L04. Particle swarm optimization (PSO): a potentially useful tool in chemometrics?

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Particle swarm optimization techniques are a family of optimization methods based on the concept of swarm intelligence, that has been developed in the last 10–15 years. In particular, it is a population-based stochastic optimization technique inspired by social behavior of bird flocking or fish schooling. If compared to other evolutionary optimization techniques as GA, PSO has a simpler algorithmic structure and fewer parameters to be adjusted, both desirable characteristics in the light of their possible application to the solution of practical problems.

However, while successful applications have been reported in different engineering, computer science or signal processing problems, yet their potential for solving chemometric problems remains almost unexplored.

In this communication, the possibility of using PSO in different chemometric ambits will be explored both theoretically and by means of selected representative examples (robust regression, clustering, optimization of learning parameters).