_h(h)\sigma_2$$

$$v'(h) = s_h(h) - s'_h(h)\sigma_2$$

$$v''(h) = 2s'_h(h) - s''_h(h)\sigma_2$$

$$\vdots$$

Similar results for the other endpoint.

Asymptotic analysis for Q_2^{F-A}

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

Reordering for $s_h(h)$, $s'_h(h)$, ...

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

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

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

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

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

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

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

Illustration

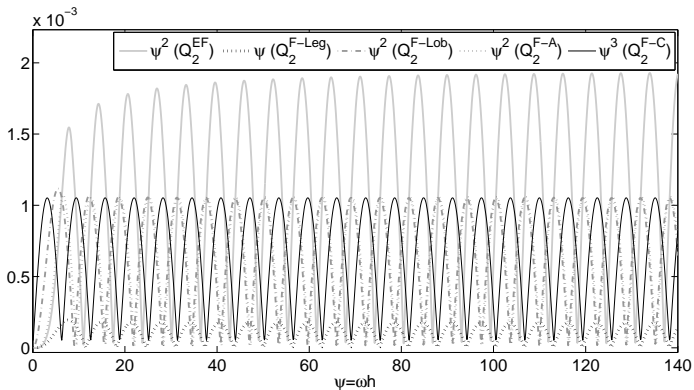


Figure: The normalised errors in some $\nu = 2$ Filon-type schemes for $f(x) = e^x$, $h = 1/10$ and different values of ω .

Error control for Q_2^{F-C}

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

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

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

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

$$\left((2 - i\psi) f\left(\frac{i}{\omega}\right) - (2 + i\psi) f\left(h + \frac{i}{\omega}\right) + (2i\psi) f\left(\frac{h}{2}\right) \right)$$

Illustration

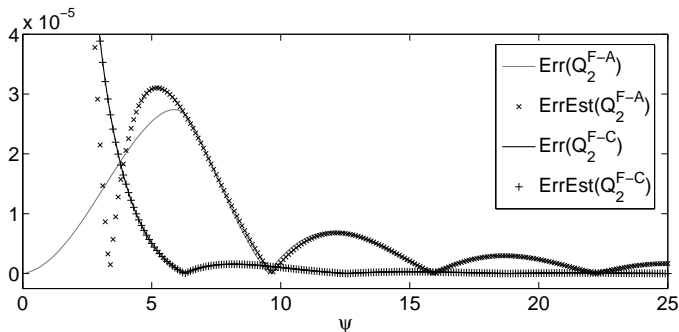


Figure: Error estimations for the Q_2^{F-A} and Q_2^{F-C} method applied on the problem with $f(x) = e^x$, $h = 2$.

Illustration

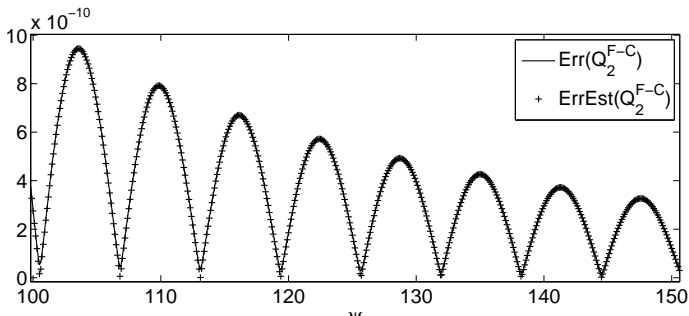


Figure: Error estimations for the Q_2^{F-A} and Q_2^{F-C} method applied on the problem with $f(x) = e^x$, $h = 2$.

Conclusions

- Filon rules, EF rules, and steepest descent rules are built up starting from different points of 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.