Fast Fourier transform at nonequispaced knots

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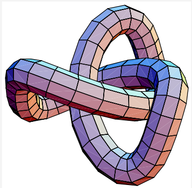


Content

- FFT, introduction
- Fourier analysis, basic properties
- NFFT
- Applications of NFFTs

FFT

The FFT is, without doubt, one of the most important algorithm in applied mathematics and engineering.

”The Fast Fourier transform (FFT) is one of the truly great computational developments of this century. It has changed the face of science and engineering so that it is not an exaggeration to say that life as we know it would be very different without FFT.” (Charles Van Loan)

1805 Carl Friedrich Gauß used an algorithm similar to FFT.
1903 Runge
1942 Danielson and Lanczos
1965 Cooley and Tukey


Gauß


Runge


Lanczos


Tukey

Problem: fast computation of

$$f(x_j) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x_j} \qquad (j = -M/2, \dots, M/2-1)$$

$$h(k) = \sum_{j=-M/2}^{M/2-1} f_j \, \mathrm{e}^{2\pi \mathrm{i} k x_j} \qquad (k = -N/2, \dots, N/2-1)$$

$$x_j \in [-1/2, 1/2)$$

for equispaced nodes x_j and $N = M$

$$x_j := \frac{j}{N} \quad (j = -N/2, \dots, N/2-1)$$

FFT in $\mathcal{O}(N \log N)$ instead of $\mathcal{O}(N^2)$ flops

Content

- Basic properties
  - Fourier series, introduction
  - From Fourier series to DFT
  - DFT
  - FFT
  - Fourier transform
  - Poisson's summation formula
  - Summary
- NFFT

Fourier series

$L^2(\mathbb{T}) = L^2([-1/2, 1/2))$ Hilbert space $\int\limits_{-1/2}^{1/2} |f(x)|^2 \, \mathrm{d}x < \infty$

$$(f,g)_{L^2(\mathbb{T})} := \int\limits_{-1/2}^{1/2} f(x) \, \overline{g(x)} \, \mathrm{d}x, \qquad \|f\|_{L^2(\mathbb{T})} = \left(\int\limits_{-1/2}^{1/2} |f(x)|^2 \, \mathrm{d}x \right)^{\frac{1}{2}}$$

orthogonality property of the functions

$$\mathrm{e}_k := \mathrm{e}^{2\pi \mathrm{i} kx} = \cos 2\pi kx + \mathrm{i} \sin 2\pi kx$$

with respect to $(\ ,\ )_{L^2(\mathbb{T})}$, because:

$$(\mathrm{e}_j, \mathrm{e}_k)_{L^2(\mathbb{T})} = \int\limits_{-1/2}^{1/2} \mathrm{e}^{2\pi \mathrm{i} jx} \, \mathrm{e}^{-2\pi \mathrm{i} kx} \, \mathrm{d}x = \int\limits_{-1/2}^{1/2} \mathrm{e}^{2\pi \mathrm{i}(j-k)x} \, \mathrm{d}x$$

$$= \frac{1}{2\pi \mathrm{i}(j-k)} \, \mathrm{e}^{2\pi \mathrm{i}(j-k)x} \Big|_{-1/2}^{1/2} = 0 \qquad (j \neq k)$$

$f \in L^2([-1/2, 1/2])$ can be represented by

$$f(x) \;=\; \sum_{k=-\infty}^{\infty} c_k(f)\;\mathrm{e}^{2\pi \mathrm{i} k x} \quad \text{(complex Fourier series)}$$

with

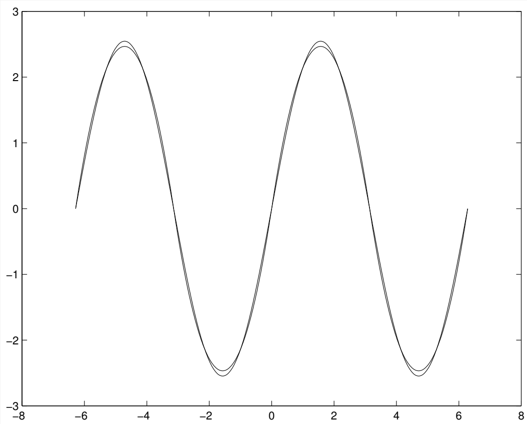
$$\begin{aligned} c_k(f) \;&=\; (f,\, \mathrm{e}_k)_{L^2(\mathbb{T})} \\ &=\; \int_{-1/2}^{1/2} f(x)\,\mathrm{e}^{-2\pi \mathrm{i} k x}\;\mathrm{d}x \quad \text{(Fourier coefficients)} \end{aligned}$$

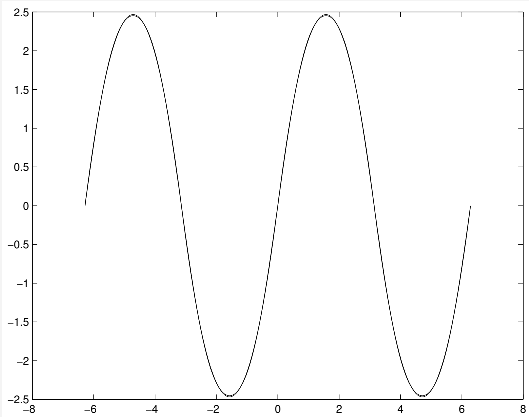
Theorem: Let f be a continuous one-periodic function with

$$\sum_{k=-\infty}^{\infty} |c_k(f)| < \infty\,,$$

then the Fourier series converges absolutely and uniformly.

Example of a Fourier series





Fourier series

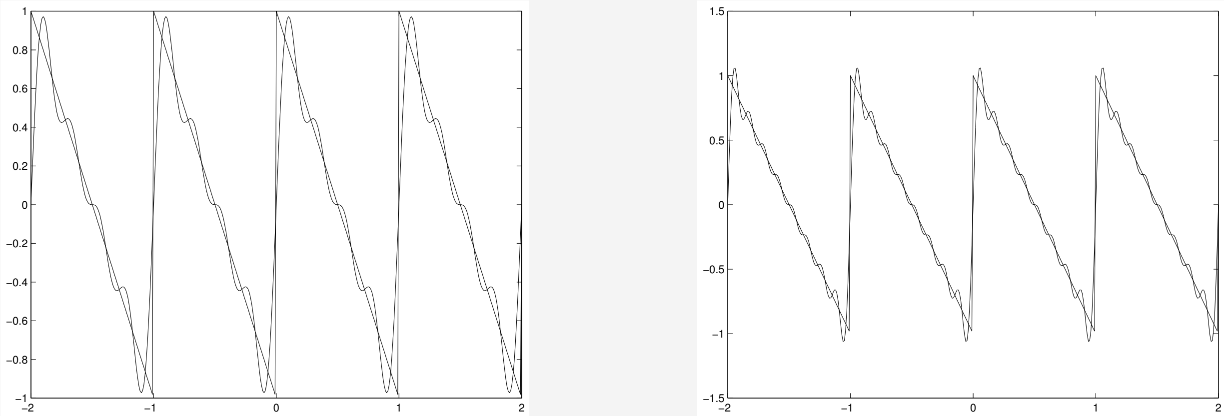
$$\frac{\pi}{8}\sum_{k=1}^{N}\frac{\sin((2k-1)x)}{(2k-1)^3}$$

of the 2π–periodic function

$$f(x)=\begin{cases} x(\pi-x) & x\in[0,\pi) \\ (\pi-x)(2\pi-x) & x\in[\pi,2\pi) \end{cases}$$

for $N=1$ and $N=2$

Example of a Fourier series



Fourier series

$$\sum_{k=1}^{N} \frac{2}{\pi} \frac{\sin(2\pi k x)}{k}$$

of the 1–periodic function

$$f(x) = -2x + 1$$

for $N = 4$ and $N = 8$

Properties of Fourier coefficients

Linearity

$$\begin{aligned} c_k(f+g) &= c_k(f) + c_k(g) \\ c_k(\lambda f) &= \lambda\, c_k(f) \end{aligned}$$

Symmetry

$$\begin{aligned} c_k(h) &= c_{-k}(f) \qquad \text{with} \quad h(x) := f(-x) \\ c_k(h) &= \overline{c_{-k}(f)} \qquad \text{with} \quad h(x) := \overline{f(x)} \end{aligned}$$

Shift Property - Modulation

$$\begin{aligned} c_k(h) &= \mathrm{e}^{2\pi \mathrm{i} x_0 k}\, c_k(f) \qquad \text{with} \quad h(x) := f(x - x_0) \\ c_k(h) &= c_{k-k_0}(f) \qquad \text{with} \quad h(x) := \mathrm{e}^{-2\pi \mathrm{i} k_0 x} f(x) \end{aligned}$$

Differentiation

$$c_k(h) = (2\pi \mathrm{i} k)^m\, c_k(f) \qquad \text{with} \quad h(x) := f^{(m)}(x)$$

Parseval's equation

Let l_2 be the Hilbert space of square-summable sequences $\boldsymbol{a} = (a_k)_{k\in\mathbb{Z}}$, such that

$$\sum_{k\in\mathbb{Z}} |a_k|^2 < \infty$$

with the inner product and norm defined by

$$(\boldsymbol{a}, \boldsymbol{b})_{l_2} := \sum_{k\in\mathbb{Z}} a_k \overline{b_k}, \quad ||\boldsymbol{a}||_{l_2} := \left(\sum_{k\in\mathbb{Z}} |a_k|^2 \right)^{\frac{1}{2}}.$$

For $f, g \in L^2(\mathbb{T})$ holds that

$$\boldsymbol{c}(f) := (c_k(f))_{k\in\mathbb{Z}}, \quad \boldsymbol{c}(g) := (c_k(g))_{k\in\mathbb{Z}} \in l_2$$

and

$$(\boldsymbol{c}(f), \boldsymbol{c}(g))_{l_2} = (f, g)_{L^2(\mathbb{T})}, \quad ||\boldsymbol{c}(f)||_{l_2} = ||f||_{L^2(\mathbb{T})}.$$

Basic properties (aliasing theorem for Fourier series)

Theorem: Let f be a one-periodic function with absolutely convergent Fourier series, i.e.,

$$f(x) = \sum_{k\in\mathbb{Z}} c_k(f)\ \mathrm{e}^{2\pi \mathrm{i} k x} \tag{1}$$

with Fourier coefficients

$$c_k(f) := \int_{-\frac{1}{2}}^{\frac{1}{2}} f(x)\ \mathrm{e}^{-2\pi \mathrm{i} k x} \mathrm{d}x. \tag{2}$$

If the $c_k(f)$ are approximated using the rectangle quadrature rule by the discrete Fourier coefficients $\frac{1}{n}\hat{f}_k$ $(k \in \mathbb{Z})$, where

$$\hat{f}_k := \sum_{j=-n/2}^{n/2-1} f\left(\frac{j}{n}\right)\ \mathrm{e}^{-2\pi \mathrm{i} j k/n} \tag{3}$$

then the following aliasing relation holds:

$$c_k(f) \approx \frac{1}{n}\hat{f}_k = c_k(f) + \tag{4}$$

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with Fourier coefficients

$$c_k(f) := \int_{-\frac{1}{2}}^{\frac{1}{2}} f(x)\ \mathrm{e}^{-2\pi \mathrm{i} k x} \mathrm{d}x. \tag{2}$$

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then the following aliasing relation holds:

$$c_k(f) \approx \frac{1}{n}\hat{f}_k = c_k(f) + \sum_{\substack{r \in \mathbb{Z} \\ r \neq 0}} c_{k+rn}(f). \tag{4}$$

Proof: Substituting the Fourier expansion of f from (1) into the definition of the $\hat{f}_k$ (given in (3)) yields

$$\frac{1}{n}\hat{f}_k = \frac{1}{n}\sum_{j=-n/2}^{n/2-1}\sum_{l\in\mathbb{Z}} c_l(f)\ \mathrm{e}^{2\pi\mathrm{i}lj/n}\ \mathrm{e}^{-2\pi\mathrm{i}jk/n}$$
$$= \sum_{l\in\mathbb{Z}} c_l(f)\,\frac{1}{n}\sum_{j=-n/2}^{n/2-1} \mathrm{e}^{2\pi\mathrm{i}j(l-k)/n}$$
$$= \sum_{l\in\mathbb{Z}} c_l(f)\,\frac{1}{n}\sum_{j=0}^{n-1} \mathrm{e}^{2\pi\mathrm{i}j(l-k)/n}. \tag{5}$$

We claim that

$$\frac{1}{n}\sum_{j=0}^{n-1} \mathrm{e}^{2\pi\mathrm{i}j(l-k)/n} = \begin{cases} 1 & \text{if } \frac{l-k}{n}\in\mathbb{Z} \\ 0 & \text{otherwise.}\end{cases} \tag{6}$$

In the case where $\frac{l-k}{n}\in\mathbb{Z}$, this holds because all terms in the sum are 1.

In the case where $\frac{l-k}{n} \notin \mathbb{Z}$, we apply the geometrical sum

$$\sum_{k=0}^{n-1} q^k = \frac{q^n - 1}{q - 1}\,.$$

This yields

$$\sum_{j=0}^{n-1} \mathrm{e}^{2\pi \mathrm{i} j(l-k)/n} = \frac{\mathrm{e}^{2\pi \mathrm{i}(l-k)} - 1}{\mathrm{e}^{2\pi \mathrm{i}(l-k)/n} - 1} = \frac{0}{\mathrm{e}^{2\pi \mathrm{i}(l-k)/n} - 1} = 0$$

because $\frac{l-k}{n} \notin \mathbb{Z}$ and thus $\mathrm{e}^{2\pi \mathrm{i}(l-k)/n} \neq 1$.
Applying (6) to (5) yields

$$\frac{1}{n}\hat{f}_k = \sum_{\substack{l \in \mathbb{Z} \\ (l-k)/n \in \mathbb{Z}}} c_l(f) = \sum_{r \in \mathbb{Z}} c_{k+rn}(f) = c_k(f) + \sum_{\substack{r \in \mathbb{Z} \\ r \neq 0}} c_{k+rn}(f).$$

■

Corollary: If f is a one-periodic function of which only the lowest n Fourier coefficients are non-zero, i.e.,

$$f(x) = \sum_{k=-n/2}^{n/2-1} c_k(f)\ \mathrm{e}^{2\pi \mathrm{i} k x},$$

then the approximation $\frac{1}{n}\hat{f}_k$ for the Fourier coefficients is exact for $k = -n/2, \ldots, n/2 - 1$. $\square$

Definitions:

Index-set

$$I_N^d := \left\{ \boldsymbol{k} \in \mathbb{Z}^d : -\frac{N}{2}\mathbf{1}_d \le \boldsymbol{k} < \frac{N}{2}\mathbf{1}_d \right\}$$

with $\mathbf{1}_d := (1, \ldots, 1)^{\mathrm{T}} \in \mathbb{Z}^d$, inequalities hold componentwise

torus $\mathbb{T}^d$

$$\mathbb{T}^d := \{\boldsymbol{x} = (x_1, \ldots, x_d)^{\mathrm{T}} \in \mathbb{R}^d ; -1/2 \le x_t < 1/2, t = 1, \ldots, d\}$$

$$\boldsymbol{x}\boldsymbol{k} = k_1 x_1 + k_2 x_2 + \ldots + k_d x_d$$

Basic properties (aliasing theorem for d-variate Fourier series)

Theorem: Let $f \in L^2(\mathbb{T}^d)$ be a one-periodic function with absolutely convergent Fourier series, i.e.

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}^d} c_{\boldsymbol{k}}(f)\ \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}$$

with Fourier coefficients

$$c_{\boldsymbol{k}}(f) := \int_{\mathbb{T}^d} f(\boldsymbol{x})\ \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}\mathrm{d}\boldsymbol{x}.$$

If the $c_{\boldsymbol{k}}(f)$ are approximated by the discrete Fourier coefficients $\hat{f}_{\boldsymbol{k}}$ $(\boldsymbol{k} \in \mathbb{Z}^d)$ as

$$\hat{f}_{\boldsymbol{k}} := \sum_{\boldsymbol{j}\in I_n^d} f\left(\frac{\boldsymbol{j}}{n}\right)\ \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{j}\boldsymbol{k}/n}$$

using the rectangle quadrature rule, then the following aliasing relation holds:

$$c_{\boldsymbol{k}}(f) \approx \frac{1}{n^d}\hat{f}_{\boldsymbol{k}} = c_{\boldsymbol{k}}(f) + \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^d\\ \boldsymbol{r}\neq\boldsymbol{0}}} c_{\boldsymbol{k}+n\boldsymbol{r}}(f).$$

Basic properties (DFT)

The discrete Fourier transform (DFT) of a vector $\boldsymbol{f} = (f_j)_{j=-n/2}^{n/2-1} \in \mathbb{C}^n$ is given by

$$\hat{f}_k := \sum_{j=-n/2}^{n/2-1} f_j \, \mathrm{e}^{-2\pi \mathrm{i} jk/n} \quad (k = -n/2, \ldots, n/2-1)\,. \tag{7}$$

matrix–vector form

$$\hat{\boldsymbol{f}} := (\hat{f}_j)_{j=-n/2}^{n/2}, \; \boldsymbol{F}_n := \left(\mathrm{e}^{-2\pi \mathrm{i} kj/n}\right)_{j=-n/2,k=-n/2}^{n/2-1,n/2-1}$$

$$\hat{\boldsymbol{f}} = \boldsymbol{F}_n \boldsymbol{f}$$

Theorem: The discrete inverse Fourier transform (IDFT) of the vector $\hat{\boldsymbol{f}} \in \mathbb{C}^n$ is given by

$$f_j = \frac{1}{n} \sum_{k=-n/2}^{n/2-1} \hat{f}_k \, \mathrm{e}^{2\pi \mathrm{i} jk/n} \quad (j = -n/2, \ldots, n/2-1)\,. \tag{8}$$

Proof: To prove that (8) holds, substitute (8) into (7).

$$\begin{aligned}
\sum_{j=-n/2}^{n/2-1} f_j \; \mathrm{e}^{-2\pi \mathrm{i} jk/n} &= \sum_{j=-n/2}^{n/2-1} \frac{1}{n} \sum_{r=-n/2}^{n/2-1} \hat{f}_r \; \mathrm{e}^{2\pi \mathrm{i} jr/n} \; \mathrm{e}^{-2\pi \mathrm{i} jk/n} \\
&= \frac{1}{n} \sum_{r=-n/2}^{n/2-1} \hat{f}_r \left(\sum_{j=-n/2}^{n/2-1} \mathrm{e}^{2\pi \mathrm{i} jr/n} \; \mathrm{e}^{-2\pi \mathrm{i} jk/n} \right) \\
&= \hat{f}_k
\end{aligned}$$

The identity follows from the orthogonality relation:

$$\sum_{j=-n/2}^{n/2-1} \mathrm{e}^{2\pi \mathrm{i} jr/n} \; \mathrm{e}^{-2\pi \mathrm{i} jk/n} = \begin{cases} n & \text{if } r = k \\ 0 & \text{otherwise} \end{cases}$$

(see (6)).

$\mathbf{F}_n$ contains only n different values;

$\mathrm{e}^{-2\pi \mathrm{i} k/n}$ $(k \in \mathbb{Z})$ is n periodic

Example:

$$\boldsymbol{F}_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \boldsymbol{F}_3 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & \theta & \theta^2 \\ 1 & \theta^2 & \theta \end{pmatrix}, \quad \boldsymbol{F}_4 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -\mathrm{i} & -1 & \mathrm{i} \\ 1 & -1 & 1 & -1 \\ 1 & \mathrm{i} & -1 & -\mathrm{i} \end{pmatrix},$$

with

$$\theta := \mathrm{e}^{-2\pi \mathrm{i}/3}$$

Basic properties (FFT)

Computation of the DFT by standard matrix-vector multiplication would take order $\mathcal{O}(n^2)$ operations. The Fast Fourier Transform (FFT) speeds up this computation to $\mathcal{O}(n \log n)$ by using a divide-and-conquer approach. Namely, the FFT reduces solving the problem of size n to two problems of size $n/2$ at the cost of only $\mathcal{O}(n)$. Since the recursive application of this method will result in approximately $\log n$ halving steps, the result is $\mathcal{O}(n \log n)$ running time. The idea behind the FFT is highlighted by the following formula:

$$\boldsymbol{F}_n = \begin{bmatrix} odd - even \\ permutation \end{bmatrix} \begin{bmatrix} \boldsymbol{F}_{n/2} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{F}_{n/2} \end{bmatrix} \begin{bmatrix} \boldsymbol{I}_{n/2} & \boldsymbol{I}_{n/2} \\ \boldsymbol{W} & -\boldsymbol{W} \end{bmatrix}$$

where $\boldsymbol{W} =$ diag$(1,\, \mathrm{e}^{-2\pi \mathrm{i} 1/n},\, \mathrm{e}^{-2\pi \mathrm{i} 2/n}, \ldots,\, \mathrm{e}^{-2\pi \mathrm{i}(n/2-1)/n})$.

Software: e.g. FFTW

FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions.

The FFTW package was developed at MIT by Matteo Frigo and Steven G. Johnson (see http://www.fftw.org/).

FFT (main idea)

$N = 2^n$ $(n \in \mathbb{N})$ divide and conquer

compute DFT(N) (= DFT of size N)

$$\begin{aligned} \hat{f}_k &= \sum_{j=0}^{N-1} f_j \, \mathrm{e}^{-2\pi \mathrm{i} jk/N} \qquad (k = 0, \ldots, N-1) \\ &= \sum_{j=0}^{N-1} f_j w_N^{jk} \qquad , \; w_N := \mathrm{e}^{-2\pi \mathrm{i}/N} \end{aligned}$$

Decimation-in-frequency or Sande-Tukey-algorithm

divide the above sum

$$\hat{f}_k = \sum_{j=0}^{\frac{N}{2}-1} f_j w_N^{jk} + \sum_{j=0}^{\frac{N}{2}-1} f_{\frac{N}{2}+j} w_N^{\left(\frac{N}{2}+j\right)k} \quad (k = 0, \ldots, N-1)$$

case 1.: $k = 2l \quad (l = 0, \dots, \frac{N}{2} - 1)$

$$\hat{f}_{2l} = \sum_{j=0}^{\frac{N}{2}-1} f_j w_N^{2jl} + \sum_{j=0}^{\frac{N}{2}-1} f_{\frac{N}{2}+j} w_N^{\left(\frac{N}{2}+j\right)2l} \quad (k = 0, \dots, N-1).$$

note that

$$w_N^{\left(\frac{N}{2}+j\right)2l} = \mathrm{e}^{-2\pi \mathrm{i}\left(\frac{N}{2}+j\right)\frac{2l}{N}} = \mathrm{e}^{-2\pi \mathrm{i} l}\, \mathrm{e}^{-2\pi \mathrm{i} jl/(N/2)} = w_{\frac{N}{2}}^{jl},$$

hence

$$\begin{aligned} \hat{f}_{2l} &= \sum_{j=0}^{\frac{N}{2}-1} f_j w_{\frac{N}{2}}^{jl} + \sum_{j=0}^{\frac{N}{2}-1} f_{\frac{N}{2}+j} w_{\frac{N}{2}}^{jl}, \\ \hat{f}_{2l} &= \sum_{j=0}^{\frac{N}{2}-1} \left(f_j + f_{\frac{N}{2}+j}\right) w_{\frac{N}{2}}^{jl} \quad (l = 0, \dots, \frac{N}{2} - 1). \end{aligned}$$

$\frac{N}{2}$ additions $f_j + f_{\frac{N}{2}+j} \quad (j = 0, \dots, \frac{N}{2} - 1)$,
compute DFT$(\frac{N}{2})$

case 2.: $k = 2l+1 \quad (l = 0, \ldots, \frac{N}{2}-1)$

$$\hat{f}_{2l+1} = \sum_{j=0}^{\frac{N}{2}-1} f_j w_N^{j(2l+1)} + \sum_{j=0}^{\frac{N}{2}-1} f_{\frac{N}{2}+j} w_N^{\left(\frac{N}{2}+j\right)(2l+1)} \quad (l = 0, \ldots, \frac{N}{2}-1).$$

note that

$$w_N^{\left(\frac{N}{2}+j\right)(2l+1)} = w_N^{\frac{N}{2}(2l+1)} w_N^{j(2l+1)} = \mathrm{e}^{-2\pi\mathrm{i}\frac{N}{2}\frac{2l+1}{N}} w_N^j w_{\frac{N}{2}}^{jl} = -w_N^j w_{\frac{N}{2}}^{jl},$$

hence

$$\begin{aligned}
\hat{f}_{2l+1} &= \sum_{j=0}^{\frac{N}{2}-1} f_j w_{\frac{N}{2}}^{jl} w_N^j - \sum_{j=0}^{\frac{N}{2}-1} f_{\frac{N}{2}+j} w_{\frac{N}{2}}^{jl} w_N^j, \\
\hat{f}_{2l+1} &= \sum_{j=0}^{\frac{N}{2}-1} \left(f_j - f_{\frac{N}{2}+j}\right) w_N^j w_{\frac{N}{2}}^{jl} \quad (l = 0, \ldots, \frac{N}{2}-1).
\end{aligned}$$

$\frac{N}{2}$ additions $(f_j - f_{\frac{N}{2}+j})$ $(j = 0, \ldots, \frac{N}{2} - 1)$ and

$\frac{N}{2}$ multiplications with **twiddle factors** w_N^j $(j = 0, \ldots, \frac{N}{2} - 1)$

compute DFT$(\frac{N}{2})$

Summary: DFT(N) can computed with
N additions, $\frac{N}{2}$ multiplications and 2 DFT$(\frac{N}{2})$
with a recursive procedure

$$\text{DFT}(N) \underbrace{\xrightarrow{1.}}_{\substack{N \text{ add.} \\ \frac{N}{2} \text{ mult.}}} 2\,\text{DFT}\left(\frac{N}{2}\right) \underbrace{\xrightarrow{2.}}_{\substack{2\cdot\frac{N}{2} \text{ add.} \\ 2\cdot\frac{N}{4} \text{ mult.}}} 4\,\text{DFT}\left(\frac{N}{4}\right) \longrightarrow \cdots \xrightarrow{n.} N \underbrace{\text{DFT}(1)}_{\text{output}}$$

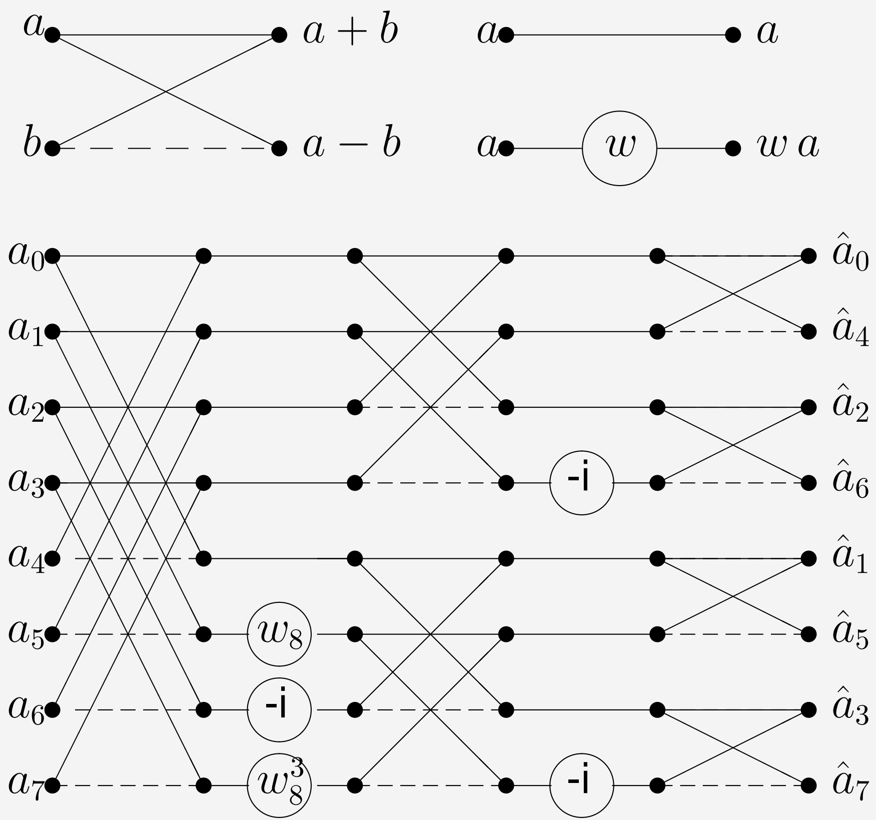
altogether

$n \cdot N$ add. + $n \cdot \frac{N}{2}$ mult., i.e.,

$\mathcal{O}(Nn) = \mathcal{O}(N \log N)$ arithmetical operations

FFT Flow Graphs

Example: decimation-in-frequency: $N = 8$



Fourier transform

$L^p = L^p(\mathbb{R})$ $(1 \le p \le \infty)$ Banach space

norm

$$||f||_{L^p} := \left(\int_{-\infty}^{\infty} |f(x)|^p \, \mathsf{d}x \right)^{1/p}$$

The Fourier transform $\hat{f}$ of $f \in L^1(\mathbb{R})$ is given by

$$\hat{f}(v) := \int_{-\infty}^{\infty} f(t)\, \mathrm{e}^{-2\pi \mathrm{i} v t} \, \mathsf{d}t \quad (v \in \mathbb{R})$$

Example:

1. **characteristic function**

$$f(x) := \begin{cases} 1 & \text{if} \quad |x| < L, \\ \frac{1}{2} & \text{if} \quad x = \pm L, \\ 0 & \quad \text{else} \end{cases} \qquad (L > 0)$$

$$\begin{aligned} \hat{f}(v) &= \int_{-L}^{L} \mathrm{e}^{-2\pi \mathrm{i} v x} \, \mathrm{d}x = -\frac{1}{2\pi \mathrm{i} v} \mathrm{e}^{-2\pi \mathrm{i} v x} \Big|_{-L}^{L} \\ &= \frac{-\mathrm{e}^{-2\pi \mathrm{i} v L} + \mathrm{e}^{2\pi \mathrm{i} v L}}{2\pi \mathrm{i} v} = \frac{2\mathrm{i} L \sin(2\pi v L)}{\mathrm{i} 2\pi v L} \\ &= 2L \operatorname{sinc}(2\pi L v) \end{aligned}$$

with **sinc-function**

$$\operatorname{sinc} x := \begin{cases} \frac{\sin x}{x} & \text{if} \quad x \neq 0, \\ 1 & \text{if} \quad x = 0. \end{cases} \tag{9}$$

Example:

1. The Gaussian function

$$f(x) = \mathrm{e}^{-x^2}$$

We claim that

$$\hat{f}(v) = \sqrt{\pi}\,\mathrm{e}^{-v^2\pi^2}\,. \tag{10}$$

Proof:

$$\left(\int_{-\infty}^{\infty} \mathrm{e}^{-t^2}\,\mathrm{d}t\right)^2 = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\,\mathrm{d}x \int_{-\infty}^{\infty} \mathrm{e}^{-y^2}\,\mathrm{d}y$$
$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-(x^2+y^2)}\,\mathrm{d}x\,\mathrm{d}y$$

with $x = r\cos\varphi,\ y = r\sin\varphi \quad (r \geq 0,\ 0 \leq \varphi < 2\pi)$

$$
\begin{aligned}
\left(\int_{-\infty}^{\infty} \mathrm{e}^{-t^2}\,\mathrm{d}t\right)^2 &= \int_0^{2\pi}\int_0^{\infty} \mathrm{e}^{-r^2} r\,\mathrm{d}r\,\mathrm{d}\varphi = \frac{1}{2}\int_0^{2\pi}\int_0^{\infty} \mathrm{e}^{-s}\,\mathrm{d}s\,\mathrm{d}\varphi \\
&= -\pi\,\mathrm{e}^{-s}\Big|_0^{\infty} \\
&= \pi
\end{aligned}
$$

hence

$$
\hat{f}(0) = \int_{-\infty}^{\infty} \mathrm{e}^{-t^2}\,\mathrm{d}t = \sqrt{\pi} \tag{11}
$$

The Fourier transform of f is given by

$$
\hat{f}(v) = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\,\mathrm{e}^{-2\pi \mathrm{i} v x}\,\mathrm{d}x\,.
$$

The exponent can be rewritten (by completing the square) as

$$
-x^2 - 2\pi \mathrm{i} v x = -(x + \pi \mathrm{i} v)^2 - \pi^2 v^2
$$

and then

$$\hat{f}(v) = \mathrm{e}^{-\pi^2 v^2} \int_{-\infty}^{\infty} \mathrm{e}^{-(x+\pi \mathrm{i} v)^2} \, \mathrm{d}x$$

put $x + \pi \mathrm{i} v = z$, so that $\mathrm{d}x = \mathrm{d}z$. Then by (11)

$$\hat{f}(v) = \mathrm{e}^{-\pi^2 v^2} \int_{-\infty}^{\infty} \mathrm{e}^{-z^2} \, \mathrm{d}z = \sqrt{\pi}\, \mathrm{e}^{-\pi^2 v^2} .$$

■

Basic properties (Poisson's summation formula)

Let $\varphi \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$ given, such that

$$\tilde{\varphi}(x) := \sum_{r \in \mathbb{Z}} \varphi(x+r)$$

has an uniformly convergent Fourier series

$$\tilde{\varphi}(x) = \sum_{k \in \mathbb{Z}} c_k(\tilde{\varphi}) \, \mathrm{e}^{2\pi \mathrm{i} k x}$$

with Fourier coefficients

$$c_k(\tilde{\varphi}) := \int_{-1/2}^{1/2} \tilde{\varphi}(x) \, \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{d}x \quad (k \in \mathbb{Z}) \, .$$

If the Fourier transform

$$\hat{\varphi}(k) := \int_{\mathbb{R}} \varphi(x) \, \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{d}x$$

of φ is known, then $c_k(\tilde{\varphi})$ can be obtained by sampling $\hat{\varphi}$ at the frequencies $k \in \mathbb{Z}$, i.e. $\hat{\varphi}(k) = c_k(\tilde{\varphi})$, because

$$
\begin{aligned}
c_k(\tilde{\varphi}) &= \int_{-1/2}^{1/2} \tilde{\varphi}(x)\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&= \int_{-1/2}^{1/2} \sum_{r\in\mathbb{Z}} \varphi(x+r)\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&= \sum_{\boldsymbol{r}\in\mathbb{Z}} \int_{-1/2}^{1/2} \varphi(x+r)\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&= \sum_{r\in\mathbb{Z}} \int_{-1/2+r}^{1/2+r} \varphi(y)\, \mathrm{e}^{-2\pi \mathrm{i} k y}\, \underbrace{\mathrm{e}^{2\pi \mathrm{i} k r}}_{=1}\, \mathrm{d}y \\
&= \int_{\mathbb{R}} \varphi(y)\, \mathrm{e}^{-2\pi \mathrm{i} k y}\, \mathrm{d}y \\
&= \hat{\varphi}(k)\,.
\end{aligned}
$$

Basic properties d-variate Poisson's summation formula

Let $\varphi \in L^2(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$ given, such that

$$\tilde{\varphi}(\boldsymbol{x}) := \sum_{\boldsymbol{r} \in \mathbb{Z}^d} \varphi(\boldsymbol{x} + \boldsymbol{r})$$

has an uniformly convergent Fourier series

$$\tilde{\varphi}(\boldsymbol{x}) = \sum_{\boldsymbol{k} \in \mathbb{Z}^d} c_{\boldsymbol{k}}(\tilde{\varphi})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\boldsymbol{x}}$$

with Fourier coefficients

$$c_{\boldsymbol{k}}(\tilde{\varphi}) := \int_{\mathbb{T}^d} \tilde{\varphi}(\boldsymbol{x})\, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{x} \quad (\boldsymbol{k} \in \mathbb{Z}^d)\,.$$

If the Fourier transform

$$\hat{\varphi}(\boldsymbol{k}) := \int_{\mathbb{R}^d} \varphi(\boldsymbol{x})\, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{x}$$

of φ is known, then $c_{\boldsymbol{k}}(\tilde{\varphi})$ can be obtained by sampling $\hat{\varphi}$ at the frequencies
$\boldsymbol{k} \in \mathbb{Z}^d$, i.e. $\hat{\varphi}(\boldsymbol{k}) = c_{\boldsymbol{k}}(\tilde{\varphi})$, because

$$
\begin{aligned}
c_{\boldsymbol{k}}(\tilde{\varphi}) &= \int_{\mathbb{T}^d} \tilde{\varphi}(\boldsymbol{x})\,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x} \\
&= \int_{\mathbb{T}^d} \sum_{\boldsymbol{r}\in\mathbb{Z}^d} \varphi(\boldsymbol{x}+\boldsymbol{r})\,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x} \\
&= \sum_{\boldsymbol{r}\in\mathbb{Z}^d} \int_{\mathbb{T}^d} \varphi(\boldsymbol{x}+\boldsymbol{r})\,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x} \\
&= \sum_{\boldsymbol{r}\in\mathbb{Z}^d} \int_{-1/2+r_1}^{1/2+r_1} \dots \int_{-1/2+r_d}^{1/2+r_d} \varphi(\boldsymbol{y})\,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}(\boldsymbol{y}-\boldsymbol{r})}\,\mathrm{d}\boldsymbol{y} \\
&= \int_{\mathbb{R}^d} \varphi(\boldsymbol{y})\,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{y}}\,\mathrm{d}\boldsymbol{y} \\
&= \hat{\varphi}(\boldsymbol{k})\,. \qquad (12)
\end{aligned}
$$

Four different Fourier transforms can be defined by sampling in time (space) and frequency domains

	continuous time	discrete time
continuous frequency		
discrete frequency		

Four different Fourier transforms can be defined by sampling in time (space) and frequency domains

	continuous time	discrete time
continuous frequency	Fourier Transform	
discrete frequency		

Four different Fourier transforms can be defined by sampling in time (space) and frequency domains

	continuous time	discrete time
continuous frequency	Fourier Transform	semidiscrete Fourier transform
discrete frequency		

Four different Fourier transforms can be defined by sampling in time (space) and frequency domains

	continuous time	discrete time
continuous frequency	Fourier Transform	semidiscrete Fourier transform
discrete frequency	Fourier series	

Four different Fourier transforms can be defined by sampling in time (space) and frequency domains

	continuous time	discrete time
continuous frequency	Fourier Transform	semidiscrete Fourier transform
discrete frequency	Fourier series	discrete Fourier transform

Fourier transform

forward:

inverse:

periodicity:

Fourier transform

forward: $$\hat{f}(v) = \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-2\pi \mathrm{i} v x}\,\mathrm{d}x$$

inverse:

periodicity:

Fourier transform

forward: $$\hat{f}(v) = \int\limits_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-2\pi \mathrm{i} v x}\,\mathrm{d}x$$

inverse: $$f(x) = \int\limits_{-\infty}^{\infty} \hat{f}(v)\,\mathrm{e}^{2\pi \mathrm{i} v x}\,\mathrm{d}x$$

periodicity:

Fourier transform

forward: $$\hat{f}(v) = \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-2\pi \mathrm{i} v x}\,\mathrm{d}x$$

inverse: $$f(x) = \int_{-\infty}^{\infty} \hat{f}(v)\,\mathrm{e}^{2\pi \mathrm{i} v x}\,\mathrm{d}x$$

periodicity: none

semidiscrete Fourier transform

forward:

inverse:

periodicity:

semidiscrete Fourier transform

forward: $$\hat{f}(v) = \sum_{j=-\infty}^{\infty} f(j)\,\mathrm{e}^{-2\pi \mathrm{i} v j}$$

inverse:

periodicity:

semidiscrete Fourier transform

forward: $$\hat{f}(v) = \sum_{j=-\infty}^{\infty} f(j)\, \mathrm{e}^{-2\pi \mathrm{i} v j}$$

inverse: $$f(j) = \int_{-1/2}^{1/2} \hat{f}(v)\, \mathrm{e}^{2\pi \mathrm{i} v j}\, \mathrm{d}v$$

periodicity:

semidiscrete Fourier transform

forward: $$\hat{f}(v) = \sum_{j=-\infty}^{\infty} f(j)\,\mathrm{e}^{-2\pi \mathrm{i} v j}$$

inverse: $$f(j) = \int_{-1/2}^{1/2} \hat{f}(v)\,\mathrm{e}^{2\pi \mathrm{i} v j}\,\mathrm{d}v$$

periodicity: $\hat{f}(v) = \hat{f}(v+1)$

Fourier series

forward:

inverse:

periodicity:

Fourier series

forward: $$c_k(f) = \int_{-1/2}^{1/2} f(x)\,\mathrm{e}^{-2\pi \mathrm{i} k x}\,\mathrm{d}x$$

inverse:

periodicity:

Fourier series

forward: $$c_k(f) = \int_{-1/2}^{1/2} f(x)\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x$$

inverse: $$f(x) = \sum_{k=-\infty}^{\infty} c_k(f)\, \mathrm{e}^{2\pi \mathrm{i} k x}\, \mathrm{d}x$$

periodicity:

Fourier series

forward: $$c_k(f) = \int_{-1/2}^{1/2} f(x)\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x$$

inverse: $$f(x) = \sum_{k=-\infty}^{\infty} c_k(f)\, \mathrm{e}^{2\pi \mathrm{i} k x}\, \mathrm{d}x$$

periodicity: $f(x) = f(x+1)$

discrete Fourier transform

forward:

inverse:

periodicity:

discrete Fourier transform

forward: $$\hat{f}_k = \sum_{j=0}^{N-1} f_j \, \mathrm{e}^{-2\pi \mathrm{i} jk/N}$$

inverse:

periodicity:

discrete Fourier transform

forward: $$\hat{f}_k = \sum_{j=0}^{N-1} f_j \, \mathrm{e}^{-2\pi \mathrm{i} jk/N}$$

inverse: $$f_j = \frac{1}{N} \sum_{k=0}^{N-1} \hat{f}_k \, \mathrm{e}^{2\pi \mathrm{i} jk/N}$$

periodicity:

discrete Fourier transform

forward: $$\hat{f}_k = \sum_{j=0}^{N-1} f_j \, \mathrm{e}^{-2\pi \mathrm{i} jk/N}$$

inverse: $$f_j = \frac{1}{N} \sum_{k=0}^{N-1} \hat{f}_k \, \mathrm{e}^{2\pi \mathrm{i} jk/N}$$

periodicity: $\hat{f}_k = \hat{f}_{k+rN} \, ; f_j = f_{j+rN}$

Content

References: G. Steidl [42]; P., G. Steidl, M. Tasche [38]; S. Kunis, P. [23]

- NFFT
  - NFFT-1D
  - NFFT-1D, algorithm
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  - NFFT-1D, error estimates
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NFFT–1D

Problem: fast computation of

$$f(x_j) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x_j} \qquad (j = -M/2, \ldots, M/2-1)$$

$$h(k) = \sum_{j=-M/2}^{M/2-1} f_j \, \mathrm{e}^{2\pi \mathrm{i} k x_j} \qquad (k = -N/2, \ldots, N/2-1)$$

$$x_j \in [-1/2, 1/2)$$

for equispaced nodes x_j and $N = M$

$$x_j := \frac{j}{N} \quad (j = -N/2, \ldots, N/2-1)$$

FFT in $\mathcal{O}(N \log N)$ flops

Problem: (NFFT) fast computation of

$$f(x_j) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x_j} \qquad (j = -M/2, \dots, M/2-1)$$

matrix–vector form

$$\hat{\boldsymbol{f}} := (\hat{f}_k)_{k=-N/2}^{N/2}, \; \boldsymbol{f} := (f(x_j))_{j=-M/2}^{M/2}, \; \boldsymbol{A} := (\mathrm{e}^{-2\pi \mathrm{i} k x_j})_{j=-M/2, k=-N/2}^{M/2-1, N/2-1}$$

$$\boldsymbol{f} = \boldsymbol{A} \hat{\boldsymbol{f}}$$

Problem: (NFFT$^{\mathsf{H}}$) fast computation of

$$h(k) = \sum_{j=-M/2}^{M/2-1} f_j \, \mathrm{e}^{2\pi \mathrm{i} k x_j} \qquad (j = -N/2, \dots, N/2-1)$$

matrix-vector multiplication with $\bar{\boldsymbol{A}}^{\mathrm{T}} = \boldsymbol{A}^{\mathsf{H}}$

Problem: (NFFT) evaluation of the 1–periodic function

$$f(x) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x}$$

at the nodes $x_j \; (j = -M/2, \ldots, M/2-1)$
Idea: approximate f by

$$s_1(x) := \sum_{l=-n/2}^{n/2-1} g_l \, \tilde{\varphi}(x - \frac{l}{n})$$

with $n := \sigma N \; (\sigma > 1)$, $\tilde{\varphi}$ is 1–periodic function
switching to the frequency domain

$$s_1(x) = \sum_{k=-\infty}^{\infty} c_k(s_1) \, \mathrm{e}^{-2\pi \mathrm{i} k x}$$

$$c_k(s_1) := \int_{-1/2}^{1/2} s_1(x) \mathrm{e}^{2\pi \mathrm{i} k x} \, \mathrm{d}x \quad (k \in \mathbb{Z})$$

$$
\begin{aligned}
c_k(s_1) &:= \int\limits_{-1/2}^{1/2} s_1(x)\mathrm{e}^{2\pi \mathrm{i} kx}\,\mathrm{d}x \quad (k \in \mathbb{Z}) \\
&= \int\limits_{-1/2}^{1/2} \sum_{l=-n/2}^{n/2-1} g_l\, \tilde{\varphi}(x - \frac{l}{n})\mathrm{e}^{2\pi \mathrm{i} kx}\,\mathrm{d}x \\
&= \sum_{l=-n/2}^{n/2-1} g_l \int\limits_{-1/2}^{1/2} \tilde{\varphi}(\underbrace{x - \frac{l}{n}}_{y})\mathrm{e}^{2\pi \mathrm{i} kx}\,\mathrm{d}x \\
&= \sum_{l=-n/2}^{n/2-1} g_l \mathrm{e}^{2\pi \mathrm{i} kl/n} \int\limits_{-1/2-l/n}^{1/2-l/n} \tilde{\varphi}(y)\mathrm{e}^{2\pi \mathrm{i} ky}\,\mathrm{d}y \\
&= \hat{g}_k\, c_k(\tilde{\varphi})
\end{aligned}
$$

hence

$$s_1(x) = \sum_{k=-\infty}^{\infty} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k x}$$

with discrete Fourier coefficients of g_l

$$\hat{g}_k := \sum_{l=-n/2}^{n/2-1} g_l \, \mathrm{e}^{2\pi \mathrm{i} k l / n}$$

and Fourier coefficients of $\tilde{\varphi}$

$$c_k(\tilde{\varphi}) := \int_{-1/2}^{1/2} \tilde{\varphi}(x) \mathrm{e}^{2\pi \mathrm{i} k v} \, \mathrm{d}x \quad (k \in \mathbb{Z})$$

note (12)

$$c_k(\tilde{\varphi}) = \hat{\varphi}(k)$$

compare

$$f(x) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x}$$

and

$$\begin{aligned} s_1(x) &= \sum_{k=-\infty}^{\infty} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k x} \\ &= \sum_{r=-\infty}^{\infty} \sum_{k=-n/2}^{n/2-1} \\ &= \end{aligned}$$

compare

$$f(x) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x}$$

and

$$\begin{aligned} s_1(x) &= \sum_{k=-\infty}^{\infty} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k x} \\ &= \sum_{r=-\infty}^{\infty} \sum_{k=-n/2}^{n/2-1} \underbrace{\hat{g}_{k+nr}}_{\hat{g}_k} \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} (k+nr) x} \\ &= \end{aligned}$$

compare

$$f(x) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x}$$

and

$$\begin{aligned} s_1(x) &= \sum_{k=-\infty}^{\infty} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k x} \\ &= \sum_{r=-\infty}^{\infty} \sum_{k=-n/2}^{n/2-1} \underbrace{\hat{g}_{k+nr}}_{\hat{g}_k} \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i}(k+nr)x} \\ &= \sum_{k=-n/2}^{n/2-1} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k x} + \end{aligned}$$

compare

$$f(x) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x}$$

and

$$\begin{aligned} s_1(x) &= \sum_{k=-\infty}^{\infty} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k x} \\ &= \sum_{r=-\infty}^{\infty} \sum_{k=-n/2}^{n/2-1} \underbrace{\hat{g}_{k+nr}}_{\hat{g}_k} \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i}(k+nr)x} \\ &= \sum_{k=-n/2}^{n/2-1} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k x} + \sum_{\substack{r=-\infty \\ r \neq 0}}^{\infty} \sum_{k=-n/2}^{n/2-1} \hat{g}_k \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i}(k+nr)x} \end{aligned}$$

$$\hat{g}_k := \hat{g}_{k+rn} = \begin{cases} \hat{f}_k / c_k(\tilde{\varphi}) & k = -N/2, \ldots, N/2-1, \\ 0 & k = -n/2, \ldots, -N/2-1; N/2, \ldots, n/2-1 \end{cases} \tag{13}$$

$$s_1(x) = \sum_{l=-n/2}^{n/2-1} g_l \, \tilde{\varphi}(x - \frac{l}{n}).$$

suppose $\tilde{\varphi}$ is small outside $[-m/n, m/n]$ $(m << n)$
approximate φ by compactly supported function

$$\psi(x) := \begin{cases} \varphi(x) & \text{if } x \in [-m/n, m/n], \\ 0 & \text{else,} \end{cases} \tag{14}$$

and approximate $\tilde{\varphi}$ by 1–periodic function

$$\tilde{\psi}(x) := \sum_{r \in \mathbb{Z}} \psi(x + r) \, \in L^2(\mathbb{T}).$$

for $j = -M/2, \ldots, M/2 - 1$ compute

$$f(x_j) \approx s_1(x_j) \approx s(x_j) := \sum_{l=\lfloor x_j n \rfloor - m}^{\lceil x_j n \rceil + m} g_l \, \tilde{\psi}\left(x_j - \frac{l}{n}\right)$$

Algorithm (NFFT)

1. For $k = -N/2, \ldots, N/2-1$ compute

$$\hat{g}_k := \hat{f}_k / c_k(\tilde{\varphi}).$$

2. For $l = -n/2, \ldots, n/2-1$ compute by FFT(n)

$$g_l := \frac{1}{n} \sum_{k=-N/2}^{N/2-1} \hat{g}_k \, \mathrm{e}^{-2\pi \mathrm{i} k l / n}. \tag{15}$$

3. For $j = -M/2, \ldots, M/2-1$ compute

$$s(x_j) := \sum_{l=\lfloor x_j n \rfloor - m}^{\lceil x_j n \rceil + m} g_l \, \tilde{\psi}\left(x_j - \frac{l}{n}\right).$$

arithmetic operations

$$\mathcal{O}(N + n \log n + (2m+1)M) = \mathcal{O}(n \log n + mM)$$

NFFT, matrix-vector form:

$\boldsymbol{A}$ may be factorised approximately as follows:

$$\boldsymbol{A} \approx \boldsymbol{B}\boldsymbol{F}\boldsymbol{D},$$

where each of the three matrices corresponds to a step in the NFFT algorithm:

1. $\boldsymbol{D} \in \mathbb{R}^{N\times N}$ is a diagonal matrix:

$$\boldsymbol{D} := \text{diag}\left(\frac{1}{n\, c_k(\tilde{\varphi})}\right)_{k=-N/2}^{N/2-1}$$

2. $\boldsymbol{F} \in \mathbb{R}^{n\times N}$ is a truncated Fourier matrix:

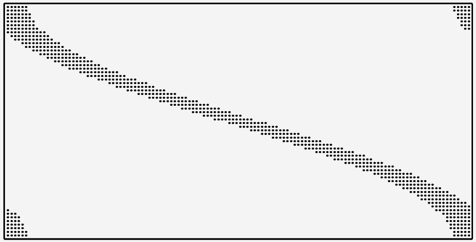
$$\boldsymbol{F} := \left(\mathrm{e}^{-2\pi \mathrm{i} kl/n}\right)_{l=-n/2,\; k=-N/2}^{n/2-1 \quad N/2-1}$$

3. $\boldsymbol{B} \in \mathbb{R}^{M \times n}$ is a sparse band matrix with $2m+1$ non-zero entries per row:

$$\boldsymbol{B} := (b_{j\,l})_{j=-M/2,\ l=-n/2}^{M/2-1\quad n/2-1}$$

where

$$b_{j\,l} = \begin{cases} \tilde{\psi}\left(x_j - \frac{l}{n}\right) & \text{if } l \in \{\lfloor x_j n \rfloor - m, \ldots, \lceil x_j n \rceil + m\} \\ 0 & \text{otherwise.} \end{cases}$$



Structure of the matrix $\boldsymbol{B}$. Non-zero entries are indicated by dots. The row index j runs from $-M/2$ to $M/2-1$, the column index l runs from $-n/2$ to $n/2-1$. Parameters used were $M = N = 64$, $n = 128$ and $m = 5$; Legendre nodes were used for the x_j.

Algorithm (NFFT$^{\mathsf{H}}$-1D)

The factorisation that was derived for $\boldsymbol{A}$ allows us to derive an NFFT$^{\mathsf{H}}$ algorithm simply by transposing $\boldsymbol{A}$:

$$\boldsymbol{A}^{\mathsf{H}}\boldsymbol{h} \approx \boldsymbol{D}^{\mathsf{H}}\boldsymbol{F}^{\mathsf{H}}\boldsymbol{B}^{\mathsf{H}}\boldsymbol{h}.$$

We thus propose implementing the operation $\boldsymbol{g} = \boldsymbol{B}^{\mathsf{H}}\boldsymbol{h}$ like this:

$\texttt{for}\ l = -n/2, \ldots, n/2 - 1$
    $g_l := 0$
$\texttt{end}$
$\texttt{for}\ j = -M/2, \ldots, M/2 - 1$
    $\texttt{for}\ l = \lfloor x_j n \rfloor - m, \ldots, \lceil x_j n \rceil + m$
        $g_l := g_l + h_j\, b_{jl}$
    $\texttt{end}$
$\texttt{end}$

Error estimates:

$$E(x_j) := |f(x_j) - s(x_j)| \;\le\; E_\mathrm{a}(x_j) + E_\mathrm{t}(x_j)$$

aliasing error $E_\mathrm{a}(x_j) := |f(x_j) - s_1(x_j)|$

truncation error $E_\mathrm{t}(x_j) := |s_1(x_j) - s(x_j)|$

Theorem : Let $\|\hat{\boldsymbol{f}}\|_1 := \sum_{k=-N/2}^{N/2-1} |\hat{f}_k|$, then the errors can be estimated as

$$E_\mathrm{a}(x_j) \le \|\hat{\boldsymbol{f}}\|_1 \max_{k=-N/2,\dots,N/2-1} \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \left| \frac{c_{k+nr}(\tilde{\varphi})}{c_k(\tilde{\varphi})} \right| \tag{16}$$

and

$$E_\mathrm{t}(x_j) \le \frac{\|\hat{\boldsymbol{f}}\|_1}{n} \max_{k \in I_N^1} \frac{1}{|c_k(\tilde{\varphi})|} \sum_{\left|x_j + \frac{r}{n}\right| \ge \frac{m}{n}} \left| \varphi\left(x_j + \frac{r}{n}\right) \right| \tag{17}$$

Proof:

$$
\begin{aligned}
E_{\mathrm{a}}(x_j) &:= |f(x_j) - s_1(x_j)| \\
&= \\
&= \\
&\leq \\
&\leq
\end{aligned}
$$

Proof:

$$\begin{aligned}
E_{\mathrm{a}}(x_j) &:= |f(x_j) - s_1(x_j)| \\
&= \left| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \sum_{k=-n/2}^{n/2-1} \hat{g}_k \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i}(k+nr)x} \right| \\
&= \\
&\leq \\
&\leq
\end{aligned}$$

Proof:

$$
\begin{aligned}
E_{\mathrm{a}}(x_j) &:= |f(x_j) - s_1(x_j)| \\
&= \left| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \sum_{k=-n/2}^{n/2-1} \hat{g}_k \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi\mathrm{i}(k+nr)x} \right| \\
&= \left| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \sum_{k=-N/2}^{N/2-1} \frac{\hat{f}_k}{c_k(\tilde{\varphi})} \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi\mathrm{i}(k+nr)x} \right| \\
&\leq \\
&\leq
\end{aligned}
$$

Proof:

$$
\begin{aligned}
E_{\mathrm{a}}(x_j) &:= \left|f(x_j) - s_1(x_j)\right| \\
&= \left| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \sum_{k=-n/2}^{n/2-1} \hat{g}_k \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i}(k+nr)x} \right| \\
&= \left| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \sum_{k=-N/2}^{N/2-1} \frac{\hat{f}_k}{c_k(\tilde{\varphi})} \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i}(k+nr)x} \right| \\
&\leq \sum_{k=-N/2}^{N/2-1} \left|\hat{f}_k\right| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \left| \frac{c_{k+nr}(\tilde{\varphi})}{c_k(\tilde{\varphi})} \right| \\
&\leq
\end{aligned}
$$

Proof:

$$
\begin{aligned}
E_{\mathrm{a}}(x_j) &:= |f(x_j) - s_1(x_j)| \\
&= \left| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \sum_{k=-n/2}^{n/2-1} \hat{g}_k \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi\mathrm{i}(k+nr)x} \right| \\
&= \left| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \sum_{k=-N/2}^{N/2-1} \frac{\hat{f}_k}{c_k(\tilde{\varphi})} \, c_{k+nr}(\tilde{\varphi}) \, \mathrm{e}^{-2\pi\mathrm{i}(k+nr)x} \right| \\
&\leq \sum_{k=-N/2}^{N/2-1} \left| \hat{f}_k \right| \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \left| \frac{c_{k+nr}(\tilde{\varphi})}{c_k(\tilde{\varphi})} \right| \\
&\leq \|\hat{\boldsymbol{f}}\|_1 \max_{k=-N/2,\ldots,N/2-1} \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \left| \frac{c_{k+nr}(\tilde{\varphi})}{c_k(\tilde{\varphi})} \right|
\end{aligned}
$$

$$E_{\mathrm{t}}(x_j) = \left| \sum_{l=-n/2}^{n/2-1} g_l \left(\tilde{\varphi}\left(x_j - \frac{l}{n}\right) - \tilde{\psi}\left(x_j - \frac{l}{n}\right)\right)\right| .$$

note

$$g_l = \frac{1}{n} \sum_{k \in I_N^1} \frac{\hat{f}_k}{\hat{\varphi}(k)} \, \mathrm{e}^{-2\pi \mathrm{i} k l/n},$$

hence

$$E_{\mathrm{t}}(x_j) \;\le\; \frac{1}{n} \left| \sum_{l \in I_n^1} \sum_{k \in I_N^1} \frac{\hat{f}_k}{\hat{\varphi}(k)} \, \mathrm{e}^{-2\pi \mathrm{i} k l/n} \left(\tilde{\varphi}\left(x_j - \frac{l}{n}\right) - \tilde{\psi}\left(x_j - \frac{l}{n}\right)\right)\right|$$

$$
\begin{aligned}
E_{\mathrm{t}}(x_j) &\le \frac{1}{n}\left|\sum_{k\in I_N^1}\frac{\hat{f}_k}{\hat{\varphi}(k)}\sum_{l\in I_n^1}\left(\tilde{\varphi}\left(x_j-\frac{l}{n}\right)-\tilde{\psi}\left(x_j-\frac{l}{n}\right)\right)\,\mathrm{e}^{-2\pi\mathrm{i}kl/n}\right| \\
&\le \frac{\|\hat{\boldsymbol{f}}\|_1}{n}\max_{k\in I_N^1}\frac{1}{|\hat{\varphi}(k)|}\left|\sum_{l\in I_n^1}\left(\tilde{\varphi}\left(x_j-\frac{l}{n}\right)-\tilde{\psi}\left(x_j-\frac{l}{n}\right)\right)\,\mathrm{e}^{-2\pi\mathrm{i}kl/n}\right|.
\end{aligned}
$$

consider sum over l

$$
\tilde{\varphi}(x)-\tilde{\psi}(x)=\sum_{r\in\mathbb{Z}}\varphi(x+r)-\varphi(x+r)\,\chi_{[-\frac{m}{n},\frac{m}{n}]}(x+r).
$$

$$
\begin{aligned}
& \sum_{l\in I_n^1}\left(\tilde{\varphi}\left(x_j-\frac{l}{n}\right)-\tilde{\psi}\left(x_j-\frac{l}{n}\right)\right)\,\mathrm{e}^{-2\pi\mathrm{i}kl/n} \\
= & \sum_{l\in I_n^1}\left(\sum_{r\in\mathbb{Z}}\varphi\left(x_j-\frac{l}{n}+r\right)\right. \\
& \left.-\varphi\left(x_j-\frac{l}{n}+r\right)\,\chi_{[-\frac{m}{n},\frac{m}{n}]}\left(x_j-\frac{l}{n}+r\right)\right)\mathrm{e}^{-2\pi\mathrm{i}kl/n} \\
= & \sum_{r\in\mathbb{Z}}\left(\varphi\left(x_j+\frac{r}{n}\right)-\varphi\left(x_j+\frac{r}{n}\right)\,\chi_{[-\frac{m}{n},\frac{m}{n}]}\left(x_j+\frac{r}{n}\right)\right)\,\mathrm{e}^{-2\pi\mathrm{i}kr/n} \\
= & \sum_{|x_j+\frac{r}{n}|\geq\frac{m}{n}}\varphi\left(x_j+\frac{r}{n}\right)\,\mathrm{e}^{-2\pi\mathrm{i}kr/n}
\end{aligned}
$$

finally

$$
\begin{aligned}
E_{\mathrm{t}}(x_j) \;&\le\; \frac{\|\hat{\boldsymbol{f}}\|_1}{n} \max_{k \in I_N} \frac{1}{|\hat{\varphi}(k)|} \left| \sum_{\left|x_j + \frac{r}{n}\right| \ge \frac{m}{n}} \varphi\left(x_j + \frac{r}{n}\right) \mathrm{e}^{-2\pi \mathrm{i} k r/n} \right| \\
&\le\; \frac{\|\hat{\boldsymbol{f}}\|_1}{n} \max_{k \in I_N^1} \frac{1}{|\hat{\varphi}(k)|} \sum_{\left|x_j + \frac{r}{n}\right| \ge \frac{m}{n}} \left| \varphi\left(x_j + \frac{r}{n}\right) \right|
\end{aligned}
$$

■

Corollary: For even, monotone decreasing $\varphi \ge 0$ holds

$$
E_{\mathrm{t}}(x_j) \le \frac{\|\hat{\boldsymbol{f}}\|_1}{n} \max_{k \in I_N^1} \frac{2}{|\hat{\varphi}(k)|} \left(\varphi\left(\frac{m}{n}\right) + \int_m^{\infty} \varphi\left(\frac{x}{n}\right) \mathrm{d}x \right). \tag{18}
$$

Multivariate functions

$$\varphi : \mathbb{R}^d \to \mathbb{R} \quad \text{by} \quad \varphi(\boldsymbol{x}) := \prod_{t=1}^{d} \varphi(x_t)$$

with $\boldsymbol{x} = (x_1, x_2, \ldots, x_d)^{\mathrm{T}}$
note

$$\hat{\varphi}(\boldsymbol{k}) = \prod_{t=1}^{d} \hat{\varphi}(k_t) \text{ with } \boldsymbol{k} := (k_1, \ldots, k_d)^{\mathrm{T}}$$

Content

- NFFT, Window functions
  - B-splines ($E_{\mathrm{t}} = 0$)
  - Gaussian bells ($E_{\mathrm{t}} \approx E_{\mathrm{a}}$)
  - Sinc, Kaiser-Bessel ($E_{\mathrm{a}} = 0$)
- NFFT, Window functions, Summary
- NFFT, Software, Numerical examples
- NFFT, further topics

B-splines ($E_{\mathrm{t}} = 0$)

References: G. Beylkin [2]; G. Steidl [42]

centered cardinal B-spline of order m

$$M_1(x) := \begin{cases} 1 & \text{if} \quad x \in [-1/2, 1/2), \\ 0 & \text{else}, \end{cases}$$

$$M_{m+1}(x) := \int_{-1/2}^{1/2} M_m(x-t)\,\mathrm{d}t \qquad (m = 1, 2, \ldots)$$

$$\text{supp} M_m = [-m/2, m/2]$$

by (9) follows

$$\hat{M}_1(v) = \int_{-1/2}^{1/2} \mathrm{e}^{-2\pi\mathrm{i}vx}\,\mathrm{d}x = \text{sinc}(\pi v)$$

Lemma: We claim that

$$\hat{M}_m(k) = (\mathsf{sinc}(\pi k))^m \qquad (m \in \mathbb{N}).$$

Proof: by induction

$$\begin{aligned}
\hat{M}_{m+1}(k) &= \int_{\mathbb{R}} M_{m+1}(x)\, \mathrm{e}^{-2\pi \mathrm{i} x k}\, \mathrm{d}x \\
&= \int_{\mathbb{R}} \int_{-1/2}^{1/2} M_m(\underbrace{x-t}_{y})\, \mathrm{e}^{-2\pi \mathrm{i} x k}\, \mathrm{d}t\, \mathrm{d}x \\
&= \int_{-1/2}^{1/2} \underbrace{\int_{\mathbb{R}} M_m(y)\, \mathrm{e}^{-2\pi \mathrm{i} y k}\, \mathrm{d}y}_{\hat{M}_m(k)}\, \mathrm{e}^{-2\pi \mathrm{i} t k}\, \mathrm{d}t \\
&= (\mathsf{sinc}(\pi k))^m\, \mathsf{sinc}(\pi k) \\
&= (\mathsf{sinc}(\pi k))^{m+1}
\end{aligned}$$

■

Lemma: For $0 < u < 1$ with $m \in \mathbb{N}$ it holds that

$$\sum_{r \in \mathbb{Z} \setminus \{0\}} \left(\frac{u}{u+r} \right)^{2m} < \frac{4m}{2m-1} \left(\frac{u}{u-1} \right)^{2m} .$$

Proof: For $r \geq 0$ holds

$$\left(\frac{u}{u+r} \right)^{2m} \leq \left(\frac{u}{u-r} \right)^{2m}$$

and

$$\begin{aligned}
\sum_{r \in \mathbb{Z}} \left(\frac{u}{u+r} \right)^{2m} &\leq 1 + 2 \left(\frac{u}{u-1} \right)^{2m} + 2 \sum_{r=2}^{\infty} \left(\frac{u}{u-r} \right)^{2m} \\
&\leq 1 + 2 \left(\frac{u}{u-1} \right)^{2m} + 2 \int_1^{\infty} \left(\frac{u}{u-x} \right)^{2m} \mathrm{d}x \\
&= 1 + 2 \left(\frac{u}{u-1} \right)^{2m} \left(1 + \frac{1-u}{2m-1} \right) \\
&< 1 + 2 \left(\frac{u}{u-1} \right)^{2m} \left(1 + \frac{1}{2m-1} \right) .
\end{aligned}$$

■

Theorem:
Let $f(x_j)$ $(j = -M/2, \ldots, M/2-1)$ be approximately computed by the NFFT with

$$\varphi(x) := M_{2m}(nx)$$

and $n := \sigma N$ $(\sigma > 1)$. Then the approximation error can be estimated by

$$E_\infty := \max_{j \in I_M^1} E(x_j) \le \|\hat{\boldsymbol{f}}\|_1 \frac{4m}{2m-1} \left(\frac{1}{2\sigma - 1}\right)^{2m},$$

where $\hat{\boldsymbol{f}} := (\hat{f}_k)_{k \in I_N^1}$.

Proof:

$$\text{supp}\quad \varphi \subseteq [-\frac{m}{\sigma N}, \frac{m}{\sigma N}] \Rightarrow E_{\mathrm{t}} = 0 \quad \text{(see } (14))$$

$$\begin{aligned}
\hat{\varphi}(k) = c_k(\tilde{\varphi}) &= \int_{\mathbb{R}} \varphi(x)\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&= \int_{\mathbb{R}} M_{2m}(\underbrace{\sigma N x}_{y})\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&= \frac{1}{\sigma N} \int_{\mathbb{R}} M_{2m}(y)\, \mathrm{e}^{2\pi \mathrm{i} k y/(\sigma N)}\, \mathrm{d}y \\
&= \frac{1}{\sigma N} \left(\text{sinc} \frac{\pi k}{\sigma N} \right)^{2m}
\end{aligned}$$

with

$$\begin{aligned}\sigma N\hat{\varphi}(k+r\sigma N) &= \left(\frac{\sin(k\pi/(\sigma N))}{k\pi/(\sigma N)+r\pi}\right)^{2m}\\ &= \left(\frac{\sin(k\pi/(\sigma N))}{k\pi/(\sigma N)}\right)^{2m}\left(\frac{k\pi/(\sigma N)}{k\pi/(\sigma N)+r\pi}\right)^{2m}\\ &= \sigma N\hat{\varphi}(k)\left(\frac{k/(\sigma N)}{k/(\sigma N)+r}\right)^{2m}\end{aligned}$$

follows by (16) and Lemma

$$E_\infty \le \|\hat{\boldsymbol{f}}\|_1 \, \frac{4m}{2m-1} \max_{k=-N/2,\ldots,N/2-1} \frac{(k/(\sigma N))^{2m}}{(k/(\sigma N)-1)^{2m}} \, .$$

The right-hand side increases since

$$u^{2m}/(u-1)^{2m}$$

increases for $u \in [0,1/2]$ and $|k| \le N/2$. The assertion follows for $k = N/2$. ■

Gaussian bells ($E_{\mathrm{t}} \approx E_{\mathrm{a}}$)

References: A. Dutt and V. Rokhlin [9], G. Steidl [42], [38], L. Greengard and J. Lee [15]

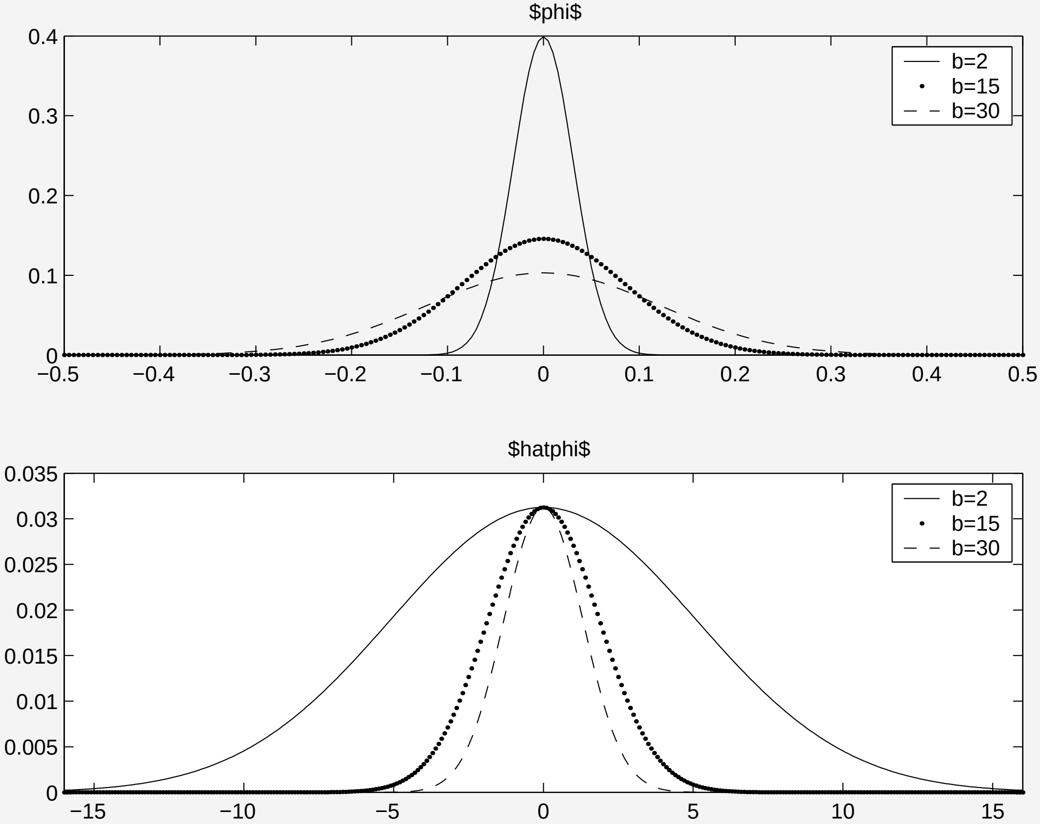
Theorem:
Let $f(x_j)$ $(j = -M/2, \ldots, M/2-1)$ be approximately computed by the NFFT with

$$\varphi(x) := \frac{1}{\sqrt{\pi b}}\, \mathrm{e}^{-(\sigma N x)^2/b} \quad (b \in \mathbb{R}^+)$$

and $\sigma \geq 3/2$, $b := \frac{2\sigma}{2\sigma-1}\frac{m}{\pi}$. Then the approximation error can be estimated

$$E_\infty = \max_{j \in I_M^1} E(x_j) \leq 4\|\hat{\boldsymbol{f}}\|_1\, \mathrm{e}^{-m\pi\left(1-\frac{1}{2\sigma-1}\right)}$$

where $\hat{\boldsymbol{f}} := (\hat{f}_k)_{k \in I_N^1}$.



Gaussian bells φ and $\hat{\varphi}$ for $\sigma N = 32$ and different parameters $b \in \{2, 15, 30\}$.

Proof: by (10)

$$\int_{\mathbb{R}} \mathrm{e}^{-x^2}\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x = \sqrt{\pi}\, \mathrm{e}^{-\pi^2 k^2}$$

$$c_k(\tilde{\varphi}) = \hat{\varphi}(k) = \frac{1}{\sigma N}\, \mathrm{e}^{-\left(\frac{\pi k}{\sigma N}\right)^2 b} \tag{19}$$

we frequently use for $a > 0$, $c > 0$

$$\int_a^\infty \mathrm{e}^{-cx^2}\, \mathrm{d}x = \int_0^\infty \mathrm{e}^{-c(x+a)^2}\, \mathrm{d}x \le \mathrm{e}^{-ca^2} \int_0^\infty \mathrm{e}^{-2acx}\, \mathrm{d}x = \frac{\mathrm{e}^{-ca^2}}{2ac} \tag{20}$$

consider E_{a}, with (19) and (16) follows

$$E_{\mathrm{a}}(x_j) \le \|\hat{\boldsymbol{f}}\|_1 \max_{k \in I_N^1} \sum_{r \in \mathbb{Z} \setminus \{0\}} \mathrm{e}^{-b\pi^2\left(\frac{2k}{\sigma N} r + r^2\right)}.$$

since

$$\max_{k \in I_N^1} \mathrm{e}^{-b\pi^2\left(\frac{2k}{\sigma N} r + r^2\right)} \le \mathrm{e}^{-b\pi^2\left(\frac{N}{\sigma N} r + r^2\right)}$$

$$
\begin{aligned}
E_{\mathrm{a}}(x_j) &\le \|\hat{\boldsymbol{f}}\|_1 \sum_{r=1}^{\infty} \left(\mathrm{e}^{-b\pi^2\left(r^2 - \frac{N}{\sigma N} r\right)} + \mathrm{e}^{-b\pi^2\left(r^2 + \frac{N}{\sigma N} r\right)} \right) \\
&\le ||\hat{\boldsymbol{f}}||_1 \left(\mathrm{e}^{-b\pi^2\left(1 - \frac{1}{\sigma}\right)} \left(1 + \mathrm{e}^{-\frac{2b\pi^2}{\sigma}}\right) + \mathrm{e}^{b\left(\frac{\pi}{2\sigma}\right)^2} \sum_{r=2}^{\infty} \left(\mathrm{e}^{-b\pi^2\left(r - \frac{1}{2\sigma}\right)^2} + \mathrm{e}^{-b\pi^2\left(r + \frac{1}{2\sigma}\right)^2} \right) \right) \\
&\le ||\hat{\boldsymbol{f}}||_1 \left(\mathrm{e}^{-b\pi^2\left(1 - \frac{1}{\sigma}\right)} \left(1 + \mathrm{e}^{-\frac{2b\pi^2}{\sigma}}\right) + \mathrm{e}^{b\left(\frac{\pi}{2\sigma}\right)^2} \int_1^{\infty} \mathrm{e}^{-b\pi^2\left(x - \frac{1}{2\sigma}\right)^2} + \mathrm{e}^{-b\pi^2\left(x + \frac{1}{2\sigma}\right)^2} \, \mathrm{d}x \right)
\end{aligned}
$$

finally with (20)

$$
E_{\mathrm{a}}(x_j) \le ||\hat{\boldsymbol{f}}||_1 \, \mathrm{e}^{-b\pi^2\left(1 - \frac{1}{\sigma}\right)} \left(1 + \frac{\sigma}{(2\sigma - 1)b\pi^2} + \mathrm{e}^{-2b\pi^2/\sigma} \left(1 + \frac{\sigma}{(2\sigma + 1)b\pi^2}\right)\right)
$$

consider E_t

$$\varphi\left(\frac{m}{n}\right) = \frac{1}{\sqrt{\pi b}}\,\mathrm{e}^{-m^2/b}; \qquad \max_{k\in I_N^1}\frac{1}{|\hat{\varphi}(k)|} = \frac{1}{|\hat{\varphi}(N/2)|} = \sigma N\,\mathrm{e}^{b(\pi/(2\sigma))^2}$$

with (18)

$$E_\mathrm{t}(x_j) \;\le\; ||\hat{\boldsymbol{f}}||_1 \frac{2}{\sqrt{\pi b}}\,\mathrm{e}^{b\left(\frac{\pi}{2\sigma}\right)^2}\left(\mathrm{e}^{-m^2/b} + \int_m^\infty \mathrm{e}^{-x^2/b}\,\mathrm{d}x\right).$$

with (20)

$$E_\mathrm{t}(x_j) \le ||\hat{\boldsymbol{f}}||_1 \frac{2}{\sqrt{\pi b}}\left(1 + \frac{b}{2m}\right)\,\mathrm{e}^{-b\pi^2\left(\left(\frac{m}{b\pi}\right)^2 - \left(\frac{1}{2\sigma}\right)^2\right)}$$

since $b = \frac{2\sigma}{2\sigma-1}\frac{m}{\pi}$

$$\left(\frac{m}{b\pi}\right)^2 - \left(\frac{1}{2\sigma}\right)^2 = 1 - \frac{1}{\sigma}$$

$$E_\mathrm{t}(x_j) \le ||\hat{\boldsymbol{f}}||_1 \frac{2}{\sqrt{\pi b}}\left(1 + \frac{\sigma}{(2\sigma-1)\pi}\right)\,\mathrm{e}^{-b\pi^2\left(1-\frac{1}{\sigma}\right)}$$

finally $E \le E_\mathrm{t} + E_\mathrm{a}$

$$E_\infty \le ||\hat{\boldsymbol{f}}||_1 \; \mathrm{e}^{-b\pi^2\left(1-\frac{1}{\sigma}\right)} \underbrace{\left[1 + \frac{1}{2m\pi} + \mathrm{e}^{\frac{-4m\pi}{2\sigma-1}}\left(1 + \frac{2\sigma-1}{2(2\sigma+1)m\pi}\right) + \frac{1+\frac{\sigma}{(2\sigma-1)\pi}}{\sqrt{\frac{\sigma m}{2(2\sigma-1)}}}\right]}_{A}$$

A is increasing for for fixed $m \ge 1$ and increasing σ
A is decreasing for fixed σ and increasing m

$$A \to 2 + \frac{\sqrt{m} + m + 2m\pi}{m^{3/2}\pi} \quad \text{for} \quad \sigma \to \infty$$

assertion follows for $m \ge 2$ with

$$\begin{aligned} E_\infty &\le 4\,||\hat{\boldsymbol{f}}||_1 \; \mathrm{e}^{-b\pi^2\left(1-\frac{1}{\sigma}\right)} \\ &= 4\,||\hat{\boldsymbol{f}}||_1 \; \mathrm{e}^{-m\pi\left(1-\frac{1}{2\sigma-1}\right)}. \end{aligned}$$

■

Sinc functions ($E_\mathrm{a} = 0$)

$$\hat{\varphi}(k) := M_{2m}\left(\frac{2mk}{(2\sigma-1)N}\right) \tag{21}$$

since

$$\text{supp} M_{2m} = [-m, m]$$

from

$$\left|\frac{2mk}{(2\sigma-1)N}\right| \leq m$$

follows that

$$|k| \leq \frac{(2\sigma-1)N}{2} = \sigma N\left(1 - \frac{1}{2\sigma}\right)$$

hence

$$\hat{\varphi}(k) = 0 \quad \text{for} \quad |k| \geq \sigma N\left(1 - \frac{1}{2\sigma}\right)$$

$$\Rightarrow \quad E_\mathrm{a}(x_j) = 0$$

compute φ such that $\hat{\varphi}$ is given in (21) note

$$\int_{\mathbb{R}} M_{2m}(Nx)\,\mathrm{e}^{-2\pi \mathrm{i} x w}\,\mathrm{d}x = \frac{1}{N}\left(\text{sinc}\left(\frac{\pi w}{N}\right)\right)^{2m}$$

substitute $x = \frac{2mk}{(2\sigma-1)N^2}$ and let $w = \frac{N^2 s(2\sigma-1)}{2m}$

$$\int_{\mathbb{R}} M_{2m}\left(\frac{2mk}{(2\sigma-1)N}\right)\mathrm{e}^{-2\pi \mathrm{i} k s}\,\mathrm{d}k = \frac{N(2\sigma-1)}{2m}\left(\text{sinc}\left(\frac{\pi N s(2\sigma-1)}{2m}\right)\right)^{2m}$$

hence

$$\varphi(x) = \frac{N(2\sigma-1)}{2m}\left(\text{sinc}\left(\frac{\pi N x(2\sigma-1)}{2m}\right)\right)^{2m} \tag{22}$$

Theorem:

Let $f(x_j)$ $(j = -M/2, \ldots, M/2-1)$ be approximately computed by the NFFT with φ given in (22) and $\sigma > 1$. Then the approximation error can be estimated

$$E_\infty := \max_{j \in I_M^1} E(x_j) \le ||\hat{\boldsymbol{f}}||_1 \frac{1}{2m-1} \left(\frac{4}{\sigma^{2m}} + \left(\frac{\sigma}{2\sigma - 1} \right)^{2m-1} \right)$$

where $\hat{\boldsymbol{f}} := (\hat{f}_k)_{k \in I_N^1}$.

Proof:

$$\max_{k \in I_N^1} \frac{1}{\hat{\varphi}(k)} = \frac{1}{\hat{\varphi}\left(\frac{N}{2}\right)} = \frac{1}{M_{2m}\left(\frac{m}{2\sigma-1}\right)}$$

note

$$M_{2m}\left(\frac{2mk}{(2\sigma-1)N}\right) = \frac{N(2\sigma-1)}{2m} \int_{\mathbb{R}} \left(\text{sinc}\left(\frac{\pi N s(2\sigma-1)}{2m}\right)\right)^{2m} \mathrm{e}^{2\pi \mathrm{i} k s}\, \mathrm{d}s$$

hence

$$\hat{\varphi}\left(\frac{N}{2}\right) = M_{2m}\left(\frac{m}{2\sigma-1}\right) = \frac{N(2\sigma-1)}{m} \int_{\mathbb{R}} \left(\text{sinc}\left(\frac{\pi N s(2\sigma-1)}{m}\right)\right)^{2m} \mathrm{e}^{\pi \mathrm{i} N s}\, \mathrm{d}s$$

with $\sin(x) \geq \frac{2}{\pi} x$ for $x \in [0, \pi/2]$

$$M_{2m}\left(\frac{m}{2\sigma-1}\right) \geq \frac{N(2\sigma-1)}{m} \int_{-\frac{m}{2(2\sigma-1)N}}^{\frac{m}{2(2\sigma-1)N}} \left(\frac{2}{\pi}\right)^{2m} \mathrm{d}s$$

$$= \left(\frac{2}{\pi}\right)^{2m}$$

finally

$$\max_{k\in I_N^1} \frac{1}{\hat{\varphi}(k)} \leq \left(\frac{\pi}{2}\right)^{2m}$$

furthermore

$$\begin{aligned}
\int_m^\infty \varphi\left(\frac{x}{\sigma N}\right)\,\mathrm{d}x &= \frac{N(2\sigma-1)}{2m}\int_m^\infty \left(\text{sinc}\left(\frac{\pi x(2\sigma-1)}{2m\sigma}\right)\right)^{2m}\,\mathrm{d}x \\
&\leq \frac{N(2\sigma-1)}{2m}\int_m^\infty \left(\frac{2\sigma m}{\pi x(2\sigma-1)}\right)^{2m}\,\mathrm{d}x \\
&= \left(\frac{2}{\pi}\right)^{2m}\frac{2\sigma-1}{2}\frac{N}{2m-1}\left(\frac{\sigma}{2\sigma-1}\right)^{2m} \\
&= \left(\frac{2}{\pi}\right)^{2m}\frac{N\sigma}{4m-2}\left(\frac{\sigma}{2\sigma-1}\right)^{2m-1}
\end{aligned}$$

estimate $\varphi\left(\frac{m}{\sigma N}\right)$
by definition of (22)

$$\varphi\left(\frac{m}{\sigma N}\right) = \frac{N(2\sigma - 1)}{2m}\left(\text{sinc}\frac{(2\sigma-1)\pi}{2\sigma}\right)^{2m}$$

for $\sigma > 1$ holds $\frac{\pi}{2} < \frac{2\sigma-1}{2\sigma}\pi < \pi$ and

$$|\sin(x)| < -\frac{4}{\pi^2}x^2 + \frac{4}{\pi}x \quad \text{for} \quad x \in (\frac{\pi}{2}, \pi)$$

we obtain

$$\left(\text{sinc}\left(\frac{2\sigma-1}{2\sigma}\pi\right)\right)^{2m} \; < \; \left(\frac{2}{\pi\sigma}\right)^{2m}$$

and

$$\varphi\left(\frac{m}{\sigma N}\right) < \frac{N(2\sigma - 1)}{2m}\left(\frac{2}{\pi\sigma}\right)^{2m}$$

finally for E_{t} see (18)

$$E_\infty \leq 2||\hat{\boldsymbol{f}}||_1 \frac{1}{\sigma N}\left(\frac{\pi}{2}\right)^{2m}\left[\frac{N(2\sigma-1)}{2m}\left(\frac{2}{\pi\sigma}\right)^{2m}+\left(\frac{2}{\pi}\right)^{2m}\frac{N\sigma}{4m-2}\left(\frac{\sigma}{2\sigma-1}\right)^{2m-1}\right]$$

$$= ||\hat{\boldsymbol{f}}||_1 \left[\frac{2\sigma-1}{m}\frac{1}{\sigma^{2m+1}}+\frac{1}{2m-1}\left(\frac{\sigma}{2\sigma-1}\right)^{2m-1}\right] \qquad \blacksquare$$

Kaiser-Bessel functions ($E_{\mathrm{a}} = 0$)

References: K. Fourmont [13, 14], [35]

$$\varphi(x) := \begin{cases} \dfrac{\sinh(b\sqrt{m^2 - (\sigma N)^2 x^2})}{\pi\sqrt{m^2 - (\sigma N)^2 x^2}} & \text{for} \quad |x| < \frac{m}{\sigma N} \qquad \left(b := \pi\left(2 - \frac{1}{\sigma}\right)\right), \\ \dfrac{b}{\pi} & \text{for} \quad |x| = \frac{m}{\sigma N}, \\ \dfrac{\sin(b\sqrt{(\sigma N)^2 x^2 - m^2})}{\pi\sqrt{(\sigma N)^2 x^2 - m^2}} & \text{else} \end{cases} \tag{23}$$

$$\hat{\varphi}(k) = \begin{cases} \frac{1}{\sigma N} I_0(m\sqrt{b^2 - (2\pi k/(\sigma N))^2}) & \text{for } k = -\sigma N\left(1 - \frac{1}{2\sigma}\right), \ldots, \sigma N\left(1 - \frac{1}{2\sigma}\right), \\ 0 & \text{else.} \end{cases}$$

where I_0 denotes the modified zero-order Bessel function

Theorem: [30]

Let $f(x_j)$ $(j = -M/2, \ldots, M/2-1)$ be approximately computed by the NFFT with φ given in (23) and $\sigma > 1$. Then the approximation error can be estimated

$$E_\infty := \max_{j \in I_M^1} E(x_j) \le \|\hat{\boldsymbol{f}}\|_1 \, 4\pi(\sqrt{m} + m)\sqrt[4]{1 - \frac{1}{\sigma}} \; \mathrm{e}^{-2\pi m \sqrt{1-1/\sigma}}$$

where $\hat{\boldsymbol{f}} := (\hat{f}_k)_{k \in I_N^1}$.

Window functions, Summary

Theorem: Let $f(x_j)$ $(j = -M/2, \ldots, M/2-1)$ be approximately computed by the NFFT. Then the approximation error

$$E(x_j) := |f(x_j) - s(x_j)| \le C(\sigma, m) ||\hat{\boldsymbol{f}}||_1$$

can be estimated with

$$C(\sigma, m) := \begin{cases} 4\left(\frac{1}{2\sigma-1}\right)^{2m} & \text{for } B\text{-Splines}, \\ 4\,\mathrm{e}^{-m\pi(1-1/(2\sigma-1))} & \text{for Gaussian bells}, \\ \frac{3}{m-1}\left(\frac{\sigma}{2\sigma-1}\right)^{2m-1} & \text{for sinc-functions}, \\ 4\pi(\sqrt{m}+m)\sqrt[4]{1-\frac{1}{\sigma}}\,\mathrm{e}^{-m2\pi\sqrt{1-1/\sigma}} & \text{for Kaiser-Bessel-functions.} \end{cases}$$

Corollary: In order to achieve a precision ϵ of the relative approximation error E we have for fixed $\sigma > 1$ to choose m at least as $m \sim \log(1/\epsilon)$.

Software available:

NFFT – C subroutine library (Keiner, Kunis, P. 2002–2010)

http://www.tu-chemnitz.de/∼potts/nfft

Generalization

Time and frequency nonequispaced, nonequispaced DCT/DST, yyperbolic cross, NFFT on the sphere, iterative solution of the inverse transforms

Applications

fast summation, fast Gauss transform, summation on the sphere, MRI, polar FFT, Radon transform, CT, ridgelet transform

Documentation

NFFT3 Tutorial (Keiner, Kunis, P.) [19]

Content

- NFFT, further topics
  - Approximate factorizations of NDFT matrices
  - Fourier matrices with nonuniform knots in both time and frequency
  - Fast trigonometric transforms at nonequispaced nodes (NDCT, NDST)
  - Roundoff errors
- ”inverse” NFFT

Approximate factorizations of NDFT matrices

References: A. Nieslony and G. Steidl [28]

aim: reduce the approximation error by choosing a sparse factorization of $\boldsymbol{A}$ of the form

$$\boldsymbol{A} \approx \boldsymbol{B}\boldsymbol{F}_n\tilde{\boldsymbol{D}},$$

with different entries of the matrix $\boldsymbol{B}$

$$||\boldsymbol{A}\boldsymbol{f} \;-\; \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}\,\boldsymbol{f}||_2 \leq ||\boldsymbol{A} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}||_F\,||\boldsymbol{f}||_2\,,$$

where $||\boldsymbol{A}||_F$ denotes the Frobenius norm of $\boldsymbol{A}$

since $||\boldsymbol{x}||_\infty \leq ||\boldsymbol{x}||_2 \leq ||\boldsymbol{x}||_1$ this also implies

$$||\boldsymbol{A}\boldsymbol{f} \;-\; \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}\,\boldsymbol{f}||_\infty \leq ||\boldsymbol{A} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}||_F\,||\boldsymbol{f}||_1$$

we intend to choose the $(2m+1)N$ nonzero entries of $\boldsymbol{B}$ such that

$$||\boldsymbol{A} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}||_F$$

becomes minimal

by

$$||\boldsymbol{A}_f - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}||_F^2 = \sum_{j=-N/2}^{N/2-1} \sum_{k=-N/2}^{N/2-1} \left| \mathrm{e}^{-2\pi \mathrm{i} k x_j} - \sum_{l=[nx_j]-m}^{[nx_j]+m} b_{j,l \bmod n} \mathrm{e}^{-2\pi \mathrm{i} kl/n} \frac{1}{n\hat{\varphi}(k)} \right|^2$$

it follows with

$$\boldsymbol{e}_j = \left(\mathrm{e}^{-2\pi \mathrm{i} k x_j}\right)_{k=-N/2}^{N/2-1}, \quad \boldsymbol{b}_j = (b_{j,l})_{l=[nx_j]-m}^{[nx_j]+m}, \quad \boldsymbol{T}_j = \left(\mathrm{e}^{-2\pi \mathrm{i} kl/n}\right)_{k=-N/2,l=[nx_j]-m}^{N/2-1,[nx_j]+m}$$

$$\tilde{\boldsymbol{D}} = \left(\mathbf{0}_{N,(n-N)/2} \,|\boldsymbol{D}|\, \mathbf{0}_{N,(n-N)/2}\right)^T, \quad \boldsymbol{D} = (\mathrm{diag}(1/(n\hat{\varphi}(k))))_{k=-N/2}^{N/2-1}$$

with the $(N,(n-N)/2)$–zero matrices $\mathbf{0}_{N,(n-N)/2}$, that

$$||\boldsymbol{A} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}||_F^2 = \sum_{j=-N/2}^{N/2-1} ||\boldsymbol{e}_j - \boldsymbol{D}\boldsymbol{T}_j\boldsymbol{b}_j||_2^2 \,.$$

The above expression becomes minimal iff

$$||\boldsymbol{e}_j - \boldsymbol{D}\boldsymbol{T}_j\boldsymbol{b}_j||_2^2 = \min \tag{24}$$

for all $j = -N/2, \ldots, N/2-1$.

The solution of (24) is given by

$$\boldsymbol{b}_j = \left(\bar{\boldsymbol{T}}_j^T \boldsymbol{D}^2 \boldsymbol{T}_j\right)^{-1} \bar{\boldsymbol{T}}_j^T \boldsymbol{D} \boldsymbol{e}_j \,. \tag{25}$$

The matrix $\bar{\boldsymbol{T}}_j^T \boldsymbol{D}^2 \boldsymbol{T}_j$ is the $(2m+1) \times (2m+1)$ Toeplitz matrix

$$\bar{\boldsymbol{T}}_j^T \boldsymbol{D}^2 \boldsymbol{T}_j = \left(\sum_{k=-N/2}^{N/2-1} \left(\frac{1}{n\hat{\varphi}(k)}\right)^2 \mathrm{e}^{-2\pi \mathrm{i} k(r-s)/n} \right)_{r,s=0}^{2m}$$

which is independent of j and can be precomputed once for all j. Note again that the entries $b_{k,l}$ are treated n–periodically with respect to l.

Remark: A similar algorithm for the fast multiplication with $\boldsymbol{A}$ was introduced by Ngyuen and Liu [27]. Instead of (24) these authors suggested to minimize

$$||\boldsymbol{D}^{-1}\boldsymbol{e}_j - \boldsymbol{T}_j \boldsymbol{b}_j||_2^2$$

for all $j = -N/2, \ldots, N/2-1$.

Numerical examples

References: A. Nieslony and G. Steidl [28]

The following table presents the Frobenius norm

$$||\boldsymbol{A}_f - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}||_F$$

and the corresponding error

$$||\boldsymbol{A}_f\boldsymbol{f} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}\boldsymbol{f}||_2/||\boldsymbol{f}||_2$$

for the three different choices of $\boldsymbol{B}$ according to ALGauss, NLGauss and FRGauss.

The figures show the arithmetic means of the errors

$$\hat{E}_2 = ||\boldsymbol{A}_f\boldsymbol{f} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}\boldsymbol{f}||_2/||\boldsymbol{A}_f\boldsymbol{f}||_2$$

and

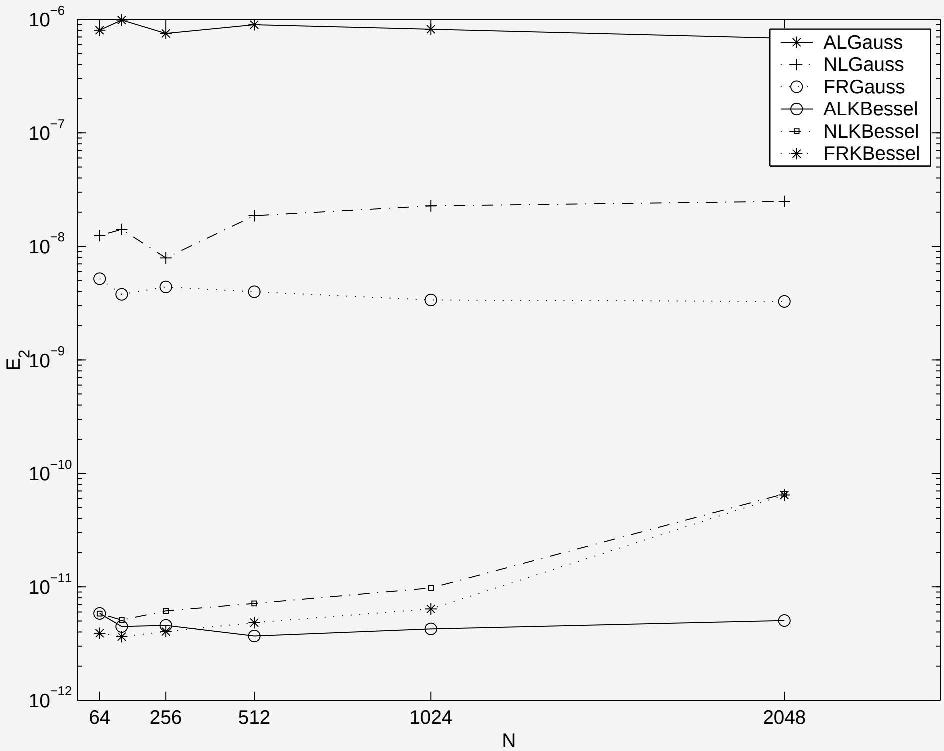
$$E_\infty = ||\boldsymbol{A}_f\boldsymbol{f} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}\boldsymbol{f}||_\infty/||\boldsymbol{f}||_1$$

taken over 10 runs of the algorithm.

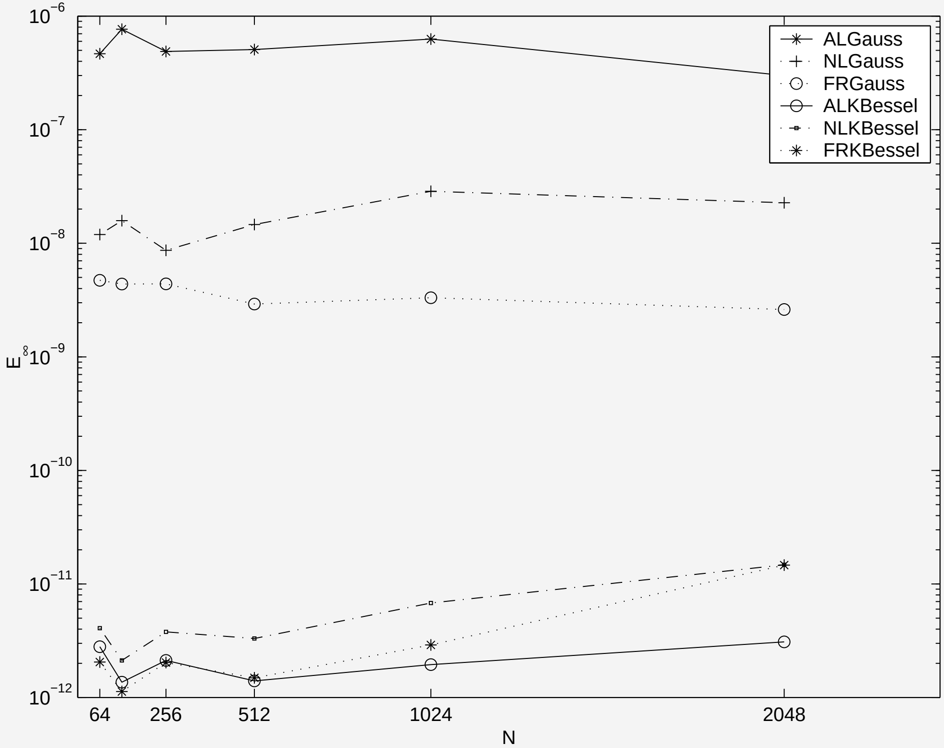
- ALGauss: algorithm with function values of $\tilde{\psi}$ as entries of $\boldsymbol{B}$ and Gaussian window function
- ALKBessel: algorithm with function values of $\tilde{\psi}$ as entries of $\boldsymbol{B}$ and Kaiser–Bessel window function
- NLGauss: algorithm of Ngyuen and Liu with Gaussian window function
- NLKBessel: algorithm of Ngyuen and Liu with Kaiser–Bessel window function
- FRGauss: algorithm with minimal Frobenius norm of the difference matrix and Gaussian window function
- FRKBessel: algorithm with minimal Frobenius norm of the difference matrix and Kaiser–Bessel window function

m	ALGauss		NLGauss		FRGauss	
	E_F	E_2	E_F	E_2	E_F	E_2
2	2.40e-01	8.52e-02	6.47e-02	5.01e-03	2.16e-02	4.81e-03
3	2.91e-02	8.46e-03	3.02e-03	2.35e-04	8.56e-04	2.12e-04
4	3.74e-03	8.54e-04	1.48e-04	1.13e-05	4.69e-05	9.56e-06
5	4.53e-04	9.21e-05	4.94e-06	3.86e-07	1.68e-06	3.55e-07
6	5.53e-05	9.25e-06	3.28e-07	2.30e-08	9.42e-08	2.28e-08
7	6.86e-06	1.15e-06	1.26e-08	9.63e-10	3.18e-09	6.13e-10
8	8.52e-07	1.27e-07	3.88e-08	2.92e-09	3.00e-09	5.87e-10

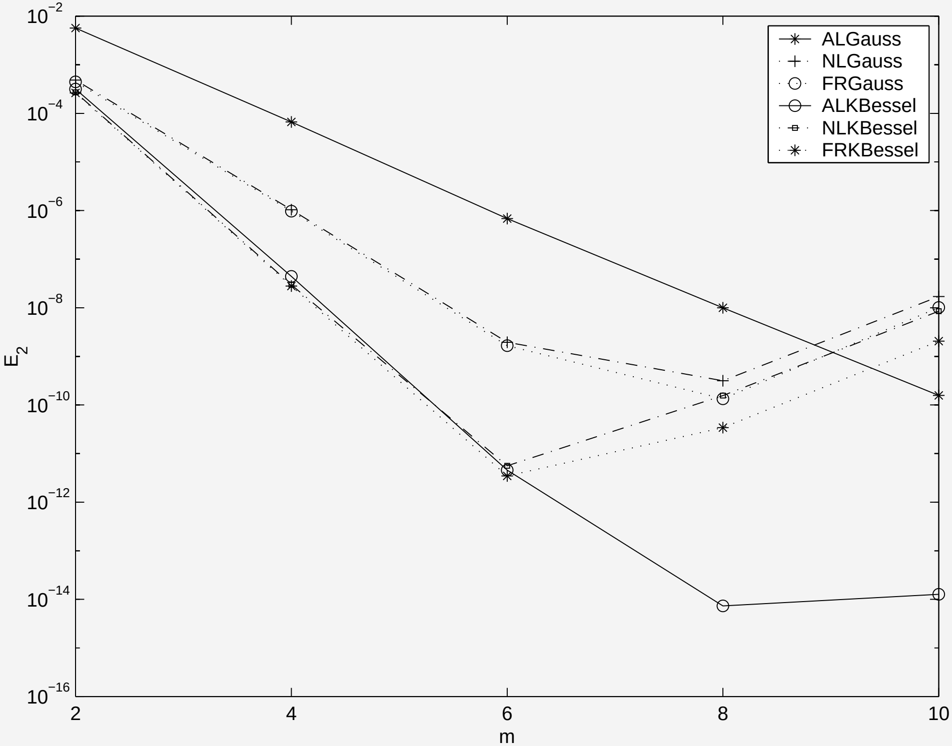
Comparison of $||\boldsymbol{A} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}||_F$ (E_F) and $||\boldsymbol{A}\boldsymbol{f} - \boldsymbol{B}\,\boldsymbol{F}_n\,\tilde{\boldsymbol{D}}\boldsymbol{f}||_2/||\boldsymbol{f}||_2$ (E_2) for $\boldsymbol{B}$ in ALGauss, NLGauss and FRGauss, where $\alpha = 2$ and $N = 256$.



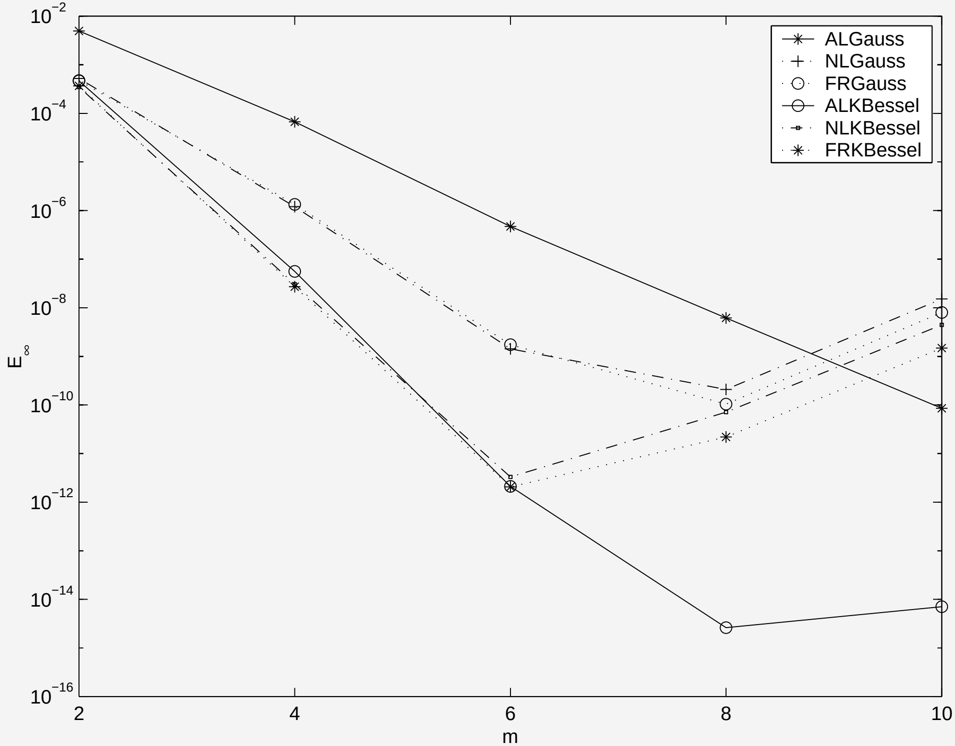
Comparison of the approximation error $\hat{E}_2$ of the three algorithms with Gaussian window function and Kaiser–Bessel window function for $\alpha = 2$, $m = 6$ and different transform lengths N.



Comparison of the approximation error E_∞ of the three algorithms with Gaussian window function and Kaiser–Bessel window function for $\alpha = 2$, $m = 6$ and different transform lengths N.



Comparison of the approximation error $\hat{E}_2$ of the three algorithms with Gaussian window function and Kaiser–Bessel window function for $\alpha = 2$, $N = 256$ and different 'band widths' m.



Comparison of the approximation error E_∞ of the three algorithms with Gaussian window function and Kaiser–Bessel window function for $\alpha = 2$, $N = 256$ and different 'band widths' m.

Fourier matrices with nonuniform knots in both time and frequency

References: A. Elbel and G. Steidl [10, 38, 28]

fast evaluations of sums of the form

$$\hat{f}(v_j) = \sum_{k=-N/2}^{N/2-1} f_k \, \mathrm{e}^{-2\pi \mathrm{i} x_k v_j / N} \qquad (j = -N/2, \ldots, N/2-1)\,, \tag{26}$$

i.e. fast matrix–vector multiplications

$$\hat{\boldsymbol{f}} = \boldsymbol{A}_{tf}\, \boldsymbol{f}\,, \quad \boldsymbol{A}_{tf} = \left(\mathrm{e}^{-2\pi \mathrm{i} x_k v_j / N}\right)_{j,k=-N/2}^{N/2-1}\,, \tag{27}$$

where $\boldsymbol{f} = (f_k)_{k=-N/2}^{N/2-1}$ and $\hat{\boldsymbol{f}} = \left(\hat{f}(v_j)\right)_{j=-N/2}^{N/2-1}$,

$$x_k, v_j \in [-N/2, N/2)$$

equispaced data $x_k = k$ and $v_j = j$, the matrix–vector multiplication (27) coincides with the uniform discrete Fourier transform

aim: sparse factorization of $\boldsymbol{A}_{tf}$

main difference: $\{e^{-2\pi i k \cdot} : k \in \mathbb{Z}\}$ is related to periodic functions
$\{e^{-2\pi i v \cdot} : v \in \mathbb{R}\}$ corresponds to functions defined on $\mathbb{R}$

let $\varphi_1 \in L_2(\mathbb{R})$ denote a sufficiently smooth and even function with Fourier transform

$$\hat{\varphi}_1(v) = \int\limits_{\mathbb{R}} \varphi_1(x) \mathrm{e}^{-2\pi \mathrm{i} v x} \mathrm{d}x \,,$$

where $\hat{\varphi}_1(v) \neq 0$ for all $v \in [-N/2, N/2)$. Then we obtain for

$$G(x) = \sum_{k=-N/2}^{N/2-1} f_k \, \varphi_1 \left(x - \frac{x_k}{N} \right) \tag{28}$$

that

$$\frac{\hat{G}(v)}{\hat{\varphi}_1(v)} = \sum_{k=-N/2}^{N/2-1} f_k \, \mathrm{e}^{-2\pi \mathrm{i} x_k v/N} = \hat{f}(v) \quad (v \in [-N/2, N/2)) \,. \tag{29}$$

By (26), we have to ask for a fast computation of

$$\hat{G}(v_j) \quad (j = -N/2, \ldots, N/2-1) \,.$$

Let $n_1 = \sigma_1 N$ $(\sigma_1 > 1)$ and $m_1 << N$. We approximate φ_1 by a function ψ_1 with support in $[-(m_1+1/2)/n_1, (m_1+1/2)/n_1]$. Then we obtain for all $x_k \in [-N/2, N/2)$ that

$$\text{supp}\,\psi_1(x - \frac{x_k}{N}) \subseteq \left[\frac{x_k}{N} - \frac{m_1 + 1/2}{n_1}, \frac{x_k}{N} + \frac{m_1 + 1/2}{n_1}\right] \subseteq \left[-\frac{a}{2}, \frac{a}{2}\right],$$

where

$$a = 1 + \frac{2m_1 + 1}{n_1}\,.$$

Now we conclude by (29) and (28) that

$$\begin{aligned} \hat{f}(v_j)\hat{\varphi}_1(v_j) &= \sum_{k=-N/2}^{N/2-1} f_k \int_{\mathbb{R}} \varphi_1(x - \frac{x_k}{N})\,\mathrm{e}^{-2\pi \mathrm{i} x v_j}\,\mathrm{d}x \\ &\approx \sum_{k=-N/2}^{N/2-1} f_k \int_{-a/2}^{a/2} \psi_1(x - \frac{x_k}{N})\,\mathrm{e}^{-2\pi \mathrm{i} x v_j}\,\mathrm{d}x\,. \end{aligned}$$

Evaluating the integral by the rectangular rule we obtain

$$\hat{f}(v_j)\hat{\varphi}_1(v_j) \approx \sum_{k=-N/2}^{N/2-1} f_k \frac{1}{n_1} \sum_{l=-an_1/2}^{an_1/2-1} \psi_1\left(\frac{l}{n_1} - \frac{x_k}{N}\right) \mathrm{e}^{-2\pi \mathrm{i} l v_j/n_1}.$$

Here we have to ensure that $an_1/2 = a\sigma_1 N/2 \in \mathbb{Z}$. Finally this can be rewritten as

$$\hat{f}(v_j)\hat{\varphi}_1(v_j) n_1 = \sum_{l=-an_1/2}^{an_1/2-1} \left(\sum_{k\in I_l} f_k \, \psi_1\left(\frac{l}{n_1} - \frac{x_k}{N}\right)\right) \mathrm{e}^{-2\pi \mathrm{i} l a v_j/(an_1)}, \qquad (30)$$

where

$$I_l = \{k : l - (m_1 + \frac{1}{2}) \le x_k n_1/N \le l + (m_1 + \frac{1}{2})\}.$$

After the computation of the inner sums the computation of (30) reduces to the NFFT.

matrix–vector form

$$\boldsymbol{A}_{tf} \approx \boldsymbol{D}_1 \, \boldsymbol{A}_f \boldsymbol{B}_1^T \,, \tag{31}$$

$$\boldsymbol{D}_1 = \operatorname{diag}\left(1/(n_1 \hat{\varphi}_1(v_j))\right)_{j=-N/2}^{N/2-1} \,, \;\; \boldsymbol{A}_f = \left(\mathrm{e}^{-2\pi \mathrm{i} l v_j / n_1}\right)_{j=-N/2, l=-a n_1/2}^{N/2-1, a n_1/2-1}$$

$$\boldsymbol{B}_1 = (b_{1,k,l})_{k=-N/2, l=-a n_1/2}^{N/2-1, a n_1/2-1}$$

with

$$b_{1,k,l} = \begin{cases} \psi_1\left(\frac{l}{n_1} - \frac{x_k}{N}\right) & l = \left[\frac{n_1 x_k}{N}\right] - m_1, \ldots, \left[\frac{n_1 x_k}{N}\right] + m_1 \,, \\ 0 & \text{otherwise.} \end{cases}$$

Note that in contrast to the entries of the matrix $\boldsymbol{B}$, the entries of $\boldsymbol{B}_1$ were not arranged periodically. For $a = 1$ and periodic or non–periodic entries of $\boldsymbol{B}_1$, the algorithm doesn't work.

Fast trigonometric transforms at nonequispaced nodes (NDCT, NDST)

References: M. Fenn and P. [11, 29]

Problem: fast computation of

$$f^{\mathrm{C}}(x) := \sum_{k=0}^{N-1} \hat{f}_k^{\mathrm{C}} \cos(2\pi k x) \tag{32}$$

at knots

$$x_j \in [0, 1/2] \quad (j = 0, \ldots, M-1)$$

for equispaced nodes x_j and $N = M$

$$x_j := \frac{j}{N} \quad (j = -N/2, \ldots, N/2)$$

DCT in $\mathcal{O}(N \log N)$ flops

DCT-I

$$\boldsymbol{x} = \boldsymbol{C}_{N+1}^{I} \hat{\boldsymbol{x}}, \qquad \boldsymbol{C}_{N+1}^{I} := \left(\varepsilon_{N,j} \cos \frac{jk\pi}{N} \right)_{k,j=0}^{N} \tag{33}$$

with $\varepsilon_{N,0} = \varepsilon_{N,N} = 1/2$, $\varepsilon_{N,j} = 1$ $(j = 1, \ldots, N-1)$

approach based on the NFFT

φ even with $\varphi \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$

$$s_1(x) := \sum_{l=0}^{\sigma N} g_l \tilde{\varphi}\left(x - \frac{l}{2\sigma N}\right) \tag{34}$$

compute $g_l \in \mathbb{R}$ $(l = 0, \ldots, \sigma N)$ such that $s_1 \approx f^{\mathrm{C}}$

$$f(x) := \sum_{k=-N}^{N-1} \hat{f}_k \, \mathrm{e}^{2\pi \mathrm{i} k x} \tag{35}$$

chose $\hat{f}_k \in \mathbb{R}$ $(k = 0, \ldots, N-1)$ with $\hat{f}_k = \hat{f}_{-k}$ and $\hat{f}_{-N} = 0$

then

$$f^{\mathrm{C}}(x) = f(x) \quad \text{if} \quad \hat{f}_k^{\mathrm{C}} = 2\varepsilon_{N,k} \hat{f}_k$$

since $\tilde{\varphi}$ is even $c_k(\tilde{\varphi}) = c_{-k}(\tilde{\varphi})$ and with (13) follows $\hat{g}_k = \hat{g}_{-k}$.

to take into account this symmetries in (15)

$$g_l = \text{Re}(g_l) = \frac{1}{\sigma N} \sum_{k=0}^{\sigma N} \varepsilon_{\sigma N,k}\, \hat{g}_k \cos(\frac{2\pi kl}{\sigma N}) \quad (l = 0, \ldots, \sigma N)$$

note $g_l = g_{2\sigma Nr-l}$ $(r \in \mathbb{Z})$ i.e., g_l in (34) with DCT-IσN finally

$$s(x) := \sum_{l=\lfloor 2\sigma Nx \rfloor - m}^{\lceil 2\sigma Nx \rceil + m} g_l \tilde{\psi}\left(x - \frac{l}{2\sigma N}\right) \tag{36}$$

Algorithm: (NFCT)

Input: $N, M \in \mathbb{N}$, $\sigma > 1$, $\hat{f}_k^{\mathrm{C}} \in \mathbb{R}$ $(k = 0, \ldots, N-1)$,
$v_j \in [0, 1/2]$ $(j = 1, \ldots, M)$.

Precomputation: $c_k(\tilde{\varphi})$ $(k = 0, \ldots, N-1)$,
$\tilde{\varphi}\left(v_j - \frac{l}{2\sigma N}\right)$ $(j = 1, \ldots, M;$
$(l = \lfloor 2\sigma N v_j \rfloor - (m-1), \ldots, \lceil 2\sigma N v_j \rceil + (m-1))$

1. For $k = 0, \ldots, N-1$ compute $\hat{g}_k := \dfrac{\hat{f}_k^{\mathrm{C}}}{2\varepsilon_{N,k} c_k(\tilde{\varphi})}$ and for $k = N, \ldots, \sigma N$ set $\hat{g}_k := 0$.
2. For $l = 0, \ldots, \sigma N$ compute g_l by a fast DCT–I of length σN.
3. For $j = 1, \ldots, M$ compute $s(v_j)$.

Output: $s(v_j)$ approximate values for $f^{\mathrm{C}}(v_j)$.

NDST

Problem: fast computation of

$$f^{\mathrm{S}}(x) = \sum_{k=1}^{N-1} \hat{f}_k^{\mathrm{S}} \sin(2\pi k x) \tag{37}$$

$$x_j \in [0, 1/2] \quad (j = 0, \ldots, M-1)$$

for equispaced nodes x_j and $N = M$

$$x_j := \frac{j}{N} \quad (j = -N/2, \ldots, N/2)$$

DST in $\mathcal{O}(N \log N)$ flops

approach based on the NFFT
$\hat{f}_k \in \mathbb{R}$ with $\hat{f}_{-k} = -\hat{f}_k$ $(k = 1, \ldots, N-1)$ and $\hat{f}_0 = \hat{f}_{-N} = 0$
then in (35)

$$f(x) = \sum_{k=-N}^{N-1} \hat{f}_k \; \mathrm{e}^{2\pi \mathrm{i} k x} = \mathrm{i} \sum_{k=1}^{N-1} 2\hat{f}_k \sin(2\pi k x).$$

we obtain for $\hat{f}_k^{\mathrm{S}} = 2\hat{f}_k$ that $f^{\mathrm{S}}(x) = \mathrm{i} f(x)$
compute g_k in (13)
$\hat{g}_k = -\hat{g}_{-k}$ $(k = 1, \ldots, \sigma N - 1)$ and for $l = 0, \ldots, \sigma N$

$$-\mathrm{i} g_l = \frac{-\mathrm{i}}{2\sigma N} \sum_{k=-\sigma N}^{\sigma N - 1} \hat{g}_k \; \mathrm{e}^{\pi \mathrm{i} k l/(\sigma N)} = \frac{1}{\sigma N} \sum_{k=1}^{\sigma N - 1} \hat{g}_k \sin\left(\frac{\pi k l}{\sigma N}\right). \tag{38}$$

note $g_{2\sigma N r - l} = -g_l$ $(r \in \mathbb{Z})$
finally

$$\mathrm{i} s(x_j) := \sum_{l=\lfloor 2\sigma N x_j \rfloor - m}^{\lceil 2\sigma N x_j \rceil + m} \mathrm{i} g_l \, \tilde{\psi}\left(x_j - \frac{l}{2\sigma N}\right) \tag{39}$$

with $f^{\mathrm{S}}(x_j) = \mathrm{i} f(x_j) \approx \mathrm{i} s(x_j)$.

Algorithm: (NFST)

Input: $N, M \in \mathbb{N}$, $\sigma > 1$, $\hat{f}_k^{\mathrm{S}} \in \mathbb{R}$ $(k = 1, \ldots, N-1)$,
$v_j \in [0, 1/2]$ $(j = 1, \ldots, M)$.
Precomputation: $c_k(\tilde{\varphi})$ $(k = 1, \ldots, N-1)$,
$\tilde{\varphi}\left(v_j - \frac{l}{2\sigma N}\right)$ $(j = 1, \ldots, M;$
$l = \lfloor 2\sigma N v_j \rfloor - (m-1), \ldots, \lceil 2\sigma N v_j \rceil + (m-1))$

1. For $k = 1, \ldots, N-1$ compute $\hat{g}_k := \dfrac{\hat{f}_k^{\mathrm{S}}}{2c_k(\tilde{\varphi})}$ and for $k = 0, N, \ldots, \sigma N$ set $\hat{g}_k := 0$.
2. For $l = 0, \ldots, \sigma N$ compute g_l by (38) by a fast DST–I of length σN.
3. For $j = 1, \ldots, M$ compute i$s(v_j)$ by (39).

Output: i$s(v_j)$ approximate values for $f^{\mathrm{S}}(v_j)$.

Roundoff errors

References: P., Steidl, Tasche [38, 39]

classical FFT [40, 17] is robust with respect to roundoff errors

Problem: Is the NFFT robust ?

Let us call an algorithm *robust*, if for all $\boldsymbol{f} \in \mathbb{R}^N$ there exists a positive constant k_N with $k_N\, u \ll 1$ such that

$$||\mathrm{fl}(\tilde{\boldsymbol{f}}) - \tilde{\boldsymbol{f}}||_2 \le (k_N u + \mathcal{O}(u^2))\, ||\boldsymbol{f}||_2$$

with $\tilde{\boldsymbol{f}} = \boldsymbol{A}\boldsymbol{f}$.

standard model of real floating point arithmetic (see [17], p. 44):
For arbitrary $\xi, \eta \in \mathbb{R}$ and any operation $\circ \in \{+, -, \times, /\}$ the exact value $\xi \circ \eta$ and the computed value $\mathrm{fl}(\xi \circ \eta)$ are related by

$$\mathrm{fl}(\xi \circ \eta) = (\xi \circ \eta)\,(1 + \delta) \quad (|\delta| \le u)\,,$$

where u denotes the *unit roundoff* (or machine precision).

Example: single precision (24 bits for the mantissa (with 1 sign bit), 8 bits for the exponent)

$$u = 2^{-24} \approx 5.96 \times 10^{-8}$$

double precision (53 bits for the mantissa (with 1 sign bit), 11 bits for the exponent)

$$u = 2^{-53} \approx 1.11 \times 10^{-16}.$$

complex arithmetic is implemented using real arithmetic
the complex floating point arithmetic is a consequence of the corresponding real arithmetic (see [17], pp. 78 – 80):

For arbitrary $\xi, \eta \in \mathbb{C}$, we have

$$\mathrm{fl}(\xi + \eta) \;=\; (\xi + \eta)\,(1 + \delta) \quad (|\delta| \leq u)\ , \tag{40}$$

$$\mathrm{fl}(\xi\,\eta) \;=\; \xi\,\eta\,(1 + \delta) \quad (|\delta| \leq \frac{2\sqrt{2}\,u}{1 - 2u})\ . \tag{41}$$

In particular, if $\xi \in \mathbb{R} \cup \mathrm{i}\mathbb{R}$ and $\eta \in \mathbb{C}$, then

$$\mathrm{fl}(\xi\eta) = \xi\eta\,(1 + \delta) \quad (|\delta| \leq u)\ . \tag{42}$$

compute

$$\hat{\boldsymbol{f}} := \boldsymbol{A}_N \boldsymbol{f}$$

by conventional multiplication and cascade summation

$$|\mathrm{fl}(\hat{f})_j - \hat{f}_j| \le \frac{(\lceil \log_2 N \rceil + 1)\, u}{1 - (\lceil \log_2 N \rceil + 1) u} \, \|\boldsymbol{f}\|_1$$

and by taking the Euclidean norm

$$\|\mathrm{fl}(\hat{\boldsymbol{f}}) - \hat{\boldsymbol{f}}\|_2 \le \big(u\, N \,(\lceil \log_2 N \rceil + 1) + \mathcal{O}(u^2)\big) \, \|\boldsymbol{f}\|_2 \, .$$

In particular, we have for $\hat{\boldsymbol{f}} := \boldsymbol{F}_N \boldsymbol{f}$ that

$$\|\mathrm{fl}(\boldsymbol{F}_N \boldsymbol{f}) - \boldsymbol{F}_N \boldsymbol{f}\|_2 \le \big(u\, N \,(\lceil \log_2 N \rceil + 1) + \mathcal{O}(u^2)\big) \, \|\boldsymbol{f}\|_2 \, .$$

If we compute $\hat{\boldsymbol{f}} = \boldsymbol{F}_N \boldsymbol{f}$ ($\boldsymbol{f} \in \mathbb{R}$, N power of 2) by the radix–2 Cooley–Tukey FFT, then, following the lines of the proof in [44] and using (40) – (41), the roundoff error estimate can be improved by the factor $\sqrt{N}$, more precisely

$$\|\mathrm{fl}(\boldsymbol{F}_N \boldsymbol{f}) - \boldsymbol{F}_N \boldsymbol{f}\|_2 \le \left(u\,(4+\sqrt{2})\sqrt{N}\,\log_2 N \;+\; \mathcal{O}(u^2)\right)\, \|\boldsymbol{f}\|_2 \,.$$

The following theorem states that the roundoff error introduced by NFFT can be estimated as the FFT error up to a constant factor, which depends on m and α.

Theorem: Let $m, N \in \mathbb{N}$ and let $n := \alpha N$ $(\alpha > 1)$ be a power of 2 with $2m \ll n$. Furthermore let the nodes $w_j := \frac{v_j}{N} \in [-\frac{1}{2}, \frac{1}{2})$, $w_j \pm 1$ $(j \in I_N)$ be distributed such that each "window" $\left[-\frac{m}{n} + \frac{l}{n}, \frac{m}{n} + \frac{l}{n}\right)$ $(l \in I_n)$ contains at most γ/α nodes. If

$$\tilde{\boldsymbol{f}} := \boldsymbol{B}\,\boldsymbol{F}_n\,\boldsymbol{D}\,\boldsymbol{f} \quad (\boldsymbol{f} \in \mathbb{R}^N)\,,$$

is computed by with the NFFT, then the roundoff error can be estimated by

$$\|\mathrm{fl}(\hat{\boldsymbol{f}}) - \tilde{\boldsymbol{f}}\|_2 \le \beta\,\sqrt{\gamma}\left(u(4+\sqrt{2})\,\sqrt{N}\,(\log_2 N + \log_2 \alpha + \frac{2m+1}{4+\sqrt{2}}) + \mathcal{O}(u^2)\right)\|\boldsymbol{f}\|_2$$

with

$$\beta := \frac{(\hat{\varphi}^2(0) + ||\hat{\varphi}||_{L_2}^2)^{1/2}}{|\varphi(\pi/\alpha)|}\,.$$

Content

- ”inverse” NFFT
  - Linear system of equations - iNFFT
  - Interpolation problem
  - Approximation problem
  - Iterative methods
  - ”Probabilistic” condition number
- Applications of NFFTs

Linear system of equations - iNFFT

inverse problem, $\boldsymbol{f} \in \mathbb{C}^M$ given in

$$\boldsymbol{A}\hat{\boldsymbol{f}} \approx \boldsymbol{f}$$

Moore-Penrose pseudo-inverse solution $\hat{\boldsymbol{f}}^\dagger = \boldsymbol{A}^\dagger \boldsymbol{f}$ fulfills

$$\| \overbrace{\boldsymbol{A}\hat{\boldsymbol{f}}^\dagger - \boldsymbol{f}}^{\text{residual}} \|_2 \le \|\boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f}\|_2 \qquad \text{for all} \quad \hat{\boldsymbol{f}} \in \mathbb{C}^N$$

$\leadsto$ approximation problem

$$\|\hat{\boldsymbol{f}}^\dagger\|_2 \le \|\hat{\boldsymbol{f}}\|_2 \qquad \text{for all} \quad \hat{\boldsymbol{f}} \text{ with } \|\boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f}\|_2 = \min$$

$\leadsto$ minimization problem

special case IDFT, Gauß quadrature, $M = N,\ x_j = \frac{j}{M} - 0.5$

$$\boldsymbol{A}^{\mathsf{H}} \underbrace{\boldsymbol{W}}_{\frac{1}{M}\boldsymbol{I}} \boldsymbol{A} = \boldsymbol{I} \quad \Rightarrow \quad \hat{\boldsymbol{f}} = \boldsymbol{A}^{\mathsf{H}}\boldsymbol{W}\boldsymbol{f}$$

Interpolation problem

vanishing residual, i.e. $\boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f} = \boldsymbol{0}$, $\rightsquigarrow$ interpolation problem

damped minimisation problem, $\hat{\omega}_k > 0$, $\hat{\boldsymbol{W}} := \operatorname{diag}(\hat{\omega}_k)_{k=-\frac{N}{2}}^{\frac{N}{2}-1}$,

$$\left(\sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{\omega}_k^{-1} |\hat{f}_k|^2\right)^{\frac{1}{2}} =: \|\hat{\boldsymbol{f}}\|_{\hat{\boldsymbol{W}}^{-1}} \stackrel{\hat{\boldsymbol{f}}}{\to} \min \quad \text{subject to} \quad \boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f}$$

substitute

$$\hat{\boldsymbol{f}}^{\omega} := \hat{\boldsymbol{W}}^{-\frac{1}{2}} \hat{\boldsymbol{f}}$$

$$\|\hat{\boldsymbol{f}}^{\omega}\|_2 \stackrel{\hat{\boldsymbol{f}}^{\omega}}{\to} \min \quad \text{subject to} \quad \boldsymbol{A}\hat{\boldsymbol{W}}^{\frac{1}{2}} \hat{\boldsymbol{f}}^{\omega} = \boldsymbol{f}$$

damped normal equation of second kind

$$\boldsymbol{A}\hat{\boldsymbol{W}}\boldsymbol{A}^{\mathsf{H}}\tilde{\boldsymbol{f}} = \boldsymbol{f}, \qquad \hat{\boldsymbol{f}} = \hat{\boldsymbol{W}}\boldsymbol{A}^{\mathsf{H}}\tilde{\boldsymbol{f}}$$

Towards normal equation of second kind (1)

standard minimisation problem, i.e. $\hat{\boldsymbol{W}} = \boldsymbol{I}$,

$$\|\hat{\boldsymbol{f}}\|_2 \xrightarrow{\hat{\boldsymbol{f}}} \min \quad \text{subject to} \quad \boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f}$$

null space and range of $\boldsymbol{A}$

$$\mathcal{N}(\boldsymbol{A}) := \left\{\hat{\boldsymbol{f}} \in \mathbb{C}^N : \boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{0}\right\}, \quad \mathcal{R}(\boldsymbol{A}) := \left\{\boldsymbol{f} = \boldsymbol{A}\hat{\boldsymbol{f}} : \hat{\boldsymbol{f}} \in \mathbb{C}^N\right\}$$

equivalent problem

$$\hat{\boldsymbol{f}} \perp \mathcal{N}(\boldsymbol{A}) \quad \text{subject to} \quad \boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f}$$

furthermore

$$\mathcal{N}(\boldsymbol{A})^{\perp} \overset{[3]}{=} \mathcal{R}\left(\boldsymbol{A}^{\mathsf{H}}\right) \quad \Rightarrow \quad \exists \tilde{\boldsymbol{f}} \in \mathbb{C}^M : \hat{\boldsymbol{f}} = \boldsymbol{A}^{\mathsf{H}}\tilde{\boldsymbol{f}}$$

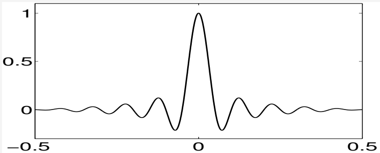
normal equation of second kind

$$\boldsymbol{A}\boldsymbol{A}^{\mathsf{H}}\tilde{\boldsymbol{f}} = \boldsymbol{f}, \qquad \hat{\boldsymbol{f}} = \boldsymbol{A}^{\mathsf{H}}\tilde{\boldsymbol{f}}$$

Towards normal equation of second kind (2)

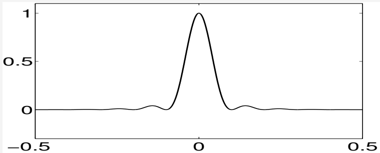
interpolation with polynomial kernels

$$K_N(x-y) := \sum_{k\in I_N^1} \mathrm{e}^{-2\pi \mathrm{i} k y} \hat{\omega}_k \, \mathrm{e}^{2\pi \mathrm{i} k x},$$



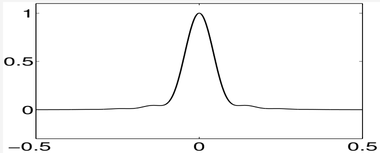
Dirichlet

$\hat{\omega}_k = 1/N$



Fejer

$\hat{\omega}_k = \frac{1}{2} + \frac{1}{N} - \frac{|k|}{N}$



'Gauß'

$\hat{\omega}_k = \mathrm{e}^{-k^2/N}/N$

linear combination

$$\sum_{j=0}^{M-1} \tilde{f}_j K_N(\cdot - x_j) = f, \qquad \hat{\boldsymbol{f}} = \hat{\boldsymbol{W}} \boldsymbol{A}^{\mathsf{H}} \tilde{\boldsymbol{f}}$$

discrete version - damped normal equation of second kind

$$\boldsymbol{A}\hat{\boldsymbol{W}}\boldsymbol{A}^{\mathsf{H}}\tilde{\boldsymbol{f}} = \boldsymbol{f}, \qquad \boldsymbol{A}\hat{\boldsymbol{W}}\boldsymbol{A}^{\mathsf{H}} = \left(K_N\left(y_l - x_j\right)\right)_{j=0,l=0}^{M-1,M-1}$$

Interpolation - eigenvalues

compare $\boldsymbol{f} \in \mathbb{C}^M$ and $f \in L_N := \operatorname{span}\{\mathrm{e}^{2\pi\mathrm{i}k\cdot} : k \in I_N^1\}$ with $f(x_j) = f_j$ and $\|f\|_{\hat{\boldsymbol{W}}^{-1}}$ minimal (Marcinkiewicz-Zygmund)

$$\xi \|\boldsymbol{f}\|_2^2 \leq \|f\|_{\hat{\boldsymbol{W}}^{-1}}^2 \leq \Xi \|\boldsymbol{f}\|_2^2$$

best possible constants

$$\xi = \left(\lambda_{\max}\left(\boldsymbol{A}\hat{\boldsymbol{W}}\boldsymbol{A}^{\mathrm{H}}\right)\right)^{-1}, \quad \Xi = \left(\lambda_{\min}\left(\boldsymbol{A}\hat{\boldsymbol{W}}\boldsymbol{A}^{\mathrm{H}}\right)\right)^{-1}$$

for $\hat{\omega}_k = 1$ with the theorem of Gershgorin

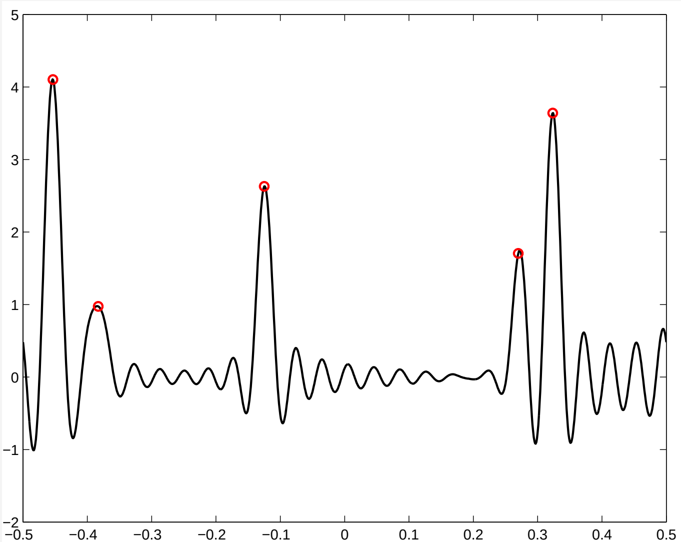
$$\begin{aligned} \left|\lambda\left(\boldsymbol{A}\boldsymbol{A}^{\mathrm{H}}\right) - 1\right| &\leq \sum_{j=0;j\neq l}^{M-1} |D_N(x_j, x_l)| \\ &\leq \frac{1}{q}\left(1 + \ln\frac{M}{2}\right) \end{aligned}$$

with

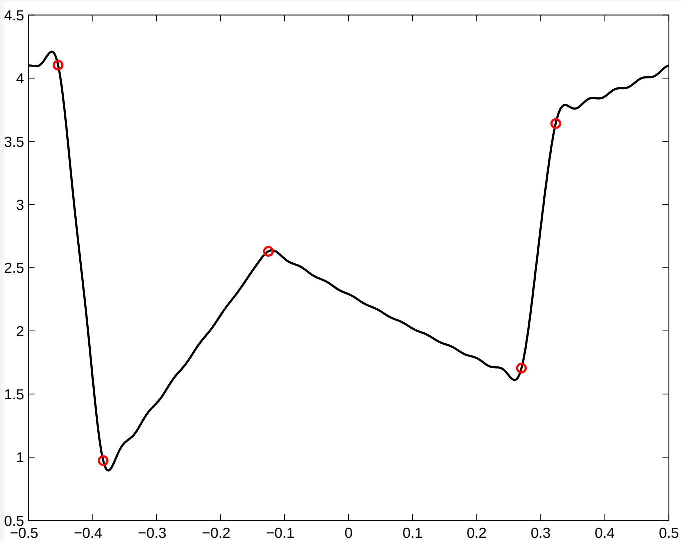
$$q = q_{\boldsymbol{X}} := \min_{j=0,\ldots,M-1} \operatorname{dist}(x_j, x_{j+1}), \qquad \operatorname{dist}(x, y) := \min_{j\in\mathbb{Z}} |x - (y + j)|$$

Interpolation example - Sobolev norm

real part of interpolation with polynomials, $M = 5,\ N = 50$
interpolation conditions are given by circles
damped factors $\hat{\omega}_k = (1 + (2\pi k)^2)^{-1}$



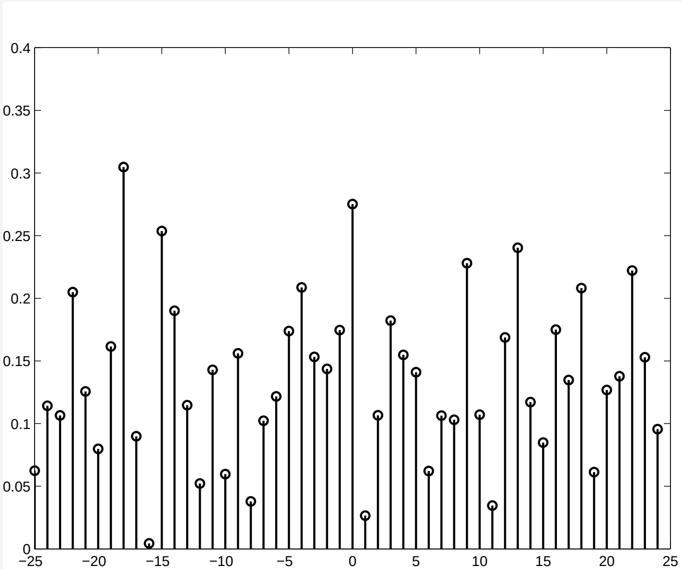
$$\|f\|_{L^2(\mathbb{T})} = \|\hat{\boldsymbol{f}}\|_2$$



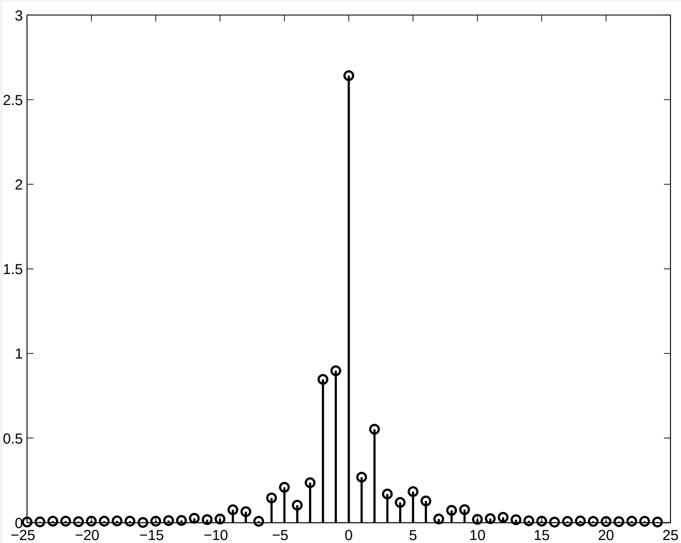
$$\|f\|_{W_1^2} = \|f\|_{L^2(\mathbb{T})} + \|f'\|_{L^2(\mathbb{T})} = \|\hat{\boldsymbol{f}}\|_{\hat{\boldsymbol{W}}}$$

Interpolation example - Sobolev-norm

absolute value of Fourier coefficients $\hat{f}_k, \; k = -25, \ldots, 24$



$\|\hat{\boldsymbol{f}}\|_2$ minimal



$\|\hat{\boldsymbol{f}}\|_{\hat{W}}$ minimal

Lemma [22]: Let $M \in \mathbb{N}$, $N \in 2\mathbb{N}$, and let $\mathcal{X}$ contain arbitrary sampling nodes with separation distance $q = \min_{j \neq l} \operatorname{dist}(x_j, x_l)$. If for some $\beta > 1$ the kernel K_N fulfils the conditions

1. $K_N(0) = 1$,
2. $|K_N(x)| \le \frac{C_\beta}{N^\beta |x|^\beta}$ for $x \in \left[-\frac{1}{2}, \frac{1}{2}\right] \setminus \{0\}$,

then the spectrum of the matrix

$$\boldsymbol{A}\hat{\boldsymbol{W}}\boldsymbol{A}^{\mathrm{H}} = \boldsymbol{K}_N = \left(K_N(x_j - x_l)\right)_{j,l=0,\ldots,M-1}$$

is bounded by

$$\sigma(\boldsymbol{K}_N) \subseteq \left[1 \pm \frac{2\,\zeta(\beta)\,C_\beta}{N^\beta q^\beta}\right].$$

Proof:

Let $\lambda_\star$ be an arbitrary eigenvalue of $\boldsymbol{K}$. Then, for some index $j \in \{0, \ldots, M-1$ assumption 1. and Geršgorin's circle theorem yield

$$|\lambda_\star - 1| \leq \sum_{l=0; l \neq j}^{M-1} |K_N(x_j - x_l)| \, .$$

Furthermore, by using that the separation distance of the sampling set is q, and by assuming 2. for the kernel K_N, we obtain

$$|\lambda_\star - 1| \; \leq \; \frac{C_\beta}{N^\beta} \sum_{l=0; l \neq j}^{M-1} \frac{1}{|x_j - x_l|^\beta} \leq \frac{2\, C_\beta}{N^\beta q^\beta} \sum_{l=1}^{\lfloor M/2 \rfloor} l^{-\beta} < \frac{2\, \zeta(\beta) C_\beta}{N^\beta q^\beta}.$$

Interpolation - multivariate setting

Lemma: Let $M \in \mathbb{N}$, $N \in 2\mathbb{N}$, and let $\mathcal{X}$ contain arbitrary sampling nodes with separation distance q, where dist $(\boldsymbol{x}, \boldsymbol{y}) := \min_{\boldsymbol{j} \in \mathbb{Z}^d} \|(\boldsymbol{x} + \boldsymbol{j}) - \boldsymbol{y}\|_\infty$ If for some $\beta > 1$ the multivariate kernel K_N fulfils the conditions

1. $K_N(\mathbf{0}) = 1$,
2. $|K_N(\boldsymbol{x})| \leq \frac{C_\beta}{N^\beta \|\boldsymbol{x}\|_\infty^\beta}$ for $\boldsymbol{x} \in \left[-\frac{1}{2}, \frac{1}{2}\right]^d \setminus \{\mathbf{0}\}$,

then the spectrum of the kernel matrix $\boldsymbol{K}_N = (K_N(\boldsymbol{x}_j - \boldsymbol{x}_l))_{j,l=0,\ldots,M-1}$ is bounded by

$$\sigma(\boldsymbol{K}_N) \subseteq \left[1 \pm \frac{2d\zeta(\beta) C_\beta}{N^\beta q^{\beta+d-1}}\right].$$

Approximation problem

weighted approximation problem, $\omega_j > 0,\ \boldsymbol{W} = \operatorname{diag}\left(\omega_j\right)_{j=0}^{M-1}$,

$$\|\boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f}\|_{\boldsymbol{W}} \xrightarrow{\hat{\boldsymbol{f}}} \min$$

substitute

$$\boldsymbol{A}^{\omega} := \boldsymbol{W}^{\frac{1}{2}}\boldsymbol{A}, \qquad \boldsymbol{f}^{\omega} := \boldsymbol{W}^{\frac{1}{2}}\boldsymbol{f}$$

$$\|\boldsymbol{A}^{\omega}\hat{\boldsymbol{f}} - \boldsymbol{f}^{\omega}\|_2 \xrightarrow{\hat{\boldsymbol{f}}} \min$$

weighted normal equation of first kind

$$\underbrace{\boldsymbol{A}^{\mathsf{H}}\boldsymbol{W}\boldsymbol{A}}_{\text{Toeplitz}}\,\hat{\boldsymbol{f}} = \boldsymbol{A}^{\mathsf{H}}\boldsymbol{W}\boldsymbol{f}$$

Towards normal equation of first kind

standard approximation problem, i.e. $\boldsymbol{W} = \boldsymbol{I}$,

$$\|\boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f}\|_2 \xrightarrow{\hat{\boldsymbol{f}}} \min$$

equivalent problem

$$\boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f} \perp \mathcal{R}\left(\boldsymbol{A}\right)$$

furthermore

$$\mathcal{R}\left(\boldsymbol{A}\right)^{\perp} \overset{[3]}{=} \mathcal{N}\left(\boldsymbol{A}^{\mathsf{H}}\right) \quad \Rightarrow \quad \boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f} \in \mathcal{N}\left(\boldsymbol{A}^{\mathsf{H}}\right)$$

normal equation of first kind

$$\boldsymbol{A}^{\mathsf{H}}\left(\boldsymbol{A}\hat{\boldsymbol{f}} - \boldsymbol{f}\right) = \boldsymbol{0}$$

Sampling set - eigenvalues

compare $f \in L_N := \operatorname{span}\left\{ \mathrm{e}^{2\pi \mathrm{i} k \cdot} : k \in I_N^1 \right\}$ and $\boldsymbol{f} = \left(f\left(x_j\right)\right)_{j=0}^{M-1}$, (Marcinkiewicz-Zygmund),

$$\xi \|f\|_{L^2(\mathbb{T})}^2 \leq \|\boldsymbol{f}\|_{\boldsymbol{W}}^2 \leq \Xi \|f\|_{L^2(\mathbb{T})}^2$$

best possible constants

$$\xi = \lambda_{\min}\left(\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A}\right), \quad \Xi = \lambda_{\max}\left(\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A}\right), \quad \text{cond}_2\left(\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A}\right) \leq \frac{\Xi}{\xi}$$

Parseval $\|f\|_{L^2(\mathbb{T})} = \|\hat{\boldsymbol{f}}\|_2$, $\boldsymbol{f} = \boldsymbol{A}\hat{\boldsymbol{f}}$, Rayleigh coefficients of $\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A}$

$$\xi \leq \underbrace{\frac{\hat{\boldsymbol{f}}^{\mathsf{H}} \boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A} \hat{\boldsymbol{f}}}{\hat{\boldsymbol{f}}^{\mathsf{H}} \hat{\boldsymbol{f}}}}_{\in \left[\lambda_{\min}\left(\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A}\right), \lambda_{\max}\left(\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A}\right)\right]} \leq \Xi$$

Simple example, worst sampling set (1)

equidistant points $M \geq N,\ x_j = \frac{j}{M} - \frac{1}{2},\ \omega_j = \frac{1}{M}$

$$\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A} = \boldsymbol{I}$$

lower bound ξ

$$f \neq 0 \text{ and } \forall j : \ f(x_j) = 0 \quad \Rightarrow \quad \xi = 0$$

weak conditions

1. $M \geq N$ arbitrary distinct sampling nodes in $\mathbb{T}$ guarantees $\xi > 0$.
2. $M \geq N$ independent uniform distributed sampling nodes in $\mathbb{T}^d$ ensures almost surely $\xi > 0$.

Worst sampling set (2)

upper bound Ξ, Nikol'skii,

$$\begin{aligned}
D_N(\cdot) &:= \sum_{k \in I_N^1} \mathrm{e}^{2\pi \mathrm{i} k \cdot}, \\
\|f\|_\infty \le \int_{\mathbb{T}} |f(t)|\,|D_N(t-x)|\,\mathrm{d}t &\le \|f\|_{L^2(\mathbb{T})} \|D_N\|_{L^2(\mathbb{T})}, \\
\|f\|_\infty &\le \sqrt{N} \|f\|_{L^2(\mathbb{T})}, \\
\|D_N\|_\infty = \sqrt{N} \|D_N\|_{L^2(\mathbb{T})} &= N, \\
\|\boldsymbol{f}\|_{\boldsymbol{W}}^2 = \sum_{j=0}^{M-1} \omega_j |f(x_j)|^2 \le \sum_{j=0}^{M-1} \omega_j \|f\|_\infty^2 &\le N \|\boldsymbol{\omega}\|_1 \|f\|_{L^2(\mathbb{T})}^2, \\
f = D_N \text{ and } \forall j: \; f(x_j) = \|f\|_\infty &\Rightarrow \Xi = N \|\boldsymbol{\omega}\|_1
\end{aligned}$$

Towards dense sampling set - partition

$$\text{dist}\,(x,y) := \min_{j\in\mathbb{Z}} |x-(y+j)|$$

mesh–norm, Mhaskar, δ-dense

$$\delta_{\boldsymbol{X}} = \max_{x\in\mathbb{T}} \min_{j=0,\dots,M-1} \text{dist}\,(x,x_j)\,, \qquad \delta_{\boldsymbol{X}} < \delta \in \mathbb{R}^+$$

Voronoi partition

$$R_{\mathsf{V},j} := \left\{ x\in\mathbb{T} : \arg\min_{l=0,\dots,M-1} \text{dist}\,(x,x_l) = j \right\},$$

$$\boldsymbol{R}_{\mathsf{V}} := \{R_{\mathsf{V},j} : j=0,\dots,M-1\}\,, \qquad \omega_j := \int_{R_{\mathsf{V},j}} \mathrm{d}x$$

Dense sampling set

Feichtinger, Gröchenig, Strohmer
δ-dense sampling set $\boldsymbol{X}$, Voronoi weights ω_j, $N < \frac{1}{\delta}$

$$(1-\delta N)^2 \, ||f||^2_{L^2(\mathbb{T})} \leq ||\boldsymbol{f}||^2_{\boldsymbol{W}} \leq (1+\delta N)^2 \, ||f||^2_{L^2(\mathbb{T})}$$

weighted normal equation of first kind

$$\text{cond}_2 \left(\boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{A}\right) \leq \left(\frac{1+\delta N}{1-\delta N}\right)^2$$

Summary

given samples $f_j = f(x_j) \in \mathbb{C},\ j = 0, \ldots, M-1$

$$f \in L_N, \qquad N \in \mathbb{N},$$

damped and weighted normal equation of second kind, interpolation,

$$\underbrace{\boldsymbol{W}^{\frac{1}{2}} \boldsymbol{A} \hat{\boldsymbol{W}}^{\frac{1}{2}}}_{\boldsymbol{A}^{\omega}} \hat{\boldsymbol{W}}^{\frac{1}{2}} \boldsymbol{A}^{\mathsf{H}} \boldsymbol{W}^{\frac{1}{2}} \tilde{\boldsymbol{f}} = \underbrace{\boldsymbol{W}^{\frac{1}{2}} \boldsymbol{f}}_{\boldsymbol{f}^{\omega}}, \qquad \hat{\boldsymbol{f}} = \hat{\boldsymbol{W}} \boldsymbol{A}^{\mathsf{H}} \boldsymbol{W}^{\frac{1}{2}} \tilde{\boldsymbol{f}}$$

damped and weighted normal equation of first kind, approximation,

$$\hat{\boldsymbol{W}}^{\frac{1}{2}} \boldsymbol{A}^{\mathsf{H}} \boldsymbol{W}^{\frac{1}{2}} \underbrace{\boldsymbol{W}^{\frac{1}{2}} \boldsymbol{A} \hat{\boldsymbol{W}}^{\frac{1}{2}}}_{\boldsymbol{A}^{\omega}} \underbrace{\hat{\boldsymbol{W}}^{\frac{1}{2}} \hat{\boldsymbol{f}}}_{\hat{\boldsymbol{f}}^{\omega}} = \hat{\boldsymbol{W}}^{\frac{1}{2}} \boldsymbol{A}^{\mathsf{H}} \boldsymbol{W} \boldsymbol{f}$$

Iterative methods

residuals

$$\boldsymbol{r}_l = \boldsymbol{f} - \boldsymbol{A}\hat{\boldsymbol{f}}_l, \qquad \hat{\boldsymbol{z}}_l = \boldsymbol{A}^{\mathsf{H}}\boldsymbol{W}\boldsymbol{r}_l$$

Landweber iteration (Neumann series of $\boldsymbol{A}^{\mathsf{H}}\boldsymbol{W}\boldsymbol{A}$)

$$\hat{\boldsymbol{f}}_{l+1} = \hat{\boldsymbol{f}}_l + \alpha\hat{\boldsymbol{W}}\hat{\boldsymbol{z}}_l$$

steepest descent

$$\boldsymbol{v}_l = \boldsymbol{A}\hat{\boldsymbol{W}}\hat{\boldsymbol{z}}_l, \qquad \alpha_l^{\omega} = \frac{\hat{\boldsymbol{z}}_l^{\mathsf{H}}\hat{\boldsymbol{W}}\hat{\boldsymbol{z}}_l}{\boldsymbol{v}_l^{\mathsf{H}}\boldsymbol{W}\boldsymbol{v}_l}$$

CG–type methods

CG–type methods, see e.g. [3, 16]

hermitian, positive semidefinite matrices

$$\boldsymbol{A}^{\omega\,\mathsf{H}}\boldsymbol{A}^{\omega}, \qquad \boldsymbol{A}^{\omega}\boldsymbol{A}^{\omega\,\mathsf{H}}$$

substitute $\hat{\boldsymbol{z}}_l^{\omega} = \hat{\boldsymbol{W}}^{-\frac{1}{2}}\hat{\boldsymbol{z}}_l = \hat{\boldsymbol{W}}^{-\frac{1}{2}}\boldsymbol{A}^{\mathsf{H}}\boldsymbol{W}\boldsymbol{r}_l$

$$\begin{aligned}
\mathcal{K}_l^{\omega}\left(\boldsymbol{A}, \hat{\boldsymbol{r}}_0\right) &:= \hat{\boldsymbol{W}}^{\frac{1}{2}}\mathcal{K}_l\left(\boldsymbol{A}^{\omega\,\mathsf{H}}\boldsymbol{A}^{\omega}, \hat{\boldsymbol{z}}_0^{\omega}\right) \\
&= \hat{\boldsymbol{W}}^{\frac{1}{2}}\mathrm{span}\left(\hat{\boldsymbol{z}}_0^{\omega}, \boldsymbol{A}^{\omega\,\mathsf{H}}\boldsymbol{A}^{\omega}\hat{\boldsymbol{z}}_0^{\omega}, \ldots, \left(\boldsymbol{A}^{\omega\,\mathsf{H}}\boldsymbol{A}^{\omega}\right)^{l-1}\hat{\boldsymbol{z}}_0^{\omega}\right)
\end{aligned}$$

CG–type methods

CG applied to the normal equation of first kind, CGNR

$$\boldsymbol{A}^{\omega\,\mathsf{H}}\boldsymbol{A}^{\omega}\hat{\boldsymbol{f}}^{\omega} = \boldsymbol{A}^{\omega\,\mathsf{H}}\boldsymbol{f}^{\omega}$$

the iterates $\hat{\boldsymbol{f}}_l \in \mathcal{K}_l^{\omega}\left(\boldsymbol{A}, \hat{\boldsymbol{r}}_0\right)$ minimise the residual

$$E_1^{\omega}\left(\hat{\boldsymbol{f}}_l\right) := ||\boldsymbol{r}_l||_{\boldsymbol{W}} - ||\boldsymbol{r}^{\dagger}||_{\boldsymbol{W}}$$

CG applied to the normal equation of second kind, CGNE

$$\boldsymbol{A}^{\omega}\boldsymbol{A}^{\omega\,\mathsf{H}}\tilde{\boldsymbol{f}}^{\omega} = \boldsymbol{f}^{\omega}, \qquad \hat{\boldsymbol{f}}^{\omega} = \boldsymbol{A}^{\omega\,\mathsf{H}}\tilde{\boldsymbol{f}}^{\omega}$$

the iterates $\hat{\boldsymbol{f}}_l \in \mathcal{K}_l^{\omega}\left(\boldsymbol{A}, \hat{\boldsymbol{r}}_0\right)$ minimise the error

$$E_0^{\omega}\left(\hat{\boldsymbol{f}}_l\right) := ||\hat{\boldsymbol{f}}^{\dagger} - \hat{\boldsymbol{f}}_l||_{\hat{\boldsymbol{W}}^{-1}}$$

Summary

Approximation problem, $N \leq M$

$$\boldsymbol{A}^{\mathrm{H}}\boldsymbol{W}\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{A}^{\mathrm{H}}\boldsymbol{W}\boldsymbol{f}$$

ACT, CGNR (Feichtinger, Gröchenig, Strohmer) $(N < \frac{1}{\delta})$

$$\|\boldsymbol{r}_l - \boldsymbol{r}^{\dagger}\|_{\boldsymbol{W}} \leq 2\left(\frac{2\delta N}{1+(\delta N)^2}\right)^l \|\boldsymbol{r}_0 - \boldsymbol{r}^{\dagger}\|_{\boldsymbol{W}}$$

Interpolation problem, $N \geq M$

$$\boldsymbol{A}\hat{\boldsymbol{W}}\boldsymbol{A}^{\mathrm{H}}\tilde{\boldsymbol{f}} = \boldsymbol{f}, \qquad \hat{\boldsymbol{f}} = \hat{\boldsymbol{W}}\boldsymbol{A}^{\mathrm{H}}\tilde{\boldsymbol{f}}$$

CGNE ($\hat{w}_k = 1$, i.e. Dirichlet kern) $N \geq \frac{1}{h}\left(1 + \ln\frac{M}{2}\right)$

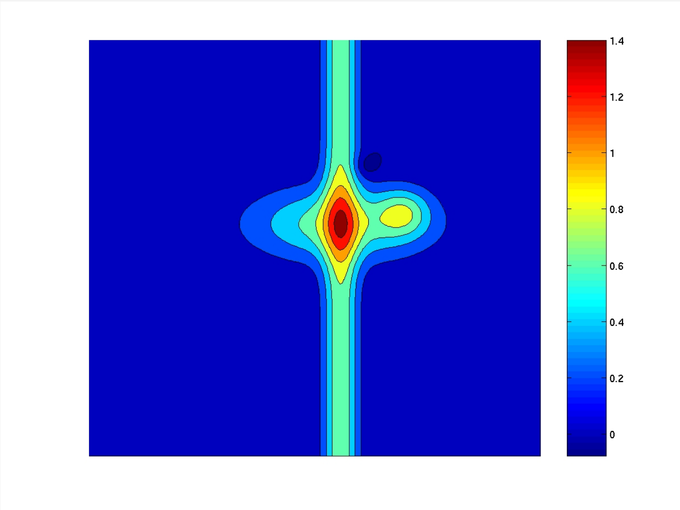
$$\|\hat{\boldsymbol{f}}_l - \hat{\boldsymbol{f}}^{\dagger}\|_{\hat{\boldsymbol{W}}^{-1}} \leq 2\left(\frac{1 + \ln\frac{M}{2}}{Nh}\right)^l \|\hat{\boldsymbol{f}}_0 - \hat{\boldsymbol{f}}^{\dagger}\|_{\hat{\boldsymbol{W}}^{-1}}$$

CGNE ($\hat{w}_k = \frac{N}{2} + 1 - |k|$, i.e. Fejer kern) $N \geq \frac{2}{h}$

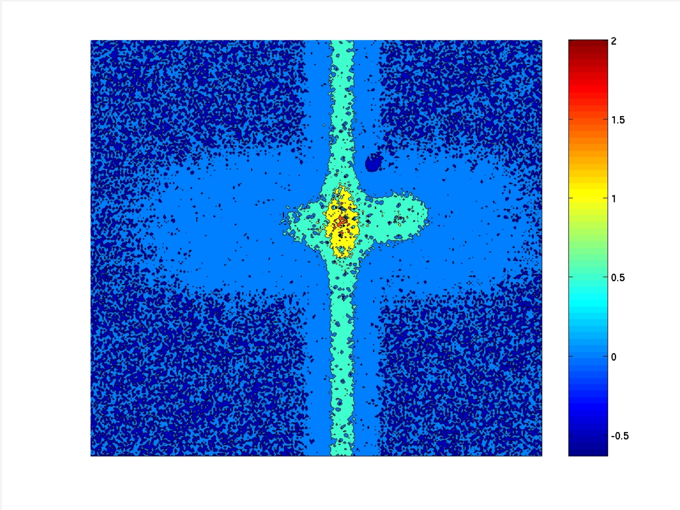
$$\|\hat{\boldsymbol{f}}_l - \hat{\boldsymbol{f}}^{\dagger}\|_{\hat{\boldsymbol{W}}^{-1}} \leq 2\left(\frac{2}{Nh}\right)^l \|\hat{\boldsymbol{f}}_0 - \hat{\boldsymbol{f}}^{\dagger}\|_{\hat{\boldsymbol{W}}^{-1}}$$

Franke function

$[-2,2]^2 \to [-\frac{1}{4},\frac{1}{4}]^2$,
$M = 100000$ random sampling nodes,
$N = 512,\ \dim(L_N) = 262144$, CGNE, 10 iterations



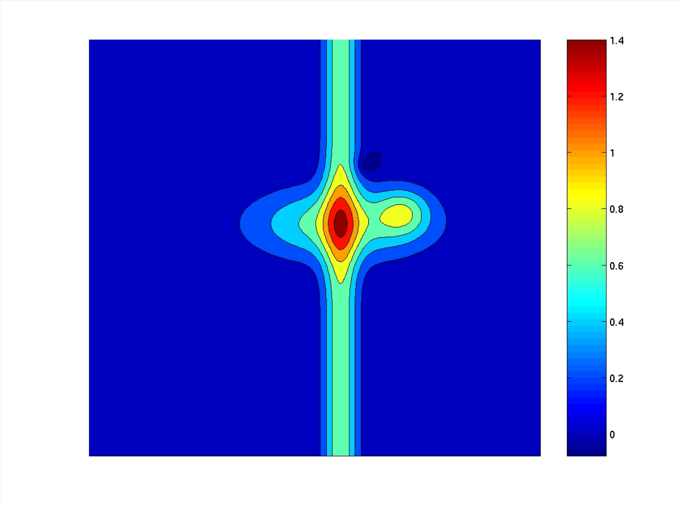
original



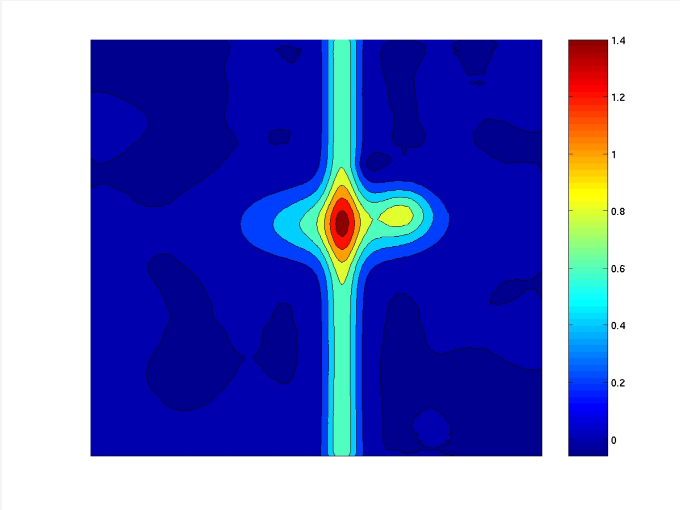
undamped reconstruction

Franke function

Sobolev-like damping factors $\hat{\omega}_{\boldsymbol{k}} = ((1 + |k_1|)\,(1 + |k_2|))^{-1/2}$



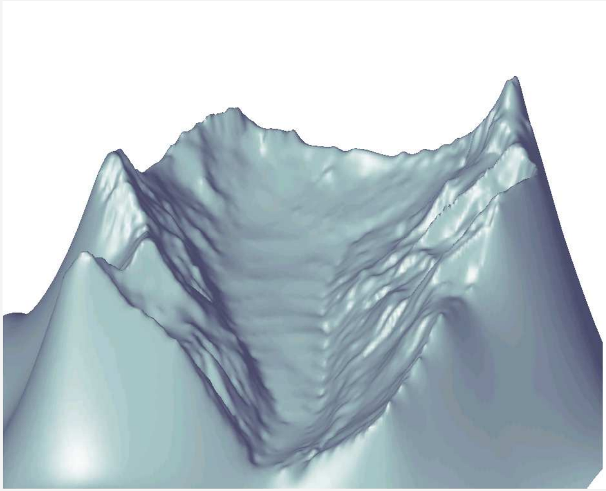
original

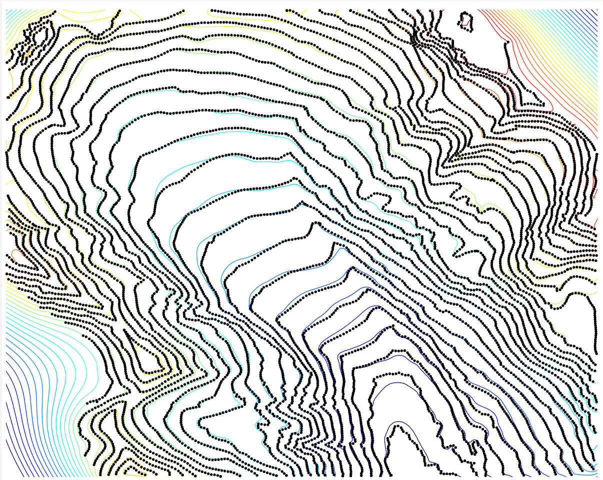


damped reconstruction

Example - glacier

glacier contour data, $M = 8345$ points, $N = 256$, multiquadric-type $\hat{\boldsymbol{W}}$





”Probabilistic” condition number

References: R. Bass and K. Gröchenig [1]; Böttcher, P., D. Wenzel [6, 7]

Observation: in practice theoretically ill-conditioned systems often behave better than one would expect
Idea: probabilistic arguments

suppose $\boldsymbol{p}$ ist independently and randomly drawn from

$$\{\boldsymbol{q} \in \mathbb{C}^N : \|\boldsymbol{q}\| \leq \varrho\},$$

with the uniform distribution
we consider (cf. MZ inequality)

$$\mathbb{P}\Big(\alpha\|\boldsymbol{p}\| \leq \|\boldsymbol{A}\boldsymbol{p}\| \leq \beta\|\boldsymbol{p}\|\Big) \geq 1 - \theta,$$

where

$\mathbb{P}(E)$ is the probability of the event $E, \theta \in [0, 1),$ and $\alpha, \beta \in (0, \infty)$

By A. Böttcher, S. Grudsky [5] it was shown that if $\boldsymbol{p}$ is randomly drawn from the uniform distribution

$$\mathbb{P}\left(\left(\frac{\|\boldsymbol{A}\|_{\mathrm{F}}^2}{N} - \varepsilon\|\boldsymbol{A}\|^2\right)\|\boldsymbol{p}\|^2 \le \|\boldsymbol{A}\boldsymbol{p}\|^2 \le \left(\frac{\|\boldsymbol{A}\|_{\mathrm{F}}^2}{N} + \varepsilon\|\boldsymbol{A}\|^2\right)\|\boldsymbol{p}\|^2\right)$$

$$\ge 1 - \frac{2}{(N+2)\varepsilon^2}$$

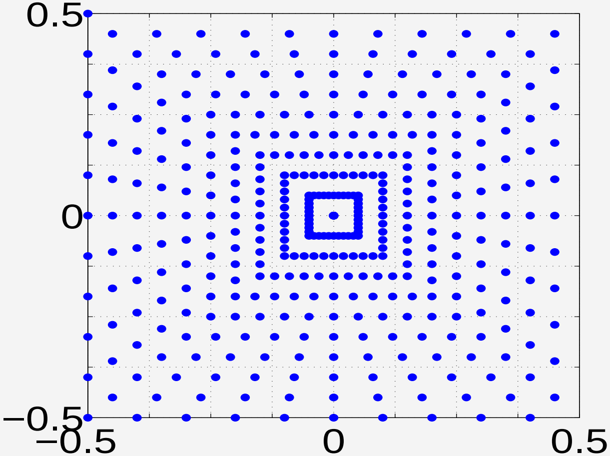
We consider the system $\boldsymbol{A}\boldsymbol{p} = \boldsymbol{y}$ and a sequence of sampling knots governed by a constraint for the separation distance q.

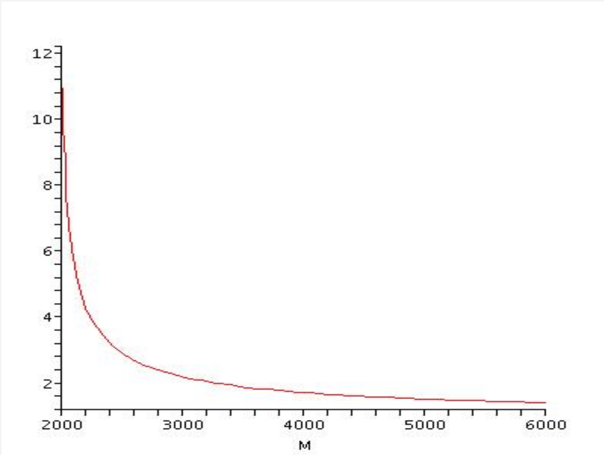
Theorem: If $q \geq \gamma_1 M^{-1/d}$ and $\gamma_2 N^{1/2+\eta} \leq M^{1/d} \leq \gamma_3 \exp \sqrt[3]{N}$ with positive constants γ_1, γ_2, γ_3, η, then there are two sequences $\{C_N\}_{N=1}^{\infty}$ (the "probabilistic" condition number) and $\{P_N\}_{N=1}^{\infty}$ such that

$$C_N > 1, \quad \lim_{N\to\infty} C_N = 1, \quad P_N < 1, \quad \lim_{N\to\infty} P_N = 1$$

and $\mathbb{P}\Big(\|\delta \boldsymbol{p}\| \leq C_N \|\delta \boldsymbol{y}\| \Big) \geq P_N$.

Example:





Left: Linogram grid; Right: "probabilistic" condition number C_N with a probability of at least 0.9

Content

- Applications of NFFTs
  - Fast summation Algorithms
  - Poisson solvers on nonequispaced grids
  - Algorithms for computerized tomography
  - Applications on the sphere
  - Applications for MRI and NMR

Content

- Fast summation algorithms
  - Introduction
  - Fast summation at equispaced knots
  - Fast summation at nonequispaced knots
  - Error estimates
  - Fast summation at multidimensional knots
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- Particle Simulation

Fast summation algorithms, introduction

Problem: fast computation of

$$f(\boldsymbol{y}_j) := \sum_{k=1}^{N} \alpha_k \mathcal{K}(\boldsymbol{y}_j - \boldsymbol{x}_k) \qquad (j = 1, \ldots, M)$$

nodes $\boldsymbol{y}_j, \boldsymbol{x}_k \in \mathbb{R}^d$, $\mathcal{K}(\boldsymbol{x}) = K(\|\boldsymbol{x}\|)$ radial basis functions

$$\boldsymbol{f} = \boldsymbol{K}\boldsymbol{\alpha}$$

K are special kernels

singular kernels $\dfrac{1}{x}, \; \dfrac{1}{x^2}, \; \log|x|, \; x^2 \log|x|$

nonsingular kernels $(x^2 + c^2)^{\pm 1/2}, \mathrm{e}^{-\delta x^2}$

Applications: integral equations, scattered data approximation, image processing, discrete Gauss transform, . . .

known Methods for
products of vectors with special structured dense matrices

$$\boldsymbol{f} = \boldsymbol{K}\boldsymbol{\alpha}$$

panel clustering, fast multipole method, wavelet methods,
mosaic–skeleton approximations,
H-matrices

standard algorithm for equispaced nodes

$\boldsymbol{K}$ – Toeplitz matrix

$$\boldsymbol{f} = \text{FFT}(\ \text{diag}(\boldsymbol{b})\ \text{FFT}^H(\boldsymbol{\alpha}))$$

Idea for nonequispaced nodes
replace FFT by NFFT

$$\boldsymbol{f} = \text{NFFT}(\ \text{diag}(\tilde{\boldsymbol{b}})\ \text{NFFT}^H(\boldsymbol{\alpha})) + \text{nearfield}$$

Fast summation at equispaced nodes

equally spaced points in $[-1/4, 1/4)$

$$x_k := -1/4 + (k-1)/(2N), \quad (k = 1, \ldots, N)$$

and

$$y_j := -1/4 + (j-1)(2M), \quad (j = 1, \ldots M)$$

set $K(0) := 0$ if K has a singularity at the origin
fast summation of

$$f(y_j) := \sum_{k=1}^{N} \alpha_k K\left(\frac{j-1}{2M} - \frac{k-1}{2N}\right) \qquad (j = 1, \ldots, M), \tag{43}$$

let $n := 2\,\mathrm{lcm}(N, M)$ and $\tilde{K}$ be any smooth 1–periodic function with

$$\tilde{K}(j/n) = K(j/n) \qquad (j = -n/2 + 1, \ldots, n/2 - 1)$$

and with an arbitrary boundary value $\tilde{K}(-1/2)$

by aliasing formula (4)

$$c_l(\tilde{K}) = b_l - \sum_{\substack{r\in\mathbb{Z}\\ r\neq 0}} c_{l+rn}(\tilde{K})$$

where

$$b_l := \frac{1}{n} \sum_{j=-n/2}^{n/2-1} \tilde{K}\left(\frac{j}{n}\right) \mathrm{e}^{-2\pi \mathrm{i} jl/n} \tag{44}$$

$$\begin{aligned}
\tilde{K}(x) &= \sum_{l\in\mathbb{Z}} c_l(\tilde{K})\,\mathrm{e}^{2\pi \mathrm{i} lx} \\
&= \sum_{l=-n/2}^{n/2-1} c_l(\tilde{K})\,\mathrm{e}^{2\pi \mathrm{i} lx} + \sum_{l=-n/2}^{n/2-1} \sum_{\substack{r\in\mathbb{Z}\\ r\neq 0}} c_{l+rn}(\tilde{K})\,\mathrm{e}^{2\pi \mathrm{i}(l+rn)x} \\
&= \sum_{l=-n/2}^{n/2-1} b_l\,\mathrm{e}^{2\pi \mathrm{i} lx} + \sum_{l=-n/2}^{n/2-1} \sum_{\substack{r\in\mathbb{Z}\\ r\neq 0}} c_{l+rn}(\tilde{K})\,\mathrm{e}^{2\pi \mathrm{i} lx}(\,\mathrm{e}^{2\pi \mathrm{i} nrx} - 1),
\end{aligned} \tag{45}$$

for

$$x := (j-1)/(2M) - (k-1)/(2N)\,,$$

we see by definition of n that $\mathrm{e}^{2\pi\mathrm{i}nrx} - 1$ vanishes
thus

$$\begin{aligned}\tilde{K}\left(\frac{j-1}{2M} - \frac{k-1}{2N}\right) &= K\left(\frac{j-1}{2M} - \frac{k-1}{2N}\right) \\ &= \sum_{l=-n/2}^{n/2-1} b_l\,\mathrm{e}^{2\pi\mathrm{i}l((j-1)/(2M)-(k-1)/(2N))}\end{aligned}$$

and by (43)

$$\begin{aligned}f\left(y_j\right) &= \sum_{k=1}^{N} \alpha_k \sum_{l=-n/2}^{n/2-1} b_l\,\mathrm{e}^{2\pi\mathrm{i}l((j-1)/(2M)-(k-1)/(2N))} \\ &= \sum_{l=-n/2}^{n/2-1} b_l \left(\sum_{k=1}^{N} \alpha_k\,\mathrm{e}^{-2\pi\mathrm{i}l(k-1)/(2N)}\right) \mathrm{e}^{2\pi\mathrm{i}l(j-1)/(2M)}\end{aligned}$$

Algorithm

Precomputation: Computation of $(b_l)_{l=-n/2}^{n/2-1}$ by (44).

1. For $l = -n/2, \ldots, n/2-1$ compute

$$a_l := \sum_{k=1}^{N} \alpha_k \, \mathrm{e}^{-2\pi \mathrm{i} l (k-1)/(2N)}$$

by FFT($2N$) and applying that $a_{l+2Ns} = a_l$ for $s = -(n-2N)/(4N), \ldots, (n-2N)/(4N)$.

2. For $l = -n/2, \ldots, n/2-1$ compute the products

$$d_l := a_l b_l .$$

3. For $j = 1, \ldots, M$ compute

$$f\,(y_j) = \sum_{l=-n/2}^{n/2-1} d_l \, \mathrm{e}^{2\pi \mathrm{i} l (j-1)/(2M)} = \sum_{l=-M}^{M-1} \left(\sum_{s=-(n-2M)/(4M)}^{(n-2M)/(4M)} d_{l+2Ms} \right) \mathrm{e}^{2\pi \mathrm{i} l (j-1)/(2M)}$$

by IFFT($2M$).

Remark:

For $M = N$ we have that

$$\boldsymbol{K}_N := \left(K(\frac{j-k}{2N}) \right)_{j,k=1}^{N}$$

is an N by N Toeplitz matrix. In this case the method coincides with the standard Toeplitz matrix – vector multiplication algorithm based on embedding $\boldsymbol{K}_N$ into an $2N$ by $2N$ circulant matrix, and than carrying out the multiplication by using the fast Fourier transform.

Fast summation at nonequispaced nodes

$$f(x) := \sum_{k=1}^{N} \alpha_k K(x - x_k) \tag{46}$$

aim: fast evaluation of $f(y_j)$ ($|x_k|, |y_j| \leq \frac{1}{4} - \frac{\varepsilon_B}{2}$)

restrict to even kernels $K \in C^\infty$ except for the origin

note

$$|y_j - x_k| \leq \frac{1}{2} - \varepsilon_B$$

regularize K near 0 and near the boundary $\pm 1/2$ to obtain a 1–periodic smooth kernel $\tilde{K}$ in the Sobolev space $H^p(\mathbb{T})$

$$\tilde{K}(x) := \begin{cases} K_I(x) & \text{for } x \in [-\varepsilon_I, \varepsilon_I], \\ K_B(x) & \text{for } x \in [-\frac{1}{2}, -\frac{1}{2} + \varepsilon_B] \cup [\frac{1}{2} - \varepsilon_B, \frac{1}{2}], \\ K(x) & \text{else}, \end{cases} \tag{47}$$

where $0 < \varepsilon_I < \frac{1}{2} - \varepsilon_B < \frac{1}{2}$

approximate $\tilde{K}$ by the Fourier series $\mathcal{T}_n(\tilde{K})$ given by

$$\mathcal{T}_n(\tilde{K})(x) := \sum_{l=-n/2}^{n/2-1} b_l \, \mathrm{e}^{2\pi \mathrm{i} l x}, \tag{48}$$

where $n \leq 2N$ and (see (44))

$$b_l := \frac{1}{n} \sum_{j=-n/2}^{n/2-1} \tilde{K}\left(\frac{j}{n}\right) \mathrm{e}^{-2\pi \mathrm{i} j l / n} \qquad (l = -n/2, \dots n/2 - 1) \tag{49}$$

regarding that

$$K = \underbrace{(K - \tilde{K})}_{K_{\mathrm{NE}}} + \underbrace{(\tilde{K} - \mathcal{T}_n(\tilde{K}))}_{K_{\mathrm{ERR}}} + \mathcal{T}_n(\tilde{K}) \; = \; K_{\mathrm{NE}} + K_{\mathrm{ERR}} + \mathcal{T}_n(\tilde{K}), \quad (50)$$

and assuming that K_{ERR} becomes sufficiently small

approximate K by $K_{\mathrm{NE}} + \mathcal{T}_n(\tilde{K})$ and consequently f by

$$\tilde{f}(x) := \sum_{k=1}^{N} \alpha_k K_{\mathrm{NE}}(x - x_k) + \mathcal{T}_n(f)(x) \quad (51)$$

where

$$\mathcal{T}_n(f)(x) := \sum_{k=1}^{N} \alpha_k \mathcal{T}_n(\tilde{K})(x - x_k) \quad (52)$$

Instead of f we intend to evaluate $\tilde{f}$ at the points y_j.

suppose that every interval of length $2\varepsilon_I$ contains at most ν of the points x_k or of the points y_j i.e. ε_I depends linearly on $1/N$, respectively $1/M$.

In the following we restrict our attention to the case

$$\varepsilon_I \approx \frac{\nu}{2N}. \tag{53}$$

Then, since $|y_j - x_k| < \frac{1}{2} - \varepsilon_B$ and supp$(K - \tilde{K}) \cap [-\frac{1}{2} + \varepsilon_B, \frac{1}{2} - \varepsilon_B] = [-\varepsilon_I, \varepsilon_I]$, the evaluation of

$$\sum_{k=1}^{N} \alpha_k K_{\mathrm{NE}}(y_j - x_k) \qquad (j = 1, \ldots, M)$$

requires $\leq \nu M$, i. e. $\mathcal{O}(M)$ arithmetic operations.

by (48) rewrite (52) as

$$\mathcal{T}_n(f)(x) = \sum_{k=1}^{N} \alpha_k \sum_{l=-n/2}^{n/2-1} b_l \, \mathrm{e}^{2\pi \mathrm{i} l (x-x_k)}$$

which further implies

$$\mathcal{T}_n(f)(y_j) = \underbrace{\sum_{l=-n/2}^{n/2-1} b_l \underbrace{\left(\sum_{k=1}^{N} \alpha_k \, \mathrm{e}^{-2\pi \mathrm{i} l x_k} \right)}_{\text{NFFT}^{\mathrm{H}}(n)} \mathrm{e}^{2\pi \mathrm{i} l y_j}}_{\text{NFFT}(n)}$$

In summary, our summation algorithm requires

$$\mathcal{O}(M + N + n \log n)$$

arithmetic operations.
aim: relation between M, N and n, p determined by the approximation error

Kernel Regularization

K is even, we have that $K^{(j)}(x) = (-1)^j K^{(j)}(-x)$. To ensure that

$$\tilde{K}(x) := \begin{cases} K_I(x) & \text{for } x \in [-\varepsilon_I, \varepsilon_I], \\ K_B(x) & \text{for } x \in [-\frac{1}{2}, -\frac{1}{2} + \varepsilon_B] \cup [\frac{1}{2} - \varepsilon_B, \frac{1}{2}], \\ K(x) & \text{else}, \end{cases}$$

is in $H^p(\mathbb{T})$, we need that the function K_I fulfills the conditions

$$\begin{aligned} K_I^{(j)}(\varepsilon_I) &= K^{(j)}(\varepsilon_I), \\ K_I^{(j)}(-\varepsilon_I) &= K^{(j)}(-\varepsilon_I) = (-1)^j K^{(j)}(\varepsilon_I) \end{aligned} \tag{54}$$

for all $j = 0, \ldots, p-1$,

and the function K_B the conditions

$$
\begin{aligned}
K_B^{(j)}\left(\frac{1}{2}-\varepsilon_B\right) &= K^{(j)}\left(\frac{1}{2}-\varepsilon_B\right), \\
K_B^{(j)}\left(\frac{1}{2}+\varepsilon_B\right) &= K^{(j)}\left(-\frac{1}{2}+\varepsilon_B\right) = (-1)^j K^{(j)}\left(\frac{1}{2}-\varepsilon_B\right)
\end{aligned}
\tag{55}
$$

for all $j = 0, \ldots, p-1$. Then, the periodicity of $\tilde{K}$ follows by setting

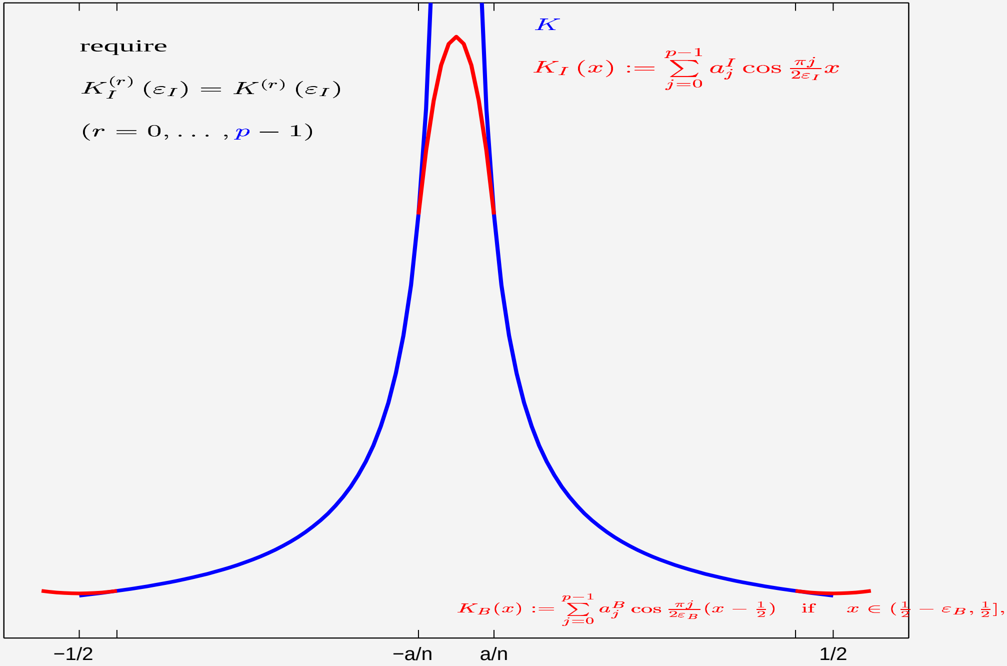
$$
K_B\left(-\frac{1}{2}+x\right) := K_B\left(\frac{1}{2}+x\right) \qquad (x \in [0, \varepsilon_B]).
$$

regularizing functions K_I and K_B

– trigonometric polynomials [35],

– algebraic polynomials [12],

– splines [12]


require
$K_I^{(r)}(\varepsilon_I) = K^{(r)}(\varepsilon_I)$
$(r = 0, \ldots, p-1)$
K
$K_I(x) := \sum_{j=0}^{p-1} a_j^I \cos \frac{\pi j}{2\varepsilon_I} x$
$K_B(x) := \sum_{j=0}^{p-1} a_j^B \cos \frac{\pi j}{2\varepsilon_B}(x - \frac{1}{2}) \quad \text{if} \quad x \in (\frac{1}{2} - \varepsilon_B, \frac{1}{2}],$
−1/2
−a/n
a/n
1/2

Regularization by polynomial interpolation

construct polynomials K_I and K_B of degree $2p-1$

two-point Taylor interpolation

For given a_j, b_j ($j = 0, \ldots, p-1$) there exists a unique polynomial P of degree $2p-1$ which satisfies the interpolation conditions

$$P^{(j)}(m-r) = a_j, \qquad P^{(j)}(m+r) = b_j \qquad (j = 0, \ldots, p-1)$$

at the endpoints of an interval $[m-r, m+r]$ ($r > 0$). This polynomial can be written as

$$P(x) = \sum_{j=0}^{p-1} \sum_{k=0}^{p-1-j} \binom{p-1+k}{k} \left(\frac{(x-m+r)^j}{j!} \left(\frac{x-m-r}{-2r} \right)^p \left(\frac{x-m+r}{2r} \right)^k a_j + \frac{(x-m-r)^j}{j!} \left(\frac{x-m+r}{2r} \right)^p \left(\frac{x-m-r}{-2r} \right)^k b_j \right).$$

Regularization by spline interpolation

normalized cardinal B-splines N_p of degree p

$$N_0(x) := \begin{cases} 1 & \text{for } x \in [0,1), \\ 0 & \text{otherwise} \end{cases}$$

and

$$N_p(x) := \frac{x}{k} N_{p-1}(x) + \frac{p+1-x}{k} N_{p-1}(x-1) \qquad (p \in \mathbb{N}).$$

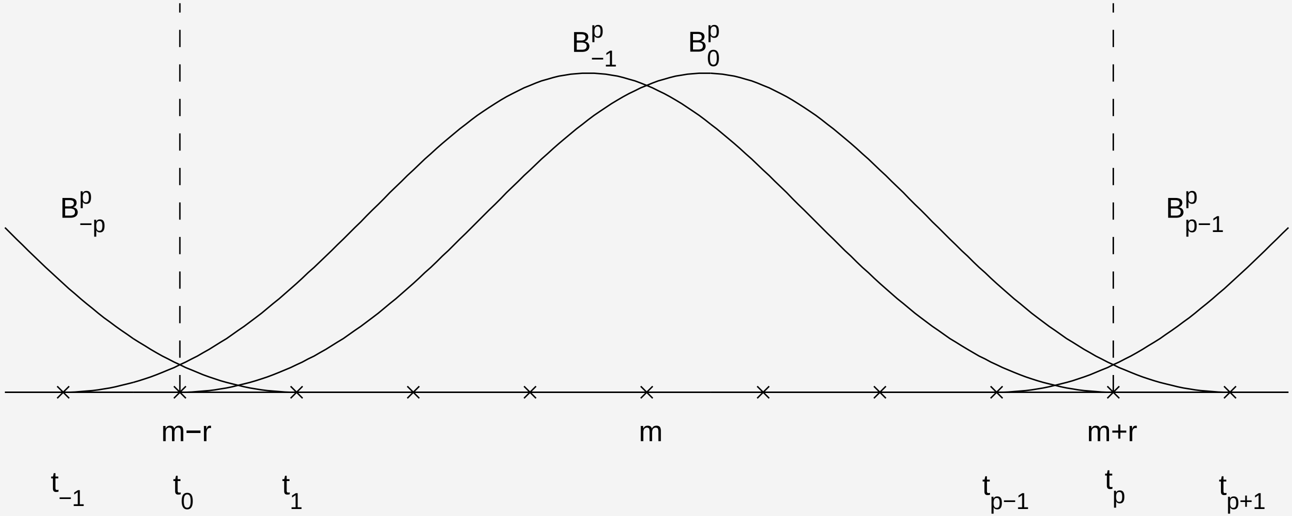
$$\text{supp} N_p = [0, p+1]$$

At the interval $[m-r, m+r]$ we choose the equispaced nodes

$$\Delta := \{t_k = m - r + \frac{2r}{p} k : \; k = -p, \dots, 2p\}$$

and introduce the dilated and translated versions of N_p with respect to these spline nodes

$$B_k^p(x) := N_p\left(\frac{p(x-m+r)}{2r} - k\right).$$



The set of B-splines $\{B_k^p\}_{k=-p}^{p-1}$ forms a basis of the spline space

$$S_p(\Delta) := \{s \in C^{p-1}[m-r, m+r] \,:\, s|_{[t_k,t_{k+1}]} \in \Pi_p, k = 0, \ldots, p-1\}.$$

Theorem: For given a_j, b_j ($j = 0, \ldots, p-1$) there exists a unique spline $S \in S_p(\Delta)$ which satisfies the interpolation conditions

$$S^{(j)}(m-r) = a_j, \qquad S^{(j)}(m+r) = b_j \qquad (j = 0, \ldots, p-1)$$

at the endpoints of an interval $[m-r, m+r]$ ($r > 0$). This spline can be written as

$$S(x) = \sum_{k=-p}^{p-1} c_k B_k^p(x)$$

where the coefficients c_k are the solution of the two $p \times p$ linear systems

$$\begin{aligned} \sum_{k=1}^{p} c_{-k} (B_{-k}^p)^{(j)}(m-r) &= a_j, \\ \sum_{k=1}^{p} c_{k-1} (B_{-k}^p)^{(j)}(m-r) &= (-1)^j b_j \qquad (j = 0, \ldots, p-1) \end{aligned}$$

with the same coefficient matrix.

Error Estimates

By (51) and (46), we obtain for $|y| \le \frac{1}{4} - \frac{\varepsilon_B}{2}$ that

$$\left|f(y) - \tilde{f}(y)\right| = \left|\sum_{k=1}^{N} \alpha_k \left(\tilde{K}(y - x_k) - \mathcal{T}_n(\tilde{K})(y - x_k)\right)\right| \le \sum_{k=1}^{N} |\alpha_k| \, \|K_{\mathrm{ERR}}\|_\infty,$$

where

$$\|K_{\mathrm{ERR}}\|_\infty := \max_{|x| \le \frac{1}{2}} |K_{\mathrm{ERR}}(x)|, \quad K_{\mathrm{ERR}}(x) := \tilde{K}(x) - \mathcal{T}_n(\tilde{K})(x). \tag{56}$$

Lemma: Let K be an even kernel and let $\tilde{K} \in H^p(\mathbb{T})$ be defined by (47). Then, for $2 \le p \ll n$, the following estimate holds true:

$$\|K_{\mathrm{ERR}}\|_\infty \le \frac{C}{(p-1)\pi^p n^{p-1}} \int_0^{\frac{1}{2}} |\tilde{K}^{(p)}(x)| \, \mathrm{d}x.$$

Proof: By Fourier expansion of $\tilde{K}$ and (48) we obtain for $x \in [-\frac{1}{2}, \frac{1}{2}]$ that

$$K_{\mathrm{ERR}}(x) = \sum_{k \in \mathbb{Z}} c_k(\tilde{K})\, \mathrm{e}^{2\pi \mathrm{i} k x} - \sum_{l \in I_n^1} b_l\, \mathrm{e}^{2\pi \mathrm{i} l x},$$

and hence by (45)

$$K_{\mathrm{ERR}}(x) = \sum_{k \in I_n^1} \sum_{\substack{r \in \mathbb{Z} \\ r \neq 0}} c_{k+rn}(\tilde{K})\, \mathrm{e}^{2\pi \mathrm{i} k x} (\, \mathrm{e}^{2\pi \mathrm{i} r n x} - 1).$$

Since $\tilde{K}$ is even, we can estimate

$$\|K_{\mathrm{ERR}}\|_\infty \leq 4 \sum_{k=\frac{n}{2}}^{\infty} |c_k(\tilde{K})|.$$

By construction we have that $\tilde{K} \in H^p(\mathbb{T})$ which implies that

$$c_k(\tilde{K}) = (2\pi \mathrm{i} k)^{-p}\, c_k(\tilde{K}^{(p)})$$

so that

$$\|K_{\mathrm{ERR}}\|_\infty \leq 4 \left(\sum_{k=\frac{n}{2}}^{\infty} (2\pi k)^{-p} \right) \int_{-\frac{1}{2}}^{\frac{1}{2}} |\tilde{K}^{(p)}(x)| \, \mathrm{d}x.$$

For $p \geq 2$ the sum can be estimated by an upper integral

$$\begin{aligned} \sum_{k=\frac{n}{2}}^{\infty} k^{-p} < \left(\frac{n}{2}\right)^{-p} + \int_{n/2}^{\infty} x^{-p} \, \mathrm{d}x &= \left(\frac{n}{2}\right)^{-p} + \frac{x^{1-p}}{1-p} \Bigg|_{x=n/2}^{\infty} \\ &< \frac{2^p \left(\frac{p-1}{n} + \frac{1}{2}\right)}{n^{p-1}(p-1)} \end{aligned}$$

and so

$$\|K_{\mathrm{ERR}}\|_\infty \leq \frac{2\left(1 + \frac{2(p-1)}{n}\right)}{(p-1)\pi^p n^{p-1}} \int_{-\frac{1}{2}}^{\frac{1}{2}} |\tilde{K}^{(p)}(x)| \, \mathrm{d}x.$$

Since $p \ll n$, this implies the assertion with a constant $C \approx 4$. $\square$

Theorem: For $\beta \in \mathbb{N}_0$, let $K = K_\beta$ be defined by

$$K_0(x) = \log|x|,\ K_\beta(x) = \frac{1}{|x|^\beta} \qquad (\beta \in \mathbb{N})$$

and $\tilde{K}$ by (47) with K_I and K_B, where $\varepsilon_I \le \min\{\varepsilon_B, \frac{1}{2} - \varepsilon_B\}$. Then, for $2 \le p \ll n$, the error $\|K_{\mathrm{ERR}}\|_\infty$ in (56) can be estimated by

$$\|K_{\mathrm{ERR}}\|_\infty \le C(K_I, K_B) + \left(\frac{p+\beta-2}{\mathrm{e}\varepsilon_I}\right)^\beta \left(\frac{p+\beta-2}{\pi n \varepsilon_I}\right)^{p-1} \tag{57}$$

Proof: We obtain by the definition of $\tilde{K}$ that

$$\int_0^{\frac{1}{2}} |\tilde{K}^{(p)}(x)|\,\mathrm{d}x = \int_0^{\varepsilon_I} |K_I^{(p)}(x)|\,\mathrm{d}x + \int_{\varepsilon_I}^{\frac{1}{2}-\varepsilon_B} |K^{(p)}(x)|\,\mathrm{d}x + \int_{\frac{1}{2}-\varepsilon_B}^{\frac{1}{2}} |K_B^{(p)}(x)|\,\mathrm{d}x\,.$$

and consider only the ”main” integral of $\int_{\varepsilon_I}^{\frac{1}{2}-\varepsilon_B}$. For details see [35, 12].

By

$$\left|K_\beta^{(j)}(x)\right| = \frac{(j+\beta-1)!}{(\beta-1)!}\,|x|^{-(j+\beta)} \qquad (x \neq 0; \beta \in \mathbb{N}_0),$$

where we set $(-1)! := 1$ in case $\beta = 0$. We obtain that

$$\begin{aligned}
\int_{\varepsilon_I}^{\frac{1}{2}-\varepsilon_B} |K^{(p)}(x)| \,\mathrm{d}x &= \frac{(p+\beta-1)!}{(\beta-1)!} \int_{\varepsilon_I}^{\frac{1}{2}-\varepsilon_B} |x|^{-(p+\beta)} \,\mathrm{d}x \\
&= \frac{(p+\beta-1)!}{(\beta-1)!} \left(- \frac{|x|^{-(p+\beta-1)}}{p+\beta-1} \Bigg|_{x=\varepsilon_I}^{\frac{1}{2}-\varepsilon_B} \right) \\
&\leq \frac{(p+\beta-2)!}{(\beta-1)!}\,\varepsilon_I^{-(p+\beta-1)}\,.
\end{aligned}$$

With Stirling formula

$$\sqrt{2\pi p}\,\left(\frac{p}{\mathrm{e}}\right)^{p} < p! < 1.1\,\sqrt{2\pi p}\,\left(\frac{p}{\mathrm{e}}\right)^{p}$$

holds

$$\begin{aligned}\frac{(p+\beta-2)!}{(\beta-1)!} \;&\le\; 1.1\,\frac{\sqrt{\pi\;(p+\beta-2)}\left(\frac{p+\beta-2}{\mathrm{e}}\right)^{p+\beta-2}}{\sqrt{\pi\;(\beta-1)}\left(\left(\frac{\beta-1}{\mathrm{e}}\right)^{\beta-1}\right)}\\ &=\; 1.1(p+\beta-2)^{-3/2+p+\beta}\;\mathrm{e}^{-p+1}\,(\beta-1)^{1/2-\beta}\end{aligned}$$

and we can rewrite our error estimate as

$$\int_{\varepsilon_I}^{\frac{1}{2}-\varepsilon_B} |K^{(p)}(x)|\;\mathrm{d}x \;<\; 1.1(p+\beta-2)^{-1/2}\;\mathrm{e}^{-p+1}\,(\beta-1)^{1/2-\beta}\left(\frac{p+\beta-2}{\varepsilon_I}\right)^{p+\beta-1}.$$

Combining these estimates with the above Lemma we obtain

$$\|K_{\mathrm{ERR}}\|_\infty \le C(K_I, K_B) + \frac{4.4\,(\beta-1)^{1/2-\beta}}{(p-1)\pi\sqrt{p+\beta-2}} \left(\frac{p+\beta-2}{\mathrm{e}\varepsilon_I}\right)^{\beta} \left(\frac{p+\beta-2}{\pi n \varepsilon_I}\right)^{p-1}$$

and finally the assertion. ■

Thus, choosing ε_I such that $\frac{p+\beta-2}{\mathrm{e}\,\pi\,\varepsilon_I n} < 1$, our error decays exponentially in p. In our numerical examples we choose

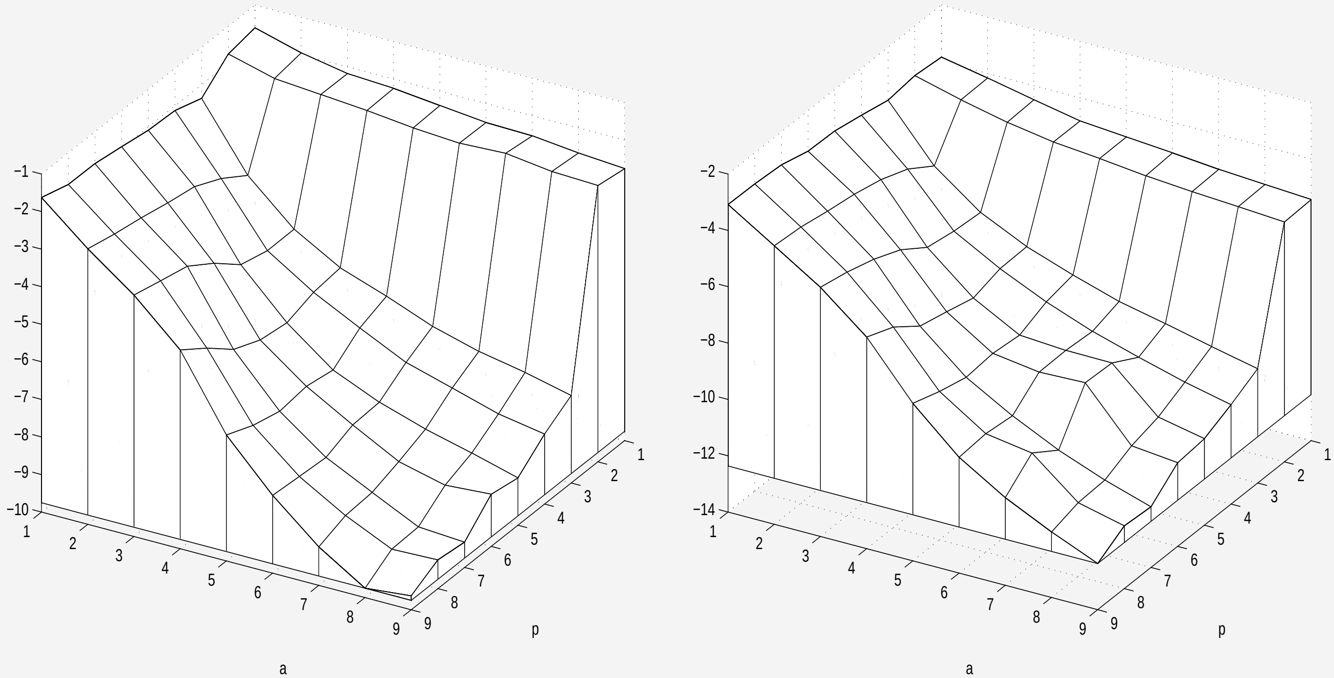
$$\varepsilon_I = \frac{p}{n}.$$

Numerical Results

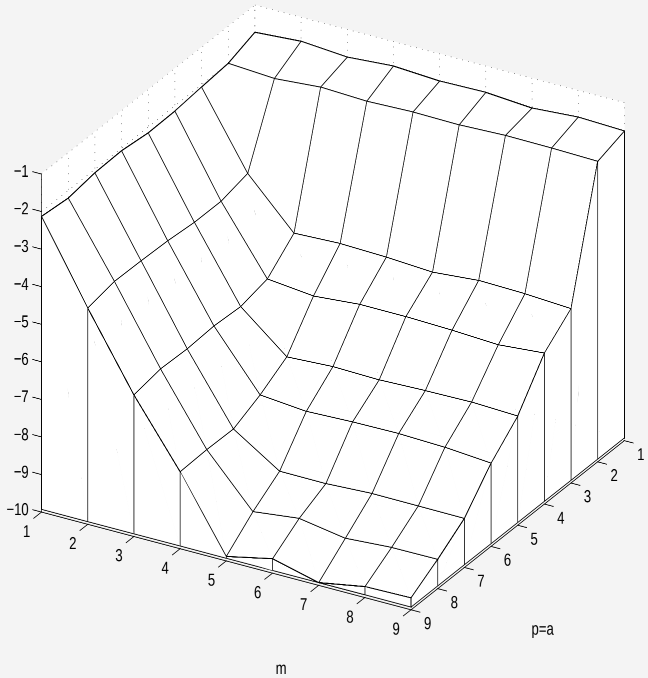
$$f(x_j) := \sum_{\substack{k=1 \\ k \neq j}}^{N} \alpha_k K(x_j - x_k) \qquad (j = 1, \ldots, N)$$

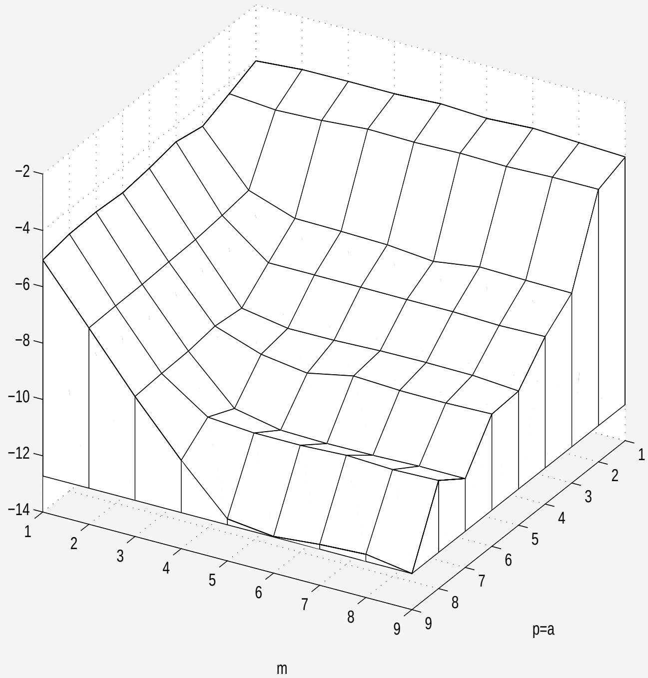
- α_k were randomly distributed in $[0, 1]$
- every figure presents the arithmetic mean of 20 runs of the algorithm

$$E := \max_{j=1,\ldots,N} \frac{|f(x_j) - \tilde{f}(x_j)|}{|f(x_j)|}.$$



Error $\log_{10} E$ for $K(x) = 1/|x|$ (left) and $K(x) = 1/|x|^2$ (right) for $N = 512$, $m = 12$ and $(p, a) \in \{1, \ldots, 9\}^2$ $n = N = 512$, $\varepsilon = a/n$.





Error $\log_{10} E$ for $K(x) = 1/|x|$ (left) and $K(x) = 1/|x|^2$ (right) for $(a, m) \in \{1, \ldots, 9\}^2$ and $a = p$, $n = N = 512$, $\varepsilon = a/n$.

Fast summation at multidimensional nodes

rotation-invariant kernels $\mathcal{K}(\boldsymbol{x}) = K(\|\boldsymbol{x}\|_2)$

$$f(\boldsymbol{y}_j) := \sum_{k=1}^{N} \alpha_k \mathcal{K}(\boldsymbol{y}_j - \boldsymbol{x}_k) = \sum_{k=1}^{N} \alpha_k K(\|\boldsymbol{y}_j - \boldsymbol{x}_k\|_2) \qquad (\boldsymbol{x}_k, \boldsymbol{y}_j \in \mathbb{R}^d) \quad (58)$$

for $j = 1, \ldots, M$

regularize $\mathcal{K}$ near 0 and near the boundary of $[-\frac{1}{2}, \frac{1}{2})^d$ to obtain a smooth periodic kernel $\tilde{\mathcal{K}}$:

$$\tilde{\mathcal{K}}(\boldsymbol{x}) := \begin{cases} K_I(\|\boldsymbol{x}\|_2) & \text{if } \|\boldsymbol{x}\|_2 \le \varepsilon_I, \\ K_B(\|\boldsymbol{x}\|_2) & \text{if } \frac{1}{2} - \varepsilon_B < \|\boldsymbol{x}\|_2 < \frac{1}{2}, \\ K_B(\frac{1}{2}) & \text{if } \|\boldsymbol{x}\|_2 \ge \frac{1}{2}, \\ K(\|\boldsymbol{x}\|_2) & \text{otherwise.} \end{cases}$$

require that the polynomial K_B fulfills the conditions

$$K_B^{(j)}\left(\frac{1}{2}-\varepsilon_B\right) = K^{(j)}\left(\frac{1}{2}-\varepsilon_B\right) \quad (j=0,\ldots,p-1),$$
$$K_B^{(j)}\left(\frac{1}{2}\right) = \delta_{0,j}\, K\left(\frac{1}{2}\right), \qquad (j=0,\ldots,p-1)$$

approximate $\tilde{\mathcal{K}}$ by the Fourier series

$$\mathcal{T}_n(\tilde{\mathcal{K}})(\boldsymbol{x}) := \sum_{\boldsymbol{l}\in I_n^d} b_l\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{l}\boldsymbol{x}},$$

where

$$b_{\boldsymbol{l}} := \frac{1}{n^d}\sum_{\boldsymbol{j}\in I_n^d} \tilde{\mathcal{K}}\left(\frac{\boldsymbol{j}}{n}\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{j}\boldsymbol{l}/n} \qquad (\boldsymbol{l}\in I_n^d).$$

decompose the kernel as

$$\mathcal{K} = (\mathcal{K}-\tilde{\mathcal{K}}) + \big(\tilde{\mathcal{K}} - \mathcal{T}_n(\tilde{\mathcal{K}})\big) + \mathcal{T}_n(\tilde{\mathcal{K}})$$

neglecting the summand in the middle and approximate f by

$$\tilde{f}(\boldsymbol{x}) := \sum_{k=1}^{N} \alpha_k (\mathcal{K} - \tilde{\mathcal{K}})(\boldsymbol{x} - \boldsymbol{x}_k) + \sum_{k=1}^{N} \alpha_k \mathcal{T}_n(\tilde{\mathcal{K}})(\boldsymbol{x} - \boldsymbol{x}_k).$$

1) Near field computation

To achieve the desired complexity of our algorithm we suppose that either the N points $\boldsymbol{x}_k$ or the M points $\boldsymbol{y}_j$ are "sufficiently uniformly distributed" in the ball with radius $\frac{1}{2} - \varepsilon_B$, i. e., we suppose that there exists a small constant $\nu \in \mathbb{N}$ such that each ball with radius ε_I contains at most ν of the points $\boldsymbol{x}_k$ or of the points $\boldsymbol{y}_j$, respectively. This implies that ε_I depends linearly on $N^{-1/d}$, respectively $M^{-1/d}$. In the following we restrict our attention to the case

$$\varepsilon_I \approx \frac{1}{2} \left(\frac{\nu}{N} \right)^{1/d}.$$

Then, as in one dimension, the computation of the first sum requires only $\leq \nu\, M$ arithmetic operations.

2) NFFT based summation

The evaluation of the second sum is done exactly in the same way as in one dimension, but with d-dimensional NFFTs of size n now.

$$\mathcal{T}(f)(\boldsymbol{y}_j) = \underbrace{\sum_{\boldsymbol{l}\in I_n^d} b_{\boldsymbol{l}} \underbrace{\left(\sum_{k=1}^{N} \alpha_k \,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{l}\boldsymbol{x}_k}\right)}_{\text{NFFT}^{\mathrm{H}}(n)} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{l}\boldsymbol{y}_j}}_{\text{NFFT}(n)}$$

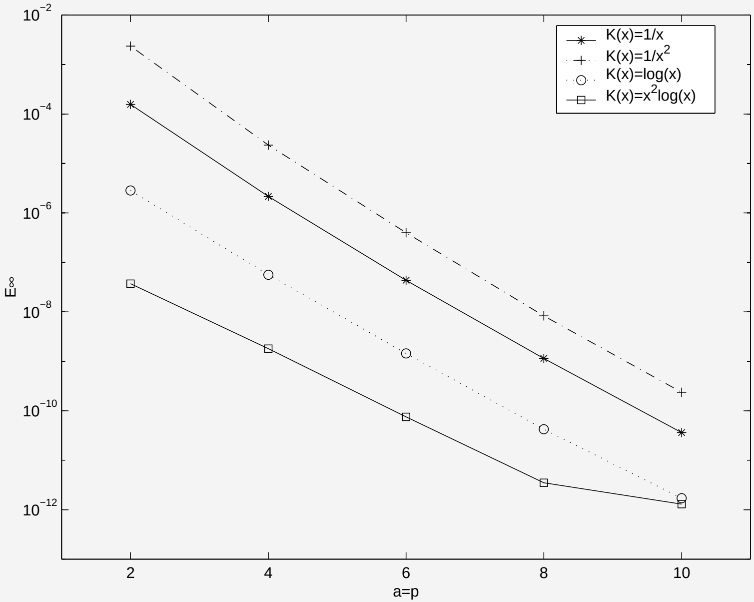
This computation part requires

$$\mathcal{O}(n^d \log n + N + M)$$

arithmetic operations.

To obtain an exponential error decay in p, we have to choose again $\varepsilon_I \approx \frac{p}{n}$.

Numerical examples



Error E_∞ in dependence on $\varepsilon_I = p/n$ for singular kernels, where $n = 256$, $N = 40000$, $m = 8$ and $d = 2$.

$$E_\infty := \max_{j=1,\dots,N} \frac{|f(\boldsymbol{x}_j) - \tilde{f}(\boldsymbol{x}_j)|}{|f(\boldsymbol{x}_j)|}$$

Parameter		Computational Time			Error
n	N	t_{slow}	t_{apr}	$\%$	E_∞
32	1000	2.950e-01	5.700e-01	193	1.184e-05
64	4000	4.755e+00	2.305e+00	48	4.820e-06
128	16000	7.699e+01	1.166e+01	15	2.815e-06
256	65000	1.502e+03	5.144e+01	3.42	1.757e-06
512	65000	1.496e+03	3.314e+01	2.21	1.754e-06
512	260000	2.885e+04	2.138e+02	0.74	1.026e-06

Comparison of the computational time and of the approximation error for $\mathcal{K}(\boldsymbol{x}) = 1/||\boldsymbol{x}||$, $p = m = 4$ and $d = 2$.

Nonsingular Kernels

smooth kernels as

$$(x^2 + c^2)^{\pm 1/2},\ \mathrm{e}^{-\delta x^2}\,.$$

Here no regularization at the neighborhood of $\mathbf{0}$ is necessary and our computation doesn't require a "near field" correction. If the kernel K is very small at the boundary, e.g. for large values δ in the Gaussian, we also don't need a regularization at the boundary, i.e. we can set $\tilde{\mathcal{K}} := \mathcal{K}$. Otherwise we use

$$\tilde{\mathcal{K}}(\boldsymbol{x}) = \begin{cases} T_B(\|\boldsymbol{x}\|) & \text{if} \quad \varepsilon_B < \|\boldsymbol{x}\| < \frac{1}{2}, \\ T_B(\frac{1}{2}) & \text{if} \quad \frac{1}{2} \le \|\boldsymbol{x}\|, \\ K(\|\boldsymbol{x}\|) & \text{otherwise.} \end{cases}$$

- parameter-dependent generalized multiquadrics (see [12])

$$K_{-1}(x;c) = (|x|^2 + c^2)^{\frac{1}{2}},\ K_\beta(x;c) = (|x|^2 + c^2)^{-\frac{\beta}{2}} \qquad (\beta \in \mathbb{N};\ \text{odd})$$

Theorem: (Fast Gauß transform, for $\delta \in \mathbb{C}$ see [24])
Let $\delta \geq 2$ and $\mathcal{K}(\boldsymbol{x}) := \mathrm{e}^{-\delta||\boldsymbol{x}||^2}$ $(x \in R^2)$. Further let $\mathcal{K}_{\mathrm{ERR}} := \mathcal{K} - \mathcal{T}_n(\tilde{\mathcal{K}})$, where $\mathcal{T}_n(\tilde{\mathcal{K}})$ denotes the finite Fourier series of $\mathcal{K}$ consisting of n^2 summands. Let $\eta := \frac{\pi n}{2\sqrt{\delta}} \geq 1$. Then the following estimate holds true

$$\|\mathcal{K}_{\mathrm{ERR}}\|_\infty \leq 20 \max\{\frac{1}{\eta}, \frac{1}{\sqrt{\delta}}\} \, \mathrm{e}^{-\eta^2} \; + \; 40\frac{\sqrt{\delta}}{\eta} \, \mathrm{e}^{-\delta/4}. \qquad (59)$$

Proof: The Fourier transform of the univariate Gaussian is given by (10)

$$\int\limits_{-\infty}^{\infty} \mathrm{e}^{-\delta x^2} \, \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{d}x = \sqrt{\frac{\pi}{\delta}} \, \mathrm{e}^{-k^2\pi^2/\delta}.$$

Further we will use the following simple estimates:

$$\sum_{k=1}^{n/2} \frac{1}{k^2} \;\le\; \sum_{k=1}^{\infty} \frac{1}{k^2} \;=\; \frac{\pi^2}{6}, \tag{60}$$

$$\sum_{k=1}^{n/2} \mathrm{e}^{-k^2\pi^2/\delta} \;\le\; \int_0^{\infty} \mathrm{e}^{-x^2\pi^2/\delta}\,\mathrm{d}x \;=\; \frac{1}{2}\sqrt{\frac{\delta}{\pi}}, \tag{61}$$

$$\sum_{k=n/2+1}^{\infty} \frac{1}{k^2} \;\le\; \int_{n/2}^{\infty} \frac{1}{x^2}\,\mathrm{d}x \;=\; \frac{2}{n}, \tag{62}$$

$$\sum_{k=n/2+1}^{\infty} \mathrm{e}^{-k^2\pi^2/\delta} \;\le\; \int_{n/2}^{\infty} \mathrm{e}^{-x^2\pi^2/\delta}\,\mathrm{d}x \;\le\; \frac{\delta}{n\pi^2}\,\mathrm{e}^{-\pi^2 n^2/(4\delta)}, \tag{63}$$

where the last inequality follows by

$$\int_a^{\infty} \mathrm{e}^{-cx^2}\,\mathrm{d}x \le \int_0^{\infty} \mathrm{e}^{-c(x+a)^2}\,\mathrm{d}x \le\; e^{-ca^2} \int_0^{\infty} \mathrm{e}^{-2acx}\,\mathrm{d}x = \frac{e^{-ca^2}}{2ac}.$$

By applying two times integration by parts, we obtain for the univariate Gaussian and $k \neq 0$ that

$$
\begin{aligned}
c_k\left(\mathrm{e}^{-\delta x^2}\right) &:= \int_{-1/2}^{1/2} \mathrm{e}^{-\delta x^2}\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&= (-1)^{k+1} \frac{\delta}{2\pi^2 k^2}\, \mathrm{e}^{-\delta/4} + \frac{\delta}{2\pi^2 k^2} \int_{-1/2}^{1/2} (1 - 2\delta x^2)\, \mathrm{e}^{-\delta x^2}\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&= (-1)^{k+1} \frac{\delta}{2\pi^2 k^2}\, \mathrm{e}^{-\delta/4} - \frac{1}{4\pi^2 k^2} \int_{-\infty}^{\infty} (\mathrm{e}^{-\delta x^2})''\, \mathrm{e}^{-2\pi \mathrm{i} k x}\, \mathrm{d}x \\
&\quad - \frac{\delta}{\pi^2 k^2} \int_{1/2}^{\infty} (1 - 2\delta x^2)\, \mathrm{e}^{-\delta x^2}\, \cos(2\pi k x)\, \mathrm{d}x
\end{aligned}
$$

and consequently, for $\delta \geq 2$,

$$|c_k\left(\mathrm{e}^{-\delta x^2}\right)| \;\leq\; \frac{\delta}{2\pi^2 k^2}\,\mathrm{e}^{-\delta/4} \;+\; \sqrt{\frac{\pi}{\delta}}\,\mathrm{e}^{-k^2\pi^2/\delta} \;+\; \frac{\delta}{\pi^2 k^2}\int_{1/2}^{\infty}(2\delta x^2-1)\,\mathrm{e}^{-\delta x^2}\,\mathrm{d}x$$

$$= \;\sqrt{\frac{\pi}{\delta}}\,\mathrm{e}^{-k^2\pi^2/\delta} \;+\; \frac{\delta}{\pi^2 k^2}\,\mathrm{e}^{-\delta/4}. \qquad (64)$$

By the aliasing formula we have to estimate the right–hand side of

$$|\mathcal{K}_{ER}(\boldsymbol{x})| \;\leq\; 2\sum_{k=-n/2}^{n/2}\left(|c_{(n/2,k)}(\mathcal{K})| + |c_{(k,n/2)}(\mathcal{K})|\right) \;+\; 2\sum_{\substack{\boldsymbol{k}\in\mathbb{Z}^2\\ \|\boldsymbol{k}\|_\infty \geq n/2+1}} |c_{\boldsymbol{k}}(\mathcal{K})|$$

$$=:\; 2\,S_1 \;+\; 2\,S_2.$$

Using the tensor product structure of the bivariate Gaussian, i.e. the splitting

$$c_{\boldsymbol{k}}(\mathcal{K}) = c_{k_1}(\,\mathrm{e}^{-\delta x_1^2})c_{k_2}(\,\mathrm{e}^{-\delta x_2^2})\,,$$

where $\boldsymbol{k} := (k_1, k_2)^{\mathrm{T}}$ and $\boldsymbol{x} := (x_1, x_2)^{\mathrm{T}}$, and (64) we get for the first sum

$$S_1 \le 2 \left(\sqrt{\frac{\pi}{\delta}}\, \mathrm{e}^{-n^2\pi^2/(4\delta)} + \frac{4\delta}{\pi^2 n^2}\, \mathrm{e}^{-\delta/4} \right) \left(\sum_{\substack{k=-n/2 \\ k\neq 0}}^{n/2} \left(\sqrt{\frac{\pi}{\delta}}\, \mathrm{e}^{-k^2\pi^2/\delta} + \frac{\delta}{\pi^2 k^2}\, \mathrm{e}^{-\delta/4} \right) \, + \, \sqrt{\frac{\pi}{\delta}} \right)$$

and further by (60) and (61)

$$S_1 \le 2\, C \, \left(\sqrt{\frac{\pi}{\delta}}\, \mathrm{e}^{-\eta^2} + \frac{1}{\eta^2}\, \mathrm{e}^{-\delta/4} \right),$$

where $C := \left(1 + \frac{\delta}{3}\, \mathrm{e}^{-\delta/4} + \sqrt{\frac{\pi}{\delta}}\right)$. The second sum splits as

$$S_2 \le 4 \sum_{k_1=n/2+1}^{\infty} \sum_{k_2=n/2+1}^{\infty} |c_{(k_1,k_2)}(\mathcal{K})| \, + \, 4 \sum_{k_1=-n/2}^{n/2} \sum_{k_2=n/2+1}^{\infty} |c_{(k_1,k_2)}(\mathcal{K})|.$$

Estimating the right–hand side by (64), (62) and (63) we arrive at

$$S_2 \le 4\, A(n,\delta)\, \left(A(n,\delta) + C\right),$$

where

$$A(n,\delta) := \frac{1}{2\sqrt{\pi}\eta}\,\mathrm{e}^{-\eta^2} \;+\; \frac{\sqrt{\delta}}{\pi\eta}\,\mathrm{e}^{-\delta/4}.$$

In summary we obtain

$$\|\mathcal{K}_{ER}\|_\infty \le C_1 \max\{\frac{1}{\eta}, \frac{1}{\sqrt{\delta}}\}\,\mathrm{e}^{-\eta^2} \;+\; C_2\frac{\sqrt{\delta}}{\eta}\,\mathrm{e}^{-\delta/4},$$

where

$$C_1 := \max\{4\,C\sqrt{\pi}, 4(A(n,\delta)+C)/(\sqrt{\pi})\}\;,$$
$$C_2 := \max\{8\,C/(\pi n), 8(A(n,\delta)+C)/(\pi)\}.$$

The assertion follows with $C < 2.7$ and $A(n,\delta) < 0.4$. ■

The first summand in (59) decreases with increasing η. The second summand is negligible for larger δ, e.g. we have that $\sqrt{\delta}\,\mathrm{e}^{-\delta/4} < 2.7\times 10^{-6}$ for $\delta \ge 60$.

Parameter			Computational Time		Error
δ	n	N	t_{slow}	t_{apr}	E_∞
1	32	25000	7.384e+01	1.340e-01	3.659e-05
1	32	50000	2.965e+02	2.700e-01	3.808e-05
1	32	100000	1.187e+03	5.400e-01	3.647e-05
100	64	25000	7.392e+01	1.560e-01	3.354e-07
100	64	50000	2.968e+02	2.960e-01	3.407e-07
100	64	100000	1.189e+03	5.780e-01	3.525e-07
10000	512	25000	1.238e+02	7.372e+00	3.538e-07
10000	512	50000	4.977e+02	7.584e+00	3.384e-07
10000	512	100000	1.983e+03	8.242e+00	3.523e-07

Comparison of the computational time and of the approximation error without boundary regularization for $\mathcal{K}(\boldsymbol{x}) = \mathrm{e}^{-\delta\|2\boldsymbol{x}\|_2^2}$ and $m = 4$.

Poisson solvers on nonequispaced grids

(G. Pöplau, 95, 03): $W_2^s(\mathbb{T}^3)$ periodic Sobolev space of order $s \in \mathbb{R}$

$$\|f\|_{s,2} := \left(\sum_{\boldsymbol{k} \in \mathbb{Z}^3} \left(1 + \|2\pi \boldsymbol{k}\|_2^2\right)^s |c_{\boldsymbol{k}}(f)|^2 \right)^{1/2}$$

Problem: find $u \in W_2^s(\mathcal{T}^3)$ which satisfies the differential equation

$$\begin{aligned} -\Delta u &= f \quad \text{in} \quad \Omega \subset \mathbb{R}^3 \\ u &= g \quad \text{on} \quad \partial\Omega \end{aligned}$$

i.e. find $\hat{u}_{\boldsymbol{k}}$ of

$$u(\boldsymbol{v}) = \sum_{\boldsymbol{k} \in I_N^3} \hat{u}_{\boldsymbol{k}} \left(1 + \|2\pi \boldsymbol{k}\|_2^2\right)^{-s} \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{v}} \,.$$

(Index-set $I_N^d := \{\boldsymbol{k} = (k_1, \dots, k_d)^{\mathrm{T}} \in \mathbb{Z}^d : -\frac{N}{2} \leq k_j < \frac{N}{2}; j = 1, \dots, d\}$) such that

$$\begin{aligned} \Delta\, u(\boldsymbol{v}_j) &= f(\boldsymbol{v}_j) \qquad (j \in I_M^1) \\ u(\boldsymbol{w}_j) &= g(\boldsymbol{w}_j) \qquad (j \in I_R^1) \end{aligned}$$

matrix vector notation

$$\boldsymbol{A}\boldsymbol{W}\hat{\boldsymbol{u}}_N = \boldsymbol{f}^1_M,$$

$$\boldsymbol{A} := \left(\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{v}_j}\right)_{j\in I^1_M, \boldsymbol{k}\in I^3_N}, \quad \hat{\boldsymbol{u}}_N := (\hat{u}_{\boldsymbol{k}})_{\boldsymbol{k}\in I^3_N}, \quad \boldsymbol{f}^1_M := (f(v_j))_{j\in I^1_M}$$

$$\boldsymbol{W} := \text{diag}\left(\frac{-\|2\pi\boldsymbol{k}\|_2^2}{(1+\|2\pi\boldsymbol{k}\|_2^2)^s}\right)_{\boldsymbol{k}\in I^3_N}$$

and

$$\boldsymbol{A}_{\mathsf{B}}\boldsymbol{W}_{\mathsf{B}}\hat{\boldsymbol{u}}_N = \boldsymbol{g}^1_R,$$

$$\boldsymbol{A}_{\mathsf{B}} := \left(\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{w}_j}\right)_{j\in I^1_R, \boldsymbol{k}\in I^3_N} \quad \boldsymbol{g}^1_R := (g_j)_{j\in I^1_R}$$

$$\boldsymbol{W}_{\mathsf{B}} := \text{diag}((1+\|2\pi\boldsymbol{k}\|_2^2)^{-s})_{\boldsymbol{k}\in I^3_N},$$

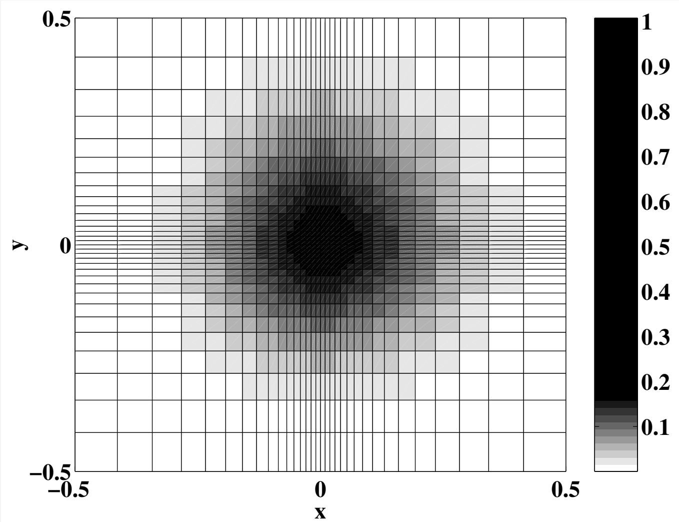
Kansa's method

$$\begin{bmatrix} \boldsymbol{A}\boldsymbol{W} \\ \boldsymbol{A}_{\mathsf{B}}\boldsymbol{W}_{\mathsf{B}} \end{bmatrix} \hat{\boldsymbol{u}}_N = \begin{bmatrix} \boldsymbol{f}^1_M \\ \boldsymbol{g}^1_R \end{bmatrix}$$

solve by CG-type method

Numerical examples

simulations of the behaviour of charged particles in accelerators



Potential given on the nonequidistant grid: (x, z)-plane with $y = 0$

$$E := \max_{j=1,\ldots,M} \frac{|f(\boldsymbol{v}_j) - \tilde{f}(\boldsymbol{v}_j)|}{|f(\boldsymbol{v}_j)|},$$

	multigrid method		Fourier method	
M	time in sec.	E	time in sec.	E
16^3	0.04	3.33e-02	0.68	2.95e-01
32^3	0.17	8.60e-03	5.76	5.19e-02
64^3	1.43	1.05e-02	41.44	3.34e-02
128^3	12.1	1.07e-02	217.8	4.85e-02

Approximation error and computational time

NFFT (iNFFT)

$$\Delta u = f \quad (u \in \Omega)$$
$$u \quad \text{periodic}$$

Fast summation, Method of fundamental solution

$$\begin{aligned} \Delta u &= 0 \\ u &= g \quad (u \in \delta\Omega) \end{aligned}$$

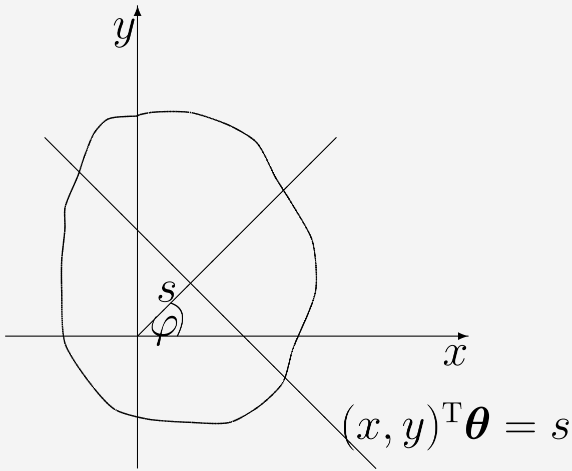
Content

- Fourier reconstruction algorithms for computerized tomography
  - Introduction (Radon transform, Fourier slice theorem)
  - Fourier reconstruction algorithms on standard grid
  - Fourier reconstruction algorithms on non-standard grid
- Applications on the sphere

Radon transform

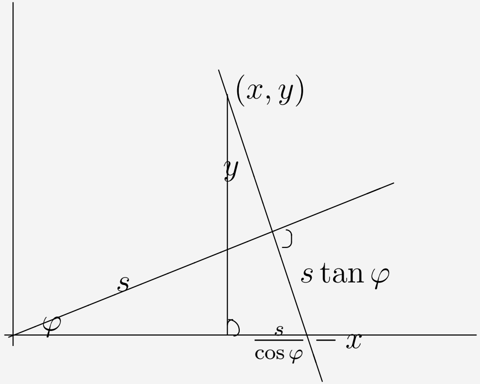
$$R : \mathcal{S}(\mathbb{R}^2) \to \mathcal{S}(\mathbb{R} \times \mathbb{T})$$

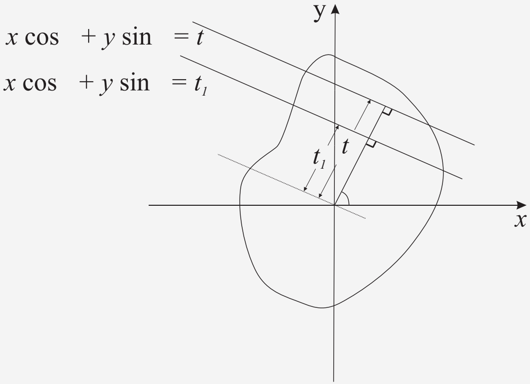
$$Rf(s,\varphi) := \int\limits_{\boldsymbol{x}\boldsymbol{\theta}=s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad \left(\boldsymbol{\theta} := \begin{pmatrix}\cos\varphi \\ \sin\varphi\end{pmatrix}\right)$$



X–ray in parallel beam tomography

Equation of line

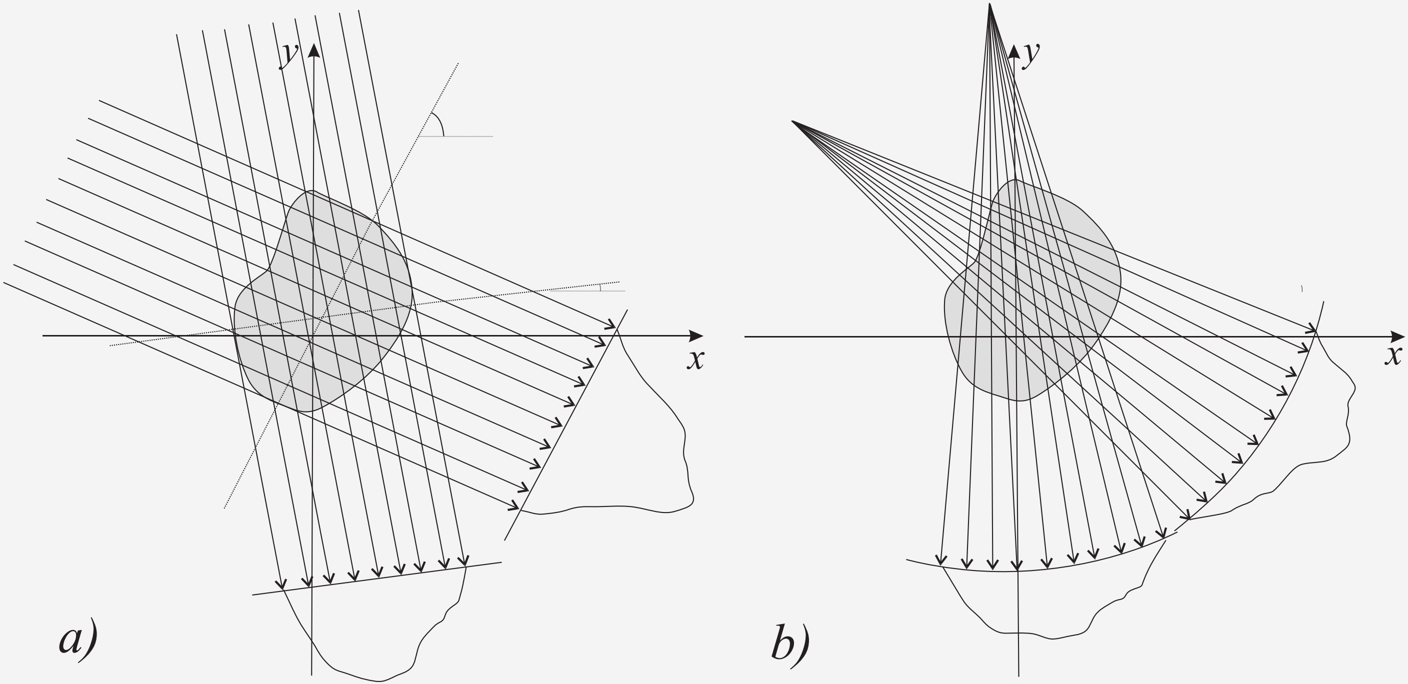




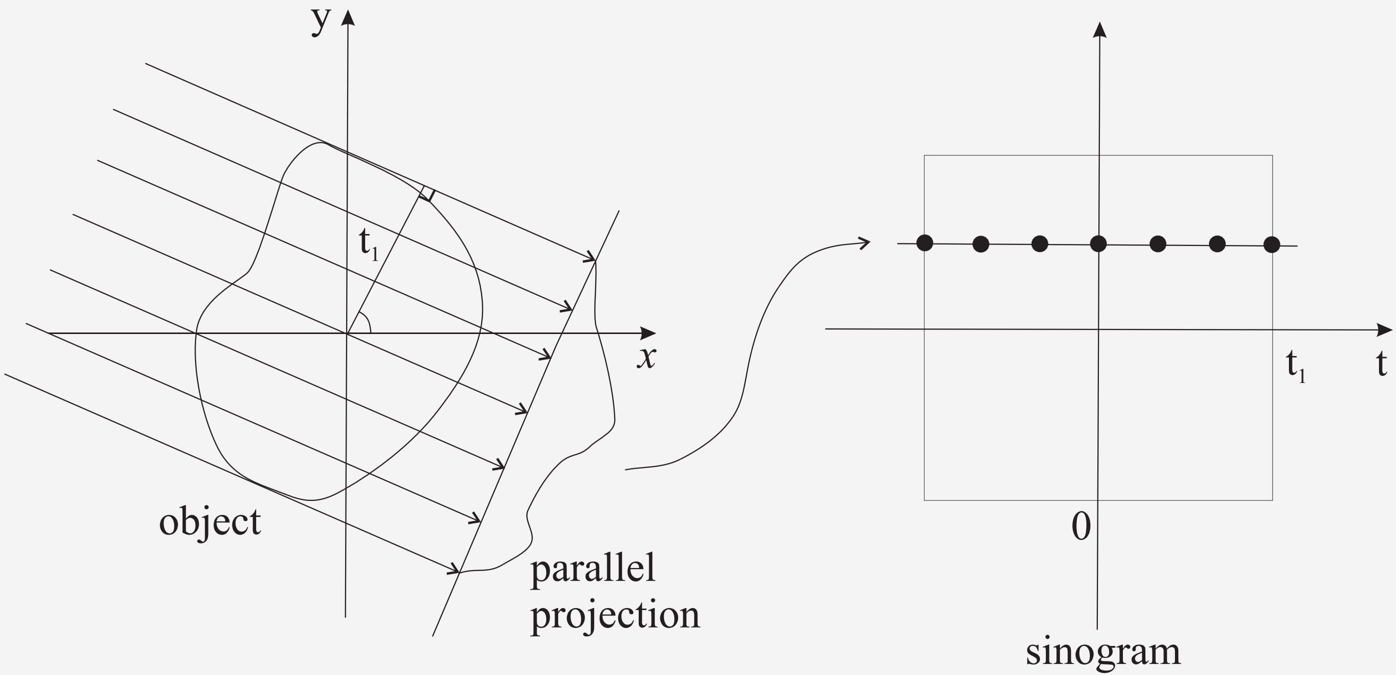
$$\frac{y}{s} = \frac{\frac{t}{\cos\varphi} - x}{s\tan\varphi}$$

$$ys\tan\varphi = \frac{s^2}{\cos\varphi} - xs \qquad \Big| \cdot \frac{\cos\varphi}{s}$$

$$y\sin\varphi + x\cos\varphi = \boldsymbol{x\theta} = s$$



Parallel projections are taken by measuring a set of parallel rays for a number of different angles (left).
A fan beam projection is collected if all rays meet in one location (right).



Parallel projection for a fixed θ and the points in sinogram.

Fourier slice theorem

Fourier transform of $f \in L_2(\mathbb{R}^n)$, $(n = 1, 2)$

$$\hat{f}(\boldsymbol{\xi}) := \int_{\mathbb{R}^n} f(\boldsymbol{x})\, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{x}\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{x}$$

Theorem:

If $f \in \mathcal{S}(\mathbb{R}^2)$, then

$$\hat{f}(\sigma\boldsymbol{\theta}) = \int_{\mathbb{R}} Rf(s, \varphi)\, \mathrm{e}^{-2\pi \mathrm{i} s\sigma}\, \mathrm{d}s = \widehat{Rf}(\sigma, \varphi) \quad (\boldsymbol{\theta} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix}).$$

Proof: Fourier transform of Rf with respect to s

$$\widehat{Rf}(\sigma,\varphi) = \int_{-\infty}^{\infty} Rf(s,\varphi)\,\mathrm{e}^{-2\pi\mathrm{i}\sigma s}\,\mathrm{d}s. \tag{65}$$

rotate by φ

$$\begin{bmatrix} s \\ t \end{bmatrix} = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

f_{r} is the rotated function of f with

$$f(x\cos\varphi + y\sin\varphi, -x\sin\varphi + y\cos\varphi) = f_{\mathrm{r}}(s,t)$$

substituting

$$Rf(s,\varphi) = \int\limits_{\boldsymbol{x}\boldsymbol{\theta}=s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_{-\infty}^{\infty} f_{\mathrm{r}}(s,t)\,\mathrm{d}t.$$

in (65)

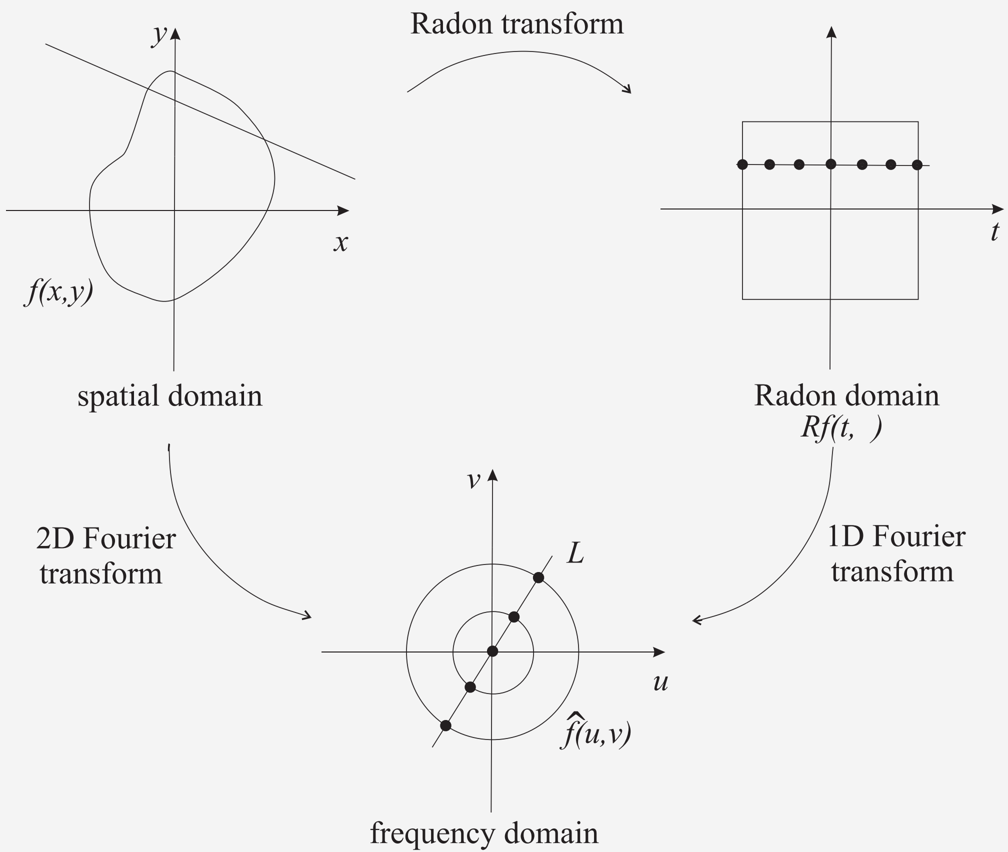
$$\begin{aligned} \widehat{Rf}(\sigma,\varphi) &= \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f_{\mathrm{r}}(s,t)\,\mathrm{d}t\right] \mathrm{e}^{-2\pi\mathrm{i}\sigma s}\,\mathrm{d}s \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_{\mathrm{r}}(s,t)\,\mathrm{e}^{-2\pi\mathrm{i}\sigma s}\,\mathrm{d}t\,\mathrm{d}s \end{aligned}$$

note

$$\begin{vmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{vmatrix} = 1$$

but this means $\mathrm{d}s\,\mathrm{d}t = \mathrm{d}x\,\mathrm{d}y$ and we obtain

$$\begin{aligned} \widehat{Rf}(\sigma,\varphi) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y)\,\mathrm{e}^{-2\pi\mathrm{i}\sigma(x\cos\varphi+y\sin\varphi)}\,\mathrm{d}x\,\mathrm{d}y \\ &= \int_{\mathbb{R}^2} f(\boldsymbol{x})\,\mathrm{e}^{-2\pi\mathrm{i}\sigma\boldsymbol{x}\boldsymbol{\theta}}\,\mathrm{d}\boldsymbol{x} \\ &= \hat{f}(\sigma\boldsymbol{\theta}) \end{aligned} \qquad \blacksquare$$



Radon transform
y
x
f(x,y)
spatial domain
t
Radon domain
Rf(t,)
2D Fourier
transform
1D Fourier
transform
v
L
u
f̂(u,v)
frequency domain

Fourier reconstruction on standard grid

References: P. and G. Steidl [32, 33]

$$\operatorname{supp} f \subseteq \Omega := \{\boldsymbol{x} \in \boldsymbol{R}^2 : ||\boldsymbol{x}||_2 \leq 1\}$$

reconstruct f on the grid

$$(x_j, y_k) := \left(j\frac{2}{N}, k\frac{2}{N}\right)$$

$$(j, k = -\frac{N}{2}, \ldots \frac{N}{2} - 1)$$

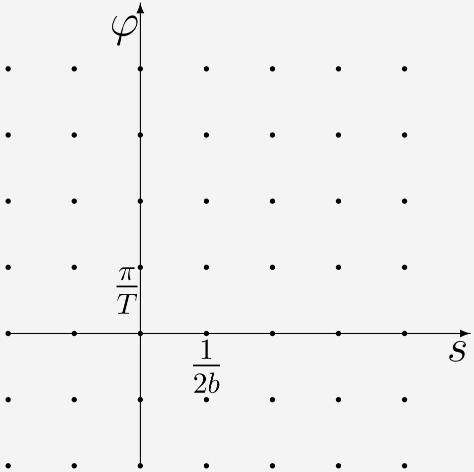
Rf given at the grid points

$$(s_r, \varphi_t) = \left(r\frac{2}{R}, t\frac{\pi}{T}\right)$$

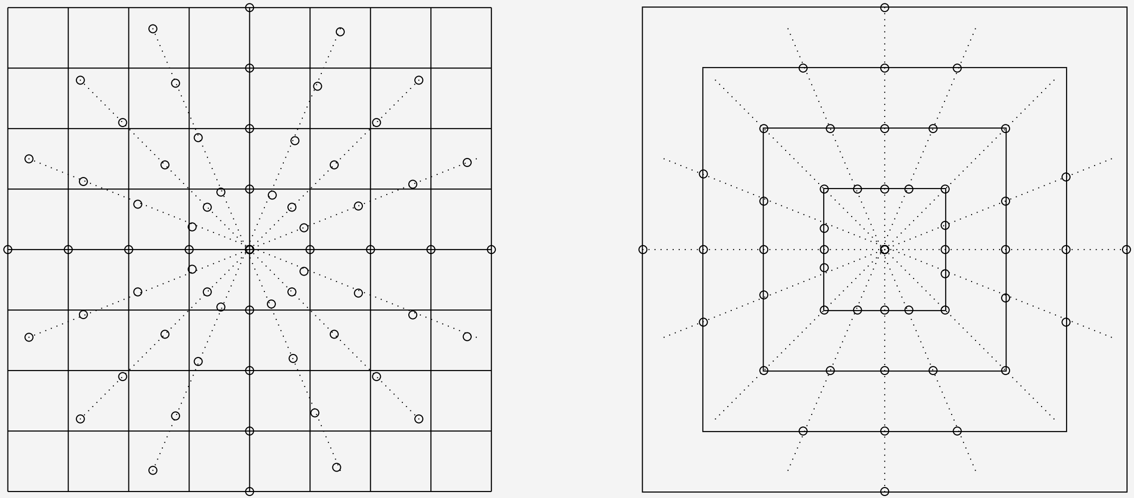
$$(t = 0, \ldots, T-1; r = -\frac{R}{2}, \ldots, \frac{R}{2} - 1),$$

Shannon's sampling theorem

$R \geq N$ and $T \geq \frac{\pi R}{2}$



standard grid in Radon domain



Polar grid (left) and linogram (right) in Fourier domain

Algorithm based on the polar grid

1. Computation of

$$\hat{f}(\frac{m}{\gamma}\,\boldsymbol{\theta}_t) \approx \frac{2}{R} \sum_{r=-\frac{R}{2}}^{\frac{R}{2}-1} Rf(r\frac{2}{R}, \varphi_t)\mathrm{e}^{-2\pi \mathrm{i} rm/\left(\frac{R\gamma}{2}\right)}$$

$$(m = -\frac{R\gamma}{4}, \ldots, \frac{R\gamma}{4} - 1; t = 0, \ldots, T-1)$$

by T univariate FFT's of length $\frac{R\gamma}{2}$ $(\frac{\gamma}{2} \geq 1)$.

2. Computation of $f(x_j, y_k) \approx$

$$\frac{\pi}{\gamma^2 T} \sum_{m=0}^{\frac{R\gamma}{4}-1} \sum_{t=-T}^{T-1} \nu_m \, \hat{f}(\frac{m}{\gamma}\boldsymbol{\theta}_t)\, \mathrm{e}^{2\pi \mathrm{i}(jm\cos\varphi_t + km\sin\varphi_t)/\left(\frac{\gamma N}{2}\right)} \qquad (j, k = -\frac{N}{2}, \ldots, \frac{N}{2} - 1)$$

by bivariate NFFT, where

$$\nu_m := \begin{cases} \frac{1}{12} & m = 0\,, \\ m & m = 1, \ldots, \frac{R\gamma}{2} - 1\,. \end{cases}$$

First step

$h(s) := Rf(s,\varphi_t)$; $\hat{h}(\sigma) := \hat{Rf}(\sigma,\varphi_t)$

$$\hat{h}(\sigma) = \int_{-1}^{1} h(s)\mathrm{e}^{-2\pi\mathrm{i}s\sigma}\,\mathrm{d}s$$

by Poisson's summation formula

$$\hat{h}(\sigma) + \sum_{\substack{n\in Z\\ n\neq 0}} \hat{h}(\sigma + n\frac{R}{2}) = \frac{2}{R}\sum_{r=-\frac{R}{2}}^{\frac{R}{2}-1} h(r\frac{R}{2})\mathrm{e}^{-2\pi\mathrm{i}r\sigma/(\frac{R}{2})}$$

is a good approximation of $\hat{h}(\sigma)$ for $\sigma \in [-\frac{R}{4}, \frac{R}{4}]$.

Second step

$$f(x, y) =$$

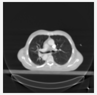
$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{f}(u, v) \mathrm{e}^{2\pi \mathrm{i}(ux+vy)} \, \mathsf{d}u \mathsf{d}v =$$

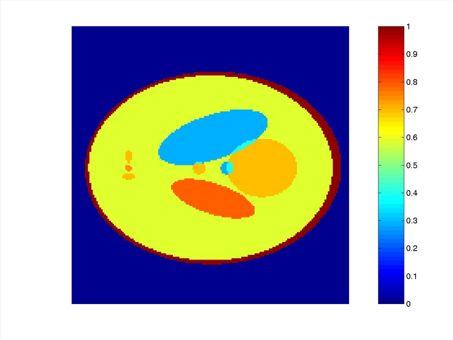
$$\int_{0}^{\infty} \sigma \int_{-\pi}^{\pi} \hat{f}(\sigma \cos \varphi, \sigma \sin \varphi) \mathrm{e}^{2\pi \mathrm{i} \sigma (x \cos \varphi + y \sin \varphi)} \, \mathsf{d}\varphi \mathsf{d}\sigma$$

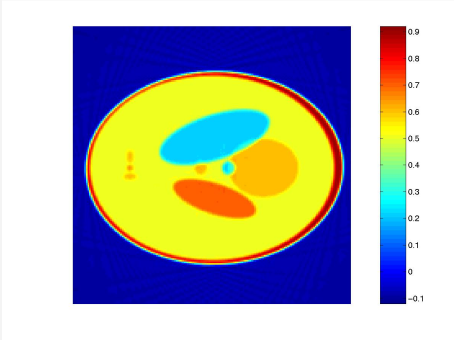
	R	T	N	time in s
FB	180	600	180	20.2
NFFTL	180	600	180	2.08
NFFT/NFFT^T	180	600	180	3.5
NFFT2D	180	600	180	9.1
FB	362	900	362	127.81
NFFTL	362	900	362	8.44
NFFT/NFFT^T	362	900	362	10.59
NFFT2D	362	900	362	31.3

Computation time of the filtered back projection and of different Fourier algorithms

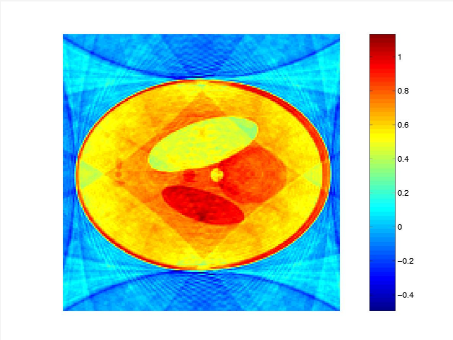
Numerical examples

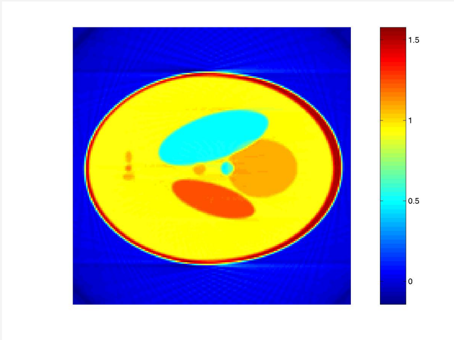






Shepp-Logan phantom   reconstruction with FB (20 sec.)





FFT reconstruction (2 sec.)   NFFT reconstruction (3 sec.)

Fourier reconstruction on nonstandard grid

References: P. and G. Steidl [34]

sample Rf on a grid

$$\mathcal{G} := \{\boldsymbol{A}\,\boldsymbol{k} : \boldsymbol{k} \in \mathbb{Z}^2\} \subseteq \mathbb{R} \times \mathbb{T}$$

dual grid $\hat{\mathcal{G}} := \{\hat{\boldsymbol{A}}\,\boldsymbol{k} : \boldsymbol{k} \in \mathbb{Z}^2\} \subseteq \mathbb{R} \times \mathbb{Z}$

$$\hat{\boldsymbol{A}} := \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \in \mathbb{R}^{2\times 2}; \quad (a_{21}, a_{22} \in \mathbb{Z})$$

$$\boldsymbol{A} := \frac{1}{\det(\hat{\boldsymbol{A}})} \begin{pmatrix} a_{22} & -a_{21} \\ -2\pi a_{12} & 2\pi a_{11} \end{pmatrix}$$

filtered back projection algorithm – Kruse (1989)
algebraic reconstruction algorithms – Klaverkamp (1991)

Theorem: (Natterer [26])
$f \in C_0^\infty(\Omega)$, $Rf \in \mathcal{S}(\mathbb{R} \times \mathbb{T})$
For $\nu \in (0,1)$ and $b \geq 1$ define the set K by
$K := \{(\sigma, k) \in \mathbb{R} \times \mathbb{Z} : |\sigma| < b,$
$|k| < 2\pi \max\left\{\frac{|\sigma|}{\nu}, \left(\frac{1}{\nu} - 1\right) b\right\}\}.$
Let $\hat{\boldsymbol{A}}$ be given so that the sets

$$K + \hat{\boldsymbol{A}}\,\boldsymbol{k} \quad (\boldsymbol{k} \in \mathbb{Z}^2)$$

are mutually disjoint. If $Rf(\boldsymbol{A}\,\boldsymbol{k}) = 0$ for all $\boldsymbol{k} \in \mathbb{Z}^2$, then we have for $b \geq B(\nu) \geq 1$ that

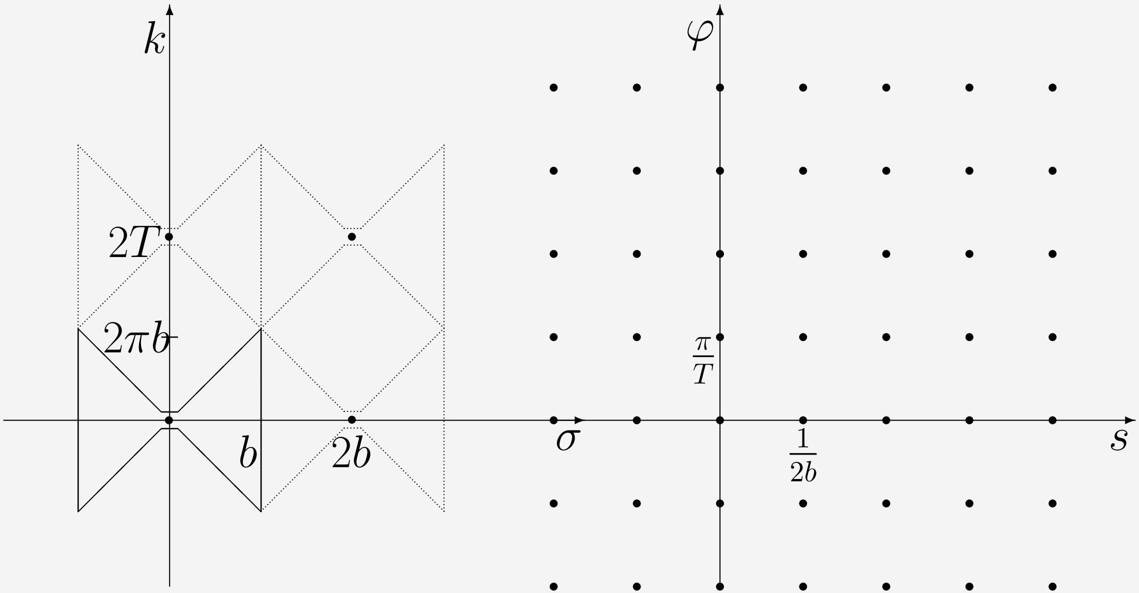
$$\|Rf\|_{L_\infty(\mathbb{R}\times\mathbb{T})} \leq C(\nu)\, \mathrm{e}^{-\lambda(\nu) b} \|f\|_{L_1(\Omega)} + \frac{8}{\pi\nu} \varepsilon_0(f, b).$$

Here $C(\nu)$ and $\lambda(\nu)$ are positive constants and

$$\varepsilon_0(f, b) := \int_{|\xi| \geq b} |\hat{f}(\xi)|\, \mathrm{d}\xi.$$

Standard grid with generating matrix

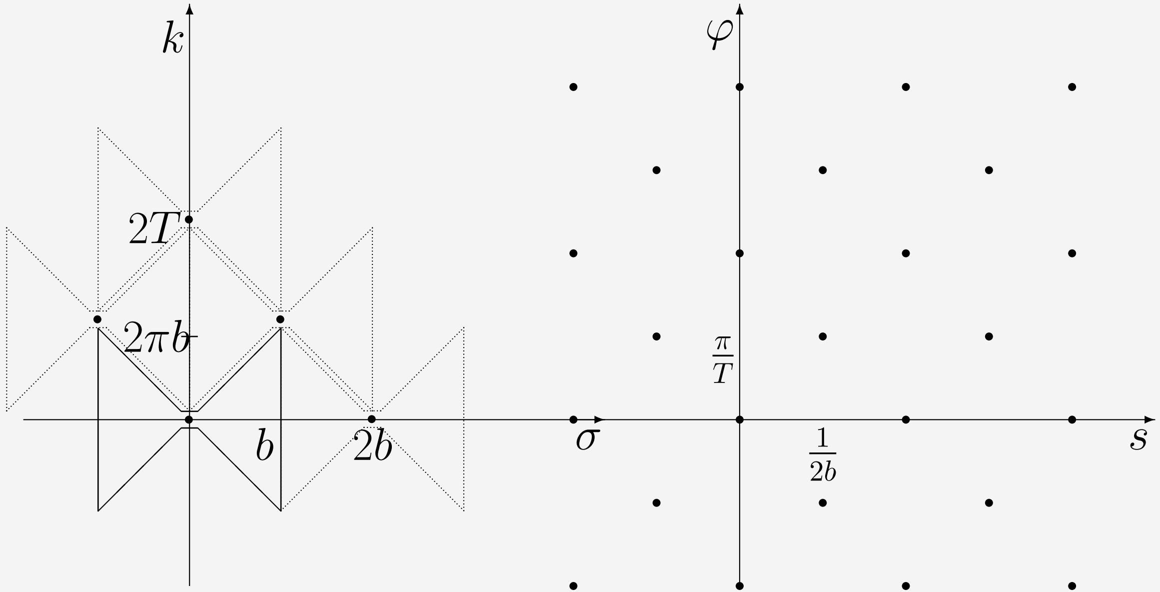
$$\boldsymbol{A} = \begin{pmatrix} \frac{1}{2b} & 0 \\ 0 & \frac{\pi}{T} \end{pmatrix}, \quad \hat{\boldsymbol{A}} = \begin{pmatrix} 2b & 0 \\ 0 & 2T \end{pmatrix} \quad (T > 2b\pi)$$



Dual standard grid with four sets $K + \hat{\boldsymbol{A}}\boldsymbol{k}$ (left) and standard grid (right), where $T = \frac{2\pi b}{\nu}$ ($\nu \approx 0.95$).

Interlaced grid with generating matrix

$$\boldsymbol{A} := \begin{pmatrix} \frac{1}{b} & \frac{1}{2b} \\ 0 & \frac{\pi}{T} \end{pmatrix}, \ \hat{\boldsymbol{A}} = \begin{pmatrix} b & 0 \\ -T & 2T \end{pmatrix} \quad (T > 2b\pi),$$



Dual interlaced grid with five sets $K + \hat{\boldsymbol{A}}\boldsymbol{k}$ (left) and interlaced grid (right), where $T = \frac{2\pi b}{\mu}$ ($\mu < \nu$; $\nu \approx 0.95$).

For $t = -T, \dots, T-1$, we set

$$\varphi_t := \varphi_{j,k} := \frac{\pi}{T}(ja + k)$$

$$\left(k = 0, \dots, a-1;\ j = -\frac{T}{a}, \dots, \frac{T}{a} - 1\right)$$

$$\boldsymbol{\theta}_{j,k} := \left(\cos\varphi_{j,k}, \sin\varphi_{j,k}\right)^{\mathrm{T}}$$

$$s_{n,k} := \frac{(kc)_a + na}{M} \quad \left(n = -\frac{M}{a}, \dots, \frac{M}{a} - 1\right)$$

$(k)_a$ nonnegative residue of k modulo a

Rf of f given at the grid points $(s_{n,k}, \varphi_{j,k})$

Aim: reconstruct f with on the grid

$$(x_j, y_k) = \left(j\frac{2}{N}, k\frac{2}{N}\right) \quad \left(j, k = -\frac{N}{2}, \dots, \frac{N}{2} - 1\right)$$

i.e. we are interested in details of size $\geq \frac{2}{N}$

First step

$$\widehat{Rf}(\sigma,\varphi) = \hat{f}(\sigma\boldsymbol{\theta}) = \int_{-1}^{1} Rf(s,\varphi)\, \mathrm{e}^{2\pi \mathrm{i} s\sigma}\, \mathrm{d}s$$

using $Rf(s_{n,k},\varphi_{j,k})$, the trapezoidal rule and for oversampling factor $\gamma \in \mathbb{N}$,

$$\hat{g}\left(\frac{m}{\gamma},\varphi_{j,k}\right) = \mathrm{e}^{-2\pi\mathrm{i}(kc)_a m/(\gamma M)} \frac{a}{M} \sum_{n=-\frac{M}{a}}^{\frac{M}{a}-1} Rf(s_{n,k},\varphi_{j,k})\, \mathrm{e}^{-2\pi\mathrm{i} nm/\left(\frac{M\gamma}{a}\right)}$$

we have for

$$m = u\frac{M\gamma}{a} + v \quad \left(u \in \mathbb{Z}, v \in \left\{-\frac{M\gamma}{2a},\ldots,\frac{M\gamma}{2a}-1\right\}\right)$$

that

$$\hat{g}\left(\frac{m}{\gamma},\varphi_{j,k}\right) = \mathrm{e}^{-2\pi\mathrm{i}(kc)_a u/a}\, \hat{g}\left(\frac{v}{\gamma},\varphi_{j,k}\right)$$

Second step as before

$$(f * W_b)(\boldsymbol{x}) = \int\limits_0^b \sigma \int\limits_{-\pi}^{\pi} \hat{f}(\sigma\boldsymbol{\theta})\, \mathrm{e}^{2\pi \mathrm{i} \sigma \boldsymbol{\theta} \boldsymbol{x}}\, \mathrm{d}\varphi\ \mathrm{d}\sigma$$

where

$$\hat{W}_b(\xi) = 1_{[-b,b]}(|\xi|) \quad (\xi \in \mathbb{R}^2).$$

$$(f * W_b)^{(\mathrm{i})}(x) := \int\limits_0^b \sigma \frac{\pi}{T} \sum_{t=-T}^{T-1} \hat{g}(\sigma, \varphi_t)\, \mathrm{e}^{2\pi \mathrm{i} \sigma \boldsymbol{\theta}_t \boldsymbol{x}}\ \mathrm{d}\sigma$$

outer integral with $b := \frac{N}{4}$ to

$$\left(f * W_{\frac{N}{4}}\right)^{(\mathrm{ii})}(x_j, y_k) \ = \ \frac{\pi}{\gamma T} \sum_{m=0}^{\frac{N\gamma}{4}} \sum_{t=-T}^{T-1} \nu_m \hat{g}\left(\frac{m}{\gamma}, \varphi_t\right) \times \ \mathrm{e}^{2\pi \mathrm{i} m \boldsymbol{\theta}_t \binom{j}{k} / \left(\frac{N\gamma}{2}\right)}$$

where

$$\nu_m := \begin{cases} \frac{1}{12} & m = 0, \\ m & \text{otherwise} \end{cases}$$

Theorem: Let $f \in C_0^\infty(\Omega)$ and let $Rf \in \mathcal{S}(\mathbb{R} \times T)$ be sampled with respect to the grid generated by the matrix

$$\boldsymbol{A} := \begin{pmatrix} \frac{a}{M} & \frac{1}{M} \\ 0 & \frac{\pi}{T} \end{pmatrix} \quad (a, M, T \in \mathbb{N}; \quad a, M, T > 0)$$

If $M, T \in \mathbb{N}$ satisfy one of the following conditions

$$\begin{aligned}
&\text{i)} && 2b \leq M < \frac{2ab}{a-1} \text{ and } T > \pi M(a-1);\ (a \geq 3),\\
&\text{ii)} && \frac{2ab}{a-1} \leq M < ab \text{ and } T > \pi(2ab - M);\ (a \geq 4),\\
&\text{iii)} && ab \leq M < 2ab \text{ and } T > \pi M;\ (a \geq 2),\\
&\text{iv)} && M \geq 2ab \text{ and } T > 2\pi b;\ (a \geq 1),
\end{aligned}$$

then

$$\|f * W_b - (f * W_b)^{(\mathrm{i})}\|_{L_\infty(\Omega)} \leq \pi ab\, \varepsilon_0(f, b) +$$

$$C \|f\|_{L_1(\Omega)}\, a\sqrt{b}\, (1 - \tau^2)^{-\frac{1}{4}}\, \mathrm{e}^{-\frac{2\pi}{3} b (1-\tau^2)^{\frac{3}{2}}}\ ,$$

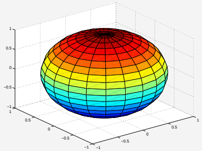
where C denotes a positive constant and

$$\tau := \begin{cases} \frac{\pi}{T} M(a-1) & \text{in case i)}, \\ \frac{\pi}{T}(2ab - M) & \text{in case ii)}, \\ \frac{\pi}{T} M & \text{in case iii)}, \\ \frac{\pi}{T} 2b & \text{in case iv)}. \end{cases}$$

Content

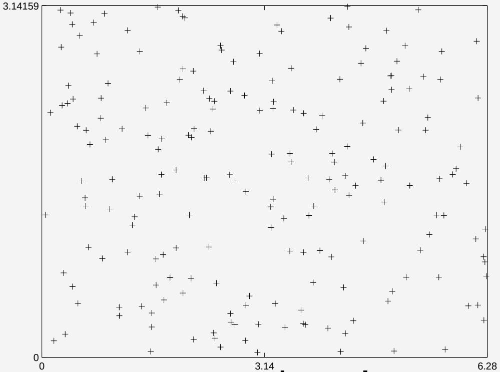
- Applications on the sphere
  - Scattered data approximation on the sphere
  - Fourier algorithms on the sphere
  - Fast summation algorithms on the sphere
  - Spherical Filter and Wavelet Decomposition
- Applications

Scattered data approximation on the sphere



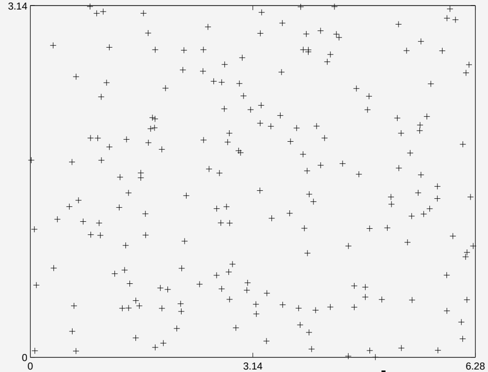
map

north pole



blend

east pole



south pole

west pole

The map:

standard latitude/longitude mapping from

$$M_1(\theta, \phi) := (\cos(\phi)\cos(\theta), \sin(\phi)\cos(\theta), \sin(\theta))^{\mathrm{T}}$$

inverse mapping of M_1

$$\tilde{M}_1(\boldsymbol{x}) := \begin{cases} \left(\arccos\left(\frac{x_1}{\sqrt{1-x_3^2}}\right), \arcsin(x_3)\right)^{\mathrm{T}} & \text{for } x_2 \geq 0\,, \\ \left(-\arccos\left(\frac{x_1}{\sqrt{1-x_3^2}}\right), \arcsin(x_3)\right)^{\mathrm{T}} & \text{for } x_2 < 0 \end{cases}$$

similar mapping based upon east pole and west pole

$$M_2(\theta, \phi) := (-\cos(\phi)\cos(\theta), \sin(\theta), \sin(\phi)\cos(\theta))^{\mathrm{T}}$$

inverse mapping

$$\tilde{M}_2(\boldsymbol{x}) := \begin{cases} \left(\arccos\left(\frac{x_1}{\sqrt{1-x_2^2}}\right), \arcsin(x_2)\right)^{\mathrm{T}} & \text{for } x_3 \geq 0\,, \\ \left(-\arccos\left(\frac{x_1}{\sqrt{1-x_2^2}}\right), \arcsin(x_2)\right)^{\mathrm{T}} & \text{for } x_3 < 0 \end{cases}$$

The map and blend approximation:

blend of two bivariate polynomials p and q

$$p(\theta,\phi) = \sum_{k_1=0}^{N-1}\sum_{k_2=0}^{N-1} \hat{p}_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}(k_1\phi+2\,k_2\theta)}$$

and

$$q(\theta,\phi) = \sum_{k_1=0}^{N-1}\sum_{k_2=0}^{N-1} \hat{q}_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}(k_1\phi+2\,k_2\theta)}$$

defined over a planar domain

$$F(\boldsymbol{x}) = W_1(\boldsymbol{x}) p(\tilde{M}_1(\boldsymbol{x})) + W_2(\boldsymbol{x}) q(\tilde{M}_2(\boldsymbol{x})) \quad (\boldsymbol{x} \in \mathcal{S})$$

with

$$W_1(\boldsymbol{x}) + W_2(\boldsymbol{x}) = 1 \quad (\boldsymbol{x} \in \mathcal{S})$$

Theorem: (P., 01 [31])
Let the weight functions given as

$$W(\theta,\phi)^{\mathrm{T}} := W(\theta) := \begin{cases} \mathrm{e}^{\frac{\pi^2}{4\theta^2-\pi^2}} & -\frac{\pi}{2} < \theta < \frac{\pi}{2}\,, \\ 0 & \theta = \pm\frac{\pi}{2} \end{cases}$$

$$\tilde{W}_1(\theta,\phi) := W_1(M_1(\theta,\phi)) = \frac{W(\theta)}{W(\theta) + W(\arcsin(\sin(\phi)\cos(\theta))}\,,$$

$$\tilde{W}_2(\theta,\phi) := W_2(M_2(\theta,\phi)) = \frac{W(\arcsin(\sin(\phi)\cos(\theta))}{W(\theta) + W(\arcsin(\sin(\phi)\cos(\theta))}$$

then for $l \in \{1,2\}$

i) $\tilde{W}_l$ are nonnegative functions,

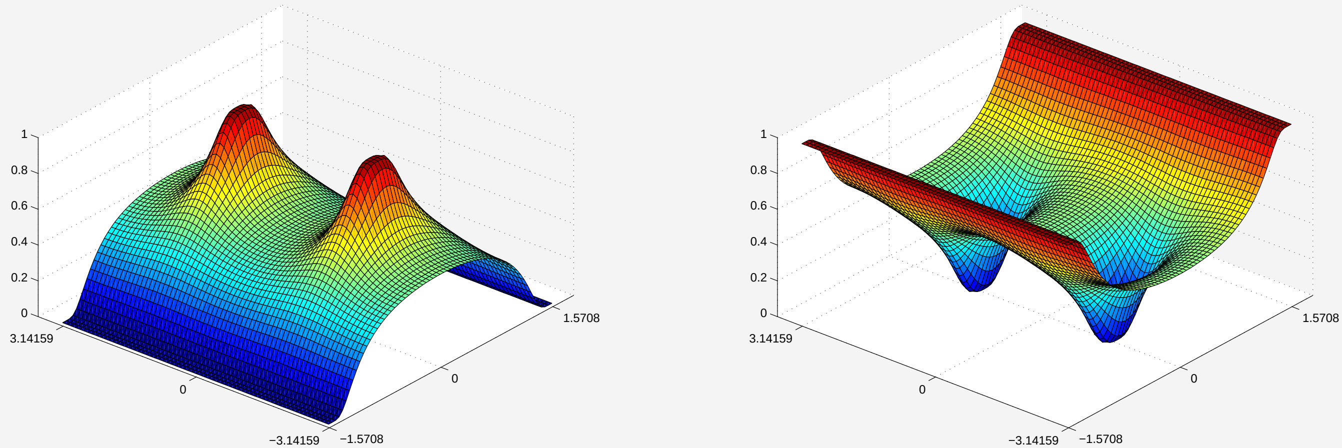
ii) $\tilde{W}_1(\theta,\phi) + \tilde{W}_2(\theta,\phi) = 1$,

iii) $\tilde{W}_l(\theta,\phi)$ are 2π periodic with respect to ϕ,

iv) $\lim\limits_{\theta\to-\pi/2+} \frac{\mathrm{d}^n}{\mathrm{d}\theta^n}\tilde{W}_1(\theta,\phi) = \lim\limits_{\theta\to\pi/2-} \frac{\mathrm{d}^n}{\mathrm{d}\theta^n}\tilde{W}_1(\theta,\phi) = 0 \quad (n \in \mathbb{N}_0)$,

$\lim\limits_{\theta\to-\pi/2+} \tilde{W}_2(\theta,\phi) = \lim\limits_{\theta\to\pi/2-} \tilde{W}_2(\theta,\phi) = 1\,,$

$\lim\limits_{\theta\to-\pi/2+} \frac{\mathrm{d}^n}{\mathrm{d}\theta^n}\tilde{W}_2(\theta,\phi) = \lim\limits_{\theta\to\pi/2-} \frac{\mathrm{d}^n}{\mathrm{d}\theta^n}\tilde{W}_2(\theta,\phi) = 0 \quad (n \in \mathbb{N})$.



Weight function $\tilde{W}_1(\theta, \phi)$ (left) and $\tilde{W}_2(\theta, \phi)$ (right)

discrete Problem:

minimize the discrete least–squares error

$$\sqrt{\sum_{j \in I_M^1} |f_j - W_1(\boldsymbol{x}_j)\, p(\tilde{M}_1(\boldsymbol{x}_j) - W_2(\boldsymbol{x}_j) q(\tilde{M}_2(\boldsymbol{x}_j))|^2}$$

rewrite

$$\|\boldsymbol{W}_1 \boldsymbol{A}_1 \hat{\boldsymbol{p}}_N^2 + \boldsymbol{W}_2 \boldsymbol{A}_2 \hat{\boldsymbol{q}}_N^2 - \boldsymbol{f}_M^1\|_2$$

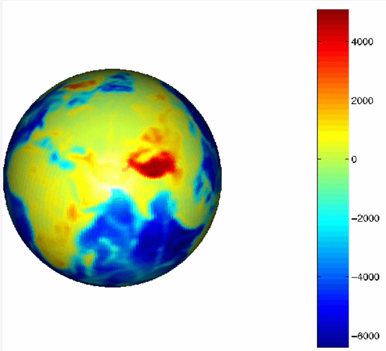
$$\boldsymbol{W}_1 := \text{diag}(W_1(\boldsymbol{x}_j))_{j \in I_M^1}, \quad \boldsymbol{W}_2 := \text{diag}(W_2(\boldsymbol{x}_j))_{j \in I_M^1}$$

$$\boldsymbol{A}_l := \left(\mathrm{e}^{-\mathrm{i}(k_1 \phi_j + 2\, k_2 \theta_j)}\right)_{j \in I_M^1, \boldsymbol{k} \in I_N^2}, \quad (\phi_j, \theta_j)^{\mathrm{T}} := \tilde{M}_l(\boldsymbol{x}_j) \quad (l = 1, 2)$$

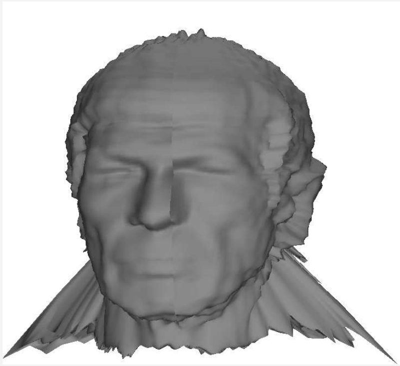
apply the CGNR method to the equation

$$[\boldsymbol{W}_1 \boldsymbol{A}_1, \boldsymbol{W}_2 \boldsymbol{A}_2] \begin{bmatrix} \hat{\boldsymbol{p}}_N^2 \\ \hat{\boldsymbol{q}}_N^2 \end{bmatrix} = \boldsymbol{f}_M^1$$

Numerical Example



earth (65536 points)



Spock (9508 points)

Fourier algorithms on the Sphere Kunis, P. [21]; Keiner, P. [20]

$$Y_k^n(\theta,\phi) := P_k^{|n|}(\cos(\theta))\,\mathrm{e}^{in\phi}$$

$$P_k^{|n|}(x) := \left(\frac{(k-n)!}{(k+n)!}\right)^{1/2}(1-x^2)^{n/2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}P_k(x)$$

Problem: fast computation of

$$f(\theta,\phi) = \sum_{k=0}^{M-1}\sum_{n=-k}^{k} a_k^n Y_k^n(\theta,\phi)$$

at arbitrary nodes $(\theta_d,\phi_d)\in\mathcal{S}$ $(d=0,\ldots,D-1)$
discrete spherical Fourier transform (FFT on the Sphere, FSFT)

$$(\theta_{d_1},\phi_{d_2}) := \left(\tfrac{d_1\pi}{D_1},\tfrac{2d_2\pi}{D_2-1}\right) \quad d_1=0,\ldots,D_1-1,\ d_2,\ldots,D_2-1$$

Driscoll, Healy (94) [8]; P., Steidl, Tasche (98) [37]; Mohlenkamp (99) [25]; Suda, Takami (01) [43]; Rokhlin, Tygert[41]

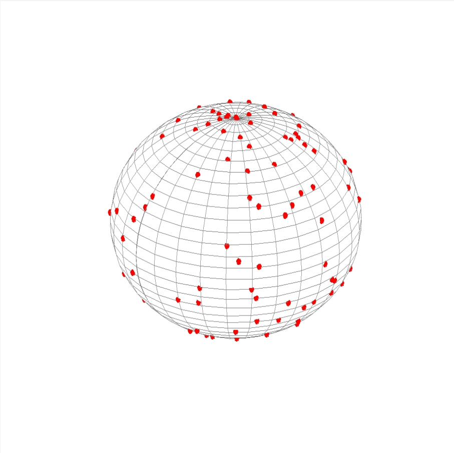
direct computation ($M = \sqrt{D}$)

$$h_n(\cos\theta) = \sum_{k=|n|}^{M} a_k^n P_k^{|n|}(\cos\theta)\ , \qquad f(\theta,\phi) = \sum_{n=-M}^{M} h_n(\cos\theta)\,\mathrm{e}^{\mathrm{i}n\phi}$$

1. arbitrary knots

$(f(\theta_d, \phi_d))$

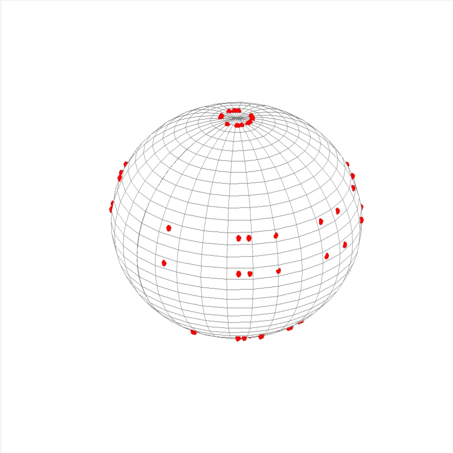
$\mathcal{O}(D^2)$



2. arbitrary grids

$(f(\theta_s, \phi_t))$

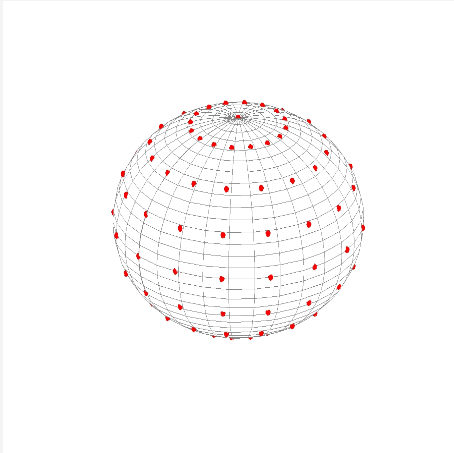
$\mathcal{O}\left(D^{3/2}\right)$



3. equispaced grids

$\left(f\left(\frac{s\pi}{N}, \frac{t\pi}{2N}\right)\right)$

$\mathcal{O}\left(D \log^2 D\right)$



Problem: NFFT on the sphere (NFSFT)

Idea:

$$
\begin{aligned}
f(\theta,\phi) &= \sum_{k=0}^{M-1} \sum_{n=-k}^{k} a_k^n Y_k^n(\theta,\phi) \\
&= \sum_{n=-M+1}^{M-1} \sum_{k=|n|}^{M-1} a_k^n Y_k^n(\theta,\phi) \\
&= f_e(\theta,\phi) + \sin(\theta)\, f_o(\theta,\phi)
\end{aligned}
$$

with

$$
f_e(\theta,\phi) := \sum_{\substack{n=-M+1 \\ n \text{ even}}}^{M-1} \sum_{k=|n|}^{M-1} a_k^n Y_k^n(\theta,\phi)
$$

$$
f_o(\theta,\phi) := \frac{1}{\sin(\theta)} \sum_{\substack{n=-M+1 \\ n \text{ odd}}}^{M-1} \sum_{k=|n|}^{M-1} a_k^n Y_k^n(\theta,\phi)
$$

$$f_e(\theta,\phi) = \sum_{\substack{n=-M+1 \\ n \text{ even}}}^{M-1} \sum_{k=|n|}^{M-1} a_k^n Y_k^n(\theta,\phi)$$

$$= \sum_{\substack{n=-M+1 \\ n \text{ even}}}^{M-1} g_n(\theta)\, \mathrm{e}^{\mathrm{i}n\phi},$$

$$g_n(\theta) := \sum_{k=|n|}^{M-1} a_k^n P_k^{|n|}(\cos(\theta)) \qquad \in \Pi_{M-1}$$

apply the Discrete Polynomial Transform (P., Steidl, Tasche 1998 [36])

$$g_n(\theta) = \sum_{k=0}^{M-1} \tilde{a}_k^n T_k(\cos(\theta))$$

Algorithm (NFFT on the sphere, NFSFT)

1. From

$$f(\theta,\phi) \;=\; \sum_{k=0}^{M-1}\sum_{n=-k}^{k} a_k^n Y_k^n(\theta,\phi)$$

   compute with the Discrete Polynomial Transform

$$f(\theta,\phi) \;=\; \sum_{n=-M+1}^{M-1}\sum_{k=-M+1}^{M-1} c_k^n \,\mathrm{e}^{\mathrm{i}k\theta}\,\mathrm{e}^{\mathrm{i}n\phi}\,.$$

2. Compute with the bivariate NFFT

$$f(\theta_d,\phi_d) \qquad (d=0,\dots,D-1)\,.$$

arithmetic operations

$$\mathcal{O}\left(M^2\log^2 M + (\alpha M)^2\log M + m^2 D\right) = \mathcal{O}\left(M^2\log^2 M + D\right)$$

How to obtain the fast adjoint NFSFT algorithm?

(Keiner, P., 08)

$$a_k^n := \sum_{j=0}^{M-1} \omega_j f(\theta_j, \phi_j) Y_k^{-n}(\theta_j, \phi_j) \quad (k = 0, \ldots, N; n = -k, \ldots, k)$$

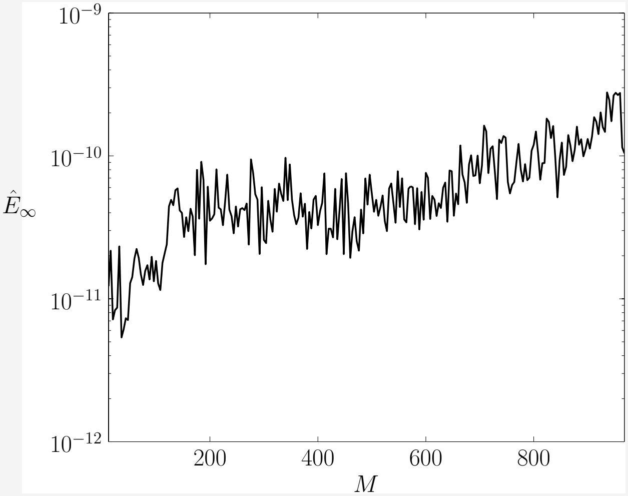
$$\mathbf{Y} := \left(Y_k^{-n}(\theta_j, \phi_j)\right)_{j;(k,n)}$$

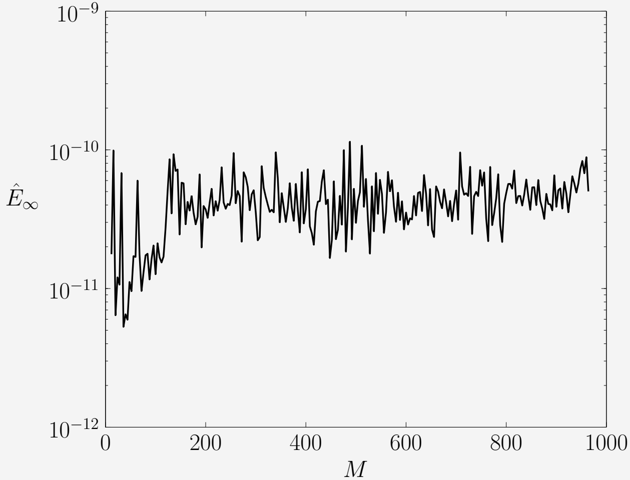
fast NFSFT algorithm $\quad ? \rightarrow ? \quad$ fast adjoint NFSF algorithm

$\downarrow$ $\qquad\qquad\qquad\qquad$ $\uparrow$

factorization of $\mathbf{Y}$ $\quad \rightarrow \quad$ factorisation of $\mathbf{Y}^{\mathrm{H}}$

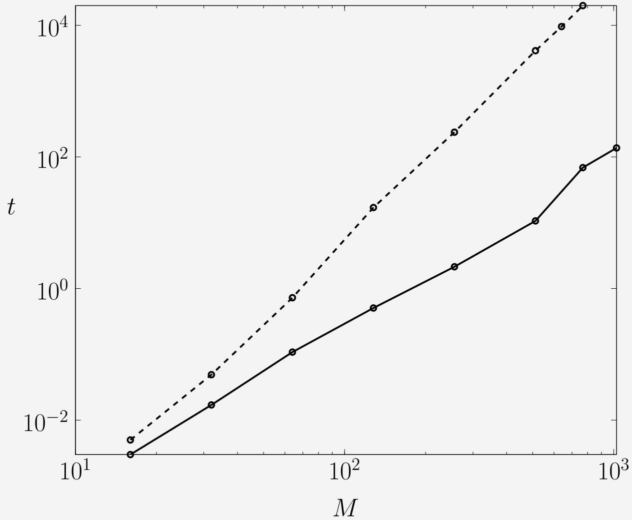
Accuracy of the NFSFT





The error $\hat{E}_\infty$ for the Gauß-Legendre (left) and the Clenshaw-Curtis quadrature (right) as a function of the bandwidth N.

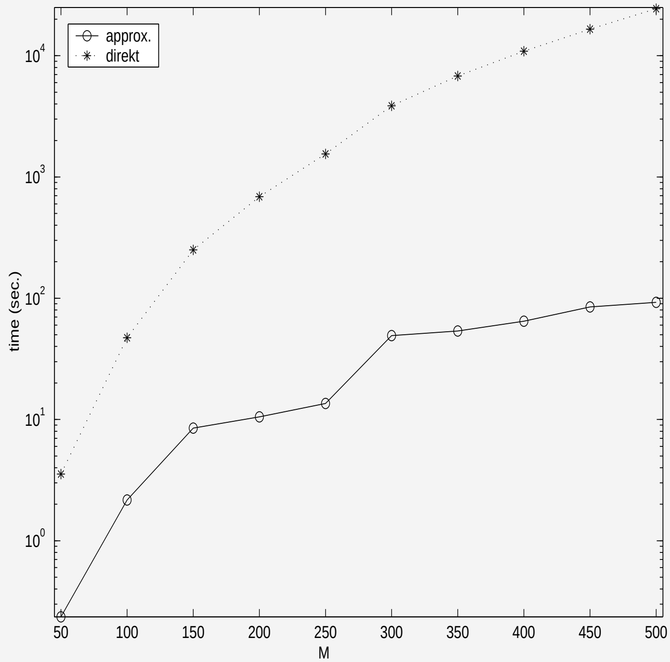
Performance of the NFSFT



The time t in seconds for NDSFT transforms using the direct NDSFT algorithm (dashed), and the NFSFT algorithm (solid) as a function of the bandwidth N for $M = N^2$ nodes.

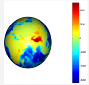
Numerical example:

Computational time for various bandwidth $M = 50, \ldots, 500$

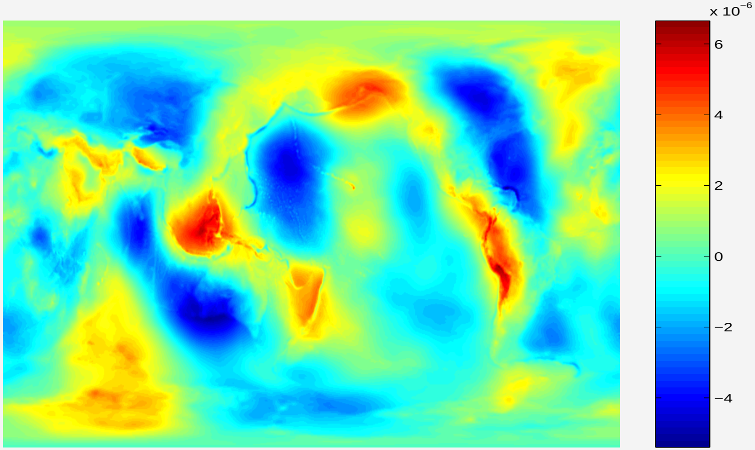


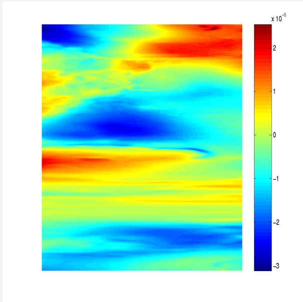
number of points $D = M^2$, $\alpha = 2, m = 4$

Gravitation field 1996 (EGM96)



spherical harmonics, M=360.





EGM96

EGM96 sector

DPT (discrete polynomial transform)

DPT$(N+1, M+1) : \mathbb{R}^{N+1} \to \mathbb{R}^{M+1}$

$$\hat{a}_j := \sum_{k=0}^{N} a_k P_k(c_j^M) \quad (j = 0, \ldots, M)$$

- Applications:

– numerical solution of differential– and integral equations

– polynomial wavelets

– Fourier transforms on S

- Fast polynomial transform for $P_k = T_k$

$$
\begin{aligned}
T_0(x) &:= 1\,, \quad T_1(x) := x\,, \\
T_n(x) &= 2x\,T_{n-1}(x) - T_{n-2}(x) \quad (n = 2, 3, \ldots)\,.
\end{aligned}
$$

with DCT in $\mathcal{O}(N \log N)$ flops

$$
\begin{aligned}
P\,(c_j^N) &= \sum_{k=0}^{N} a_k\, T_k(c_j^N) \\
&= \sum_{k=0}^{N} a_k\, \cos(\frac{jk\pi}{N})
\end{aligned}
$$

Chebyshev nodes

$$
c_j^N := \cos\frac{j\pi}{N} \qquad (j = 0, \ldots, N)\,.
$$

• Let $P \in \Pi_n$ $(n \in \mathbb{N})$ be given w.r.t. the basis of Chebyshev polynomials, i.e.

$$P \;=\; \sum_{k=0}^{n} a_k\, T_k \;.$$

• Further, let $Q \in \Pi_m$ $(m \in \mathbb{N})$ be a fixed polynomial with known values $Q(c_{2j+1}^{2M})$ for $j = 0, \ldots, M-1$, where $M = 2^s$ $(s \in \mathbb{N})$ with $M/2 \le m+n < M$ is chosen.

• Then compute b_k in

$$R \;:=\; P\,Q \;=\; \sum_{k=0}^{n+m} b_k\, T_k$$

by the following procedure:

Fast polynomial multiplication

Input: $M = 2^s$ $(s \in \mathbb{N})$ with $M/2 \le m + n < M$,
$Q(c_{2j+1}^{2M}) \in \mathbb{R}$ $(j = 0, \ldots, M-1)$ with $Q \in \Pi_m$,
$a_k \in \mathbb{R}$ $(k = 0, \ldots, n)$.

1. Compute

$$(P(c_{2j+1}^{2M}))_{j=0}^{M-1} \;:=\; \tilde{\boldsymbol{C}}_M^{\mathsf{T}}\,(a_k)_{k=0}^{M-1}$$

by fast DCT–III (M) of $(a_k)_{k=0}^{M-1}$ with $a_k := 0$ $(k = n+1, \ldots, M-1)$.

2. Evaluate the M products

$$R(c_{2j+1}^{2M}) \;:=\; P(c_{2j+1}^{2M})\,Q(c_{2j+1}^{2M}) \quad (j = 0, \ldots, M-1)\,.$$

3. Compute

$$(b_k)_{k=0}^{M-1} \;:=\; \frac{2}{M}\,\tilde{\boldsymbol{D}}_M\,\tilde{\boldsymbol{C}}_M\,(R(c_{2j+1}^{2M}))_{j=0}^{M-1}$$

by fast DCT–II (M) of $(R(c_{2j+1}^{2M}))_{j=0}^{M-1}$.
Output: b_k $(k = 0, \ldots, m+n)$.

- three–term recurrence relation

$$
\begin{aligned}
P_{-1}(x) &:= 0\,, \quad P_0(x) := 1\,, \\
P_{c+1}(x) &= (\alpha_{c+1}x + \beta_{c+1})\,P_c(x) + \gamma_{c+1}P_{c-1}(x) \\
& \quad (c = 0, 1, \ldots)
\end{aligned}
$$

- generalization

$$
\begin{aligned}
P_{c+n}(x) &= P_n(x,c)\,P_c(x) \\
&+ \gamma_{c+1}P_{n-1}(x,c+1)P_{c-1}(x)
\end{aligned}
$$

- associated polynomials of $P_n(x)$

$$
\begin{aligned}
P_{-1}(x,c) &:= 0\,, \quad P_0(x,c) := 1\,, \\
P_n(x,c) &:= (\alpha_{n+c}x + \beta_{n+c})\,P_{n-1}(x,c) \\
&+ \gamma_{n+c}P_{n-2}(x,c) \quad (n = 1, 2, \ldots)
\end{aligned}
$$

- Fast DPT

$$P \;:=\; \sum_{k=0}^{N} a_k \, P_k \;\in \Pi_N$$

with $a_k \in \mathbb{R}$ given.

- Idea: basis exchange

$$P \;=\; \sum_{k=0}^{N} \tilde{a}_k \, T_k$$

- Compute $\tilde{a}_k \quad (k = 0, \ldots, N)$ in $\mathcal{O}(N(\log N)^2)$ flops.

1. step:

$$P = \sum_{k=0}^{N-1} a_k^{(0)} P_k = \sum_{k=0}^{N/4-1} \left(\sum_{l=0}^{3} a_{4k+l}^{(0)} P_{4k+l} \right)$$

with

$$\begin{aligned} a_k^{(0)}(x) &:= a_k \quad (k = 0, \ldots, N-3), \\ a_{N-2}^{(0)}(x) &:= a_{N-2} + \gamma_{N-1} a_N , \\ a_{N-1}^{(0)}(x) &:= a_{N-1} + \beta_{N-1} a_N + \alpha_{N-1} a_N T_1(x) \end{aligned}$$

2. step:

$$P = \sum_{k=0}^{N/4-1} \left(a_{4k}^{(1)} P_{4k} + a_{4k+1}^{(1)} P_{4k+1} \right)$$

with

$$\begin{pmatrix} a_{4k}^{(1)} \\ a_{4k+1}^{(1)} \end{pmatrix} := \begin{pmatrix} a_{4k}^{(0)} \\ a_{4k+1}^{(0)} \end{pmatrix} + \boldsymbol{U}_1(\,\cdot\,, 4k+1) \begin{pmatrix} a_{4k+2}^{(0)} \\ a_{4k+3}^{(0)} \end{pmatrix},$$

and

$$\boldsymbol{U}_n(x,c) := \begin{pmatrix} \gamma_{c+1} P_{n-1}(x, c+1) & \gamma_{c+1} P_n(x, c+1) \\ P_n(x,c) & P_{n+1}(x,c) \end{pmatrix}$$

Note
$a_{4k}^{(1)}, a_{4k+1}^{(1)} \in \Pi_3 \; (k = 0, \ldots, N/4-1)$

Numerical Example

- ultraspherical polynomials P_n^λ $(\lambda > -1/2)$ given by:

$$\begin{aligned} P_{-1}^\lambda(x) &:= 0\,, \quad P_0^\lambda(x) := 1\,, \\ P_n^\lambda(x) &:= \frac{2(n+\lambda-1)}{n} x P_{n-1}^\lambda(x) \\ &- \frac{n+2\lambda-2}{n} P_{n-2}^\lambda(x) \end{aligned}$$

- Compute for $a_k \in [-0.5, 0.5]$

$$\hat{a}_j = \sum_{k=0}^{N} a_k \, P_k^\lambda(c_j^N) \quad (j = 0, \ldots, N)$$

Numerical Example

N	λ	t(CA)	t(FPT)	$\tilde{\varepsilon}$(FPT)
128	0.5	0.05	0.04	$3.59E-14$
256	0.5	0.21	0.07	$4.35E-12$
512	0.5	0.82	0.19	$4.93E-12$
1024	0.5	3.27	0.39	$5.78E-11$
2048	0.5	13.70	0.85	$2.09E-10$
4096	0.5	55.41	1.92	$1.04E-09$
8192	0.5	220.05	4.26	$5.04E-08$
4096	2.5	55.43	1.91	$1.72E-09$
4096	4.0	55.42	1.91	$6.41E-10$
4096	5.0	55.42	1.92	$3.35E-10$

Fast summation algorithms on the sphere

$\sum$

Problem: fast computation of

$$f(\boldsymbol{\xi}_{d_2}) := \sum_{d_1=1}^{D_1} \alpha_{d_1} \mathcal{K}(\boldsymbol{\xi}_{d_2} \cdot \boldsymbol{\eta}_{d_1}) \qquad (d_2 = 1, \ldots, D_2)$$

knots $\boldsymbol{\xi}_{d_2}, \boldsymbol{\eta}_{d_1} \in \mathbb{S}^2$, $\mathcal{K}$ spherical radial basis functions

$$\boldsymbol{f} = \boldsymbol{K}\boldsymbol{\alpha}$$

$\mathcal{K}$ special kernels, e.g.

Gauss Kernel: $\mathcal{K}(t) = \mathcal{K}(\sigma, t) = \mathrm{e}^{-2\sigma(t-1)}$

Abel-Poisson Kernel: $\mathcal{K}(t) = \mathcal{K}(h, t) = \dfrac{1}{4\pi} \dfrac{1 - h^2}{(1 + h^2 - 2rt)^{3/2}}$

Applications: geophysics, tomography, crystallography

known methods for
products of vectors with specially structured dense matrices

$$\boldsymbol{f} = \boldsymbol{K}\boldsymbol{\alpha}$$

panel clustering, fast multipole method

W. Freeden, O. Glockner, M. Schreiner; Spherical panel clustering,
J. Geodesy 72, (1998).

Fourier method

approximate $\mathcal{K}$

$$\mathcal{K}(t) = \sum_{k=0}^{\infty} b_k P_k(t) \qquad \text{by} \qquad \mathcal{K}_M(t) := \sum_{k=0}^{M} b_k P_k(t)$$

choose M such that

$$|\mathcal{K}_M - \mathcal{K}| \leq \sum_{k=M+1}^{\infty} |b_k| < \varepsilon$$

approximate f by f_M at D_2 different knots $\boldsymbol{\xi} = \boldsymbol{\xi}_{d_2} \in \mathbb{S}^2$

$\sum$

$$f(\boldsymbol{\xi}) := \sum_{d_1=1}^{D_1} \alpha_{d_1} \mathcal{K}(\boldsymbol{\xi} \cdot \boldsymbol{\eta}_{d_1}); \qquad f_M(\boldsymbol{\xi}) := \sum_{d_1=1}^{D_1} \alpha_{d_1} \mathcal{K}_M(\boldsymbol{\xi} \cdot \boldsymbol{\eta}_{d_1})$$

$$\begin{aligned} f_M(\boldsymbol{\xi}_{d_2}) &= \sum_{d_1=1}^{D_1} \alpha_k \sum_{k=0}^{M} b_k P_k(\boldsymbol{\xi}_{d_2} \cdot \boldsymbol{\eta}_{d_1}) \qquad (d_2 = 0, \ldots, D_2 - 1) \\ &= \sum_{d_1=1}^{D_1} \alpha_k \sum_{k=0}^{M} b_k \sum_{n=-k}^{k} Y_k^n(\boldsymbol{\xi}_{d_2}) \overline{Y_k^n(\boldsymbol{\eta}_{d_1})} \\ &= \underbrace{\sum_{k=0}^{M} \sum_{n=-k}^{k} b_k \underbrace{\left(\sum_{d_1=1}^{D_1} \alpha_{d_1} \overline{Y_k^n(\boldsymbol{\eta}_{d_1})} \right)}_{\text{NFSFT}^H} Y_k^n(\boldsymbol{\xi}_{d_2})}_{\text{NFSFT}} \end{aligned}$$

Complexity: $\mathcal{O}(M^2 \log^2 M + D_1 + D_2)$

Fast summation scheme

error estimate

$$\begin{aligned} \|f - f_M\|_\infty &\leq \|\boldsymbol{\alpha}\|_1 \, \|(K - K_M)(\cdot\, \boldsymbol{\eta})\|_\infty \\ &\leq \|\boldsymbol{\alpha}\|_1 \sum_{k>M} \frac{2k+1}{4\pi} \left|K^\wedge(k)\right| \end{aligned}$$

where

$$K^\wedge(k) = 2\pi \int_{-1}^{1} K(x)\, P_k(x)\, \mathrm{d}x$$

typically

$$M \approx \frac{\log \varepsilon}{\log h}$$

Fast summation scheme, examples

1. Gauss kernel, $\sigma \in \mathbb{R}_+$,

$$K_\sigma(x) = \mathrm{e}^{2\sigma(x-1)}$$

has symbol $K_\sigma^\wedge(k) = \frac{1}{2\pi}\int_{-1}^{1} \mathrm{e}^{2\sigma(x-1)} P_k(x) \, \mathrm{d}x = 2\sigma^{-\frac{1}{2}} \mathrm{e}^{-2\sigma} \pi^{\frac{3}{2}} I_{k+\frac{1}{2}}(2\sigma)$ and yields

$$\frac{\|f - f_M\|_\infty}{\|\boldsymbol{\alpha}\|_1} \leq \frac{\sqrt{\pi\sigma}\,(\mathrm{e}^\sigma - 1)\,\sigma^{M-\frac{1}{2}}}{\Gamma\left(M + \frac{1}{2}\right)}$$

2. Abel-Poisson kernel, $h \in (0,1)$,

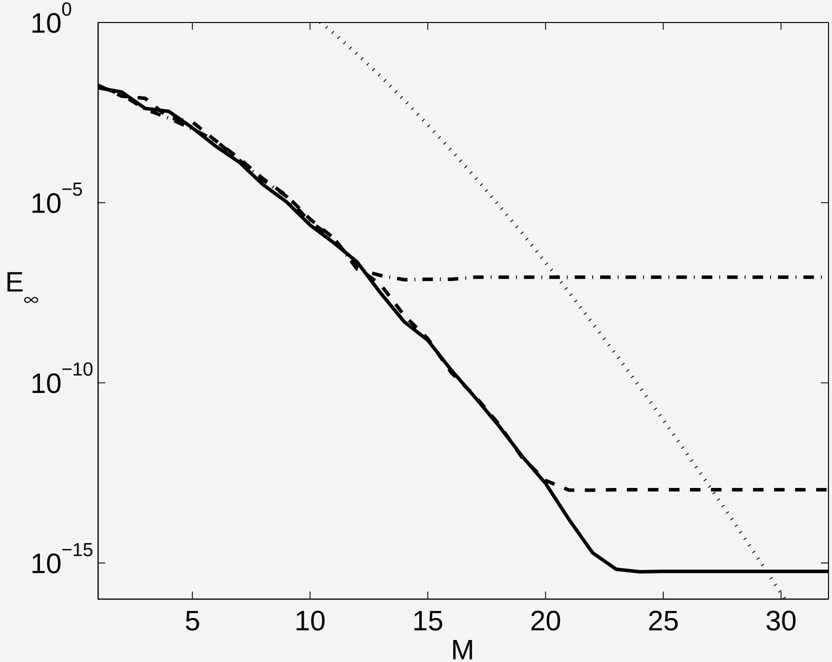
$$Q_h(x) = \frac{1}{4\pi} \frac{1 - h^2}{(1 + h^2 - 2hx)^{3/2}}$$

has symbol $Q_h^\wedge(k) = h^k$ and yields

$$\frac{\|f - f_M\|_\infty}{\|\boldsymbol{\alpha}\|_1} \leq \frac{h^{M+1}}{4\pi} \left(\frac{2M+1}{1-h} + \frac{2}{(1-h)^2} \right),$$

Fast spherical Gauss transform

$L = M = 1000$ pseudo random nodes and coefficients, $\sigma = 5$



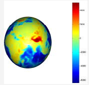
NDSFT (solid), NFSFT, $m = 3$ (dash-dot),
NFSFT, $m = 6$ (dashed), Error estimate (dotted)

Computation time

$L = D$	direct alg.	w/pre-comp.	FS, NFSFT	error E_∞
2^6	0.00001 s	0.00008 s	0.62 s	$7.7 \cdot 10^{-14}$
2^8	0.00025 s	0.0014 s	0.62 s	$4.1 \cdot 10^{-14}$
2^{10}	0.04 s	0.021 s	0.65 s	$3.6 \cdot 10^{-14}$
2^{12}	6.4 s	0.35 s	0.72 s	$1.3 \cdot 10^{-14}$
2^{14}	1.6 min	*5.6 s	1.0 s	$5.5 \cdot 10^{-15}$
2^{16}	27.6 min	*1.5 min	2.3 s	$2.9 \cdot 10^{-15}$
2^{18}	7.2 h	*23.3 min	7.5 s	$1.9 \cdot 10^{-15}$
2^{20}	*4.8 d	*6.4 h	28 s	—
2^{21}	*19.7 d	*1.0 d	55 s	—

* = estimated

Spherical Filter and Wavelet Decomposition



Jakob-Chien and Alpert 97 [18], N. Yarvin and V. Rokhlin 98 [45]

$$f_N(\theta,\phi) = \sum_{k=0}^{N-1} \sum_{n=-k}^{k} a_k^n \, Y_k^n(\theta,\phi) \qquad (a_k^n \in \mathbb{C}).$$

$$f_{N/2}(\theta,\phi) = \sum_{k=0}^{N/2-1} \sum_{n=-k}^{k} a_k^n \, Y_k^n(\theta,\phi).$$

$$g_{N/2}(\theta,\phi) = \sum_{k=N/2}^{N-1} \sum_{n=-k}^{k} a_k^n \, Y_k^n(\theta,\phi).$$

Problem:

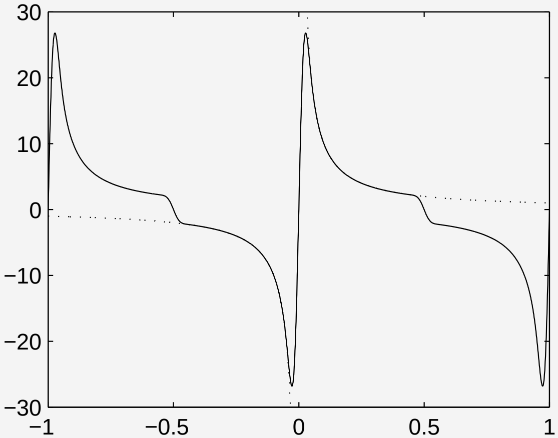
given $f_N(\theta_s,\varphi_t)$ ($s = 0,\ldots,N-1$, $t = 0,\ldots,N-1$)
with $\theta_s := \mathrm{arccos}(x_s)$ (x_s – Gauss Legendre nodes), $\varphi_t := \frac{t\pi}{N}$
compute $f_{N/2}(\theta_s,\varphi_t)$ and $g_{N/2}(\theta_s,\varphi_t)$

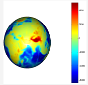
Idea: • compute a_k^n by quadrature rules
• apply Christoffel–Darboux formula

Compute sums of the form

$$\hat{f}_\sigma = \sum_{k=0}^{N-1} \frac{f_k}{x_k - x_\sigma} \quad (\sigma = 0, \ldots, N-1)$$

by a fast summation algorithm with the kernel $1/x$.





$$a_k^n = \langle f, Y_k^n \rangle \; = \; \frac{1}{2\pi} \int_0^\pi \int_0^{2\pi} f(\theta,\phi)\; P_k^{|n|}(\cos\theta) \mathrm{e}^{-\mathrm{i}n\phi} \sin\theta \; \mathrm{d}\phi \; \mathrm{d}\theta$$

$$\tilde{a}_k^n := \sum_{s=0}^{M} \sum_{t=0}^{M_s-1} \omega_{t,s} f(\theta_s, \phi_{t,s}) Y_k^{-n}(\theta_s, \phi_{t,s})$$

$$\tilde{f}^N(\tilde{\theta}, \tilde{\phi}) = \sum_{k=0}^{N} \sum_{n=-k}^{k} \tilde{a}_k^n \, Y_k^n(\tilde{\theta}, \tilde{\phi})$$

Theorem (Christoffel–Darboux formula):
The sum

$$S_N^n(x,y) := \sum_{k=n}^{N} P_k^n(x)\; P_k^n(y) \tag{66}$$

possesses the closed form

$$S(x,y) = \begin{cases} \frac{\alpha_N^n \left(P_N^n(x)P_{N-1}^n(y) - P_{N-1}^n(x)P_N^n(y)\right)}{x-y} & \text{if} x \neq y \\ \alpha_N^n \left(P_N^{n\prime}(x)P_{N-1}^n(x) - P_{N-1}^{n\prime}(x)P_N^n(x)\right) & \text{if} x = y, \end{cases}$$

where the α_k^n are the constants from the three-term recurrence

$$xP_k^n = \alpha_k^n P_{k-1}^n + \alpha_{k+1}^n P_{k+1}^n$$

with

$$\alpha_k^n := \left(\frac{(k-n)(k+n)}{(2k-1)(2k+1)}\right)^{\frac{1}{2}}$$

for $k \geq n$ and $\alpha_k^n := 0$ otherwise.

Proof:

We first examine the case where $x \neq y$. Applying the three-term recurrence to equation (66) yields

$$xS(x,y) = \sum_{k=n}^{N-1} \left(\alpha_k^n P_{k-1}^n(x) + \alpha_{k+1}^n P_{k+1}^n(x)\right) P_k^n(y)$$

and

$$yS(x,y) = \sum_{k=n}^{N-1} P_k^n(x) \left(\alpha_k^n P_{k-1}^n(y) + \alpha_{k+1}^n P_{k+1}^n(y)\right).$$

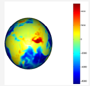
Taking the difference of these two equations yields

$$
\begin{aligned}
(x-y)S(x,y) &= \sum_{k=n}^{N-1} \quad \alpha_k^n P_{k-1}^n(x)P_k^n(y) + \alpha_{k+1}^n P_{k+1}^n(x)P_k^n(y) \\
&\quad - \quad\quad \alpha_k^n P_k^n(x)P_{k-1}^n(y) - \alpha_{k+1}^n P_k^n(x)P_{k+1}^n(y) \\
&= \sum_{k=n}^{N-1} \quad \alpha_k^n P_{k-1}^n(x)P_k^n(y) - \alpha_k^n P_k^n(x)P_{k-1}^n(y) \\
&\quad + \sum_{k=n}^{N-1} \quad \alpha_{k+1}^n P_{k+1}^n(x)P_k^n(y) - \alpha_{k+1}^n P_k^n(x)P_{k+1}^n(y) \\
&= \sum_{k=n}^{N-1} \quad \alpha_k^n P_{k-1}^n(x)P_k^n(y) - \alpha_k^n P_k^n(x)P_{k-1}^n(y) \\
&\quad + \sum_{k=n+1}^{N} \quad \alpha_k^n P_k^n(x)P_{k-1}^n(y) - \alpha_k^n P_{k-1}^n(x)P_k^n(y) \\
&= \underbrace{\alpha_n^n P_{n-1}^n(x)P_n^n(y) - \alpha_n^n P_n^n(X)P_{n-1}^n(y)}_{=0 \text{ because } P_k^n \equiv 0 \text{ for } k<n} \\
&\quad + \alpha_N^n P_N^n(x)P_{N-1}^n(y) - \alpha_N^n P_{N-1}^n(x)P_N^n(y) \\
&= \alpha_N^n \left(P_N^n(x)P_{N-1}^n(y) - P_{N-1}^n(x)P_N^n(y)\right).
\end{aligned}
$$

Dividing by $x-y$ yields the proposition.

We now turn to the case $x = y$. Using l'Hôpital's rule, we obtain

$$\begin{aligned}
\lim_{y \to x} S(x, y) &= \lim_{y \to x} \frac{\alpha_N^n \left(P_N^n(x) P_{N-1}^n(y) - P_{N-1}^n(x) P_N^n(y)\right)}{x - y} \\
&= \lim_{y \to x} \frac{\alpha_N^n \left(P_N^n(x) {P_{N-1}^n}'(y) - P_{N-1}^n(x) {P_N^n}'(y)\right)}{-1} \\
&= \alpha_N^n \left(P_{N-1}^n(x) {P_N^n}'(x) - P_N^n(x) {P_{N-1}^n}'(x)\right). \qquad \blacksquare
\end{aligned}$$



$$
\begin{aligned}
&\tilde{f}^N(\tilde{\theta},\tilde{\phi}) \\
=\;& \sum_{n=-N}^{N}\sum_{k=|n|}^{N} \tilde{a}_k^n\, Y_k^n(\tilde{\theta},\tilde{\phi}) \\
=\;& \sum_{n=-N}^{N}\sum_{k=|n|}^{N}\sum_{s=0}^{M}\sum_{t=0}^{M_s-1} \omega_{t,s} f(\theta_s,\phi_{t,s}) P_k^{|n|}(\cos\theta_s)\,\mathrm{e}^{-\mathrm{i}n\phi_{t,s}} P_k^{|n|}(\cos\tilde{\theta})\,\mathrm{e}^{\mathrm{i}n\tilde{\phi}} \\
=\;& \underbrace{\sum_{n=-N}^{N}\left(\sum_{s=0}^{M}\underbrace{\left(\underbrace{\left(\sum_{t=0}^{M_s-1}\omega_{t,s} f(\theta_s,\phi_{t,s})\,\mathrm{e}^{-\mathrm{i}n\phi_{t,s}}\right)}_{\text{NFFT}} S_N^n(\theta_s,\tilde{\theta})\right)}_{\sum}\right)\mathrm{e}^{\mathrm{i}n\tilde{\phi}}}_{\text{NFFT}}
\end{aligned}
$$

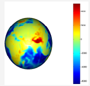
Lemma:(Böhme, P., 02 [4])

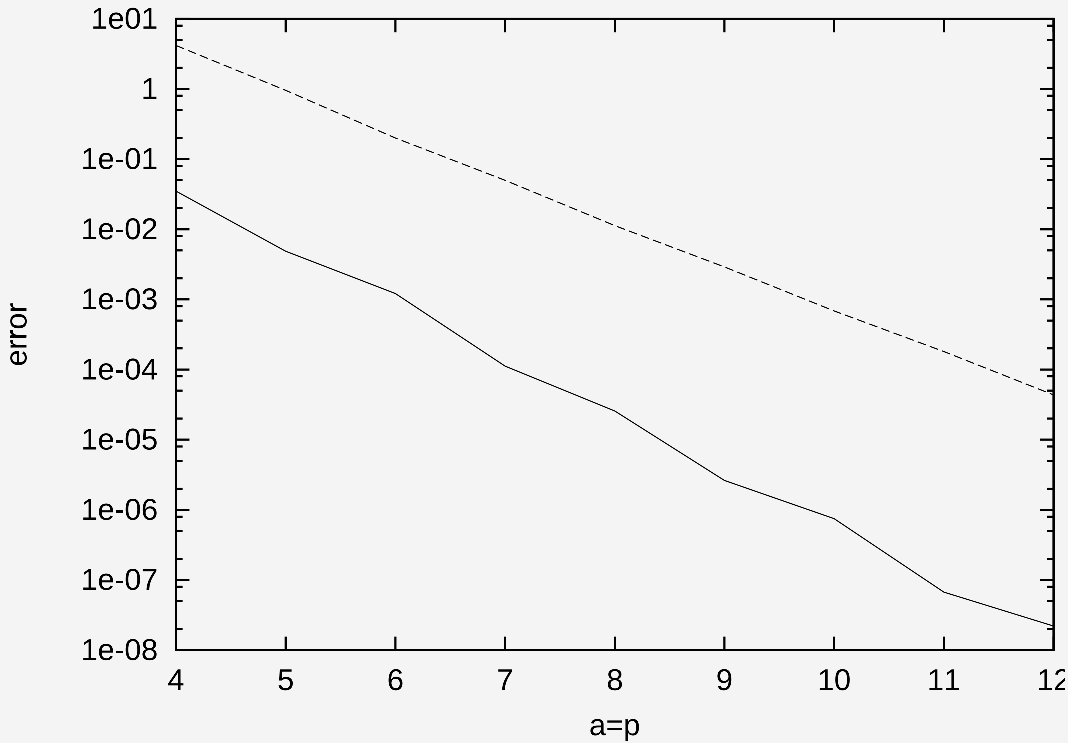
If the NFFT summation algorithm is used with
Legendre nodes x_k ($k = 1, \ldots, N$, with N an integer multiple of 4),
if $M = N$ and $y_k = x_k$ ($k = 1, \ldots, N$) and the parameters a and n satisfy

$$\frac{a}{n} < \frac{1}{\sqrt{2}},$$

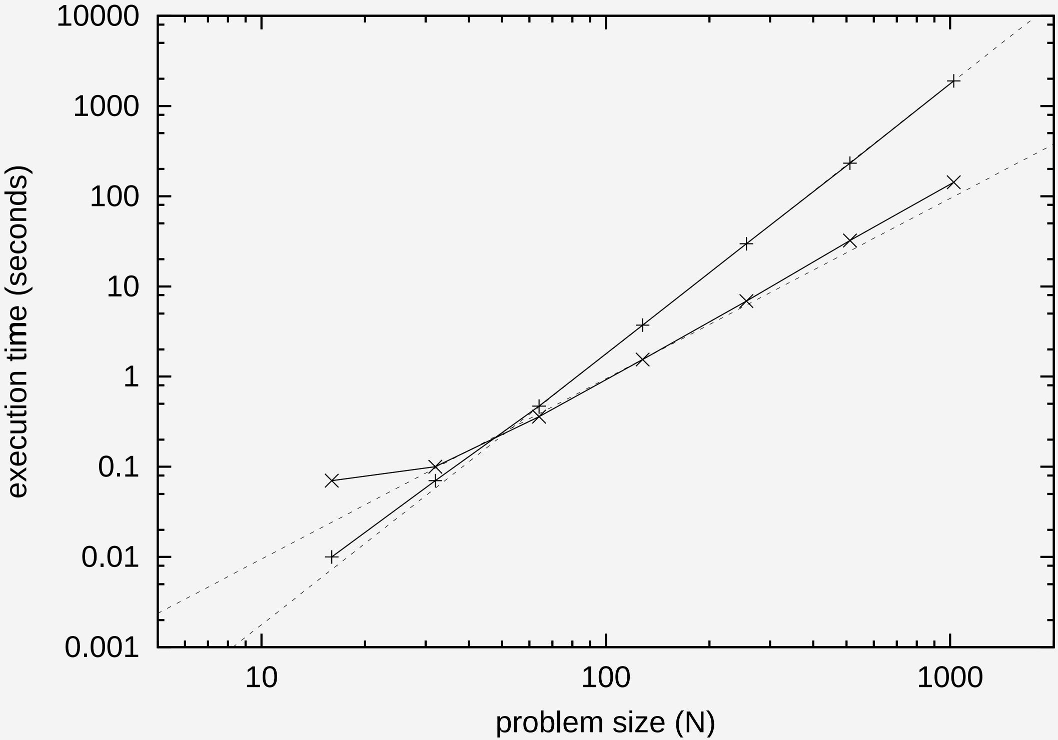
then the number of near-field evaluations required in the algorithm is not greater than

$$\frac{a(2N+1)^2}{n}\left(\frac{7}{24} + \frac{1}{2\pi}\ln\frac{4N+2}{3\pi}\right) \quad \sim \quad \mathcal{O}(aN\log N)\,.$$





Predicted maximum error (dashed) and actual maximum error (solid) for the NFFT summation algorithm (N=1024).

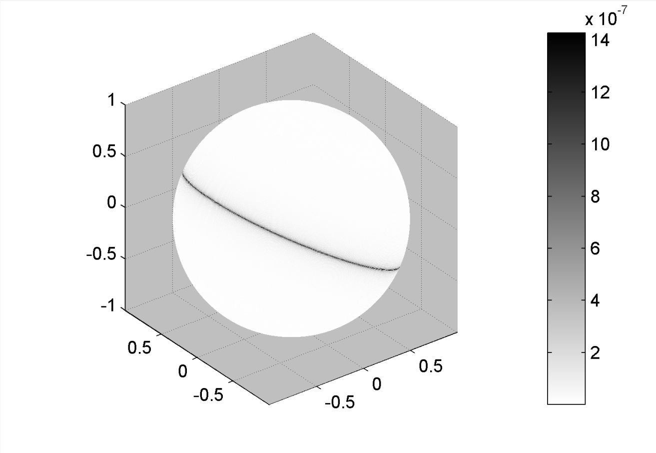


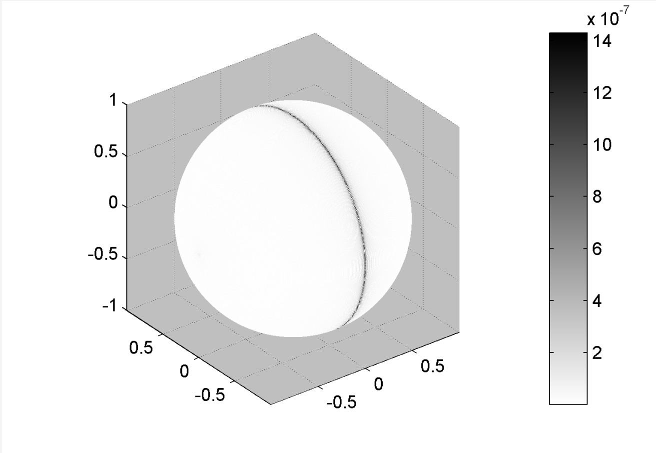
Execution times of the exact algorithm (plus signs) and the approximate algorithm (crosses). The dashed lines show time complexities of $\mathcal{O}(N^2)$ and $\mathcal{O}(N^3)$; they intercept the plots at $N = 128$.

Wavelet Decomposition on the Sphere

$$f_{\text{test}}(\theta, \phi) := \begin{cases} 1 & \text{if} \quad \theta \in [0, \pi/2] \\ (1 + 3\cos^2\theta)^{-1/2} & \text{if} \quad \theta \in (\pi/2, \pi] \end{cases}$$

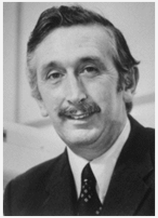
$$N = 1024,\ a = p = 10,\ m = 7$$

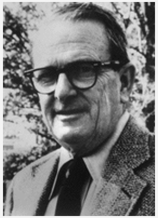




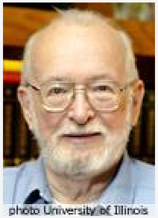
Nobelpreise für bildgebende Verfahren

W. C. Röntgen
Physik
Nobelpreis 1901



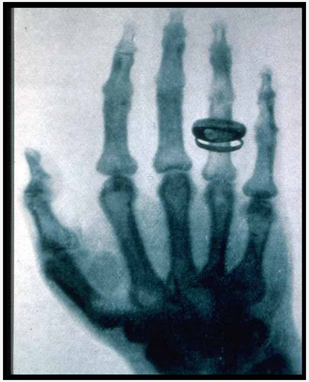


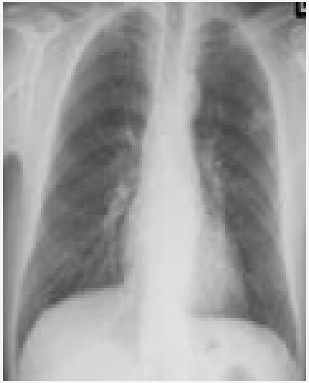
G.H. Hounsfield
A.M.Cormack
Medizin Nobelpreis 1979



P. C. Lauterbur P. Mansfield
Medizin Nobelpreis 2003

Wilhelm Conrad Röntgen (1845-1923) war der erste Nobelpreisträger für Physik.





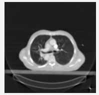
Hand, aufgenommen von Prof. Röntgen am 23. Januar 1896
Historisches Röntgengerät
Röntgenbild eines Oberkörpers

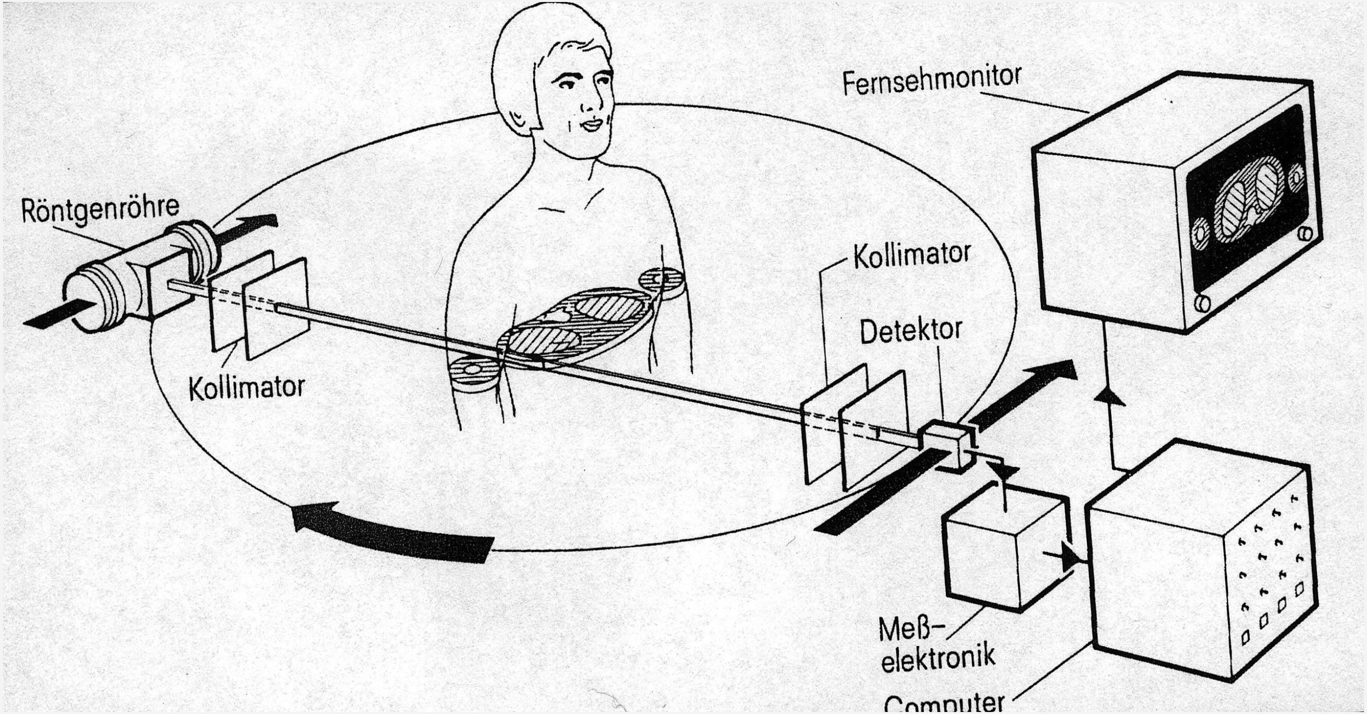
Röntgendiagnostik: Die unterschiedlich dichten Gewebe des menschlichen (oder tierischen) Körpers absorbieren die Röntgenstrahlen unterschiedlich stark, so dass man eine Abbildung des Körperinneren erreicht.
weitere Anwendungen: Materialprüfung, Qualitätssicherung, Archäologie, Röntgen-Strukturanalyse

Computertomographie

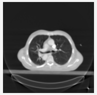
- Die Computertomographie basiert auf einem mathematischen Verfahren, das 1917 von dem Mathematiker **Johann Radon** entwickelt wurde.
- Die Radon–Transformation ermöglicht die zerstörungsfreie räumliche Aufnahme eines Objektes mit seinen gesamten Innenstrukturen.
- Nach Vorarbeiten des Physikers Allan M. Cormack in den 1960er Jahren realisierte der Elektrotechniker Godfrey Hounsfield mehrere Prototypen. Die erste CT-Aufnahme wurde 1971 an einem Menschen vorgenommen. Beide erhielten für ihre Arbeiten 1979 gemeinsam den Nobelpreis in Medizin.

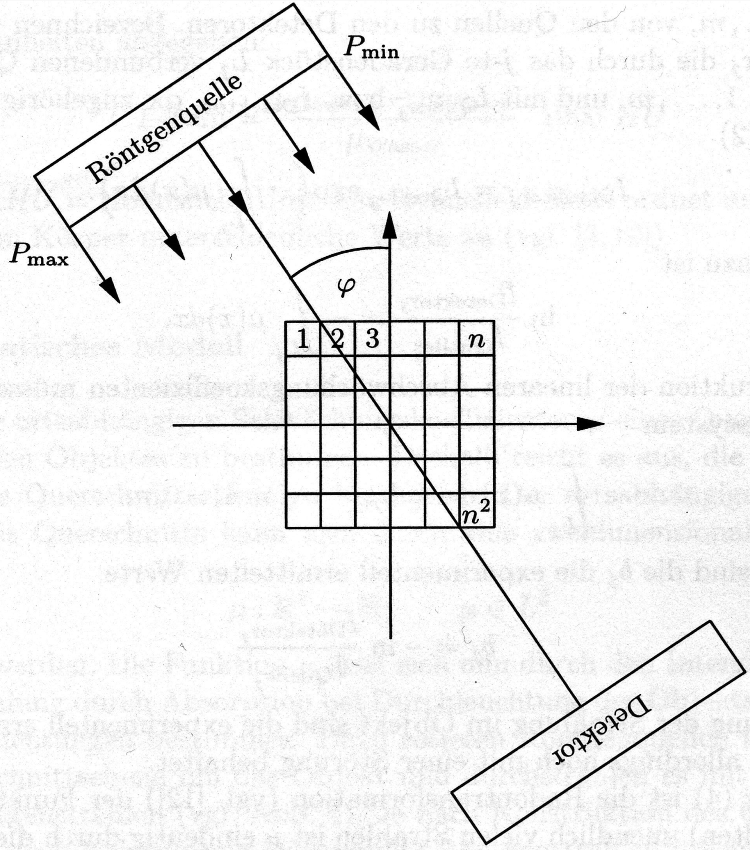
Meßanordnung eines einfachen Translations-Rotations-Scanners

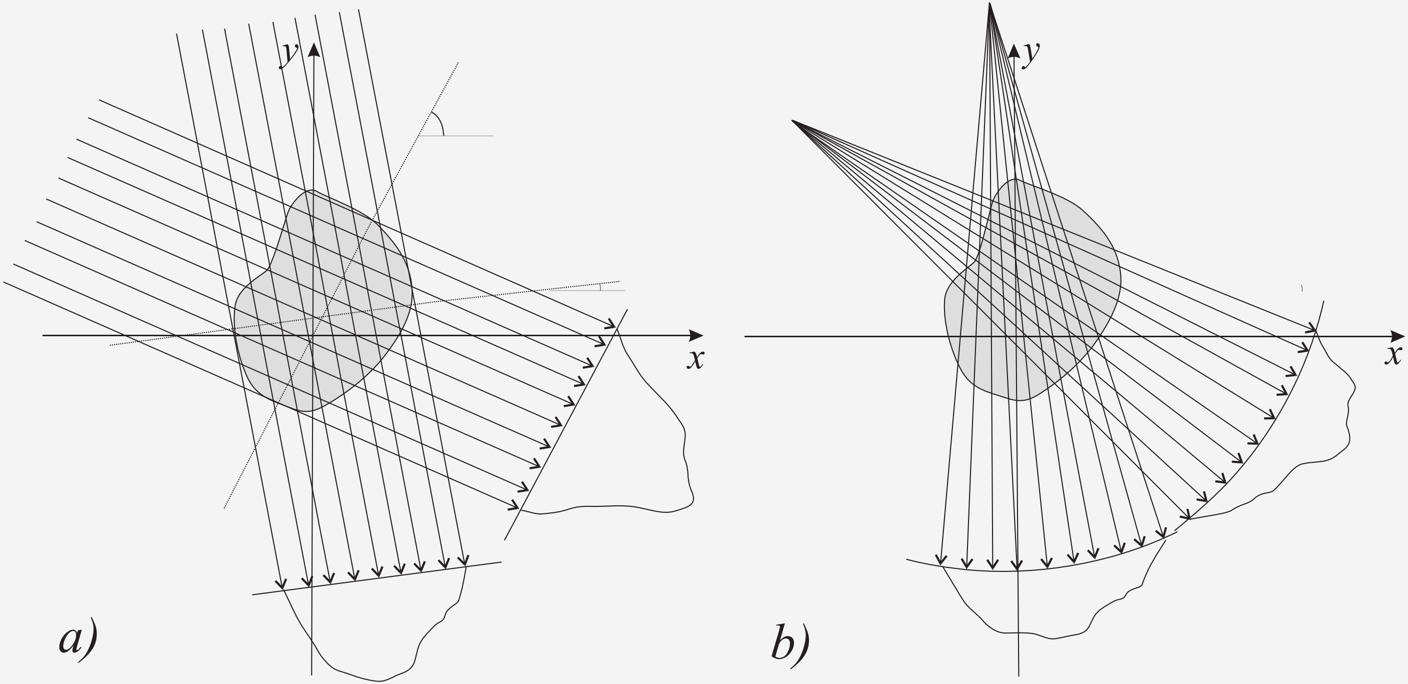


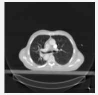


Idee der CT







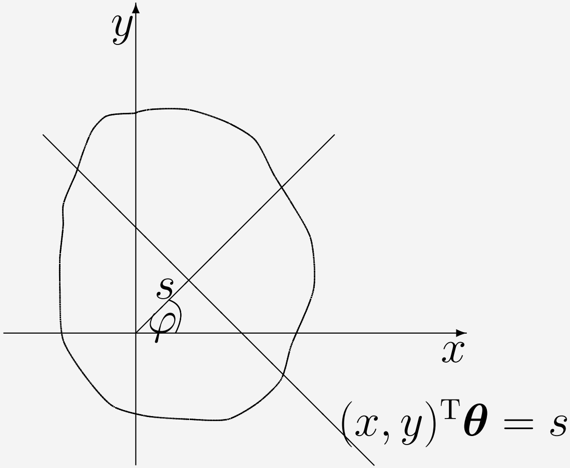


Parallel-Projektionen (links), Fächerstrahl-Projektionen (rechts).

Radon-Transformation

$$R : \mathcal{S}(\mathbb{R}^2) \to \mathcal{S}(\mathbb{R} \times \mathbb{T})$$

$$Rf(s,\varphi) := \int\limits_{\boldsymbol{x}\boldsymbol{\theta}=s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad \left(\boldsymbol{\theta} := \begin{pmatrix}\cos\varphi \\ \sin\varphi\end{pmatrix}\right)$$



Fourier-Projektionssatz

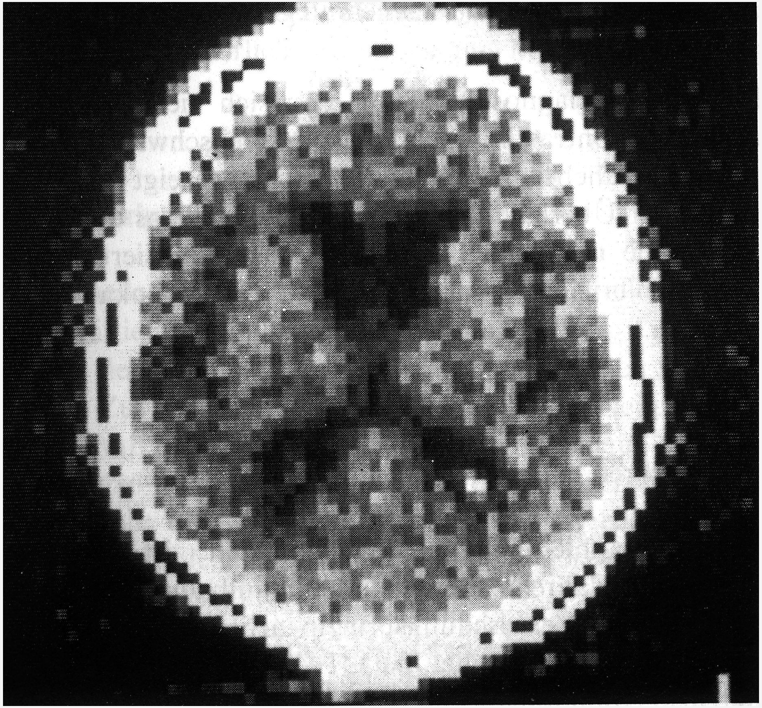
Fourier–Transformation von $f \in L_2(\mathbb{R}^n)$, $(n = 1, 2)$

$$\hat{f}(\boldsymbol{\xi}) := \int_{\mathbb{R}^n} f(\boldsymbol{x})\, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{x}\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{x}$$

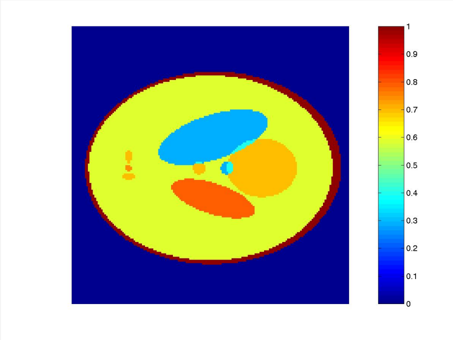
Satz:
Falls $f \in \mathcal{S}(\mathbb{R}^2)$, dann

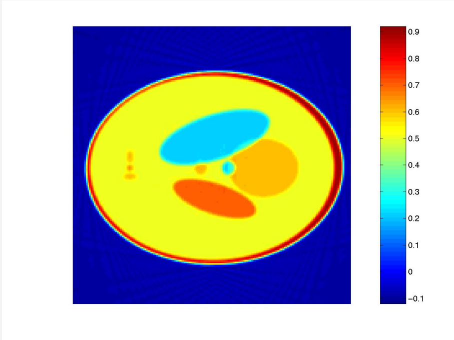
$$\hat{f}(\sigma\boldsymbol{\theta}) = \int_{\mathbb{R}} Rf(s,\varphi)\, \mathrm{e}^{-2\pi \mathrm{i} s\sigma}\, \mathrm{d}s = \widehat{Rf}(\sigma,\varphi) \quad \left(\boldsymbol{\theta} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix}\right).$$

Qualität der ersten CT-Aufnahmen, 1974

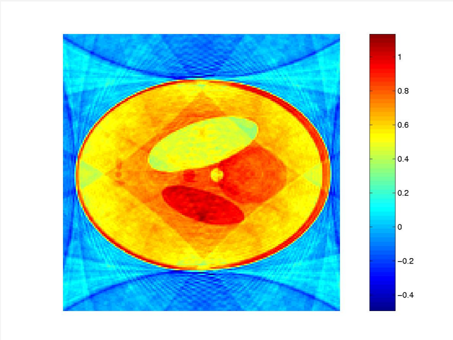


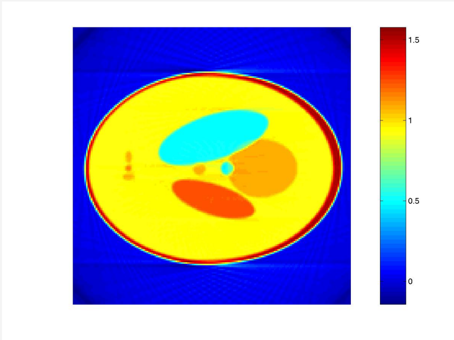
Numerische Beispiele





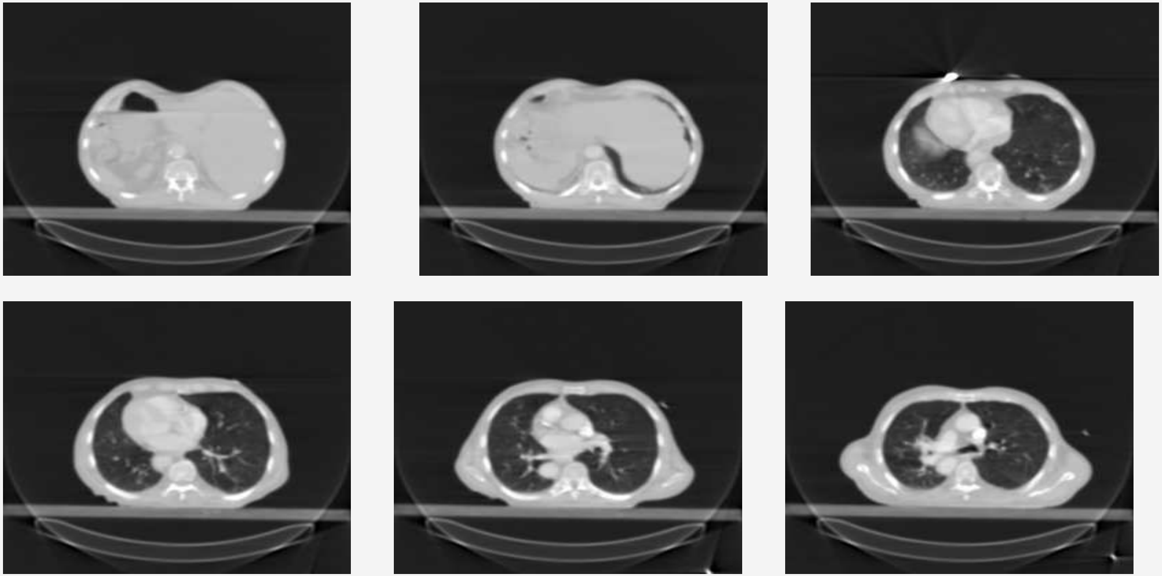
Shepp-Logan Phantom   Rekonstruktion mit FB (20 Sek.)



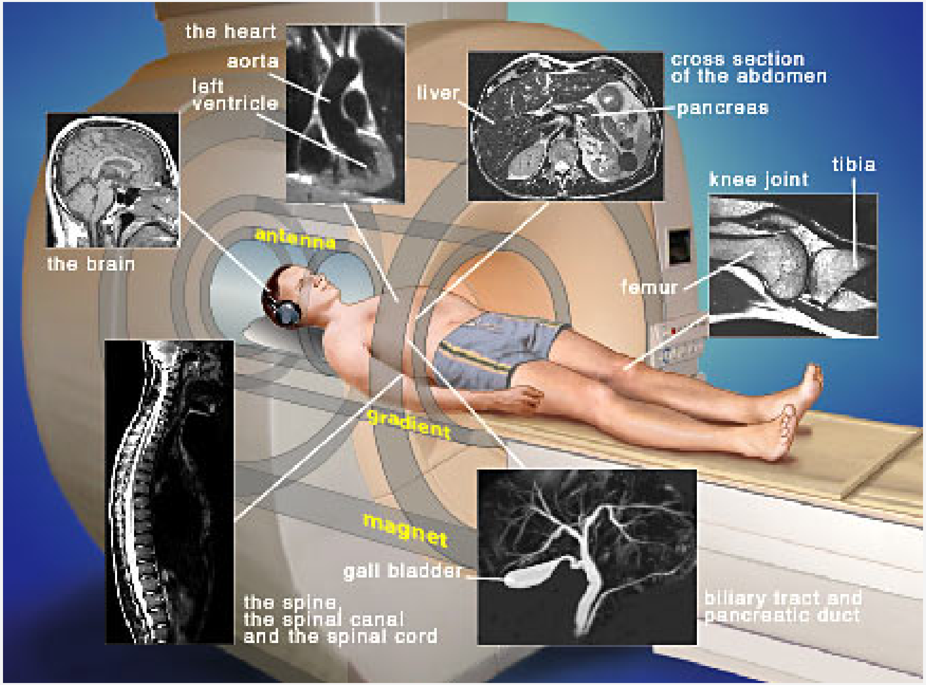


FFT–Rekonstruktion (2 Sek.)   NFFT-Rekonstruktion (3 Sek.)


SOMATOM Plus 4

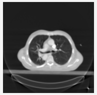


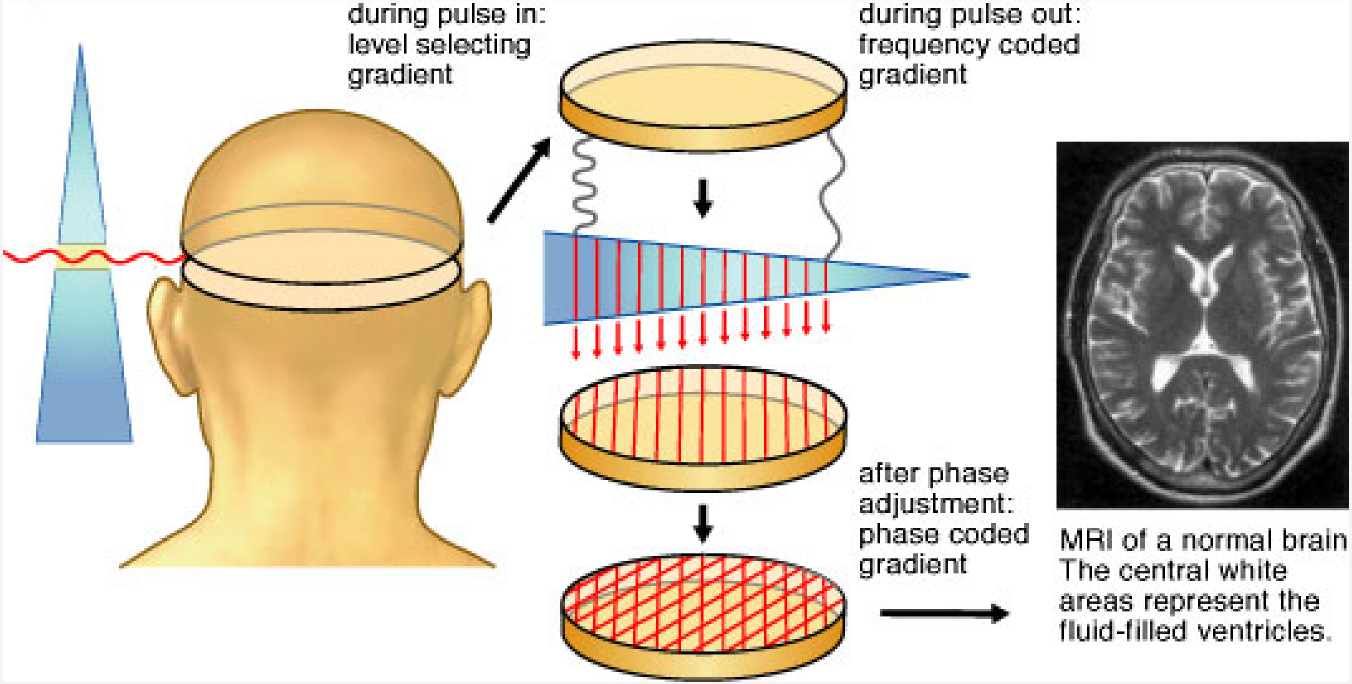
Magnetresonanztomographie



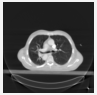
Magnetresonanztomographie

- Die physikalische Grundlage der Magnetresonanztomographie (MRT) bildet die Kernspinresonanz. Hier nutzt man die Tatsache, dass Protonen einen Eigendrehimpuls (Spin) besitzen und Atomkerne dadurch ein magnetisches Moment erhalten.
- Ein Atomkern kann als ein magnetischer Kreisel angesehen werden.




during pulse in:
level selecting
gradient
during pulse out:
frequency coded
gradient
after phase
adjustment:
phase coded
gradient
MRI of a normal brain
The central white
areas represent the
fluid-filled ventricles.

Magnetresonanztomographie, Modell



$$s\left(t\right) = \int_{\mathbb{R}^2} m\left(\boldsymbol{r}\right) \mathrm{e}^{\mathrm{i}\boldsymbol{k}(t)\boldsymbol{r}} \,\mathrm{d}\boldsymbol{r}$$

$$s_\kappa \approx \tilde{s}_\kappa := \sum_{\rho=0}^{N_1 N_2 - 1} m_\rho \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\kappa \boldsymbol{r}_\rho}$$

$$\boldsymbol{A} := \left(\mathrm{e}^{\mathrm{i}\boldsymbol{k}_\kappa \boldsymbol{r}_\rho}\right)_{\kappa=0;\ \rho=0}^{M-1;\ N_1 N_2 - 1}$$

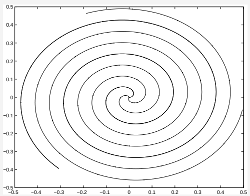
$$\boldsymbol{s} \approx \boldsymbol{A}\boldsymbol{m}$$

$$s\left(t\right) = \int_{\mathbb{R}^2} m\left(\boldsymbol{r}\right) \mathrm{e}^{\mathrm{i}\omega(\boldsymbol{r})t} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(t)\boldsymbol{r}} \,\mathrm{d}\boldsymbol{r}$$

$$s_\kappa \approx \tilde{s}_\kappa := \sum_{\rho=0}^{N_1 N_2 - 1} m_\rho \mathrm{e}^{\mathrm{i}\omega_\rho t_\kappa} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\kappa \boldsymbol{r}_\rho}$$

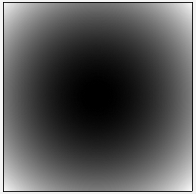
$$\boldsymbol{H} := \left(\mathrm{e}^{\mathrm{i}\omega_\rho t_\kappa} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\kappa \boldsymbol{r}_\rho}\right)_{\kappa=0\ ;\rho=0}^{M-1;\ N_1 N_2 - 1}$$

$$\boldsymbol{s} \approx \boldsymbol{H}\boldsymbol{m}$$



Beispiel 1

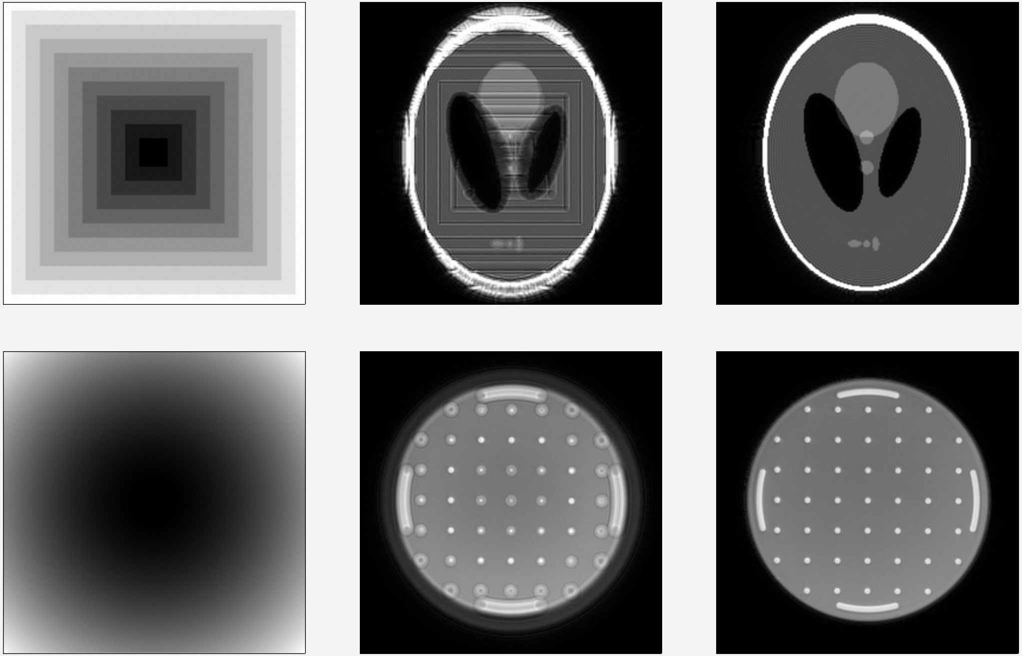
Beispiel 2



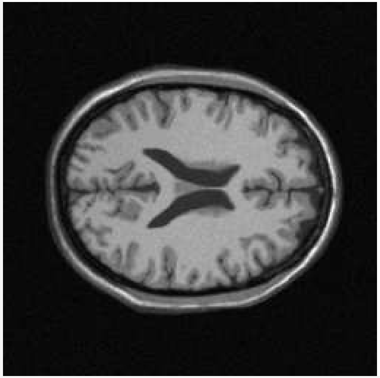
$$\mathrm{e}^{2\pi \mathrm{i} k x} \approx \frac{1}{\alpha N \hat{\varphi}(x)} \sum_{l=-\alpha N/2}^{\alpha N/2 - 1} \psi\left(k - \frac{l}{\alpha N}\right) \mathrm{e}^{2\pi \mathrm{i} \frac{l x}{\alpha N}},$$

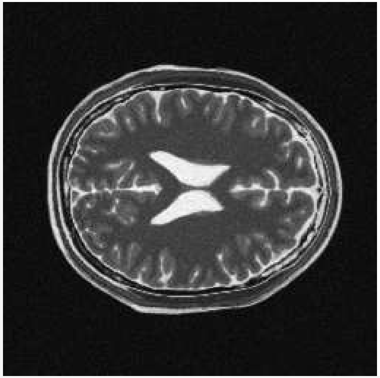
Magnetresonanztomographie, Ergebnisse

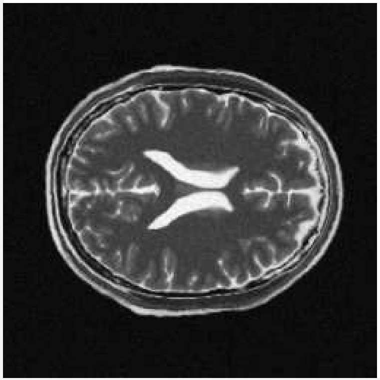
(H. Eggers, T. Knopp, P.)



weitere Anwendung: Bildregistrierung







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