The Center of Curvature Collectice Variable

21 January 2025

1 Introduction

The code is a collective variable for finding the center of curvature. The center of of the circle is the intersection of the perpendicular bisectors of any two segments formed by the three points. Below is the mathematical workout

2 Theory

Given 3 points $\mathbf{p}_1$, $\mathbf{p}_2$, and $\mathbf{p}_3$, the line segments $\mathbf{v}$ can be constructed as:

$$\mathbf{v}_{12} = \mathbf{p}_2 - \mathbf{p}_1, \quad \mathbf{v}_{23} = \mathbf{p}_3 - \mathbf{p}_2$$

To calculate the perpendicular vectors to these bisectors, calculate $\mathbf{N}$, a vector perpendicular to the plane formed by $\mathbf{v}_{12}$ and $\mathbf{v}_{23}$.

$$\mathbf{N} = \mathbf{v}_{12} \times \mathbf{v}_{23}$$

The vector $\mathbf{v}_{12}^{\perp}$, which is perpendicular to $\mathbf{v}_{12}$, can be calculated as:

$$\mathbf{v}_{12}^{\perp} = \mathbf{v}_{12} \times \mathbf{N}$$

$$\mathbf{v}_{23}^{\perp} = \mathbf{v}_{23} \times \mathbf{N}$$

The normalized vector $\mathbf{v}_{12}^{\perp}$ and $\mathbf{v}_{23}^{\perp}$ is given by:

$$\mathbf{v}_{12}^{\perp} = \frac{\mathbf{v}_{12}^{\perp}}{\|\mathbf{v}_{12}^{\perp}\|}, \mathbf{v}_{23}^{\perp} = \frac{\mathbf{v}_{23}^{\perp}}{\|\mathbf{v}_{23}^{\perp}\|}$$

The parametric equation of the bisector to the line segments has the form

$$\mathbf{x} = \mathbf{m}_{12} + t_1 \mathbf{v}_{12}^{\perp}$$

$$\mathbf{x} = \mathbf{m}_{23} + t_1 \mathbf{v}_{23}^{\perp}$$

where $\mathbf{m}_{12}$ and $\mathbf{m}_{23}$ are the midpoints of the segments and $\mathbf{x}$ is the center of curvature.

The relationship between the perpendicular bisectors and the midpoints is given by:

$$t_1\mathbf{v}_{12}^{\perp} - t_2\mathbf{v}_{23}^{\perp} = \mathbf{m}_{23} - \mathbf{m}_{12}$$

This can be rewritten in matrix form as:

$$\mathbf{A} \cdot \mathbf{t} = \mathbf{b}$$

and solved using the least square method.