Pattern recognition issues on anisotropic smoothed particle hydrodynamics

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Abstract. This is a preliminary theoretical discussion on the computational requirements of the state of the art smoothed particle hydrodynamics (SPH) from the optics of pattern recognition and artificial intelligence. It is pointed out in the present paper that, when including anisotropy detection to improve resolution on shock layer, SPH is a very peculiar case of unsupervised machine learning. On the other hand, the free particle nature of SPH opens an opportunity for artificial intelligence to study particles as agents acting in a collaborative framework in which the timed outcomes of a fluid simulation forms a large knowledge base, which might be very attractive in computational astrophysics phenomenological problems like self-propagating star formation.

1. Introduction
Smoothed particle hydrodynamics (SPH) has been a successful computer simulation paradigm originated in computational astrophysics since 1977 [2, 5]. Nowadays SPH is used in other areas and has gained significant improvement in accuracy and stability, not only on simulating compressible shock as also on performing high resolution incompressible fluid, solids etc, e.g. [4].

One essential issue in SPH is anisotropy, which arises naturally on performing adaptive interpolation, e.g. [7], where the dimensionality reduction to detect critical surfaces, as shock layers might be included. Anisotropy is an important subject in pattern recognition for feature extraction methods [1].

There are encouraging works on the application of artificial intelligence to reproduce real systems, mainly in the context of complex systems as in economics and many other social and life sciences, e.g. [3]. The collective phenomena of star formation, unveiled in the intermittent pattern in the spiral galaxies arms, have been proposed by means of the stochastic self-propagating star formation model, in the sense that star formation is contagious, e.g. [8].

The present work is a brief discussion on some aspects of SPH circumstanced by the concepts of pattern recognition and artificial intelligence. Several details are omitted to fulfill the limited space with no significative lost of focus on reviewing the theory in the context of intelligent computing.

2. SPH database and space representation
The SPH database comprises \( N \) instances, usually thousand hundreds or even millions particles, indexed by a descriptor table \( P_N \). Each particle is addressed by a unique label, or descriptor...
i, and as much as possible the particle object is referred as just i or i-particle. Any particle attribute, say $A_i$, is addressed by sub-indexing the same with the particle label, $A_i$.

Since a specific SPH problem is headed by the mathematical, physical and computational models, the adopted methods might be included in the database in the form of classes and module libraries, described in a commonly used data model language as for instance the XML, which may also improve the information interchange between different SPH simulation bases.

The usual 3D space description in SPH uses hierarchical spatial tessellation, as for instance by means of octrees, e.g. [6], which are the 3D version of quadtrees. Other tree-based spatial tessellation schemes are also adopted. For instance [7] proposes an approach to easily adapt earlier versions of octree-based SPH codes to covariance-based octree tessellation to improve anisotropic kernel computations, e.g. [11].

3. **Starring pattern recognition and AI in SPH**

The $k$-nearest neighbor is a mathematical relation $N_k \subseteq P_N \times P_N$, which associates $i \in P_N$ with a subset $N_k(i) = \{i_1, \ldots, i_k\} \subseteq P_N$, so that $j \in N_k(i)$ if, and only if, the adopted distance $d(\vec{x}_i, \vec{x}_j)$ from $i$ to $j$ obeys the inequality $d(\vec{x}_i, \vec{x}_j) \leq \max\{d(\vec{x}_i, \vec{x}_l)\ l \in N_k(i)\}$. The KNN algorithm is the method by which the relation $N_k$ is populated by ordered pairs $(i,j)$ in $P_N \times P_N$, given the particle-descriptor table $P_N$.

The $N_k$ relation is asymmetric and reflexive. The later comes from the fact that each point is the nearest neighbor of itself – this is called improper neighbor. The former comes from the fact that if $a$ is the proper nearest neighbor (not a reflection) of $b$, not necessarily $b$ is the nearest neighbor of $a$. For example, $a$ could be closer to a third point $c$ than $b$, which is too faraway from any other point but $a$.

The KNN asymmetry reflects imperfections on writing simpler forms of the SPH conservation equations, which require particle commutation symmetry. To workaround the asymmetry issue is necessary to introduce the symmetric closure of the KNN relation, which is known as effective neighbors

$$E_k = N_k \cup \{(i,j) \in P_N \times P_N \mid (j,i) \in N_k\}. \quad (1)$$

Of course, the KNN algorithm requires a predesign metric in the 3D space. If the metric is invariant under rotation, the KNN relation is isotropic. On the other hand, the metric relation is said anisotropic. For instance the Mahalanobis metric, as adopted in the KNN algorithm proposed by [7], is anisotropic and is used to reveal biased structures like the arms in spiral galaxy images.

The Mahalanobis distance $\xi_{ij}$ is defined in terms of the covariance tensor $\Sigma$:

$$\xi_{ij} = (\vec{x}_i - \vec{x}_j)\Sigma^{-1}(\vec{x}_i - \vec{x}_j)^T, \quad (2)$$

where $(\vec{x}_i - \vec{x}_j)^T$ is the transpose of the matrix representation of the relative position vector $(\vec{x}_i - \vec{x}_j)$.

Of course, equation (2) is not the only way of defining anisotropic distance in SPH. For instance, the positive-definite stress tensor $T$ might be eventually used to define the non-normalized anisotropic distance $\xi_{ij}$:

$$\xi_{ij} = (\vec{x}_i - \vec{x}_j)T^{-1}(\vec{x}_i - \vec{x}_j)^T. \quad (3)$$

According to equations (2) or (3), the outermost boundary for the $k$-nearest neighbors of the $i$-particle is an ellipsoid centered in the query position $\vec{x}_i$, whose principal axes are set by the respective tensor eigenvectors [7].

A cognitive interpretation for the well-known SPH interpolation formula can be illustrated as follows: given an $i$-labeled particle, say $i$-particle, one may suppose this particle has to make
an estimation, $\tilde{A}_i$, of a local fluid quantity, $A_i$, after hearing votes, e.g. \cite{1}, from its effective neighbors what impression they get regarding the same quantity.

A democratic decision is made if the $i$-particle weights the individual suggestions from its informants, giving more importance to the closest ones. The importance, or weight, comes from a compact-support smoothing kernel, which drops to zero outside the influence zone defined by the effective neighbors and grows up as gets closer to $i$, reaching its maximum for $i$ itself.

Each $i$-particle, $i = 1, \ldots, N$, has its own effective neighbors, $E_k(i)$. The $i$-particle asks each $j$-particle in $E_k(i)$ for suggestions, which answers accordingly to the predefined protocol, $A_j m_j / \rho_j$, whose reliability is expressed by a weight, or smoothing kernel $W_{ij}$.

The $i$-particle gets a conclusive perception $\tilde{A}_i$ from its locality by adding together all of the weighted votes, $W_{ij} A_j m_j / \rho_j$, received from its $k$-nearest neighbors:

$$\tilde{A}_i = \sum_{j \in E_k(i)} W_{ij} A_j m_j / \rho_j$$  \hspace{1cm} (4)

where $W_{ij} = W(\vec{x}_i - \vec{x}_j)$ is the smoothing kernel, whose analytical profile might be an issue regarding accuracy and stability on SPH simulations, but this particular subject will not be discussed here.

Similar election procedure applies on estimating the interpolated gradient, $\tilde{\nabla}_i A_i$, yielding

$$\tilde{\nabla}_i A_i = \sum_{j \in E_k(i)} \tilde{\nabla}_i W_{ij} A_j m_j / \rho_j$$  \hspace{1cm} (5)

where $\tilde{\nabla}_i W_{ij} = \tilde{\nabla}_i W(\vec{x}_i - \vec{x}_j)$ is the smoothing-kernel gradient.

If the kernel is symmetric, one finds from the effective neighbors symmetry that $i \in E_k(j) \iff j \in E_k(i)$, and also finds $W_{ij} = W_{ji} \neq 0$, and $\tilde{\nabla}_i W_{ij} = - \tilde{\nabla}_j W_{ji}$ if and only if $(i,j) \in E_k$.

Densities are required to perform SPH interpolations, as in equations (4) and (5), and they are estimated from equation (4) itself by means of a self-consistent replacement $A_j \rightarrow \rho_j$, yielding

$$\tilde{\rho}_i = \sum_{j \in E_k(i)} W_{ij} m_j = \rho_i.$$  \hspace{1cm} (6)

The SPH fluid equations of motion are derived from the actual fluid equations, and they must be solved by means of some integration scheme regarding accuracy and stability. The timed outcomes from the integration scheme express discrete states of the particle description. Depending on the time-integration method, each particle knows a brief history of its previous states.

The way as the SPH equations are presented usually requires rearrangement to attend to subsidiary information concerning physics, chemistry etc. For instance, in most astrophysical problems, the SPH momentum conservation equation can be written as

$$\frac{d\vec{v}_i}{dt} = - \sum_{j \in E_k(i)} \tilde{\nabla}_i W_{ij} \Pi_{ij} + \vec{F}_i,$$  \hspace{1cm} (7)

where the $\Pi_{ij}$-factor carries the pressure coefficients, which might even include anisotropic pressure as the elastic stress tensor and the Maxwell stress tensor, e.g. \cite{6}. The $\vec{F}_i$-vector term is a non-hydrodynamic acceleration as for instance the gravity field $\vec{F}_i = -\vec{g}_i$ on $i$-particle.

Time-integration scheme plays the role of particle actuators modifying their local environment, in response to the information received from their effective neighbors. Every particle contributes to a global knowledge, which might attend to a subsidiary simulation, as for
example the qualitative results of self-propagating star formation, e.g. [8], the SPH-data history constitutes a knowledge-base [10] or even a more pretentious context as in live tissue simulations [9].

Each SPH particle recognizes its surroundings by means of its effective neighbors using pattern detection techniques to identify the neighborhood morphology and consequent critical surfaces. However, particles obey a set of transition rules, according to the physics model, to decide what action they have to do against their local environment.

From the theory of intelligent agents, SPH particles might be classified as simple reflex agents [10], acting as environment modifiers in function of what they perceive in their surroundings through their effective neighbors. The particles act under the local physical conditions in response to the input they receive from their effective neighbors, ignoring the long term history of all their actions and percepts. Regarding the adopted time integration scheme embedded as actuators, only the knowledge of a recent past is required.

4. Conclusion

More than a numerical simulation technique, SPH is a very complex system that can be studied not only under applied mathematics techniques but also under the light of intelligent computing, where particles are individuals cooperatively working in behalf of a collective objective of mimicking the fluid behavior.

The SPH spirit resides in computationally reproducing the continuous fluid flow using free particles. A fluid particle moves like a marker, accordingly to the lagrangian equations of motion. Each particle is a data structure storing the specific fluid properties as density, pressure, position, velocity etc. Any particle knows its surroundings through its \( k \)-nearest neighbors (KNN), which play the role of sensors, or informants. The information mechanism is known as KNN-based kernel interpolation, which might be interpreted as a weighted voting, from the machine learning viewpoint.

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