

Appendix: Modelling checklist

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Stating the objectives

1. Have you stated clearly and explicitly the objectives of the research and the reasons for doing it?
2. Have you translated these objectives into precise questions that the research may be expected to answer?

Relevance of Modelling

3. Are you satisfied that modelling of some part of the system through a formal statement of relationships in physical or mathematical terms will help in the achievement of the objectives of the research?
4. Are sufficient accurate data available to allow models to be tested? If not, can such data be collected?
5. Are the relationships envisaged by this research complex in the sense that they involve feedback and non-linearity?
6. Is the model intended to provide a simulation of the natural system for further experimentation and as a synthesis to guide further research?
7. Is the model intended to help with the making of decisions about the natural system?
8. Is the model intended to integrate and test the compatibility of information about the system which has already been collected?
9. Do you have any doubts about the feasibility of modelling the system which relates to the research objectives?
10. If so, have you consulted someone with modelling expertise in your field of research in order to confirm the feasibility of the modelling approach to your particular problem?
11. Have you estimated the time and cost of producing models and established that the requisite resources are available?

Word model

12. Have you identified and defined the boundaries of the problem and of the system to be modelled?
13. Have you written a verbal description of the assumed relationships between the various entities of the problem, using the simplest language possible?

14. Has this verbal description been seen by a cross-section of appropriate experts and been agreed by them as an adequate description?
15. Does the verbal description identify the parameters which you consider to be essential to the solution of the problem and give some preliminary indication of the relative importance of these parameters?
16. Does the verbal description give any indication of possible qualitative solutions which might subsequently be compared with the quantitative solutions to be derived from modelling?
17. Have you translated the relationships described in the word model into diagrams, using one of the established conventions for such diagrams?
18. Have you identified distinct sub-systems in the problem which can be examined separately, but which need to be connected together?

Dynamic models

19. Have you considered the possibility of modelling the relationships described in the word model by one or more differential or difference equations?
20. Have you identified the necessary input, state and output variables for such equations?
21. Have you identified the appropriate time steps for the solution of the equations?
22. Does the word model make explicit the non-linearity of the relationships between the model parameters?
23. If not, are there some alternative ways of expressing this non-linearity which you would like to test?
24. Do the equations express the necessary degree of feedback to meet the requirements described by the word model?

Matrix models

25. Have you considered the formulation of the model in terms of a matrix or matrices?
26. If so, do any of the well-known matrix formulations meet the requirements described by the word model? Does the matrix notation simplify the mathematical presentation and solution of the problem?
27. Do eigenvalue and eigenvector solutions of the component matrices define properties of the model which are relevant to the solution of the original problem?

Markov models

28. Does a Markov model, as a special type of matrix model, have any application in the solution of the original problem?
29. If so, do you have any appropriate procedure for estimating the probabilities for the transitions from one state to another?
30. Does the model have closed states, i.e. is it an absorbing Markov chain?
31. If so, are you concerned to estimate the absorption times and probabilities?
32. If the model does not have absorbing states, i.e. is an ergodic Markov chain, are you concerned to estimate the limiting probabilities and the mean passage times from one state to another?

Stochastic models

33. Does the model formulation envisaged by the word model require the introduction of stochastic elements?

34. If so, can these stochastic elements be estimated for non-linear relationships?
35. Does the model require the estimation of several variances?
36. If so, do you know how to structure the collection of data so as to obtain unbiased estimates of those variances?
37. Can your model be structured so as to make use of the well-tested methods of least-squares estimation, e.g. analysis of variance or multiple regression analysis?
38. Are the estimates of the parameter values derived from your model independent of each other?

Multivariate models

39. Does your word model envisage the simultaneous evaluation of many variables or attributes?
40. If so, is the main purpose of your model to derive the most parsimonious representation of the variables in multivariate space, and a subsequent ordination of the model elements in the essential dimensions of that space?
41. Is the main purpose of your model to discriminate between *a priori* groupings of the model elements, and to allocate new elements to those groupings?
42. Is the main purpose of your model to find discontinuities in the multivariate space required to describe the variation of the model elements, and so to perform a cluster analysis of those elements?
43. Is the main purpose of your model to investigate the relationships between two or more groups of variables, for example by canonical correlation analysis?

Optimization models

44. Can the essential criteria of the word model be expressed in terms of game theory?
45. If so, can you evaluate the outcomes of the various strategies which are available to the opponents in the game model?
46. Does a saddle-point exist in the choice of strategies, i.e. a single strategy for each opponent which should always be played?
47. If not, what combination of strategies represents the optimum response to the conflict of issues between the opponents?
48. Can the search for an optimum strategy be developed within the constraints of a mathematical programming model?
49. If so, can the objective function and the constraints be expressed as linear equations or inequalities?
50. If either the objective function or the constraints have to be expressed as non-linear equations or inequalities, does an appropriate method of solution exist?
51. Does the search for an optimum solution have to take into account the need to retain the widest possible range of options for future solutions, i.e. indicate the need for a dynamic programming solution?

Catastrophe theory

52. Does the word model indicate any of the useful properties of catastrophe theory models, i.e. bimodality, discontinuity, hysteresis and divergence?
53. Can the delay in the jump from one state of the system to another, i.e. the

hysteresis, be expressed as a crossing of a singularity in the catastrophe surface?

54. Can the divergence between the outcomes of changes in the control variables be shown to arise from paths on either side of a catastrophe manifold?

Sensitivity analysis

55. Will you test the sensitivity of your model to small changes in the basic parameters of the model?
56. If so, will marked differences in the sensitivity of the output variables to these small changes help to identify those variables for which increased precision of estimation is desirable?
57. Will the sensitivity analysis be extended to the simultaneous alteration of parameters and coefficients so as to test the interaction of such changes?
58. Are you aware of the experimental designs which enable such tests to be made efficiently and without bias?
59. Will the sensitivity analysis be incorporated as a regular feature of the modelling procedure from the very beginning?
60. Will the sensitivity analysis identify any discontinuities in the performance of the model which would limit the practical use of the model?

Verification

61. Will you develop several models simultaneously, preferably from different model families, so that you can compare the output from the models under broadly comparable conditions?
62. Will these models behave in a way which fits broadly with your expectations?
63. If not, is this likely to be because of some fault with the model(s)?
64. Is it possible that the real system which you are seeking to model behaves in a counter-intuitive way?
65. Will verification of the model suggest any improvements which could be made to the research and to the modelling procedure?

Validation

66. Have you established which data are to be used in your model and ensured that independent data will be used to test the validity of your model?
67. Will the model which you construct suggest any explicit tests of hypotheses which might be made on the real system?
68. If so, are any of these tests critical in the sense that they significantly advance the research towards the originally-defined objectives.
69. Are you aware of the experimental designs which may improve the efficiency of these tests of the real system?

Computing

70. Have you investigated the computer facilities which are available to help with the modelling of your problem?
71. Do these facilities include any special-purpose modelling languages?
72. If so, have you investigated the applicability of these languages to your particular problem?
73. Are you intending to use a general-purpose computer language (e.g. BASIC, FORTRAN, APL, ALGOL) for the modelling of your problem?

74. If so, have you enquired about the existence of subroutines and algorithms which might simplify the task of programming your application?
75. Does the computer you intend to use provide for interactive facilities. e.g. through a computer terminal?
76. If not, is the time between submitting a request for a run and receiving the results short enough to allow you to make progress with the modelling task, i.e. less than 1–2 hours?

Exploration of model

77. When one or more models are complete, have you planned the uses of the models and the exploration of the consequences of changes in the input variables?
78. If so, are you aware of the experiment designs which may considerably simplify the exploration?
79. Have you thought through the possible uses of the simulation you hope to achieve?

Documentation

80. Have you provided for adequate documentation of the various stages of the modelling so that other research workers can benefit from your experience?
81. Have you planned the form of publication of the results of the modelling so that these results will be useful to decision-makers and administrators (if appropriate) as well as to scientists?

The final (and most important) question

82. If you are in any doubt about the purpose of any of the questions in this checklist, should you not obtain some advice from a modeller with experience of your field of research before continuing?

There is usually little that an expert advisor can do to help you once you have committed yourself to a particular approach.

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Index

- Aberdeen, 19
- Absence, 10, 11, 21, 50
- Absorption, 46
- Achnashellach, 19
- Age structure, 40
- Agriculture, 16
- Airborne sulphur, 12
- Alcohol, 22
- Algebra, 9, 33–36, 41, 46
- ALGOL, 61
- Algorithm, 8, 30, 52, 55, 61, 62, 64
- Ambleside, 19
- Ammophila arenaria*, 20
- Analogue, 7, 41
- Analysis of variance, 19, 22, 43, 44, 45
- Animal, 27, 31, 40, 42
- APL, 61
- Arenicola marina*, 53
- Arithmetic, 33, 34, 62
- Array, 35
- Association, 48
 - analysis, 50

- Bacteria, 17, 23
- BASIC, 56, 61, 62
- Beetle, 15
- Bimodality, 20, 21, 56
- Binomial distribution, 43
- Biology, 31, 39, 41
- Biological process, 31
- Biomass, 27, 31
- Birmingham, 19
- Bog, 13, 17
- Bognor Regis, 19
- Boolean, 35, 36
- Bounding of problem, 25, 26, 27
- Broom, 51

- Calcium, 53
- Calculation, 7, 29, 40, 46, 48, 59, 62, 63
- Calculus, 7, 27, 34, 36
- Calluna*, 13
- Cambridge, 19
- Canonical analysis, 47
 - correlation, 52, 53
 - variate, 47, 52
 - variate analysis, 47, 52
- Cardiff, 19

- Carrying capacity, 10, 11, 17
- Cartesian product, 35
- Catastrophe theory, 21, 36, 37, 56, 57
- Chemical, 39
- Chi-square, 43
- Classification, 49
- Climate, 15, 17, 45
- Climatology, 27
- Cluster analysis, 47, 48–50
- Coefficient, 11, 27, 48, 49, 51, 55, 66, 68
- COMAL, 61
- Communication, 16, 29, 38, 63, 64
- Compatibility, 16, 21, 23
- Competition, 15, 16, 19, 21
- Complexity, 8, 15, 16–21, 25, 28, 34, 41
- Computation, 8, 41, 52, 56, 60, 63, 64
- Computer, 8, 21, 29, 30, 35, 36, 37, 39,
 - 54, 56, 59–64
- Conceptual, 8, 30, 65–67
- Confidence, 44, 51, 67
- Consistency of data, 21
- Constant, 10, 11, 15, 17, 27, 29, 30, 34,
 - 35, 40, 42, 45
- Convergence, 46
- Corophium volutator*, 53
- Correlation, 47, 48, 49, 52, 53
- Covariance, 22
- Crop species, 16
- Crucianella maritima*, 20
- CSMP, 61
- Cumbria, 49
- Curve, 35, 66, 67
- Cusp, 57
- Cycling, 38, 41

- Data bank, 21
- Data-base, 63
- Decision-making, 23
- Decomposer, 31
- Definition
 - model, 7, 10
 - objectives, 68
 - parameters, 27
 - population, 27
 - problem, 25, 26, 28, 55
 - sample, 27
 - state variable, 27
 - variable, 46

- Definition *cont.*
 variate, 46
 Dendrogram, 49, 50
 Dependent, 11, 43, 45
 Dependent variable, 27, 56
 Deposition, 12, 49
 Descriptive model, 47, 50
 Desert, 20
 Design
 experimental, 16, 19, 45, 66, 68
 model, 39, 62
 Deterministic, 39, 40, 41
 exponential model, 40, 41
 Detritus, 31
 Deviation, 11, 12
 Diagram, 28, 29, 30, 38, 49
 Differential calculus, 27, 34
 equation, 10, 34, 35, 41
 Differentiation, 34
 Dimension, 7, 9, 16, 21, 22, 36, 47, 48
 Discontinuity, 17, 20, 21, 28, 38, 56, 67
 Discriminant analysis, 47
 coefficient, 51
 function, 51, 52
 Disease, 57
 Distribution, 42, 43
 model, 42
 Divergence, 20, 21, 56, 57
 Dover, 19
 Driving variable, 27, 28, 29, 38, 67
 Dry matter production, 17, 18, 19, 29
 Durham, 19
 Dynamic
 interactions, 15
 model, 36, 37–39, 41
 populations, 21
 processes, 41
 programming, 55, 56
 simulation, 53
 Dynamics, seasonal, 27
 DYNAMO, 61

Echinops spinosissimus, 20
 Ecosystem, 16, 27, 41
 Eigenvalue, 48, 49, 52
 Eigenvector, 48
Elymus farctus, 20
 Enchytraeid worm, 16
 Energy, 30, 31, 37, 41, 60
 Environment, 7, 15, 16, 23, 43, 53, 54, 56
 Environmental change, 40
 impact, 23, 56
 management, 16
 planning, 56
 Equalities, 33
 Equation, differential, 10, 34, 35, 41
 Equilibrium, 13

Euphorbia paralias, 20
 Exogeneous variable, 29
 Experiment, 8, 16, 19, 23, 38, 40, 45, 55,
 63, 66, 67, 68
 Experimental design, 16, 19, 45, 66, 68
 Exponential growth, 10, 17, 18, 38, 40
 Expression, 7, 10, 28, 30, 34, 37, 39, 45,
 46, 54, 67
 Extractable ion, 50
 Extrapolation, 66, 67

 Factorial model, 44, 45
 Families of models, 22, 36, 38, 39, 41,
 65, 68
 Fecundity, 40
 Feedback, 9, 15, 17, 19, 28, 31, 37, 38, 68
 Fertilizer, 45
 Fitting curves, 67
 Flour, 16
 Flow, 29, 30, 31, 41
 charts, 29
 energy, 41
 Forests, 41
 Forestry, 16
 FORTRAN, 61
 Frequency, 42, 43, 46, 51

 Game theory, 37, 56
 Geometry, 7, 34, 36, 50
 Goal, 26, 27, 36
 Goodness of fit, 43
 Graph, 30
 Graphical method, 54, 55
 Grasshopper, 51
 Grazing, 13, 27
 Grid co-ordinate, 12
 Growth, 10, 15, 17, 19, 21–23, 38, 40, 60

 Habitat, 13, 15, 16
 Harmonic, 34
 Harvesting, 40, 41
 Heat, 31
 Heath, 13
 Hierarchy, 26, 49
Hydrobia ulvae, 53
 Hypothesis, 16, 21, 23, 38, 42, 68
 Hysteresis, 20, 21, 56

 Immigration, 40
 Impedence, 30
 Independent, 13, 15, 22, 27, 34, 35, 42,
 44, 45, 48, 68
 variable, 27, 34, 35
 Indices, 34, 48, 50
 Industrial system, 29
 Inequality, 33, 34, 54
 Information, 8, 9, 16, 21, 23, 26, 29, 30, 31

Input, 29, 38, 41, 47, 48, 63
 variable, 38
 Insect, 57
 Integral, 35
 calculus, 34
 Integration, 16, 21, 23, 34
 Interaction, 10, 15, 16, 17, 19, 23, 28, 38,
 44, 66, 68
 Interference, 22
 Invertebrate, 43, 53

 Junction, 30

 Lake, 43
 Lake District, 50
 Land use, 16
 Language, 7, 8, 9, 15, 27, 31, 33, 60, 61,
 62, 64
 Leaf, 22, 42
 Life cycle, 41
 Line-printer, 59
 Linear, 11, 17, 19, 28, 34, 44, 45, 47, 48,
 51, 54, 55
 expression, 34
 model, 44, 45
 objective function, 55
 programming, 54, 55
 stochastic model, 51
 Logic, 10, 29, 40, 53, 60, 67
 Logistic, 10, 17, 18, 38
 growth function, 17
 London, 19
 Loss of ignition, 50, 53

Macoma balthica, 53
 Management, 16, 26, 27, 41, 45, 46, 54,
 55, 68
 Manchester, 19
 Map, 18, 42
 Markov, 13, 41, 45, 46
 Material flow, 30
 Mathematical model, 7, 8, 28, 29, 35–39,
 42, 43, 53
 Mathematical programming, 54, 56
 Matrix, 35, 36, 39, 40, 41, 45, 46, 48, 52
 Matter, dry, 17, 18, 19, 29
 Measurement, 12, 22, 43, 46, 47, 51
 Median, 19, 20
 Metaphysics, 68
 Meteorology, 27
 Micro-processor, 60
 Minimum spanning tree, 50
 Model families, 22, 36, 38, 39, 41, 65, 68
 Moisture content, 20
 Morecambe bay, 53
 Multiple linear regression, 11
 Multiple regression, 12

 Multivariate analysis, 21
 Multivariate model, 22, 37, 46, 47, 48,
 50, 52
 Mythology, 68

 Natural resource, 55
 Nature, 56, 68
Nephtys homerbergii, 53
Nereis diversicolor, 53
 Newton, 7
 Nitrogen, 50, 53
 Non-linear, 9, 17, 19, 28, 37, 38, 45, 55
 Normal distribution, 43–45
 Northern England, 19
 Notation, 8, 31, 33–36
 Nutrient, 27, 41

 Objectives, 25, 26, 27, 36, 46, 47, 48, 65,
 66, 67, 68
 Objective function, 54, 55
Ononis vaginalis, 20
 Operational, 48, 54
 Optimization, 37, 54–56
 Ordination, 50
 Organism, 15, 16, 18, 20, 22, 23, 27, 31,
 37, 42, 43
 Orreries, 7
 Orthogonal, 48
 Oscillation, 10, 11, 40
 Output, 21, 27, 28, 29, 31, 41, 54, 59, 66

 Package programs, 60–62
Pancreatium arabicum, 20
 Parameter, 22, 27, 29, 35, 38, 39, 41–45,
 57, 66, 68
 Partitioning, 53
 PASCAL, 61
 Pathway, 30
 Pattern, 42, 43
 Penzance, 19
 pH, 50
 Phosphatase, 50
 Phosphorus, 50, 53
 Physical, 7, 8, 9, 10, 28, 39, 41, 53
 Physiology, 28
 Planning, 22, 23, 56
 Plant, 30, 31, 36, 42, 51, 57
 Plot, 44
 Plotter, 59
 Plymouth, 19
 Point set, 35
 Poisson, 42
 Polynomial, 45
 Poplar, 22, 52
 Population density, 17, 21
 Precipitation, 12, 17, 19
 Predation, 10, 15

Predator, 10, 11, 40, 55
 Prediction, 7, 10, 19, 29, 40, 68
 Predictive model, 47, 51
 Presence, 15, 20, 42, 45, 50
 PRESTEL, 63
 Prey, 10, 11, 40
 Primary productivity, 17, 18
 Principal component analysis, 47, 48, 50
 Probability, 42, 43, 46, 51
 Production, 15, 17, 18, 19, 22, 29
 Productivity, 17, 18, 19
 Pythagoras, 7

Quadrat, 27, 50

Radiation, 49
 Radionuclide, 49
 Random, 13, 40, 42, 43
 Random variable, 11, 45, 46
 Ratio, 10, 40, 47
 Realism, 41
 Reality, 10, 21, 38, 39, 40, 53, 65
 Reciprocal averaging, 50
 Redundancy of data, 21, 22
 Regression model, 11, 12, 23, 45, 51, 68
 Regressor, 27, 51
 Reproduction, 15
 Residual, 20, 44, 45
 Respiration, 23, 31
 Response, 15, 16, 20, 34, 37, 38, 41, 59, 66, 67
 Root, 20

Saccharomyces, 22
 Sample, 22, 27, 43, 44, 45, 48
 Sampling, 23, 42, 43, 47, 48
 Scalar, 35
 Scaled, 47, 53
Schizosaccharomyces, 22
 Scotland, 12
 Seasonal, 27, 40
 Seed, 42
 Sensitivity, 66, 67
 Servo-mechanism theory, 37
 Sex, 20, 40, 46
 Shoot, 20
 Significance, 44, 45
 Simplex, 54
 Simplification, 16, 25, 65
 SIMULA, 61
 Simulation, 16, 23, 28, 37, 53, 68
 Sink, 30
 Size, 10, 17, 36, 40, 41, 43, 55
 Soil, 16, 23, 50
 Solar system, 7
 Source, 30

Space, 7, 8, 26, 35, 36, 48, 56
 Spatial, 42, 43
 Species, 10, 11, 16, 20, 22, 36, 41, 43, 50, 53
 Speed, 8, 37, 62, 63, 64
 Stability, 39, 40, 41, 46
 State, 11, 13, 17, 20, 21, 36, 45, 46, 57
 variable, 27, 28, 29, 30, 31, 38
 Stochastic, 37, 39, 41, 42, 43, 45, 46, 51
 Storage, 30
 Stornaway, 19
 Stream, 43
 Structure, 22, 38, 39, 40, 41, 47, 48, 52, 53, 67, 68
 Subroutine, 61, 62
 Subscripts, 34, 35
 Subset, 15, 26, 27
 Succession, 13
 Successive, 38, 39
 Sugar, 31
 Sulphur, 12
 Survival, 40
 Symbol, 8, 29, 30
 Synthesis, 16, 23, 67

Taxonomy, 22
Tellina tenuis, 53
 Temperature, 17, 19, 23
 Terminal, 59
 Test, 10, 16, 21, 23, 38, 42, 43, 44, 45, 66, 67, 68
 Time, 7, 10, 13, 15, 16, 17, 18, 19, 20, 26, 27, 36, 37, 38, 40, 45, 46, 56
 scale, 16
 step, 13, 45
 Topology, 36, 56
 Transaction, 30
 Transition, 13, 45, 46
 Tree, 22, 41
 Trigonometry, 36
 Trophic level, 41

Validation, 10, 67
 Valve, 30
 Variability, 12, 15, 16, 22, 39, 41, 42, 47, 48
 Variance, 11, 19, 22, 42, 43, 44, 45, 68
 Variate, 46, 47, 50, 51, 52
 Vector, 48, 51, 53, 57
 Vegetation, 27, 29
 Verification, 67

Water, 27
 Weight, 18, 37, 46, 48
 Wick, 19
 Woodland, 13