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# Cloud of points as discrete measures for Gaussian models and stochastic optimization 

 Babacar SOW (EMSE, LIMOS), Rodolphe LE RICHE (CNRS LIMOS)Julien PELAMATTI(EDF R\&D), Merlin KELLER (EDF R\&D), Sanaa ZANNANE (EDF R\&D) Universités: Ecole Nationale Supérieure des Mines de Saint-Etienne(EMSE), Université Clermont Auvergne(UCA)

Context and problem



- A cloud of points is a sample of $n$ unordered points $X=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}$ with $\mathbf{x}_{i} \in$ $\mathbf{R}^{d}$.
- Metamodel functions defined over clouds of points using Gaussian process.
- Design stochastic, evolutionary, algorithms with operators based on Wasserstein barycenter.
- Note the set of clouds of points as $\mathcal{X}$ and the set of finite discrete measures defined over $\mathbf{R}^{d}$ as $\mathcal{P}$


## An evolutionary algorithm

- Clouds can be viewed as measures through the bijective mapping : $\varphi: \mathcal{X} \longrightarrow \mathcal{P}$ $X=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\} \longmapsto P_{X}=\frac{1}{n} \sum_{i=1}^{n} \delta_{\mathbf{x}_{i}}$
- Given two clouds of points $X$ and $X^{\prime}$, we denote $W_{2}^{2}\left(P_{X}, P_{X^{\prime}}\right)$ the 2-Wasserstein distance between $P_{X}$ and $P_{X^{\prime}}$ (see [3] for details)

A stochastic (evolutionary) optimizer over clouds of points is defined by the following:

- Crossover as Wasserstein barycenter: $\quad X^{\prime \prime}=\mathbf{W}$-barycenter $\left(X, X^{\prime}\right)$ where $X^{\prime \prime}$ is the discrete measure minimizing $\frac{1}{2}\left(W_{2}^{2}\left(P_{X^{\prime \prime}}, P_{X}\right)+\right.$ $\left.W_{2}^{2}\left(P_{X^{\prime \prime}}, P_{X^{\prime}}\right)\right)$.
$X^{\prime \prime}$ can have different sizes according to $X$ and $X^{\prime}$ (see [2] for details).
- Mutation: with probability $p$, do $X^{\prime \prime \prime}=$ W-barycenter $\left(X^{\prime \prime},\left(X^{\prime \prime} \cup D o m\right)\right) . D o m$ is a set of points at the domain boundary. For a square domain, Dom can be the corners.
The crossover promotes recombination of shapes while the mutation increases the spread of clouds.


## Wind-farm test functions

$F_{90}, F_{45}, F_{0}$ and $F_{40 d}$ are analytical functions $\mathcal{X} \rightarrow \mathbb{R}$ mimicking the power production of wind farms with wind directions $90^{\circ}, 45^{\circ}, 0^{\circ}$ and 40 averaged directions, respectively.

## References

[1] Muandet, Krikamol and Fukumizu, Kenji and Sriperumbudur, Bharath and Schölkopf, Bernhard and others: Kernel mean embedding of distributions: A review and beyond, Foundations and Trends $®$ in Machine Learning
[2] Cuturi, Marco and Doucet, Arnaud Fast computation of Wasserstein barycenters. International conference on machine learning
[3] Panaretos, Victor M and Zemel, Yoav, Statistical aspects of Wasserstein distances. Annual review of statistics and its application

## MMD-based Gaussian process through measure modeling

- Let $\mathcal{H}$ be a Reproducing Kernel Hilbert Space with a characteristic kernel $k_{\mathcal{H}}$ such as Matérn $5 / 2$. The characteristic nature guarantees the injectivity of the embedding map [1]: $P_{X} \longmapsto$ $\mu_{X}=\int P_{X}(x) k_{\mathcal{H}}(x,)$.$\mathrm{d} x . \theta_{1}$ and $\theta_{2}$ are 2 hyper-parameters scaling the dimensions between two points $\mathbf{x}$ and $\mathbf{x}^{\prime}$ through $\left|x_{1}-x_{1}^{\prime}\right| / \theta_{1}$ and $\left|x_{2}-x_{2}^{\prime}\right| / \theta_{2}$.
- The correlation kernel $K\left(X, X^{\prime}\right)=\sigma \exp \left(-\frac{\left\|\mu_{X}-\mu_{X^{\prime}}\right\|_{\mu_{H}}^{2}}{2 \theta^{2}}\right)$ is symmetric and semi-definite positive.
- Learned on 300 clouds of points, we get the following correspondence between the vector $\theta$ and the functions. The $Q 2$ values obtained by prediction on 1000 unseen (but of same type ) clouds of points are

| Functions | $F_{90}$ | $F_{45}$ | $F_{0}$ | $F_{40 d}$ |
| :--- | :--- | :--- | :--- | :--- |
| $Q 2$ | 0.899 | 0.868 | 0.906 | 0.906 |



Figure 1: Vectors of length scales of the MMD embedding kernel learned by maximum likelihood on the wind farm proxy for various wind directions. Left: reminder of the turbine contributions for winds at $90^{\circ}, 45^{\circ}, 0^{\circ}$ and 40 directions (left to right, top to bottom). Right: $\left(\theta_{1}, \theta_{2}\right)^{\top}$ vectors of length scales of the embedding kernel.

## Best designs found with the evolutionary optimizer

- We add the two following test functions $F_{\text {inert }}\left(\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}\right)=\sum_{i=1}^{n}\left\|\mathbf{x}_{i}-\bar{X}\right\|^{2}$ and $F_{\text {minDist }}\left(\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}\right)=\min _{i \neq j}\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|$.
- The following designs correspond to the ones found respectively on $F_{0}, F_{45}, F_{90}, F_{40 d}, F_{\text {inert }}$ and $F_{\text {minDist }}$. The inputs are clouds of points (in squares) with varying size (10 to 20).
- We observe an adaptation of the returned designs to the optimized functions. The points are placed optimally according to the wind's direction for wind-farms analytical functions. The algorithm returns also the optimal design for $F_{\text {inert }}$.
- These results illustrate that modeling clouds of points as finite discrete measures allow their processing without loss of geometrical information.


Figure 2: The designs correspond respectively to $F_{0}, F_{45}, F_{90}, F_{40 d}, F_{\text {inert }}$ and $F_{\text {minDist }}$ (left to right, top to bottom).

