

The Hidden Model Problem: When a Good Fit Becomes a Mechanism and an Optimum

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Abstract

A model can describe observed data accurately without uniquely identifying the mechanism that generated them. Flexible models can fit several competing explanations; empirical parameters can absorb multiple physical effects; and an optimum computed from a fitted surface can lie in a region where the experiment provided little information. The hidden model problem begins when descriptive success is promoted into mechanistic truth or when a mathematical optimum is treated as a physical optimum without checking model adequacy, parameter identifiability, uncertainty and domain. This methodological article separates representation, interpolation, prediction, mechanism and optimisation. The central proposition is that fit is evidence about the relation between a model and a dataset, not automatic evidence that the model's internal story is true.

Keywords: model; mechanism; goodness of fit; identifiability; extrapolation; optimization; response surface; prediction; parameter

1. Purpose and evidence boundary

HEB-001 distinguishes pure error from lack of fit and places model validation after measurement qualification and replication [1]. HEB-013 develops the epistemic boundary between useful representation and mechanistic claim.

2. A fitted equation has several possible roles

An equation can summarise data, interpolate within a region, predict future observations, estimate a parameter with physical meaning, or represent a proposed mechanism. These roles have different evidence requirements. A polynomial response surface can be valuable for local optimisation while making no claim that the underlying system is literally polynomial.

3. Goodness of fit is not uniqueness

Two different models can fit the same finite dataset similarly well. A high coefficient of determination or small residual sum of squares therefore does not show that one mechanism is uniquely supported. Discrimination requires predictions or interventions on which the competing models differ.

4. Parameters can be non-identifiable

When parameters are strongly correlated, several combinations can produce nearly the same curve. The fitted values may look precise because software returns digits, yet the experiment may not have independently constrained them. Parameter uncertainty and correlation are therefore part of interpretation, not optional diagnostics. NIST/SEMATECH treats parameter uncertainty, correlation and model diagnostics as distinct parts of regression analysis [2].

5. Residuals test the representation, not the story

Residual structure can reveal curvature, heteroscedasticity, missing interactions or time dependence. Random-looking residuals support adequacy of the representation within the observed domain, but they do not prove the mechanistic interpretation of each term. A model can be empirically adequate and mechanistically wrong.

6. Interpolation and extrapolation are different acts

Within a densely sampled region, a fitted model can interpolate with bounded uncertainty. Outside that region, the result depends increasingly on the assumed functional form. Extrapolation should therefore be labelled explicitly and challenged against physical limits, alternative models and new measurements.

7. Model-based optima are conditional

An optimum is defined by the chosen response, constraints, model and domain. Changing any of them can move the optimum. In multi-response problems, the result is often a compromise region rather than one privileged point. A mathematically stationary point is not automatically robust to experimental noise or model uncertainty. Mixture-model optimisation makes this dependence on model and constrained domain explicit [3].

8. Mechanism requires perturbation

Mechanistic confidence increases when changing a variable predicted by the mechanism produces the expected specific response while plausible alternatives fail. Correlation alone is weak because hidden variables can generate the same pattern. The most informative experiment is often one designed to separate competing models rather than to improve the fit of the preferred one.

9. Physical constraints are valuable but not magical

Conservation laws, bounds, symmetry and known monotonicities can reduce implausible models. Yet a constrained model can still be incomplete. Physical plausibility is a filter on inference, not a substitute for discriminating evidence.

10. Practical model discipline

State the model's role, fitting domain, parameter meanings, uncertainty, residual behaviour and extrapolation boundary. Compare plausible alternatives where the conclusion depends on model form. Validate predictions on data not used to fit the model when feasible. For optimisation, verify the predicted region experimentally and test robustness around it rather than publishing only the computed maximum.

11. Equifinality: different mechanisms can produce the same observable

Many physical systems are equifinal: distinct causal routes lead to similar final measurements. A decrease in conversion can arise from lower delivered light, stronger inhibition, different photoinitiator efficiency, attenuation, temperature or composition; a dimensional error can arise from cure spread, shrinkage, mechanics or measurement bias. Fitting one mechanistic model to the final response does not eliminate these alternatives. ER-184 treats competing defect mechanisms explicitly and accepts unresolved attribution as a legitimate outcome [4]. HEB-013 generalises that discipline: when several mechanisms predict the same observable, the experiment must add a discriminating measurement rather than award truth to the best-fitting narrative.

12. Overfitting can hide behind excellent residuals

A sufficiently flexible model can follow noise and local idiosyncrasies in the calibration data. Training residuals then shrink while predictive performance deteriorates on new observations. The cure is not one universal complexity penalty; it is separation between model construction and model challenge. Hold-out validation, replicated confirmation runs, pre-specified model forms or external datasets can all test whether apparent structure generalises. A model that cannot survive data it did not help explain is a weak basis for mechanism or optimisation.

13. Prediction and explanation should be evaluated separately

A black-box empirical model can predict well within a bounded domain without offering a convincing physical mechanism. A mechanistic model can explain qualitative behaviour while remaining too uncertain for precise prediction. These are different scientific achievements. Confusion arises when predictive accuracy is used as proof of mechanism or when mechanistic plausibility is used as proof of quantitative prediction. Reports should state which role matters to the decision and evaluate the model against that role.

14. Conclusions

A model earns trust by surviving appropriate tests, not by looking smooth or fitting closely. Good fit supports representation within a declared domain; mechanism requires discriminating evidence; extrapolation adds assumptions; and an optimum is conditional on the model and objective. The hidden model problem is controlled when mathematical convenience and physical claim remain explicitly separated.

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Knowledge boundary

HEB-013 owns the general distinction between fit, prediction, mechanism and model-based optimisation. Application-specific mechanistic models and qualification criteria remain with their relevant ERs.

Limitations

This methodological article is a bounded synthesis of the controlled HEB and Engineering Review corpus. It does not report a new experimental dataset, does not establish universal numerical thresholds, and does not convert examples from one domain into application-wide specifications. Claims that require application-specific qualification remain with the corresponding technical review or primary study.