Traditional and novel tensor formats

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Setting - Tensors of order $d$

**Goal:** Generic perspective on methods for high-dimensional problems, i.e. problems posed on tensor spaces,

\[ \mathcal{V} := \bigotimes_{i=1}^{d} V_i, \quad \text{today:} \quad \mathcal{V} = \bigotimes_{i=1}^{d} \mathbb{R}^n = \mathbb{R}^{(n^d)} \]

**Notation:** $(x_1, \ldots, x_d) \mapsto U = U(x_1, \ldots, x_d) \in \mathcal{V}$

**Main problem:**

\[ \dim \mathcal{V} = \mathcal{O}(n^d) \quad – \quad \text{Curse of dimensionality!} \]

e.g. $n = 100, d = 10 \leadsto 100^{10}$ basis functions, 
\[ \leadsto \text{coefficient vectors of } 800 \times 10^{18} \text{ Bytes} = 800 \text{ Exabytes} \]

**Approach:** Some higher order tensors can be constructed (data-) sparsely from lower order quantities.

**As for matrices, incomplete SVD:**

\[ A(x_1, x_2) \approx \sum_{k=1}^{r} \sigma_k (u_k(x_1) \otimes v_k(x_2)) \]
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**Approach:** Some higher order tensors can be constructed (data-) sparsely from lower order quantities.

$$ \leadsto \text{Canonical decomposition for order-}d\text{-tensors:} $$

$$ U(x_1, \ldots, x_d) \approx \sum_{k=1}^{r} \sigma_k \left( \bigotimes_{i=1}^{d} u_{i,k}(x_i) \right). $$
Setting - Tensors

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

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

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.

\[ k \mapsto U(k_1, \ldots, k_d) = (U_{k_1, \ldots, k_d}) \quad , \quad k_i = 1 \ldots, n_i . \]

Or in index (vectorial) notation

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

\[ \dim \mathcal{H} = n^d \quad \text{curse of dimensions!!!} \]

E.g. wave function \( \psi(r_1, s_1, \ldots, r_N, s_N) \)
Tensors, basis vectors and linear operators

Tensor product basis from uni-variate basis

\[ \{ v_i \in V_i : i = 1, \ldots, n_i \} : \]

\[ \{ \mathbf{V}_{k_1, \ldots, k_d} = \mathbf{v}_{k_1} \otimes \ldots \otimes \mathbf{v}_{k_d} = \bigotimes_{i=1}^{d} \mathbf{v}_{k_i} \in \mathcal{H} : 1 \leq k_i \leq n_i, 1 \leq i \leq d \} \]

Linear operators \( A : \mathcal{H} \to \mathcal{H} \) in index notation

\[ A =: \left( A^y_x \right) = \left( A^{y_1, \ldots, y_l}_{x_1, \ldots, x_d} \right) \]

and vectorized (tensorized)

\[ (x_1, \ldots, x_d, y_1, \ldots, y_l) \to A(x_1, \ldots, x_d, y_1, \ldots, y_l) \in \mathcal{H}_x \otimes \mathcal{H}_y . \]

Matricisation or unfolding:

\[ A =: \left( A^k_x \right), \quad A = \left( A^{k_1, \ldots, k_l}_{x_1, \ldots, x_d} \right) := \left( a_{x_1, \ldots, x_d; k_1, \ldots, k_l} \right) . \]
Canonical format

\[ \mathcal{H} \simeq \{ \mathbf{x} = (x_1, \ldots, x_d) \mapsto U(x_1, \ldots, x_d) \in \mathbb{R}, x_i = 1, \ldots, n_i \} . \]

Single tensor product

\[ (x_1, \ldots, x_d) \mapsto U(x_1, \ldots, x_d) = \prod_{i=1}^{d} u_{i,k}(x_i) = \prod_{i=1}^{d} u_i(x_i, k) , \]

\[ U = \bigotimes_{i=1}^{d} u_{k,i} . \]

Canonical (CP) format, PARAFAC or r-term expansion,

\[ U(x_1, \ldots, x_d) = \sum_{k=1}^{r_C} U_k(x) = \sum_{k=1}^{r_C} \prod_{i=1}^{d} u_{i,k}(x_i) . \]

or

\[ U = \sum_{k=1}^{r_C} U_k = \sum_{k=1}^{r_C} \bigotimes_{i=1}^{d} u_{i,k} . \]
Canonical format - pros
Definition (Canonical format)

\[ U(x_1, \ldots, x_d) = \sum_{k=1}^{r} \bigotimes_{i=1}^{d} u_{i,k}(x_i) = \sum_{i=1}^{r} \bigotimes_{\nu=1}^{d} u_i(x_i, k). \]

\( r \) - canonical rank (?

Let \( n := \max\{n_i : 1 \leq i \leq d\} \).

- Number of terms \( r = r_c \) (canonical rank (?)) is invariant w.r.t. basis transformations
- canonical rank \( r \leq \# \text{ DOF} \) for a given tensor product basis - best \( N \)-term approximation (super adaptivity)!
- there is an additional cost storing the components \( u_{i,k_i} \)
- degrees of freedom (DOF) or better storage complexity: \( \mathcal{O}(drn) \)
- complexity scaling is \( \mathcal{O}(drn) \) instead of \( \mathcal{O}(n^d) \) for the full tensor!
Counter example of Silva and Lim

Let \( A = \bigotimes_{i=1}^{d} a_i \), \( B = \bigotimes_{i=1}^{d} b_i \in \mathcal{H} \), (possibly \( \langle a_i, b_i \rangle = 0 \ \forall i \)).

Let 

\[
\begin{align*}
U(x_1, \ldots, x_d) &:= U_1(x_1, \ldots, x_d) + \ldots + U_d(x_1, \ldots, x_d) , \quad (U_i \perp U_j) \\
&:= b_1(x_1)a_2(x_2)\ldots a_d(x_d) + \cdots + a_1(x_1)\ldots a_{d-1}(x_{d-1})b_d(x_d) \\
&= \frac{1}{\epsilon}(a_1(x_1) + \epsilon b_1(x_1)) \cdots (a_d(x_d) + \epsilon b_d(x_d)) \\
&\quad - \frac{1}{\epsilon} a_1(x_1) \cdots a_d(x_d) + \mathcal{O}(\epsilon) \\
&=: V_\epsilon(x_1, \ldots, x_d) + \mathcal{O}(\epsilon) , \quad \text{product -rule for } A'.
\end{align*}
\]

\( V_\epsilon \to U \) as \( \epsilon \to 0 \), but rank \( r_c(U) = d \neq r_c(V_\epsilon) = 2 \) if \( d \geq 3 \)

\[ \Rightarrow \]

\[ \mathcal{K}^{\leq r} := \{ U \in \mathcal{H} : U = \sum_{k=1}^{r} U_k \} \text{ is not closed.} \]

(nor weakly closed)

\[ \Rightarrow \text{The notion of canonical rank is not well defined! Border rank problem.} \]

Remark: The above example shows the product rule for the directional derivative
Optimization Problems

Problem (Generic optimization problem (OP))

Given a cost functional \( F : \mathcal{H} \rightarrow \mathbb{R} \) and an admissible set \( \mathcal{M} \subset \mathcal{H} \) finding

\[
\arg\min \{ F(W) : W \in \mathcal{M} \}.
\]

Problem (Tensor product optimization problem (TOP))

\[
U := \arg\min \{ F(W) : W \in \mathcal{M} \cap \mathcal{K}^{\leq r} \} \tag{1}
\]

Here we consider a modified optimization problem where the original admissible set is confined to tensors of rank at most \( r \). Most problems can cast into this form.
Example

1. Approximation: for given $U \in \mathcal{H}$ minimize

$$F(W) = \| U - W \|_{\mathcal{H}}^2 = \| U - W \|^2, \ W \in \mathcal{K}^r$$

2. solving equations: where $A, g : \mathcal{V} \to \mathcal{H}$,

$$AU = B \text{ or } g(U) = 0$$

here

$$F(W) := \| AW - B \|^2 \text{ resp. } F(W) := \| g(W) \|^2.$$ 

3. or, if $A : \mathcal{V} \to \mathcal{V}'$ is symmetric and $B \in \mathcal{V}'$, $\mathcal{V} \subset \mathcal{H} \subset \mathcal{V}'$,

$$F(W) := \frac{1}{2} \langle AW, W \rangle - \langle B, W \rangle$$

4. computing the lowest eigenvalue of a symmetric operator $A : \mathcal{V} \to \mathcal{V}'$,

$$U = \text{argmin} \left\{ F(W) = \langle AW, W \rangle : \langle W, W \rangle = 1 \right\}.$$ 

In many cases $\mathcal{M} \cap \mathcal{K}^{\leq r} = \mathcal{K}^{\leq r}$, and most $F$ are quadratic.
Tensor optimization problem

\[ U = \arg\min \ F(W) \text{ means finding } u_{i,k} \in V \text{ s. t.} \]
\[ U = \sum_{k=1}^{r} \bigotimes_{i=1}^{d} u_{i,k} \]

The unknown components are

\[ u := (u_{i,k})_{k=1,...,r,i=1,...,d} \in V^{r \times d} = \times_{i=1}^{d} \times_{k=1}^{r} V. \]

Definition

We introduce the (multi-linear) mapping

\[ T : V^{r \times d} \to \mathcal{H} = \bigotimes_{\nu=1}^{d} V, \ u \mapsto U = T(u) := \sum_{k=1}^{r} \bigotimes_{k=1}^{d} u_{i,k}. \]

Then our original optimization problem takes the form TOP1:
Finding

\[ u = \arg\min \{ J(w) := F(T(w)) : T(w) \in \mathcal{M}, w \in V^{r \times d} \}. \]

Even, if OP is well posed, TOP, or equivalently TP1, will be no longer be well posed!
Canonical format - cons

In order to get rid of the non-closedness, further assumptions are required

- assuming an upper bound $\|U_k\| \leq C$, by penalization, see Espig et al.
- assuming positivity $U_k(x) \geq 0$, by inequality constraints
- assuming orthogonality $\langle U_k, U_l \rangle = 0$, $k \neq l$, (???? not yet clear how to do this).

Redundancy could only partially be removed. Obvious redundancy could be avoided, see Espig etc.

Approximation or optimization suffer from all kind of troubles:

- no uniqueness
- often trapped by local minima
- Canonical rank $r$ is not low, in real applications.
- Usually, it becomes worse with increasing ranks.
- there is no dynamical formulation

Canonical format cannot be recommended without serious warnings!
Algorithmic treatment of (TP3)

**Goal:** First/second order methods for (TP3).

Directional derivatives of $T(u) := \sum_{i=1}^{r} \bigotimes_{\nu=1}^{d} u_{i,\nu}$ w.r.t. $u_{k,\alpha}$, $u_{\ell,\beta}$:

$$[ T'_{(k,\alpha)}(u) ](v) = (\bigotimes_{\nu=1}^{\alpha-1} u_{k,\nu}) \otimes v \otimes (\bigotimes_{\nu=\alpha+1}^{d} u_{k,\nu}),$$

$$[ T''_{(k,\alpha), (\ell,\beta)}(u) ](v, w) = \delta_{k,\ell} (1 - \delta_{\alpha,\beta}) (\bigotimes_{\nu=1}^{\alpha-1} u_{k,\nu}) \otimes v \otimes (\bigotimes_{\nu=\alpha+1}^{\beta-1} u_{k,\nu}) \otimes w \otimes (\bigotimes_{\nu=\beta+1}^{d} u_{k,\nu}).$$

Directional derivatives of $J(u) := F(T(u))$:

$$[ J'_{(k,\alpha)}(u) ](v) = \left\langle F'(T(u)), [ T'_{(k,\alpha)}(u) ](v) \right\rangle,$$

$$[ J''_{(k,\alpha), (\ell,\beta)}(u) ](v, w) = \left\langle F''(T(u))[ T'_{(\ell,\beta)}(u) ](w), [ T'_{(k,\alpha)}(u) ](v) \right\rangle$$

$$+ \left\langle F'(T(u)), [ T''_{(k,\alpha), (\ell,\beta)}(u) ](v, w) \right\rangle.$$
Example: Second order methods, linear equation

\[ AU = B \quad \text{for} \quad A = \sum_{j=1}^{R} \bigotimes_{\nu=1}^{d} A_{j,\nu}, \quad B = \sum_{j=1}^{s} \bigotimes_{\nu=1}^{d} b_{j,\nu}. \]

\[
\begin{align*}
[F'(U)](V) &= \langle AU, V \rangle - \langle B, V \rangle, \\
[F''(U)](V, W) &= \langle AU, V \rangle.
\end{align*}
\]

Gradient of \( J(u) := F(T(u)) \):

\[
[J'_{(k,\alpha)}(u)](\cdot) = \sum_{i=1}^{r} \sum_{j=1}^{R} \left( \prod_{\nu \neq \alpha} \langle A_{j,\nu} u_i, \nu, u_k, \nu \rangle \right) A_{j,\alpha} u_i,\alpha - \sum_{j=1}^{s} \left( \prod_{\nu \neq \alpha} \langle b_{j,\nu}, u_k, \nu \rangle \right) b_{j,\alpha}
\]

Approximate Hessian of \( J(u) \):

\[
[J''_{(k,\alpha),(\ell,\beta)}(u)](V, W) = \delta_{\alpha,\beta} \cdot \sum_{j=1}^{R} \left( \prod_{\nu \neq \alpha} \langle A_{j,\nu} u_k, \nu, u_{\ell,\nu} \rangle \right) \langle A_{j,\alpha} V, W \rangle \\
+ (1 - \delta_{\alpha,\beta})[\ldots]
\]
Example: Second order methods, linear equation

Solve \( AU = B \) for \( A = \sum_{j=1}^{R} \bigotimes_{\nu=1}^{d} A_{j,\nu} \), \( B = \sum_{j=1}^{s} \bigotimes_{\nu=1}^{d} b_{j,\nu} \).

\[
[F'(U)](V) = \langle AU, V \rangle - \langle B, V \rangle, \quad [F''(U)](V, W) = \langle AU, V \rangle.
\]

**Gradient of \( J(u) \):**

\[
[J'_{(k,\alpha)}(u)](.) = \sum_{i=1}^{r} \sum_{j=1}^{R} (\prod_{\nu \neq \alpha} \langle A_{j,\nu} u_i,\nu, u_k,\nu \rangle) A_{j,\alpha} u_i,\alpha - \sum_{j=1}^{s} (\prod_{\nu \neq \alpha} \langle b_{j,\nu}, u_k,\nu \rangle) b_{j,\alpha}
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$$

**Approximate Hessian of $J(u)$:**

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+ (1 - \delta_{\alpha,\beta})[\ldots]
$$
Greedy algorithm

Best $\mathcal{H}$ approximation: Given tensor $U \in \mathcal{H}$ find $T(u) \in \mathcal{K}^\leq r$, which approximates

$$\|U - T(u)\| \rightarrow 0, \quad r \rightarrow \infty.$$ 

Start $V_1 := U$ For $k = 1, \ldots, r$

- Find best rank one approximation
  $$\text{argmin}\{\|U_k - V_k\| : U_k = \bigotimes_{i=1}^d u_{k,i}\}$$
- $V_{k+1} := V_k - U_k$
- repeat

Ehrlacher et al. have shown convergence of the greedy method for strongly convex $F$.

Result from Lim:

**Theorem**

For $d \geq 3$, computing a minimizer

$$\text{argmin}\{\|U_k - V_k\| : U_k = \bigotimes_{i=1}^d u_{k,i}\}$$ is NP hard.
Remarks and conclusions

Further remarks:

1. Sum of exponentials (e.g. discretized Laplace-Transform)

\[
\frac{1}{x_1 + \ldots + x_d} = \int_0^\infty e^{-s(x_1+\ldots+x_d)} ds \approx \sum_k \omega_k e^{-s_k(x_1+\ldots+x_d)}, \quad x_i > 0, \quad 1 \leq i \leq d.
\]

2. Sufficient conditions for uniqueness of the CP format are stated by Kruskal.

3. For symmetric tensors a recovery scheme has been provided by P. Comon.

4. The canonical format is often considered as the true tensor product format.

5. Its complexity scaling is ideal \(O(n d r)\)!

6. .... there is much more to tell you ...

Conclusion:

The canonical format is like a \textit{Queen of Night}, you and everybody like to dance with. But you must be an extremely good dancer, not to get dissapointed.
Tucker format - subspace approximation

**Tucker format**

\[
U(x_1, \ldots, x_d) = \sum_{k_1=1}^{r_1} \ldots \sum_{k_d=1}^{r_d} V(k_1, \ldots, k_d) \bigotimes_{i=1}^{d} u_{k_i}(x_i)
\]

\[r = (r_1, \ldots, r_d) \text{ rank (array) } r := \max\{r_i : 1 \leq i \leq d\} - \text{ max. Tucker rank.}
\]

\[(k_1, \ldots, k_d) \rightarrow V(k_1, \ldots, k_d) - \text{ core tensor in } \mathbb{R}^{r_1 \times \cdots \times r_d}.
\]

Tucker format is a subspace approximation:
\[V_i = \text{span } \{u_{k_i} : k_i = 1, \ldots, r_i\} \text{ univariate basis } x_i \mapsto u_{k_i}(x_i) \text{ can be choosen to ONB } \langle u_{i,k_i}, u_{i,l_i} \rangle = \delta_{l,k}.
\]

\[
U = \sum_{k_1=1}^{r_1} \ldots \sum_{k_d=1}^{r_d} V(k_1, \ldots, k_d) \bigotimes_{i=1}^{d} u_{k_i}
\]

Remark: The two formats are identical if \(d = 2\) or \(r_c = 1\).
Tucker format

Degr. of freedom (DOF): \[ \text{DOF} : \mathcal{O}(r_{\text{max}}^{d} + d r_{\text{max}} n) \], \( n : = \max\{n_i : 1 \leq i \leq d\} \).

If \( d = 2 \) or \( r = 1 \) it is \( \approx \) canonical format. **Curse of dimensionality!**

But: \( \mathcal{T}^{\leq r} = \bigcup_{s_i=1}^{r_i} \mathcal{T}^{s} = \text{clos} \ \mathcal{T}^{r} \) is closed (Falco & Hackbusch)-Segre variety

\( \mathcal{T}^{r} \) is an **embedded manifold** (Lubich et al.)

Tucker format is well established in physics: in particular for anti-(symmetric) functions. It allows the treatment of dynamical problems.

Examples: MCSCF (Multi configuration self-consistent field), Analysis: infinite-dim.: Friesecke, M. Lewin, TDMCH (time dep. multi-configurational Hartree approximation)

Stable (submanifold), But \[ \text{DOF} : \mathcal{O}(r_{\text{max}}^{d} + d r_{\text{max}} n) \], **Curse of dimensionality!**

- Is there a format breaking the curse of dimensionality, and inheriting the properties of the Tucker format?
Hierarchical Tucker (HT) format
Hackbusch & Kühn (2009), Grasedyck (2010)

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

TT-representation of $U$

$$U(x) = U_1(x_1) \cdots U_i(x_i) \cdots U_d(x_d)$$

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

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

DOFs: $O(ndr^2)$, TT and HT inherits nice properties from the Tucker format!
Thank you
for your attention.

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