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Estimating parameters of soil hydraulic functions by nonlinear programming

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Parameter values, say $\boldsymbol{x}$, of soil hydraulic functions (SHF) are routinely identified from lab and field measurements $\boldsymbol{y}$ of soil water potential, content and flux by nonlinear regression techniques. The resulting parameter values maximize a goodness-of-fit criterion $Q(\boldsymbol{y}, \boldsymbol{x})$ that captures the discrepancy (e.g. mean squared difference) between measured and modeled values of the responses $\boldsymbol{y}$. Unfortunately, maximizing goodness-of-fit without further measures may result in values of $\boldsymbol{x}$ that yield unrealistic predictions of physical quantities such as the maximum length of capillary flow to sustain stage-I evaporation (evaporation characteristic length L_c) or the time t_p to ponding in an infiltration experiment. We therefore need estimation procedures that honor (nonlinear) inequality constraints of the form $\boldsymbol{x}_\mathrm{l} < \boldsymbol{x} \leq \boldsymbol{x}_\mathrm{u}$, $L_\mathrm{l} < L_\mathrm{c}(\boldsymbol{x}) \leq L_\mathrm{u}$ and $t_\mathrm{l} < t_\mathrm{p}(\boldsymbol{x}) \leq t_\mathrm{u}$ when maximizing $Q(\boldsymbol{y}, \boldsymbol{x})$. Various approaches developed in nonlinear programming (active set, penalty, barrier methods, etc.) exist to estimate $\boldsymbol{x}$ by maximizing $Q(\boldsymbol{y}, \boldsymbol{x})$ subject to such constraints. We explored robustness and ease of use of selected approaches by applying them on different soil hydraulic data sets. We present recommendations what method to use and discuss the effect of constrained estimation of $\boldsymbol{x}$ on modeled SHF.