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Modified Fourier expansions and spectral problems for highly oscillatory Fredholm operators

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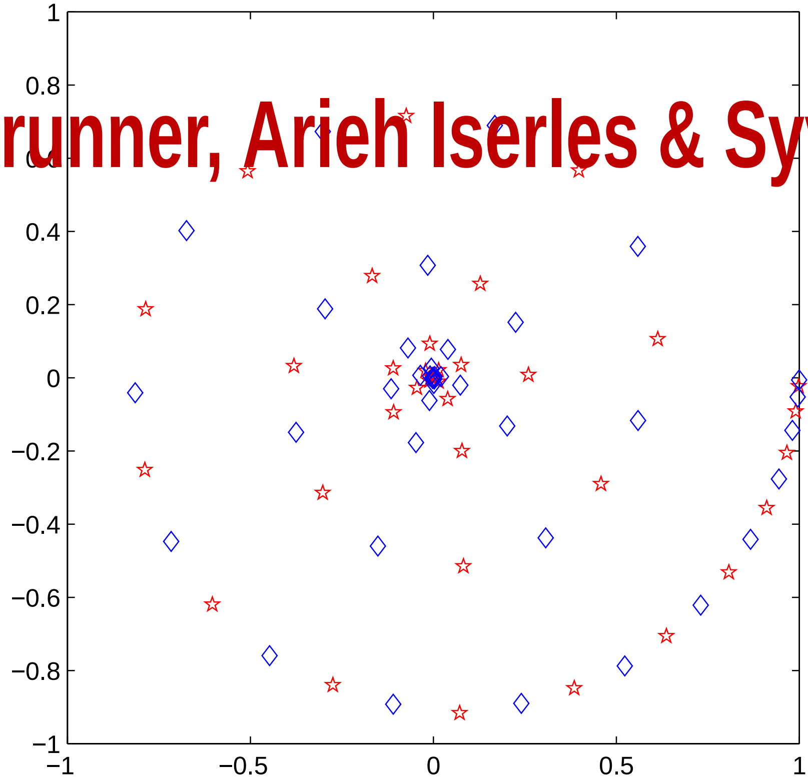

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THE FINITE SECTION METHOD

Fredholm spectral problems

Given $g \in \mathrm{C}[-1,1]$ and $\omega > 0$, we seek the solution of the *Fredholm spectral problem*

$$\int_{-1}^{1} f(x)\mathrm{e}^{\mathrm{i}\omega g(x-y)}\mathrm{d}x = \lambda f(y), \qquad y \in [-1,1].$$

- The Fredholm operator is compact, hence it has solely eigenvalues (i.e., point spectrum), which accumulate at the origin.
- The operator is symmetric, but not self adjoint (it is complex-valued!).
- $\omega > 0$ might be large, in which case the kernel is highly oscillatory. This isn't essential to our argument! High oscillation will arise in our analysis regardless of the size of ω.

The finite section method I: The naive approach

Approximate the integral by quadrature. This leads to the algebraic eigenvalue problem

$$\sum_{k=-N}^{N} b_k f_k \mathrm{e}^{\mathrm{i}\omega g(c_k - c_m)} = \lambda f_m, \qquad -N \le m \le N,$$

where c_k and b_k are the nodes and the weights respectively, while $f_k \approx f(c_k)$.

SHORTCOMINGS:

1. The k, m element of the matrix is of size $|b_k| = \mathcal{O}\left(N^{-1}\right)$, hence decays very slowly with N. Therefore, we require very large matrix!

2. If $\omega \gg 0$ then the elements of the matrix exhibit high oscillation, unless N is really huge! This further increases the size of the matrix.

3. For practical purposes, when N is really large, we are compelled to take equally-spaced points: $c_k = \frac{k}{N}$ and $b_k \equiv \frac{2}{2N+1}$. No benefits of “clever” quadrature!

The finite section method II: Orthogonal basis

Let $\mathcal{B} = \{\varphi_1, \varphi_2, \ldots\}$ be an orthonormal basis of $\mathrm{L}_2[-1,1]$. We seek to represent the eigenfunction f within this basis,

$$f(x) = \sum_{k=1}^{\infty} f_k \varphi_k(x).$$

Substituting into the Fredholm equation, multiplying by φ_m, integrating and exploiting orthogonality, we obtain an infinite-dimensional algebraic eigenvalue problem

$$\sum_{k=1}^{\infty} A_{m,k} f_k = \lambda f_m, \qquad m \in \mathbb{N},$$

where

$$A_{m,k} = \int_{-1}^{1} \int_{-1}^{1} \varphi_k(x) \varphi_m(y) \mathrm{e}^{\mathrm{i}\omega g(x-y)} \mathrm{d}x \mathrm{d}y.$$

The main idea is to truncate the matrix A (hence "finite section"), under the assumption that the eigenvalues of the finite section are near the true eigenvalues – this assumption is justified by compactness.

THE MATRIX A

The asymptotics of A

How large are the elements of the matrix A? Or, more to the point, *how to choose the basis $\mathcal{B}$ so that the elements of A are most suitable to the task at hand?*

We partition A into four sub-matrices,

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix},$$

where $A_{1,1}$ is $r \times r$, hence $A_{1,2}$ is $r \times \mathbb{N}$, $A_{2,1}$ is $\mathbb{N} \times r$ and $A_{2,2}$ is $\mathbb{N} \times \mathbb{N}$.

Note that we have two highly oscillatory processes to reckon with: Firstly, if ω is large, the kernel of the integral operator oscillates. Secondly, being orthogonal functions, in natural ordering each φ_m has $m-1$ zeros in $(-1,1)$, hence $\mathcal{B}$ consists of highly oscillatory functions.

The asymptotics of $A_{1,1}$

We henceforth assume that $g'(0)=0$, $g''(0)\neq 0$ and that $g'\neq 0$ elsewhere in $[-1,1]$.

This isn't essential but makes life easier – incidentally, assuming that g is strictly monotone would have made matters too trivial and specialised.

Our setting means that $\nabla g \equiv 0$ along the line $x=y$: a *line* of stationary points. On the other hand, we don't need to worry about resonance points.

After easy manipulation, we have

$$\int_{-1}^{1}\int_{-1}^{1} f(x,y)\mathrm{e}^{\mathrm{i}\omega g(x-y)}\mathrm{d}x = \int_{-2}^{0} h^{[-]}(t)\mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t + \int_{0}^{2} h^{[+]}(t)\mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t,$$

where

$$h^{[-]}(t) = \int_{-1-t}^{1} f(t+y,y)\mathrm{d}y, \qquad h^{[+]}(t) = \int_{-1}^{1-t} f(t+y,y)\mathrm{d}y.$$

We expand the two univariate highly oscillatory integrals using the standard asymptotic expansion (AI & Nørsett):

$$\int_0^2 h^{[+]}(t)\mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t \sim -\sum_{m=0}^{\infty}\frac{1}{(-\mathrm{i}\omega)^{m+1}}\left[\frac{h_m^{[+]}(2)-h_m^{[+]}(0)}{g'(2)}\mathrm{e}^{\mathrm{i}\omega g(2)} - \frac{h_m^{[+]\prime}(0)}{g''(0)}\mathrm{e}^{\mathrm{i}\omega g(0)}\right] + \int_0^2 \mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t \sum_{m=0}^{\infty}\frac{h_m^{[+]}(0)}{(-\mathrm{i}\omega)^m},$$

$$\int_{-2}^0 h^{[-]}(t)\mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t \sim \sum_{m=0}^{\infty}\frac{1}{(-\mathrm{i}\omega)^{m+1}}\left[\frac{h_m^{[-]}(-2)-h_m^{[-]}(0)}{g'(-2)}\mathrm{e}^{\mathrm{i}\omega g(-2)} - \frac{h_m^{[-]\prime}(0)}{g''(0)}\mathrm{e}^{\mathrm{i}\omega g(0)}\right] + \int_{-2}^0 \mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t \sum_{m=0}^{\infty}\frac{h_m^{[-]}(0)}{(-\mathrm{i}\omega)^m}.$$

Here

$$h_0^{[\pm]}(t) = h^{[\pm]}(t), \qquad h_{m+1}^{[\pm]}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\frac{h_m^{[\pm]}(t)-h_m^{[\pm]}(0)}{g'(t)}, \quad m \in \mathbb{N}.$$

Thus, letting $f(x,y) = \varphi_k(x)\varphi_m(y)$ and observing that

$$\int_{-2}^{0} \mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t, \int_{0}^{2} \mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t = \mathcal{O}\left(\omega^{-\frac{1}{2}}\right),$$

we deduce, using orthogonality, that

$$A_{k,k} \sim \int_{-2}^{2} \mathrm{e}^{\mathrm{i}\omega g(t)}\mathrm{d}t \sim \mathcal{O}\left(\omega^{-\frac{1}{2}}\right),$$

$$A_{k,m} \sim \frac{1}{\mathrm{i}\omega}\frac{\varphi_k(-1)\varphi_m(-1) + \varphi_k(1)\varphi_m(1)}{g''(0)}\mathrm{e}^{\mathrm{i}\omega g(0)} \sim \mathcal{O}\left(\omega^{-1}\right), \qquad k \neq m.$$

Note that if $\varphi_k(-1)\varphi_m(-1) + \varphi_k(1)\varphi_m(1) = 0$ then $A_{k,m} \sim \mathcal{O}\left(\omega^{-2}\right)$ for $k \neq m$. For reasons that will be clear soon, we don't pursue this route.

The important fact to remember is that, as ω grows, the entries of $A_{1,1}$ decay gently along the diagonal, more rapidly away from the diagonal.

The asymptotics of $A_{2,2}$

Suppose now that $k, m \gg \omega^{\frac{1}{2}}$. We assume in the sequel that the φ_ks can be expressed as linear combinations of exponentials. This will cover all the cases of interest. Let

$$\rho(x) = \mathrm{e}^{\mathrm{i}\omega g(x)}, \qquad e(a,b,\omega) = \int_{-1}^{1}\int_{-1}^{1} \mathrm{e}^{\mathrm{i}(ax+by)}\rho(x-y)\mathrm{d}x\mathrm{d}y.$$

We expand asymptotically *a la* (Al & Nørsett):

$$e(a,b,\omega) \sim \sum_{j=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^n}{(-\mathrm{i}a)^{j+1}(-\mathrm{i}b)^{n+1}}[2\cos(a+b)\rho^{(m+n)}(0) - \mathrm{e}^{\mathrm{i}(a+b)}\rho^{(m+n)}(2) - \mathrm{e}^{-\mathrm{i}(a+b)}\rho^{(m+n)}(-2)].$$

MODIFIED FOURIER EXPANSIONS

Fourier and modified Fourier bases

Given two strictly monotone sequences $\{a_n\}_{n\in\mathbb{Z}_+}$ and $\{b_n\}_{n\in\mathbb{Z}_+}$, we let

$$c_{m,n} = \int_{-1}^{1}\int_{-1}^{1} \cos a_m x \cos a_n y \mathrm{e}^{\mathrm{i}\omega g(x-y)} \mathrm{d}x \mathrm{d}y,$$
$$p_{m,n} = \int_{-1}^{1}\int_{-1}^{1} \cos a_m x \sin b_n y \mathrm{e}^{\mathrm{i}\omega g(x-y)} \mathrm{d}x \mathrm{d}y,$$
$$q_{m,n} = \int_{-1}^{1}\int_{-1}^{1} \sin b_m x \cos a_n y \mathrm{e}^{\mathrm{i}\omega g(x-y)} \mathrm{d}x \mathrm{d}y,$$
$$s_{m,n} = \int_{-1}^{1}\int_{-1}^{1} \sin b_m x \sin b_n y \mathrm{e}^{\mathrm{i}\omega g(x-y)} \mathrm{d}x \mathrm{d}y.$$

Note that $a_n = b_n = \pi n$ corresponds to the Fourier basis, while $a_n = \pi n$, $b_n = \pi(n - \frac{1}{2})$ to modified Fourier basis.

We exploit the asymptotic expansion of the $e(a, b, \omega)$s to construct expansions for the the above coefficients. We will do so explicitly just for $c_{m,n}$.

We have

$$
\begin{aligned}
c_{m,n} \sim & \sin a_m \sin a_n \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l}}{a_m^{2k+1} a_n^{2l+1}} [\rho^{(2k+2l)}(2) + \rho^{(2k+2l)}(-2) \\
& + 2\rho^{(2k+2l)}(0)] \\
& + \sin a_m \cos a_n \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l}}{a_m^{2k+1} a_n^{2l+2}} [\rho^{(2k+2l+1)}(2) - \rho^{(2k+2l+1)}(-2)] \\
& + \cos a_m \sin a_n \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l}}{a_m^{2k+2} a_n^{2l+1}} [\rho^{(2k+2l+1)}(2) - \rho^{(2k+2l+1)}(-2)] \\
& + \cos a_m \cos a_n \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l}}{a_m^{2k+2} a_n^{2l+2}} [\rho^{(2k+2l+2)}(2) \\
& + \rho^{(2k+2l+2)}(-2) - 2\rho^{(2k+2l+2)}(0)].
\end{aligned}
$$

Thus, the best choice is $a_n = \pi n$, which kills all but the fourth double sum and results in

$$c_{m,n} \sim \mathcal{O}\left(m^{-2} n^{-2}\right).$$

Once we also wish for the remaining coefficients to be $\mathcal{O}\left(m^{-2}n^{-2}\right)$, we need also $b_m = \pi(m - \frac{1}{2})$. Thus,

Modified Fourier basis is optimal!

The asymptotics of $A_{1,2}$ and $A_{2,1}$

Now one of the φ_ms dominates. Again, for Fourier basis we obtain $\mathcal{O}\left(m^{-1}\right)$ decay, but for modified Fourier it becomes $\mathcal{O}\left(m^{-2}\right)$.

Even oscillator g

If the function g is even then modified Fourier expansions have another advantage: the eigenfunctions are either even or odd functions, $p_{m,n}, q_{m,n} \equiv 0$ and the matrix A partitions (in a checkerboard manner) into two matrices: $\{c_{m,n}\}$ for the even eigenfunctions and $\{s_{m,n}\}$ for the odd ones.

The hyperbolic cross

We conclude that

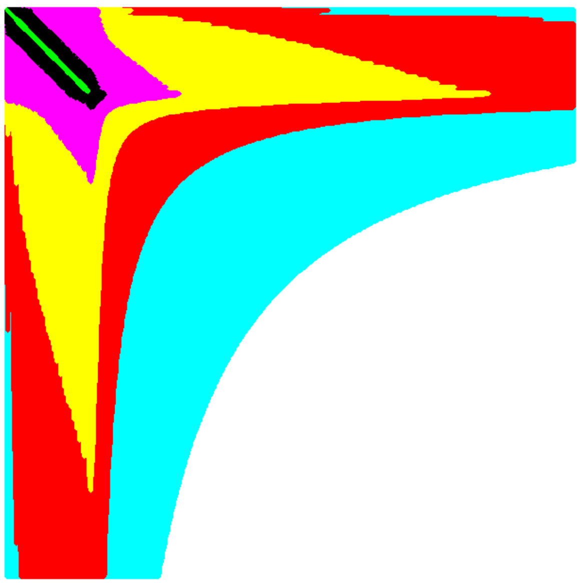
- The elements of $A_{1,1}$ decay like $\mathcal{O}\left(\omega^{-\frac{1}{2}}\right)$ along the diagonal, $\mathcal{O}\left(\omega^{-1}\right)$ elsewhere;
- The elements of $A_{1,2}$ decay like $\mathcal{O}\left(m^{-2}\right)$;
- The elements of $A_{2,1}$ decay like $\mathcal{O}\left(k^{-2}\right)$;
- The elements of $A_{2,2}$ decay like $\mathcal{O}\left(k^{-2}m^{-2}\right)$.

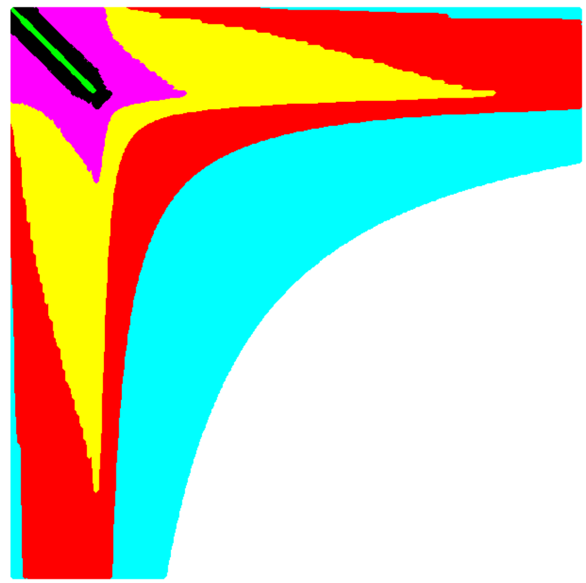
Thus, provided that r (the size of $A_{1,1}$) is large enough (roughly, $r \sim \omega$), the elements of $A_{2,2}$ are much smaller then the remaining elements of the matrix. This has important implications.

The Fox–Li equation

$$\sqrt{\frac{-\mathrm{i}\omega}{\pi}}\int_{-1}^{1} f(x)\mathrm{e}^{\mathrm{i}\omega(x-y)^2}\mathrm{d}x = \lambda f(y)$$

with $\omega = 100$.





The hyperbolic cross: The size of cosine and sine elements in 800×800 matrices.

[cyan] $\rightsquigarrow > 10^{-6}$, [red] $\rightsquigarrow > 10^{-5}$, [yellow] $\rightsquigarrow > 10^{-4}$, [magenta] $\rightsquigarrow > 10^{-3}$, [black] $\rightsquigarrow > 10^{-2}$, [green] $\rightsquigarrow > 10^{-1}$.

Exploiting the hyperbolic cross

The phenomenon of hyperbolic cross – coefficients being substantially larger near the axes – has been noticed a long time ago by Babenko and it has many uses in computation. In our case it can be exploited by setting the matrix $A_{2,2}$ to zero. This yields a new matrix,

$$\tilde{A} = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & O \end{bmatrix}.$$

LEMMA *The matrix $\tilde{A}$ is of rank $\leq 2r$.*

In other words, once we replace A by $\tilde{A}$ (our only discretization step so far!) we obtain a new matrix which, although infinite, may have at most $2r$ nonzero eigenvalues!

Recall that the eigenvalues of A accumulate at the origin. Our approach essentially sets all but the $2r$ largest eigenvalues to zero. Since the $(2r+1)$st eigenvalue is minute, we incur *very* small error.

Computing the spectrum of $\tilde{A}$

Let $G = A_{1,2}A_{2,1}$. Note that G is $r \times r$: its computation requires the truncation of infinite sums (which can be performed adaptively) – this is the second discretization step!

THEOREM *Let $G = G_1 G_2$, where both G_1 and G_2 are $r \times r$. Assume further that $\operatorname{rank} G_1 = r$ and $\operatorname{rank} G_2 = \operatorname{rank} G$. Finding the nonzero eigenvalues of $\tilde{A}$ is equivalent to finding the eigenvalues of the $(2r) \times (2r)$ matrix*

$$B = \begin{bmatrix} A_{1,1} & G_1 \\ G_2 & O \end{bmatrix}.$$

The proof is easy. Obvious choice is $G_1 = I$, $G_2 = G$. Alternatively, $G_1 = Q$, $G_2 = R$, where QR is the QR factorization of G.

To conclude...

To find the spectrum of a Fredholm operator, we need the following steps:

1. Choose sufficiently large N and $r \ll N$. Compute $A_{k,m}$ for $1 \leq k, m \leq N$ and $\max\{m, n\} \leq r$.

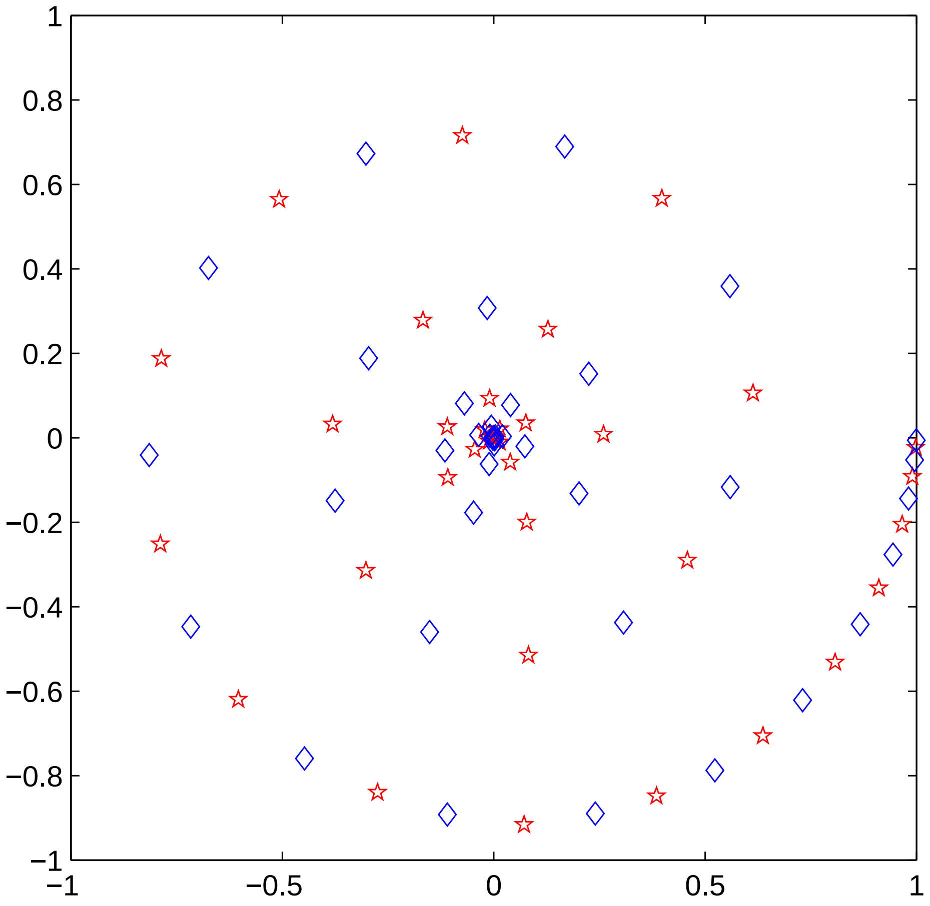
   Often – e.g. for Fox–Li – this can be done explicitly. Otherwise we can use highly oscillatory quadrature at a cost linear in $r(2N - r)$, the number of coefficients that we need to compute.

2. Compute the $r \times r$ matrix $G = A_{1,2}A_{2,1}$ and QR-factorize it. The outcome is the $(2r) \times (2r)$ matrix B.

3. Compute the eigenvalues (and, if required, eigenvectors) of B.

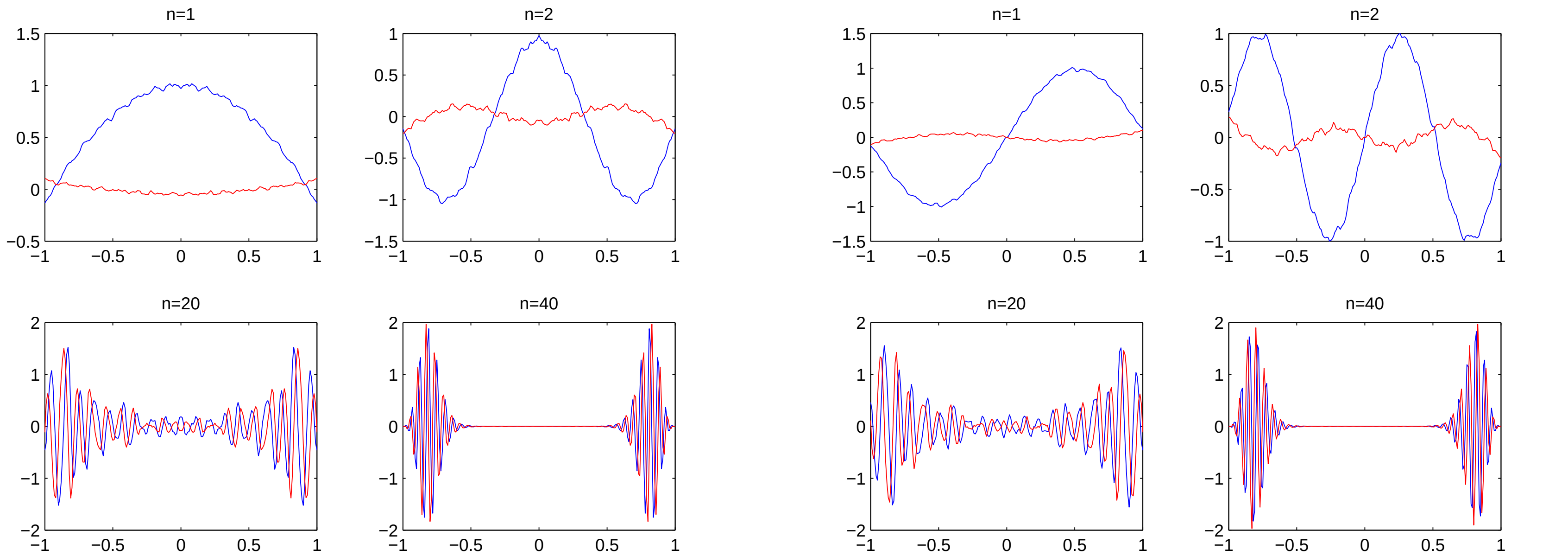
Of course, we are always on the lookout for additional structure: e.g. the evenness of g simplifies matters a great deal.

Fox–Li eigenvalues



$\omega = 100$, $r = 127$. $\diamond$ corresponds to ‘odd’ eigenvalues and $\star$ to ‘even’.

Fox–Li eigenvectors



Real and imaginary parts – even eigenfunctions to the left. Note that for small n the eigenfunctions are almost trigonometric, for large n they resemble wave packets. This is consistent with an interpretation of Fox–Li as a perturbed Schrödinger problem.