

Things I've tried to get sensitivity analysis working

- In sundials you can manually differentiate your equations wrt the parameters and analytically provide these as a user supplied call back function. Look at SimpleFluxWithUserSuppliedFunctions.c
 - This works. But isn't useful to us because roadrunner has no way of providing the equations for differentiation.
 - Incidentally I think this would be a very useful addition to roadrunner and this is something I'd quite like to do.
 - We could use ginac as a dependency and create equations from the sbml. This can be used for sensitivities, providing equations in latex and structural identifiability analysis. And probably more.
- Alternatively, sundials falls back on the finite differences approximation - and there are several options. See SimpleFluxWithFiniteDifferences.c. Basically we remove the user supplied call back function and provide the parameter values. I haven't been able to get this to work.
- I thought there could be a problem with the model, in the same way that this model wouldn't solve for steady state because of the moiety conservation. So I tried another model - see VenkatramanFSAWithFiniteDifferences.c. Same problem.
- The finite differences approx is not well represented in the sundials examples. See cvsAdvDiff_FSA_non.c for the only relevant example.
- Another sensitivities example cvsRoberts_FSA_dns.c provides the analytical rhs to the sensitivity equations. I was able to replace this with the finite differences approximation, using their model (but not my own). See cvsRoberts_FSA_dns_cw.c.
- I thought that the problem might be something to do with the sensitivity initial conditions, which do affect the output despite all being wrong. So I tried approximating the first step with manual computed finite differences: $\text{fabs}(y1 - y2)/\text{step size}$. Output is still 0.
- I took the example that works with finite differences and copied into new .c file. Then I minimally changed the problem that was being solved to the venkatraman model. Still get 0's. So the setup for the example is not appropriate for the venkatraman model?