Multi-scale tensorization - the blessing of dimensions

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Anouncement

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Max-Planck-Institut für Physik komplexer Systeme

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Setting - Tensors

$$V_\nu := \mathbb{R}^n \ , \ \ \mathcal{H}_d = \mathcal{H} := \bigotimes_{\nu=1}^{d} V_\nu$$ d-fold tensor product Hilbert-s.,

$$\mathcal{H} \simeq \{(x_1, \ldots, x_d) \mapsto U(x_1, \ldots, x_d) \in \mathbb{R} : x_i = 1, \ldots, n_i\} \ .$$

The function $U \in \mathcal{H}$ will be called an order d-tensor.
For notational simplicity, we often consider $n_i = n$. Here
$x_1, \ldots, x_d \in \{1, \ldots, n\}$ will be called variables or indices.

$$\mathbf{k} \mapsto U(\mathbf{k}) = U(k_1, \ldots, k_d) = (U_{k_1,\ldots,k_d}) \ \ , \ \ k_i = 1 \ldots, n_i \ .$$

Or in index (vectorial) notation

$$\mathbf{U} = \left(U_{k_1,\ldots,k_d}\right)_{k_i=0, 1\leq i\leq d}^{n_i}$$

$\dim \mathcal{H} = n^d$ curse of dimensions!!!

E.g. wave function $\Psi(\mathbf{r}_1, s_1, \ldots, \mathbf{r}_N, s_N)$

Vector-Tensorization - e.g. Binary coding

1D example: vector, e.g. signal

$$k \to f(k) \,, \ \left(\text{ or } \ g(\frac{k}{2^d}) \right) \,, \ k = 0, \ldots, 2^d - 1 \ .$$

Labeling of indices $k \simeq \mu \in \mathcal{I}$ by an binary string of length d,

$$\boldsymbol{\mu} = \mu(k) \ = \ (0,0,1,1,0,\ldots) \simeq \sum_{j=0}^{d-1} \mu_i 2^j = k(\boldsymbol{\mu}) \,, \ \mu_i = 0, 1 \ .$$

Tensorization

$$\boldsymbol{\mu} \mapsto U(\boldsymbol{\mu}) := f(k(\boldsymbol{\mu})) \in \bigotimes_{j=0}^{d-1} \mathbb{R}^2 \ , \quad \text{or} \ \bigotimes_{j=0}^{d-1} \mathbb{C}^2 .$$

This provides an isomorphm $T : \mathbb{R}^{2^d} \leftrightarrow \bigotimes_{j=0}^{d-1} \mathbb{R}^2$ by $Tf := U$.
So far no information is lost, $N = 2^d$ or $d = \log_2 N$.

Hierarchical Tucker (HT) format

Hackbusch & Kühn (2009), Grasedyck (2010)

Hierarchical MCTDH *Mayer et al.* (2000) Matrix product states (1992) – (Tree) Tensor networks: e.g. *Vidal, Schollwöck etc. (2003)*

Noteable special case of HT: TT format , Oseledets & Tyrtyshnikov

TT- or matrix product representation of U

$$\boxed{U(\mathbf{x}) = \mathbf{U}_1(x_1)\cdots\mathbf{U}_i(x_i)\cdots\mathbf{U}_d(x_d)}$$

$$= \sum_{k_1=1}^{r_1} .. \sum_{k_{d-1}=1}^{r_{d-1}} U_1(x_1,k_1)U_2(k_1,x_2,k_2)...U_{d-1}(k_{d-2}x_{d-1},k_{d-1})U_d(k_{d-1},x_d,k_d)$$

- component tensors $U_i(k_{i-1},x_i,k_i) \in \mathbb{R}^{r_{i-1}\times n_i\times r_i}$,

if $r := \max\{r_1,\dots,r_{d-1}\}$, here $n = 2$, (or $4,\dots$ small!)

storage complexity DOFs: $\leq\ ndr^2$,

Binary coding - signal compression - 1 D functions

Quantized TT - Oseledets (2009), Khoromskij (2009) :

TT approximation of U

- Storage complexity N is reduced to $2r^2 \log_2 N$! (linear in $d = \log_2 N$)
- Allow extreme fine grid size $h = o(\epsilon) = 2^{-d} = \frac{1}{N}$.
  Example: $d = 50$, then $h \leq 10^{-15}$

Basic question: when is r small or moderate?

(Grasedyck (2010), Hackbusch (2010), Oseledets (2010))

Examples:

1. For Kronecker $\delta_{i,j}$ (Dirac function) is $r = 1$.
2. For plane wave (fixed $k = \sum_{j=1}^{d} \nu_j 2^{j-1}$)

$$e^{2\pi ik} = e^{2\pi i \sum_{j=1}^{d} \nu_j 2^{j-1}} = \Pi_{j=1}^{d} e^{2\pi i \nu_l 2^{j-1}} \ , \ \nu_j = 0, 1,$$

again (complex) $r = 1$, or (real $r = 2$) .

TT representation of tensorized f

The TT ranks r_i, $\underline{r} = (r_1, \ldots, r_{d-1})$, of the TT decomposition of $U = T(f)$ are the ranks of the following matrices, $i = 1, \ldots, d-1$

$$r_i = \text{rank of } \mathbf{A}_i = U^{\mu_{i+1},\ldots,\mu_d}_{\mu_1,\ldots,\mu_i} = U^{(1,0,\ldots)}_{(0,1,\ldots)} .$$

or

$$\mathbf{A}_i = U^q_p \ , p = p(\mu_1, \ldots, \mu_i) \text{ and } q = q(\mu_{i+1}, \ldots, \mu_d)$$

consider $g : [0,1] \to \mathbb{R}$, $x = \frac{k}{2^d}$, $k = 0, \ldots, 2^d - 1$, $f(k) = g(\frac{k}{2^d})$, then k_1 is the number of the subinterval

$$I^i_{k_1} := [\frac{k_1 - 1}{2^i}, \frac{k_1}{2^i}]$$

and $\{\frac{k_1-1}{2^i} + \frac{1}{2^d}[0, \ldots, k_2, \ldots, 2^{d-i} - 1] : k_2 = 0, \ldots, 2d - i - 1\}$ the corresponding grid.

Two-scale decomposition-similarity rank

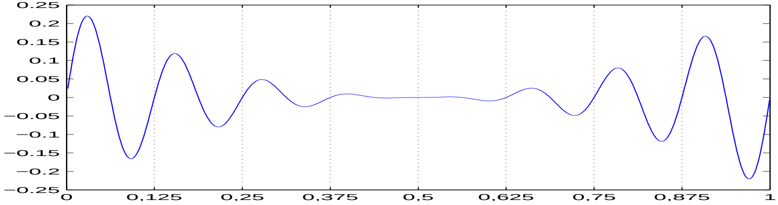
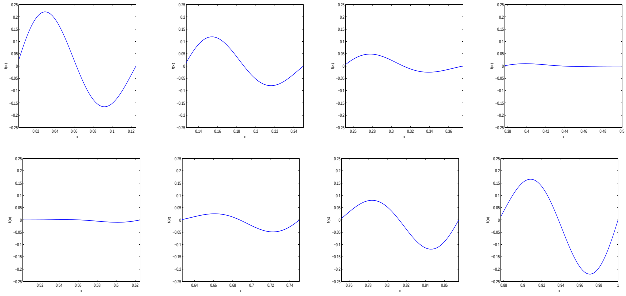


Figure: Function$g(x) = x^2 \sin \frac{8x}{2\pi}$ and translated functions g_k^3



Similarity rank and Multi-scale decomposition

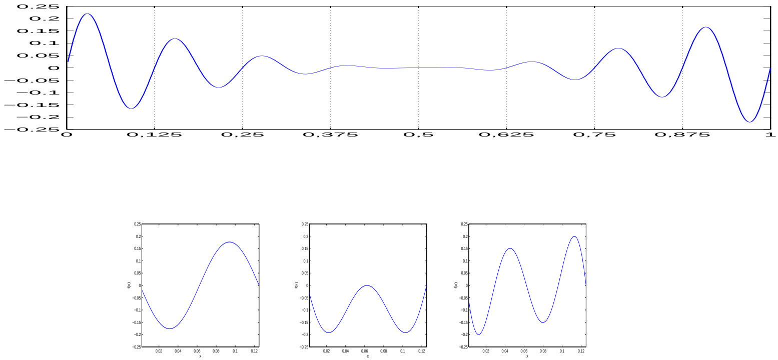


Figure: PCA principal component analysis (SVD) functions g_k^3, $k = 1, \dots 3$

Recursively performed SVD from level to level (Vidal-decomposition) $\Rightarrow$ multiscale decomposition, i.e. a TT representation of U.

Examples for admitting low rank representations

Low ranks

1. (Piecewise) polynomials of degree p.
2. $e^{i\langle \mathbf{k}, \mathbf{x} \rangle}$, i.e. Fourier polynomials
3. Splines, wavelets etc.
4. adaptive - best n-term approximation
   For homogenization:
5. Let $\phi : \mathbb{R} \to \mathbb{K}$ be 2^{-j}-periodic, then $\phi|_\Omega$ is if rank $_i\phi = 1$.
6. Let $f : [0, 1] \to \mathbb{K}$ has sim rank$f = p$, and ϕ 1-periodic, then the modulated function $x \mapsto g(x) := f(x)\phi(\frac{x}{2^{-j}})$ has ranks rank $_ig \le p$.

see e.g. appendix.

Low TT rank approximation

Theorem

1. $f \in H^s(\Omega_k^j)$, $k \in \Delta_j$, $(\Omega \subset \mathbb{R}^D)$. *There exists* f_ϵ *with rank* r_j *on level* j *satisfying*

$$\|f - f_\epsilon\|^2 \lesssim r_j^{-s/D} \sum_{k \in \Delta_j} |f|^2_{H^s} \ . \tag{1}$$

2. f *analytic on the domains* Ω_k^j, $k \in \Delta_j$

$$\|f - f_\epsilon\| \lesssim e^{-\alpha r_j} \ , \quad \textit{for some } \alpha > 0 \ . \tag{2}$$

3. *Let* f *be a piecewise analytic function on* $\Omega \setminus \{x_0\}$ *satisfying*

$$|\partial^{\boldsymbol{\alpha}} f(\mathbf{x})| \leq c_{\boldsymbol{\alpha}} |\mathbf{x} - \mathbf{x}_0|^{\gamma - |\boldsymbol{\alpha}|} \boldsymbol{\alpha}!$$

then there exists $\alpha > 0$ *s.t.*

$$\|f - f_\epsilon\| \lesssim e^{-\alpha r_j} \ . \tag{3}$$

Examples for admiting low rank representations

- From this perspective, the approach can be easily extended to 2D and 3D Finite Elements with uniform refinement.
- Black-box algorithm: The multi-level scheme corresponds to a (multi-) wavelet packet decomposition.
- The two-scale relations are not fixed, but optimized in each component (such that no wavelets appears).
- ranks $r_j \leq cN$ for best N-term approximation (e.g. Fourier, wavelets etc.), even with $c << 1$ but scaling is $\mathcal{O}(r^2)$!

Two-scale decomposition - matricisation

Reference domain Ω_0 and $\Omega = \bigcup_{k \in \Delta_j} \Omega_k^j$, above example $\Omega = \Omega_0$, $\Omega_k^j = [k2^{-j}, (k+1)2^{-j}]$ together with isomorphisms (renormalization group)

$$\boxed{T_k^j : \Omega_k^j \to \Omega_0 \ \ , \Omega = \bigcup_{k \in \Delta_j} \Omega_k^j \ .}$$

$f_l := \sum_{k \in \Delta_j} f_l|_{\Omega_k^j} : \Omega \to \mathbb{K}$, $l = 1, \dots, m$ simultanously,

$$f_{k,l}^j : \Omega_k^j \to \mathbb{K} \, , \; x \mapsto f_{k,l}^j(x) := f_l\big((T_k^j)^{-1} x\big) = f_l \circ (T_k^j)^{-1}(x) \, , \; x \in \Omega_0 \, .$$

The *similarity rank* of f at level j

$$\boxed{\text{sim rank}_j f := \dim \text{span}\{f_{k,l}^j : k \in \Delta_j \; l = 1, \dots, n\} = r_j \ .}$$

is equal to the TT Rank r_j of U.

Multi-scale decomposition by recursion

$$\Omega_0^j = \bigcup_{\mu_j=0}^{n_j-1} \Omega_{\mu_j}^{j+1} \ , \quad T_{\mu_j}^j : \Omega_{\mu_j}^{j+1} \to \Omega_0^{j+1} \ , \ \mu_j = 0, \ldots, n_j$$

$k \in \Delta_{j+1}$ can be encoded by a multi-index
$\boldsymbol{\mu} = \boldsymbol{\mu}(k) = (\mu_0, \ldots, \mu_j) \in \mathcal{I}_0 \times \cdots \times \mathcal{I}_j, \mathcal{I}_j = 0, \ldots, n_j - 1,$

We define multi-scale scaling functions (see multi -wavelets)

$$x \mapsto \varphi_{\alpha_{j-1}}^j(x), x \in \Omega_0 \ .$$

Two-scale relation

$$\varphi_{\alpha_{j-1}}^j(x) = \sum_{\mu_j=1}^{n_j} \sum_{\alpha_j=1}^{r_d} U_j(\alpha_{j-1}, \mu_j, \alpha_j) \varphi_{\alpha_j}^{j+1}(T_{\mu_j}^j x) \ , \ x \in \Omega_0 \ .$$

Multi-scale decomposition by recursion

Iterating

$$T_k^{j+1} = T_{k(\boldsymbol{\mu})}^{j+1} = T_{\mu_0}^0 \circ \cdots \circ T_{\mu_j}^j \ .$$

yields nonlinear (multi wavelet (packets)-) subdivison scheme reconstructing A vector, resp. function f corresponds to a tensor U

$$x \mapsto f(x), x \in \Omega_0 \ , \ (\boldsymbol{\mu}) \mapsto U(\boldsymbol{\mu}) = U(\mu_0, \ldots, \mu_d) \ ,$$

$$\Rightarrow \quad f(x) = \sum_{\boldsymbol{\mu}: k(\boldsymbol{\mu}) \in \Delta_d} U(\boldsymbol{\mu}) \varphi^d (T_{k(\boldsymbol{\mu})}^d x) \ , \ x \in \Omega_0 \ .$$

$$U(\boldsymbol{\mu}, \alpha_d) = \sum_{\alpha_0=1}^{r_0} \cdots \sum_{\alpha_{d-1}}^{r_{d-1}} U_i(\alpha_{i-1}, \mu_i, \alpha_i) \ .$$

U_i computed e.g. sequentially by SVDs (opt. - black box)

Binary coding - linear operators and matrices

$\mathbf{A} = \left[a(k_1, k_2)\right] : \bigotimes_{j=1}^{d} \mathbb{K}^2 \to \bigotimes_{j=1}^{d} \mathbb{K}^2 \simeq \mathbb{K}^{2^d}$. coding
$\boldsymbol{\theta} = (\theta_1, \ldots \theta_{2d}) := \big((\mu_1, \nu_1), \ldots, (\mu_d, \nu_d)\big)$.

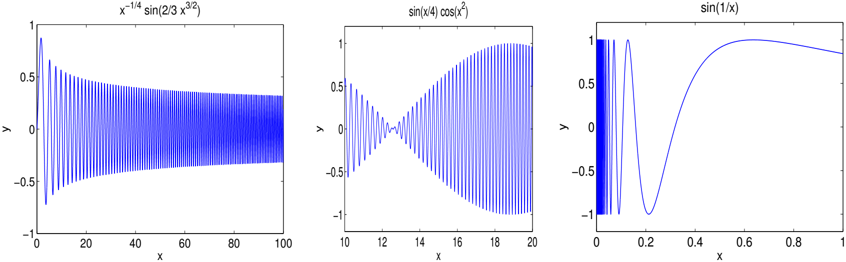
$$\big((\mu_1, \nu_1), \ldots, (\mu_d, \nu_d)\big) \mapsto A(\boldsymbol{\theta}) := a\big(\mathbf{k}(\boldsymbol{\theta})\big) \in \bigotimes_{j=1}^{d} \mathbb{K}^{2\times 2} ,$$

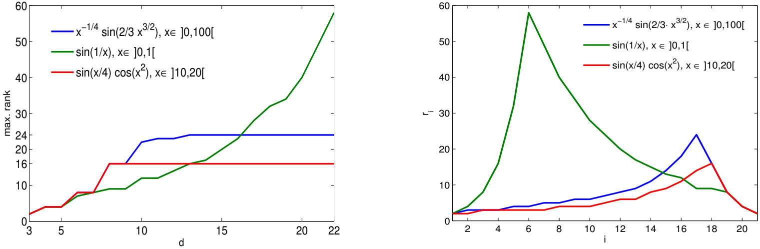
Example:

1. Bit reversal is a permutation of tensor variables.
2. Identity matrix
$$\mathbf{I} = \mathbf{I}_{2\times 2} \otimes \cdots \otimes \mathbf{I}_{2\times 2} \ .$$
3. The Hadamar-Walsh transform is given by
$$\mathbf{W} = \bigotimes_{j=1}^{d} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
4. finite differences, e.g. $\frac{d^2 f}{dx^2} \approx \frac{f(x_{k-1}) - 2f(x_k) + f(x_{l+1})}{2h^2}$, $h = 2^{-d}$, has ranks $r_j \leq 3$.
5. (quantum) Fourier transform

Examples: TT approximation of tensorized functions

Airy function: $f(x) = x^{1/4} \sin \frac{2x^{2/3}}{3}$, chirp: $f(x) = \sin \frac{x}{4} \cos(x^2)$ and $f(x) = \sin \frac{1}{x}$





Comparison: quantum information theory - $\bigotimes_{i=1}^{d} \mathbb{C}^2$

$$\mathcal{H} = \mathbb{C}^{2^d} \eqsim L_2(\{1, \ldots, 2^d\}, \mathbb{C}) \eqsim L_2(\{0,1\}^d, \mathbb{C}) \eqsim \bigotimes_{i=1}^{d} \mathbb{C}^2$$

all equipped with L_2 resp. Froebenius norms.

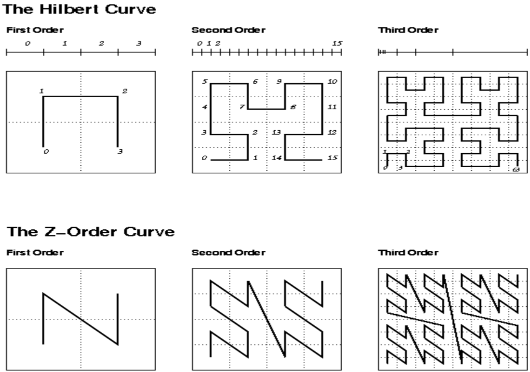
- here we have the same configuration space
- here we do not confine to $U \in H$ with $\|U\| = 1$
- not necessarily a probabilistic interpretation
- we do not confine to unitary operator $A : \mathcal{H} \to \mathcal{H}$
- But: TT ranks must be moderate!

The treatment of quantum mechanical problems with MPS willl be presented later!

Ordering of indices - space filling curves

There are various possibilities for higher-dimensional functions

1. lexigraphical ordering $(k_1, k_2, \ldots) \to \bigotimes_{i=1}^{D} \otimes_{l=1}^{n_i} \mathbb{R}^2$
2. Z-curve ordering, multi-level octree ordering
   $(k_1, k_2, \ldots) \to \bigotimes \mathbb{R}^{2^D}$
3. Hilbert space filling curves



Appendix: Translation invariant operators and spaces

$$v \mapsto L^{(p)}v := v^{(p)} + a_{p-1}v^{(p-1)} + \cdots + a_0 \ .$$

The kernel of the linear differential operator $L^{(p)}$

$$V_p := \{v \in H^p_{loc}(\mathbb{R}) : L^{(p)}v = 0\} \ .$$

The space V_p is translation invariant, i.e.

$$f(\cdot) \in V_p \Rightarrow f(\cdot - a) \in V_p \ , \forall a \in \mathbb{R} \ , \ \ \dim \ V_p = p \ .$$

Let $L^{(p)}$ be a linear partial differential operator of order p,

$$v \mapsto L^{(p)}v := \sum_{|\alpha| \leq p} a_\alpha D^\alpha v.$$

Then $V_p := \{v \in H^p_{loc}(\mathbb{R}) : L^{(p)}v = 0\}$, is translation invariant.

$$S^p = \bigoplus_{k \in \Delta_j} V_p|_{\Omega^j_k} \ \Rightarrow \text{sim rank} S^p = \dim \ V_p \ .$$

Examples

1. $L^{(2)}v = v''$ then V_p contains polynomials of degree $p = 2$.
2. $L^{(1)}v = v' + a$, $a \in \mathbb{C}$ then $v(x) = ce^{-ax}$.
3. $L^{(2)}v = v'' + a^2$, $a \in \mathbb{R}$, then $v(x) = c_1 \cos ax + c_2 \sin ax$ or $v(x) = ce^{i\sqrt{a}x}$.
4. harmonic polynomials for the Laplacian $L = \Delta$,
5. $e^{i\langle \mathbf{k},\mathbf{x}\rangle}$ or Fourier Bessel function for the Helmholtz operator, (Treftz method)
6. advection equation (Demkovich et al.)

Corollary

- $S^p := \bigoplus S^p(\Omega_j^k)$,
  $S^p(\Omega_j^k) = \{f : \Omega_k^j : \mathbb{R} : f$ *is a polynomial of degree* $\leq p\}$
  $p_n = \sum_{k=0}^{p} a_k x^k$ *are of similarity rank* $\leq (p+1)^D$.
- *Assume* $f = \sum_{|k|\leq p} \hat{f}_k e^{2\pi ikx}$, *is piecewise bandlimited, and* $l \leq j$ *sufficiently large. Then* f *has rank* $r_l \leq 2p+1$.

Appendix - examples

Let $T_k : \mathbb{R}^D \to \mathbb{R}^D$. We will call a function space V_T of functions T_k *-invariant* if $\forall\ k \in \Delta_j$ and transformations T_k
$f \in V_T \Rightarrow f \circ T_k \in V_T$.

1. If V_T is a T_k invariant space of dimension $\dim V_T$ then the similarity rank of a function $f \in V_T$ is $\leq \dim V_T$.
2. T_k-translation invariant space V_j generated by $\varphi_k(x) = \varphi(x-k)$ has similarity rank $p \leq \sharp\{\text{supp } \varphi_k \cap \Omega_0^j \neq \emptyset\}$.
3. Multiresolution spaces $V^l = V^0 \oplus \bigoplus_{i=0}^{l-1} W^i$, where $l \leq j$ have similarity rank $\leq p$.

Homogenization

1. Let $\phi : \mathbb{R} \to \mathbb{K}$ be 2^{-J}-periodic, $J \geq j$ then $\phi|_\Omega$ is if sim rank $\phi = 1$.
2. Let $f : [0,1] \to \mathbb{K}$ has sim rank$f = p$, and ϕ 1-periodic, than $x \mapsto g(x) := f(x)\phi(\frac{x}{2^{-j}})$ has similarity rank sim rank $g = p$.

Two-scale decomposition

Theorem

1. *Let us consider*

$$f = \sum_{j=0}^{d-1} \sum_{k \in \mathcal{I}^j} \sum_{i=1}^{p} a^j_{k,i} \varphi^j_{k,i}$$

   to be a piecewise polynomial function with polynomial degree $\leq p-1$*. Let* N_j *be the number of domains* Ω^j_k *where* $f|_{\Omega^j_k}$ *is not a polynomial. Then the similarity rank of f at level j satisfy*

$$\textit{sim rank}_j\ f \leq N_j + p\ .$$

2. *(Best N-term representation) Let f be expanded by multiwavelets of degree p within N terms, then the similarity rank is bounded by*

$$\textit{sim rank}_j\ f \leq \max\{N, p+1\}\ .$$

Thank you
for your attention.

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