

nlmixr2: an open-source package for pharmacometric modelling in R

Course material nlmixr2 PMxAfrica 2025

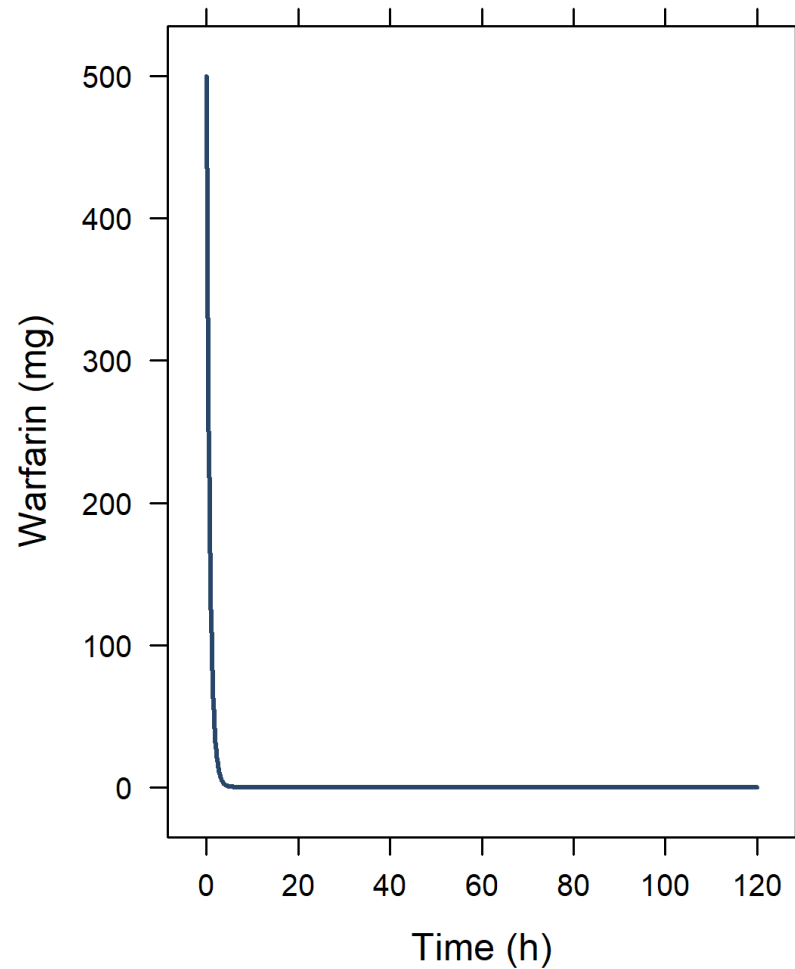
Rik Schoemaker, PhD

07 August 2025

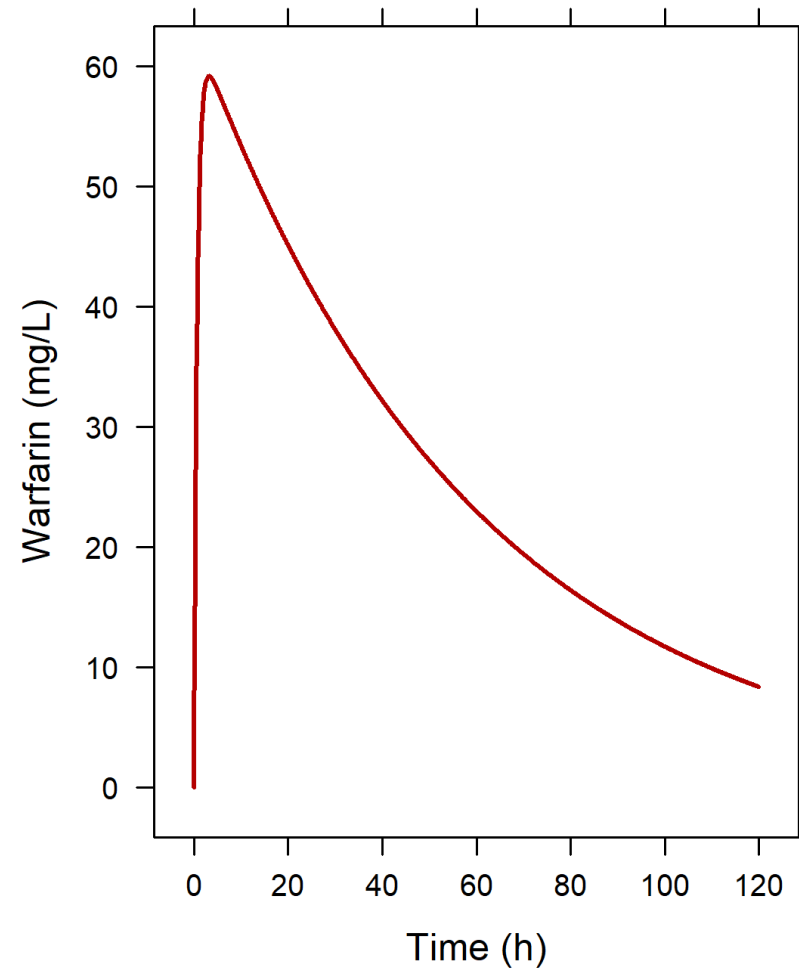


Simulation of a single (warfarin concentration) curve with a single dose

Depot compartment amounts

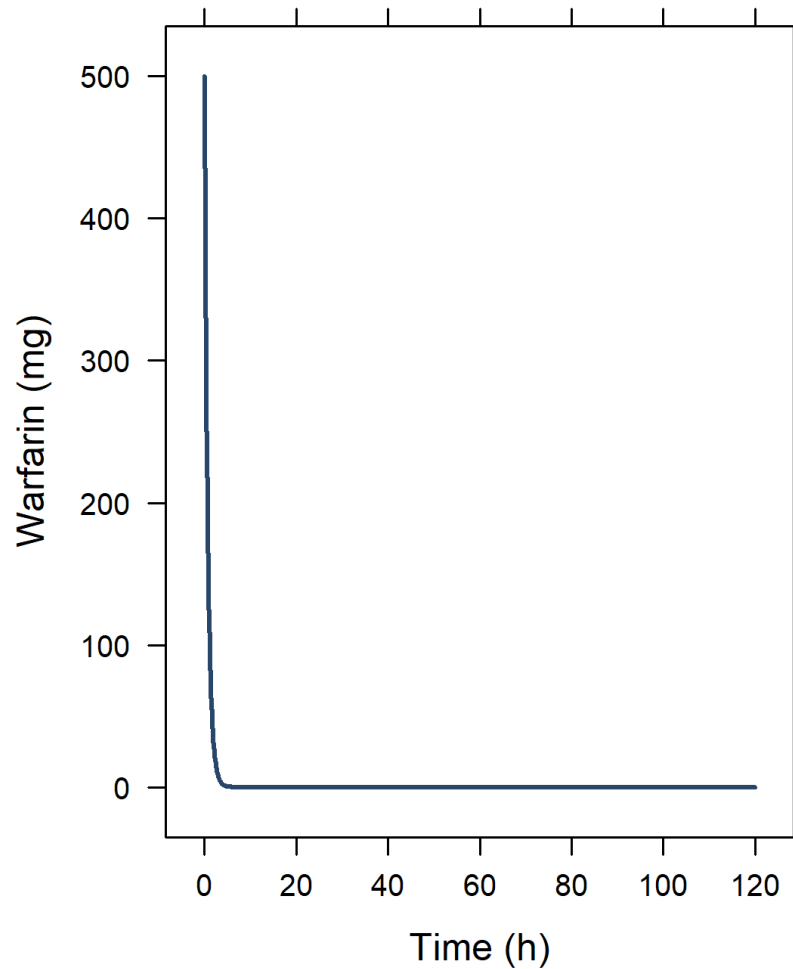


Central compartment concentrations

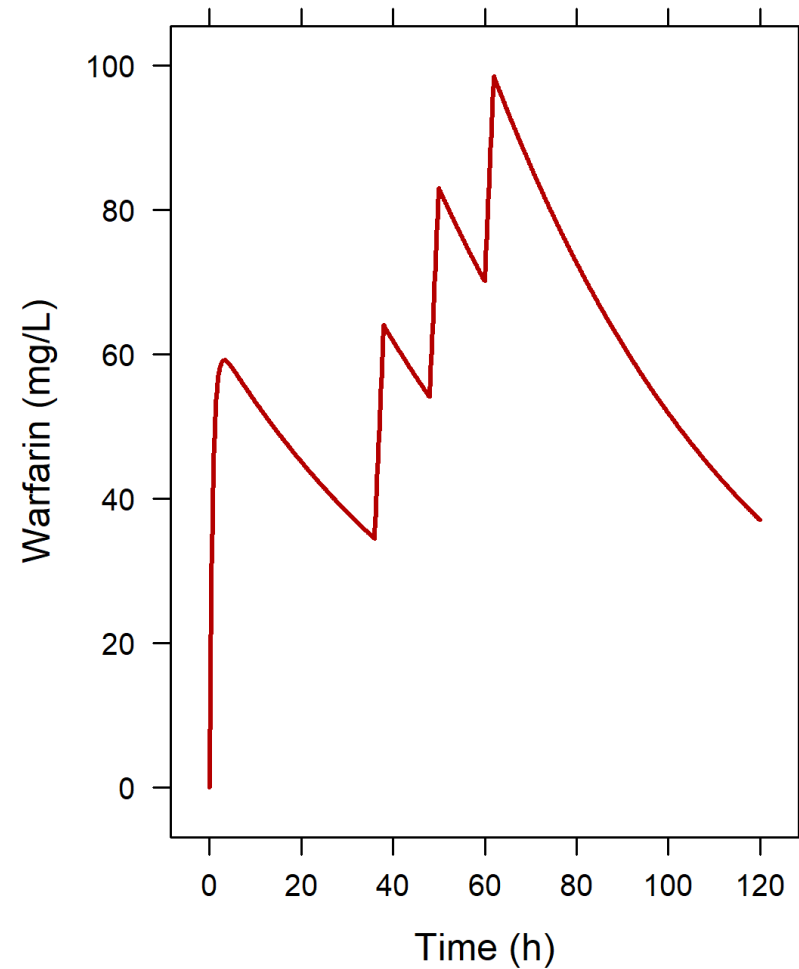


...and simulating three additional infusions in the central compartment

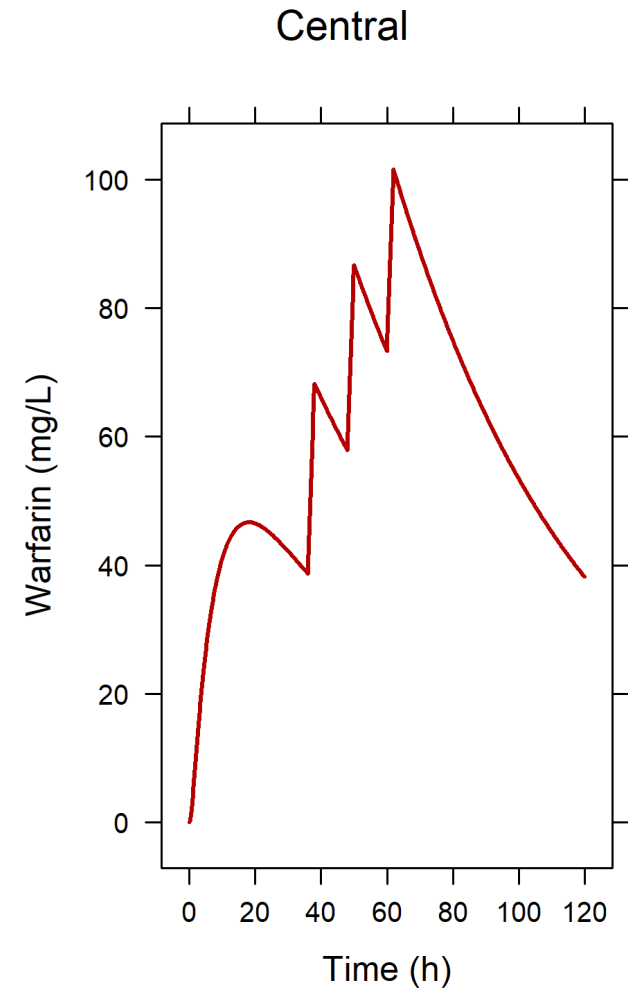
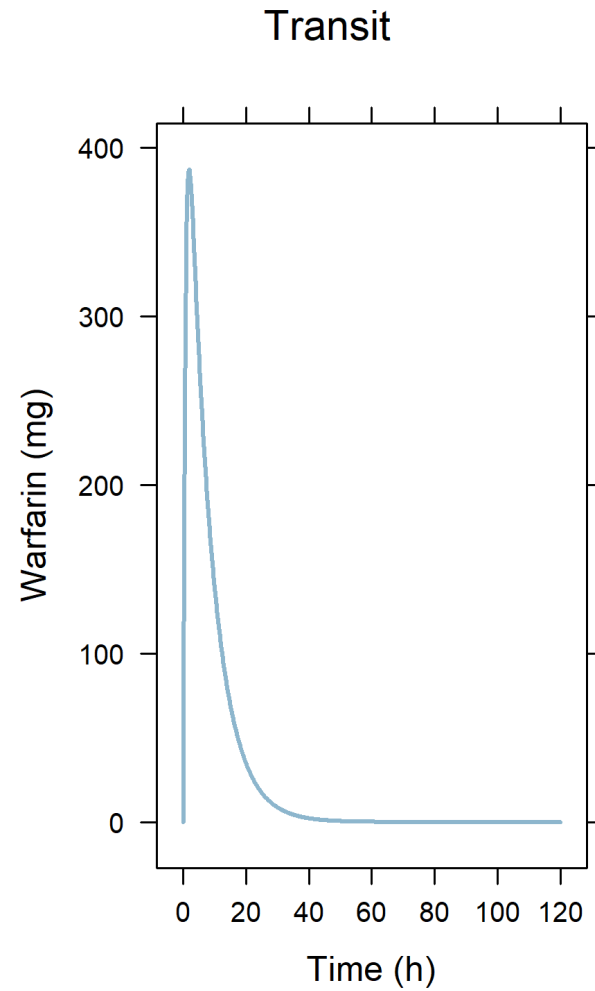
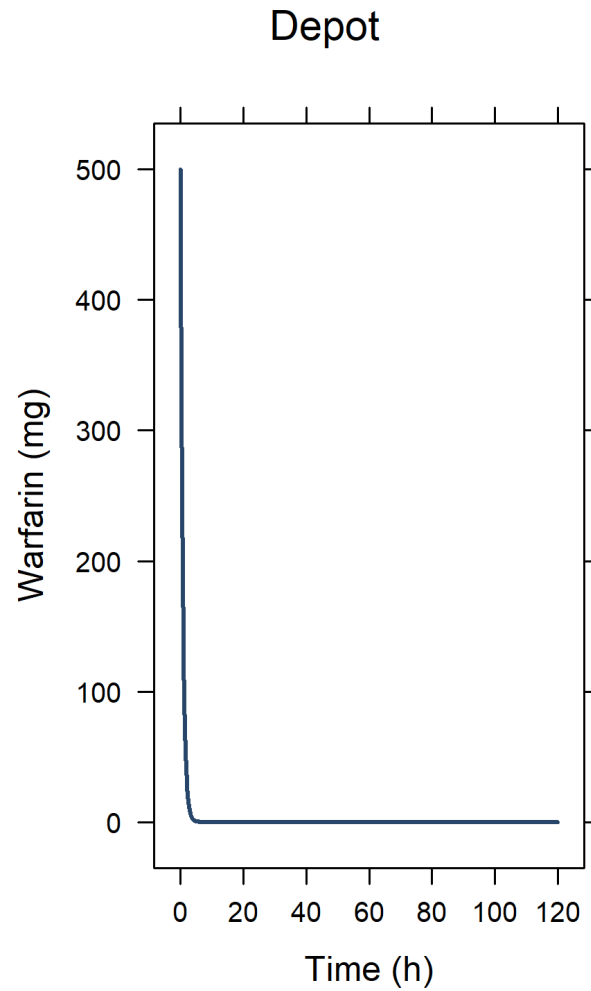
Depot compartment amounts



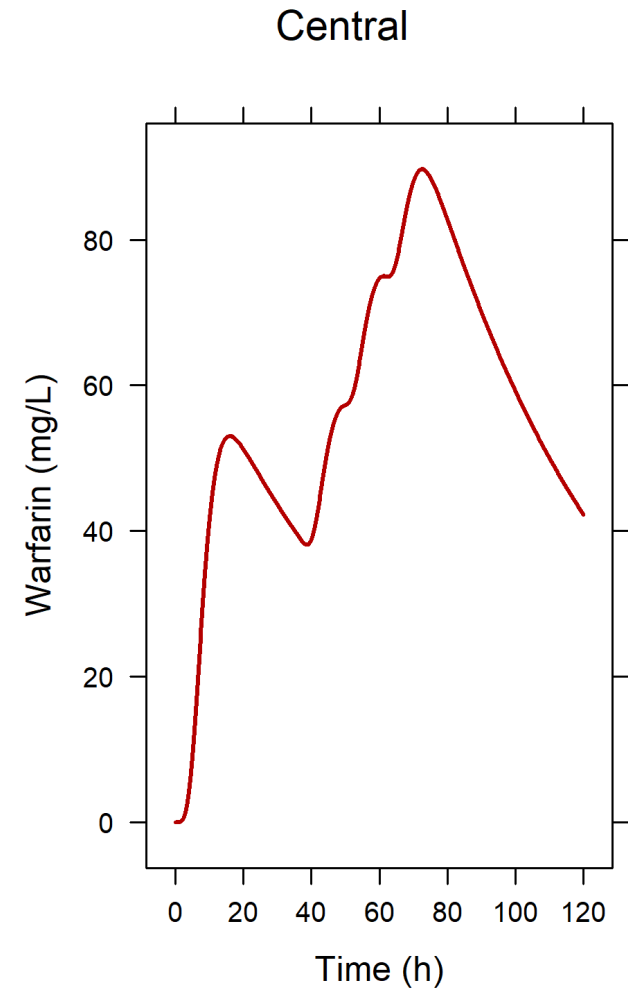
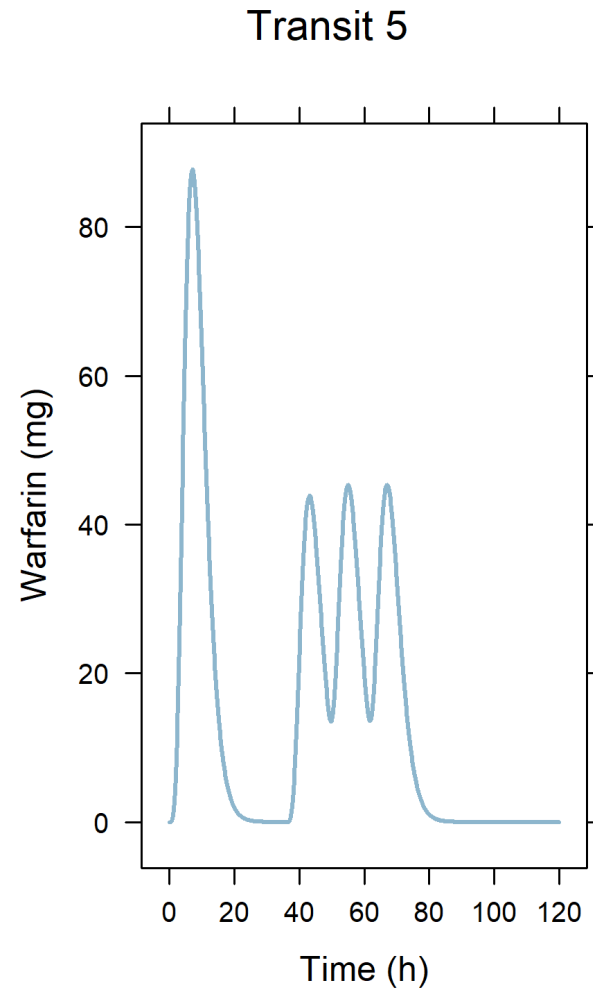
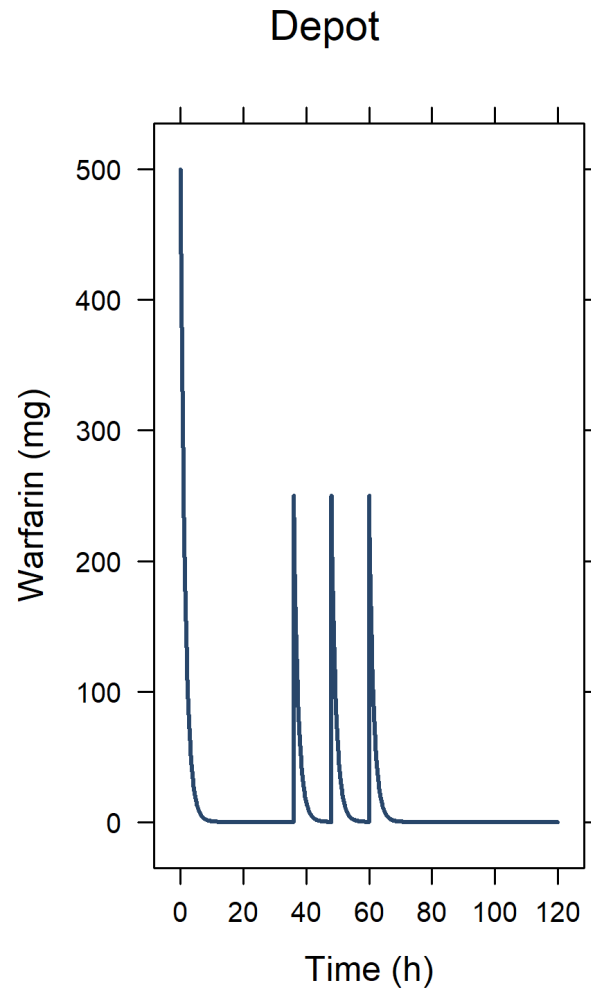
Central compartment concentrations



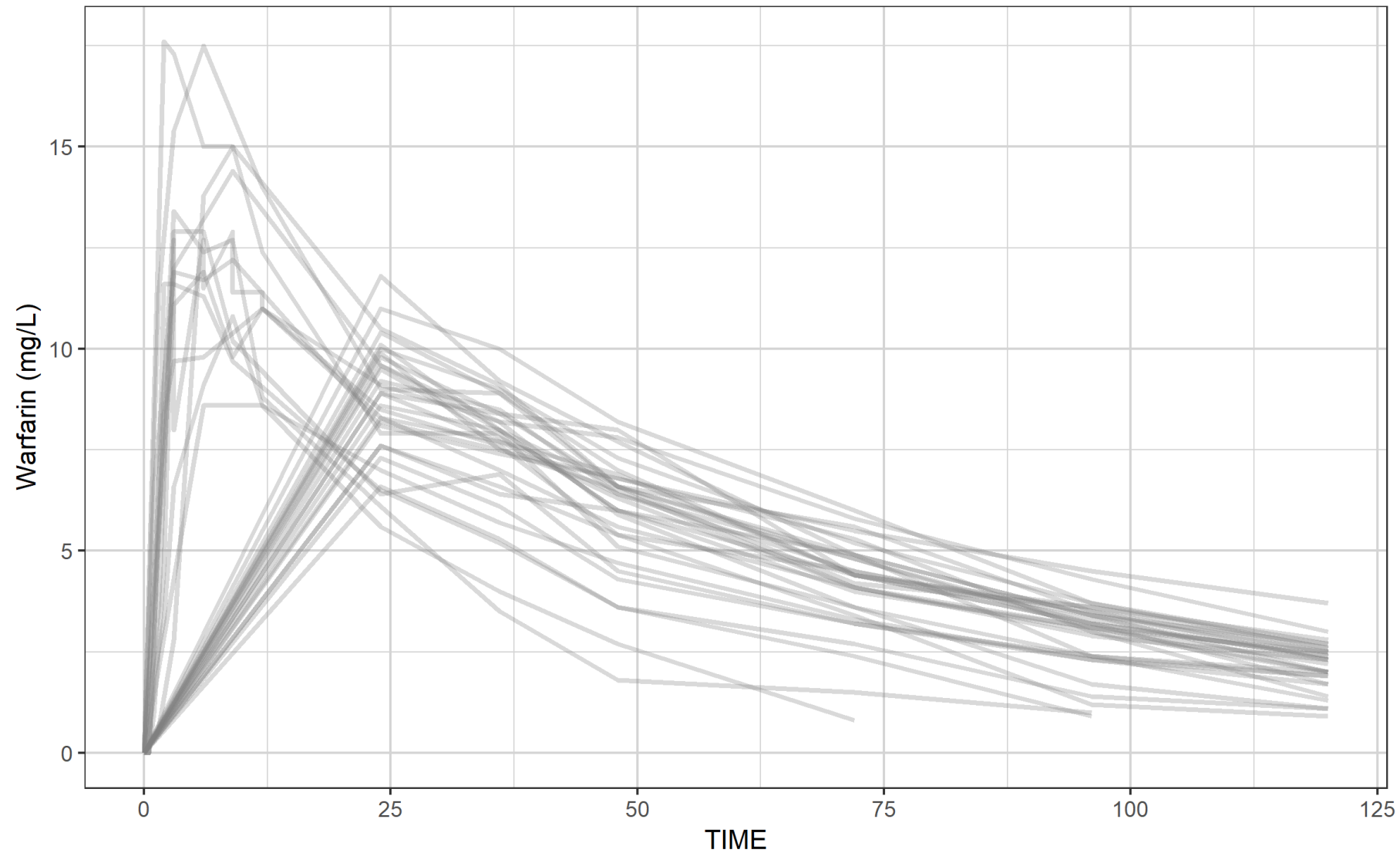
...adding a transit compartment between depot and central



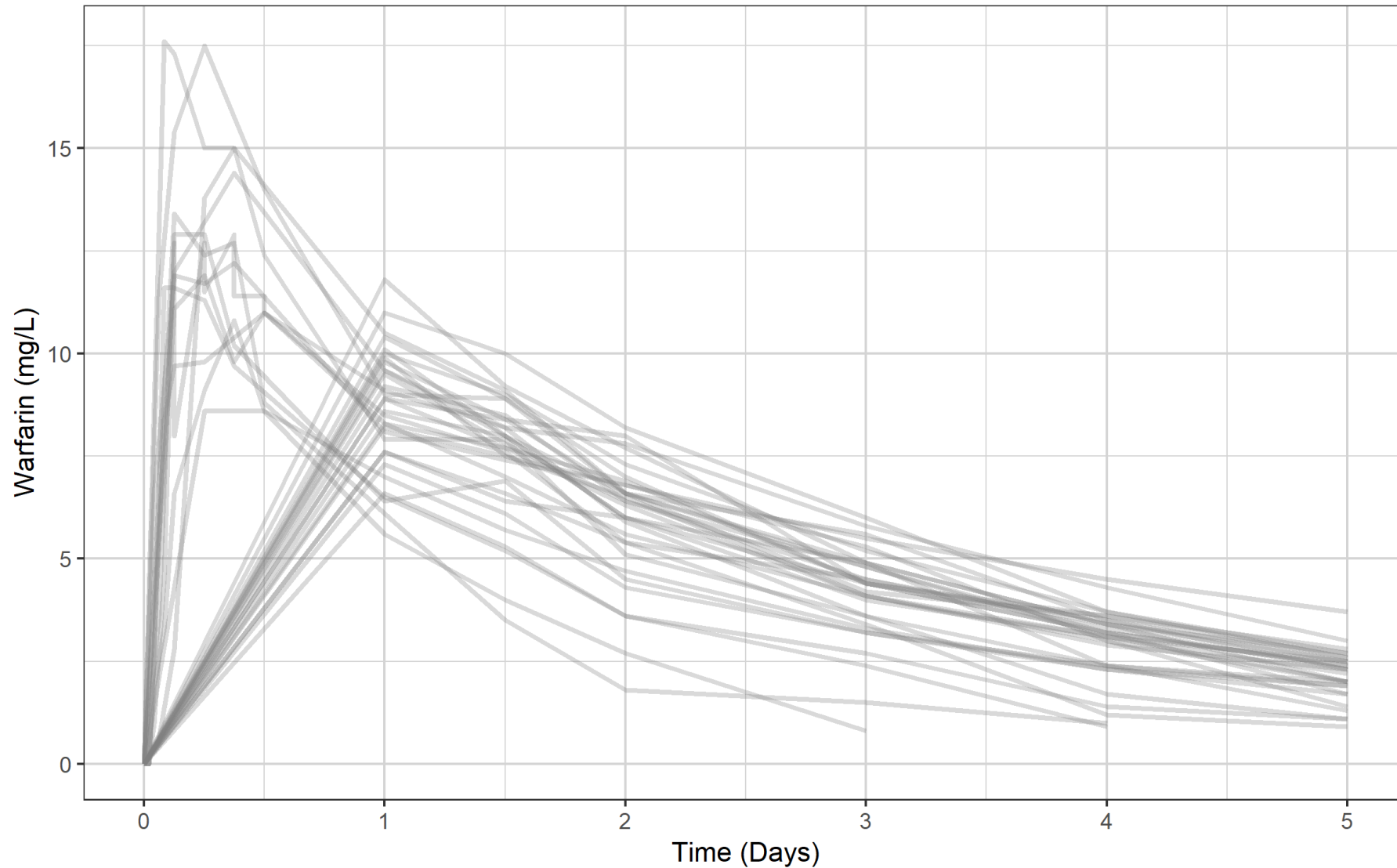
...adding 5 transit compartments between depot and central and giving 4 bolus doses in the 1st compartment



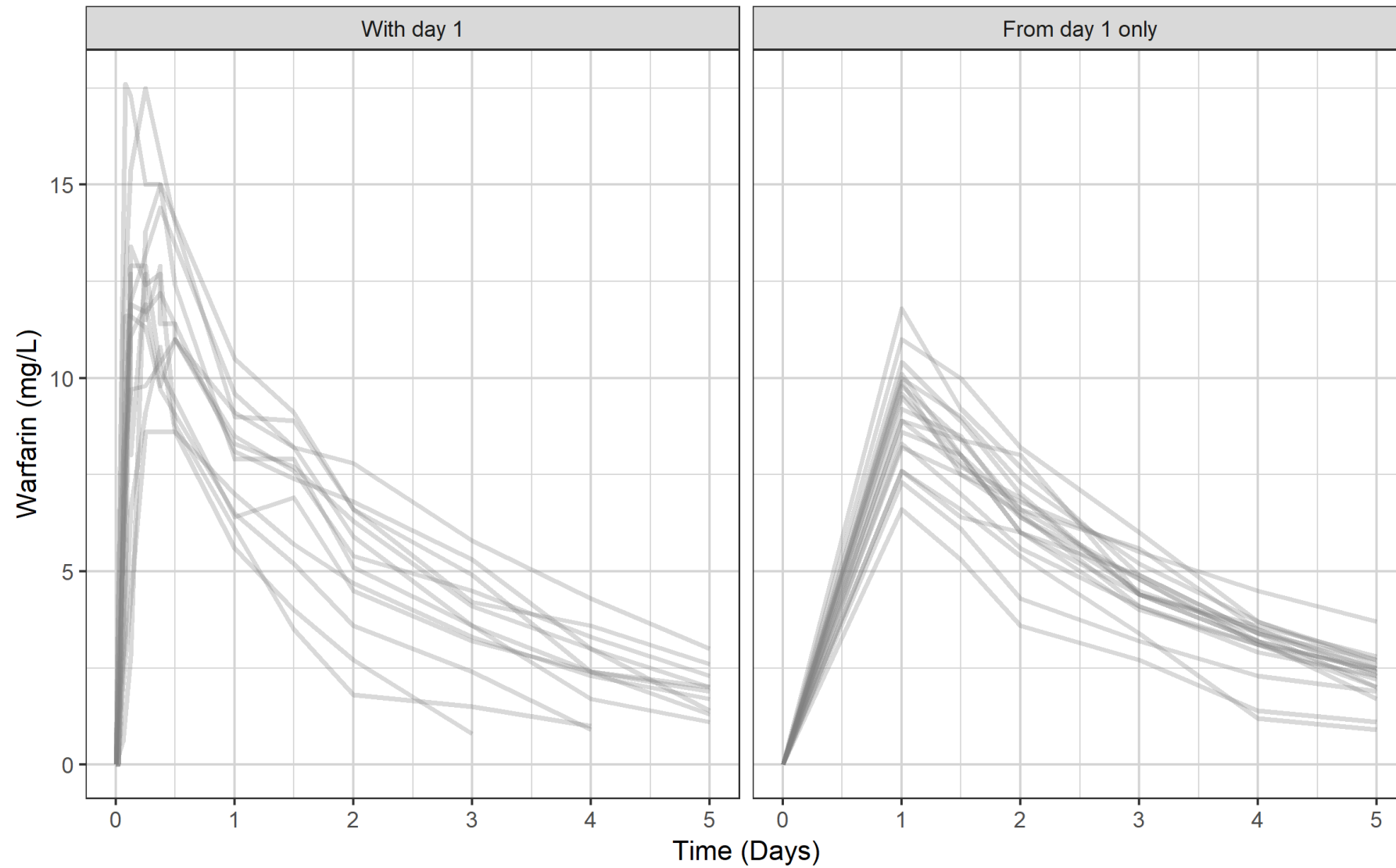
Our warfarin data file: a ggplot to provide an impression



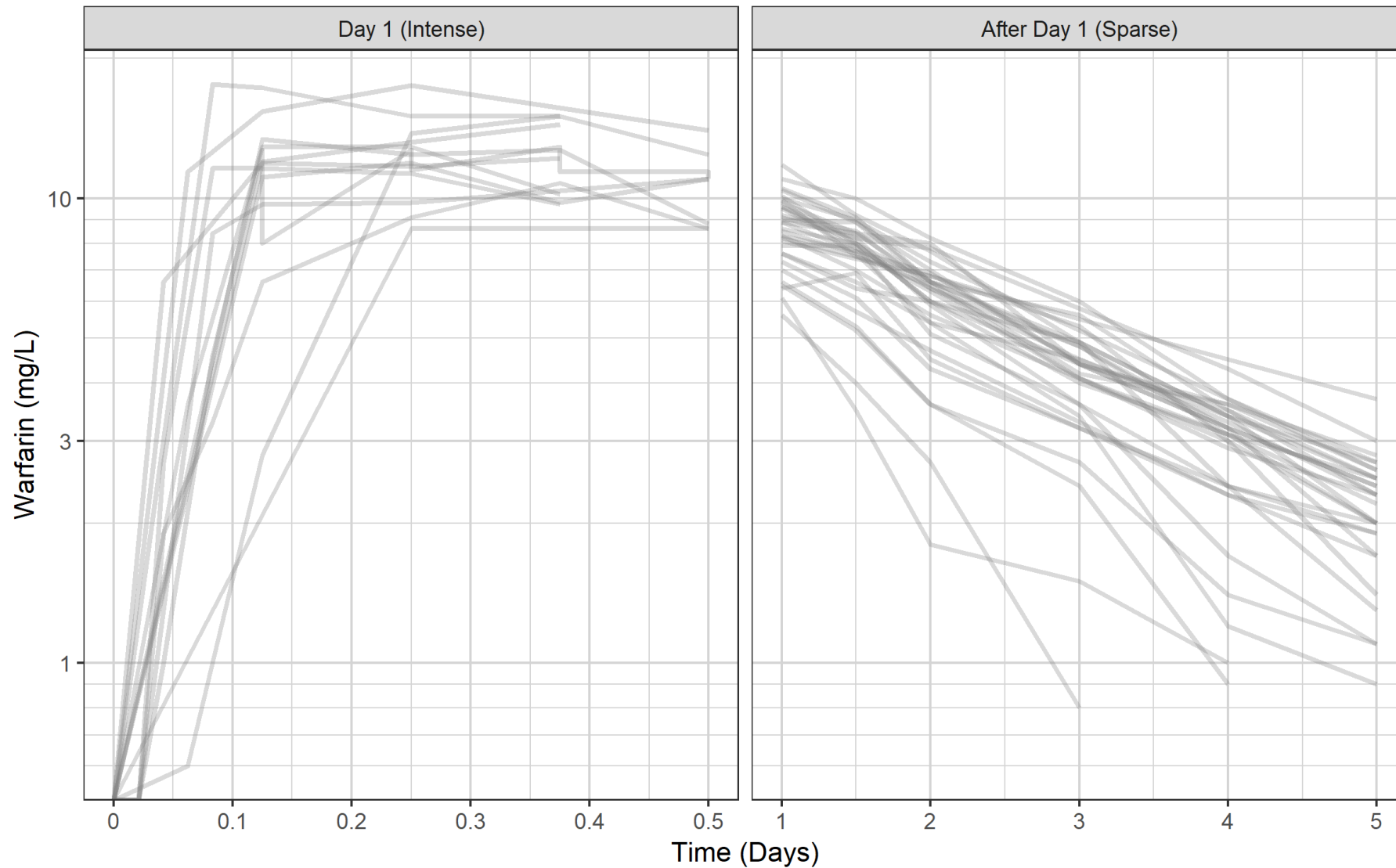
Change the x-axis from hours to days and add a proper label using the xgx helper `xgx_scale_x_time_units(units_dataset = "hours", units_plot = "days")`



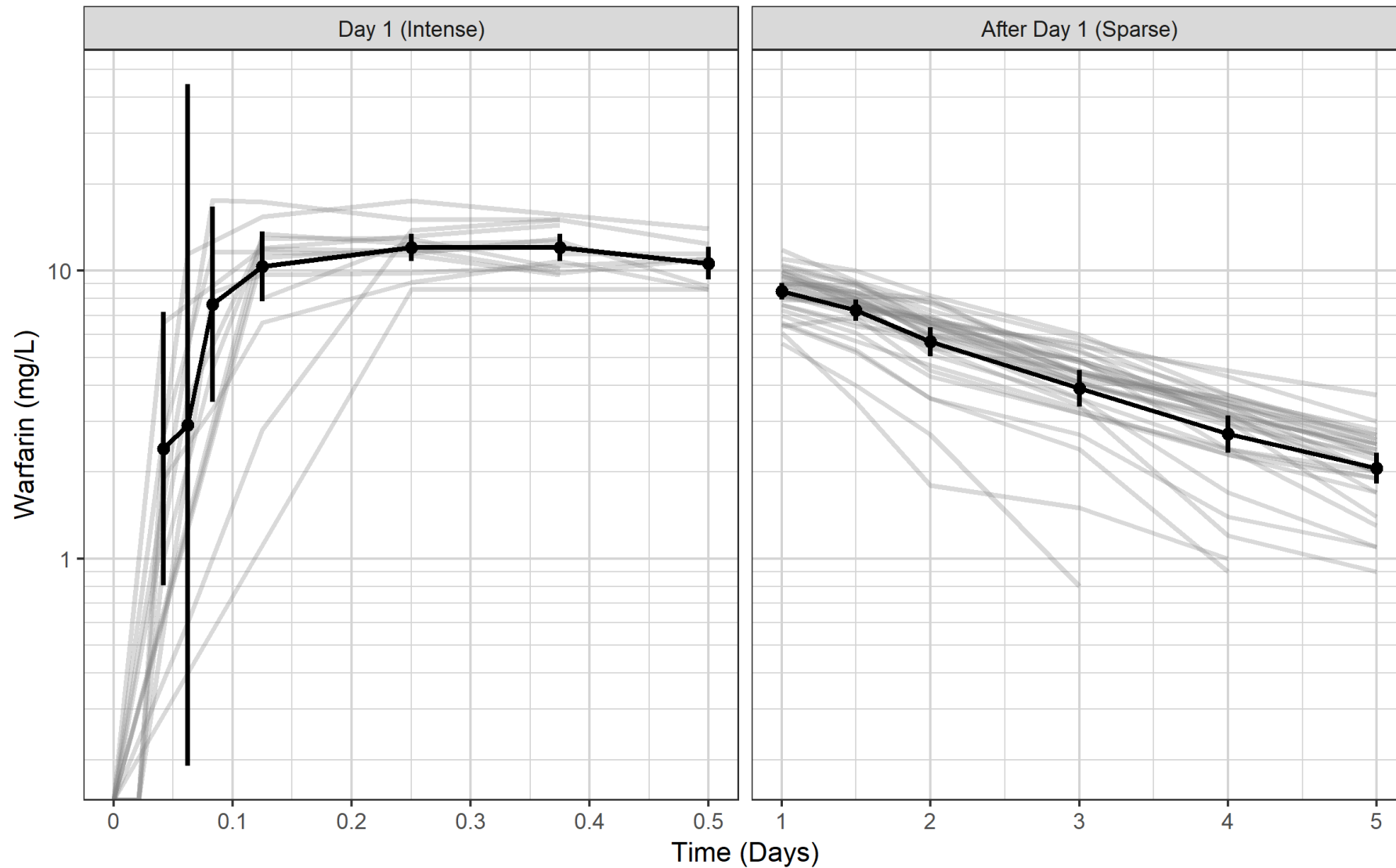
The data set has two types of profiles



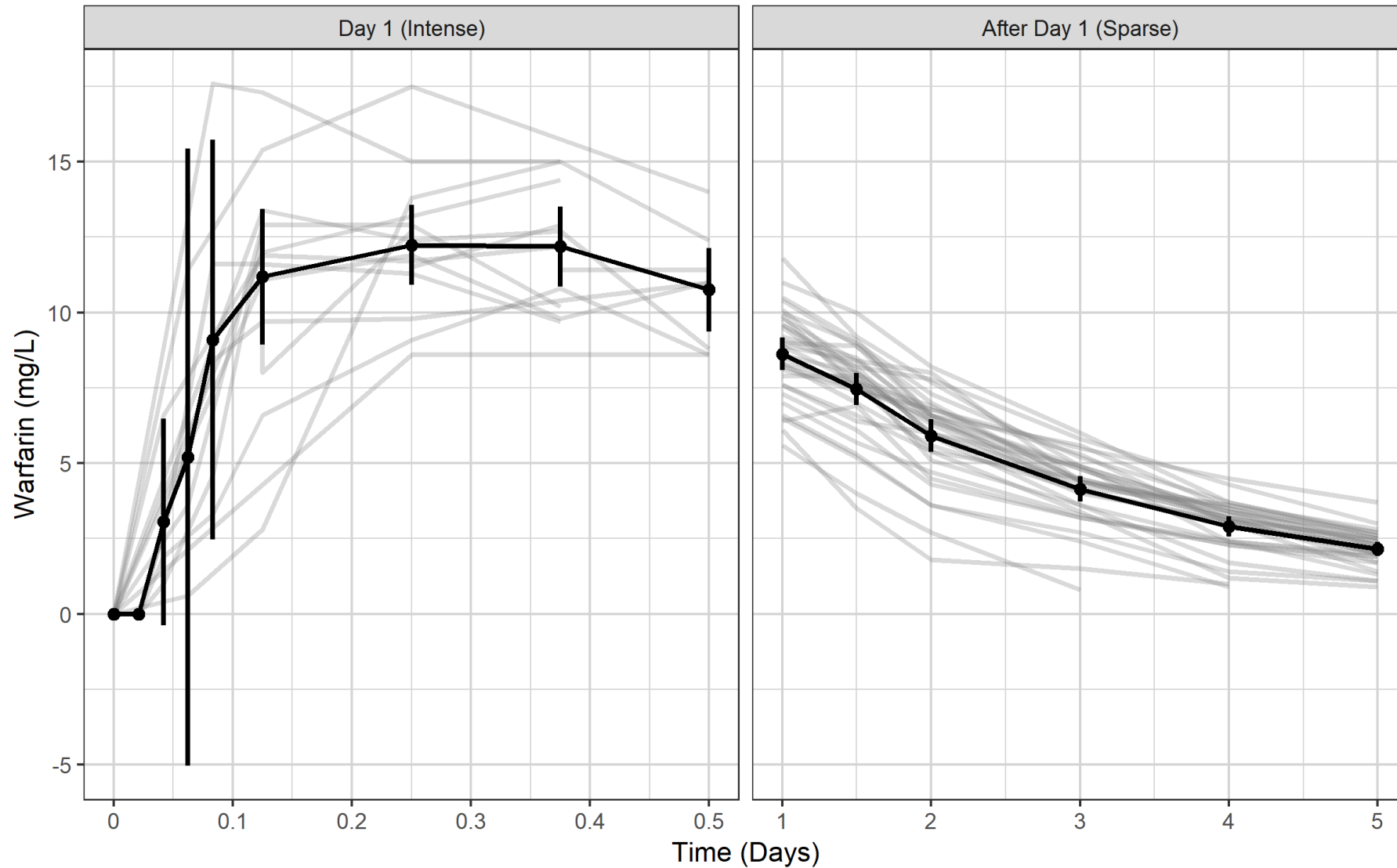
Switch to semi-log scale using xgx helper `xgx_scale_y_log10()`
Any clues to what model we should use?



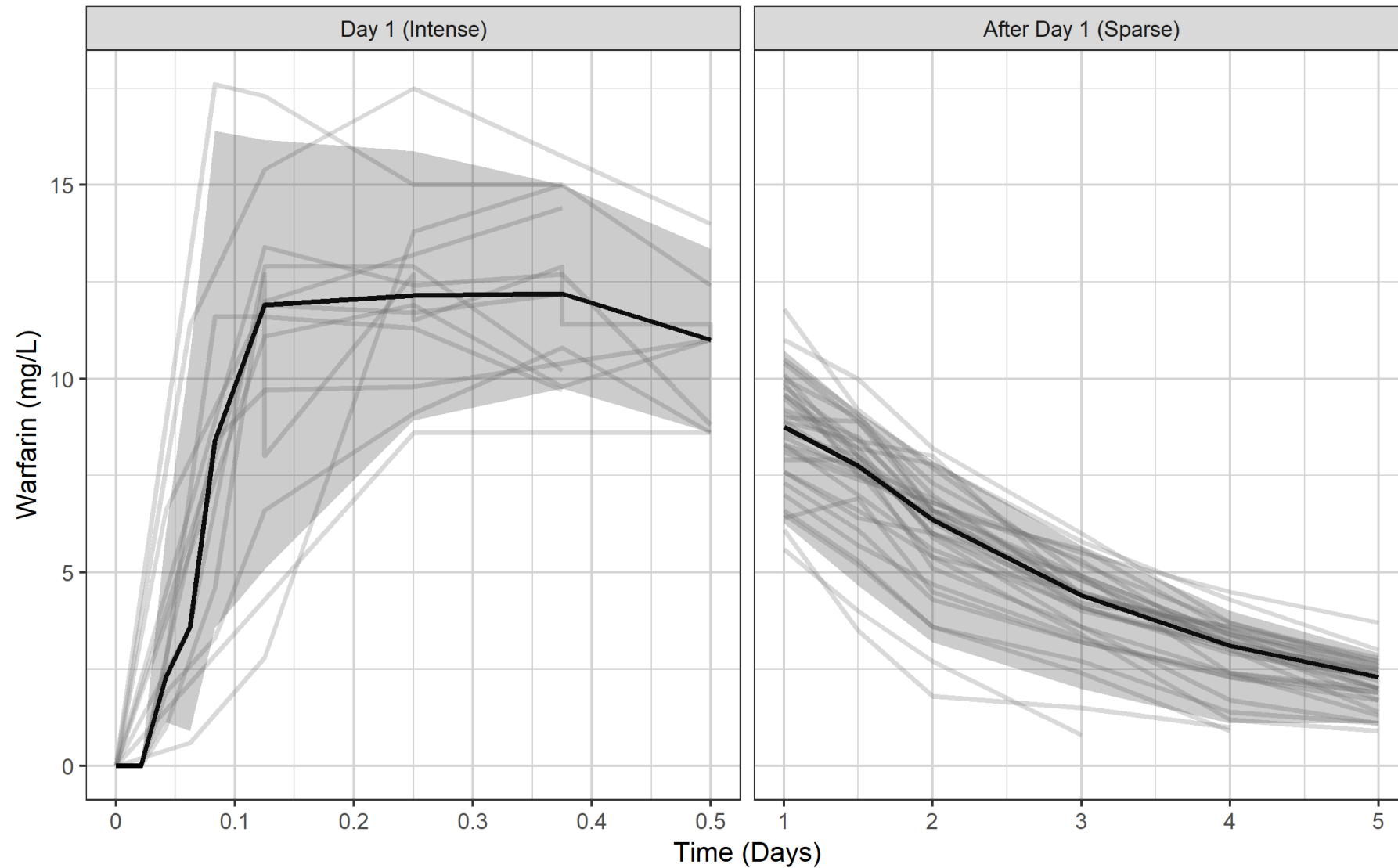
xgx can also add nice summary information if data has nominal times: summaries of mean plus 95% CI
`xgx_geom_ci(aes(x = TIME, color = NULL, group = NULL, shape = NULL), conf_level = 0.95)`



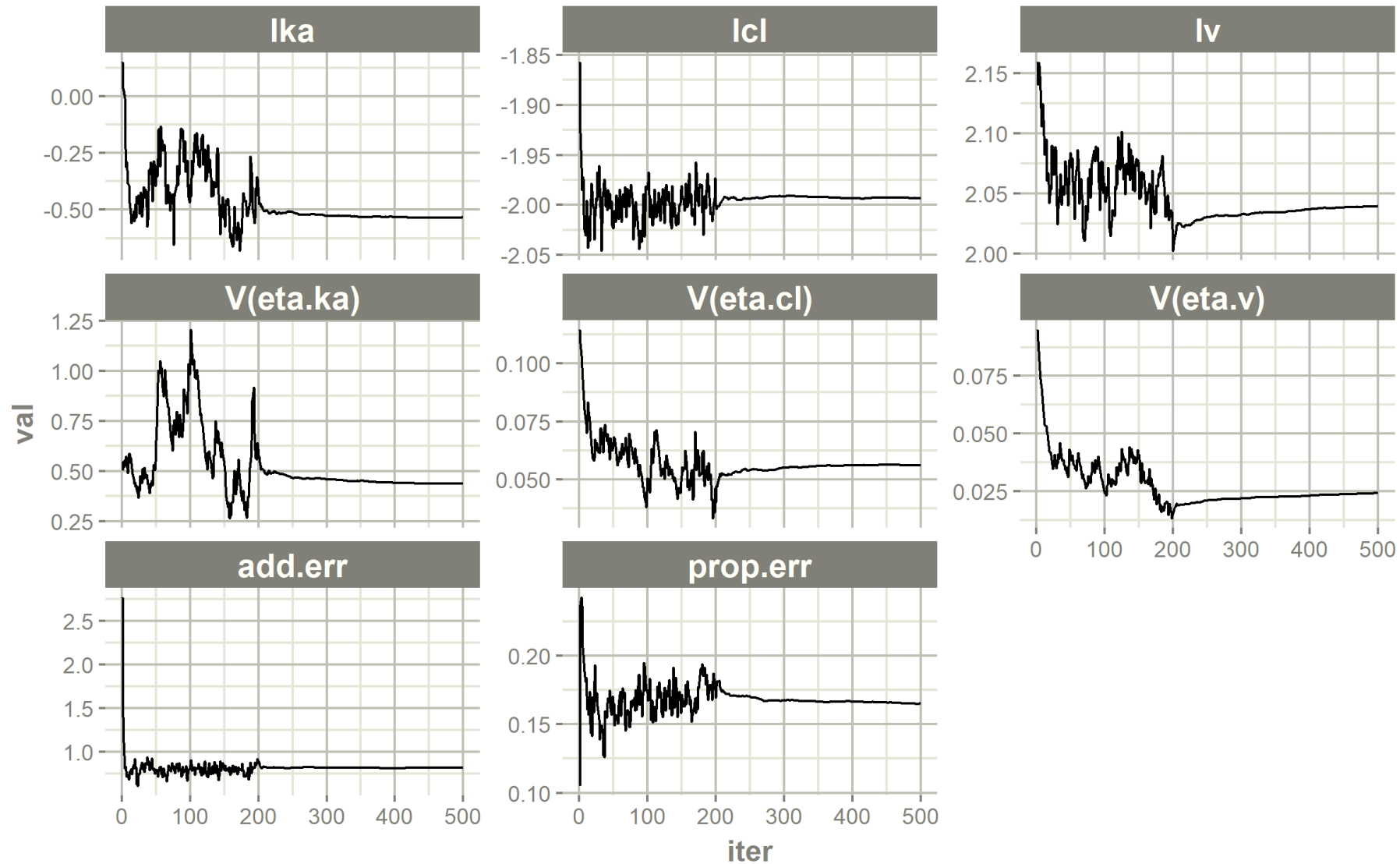
On linear scale this would result in a CI crossing zero because CIs are assumed symmetrical



...so perhaps a median and 95% of the data would be more suitable
`xgx_geom_pi(aes(x = TIME, color = NULL, group = NULL, shape = NULL))`



Traceplot for SAEM parameter estimates using nlmixr2 command



NPDE vs PRED plot using ggPMX

ctr %>% pmx_plot_npde_pred or pmx_plot_npde_pred(ctr)

