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OptiDose: An advanced approach to compute optimal drug dosing schemes for a PKPD model using optimal control theory

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Abstract. Providing the optimal dosing strategy of a drug for the individual patient is one of the main objectives in pharmaceutical sciences and daily clinical application. Drug administration at certain time points gives a finite number of discrete controls, the drug doses, determining the drug concentration and its effect on the disease state. An objective function quantifying the difference between a desired disease state and the actual state generated by a certain treatment is minimized. With Karush-Kuhn-Tucker theory the adjoint state and the gradient of the objective are computed. This technique admits to apply robust descent methods from finite-dimensional optimization theory to solve the optimal control problem. The code was validated for various pharmacokinetics-pharmacodynamics problems, e.g. slow hormone level adjustment in hyperthyroidism and tumor stasis or eradication in oncology.