Dealing with Data Gradients: Calibration 2

Nathaniel Osgood CMPT 858 March 31, 2011

A Key Deliverable! Mental Model Knowledge Qualitative Problem Model Testing Policy Evaluation Model Problem Model Calibration Translation Formulation Conceptualization Mapping Reference mode Specification & Learning Parameter sensitivity Specification of reproduction investigation of environm analysis Model scope/boundary Causal loop diagrams intervention scenarios ents/Mic Matching of selection. Stock & flow diagrams Parameters **Cross-validation** Investigation of roworlds intermediate time Model time horizon **Policy structure** Robustness&extreme case Quantitative causal /flight Identification of diagrams series relations conditions simulator tests key variables Matching of S Reference modes for •Decision rules Cross-scenario observed data point nit checking comparisons (e.g. CEA) explanation Problem domain tests Initial conditions Constrain to sensible Group model building bounds Structural sensitivity analysis

Some elements adapted from H. Taylor (2001)

Recall: Dealing with Data Gradients

- Often we don't have reliable information on some parameters, but do have other data
 - Some parameters may not be observable, but some closely related observable data is available
 - Sometimes the data doesn't have the detailed breakdown needed to specifically address one parameter
 - Available data could specify sum of a bunch of flows or stocks
 - Available data could specify some function of several quantities in the model (e.g. prevalence)
- Some parameters may implicitly capture a large set of factors not explicitly represented in model
- There are two big ways of dealing with this: manually "backing out", and automated calibration

Recall: Calibration: "Triangulating" from Diverse Data Sources

- Calibration involves "tuning" values of less well known parameters to best match observed data
 - Often try to match against *many* time series or pieces of data at once
 - Idea is trying to get the software to answer the question:
 "What must these (less known) parameters be in order to explain all these different sources of data I see"
- Observed data can correspond to complex combination of model variables, and exhibit "emergence"
- Frequently we learn from this that our model structure just can't produce the patterns!

Recall: Calibration: A Bit of the How

- Calibration uses a (global) optimization algorithm to try to adjust unknown parameters so that it automatically matches an arbitrarily large set of data
- The data (often in the form of time series) forms constraints on the calibration
- The optimization algorithm will run the model many (minimally, thousands, typically 100K or more) times to find the "best" match for all of the data

Recall: Required Information for Calibration

- Specification of what to match (and how much to care about each attempted match)
 - Involves an "error function" ("penalty function", "energy function") that specifies "how far off we are" for a given run (how good the fit is)
 - Alternative: specify "payoff function" ("objective function")
- A statement of what parameters to vary, and over what range to vary them (the "parameter space")
- Characteristics of desired tuning algorithm

 Single starting point of search?

Recall: Example Global Optimization Algorithm

- Starts at random position, tries to improve match (minimize error) by
 - Adjusting parameters
 - Running Model
 - Recording error function
- Keeps on improving until reaches "local minimum" in error of fit
 - May add some randomness to knock out of local minima

Running Calibrations in Vensim: (Under Model/Simulate Commands)

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Optimization Control



Payoff Definition



The Pieces of the Elephant Example Model of Underlying Process & Time Series It Must Match



Single Model Matches Many Data Sources





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Example: Iteration & Calibration





From Sterman

Expanding the Boundary: Behavioral Feedbacks



From Sterman

Cumulative Cases



Pieces of the Elephant: STI







Hands on Model Use Ahead



Load Sample Model: SIR Agent Based Calibration

(Via "Sample Models" under "Help" Menu)

An Optimization Experiment in AnyLogic



Defining a Payoff Function Caveat: Non-Analytic, Non-Concave



Historic Data Captured via Table Function



Stochastics in Agent-Based Models

- Recall that ABMs typically exhibit significant stochastics
 - Event timing within & outside of agents
 - Inter-agent interactions
- When calibrating an ABM, we wish to avoid attributing a good match to a particular set of parameter values simply due to chance
- To reliably assess fit of a given set of parameters, we need to repeatedly run model realizations
 - We can take the mean fit of these realizations

Distinction

Replication/"Run": One realization

Particular random number seed

Iteration: Evaluation of a particular parameter set

- This can contain many realizations ("replications")

• Confusingly, the term "simulation" appears to sometimes be used for either of the above

Populating the Appropriate Datasets



Running Calibration in AnyLogic



Optimization Constraints – Tests on Legitimacy of Parameter Values



Optimization Requirements – Tests on Emergent results to Sense Validity

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Enabling Multiple Realizations ("Replications","Runs") per Iteration



Fixed Number of Replications per Iteration



Example



Terminates

Automatic Throttling of Replications Based on Empirical Fractiles for the Average of the Differences between Best and Current

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Enabling Random Variation Between Realizations ("Replications")



Understanding Replications: Report Results for Each Replication!



During First Several Realizations

("Replications", "Runs"), No Results Appear

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Run calibration	AnyLogic and this model is (c) XJ Technologies, www.anylogic.com. All rights reserved.
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Parameters ContactRate 1.75 InfectionProbability 0.45 Copy the best solution to the clipboard Copy In this applet OptQuest optimizer is used to calibrate an agent based model of epidemic spread developed with AnyLogic. In that model each person is represented as a active object (agent) with 4 possible states: Susceptible, Exposed, Infectious and Recovered (SEIR). Initially all but few people are susceptible, and few – exposed. A person can contact another person, and in case one is susceptible and another – exposed or infectious, the first may get infected with a certain probability. The objective is to find the parameters of the agents (contact frequencies and infection probabilities) so that the output of the simulation model fits best with the historical data (in this case – the dynamics of infectious population). As the model is stochastic, the optimization is done under uncertainty, and simulation replications	Historic data, best fitting and current simulation output
Run: 2 💟 Running Experiment: 0%	Simulation: 21% Q. 4.6 sec

Report on Iteration 1 Appears after a Count of Runs Equal to Replications per Iteration

Reports best payoff (objective) yet reached (lower is better), but from where did this number Come?



In this applet OptQuest optimizer is used to calibrate an agent based model of epidemic spread developed with AnyLogic. In that model each person is represented as a active object (agent) with 4 possible states: Susceptible. Exposed, Infectious and Recovered (SEIR). Initially all but few people are susceptible, and few - exposed. A person can contact another person, and in case one is susceptible and another - exposed or infectious, the first may get infected with a certain probability. The objective is to find the parameters of the agents (contact frequencies and infection probabilities) so that the output of the simulation model fits best with the historical data (in this case - the dynamics of infectious population). As the model is stochastic, the optimization is done under uncertainty, and simulation replications are used.

Experiment:

096

Run: 11 🕕

Paused



🧏 AnyLogic

Output



Average of Results for Replications is the Reported Score for the Iteration!

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