Chapter 1: No model without a Purpose

Modelling Purposes in the context of research

* **Explain** X (Why is X the case?): An explanation assumes the presence of some accepted theory in which the explanation should make sense
* **Predict** X (When will X happen (if)? What will happen to X (if)?)
* **Compress** X (How can X be written down in a more compact form?)
* **Abstract** X (What is essential in X?): gives an explanation
* **Unify** (What do X and Y have in common?): providing a representation that allows explanations and predictions in two domains that initially were thought unrelated. Unification is a special case of abstraction; leaving out details in the hope that the remaining essentials allow for generic explanation, applying to two (or more) domains.
* **Analyse** X (What is the relation between X and Y?): analysis (deduce properties) or do predictions. To do predictions some analysis is required, not all analysis lead to prediction

Modelling purposes in the context of design

* **Data compression**: al large and heterogeneous amount of information should be condensed into a structured and accessible format
* **Communicate** (How do I make sure person P knows X?)
* **Specify** (Which requirements should X (which does not yet exist) fulfil?)
* **Exploration** (What are the various possibilities for X?): closed = all possible outcomes are fully known beforehand. Open = the designer has to invent the alternatives
* **Optimization** (What should we choose for Y such that X is as large or as small as possible?)
* **Decide** (What do I choose for X so that some condition is fulfilled?)
* **Verify** X (Is it true that X holds?)
* **Steer and control** (What interventions should take place in X such certain conditions hold?)
* **Train** (How could a prospective user learn to operate X without actual dealing with X?)

Model Dimensions

* **Material – Immaterial**
	+ Material: Models involving material objects (natural object (guinea pig) or artefact (scaled down model))
	+ Immaterial: formal models such as mathematical, logical or software models
* **Static – Dynamic**
	+ Static: involves only stationary quantities
	+ Dynamic: models that involve time
* **Continuous – Discreet**
	+ Continuous: quantity can assume any value (weight, height, speed)
	+ Discreet: Quantity that can only occur as an integer (number of people, cars, etc)
* **Numerical – Symbolic**
	+ Symbolic: Uses mathematical analysis
	+ Numerical: Apply Iterative Algorithm (determine Y for many values of X and pick the most appropriate)
* **Geometric – Non Geometric**
	+ Geometric: models hinging on space related quantities (coordinates)
	+ Non geometric: space related quantities do not occur
* **Deterministic – Stochastic**
	+ Deterministic: The outcome leaves no room for uncertainty if the initial configuration is known with 100% accuracy
	+ Stochastic: Random components make the results unpredictable. By bulk quantity of the ensemble an deterministic quantity can emerge (averaging out)
* **Calculating – Reasoning**
	+ Calculating: involve calculations with numbers or symbols
	+ Reasoning: logical expressions such as ‘AND’,’OR’, ‘IMPLIES’ give value TRUE or FALSE
* **Black Box – Glass Box**
	+ Black Box: We know how the model behaves, but not why it behaves like this
	+ Glass (White) Box: We postulate a theory of how the model behaves, but are not sure this is right
	+ Grey Box: A combination of a black and white box for the same system

Stages in the modelling process (also see next table)

* **Definition**
	+ State initial problem and formulate purpose
	+ *Verify if the new, redefined version of the problem is still in accordance with the problem owner’s intentions*
* **Conceptualisation**
	+ Collection of entities, their properties, relations between them (not in mathematical form)
	+ Entity relation graph
	+ *Verify the conceptual model reflects our intuition about the things that matter. Did we forget anything? Is there not too much detail? Are the relations we identified adequate for the purpose of the model?*
* **Formalization**
	+ Quantities and quantitative relations connecting them. A formal form no longer relies on human interpretation
	+ Collection of data that serves as input: raw data or processed/aggregated data
	+ Glass box 🡪 knowledge about the mechanisms inside the modelled system. Black Box 🡪 hypotheses
	+ Introduce assumptions to assist to assess or limit the plausibility of the model’s result and inspire to do model refinement
	+ *Seek arguments to support the conclusion that the formulas are good enough for the model’s purpose. Validation and verification*
* **Execution**
	+ Do operations with the model (run a computer program if the model involves a computer)
	+ Obtain a result (the value of a quantity, a set of numbers, a graph)
	+ *Verify the numerical outcomes fall in the regimes that were assumed in the various parts of the calculations. (Regime: a range of values for the quantities in the model such that the model behaves similarly, or a rage of values for the quantities in a model such that the same set of assumptions hold. In general conclusions obtained in one regime cannot be carried over to another regime)*
* **Conclusion**
	+ Translate the results to the problem domain
	+ Present the results
	+ Interpret the result
	+ *Did we solve the initial problem? Did we do a proper presentation of our results and is our interpretation of the results adequate?*
* **Evaluation**
	+ Reflection



**Summary from Lecture notes chapter 1**

* A model can only be meaningful with a clearly defined purpose;
	+ purposes come from research (aim: to produce knowledge or understanding) or design (aim: to create or add value)
	+ purposes are: explanation, prediction (unconditional, conditional), compression, abstraction, unification, communication, analysis, verification, exploration, decision, optimization, specification, steering and control, training.
* Modelling approaches can be distinguished on a number of dimensions:
	+ material - immaterial: does the model involve material objects?
	+ static - dynamic: does time play a role?
	+ continuous - discrete: does the modelled system involve 'counting' or 'measuring'?
	+ numerical - symbolic: do results follow from operations on numbers or on expressions?
	+ geometric - non-geometric: do features from 2D or 3D space play a role?
	+ deterministic - stochastic: does probability play a role?
	+ calculating - reasoning: does the purpose rely on numbers or on propositions?
	+ black box - glass box: does the model start from data or from mechanisms?
* Modelling is a process involving 5 stages, each stage consisting of one or two activities (=subsequent blocks in Table 1.3) and a reflection:
	+ definition: establish the purpose
	+ conceptualization: devise a representation of the modelled system in terms of concepts, properties and relations
	+ formalization: devise a representation of the conceptual relations in terms of mathematical expressions
	+ execution: perform the appropriate operations (often involves running a computer program)
	+ conclusion: devise an adequate presentation and interpretation

Chapter 2: The Art of Omitting

* **Concept**:
	+ A placeholder for an entity in the system that is being modelled; refers to entities in the modelled system
	+ Defined as a bundle of properties, *e.g. a vector*
* **Property**
	+ A means to distinguish concepts from each other.
	+ Carries part of the information in a concept; a chunk of information about the concept
	+ Comes in the form of a name and a set of values
* **Type**
	+ The set of values a property can have
	+ Singleton {4}, {red}
	+ Set {1,2,3,4,5}, {red, blue, green}
	+ Range {1 … 5}, (lightGreen ... darkGreen}
* **Value**
	+ The type of a property, if a properties type is a singleton
* **Relation**
	+ Connects concepts or properties of concepts
	+ Prepositions (near, above, in)
	+ Verbs (produces, likes, wait)
	+ Can be seen as functions *e.g. smarter(John, Peter)* with a domain *e.g. the set of pairs of humans* and range *e.g. the set {true,false}*

**Constructing a Conceptual Model**

* Establish concepts
* Establish properties
* Establish types of the properties
* Establish relations

**Quantity**

* The property of an unknown concept, *e.g. radius, height, temperature*
* In other texts: parameter, variable, factor, term, coefficient
* Elementary types
	+ Booleans {true, false}
	+ Strings
	+ Real numbers
	+ Enumerated list of constants {wood, plastic, metal, cement} or {1,2,3,4,5}
* Compound types *(eg rectangle; compound of length& height or area& perimeter)*
	+ Properties should be consistent (logically possible)
	+ Properties should be independent

**Kinds of Ordering and mathematical operations that are allowed**

* Nominal: quantities that cannot be ordered {red, blue, green}, {wood, plastic, metal}
* Ordinal: quantities that can be ordered (transitive: if a<b and b<c 🡪 a<c)
	+ Partial Ordering
		- Only applies to some pairs
	+ Total Ordering
		- Applies to any two elements in the set
			* Ordinal scale: ranking (*eg military ranks*)
			* Interval scale: difference has a meaning *(eg temp in ⁰C)*
			* Ratio Scale: has a meaningful 0 (*eg temp in K)*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| OK to compute … | Nominal | Ordinal  | Interval | Ratio |
| Frequency distribution | Yes | Yes | Yes | Yes |
| Median | No | Total: yes, Partial: no | Yes | Yes |
| Add, subtract, mean | No | No | Yes | Yes |
| ratio | no | no | no | Yes |

**Mathematical operations on units and the rules that apply**

* Unit symbols are algebraic factors that are part of the expression, and should be manipulated as such when doing algebra with the quantities
* Adding two quantities with different units *(u1=cm, u2=km*) is not forbidden, but if the result should be expressed as a quantity with a single unit *(u=m*), then u­1 and2 should have a constant ratio (*u1/100=u2\*1000=u*)

**Dimension, dimension analysis & dimension synthesis**

* Dimension: class of all units that have constant ratio’s (equivalent units) *eg units: seconds, minutes and hours*🡪 *dimension: Time* and *units: gram, kg and pound*🡪 *dimension: Mass*
* If two quantities are equal, their dimensions are also equal. This means we can, to a large extent, guess the form a mathematical expressions, merely by observing dimensions.

**Summary from Lecture Notes chapter 2**

* The conceptual model is constructed in stage 2 (conceptualization) of the modelling process;
* The conceptual model consists of concepts; entities in the modelled system are represented by concepts;
* A concept is a bundle of properties, every property consisting of a name and a set of values: this set is the type of the property;
* Concepts can have relations; the concepts and relations together form the conceptual model, usually drawn as an entity-relation graph. Relations can also exist between the properties of concepts. The conceptual model is constructed in 4 steps:
	+ establish concepts;
	+ establish properties;
	+ establish types of properties;
	+ establish relations.
* Sets of values can be bound in different ways to properties, e.g. as choices, as results from

measurements, or as desired outcomes;

* Values, occurring in the type of a property, can be concepts of their own;
* Quantities are properties, where the concept they are properties of is disregarded;
* Allowed mathematical operations on quantities depend on their ordering ; we distinguish nominal (no order), partial ordering or total ordering. For totally ordered scales, we further distinguish interval scale and ratio scale;
* Measuring amounts to counting the number of units of some sort that fit in the measured item. Units can have constant ratio's (e.g., 1m=100cm);
* Sets of units that have a constant ratio are called equivalent. A dimension is an equivalence class on units;
* Operations on units follow the operations on quantities (dimensional analysis);
* Using the dimension of quantities, the form of a mathematical relation between them can often be derived (dimensional synthesis).

Chapter 3: Time for Change

State

* Described in terms of concepts, properties, values and relations
* States differ with respect to which values are currently assumed by the properties (binding: “value v is currently bound to property p”)

State space

* All states of a system together
* Number of states in a system of *n* properties with *m* values per property = *m1\*m2\*...\*mn*
* Number of possible routes of length L in a state space=(Number of states)L
* State space reduction
	+ Spatial symmetry or temporal symmetry
	+ Projection: limiting the number of properties, or the number of values for properties
		- By leaving out quantities
		- By hiding properties (*eg not showing the seconds hand of a clock*) or values. Only transitions of exposed properties are considered, but hidden states still change. This may mean that the modelled system can no longer be fully understood.

State chart/diagram

* Graphical means to denote things that take place over time
* A collection of states

Applying state charts:

* Verify there are no deadlocks
* Verify that states that should be reached can be reached
* Verify that states that should be reached in some order are reached in that order
* Verify occurring transitions are expected or admitted while monitoring a system
* Verify that eventually the behaviour of a system will have certain properties
* Argue about the synchronisation of events

Transition

* The system goes from one state to another state, this corresponds to a change in binding
* The maximal number of possible transitions for N states is N2, including transitions from a state to the same state. The number of allowed transitions is often a lot less.
* We assume transitions take no time
* Internal transitions: occur as a result of a transition of a hidden property

Process

* Formed by cause, effect and the advance of time
* Consider:
	+ the sequence of steps (one thing happens after the other)
	+ Causative effect (one is a result of the other)
	+ Unrelated steps
	+ Time dependent steps
	+ Repeated steps
	+ Wait for a known amount of time till next step
	+ Wait for an unknown amount of time till next step (wait till something else happens)

Behaviour/Trace

* A route through a state space

Event

* Something that happens outside the modelled system which affects its state
* Examples: a telephone ringing, insertion of a coin into a coffee machine, a billiard ball colliding with something

State space explosion

* Because the number of routes through a state space grow exponentially with the number of transitions, the number of properties and the number of values one property can assume, it is intractable to account for all possible routes explicitly

Deadlock

* Dead end state: a state that has no outgoing transitions
* Lifelock: a small collection of permitted states, but none of these states has a transition to any state outside the collection

Types of time models

* partially ordered time
* total ordered time
	+ with equal time intervals (periodicity)
	+ without equal time intervals

Recursive functions

* the numerical solution of a differential equation
* recursion = defining something in terms of earlier versions of itself
* sampling = capturing the characteristics of a large set by looking at a small number of elements of this set
* the error of a recursive function is larger when ∆ is larger 🡪 for an accurate simulation, ∆ should be sufficiently small, and the approximation deviates more when time proceeds

**Summary of Lecture Notes chapter 3**

* A state is a snapshot of a conceptual model at some time point;
* The state space is the collection of all states of a modelled system;
* Change comes in the form of transitions between states; a state chart is a graph where nodes are states and arrows are transitions;
* A behaviour is a path through state space; a process is the set of all behaviours. The size of state spaces is huge, causing practical problems for state space models; this is called state space explosion. Two methods to mitigate state space explosion:
	+ symmetry: some parts of state space are identical and therefore redundant;
	+ projection: distinguish exposed and hidden properties or value sets and if possible limit the state space to exposed properties only;
* Multiple flavours of time:
	+ partially ordered time, for instance for specification and verification;
	+ totally ordered time, for instance for prediction, steering and control;
	+ a recursive function of the form Qi+1 = F(Qi;Qi-1;Qi-2; … ; Pi; Pi-1; Pi-2; …) is used to evaluate or unroll a behaviour;
* arbitrary, perhaps unequal intervals: often no methods for closed form evaluation; unrolling is the only approach;
* equal intervals: the possibility for closed form evaluation (example: periodic financial transactions); sampling;
* equal, small intervals: approximation, sampling error (examples: moving point mass, rotating dumbbell, mass-spring system, dissipation);
* infinitesimal intervals: continuous time, differential equations (examples: motion of a point mass with or without force); contrast between numerical and symbolic approach
* Numerical methods for differential equations:
	+ construction and interpretation of a direction field;
	+ Euler's method to find approximate solutions of first-order differential equations;
	+ equilibrium solutions.

Chapter 4 The function of functions

Extended Summary from lecture notes

* It is necessary to translate a conceptual model to a formal model, so it is no longer dependent on interpretation
* Translating a conceptual model to a formal model cannot be done in a formally provable way; it requires interpretation and imagination
* A heuristic approach has the following 4 elements:
	+ The good practice of naming convention
	+ The use of dimensional analysis to derive plausible formulas
	+ The use of the to-do-list
	+ The role of the wisdom of the crowds
	+ appropriate naming; names should:
		- be unambiguous
		- not conflict with standard usage
		- not rely on the distinction between UPPERCASE and lowercase or between o (letter) and 0 (digit)
		- not start with a digit
		- be transliterated (β becomes beta)
		- self explanatory
		- long strings should be CamelCased to improve readability
	+ structure
		- chain of dependencies: the formal model as a directed acyclic graph (DAG);
			* What mechanism?
			* What quantities drive this mechanism?
			* What is the qualitative behavior of the mechanism?
			* What is the mathematical expression to describe this mechanism?
		- to-do-list to ensure that all intermediate quantities are found and elaborated in turn;
	+ formation of mathematical expressions:
		- dimensional analysis can give mathematical expressions, e.g for proportionality and inverse proportionality;
		- the Relation Wizard can help to find appropriate fragments of mathematics;
		- the Function Selector can help to find an appropriate expression for a desired (visual) behavior;
			* The notion of ramp functions to formalize monotonic, saturating behavior;
			* The logistic function as a smooth approximation to the ramp function;
	+ wisdom of the crowds can help improve the accuracy of values that have to be guessed;

Additional Notes:

DAG (Directed Acyclic Graph)

* Every arrow designated the relation depensOn
* Roots: Nodes with only outgoing arrows; a quantity we are interested in (cat. II)
* Leaves: Nodes without outgoing arrows: a constant (cat. III) or quantity that can be freely chosen (cat. I)
* All other nodes are category IV

Expanding a DAG:

1. Think of the simplest mechanism that causes x to take its value (what is the mechanism?)
2. Express this mechanism in terms of other quantities (What are the quantities this mechanism depends on?)
3. State qualitatively what this dependency looks like (What is the qualitative form of the mechanism?)
4. Translate this qualitative statement into a mathematical statement (What is the quantitative form of the mechanism?)
	1. Assumptions are crucial in determining the arity of a relation
	2. Assumptions may give conceptual simplicity and more efficient execution of the model, but if the assumptions do not hold we have to recalculate
	3. The modeller should investigate whether simplifying assumptions are acceptable
	4. The simplifying assumptions must be communicated and validated. If the assumptions are so restrictive the model’s outcomes have nothing to say about the problem at hand, the entire modelling effort is in vain.

To do list

* A simple device to keep track of intermediate quantities
* It helps building a DAG in a systematic way
* It indicates the moment when a DAG is executable; when all occurring values van be computed from known data.

Relation Wizard

Starts from a qualitative relation and helps to find appropriate mathematical terminology using a number of question and answer steps.

Function selector

Uses the visual features of a graph or a data set as input and suggests a possible parameterization to reproduce these.

Chapter 5

 Summary from lecture notes

* A functional model helps to distinguish input and output
	+ Desired output follows from purpose
	+ Input, if present, represents modeller’s or designer's choices;
* Building a functional model in the form of a DAG according to Section 5.2.1 reveals the roles of quantities. These are:
	+ Cat.-I : free to choose;
		- Models for (design) decision support: the notion of design space;
		- Choice of cat.-I quantities: no dependency-by-anticipation;
		- The necessity of avoiding causal loops;
	+ Cat.-II : represents the intended output;
		- The advantages and disadvantages of lumping and penalty functions;
		- The distinction between requirements, desires, and wishes;
		- The notion of dominance to express multi-criteria comparison;
		- The Pareto-front as the hyper surface of non-dominated points in cat.-II space;
	+ Cat.-III : represents constraints from context;
	+ Cat.-IV : intermediate quantities;
* For the purpose optimisation, an evolutionary approach can be used to deal with arbitrary functional models and multiple cat.-II quantities;
	+ The Pareto front can be approximated by evolutionary approach using the SPEA-algorithm;
	+ Local search can be used for post-processing.



Additional notes:

The **Cartesian Product** of all value sets of all cat I quantities is called **cat-I space**. If the functional model serves to support design decisions, it is called **design space**.

Proposition: a sentence that is either True of Fals

Predicate: a proposition with an argument, or a function with {True/False} as range.

Requirement: Predicates on Cat-II quantities

* Any requirement that yields False renders the ATBD (artefact to be designed) unacceptable. So requirements reduce the design space to a limited, and perhaps empty, subspace.

Desire: False is acceptable

* There is no logical difference between requirement and desire.

Wishes: Conditions that are not Predicates

* Usually an optimisation (as little as possible, as cheap as possible)
* It would require the impossible: a complete design space and an exhaustive search over this design space.

Penalty function

* A quantity depending in cat-I quantities, that expresses how successful our ATBD is.
* Nonnegative function, the larger the worse the ATBD performs with respect to the penalty

Lumping: evaluating multiple penalties as one

* Not unique: sum / sum of squares / any nonnegative combination
* Must have the same dimensions
* Relative contribution: one penalty may be more important than others, even if they have the same dimension
* Always introduces additional assumptions, which are difficult to formulate and even more difficult to verify
* Alternative is having more cat-II quantities (every penalty is a cat-II quantity)

Injective: preserve distinctiveness (any two different argument values produce different result values)

Surjective: all values in the range set are reached

In general, the functional model is not injective and not surjective

Dominance: ATBD1 dominates ATBD2 if for **all** cat-II quantities, 1 is better than 2.

An ATBD that is dominated should not be considered for realisation.

For n independent cat-II quantities, the chance that an ATBD is dominated is 2­­­-n.

The non-dominated solutions form the **Pareto Front**. In case of n cat-II quantities, these points are on a n-1-dimensional hyper surface in cat-II space. Moving within the Pareto front means exploring trade-offs. Moving perpendicular to the Pareto front means considering either superior or inferior solutions.

Pareto Optimisation:

* Helps to reduce the number of possible solutions to those that are non-dominated
* No weights have to be thought of, so much subjectivity is avoided and therefore discussions related to weight-factors can be postponed or avoided.
* The number of cat-II quantities should not exceed 4 to limit the collections of solutions and keep the effectiveness of the Pareto front.

SPEA: Strength Pareto Evolutionary Algorithm

1. Create a set of individuals in a random way 🡪 population
2. Determine the fitness of the individuals (number of solutions by which it is dominated, the lower the fitter). Relates to the quantity Strength of which SPEA derives its name.
3. Eliminate, randomly, a certain percentage of the non-fit ones. Not all, since there might be latent strong properties.
4. Generate additional new individuals using a number of different schemes
* Random mutations
* Crossing over: combine successful values for cat-I quantities from 2 individuals
* Re-introduce a few of the eliminated candidate solutions with different values for some of their attributes

After step 4 return to step 1

Reasons for the Pareto front to stop improving and their solutions:

* The approximated front is sufficiently close to the theoretical front
* There are not enough non-dominated solutions left to generate new mutants
	+ Consider increasing the population
	+ Eliminate some of the individuals from the Pareto front; only if there are other individuals sufficiently nearby to avoid deterioration
* The entire population occupies a niche (gets stuck in a local extreme)
	+ Increase the size of the population
	+ Increase the relative probability of random mutations

Pareto Post Processing

* Checking for al cat-I quantities if an individual solution can be improved.
* Do at least one further round of SPEA to verify the improved solution do not dominate another solution previously on Pareto front

Last resorts if Pareto-evolutionary optimisation gives insufficient results:

* Splitting cat-I space (use several separate models instead of an integral model)
* Fixing some of the cat-IV quantities (treat as if in cat-III). Afterwards we have to re-calculate for the original cat-IV quantities, to get a more accurate estimate, and redo the entire calculation.

Chapter 6

Extended summary from lecture notes

Confidence in the outcome of a model depends on the model, the modeled system, and the

purpose of the model:

* Verification: is model X correct? Is it 'true' enough to be convincing?
	+ Consistency of the model (dimensional consistency of expressions, obtained values fall within the types given during conceptualisation)
	+ The functional model is a DAG (contains no cycle)
	+ Logical structure of assumptions (there should be sufficiently many assumptions such that formal expressions uniquely follow from the assumptions)
* Validation: is X the correct model? Is it `strong' enough to satisfy the purpose?
	+ Logical structure of assumptions ( All assumptions must be true)
	+ 'are the values of cat.-III quantities reliable, given the modelled system?
	+ 'are the obtained values for cat.-II quantities conclusive, given the purpose?'
	+ 'do predictions of the model match with empirical observations within tolerance?’
	+ 'are assumptions about the modelled system true?'.
* Large tolerance = weak assumptions = large range of applicability = small strength of conclusions (the model may not be precise enough to fulfil the purpose)

Modeling involves uncertainty because of different causes:

* Accuracy relates to:
	+ Bias
	+ Systemic error
	+ Offset
	+ The agreement (or deviation) between values, resulting from a model, and from the modeled system
		- Can only be improved if sources of systematic deviation are removed
* Precision relates to:
	+ Noise
	+ Random error
	+ Statistical spreading
	+ Reproducibility
		- Can be improved with effort, e.g., repeating a measurement more often, or taking more digits or more terms into account

All forms of uncertainty cause distributions of values rather than a single value;

* The normal distribution: smooth, peaked, and with infinite wide support;
* The uniform distribution: non-smooth, non-peaked, and with finite support;

The notions of distance and similarity;

* Similarity is related to distance
	+ Distance is always positive
	+ Similarity has a value between -1 (opposite) and 1 (similar).

The meaning of confidence for black box models:

* Commonly occurring features of aggregation:
	+ Average / arithmetic mean $\hat{μ}=\frac{1}{n}\sum\_{i=1}^{n}s\_{i}$
	+ Geometric mean $\hat{μ}=(\prod\_{i=1}^{n}s\_{i})^{^{1}/\_{n}}$
	+ Standard deviation (a measure for the spreading of the values)

 $σ=\sqrt{\frac{1}{n}\sum\_{i=1}^{n}s\_{i}^{2}}$ σ2 is called the variance

* + Correlation (ρ) informs about the linear similarity between 2 vectors
		- Value between -1 and 1 (no correlation=0)
* Linear least squares fit: the regression line with the smallest sum of squares of residues; an example of aggregation
* Residue: measured y minus predicted y on basis of the model (regression line)
* Validation of a black box model:
	+ Residual error : how much of the behavior of the data is captured in the model?
	+ Distinctiveness: to what extent can the model distinguish between different modelled systems?
	+ Common sense: how plausible are conclusions, drawn from a black box model?

The meaning of confidence for glass box models:

* We define a glass box model as valid if:
	+ The possible outcomes of the modelled system do not fall outside the uncertainty interval of the output quantities of the model
	+ The uncertainty interval of the output quantities is narrow enough to fulfil the purpose
* Structural validity: do we believe the behavior of the mechanism inside the glass box?
	+ There must be no mistakes in the calculation of the uncertainty intervals, and they must be sufficiently narrow to fulfil the purpose
	+ Ensure the model has the right functional dependencies
		- Divide and conquer (confirm behaviour of cat-IV quantities)
		- Asymptotic analysis (verify simpler configurations)
		- Singular cases (behaviour near zero crossings)
		- Check convergence (check step size/number of steps is adequate/sufficient for iterative calculations)
* Quantitative validity: what is the numerical uncertainty of the model outcome?
	+ Sensitivity analysis and the propagation of uncertainty in input data;
		- Error propagation regards the way uncertainties in inputs determine uncertainties in outputs of a functional model
	+ Sensitivity analysis (=calculation of condition numbers) to decide if a model should be improved.
		- A large value in a condition number indicates there could be a problem with stability; a small change in input causes a problematic large change in output
		- Condition numbers are dependent on x and may vary over the input space

Chapter 7

Extended summary from lecture notes

* Leading question: to what extent has the initial problem been solved?
* Approach: define criteria to assess the quality of the modeling process as a whole
* A taxonomy to make criteria for modeling quality:
	+ Input or output side?
	+ Inside (=model, modeled system) or outside (=context, stakeholders)?
	+ Qualitative or quantitative?



* Resulting criteria:
	+ Genericity: how many different modeled systems can we handle?
		- The model is better if it works for more different kinds of situations
	+ Scalability: how large can the size of the problem be?
		- A better model works well for modelled systems with a larger number of components
		- Depends on:
			* Solution time
			* Required memory space in a computer
	+ Specialization (level of specialisation of intended problem owner): how much should the intended audience know?
		- The model performs better if the users of the model need to know less
			* The importance of presentation (data visualisation)
			* Limiting the claims (be more conservative with the interpretation when the problem owner is less experienced)
			* Biased stakeholders
				+ Detailed account of assumptions and approximations in the final report
				+ Insisting the entire report is kept as an indivisible document
				+ Refrain from providing ‘easy to misapprehend’results that might support known stakeholders’ biases
				+ Seek assistance from a neutral colleague or ask an independent second opinion
			* Self-fulfilling and self-denying prophecies;
				+ Wicked problems are changed by their own solution
	+ Audience (number of intended stakeholders): how large can the intended audience be?
		- For a model to score high on audience, special attention has to be paid to robustness, ease of use and performance
	+ Convincingness: how plausible are the assumptions?
		- Assumptions that are verified using formal reasoning or mathematics
		- The assumption is an instance of a law or theory in a well-accepted discipline (physics, economy)
		- The current system can be compared to a plausible Formal Model System (FMS)
		- The assumption is supported by an Empirical Model System (EMS) together with a similarity argument
		- The assumption is consistent with intuition
	+ Distinctiveness (the power of distinction): e.g., how accurate, how certain, how decisive can the model outcome be?
		- Unification, abstraction, exploration do not relate to distinctiveness
		- False positive: the situation where we take an action that should not have been taken
		- False negative: the situation where we should take action, but omit to do so
		- The narrower the distribution of uncertainty in the output quantities, the larger the distinctiveness of the model
	+ Surprise: to what extent can the model outcome give new insight?
	+ Impact: how big can the consequences of the model outcome be?

$$ρ=\frac{(\left(r\_{2}-r\_{1}\right)-\left(c\_{2}-c\_{1}\right))}{(|r\_{2}-r\_{1}|+\left|c\_{2}-c\_{1}\right|)}$$

r1 the profit in present situation

r2 the profit with model outcome

c1 the cost in current situation

c2 the cost with model outcome

* + - It depends on the modellers purpose whether an smaller or bigger impact is better
* Criteria for modelling quality are related to purposes; every purpose has its own dominant criteria.
	+ Prediction: Convincingness, distinctiveness, impact
	+ Compression: Scalability, Audience, Distinctiveness
	+ Inspiration: Surprise
	+ Unification: genericity, convincingness, surprise
	+ Abstraction: Convincingness, surprise, distinctiveness
	+ Verification: Scalability, convincingness, impact
	+ Exploration: genericity, surprise
	+ Decision: convincingness, distinctiveness, impact
	+ Optimisation: genericity, scalability, convincingness, impact
	+ Specification: genericity, distinctiveness
	+ Realisation: genericity, distinctiveness, impact
	+ Steering and control: distinctiveness
1. From the problem definition, analyse which purpose the model should fulfil
2. From this purpose, identify which criteria are most central to the current problem setting
3. Develop the model
4. Using the selected criteria, asses if the model outcome fulfils the purpose. If not, the criterion for which the model outcome is insufficient may hint at a direction for improvement
5. Interpret the model outcome and formulate a solution of the initial problem; pay special attention to those aspects of the model that account for the selected criteria.

Math

Absolute uncertainty for given x = y’(x)

Uncertainty in y with given uncertainty in x =y’(x) \* uncertainty in x

Condition number =
$$\left|F^{'}\left(x\right)\*\frac{x}{F(x)}\right|$$

Condition number for multiple variables=

$$\left|\frac{f^{1}\left(x\_{1},\cdots ,x\_{n}\right)+\cdots +f^{n}(x\_{1},\cdots ,x\_{n})}{f(x\_{1,\cdots ,}x\_{n)}}\right|\*max\left\{\left|x\_{1}\right|,\cdots ,\left|x\_{n}\right|\right\}$$

Uncertainty in y (%) with given uncertainty in x(%) = condition number \* uncertainty in x

Equation of tangent plain to f(x,y):

$$\frac{∂z}{∂x}\*\left(x-x\_{coordinaat}\right)+\frac{∂z}{∂y}\*\left(y-y\_{coordinaat}\right)-\left(z-z\_{coordinaat}\right)=0$$

Equation of tangent plain to f(x,y,z):

$$\frac{∂f}{∂x}\*\left(x-x\_{coordinaat}\right)+\frac{∂f}{∂y}\*\left(y-y\_{coordinaat}\right)+\frac{∂f}{∂z}\*\left(z-z\_{coordinaat}\right)=0$$

Rate of change in the direction of vector **v**:

$$\frac{∇f\*\overline{v}}{\sqrt{\overline{v}\*\overline{v}}}$$

The maximum change is in the direction of $∇f$, so $∇f=\overline{v}$

If
$$x=\frac{-b+\sqrt{b^{2}-4ac}}{2a}$$

Then
$$\frac{∂x}{∂a}=\frac{-c}{a\sqrt{b^{2}-4ac}}-\frac{b+\sqrt{b^{2}-4ac}}{2a^{2}}$$

$$\frac{∂x}{∂b}=\frac{1+\frac{b}{\sqrt{b^{2}-4ac}}}{2a}$$

$$\frac{∂x}{∂c}=\frac{-1}{\sqrt{b^{2}-4ac}}$$