Rank-1 Lattice Based
High-dimensional Approximation
and sparse FFT

Toni Volkmer

joint work with Lutz Kämmerer, Daniel Potts, and Tino Ullrich
Introduction
Approximation of periodic functions based on samples

- torus $\mathbb{T} \simeq [0, 1)$, $\{e^{2\pi ikx}\}_{k \in \mathbb{Z}}$ orthonormal basis of $L_2(\mathbb{T})$
- function $f \in L_2(\mathbb{T})$, $f(x) = \sum_{k \in \mathbb{Z}} \hat{f}_k e^{2\pi ikx}$, $\hat{f}_k = \int_{\mathbb{T}} f(x) e^{-2\pi ikx} \, dx \in \mathbb{C}$
- smooth function $f \implies$ fast decay of Fourier coefficients $\hat{f}_k$
- truncated Fourier series $S_I f(x) = \sum_{k \in I} \hat{f}_k e^{2\pi ikx} \approx f(x)$
- $\hat{f}_k = \int_{\mathbb{T}} f(x) e^{-2\pi ikx} \, dx \approx \tilde{\hat{f}}_k := \frac{1}{2N} \sum_{j=0}^{2N-1} f(x_j) e^{-2\pi ikx_j}$, $x_j := \frac{j}{2N}$

$\implies$ transfer to multivariate case (tensorization)

\[
\begin{align*}
\hat{f}_k & \in \mathbb{C} \\
\tilde{\hat{f}}_k & \approx \frac{1}{2N} \sum_{j=0}^{2N-1} f(x_j) e^{-2\pi ikx_j}
\end{align*}
\]

$\mathcal{O}(N \log N)$

[Gauß 1866] [Cooley, Tukey 1965]
Introduction
Approximation of periodic functions based on samples

- **torus** $\mathbb{T} \simeq [0, 1)$, \( \{ e^{2\pi i k x} \}_{k \in \mathbb{Z}} \) orthonormal basis of \( L_2(\mathbb{T}) \)
- **function** \( f \in L_2(\mathbb{T}), \ f(x) = \sum_{k \in \mathbb{Z}} \hat{f}_k e^{2\pi i k x}, \ \hat{f}_k = \int_{\mathbb{T}} f(x) e^{-2\pi i k x} \, dx \in \mathbb{C} \)
- **smooth function** \( f \implies \) fast decay of Fourier coefficients \( \hat{f}_k \)
- **truncated Fourier series** \( S_I f(x) = \sum_{k \in I} \hat{f}_k e^{2\pi i k x} \simeq f(x) \)
- **transfer to multivariate case (tensorization)**

\[
\begin{align*}
\hat{f}_k &= \int_{\mathbb{T}} f(x) e^{-2\pi i k x} \, dx \approx \hat{f}_k := \frac{1}{2N} \sum_{j=0}^{2N-1} f(x_j) e^{-2\pi i k x_j}, \ x_j := \frac{j}{2N} 
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$|\hat{f}_k|$

$\mathcal{O}(N \log N)$

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$\implies$ transfer to multivariate case (tensorization)

- full grid in frequency domain
- equispaced full grid in spatial domain

$\mathcal{O}(N^d \log N)$
curse of dimensionality

$\implies$ assumption: sparsity or smoothness
In this talk

first part:

▶ fast reconstruction of arbitrary high-dimensional trigonometric polynomials

\[ p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \] using 1-dimensional FFTs

spatial domain: general known frequency index set \( I \subset \mathbb{Z}^d \)
multiple rank-1 lattice

\[ \mathcal{O}(|I| (d + \log |I|) \log^3 |I|) \]

▶ fast approximation \( f(x) \approx \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \) of functions from samples

second part:

▶ unknown frequency index set \( I \) / weights / function space in high dimensions

⇒ dimension-incremental sparse FFT using multiple rank-1 lattices
Multivariate trigonometric polynomials

\[ p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x) \]

Fast reconstruction of \( \hat{p}_k \) and approximation of \( f \) using rank-1 lattices

\[ f(x) = p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \] arbitrary freq. index set \( I \subset \mathbb{Z}^d, |I| < \infty \)

rank-1 lattice \( R1L(z, M) := \{ x_j := \frac{j}{M} z \text{ mod } 1 \}_{j=0}^{M-1}, z \in \mathbb{Z}^d, M \in \mathbb{N} \), as discretization in spatial domain

\[ z = (1, 4) \]
\[ M = 11 \]

Korobov '59
Maisonneuve '72
Sloan & Kachoyan '84,'87,'90
Temlyakov '86
Lyness '89
Sloan & Joe '94
Sloan & Reztsov '01
Li & Hickernell '03
Kämmerer & Kunis & Potts '12
Multivariate trigonometric polynomials $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x)$

Fast reconstruction of $\hat{p}_k$ and approximation of $f$ using rank-1 lattices

- $f(x) = p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x}$, arbitrary freq. index set $I \subset \mathbb{Z}^d$, $|I| < \infty$

- rank-1 lattice $R1L(z, M) := \{ x_j := \frac{j}{M} z \text{ mod } 1 \}_{j=0}^{M-1}$, $z \in \mathbb{Z}^d$, $M \in \mathbb{N}$

- Fast reconstruction of $\hat{p}_k$ using 1-dim. FFT? $\hat{p}_k \overset{?}{=} \frac{1}{M} \sum_{j=0}^{M-1} p_I(x_j) e^{-2\pi i k \cdot x_j}$
Multivariate trigonometric polynomials $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x)$

Fast reconstruction of $\hat{p}_k$ and approximation of $f$ using rank-1 lattices

$\Rightarrow$ reconstruction property: [Kämmerer, Kunis, Potts '12] [Kämmerer '12]

$k \cdot z \not\equiv k' \cdot z \pmod{M}$ for all $k, k' \in I$, $k \neq k'$
Multivariate trigonometric polynomials \( p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x) \)

Fast reconstruction of \( \hat{p}_k \) and approximation of \( f \) using rank-1 lattices

- \( f(x) \approx p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \), arbitrary freq. index set \( I \subset \mathbb{Z}^d, |I| < \infty \)

- rank-1 lattice \( R_{1L}(z, M) := \{ x_j := \frac{j}{M} z \mod 1 \}_{j=0}^{M-1}, z \in \mathbb{Z}^d, M \in \mathbb{N} \)

- fast reconstruction of \( \hat{p}_k \) using 1-dim. FFT

  \[ \Rightarrow \text{reconstruction property: } [\text{Kalmerer, Kunis, Potts '12}] \ [\text{Kalmerer '12}] \]

  \[ \forall k, k' \in I, k \neq k' \quad k \cdot z \not\equiv k' \cdot z \pmod{M} \]

- fast approximation of \( f \in L_2(\mathbb{T}^d) \cap C(\mathbb{T}^d) \) using rank-1 lattice sampling

  error estimates in \[ [\text{Byrenheid, Kalmerer, Ullrich, V. '17}] \ [V. '17] \]

\[ O(M \log M + d |I|) \]
Multivariate trigonometric polynomials $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x)$

Example – function from Sobolev space of dominating mixed smoothness

$\triangleright f(x) := \prod_{s=1}^{d} (2 + \text{sgn}(x_s \mod 1 - \frac{1}{2}) \sin(2\pi x_s)^3),$

$\triangleright$ hyperbolic cross $I := \{k \in 2\mathbb{Z}^d : \prod_{s=1}^{d} \max(1, |k_s|) \leq N\}$

$\begin{align*}
\quad f\left((x_1, x_2)^\top\right), \\
\quad \log_{10} \left| \hat{f}(k_1, k_2)^\top \right|, \\
\quad \text{Relative } L_2(T^d) \text{ error}
\end{align*}$
Multivariate trigonometric polynomials $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x)$

Single vs. multiple rank-1 lattices

- (reconstructing) rank-1 lattice:
  - number of samples $M$: $|I| \leq M \leq |I|^2$, construction: $O(d |I|^3)$, ($|I| \gtrapprox N$)
  - no additional dependence on spatial dimension $d$ in $M$
  - very easy and fast computation of Fourier coefficients (single 1-dim. FFT)

\[ \Rightarrow \text{two lines of MATLAB code:} \]
\[ g_{\text{hat}} = \text{fft}(\text{samples})/M; \]
\[ p_{\text{hat}} = g_{\text{hat}}(\text{mod}(I*z',M)+1); \]

- improvements? Use more than one rank-1 lattice! (union of several)

\[ \Rightarrow \text{multiple rank-1 lattice sampling [Kämmerer '16] [Kämmerer '17],} \]
\[ \text{complexities linear in } d, \text{ almost linear in sparsity } |I| \text{ (for } |I| \gtrapprox N): \]

- samples: \[ \leq C |I| \log^2 |I| \text{ (w.h.p.)} \]
- construct lattice: \[ \leq C |I| (d + \log |I|) \log^3 |I| \text{ (w.h.p.)} \]
- reconstruction / approximation: \[ \leq C |I| (d + \log |I|) \log^3 |I| \]
Multivariate trigonometric polynomials \( p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x) \)

Single vs. multiple rank-1 lattices

▸ (reconstructing) rank-1 lattice:

- number of samples \( M \): \(|I| \leq M \leq |I|^2\), construction: \( O(d|I|^3) \), \(|I| \gtrsim N\)
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\[ \Rightarrow \text{multiple rank-1 lattice sampling} \ [\text{Kämmerer '16}] \ [\text{Kämmerer '17}], \]
complexities linear in \( d \), almost linear in sparsity \(|I|\) (for \(|I| \gtrsim N\)):

- samples: \( \leq C |I| \log^2 |I| \) (w.h.p.)
- construct lattice: \( \leq C |I| (d + \log |I|) \log^3 |I| \) (w.h.p.)
- reconstruction / approximation: \( \leq C |I| (d + \log |I|) \log^3 |I| \)
Multivariate trigonometric polynomials $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \approx f(x)$

Example — fast approximation

kink function $g_d : \mathbb{T}^d \rightarrow \mathbb{R}$,

$$g_d(x) = \prod_{s=1}^{d} \left( \frac{5^{3/4} 15}{4\sqrt{3}} \max \left\{ \frac{1}{5} - (x_s - \frac{1}{2})^2, 0 \right\} \right)$$

- error estimates for (multiple) rank-1 lattice sampling
  in [Byrenheid, Kämmerer, Ullrich, V. '17] [V. '17] [Kämmerer, V. '18]
Interlude

first part:

- fast reconstruction of arbitrary high-dimensional trigonometric polynomials
  \[ f(x) = p_I(x) = \sum_{\mathbf{k} \in I} \hat{p}_\mathbf{k} e^{2\pi i \mathbf{k} \cdot x} \] using 1-dimensional FFTs

  spatial domain: general known frequency index set \( I \subset \mathbb{Z}^d \)

- fast approximation
  \[ f(x) \approx \sum_{\mathbf{k} \in I} \hat{p}_\mathbf{k} e^{2\pi i \mathbf{k} \cdot x} \] of functions from samples

  \[ \mathcal{O}(|I| (d + \log |I|) \log^3 |I|) \]

second part:

- unknown frequency index set \( I \) / weights / function space in high dimensions
  \[ \Rightarrow \] dimension-incremental sparse FFT using multiple rank-1 lattices
High-dimensional dimension-incremental sparse FFT
Method [Potts, V. '15] [V. '17] [Potts, Kämmerer, V. '17], $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2 \pi i k \cdot x}$

$I \subset \Gamma = \hat{G}^3_8 := \{-8, -7, \ldots, 8\}$

$k_1 = -8, \ldots, 8$

$p_{k_1} := \frac{1}{17} \sum_{\ell=0}^{16} p\left(\begin{pmatrix} \ell/17 \\ x_2' \\ x_3' \end{pmatrix}\right) e^{-2\pi i \frac{\ell k_1}{17}}$

frequency candidates

sampling nodes $\left\{\left(\frac{\ell}{17}, x_2', x_3'\right)\right\}_{\ell=0}^{16}$
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construct sampling set

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1-dim. FFT

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\[ \hat{p}_k := \frac{1}{17} \sum_{\ell=0}^{16} p \left( \begin{pmatrix} \ell/17 \\ x'_2 \\ x'_3 \end{pmatrix} \right) e^{-2\pi i \frac{\ell k_1}{17}} \]

\[ = \sum_{(h_2,h_3) \in \{-8,...,8\}^2} \hat{p} \begin{pmatrix} k_1 \\ h_2 \\ h_3 \end{pmatrix} e^{2\pi i (h_2 x'_2 + h_3 x'_3)}, \]

\[ k_1 = -8,...,8 \]

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\[ = \sum_{(h_2,h_3) \in \{-8,\ldots,8\}^2} \hat{p} \left( \begin{pmatrix} k_1 \\ h_2 \\ h_3 \end{pmatrix} \right) e^{2\pi i (h_2 x_2' + h_3 x_3')}, \]

\[ k_1 = -8, \ldots, 8 \]

\[ I \subset \Gamma = \hat{G}_8^3 := \{-8,-7,\ldots,8\} \]

\[ 1 \text{-dim. FFT} \]

detected frequencies \( I^{(1)} \)

\[ + \text{ repeat (} r \text{ detection iterations)} \]

sampling nodes \( \left\{ \left( \frac{\ell}{17}, x_2', x_3' \right) \right\}_{\ell=0}^{16} \)
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construct sampling set

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\( I^{(2)} \)

reconstructing multiple rank-1 lattice

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$\mathcal{I} \subset \Gamma = \hat{G}_8^3 \equiv \{-8,-7,\ldots,8\}$

detected frequencies $\mathcal{I}^{(1)}$

detected frequencies $\mathcal{I}^{(2)}$

frequency candidates $\mathcal{I}^{(1)} \times \mathcal{I}^{(2)}$
High-dimensional dimension-incremental sparse FFT

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detected frequencies $I^{(1)}$

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$1$-dim. $\leftarrow$ FFTs

detected frequencies $I^{(1,2)}$
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+ repeat \((r\) detection iterations\)

sampling nodes
High-dimensional dimension-incremental sparse FFT Method [Potts, V. ’15] [V. ’17] [Potts, Kämmerer, V. ’17], $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x}$

$I \subset \Gamma = \hat{G}_8^3 := \{-8, -7, \ldots, 8\}$

- detected frequencies $I^{(1)}$
- detected frequencies $I^{(2)}$

$+ \text{ repeat (r detection iterations)}$
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High-dimensional dimension-incremental sparse FFT Method \cite{Potts:2015a, Potts:2017a, Potts2017a, Kammerer2017a}

\[ p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \]

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\( \rightarrow \) construct sampling set

\( \rightarrow \) sampling nodes

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1-dim. ← FFT

sampling nodes

Toni Volkmer 12 / 16 https://www.tu-chemnitz.de/~tovo/
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1-dim. FFT

sampling nodes
High-dimensional dimension-incremental sparse FFT

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detected frequencies \( I^{(1,2)} \)

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\[ \text{sampling nodes} \]

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reconstructing multiple rank-1 lattice

sampling nodes
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\[ I^{(1,2,3)} = I \]

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detected frequencies $I^{(1,2)}$

$1$-dim. $\leftrightarrow$ FFTs

detected frequencies $I^{(1,2,3)} = I$

sampling nodes
reconstruction of \( p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x} \) with unknown \( I \)

using multiple rank-1 lattices:

\begin{itemize}
  \item sparsity \( s = |I| \), search domain \( \Gamma = \hat{G}_N^d := \{-N, \ldots, N\}^d \supset I \),
  \end{itemize}

\begin{table}
\begin{tabular}{l|c|c}
  & theory & in practice \\
  \hline
  samples & \( \leq C d s^2 N \log^3(sN) \) (w.h.p.) & \( \leq C d sN \log^2(sN) \) \\
  arithmetic op. & \( \leq C d^2 s^2 N \log^5(sN) \) (w.h.p.) & \( \leq C d^2 sN \log^4(sN) \)
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\begin{itemize}
  \item MATLAB implementation
  \item numerically tested for up to 30 spatial dimensions
\end{itemize}
reconstruction of $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x}$ with unknown $I$

using multiple rank-1 lattices:

- sparsity $s = |I|$, search domain $\Gamma = \hat{G}_N^d := \{-N, \ldots, N\}^d \supset I$,

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- MATLAB implementation
- numerically tested for up to 30 spatial dimensions
High-dimensional dimension-incremental sparse FFT
Example — 10-dimensional test function

- approximate reconstruction of a function \( f \in L_2(\mathbb{T}^d) \cap C(\mathbb{T}^d) \)
- \( f(x) := \prod_{t \in \{1, 3, 8\}} B_2(x_t) + \prod_{t \in \{2, 5, 6, 10\}} B_4(x_t) + \prod_{t \in \{4, 7, 9\}} B_6(x_t), \)
  \( B_m(x) = \sum_{k \in \mathbb{Z}} C_m \text{sinc} \left( \frac{\pi m k}{m} \right) (-1)^k e^{2\pi i k x} \)
  univariate B-spline of order \( m \in \mathbb{N} \)
- dimension-incremental sparse FFT for \( \Gamma = \hat{G}_{64}^{10} \) (\( |\hat{G}_{64}^{10}| \approx 1.28 \cdot 10^{21} \)):
Conclusion

- known frequency index set \( I \subset \mathbb{Z}^d \), multiple rank-1 lattice
  - fast reconstruction of high-dim. trigonometric polynomials \( p_I \)
    [Kämmerer '16] [Kämmerer '17]
  - fast approximation (error estimates for Sobolev-Hilbert type spaces)
    [Kämmerer, Potts, V. '15] [Byrenheid, Kämmerer, Ullrich, V. '17] [V. '17] [Kämmerer, V. '18]

- unknown \( I \subset \mathbb{Z}^d \), sampling along (multiple) rank-1 lattices
  - high-dimensional dimension-incremental sparse FFT
    [Potts, V. '16] [V. '17] [Kämmerer, V. '17]
  - very good numerical results
    for high-dimensional sparse trigonometric polynomials and
    for high-dimensional functions (non-sparse in frequency domain)
  - can be transferred to non-periodic case (tensor product Chebyshev bases)

- see also


T. V. Multivariate Approximation and High-Dimensional Sparse FFT Based on Rank-1 Lattice Sampling. Dissertation (PhD thesis), Faculty of Mathematics, Chemnitz University of Technology, 2017.


Software: MATLAB toolboxes (for single rank-1 lattices) https://www.tu-chemnitz.de/~tovo