Summary of Simode Experiments

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# Introduction

We want to understand the performance of the simode R package. To that end, we used simode to solve a collection of initial value problems. We chose some models with only linear parameters, and others with both linear and non-linear parameters. Our goals are exploratory, in order to come up with hypotheses about the performance profile of the separable least squares (SLS) method of finding the parameters of IVPs, and comparing it with non-linear least squares (SLS) regression. In particular, we are interested in the following questions:

1. Does SLS perform well in determining the linear and non-linear parameters of IVPs?
2. Under what conditions does SLS perform better than NLS, and vice versa?

# Setup:

MacBook Pro 2014

RStudio

R 3.4

# Method

We ran sets of simulations, based on the following known models of IVPs:

* S-Systems
* Lotka-Volterra
* Lotka-Volterra with sinusoidal seasonal adjustment
* FitzHugh-Nagumo
* SIR semi-linear.

Our experiments generated random observations based on a gaussian error distribution, centered at the “true” parameter values. We then used both SLS and NLS to compute estimate the parameters using integral matching.

In most cases, we varied the “prior information”, meaning the initial guess for the parameter values. Higher quality “prior information” means that the initial guesses of the parameter values is closer to the truth.

Sometimes, the integral matching loss is the same for SLS and SLS. In such cases, we looked at the variance of the parameter estimates over the simulations.

# Results

## FitzHugh-Nagumo

We tried two experiments, varying the value of the V parameter. With V=-1, R=1, we saw that the variance of the parameter estimates using SLS was less than 0.5 times the NLS. When we changed V=-0.5, the variance of the parameter estimates was lower for most cases.





## S-Systems

We tried an S-System example, with 4 differential equations and 4 unknowns. The equations were:

x1’ = alpha1\*(x3^g13)-beta1\*(x1^h11)

x2’ = alpha2\*(x1^g21)-beta2\*(x2^h22)

x3’ = alpha3\*(x2^g32)-beta3\*(x3^h33)\*(x4^h34)

x4’ = alpha4\*(x1^g41)-beta4\*(x4^h44)

We compared the integral matching loss function using NLS and SLS, with the SLS error being significantly lower when the quality of the prior information was low.



## SIR model

We next tried a semi-linear SIR model over 5 years for 2 age groups. Our non-linear parameters were the initial values of S during the 5 years. We measured the integral matching errors of the simulations, and found that SLS and NLS performed the same. We then compared the variance of the parameter estimates, and it too was the same, as indicated by the ratio of 1.





## Lotka-Volterra

The Lotka-Volterra predator-prey model has only linear parameters. We show the variance ratio of SLS/NLS for the variance of the linear parameters. It is exactly 1, independent of prior information. We ran simulations using sigma=0.1 and sigma=0.4. This suggests that the performance of SLS and NLS may be the same when all of the parameters are linear.





## Lotka-Volterra Seasonal

Finally, we add seasonal variation to the Lotka-Volterra system in the form of sinusoidal non-linear parameters. In this instance, we can see from the variance ratio graph that the *linear* parameters estimates have much lower variance using SLS, whereas the *nonlinear* parameters are much more similar for both techniques. This is further emphasized in the bar charts below.



 

We next examine the effect of sample size on the integral matching loss It appears that the sample size does not affect the integral matching error in any significant way.



# Discussion

From our preliminary tests, it appears that SLS performs as well or better than NLS for estimating the parameters of IVPs. This is true for both linear and non-linear parameters. For the Lotka-Volterra IVP, we observed that when estimating linear parameters, the two techniques were equivalent. However, when we added non-linear seasonal parameters we observed that SLS performed significantly better than NLS on the linear parameter estimates.