Mathematical Modeling I

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- There is no one modeling technique that is suitable for all problems.
- Different problems call for different approaches.
- Researchers should know a reasonable amount about many techniques, rather than very much about a single one.

Simulation vs. Analytic Results

- The ideal result of any mathematical modeling activity is a single, closed form formula that states in a compact way the relationship between the relevant variables of a system.
- Such analytical solutions provide global insight into behavior of the system.
- In real world these models are not realistic.
- In the vast of majority of cases, mathematical models in real world need to be solved numerically.
- The down side is that much of the beauty and generality of analytic results become lost when numerical results are used.

- This means that the relationship between variables, and how this depend on parameters, can no longer be seen directly from an individual solution, but must be inferred from extensive sweeps through the parameter space.
- Relative small models is often possible to explore the space of parameters, at least the space of parameters.
- This is a tedious exercise but can lead to robust insights.
- In many cases one find that there are only a few parameters that actually make a qualitative difference in behavior of the system.

- The sensitivity of the model to changes of parameters must be explored by the modeler.
- A common method for dealing with unknown parameters is to fit the model to measured data.
- A good fit with experiment is not sufficient but it is necessary.
- Results from fitted models have be treated with appropriate caution.

- There are situations in modeling when even numerical solutions cannot be obtained.
- This can be either because the system of equations to be solved is to complicated to even be formulated or because the modeling is not amenable to a mathematical description.
- Evolutionary systems are more expressed using rules(logic) rather than equations. eg. when born, then mutate.
- It is difficult to capture stochastic behavior using mathematical formulas. True, there are methods to estimate the statistical properties of stochastic systems using mathematical tools.

- Many of these problems can be addressed by computer simulations.
- Simulations can be powerful tools and are able to capture accurate models of nearly limitless complexity.
- In practice there is the problem of finding the correct parameters.

Two serious limitation

- Simulation models must be specified in a suitable form that a computer can understand-often a programming language.
- This process above takes time.
- Limitation in practical applications is that arising from run time requirements.

Simplification of a model

- A common approach is to remove spatial arrangements from consideration. perfect mixing, where it is assumed that every entity interacts with every other entity with equal probability.
- dimension of the model to add to complexity of the model.

Stochastic

(1) The insight that various phenomena in nature need to be described stochastically is deep rooted in many branches of physics; quantum mechanics or statistical physics are inherently about the random in nature.

(2) Stochastic thinking is even more important in biology.

(3) Mathematical and computational modeling are central to understand stochastic of systems.

(4) Nearly all systems in nature exhibit some sort of noise.

Deterministic

(1) Systems free of noise can be modeled by differential equations. The called deterministic models.

(2) Deterministic models are often a good strategy at the start of a modeling project.

Two vital ingredients for modeling

(1) Skill
(2) Technique.

Technique

(1) The ability to formulate a model mathematically, or
(2) to program computational simulation models

Skill

- The ability to ask the correct, field(biology, engineering, ...) question;
- to find the right level of abstraction that captures the essence of the question while leaving out irrelevant detail.
- One of the common misconceptions about modeling is the, More-detailed models are better models principle.

Why simplification is a virtue in modeling

- Modeler's ability to program/formulate detailed models is limited.
- Bigger models are not necessary better models.

A general success principle

- Start with a bare-bones model that contains only basic interaction in the system.
- If the predictions of this bare-bone model in any realistic or even relevant of reality then this is a good indicator that the model is too complicated and needs to be trimmed further.
- A bare-bone model is easy to analyze.
- Only when the behavior and the properties of the bare-bones model are fully understood should the modeler consider extending it and add more realism.

- Any new step of complexity should only be made when consequences of the previous step is well understood.
- The quality of the model is its ability to make predictions and levels of predictions.

Once the modeler has finished a model

- It is important for the modeler to give a detailed justification as why the model is relevant.
- All models are simplified version of reality.
- In practice, simplifying assumptions can sometimes become the sticking point for reviewers who will insist on better justifications.
- One possible way to justify particular modeling choices is to show that they do not materially change the result.
- If the modeler can demonstrate that a particular simplification barely makes any difference to the results but yields a massively simplified model , then this provides a strong basis from which one can pre-empt or answer referees' objections.

How to choose a useful model

- George Box: "Essentially, all models are wrong, but some are useful."
- It has been discussed already that a model that is correct, in the sense that it represents every part of the real systems, would be useless.
- Being "wrong" is not a flaw of a model but an essential attribute.
- There are many models that are, indeed, both wrong and useless.
- The question then is, how can one choose useful ones, or better, the most useful one from among all the possible wrong ones?

Classify Models

- Predictive.
- Explanatory.
- toy models.

Predictive Model

- Predictive models are primary used for the purpose of predicting the future behavior of a system.
- Predictive models must adhere to the most exact standards of rigor. There is no arguing with data.
- Predictive model is the most valid one; is some sense the most correct one.
- In practice predictions is useful, but is one criterion, not always the most important one, and never sufficient to make a model useful.

Predictive Model

- A well know class of models that are predictive, but otherwise quite uninformative, are the so called empirical formula.
- These are quite common in physics.
- Sometimes, these empirical models even make assumptions that are known to be completely incorrect, but they still used in some circumstances, simply for predicting certain values.

Explanatory Model

- Do explain reality in some way, and are very important in science.
- Primary purpose is to show how certain aspects of nature that have been observed experimentally can be made sense of.
- Explanatory models are predictive.
- There are explanatory models that do not predict reality correctly, especially in Biology, this is due to the chronic difficulty of measuring the correct parameters of systems. A quantification prediction is then often impossible. Settle for qualitative prediction.
- The main evaluation criterion for explanatory models is how well they illuminate a particular phenomenon in nature.

Explanatory Model

- prediction is one way to assess this, but another is the structural congruence between model and reality.
- Explanatory models are often used to ask whether a certain subset of ingredients is sufficient to explain a specific observed behavior.

Toy Model

- A subclass of explanatory models are "toy models".
- These are models that are primarily used to demonstrate some general principle without making specific reference to any particular system .

In summary

- There is no single criterion to assess the quality or usefulness of a model.
- In every modeling enterprize, the specific choices made to produce the model must be justified each time.
- Predictive power in a model is a good thing, but it is not the only criterion.

References

- David J. Barnes and Dominique Chu, Introduction to modeling for Biosciences, Springer 2010.
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