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Highly oscillatory quadrature and its applications

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Part I:
Quadrature of HiOsc integrals

Suppose that the kernel

$$K(x,\omega) \in \mathrm{L}[[0,1] \times \mathbb{R}_+]$$

oscillates rapidly for $\omega \gg 1$, e.g.

- The Fourier oscillator $\mathrm{e}^{\mathrm{i}\omega x}$;
- The irregular oscillator $\mathrm{e}^{\mathrm{i}\omega g(x)}$, where g is real;
- The singular oscillator $\mathrm{e}^{\mathrm{i}\omega|x-y|}/|x-y|^{\alpha}$, where $y \in [0,1]$ and $\alpha < 1$;
- The Bessel oscillator $\mathrm{J}_\nu(\omega x)$, $\nu \in \mathbb{R}$;
- The Airy oscillator $\mathrm{Ai}(-\omega x)$.

We are interested in approximating

$$I[f] = \int_0^1 f(x) K(x,\omega) \mathrm{d}x.$$

What's wrong with Gaussian quadrature?

Gauss–Christoffel quadrature:

$$I[f] \approx Q^{\mathrm{GC}}[f] = \int_0^1 \phi(x)\mathrm{d}x = \sum_{l=1}^{\nu} b_l f(c_l) K(c_l, \omega),$$

where ϕ is the $(\nu - 1)$-degree polynomial that interpolates $f(x)K(x,\omega)$ at the quadrature nodes

$$c_1 < c_2 < \cdots < c_\nu \qquad \text{in} \qquad [0,1].$$

In particular: $c_1, c_2, \ldots, c_\nu$ zeros of $\mathrm{P}_\nu(2x-1) \Rightarrow$ the quadrature is of maximal order 2ν: this is the Gauss–Legendre quadrature.

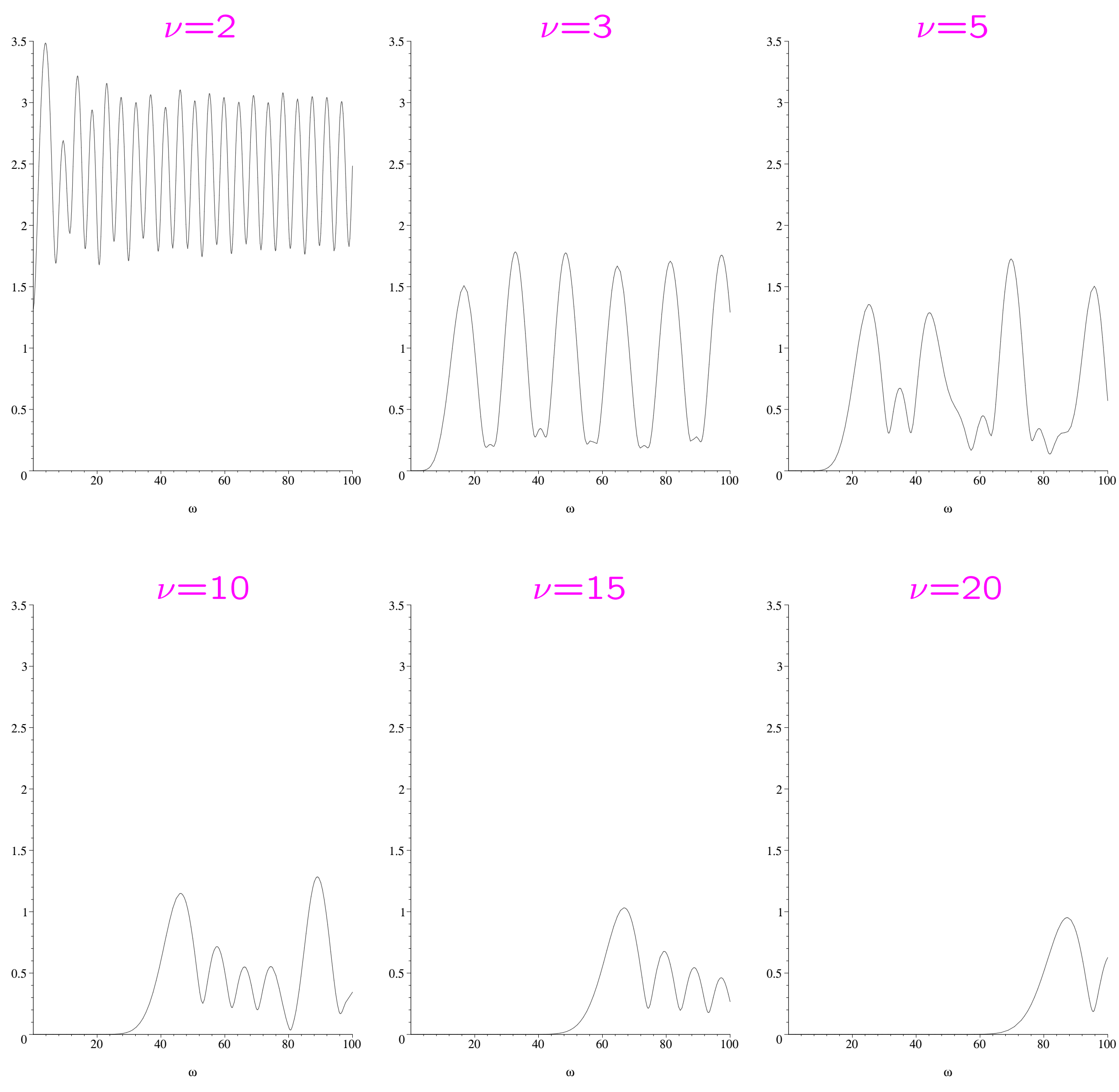
Suppose for simplicity that $K(x,\omega) = \mathrm{e}^{\mathrm{i}\omega x}$.
For $\omega \gg 1$ and fixed $x \neq 0$ the value $\mathrm{e}^{\mathrm{i}\omega x}$ is, to all intents and purposes, a random number on the complex unit circle $|z| = 1$. Therefore, for fixed ν

$$Q^{\mathrm{GC}}[f] = \sum_{l=1}^{\nu} b_l f(c_l) \mathrm{e}^{\mathrm{i}\omega c_l} \sim \mathcal{O}(1), \qquad \omega \to \infty.$$

On the other hand, Riemann–Lebesgue implies that

$$\lim_{\omega \to \infty} I[f] = 0, \qquad f \in \mathrm{L}_1[0,1].$$

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



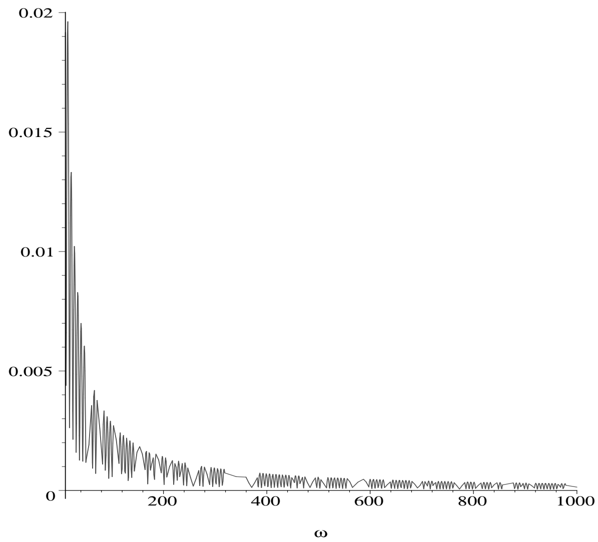
Generalising the Filon method

Instead of interpolating the integrand $f(x)K(x,\omega)$ at the quadrature nodes, we interpolate the values of $f(x)$ there by the polynomial $\tilde{\phi}$:

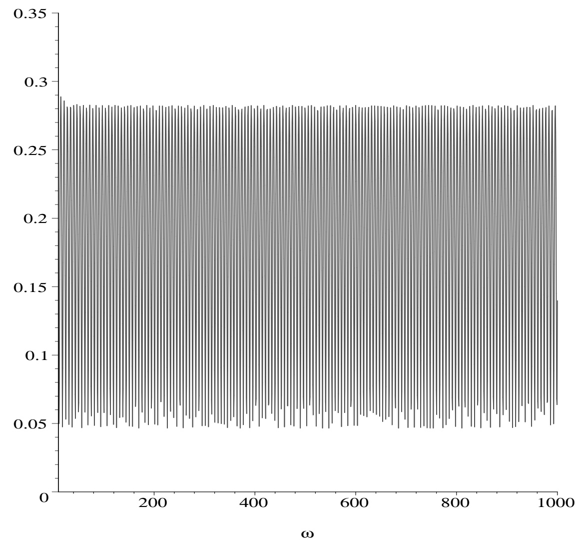
$$I[f] \approx Q^{\mathsf{F}}[f] = \int_0^1 \tilde{\phi}(x) K(x,\omega)\,\mathrm{d}x = \sum_{l=1}^{\nu} b_l(\omega) f(c_l).$$

Note that the weights depend on the frequency ω.

Filon–Legendre: $\nu = 2$, $\boldsymbol{c} = [\frac{1}{2} - \frac{\sqrt{6}}{3}, \frac{1}{2} + \frac{\sqrt{6}}{3}]$.



$|Q^{\mathsf{F}}[\mathrm{e}^x] - I[\mathrm{e}^x]|$

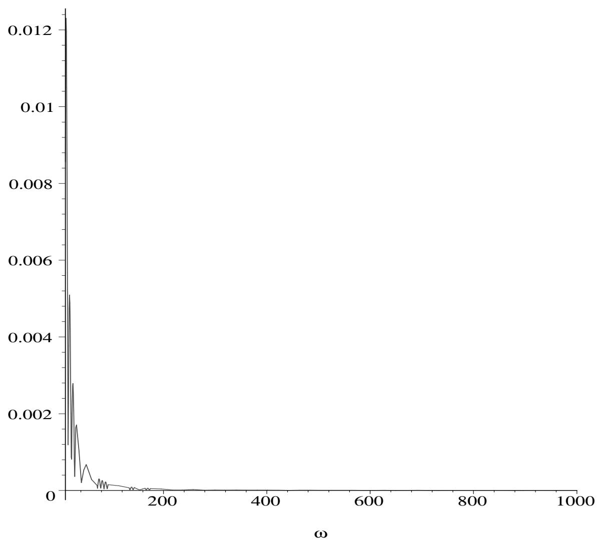


$\omega|Q^{\mathsf{F}}[\mathrm{e}^x] - I[\mathrm{e}^x]|$

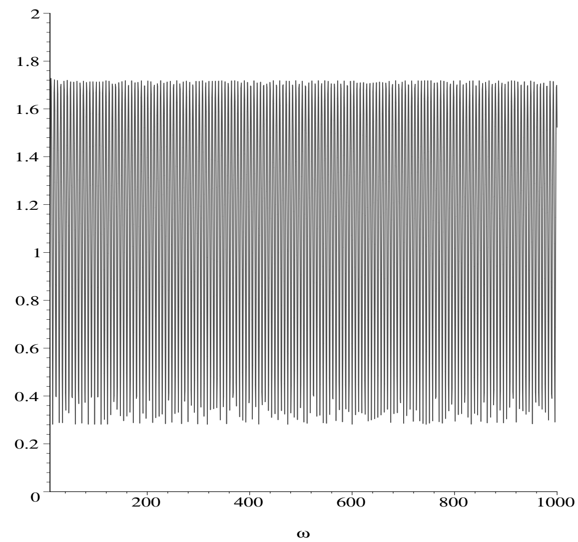
Just two quadrature points…

...but we can do even better!

Choose instead Lobatto points: $\nu = 2$, $c = [0, 1]$:



$|Q^F[e^x] - I[e^x]|$



$\omega^2 |Q^F[e^x] - I[e^x]|$

The wonder-method is

$$\int_0^1 f(x) e^{i\omega x} dx \approx b_1(\omega) f(0) + b_2(\omega) f(1),$$

where

$$b_1(\omega) = \frac{1}{-i\omega} + \frac{e^{i\omega} - 1}{(-i\omega)^2},$$

$$b_2(\omega) = -\frac{e^{i\omega}}{-i\omega} - \frac{e^{i\omega} - 1}{(-i\omega)^2}.$$

But why does it work so well?

Asymptotic expansion

Let $K(x,\omega) = \mathrm{e}^{\mathrm{i}\omega g(x)}$, where g is real and smooth.
In addition, we require that $g' \neq 0$ in $[0,1]$.
Integrating by parts,

$$
\begin{aligned}
I[f] &= \frac{1}{\mathrm{i}\omega}\int_0^1 \frac{f(x)}{g'(x)}\frac{\mathrm{d}\mathrm{e}^{\mathrm{i}\omega g(x)}}{\mathrm{d}x}\mathrm{d}x \\
&= \frac{1}{\mathrm{i}\omega}\left[\mathrm{e}^{\mathrm{i}\omega g(1)}\frac{f(1)}{g'(1)} - \mathrm{e}^{\mathrm{i}\omega g(0)}\frac{f(0)}{g'(0)}\right] \\
&\quad - \frac{1}{\mathrm{i}\omega} I[\mathrm{d}(f/g')/\mathrm{d}x].
\end{aligned}
$$

We continue by induction. Let

$$
\begin{aligned}
\sigma_0(x) &= f(x), \\
\sigma_{m+1}(x) &= \frac{\mathrm{d}}{\mathrm{d}x}\frac{\sigma_m(x)}{g'(x)}, \qquad m \in \mathbb{Z}_+.
\end{aligned}
$$

Then, in the limit,

$$
\begin{aligned}
I[f] \sim \sum_{m=0}^{\infty} \frac{1}{(-\mathrm{i}\omega)^{m+1}} &\left[\frac{\sigma_m(0)}{g'(0)}\mathrm{e}^{\mathrm{i}\omega g(0)}\right. \\
&\left. - \frac{\sigma_m(1)}{g'(1)}\mathrm{e}^{\mathrm{i}\omega g(1)}\right].
\end{aligned}
$$

We have

$$\sigma_0 = f,$$
$$\sigma_1 = -\frac{g''}{g'^2} f + \frac{1}{g'} f',$$
$$\sigma_2 = \frac{3g''^2 - gg'''}{g'^4} f - 3\frac{g''}{g'^3} f' + \frac{1}{g'^2} f''$$

and so on.

Asymptotic quadrature

Let

$$Q_s^{\mathrm{A}}[f] = \sum_{m=0}^{s-1} \frac{1}{(-\mathrm{i}\omega)^{m+1}} \left[\frac{\sigma_m(0)}{g'(0)} \mathrm{e}^{\mathrm{i}\omega g(0)} - \frac{\sigma_m(1)}{g'(1)} \mathrm{e}^{\mathrm{i}\omega g(1)} \right].$$

The method uses $s-1$ derivatives of f and

$$Q_s^{\mathrm{A}}[f] - I[f] \sim \mathcal{O}\left(\omega^{-s-1}\right), \qquad \omega \to \infty.$$

For $g(x) = x$ we have

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

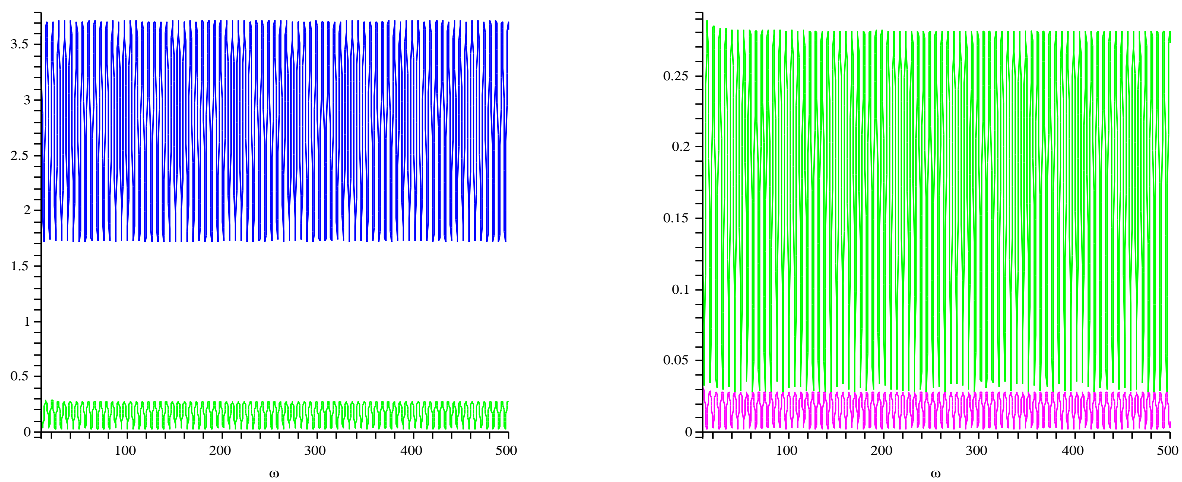
Filon-type methods

Given nodes $c_1, < \cdots < c_\nu$ and $n_1, \ldots, n_\nu \in \mathbb{N}$, we choose the unique polynomial $\tilde{\phi}$ of degree $\sum_l n_l - 1$ such that for all $l = 1, \ldots, \nu$

$$\tilde{\phi}^{(j)}(c_l) = f^{(j)}(c_l), \qquad j = 0, \ldots, n_l - 1.$$

A Filon-type method is

$$Q^{\mathsf{F}}[f] = I[\tilde{\phi}].$$



$\omega^3 |Q^{\mathsf{F}}[\mathrm{e}^x] - I[\mathrm{e}^x]|$

BLUE: Q_2^{A};

GREEN: Q^{F}, $\nu = 2$, $n_1 = n_2 = 2$, $c_1 = 0$, $c_2 = 1$;

MAGENTA: Q^{F}, $\nu = 3$, $n_1 = n_3 = 2$, $n_2 = 1$, $c_1 = 0$, $c_2 = \frac{1}{2}$, $c_3 = 1$.

THEOREM *If* $c_1 = 0$, $c_\nu = 1$ *and* $n_1 = n_\nu = s$ *then* $Q^{\mathsf{F}}[f] - I[f] \sim \mathcal{O}\left(\omega^{-s-1}\right)$ *when* $\omega \to \infty$.

Proof Since $Q^{\mathsf{F}}[f] - I[f] = I[\tilde{\phi} - f]$ and

$$\tilde{\phi}^{(j)}(0) = f^{(j)}(0), \qquad \tilde{\phi}^{(j)}(1) = f^{(j)}(1),$$

for $j = 0, 1, \ldots, s-1$, the proof follows from the asymptotic expansion of $I[\tilde{\phi} - f]$. $\square$

Thus, Filon has the same asymptotic order as the asymptotic method. Typically it has a smaller error constant, which can be further decreased, by adding extra nodes in $(0, 1)$.

All this is true as long as there are no stationary points of the oscillator in $[0, 1]$, i.e. $g' \neq 0$ in the interval.

Stationary points

Suppose first that $g'(y) = 0$, $g''(y) \neq 0$, for some $y \in [0, 1]$ and that $g' \neq 0$ elsewhere.

Naive integration by parts breaks down, since division by g' introduces a polar singularity. An alternative is the method of stationary phase (Cauchy, Stokes, Kelvin), except that, while requiring nasty contour integration, it does not deliver all the information we need. Instead, let

$$\mu_0(\omega) = \int_0^1 \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x$$

and

$$\begin{aligned} I[f] &= f(y)\mu_0(\omega) + \frac{1}{\mathrm{i}\omega} \int_0^1 \frac{f(x) - f(y)}{g'(x)} \frac{\mathrm{d}\mathrm{e}^{\mathrm{i}\omega g(x)}}{\mathrm{d}x} \mathrm{d}x \\ &= f(y)\mu_0(\omega) + \frac{1}{\mathrm{i}\omega} \left[\mathrm{e}^{\mathrm{i}\omega g(1)} \frac{f(1) - f(y)}{g'(1)} \right. \\ &\qquad \left. - \mathrm{e}^{\mathrm{i}\omega g(0)} \frac{f(0) - f(y)}{g'(0)} \right] \\ &\qquad - \frac{1}{\mathrm{i}\omega} \int_0^1 \left[\frac{\mathrm{d}}{\mathrm{d}x} \frac{f(x) - f(y)}{g'(x)} \right] \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x. \end{aligned}$$

We continue by induction. Letting

$$\sigma_0(x) = f(x),$$
$$\sigma_{m+1}(x) = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\sigma_m(x) - \sigma_m(y)}{g'(x)}, \qquad m \in \mathbb{N},$$

we have

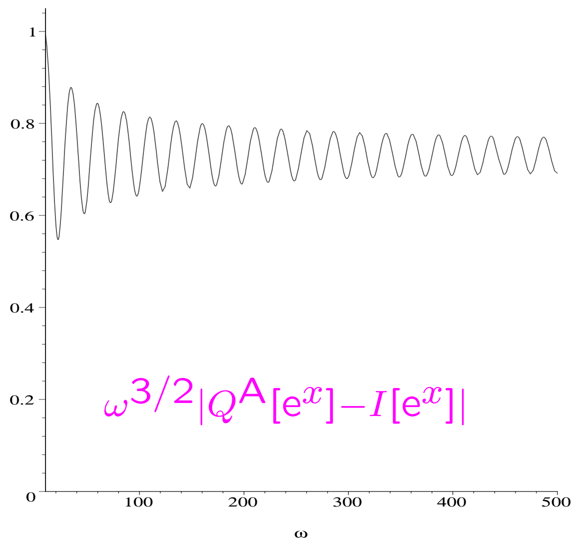
$$I[f] \sim \mu_0(\omega) \sum_{m=0}^{\infty} \frac{\sigma_m(y)}{(-\mathrm{i}\omega)^m}$$
$$+ \sum_{m=0}^{\infty} \frac{1}{(-\mathrm{i}\omega)^{m+1}} \left[\mathrm{e}^{\mathrm{i}\omega g(0)} \frac{\sigma_m(0) - \sigma_m(y)}{g'(0)} - \mathrm{e}^{\mathrm{i}\omega g(1)} \frac{\sigma_m(1) - \sigma_m(y)}{g'(1)} \right].$$

The van der Corput lemma $\Rightarrow$ $\mu_0(\omega) = \mathcal{O}\left(\omega^{-1/2}\right)$. Therefore, using the first s derivatives at 0, y and 1 gives an asymptotic method with an asymptotic error of $\mathcal{O}\left(\omega^{-s-\frac{3}{2}}\right)$.

Easy generalisation to several stationary points and to $g'(y) = \cdots = g^{(r)}(y) = 0$, $g^{(r+1)}(y) \neq 0$, $r \geq 1$.

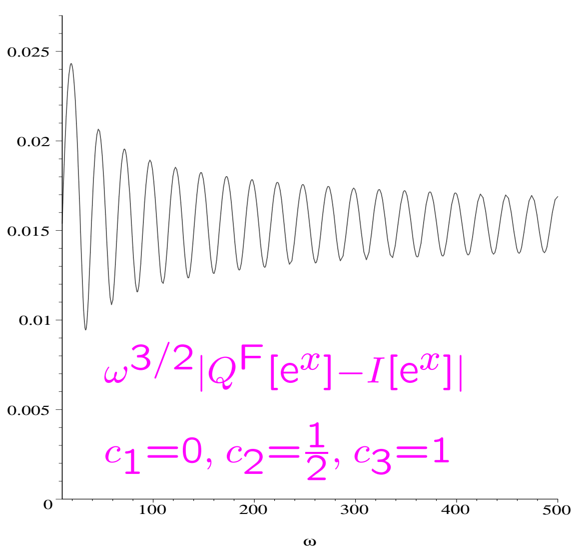
Filon again…

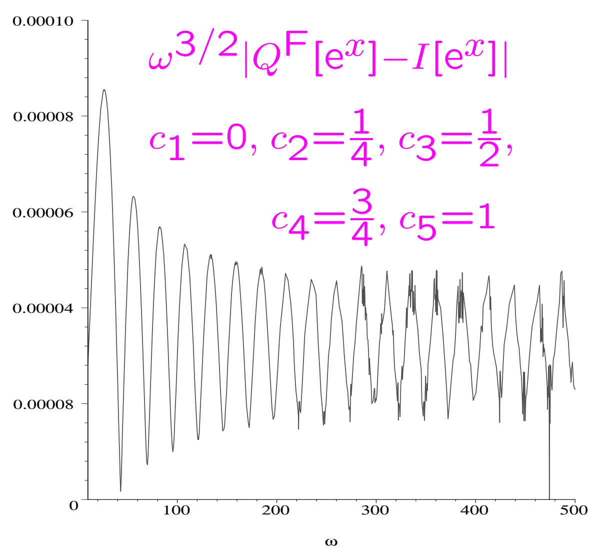
The Filon method can be generalised to cater for stationary points. Again, the idea is to interpolate to f and its derivatives at $\{0, y_1, y_2, \ldots, y_n, 1\}$, where $y_1, \ldots, y_n$ are the stationary points.



$g(x) = x(1-x)$

$y=\frac{1}{2}, \quad s=0$





‘Exotic’ oscillators

Most results can be extended to more ‘exotic’ oscillators, for example

$$\mathrm{J}_\nu(\omega x) \qquad \text{and} \qquad \mathrm{Ai}(-\omega x)$$

but, clearly, much remains to be done.

Computation of special functions

In the stage of tentative ideas: using Filon quadrature for fast computation of special functions (e.g. hypergeometric and Bessel functions) for large arguments, (hopefully) more precise than using standard asymptotic formulæ.

Singular integrals (Hermann Brunner, AI & SPN)

Similar techniques have been applied to the kernels

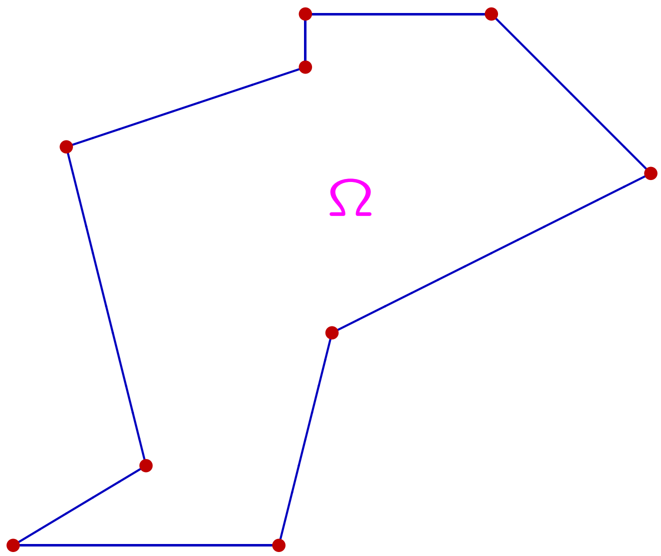
$$\frac{\mathrm{e}^{\mathrm{i}\omega|x-y|}}{|x-y|^\alpha} \qquad \text{and} \qquad \mathrm{e}^{\mathrm{i}\omega|x-y|}\log|x-y|,$$

where $\alpha < 1$ and $y \in [0,1]$. The asymptotic expansion is more difficult, mainly since σ_m need not be smooth at y, but an important observation is that singularities play similar role to stationary points.

Multivariate integrals

This is perhaps the most fascinating chapter of our work!

RESULT 1 Let $\Omega \subset \mathbb{R}^d$ be a compact domain with piecewise-linear boundary,



Then, as long as $\nabla g(\boldsymbol{x}) \neq \mathbf{0}$ in $\mathrm{cl}\,\Omega$,

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

where each functional $a_{m,k}$, a periodic function in ω, depends just on f and its first m derivatives at the kth vertex.

Consequently, we again have two options, both resulting in an $\mathcal{O}\left(\omega^{-s-d}\right)$ quadrature: either truncate the asymptotic expansion at $m = s$ or replace f by Hermite interpolation to the function and its first s directional derivatives at the vertices.

RESULT 2 Let $\Omega \subset \mathbb{R}^d$ be a compact domain with piecewise-smooth boundary and without cusps. Suppose again that there are no critical points in $\operatorname{cl}\Omega$, i.e. that $\nabla g \neq \mathbf{0}$ there. Then

$$\int_\Omega f(\boldsymbol{x})\mathrm{e}^{\mathrm{i}\omega g(\boldsymbol{x})}\mathrm{d}V = \frac{1}{\mathrm{i}\omega}\int_{\partial\Omega}\frac{f(\boldsymbol{x})}{\|\nabla g(\boldsymbol{x})\|^2}\boldsymbol{n}(\boldsymbol{x})^\top\nabla g(\boldsymbol{x})\mathrm{e}^{\mathrm{i}\omega g(\boldsymbol{x})}\mathrm{d}S - \frac{1}{\mathrm{i}\omega}\int_\Omega \nabla^\top\frac{f(\boldsymbol{x})}{\|\nabla g(\boldsymbol{x})\|^2}\nabla g(\boldsymbol{x})\mathrm{e}^{\mathrm{i}\omega g(\boldsymbol{x})}\mathrm{d}V,$$

where $\boldsymbol{n}$ is the outward unit normal.

This can be converted into an asymptotic expansion, a Stokes-type theorem, “pushing” the integral from Ω to the boundary. All this can be extended to cater for nondegenerate critical points $\boldsymbol{x}_0 \in \Omega$, where $\nabla g(\boldsymbol{x}_0) = \mathbf{0}$, $\det \nabla\nabla^\top g(\boldsymbol{x}_0) \neq 0$.

Part II:
Fredholm equations of the 2nd kind

(Hermann Brunner, AI & SPN)

Consider the problem

$$\mathcal{K}[\phi](y) = \lambda\phi(y) - g(y), \qquad y \in [0,1],$$

where g is given,

$$\mathcal{K}[\phi](y) = \int_0^1 \phi(x)\mathrm{e}^{\mathrm{i}\omega|x-y|}\mathrm{d}x$$

and $\lambda \notin \sigma(\mathcal{K})$.

A naive approach Cover $[0,1]$ with the grid

$$0 = y_0 < y_1 < \cdots < y_{N-1} < y_N = 1.$$

Let $\phi_k \approx \phi(y_k)$ and replace integrals with Filon. We obtain a linear system of the form

$$\sum_{l=0}^{N} b_{k,l}(\omega)\phi_l = \lambda\phi_k - g_k, \quad k = 0, 1, \ldots, N.$$

This will not work, since the solution ϕ also oscillates with frequency ω, and this means that our asymptotics break down.

An alternative We seek complex numbers λ_m and complex-valued functions ϕ_m s.t.

$$\mathcal{K}[\phi_m] = \lambda_m \phi_m.$$

Since

$$\mathcal{K}[\phi](y) = \int_0^y \phi(x) \mathrm{e}^{\mathrm{i}\omega(y-x)} \mathrm{d}x + \int_y^1 \phi(x) \mathrm{e}^{\mathrm{i}\omega(x-y)} \mathrm{d}x,$$

we have

$$\begin{aligned}\frac{\mathrm{d}\mathcal{K}[\phi](y)}{\mathrm{d}y} &= \mathrm{i}\omega \left[\int_0^y \phi(x) \mathrm{e}^{\mathrm{i}\omega(y-x)} \mathrm{d}x \right. \\ &\qquad \left. - \int_y^1 \phi(x) \mathrm{e}^{\mathrm{i}\omega(x-y)} \mathrm{d}x \right], \\ \frac{\mathrm{d}^2\mathcal{K}[\phi](y)}{\mathrm{d}y^2} &= (\mathrm{i}\omega)^2 \mathcal{K}[\phi](y) + 2\mathrm{i}\omega\phi(y).\end{aligned}$$

But

$$\frac{\mathrm{d}\mathcal{K}[\phi](y)}{\mathrm{d}y} = \lambda\phi'(y), \qquad \frac{\mathrm{d}^2\mathcal{K}[\phi](y)}{\mathrm{d}y^2} = \lambda\phi''(y).$$

Therefore

$$\lambda\phi'' = (\mathrm{i}\omega)^2\lambda\phi + 2\mathrm{i}\omega\phi.$$

Let

$$\theta(\omega) = \sqrt{\omega^2 - \frac{2\mathrm{i}\omega}{\lambda}},$$

then

$$\phi'' + \theta^2\phi = 0.$$

Moreover,

$$\lambda\phi'(0) = \frac{\mathrm{d}\mathcal{K}[\phi](0)}{\mathrm{d}y} = -\mathrm{i}\omega\lambda\phi(0),$$
$$\lambda\phi'(1) = \frac{\mathrm{d}\mathcal{K}[\phi](1)}{\mathrm{d}y} = \mathrm{i}\omega\lambda\phi(1).$$

The condition at $y = 0$ results (up to normalization) in

$$\phi(x) = (\theta - \omega)\mathrm{e}^{\mathrm{i}\theta x} + (\theta + \omega)\mathrm{e}^{-\mathrm{i}\theta x}.$$

Note however that θ depends on the unknown eigenvalue λ.

Using the boundary condition at $y = 1$ we obtain

$$(\theta - \omega)^2 \mathrm{e}^{\mathrm{i}\theta} = (\theta + \omega)^2 \mathrm{e}^{-\mathrm{i}\theta}.$$

Therefore

$$(\theta - \omega)\mathrm{e}^{\frac{1}{2}\mathrm{i}\theta} = \pm(\theta + \omega)\mathrm{e}^{-\frac{1}{2}\mathrm{i}\theta},$$

Taking the plus sign we obtain the transcendental equation

$$\mathrm{i}\theta \tan\frac{\theta}{2} = \omega,$$

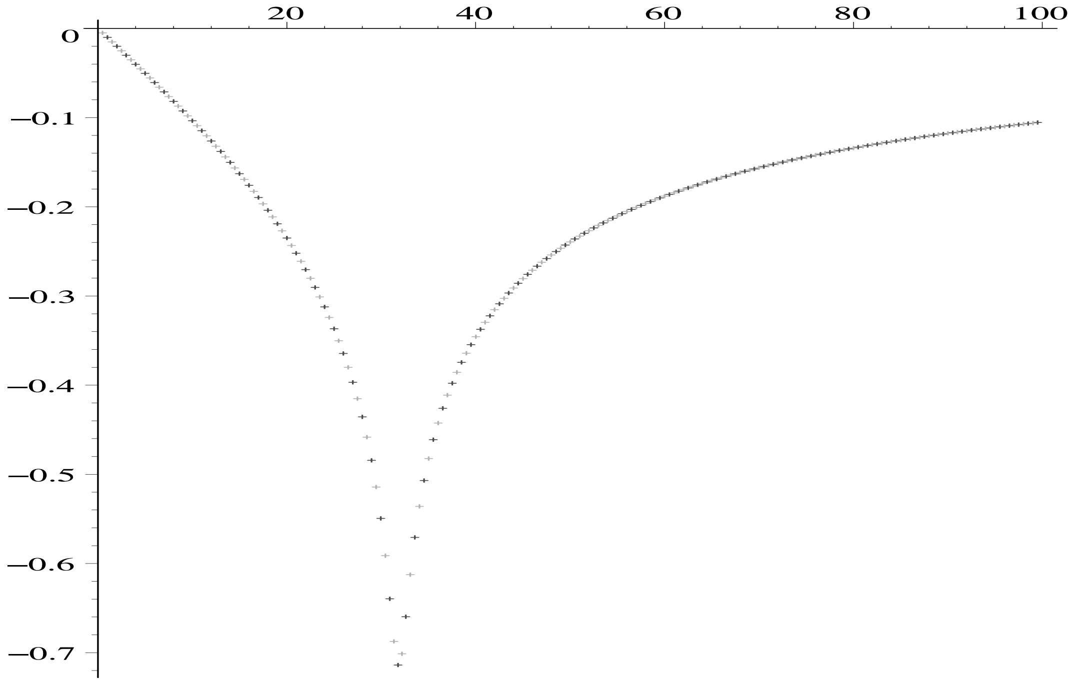
while the minus sign yields

$$\mathrm{i}\theta \cot\frac{\theta}{2} = \omega.$$

The solutions of these equations interlace: the first has a solution for $\mathrm{Re}\,\theta \in (2m\pi, (2m+1)\pi)$ and the second in $\mathrm{Re}\,\theta \in ((2m+1)\pi, (2m+2)\pi)$. We observe that

The real part of θ behaves like $\mathcal{O}(m)$,

The imaginary part of θ is $\mathcal{O}(1)$ and small.



The values of $\theta_m/(2\pi)$ in the complex plane for $1 \le m \le 200$.

How is this going to help?

Let (with greater generality)

$$\mathcal{K}[f](y) = \int_0^1 f(x)K(x,y)\mathrm{d}x, \qquad y \in [0,1].$$

Then the Hilbert–Schmidt theory tells us that $\mathcal{K}$ has a countable number of distinct eigenvalues and eigenfunctions $\{\lambda_m, \phi_m\}$. Let

$$\langle f, g \rangle = \int_0^1 f(x)g(x)\mathrm{d}x$$

be the standard real L_2 inner product.

For $m \neq n$

$$\lambda_m \phi_m(y) = \int_0^1 \phi_m(y) K(x,y) \mathrm{d}x$$

$$\Rightarrow \lambda_m \langle \phi_m, \phi_n \rangle = \int_0^1 \int_0^1 \phi_m(x) \phi_n(x) K(x,y) \mathrm{d}x \mathrm{d}y.$$

By symmetry, also

$$\lambda_n \langle \phi_m, \phi_n \rangle = \int_0^1 \int_0^1 \phi_m(x) \phi_n(x) K(x,y) \mathrm{d}x \mathrm{d}y$$

and we just deduce L_2 orthogonality of the eigenfunctions,

$$\langle \phi_m, \phi_n \rangle = 0, \qquad m \neq n.$$

Note that $\langle \cdot \, , \, \cdot \rangle$ is not a positive definite inner product: it is complex-valued and it is entirely possible that

$$\langle f, f \rangle = 0, \qquad f \neq 0.$$

However, $\langle \phi_m, \phi_m \rangle \neq 0$, and that's all we need.

A spectral method

We expand

$$f(y) = \sum_{m=0}^{\infty} f_m \phi_m(y).$$

Therefore,

$$f_m = \frac{g_m}{\lambda - \lambda_m}, \qquad m \geq 0,$$

where

$$g_m = \frac{\langle g, \phi_m \rangle}{\langle \phi_m, \phi_m \rangle} = \frac{\langle g, \phi_m \rangle}{2(\lambda_m^2 - 2\mathrm{i}\omega - \omega^2)}.$$

We thus need to compute $\langle g, \phi_m \rangle$ for a large number of ms. However, if

$$\theta_m = \alpha_m - \mathrm{i}\beta_m$$

then

$$\langle g, \phi_m \rangle = (\theta_m - \omega) \int_0^1 g(x) \mathrm{e}^{(\beta_m + \mathrm{i}\alpha_m)x} \mathrm{d}x + (\theta_m + \omega) \int_0^1 g(x) \mathrm{e}^{-(\beta_m + \mathrm{i}\alpha_m)x} \mathrm{d}x.$$

Recall: while $\alpha_m \approx 2\pi m$ is large, $|\beta_m|$ is small. Moreover, g is nonoscillatory. Therefore

All the integrals can be computed very fast and accurately by either the asymptotic method or a Filon-type method.

An ongoing challenge is to generalize all this to other Fredholm kernels, e.g.

$$\mathcal{K}[f](y) = \int_0^1 f(x) x^\gamma \mathrm{e}^{\mathrm{i}\omega|x-y|} \mathrm{d}x$$

for $\gamma > -1$ and

$$\mathcal{K}[f](y) = \int_0^1 f(x) \frac{\mathrm{e}^{\mathrm{i}\omega|x-y|}}{|x-y|^\gamma} \mathrm{d}x$$

for $\gamma \in (0, 1)$.

Part III:
Solving HiOsc differential equations

We commence from the linear ODE

$$\boldsymbol{y}' = A(t)\boldsymbol{y}, \quad t \geq 0, \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0.$$

Suppose that its solution oscillates fast, e.g. that all the eigenvalues of A live in $\mathrm{cl}\,\mathbb{C}_-$ and there are large eigenvalues on $\mathrm{i}\mathbb{R}$.

Standard numerical methods perform very poorly, the reason being that the principal error term of a p th-order classical method is of the form

$$h^{p+1}\mathcal{D}_{p+1}(\boldsymbol{y}(t_N)),$$

where $\mathcal{D}_{p+1}$ is a linear combination of elementary differentials of order $p+1$.

$\boldsymbol{y}(t)$ oscillates with frequency $\omega \Rightarrow$

$$\|\boldsymbol{y}^{(p+1)}(t)\| \sim \omega^{p+1}\|\boldsymbol{y}(t)\|,$$

hence $\|\mathcal{D}_{p+1}\|$ is very large!

An alternative: Change of variables

To time-step from t_N to $t_{N+1} = t_N + h$, set

$$\boldsymbol{y}(t) = \mathrm{e}^{(t-t_N)\tilde{A}} \boldsymbol{x}(t - t_N), \qquad t \geq t_N,$$

where $\tilde{A} = A(t_{N+\frac{1}{2}})$. Then

$$\boldsymbol{x}' = B(t)\boldsymbol{x}, \quad t \geq 0, \qquad \boldsymbol{x}(0) = \boldsymbol{y}_N,$$

where

$$B(t) = \mathrm{e}^{-t\tilde{A}}[A(t) - \tilde{A}]\mathrm{e}^{t\tilde{A}}.$$

Since $\mathrm{e}^{\pm t\tilde{A}}$ oscillates rapidly, so does $B(t)$.
We have already seen that high oscillation can be turned to our advantage. The main idea is to 'invert' the reason for the failure of classical methods:

Integrate, don't differentiate!

Specifically, for an s-fold integral and $\mathcal{B}(\boldsymbol{x})$ a product of s terms from $\{B(x_1), \ldots, B(x_s)\}$,

$$\left\| \int \cdots \int \mathcal{B}(\boldsymbol{x}) \mathrm{d}x_s \cdots \mathrm{d}x_1 \right\| \sim \mathcal{O}\left(\omega^{-s}\right).$$

The Magnus method Letting

$$\boldsymbol{x}(t) = \mathrm{e}^{\Omega(t)}\boldsymbol{x}_0,$$

we have

$$\begin{aligned}\Omega(t) = {} & \int_0^t B(x)\mathrm{d}x \\ & - \tfrac{1}{2}\int_0^t \int_0^{x_1} [B(x_2), B(x_1)]\mathrm{d}x_2\mathrm{d}x_1 \\ & + \tfrac{1}{4}\int_0^t \int_0^{x_1}\int_0^{x_2} [[B(x_3), B(x_2)], B(x_1)]\mathrm{d}x_3\mathrm{d}x_2\mathrm{d}x_1 \\ & + \tfrac{1}{12}\int_0^t \int_0^{x_1}\int_0^{x_1} [B(x_3), [B(x_2), B(x_1)]]\mathrm{d}x_3\mathrm{d}x_2\mathrm{d}x_1 \\ & + \cdots .\end{aligned}$$

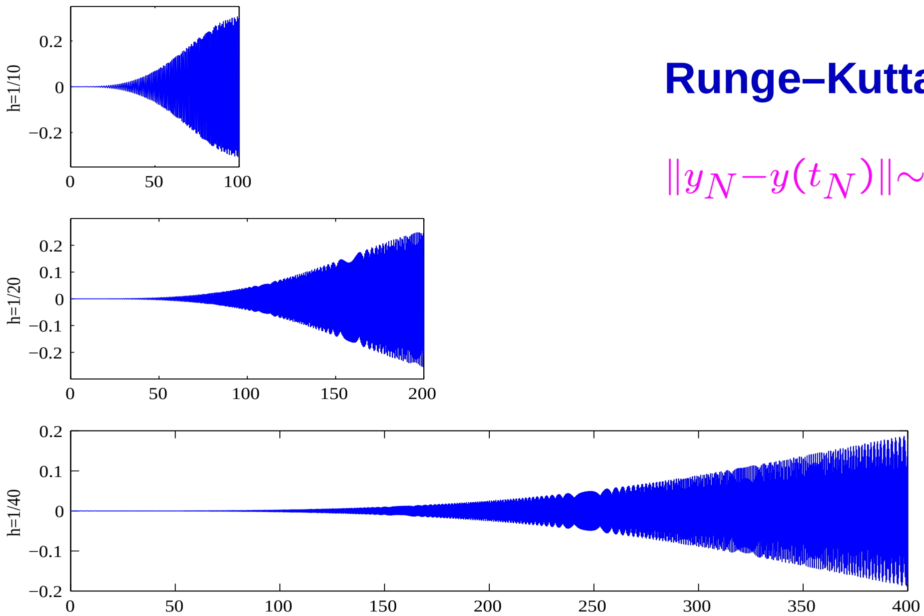
Thus, repeated integration. . . .

An advantage of Magnus: If $A(t)$ lives in a Lie algebra $\mathfrak{g}$ then $\boldsymbol{y}(t)$ evolves on a homogeneous space $\mathcal{M}$, acted upon by the corresponding Lie group $\mathcal{G}$. Using Magnus (with or without change of variables) ensures $\boldsymbol{y}_N \in \mathcal{M}$, $N \geq 0$.

An example: The Airy equation Let $y'' + ty = 0$.

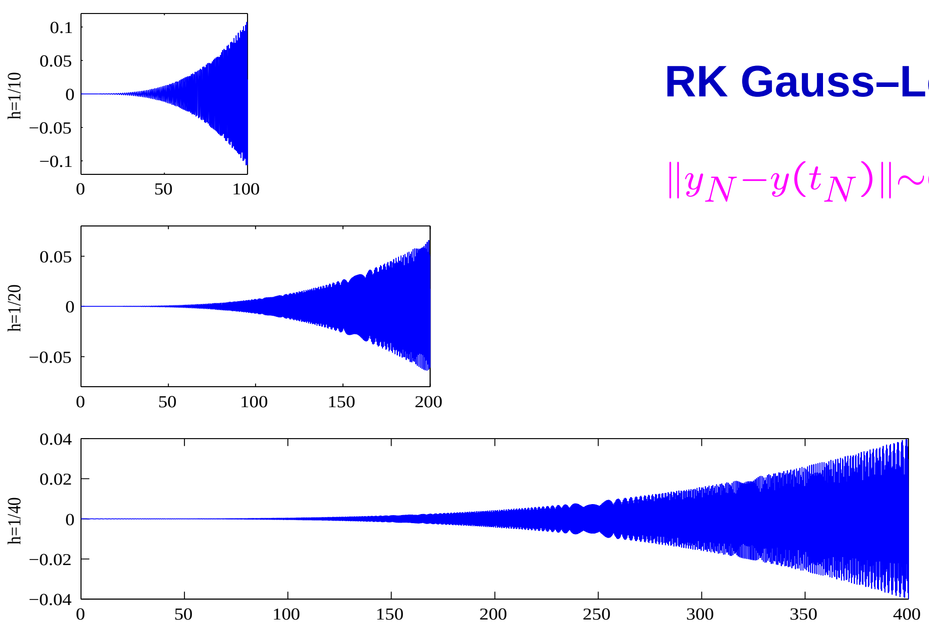
Runge–Kutta 4

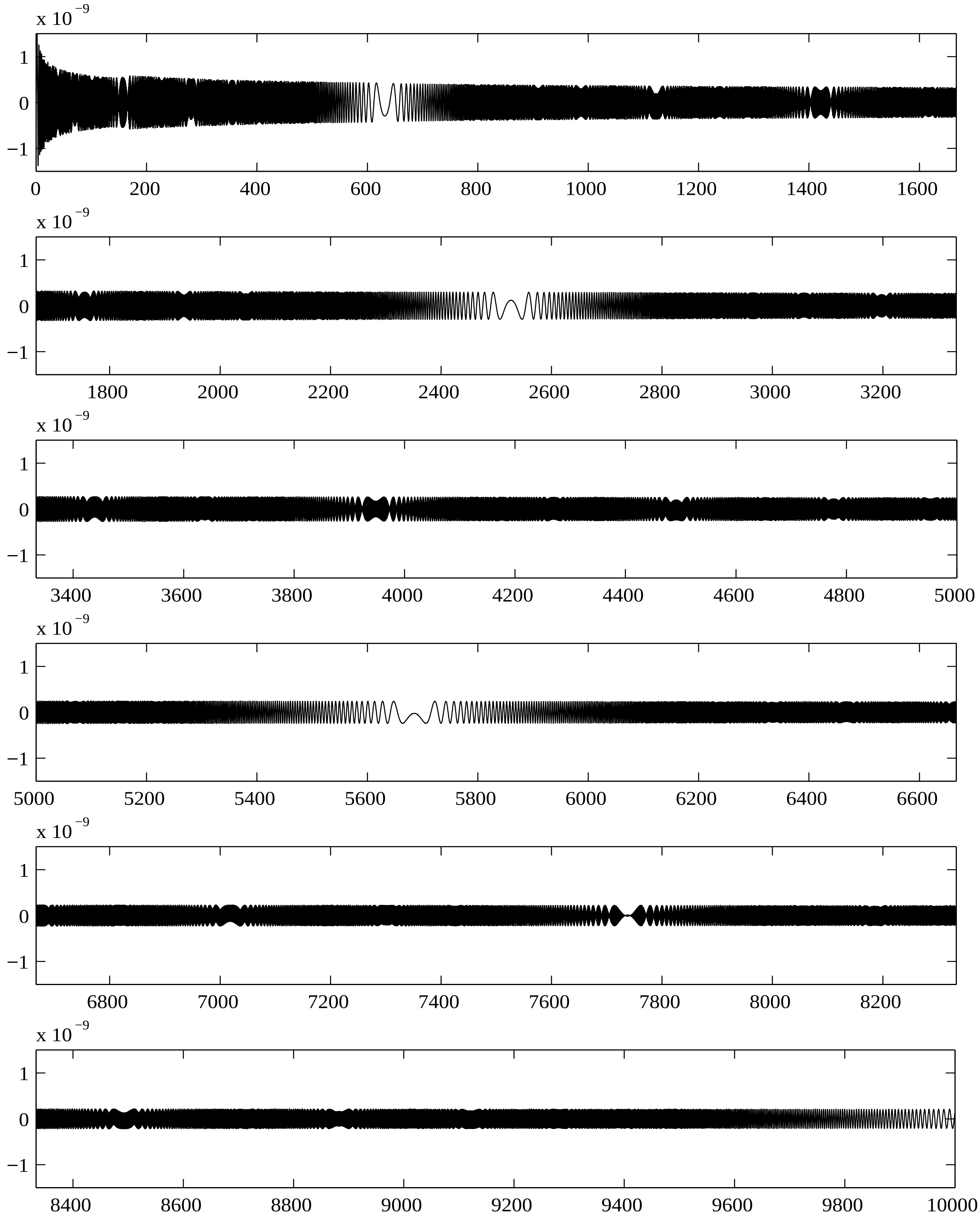
$\|y_N - y(t_N)\| \sim \mathcal{O}(h^4 t^{13/4})$



RK Gauss–Legendre 4

$\|y_N - y(t_N)\| \sim \mathcal{O}(h^4 t^{13/4})$





Modified Magnus, $h = \frac{1}{4}$, $\|y_N - y(t_N)\| \sim \mathcal{O}(h^3 t^{-1/4})$

Calculating integrals: We use Filon: all (multivariate) integrals can be calculated to high precision using just $B(0)$ and $B(h)$. As before, high oscillation helps computation!

A disadvantage of Magnus: We need to calculate two exponentials per step:

$$e^{\pm h\tilde{A}} \qquad \text{and} \qquad e^{\Omega(h)}.$$

This can be problematic when the dimension is large. However, while Ω is typically unstructured, this is not the case with $\tilde{A}$.

Suppose that the ODE originates in a semidiscretized PDE. Then often $\tilde{A}$ is block Toeplitz and $e^{\pm\tilde{A}}$ can be calculated very fast by FFT. The challenge is thus to do away with the need for the calculation of $e^{\Omega(h)}$.

The Neumann method To avoid the calculation of the second exponential, we abandon Magnus in favour of the Neumann expansion

$$\boldsymbol{x}(t) = \sum_{m=0}^{\infty} \mathcal{N}_k(t)\boldsymbol{y}_N,$$

where $\mathcal{N}_0(t) \equiv I$ and

$$\mathcal{N}_m(t) = \int_0^t \int_0^{x_1} \cdots \int_0^{x_{m-1}} B(x_1)\cdots B(x_m)\mathrm{d}x_m \cdots \mathrm{d}x_1.$$

Because of high oscillation, $\|\mathcal{N}_m(h)\| \sim \mathcal{O}((h/\omega)^m)$, hence very rapid convergence.

Multivariate integrals can be computed in a very small number of function evaluations, similarly to Magnus integrals. Again, high oscillation of B means that Filon methods are very precise.

Numerical results for Airy are virtually identical to Magnus, but the method comes into its own for HiOsc PDEs, e.g. the Schrödinger equation.

Nonlinear equations Suppose that

$$\boldsymbol{y}' = A(t)\boldsymbol{y} + \boldsymbol{g}(\boldsymbol{y})$$

is highly oscillatory. Transforming as before, but letting $\tilde{A} = A(t_N)$, we have

$$\boldsymbol{x}' = B(t)\boldsymbol{x} + \mathrm{e}^{-t\tilde{A}}\boldsymbol{g}(t_N + t, \mathrm{e}^{t\tilde{A}}\boldsymbol{x}).$$

Let

$$\Phi' = B(t)\Phi, \quad t \geq 0, \qquad \Phi(0) = I.$$

Note that we can evaluate Φ by either Magnus or Neumann. Then

$$\begin{aligned}\boldsymbol{x}(t) &= \Phi(t)\boldsymbol{y}_N \\ &\quad + \int_0^t \Phi(t-\xi)\mathrm{e}^{\xi\tilde{A}}\boldsymbol{g}(t_N + \xi, \mathrm{e}^{\xi\tilde{A}}\boldsymbol{x}(\xi))\mathrm{d}\xi.\end{aligned}$$

This motivates the waveform relaxation approach,

$$\begin{aligned}\boldsymbol{x}^{[0]}(t) &\equiv \boldsymbol{y}_N, \\ \boldsymbol{x}^{[m+1]}(t) &= \Phi(t)\boldsymbol{y}_N \\ &\quad + \int_0^t \Phi(t-\xi)\mathrm{e}^{\xi\tilde{A}}\boldsymbol{g}(t_N + \xi, \mathrm{e}^{\xi\tilde{A}}\boldsymbol{x}^{[m]}(\xi))\mathrm{d}\xi.\end{aligned}$$

Next steps...

- Filon without derivatives: Work in progress. Letting nodes depend on ω, it is possible to obtain arbitrary degree of error attenuation without using derivatives;

- Exotic oscillators: For starters, how to compute $\int_0^1 f(x)\sin(\omega \sin \pi x)\mathrm{d}x$?

- Multivariate HiOsc integrals: What are the implications of the Stokes-type theorem?

- Volterra HiOsc equations: The current approach doesn't scale up e.g. to singular kernels;

- HiOsc PDEs: Much further work required for specific PDEs, e.g. Schrödinger and Hamilton–Jacobi;

- Stochastic DEs: Perhaps...