Directional Queries and Multi-Objective Optimization

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1 Notes

Let us start by defining a preference vector $\vec{w}$ s.t. $\sum_i w_i = 1$ and $w_i > 0$ and the equal contribution vector $\vec{\bar{w}}$, s.t. $\bar{w}_i = 1/w_i$. We consider a family of scoring functions

$$\mathcal{L}_p = \left\{ f | f(x) = \left(\sum_{i=1}^{d} w_i x_i^p \right)^{1/p} \right\}$$

Given a point $\vec{A} \in \mathbf{R}^d$ and the line r parametrized by $r_i = \bar{w}_i t$, $t \in \mathbf{R}$, the point $\vec{P} \in r$ minimizing the Euclidean distance from $\vec{A}$ is given by:

$$P : P_i = \frac{\bar{w}_i \sum_j x_j \bar{w}_j}{\sum_j \bar{w}_j^2}$$

The Euclidean norm of the segment $\vec{PA}$ is then

$$|\vec{PA}| = \sqrt{\sum_i \left(A_i - \frac{\bar{w}_i \sum_j A_j \bar{w}_j}{\sum_j \bar{w}_j^2} \right)^2}$$

A directional query $\mathcal{U}(w, \beta)$ is then defined and a convex sum between a linear query ($\mathcal{L}_1$) and a fairness contribution identified by $|\vec{Px}|$:

$$\mathcal{U}(w, \beta) = \beta \sum_{i=1}^{d} w_i x_i + (1 - \beta) \sqrt{\sum_i \left(x_i - \frac{\bar{w}_i \sum_j x_j \bar{w}_j}{\sum_j \bar{w}_j^2} \right)^2}$$

where $\beta \in [0, 1]$.

However, this notation may induce some undesirable bias as the weight vector $\vec{w}$ and the fairness vector $\vec{\bar{w}}$ have been normalized differently. In fact, the fairness vector has been implicitly normalized to unit Euclidean norm while the preference vector is normalized using the L^1 norm. To better balance between the two contributions, we can just transform the preference vector into a preference unit vector: $\vec{u} = \vec{w}/|\vec{w}|_2$. To ease notation, we can apply the same transformation to get the preference unit vector, $\vec{\bar{u}} = \vec{\bar{w}}/|\vec{\bar{w}}|_2$, and rewrite the directional query as:

$$\mathcal{U}(u, \beta) = \beta \sum_{i=1}^{d} u_i x_i + (1 - \beta) \sqrt{\sum_i \left(x_i - \bar{u}_i \sum_j x_j \bar{u}_j \right)^2}$$

To see the different behavior of the original and unit vector-based formulation see Figure 1.

2 A metric formulation

Let us consider the case where we want to transform the directional query into a metric induced in the objective space. A metric tensor $g(x)$ on a vector space (or manifold) is a smoothly varying positive

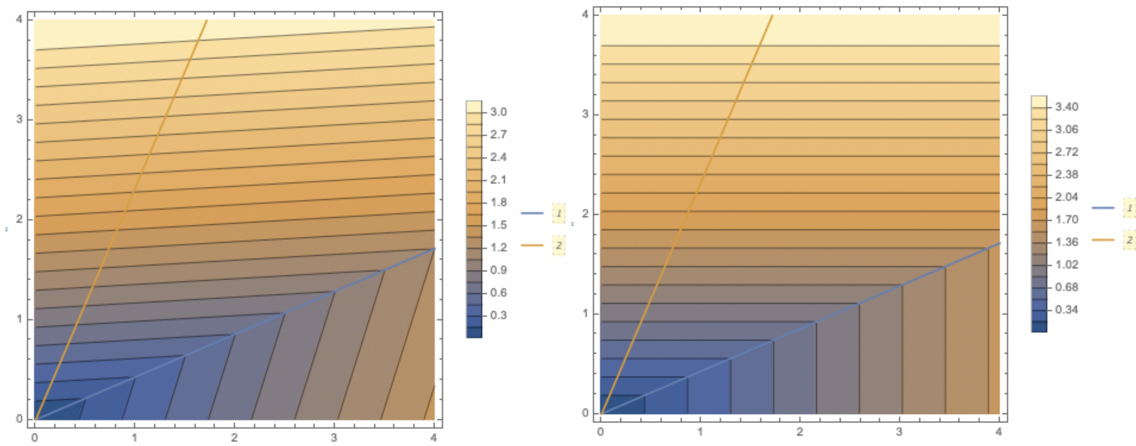

Figure 1: Left: original directional query with $\beta = 0.5$. Right: directional query with $\beta = 0.5$ after versor definition. The blue line represents the fairness vector and the orange line represents the preference vector.

definite bilinear form that defines an inner product on each tangent space. It is usually required to be quadratic in differentials (as in Riemannian geometry, where $ds^2 = g_{ij}dx^i dx^j$ leads to an L^2-type norm). While we can in principle adapt this formulation to get a metric tensor in L^1 using a Finsler metric, let us set this aside for a moment for the sake of simplicity.[1] Let us now reformulate the directional query so that it does not change its behavior in the limit cases, $\beta = 0$ and $\beta = 1$, but it allows for the introduction of a metric tensor in the objective space:

$$\tilde{\mathcal{U}}(w, \beta) = \sqrt{\beta \sum_{i=1}^{d} u_i^2 x_i^2 + (1-\beta) \sum_i \left(x_i - \bar{u}_i \sum_j x_j \bar{u}_j \right)^2}$$

The terms under the square root can be reformulated as an inner product given a certain metric:

$$\tilde{\mathcal{U}}(w, \beta) = \sqrt{\mathbf{x}^T \cdot \mathbf{G} \cdot \mathbf{x}}.$$

A straightforward calculation shows that

$$G_{ii} = \beta u_i^2 + (1-\beta)(1-\bar{u}_i^2)\,, \qquad G_{ij} = -(1-\beta)\bar{u}_i\bar{u}_j$$

Given that $\mathbf{G}$ is not trivial but contains only constant terms, the resulting space is still flat (no curvature is induced). Moreover, to re-establish a fair balancing of the utility and fairness term, I advise replacing β with γ^2 ($\gamma \in [0, 1]$) as it makes the transitioning between extreme behaviors more gradual.

3 Coulomb on non-trivial metrics

We have seen that the straightforward application of directional queries in multi-objective optimization may lead to redundant and overlapping results. This is because the is no general formalism enforcing some kind of diversity in the evolved population. To this aim, we can introduce the most well-known short-range interaction, i.e., the Coulomb interaction, between solutions in the current population. This will disfavor the evolution of particles in already populated regions of the objective space. Moreover, we would like this repelling force to follow the utility-fairness metric, to comply with the user-defined preference vector. This new ingredient implies that the utility function is not universal but changes from particle to particle according to the distribution of solutions in the current population. Calling

[1] Also note that, when considering a metric tensor in L^1, the formulation of the fairness term in the directional query should be changed as it relies on the L^2 norm.

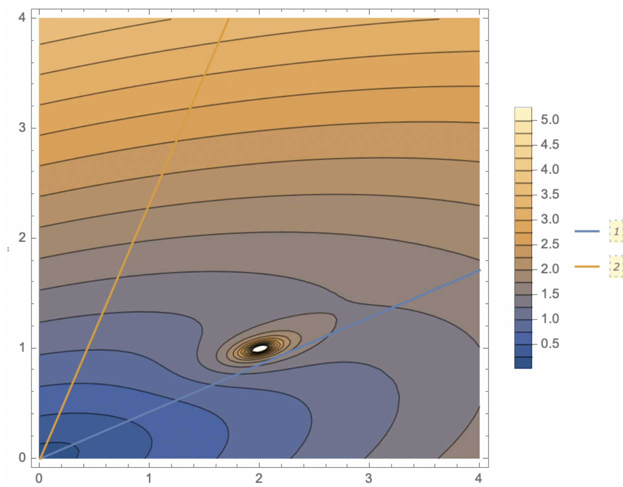

Figure 2: Potential felt by a particle when another particle is placed at coordinates (2,1). The blue line represents the fairness direction and the orange line represents the preference direction.

$S = \{\mathbf{s_1}, \mathbf{s_2}, \ldots, \mathbf{s_p}\}$ the set coordinate vectors of solutions in the current population, we have that their utility function can be expressed by:

$$\tilde{\mathcal{U}}(w, \beta, \mathbf{s}_k) = \sqrt{\mathbf{s}_k^T \cdot \mathbf{G} \cdot \mathbf{s}_k} + \sum_{q \in [1, \ldots, p], q \neq k} \frac{\rho}{|\mathbf{s}_k - \mathbf{s}_q|_G}$$

where $|\mathbf{s}_k - \mathbf{s}_q|_G = \sqrt{(\mathbf{s}_k - \mathbf{s}_q)^T \cdot \mathbf{G} \cdot (\mathbf{s}_k - \mathbf{s}_q)}$. An example of a utility function perceived by a particle when another one is placed at coordinates (2,1) in a 2-dimensional objective space is depicted in Figure 3.

4 Rephrasing from the beginning

We aim to find solutions in high dimensions focusing (more or less) on highly fair regions, given some reference weights in the objective space. To this aim, in principle, we could use some weighted norm approach expressed as:

$$\mathcal{U}(\mathbf{x}, \mathbf{w}, p) = \left(\sum_{i=1}^{N} (w_i |x_i - x_i^*|)^p \right)^{1/p} . \tag{1}$$

For a given p and a given $\mathbf{w}$, this reduces to find the intersection between the Pareto front and the metric isocurves stemming form stemming from the origin. At infinite p values, the method reduces to an optimization using the Chebyshev norm. However, it is well known that the method is unstable for high p values and may lead to non-Pareto solutions. For this reason, we aim to obtain the same behavior while keeping the objective space norm fixed (Euclidean metric). To do so, we need two ingredients: i) a diagonal metric describing an ellipsoid and ii) a rotation of the coordinate space. An ellipsoid is a quadratic form described, in its trivial diagonal version, by the following equation:

$$\sum_{i=1}^{N} z_i^2 / a_i^2 = 1 \tag{2}$$

where $a_i \in R^{>0}$ are the semi-axis distances. For this reason, using a linear algebra formulation we get the equivalent representation

$$\mathbf{z}^T \mathbf{A} \mathbf{z} = 1 \qquad A_{ij} = \delta_{ij} / a_i^2 \tag{3}$$

To reproduce the behavior or the directional queries, we would like to consider an ellipsoid having a single tunable semi-axis and unit semi-axes in every other dimensions: $A_{11} = 1/\epsilon^2$ and $A_{jj} = 1$ for $j \neq 1$. In particular, we would like the tunable semi-axis direction to coincide with the fair unit vector described above $\bar{\mathbf{u}}$. In the end, we will need to express the shape of such an ellipsoid in the canonical Euclidean basis $\mathbf{e}_i$ of $\mathbf{R}^N$. To identify a basis of R^n that includes the unit vector $\bar{\mathbf{u}}$ we can rely on the Gram-Schmitt procedure. Starting from a basis $\{\bar{\mathbf{u}}, \mathbf{e}_2, \mathbf{e}_3, \ldots, \mathbf{e}_N\}$ we can create an orthonormal basis $\mathbf{z}_i$ by following the procedure:

$$\begin{aligned}
\mathbf{z}_1 &= \bar{\mathbf{u}} \\
\mathbf{v}_k &= \mathbf{e}_k - \sum_{i=1}^{k-1} \left(\frac{\mathbf{e}_k \cdot \mathbf{z}_i}{\mathbf{z}_i \cdot \mathbf{z}_i} \right) \mathbf{z}_i \\
\mathbf{z}_k &= \mathbf{v}_k / ||\mathbf{v}_k||
\end{aligned} \tag{4}$$

In the end, the matrix $\mathbf{T}$ having the $\mathbf{z}_i$ vector as the i-th column, will represent the change of basis matrix between the standard Euclidean basis and an orthonormal basis containing $\mathbf{u}$ as the first coordinate:

$$\mathbf{T} : \{\mathbf{x}\} \rightarrow \{\mathbf{z}\} \tag{5}$$

$$\mathbf{T^{-1}} : \{\mathbf{z}\} \rightarrow \{\mathbf{x}\} \tag{6}$$

Given these ingredients, we can obtain the formulation of the ellipsoid with a tunable semi-axis along the $\bar{\mathbf{u}}$ direction in the standard eulidean coordinates as:

$$\mathbf{z}^T \mathbf{A} \mathbf{z} = \mathbf{x}^T \mathbf{T^{-1}}^T \mathbf{A} \mathbf{T^{-1}} \mathbf{x} = 1 \tag{7}$$

For this reason, the metric induced in the objective space is given by

$$\mathbf{G} = \mathbf{T^{-1}}^T \mathbf{A} \mathbf{T^{-1}} \tag{8}$$

and we can formulate the metric-based directional query with Coulomb repulsion as follows. Calling $S = \{\mathbf{s_1}, \mathbf{s_2}, \ldots, \mathbf{s_p}\}$ the set coordinate vectors of solutions in the current population, we have that their utility function can be expressed by:

$$\tilde{\mathcal{U}}(w, \epsilon, \mathbf{s}_k) = \sqrt{\mathbf{s}_k^T \cdot \mathbf{G} \cdot \mathbf{s}_k} + \sum_{q \in [1, \ldots, p], q \neq k} \frac{\rho}{|\mathbf{s}_k - \mathbf{s}_q|_G}$$

where $|\mathbf{s}_k - \mathbf{s}_q|_G = \sqrt{(\mathbf{s}_k - \mathbf{s}_q)^T \cdot \mathbf{G} \cdot (\mathbf{s}_k - \mathbf{s}_q)}$. Mind that the form of the $\mathbf{A}$ matrix is

$$\mathbf{A} = \begin{pmatrix} \frac{1}{\epsilon^2} & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ & & \ldots & & \\ & & \ldots & & \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}. \tag{9}$$

Changing the value of ϵ is equivalent to changing the power p in the weighted metric formulation but avoids numerical instability. Moreover, the Coulomb repulsion formulation enables finding a set of optimal solutions in a single run of the multi-objective algorithm.

Adaptive Coulomb force To understand the wanted scaling of the Coulomb force intensity, we can refer to the following simplified setup. Let us consider that a reference point $\vec{r}$ lies on the fairness line, i.e.,

$$\vec{r} = \bar{\mathbf{u}}\, t_0 \quad s.t. \quad t_0 > 0$$

Let us then consider another vector $\vec{p}$ that can be expressed as: $\vec{p} = \vec{r} + \vec{d}$ where $\vec{d} \cdot \bar{\mathbf{u}} = 0$ (i.e., $\vec{\delta}$ is orthogonal to the fairness line). As we are studying a scalar utility function, the coordinate system used to compute it is irrelevant. For this reason, we focus on the $\{\mathbf{z}\}$ basis where we can write $\vec{r} = (t_0, 0, \ldots, 0)$ and we can assume for simplicity that $\vec{d} = (0, t_0\delta, \ldots, t_0\delta)$. We will consider cases where $\delta < 1$ as we want to find scaling rule that works best nearby the fairness line. Now, the utility function perceived by a particle in $\vec{r}$ when another particle is placed at $\vec{p}$ can be written as:

$$\mathcal{U}(w, \epsilon, \vec{r}) = \frac{t_0}{\epsilon} + \frac{\rho}{\delta t_0 \sqrt{d-1}}$$

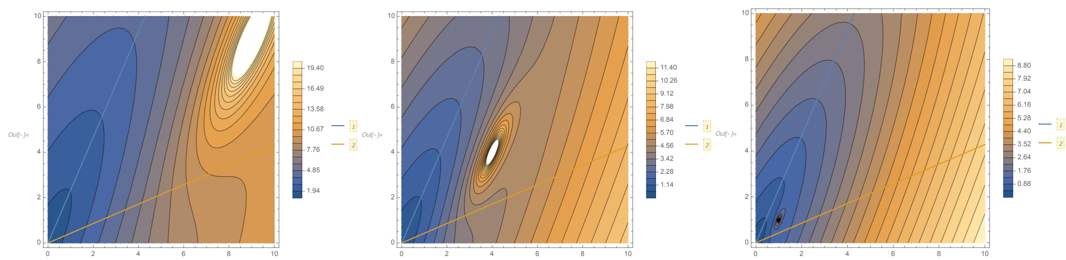

Figure 3: Potential felt by a particle when another particle is placed at coordinates {9,9} (left), {4,4} (center), and {1,1} (right). The ellipsoid potential is obtained using weights $w = \{0.7, 0.3\}$ and considering the major semi-axis $\epsilon = 4$. The parameter α is fixed to $\alpha = 0.2$

Asking that the ratio between the Coulomb force and the Utility function is fixed at $q < 1$, we get

$$\mathcal{U}(w, \epsilon, \vec{r}) = \frac{t_0}{\epsilon}\left(1 + \frac{\epsilon\rho}{\delta t_0^2 \sqrt{d-1}}\right)$$

$$q = \frac{\epsilon\rho}{\delta t_0^2 \sqrt{d-1}}$$

$$\rho = \alpha \frac{t_0^2 \sqrt{d-1}}{\epsilon} \qquad \text{where} \quad \alpha = q\delta \ll 1$$

If we want to fix the cutoff for the contribution of all other $P-1$ Coulomb particles interactions, we get:

$$\rho = \alpha \frac{t_0^2 \sqrt{d-1}}{(P-1)\epsilon} \sim \alpha \frac{t_0^2 \sqrt{d}}{P\epsilon}$$

Given the desired scaling of ρ, we can reformulate the original optimization problem as follows. Calling $S = \{\mathbf{s_1}, \mathbf{s_2}, \ldots, \mathbf{s_p}\}$ the set coordinate vectors of solutions in the current population, we have that their utility function can be expressed by:

$$\tilde{\mathcal{U}}(w, \epsilon, \mathbf{s}_k) = \sqrt{\mathbf{s}_k^T \cdot \mathbf{G} \cdot \mathbf{s}_k} + \sum_{q \in [1,\ldots,p], q \neq k} \alpha \frac{\tau_0^2 \sqrt{d}}{P\epsilon} \frac{1}{|\mathbf{s}_k - \mathbf{s}_q|_G}$$

where $|\mathbf{s}_k - \mathbf{s}_q|_G = \sqrt{(\mathbf{s}_k - \mathbf{s}_q)^T \cdot \mathbf{G} \cdot (\mathbf{s}_k - \mathbf{s}_q)}$ and $\tau_0 = \frac{1}{P}\sum_i \mathbf{s}_i \cdot \bar{\mathbf{u}}$.

Preliminary Results To evaluate the algorithm's behavior, we conducted comparisons with a well-established multi-objective evolutionary algorithm known as RVEA [CJOS16]. In Figure 4, we analyze the impact of both fixed and adaptive Coulomb forces within a 3-dimensional objective space. Notably, employing a fixed Coulomb force results in solutions that deviate significantly from the optimal Pareto front, possibly due to the challenge of precisely calibrating the force to keep all particles within the desired region. Additionally, Figure 5 demonstrates the application of two different preference lines, highlighting the algorithm's capability to focus on specific preferred regions compared to RVEA.

Figures 6 and 7 extend these findings into a 10-dimensional space. It is worth noting that when $\epsilon = 1$, it is equivalent to a linear query, as seen in the first example of Figure 7. In this case, the preference is ignored.

References

[CJOS16] Ran Cheng, Yaochu Jin, Markus Olhofer, and Bernhard Sendhoff. A reference vector guided evolutionary algorithm for many-objective optimization. *IEEE transactions on evolutionary computation*, 20(5):773–791, 2016.

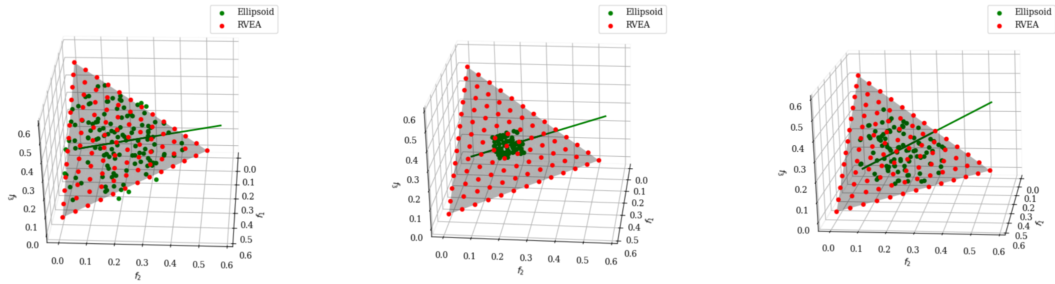

Figure 4: Comparison in a 3-dimensional objective space: (Left) fixed Coulomb force, (Center) adaptive Coulomb force with ellipsoid potential using weights $w = \{0.33, 0.33, 0.33\}$ and major semi-axis $\epsilon = 3$, and (Right) adaptive Coulomb force with $\epsilon = 1$. The parameter α is set to $\alpha = 0.1$ for the adaptive Coulomb force and $\alpha = 10^{-4}$ for the fixed Coulomb force.

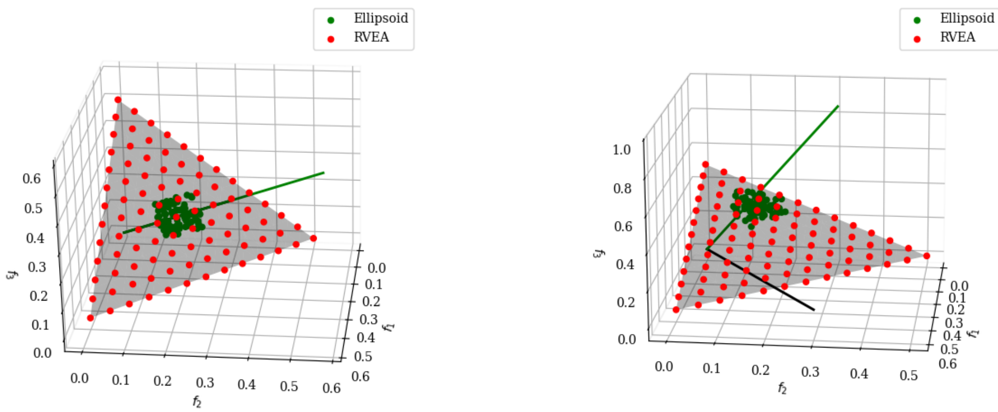

Figure 5: Comparison in a 3-dimensional objective space: (Left) adaptive Coulomb force using weights $w = \{0.33, 0.33, 0.33\}$, and (Right) adaptive Coulomb force using weights $w = \{0.6, 0.3, 0.1\}$. The parameter α is set to $\alpha = 0.1$ for the adaptive Coulomb force, and the major semi-axis is set to $\epsilon = 3$.

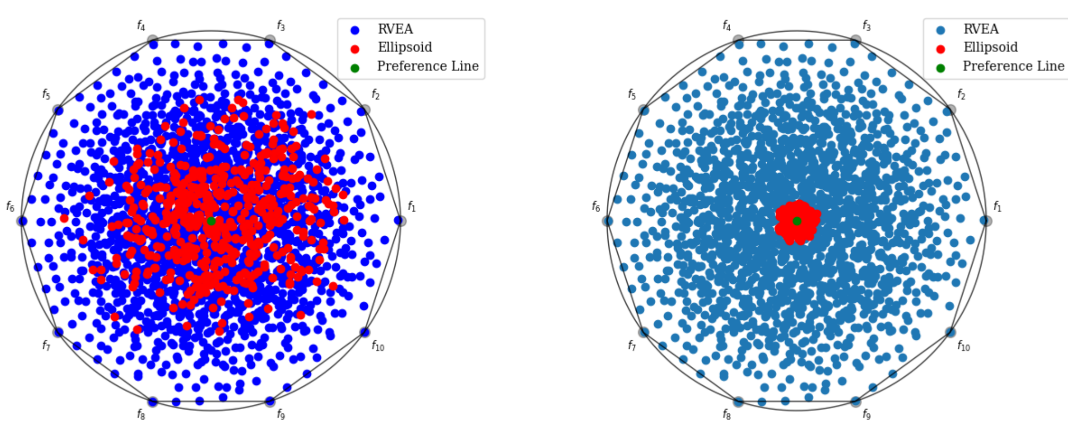

Figure 6: Comparison between the fixed and the adaptive Coulomb force in a 10-dimensional objective space. The parameter α is set to $\alpha = 0.1$ for the adaptive Coulomb force, and the major semi-axis is set to $\epsilon = 3$.

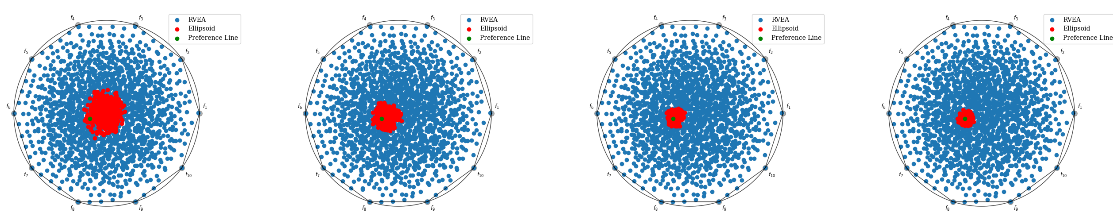

Figure 7: Solutions distribution with $\epsilon = \{1, 2, 3, 4\}$ and the adaptive Coulomb force set to $\alpha = 0.1$. The weights are set to $w_0 = w_1 = 0.3$ and $w_{2..9} = 0.05$.