Advanced Scientific Computing: Stochastic Methods for Data Analysis, Inference and Optimization

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Set 3 - Stochastic Optimization

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Question 1: Gradient based against evolution strategy

Consider the Ackley function in two dimensions:

$$f(x,y) = -20\exp\left(-0.2\sqrt{0.5(x^2+y^2)}\right) - \exp\left(0.5\left(\cos 2\pi x + \cos 2\pi y\right)\right) + 20 + e,$$

where e is the Euler number.

a) With an initial mean at $(5,5)$ and initial standard deviation of 5, minimize the Ackley function with CMA-ES. Use the `korali` python interface. An example optimization problem can be found here. Report the minimum and the convergence plot created with

```
python -m korali.plot --dir ./resultdir/
```

b) With a starting point at $(5,5)$, use a gradient based optimizer of your choice. Report the minimum and the convergence plot. How does the gradient based solver perform compared to CMA-ES?

Question 2: Corridor design for pedestrian traffic

The social force model describes pedestrian motion. Each pedestrian is affected by "social forces" which represent the internal motivations of the individuals to perform certain movements. The change in velocity of a pedestrian i is

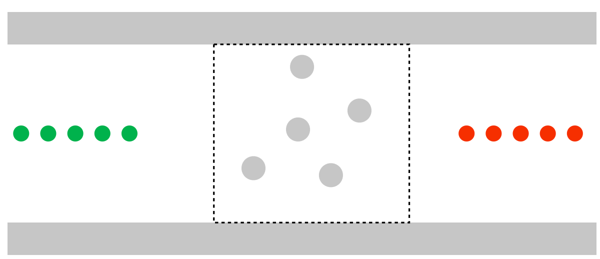
$$\frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i,$$

where $\mathbf{F}_i$ is the sum of all forces acting on the pedestrian i,

$$\mathbf{F}_i = \frac{1}{\tau}\left(\mathbf{v}_i^0 - \mathbf{v}_i\right) + \sum_{j\neq i}\mathbf{F}_{ij} + \sum_{k}\mathbf{F}_{ik},$$

where $\mathbf{v}_i$ is the velocity of the pedestrian i, $\mathbf{v}_i^0$ their desired velocity and $\mathbf{F}_{ij}$, $\mathbf{F}_{ik}$ are repulsive forces from another pedestrian j and an obstacle k. The magnitudes of the forces decrease exponentially with the relative distance

$$\mathbf{F}_{ij} = A\exp\left(-\frac{r_{ij}}{B}\right)\frac{\mathbf{x}_i - \mathbf{x}_j}{r_{ij}}, \qquad \mathbf{F}_{ik} = C\exp\left(-\frac{r_{ik}}{D}\right)\frac{\mathbf{x}_i - \mathbf{x}_k}{r_{ik}}.$$



Advance the positions and the velocities of the pedestrians using the following scheme:

$$\mathbf{x}_i \leftarrow \mathbf{x}_i + \mathbf{v}_i\,\Delta t,$$
$$\mathbf{v}_i \leftarrow \mathbf{v}_i + \mathbf{F}_i\,\Delta t.$$

If a pedestrian penetrates the walls, place it at the nearest position that is inside the domain. The corridor has a length 60 and a width 6. The horizontal length of the dashed rectangle is 10. The initial x coordinates are -28.5, -27.0, -25.5, -24.0, -22.5 for the left group of the pedestrians, and are 22.5, 24.0, 25.5, 27.0, 28.5 for the right group (the origin is at the center of the dashed rectangle).

a) Implement the model in C++.

b) Find the positions of the five obstacles that maximize the average displacement in the x direction for all pedestrians after a duration 50. Use the differential evolution algorithm. Ensure that obstacles do not overlap with walls and with other obstacles.

Use $\mathbf{v}_i^0 = (1,\,0)$ for the left group, $\mathbf{v}_i^0 = (-1,\,0)$ for the right group, $\tau = 0.2$, $A = 20$, $B = 0.5$, $C = 10$, $D = 0.6$ and $\Delta t = 0.05$.

Question 3: Optimal atoms configuration

Write a Python program to find the configuration with smallest energy for N atoms. The energy E of the atoms is the sum of all pairwise energies given by

$$E = 4 \sum_{i=1}^{N} \sum_{j=i+1}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right),$$

where r_{ij} is the distance between atom i and atom j. Compare the solutions you find with (i) a gradient based method and (ii) a stochastic optimization method of your choice for 8, 16, and 32 atoms. Report the positions, energies, and hand in your code. The file `lj.py` computes the energy and the Jacobian of the energy. Compare your program's output with the references:

```
N = 2, E = -1.000000
         0.0000000000        0.0000000000        0.0000000000
         1.1224620483        0.0000000000        0.0000000000

N = 3, E = -3.000000
         0.4391356726        0.1106588251       -0.4635601962
        -0.5185079933        0.3850176090        0.0537084789
         0.0793723207       -0.4956764341        0.4098517173

N = 5, E = -9.103852
        -0.2604720088        0.7363147287        0.4727061929
         0.2604716550       -0.7363150782       -0.4727063011
        -0.4144908003       -0.3652598516        0.3405559620
        -0.1944131041        0.2843471802       -0.5500413671
         0.6089042582        0.0809130209        0.2094855133
```

Note that due to symmetry of the problem many optimal solutions exist. The provided coordinates help you to select the initial range of the parameters. We will grant a bonus point for the top performing solutions for 38 atoms. Report the hyper-parameters and the random seed you used.