Constrained Constructive Optimization implementation
Reproducing Rudolph Karch paper

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Abstract

Implement CCO in 2D, then 3D based on Karch's work [1]. In another step consider implementation for convex volume. Combination of CFD laws, geometry, and optimization. Encapsulated articles : requires summary in one paper.

Keywords: constrained constructive optimization, implementation

Contents

Introduction

Constrained constructive optimization consists of growing a tree governed by minimizing a target function.

In Karch's method the tree is constrained into a given convex perfusion volume, and the target function minimizes the total tree volume during growth. Segment are added one by one and fulfill both local optimization (single bifurcation scale) and global optimization (tree scale). The local optimization is based on Kamiya's work [2], whereas the global optimization has been implemented first by Schreiner in 2D [3].

1 Global optimization

Initialization of the method requires physiological parameters inputs, and a randomized starting point.

Then Karch's protocol consists of a complete loop for each added segment. A random location is picked under some constraints (geometry and physiology), to use it as a segment end candidate. Its connection is tested with neighbor segments, producing a bifurcation under topological, structural and functional constraints. In view of this new branch impact on the whole tree (induced by fluid mechanics laws), the optimal connection is selected according to a target function (minimal volume of the total tree).

1.1 Assumptions and boundary conditions

The vascular tree is grown under specific assumptions and boundary conditions.

The perfused volume is convexe and supposed homogeneously filled. The terminal segments correspond to pre-arteriole level, that feed a non modeled micro-vasculature. The blood is an incompressible, homgeneous Newtonian fluid, studied at steady state and in laminar flow conditions.

The resistance and the pressure drop of a segment j are defined by:

$$R_j = \frac{8\nu}{\pi} \frac{l_j}{r_j^4} \tag{1}$$

$$\Delta P_j = R_j Q_j \tag{2}$$

The total resistance of the tree is calculated recursively by tree decomposition, considering parallel and serial arrangements.

The physiological parameters are defined such as in the following table:

The pressure at distal end of terminal segment,P_{term}, are equal and inflow pressure to the micro-circulation. The terminal flows $Q_{term,j}$ are equals, and delivered into the micro-circulation agains P_{term}. Because of flow conservation their sum correspond to the perfusion flow at the root Q_{perf}. The laminar flow resistance of the whole tree induces a given total Q_{perf} accross ΔP.Q_{perf} is the same for each step of the tree generation.

The tree grown is dichotomic, so that the total number of segments is calculated from:

$$N_{tot} = 2N_{term} - 1 \tag{3}$$

This tree follows Murray's law, with a coefficient equal to 3.

1.2 Initialization step

Inputs:

- convexe perfusion surface or volume definition: position and shape
- number of terminal segments, N_{term}
- location of the root (in our case at the border of the perfusion territory)
- a random location inside the perfusion territory for the first segment end

1.3 Loop to add new segment

1.3.1 Constrained new location

A random position is picked, that has to fulfill two constraints: belong to the perfusion territory and respect a distance criteria. This criteria is defined based on the final and current size of the tree:

$$d_{thresh} = (\pi r_{supp}^2 / k_{term})^{\frac{1}{2}} \tag{4}$$

with k_{term} the number of terminal segment at the current step, and r_{supp} defined from the estimated size of a micro-circulatory black-box area, knowing the total perfused area A_{perf}:

$$\pi r_{supp}^2 = A_{perf} / N_{term} \tag{5}$$

In 3D this criteria is defined as:

$$d_{thresh} = (\frac{4}{3}\pi r_{supp}^3 / k_{term})^{\frac{1}{3}} \tag{6}$$

with

$$\frac{4}{3}\pi r_{supp}^3 = V_{perf} / N_{term} \tag{7}$$

1.3.2 Test connection

if single bifurcation can be optimized
 if no segment has degenerated to 0
 if result doesn't overlap any other segments

1.3.3 Propagate impact on whole tree

Propagate resistance change (balancing ratio)

1.3.4 Measure target function

Mesure total tree volume

1.3.5 Select best connection between neighbors

store result in cet: volume, betas, position

compare

add the best one,then update flow, resistance, distance criteria and start again

1.4 Example of results

1.4.1 2D

1.4.2 3D

Output: images decrease of radius, to maintain constant resistance

2 Local optimization: single bifurcation scale

Kamiya proposes a numerical solution to determine minimum volume bifurcation under restriction of physiological parameters, determinant pressure and flow, and locations at origin and terminals.

This method built in 2D assumes the flow to be laminar and vessels are composed of straight ducts lying on a plane.

Note: Karch found that the optimum positions of the bifurcations in their 3D model trees were always found to lie in the plane defined by the endpoints of the respective three neighboring segments, which is consistent with the literature [4].

Process: iterative nested loops

Defining a starting position as the convex average of origin and terminal locations, weighted by respective flows.

$$(x, y) = \left(\frac{f_0 x_0 + f_1 x_1 + f_2 x_2}{2 f_0}, \frac{f_0 y_0 + f_1 y_1 + f_2 y_2)}{2 f_0}\right) \tag{8}$$

Calculate each segment length.

$$l_i^2 = (x - x_i)^2 + (y - y_i)^2 \tag{9}$$

Numerically calculate the new radii r_0, r_1,r_2. These ones are expected to satisfy both Hagen-Poiseuille's law and volume minimization.

When location of origin and two terminals segments, their pressure, and their flows are given, according to Hagen - Poiseuille's law:

$$\Delta P_1 = P_1 - P_0 = \kappa(\frac{f_0 l_0}{r_0^4} + \frac{f_1 l_1}{r_1^4}), \tag{10}$$

$$\Delta P_2 = P_2 - P_0 = \kappa(\frac{f_0 l_0}{r_0^4} + \frac{f_2 l_2}{r_2^4}) \tag{11}$$

According to Kamiya, differentiating the tree volume with x, y and r_0 and equating them to zero, one obtains:

$$\frac{r_0^6}{f_0} = \frac{r_1^6}{f_1} + \frac{r_2^6}{f_2} \tag{12}$$

and

$$x = \frac{x_0 r_0^2/l_0 + x_1 r_1^2/l_1 + x_2 r_2^2/l_2}{r_0^2/l_0 + r_1^2/l_1 + r_2^2/l_2}, y = \frac{y_0 r_0^2/l_0 + y_1 r_1^2/l_1 + y_2 r_2^2/l_2}{r_0^2/l_0 + r_1^2/l_1 + r_2^2/l_2} \tag{13}$$

The details of the path to these equations is provided in appendix.

Using $R = r^2$ in (2), we can express R_0 as:

$$R_0^3 = f_0(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2}) \tag{14}$$

Substituting this inside (2), one obtains the non linear system:

$$\begin{cases} \frac{\Delta P_1}{\kappa} R_1^2 \left(f_0(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2})\right)^{\frac{2}{3}} - f_0 l_0 R_1^2 - f_1 l_1 \left(f_0(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2})\right)^{\frac{2}{3}} = 0 \\ \frac{\Delta P_2}{\kappa} R_2^2 \left(f_0(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2})\right)^{\frac{2}{3}} - f_0 l_0 R_2^2 - f_2 l_2 \left(f_0(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2})\right)^{\frac{2}{3}} = 0 \end{cases} \tag{15}$$

We are looking for the root satisfying these equations using a non linear solver. If the solution converges, we get the new radii, that are needed to calculate the new position of the branching point in (2). This locations is a new input for the loop to iterate again (calculating length (2), then new radii (2), new location (2) and so on). If this iterative loop converges and the bifurcation total volume decreases, the bifurcation is solved and provided with optimal radii and position.

Note: in CCO the pressure is not determined all along vessels (only at the root and terminal segments). In order to adapt to our situation, we use an estimated radius to calculate the pressure drops using (2). At the first iteration the estimated radii are all equal to the segment's radius on which is connected the branch: $r_0 = r_1 = r_2 = r_{ori}$. Then, we will use the previously calculated radii to update the pressure drops at each iteration.

Example of results

Example of results on different type of bifurcations. For these example we used a tolerance of 0.01 and maximum number of iteration of 100.

In the figure 1 (a), for symetric flows and child locations: the optimal bifurcation point corresponds to convex average.

The figure 1 (b) illustrates well Steiner solutions to optimal network [5]: it is more advantageous to transport flows together by delaying bifurcation. In the fluid mechanics context, this subadditivity follows from PoiseuilleâĂŹs law, according to which the resistance of a tube increases when it gets thinner.

The figure 1 (c) shows influence of blood demand on the bifurcation geometry: because flow is more important on the right child, the radius is bigger and the bifurcation is dragged toward this child. Also, we note the bifurcation is less delayed than for symmetrical flows.

The figure 1 (d) shows influence of both destination and demand.

Karch implementation

Karch added lower and upper bounds to Kamiya's algorithm that ensures: bifurcation position within the perfusion volume the bifurcation not to degenerate to zero (by constraining segment length over segment diameter).

Conclusion

Appendices

Equation (2), from Kamiya & Togawa 1972 equation (6)

Kamiya uses Murray definition at equation (7) from Physiological principle of minimum work[6] that he calls the simplest requirement for efficiency in the circulation:

$$f = kr^3$$

With k being a constant, so that the flow of blood past any section shall everywhere bear the same relation to the cube of the radius of the vessel at that point. Using it as:

$$r_i^3 = \frac{r_i^6 k}{f_i}$$

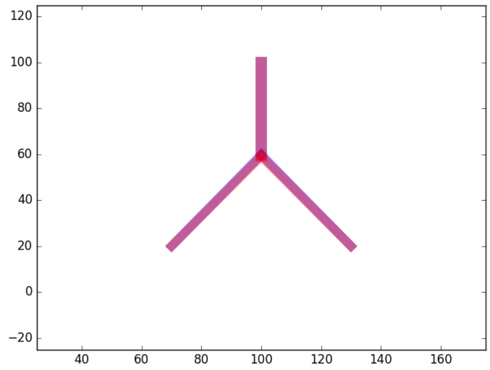
and combining it this with the famous Murray's law,

$$r_0^\gamma = r_1^\gamma + r_2^\gamma \text{ with } \gamma = 3$$

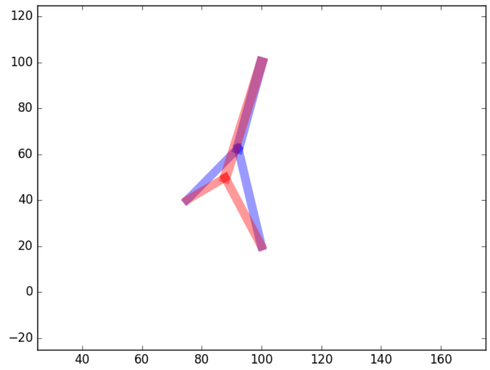
where r_0 is the parent radius, r_1 and r_2 are the children radii, one obtains:

$$\frac{kr_0^6}{f_0} = \frac{kr_1^6}{f_1} + \frac{kr_2^6}{f_2}$$

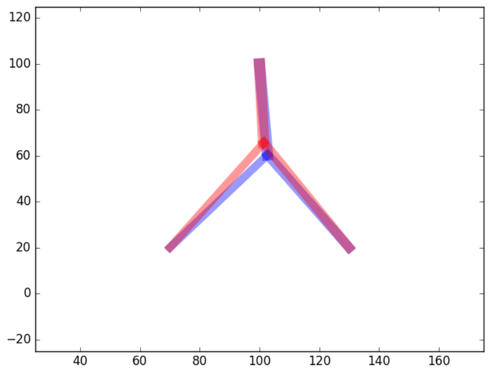
that can be simplified into equation (2).



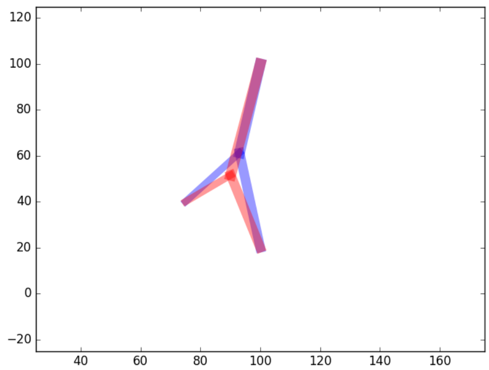
(a) $Q_l = Q_r = \frac{1}{2}Q_p$



(b) Random child locations and $Q_l = Q_r = \frac{1}{2}Q_p$



(c) $Q_l = \frac{1}{4}Q_p$ and $Q_l = \frac{3}{4}Q_p$



(d) Random child locations and $Q_l = \frac{1}{4}Q_p$, $Q_l = \frac{3}{4}Q_p$

Figure 1: In blue the starting bifurcation (convex average position), in red the final bifurcation after Kamiya's algorithm convergence reached (tolerance = 0.01). Convergence was reached at 15th, 24th, 31st and 21st iteration respectively in (a),(b),(c),(d). Q_p is the flow in parent branch, Q_l and Q_r are flows in left and right children.

Equation (2), from Kamiya & Togawa 1972 equation (7)

We have

$$V = \pi(r_0^2 l_0 + r_1^2 l_1 + r_2^2 l_2) \tag{16}$$

and

$$\begin{aligned} l_0^2 &= (x - x_0)^2 + (y - y_0)^2 \\ l_1^2 &= (x - x_1)^2 + (y - y_1)^2 \\ l_2^2 &= (x - x_2)^2 + (y - y_2)^2 \end{aligned}$$

We rewrite (2)

$$V = \pi(r_0^2\sqrt{(x-x_0)^2+(y-y_0)^2} + r_1^2\sqrt{(x-x_1)^2+(y-y_1)^2} + r_2^2\sqrt{(x-x_2)^2+(y-y_2)^2})$$

We derive each term with respect to x.

$$\frac{\partial}{\partial x}\sqrt{(x-x_0)^2+(y-y_0)^2} = \frac{x-x_0}{\sqrt{(x-x_0)^2+(y-y_0)^2}} = \frac{x-x_0}{l_0},$$

same for the x_1 and x_2 term, so we have

$$\frac{\partial V}{\partial x} = \pi\left[\frac{r_0^2(x-x_0)}{l_0} + \frac{r_1^2(x-x_1)}{l_1} + \frac{r_2^2(x-x_2)}{l_2}\right] = 0$$

Discarding the π factor and separating the terms,

$$x\frac{r_0^2}{l_0} + x\frac{r_1^2}{l_1} + x\frac{r_2^2}{l_2} = x_0\frac{r_0^2}{l_0} + x_1\frac{r_1^2}{l_1} + x_2\frac{r_2^2}{l_2}$$
$$x(\frac{r_0^2}{l_0} + \frac{r_1^2}{l_1} + \frac{r_2^2}{l_2}) = x_0\frac{r_0^2}{l_0} + x_1\frac{r_1^2}{l_1} + x_2\frac{r_2^2}{l_2}$$

and so

$$x = \frac{x_0\frac{r_0^2}{l_0} + x_1\frac{r_1^2}{l_1} + x_2\frac{r_2^2}{l_2}}{\frac{r_0^2}{l_0} + \frac{r_1^2}{l_1} + \frac{r_2^2}{l_2}}$$

This is one half of Eq.(7) in Kamiya & Togawa. The other half is obtained by substituting x with y everywhere. This is correct but not 100% satisfying since the l_i depend on x and y.

References

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