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Bridging continuous and discrete tensor representations of multivariate functions via QTT

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Chebyshev-Tucker (ChebTuck) format

Discrete and continuous tensor formats

$f:[-1,1]^D \to \mathbb{R}$, $D=3$. Approx. f with a *small number of parameters* $\rightsquigarrow$ cheap comput. with f.

1. **Grid-based methods**: discrete Tucker approximation of function related tensor $\mathbf{F}$ (contains, e.g., function values on a grid):

$$\mathbf{F} \approx \sum_{i_1=1}^{R}\sum_{i_2=1}^{R}\sum_{i_3=1}^{R}\beta_{i_1,i_2,i_3}\mathbf{a}^{(1)}_{i_1}\otimes\mathbf{a}^{(2)}_{i_2}\otimes\mathbf{a}^{(3)}_{i_3} \in \mathbb{R}^{n\times n\times n},$$
$$\mathbf{F}_{i_1,i_2,i_3} := f(t^{(1)}_{i_1}, t^{(2)}_{i_2}, t^{(3)}_{i_3}),\ t^{(\ell)}_{i_\ell} = -1+(i_\ell-1)h,\ h=2/(n-1),\ i_\ell = 1,\cdots,n. \quad (1)$$

- Storage: $\mathcal{O}(DRn+R^D)$. Disadvantage: *large* n required to achieve high accuracy.

2. **Mesh-free methods**: functional Tucker approximation of f directly:

$$f(x_1,x_2,x_3) \approx f_{\mathbf{m}}(x_1,x_2,x_3) := \sum_{i_1=1}^{R}\sum_{i_2=1}^{R}\sum_{i_3=1}^{R}\beta_{i_1,i_2,i_3}v^{(1)}_{i_1}(x_1)v^{(2)}_{i_2}(x_2)v^{(3)}_{i_3}(x_3)$$
$$v^{(\ell)}_{i_\ell}(x_\ell) = \sum_{j_\ell=1}^{m} V^{(\ell)}_{j_\ell,i_\ell}T_{j_\ell-1}(x_\ell),\ V^{(\ell)}\in\mathbb{R}^{m\times R},\ T_{j}(x)=\cos(j_\ell \arccos(x)). \quad (2)$$

- Storage: $\mathcal{O}(DRm+R^D)$. $m \ll n$ for the same accuracy as grid-based methods.
- We call it **ChebTuck format**. It is also the format Chebfun3 [3] assumes.

Three natural tasks	Input	Output	Note
Function to ChebTuck (See [1,3])	$f:[-1,1]^3\to\mathbb{R}$	ChebTuck $f_{\mathbf{m}}$	f can be evaluated freely in $[-1,1]^3$
Grid to ChebTuck (See [1])	grid-based $\mathbf{F}$ of f	ChebTuck $f_{\mathbf{m}}$	Preferably $m \ll n$
ChebTuck to Grid (our focus)	ChebTuck $f_{\mathbf{m}}$ of f	grid-based $\mathbf{F}$	$n \gg m$, but storage largely reduced by QTT

ChebTuck to Grid-based tensor

- Given ChebTuck $f_{\mathbf{m}}$ (2) of f, to get a grid-based tensor, naive approach yields a discrete Tucker:
$\mathbf{F}_{\mathbf{m}}(i_1,i_2,i_3) := f_{\mathbf{m}}(t^{(1)}_{i_1}, t^{(2)}_{i_2}, t^{(3)}_{i_3}) \Rightarrow \mathbf{F}_{\mathbf{m}} = \beta\times_1 U_1\times_2 U_2\times_3 U_3,\ U_\ell(i_\ell,j_\ell) = v^{(\ell)}_{j_\ell}(t^{(\ell)}_{i_\ell})$ (c.f. (1)),
i.e., each column of U_ℓ contains the discretization of a polynomial $v^{(\ell)}_{j_\ell}(x_\ell)$ on grid $\{t^{(\ell)}_{i_\ell}\}$.
- **Additional storage**: $\mathcal{O}(DRn)$. **Remedy**: store columns of U_ℓ as QTT [Khoromskij'11].

Definition (Quantized Tensor Trains (QTT) format of a univariate function)

Let $p:[-1,1]\to\mathbb{R}$ be a univariate function. Discretizing it on a uniform grid $\{x_i := -1+(i-1)h\}_{i=1}^n$ with $h=2/(n-1)$, $n=2^d$ yields $\mathbf{p}=[p(x_i)]_{i=1}^n\in\mathbb{R}^n$.
The multi-index mapping $(i_1,\cdots,i_D)\mapsto i_{\le d} = 1+(i_1-1)+2\cdot(i_2-1)+\cdots+2^{d-1}\cdot(i_d-1)$ for $i_\ell=1,2$ reshapes $\mathbf{p}$ into a d-dimensional tensor $\mathbf{P}\in\mathbb{R}^{2\times\cdots\times 2}$:

$$\mathbf{P}(i_1,\cdots,i_d) = p(x_{i_{\le d}}) = p\Big(\underbrace{-1+(i_1-1)h}_{=:x^{(1)}_{i_1}} + \underbrace{2\cdot(i_2-1)h}_{=:x^{(2)}_{i_2}}+\cdots+\underbrace{2^{d-1}\cdot(i_d-1)h}_{=:x^{(d)}_{i_d}}\Big).$$

QTT of p is defined as a TT (with cores $\mathbf{G}_\ell(i_\ell)\in\mathbb{R}^{r_{\ell-1}\times r_\ell}$ and ranks $r_\ell\le r$) of $\mathbf{P}$:

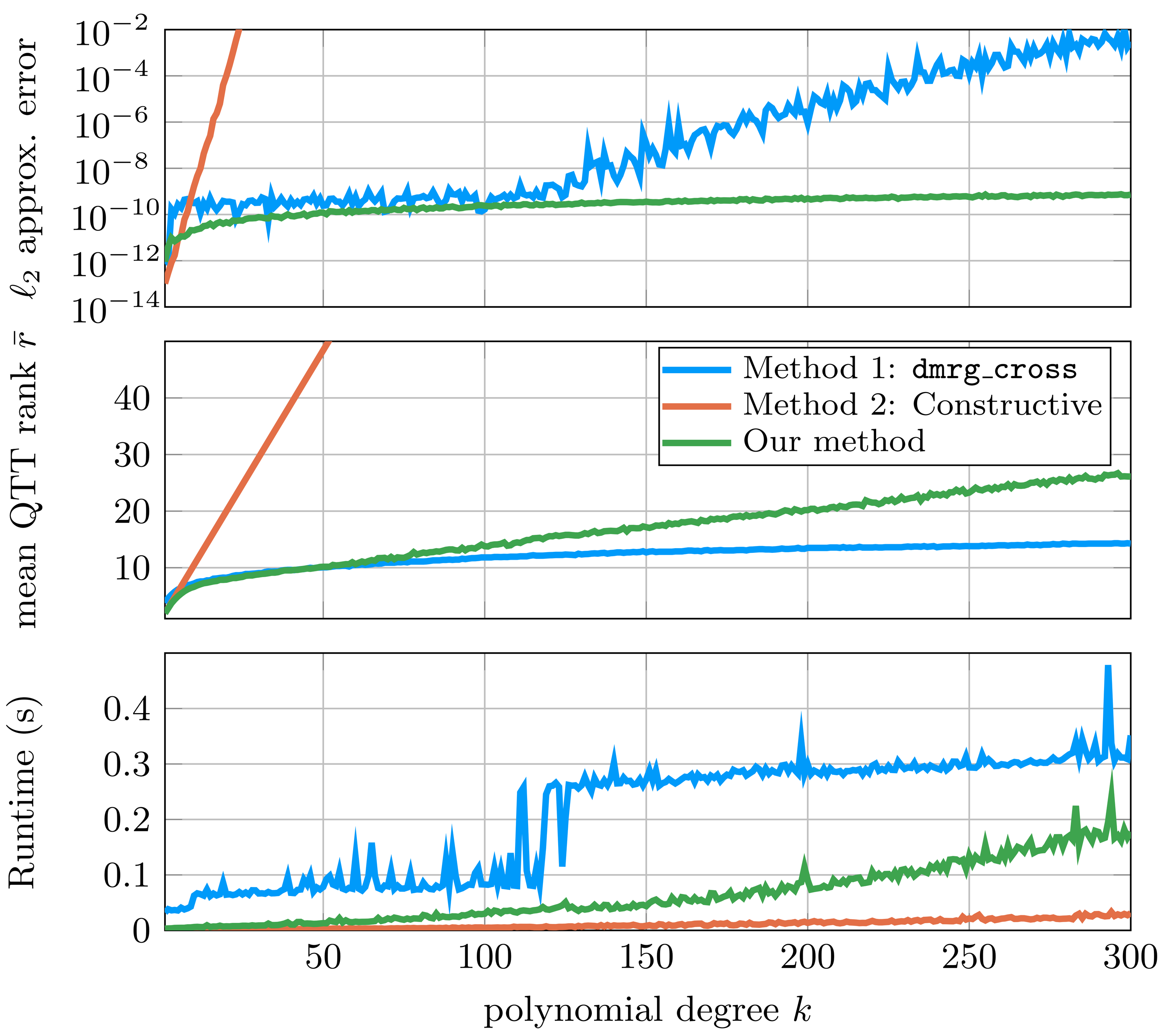
$$p(x^{(1)}_{i_1}+x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) = \mathbf{P}(i_1,\cdots,i_d) = \mathbf{G}_1(i_1)\mathbf{G}_2(i_2)\cdots\mathbf{G}_d(i_d) \text{ for } i_1,\cdots,i_d = 1,2.$$

- Storage of U_ℓ in QTT: $\mathcal{O}(DRdr^2) = \mathcal{O}(DRr^2\log n)$.
- **Classical result**: QTT ranks of degree m polynomials $\le m+1$ [Khoromskij'11, Oseledets'13] (numerically even $\log m$) $\rightsquigarrow$ reduces storage of U_ℓ from $\mathcal{O}(DRn)$ to $\mathcal{O}(DRm^2\log n)$ (numerically $\mathcal{O}(DR\log^2 m\log n)$).
- **Fundamental task**: approximate a polynomial p in QTT format efficiently $\rightsquigarrow$ our focus

Numerical experiments

Approximating Chebyshev polynomials $T_k(x)$ in QTT

- Similar results are obtained for other class of polynomials, e.g., random linear combinations of monomials/Chebyshev polynomials.



Approximation of a polynomial in QTT format

Computational methods for the TT format of $\mathbf{P}$

1. **Direct method**: apply directly the adaptive TT cross, e.g., `dmrg_cross` [Savostyanov/Oseledets'11].
   - Disadvantage: heuristic; doesn't exploit the 1D nature of the problem, just view $\mathbf{P}$ as a black box tensor.
2. **Constructive method**: $\exists$ an analytic formula [Oseledets'13] for the cores $\mathbf{G}_\ell(i_\ell)\in\mathbb{R}^{(m+1)\times(m+1)}$.
   - Disadvantage: is numerically unstable even for moderate $m>20$ & produces pessimistic TT ranks $m+1$.

Our novel method: Constructive (thus faster than Method 1), stable and rank adaptive.

Recall Oseledets' constructive method for $p(x) = p_0+p_1x+\cdots+p_mx^m$

Introduce the notation: $X_{\le k}(x) := [1,x,\cdots,x^k]^\top\in\mathbb{R}^{k+1}$

1. Notice that with $M(\alpha+1,\beta+1) = p_{\alpha+\beta}C^{\alpha}_{\alpha+\beta}$ for $\alpha+\beta\le m$ otherwise 0 (M is skew-upper triangular), it holds

$$p(x+y) = \sum_{\alpha=0}^{m}\sum_{\beta=0}^{m} M(\alpha+1,\beta+1)x^\alpha y^\beta \implies p(x+y) = X_{\le m}(x)^\top M X_{\le m}(y). \quad (3)$$

2. Let $x = x_{i_1}$ and $y = x_{i_2}+\cdots+x_{i_d}$, then separate x_{i_1} from the rest:

$$p(x^{(1)}_{i_1}+x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) = \underbrace{X_{\le m}(x^{(1)}_{i_1})^\top M}_{=\mathbf{G}_1(i_1)} X_{\le m}(x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}). \quad (4)$$

3. Similarly, $\mathbf{G}_2(i_2)$ is constructed such that $X_{\le m}(x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) = \mathbf{G}_2(i_2)X_{\le m}(x^{(3)}_{i_3}+\cdots+x^{(d)}_{i_d})$ holds,

$$\implies \mathbf{P}(i_1,i_2,\cdots,i_d) = \mathbf{G}_1(i_1)\mathbf{G}_2(i_2)X_{\le m}(x^{(3)}_{i_3}+\cdots+x^{(d)}_{i_d}).$$

4. Other cores $\mathbf{G}_3(i_3),\cdots,\mathbf{G}_d(i_d)$ are constructed similarly.

Disadvantage: Unstable since M contains large binomial coefficients & small powers e.g. $(x^{(1)}_{i_1})^\alpha$
Fixing idea: Replace x^α, y^β by Chebyshev polynomials!

$$p(x+y) = \sum_{\alpha=0}^{m}\sum_{\beta=0}^{m} M^c(\alpha+1,\beta+1)T_\alpha(x)T_\beta(y) \quad (5)$$

- A subtle but crucial difference between (3) and (5): (3) holds for all $x,y\in\mathbb{R}$ for fixed coefficients M, while (5) only holds for $x\in I_x$ and $y\in I_y$ with some intervals I_x, I_y and the coefficients M^c depend accordingly on these intervals.
- For an interval $I=[a,b]$, introduce the notation:
$T^I_\ell(x) := T_\ell((2x-(a+b))/(b-a))$, $T^I_{\le k}(x) := [1, T^I_1(x),\cdots,T^I_k(x)]^\top\in\mathbb{R}^{k+1}$ for $x\in I=[a,b]$.

Our novel method: constructive, stable & rank adaptive

Recall: 1D Chebyshev interpolation

Let $p: I\to\mathbb{R}$ be a univariate function. Then its Chebyshev interpolation of degree m is given by

$$p(x)\approx g_m := \sum_{\ell=0}^{m} c_\ell T^I_\ell(x) = \mathbf{c}^\top T^I_{\le m}(x) \text{ with } \mathbf{c} = W\mathbf{p},\ W \text{ being an inverse DCT matrix}$$

and $\mathbf{p}\in\mathbb{R}^{m+1}$ containing the function values of p at the Chebyshev points on I. In particular if p is a polynomial of degree $\le m$, then the interpolation is **exact**: $p(x) = g_m(x)$ for all $x\in I$.

- Let $I_{\ge k} = [\sum_{\ell=k}^{d} x^{(\ell)}_1, \sum_{\ell=k}^{d} x^{(\ell)}_2]$, then we have $x^{(k)}_{i_k}+x^{(k+1)}_{i_{k+1}}+\cdots+x^{(d)}_{i_d}\in I_{\ge k}$.

1. Let $M^c_{i_1}\in\mathbb{R}^{1\times(m+1)}$ be the Chebyshev coefficients of the function $I_{\ge 2}\ni x\mapsto p(x^{(1)}_{i_1}+x)$:

$$p(x^{(1)}_{i_1}+x) = M^c_{i_1}T^{I_{\ge 2}}_{\le m}(x) \text{ for } x\in I_{\ge 2},\ i_1=1,2, \text{ and in particular} \quad (6)$$
$$\mathbf{P}(i_1,i_2,\cdots,i_d) = p(x^{(1)}_{i_1}+x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) = M^c_{i_1}T^{I_{\ge 2}}_{\le m}(x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) \quad (7)$$

We can already set here $\mathbf{G}(i_1) := M^c_{i_1}$ to obtain the first QTT core (c.f. Eq. (4))

2. Yet to make it rank adaptive, we compute a LRA (e.g. SVD) of the Chebyshev coefficients:

$$\begin{bmatrix} M^c_1 \\ M^c_2\end{bmatrix} \approx U_1V_1^\top \text{ with } U_1\in\mathbb{R}^{2\times r_1},\ V_1\in\mathbb{R}^{(m+1)\times r_1}.$$

3. Let $U_{1,i_1} := U_1(i_1,:)\in\mathbb{R}^{1\times r_1}$, then $M^c_{i_1}\approx U_{1,i_1}V_1^\top$. Then Eq. (7) becomes

$$\mathbf{P}(i_1,i_2,\cdots,i_d)\approx U_{1,i_1}V_1^\top T^{I_{\ge 2}}_{\le m}(x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) = U_{1,i_1}v^{(2)}_{\le r_1}(x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) \quad (8)$$

where we have defined the polynomial vector $v^{(2)}_j(y)$ on the interval $I_{\ge 2}$ as

$$v^{(2)}_{\le r_1}(y) := [v^{(2)}_1(y),\cdots,v^{(2)}_{r_1}(y)]^\top\in\mathbb{R}^{r_1} \text{ with } v^{(2)}_j(y) := V_1(:,j)^\top T^{I_{\ge 2}}_{\le m}(y) \text{ for } j=1,\cdots,r_1,\ y\in I_{\ge 2}.$$

The first QTT core can thus be taken as $\mathbf{G}_1(i_1) = U_{1,i_1}$.

4. For the 2nd QTT core, note that each $I_{\ge 3}\ni x\mapsto v^{(2)}_j(x^{(2)}_{i_2}+x)$ for $j=1,\cdots,r_1$ and $i_2=1,2$ is a polynomial of degree $\le m \implies$ has $\le m+1$ non-zero Cheb. coeff. denoted by $C^c_{2,i_2}(j,:)\in\mathbb{R}^{m+1}$:

$$v^{(2)}_{\le r_1}(x^{(2)}_{i_2}+\cdots+x^{(d)}_{i_d}) = C^c_{2,i_2}T^{I_{\ge 3}}_{\le m}(x^{(3)}_{i_3}+\cdots+x^{(d)}_{i_d}). \quad (9)$$

We then compute a LRA of $\begin{bmatrix} C^c_{2,1}\\ C^c_{2,2}\end{bmatrix}\approx U_2V_2^\top$ with $U_2\in\mathbb{R}^{2r_1\times r_2}$, $V_2\in\mathbb{R}^{(m+1)\times r_2}$.

Let us denote $U_{2,i_2} := U_2(r_1(i_2-1)+1:r_1i_2,:)\in\mathbb{R}^{r_1\times r_2}$, then $C^c_{2,i_2}\approx U_{2,i_2}V_2^\top$. Thus

$$\mathbf{P}(i_1,i_2,\cdots,i_d)\approx U_{1,i_1}C^c_{2,i_2}T^{I_{\ge 3}}_{\le m}(x^{(3)}_{i_3}+\cdots+x^{(d)}_{i_d})\approx U_{1,i_1}U_{2,i_2}V_2^\top T^{I_{\ge 3}}_{\le m}(x^{(3)}_{i_3}+\cdots+x^{(d)}_{i_d}) \quad (10)$$

The second QTT core is therefore $\mathbf{G}_2(i_2) = U_{2,i_2}$. Other cores are constructed similarly.

References

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