Optimization methods

OBS: All examples considered the feeding happening on the first high concentration point after decreasing

MCMC + Metropolis-Hasting

A priori distribution

kcat1	0.181
kcat2	0.390
Km1	5.449
Km2	1.694
Tmax	0.824
Ken	7.947
kAB	0.682
kAN	1.989
kAOH	9.856
kNH	9.763

Results

kcat1	0.1302
kcat2	0.0504
Km1	1.4233
Km2	2.0499
Tmax	0.6019
Ken	6.8660
kAB	0.5174
kAN	1.6521
kAOH	3.6890
kNH	16.256

Solver: ode15s.

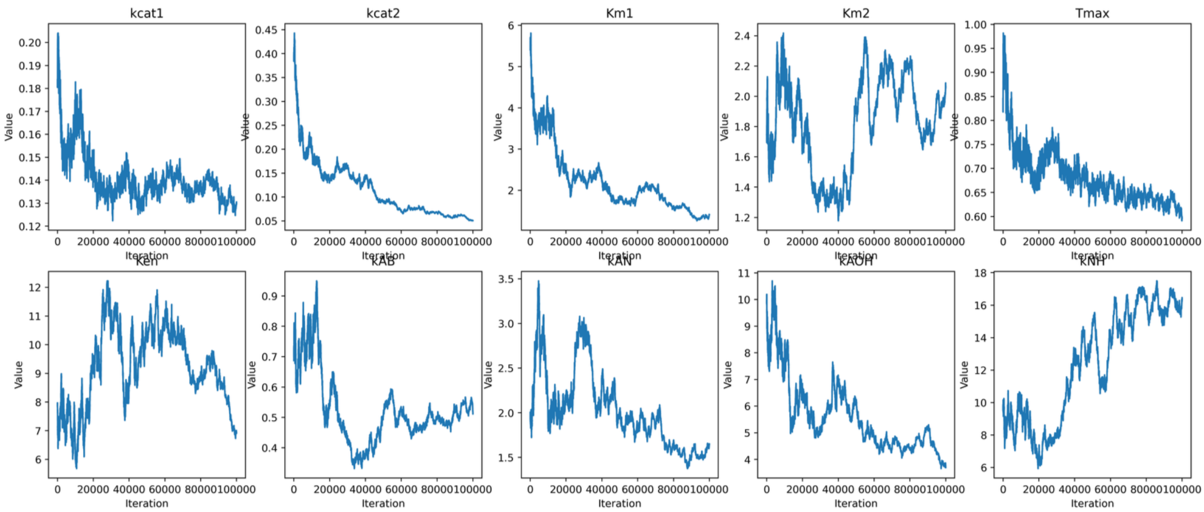
N. chain states: 100000 (100k).

Gaussian:

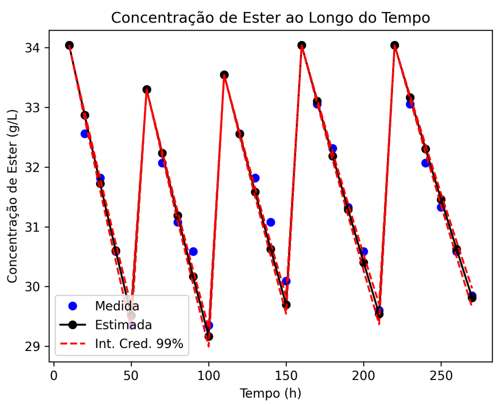
mean = 1;

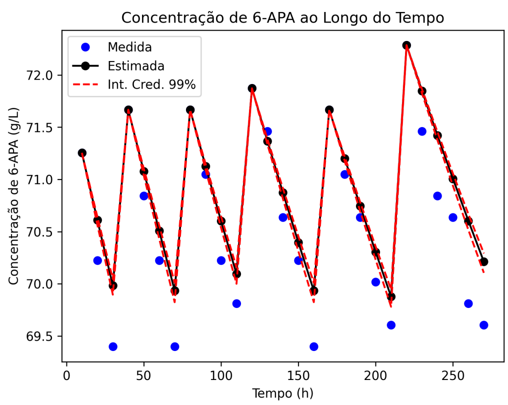
dp = 0.6.

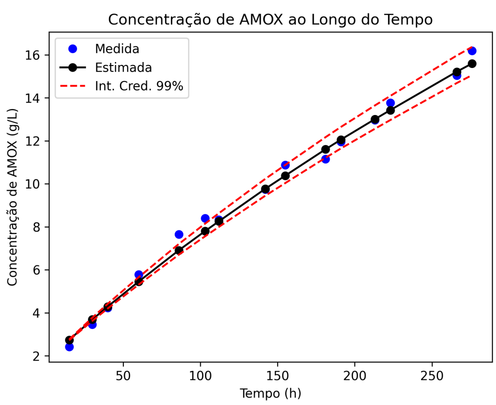
Evolution

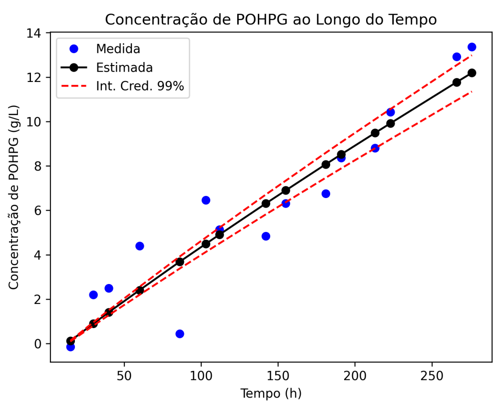


Performance









Nelder-Mead

The Nelder–Mead method is a numerical method used to find the minimum or maximum of an objective function in a multidimensional space. It's a direct search method (based on function comparison) and is often applied to nonlinear optimization problems for which derivatives may not be known. However, this technique is a heuristic search method that can converge to non-stationary points on problems that can be solved by alternative methods.

Initial guess

kcat1	0.181
kcat2	0.390
Km1	5.449
Km2	1.694
Tmax	0.824
Ken	7.947
kAB	0.682
kAN	1.989
kAOH	9.856
kNH	9.763

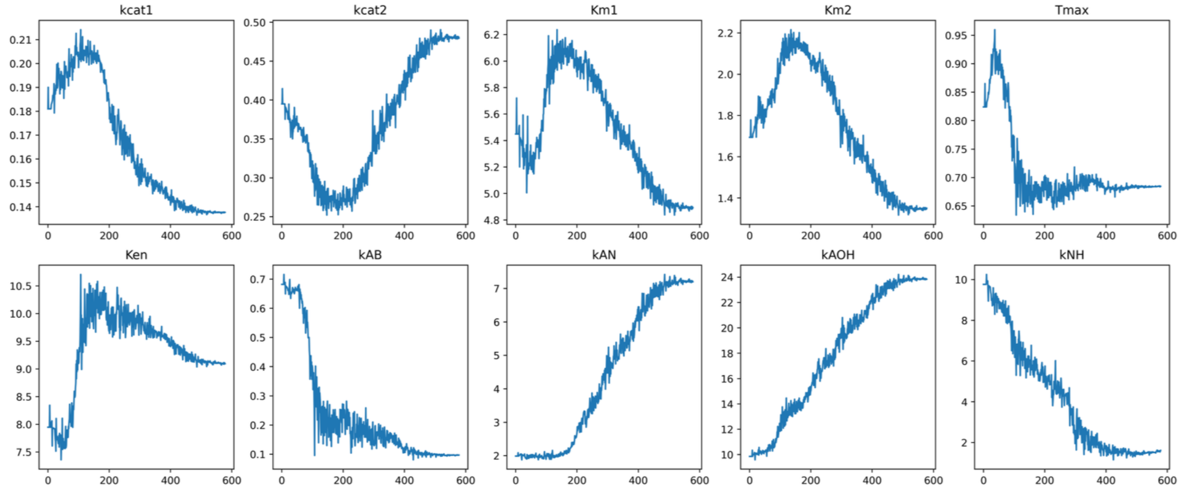
Results

kcat1	0.1377
kcat2	0.4786
Km1	4.8977
Km2	1.3540
Tmax	0.6842
Ken	9.1017
kAB	0.0972
kAN	7.1871
kAOH	23.819
kNH	1.6204

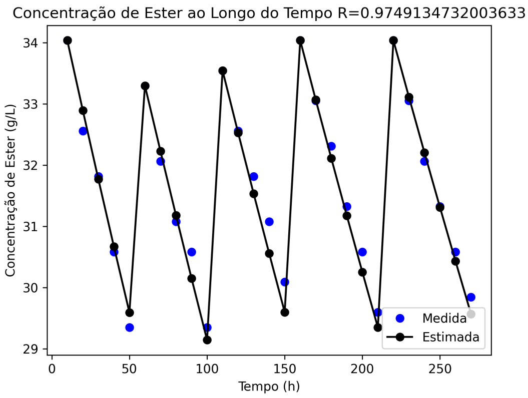
Iter = 540

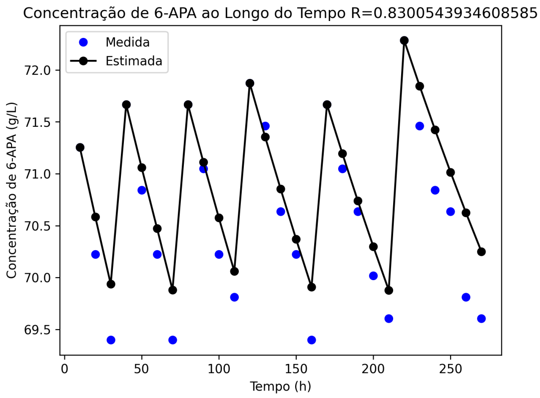
Boundaries = (0.001, inf)

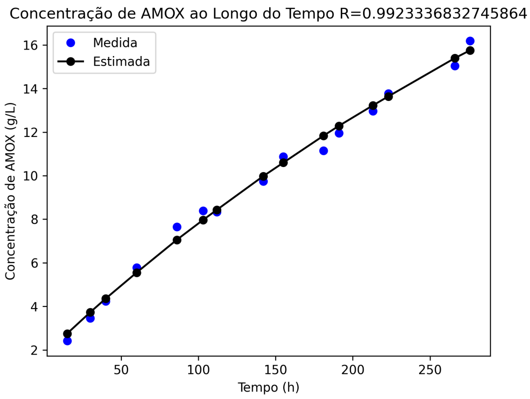
Evolution

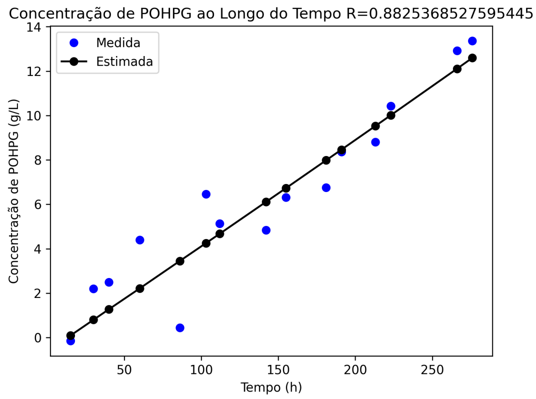


Performance









L-BFGS_B

Limited-memory BFGS (L-BFGS or LM-BFGS) is an optimization algorithm in the family of quasi-Newton methods that approximates the Broyden–Fletcher–Goldfarb–Shanno algorithm (BFGS) using a limited amount of computer memory. It is a popular algorithm for parameter estimation in machine learning. The algorithm's target problem is to minimize $f(x)$ over unconstrained values of the real-vector x where f is a differentiable scalar function.

Iter = 540

Boundaries = (0.001, inf)

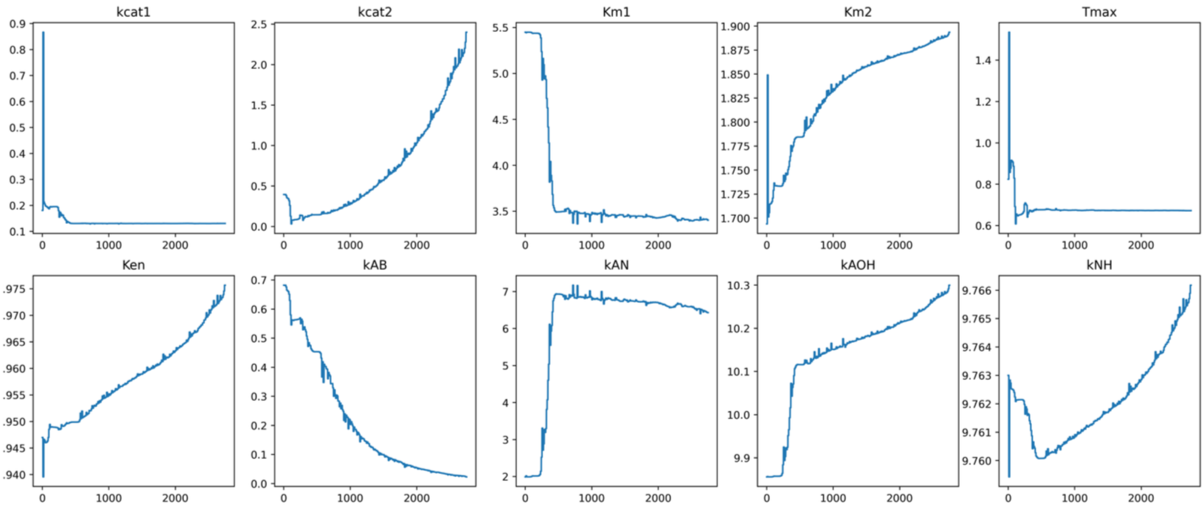
Initial guess

Results

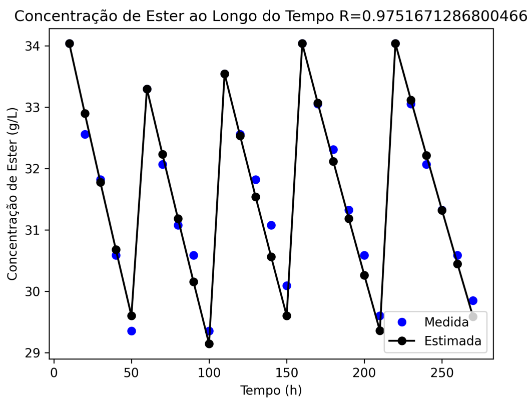
kcat1	0.181
kcat2	0.390
Km1	5.449
Km2	1.694
Tmax	0.824
Ken	7.947
kAB	0.682
kAN	1.989
kAOH	9.856
kNH	9.763

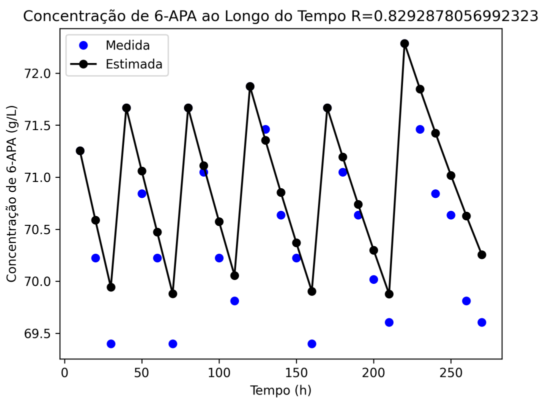
kcat1	0.1307
kcat2	2.4006
Km1	3.4037
Km2	1.8936
Tmax	0.6724
Ken	7.9757
kAB	0.0229
kAN	6.4322
kAOH	10.299
kNH	9.7661

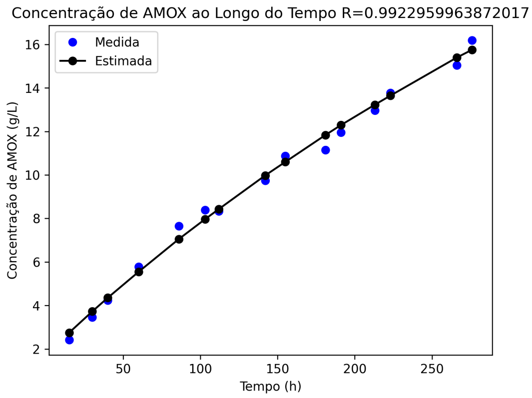
Evolution

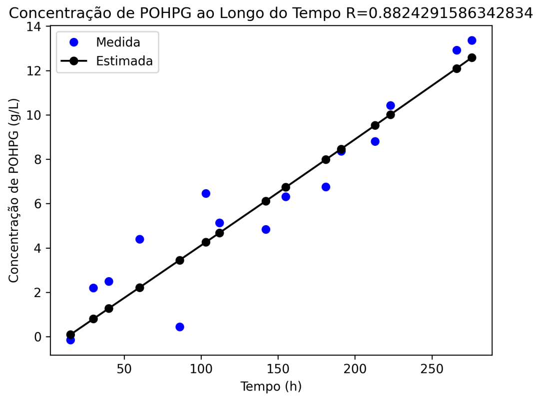


Performance









Genetic Algorithm

tournsize = 3

blend: alfa = 0.5

mutGaussian:

    mu = 0

    sigma = 0.1

    indpb = 0.2

generations = 1000

population = 50

Boudaries

kcat1	0.05, 0.22
kcat2	0.1, 0.55
Km1	4.5, 6.5
Km2	1, 2.5
Tmax	1.1, 0.4
Ken	6, 11
kAB	0.1, 0.8
kAN	1.6, 8
9.5,17	9.5,17

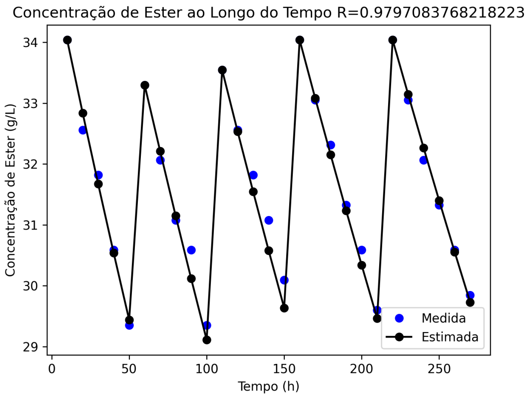
Results

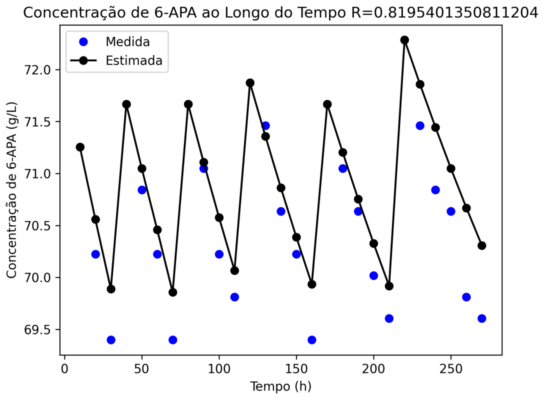
kcat1	0.1534
kcat2	0.5411
Km1	6.2420
Km2	2.0985
Tmax	0.6771
Ken	9.3321
kAB	0.1086
kAN	5.6608
kAOH	26.975

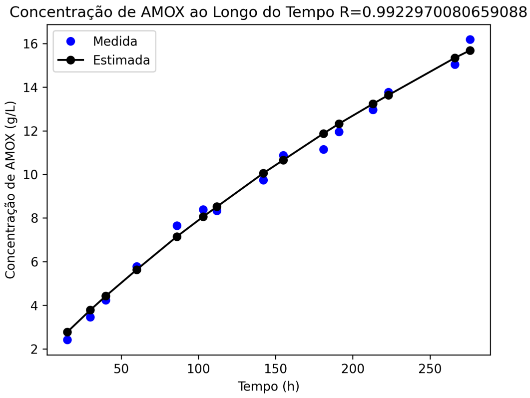
kNH	10, 2

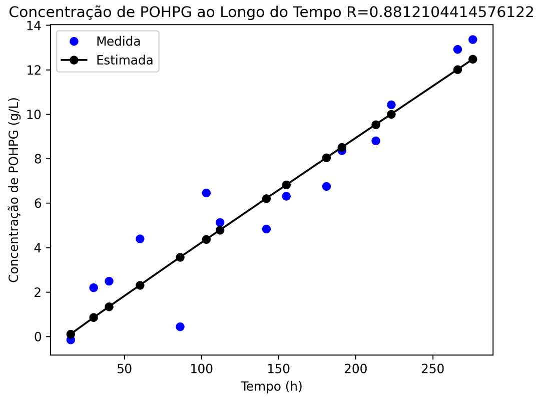
kNH	6.5178

Performance









Conclusions

- More data to validate values and reduce nonlinear redundancy
- Boundaries information are needed
- 6-APA equation is not capable of reaching the decrease level of experimental data
- POHPG experimental data / equation feels odd
- Kcat1 and Tmax tends towards an equal value
- kAOH and kNH are unstable

PARAMETER	MCMC	NELDER-MEAD	GA	L-BFGS-B
kcat1	0.1302	0.1377	0.1534	0.1307
kcat2	0.0504	0.4786	0.5411	2.4006
Km1	1.4233	4.8977	6.2420	3.4037
Km2	2.0499	1.3540	2.0985	1.8936
Tmax	0.6019	0.6842	0.6771	0.6724
Ken	6.8660	9.1017	9.3321	7.9757
kAB	0.5174	0.0972	0.1086	0.0229
kAN	1.6521	7.1871	5.6608	6.4322
kAOH	3.6890	23.819	26.975	10.299
kNH	16.256	1.6204	6.5178	9.7661
Score				