A machine learning approach of finding the optimal anisotropic SPH kernel

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Abstract. It is presented a machine learning approach to find the optimal anisotropic SPH kernel, whose compact support consists of an ellipsoid that matches with the convex hull of the self-regulating k-nearest neighbors of the smoothing particle (query).

1. Introduction
One of the main problems of SPH concerns the best morphology of the smoothing volume, regarding the optimal spatial resolution. A first attempt to improve spatial resolution is to consider each simulation particle (say, query particle) as the center of its \( k \)-nearest neighbors [1], which in turn is a variant of the Parzen window [2]. In such estimation technique the smoothing kernel is spherical, with smoothing length proportional to \( \rho^{-1/3} \). Therefore, the orthodox adaptive SPH is in fact a density-adaptive scheme, which in principle disregard the multivariate distribution of the simulation particles.

A second advance made in order to obtain a more complete spatial adaptability, both in density and in the preferential direction of deformation of the smoothing volume, was proposed by [3], hereafter MSVK, which named the adaptive technique as ASPH. The authors introduced a tensor version of the smoothing length, namely, the smoothing tensor \( H \), whose components change in space and time according to the estimated deformation-rate tensor, \( \nabla v \).

In present work, the smoothing tensor is proportional to the squared root of the covariance tensor, namely \( H = \gamma_{\text{max}} \Sigma^{1/2} \), where \( \gamma_{\text{max}} \) is the Mahalanobis distance from the query particle to the outermost one in the self-regulating \( k \)-NN cluster. Thus, \( H \) is the tensor whose eigenvalues/eigenvectors sets up the minimal ellipsoid hull of the self-regulating \( k \)-NN cluster.

2. Self-regulating kNN cluster
Let \( C \) be a cluster of SPH particles. The cluster’s covariance tensor [2] is defined as

\[
\Sigma_C = \frac{1}{M_C} \sum_{j \in C} m_j (r_j - r_C)(r_j - r_C)^t
\]

(1)

where \( M_C \) is the cluster total mass and \( r_C \) is the cluster center of mass.

The diagonal representation of the inverse covariance tensor can be written as

\[
\Sigma_C^{-1} = \frac{1}{\sigma_1^2} e_1 e_1^t + \frac{1}{\sigma_2^2} e_2 e_2^t + \frac{1}{\sigma_3^2} e_3 e_3^t
\]

(2)
from which is computed the Mahalanobis distance:

$$\delta^2 = (r - r_C)^t \Sigma_C^{-1} (r - r_C)$$  \hfill (3)

The collection of points in $\mathbb{R}^3$ whose Mahalanobis distance to the origin equals the unit is defined as the confidence ellipsoid. Particularly, doing the following transform

$$\xi_1 = \frac{(r - r_C) \cdot e_1}{\sigma_1}, \quad \xi_2 = \frac{(r - r_C) \cdot e_2}{\sigma_2}, \quad \xi_3 = \frac{(r - r_C) \cdot e_3}{\sigma_3},$$  \hfill (4)

we have

$$\xi_1^2 + \xi_2^2 + \xi_3^2 = 1,$$  \hfill (5)

which is the equation of a unit sphere $\mathbb{S}_1$ in the uncorrelated vector space

$$\mathbb{U}_3^2 = \{ \xi \mid \xi = \Sigma_C^{-1/2} (r - r_C) \}$$  \hfill (6)

It has been used in equation (6) the square root of the covariance tensor, which can be written in the diagonal form as

$$\Sigma_C^{1/2} \equiv \sigma_1 e_1 e_1^t + \sigma_2 e_2 e_2^t + \sigma_3 e_3 e_3^t,$$  \hfill (7)

whose inverse $\Sigma_C^{-1/2}$ can be easily written as

$$\Sigma_C^{-1/2} \equiv \frac{e_1 e_1^t}{\sigma_1} + \frac{e_2 e_2^t}{\sigma_2} + \frac{e_3 e_3^t}{\sigma_3}.$$  \hfill (8)

It is presumed that we already have an anisotropic kNN function as the method prescribed by [4], namely,

$$\mathcal{N}(q_0) = \{ q_0, q_1, ..., q_k \},$$  \hfill (9)

given the index $q_0$ of the query particle located at position $r_{q_0}$, and a predicted covariance tensor $\Sigma$ to perform the search according to the Mahalanobis metric.

The positive closure $\mathcal{N}^+$ of the anisotropic kNN is given by the subset $\mathcal{N}^+(q_0) = \mathcal{N}(q_0) - \{ q_0 \} = \{ q_1, ..., q_k \}$, which is the index set of the first $k$ nearest proper neighbors from $q_0$. Moreover, $\mathcal{N}(q_0)$ is ordered by Mahalanobis distances, namely, $\delta(r_{q_1}, r_{q_0}) \leq \delta(r_{q_2}, r_{q_0}) \leq \cdots \leq \delta(r_{q_k}, r_{q_0})$. If the particles are randomly distributed, the equality would very difficultly occur.

The initial step of the first training is made by using the identity tensor $\mathbf{1}$ in place of the predicted covariance tensor $\Sigma$. By first training we mean the start approach in the SPH simulation, before performing the integration scheme. Of course, such initialization switches the distance from anisotropic to euclidean. Thus, it gets the first attempt

$$\mathcal{C}_k^{(1)} \equiv \mathcal{N}(q_0|\mathbf{1}) = \{ q_0, q_1, ..., q_k \},$$  \hfill (10)

which is of course isotropic. Thus, the $\mathcal{C}_k^{(1)}$ morphology is almost spherical if it is within $\mathcal{D}$ and far from its borders.

The next approach consists of iteratively computing the covariance tensor for the newly found anisotropic neighborhood to predict a neighborhood closer to the objective that is the self-regulating kNN cluster. Thus, as it has been computed $\mathcal{C}_k^{(n)}$ at iteration $n$, compute the covariance tensor $\Sigma_{\mathcal{C}_k}^{(n)}$ for the newly found kNN cluster, and then estimate an ever more refined kNN list, namely

$$\mathcal{C}_k^{(n+1)} \leftarrow \mathcal{N}(q_0|\Sigma_{\mathcal{C}_k}^{(n)}).$$  \hfill (11)

The method converges in about 10 iterations.
3. The ellipsoidal hull for the self-regulating kNN cluster and the smoothing tensor

The convex hull of the self-regulating kNN cluster is the smallest ellipsoid whose semi-major axes are proportional to the square root of the eigenvalues of the covariance tensor computed from the self-regulating kNN. The query \( q \) itself is the geometric center of the ellipsoidal hull. Alternatively, such an envelope corresponds to the smallest sphere with radius \( \zeta_{\text{max}}(q) \) in the uncorrelated space \( \mathbb{U}^3 \), where \( \zeta_{\text{max}}(q) \) is computed as the maximum Mahalanobis distance amongst the \( k \)-nearest neighbors:

\[
\zeta_{\text{max}}(q) = \sqrt{\max_{p \in C_k(q)} \left\{ \zeta_p^2 = (r_p - r_q)^t \Sigma_{C_k(q)}^{-1} (r_p - r_q) \right\}}
\] (11)

where \( r_q \) is the query position and \( p \neq q \) stands for some of the proper \( k \)-nearest neighbors of \( q \). Thus, the kNN-cluster’s convex hull is the ellipsoid whose equation can be rewritten as

\[
(r_p - r_q)^t H^{-2} (r_p - r_q) = 1
\] (12)

where it is defined the smoothing tensor, \( H \), given the kNN cluster, \( C_k(q) \) and the query particle \( q \):

\[
H \equiv \zeta_{\text{max}} \Sigma_{C_k(q)}^{1/2}
\] (13)

whose spectral decomposition, known the \( \Sigma_{C_k(q)} \) eigenvalues/eigenvectors, is given by

\[
H = h_1 e_1 e_1^t + h_2 e_2 e_2^t + h_3 e_3 e_3^t
\] (14)

where

\[
h_1 = \zeta_{\text{max}} \sigma_1, 
\quad h_2 = \zeta_{\text{max}} \sigma_2, 
\quad h_3 = \zeta_{\text{max}} \sigma_3
\] (15)

The quadratic form expressed on the left-hand side of equation (12) induces the definition of the \( H \)-normalized, particle to query distance according to the following equation:

\[
\delta_p = \sqrt{(r_p - r_q)^t H^{-2} (r_p - r_q)}
\] (16)

where \( p \) is the generic particle index and \( H^{-1} \), the inverse of the smoothing tensor, can be easily computed as

\[
H^{-2} = \frac{e_1 e_1^t}{h_1} + \frac{e_2 e_2^t}{h_2} + \frac{e_3 e_3^t}{h_3}
\] (17)

Of course, \( H \) has the same normalized eigenvectors as does \( \Sigma_{C_k(q)} \). For brevity, we call hereafter the \( H \)-normalized distance as simply \( H \)-distance. Thus, the outermost neighbor in \( C_k(q) \) is the particle whose query’s \( H \)-distance is exactly \( \delta_p = 1 \).

4. Anisotropic smoothing kernel

The anisotropic smoothing kernel, \( W_H : \mathbb{E}^3 \mapsto \mathbb{R}_+ \), can be conveniently defined in terms of a spherical, dimensionless smoothing function \( K \), regarding equation (17)

\[
W_H(r) = \frac{1}{\det H} K(Hr),
\] (18)

as already mentioned at the end of the previous section. The smoothing kernel is a non-negative function whose domain is the original simulation space, namely, \( W_H : \mathbb{E}^3 \mapsto \mathbb{R}_+ \). While the kernel function is spherical symmetric and defined in the smoothing space, \( K : \mathcal{S}_q^3 \mapsto \mathbb{R}_+ \). As a rule, we adopt the kernel function \( K \) as having compact support, defined as the unit sphere \( \mathcal{S}_1 \).
centered on the origin, in the smoothing space $S^3_q$. Consequently, the smoothing kernel $W_H(r)$ is also a compact support function, whose support is the smoothing ellipsoid, centered on the query particle.

Since the kernel function $K$ is presumed spherically symmetric in the smoothing space $S^3_q$, we can write the kernel effect of particle $q$ over particle $p$ as

$$W_H(r_p - r_q) = \det H^{-1}K(\xi_{pq}) = \frac{1}{h_1h_2h_3}K(\xi_{pq})$$  \hfill (19)

where,

$$\xi_{pq} = |H^{-1}(r_p - r_q)| = \sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}$$  \hfill (20)

with

$$\xi_j = \frac{e_j \cdot (r_p - r_q)}{h_j}, \ j = 1, 2, 3$$  \hfill (21)

In order to perform the SPH interpolation equations, the knowledge of the kernel gradient $\nabla W_H$ is required. If one adopts the kernel formulation (19), one has from (20) and (21) the following equation

$$\nabla W_H(r) = \det H^{-1} \frac{1}{\xi} K'(\xi) H^{-2}r$$  \hfill (22)

where

$$\xi = |H^{-1}r|$$

5. Conclusion

What is new in this work is that the anisotropic kernel is defined only by multivariate arguments, involving the properties of the covariance tensor, without taking into account the ASPH technique. In summary, covariance-based SPH is based solely on the multivariability of the particle distribution, while in ASPH the smoothing tensor is defined according to the dynamics of the simulated fluid, via deformation rate tensor.

A more extensible version of the present work showing more details and results from the covariance-based SPH is being submitted.

References

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