NCA Tutorial

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1 Introduction

This is an introduction to NCA.jl, a software for noncompartmental analysis (NCA). In this tutorial we will show how to use NCA.jl to analysis data.

1.1 Installation

Currently, NCA.jl is a submodule in PuMaS.jl, so you only need to install PuMaS.jl, and everything will be ready to go.

1.2 Getting Started

To load the package, use

```
using PuMaS.NCA
```

First, let's load the example NCA data inside PuMaS.jl. This data have 24 individuals, and each of them has 16 data points.

```
using PuMaS, CSV

file = PuMaS.example_nmtran_data("nca_test_data/dapa_IV")
data = CSV.read(file)

here is what the dataset looks like

first(data, 6) # take first 6 rows
```

	ID	TIME	TAD	CObs	AMT_{IV}	AMT_ORAL	Formulation
	Int64	Float64	Float64	Float64	Float64	Float64	String
1	1	0.0	0.0	157.021	5000.0	0.0	IV
2	1	0.05	0.05	141.892	0.0	0.0	IV
3	1	0.35	0.35	116.228	0.0	0.0	IV
4	1	0.5	0.5	109.353	0.0	0.0	IV
5	1	0.75	0.75	66.4814	0.0	0.0	IV
6	1	1.0	1.0	74.7532	0.0	0.0	IV

2 Efficient Computation of Multiple NCA Diagnostics

2.1 AUC and AUMC

257.8586273987722

We can compute the area under the curve (AUC) from the first observation time to infinity. Below we are accessing the concentration and corresponding time array for the first individual.

```
NCA.auc(data[:C0bs][1:16], data[:TIME][1:16])
263.792662196049

NCA.auc(data[:C0bs][1:16], data[:TIME][1:16], method=:linuplogdown)
```

the keyword argument method can be :linear, :linuplogdown, or :linlog, and it defaults to :linear. This is a simple interface, however it is not efficient if you want to compute many quantities. The recommended way is to create an NCASubject or an NCAPopulation object first and then call the respective NCA diagnostic on the data object. To parse data to an NCAPopulation object one can call the parse_ncadata function and give column names of id, time, conc (concentration), amt (dosage), formulation, iv (IV bolus name). Note that, by default, the lower limit of quantization (LLQ) is 0, and concentrations that are below LLQ (BLQ) are dropped. Also, we can add units by providing timeu, concu, and amtu.

```
timeu = u"hr"
concu = u"mg/L"
amtu = u"mg"
pop = parse_ncadata(data, id=:ID, time=:TIME, conc=:CObs, amt=:AMT_IV,
    formulation=:Formulation, iv="IV",
    llq=0concu, timeu=timeu, concu=concu, amtu=amtu)
```

Here, each element of pop has the type NCASubject. It is a lazy data structure and actual computations are not performed. When we are instantiating NCASubject, it only performs data checking and cleaning. To calculate AUC, one can do:

NCA.auc(pop)

	id	auc		
	Int64	Quantity		
1	1	263.793 mg hr L-1		
2	2	323.253 mg hr L-1		
3	3	$339.848~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{\ }1$		
4	4	373.361 mg hr L - 1		
5	5	$132.145~\mathrm{mg}$ hr L -1		
6	6	$303.86~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{\ }1$		
7	7	380.275 mg hr L - 1		
8	8	$279.126~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{\ }1$		
9	9	239.831 mg hr L $\stackrel{\circ}{=}$ 1		
10	10	$260.862~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{\ }1$		
11	11	$146.864 \text{ mg hr L} \hat{1}$		
12	12	$359.489~\mathrm{mg}$ hr L -1		
13	13	522.905 mg hr L - 1		
14	14	$262.988 \text{ mg hr L} \hat{1}$		
15	15	378.993 mg hr L -1		
16	16	$206.926~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{-}1$		
17	17	$341.551 \text{ mg hr L} \hat{1}$		
18	18	195.925 mg hr L-1		
19	19	$433.443 \text{ mg hr L}^2$		
20	20	$214.27~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{\ }1$		
21	21	$232.537~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{\ }1$		
22	22	471.515 mg hr L - 1		
23	23	$292.413~\mathrm{mg}~\mathrm{hr}~\mathrm{L}\hat{\ }1$		
24	24	170.305 mg hr L-1		

AUClast is the area under the curve from the first observation to the last observation. To compute AUClast on the second individual, one would do:

```
NCA.auc(pop[2], auctype=:last)
```

302.24594 mg hr L^-1

Or to compute the AUC on every individual, one would do:

NCA.auc(pop, auctype=:last)