Fast, stable and accurate approximations with Fourier extensions

Ben Adcock
Department of Mathematics
Purdue University

Joint work with Daan Huybrechs (K. U. Leuven) and Jesús Martín–Vaquero (University of Salamanca)

Outline of the talk

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Fourier extensions

Fourier extensions in infinite precision

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Fourier extensions from equispaced data

Parameter choices

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Fourier extensions in infinite precision

Fourier extensions in finite precision

Fourier extensions from equispaced data

Parameter choices

Fourier series

Let $f : [-1,1] \to \mathbb{R}$. Its N^{th} partial Fourier series is

$$f_N(x) = \sum_{|n| \le N} \hat{f}_n \mathrm{e}^{\mathrm{i}n\pi x}, \qquad N \in \mathbb{N},$$

where

$$\hat{f}_n = \frac{1}{2} \int_{-1}^{1} f(x) \mathrm{e}^{-\mathrm{i}n\pi x} \, \mathrm{d}x, \quad n \in \mathbb{Z},$$

are the Fourier coefficients of f.

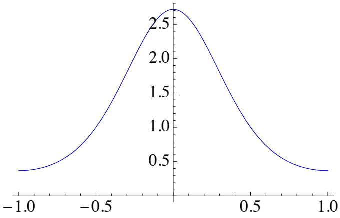
Fourier series are extremely effective tools in computations.

Reason 1: rapid convergence of Fourier series

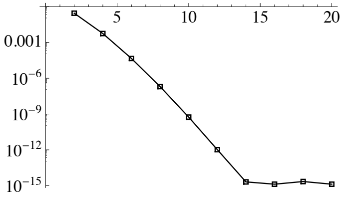
The Fourier series f_N converges geometrically fast whenever f is analytic and periodic, i.e.

$$\|f - f_N\|_\infty := \sup_{x\in[-1,1]} |f(x) - f_N(x)| \sim \rho^{-N},$$

for some $\rho > 1$.



$f(x) = \mathrm{e}^{\cos \pi x}$



$\|f - f_N\|_\infty$

Reasons 2 & 3

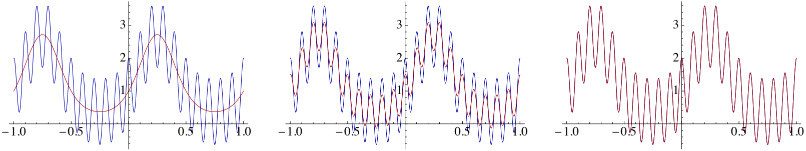
2. Computations can be carried out rapidly, in $\mathcal{O}(N \log N)$ time, with the FFT.

3. Fourier series lead to stable numerical algorithms (spectral methods) for PDEs.

Reason 4: resolution power of Fourier series

Fourier series are good at resolving periodic oscillations.

- Obtain the optimal resolution constant of 2 d.o.f. per wavelength.



10 d.o.f. ($\|f - f_N\|_\infty \approx 1$)

20 d.o.f. ($\|f - f_N\|_\infty \approx 10^{-1}$)

40 d.o.f. ($\|f - f_N\|_\infty \approx 10^{-14}$)

Graphs of $f(x) = \cos 20\pi x + \exp(\sin 2\pi x)$ (blue) and $f_N(x)$ (red).

Conversely, expansions in orthogonal polynomials (e.g. Chebyshev polynomials) have a higher resolution constant equal to π.

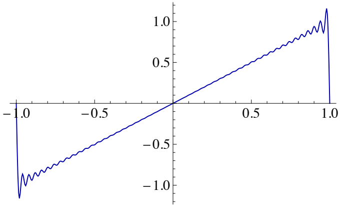
Limitations of Fourier series I

Most functions are not periodic.

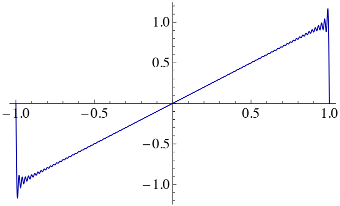
The Fourier series of a nonperiodic function gives a very poor approximation.

- Gibbs phenomenon.
- No uniform convergence.

E.g. $f(x) = x$:



$N = 50$

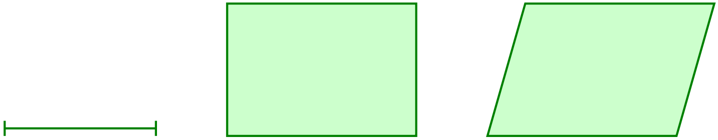


$N = 100$

Limitations of Fourier series II

Fourier series are limited to simple geometries.

- E.g. intervals, (hyper)rectangles, parallelopipeds.



- Some extensions to certain triangles and simplices. But require rather unphysical notions of periodicity.

Main question

Is there a way to retain the good properties of Fourier series of periodic functions, i.e.

(i) rapid convergence,

(ii) good resolution power,

(iii) easy manipulation via the FFT,

for nonperiodic functions, and functions defined in arbitrary domains?

Answer

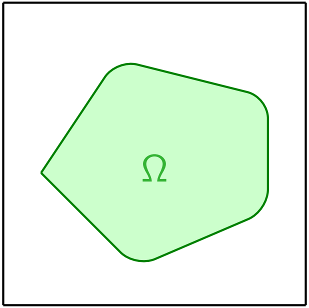
Yes! One can compute approximations of analytic, nonperiodic functions which

(i) are expressed in terms of a Fourier series,
(ii) converge rapidly,
(iii) have a resolution constant that can be made arbitrarily close to 2 by an appropriate choice of a certain parameter,
(iv) are numerically stable,
(v) in 1D at least, can be computed efficiently.

The method is based on so-called Fourier extensions.

An (old) idea

Seek to approximate a function $f : \Omega \to \mathbb{R}$ by a Fourier series on a larger, (hyper)rectangular domain.



Known as the Fourier extension problem.

The Fourier extension problem

Existence/construction of extensions:

- Whitney (1934), Hestenes (1941), Fefferman (2005),...
- However, typically cannot obtain geometric convergence this way – no analytic and periodic extension of an arbitrary analytic function.
- Throughout, we shall never explicitly calculate extensions.

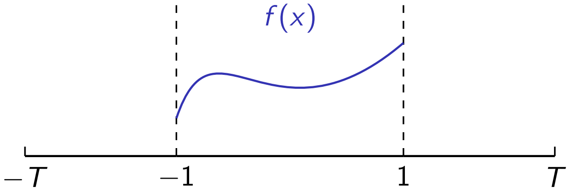
Computation of extensions:

- Boyd (2002), Bruno (2003), Bruno et al (2007), Huybrechs (2010), BA & Huybrechs (2011), BA et al (2012).
- SVD's, fast computations, smoothing of extensions: Lyon (2011, 2012).

Applications of extensions:

- Solution of PDEs in complex geometries, Lyon & Bruno (2010, 2011), Albin & Bruno (2011).

One-dimensional Fourier extensions



We seek an approximation $f_N \in \mathcal{G}_N$, where

$$\mathcal{G}_N = \operatorname{span}\left\{ \frac{1}{\sqrt{2T}} \mathrm{e}^{\mathrm{i}\frac{n\pi}{T}x} : n = -N, \ldots, N \right\},$$

is the set of Fourier series of degree N on $[-T, T]$, and $T > 1$ is fixed (up to the user).

Question: how should we compute f_N?

Least squares

Define

$$f_N := \underset{\phi \in \mathcal{G}_N}{\operatorname{argmin}} \|f - \phi\|,$$

where $\|g\|^2 = \int_{-1}^{1} |g(x)|^2 \, \mathrm{d}x$.

- Results in a linear system for the coefficients of $F_N(f)$.
- We refer to $F_N(f)$ as the continuous Fourier extension of f.

Problem: we need to know the integrals $\int_{-1}^{1} f(x) \mathrm{e}^{-\mathrm{i}\frac{n\pi}{T}x} \, \mathrm{d}x$.

Discrete least squares

Intstead, we can replace integrals by a quadrature, leading to

$$f_N := \operatorname*{argmin}_{\phi \in \mathcal{G}_N} \sum_{|n| \leq N} |f(x_n) - \phi(x_n)|^2.$$

- We refer to $\tilde{F}_N(f)$ as the discrete Fourier extension of f.

Question: what are good nodes to choose?

Fourier extensions as polynomial approximations

The set $\mathcal{G}_N$ consists of the functions

$$\cos \tfrac{k\pi}{T} x, \quad \sin \tfrac{(k+1)\pi}{T} x, \qquad k = 0, \ldots, N.$$

If $c(T) = \cos \frac{\pi}{T}$ and

$$y = y(x) := \cos \frac{\pi}{T} x, \qquad y : [0,1] \to [c(T), 1],$$

then

$$\cos \tfrac{k\pi}{T} x \in \mathbb{P}_k, \qquad \sin \tfrac{(k+1)\pi}{T} x / \sin \tfrac{\pi}{T} x \in \mathbb{P}_k.$$

Thus, any FE can be written as a sum of two polynomials expansions of degree N in the variable y, corresponding to the even and odd parts of f respectively.

Choice of nodes

Optimal nodes for polynomial interpolation in $z \in [-1, 1]$ are the Chebyshev nodes

$$z_n = \cos\left(\frac{(2n+1)\pi}{2N+2}\right), \quad n = 0, \ldots, N.$$

Mapping back to the x-domain, we get

$$x_n = \frac{T}{\pi}\cos^{-1}\left\{\frac{1}{2}(1 - c(T))\cos\left[\frac{(2n+1)\pi}{2N+2}\right] + \frac{1}{2}(1 + c(T))\right\},$$

for $n = 0, \ldots, N$, and $x_{-n} = -x_n$ otherwise.

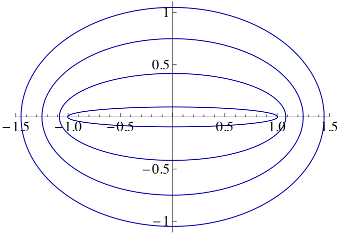
- We refer to these as mapped symmetric Chebyshev nodes.

Convergence

The expansion of an analytic function g in (almost) any orthogonal polynomial system converges geometrically fast at rate ρ, where ρ is the index of the largest Bernstein ellipse

$$\mathcal{B}(\rho) = \left\{ \tfrac{1}{2}\left(\rho \mathrm{e}^{\mathrm{i}\theta} + \rho^{-1}\mathrm{e}^{-\mathrm{i}\theta}\right) : \theta \in [-\pi, \pi) \right\}, \quad \rho \geq 1,$$

within which g is analytic.



$\mathcal{B}(\rho)$, $\rho = 1.1, 1.5, 2, 2.5$

Convergence

Let $\mathcal{D}(\rho)$ be the image of $\mathcal{B}(\rho)$ in the x-domain, and set

$$E(T) = \cot^2\left(\frac{\pi}{4T}\right).$$

Theorem (Huybrechs (2010), BA & Huybrechs (2011))

Suppose that f is analytic in $\mathcal{D}(\rho^*)$ and continuous on its boundary. Then

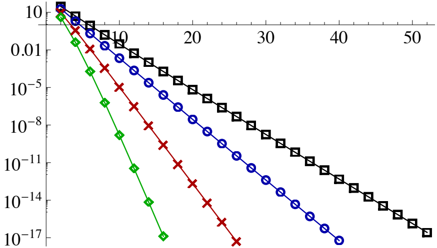
$$\|f - f_N\|_\infty \leq c_f \rho^{-N},$$

where $\rho = \min\{\rho^*, E(T)\}$ and $c_f > 0$ is proportional to $\max_{x\in\mathcal{D}(\rho)} |f(x)|$.

- The map $y = \cos\frac{\pi}{T}x$ introduces a square-root type singularity in the complex plane. This limits the maximal ρ to $E(T)$.

Numerical example

Let $T = \frac{4}{3}, \frac{3}{2}, 2, 4$:



The error $\|f - f_N\|_\infty$ for $f(x) = \mathrm{e}^{5x}$

Note that $E(T)$ is an increasing function of T, with $E(1) = 1$.

Resolution power

By analyzing the behaviour of the Fourier extension of

$$f(x) = \mathrm{e}^{\mathrm{i}\pi\omega x}, \quad x \in [-1, 1],$$

for large $\omega \gg 1$, one can show:

Theorem (BA & Huybrechs (2011))

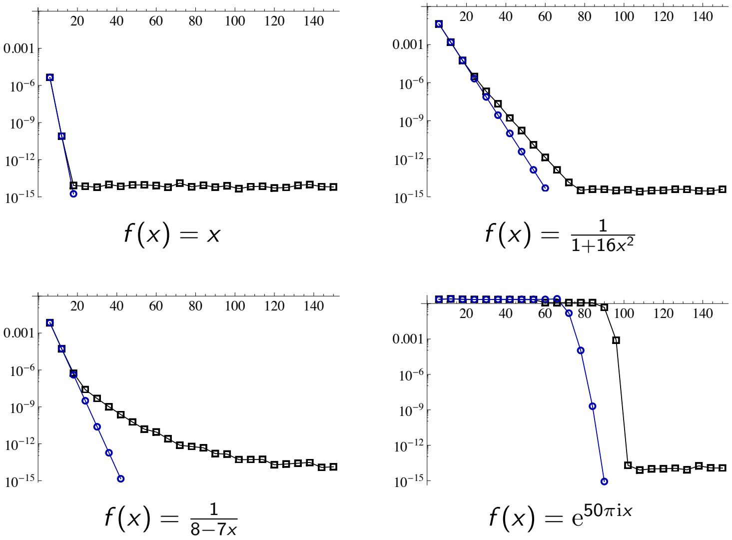
The number of points-per-wavelength $r(T)$ required to resolve the function $f(x) = \mathrm{e}^{\mathrm{i}\pi\omega x}$ satisfies

$$r(T) \leq 2T \sin\left(\frac{\pi}{2T}\right), \quad T > 1.$$

In particular, $r(T) \sim 2 + \mathcal{O}(T-1)$ as $T \to 1$.

- The PPW for standard Fourier series is the limiting value for $r(T)$.

Numerical example



The error $\|f - f_N\|_\infty$ against N, where f_N is the finite (black) or infinite (blue) precision FE with $T = 2$.

Conclusion

The differences between the infinite- and finite-precision computations suggest that either:

(i) The theorems are wrong!

(ii) The code has a bug!

(iii) The finite-precision solver does not give an extension which is 'close' to the infinite-precision FE.

Fortunately for my collaborators and me, (iii) is correct.

$\Rightarrow$ analysis of infinite-precision extensions is of limited use in understanding the results of finite-precision computations.

Ill-conditioning

The discrete FE requires solution of a linear system

$$Aa = b,$$

where $A \in \mathbb{C}^{(2N+1)\times(2N+1)}$ and $a \in \mathbb{C}^{2N+1}$ is the vector of coefficients of $\tilde{F}_N(f)$.

Theorem (BA et al. (2012))

The condition number of A satisfies

$$\kappa(A) = \mathcal{O}\left(E(T)^N\right), \quad N \to \infty.$$

Moreover, the numerical rank of A is roughly $2N/T$ for large N.

Explanation: Any function f defined on $[-1,1]$ has infinitely many extensions to $[-T,T]$. Redundancy $\Rightarrow$ numerical ill-conditioning.

Intuitive argument

1. For large N, the matrix A is highly underdetermined.

2. The numerical solver (e.g. *Matlab's* backslash) will use these degrees of freedom to seek coefficient vectors $\tilde{a}$ satisfying

$$A\tilde{a} \approx b, \qquad \|\tilde{a}\| \ll \infty.$$

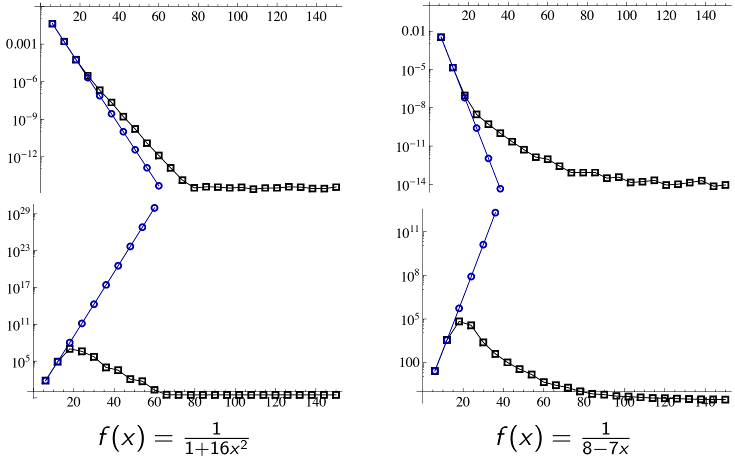
3. One can show that, if $f \in \mathcal{D}(\rho)$, then

$$\|a\| \approx (E(T)/\rho)^N.$$

4. Hence, $\|a\|$ is exponentially large in N for $\rho < E(T)$, and we must therefore have

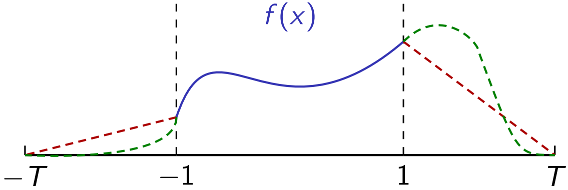
$$\tilde{a} \neq a, \quad N \text{ large.}$$

Numerical example



Top row: the error $\|f - f_N\|_\infty$ against N, where f_N is the finite (black) or infinite (blue) precision FE. Bottom row: the norms $\|\tilde{a}\|$ (black) and $\|a\|$ (blue) against N.

Existence of small-norm approximate coefficients



Lemma

Let $f \in \mathrm{H}^k(-1,1)$, $k \in \mathbb{N}$. Then there exists $\tilde{a} \in \mathbb{C}^{2N+1}$ satisfying

(i) $\|\tilde{a}\| \lesssim \|f\|_{\mathrm{H}^k}$ (*small norm*),

(ii) $\|A\tilde{a} - b\| \lesssim N^{-k}\|f\|_{\mathrm{H}^k}$ (*approximate solution*),

(iii) $\|f - \sum_{|n|\le N} a_n \phi_n\| \lesssim N^{-k}\|f\|_{\mathrm{H}^k}$ (*good approximation of f*).

Conclusion: In finite-precision, geometric convergence may be sacrificed for superalgebraic convergence for all large N.

Analysis of the finite-precision FE

Assumption 1. The result of the numerical solver is similar to that of a truncated SVD.

Assumption 2. Errors in the truncated SVD can be ignored.

- Agrees with numerical experiment.

We now consider the approximation $f \approx g_{N,\epsilon}$, where $g_{N,\epsilon}$ is the FE obtained by solving

$$Aa = b,$$

using an SVD with truncation parameter ϵ..

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Analysis of $G_{N,\epsilon}(f)$

Recall that

$$\mathcal{G}_N = \mathrm{span}\left\{ \frac{1}{\sqrt{2T}} \mathrm{e}^{\mathrm{i}\frac{n\pi}{T}x} : n = -N, \ldots, N \right\}.$$

Theorem

For any $\phi \in \mathcal{G}_N$, we have

$$\|f - g_{N,\epsilon}\|_\infty \lesssim \|f - \phi\|_\infty + \epsilon \|\phi\|_{T,\infty}, \qquad (\star)$$

where $\|\cdot\|_{T,\infty}$ is the uniform norm on $[-T, T]$.

Phases of convergence

1. Setting $\phi = f_N$ in $(\star)$ gives

$$\|f - g_{N,\epsilon}\|_\infty \lesssim c_f \rho^{-N} \left(1 + \epsilon E(T)^N\right).$$

The RHS decreases geometrically for

$$N \leq N_1 := -\frac{\log E(T)}{\log \epsilon},$$

and increases geometrically for $N > N_1$.

2. However, recall that there exist functions ϕ with small norm coefficient vectors. When substituted into $(\star)$ these give

$$\|f - g_{N,\epsilon}\|_\infty \lesssim \|f\|_{\mathrm{H}^k} \left(N^{-k} + \epsilon\right).$$

Summary

1. $N \leq N_1$. Geometric convergence in N.

2. $N = N_1$. The error satisfies

$$\|f - g_{N,\epsilon}\|_\infty \lesssim c_f \epsilon^{d_f}, \quad d_f = \frac{\log \rho}{\log E(T)} \in (0, 1].$$

3. $N > N_1$. Superalgebraic convergence down to a maximal accuracy of order ϵ.

Remarks:

- If f is sufficiently analytic, then $d_f = 1$. If c_f is also small, then convergence stops at $N = N_1$. Otherwise, there is a further regime of superalgebraic convergence.
- The breakpoint is function-independent. Up to constant factors, it is the largest N for which all singular values of A are greater than ϵ.

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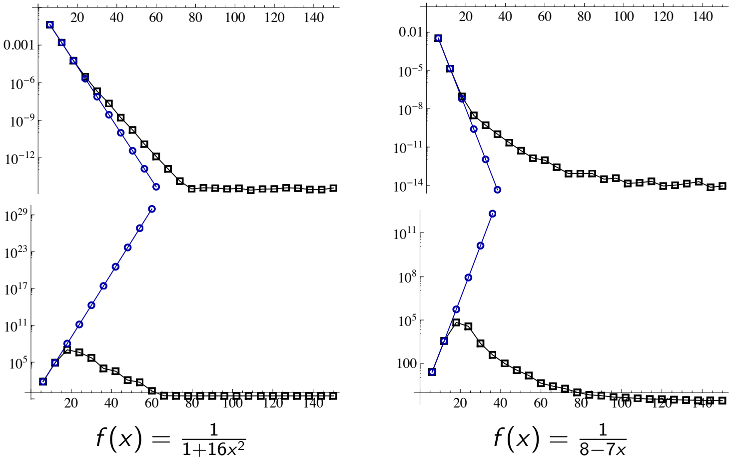
Numerical Example



Top row: the error $\|f - f_N\|_\infty$ against N, where f_N is the finite (black) or infinite (blue) precision FE. Bottom row: the norms $\|\tilde{a}\|$ (black) and $\|a\|$ (blue) against N.

Numerical stability

One can prove that the condition number of the numerical mapping $f \mapsto f_N$ satisfies $\kappa_N = \mathcal{O}(1)$ for all N.

40	80	120	160	200
1.44×10^0	1.45×10^0	1.41×10^0	1.46×10^0	1.42×10^0

The condition number κ_N for $T = 2$

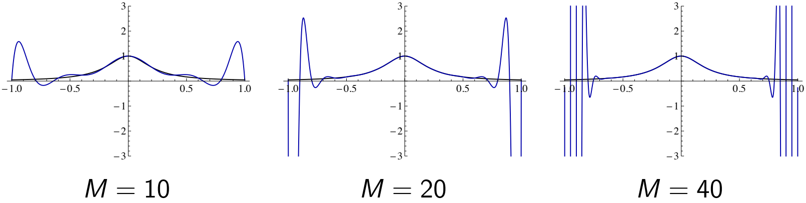
Background

In many problems one has only samples of f at equispaced points:

$$f\left(\tfrac{n}{M}\right), \quad |n| \leq M.$$

Equispaced data is difficult to handle.

Runge phenomenon: the polynomial interpolant of f at equispaced nodes diverges unless f is analytic in a sufficiently large region.



Graphs of $f(x) = \frac{1}{1+20x^2}$ (black) and its equispaced polynomial interpolant (blue).

A result of Platte, Trefethen & Kuijlaars (PTK)

Problem: given $\{f(\frac{n}{M})\}_{|n|\leq M}$, recover f to high accuracy.

Many methods have been proposed to do this. However,

Theorem (Platte, Trefethen & Kuijlaars (2011))

"Any method that recovers analytic functions f to exponential accuracy using only the grid values $\{f(\frac{n}{M})\}_{|n|\leq M}$ must be exponentially ill-conditioned. The best possible convergence for a stable method is root-exponential in M."

Fourier extensions for equispaced data

We define

$$f_{N,M} := \operatorname*{argmin}_{\phi \in \mathcal{G}_N} \sum_{|n| \leq M} |f(\tfrac{n}{M}) - \phi(\tfrac{n}{M})|^2.$$

Questions:

(i) How large does M need to be, for a given N?

(ii) What is the corresponding convergence rate and condition number, and how does this relate to Platte, Trefethen & Kuijlaars (PTK)?

(iii) Are the results for (i) and (ii) different in finite and infinite precision?

The infinite-precision FE

It is possible to show the following:

1. If $M = \gamma N$ for $\gamma \geq 1$ fixed, then
   (i) The condition number $\kappa_{N,\gamma N}$ is exponentially large in N,
   (ii) The Fourier extension $f_{N,\gamma N}$ diverges exponentially fast for any analytic function having a singularity in a certain complex region $\mathcal{R}_\gamma$ containing $[-1,1]$.

2. One requires the scaling $M = \mathcal{O}\left(N^2\right)$ to avoid (i) and (ii).

3. If $M = \mathcal{O}\left(N^2\right)$, then $f_{N,M}$ converges geometrically fast in N at the same rate as the discrete FE, and the condition number $\kappa_{N,M}$ is bounded.

$\Rightarrow$ In infinite precision, FE's attain the stability barrier of PTK.

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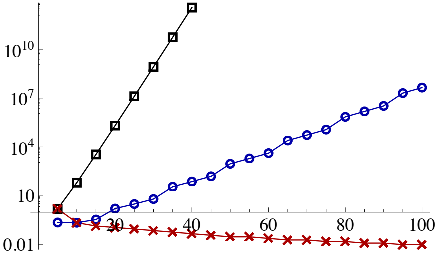
Example

Infinite precision:

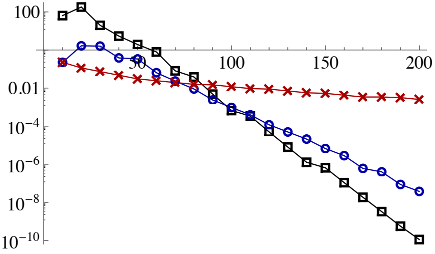


The error $\|f - f_{N,M}\|_\infty$ against M for $f(x) = \frac{1}{1+100x^2}$, where $N = M$ (black), $N = 2/3M$ (blue) and $N = 2\sqrt{M}$ (red)

Divergence for $M = \mathcal{O}(N)$.

Example

Finite precision:



The error $\|f - f_{N,M}\|_\infty$ against M for $f(x) = \frac{1}{1+100x^2}$, where $N = M$ (black), $N = 2/3M$ (blue) and $N = 2\sqrt{M}$ (red)

Convergence with $M = \mathcal{O}(N)$. The scaling $M = \mathcal{O}\left(N^2\right)$ is unnecessary.

The finite-precision FE

By analysing the truncated SVD FE, one can show the following:

1. The condition number

$$\kappa_{N,\gamma N} \lesssim \epsilon^{-a(\gamma;T)},$$

where $a(\gamma; T)$ is independent of N and satisfies

- $0 < a(\gamma; T) \leq 1$,
- $a(\gamma; T) \to 0$, $\gamma \to \infty$.

$\Rightarrow$ the condition number can be made arbitrarily close to 1 for all N by a suitable choice of γ.

The finite-precision FE

2. The error satisfies

$$\|f - f_{N,\gamma N}\|_\infty \lesssim \epsilon^{-a(\gamma;T)} \left(\|f-\phi\|_\infty + \epsilon \|\phi\|_{T,\infty} \right), \quad \forall \phi \in \mathcal{G}_N.$$

Hence

(i) $N \leq N_1$. Geometric convergence in N.

(ii) $N = N_1$. The error satisfies

$$\|f - f_{N_1,\gamma N_1}\|_\infty \lesssim c_f \epsilon^{d_f - a(\gamma;T)}, \quad d_f = \frac{\log \rho}{\log E(T)}.$$

(iii) $N > N_1$. Superalgebraic convergence down to a maximal accuracy of order $\epsilon^{1-a(\gamma;T)}$.

Relation to PTK

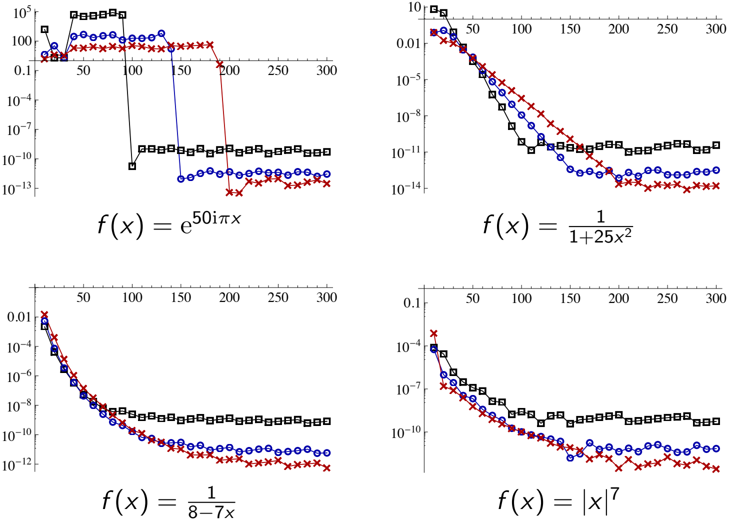
The stability barrier can be circumvented to a substantial extent.
With FE's, we have:

(i) Bounded condition numbers,

(ii) Rapid convergence, but only down to a finite tolerance.

$\Rightarrow$ No contradiction with PTK.

Examples



The error $\|f - f_{M/\gamma,M}\|_\infty$ against M, where $T = 2$ and $\gamma = 1$ (black), $\gamma = \frac{3}{2}$ (blue) or $\gamma = 2$ (red).

Parameter choices

Two parameters:

- T – the extension domain size,
- γ – the amount of oversampling.

Question: How do we best choose T and γ?

- For obvious reasons, we are most interested in function independent choices.

Factors

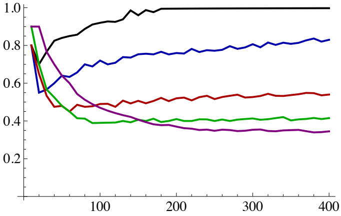
	stability	maximal accuracy	convergence
small γ	worse	worse	better
large γ	better	better	worse

	stability	maximal accuracy	convergence
small T	worse	worse	better
large T	better	better	worse

Experiment

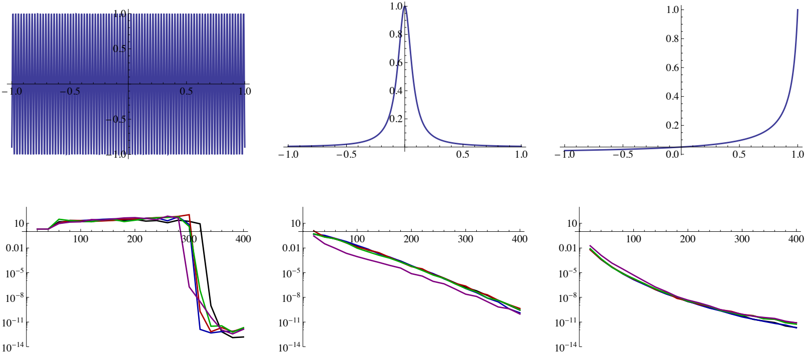
Fix T. For each M, find the largest value of N such that the condition number $\kappa_{N,M} \leq \kappa_0$, where κ_0 is some prescribed value. This gives a function

$$\Theta(M;T) = \max\{N : \kappa_{N,M} \leq \kappa_0\}, \quad M \in \mathbb{N}.$$



The function $\Theta(M;T)/M$ against M, where $T = 4, 3, 2, 3/2, 7/6$.

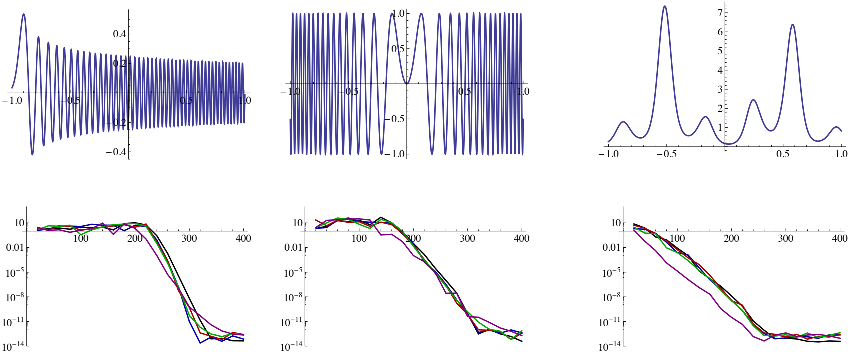
Numerical results



$f(x) = \mathrm{e}^{60\sqrt{2}\pi \mathrm{i} x}$ $\qquad f(x) = \frac{1}{1+200x^2}$ $\qquad f(x) = \frac{1}{20-19x}$

Top row: $f(x)$. Bottom row: the error $\|f - f_{\Theta(M;T),M}\|_\infty$ against M, where $T = 4, 3, 2, 3/2, 7/6$.

Numerical results



$f(x) = \mathrm{Ai}(-30x - 28)$ $\qquad$ $f(x) = \sin 100x^2$ $\qquad$ $f(x) = \mathrm{e}^{\sin(5.4\pi x - 2.7\pi) - \cos(2\pi x}$

Top row: $f(x)$. Bottom row: the error $\|f - f_{\Theta(M;T),M}\|_\infty$ against M, where
$T = 4, 3, 2, 3/2, 7/6$.

Conclusion

The choice of T makes almost no difference!

Recommendation: choose $T = 2$

Reason: fast computations in $\mathcal{O}\left(N(\log N)^2\right)$ time, Lyon (2012)

Conclusions and open problems

Despite severely ill-conditioned matrices, one can compute numerically stable, rapidly convergent Fourier extensions of arbitrary functions, even when only equispaced data is prescribed.

Challenges

- Higher dimensions: simplicial domains (triangles, tetrahedra,...)
- Higher dimensions: arbitrary domains
- Explaining the apparent γ and T independence
- Other data (nonuniform, Fourier, etc)

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