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

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## Context and problem



- A cloud of points is a sample of  $n$  unordered points  $X = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  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:  $\varphi: \mathcal{X} \rightarrow \mathcal{P}$   
 $X = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \mapsto P_X = \frac{1}{n} \sum_{i=1}^n \delta_{\mathbf{x}_i}$
- Given two clouds of points  $X$  and  $X'$ , we denote  $W_2^2(P_X, P_{X'})$  the 2-Wasserstein distance between  $P_X$  and  $P_{X'}$  (see [3] for details)
- **Crossover as Wasserstein barycenter:**  $X'' = \mathbf{W}\text{-barycenter}(X, X')$  where  $X''$  is the discrete measure minimizing  $\frac{1}{2}(W_2^2(P_{X''}, P_X) + W_2^2(P_{X''}, P_{X'}))$ .  
 $X''$  can have different sizes according to  $X$  and  $X'$  (see [2] for details).
- **Mutation:** with probability  $p$ , do  $X''' = \mathbf{W}\text{-barycenter}(X'', (X'' \cup \text{Dom}))$ .  $\text{Dom}$  is a set of points at the domain boundary. For a square domain,  $\text{Dom}$  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  $F_{40d}$  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.

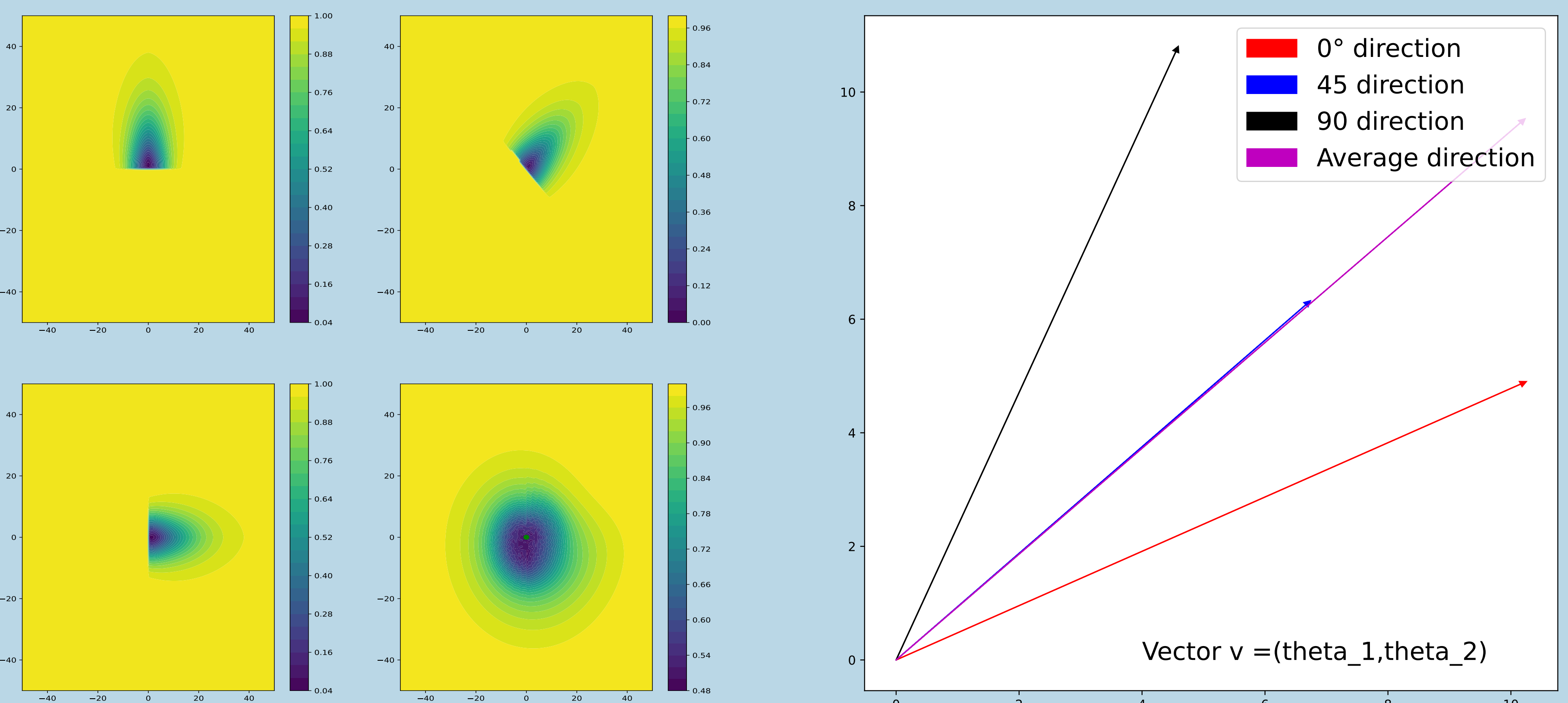
## References

- [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]:  $P_X \mapsto \mu_X = \int P_X(x)k_{\mathcal{H}}(x, \cdot)dx$ .  $\theta_1$  and  $\theta_2$  are 2 hyper-parameters scaling the dimensions between two points  $\mathbf{x}$  and  $\mathbf{x}'$  through  $|x_1 - x'_1|/\theta_1$  and  $|x_2 - x'_2|/\theta_2$ .
- The correlation kernel  $K(X, X') = \sigma \exp(-\frac{\|\mu_X - \mu_{X'}\|_{\mathcal{H}}^2}{2\theta^2})$  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  $Q2$  values obtained by prediction on 1000 unseen (but of same type) clouds of points are

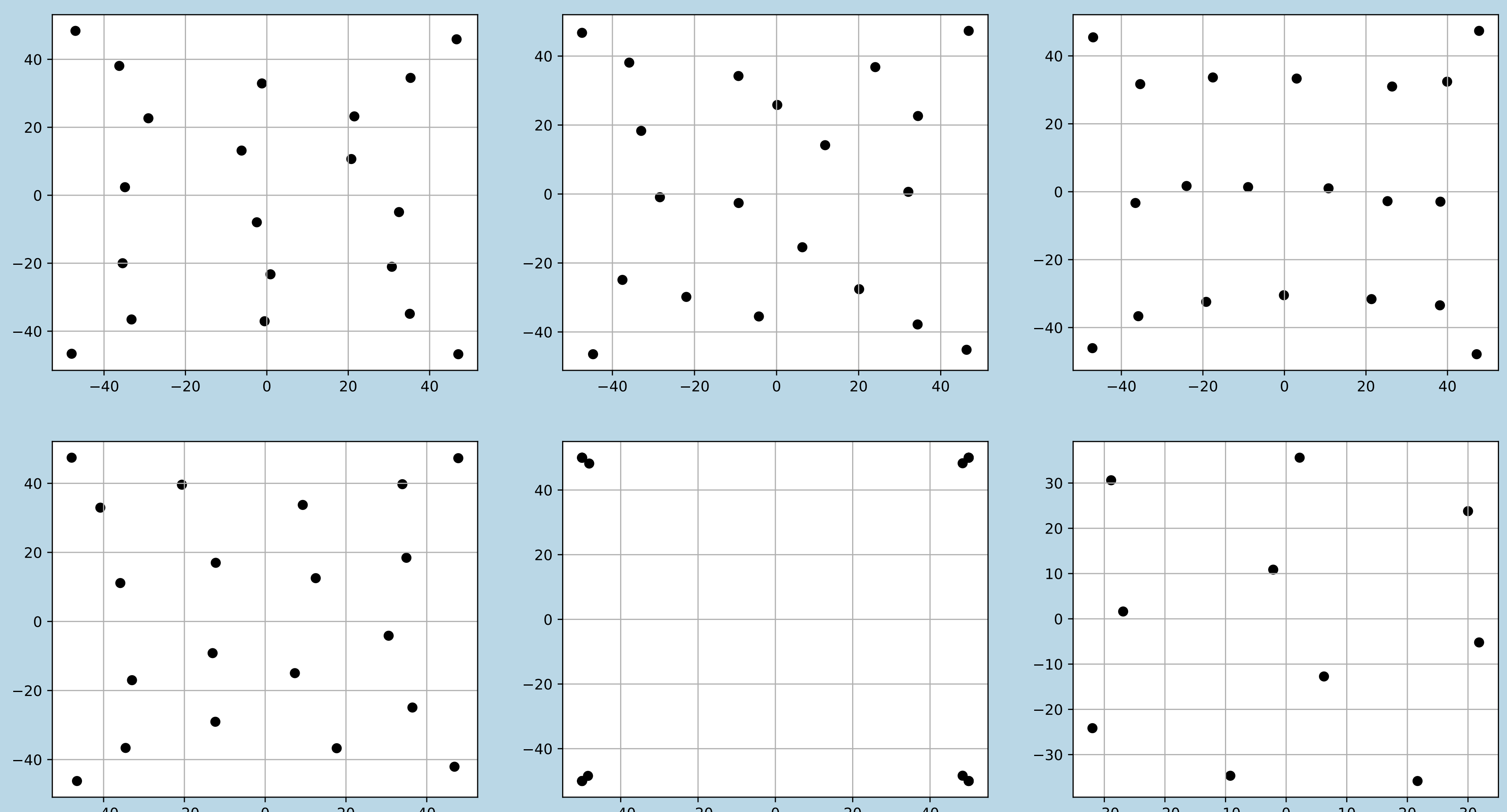
Functions	$F_{90}$	$F_{45}$	$F_0$	$F_{40d}$
$Q2$	0.899	0.868	0.906	0.906



**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:  $(\theta_1, \theta_2)^\top$  vectors of length scales of the embedding kernel.

## Best designs found with the evolutionary optimizer

- We add the two following test functions  $F_{inert}(\{\mathbf{x}_1, \dots, \mathbf{x}_n\}) = \sum_{i=1}^n \|\mathbf{x}_i - \bar{X}\|^2$  and  $F_{minDist}(\{\mathbf{x}_1, \dots, \mathbf{x}_n\}) = \min_{i \neq j} \|\mathbf{x}_i - \mathbf{x}_j\|$ .
- The following designs correspond to the ones found respectively on  $F_0$ ,  $F_{45}$ ,  $F_{90}$ ,  $F_{40d}$ ,  $F_{inert}$  and  $F_{minDist}$ . 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  $F_{inert}$ .
- **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  $F_0$ ,  $F_{45}$ ,  $F_{90}$ ,  $F_{40d}$ ,  $F_{inert}$  and  $F_{minDist}$  (left to right, top to bottom).