
PDE-constrained optimization for parameter identification in chemotaxis equations

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Abstract

In organ and tissue development, many of the mechanisms governing pattern formation and cell migration have been identified and described by systems of PDEs. However, some of the parameters or non-linear functions in these PDEs are difficult or impossible to be measured in laboratory conditions, and therefore have to be identified in a different manner. Optimal control theory, in particular PDE-constrained optimization (PDECO), provides techniques to find the solutions for the unknown parameters or functions that have driven the biological system to a particular state given by experimental data (such as an image) by posing the unknown parameter as a control variable.

In PDECO, we pose an inverse problem where we minimize the norm of the difference between the state (governed by the PDE constraint) and the desired state, while also minimising the amount of control applied.

We consider PDEs that involve chemotaxis, i.e. movement of cells up or down chemical gradients, and derive the optimality conditions which are coupled and nonlinear time-dependent PDEs that involve multiple chemotaxis equations. Several issues arise when solving chemotactic PDEs with basic numerical schemes for PDEs, such as a blow-up caused by sharp gradients, unphysical oscillations, or negative concentrations of chemicals, leading to an inaccurate solution.

We present a numerical solver for the optimality conditions that emerge from the PDECO problem, utilizing the flux-corrected transport technique combined with finite elements which addresses these challenges, promising more accurate parameter identification and deeper insights into biological mechanisms.

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