Implementation of reflecting boundary conditions on a circle

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September 4, 2025

This document describes how reflecting boundary conditions on a circle are implemented in the computer program `MonteCarloContinuous2D_BM.f90`, which is available in this GitHub repository. The program applies the Monte Carlo simulation method with resetting in [X] to a two-dimensional stochastic process confined to an annular domain, incorporating reflecting boundary conditions at the outer radius.

We consider a two-dimensional stochastic process in the (x, y) plane, confined within a circle of radius R and subject to reflecting conditions at its boundary. As illustrated in Fig. 1, let the current position of the process be $P_0 = (x_0, y_0)$, and suppose the process attempts to move to a new position P'. As P' lies outside the circle, the objective is to reflect it back to point P within the circle, whose coordinates are to be determined. To achieve this, we first identify the coordinates of point A, which lies on the boundary of the circle on the line connecting P_0 and P'. The position vector of point A can be expressed as

$$\vec{A} = \vec{P}_0 + \lambda\vec{\Delta}, \tag{1}$$

with $\vec{\Delta} = (\Delta_x, \Delta_y) = \vec{P}' - \vec{P}_0$ and $\lambda > 0$. The condition $|\vec{A}|^2 = R^2$ imposes that point A lies on the circle's boundary, leading to a quadratic equation for the parameter λ, with solution

$$\lambda = \frac{-\vec{P}_0 \cdot \vec{\Delta} + \sqrt{\left(\vec{P}_0 \cdot \vec{\Delta}\right)^2 - \left(\vec{P}_0^{\,2} - R^2\right) \cdot \vec{\Delta}^2}}{\vec{\Delta}^2}, \tag{2}$$

where we have taken the positive root of the solution, as the negative root corresponds to the opposite point A' (see Fig. 1). After some simple algebra, this expression can be rewritten as

$$\lambda = \frac{-\left(x_0\Delta_x + y_0\Delta_y\right) + \sqrt{\left(\Delta_x^2 + \Delta_y^2\right) R^2 - \left(x_0\Delta_y - y_0\Delta_x\right)^2}}{\Delta_x^2 + \Delta_y^2}. \tag{3}$$

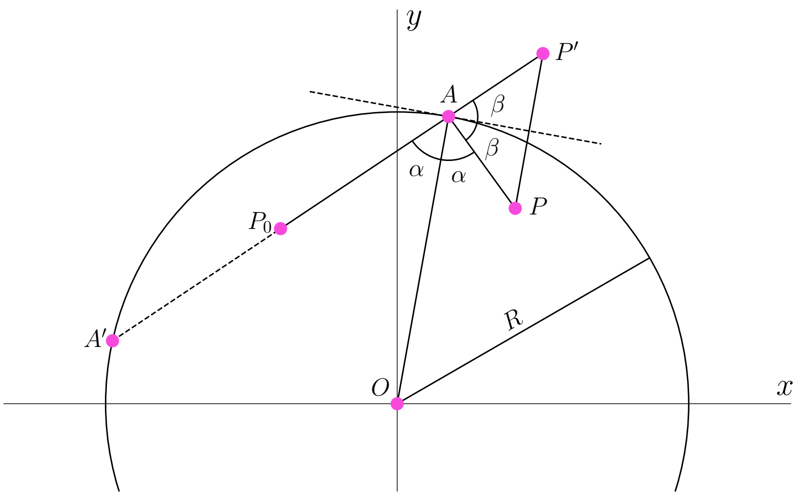

Figure 1: Scheme for the implementation of reflecting boundary conditions on a circle of radius R. P_0 denotes the initial position of the process, P' represents the position to which the process attempts to move, and P is the final position of the process resulting from applying reflecting boundary conditions. The figure also shows the following auxiliary points: the origin of coordinates, O, and points A and A', which lie on the boundary of the circle along the line connecting points P_0 and P'. The angle β is equal to $\pi/2 - \alpha$.

Once the coordinates of point A have been determined, we impose two conditions to ensure a correct reflection.

First, we ensure that the vector $\vec{A}$ is orthogonal to the vector $(\vec{P'} - \vec{A}) + (\vec{P} - \vec{A})$, which serves as a direction vector for the line tangent to the circle at point A. That is, we impose the condition

$$\vec{A} \cdot (\vec{P'} + \vec{P} - 2\vec{A}) = 0, \tag{4}$$

which leads to the relation

$$\vec{A} \cdot \vec{P} = 2R^2 - \vec{A} \cdot \vec{P'}, \tag{5}$$

where we have used that $|\vec{A}|^2 = R^2$.

Second, we ensure that the line connecting the points P and P' is parallel to the vector $\vec{A}$ by imposing

$$\vec{P'} - \vec{P} = \mu \cdot \vec{A}, \tag{6}$$

with $\mu > 0$. By multiplying the above equation by $\vec{A}$ and using the condition $|\vec{A}|^2 = R^2$ along with Eq. (5), we arrive at

$$\mu = 2\left(\frac{\vec{P'} \cdot \vec{A}}{R^2} - 1\right). \tag{7}$$

Finally, by combining Eqs. (6) and (7), we obtain the following expression for the position vector of point P:

$$\vec{P} = \vec{P'} + 2\left(1 - \frac{\vec{P'} \cdot \vec{A}}{R^2}\right) \cdot \vec{A}. \tag{8}$$

In summary, if the process attempts to move from a position P_0 to a position P' outside the circle, we reflect the process to the position P inside the circle. In order to determine the coordinates of point P using Eq. (8), we must first determine the coordinates of point A using Eqs. (1) and (3).

If both points P_0 and P' are located very close to the boundary, the reflected point P may lie outside the circle. To address this, a second reflection is applied, with $P_0^{(2)} = A^{(1)}$ and $P'^{(2)} = P^{(1)}$, where the superscripts indicate whether the points correspond to the first or the second reflection. In general, it is advisable to check that $|\vec{P}| < R$ after each reflection and to repeat the reflection procedure until this condition is satisfied.