

Model Order Reduction: A geometric approach.

Antonio Falcó



Numerical fluid dynamics: full-order and reduced-order methods
(Sevilla) 2022

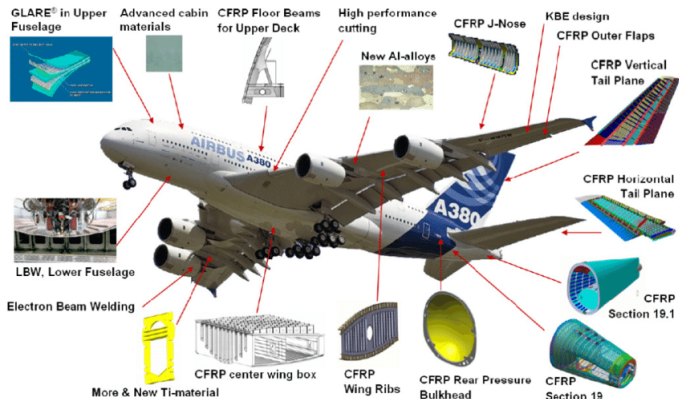
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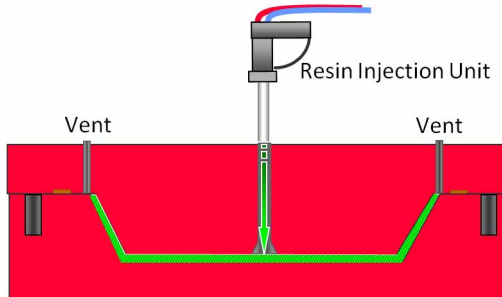
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A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modeling of complex fluids

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Abstract

Kinetic theory models involving the Fokker–Planck equation can be accurately discretized using a mesh support (finite elements, finite differences, finite volumes, spectral techniques, etc.). However, these techniques involve a high number of approximation functions. In the finite element framework, widely used in complex flow simulations, each approximation function is related to a node that defines the associated degree of freedom. When the model involves high dimensional spaces (including physical and conformation spaces and time), standard discretization techniques fail due to an excessive computation time required to perform accurate numerical simulations. One appealing strategy that allows circumventing this limitation is based on the use of reduced approximation basis within an adaptive

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Similar mathematical problem

Because of dimensions ($3N$), the direct computation of E seems rather hopeless and approximations are needed. Historically, the first method was introduced by Hartree [27] ignoring the antisymmetry (i.e. the Pauli principle) and choosing test functions in (2) of the form

$$\Phi(x_1, \dots, x_N) = \prod_{i=1}^N \varphi_i(x_i). \quad (4)$$

Later on, Fock [24] and Slater [54] proposed another class of test functions – which take into account the Pauli principle – namely the class of Slater determinants

$$\Phi(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\sigma} (-1)^{|\sigma|} \prod_{i=1}^N \varphi_{\sigma(i)}(x_i) = \frac{1}{\sqrt{N!}} \det(\varphi_i(x_j)), \quad (5)$$

where the sum is taken over all permutations σ of $\{1, \dots, N\}$ and $|\sigma|$ denotes the signature of σ . If we “restrict” the infimum in (2) to these classes of test functions, we obtain the following minimization problems

$$\inf \{ \mathcal{E}(\varphi_1, \dots, \varphi_N) / \varphi_i \in H^1(\mathbb{R}^3) \quad \forall i, \quad (\varphi_1, \dots, \varphi_N) \in K \}, \quad (6)$$

$$^1 H^1(\mathbb{R}^m) = \left\{ u \in L^2(\mathbb{R}^m), \frac{\partial u}{\partial x_i} \in L^2(\mathbb{R}^m) \quad \text{for all } 1 \leq i \leq m \right\}, \quad \text{for } m \geq 1$$

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Solutions of Hartree-Fock Equations for Coulomb Systems

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Case 1: Stampacchia's Theorem

Theorem

Let X be a reflexive Banach space and let $C \subset X$ be a non-empty, closed and convex. Given a continuous symmetric bilinear form $B : X \times X \longrightarrow \mathbb{R}$ and some $\varphi \in X^*$, define $J : X \longrightarrow \mathbb{R}$ by

$$J(x) := \frac{1}{2}B(x, x) - \langle \varphi, x \rangle_{X^* \times X}$$

and set $S = \arg \min_{x \in C} J(x)$. We have the following

- (i) If B is either positive semi-definite and C is bounded, then $S \neq \emptyset$;
- (ii) If either B is positive definite and C bounded, or B uniformly elliptic, then S is a singleton.

In any case, $\bar{x} \in S$ if, and only if, $\bar{x} \in C$ and

$$B(\bar{x}, c - \bar{x}) \geq \langle \varphi, c - \bar{x} \rangle_{X^* \times X}$$

for all $c \in C$.

Case 2: Nonlinear Laplacian

Let $\Omega = \Omega_1 \times \dots \times \Omega_d$. Given some $p > 2$, we let $X = H_0^{1,p}(\Omega)$, which is the closure of $C_c^\infty(\Omega)$ (functions in $C^\infty(\Omega)$ with compact support in Ω) in $H^{1,p}(\Omega)$ with respect to the norm in $H^{1,p}(\Omega)$. We equip $H_0^{1,p}(\Omega)$ with the norm

$$\|\mathbf{v}\| = \left(\sum_{k=1}^d \|\partial_{x_k}(\mathbf{v})\|_{L^p(\Omega)}^p \right)^{1/p}.$$

We then introduce the functional $J : X \rightarrow \mathbb{R}$ defined by

$$J(\mathbf{v}) = \frac{1}{p} \|\mathbf{v}\|^p - \langle \mathbf{f}, \mathbf{v} \rangle_{X^* \times X},$$

with $\mathbf{f} \in X^*$. Its Fréchet differential is

$$J'(\mathbf{v}) = A(\mathbf{v}) - \mathbf{f}$$

where

$$A(\mathbf{v}) = - \sum_{k=1}^d \frac{\partial}{\partial x_k} \left(\left| \frac{\partial \mathbf{v}}{\partial x_k} \right|^{p-2} \frac{\partial \mathbf{v}}{\partial x_k} \right) \quad p\text{-Laplacian.}$$

We now consider the minimization problem

$$J(u) = \min_{v \in X} J(v) \quad (\pi)$$

of a functional J on a reflexive Banach space X . Assume that we have a functional $J : X \rightarrow \mathbb{R}$ satisfying

- (A1) J is Fréchet differentiable, with Fréchet differential $J' : X \rightarrow X^*$.
- (A2) J is elliptic, i.e. there exist $\alpha > 0$ and $s > 1$ such that for all $v, w \in X$;

$$\langle J'(v) - J'(w), v - w \rangle_{X^* \times X} \geq \alpha \|v - w\|^s. \quad (1)$$

Moreover, we have set \mathcal{D} (called *dictionary*) in X satisfying:

- (B1) $\mathcal{D} \subset X$, is a weakly closed,
- (B2) for each $\mathbf{v} \in \mathcal{D}$ we have $\lambda \mathbf{v} \in \mathcal{D}$ for all $\lambda \in \mathbb{R}$, and
- (B3) $\text{span } \mathcal{D}$ is dense in X .

Algorithm to compute $u^* = \arg \min_{u \in X}(u)$.

- 1 Put $u_0 = 0$, and;
- 2 $z_n \in \arg \min_{u \in \mathcal{D}} J(u_{n-1} + u)$;
- 3 put $u_n = u_{n-1} + z_n$, and goto 2.

Observe, that

$$u_n = \sum_{k=1}^n z_k$$

and $J(0) \geq J(z_1) \geq J(z_1 + z_2) \geq \dots \geq J(u^*)$. Under some general conditions we can prove that $u_n \rightarrow u^*$.

Reference: Falcó, A., Nouy, A. Proper generalized decomposition for nonlinear convex problems in tensor Banach spaces. Numer. Math. 121, 503–530 (2012).

Let us consider the non-convex cone

$$\mathcal{D} = \{u \in L_2[0, 1] : u(x) = \alpha x^\beta \text{ where } \alpha \geq 0 \text{ and } \beta \in [0, 2]\}.$$

Then the map $\Phi : \mathbb{R}_+ \times [0, 2] \rightarrow L_2[0, 1]$, given by $\Phi(\alpha, \beta)(x) = \alpha x^\beta$, is continuous because

$$\|\Phi(\alpha, \beta) - \Phi(\alpha', \beta')\|_{L_2[0,1]}^2 \leq \frac{(\alpha - \alpha')^2}{\min(\beta, \beta')^2 + 1}.$$

Now, we assume that $\{u_n(x) = \alpha_n x^{\beta_n}\}_{n \in \mathbb{N}} \subset \mathcal{D}$ converges weakly to u in $L_2[0, 1]$. As a consequence the sequence $\{u_n\}_{n \in \mathbb{N}}$ is bounded:

$$\|u_n\|_{L_2[0,1]}^2 = \frac{\alpha_n^2}{\beta_n^2 + 1} \leq C,$$

for some $C \geq 0$ and for all $n \in \mathbb{N}$.

Also the sequence $\{(\alpha_n, \beta_n)\}_{n \in \mathbb{N}}$ is bounded in the closed set $\mathbb{R}_+ \times [0, 2]$. Hence there exists a convergent subsequence, also denoted by $\{(\alpha_n, \beta_n)\}_{n \in \mathbb{N}}$, to some $(\alpha, \beta) \in \mathbb{R}_+ \times [0, 2]$. Since

$$\lim_{n \rightarrow \infty} \|\Phi(\alpha_n, \beta_n) - \Phi(\alpha, \beta)\|_{L_2[0,1]} = 0,$$

we have that $u_n - v$, where $v(x) = \alpha x^\beta$, converges to zero in $L_2[0, 1]$. Thus $v = u$, and \mathcal{D} is weakly closed in $L_2[0, 1]$.

We can consider the Hilbert space $X = \overline{\text{span } \mathcal{D}}^{\|\cdot\|_{L_2[0,1]}}$.

Reference: V. Candela, A. Falcó and D.P. Romero. A General Framework for a Class of Non-linear Approximations with Applications to Image Restoration. Journal of Computational and Applied Mathematics. Volume 330 (2018) pp. 982–994.

- To state our results, it will be necessary to distinguish between a *neural network* as a set of weights and the associated function implemented by the network, which we call its *realization*. To explain this distinction, let us fix numbers $L, N_0, N_1, \dots, N_L \in \mathbb{N}$. We say that a family $\Phi = ((A_\ell, b_\ell))_{\ell=1}^L$ of matrix-vector tuples of the form $A_\ell \in \mathbb{R}^{N_\ell \times N_{\ell-1}}$ and $b_\ell \in \mathbb{R}^{N_\ell}$ is a **neural network**.
- We call $S := (N_0, N_1, \dots, N_L)$ the **architecture** of Φ ; furthermore $N(S) := \sum_{\ell=0}^L N_\ell$ is called the **number of neurons of S** and $L = L(S)$ is the **number of layers of S** .
- We call $d := N_0$ the **input dimension** of Φ and throughout this introduction we assume that the **output dimension** N_L of the networks is equal to one. For a given architecture S , we denote by $\mathcal{NN}(S)$ the **set of neural networks with architecture S** .

Example 2: Neural Networks

Defining the realization of such a network $\Phi = ((A_\ell, b_\ell))_{\ell=1}^L$ requires two additional ingredients: a so-called **activation function** $\varrho : \mathbb{R} \rightarrow \mathbb{R}$, and a domain of definition $\Omega \subset \mathbb{R}^{N_0}$. Given these, the **realization of the network** $\Phi = ((A_\ell, b_\ell))_{\ell=1}^L$ is the function

$$R_\varrho^\Omega(\Phi) : \Omega \rightarrow \mathbb{R}, \quad x \mapsto x_L,$$

where x_L results from the following scheme:

$$\begin{aligned} x_0 &:= x, \\ x_\ell &:= \varrho(A_\ell x_{\ell-1} + b_\ell), \quad \text{for } \ell = 1, \dots, L-1, \\ x_L &:= A_L x_{L-1} + b_L, \end{aligned}$$

and where ϱ acts componentwise; that is,
 $\varrho(x_1, \dots, x_d) := (\varrho(x_1), \dots, \varrho(x_d)).$

Before we continue, let us note that the set $\mathcal{NN}(S)$ of all neural networks (that is, the network weights) with a fixed architecture forms a finite-dimensional vector space, which we equip with the norm

$$\|\Phi\|_{\mathcal{NN}(S)} := \|\Phi\|_{\text{scaling}} + \max_{\ell=1,\dots,L} \|b_\ell\|_{\max}$$

$$\text{for } \Phi = ((A_\ell, b_\ell))_{\ell=1}^L \in \mathcal{NN}(S),$$

where $\|\Phi\|_{\text{scaling}} := \max_{\ell=1,\dots,L} \|A_\ell\|_{\max}$. If the specific architecture of Φ does not matter, we simply write $\|\Phi\|_{\text{total}} := \|\Phi\|_{\mathcal{NN}(S)}$. In addition, if ϱ is continuous, we denote the **realization map** by

$$\mathbf{R}_\varrho^\Omega : \mathcal{NN}(S) \rightarrow C(\Omega; \mathbb{R}^{N_L}), \quad \Phi \mapsto \mathbf{R}_\varrho^\Omega(\Phi). \quad (2)$$

Consider the following set:

$$\mathcal{D} := \mathbf{R}_\varrho^\Omega(\mathcal{NN}(S)) \subset C(\Omega; \mathbb{R}^{M_L}).$$

Given, $\Phi \in \mathcal{NN}(S)$ then $\lambda \mathbf{R}_\varrho^\Omega(\Phi) \in \mathcal{D}$ for all $\lambda \in \mathbb{R}$.

Observe that $\lambda \mathbf{R}_\varrho^\Omega(\Phi)(x) = \lambda x_L$ and

$$\begin{aligned} x_0 &:= x, \\ x_\ell &:= \varrho(A_\ell x_{\ell-1} + b_\ell), \quad \text{for } \ell = 1, \dots, L-1, \\ \lambda x_L &:= \lambda(A_L x_{L-1} + b_L), \end{aligned}$$

Thus, $\lambda \mathbf{R}_\varrho^\Omega(\Phi) = \mathbf{R}_\varrho^\Omega(\Phi_\lambda)$ where

$$\Phi_\lambda = ((A_1, b_1), \dots, (A_{L-1}, b_{L-1}), (\lambda A_L, \lambda b_L)),$$

and hence $\lambda \mathbf{R}_\varrho^\Omega(\Phi) \in \mathcal{D}$ for all $\lambda \in \mathbb{R}$.

Proposition

Let $\Omega \subset \mathbb{R}^d$ be compact and let $S = (d, N_1, \dots, N_L)$ be a neural network architecture. If the activation function $\varrho : \mathbb{R} \rightarrow \mathbb{R}$ is continuous, then the realization map from Equation (2) is continuous. If ϱ is locally Lipschitz continuous, then so is R_ϱ^Ω .

Finally, if ϱ is globally Lipschitz continuous, then there is a constant $C = C(\varrho, S) > 0$ such that

$$\text{Lip}(R_\varrho^\Omega(\Phi)) \leq C \cdot \|\Phi\|_{\text{scaling}}^L \quad \text{for all } \Phi \in \mathcal{NN}(S).$$

Proposition

Let $S = (d, N_1, \dots, N_L)$ be a neural network architecture, let $\Omega \subset \mathbb{R}^d$ be compact, let furthermore $p \in (0, \infty)$, and let $\varrho : \mathbb{R} \rightarrow \mathbb{R}$ be continuous. For $C > 0$, let

$$\Theta_C := \{\Phi \in \mathcal{NN}(S) : \|\Phi\|_{\text{total}} \leq C\}.$$

Then the set $R_\varrho^\Omega(\Theta_C)$ is compact in $C(\Omega)$ as well as in $L^p(\mu)$, for any finite Borel measure μ on Ω and any $p \in (0, \infty)$.

Let $\Omega \subset \mathbb{R}^d$ be compact and fix $C > 0$. Consider the cone

$$\mathcal{D} := \{ \lambda R_\varrho^\Omega(\Phi) : \lambda \in \mathbb{R} \text{ and } R_\varrho^\Omega(\Phi) \in R_\varrho^\Omega(\Theta_C) \}$$

Proposition

Let $S = (d, N_1, \dots, N_L)$ be a neural network architecture, let $C > 0$, and let $\Omega \subset \mathbb{R}^d$ be Borel measurable and compact. Finally, assume ϱ continuous.

Then the set \mathcal{D} is weakly closed in $L^p(\mu; \mathbb{R}^{N_L})$ for every $p \in [1, \infty]$ and any finite Borel measure μ on Ω . Moreover, \mathcal{D} is also weakly closed in $C(\Omega; \mathbb{R}^{N_L})$.

- We can now easily show that the set \mathcal{D} is weakly closed in $L^p(\mu; \mathbb{R}^{N_L})$ and in $C(\Omega; \mathbb{R}^{N_L})$: Let \mathcal{Y} denote either $L^p(\mu; \mathbb{R}^{N_L})$ for some $p \in [1, \infty]$ and some finite Borel measure μ on Ω , or $C(\Omega; \mathbb{R}^{N_L})$, where we assume in the latter case that Ω is compact and set $\mu = \delta_{x_0}$ for a fixed $x_0 \in \Omega$. Note that we can assume $\mu(\Omega) > 0$, since otherwise the claim is trivial.
- Let $(f_n)_{n \in \mathbb{N}}$ be a sequence in \mathcal{D} which satisfies $f_n \rightharpoonup f$ for some $f \in \mathcal{Y}$, with convergence in \mathcal{Y} . Thus, $f_n = \lambda_n R_\varrho^\Omega(\Phi_n)$ for suitable sequences $(\Phi_n)_{n \in \mathbb{N}}$ in Θ_C and $(\lambda_n)_{n \in \mathbb{N}}$ in \mathbb{R} .
- Since $(f_n)_{n \in \mathbb{N}} = (\lambda_n R_\varrho^\Omega(\Phi_n))_{n \in \mathbb{N}}$ is weakly convergent in \mathcal{Y} , it is also bounded in \mathcal{Y} . In particular, $(\lambda_n)_{n \in \mathbb{N}}$ and $(R_\varrho^\Omega(\Phi_n))_{n \in \mathbb{N}}$ are bounded in \mathbb{R} and \mathcal{Y} , respectively.
- Since $((\lambda_n, \Phi_n))_{n \in \mathbb{N}}$ is bounded in the closed set $\mathbb{R} \times \Theta_C$ there exists subsequence, also denoted by $((\lambda_n, \Phi_n))_{n \in \mathbb{N}}$, such that $(\lambda_n, \Phi_n) \rightarrow (\lambda, \Phi) \in \mathbb{R} \times \Theta_C$.

- Since Ω is compact the realization map

$$R_\varrho^\Omega : \mathcal{NN}(S) \rightarrow C(\Omega; \mathbb{R}^{N_L}), \Phi \mapsto R_\varrho^\Omega(\Phi)$$

is continuous and hence the map

$$\Phi : \mathbb{R} \times \mathcal{NN}(S) \rightarrow C(\Omega; \mathbb{R}^{N_L}), (\lambda, \Phi) \mapsto \lambda R_\varrho^\Omega(\Phi)$$

is also continuous.

- Thus, $f_n = \lambda_n R_\varrho^\Omega(\Phi_n) \rightarrow \lambda R_\varrho^\Omega(\Phi)$ as $n \rightarrow \infty$, with uniform convergence. This easily implies $f_n = \lambda_n R_\varrho^\Omega(\Phi_n) \rightarrow \lambda R_\varrho^\Omega(\Phi)$, with convergence in \mathcal{Y} as $n \rightarrow \infty$. Hence, $\lambda R_\varrho^\Omega(\Phi) = f \in \mathcal{D}$. \square

In this case, we consider $X = \overline{\text{span } \mathcal{D}}^{\|\cdot\|}$.

Reference: Petersen, P., Raslan, M. & Voigtlaender, F. Topological Properties of the Set of Functions Generated by Neural Networks of Fixed Size . Found Comput Math 21, 375–444 (2021).

We first consider the definition of the algebraic tensor space ${}_a \bigotimes_{j=1}^d V_j$ generated from Banach spaces V_j ($1 \leq j \leq d$) equipped with norms $\|\cdot\|_j$. As underlying field we choose \mathbb{R} , but the results hold also for \mathbb{C} . The suffix 'a' in ${}_a \bigotimes_{j=1}^d V_j$ refers to the 'algebraic' nature. By definition, all elements of

$$\mathbf{v} := {}_a \bigotimes_{j=1}^d V_j$$

are *finite* linear combinations of elementary tensors $\mathbf{v} = \bigotimes_{j=1}^d v^{(j)}$ ($v^{(j)} \in V_j$).

A typical representation format is the Tucker or tensor subspace format

$$\mathbf{u} = \sum_{\mathbf{i} \in \mathbf{I}} \mathbf{a}_{\mathbf{i}} \bigotimes_{j=1}^d b_{i_j}^{(j)}, \quad (3)$$

where $\mathbf{I} = I_1 \times \dots \times I_d$ is a multi-index set with $I_j = \{1, \dots, r_j\}$, $r_j \leq \dim(V_j)$, $b_{i_j}^{(j)} \in V_j$ ($i_j \in I_j$) are linearly independent (usually orthonormal) vectors, and $\mathbf{a}_{\mathbf{i}} \in \mathbb{R}$. Here, i_j are the components of $\mathbf{i} = (i_1, \dots, i_d)$. The data size is determined by the numbers r_j collected in the tuple $\mathbf{r} := (r_1, \dots, r_d)$.

The set of all tensors representable by (3) with bounded tensor rank \mathbf{r} is

$$\mathcal{T}_{\leq \mathbf{r}}(\mathbf{V}) := \left\{ \mathbf{v} \in \mathbf{V} : \begin{array}{l} \text{there are subspaces } U_j \subset V_j \text{ such that} \\ \dim(U_j) = r_j \text{ and } \mathbf{v} \in \mathbf{U} := \bigotimes_{j=1}^d U_j. \end{array} \right\} \quad (4)$$

satisfy that

$$\lambda \mathcal{T}_{\leq \mathbf{r}}(\mathbf{V}) \subset \mathcal{T}_{\leq \mathbf{r}}(\mathbf{V})$$

for all $\lambda \in \mathbb{R}$, and hence it is a cone. To simplify the notations, the set of bounded rank-one tensors (elementary tensors) will be denoted by

$$\mathcal{R}_1(\mathbf{V}) := \mathcal{T}_{\leq (1, \dots, 1)}(\mathbf{V}) = \left\{ \bigotimes_{k=1}^d w^{(k)} : w^{(k)} \in V_k \right\}.$$

We say that $\mathbf{V}_{\|\cdot\|}$ is a *Banach tensor space* if there exists an algebraic tensor space \mathbf{V} and a norm $\|\cdot\|$ on \mathbf{V} such that $\mathbf{V}_{\|\cdot\|}$ is the completion of \mathbf{V} with respect to the norm $\|\cdot\|$, i.e.

$$\mathbf{V}_{\|\cdot\|} := \overline{\|\cdot\| \bigotimes_{j=1}^d V_j} = \overline{\bigotimes_{j=1}^d V_j}_{\|\cdot\|}.$$

If $\mathbf{V}_{\|\cdot\|}$ is a Hilbert space, we say that $\mathbf{V}_{\|\cdot\|}$ is a *Hilbert tensor space*. Moreover,

$$\overline{\text{span} \mathcal{T}_{\leq(1,\dots,1)}(\mathbf{V})} = \overline{\text{span} \mathcal{T}_{\leq r}(\mathbf{V})} = \mathbf{V}_{\|\cdot\|}$$

Thus, the sets $\mathcal{D} = \mathcal{T}_{\leq r}(\mathbf{V})$ are good candidates to be dictionaries.

Now, we introduce the following norm.

Definition

Let V_j be Banach spaces with norms $\|\cdot\|_j$ for $1 \leq j \leq d$. Then for $\mathbf{v} \in \mathbf{V} = \bigotimes_{j=1}^d V_j$, we define the norm $\|\cdot\|_{\mathbf{V}}$ by

$$\|\mathbf{v}\|_{\mathbf{V}} := \sup \left\{ \frac{|(\varphi^{(1)} \otimes \varphi^{(2)} \otimes \dots \otimes \varphi^{(d)}) (\mathbf{v})|}{\prod_{j=1}^d \|\varphi^{(j)}\|_j^*} : 0 \neq \varphi^{(j)} \in V_j^*, 1 \leq j \leq d \right\}. \quad (5)$$

Proposition

Let $\mathbf{V}_{\|\cdot\|}$ be a Banach tensor space with a norm satisfying $\|\cdot\| \gtrsim \|\cdot\|_{\mathbf{V}}$ on \mathbf{V} . Then the set $\mathcal{T}_{\mathbf{r}}(\mathbf{V})$ is weakly closed.

Reference: Falcó, A., Hackbusch, W. On Minimal Subspaces in Tensor Representations. Found Comput Math 12, 765–803 (2012).

We now consider the minimization problem

$$J(u) = \min_{v \in X} J(v) \quad (\pi)$$

of a functional J on a reflexive Banach space X . Assume that we have a functional $J : X \rightarrow \mathbb{R}$ satisfying

- (A1) J is Fréchet differentiable, with Fréchet differential $J' : X \rightarrow X^*$.
- (A2) J is elliptic, i.e. there exist $\alpha > 0$ and $s > 1$ such that for all $v, w \in X$;

$$\langle J'(v) - J'(w), v - w \rangle_{X^* \times X} \geq \alpha \|v - w\|^s. \quad (6)$$

Moreover, we have set \mathcal{D} (called *dictionary*) in X satisfying:

- (B1) $\mathcal{D} \subset X$, is a weakly closed,
- (B2) for each $\mathbf{v} \in \mathcal{D}$ we have $\lambda \mathbf{v} \in \mathcal{D}$ for all $\lambda \in \mathbb{R}$, and
- (B3) $\text{span } \mathcal{D}$ is dense in X .

Thank you for your attention !