Validation levels and standards depending on models types and functions

J. Raimbault[1,2,3,*]

[1] CASA, UCL
[2] UPS CNRS 3611 ISC-PIF
[3] UMR CNRS 8504 Géographie-cités

[*] juste.raimbault@polytechnique.edu

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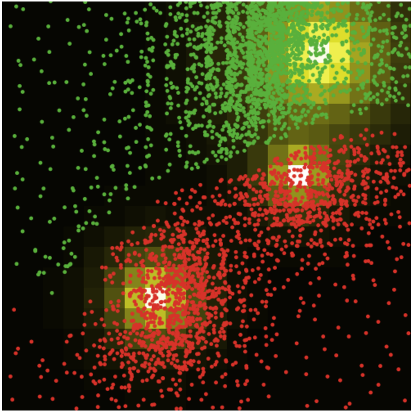
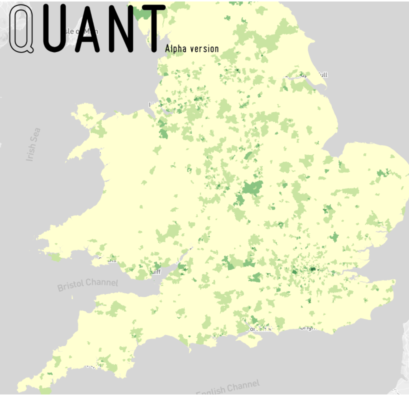


Schelling model (toy model)



Quant model (operational models)

Proposed definition: *increasing the confidence in a model to fit its purpose*

Depends on:

- model nature/type
- model purpose
- discipline
- particular problem or application case
- expected standards
- background or mood (!) of the reviewer/reader/listener
- ...

Model validation

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→ Validation has very different implications depending on epistemological positioning: from an objective procedure (reductionism) to a more conversational and reflexive process (holistic) [Barlas and Carpenter, 1990]

→ How disciplines are positioned, political relations, effective citation practices, etc. are all aspects of implicit "social" model validation

In geosciences (hydrology e.g. [Legates and McCabe Jr, 1999]), quantitative agreement between model and data

→ choice among numerous indicators to quantify the agreement

→ robust indicators? choice can be validated itself

In practice, not systematically done, as for example for land-use change models [van Vliet et al., 2016]

Microsimulation models enter a similar context (e.g. [Park and Schneeberger, 2003] for the Vissim traffic model), in a slightly different way than agent-based models

Statistical models

Statistical models exhibit different measures of “model quality”:

- predictive power (explained variance)
- p-value (alpha errors) and beta power (false positives)

Following [Saltelli, 2019], mathematical modeling may benefit similar standards as in statistics

Analytical models

$\rightarrow$ to what extent of analytical resolution is a model "validated"? (limit theorem, restricting assumptions, unfeasible ranges in practice, ...)

$\rightarrow$ finally most of the time coupled with numerical simulation? see coupling of machine learning and mathematical modeling [Butler et al., 2018] or statistical inference [Bzdok et al., 2018]

$\rightarrow$ computational turn of science [Arthur, 2013]?

On the link with simulation models:

- Formal proof systems remain limited
- Undecidability of the Turing machine Halting problem

Simulation models

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Overview of simulation model validation methods and processes by [Sargent, 2010]

1. independent validation and verification (modelers as cognitive agents [Giere, 1990]
2. iterative process between conceptual, computerized models, and the system itself
3. Numerous validation techniques: comparison, extreme conditions, historical data, internal validity, sensitivity analysis, predictive performance, Turing test
4. Specific techniques for operational validity
5. Documentation of the validation process is crucial
6. Accreditation: science as a social process

[Landry et al., 1983] similar in operations research

Simulation models as generative models

Simulating the evolution of a system in a generative way: [Epstein and Axtell, 1996]: "*if you did not grow it, you did not explained it*"

→ similar to *Pattern Oriented Modeling* [Grimm et al., 2005]: reconstruct (macro) patterns from the bottom-up

Implications for validation:

- Crucial role of indicator choice (see e.g. link prediction vs. network structure reconstruction)
- fine understanding of model behavior
- role of processes and parameters
- controlled experiments (*virtual laboratories*)

→ typical example of **explication/comprehension** models (but which can also be statistical, analytical)

→ Sensitivity analysis is part of a model validation process [Saltelli et al., 2010]: how does a model behave in response to variations in its parameters/variables/input data?

→ Articulation of complementary methods [Cariboni et al., 2007] (validation is then the full cascade of successive methods applied)

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Design of Experiments

	Coverage	Interpretability	Budget
One factor at a time	✗	✓	✓
Complete plan	✓	✓	✗
LHS/Sobol	✓	✗	✓

Sensitivity analysis

	Coverage	Interpretability	Budget
Morris	✗	✓	✓
Saltelli	✓	✓	✗

Model exploration is running a simulation model, following a *design of experiments*, to gain knowledge about *model properties*.

e.g. : sensitivity analysis

Recent and significant increase in the development of methods to explore, calibrate and optimize (geo)simulation models.

→ part of model validation also

Explicative / comprehensive models are mostly made useful by their exploration

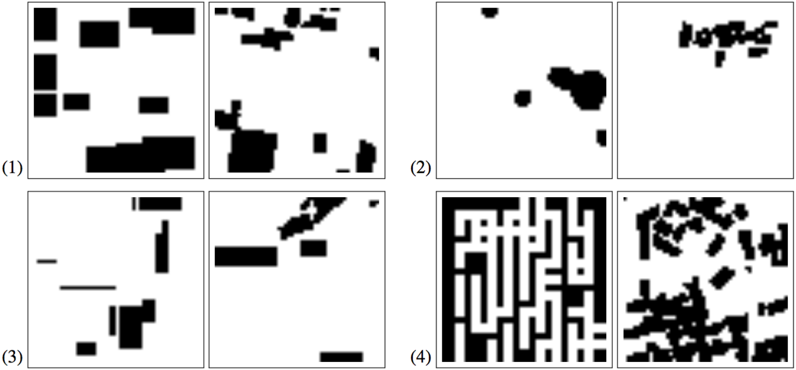
Example of validation methods included in OpenMOLE:
Calibration: Evolutionary (GA) and Bayesian (ABC) methods

Diversity Search: unveil the variety of obtainable patterns in output space: can the model produce unexpected patterns, and if so what does it means for its mechanisms ?

Origin Search: inverse problem, tackling the problem of equifinality

Spatial sensitivity analysis techniques

Example: generators of synthetic urban districts [Raimbault and Perret, 2019]



$\rightarrow$ Validation of submodels to foster diverse questions and approaches

$\rightarrow$ Validation of coupled models remains an open question (e.g. error propagation techniques)

$\rightarrow$ Comparison of the model with alternative formalisms: for example agent-based modeling against differential equations

$\rightarrow$ Importance of systematic model benchmarks/classifications

Validation and model functions

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Varenne's model function families [Varenne, 2017]:

- **Perception and observation**: perception medium, visualization, experimental medium
- **Understanding**: description, prediction, explication, comprehension
- **Theory construction**: interpretation of a theory, test of internal coherence, applicability, co-computability
- **Communication**: scientific communication, stakeholders involvement
- **Decision-making**: planning, decision-making, self-fulfilling system prescription

Validation and model functions

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- **Perception and observation**: how much information is extracted
- **Description**: how much information is contained within
- **Prediction**: predictive power (quantitative indicators or qualitative behavior)
- **Explication and comprehension**: how much of the causal structure of the system is grasped
- **Theory construction**: how does the model contributes to the theory, to coupling of its components (e.g. medium for interdisciplinarity)
- **Communication**: how much information is conveyed and to which agents
- **Decision-making**: how are decision supported, which benefits and for what dimension (societal, environmental, etc.)?

Validation and model type

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- **Statistical**: model fit/statistical power
- **Machine learning**: predictive power
- **Analytical**: level of resolution, genericity
- **Simulation/generative**: model behavior, sensitivity analysis, pattern reconstruction, causal processes
- **Operational**: planning/decision-making relevance
- ...

Rq: classification of "model types" can neither be exhaustive nor consistent

- Acceptance and impact within the discipline/specific subject of study
- Impact in other disciplines
- Impact outside of science
- Interdisciplinary/bridging/integrative role [Raimbault and Pumain, 2019]
- Different dimensions: complex and multidimensional nature of scientometrics [Raimbault and Pumain, 2019] [Cronin and Sugimoto, 2014]
- ...

Epistemological foundations of a knowledge framework for integrated approaches to complex systems [Raimbault, 2017], coined by [Raimbault and Pumain, 2019] as **Applied Perspectivism**:

Giere's cognitive approach to science [Giere, 1990] : cognitive agents have *perspectives* on aspects of the real world.

Scientific perspectivism [Giere, 2010] : *cognitive agents* use *media*, the models, to represent something with a certain purpose.

[Varenne, 2017]'s classification of main model functions : perception and observation, understanding, theory building, communication, decision making.

Knowledge domains

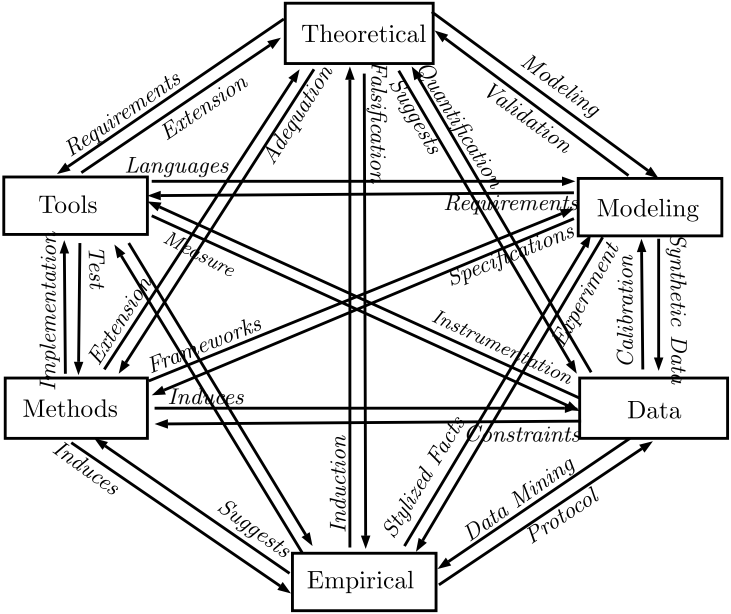
Definition of Knowledge Domains :

- **Empirical.** Empirical knowledge of real world objects.
- **Theoretical.** Conceptual knowledge, implying cognitive constructions.
- **Modeling.** The model as the formalized *medium* of the perspective.
- **Data.** Raw information that has been collected.
- **Methods.** Generic structures of knowledge production.
- **Tools.** Implementation of methods and supports of others domains.

Description of the Knowledge Framework :

1. Any scientific knowledge construction on a complex system can be understood as a perspective, decomposed into knowledge domains.
2. Contents within domains *coevolve* [Holland, 2012] between themselves and with other elements of the perspective (including cognitive agents and the purpose).
3. It implies weak emergence [Bedau, 2002] what is consistent with the existence of bodies of knowledge.

Interactions between domains



Validation within the knowledge framework

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→ Role and type/method of validation are proper to each perspective

→ Links and interaction between domains are part of the model/theory construction process and thus of validation of the perspective

→ Intrinsically iterative nature of validation

→ Cannot be dissociated (at least for the study of complex systems) to new methods and tools

Conclusion

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→ Meaning of "model validation" is indeed strongly dependant on its properties, including type, function, context of application, discipline

→ *Obvious?* Not for all seeing some debates/questions here and there. **Interdisciplinarity requires an opening to other standards/definitions/viewpoints**

→ Validation within the Applied Perspectivism knowledge framework: validation proper to each perspective and to the coupling of perspectives, intrinsically iterative

→ Construction of integrative theories and models implies this multiple view of model validation and the variety of methods and tools, in particular in the case of simulation models

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