Outline of Lecture 3 (I).

1. Additive dimension splitting.
2. Product-type separation of variables: tensor train (TT) formats.
3. Quantized tensor representation: Q-canonical and QTT formats.
4. Big picture.
5. TT/QTT appproximation of functions.
6. TT/QTT representation of matrices.
7. Tensor numerical methods: main ingredients and challenging problems.

Canonical tensors, $\mathcal{C}_R = \mathcal{C}_R(\mathbb{V})$. Storage: dRN.

V $\in \mathbb{V}_{\mathbf{n}}$ belongs to the rank-R canonical format if

$$V(i_1,\ldots,i_d) = \sum_{\alpha=1}^{R} U_1(i_1,\alpha)\ldots U_d(i_d,\alpha), \quad U_k(\cdot,\alpha) \in \mathbb{R}^{n_k}.$$

Tucker tensors, $\mathcal{T}_{\mathbf{r}} = \mathcal{T}_{\mathbf{r}}(\mathbb{V})$. Storage: $drN + r^d$, $r = \max r_\ell$.

V $\in \mathbb{V}_{\mathbf{n}}$ belongs to the rank $\mathbf{r} = [r_1,\ldots,r_d]$ Tucker format if

$$V(i_1,\ldots,i_d) = \sum_{\alpha_1,\ldots,\alpha_d=1}^{\mathbf{r}} G(\alpha_1,\ldots,\alpha_d)U_1(i_1,\alpha_1)\ldots U_d(i_d,\alpha_d).$$

Mixed Tucker-canonical tensors, $\mathcal{T}_{\mathcal{C}_R,\mathbf{r}}$. Storage: $drN + dRr$.

$$\mathbf{G} \in \mathcal{C}_R(\mathbb{R}^{r_1\times\ldots\times r_d}).$$

MPS-type dim. splitting: TT/TC formats

A matrix product states (MPS) repres. of slightly entangled systems.

MPS in quantum comput.: **[White '92; Wang, Thoss '03; Vidal '04; Cirac '06, ...]**.

In numerical analysis: TT – **Oseledets, Tyrtyshnikov, [3], [4]**, TC – **Khoromskij, [1]**.

Def. 3.1. (Tensor Train/Chain format), (TT/TC[$\mathbf{r}$]).

Given $\mathcal{J} := \times_{\ell=1}^{d} J_\ell$, $J_\ell = \{1, ..., r_\ell\}$, $J_0 = J_d$. $\mathbf{V} \in TC[\mathbf{r}] \subset \mathbb{V}_{\mathbf{n}}$ if $\mathbf{V}$ is a contracted product of tri-tensors in $\mathbb{R}^{J_{\ell-1} \times I_\ell \times J_\ell}$ over $\mathcal{J}$,

$$V(i_1, ..., i_d) = \sum_{\boldsymbol{\alpha} \in \mathcal{J}} G_1(\alpha_d, i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \cdots G_d(\alpha_{d-1}, i_d, \alpha_d) \equiv G_1(i_1) G_2(i_2) ... G_d(i_d),$$

where $G_k(i_k)$ is a $r_{k-1} \times r_k$ matrix, $1 \le i_k \le n_k$.

If $J_0 = J_d = \{1\}$ (disconnected chain), TC is the Tensor-Train (TT) form.

A tensor $\mathbf{V} \in TC[\mathbf{r}]$ is represented by a product of matrices (matrix product states (cores)), each depending on a single "physical" index: similar to Tucker, but with the localised connectivity constraints.

$d = 2$: TT is a skeleton factorization of a rank-r matrix.

Main properties of the TT model

Thm. 3.1. (Storage, rank bound, concatenation, quasioptimality).

(A) Storage: $\sum_{\ell=1}^{d} r_{\ell-1} r_\ell N \le d r^2 N$ with $r = \max_\ell r_\ell$.

(B) Rank bound: $r_\ell \le rank_{[\ell]}(\mathbf{V}) := rank(V_{[\ell]}) \le rank_C(\mathbf{V})$.
$V_{[\ell]} := [V(i_1, ..., i_\ell; i_{\ell+1}, ..., i_d)]$ is the ℓ-mode TT unfolding matr.

(C) Canonical embeddings:

$$TT[\mathbf{r}] \subset TC[\mathbf{r}]; \quad \mathcal{C}_{R,\mathbf{n}} \subset TT[\mathbf{r}, \mathbf{n}, d] \quad \text{with} \quad \mathbf{r} = (R, ..., R).$$

(D) Concatenation to higher dim.: $\mathbf{V}[d_1] \otimes \mathbf{V}[d_2] \to D = d_1 + d_2$.

(E) Quasioptimal TT[$\mathbf{r}$]-approximation of $\mathbf{V} \in \mathbb{V}_{\mathbf{n}}$, satisfy

$$\min_{\mathbf{T} \in TT[\mathbf{r}]} \|\mathbf{V} - \mathbf{T}\|_F \le \Big(\sum_{\ell=1}^{d} \varepsilon_\ell^2\Big)^{1/2}, \quad \varepsilon_\ell = \min_{rank\, B \le r_\ell} \|V_{([\ell]} - B\|_F,$$

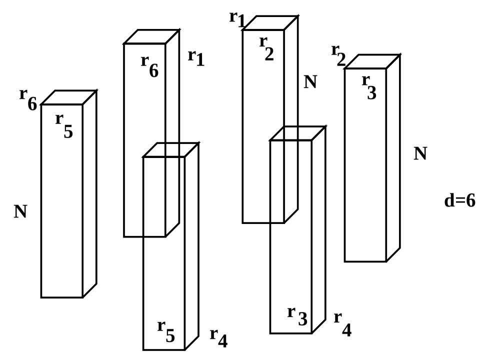
and it can be computed by QR/SVD alg.

Rem. TC approx. requires ALS-type iteration.

Benefits of the TT format

- Storage: $dr^2 N$, $\mathbf{n} = (N, ..., N)$. Rank bound $r = \max_\ell r_\ell \le rank_C(\mathbf{V})$.
- For fixed $\mathbf{r} = [r_1, \ldots, r_d]$ the parametric representations in TT[$\mathbf{r}$] define a manifold $\mathbb{T}_\mathbf{r} \subset \mathbb{V}_\mathbf{n}$, $\Rightarrow$ Dirac-Frenkel dynamics !
- Existence of best rank-$\mathbf{r}$ approximation. ALS/DMRG iteration.
- Stable quasi-optimal approximation by ℓ-mode SVD (Schmidt decomp.).

Ex. 3.1. Contracted product of tri-tensors over $J_1 \times ... \times J_6$ $(d = 6)$.



Historical remarks related to quasioptimality (E)

Numerical analysis community:

Rem. 3.1. (Quasioptimality via SVD-based approximation).

Full-to-Tucker-HOSVD – [De Lathauwer et al. 2000].

Idea of Hierarchical Dim. Split. (format only) – [BNK '06].

Canonical-to-Tucker-RHOSVD – [BNK, Khoromskaia '08].

Full-to-TT, TT-to-TT, ACA – [Oseledets, Tyrtyshnikov '09].

Hierarchical Tucker format – [Hackbusch, Kühn '09].

Quantics-TT – [BNK, Oseledets '09-'10]
(approximation, theoretical bounds on r_ℓ, numerics).

Manifolds of TT tensors – [R. Schneider, Holtz, Rohwedder '10]

Rem. 3.2. ε_ℓ can be estimated over the truncated SVD or ACA of the ℓ-mode TT unfolding of $\mathbf{V}$, $V_{[\ell]}$ $(\ell = 1, ..., d)$.

Cor. 3.1 [Oseledets, Tyrtyshnikov '09] Given a tensor $\mathbf{A}$, denote by

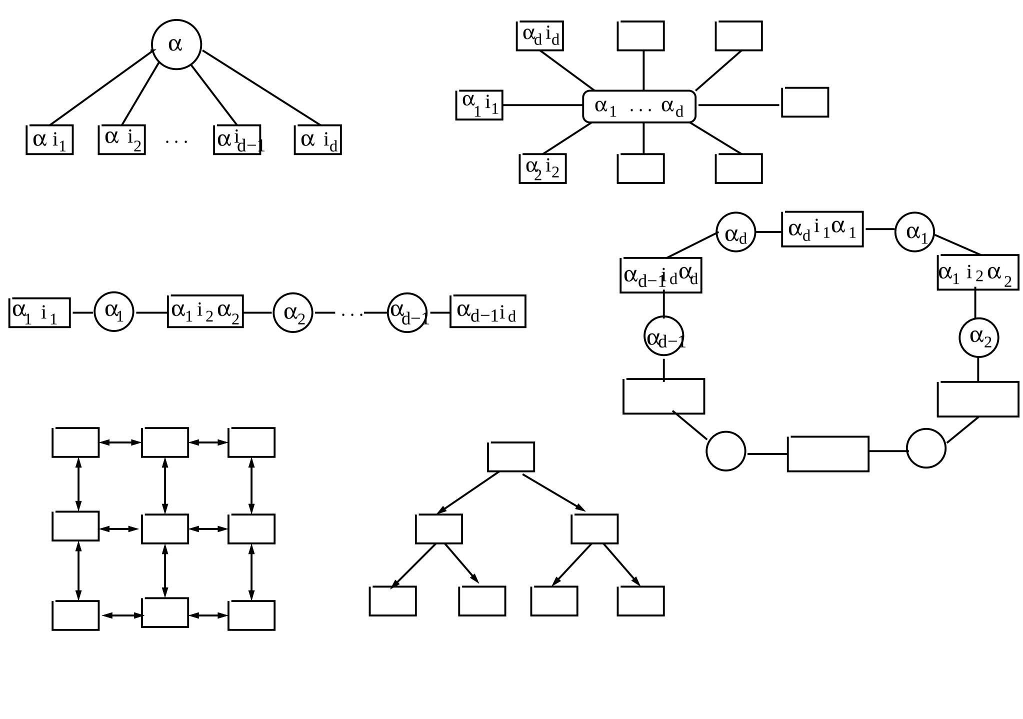
$$\varepsilon = \min_{\mathbf{B} \in TT[\mathbf{r}]} \|\mathbf{A} - \mathbf{B}\|_F.$$

Then the optimal $\mathbf{B}$ exists and the TT approx. $\mathbf{T}$ constructed in the proof of Thm. 3.1, (E), is quasi-optimal in the sense

$$\|\mathbf{A} - \mathbf{T}\|_F \leq \sqrt{d-1}\,\varepsilon.$$

Cor. 3.2. [Oseledets, Tyrtyshnikov '09] If a tensor $\mathbf{A}$ admits an R-term canonical approximation of accuracy $\varepsilon > 0$, then there exists a TT approx. with $r_k \leq R$, and accuracy $\sqrt{d-1}\varepsilon$.

Rem. 3.3. Similar to the case of product Stiefel manifold of Tucker tensors, the set of TT-tensors with fixed rank parameters, TT$[\mathbf{r}]$, can be proven to be the nonlinear manifold in the TPHS $\mathbb{V}_{\mathbf{n}}$, [R. schneider et al, '10].



Quantization (folding) of **vector/tensor** to higher (virtual) dimension !

Def. 3.2. [BNK '09] $N = q^L$, $\mathbf{n} = N^{\otimes d}$. The q-adic folding of degree L,

$$(isometry) \quad \mathcal{F}_{q,d,L} : \mathbb{V}_{\mathbf{n},d} \to \mathbb{Q}_{\mathbf{m},D}, \quad \mathbf{m} = q^{\otimes D}, \quad D = dL,$$

reshapes $\mathbf{X} \in \mathbb{V}_{\mathbf{n},d}$ to the quantized $\underbrace{q \times q \times ... \times q}_{dL}$-tensor in $\mathbb{Q}_{\mathbf{m},D}$.

- For $d = 1$, $q = 2$, a vector $\mathbf{X}_{(N,1)} = [X(i)]$, $1 \le i \le N$, is reshaped by

$$\mathcal{F}_{2,1,L} : \mathbf{X}_{(N,1)} \to \mathbf{A}_{(\mathbf{m},L)} = [A(\mathbf{j})], \quad A(\mathbf{j}) := X(i), \quad \mathbf{j} = \{j_1, ..., j_L\}.$$

$j_\nu - 1 \in \{0, 1\}$, $\nu = 1, ..., L$, gives the binary coding of $i - 1 = \sum_{\nu=1}^{L} (j_\nu - 1)2^{\nu-1}$.

- Extended to $d \ge 2$ and generalised to $q = 2, 3, ...$

Optimal choice: $q^* = 2.7...$, Euler number.

- General concept of quantized-TT (QTT) format + basic approximation results. [BNK '09], Constractive Approx., 34, 2(2011), 257-280.
- $2^L \times 2^L$ matrix reshapes to low-rank $(2 \times 2)^{\otimes L}$ $\mathbb{Q}$-matrix, [Oseledets '09]
- Contrary to Kolmogorow's paradigm ?

QTT method of log-volume storage/complexity, $N^d \to O(d \log_2 N)$.

Thm. 3.2. [BNK '09] QTT-representation of funct. related tensors.

- (a) $N = 2^L$, $L \in \mathbb{N}$, $c, z \in \mathbb{C}$. Quantized exponential N-vector

$$\mathbf{X} := \{x_n := cz^{n-1}\}_{n=1}^N \in \mathbb{C}^N,$$

is the rank-1, $2 \times 2 \times ... \times 2$-tensor,

$$\mathcal{F}_{2,L} : \mathbf{X} \mapsto \mathbf{A} = c \otimes_{p=1}^L \begin{bmatrix} 1 \\ z^{2^{p-1}} \end{bmatrix}, \quad \mathbf{A} : \{1,2\}^{\otimes L} \to \mathbb{C}, \quad (2 - L \text{ tensor}).$$

- (b) For $\forall \alpha \in \mathbb{C}$, the trigonometric N-vector

$$\mathbf{X} := \{x_n := \sin(\alpha(n-1))\}_{n=1}^N \in \mathbb{C}^N,$$

has explicit rank-2 QTT-repres. $x_p = 2^{L-p} i_p$, $i_p = 0, 1$, Hint: $\sin z = \frac{e^{iz} - e^{-iz}}{2i}$

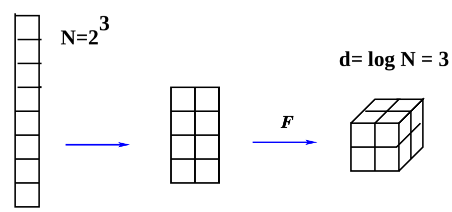
$$\mathbf{X} \mapsto [sin\, \alpha x_1 cos\, \alpha x_1] \otimes_{p=2}^{L-1} \begin{bmatrix} cos\, \alpha x_p & -sin\, \alpha x_p \\ sin\, \alpha x_p & cos\, \alpha x_p \end{bmatrix} \otimes \begin{bmatrix} cos\, \alpha x_L \\ sin\, \alpha x_L \end{bmatrix} \in \{0,1\}^{\otimes L},$$

- (c) Polynomial of degree $m \mapsto$ QTT-tensor of TT-rank $m+1$.
- (d) QTT-rank of the step function and Haar wavelet is 1 and 2, resp.
- (e) Chebyshev polyn. $T_m(x) = \cos(m \arccos x)$, sampled as a vector

$$\mathbf{X} := \{x_n := T_m(x_n)\}_{n=0}^{N} \in \mathbb{C}^N, \quad N = 2^L - 1, \ |x_n| \leq 1$$

over Chebyshev Gauss-Lobatto (CGL) nodes $x_n = \cos\frac{\pi n}{N} \in [-1,1]$, has the explicit rank-2 QTT image ($y_p = 2^{L-p} i_p - 1$, $i_p \in \{0,1\}$),

$$\mathbf{X} \mapsto [\cos y_1 \ -\sin y_1] \otimes_{p=2}^{L-1} \begin{bmatrix} \cos y_p & -\sin y_p \\ \sin y_p & \cos y_p \end{bmatrix} \otimes \begin{bmatrix} \cos y_L \\ \sin y_L \end{bmatrix} \in \{0,1\}^{\otimes L}.$$



Approximation in TT format can be based on:

(a) Analytic methods.
(b) Canonical → TT recompression, (Any canonical decomposition is a good starting point for further algebraic TT-rank approximation).
(c) SVD-based recompression of TT-tensors.

Exer. 3.1. Derive and check by the TT Toolbox, the TT representation from the $n_1 \times \cdots \times n_d$ grid representation of the rank-2 FTT decomposition of $f(x) = f_1(x_1) + f_2(x_2) + \ldots + f_d(x_d)$, using (cf. *Exer. 1.3*),

$$f(x) = \begin{pmatrix} f_1(x_1) & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ f_2(x_2) & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ f_{d-1}(x_{d-1}) & 1 \end{pmatrix} \begin{pmatrix} 1 \\ f_d(x_d) \end{pmatrix}.$$

Exer. 3.2. Apply the rank-2 TT representation of a tensor related to

$$f(x) = \sin(x_1 + \ldots + x_d) = \frac{e^{ix} - e^{-ix}}{2i} = Im(e^{ix}),$$

to approximate the exact value of the multivariate integral for $d = 5, 10, 50$,

$$I(d) = Im \int_{[0,1]^d} e^{i(x_1 + \ldots + x_d)} dx = Im\left[\left(\frac{e^i - 1}{i}\right)^d\right].$$

Hint: Use Lem. 1.3, apply simple quadrature rule on uniform $n \times \ldots \times n$ grid, and TT scalar product.

Lem. 3.1. [BNK, Oseledets '09] (QTT map of multivariate polynomials)

- A general homogeneous polynomial potential of $\mathbf{q} = (q_1, \ldots, q_d) \in \mathbb{R}^d$,

$$V(\mathbf{q}) = \sum_{i_1,\ldots,i_m=1}^{d} a(i_1,\ldots,i_m) \prod_{k=1}^{m} q_{i_k}, \quad \mathrm{rank}_{TT}(V) \le C_0 d^{[\frac{m}{2}]}.$$

- Harmonic potential: QTT-ranks are bounded by 4,

$$V(\mathbf{q}) = \sum_{k=1}^{d} w_k q_k^2, \quad rank_{TT}(V) \le 2, \; rank_{QTT}(V) \le 4$$

- Henon-Heiles potential $V(\mathbf{q}) = \frac{1}{2}\sum_{k=1}^{d} q_k^2 + \lambda \sum_{k=1}^{d-1} \left(q_k^2 q_{k+1} - \frac{1}{3} q_k^3\right)$:

$$rank_{TT}(V) \le 3, \; rank_{QTT}(V) \le 7.$$

Storage of QTT-images of functions in $\mathbb{R}^d$: $O(d\overline{r}^2 \log N)$, $\overline{r}$- average rank.

Notice: $\mathrm{rank}_{Tuck}(V) = d$ in above cases $\Rightarrow \mathcal{O}(d^d)$ complexity scaling.

Ex. 3.2. QMD: Potential energy surfaces (PES) of d-atomic syst.

Average QTT-rank: $\overline{r}^2 = \frac{1}{d}\sum_{\ell=1}^{d} r_{\ell-1} r_\ell$, Storage $\le 2d\overline{r}^2 \log N$.

Function-related N-vector: $\mathbf{F} = \{f(a + (i - \frac{1}{2})h)\}_{i=1}^{N}$, $h = \frac{b-a}{N}$, $\varepsilon = 10^{-6}$

$N \setminus \overline{r}$	$e^{-\alpha x^2}$, $\alpha = 0.1 \div 10^2$	$\frac{\sin(\alpha x)}{x}$, $\alpha = 1 \div 10^2$	$1/x$	e^{-x}/x	$x, x^{10}, \sqrt[10]{x}$
2^{12}	3.1/2.9/2.9/2.6	3.8/4.8/5.6	4.2	3.8	1.9/2.6/3.9
2^{14}	2.9/2.8/2.8/2.8	3.6/4.7/5.5	4.2	3.8	1.9/2.5/3.9
2^{16}	2.8/2.7/2.8/2.8	3.6/4.5/5.4	4.2	5.3	1.9/2.4/3.9

$N \setminus \overline{r}$	$1/(x_1 + x_2)$	$e^{-\|x\|}$	$e^{-\|x\|^2}$	$\Delta_2^{-1}\mathbf{1}$, $\varepsilon = 10^{-6}, 10^{-7}, 10^{-8}$
2^9	5.0	9.4	7.8	3.6/3.6/3.6
2^{10}	5.1	9.4	7.7	3.6/3.6/3.6
2^{11}	5.2	9.3	7.5	3.7/3.7/3.7

QTT representation of PES

Compression of **Henon-Heiles** potential vs. dimensions d.

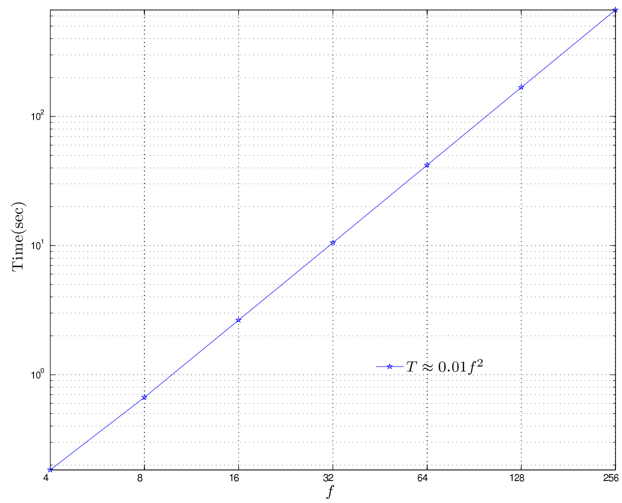


Figure 1: Timings: Can-to-QTT approx. of Henon-Heiles pot., $N = 1024$, $d = 4, \ldots, 256$.

Highest dim. considered $d = 256$, QTT-storage of V: ≤ 62.5 KB $\ll N^d$.

Logarithmic dependence on 1D grid-size $N = 2^L$, $\mathcal{O}(\log N)$.

Further Exercises

Exer. 3.3. Check the QTT rank of monomial, general polynomial and Chebyshev polynomial, all over uniform and Chebyshev grids in $[-1, 1]$.

Exer. 3.4. Test the QTT rank of $\sin$-Hemholtz kernel (scaling in κ?).

Exer. 3.5. Find the QTT rank of step-function and Haar wavelet.

In all cases look on the average rank,

$$\overline{r} := \sqrt{\frac{1}{d-1} \sum_{k=1}^{d-1} r_k r_{k+1}}.$$

Exer. 3.6. Linear-log-log scaling via quantics in auxiliary dimension: dth order Hilbert N-d tensor **A** of dimension $N^{\otimes d}$,

$$A(i_1, ..., i_d) = \frac{1}{i_1 + i_2 + ... + i_d} \approx \sum_{k=-M}^{M} c_k \bigotimes_{\ell=1}^{d} e^{-t_k i_\ell},$$

$i_1, ..., i_d = 1, ..., N = 2^L$, can be approximated by a rank-$|\log \varepsilon|$ tensor of order $D = d \log N$ and of size $2^{\otimes D}$, requiring only of

$$Q = d|\log \varepsilon| \log N \ll N^d \quad \text{reals.}$$

Using our canonical decomposition, compute its QTT aproximation applying C-to-QTT.

Numerical gain:

Matrix case: $d = 2,\ N = 2^{20} \Rightarrow Q = 40|\log \varepsilon| \ll 2^{40}$.

High dimension: $d = 2^{10},\ N = 2^{20} \Rightarrow Q = 20 \cdot 2^{10}|\log \varepsilon| \ll 2^{2 \cdot 10^4}$.

Theory.

- Exponential, polynomials, wavelets, sum/product of them: $O(\log N)$.
- Trivial extension to piecewise exponential/polynomial vectors.
- $f(x+y)$ separable with low rank.
- d-variate polynomials in $\mathbb{R}^d$: $O(d^{[m/2]})$-rank, a number of special cases.

Recent applications.

- Tucker/TT/QTT: Hartree-Fock, DFT: Green functions, Hartree, exchange potentials, electron density/orbitals.
- QTT: sPDEs, QMD (PES), FCI electron. struct., chemical master eq.
- QTT representation to retarded potentials, high-dim. integration.

Limitations.

- "Curse of ranks", dominace of rank-truncation (hope on QTT-DMRG)
- Schrödinger, Fokker-Planck hamiltonians are not (naively) separable :-(

Matrix product operators (**MPO**). A multi-way TT/QTT-matrix,

$$\boldsymbol{A} : \mathbb{X} := \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_d} \mapsto \mathbb{R}^{m_1} \times \ldots \times \mathbb{R}^{m_d} =: \mathbb{Y}$$

$$\boldsymbol{A}(i_1, j_1, \ldots, i_d, j_d) = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} U_1(i_1, j_1, \alpha_1) U_2(\alpha_1, i_2, j_2, \alpha_2) \cdot \ldots \cdot U_{D-1}(\alpha_{d-2}, i_{d-1}, j_{d-1}, \alpha_{d-1}) U_D(\alpha_{d-1}, i_d, j_d),$$

$U_k(i_k, j_k)$ is a $r_{k-1} \times r_k$ matrix.

Def. 3.4. For $\boldsymbol{A} \in \mathcal{L}(\mathbb{X} \to \mathbb{Y})$ and $\boldsymbol{X} \in \mathbb{X}$ denote the vector TT ranks of the matrix-by-vector product $\boldsymbol{AX}$ by $r_1 \ldots r_{d-1}$.

- The *operator TT rank* of $\boldsymbol{A}$ is defined by

$$\max_{\substack{k=1\ldots d-1,\\ \boldsymbol{X} \text{ is of vector TT rank } 1\ldots1}} r_k(\boldsymbol{AX}).$$

- *k-th vector TT rank* of $\boldsymbol{A}$ is the rank of its TT unfolding $\boldsymbol{A}_{[k]}$ $(1 \le k \le d-1)$ with the elements

$$\boldsymbol{A}_{[k]}(i_1 j_1 \ldots i_k j_k \,;\, i_{k+1} j_{k+1} \ldots i_d j_d) = \boldsymbol{A}(i_1 j_1 \ldots i_d j_d).$$

Rem. 3.1. $\boldsymbol{A} = u \times v$, $rank_{QTT}(u) \gtrless rank_{QTT}(v)$, apply Def. 3.4.

Ex. 3.3. d-dimensional Laplacian.

$$\Delta_d = A \otimes I_N \otimes \ldots \otimes I_N + I_N \otimes A \otimes I_N \ldots \otimes I_N + \ldots + I_N \otimes I_N \ldots \otimes A \in \mathbb{R}^{I^{\otimes d} \times I^{\otimes d}},$$

$A = \Delta_1 = \mathrm{tridiag}\{-1, 2, -1\} \in \mathbb{R}^{N \times N}$, I_N is the $N \times N$ identity.

- For the canonical rank: $rank_C(\Delta_d) = d$,
- For the Tucker rank: $rank_{Tuck}(\Delta_d) = 2$.
- Explicit rank-2 TT representation.

$$\Delta_d = \begin{bmatrix} \Delta_1 & I \end{bmatrix} \bowtie \begin{bmatrix} I & 0 \\ \Delta_1 & I \end{bmatrix}^{\otimes(d-2)} \bowtie \begin{bmatrix} I \\ \Delta_1 \end{bmatrix}.$$

The rank product operation "$\bowtie$" is defined as a regular matrix product of the two corresponding core matrices, their blocks being multiplied by means of tensor product.

- Discretized Henon-Heiles pot.: $rank_{TT}(\mathbf{V}) = 3$, $rank_{QTT}(\mathbf{V}) \le 7$.

Lem. 3.4. TT/QTT rank estimates:

- Explicit representations [Kazeev, BNK '10]:

$$rank_{QTT}(\Delta_1) = 3, \quad rank_{QTT}(\Delta_1^{-1}) \leq 5.$$

$$rank_{TT}(\Delta_d) = 2, \quad rank_{QTT}(\Delta_d) = 4.$$

- ε-rank:

$$rank_{TT}(\Delta_d^{-1}) \leq rank_C(\Delta_d^{-1}) \leq C|\log \varepsilon| \log N.$$

$$rank_{QTT}(\Delta_d^{-1}) \leq C|\log \varepsilon|^2 \log N.$$

- Variable coefficients:

$$rank_{QTT}\left(\nabla^T \operatorname{diag} a \nabla\right) \leq 7\, rank_{QTT}(a).$$

Ex. 3.4. Explicit QTT representation, $rank_{QTT}(\Delta_1) = 3$,

$$\Delta_1 = \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\otimes(d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix}.$$

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad J = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

Ex. 3.5. Reciprocal precondit. [Dolgov, BNK, Oseledets, Tyrtyshnikov '10]:

$$\Delta^{-1}\left(\nabla^T \frac{1}{a} \nabla\right) \Delta_d^{-1} \left(\nabla^T a \nabla\right) = I + R.$$

$d = 1 \Rightarrow rank(R) = 1$. Efficient for highly variable $a(x)$, $x \in \mathbb{R}^d$.

Summary: Tensor representation of operators

Theory.

- $sinc$-quadrature representation of A^{-1}, e^A, Green's functions.
- Explicit Tucker, TT, QTT representation of Δ_d related operators.
- PES, Henon-Heiles, spin Hamiltonians.
- d-dimensional convolution:
canonical/Tucker [Khoromskaia, BNK '08];
explicit QTT of $O(d \log N)$ complexity [Kazeev, BNK, Tyrtyshnikov '11].
- d-dimensional QTT-FFT, $O(d \log N)$ complex. [Dolgov, BNK, Savostyanov '11].

Recent applications.

- Operators in the Hartree-Fock eq., QMD, sPDEs, quantum comput.

Limitations.

- High cost of rank reduction, tensor represntation of the Schrödinger and Fokker-Planck hamiltonians, log-additive case of sPDEs.

Tensor numerical methods: Main ingredients

1. Discretization in tensor-product Hilbert space of N-d tensors, $\mathbf{V} = [V(i_1, ..., i_d)] \in \mathbb{V}_{\mathbf{n}} = \mathbb{R}^{n_1 \times \cdots \times n_d}$, $n_k = N$.
2. MLA in rank-$\mathbf{r}$ tensor formats $\mathcal{S} \subset \mathbb{V}_{\mathbf{n}}$:

$$\mathcal{S} \subset \{\mathcal{C}_R, \mathcal{T}_{\mathbf{r}}, \mathcal{T}_{\mathcal{C}_R,\mathbf{r}}, TT/TC[\mathbf{r}], QTT[\mathbf{r}]\}, \quad \mathbf{r} = [r_1, \ldots, r_d].$$

- Tensor truncation (projection), $T_{\mathcal{S}} : \mathcal{S}_0 \to \mathcal{S} \subset \mathcal{S}_0 \subset \mathbb{V}_{\mathbf{n}}$, based on SVD + (R)HOSVD + ALS/DMRG + multigrid.
- Scalar/Hadamard/contracted/convolution products on $\mathcal{S}$.

3. $\mathcal{S}$-tensor approximation of functions and operators.
4. Tensor-truncated solvers on low-parametr. manifold $\mathcal{S}$:

- Multilevel $\mathcal{S}$-truncated preconditioned iteration.
- Direct minimization on $\mathcal{S}$: ALS/DMRG in TT/QTT format.
- Direct $\mathcal{S}$-tensor solution operators via A^{-1}, $\exp(tA)$, Green's functions.

Conclusions and Challengin Problems

Well developed MLA on the Tucker, TT, and QTT tensors.

Representation of a broad class of functions $(+)$.

Representation of elliptic operators $(+)$.

QTT-FFT & QTT-convolution in $O(d \log N)$ complex. $(+)$.

Challenging problems:

Stochastic/parametric PDEs $(\pm)$,

Electronic Schrödinger hamiltonians, DFT $(\mp)$,

Molecular Schrödinger eq., $i\frac{\partial}{\partial t} + \mathcal{H}$, PES $(\pm)$.

Robust approximation in TC/TN formats $(?)$

Literature to Lecture 3

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2. B.N. Khoromskij, *Introduction to Tensor Numerical Methods in Scientific Computing.* Lecture Notes, Preprint 06-2011, University of Zuerich, Institute of Mathematics, 2011, pp 1 - 238. http://www.math.uzh.ch/fileadmin/math/preprints/06_11.pdf.

3. I.V. Oseledets, *Approximation of* $2^d \times 2^d$ *matrices using tensor decomposition.* SIAM J. Matrix Anal. Appl., 31(4):2130:2145, 2010.

4. I.V. Oseledets, and E.E. Tyrtyshnikov, *Breaking the Curse of Dimensionality, or How to Use SVD in Many Dimensions.* SIAM J. Sci. Comp., 31 (2009), 3744-3759.

5. I.V. Oseledets, and E.E. Tyrtyshnikov, *TT-cross approximation for multidimensional arrays.* Lin. Alg. and its Applications. 432 (2010), 70-88.

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