CEMRACS,
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Approximation and learning with tensor networks

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Tensor networks

Tensor networks are prominent tools for the representation or approximation of multivariate functions or multidimensional arrays.

- A long history in quantum physics.
- Tree tensor networks appeared independently in numerical analysis, as an extension of low-rank decompositions to high-order tensors.
- Growing use in statistics, data science and probabilistic modelling.

Computing with tensor networks

- For the approximation of a known tensor u with respect to a certain norm, we aim at finding a tensor network v with low complexity that minimizes

$$\|u - v\|.$$

  Here, the aim is the compression of u or the extraction of information from u (data analysis).

- For the solution of an equation $Au = b$ (e.g. in quantum physics, uncertainty quantification, stochastic calculus), we aim at finding a tensor network v with low complexity that minimizes some distance to u, e.g. some residual norm

$$\|Av - b\|.$$

  The aim is here to obtain an approximation of the solution u with a low computational complexity.

- In tensor completion, knowing some entries $(u(i))_{i\in\Omega}$ of a multidimensional array, we try to find a tensor network that suitably fit the data, e.g. by minimizing

$$\sum_{i\in\Omega} |u(i) - v(i)|^2,$$

The aim is here to recover (or complete) a tensor from partial information, by exploiting low-rank structures of the tensor.

- For inverse problems, we want to identify a tensor u from indirect and partial observations $y = Au$ or $y = Au + \epsilon$, where A is an observation map. We try to find a tensor network that suitably fit the observations by minimizing some distance

$$d(y, Av)$$

between observations and the prediction Av.
Exploiting low-rank structures in u allows to reduce the number of parameters to estimate and possibly makes the problem well-posed.

- Approximating a function u from evaluations $u(x^k)$ at some points x^k, e.g. by minimizing

$$\frac{1}{n}\sum_{k=1}^{n}(u(x^k) - v(x^k))^2.$$

Depending on the context, points can be given or chosen. Here we want to exploit at best the given evaluations or obtain a good approximation using a small number of evaluations.

Computing with tensor networks

- In supervised or unsupervised learning, tensor networks are used as a powerful model class for high-dimensional tasks.
- Supervised learning of the relation between a random variable Y and another random variable X. Introduction of a risk functional

$$\mathcal{R}(v) = \mathbb{E}(\ell(Y, v(X)))$$

that quantifies some expected distance between observations Y and predictions $v(X)$. In practice, using samples $\{(x_k, y_k)\}_{k=1}^{n}$, we optimize an empirical risk

$$\frac{1}{n}\sum_{k=1}^{n} \ell(y^k, v(x^k))$$

- Estimation of the density of a random variable X from samples $\{x_k\}_{k=1}^{n}$. If the density u minimizes some functional

$$\mathcal{R}(v) = \mathbb{E}(\gamma(v, X)),$$

we minimize in practice an empirical risk

$$\frac{1}{n}\sum_{k=1}^{n} \gamma(v, x^k)$$

Outline of the course

- Part I: Tensors, ranks and tensor networks
- Part II: Approximation theory of tree tensor networks
- Part III: Computational aspects

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Approximation and learning with tensor networks

Part I: Tensors, ranks and tensor networks

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Outline

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Algebraic tensors

Given d index sets $I_\nu = \{1, \dots, N_\nu\}$, $1 \le \nu \le d$, we introduce the multi-index set

$$I = I_1 \times \ldots \times I_d.$$

An element v of the vector space $\mathbb{R}^I$ is a tensor of order d.

Algebraic tensors

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$$I = I_1 \times \ldots \times I_d.$$

An element v of the vector space $\mathbb{R}^I$ is a tensor of order d.

It can be represented by a multidimensional array

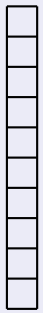
$$(v_i)_{i \in I} = (v_{i_1,\ldots,i_d})_{i_1 \in I_1,\ldots,i_d \in I_d}$$

that contains the coefficients of v in the canonical basis of $\mathbb{R}^I$, also denoted

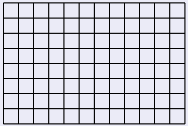
$$v(i) = v(i_1, \ldots, i_d).$$

The order d is the number of dimensions, also known as ways or modes.

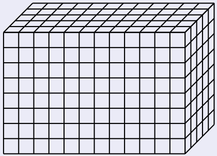
$d = 1$



$d = 2$



$d = 3$



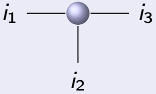
Tensor diagram notations

A tensor is represented by a solid shape and tensor indices are notated by lines emanating from this shape.

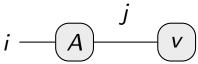
$d = 1$

$d = 2$

$d = 3$



Connecting two index lines means contraction (or summation) over the corresponding indices.



$$= \sum_j A(i,j)v(j)$$

Algebraic tensors

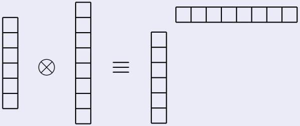
Given d vectors $v^{(\nu)} \in \mathbb{R}^{I_\nu}$, $1 \leq \nu \leq d$, the tensor product of these vectors

$$v := v^{(1)} \otimes \ldots \otimes v^{(d)}$$

is called an elementary tensor and is such that

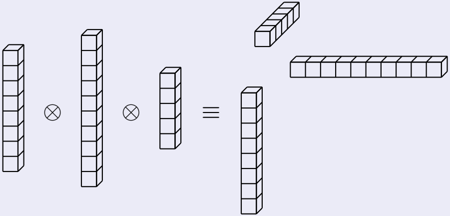
$$v(i) = v^{(1)}(i_1) \ldots v^{(d)}(i_d)$$

$d = 2$



Using matrix notations, $v \otimes w$ is identified with the matrix vw^T.

$d = 3$



Algebraic tensors

The tensor space $\mathbb{R}^I = \mathbb{R}^{I_1 \times \ldots \times I_d}$, also denoted $\mathbb{R}^{I_1} \otimes \ldots \otimes \mathbb{R}^{I_d}$, is defined by

$$\mathbb{R}^I = \mathbb{R}^{I_1} \otimes \ldots \otimes \mathbb{R}^{I_d} = \text{span}\{v^{(1)} \otimes \ldots \otimes v^{(d)} : v^{(\nu)} \in \mathbb{R}^{I_\nu}, 1 \leq \nu \leq d\}$$

The canonical norm on $\mathbb{R}^I$, also called the Frobenius norm, is given by

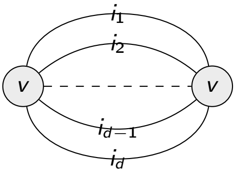
$$\|v\| = \sqrt{\sum_{i \in I} v(i)^2}$$

and makes $\mathbb{R}^I$ a Hilbert space. It coincides with the natural norm on $\ell_2(I)$. It is the only norm associated with an inner product and having the crossnorm property

$$\|v^{(1)} \otimes \ldots \otimes v^{(d)}\| = \|v^{(1)}\|_2 \ldots \|v^{(d)}\|_2.$$

In tensor diagram notations

$$\|v\|^2 = \sum_{i \in I} v(i)^2 =$$



Tensor product of functions

Let $V_\nu \subset \mathbb{R}^{\mathcal{X}_\nu}$ be a space of functions defined on $\mathcal{X}_\nu$.

$\mathcal{X}_\nu$ can be (a subset of) $\mathbb{R}$, $\mathbb{C}$, $\mathbb{N}$, $\mathbb{Z}$, or a set of vectors, sequences, graphs, images...

The tensor product of functions $v^{(\nu)} \in V_\nu$, denoted

$$v = v^{(1)} \otimes \ldots \otimes v^{(d)},$$

is a multivariate function defined on $\mathcal{X} = \mathcal{X}_1 \times \ldots \times \mathcal{X}_d$ and such that

$$v(x_1, \ldots, x_d) = v^{(1)}(x_1) \ldots v^{(d)}(x_d)$$

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Example

For $i \in \mathbb{N}_0^d$, the monomial $x^i = x_1^{i_1} \ldots x_d^{i_d}$ is an elementary tensor.

Tensor product of functions

The algebraic tensor product of spaces V_ν is defined as

$$V_1 \otimes \ldots \otimes V_d = \mathrm{span}\{v^{(1)} \otimes \ldots \otimes v^{(d)} : v^{(\nu)} \in V_\nu, 1 \leq \nu \leq d\}$$

which is the space of multivariate functions v which can be written as a finite linear combination of elementary (separated functions), i.e.

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A polynomial $\sum_i a_i x^i$ with $x^i = x_1^{i_1} \ldots x_d^{i_d}$.

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Example

A polynomial $\sum_i a_i x^i$ with $x^i = x_1^{i_1} \ldots x_d^{i_d}$.

Up to a formal definition of the tensor product $\otimes$, the above construction can be extended to more general vector spaces (not only spaces of functions), including spaces of matrices or operators.

Infinite dimensional tensor spaces

For infinite dimensional spaces V_ν, a Hilbert (or Banach) tensor space equipped with a norm $\|\cdot\|$ is obtained by the completion (w.r.t. $\|\cdot\|$) of the algebraic tensor space

$$\overline{V}^{\|\cdot\|} = \overline{V_1 \otimes \ldots \otimes V_d}^{\|\cdot\|}.$$

If the V_ν are Hilbert spaces with inner products $(\cdot,\cdot)_\nu$ and associated norms $\|\cdot\|_\nu$, a canonical inner product on V can be first defined for elementary tensors

$$(v^{(1)} \otimes \ldots \otimes v^{(d)}, w^{(1)} \otimes \ldots \otimes w^{(d)}) = (v^{(1)}, w^{(1)}) \ldots (v^{(d)}, w^{(d)})$$

and then extended by linearity to the whole space V.

The associated norm $\|\cdot\|$ is called the canonical norm.

Example (L^p spaces)

Let $1 \leq p < \infty$. If $V_\nu = L^p_{\mu_\nu}(\mathcal{X}_\nu)$, then

$$L^p_{\mu_1}(\mathcal{X}_1) \otimes \ldots \otimes L^p_{\mu_d}(\mathcal{X}_d) \subset L^p_{\mu}(\mathcal{X}_1 \times \ldots \times \mathcal{X}_d)$$

with $\mu = \mu_1 \otimes \ldots \otimes \mu_d$, and

$$\overline{L^p_{\mu_1}(\mathcal{X}_1) \otimes \ldots \otimes L^p_{\mu_d}(\mathcal{X}_d)}^{\|\cdot\|} = L^p_{\mu}(\mathcal{X}_1 \times \ldots \times \mathcal{X}_d)$$

where $\|\cdot\|$ is the natural norm on $L^p_{\mu}(\mathcal{X}_1 \times \ldots \times \mathcal{X}_d)$.

Infinite dimensional tensor spaces

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where $\|\cdot\|$ is the natural norm on $L^p_{\mu}(\mathcal{X}_1 \times \ldots \times \mathcal{X}_d)$.

Example (Bochner spaces)

Let $\mathcal{X}$ be equipped with a finite measure μ, and let W be a Hilbert (or Banach) space. For $1 \leq p < \infty$, the Bochner space $L^p_\mu(\mathcal{X}; W)$ is the set of Bochner-measurable functions $u : \mathcal{X} \to W$ with bounded norm $\|u\|_p = (\int_{\mathcal{X}} \|u(x)\|^p_W \mu(dx))^{1/p}$, and

$$L^p_\mu(\mathcal{X}; W) = \overline{W \otimes L^p_\mu(\mathcal{X})}^{\|\cdot\|_p}.$$

Example (Sobolev spaces)

The Sobolev space $H^k(\mathcal{X})$ of functions defined on $\mathcal{X} = \mathcal{X}_1 \times \ldots \times \mathcal{X}_d$, equipped with the norm

$$\|u\|_{H^k}^2 = \sum_{|\alpha|_1 \leq k} \|D^\alpha u\|_{L^2}^2,$$

is a Hilbert tensor space

$$H^k(\mathcal{X}) = \overline{H^k(\mathcal{X}_1) \otimes \ldots \otimes H^k(\mathcal{X}_d)}^{\|\cdot\|_{H^k}}.$$

The Sobolev space $H^k_{mix}(\mathcal{X})$ equipped with the norm

$$\|u\|_{H^k_{mix}}^2 = \sum_{|\alpha|_\infty \leq k} \|D^\alpha u\|_{L^2}^2,$$

is a different tensor Hilbert space

$$H^k_{mix}(\mathcal{X}) = \overline{H^k(\mathcal{X}_1) \otimes \ldots \otimes H^k(\mathcal{X}_d)}^{\|\cdot\|_{H^k_{mix}}}.$$

$\|u\|_{H^k_{mix}}$ is the canonical tensor norm on $H^k(\mathcal{X}_1) \otimes \ldots \otimes H^k(\mathcal{X}_d)$.

Tensor product basis

If $\{\phi_i^{(\nu)}\}_{i \in I_\nu}$ is a basis of V_ν, then a basis of $V = V_1 \otimes \ldots \otimes V_d$ is given by

$$\left\{ \phi_i = \phi_{i_1}^{(1)} \otimes \ldots \otimes \phi_{i_d}^{(d)} : i \in I = I_1 \times \ldots \times I_d \right\}.$$

A tensor $v \in V$ admits a decomposition

$$v = \sum_{i \in I} a_i \phi_i = \sum_{i_1 \in I_1} \ldots \sum_{i_d \in I_d} a_{i_1,\ldots,i_d} \phi_{i_1}^{(1)} \otimes \ldots \otimes \phi_{i_d}^{(d)},$$

and v can be identified with the set of its coefficients

$$a \in \mathbb{R}^I.$$

Hilbert tensor spaces

If the $\{\phi_i^{(\nu)}\}_{i\in I_\nu}$ are orthonormal bases of spaces V_ν, then $\{\phi_i\}_{i\in I}$ is an orthonormal basis of the Hilbert tensor space $\overline{V}^{\|\cdot\|}$ equipped with the canonical norm. A tensor

$$v = \sum_{i\in I} a_i \phi_i$$

is such that

$$\|v\|^2 = \sum_{i\in I} a_i^2 := \|a\|^2.$$

Therefore, the map

$$a \mapsto \sum_{i\in I} a_i \phi_i$$

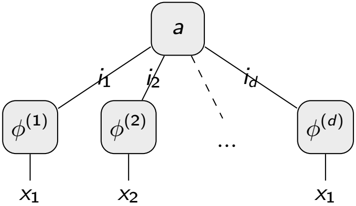
defines a linear isometry from $\ell_2(I)$ to V for finite dimensional spaces, and between $\ell_2(I)$ and $\overline{V}^{\|\cdot\|}$ for infinite dimensional spaces.

If V is a space of functions defined on $\mathcal{X} = \mathcal{X}_1 \times \ldots \times \mathcal{X}_d$, we introduce the feature map $\phi^{(\nu)}(x_\nu) = (\phi^{(\nu)}_{i_\nu}(x_\nu))_{i_\nu \in I_\nu} \in \mathbb{R}^{I_\nu}$ and the tensor product feature map $\Phi : \mathcal{X} \to \mathbb{R}^I$ such that

$$\Phi(x) = \phi^{(1)}(x_1) \otimes \ldots \otimes \phi^{(d)}(x_d) \in \mathbb{R}^I$$

and a tensor v in V admits the representation

$$v(x) = (a, \Phi(x)) =$$



Outline

Rank of order-two tensors

The rank of an order-two tensor $u \in V \otimes W$, denoted $\text{rank}(u)$, is the minimal integer r such that

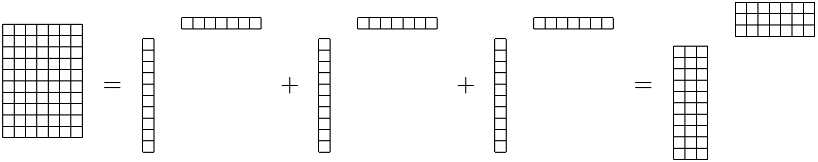
$$u = \sum_{k=1}^{r} v_k \otimes w_k$$

for some $v_k \in V$ and $w_k \in W$.

A tensor $u \in \mathbb{R}^n \otimes \mathbb{R}^m$ is identified with a matrix $u \in \mathbb{R}^{n \times m}$. The rank of u coincides with the matrix rank, which is the minimal integer r such that

$$u = \sum_{k=1}^{r} v_k w_k^T = VW^T,$$

where $V = (v_1, \ldots, v_r) \in \mathbb{R}^{n \times r}$ and $W = (w_1, \ldots, w_r) \in \mathbb{R}^{m \times r}$.



Singular value decomposition of order-two tensors

When V and W are Hilbert spaces (possibly infinite-dimensional), an algebraic tensor $u \in V \otimes W$ admits a singular value decomposition

$$u = \sum_{k \geq 1} \sigma_k v_k \otimes w_k,$$

where v_k and w_k are orthonormal vectors (singular vectors) and $\sigma_k \in \mathbb{R}^+$ are the singular values.

The rank of u is finite and coincides with the number of non-zero singular values,

$$\text{rank}(u) = \#\{k : \sigma_k \neq 0\}.$$

Example (Singular value decomposition of matrices)

For $V = \mathbb{R}^n$ and $W = \mathbb{R}^m$, u is identified with a matrix in $\mathbb{R}^{n \times m}$ and

$$u = \sum_{k=1}^{\text{rank}(u)} \sigma_k v_k w_k^T = \text{VSW}^T$$

with orthogonal matrices V and W, and a diagonal matrix S.

Singular value decomposition of order-two tensors

An algebraic tensor $u \in V \otimes W$ can be identified with a linear operator from W to V with rank equal to $\text{rank}(u)$.

For infinite dimensional Hilbert spaces, the closure $\overline{V \otimes W}^{\|\cdot\|_\vee}$ of $V \otimes W$ with respect to the injective norm (corresponding to the operator norm or spectral norm) coincides with the space of compact operators.

A tensor $u \in \overline{V \otimes W}^{\|\cdot\|_\vee}$ still admits a singular value decomposition

$$u = \sum_{k \geq 1} \sigma_k v_k \otimes w_k.$$

and the rank (number of non-zero singular values) is possibly infinite.

Singular value decomposition of order-two tensors

Example (Proper Orthogonal Decomposition)

For $\Omega \times I$ a space-time domain and V a Hilbert space of functions defined on Ω, a function $u \in L^2(I; V)$ admits a singular value decomposition

$$u(t) = \sum_{k=1}^{\infty} \sigma_k v_k w_k(t)$$

which is known as the Proper Orthogonal Decomposition (POD).

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Example (Karhunen-Loeve decomposition)

For a probability space (Ω, μ), an element $u \in L^2_\mu(\Omega; V)$ is a second-order V-valued random variable. If u is zero-mean, the singular value decomposition of u is known as the Karhunen-Loeve decomposition

$$u(\omega) = \sum_{k=1}^{\infty} \sigma_k v_k w_k(\omega)$$

where $w_k : \Omega \to \mathbb{R}$ are uncorrelated (orthogonal) random variables.

Low-rank format for order-two tensors

The set of tensors in $V \otimes W$ with rank bounded by r, denoted

$$\mathcal{R}_r = \{v : \mathrm{rank}(v) \leq r\},$$

is not a linear space nor a convex set. However, it has many favorable properties for a numerical use.

- The application $v \mapsto \mathrm{rank}(v)$ is lower semi-continuous, and therefore the set $\mathcal{R}_r$ is closed, which makes best approximation problems in $\mathcal{R}_r$ well posed.
- $\mathcal{R}_r$ is the union of smooth manifolds of tensors with fixed rank.

Canonical rank of higher-order tensors

For tensors $u \in V_1 \otimes \ldots \otimes V_d$ with $d \geq 3$, there are different notions of rank.

The canonical rank, which is the natural extension of the notion of rank for order-two tensors, is the minimal integer r such that

$$u(x_1, \ldots, x_d) = \sum_{k=1}^{r} v_k^{(1)}(x_1) \ldots v_k^{(d)}(x_d),$$

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Example

- A monomial $x^i = x_1^{i_1} \ldots x_d^{i_d}$ has rank 1.
- A polynomial $\sum_{i \in \Lambda} a_i x^i$ has rank $\#\Lambda$.
- A Gaussian function $\exp(-\alpha \|x - a\|_2^2) = \prod_{i=1}^{d} \exp(-\alpha(x_i - a_i)^2)$ has rank 1.
- The function $\frac{1}{\|x\|_2}$ has infinite rank.

Canonical format

The subset of tensors in $V = V_1 \otimes \ldots \otimes V_d$ with canonical rank bounded by r is denoted

$$\mathcal{R}_r = \{v \in V : \text{rank}(v) \leq r\}.$$

A tensor in $\mathcal{R}_r$ has a representation

$$v(x_1, \ldots, x_d) = \sum_{k=1}^{r} v_k^{(1)}(x_1) \ldots v_k^{(d)}(x_d)$$

The storage complexity of tensors in $\mathcal{R}_r$ is

$$\text{storage}(\mathcal{R}_r) = r \sum_{\nu=1}^{d} \dim(V_\nu) = O(rdn)$$

for $\dim(V_\nu) = O(n)$.

Canonical format

For $d \geq 3$, the set $\mathcal{R}_r$ looses many of the favorable properties of the case $d = 2$.

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Example

Consider the order-3 tensor

$$v = a \otimes a \otimes b + a \otimes b \otimes a + b \otimes a \otimes a$$

where a and b are linearly independent vectors in $\mathbb{R}^m$. The rank of v is 3. The sequence of rank-2 tensors

$$v_n = n(a + \frac{1}{n}b) \otimes (a + \frac{1}{n}b) \otimes (a + \frac{1}{n}b) - na \otimes a \otimes a$$

converges to v as $n \to \infty$.

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$$v = a \otimes a \otimes b + a \otimes b \otimes a + b \otimes a \otimes a$$

where a and b are linearly independent vectors in $\mathbb{R}^m$. The rank of v is 3. The sequence of rank-2 tensors

$$v_n = n(a + \frac{1}{n} b) \otimes (a + \frac{1}{n} b) \otimes (a + \frac{1}{n} b) - na \otimes a \otimes a$$

converges to v as $n \to \infty$.

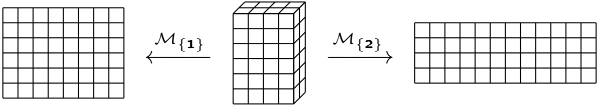
- The consequence is that for most problems involving approximation in canonical format $\mathcal{R}_r$, there is no robust method when $d > 2$.

α-rank

For a non-empty subset α of $D = \{1, \dots, d\}$, a tensor $u \in V = V_1 \otimes \dots \otimes V_d$ can be identified with an order-two tensor

$$\mathcal{M}_\alpha(u) \in V_\alpha \otimes V_{\alpha^c},$$

where $V_\alpha = \bigotimes_{\nu \in \alpha} V_\nu$, and $\alpha^c = D \setminus \alpha$. The operator $\mathcal{M}_\alpha = V \to V_\alpha \otimes V_{\alpha^c}$ is called the matricisation (or unfolding) operator.



The α-rank of u, denoted $\mathrm{rank}_\alpha(u)$, is the rank of the order-two tensor $\mathcal{M}_\alpha(u)$,

$$\mathrm{rank}_\alpha(u) = \mathrm{rank}(\mathcal{M}_\alpha(u)),$$

which is the minimal integer r_α such that

$$\mathcal{M}_\alpha(u) = \sum_{k=1}^{r_\alpha} v_k^\alpha \otimes w_k^{\alpha^c}$$

for some $v_k^\alpha \in V_\alpha$ and $w_k^{\alpha^c} \in V_{\alpha^c}$. We note that $\mathrm{rank}_\alpha(u) = \mathrm{rank}_{\alpha^c}(u)$.

A multivariate function $u(x_1, \ldots, x_d)$ with $\mathrm{rank}_\alpha(u) \leq r_\alpha$ is such that

$$u(x) = \sum_{k=1}^{r_\alpha} v_k^\alpha(x_\alpha) w_k^{\alpha^c}(x_{\alpha^c})$$

for some functions $v_k^\alpha(x_\alpha)$ and $w_k^{\alpha^c}(x_{\alpha^c})$ of groups of variables

$$x_\alpha = \{x_\nu\}_{\nu\in\alpha} \quad \text{and} \quad x_{\alpha^c} = \{x_\nu\}_{\nu\in\alpha^c}.$$

Example

- $u(x) = u^1(x_1)\dots u^d(x_d)$ can be written $u(x) = u^\alpha(x_\alpha)u^{\alpha^c}(x_{\alpha^c})$, with $u^\alpha(x_\alpha) = \prod_{\nu\in\alpha} u^\nu(x_\nu)$. Therefore, for any α, $\mathrm{rank}_\alpha(u) = 1$.

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  We deduce the following relation between α-ranks and canonical rank:

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- $u(x) = u^1(x_1) + \dots + u^d(x_d)$ can be written $u(x) = u^\alpha(x_\alpha) + u^{\alpha^c}(x_{\alpha^c})$, with $u^\alpha(x_\alpha) = \sum_{\nu \in \alpha} u^\nu(x_\nu)$. Therefore, $\text{rank}_\alpha(u) \leq 2$.

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- $u(x) = \prod_{\alpha\in T} u^\alpha(x_\alpha)$ with T a collection of disjoint subsets, is such that $\text{rank}_\alpha(u) = 1$ for all $\alpha \in T$, and $\text{rank}_\gamma(u) \le \prod_{\alpha\in T, \alpha\cap\gamma\neq\emptyset} \text{rank}_{\gamma\cap\alpha}(u^\alpha)$ for all γ.

α-ranks and minimal subspaces

For a subset α of $D = \{1, \dots, d\}$, the minimal subspace

$$U_\alpha^{min}(u)$$

of a tensor $u \in V_1 \otimes \dots \otimes V_d$ is defined as the smallest subspace

$$U_\alpha \subset V_\alpha = \bigotimes_{\nu \in \alpha} V_\nu$$

such that

$$\mathcal{M}_\alpha(u) \in U_\alpha \otimes V_{\alpha^c}.$$

The α-rank of u is the dimension of the minimal subspace $U_\alpha^{min}(u)$,

$$\mathrm{rank}_\alpha(u) = \dim(U_\alpha^{min}(u)).$$

If u admits the representation

$$u(x) = \sum_{k=1}^{\mathrm{rank}_\alpha(v)} v_k^\alpha(x_\alpha) v^{\alpha^c}(x_{\alpha^c})$$

then $U_\alpha^{min}(u) = span\{v_k^\alpha : 1 \leq k \leq \mathrm{rank}_\alpha(u)\}$.

α-ranks and minimal subspaces

For any partition $\{\alpha_1, \ldots, \alpha_m\}$ of D, an algebraic tensor u is such that

$$u \in U_{\alpha_1}^{min}(u) \otimes \ldots \otimes U_{\alpha_m}^{min}(u)$$

Moreover, for any $\alpha \subset D$ and any partition $\{\beta_1, \ldots, \beta_s\}$ of α, it holds

$$U_{\alpha}^{min}(u) \subset U_{\beta_1}^{min}(u) \otimes \ldots \otimes U_{\beta_s}^{min}(u)$$

that implies

$$\mathrm{rank}_{\alpha}(u) \leq \prod_{k=1}^{s} \mathrm{rank}_{\beta_k}(u)$$

Also, for any $p \in \{1, ..., s\}$

$$\mathrm{rank}_{\beta_p}(u) \leq \mathrm{rank}_{\alpha}(u) \prod_{\substack{k=1 \\ k \neq p}}^{s} \mathrm{rank}_{\beta_k}(u)$$

Example

The function

$$u(x_1, x_2, x_3) = \cos(x_1 + x_2) + x_1(x_2 + 2x_3) = \cos(x_1)\cos(x_2) - \sin(x_1)\sin(x_2) + x_1x_2 + 2x_1x_3$$

has for minimal subspaces and ranks

- $U_1^{min}(u) = span\{\cos(x_1), \sin(x_1), x_1\}, \quad r_1 = 3$
- $U_2^{min}(u) = span\{\cos(x_2), \sin(x_2), x_2\}, \quad r_2 = 3$
- $U_3^{min}(u) = span\{1, x_3\}, \quad r_3 = 2$
- $U_{1,2}^{min}(u) = span\{\cos(x_1 + x_2), x_1x_2, x_1\}, \quad r_{1,2} = 3$
- $U_{2,3}^{min}(u) = span\{\cos(x_2), \sin(x_2), x_2 + 2x_3\}, \quad r_{2,3} = 3$
- $U_{1,3}^{min}(u) = span\{\cos(x_1), \sin(x_1), x_1, x_1x_3\}, \quad r_{1,3} = 4$

In particular, we can check that

$$U_{1,3}^{min}(u) \subset U_1^{min}(u) \otimes U_3^{min}(u) = span\{\cos(x_1), \sin(x_1), x_1, \cos(x_1)x_3, \sin(x_1)x_3, x_1x_3\}$$

$$r_{1,3} \leq r_1 r_3, \quad r_1 \leq r_{1,3} r_3, \quad r_3 \leq r_{1,3} r_1$$

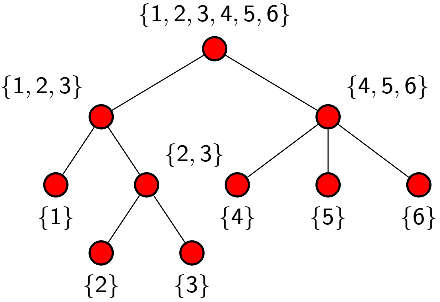
Outline

Tree-based tensor format

Tree-based (Hierarchical) tensor formats [Hackbusch-Kuhn'09] are subsets of tensors

$$\mathcal{T}_r^T = \{v \in V : \mathrm{rank}_\alpha(v) \leq r_\alpha, \alpha \in T\}$$

where $r = (r_\alpha)_{\alpha \in T}$ and where T is a dimension partition tree T over $D = \{1, \dots, d\}$, with root D and leaves $\mathcal{L}(T) = \{\{\nu\} : 1 \leq \nu \leq d\}$. All nodes in T are non empty subsets of D. The set of children of $\alpha \in T$ is either empty (for a leaf node) or is a nontrivial partition of α (for an interior node).



The tree-based rank of a tensor v is the tuple $\mathrm{rank}_T(v) = (\mathrm{rank}_\alpha(v))_{\alpha \in T}$.

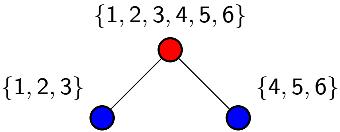
By convention, $\mathrm{rank}_D(v) = 1$.

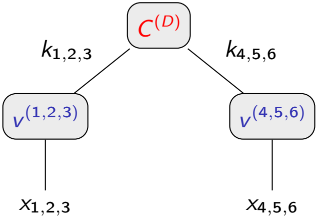
Tree-based tensor format

Elements of $\mathcal{T}_r^T$ admit an explicit representation. Let $v \in \mathcal{T}_r^T$ with T-rank $r = (r_\alpha)_{\alpha \in T}$. At the first level, v admits the representation

$$v(x) = \sum_{k_{\beta_1}=1}^{r_{\beta_1}} \dots \sum_{k_{\beta_s}=1}^{r_{\beta_s}} C^{(D)}_{k_{\beta_1},\dots,k_{\beta_s}} v^{(\beta_1)}_{k_{\beta_1}}(x_{\beta_1}) \dots v^{(\beta_s)}_{k_{\beta_s}}(x_{\beta_s})$$

where $\{\beta_1, \dots, \beta_s\} = S(D)$ are the children of the root node D, and $\{v^{(\beta)}_{k_\beta}\}_{1 \le k_\beta \le r_\beta}$ form a basis of the minimal subspace $U^{min}_\beta(v)$.

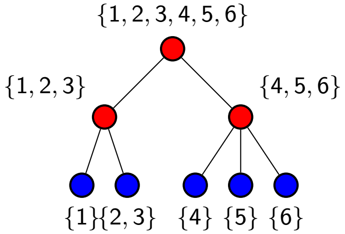


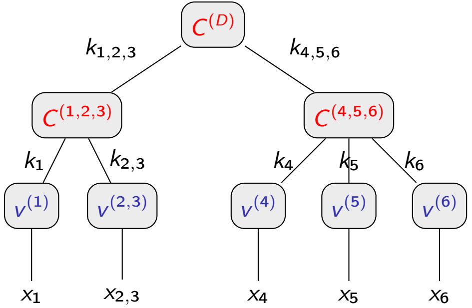


Tree-based tensor format

Then, for an interior node α of the tree, with children $S(\alpha) = \{\beta_1, \dots, \beta_s\}$, the functions (or tensors) $v^{(\alpha)}_{k_\alpha}$ admit the representation

$$v^{(\alpha)}_{k_\alpha}(x_\alpha) = \sum_{k_{\beta_1}=1}^{r_{\beta_1}} \dots \sum_{k_{\beta_s}=1}^{r_{\beta_s}} C^{(\alpha)}_{k_\alpha, k_{\beta_1}, \dots, k_{\beta_s}} v^{(\beta_1)}_{k_{\beta_1}}(x_{\beta_1}) \dots v^{(\beta_s)}_{k_{\beta_s}}(x_{\beta_s}).$$



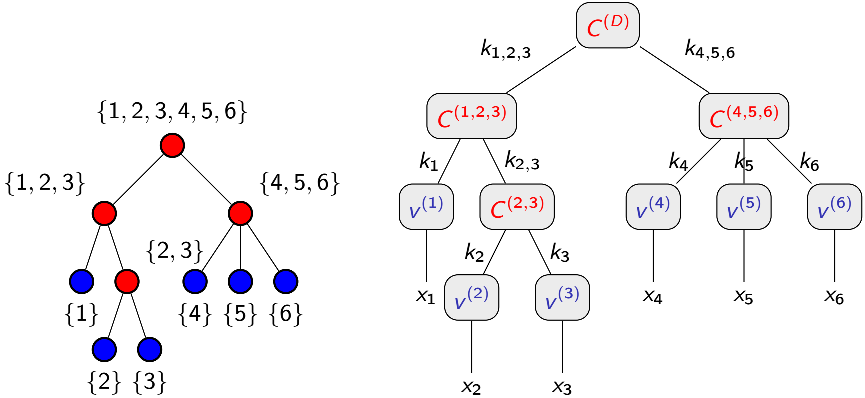


Tree-based tensor format as a tree tensor network

Finally, the tensor v admits the representation

$$v(x) = \sum_{\substack{1 \leq k_\beta \leq r_\beta \\ \beta \in T}} \prod_{\alpha \in T \setminus \mathcal{L}(T)} C^{(\alpha)}_{(k_\beta)_{\beta \in S(\alpha)}, k_\alpha} \prod_{\nu \in \mathcal{L}(T)} v^{(\nu)}_{k_\nu}(x_\nu)$$

where the parameters C^α and $v^{(\nu)}$ form a tree tensor network.

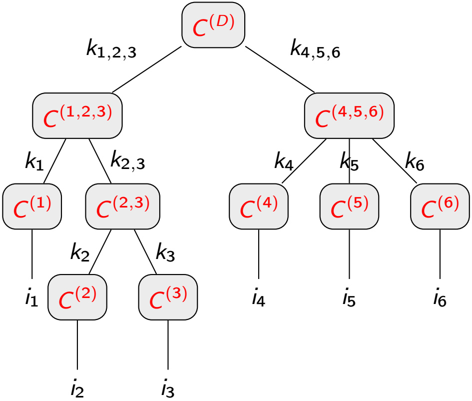


Tree-based tensor format as a tree tensor network

Given bases $\{\phi^{\alpha}_{i_\alpha}(x_\alpha)\}_{i_\alpha \in I^\alpha}$ of functions for the spaces V_α for $\alpha \in \mathcal{L}(T)$,

$$v(x) = \sum_{i_1 \in I^1} \dots \sum_{i_d \in I^d} a(i_1, \dots, i_d)\phi_{i_1}(x_1)\dots\phi_{i_d}(x_d)$$

with $a(i_1, \dots, i_d) = \sum_{\substack{1 \le k_\beta \le r_\beta \\ \beta \in T}} \prod_{\alpha \in T \setminus \mathcal{L}(T)} C^{(\alpha)}_{(k_\beta)_{\beta \in S(\alpha)}, k_\alpha} \prod_{\alpha \in \mathcal{L}(T)} C^{(\alpha)}_{i_\alpha, k_\alpha}$ or using tensor diagram notations

$a(i_1, \dots, i_d) =$ 

Representation complexity

The representation complexity for the representation of a tensor in $\mathcal{T}_r^T(V)$ is

$$C(T,r) = \sum_{\alpha \in T \setminus \mathcal{L}(T)} r_\alpha \prod_{\beta \in S(\alpha)} r_\beta + \sum_{\nu \in \mathcal{L}(T)} \# I^\alpha r_\alpha.$$

If $r_\alpha = O(R)$ and $\# I^\alpha = O(N)$,

$$C(T,r) = O(dNR + (\# T - d - 1) R^{s+1} + R^s),$$

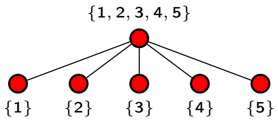
where $s = \max_{\alpha \in T \setminus \mathcal{L}(T)} \# S(\alpha)$ is the arity of the tree.

Since $\# T \leq 2d + 1$,

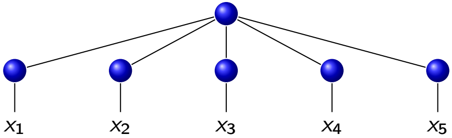
$$C(T,r) = O(dNR + dR^{s+1} + R^s)$$

Tucker format

The Tucker format [Hitchcock'27] corresponds to a trivial tree with one level, arity $s = d$, $\#T = d + 1$,



The representation of a tensor u in $\mathcal{T}_r^T$ is

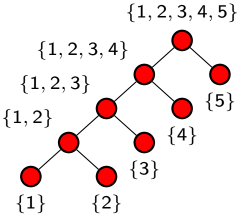


The representation complexity

$$C(T, r) = O(dNR + R^d)$$

Tensor train Tucker format

The tensor train Tucker format corresponds to a linear binary tree



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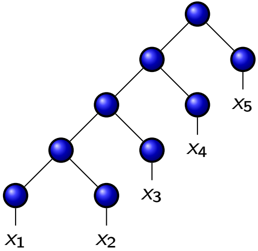
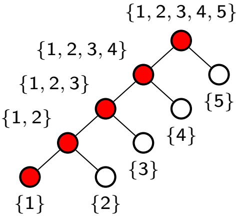


The representation complexity $C(T, r) = O(dNR + (d-2)R^3 + R^2)$.

Tensor train format

The tensor train format [Oseledets-Tyrtyshnikov'09] was discovered independently in quantum physics [Baxter'68 , Affleck'87] and coined Matrix Product State (MPS).
It corresponds to a degenerate tree-based format where T is a subset of a linear tree

$$T = \{\{1\}, \{1,2\}, \{1,2,3\}, \ldots, \{1,\ldots,d\}\}$$



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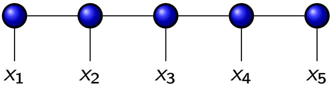


or explicitly

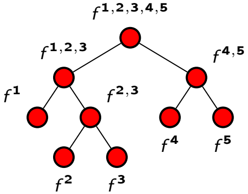
$$u(x_1,\ldots,x_d) = \sum_{k_1=1}^{r_1} \cdots \sum_{k_{d-1}=1}^{r_{1,\ldots,d-1}} v^{(1)}_{k_1}(x_1) v^{(2)}_{k_1,k_2}(x_2) \ldots v^{(d-1)}_{k_{d-2},k_{d-1}}(x_{d-1}) v^{(d)}_{k_{d-1}}(x_d)$$

The complexity is $C(T,r) = O(dNR^2)$.

By identifying a tensor $C^{(\alpha)} \in \mathbb{R}^{n_1 \times \ldots \times n_s \times r_\alpha}$ with a $\mathbb{R}^{r_\alpha}$-valued multilinear function

$$f^{(\alpha)} : \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_s} \to \mathbb{R}^{r_\alpha},$$

a function v in $\mathcal{T}_r^T$ admits a representation as a tree-structured composition of multilinear functions $\{f^{(\alpha)}\}_{\alpha \in T}$.



$$v(x) = f^D(f^{1,2,3}(f^1(\Phi^1(x_1)), f^{2,3}(f^2(\Phi^2(x_2)), f^3(\Phi^3(x_3)))), f^{4,5}(f^4(\Phi^4(x_4)), f^5(\Phi^5(x_5))))$$

where $\Phi^\nu(x_\nu) = (\phi^\nu_{i_\nu}(x_\nu))_{i_\nu \in I^\nu} \in \mathbb{R}^{\# I^\nu}$.

Tree tensor networks as feed-forward neural networks

It corresponds to a sum-product feed forward neural network with a sparse architecture (given by T), a number of hidden layers equal to $depth(T) + 1$ (including a featuring layer), and width at level ℓ related to the α-ranks of the nodes α of level ℓ.

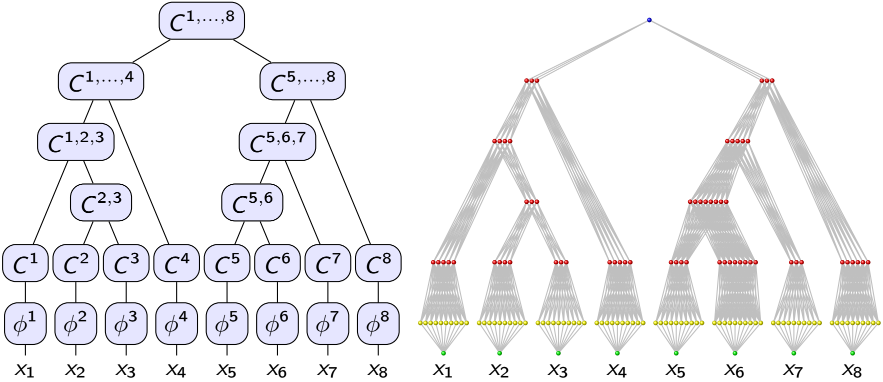


Figure: Tree tensor network and corresponding feed-forward sum-product neural network with 10 features per variable x_ν (right)

Properties of tree-based tensor formats

Many favorable properties inherited from the matrix case.

- Complexity is linear in d and polynomial in the rank for storage, evaluation, differentiation, integration...

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- Not so nonlinear approximation tool. A tensor u in tree-based format admits a multilinear parametrization with parameters $(C_\alpha)_{\alpha \in T}$ forming a tree tensor network, i.e.

  $$u = R((C_\alpha)_{\alpha \in T})$$

  with R a multilinear map.

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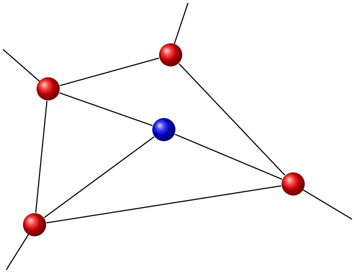
- Geometrical properties can be exploited for optimization and dynamical approximation.
- Possible extensions of singular value decomposition for u in a Hilbert tensor space V, and a way to obtain approximations u_r in $\mathcal{T}_r^T(V)$ such that

$$\|u - u_r\| \leq C_d \inf_{v \in \mathcal{T}_r^T(V)} \|u - v\|$$

  with $C_d \sim \sqrt{d}$.

General tensor networks

More general tensor networks are associated with graphs $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ with nodes (vertices) $\mathcal{N}$ and edges $\mathcal{E}$, d of the nodes being associated with variables x_ν, $1 \leq \nu \leq d$



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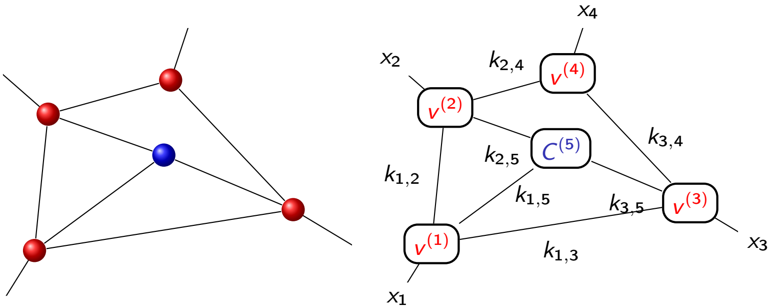


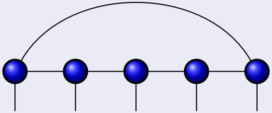
They have a multilinear parametrization of the form

$$v(x_1, \dots, x_d) = \sum_{\substack{1 \le k_e \le r_e \\ e \in \mathcal{E}}} \prod_{\nu=1}^{d} v^{(\nu)}(x_\nu, (k_e)_{e \in E_\nu}) \prod_{\nu=d+1}^{N} C^{(\nu)}((k_e)_{e \in E_\nu})$$

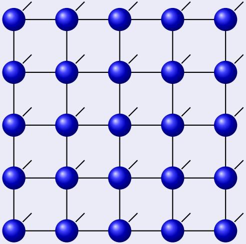
Tree tensor networks is a particular case where $\mathcal{G}$ is a tree.

Examples of tensor networks

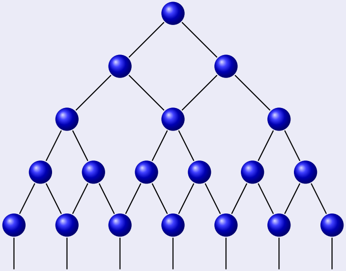
Tensor ring (MPS with periodic boundary conditions)



PEPS



MERA



General tensor networks

When the graph contains cycles,

- integers r_e (bond dimensions) may not have an interpretation as α-ranks,
- no notion of singular value decomposition,
- loss of nice geometrical and topological properties,
- computational complexity increases,
- but yet powerful for some high-dimensional applications.

Outline

Tensorization of vectors

A vector $v \in \mathbb{R}^N$ with $N = b^L$ can be identified with a tensor of order L

$$\boldsymbol{v} \in \mathbb{R}^b \otimes \ldots \otimes \mathbb{R}^b = (\mathbb{R}^b)^{\otimes L}$$

such that for $i \in \{0, \ldots, N-1\}$

$$v(i) = \boldsymbol{v}(i_1, \ldots, i_L)$$

where $(i_1, \ldots, i_L) \in \{0, \ldots, b-1\}$ are the integers of the representation of i in base b

$$i = \sum_{k=1}^{d} i_k b^{L-k} = [i_1, \ldots, i_L]_b.$$

The map which associates to v its tensorization $\boldsymbol{v}$ is a linear isometry from $\ell_2(\mathbb{R}^N)$ to $\ell_2(\mathbb{R}^b)^{\otimes L}$.

Some matrix-vector operations can be efficiently implemented using tensor algebra, such as the Hadamard transform

$$H_L v \equiv (H_1 \otimes \ldots \otimes H_1)\boldsymbol{v}$$

Tensorization of tensors

A tensor $v \in \mathbb{R}^N \otimes \ldots \otimes \mathbb{R}^N = (\mathbb{R}^N)^{\otimes d}$ with $N = b^L$ can be identified with a tensor of order dL

$$\boldsymbol{v} \in (\mathbb{R}^b)^{\otimes dL}$$

with

$$v(i_1, \ldots, i_d) = \boldsymbol{v}(i_1^1, \ldots, i_1^L, \ldots, i_d^1, \ldots, i_d^L)$$

where

$$i_\nu = [i_\nu^1 \ldots i_\nu^{L_\nu}]_b$$

Other orderings of variables can be considered, such as

$$v(i_1, \ldots, i_d) = \boldsymbol{v}(i_1^1, \ldots, i_d^1, \ldots, i_1^L, \ldots, i_d^L)$$

Tensors with different dimensions can be considered, i.e.

$$v \in \mathbb{R}^{N_1} \otimes \ldots \otimes \mathbb{R}^{N_d}, \quad N_\nu = b_\nu^{L_\nu}$$

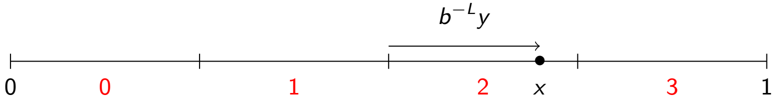
is identified with a tensor of order $\sum_{\nu=1}^d L_\nu$.

Tensorization of univariate functions

Consider a function $f \in \mathbb{R}^{[0,1)}$ defined on the interval $[0,1)$.

- For $b, L \in \mathbb{N}$, we subdivide uniformly the interval $[0,1)$ into b^L intervals. Any $x \in [0,1)$ can be written

$$x = b^{-L}(i + y), \quad i \in \{0, \dots, b^L - 1\}, \quad y \in [0,1).$$



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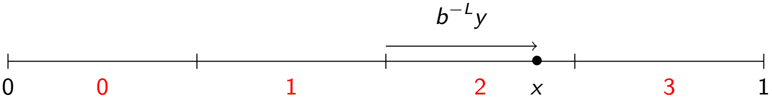
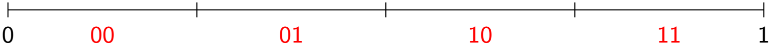


- The integer i admits a representation in base b

$$i = \sum_{k=1}^{L} i_k b^{L-k} = [i_1 \dots i_L]_b, \quad i_k \in \{0, \dots, b-1\}$$



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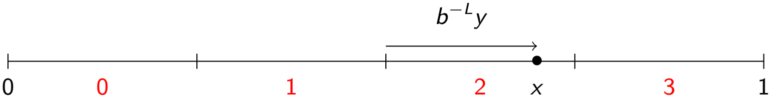

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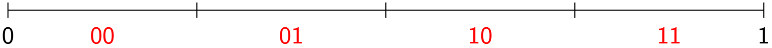
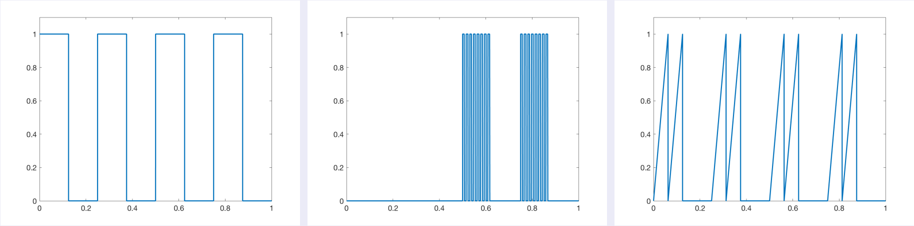


- f is thus identified with a multivariate function (tensor of order $L+1$)

$$\boldsymbol{f} \in (\mathbb{R}^b)^{\otimes L} \otimes \mathbb{R}^{[0,1)} \quad \text{such that} \quad f(x) = \boldsymbol{f}(i_1, \dots, i_L, y)$$

Tensorization of univariate functions

Examples of elementary tensors $f(x) = v^1(i_1)...v^L(i_L)v^{L+1}(y)$ $(b=2)$



(a) $\delta_{\mathbf{0}}(i_{\mathbf{3}})$ (b) $\delta_{\mathbf{1}}(i_{\mathbf{1}})\delta_{\mathbf{0}}(i_{\mathbf{3}})\delta_{\mathbf{0}}(i_{\mathbf{7}})$ (c) $\delta_{\mathbf{0}}(i_{\mathbf{1}})y$ $(L=4)$

Ranks of polynomials and splines

Polynomials

Consider a polynomial $q(x)$ of degree p. For any $\alpha \subset \{1, \dots, L\}$,

$$q(x) = q(b^{-L}(\sum_{k=1}^{L} i_k b^{L-k} + y)) = q(g(i_\alpha) + \tilde{g}(i_{\alpha^c})) = \sum_{j=0}^{p} g(i_\alpha)^j h_j(i_{\alpha^c})$$

so that $\mathrm{rank}_\alpha(\boldsymbol{q}) \leq p + 1$.

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Trigonometric polynomials

The tensorization of function $\cos(\omega x + \varphi)$ at resolution L has all ranks equal to 2.

Then a trigonometric polynomial $q(x)$ of degree p is such that for any $\alpha \subset \{1, \dots, L\}$,

$$\text{rank}_\alpha(\boldsymbol{q}) \leq 2p + 1.$$

Splines

A spline φ_N of degree p over N b-adic intervals forming a partition of $[0,1)$ is such that

$$\mathrm{rank}_{\{1,\ldots,\nu\}}(\varphi_N) \leq \begin{cases} p+N, & 1 \leq \nu < \ell. \\ p+1, & \ell \leq \nu \leq L. \end{cases}$$

where $b^{-\ell}$ is the minimal length of intervals.

Tensorization of multivariate functions

A function $f(x_1, \dots, x_d)$ defined on $[0,1)^d$ can be similarly identified with a tensor of order $(L+1)d$

$$\boldsymbol{f} \in (\mathbb{R}^b)^{\otimes Ld} \otimes (\mathbb{R}^{[0,1)})^{\otimes d}$$

such that

$$f(x_1, \dots, x_d) = \boldsymbol{f}(i_1^1, \dots, i_d^1, \dots, i_1^L, \dots, i_d^L, y_1, \dots, y_d)$$

$$\text{where} \quad x_\nu = b^{-L}(\sum_{k=1}^{L} i_\nu^k b^{L-k} + y_\nu) = b^{-L}([i_\nu^1 \dots i_\nu^L]_b + y_\nu)$$

Tensorization of multivariate functions

The map $T_{b,d}$ which associates to a function f its tensorization $\boldsymbol{f}$ is a linear isometry from $L^p([0,1)^d)$ to $L^p(\{0,\dots,b-1\}^{Ld} \times [0,1)^d)$ for any $0 < p \leq \infty$.

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