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Blending isogeometric analysis and local *maximum entropy* meshfree approximants

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ABSTRACT

We present a method to blend local maximum entropy (LME) meshfree approximants and isogeometric analysis. The coupling strategy exploits the optimization program behind LME approximation, treats isogeometric and LME basis functions on an equal footing in the reproducibility constraints, but views the former as data in the constrained minimization. The resulting scheme exploits the best features and overcomes the main drawbacks of each of these approximants. Indeed, it preserves the high fidelity boundary representation (exact CAD geometry) of isogeometric analysis, out of reach for bare meshfree methods, and easily handles volume discretization and unstructured grids with possibly local refinement, while maintaining the smoothness and non-negativity of the basis functions. We implement the method with B-Splines in two dimensions, but the procedure carries over to higher spatial dimensions or to other non-negative approximants such as NURBS or subdivision schemes. The performance of the method is illustrated with the heat equation, and linear and nonlinear elasticity. The ability of the proposed method to impose directly essential boundary conditions in non-convex domains, and to deal with unstructured grids and local refinement in domains of complex geometry and topology is highlighted by the numerical examples.

1. Introduction

Approximants selected by maximum entropy (*max-ent*) are non-negative smooth meshfree approximation schemes, optimal from an information theory viewpoint [1,2]. The non-negativity and first-order reproducing conditions endow these approximants with the structure of convex geometry [1], like linear finite element, natural neighbor method [3], subdivision approximants [4], or B-Spline and Non-Uniform Rational B-Splines (NURBS) basis functions [5]. *Max-ent* approximants have been extended to second order [6,7], and to arbitrary order by dropping non-negativity [8].

Local maximum entropy (LME) approximants allow us to flexibly control the support of the basis functions on unstructured grids of points [1,9]. Their non-negativity endow them with variation diminishing properties, as well as with a weak Kronecker-delta property on the boundary of the convex hull of the set of nodes [1], by which interior basis functions vanish at the boundary of the convex hull, and basis functions vanish at any given face unless the corresponding node belongs to that face of the boundary. Thanks to this property, essential boundary conditions can be easily imposed on polygonal convex domains, in contrast with other meshfree methods [10]. Furthermore, the evaluation of the LME basis functions is very efficient using duality methods [1]. The main drawback of these approximants is given by the inherent limitation of meshfree methods to represent complex boundaries with high fidelity. In such methods, the boundaries that can be represented by a mere collection of points are polytopes, either the convex hull or more controllable domains given by alpha shapes [11]. Furthermore, the weak Kronecker-delta property of LME approximants does not hold in non-convex parts of the domain [1].

Motivated by the recent impetus on isogeometric analysis [5,12], which aims at integrating Computer Aided Design (CAD) technologies, such as B-Splines, NURBS or subdivision surfaces [4], and engineering analysis, we propose here using such high-fidelity description of the boundary of the domain, while approximating the interior with *max-ent* methods. Remarkably, the limitations of LME approximants and of isogeometric analysis are in some sense complementary, since the main drawback of the latter is precisely the rigidity imposed by the NURBS framework on the volume meshing, which requires special techniques to go beyond tensor product meshes and accommodate trimmed surfaces, local refinement, or incongruent surface descriptions at opposing faces. Some of these issues are partially addressed in 2D with T-Spline technologies [13–17], hierarchical B-Splines [18] or trimming techniques [19], but largely open in 3D [20,21]. Three-dimensional subdivision schemes, producing

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smooth convex approximants from unstructured grids, are still the topic of current research [22].

The goal of the proposed method is to unify in a common framework the geometric fidelity of isogeometric boundary representations with the flexibility of meshfree approximants in the bulk of the domain. Since both B-Splines and LME approximants are convex schemes, we will show that they can be coupled through the constraints in a *max-ent* program. The resulting approximation scheme automatically retains the non-negativity and smoothness of the B-Spline and LME parents. Although *max-ent* approximants can be extended to higher-order consistency, at the expense of a more involved formulation [6,7], numerical experiments show that first-order consistent approximants perform very well, even in high-order partial differential equations. In [7], we showed that first-order LME approximants attain the same accuracy as 5*th*-order B-Splines for structural vibrations, and are comparable to second-order *max-ent* approximation schemes in a fourth-order phase field model [23], or in thin shell problems [24,25], where they also compete with subdivision finite elements.

In the same spirit of the method presented here, the NURBS enhanced finite element method (NEFEM) [26] adopts a NURBS boundary representation, coupled to standard finite elements in the interior of the domain. This approach exploits the high fidelity geometry representation of isogeometric analysis, but does not insist in preserving the smoothness and positivity of the basis functions, placing more emphasis in the high-order reproducibility conditions. On the other hand, Moving Least Squares (MLS) meshfree basis functions have been coupled with finite elements through the consistency conditions [27].

The paper is organized as follows. Sections 2 and 3 provide the main concepts about *max-ent* approximations schemes and the isogeometric representation of boundaries. In Section 4, we describe the proposed blending strategy, and in Section 5 we report on illustrative numerical examples. Finally, Section 6 collects the concluding remarks.

2. Maximum entropy approximation schemes

In information theory and statistical inference, the principle of *max-ent* is a means to infer the probability distribution, which best represents the current state of knowledge about a process, consistently with *a priori* information. This principle was adopted in [1,2] to generate the least biased basis functions for nodal data approximation. The key in this information theoretical viewpoint is to interpret the approximants as probability distributions. This interpretation follows from the partition of unity and the fact that we require the approximants to be non-negative.

More concretely, consider the approximation of a function in a domain $\Omega \subset \mathbb{R}^d$ as a linear combination of basis functions associated with a set of nodes $X = \{\boldsymbol{x}_a\}_{a=1,\dots,N} \subset \mathbb{R}^d$,

$$u(\boldsymbol{x}) \approx u^h(\boldsymbol{x}) = \sum_{a=1}^{N} p_a(\boldsymbol{x}) u_a.$$

Rather than defining explicitly the basis functions $p_a(\boldsymbol{x})$, we view them as unknowns, which need to fulfill the partition of unity $\sum_{a=1}^{N} p_a(\boldsymbol{x}) = 1$ and the first-order consistency condition $\sum_{a=1}^{N} p_a(\boldsymbol{x})\boldsymbol{x}_a = \boldsymbol{x}$. Additionally, we demand that $p_a(\boldsymbol{x}) \geqslant 0$. Comparing these conditions with the definition of the convex hull of the set of nodes

$$\mathrm{conv}X = \left\{ \boldsymbol{x} \in \mathbb{R}^d | \boldsymbol{x} = \sum_{a=1}^{N} \eta_a \boldsymbol{x}_a, \text{ with } \eta_a \geqslant 0, \ \sum_{a=1}^{N} \eta_a = 1 \right\},$$

it follows that such an approximation scheme can only be defined in domain satisfying $\Omega \subset \mathrm{conv}X$.

If the node set is composed of more than $d+1$ affinely independent points, there exist infinitely many convex approximation schemes, and the principle of *max-ent* emerges as a selection principle. These basis functions can be computed by maximizing the information entropy subject to the constraints given by the reproducibility conditions [1,2]. The *max-ent* framework is quite flexible and allows us to consider other related approaches. The LME approximants [1] represent the optimal compromise (in the Pareto sense) between two competing objectives: (i) maximum locality of the basis functions and (ii) maximum information entropy of the scheme.

The convex program defining the LME approximants is

$$\begin{aligned} \text{(LME)} \quad \text{For fixed } \boldsymbol{x} \text{ minimize } & \sum_{a=1}^{N} \beta_a p_a \, | \boldsymbol{x} - \boldsymbol{x}_a |^2 + \sum_{a=1}^{N} p_a \ln p_a, \\ \text{subject to } & p_a \geqslant 0, \quad a = 1, \dots, N, \\ & \sum_{a=1}^{N} p_a = 1, \quad \sum_{a=1}^{N} p_a \boldsymbol{x}_a = \boldsymbol{x}, \end{aligned}$$

where the non-negative parameters β_a weigh the relative importance given to each objective in each nodal position [9].

The above program is convex, smooth and feasible for any spatial dimension d (as long as $\boldsymbol{x} \in \mathrm{conv}X$), and produces C^∞ meshfree non-negative functions $p_a(\boldsymbol{x})$ [1]. Moreover, the constraints (consistency conditions) guarantee solutions that reproduce exactly affine functions (see [6,7,28,29] for higher-order approaches). Duality methods provide an efficient route to solving the optimization problem and computing almost explicitly $p_a(\boldsymbol{x})$ at each evaluation point $\boldsymbol{x}$. Defining the partition function

$$Z(\boldsymbol{x}, \boldsymbol{\lambda}) = \sum_{b=1}^{N} \exp\left[-\beta_b \, | \boldsymbol{x} - \boldsymbol{x}_b |^2 + \boldsymbol{\lambda} \cdot (\boldsymbol{x} - \boldsymbol{x}_b) \right],$$

the LME basis functions can be computed as

$$p_a(\boldsymbol{x}) = \frac{1}{Z(\boldsymbol{x}, \boldsymbol{\lambda}^*(\boldsymbol{x}))} \exp\left[-\beta_a \, | \boldsymbol{x} - \boldsymbol{x}_a |^2 + \boldsymbol{\lambda}^*(\boldsymbol{x}) \cdot (\boldsymbol{x} - \boldsymbol{x}_a) \right],$$

where the Lagrange multiplier for the linear consistency condition is the unique minimizer of a smooth convex unconstrained optimization problem, minimizing $\ln Z$, efficiently solved with Newton's method [1].

The parameters $\beta_a = \gamma_a / h_a^2$, where γ_a is a dimensionless aspect ratio parameter and h_a the typical nodal spacing, allow us to control the locality (the support size) of the basis functions [1,9]. The approximants become sharper and narrower as the dimensionless parameter γ_a increases, and for values close to 4 and above they are nearly indistinguishable from the affine Delaunay basis functions, as illustrated in Fig. 1 in 1D. As γ_a tends to infinity, it has been mathematically shown that the affine functions supported on the Delaunay triangulation of the node set are recovered [1]. In

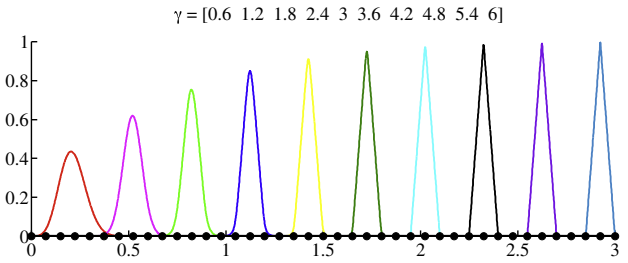

Fig. 1. LME approximants enable a seamless and smooth transition from meshfree to Delaunay affine basis functions. The transition is controlled by the non-dimensional nodal parameters γ_a, which here take linearly varying values from 0.6 (left) to 6 (right).