Testing the Sharpness of Known Error Bounds of the Fast Fourier Transform

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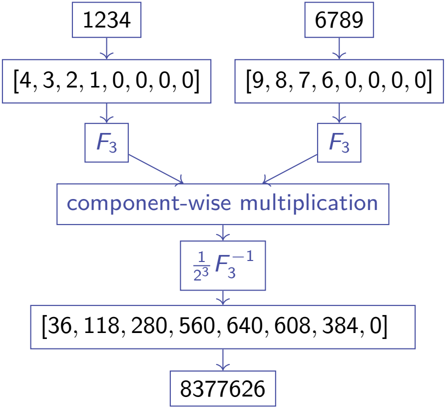
Application of FFT: fast multiplication of huge integers

Multiplication of 1234 by 6789:



Application of FFT: fast multiplication of huge integers

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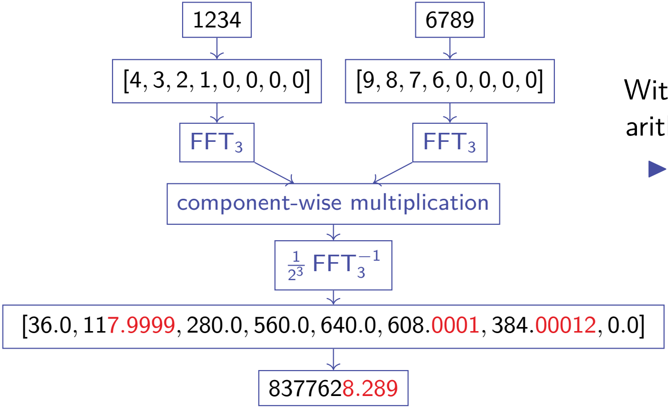

With floating-point arithmetic

- Numerical errors.

Application of FFT: fast multiplication of huge integers

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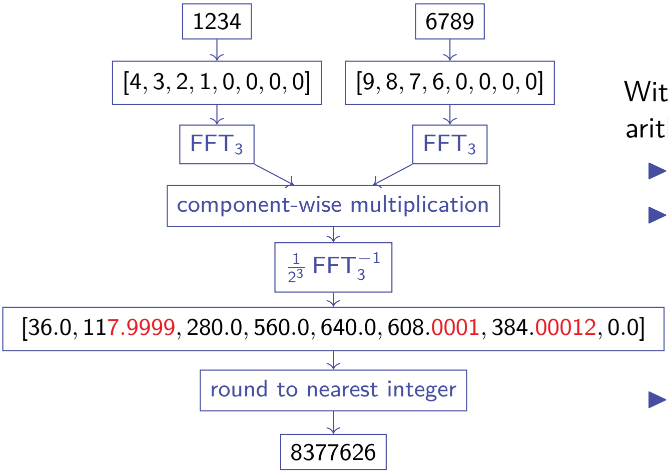


With floating-point arithmetic

- Numerical errors.
- Here, we can recover the exact result because rounding errors < 0.5.
- But, as size grows, rounding error accumulates.

Motivation

We are interested in

- Absolute bounds on FFT numerical errors
- Tight bounds for improved certification

Two approaches

- Pick a global bound from the literature, valid for all possible inputs, and use conventional floating-point arithmetic
- Use *interval arithmetic* to compute a local bound on the fly, valid only for a reduced set of inputs

Motivation

Preceding work on global bound approach

N. Brisebarre, M. Joldeș, J.-M. Muller, A.-M. Naneș, J. Picot: "Error Analysis of Some Operations Involved in the Cooley-Tukey Fast Fourier Transform", *ACM Trans. Math. Softw. 46(2)*, 2020.

Two antagonistic effects of local bounds

- Local bounds are expected to be tighter than global bound
- Interval arithmetic is prone to overestimation[1]

Goal

Compare global and local bound approaches for the [Cooley & Tukey, 1965] with numerical tests

[1] Liu & Kreinovich [2010]

Notations

$X \in \mathbb{C}^{2^n}$ *input vector* of complex, *floating-point* coefficients

$F_n X$ is the *exact* transform

$\mathrm{FFT}_n(X)$ is the *computed* transform

Measuring errors: the choice of the metric

2-norm relative error

$$e_2(X) = \frac{\left\| F_n X - \mathrm{FFT}_n(X) \right\|_2}{\| F_n X \|_2}$$

where:

$$\|Z\|_2 = \sqrt{|z_0|^2 + \cdots + |z_{2^n-1}|^2}$$

- Natural norm for Fourier transforms
- Many results on the literature are based on it
- ☹ Ill-suited to bound individual coefficients

Measuring errors: the choice of the metric

Component-wise ∞-norm *input-relative* error

$$e_\infty^\perp(X) = \frac{\|F_n X - \mathrm{FFT}_n(X)\|_\infty^\perp}{\|X\|_\infty^\perp}$$

where:

$$\|Z\|_\infty^\perp = \max_{k=0}^{2^n-1} \left\{ |u|, |v| \;\middle|\; u + i\,v \in Z \right\}$$

☺ Represent the maximum error on every FP coefficient

- $\|X\|_\infty^\perp$ removes dependency on input magnitude
- We can deduce the latter from the former:

$$e_\infty^\perp(X) \leqslant 2^n \sqrt{2}\; e_2(X)$$

Sources of error

Excerpt of the FFT algorithm

Pseudo-code

$$\mathtt{y}_j := \mathtt{x}_j + \mathtt{x}_{j+2^{s-1}} \cdot \mathtt{w}_s^j$$
$$\mathtt{y}_{j+2^{s-1}} := \mathtt{x}_j - \mathtt{x}_{j+2^{s-1}} \cdot \mathtt{w}_s^j$$

FP rounding occurs in:

1. FP operations in $+, -, \times$
2. Rounded roots

1. Radix-2, precision-p, unbounded exponent range
   For any FP number $\mathtt{x}$ and $\mathtt{y}$ and $\triangle \in \{+, -, \times\}$:

$$\left|\,\mathsf{RN}(\mathtt{x} \triangle \mathtt{y}) - (\mathtt{x} \triangle \mathtt{y})\right| \leqslant u\,|\mathtt{x} \triangle \mathtt{y}|$$

   where $u = 2^{-p}$ is unit roundoff

2. For any order s: $\left|\mathtt{w}_s^j - \omega_s^j\right| \leqslant \delta_s \leqslant \frac{\sqrt{2}}{2} u$

s	δ_s
1	0
2	0
3	$0.616u$
4	$0.616u$
11	$0.641u$
15	$0.697u$

Global error bound [Brisebarre & al., 2020]

Error bound

Best known error bound

$$e_\infty^\perp(X) \leqslant b^{\text{global}} = 2^n\sqrt{2}\left((1+u)^n \prod_{s=1}^{n}(1+g_s) - 1\right)$$

where g_s is the relative error at step s

$$\begin{cases} g_1 = g_2 = 0 \\ g_s = \delta_s + \rho(1+\delta_s) \end{cases}$$

and ρ is the relative error of the complex multiplication

$$\begin{cases} \rho = u\sqrt{5} & \text{without FMA} \\ \rho = 2u & \text{with FMA} \end{cases}$$

Global error bound [Brisebarre & al., 2020]

Bad case

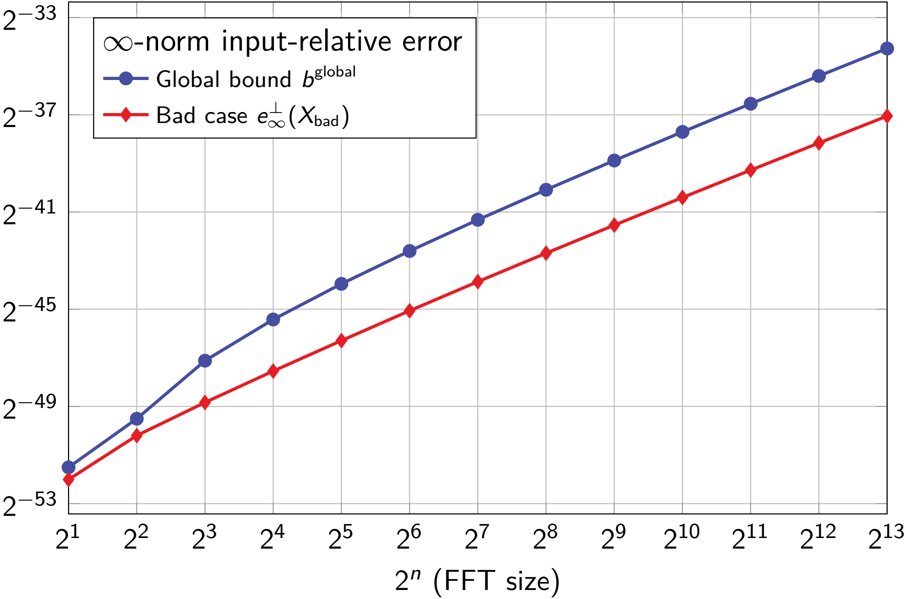
I.e. an input X_{bad} that generates large errors

- An explicit formula for the error can be computed with the help of B. Salvy and the GFUN package[2]:

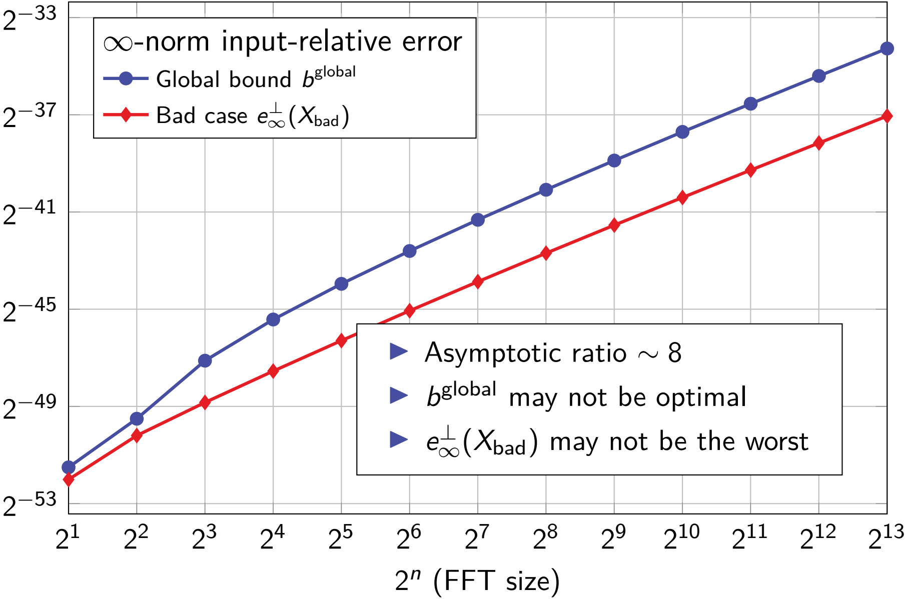
$$e_\infty^\perp(X_{\text{bad}}) = \left(\frac{2^n}{27} + (15n+14) - \frac{5}{9}\cos\left(\frac{n\pi}{3}\right) + \frac{\sqrt{3}}{9}\sin\left(\frac{n\pi}{3}\right) + \frac{(-1)^n}{27}\right)u$$

[2] Salvy & Zimmermann [1994]

Global error bound



Global error bound



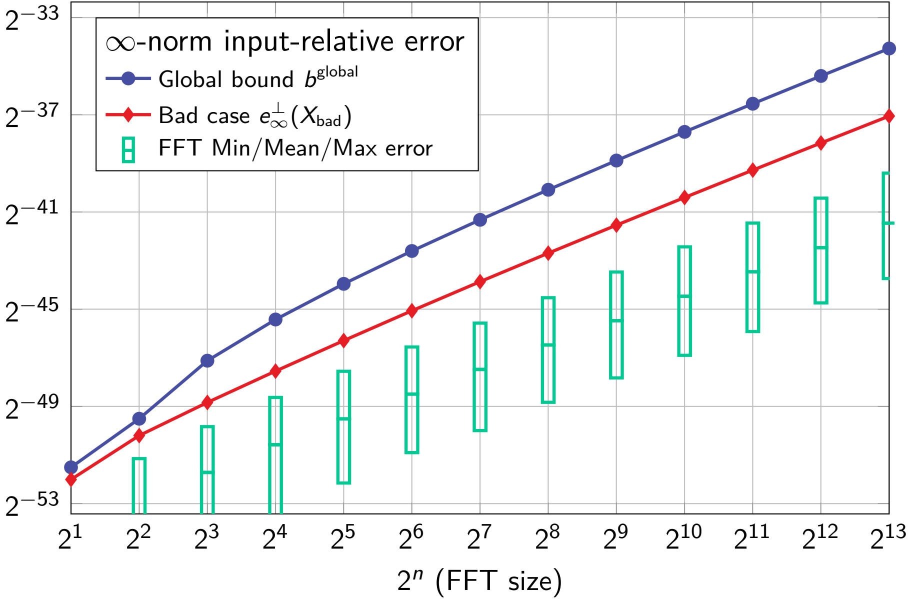
- Asymptotic ratio ~ 8
- b^{global} may not be optimal
- $e^{\perp}_{\infty}(X_{\text{bad}})$ may not be the worst

Numerical tests

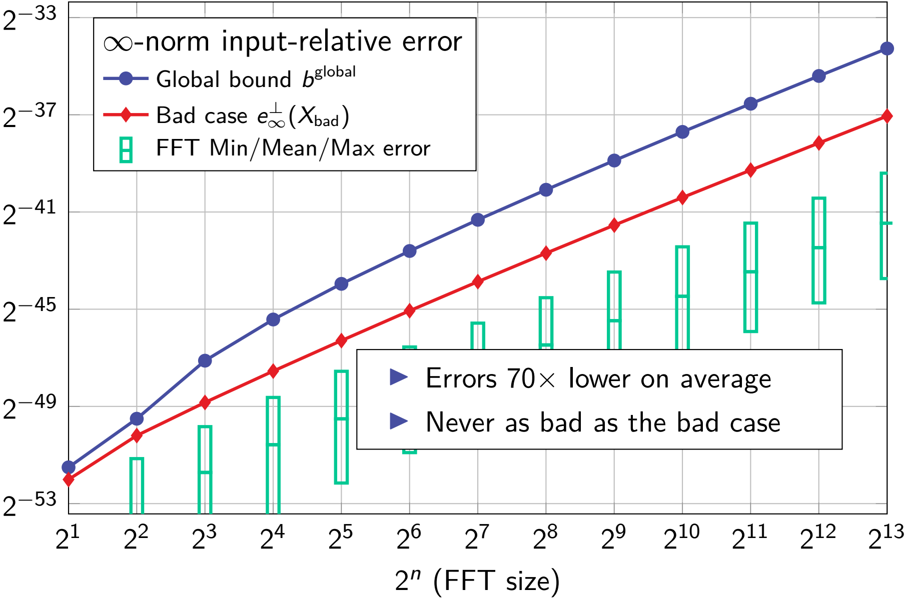
- Cooley & Tukey [1965] algorithm implemented with Julia (v1.7.2)
- FP format: binary64/double-precision arithmetic ($p = 53$)
- Random set of 65 536 input vectors for each n up to 13
- "Exact results" computed with Johansson's Arblib[3]
- For each size, we collect statistics of error values

[3] https://github.com/kalmarek/arblib.jl/tree/v0.8.1

Global error bound: numerical tests



Global error bound: numerical tests



- Errors 70× lower on average
- Never as bad as the bad case

- It seems that numerical errors are much smaller than b^{global} on average
- There is Interval Arithmetic that may produce *tighter local bounds*
- But Interval Arithmetic seems to have large overestimation on FFT
- Let's try it out

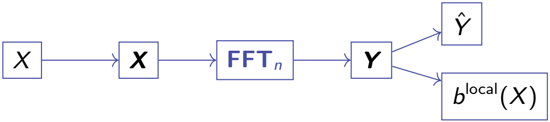
A posteriori or local error bound

Interval Arithmetic

- Each number z is replaced by an interval $\boldsymbol{z}$ of possible values
- Interval operations encloses exact and rounded values

$$x \triangle y \in \boldsymbol{x} \boldsymbol{\Delta} \boldsymbol{y} \qquad\qquad \mathrm{RN}(x \triangle y) \in \boldsymbol{x} \boldsymbol{\Delta} \boldsymbol{y}$$

- In **FFT**, operations are performed with Interval Arithmetic



where we can extract a local bound $b^{\text{local}}(X)$

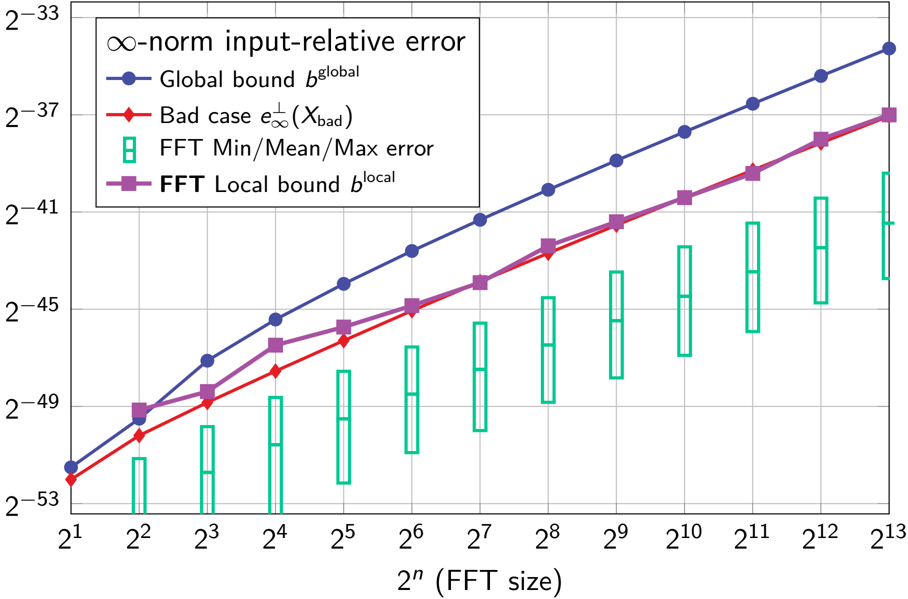
$$e_{\infty}^{\perp}(X) \leqslant b^{\text{local}}(X) = \frac{\max\left\{ \operatorname{diam}(\boldsymbol{u}), \operatorname{diam}(\boldsymbol{v}) \,\middle|\, \boldsymbol{u} + i\,\boldsymbol{v} \in \boldsymbol{Y} \right\}}{\|X\|_{\infty}^{\perp}}$$

Numerical tests

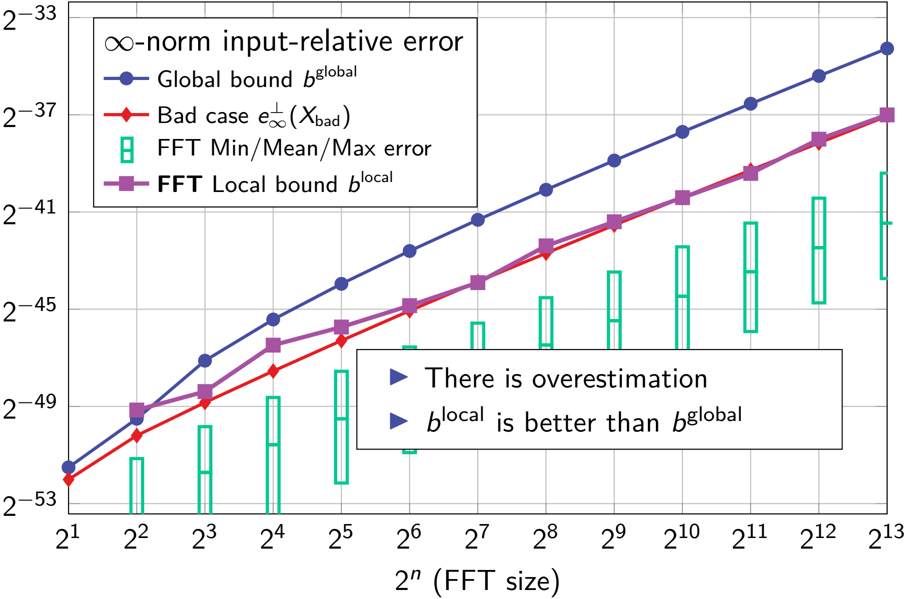
- We compute the local error bound for the same set of input
- We use the IntervalArithmetic library[4]
- Endpoints are encoded with binary64/double-precision arithmetic ($p = 53$)

[4] https://github.com/JuliaIntervals/IntervalArithmetic.jl/tree/v0.20.8

Local error bound: numerical tests

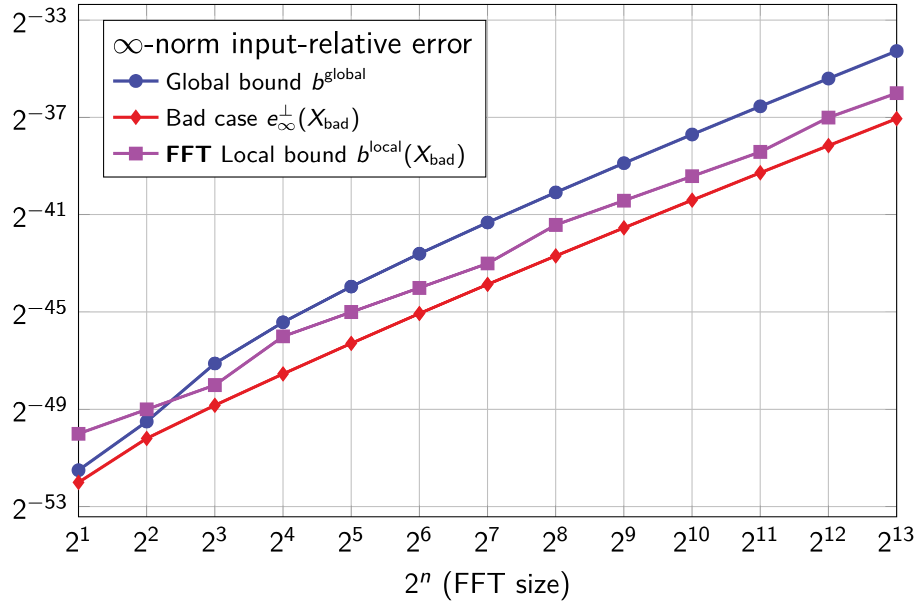


Local error bound: numerical tests



- There is overestimation
- b^{local} is better than b^{global}

Local bound applied to the bad case



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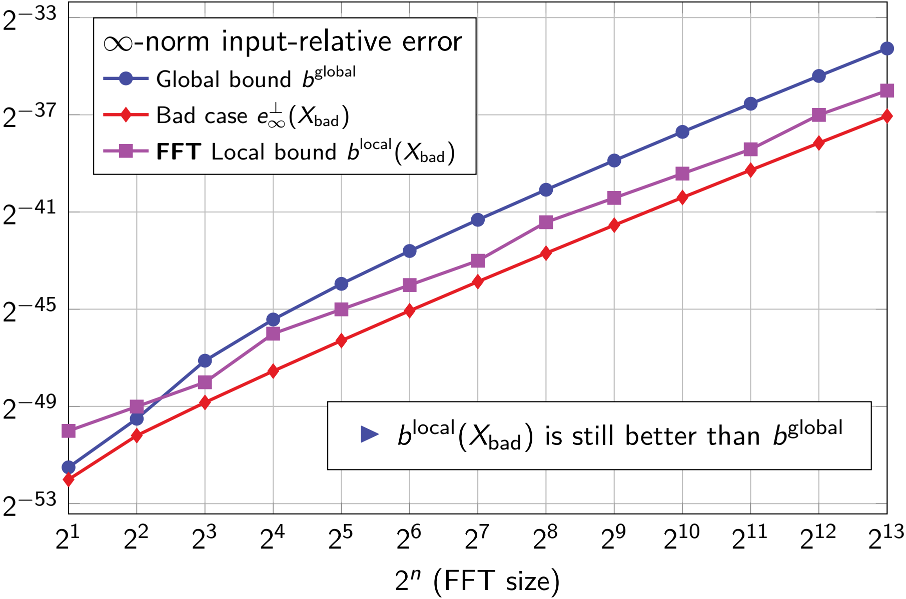


▶ $b^{\text{local}}(X_{\text{bad}})$ is still better than b^{global}

Preliminary insights

Global bound approach

- We have a global bound, and a bad case [Brisebarre & al., 2020]
- Actual errors almost always much smaller

Local bound approach

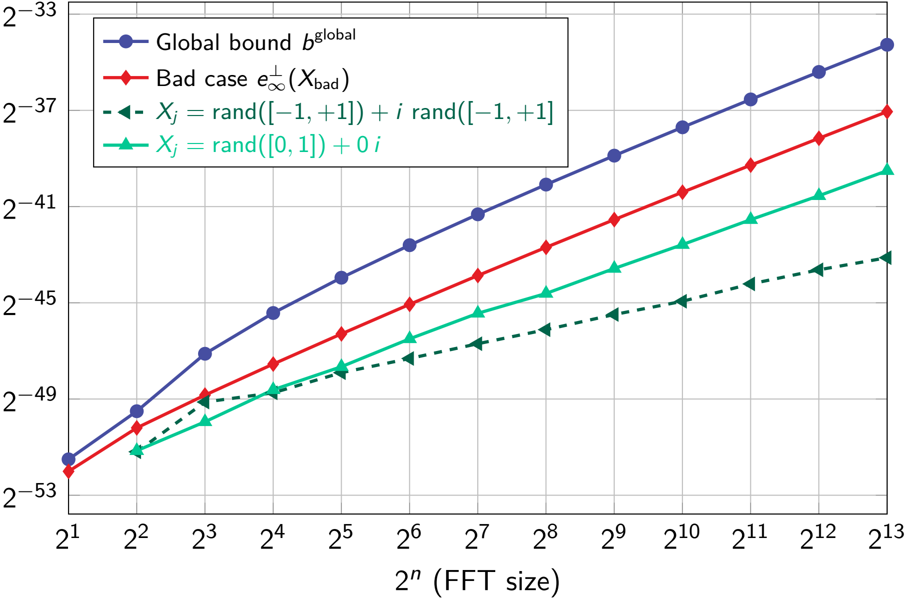
- Interval Arithmetic generate large overestimation on local bounds
- The local bound seems better for the average case

Future work

- Benchmarks should complete the choice between global and local

Thank you!

Generate random input vectors



Floating-point errors in complex numbers

- Complex numbers are implemented with real and imag. FP numbers:

$$x = \mathtt{a} + i\,\mathtt{b} \qquad\qquad y = \mathtt{c} + i\,\mathtt{d}$$

- Complex multiplication: $\hat{z} = x \otimes y = \mathtt{e} + i\,\mathtt{f}$ computed as:

Without FMA*

$$\begin{cases} \mathtt{e} = (\mathtt{a} \otimes \mathtt{c}) \ominus (\mathtt{b} \otimes \mathtt{d}) \\ \mathtt{f} = (\mathtt{a} \otimes \mathtt{b}) \oplus (\mathtt{c} \otimes \mathtt{d}) \end{cases}$$

With FMA*

$$\begin{cases} \mathtt{e} = \mathrm{fma}(\mathtt{a}, \mathtt{c}, -(\mathtt{b} \otimes \mathtt{d})) \\ \mathtt{f} = \mathrm{fma}(\mathtt{a}, \mathtt{b}, (\mathtt{c} \otimes \mathtt{d})) \end{cases}$$

*$\mathrm{fma}(\alpha, \beta, \gamma) = \circ(\alpha \times \beta + \gamma)$

- Error bounds for complex multiplication:

$$|z - \hat{z}| \leqslant u\sqrt{5}\,|z|$$

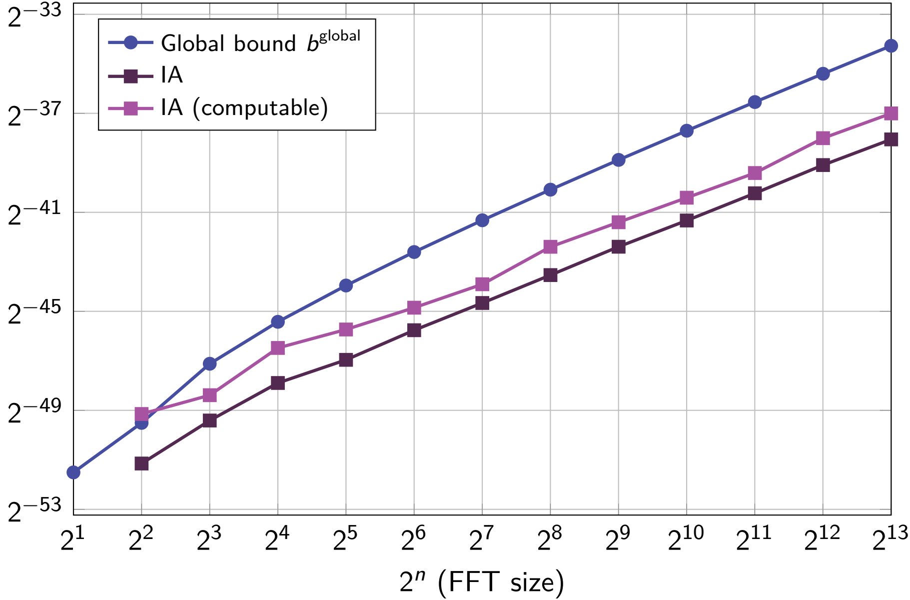
[Percival, 2002]

$$|z - \hat{z}| \leqslant 2u\,|z|$$

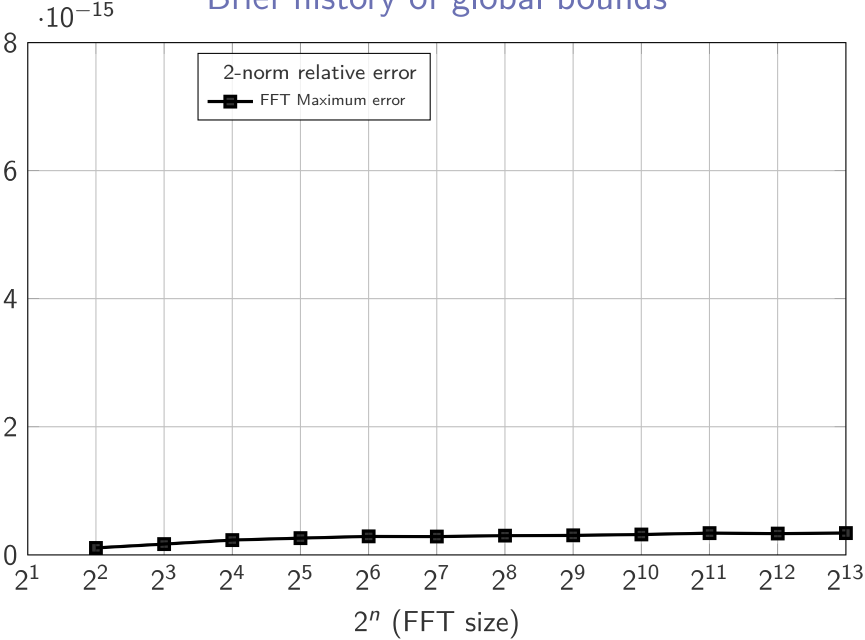
[Jeannerod & al., 2017]

- These bounds are asymptotically optimal.

Comparison between error and computable error



Brief history of global bounds



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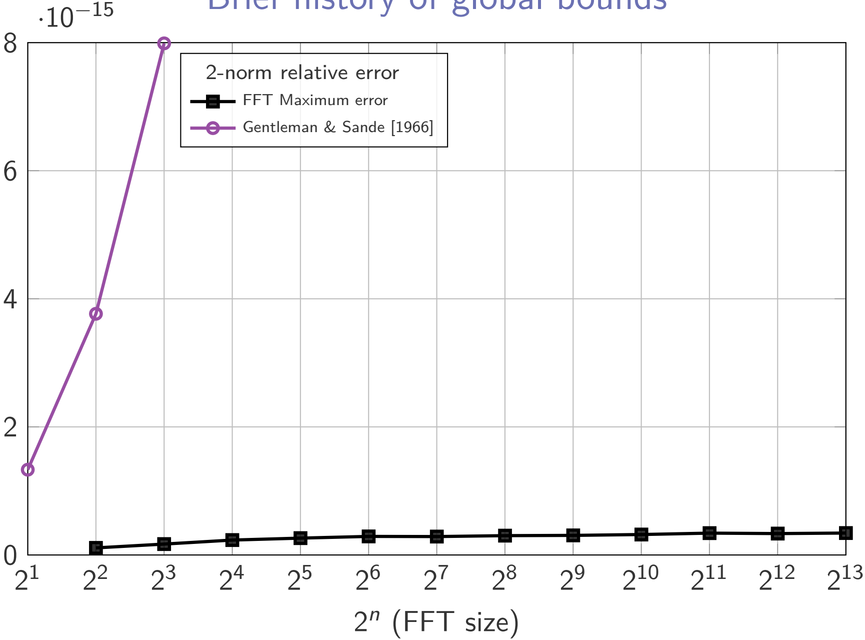

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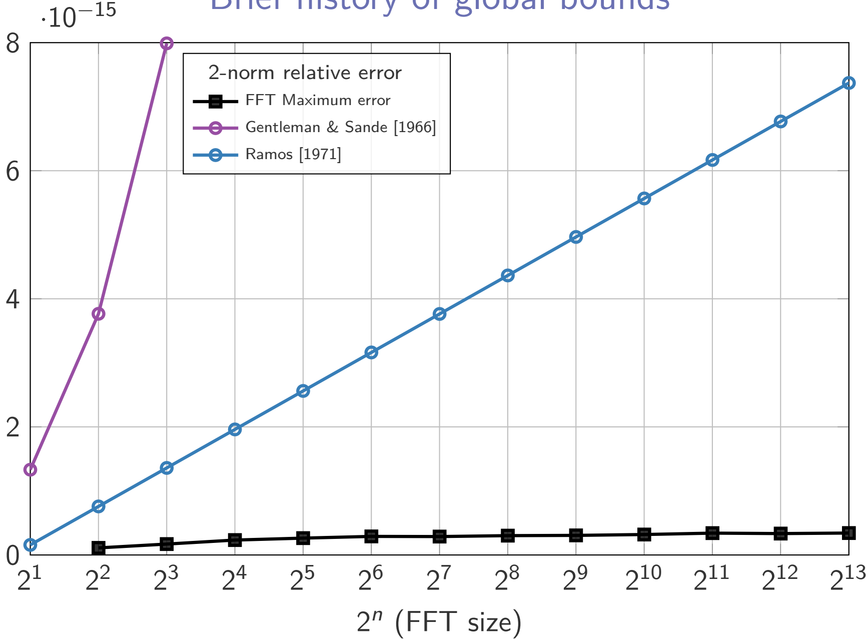

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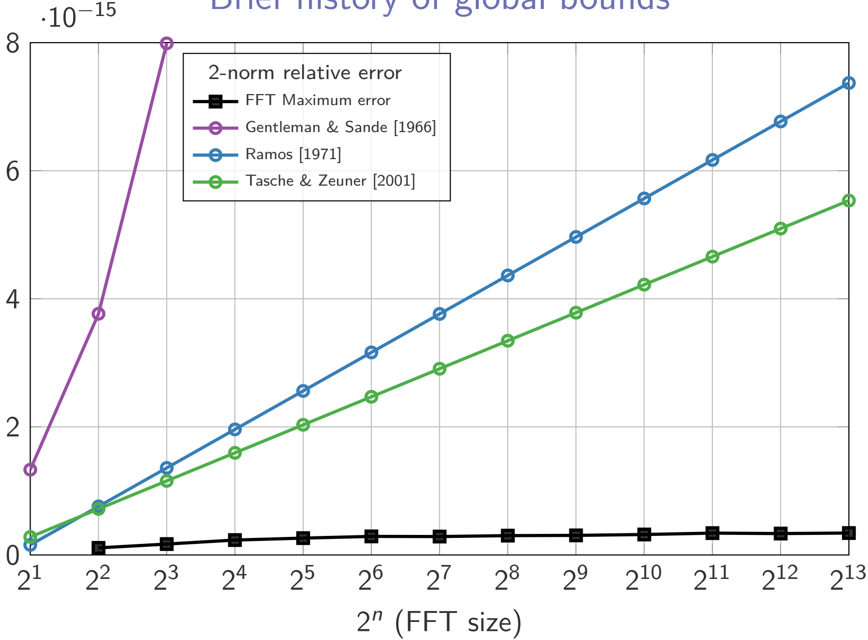

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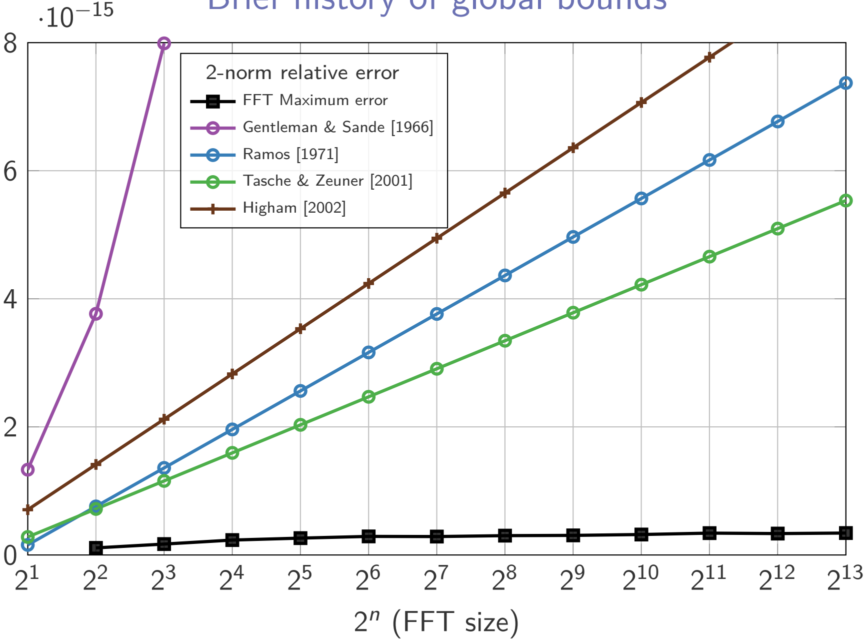

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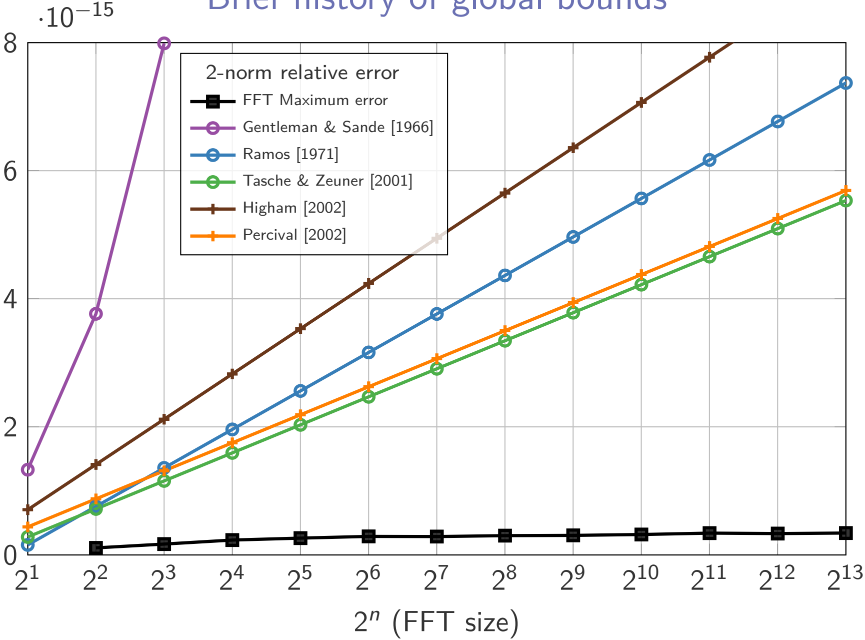

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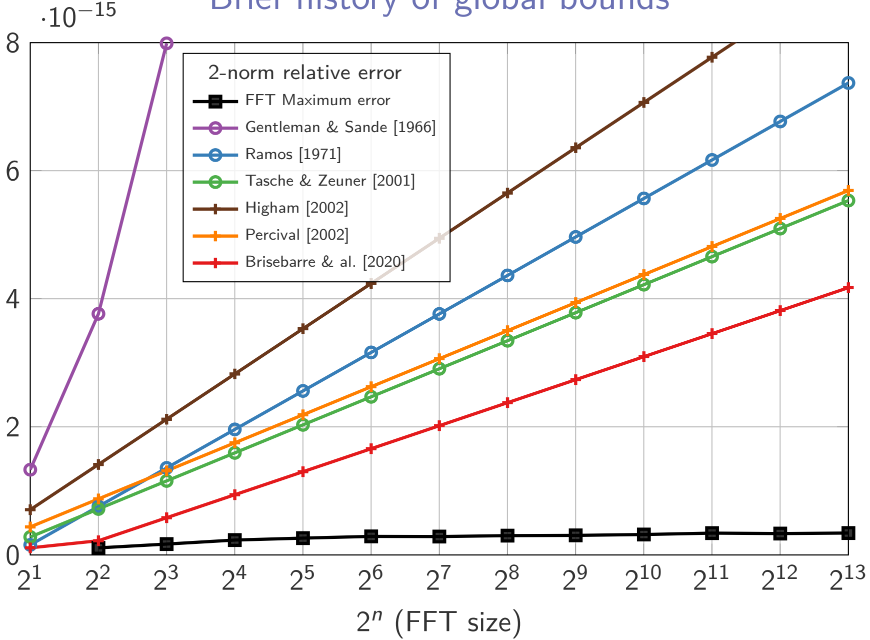

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