Using Machine Intelligence in building PK/PD and Disease Progression Models

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The analyses of time course data from clinical trials are currently performed using pharmacometrics or QSP methodologies based on differential equations. These require considerable human expertise and trial-and-error in devising the appropriate model equations. However, recent advancements in Deep Learning have led to the development of the neural ordinary differential equation (Neural-ODE) methodology, thereby opening up a new paradigm whereby the governing equations can be generated from clinical data via machine intelligence. In this presentation, we show how this methodology in conjunction with key pharmacological principles, can enable the discovery of Neural-PK/PD models from data [Lu et al, Nature Machine Intelligence (2021)]. Furthermore, we show how the Neural-ODE methodology with an encoder-decoder architecture can be utilized for Disease Progression Modeling as well. We envisage that machine intelligence has the potential to transform modeling and discuss the associated opportunities and challenges.

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