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Tools or Toys?

On specific Challenges for Modeling and the Epistemology of Models & Simulations in the Social Sciences

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- General Epistemology of Models
- Example: Simulations in Chemistry
- Opinions on Social Simulations
- The Difference, the Social Sciences make
- What we can do about it
- References

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1. The Epistemology of Models

The Role of Models in Science

Models are "Mediators" between Theory and Empirical Reality:

- **Theoretical Foundation**

  Models are derived from theories. They contain laws of nature from theories.

- **Semi-Autonomy**

  Models involve model building techniques not derived from background theories.

- **Target System**

  Models have target systems in the real world which they represent.

References: [MM99, Win03]

Sources of Credibility of Models:

- Credible background theory and background knowledge
- Well approved modeling techniques
- Successful empirical tests

Rules of Credibility

- Successful empirical tests trump background theory and modeling techniques
- The smaller the credibility of one source, the greater the strain on the others

"Same old stew"

Simulations are models (w.r.t. validation)

- Opacity?

Only the process of simulation is opaque not the algorithms.

- Computational process replaces deduction from axioms?

Models just as simulations are semi-autonomous.

- Temporal dynamics matter?

True, but introduces no new issues concerning the validation of simulation.

- Distinction between "in principle" and "in practice"?

What is possible "in practice" matters. But again, no difference to models.

References: [FR09, Hum04, Hum09]

Simulations are not experiments

- Simulations only yield results that are implied by background theories and simulation assumptions
- No causal influence from the target system on the results
- *Experimenta crusis* not replacable by simulations
- Only some experiments ("analog computations") replacable

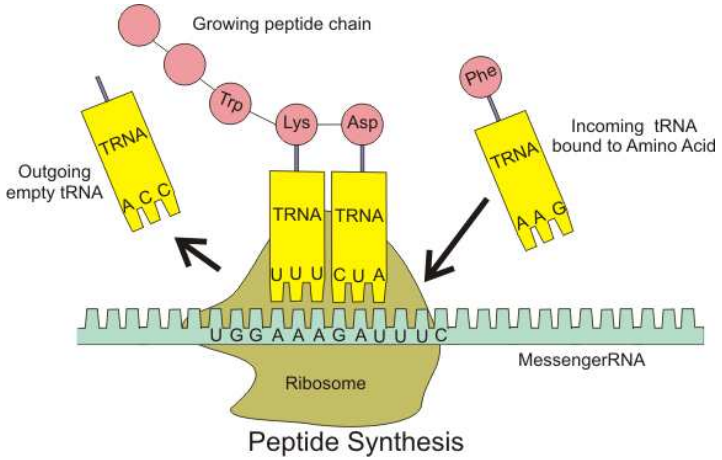
Therefore: Simulations – just like models or theories – belong to the theoretical side of science!

References: [Mä05, KL05, Win03, Mor09]

2. Example Case: Computer Simulations of Peptid Bond Formation in Chemistry

Acknowledgement: I'd like to thank Prof. Johannes Käster, Insitute of Physical Chemistry in Stuttgart, for explaining this type research to me!

Ribosomes: Protein Factories of Living Cells



The ribosome catalyzes the peptid bond formation between amino acids (image source: wikipedia)

Current research questions:

- How does the ribosome catalyze? Spatial arrangement or electrostatic influence?
- How does the reaction take place? (Different mechanisms imaginable)

Problem: Experiments can only determine the reaction energies!

References: [KS10, wik10]

Simultions of the ribosome

Approach

- QM/MM-simulations of the ribosome of the *thermus thermophilus* bacteria
- Multiple techniques for approximation and optimization to lower computing time

Results

- Electrostatic influence rather than spatial arrangement of molecules essential for catalysing the reation
- Two different reaction mechanisms possible, possibly both competing in nature

Confirmation?

- Activation energy found in simulations matches experimentally determined values
- Mismatch in one particular scenario, calling for explanation and giving rise to new research questions

References: [KS10]

Epistemological Reflections

- All three sources of credibility involved
- Powerful physical background theories exist
- Comprehensive prior knowledge about the ribosme
- Empirical data to test part of the simulation results
- Reliability of approximations and quality of experimental data may raise further questions

(Expert knowledge required to assess these)

References: [KS10]

3. The role of models & simulations in the social sciences

Brief overview of some recent accounts

Models & Simulations in the Social Sciences

Some striking, yet frequent features:

- Highly stylized and idealized
- Reliance on counterfactual or unrealistic assumptions
- Little or no empirical testing
- Few generalizable results
- Unclear epistemological role

"authors typically say very little about how their models relate to the real world" [Sug09, p.25]

References: [Sug09, Car09, Arn08, Sha05, GS94]

Accounts of Models in the Social Sciences

1. Predictive devices

But: Poor prediction qualitiy undermines this justification [Fri53, Bet06]

2. Quasi-Experiments

But: Epistemologically dangerous analogy [Mä05]

3. Isolating devices

But: Analogy limited if not misleading [Mä09, Car09, KL09]

4. Credible counterfactual worlds

But: Who determines the credibility? [Sug00, Sug09]

5. Incredible worlds

But: Strong robustness requirement [KL09]

6. Partial explanations

Good for a research design, but may not fit all modeling types [Ayd07]

7. Open Forumlae

Good for a research design, but may not fit all modeling types [Ale08]

8. Tools for conceptual exploration

Always possible fallback, but greater potential of modeling may be overlooked

No easy Solution:

Many diverse opinions, but no winner in sight

- Some of the accounts contradict each other sharply
- Most of the presented accounts relate to the same examples (e.g. Schellings neighborhood segregation model), so the incompatibility is serious
- Most of these accounts have some good reason on their side
- There is no obviously "better than all the others" account, although the "partial explanation" account seems a very strong contender.

4. Differences between the Social- and the Natural Sciences that are relevant for Modeling

Specific Features of the Social Sciences

Obstacles for Modeling?

- Lack of well confirmed background theories
- Pluralism of paradigms as a normal state
- Multiple and varying causes for the same effect
- "Wholistic" nature of social phenomena
- Difficulties of measurement and lack of quantitative data
- Pluralism of scientific styles

Lack of universal Background Theories

No empirically well confirmed background theories in the social sciences that fully cover the phenomena in their domain

(as for example Newtonian mechanics in physics).

Epistemological consequences:

- Theoretical validation insufficient, empirical validation needed
- Unknown unknowns more abundant

Unknown unknowns cannot be excluded on the grounds that they fall outside of what some theory allows. (In contrast, in Chemistry we could probably say: "Nothing can happen that quantum mechanics does not allow.")

Pluralism of Paradigms

Typical for the social sciences:
Pluralism of paradigms and multitude of competing theories

Example: In their book on the cuban misile crisis, Graham Allison and Philip Zelikow present three different paradigms, each of which encompasses a host of different theories and approaches, partly overlapping, partly contradicting and partly complementing each other [AZ99].

Epistemological consequences:

- **Phenomenological models better than theoretical models**

  For, theoretical models are more liable to merely reflect the presuppositions of the preferred paradigm.

- **Alternatives must be considered**

  The best way to avoid falling prey to the sugestiveness of one particular paradigm is consider things from the viewpoint of another paradigm.

Multiple and Varying Causes of the same Effect

Many important phenomena in the social sciences are characterized by the fact that they may be caused in many different ways (e.g. outbreak of war).

Epistemological consequences:

- A demonstrated "theoretical possibility" is just a single piece in the puzzle
- Parsimony: a vice, not a virtue
- Other "possible explanations" to be checked as well

Other possible explanations that cannot be rendered in a mathematical model should not silently be ignored.

"Wholism"

Social phenomena are often "wholistic". The effect of particular causes depends on the circumstances. There are usually no rules to determine the joint effect of several cuases.

Epistemological consequences:

- General conculsions regarding regularities or "capacities" cannot be drawn from models alone
- The use of the analytic method, i.e. breaking down a problem into its component parts is stronlgy limited.

References: [Ale08]

Difficulties of measurement

In the social sciences, many phenomena are notoriously difficult to isolate, experimentation is often not possible and many factors cannot be measured precisely.

Epistemological consequences:

- Greater strain placed on the robustness of models
- Simple models often the best choice

Increase a model's complexity only if this is rewarded by greater explanatory power as testified by comparison with measured data!

- Where measurement is not possible, modeling is not worthwhile

Models may give a false sense of understanding and precision where we really know nothing.

References: [Sha05, GS94, Hum04, Arn08]

Pluralism of Scientific Styles

Multitude of different scientific styles in the social sciences, e.g. thick narratives, stylized verbal descriptions, mathematical descriptions or hermeneutical methods.

Epistemological consequences:

- **Not only "models as mediators"**

  The "last mile" between model and the raw empirical material is typically some sort of narrative description.

- **Challenge of integrating models with other methods**

  The task of formalizing a verbal account is often highly non-trivial: Does the model really capture the essential aspects of the problem at hand? Does the formalized form still represent the verbal form? Etc.

- **Are models a reasonable option at all?**

  Should be evaluated before constructing a model.

5. Challenges and Responses

What modellers can do about it
and what philosophers of science should be aware of

Lessons for Modelers

Lessons for *problem orientated research*:

- Keep your options open: Evaluate other methods as well
- Choose wisely: If models do not work for your problem, try solutions without models.

Lessons for *method orientated research*:

- Choose the right problems for your method

i.e. problems where models work and their success can be tested.

- Keep in mind that your model needs to be validated empirically

Do not use unmeasurable parameters, mind the limits of measurement accuracy already at design stage.

- Validate your model, take failures seriously

A model that fails validation is wrong. A model that cannot be validated is unscientific.

References: [Sha05, GS94]

Lessons for Philosophers

Where modeling in the social sciences differs:

- Models "mediate" differently in the social sciences

On the theory side, there are only vage or non-unversal theories. On the empirical side models may need to link to narratives.

- Simulation-experiment analogy harder to justify

In natural sciences this analogy works (sometimes), because powerful background theories and comprehensive background knowledge allow conducting "computer experiments".

- Because of the lack of powerful background theories, empirical validation becomes even more important

- Philosophers should refrain from rationalising bad practices

If modelers themselves do not know, how their models relate to reality, then the most salient explanation is that their models are inappropriate.

Thank your very much for your attention :)

References

[Ale08] Anna Alexandrova. Making models count. *Philosophy of Science*, 75:383–404, July 2008.

[Arn08] Eckhart Arnold. *Explaining Altruism. A Simulation-Based Approach and its Limits*. ontos Verlag, Heusenstamm, 2008.

[Ayd07] N. Emrah Aydinonat. Models, conjectures and exploration: an analysis of schelling's checkerboard model of residential segregation. *Journal of Economic Methodology*, 14(4):429–454, December 2007.

[AZ99] Graham Allison and Philip Zelikow. *Essence of Decision. Explaining the Cuban Missile Crisis*. Addison Wesley Longman, 1999.

[Bet06] Gregor Betz. *Prediction or Prophecy? The Boundaries of Economic Foreknowledge and Their Socio-Political Consequences*. Deutscher Universitäts Verlag, Wiesbaden, 2006.

[Car09] Nancy Cartwright. If no capacities then no credible worlds. but can models reveal capacities? *Erkenntnis*, 70:45–58, 2009.

[FR09] Roman Frigg and Julian Reiss. The philosophy of simulation: hot new issues or same old stew? *Synthese*, 169:593–613, 2009.

[Fri53] Milton Friedman. The methodology of positive economics. In *Essays in Positive Economics*, chapter 1, pages 3–46. Chicago University Press, 1953.

[GS94] Donald P. Green and Ian Shapiro. *Pathologies of Rational Choice Theory. A Critique of Applications in Political Science*. Yale University Press, New Haven and London, 1994.

[Hum04] Paul Humphreys. *Extending Ourselves. Computational Science, Empiricism and Scientific Method*. Oxford University Press, 2004.

[Hum09] Paul Humphreys. The philosophical novelty of computer simulations. *Synthese*, 169:615–626, 2009.

References

[KL05] Günter Küppers and Johannes Lenhard. Validation of simulation: Patterns in the social and natural sciences. *Journal of Artificial Societies and Social Simulation*, 8(4):3, 2005.

[KL09] Jaakko Kourikoski and Aki Lethinen. Incredible worlds, credible results. *Erkenntnis*, 70:119–131, 2009.

[KS10] Johannes Kästner and Paul Sherwood. The ribosome catalyzes peptide bond formation by providing high ionic strength. *Molecular Physics*, pages 1–14, 2010.

[MM99] Mary S. Morgan and Margaret Morrison, editors. *Models as Mediators. Perspektives on Natural and Social Science*. Cambridge University Press, 1999.

[Mor09] Margaret Morrison. Models, measurement and computer simulation: the changing face of experimentation. *Philosophical Studies*, 143:33–57, 2009.

[Mä05] Uskali Mäki. Models are experiments, experiments are models. *Journal of Economic Methodology*, 12(2):303–315, June 2005.

[Mä09] Uskali Mäki. Missing the world. models are isolations and credible surrogate systems. *Erkenntnis*, 70:29–43, 2009.

[Sha05] Ian Shapiro. *The Flight from Reality in the Human Sciences*. Princeton University Press, Princeton and Oxford, 2005.

[Sug00] Robert Sugden. Credible worlds: the status of theoretical models in economics. *Journal of Economic Methodology*, 7(1):1–31, 2000.

[Sug09] Robert Sugden. Credible worlds, capacities and mechanisms. *Erkenntnis*, 70:3–27, 2009.

[wik10] wikipedia. Ribosome, May 2010.

[Win03] Eric Winsberg. Simulated experiments: Methodology for a virtual world. *Philosophy of Science*, 70:105–125, January 2003.