Systems Analysis for Sustainable Development

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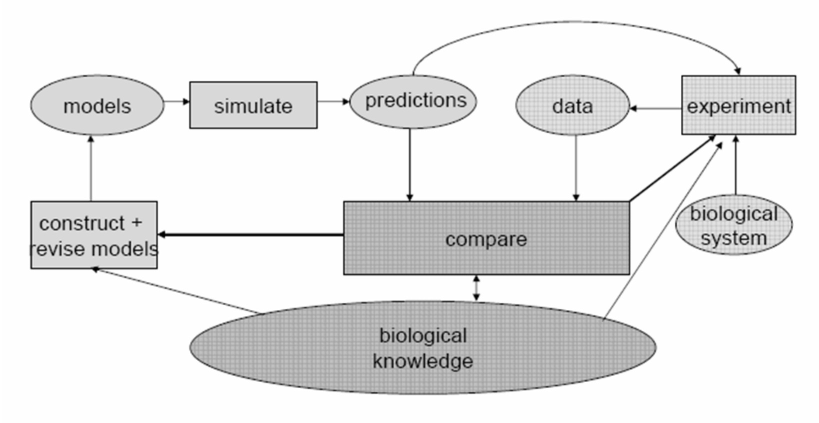
Today's session

General techniques

1. Objective function
2. Sensitivity analysis
3. Optimisation
4. Model fitting (identification)
5. Prediction

An Integrated Modeling Process



How can we trust our models?

A mathematical model is defined by a series of equations, input factors, parameters, and variables aimed to characterize the process being investigated.

Input is subject to many sources of uncertainty including *errors of measurement*, *absence of information* and *poor or partial understanding* of the driving forces and mechanisms.

This uncertainty imposes a limit on our confidence in the response or output of the model. Further, models may have to cope with the natural *intrinsic variability* of the system, such as the occurrence of stochastic events.

How can we trust our models?

Good modeling practice requires that the modeler provides an *evaluation* of the *confidence* in the model, possibly assessing the *uncertainties* associated with the modeling process and with the outcome of the model itself. Sensitivity and Stability Analysis offer valid tools for characterizing the uncertainty associated with a model.

Techniques

- Model building
  - Sensitivity analysis to test accuracy. (If a component has to be included, how accurately does it need to be known and described?)
  - Model fitting (to fit the model to the system data)
- Validation
  - Sensitivity analysis (to test if the model is sufficiently accurate)
  - Testing how well the model fits ”new” independent data from the system.
- Analysis
  - Sensitivity analysis (to study effects)
  - Optimisation (to find the best result)
  - Prediction (to predict what will happen in the future)

1. Objective function

Sensitivity analysis, optimisation , model fitting and prediction requires an objective function!

An objective function *V*, is a quantitative formulation of a purpose.

$V = f(x_1, x_2, \ldots, x_n)$, where the quantities $x_1, x_2, \ldots x_n$ may be states, flows, parameters, initial values, input values,….

Examples: (x_1 = # rabbits; x_2 = # foxes)

$V = x_1 + x_2$	(number of rabbits and foxes)
$V = 2.8\ x_1 + 8.5\ x_2$	(biomass of all rabbits and foxes)

2. Sensitivity Analysis

Sensitivity analysis is used to determine how "sensitive" a model is to changes in the value of the parameters of the model and to changes in the structure of the model.

Sensitivity Analysis

To study the sensitivity of an objective function, $V = f(x_1, x_2, \ldots x_n)$, to changes in a quantity x_i.

- *How sensitive is one quantity for a change in another?*
- *Which quantities are especially sensitive/insensitive?*
- *How accurate is our model?*

- **Absolute sensitivity:** $\Delta V / \Delta x$

  (How much does V change when x changes a little?)

- **Relative sensitivity:** $\Delta V/V / \Delta x/x$

  (What is the relative change of V (in %), when x changes by a few percent?)

Examples

– ***Parameter change:*** How much do the rabbits increase if the fertility constant increases by 0.001?

– ***Changed input:*** How many degrees will the room temperature increase if the out-door temperature increases by one degree?

– ***Change in initial conditions:*** How many percent will the share of sick potatoes increase if the share of sick seed potatoes is increased by 1 percent?

– ***Structural change:*** How many more patients can a hospital handle if the number of treatment units is increased by 1?

– **...**

Parameter sensitivity

Parameter sensitivity is usually performed as a series of tests in which the modeler sets different parameter values to see how a change in the parameter causes a change in the dynamic behaviour of the stocks.

By showing how the model behaviour responds to changes in parameter values, sensitivity analysis is a useful tool in model building as well as in model evaluation.

Parameter sensitivity

Sensitivity analysis helps to build confidence in the model by studying the uncertainties that are often associated with parameters in models. Many parameters in system dynamics models represent quantities that are very difficult, or even impossible to measure to a great deal of accuracy in the real world. Also, some parameter values change in the real world.

Therefore, when building a system dynamics model, the modeler is usually somewhat uncertain about the parameter values he chooses and must use estimates.

Sensitivity analysis allows him to determine what level of accuracy is necessary for a parameter to make the model sufficiently useful and valid. If the tests reveal that the model is insensitive, then it may be possible to use an estimate rather than a value with greater precision.

Parameter sensitivity

Sensitivity analysis can also indicate which parameter values are reasonable to use in the model. If the model behaves as expected from real world observations, it gives some indication that the parameter values reflect, at least in part, the "real world."

Parameter sensitivity

Sensitivity tests help the modeller to understand the dynamics of a system.

Experimenting with a wide range of values can offer insights into behaviour of a system in extreme situations.

Discovering that the system behaviour greatly changes for a change in a parameter value can identify a leverage point in the model — a parameter whose specific value can significantly influence the behaviour mode of the system.

Sensitivity Analysis

Sensitivity Analysis can be used to determine:

1. The model resemblance with the process under study
2. The quality of model definition
3. Factors that mostly contribute to the output variability
4. The region in the space of input factors for which the model variation is maximum
5. Optimal - or instability - regions within the space of factors for use in a subsequent calibration study
6. Interactions between factors

Sensitivity Analysis: Methodology

There are several possible procedures to perform sensitivity and stability analysis. The most common sensitivity analysis is sampling-based.

A sampling-based sensitivity is one in which the model is executed repeatedly for combinations of values sampled from the distribution (assumed known) of the input factors.

Other methods are based on the decomposition of the variance of the model output and are model independent (see references)

In general, sensitivity analysis is performed by executing the model repeatedly for combination of factor values sampled with some probability distribution. The following steps can be listed:

1. Specify the objective function and select the input of interest
2. Assign a distribution function to the selected factors
3. Generate a matrix of inputs with that distribution(s) through an appropriate design
4. Evaluate the model and compute the distribution of the objective function
5. Select a method for assessing the influence or relative importance of each input factor on the objective function.

3. Optimisation

The desire for optimality (perfection) is inherent for humans. The search for extremes inspires mountaineers, scientists, mathematicians, and many others. A beatutiful and practical mathematical theory of optimisation (i.e. search-for-optimum strategies) is developed since the sixties when computers become available. Every new generation of computers allows for attacking new types of problems and calls for new methods.

The goal of the theory is the creation of reliable methods to catch the extremum of a function by an intelligent arrangement of its evaluations (measurements). This theory is vitally important for modern engineering and planning that incorporate optimisation at every step of a complicated decision making process.

Optimisation (contd)

Naturally, one wants to produce more goods, with lowest cost and highest quality. To optimize the production, one either may *constrain* by some level the cost and the quality and *maximise* the quantity, or constrain the quantity and quality and *minimise* the cost, or constrain the quantity and the cost and *maximise* the quality. There is no way to avoid the difficult choice of the values of constraints.

"Better be healthy and wealthy than poor and ill"

Some Frivolous Remarks on Optimisation

The inherent human desire to optimize is cerebrated in the famous Dante quotation:

”*All that is superfluous displeases God and Nature*
All that displeases God and Nature is evil.”

1265 - 1321

In engineering, optimal projects are considered beautiful and rational, and the far-from-optimal ones are considered ugly and meaningless. Obviously, every engineer tries to create the best project and he/she relies on optimisation methods to achieve the goal.

Maupertuis

1698 - 1759

The *principle of least action* proclaims:

"If there occur some changes in nature, the amount of action necessary for this change must be as small as possible".

This principle proclaims that the nature always finds the "best" way to reach a goal. It leads to an interesting *inverse optimization problem*: Find the essence of optimality of a natural "project."

Optimality in Nature

The trees of Ponderosa pine and Utah Juniper in windy areas of South Utah possess spiral wood fibers that wiggle around the trunk.

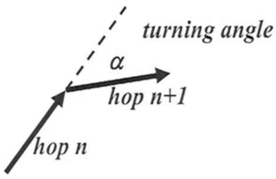
The question is: Why?

It may be postulated that morphology of a bio-structure is optimal with respect to some evolution goal, which simply means that it is best adapted to the environment.

The question is:

In what sense is the structure optimal?

Optimality in Nature



Optimal foraging by zooplankton within patches: the case of *Daphnia*.

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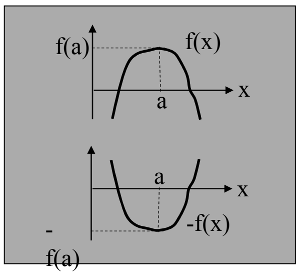
Abstract

The motions of many physical particles as well as living creatures are mediated by random influences or "noise". One might expect that over evolutionary time scales internal random processes found in living systems display characteristics that maximize fitness. Here we focus on animal random search strategies [1, 2], and we describe experiments with *the* following *Daphnia* species: *D. magna, D. galeata, D. lumholtzi, D. pulicaria,* and *D. pulex.* We observe that the animals, while foraging for food, choose turning angles from distributions that can be described by exponential functions with a range of widths. This observation leads us to speculate and test the notion that this characteristic distribution of turning angles evolved in order to enhance survival. In the case of theoretical agents, some form of randomness is often introduced into search algorithms, especially when information regarding the sought object(s) is incomplete or even misleading. In the case of living animals, many studies have focused on search strategies that involve randomness [3, 4] A simple theory based on stochastic differential equations of the motion backed up by a simulation shows that the collection of material (information, energy, food, supplies, etc) by an agent executing Brownian-type hopping motions is optimized while foraging for a finite time in a supply patch of limited spatial size if the agent chooses turning angles taken from an exponential

Optimisation (contd)

Optimisation is to find the ***maximum*** or ***minimum*** of a function that depends on a number of parameters.

Since: max(function) = - min(-function), it is sufficient to treat only one of these cases; e.g. minimisation!



Optimisation can be performed by different methods:

- Analytically (for more simple functions; $df/dx = 0$).
- Operations Research techniques like Linear Programming, Dynamic Programming, Game Theory
- Numerical search methods can be used for all kinds of models, e.g. for simulation models. (See below).

Optimisation

The term *optimisation*, or *mathematical programming*, refers to the study of problems in which one seeks to *minimise* or *maximise* a real function by systematically choosing the values of real or integer variables from within an allowed set. This problem can be represented in the following way

- *Given:* a function $f : A \to \mathbf{R}$ from some set A to the real numbers
- *Sought:* an element x_0 in A such that $f(x_0) \leq f(x)$ for all x in A ("minimisation") or such that $f(x_0) \geq f(x)$ for all x in A ("maximisation").

Such a formulation is called an *optimisation problem* or a *mathematical programming problem.* Many real-world and theoretical problems may be modeled in this general framework.

Optimisation (contd.)

Typically, A is some subset of the Euclidian space $\mathbf{R}^n$, often specified by a set of constraints, equalities or inequalities that the members of A have to satisfy. The domain A of f is called the *search space*, while the elements of A are called candidate solutions, or *feasible solutions*.

The function f is the *objective function*, or *cost function*. A feasible solution that minimises (or maximises, if that is the goal) the objective function is called an *optimal solution*.

Optimisation (contd.)

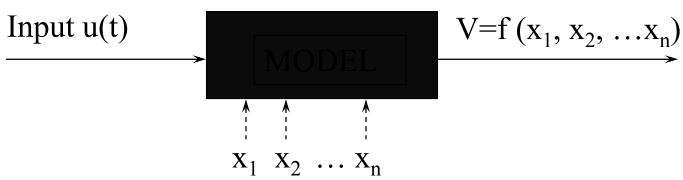
Generally, when the feasible region or the objective function of the problem does not present convexity, there may be several local minima and maxima, where a *local minimum* x* is defined as a point for which there exists some $\delta > 0$, so that for all x, such that

$$\|\mathbf{x} - \mathbf{x}^*\| \leq \delta$$

the expression $f(x^*) \leq f(x)$ holds; that is to say, on some region around x* all of the function values are greater than or equal to the value at that point. *Local maxima* are defined similarly.

Note: A large number of algorithms proposed for solving non-convex problems are not capable of making a distinction between local optimal solutions and rigorous optimal solutions, and will treat the former as actual solutions to the original problem.

Optimise *V* by finding the best combination of some quantities (parameters) $x_1, x_2, \ldots x_n$

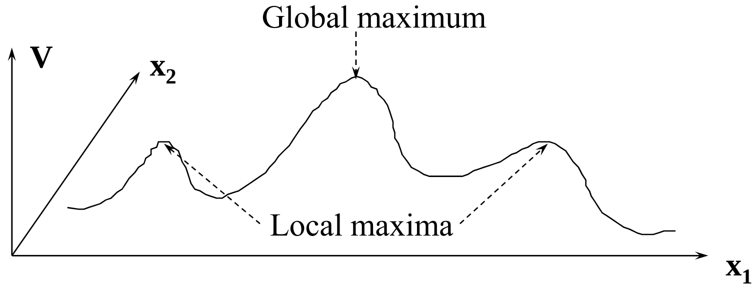


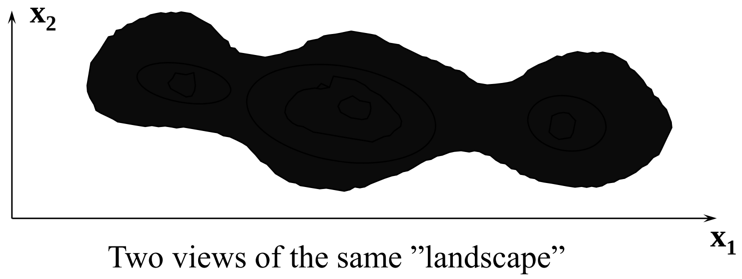
The task is to find that combination of quantity values, x_1, x_2, …x_n, that maximises/minimises the objective function V.

<u>The quantities can be</u>:

- *<u>Discrete</u>:* number of tractors, cooks, variety A or B, etc. (Test the different alternatives separately.)
- *<u>Continuous</u>:* energy price, water content, process time, amount of seed used, etc. Continuous parameters can have an "infinite" number of values. (Use a *search method*.)

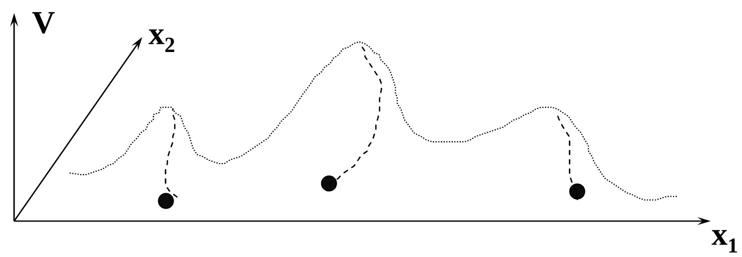
Local and global maxima





Two views of the same ”landscape”

For different parameter values (x_1, x_2) the objective function gets different values. *But the landscape is invisible*. Each simulation (fixed values of x_1 and x_2) gives only the value of $V(x_1, x_2)$ at the investigated point. (Compare mapping the depth of a lake from a boat by using a stone in a string.)



Search methods start to evaluate (simulate) the result at one point (x_1, x_2). By systematically testing new points, it searches the way up to a top (or down to a bottom). But depending on the *starting point,* it finds a local or a global optimum! (Knowledge about the system or using different starting points handle this problem.)

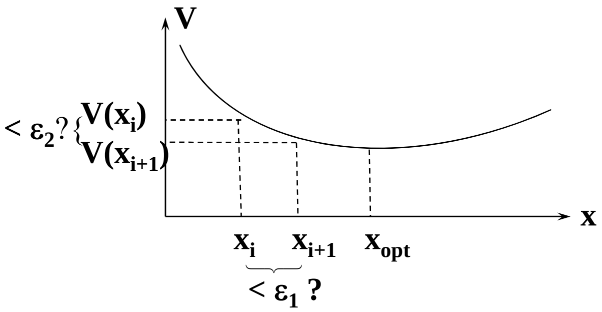
Search methods

A. Search methods for one dimension
  - *Golden section search*

B. Search methods for several dimensions
  - B1. Methods using only function values
    - *Tabulation*
    - *Search in co-ordinate directions*
    - *Simplex methods*
  - B2. Methods using function values and first derivatives
    - *Steepest descent method*
  - B3. Methods using function values, first and second derivatives
    - *Newton methods*
    - *Quasi-Newton methods*

Breaking criteria

For all search methods we need *a criterion when to end the search*. This is accomplished by specifying a number, ε, such that the search ends when: a) The improvement in parameter space is less than ε or b) The improvement of the objective function is less than ε or c) A mixed criterion based on a) and b).



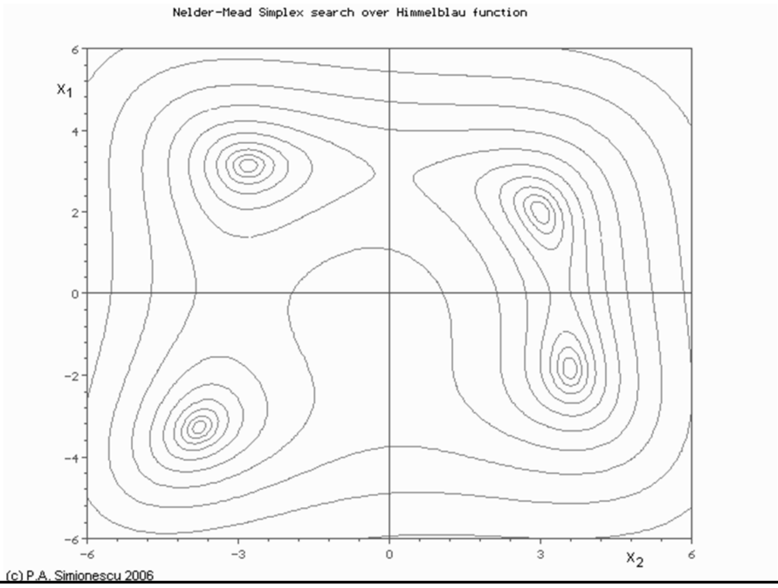
Break when:

a) $|x_{i+1} - x_i| < \varepsilon_1$

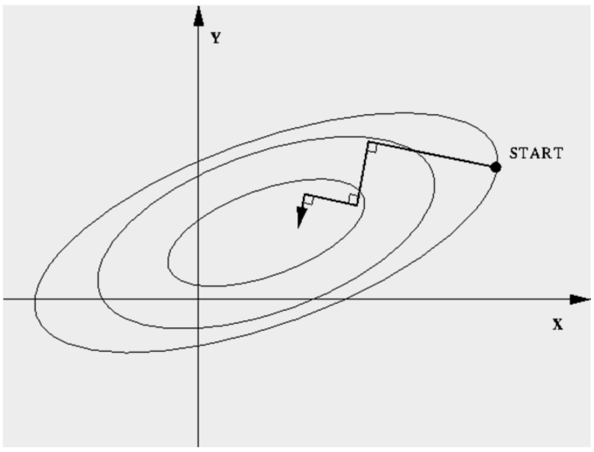
b) $|V(x_{i+1}) - V(x_i)| < \varepsilon_2$

c) Both a) and b) should be true.

Nelder-Mead simplex search of optimal points in 2-D space

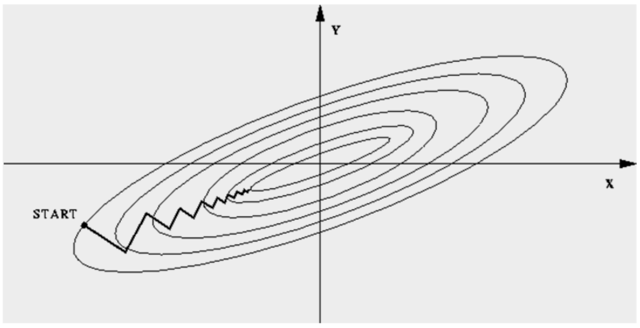


The steepest descent method



The method of Steepest Descent approaches the minimum in a zig-zag manner, where the new search direction is orthogonal to the previous.

The steepest descent method



The convergence of the method of Steepest Descent. The step size gets smaller and smaller, crossing and recrossing the valley (shown as contour lines), as it approaches the minimum.

Robustness

The search process first moves to the ”goal area”, and there it refines the search. Close to the goal the Newton and Quasi-Newton methods converge very rapidly because the curvature in that restricted area becomes well mapped by these methods.

But in a more irregular landscape (with discontinuities in the objective function or its derivatives) gradient-, Newton and Quasi-Newton methods are not very robust. They may fail.

Only when you need a very high precision are such methods recommended. For problems in biology, medicine, agriculture etc. a *simplex optimiser* is very robust and reasonably efficient. The simplex method also smoothly handles constraints.

Constraints

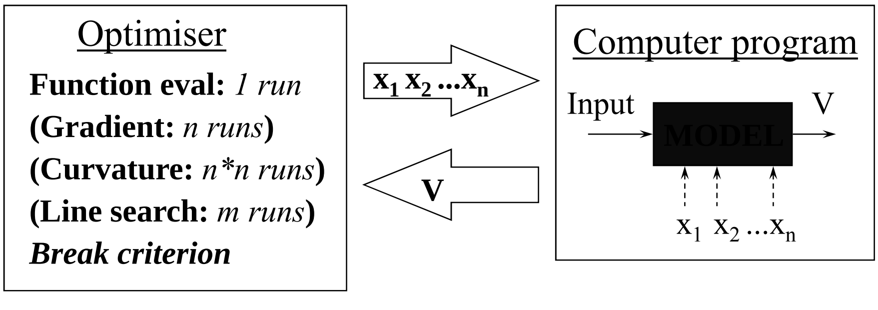
Often, you are not allowed to use any combination of the parameter values x_1, $x_{2,\ldots,}$ x_n. The parameter space is constrained.

Example: You want to maximise the economic outcome of potato cultivation which depends on harvested amount and quality. You control parameters like *amount* (**A**) and *quality* (**Q**) of seed potatoes, *time* for putting them into the soil (**T**), amount to *spray* (**S**) and *irrigation* (**I**), etc. But there are restrictions (constraints):

- Setting the seed: April 10 < T < May 20.
- Water supply is limited: I < 2600.
- Limited economic resources: k_1*A*k_2*Q + k_3*S + k_4*I < 15000

The optimiser and the model

An optimiser is a program that controls the parameter settings of the model (mathematical or simulation program) and runs the model repeatedly, using one of the methods described above. After each run the value of the objective function is returned to the optimiser which sets the values of $x_1\ x_2 \ldots x_n$ for the next run, and so on until the break criterion specified to the optimiser is fulfilled.



4. Model Fitting (Identification)

Two ways of model building:

1. Model building using physical, chemical or other ***well known laws*** which directly give the model equations.

2. ***Model fitting*** (identification). The model which behaves most like the real system is selected .

Model fitting can be performed by:

A) Non-parametric or

B) Parametric methods

Model fitting

A) Non-parametric methods: The system is *disturbed* to reveal its dynamic behaviour.

- Transient analysis (Impulse response, step response ...)
- Frequency analysis and Fourier analysis

These methods display the relations between input and output in a way that can be mathematically described (- an external model).

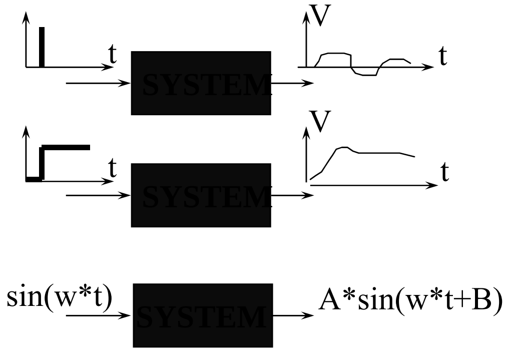
B) Parametric methods: System identification by model fitting. Identification refers to both model structure and parameters (*parameter estimation*).

Identification means specification of the model (on the basis of input and output) so that it behaves like the real system as much as possible (see below).

A) Non-parametric methods

Transient analysis - *disturb the system.*

- *Impulse*
- *Step*
- *Sinusoidal variations*



Impulse response

Step response

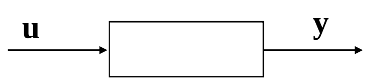
Frequency analysis

Mapping the attenuation A and the phase lag B for all frequencies w gives a description of the input-output relation.

Automatic control treats how a model structure and quantities can be deduced from these kinds of experiments.

Non-parametric methods (contd.)

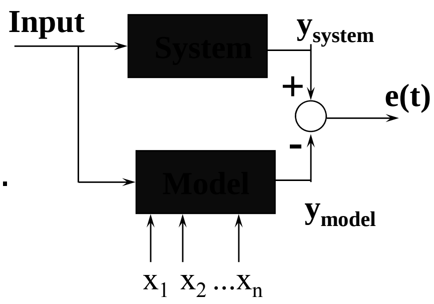
Transient analysis shows the relation between input (impulse or step) and output (impulse or step response) for a system. This gives *a black box description* of the system. The same is true for frequency analysis.



We then get a differential equation relating output, y, to input, u. But no structure of states are involved.

B) Parametric methods

1a) Choose a model structure.
1b) Fit the parameter values so that model and system behave in the same way.
2a) Try another model structure.
2b) Fit the parameter values.
Etc.



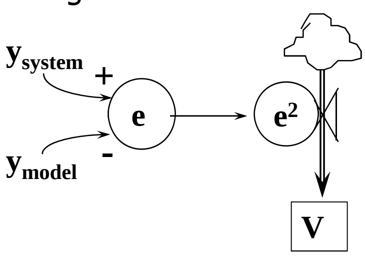
Parameter estimation is finding that set of parameters that minimises the difference between model's and system's behaviour.

The square of the difference:
$e^2 = (y_{system} - y_{model})^2$
is to be minimised
(Least-square fit)

Least-square calculations

The difference $e(t) = y_{system} - y_{model}$ is squared and integrated over the time period studied. $V = \int e^2(t)\, dt$ becomes our objective function to be *minimised* with the help of an optimiser.

In e.g. Powersim this can be done within the model:



Y_{syst}=TABLE(...)
.....
Y_{mod}= ...
.....
e.K=Y_{syst} - Y_{mod}
e2=e*e
V=V+dt*e2
V=0 (*initial value*)

Then, let an optimiser run the model over and over again searching for the set of parameter values giving the least-square value of the difference. This will minimise V.

The model you successfully fitted to the system may still be a bad model!

When you fitted the model to the system, you tuned a number of quantities (parameter values, constants, initial values etc.). The accumulated value of squared errors (V) also gave you a measure of how well the model was fitted. However, *the model structure may still be poor*. Perhaps you should try another model structure and see if that can be even better fitted to the system (giving a smaller V-value). Or perhaps you can reach the same value of V with a simpler model.

Remember: ***Fitting a model to a system also includes model structure!!!***

Over-parameterisation

You can always fit a system behaviour with a complex enough model. This will require a model with many parameters.

If the number of unknowns (parameters) in the model exceeds the information available (for model fitting and validation) we have an ***over-parameterised*** model. Such a model can give you any stupid result.

E.g. Your model is an equation-system of 5 equations that has 6 unknown quantities. Then there are infinitely many different solutions!

E.g. You fit three points with a polynomial model of degree 2 ($y=a+bx+cx^2$) and get a unique solution. But if you use a 3:rd degree polynomial ($y=a+bx+cx^2+dx^3$) you get an infinite number of different solutions.

5. Prediction

Prediction - prophesies about the future - are inherently problematic. Fitting a model to a system so that the model's behaviour agrees with the system's under (historically) known conditions is "trivial". But *fitting the model to the future* (where information about the system structure and behaviour is unknown) *is not possible*. Instead, you have to make a number of assumptions (guesses) about the future. (Especially that "nothing new" happens!)

Also validation against future data is impossible. Therefore: The calculation of the future development by drawing a trend or by simulating a model which was never fitted or validated is extremely risky.

Always be sceptical to predictions!

Is the world predictable?

Prediction (contd)

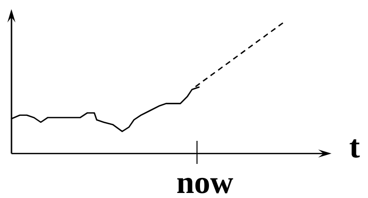
<u>However, planning requires prediction:</u>

- Weather forecast
- Economic planning
- Oil supply in 2015
- Number of school children five years from now

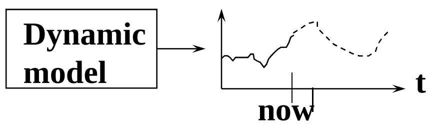
The better information you have, the more reliable the prediction.

Prediction methods

<u>Expanding the trend</u>:
(Very primitive).



<u>Simulating the future</u>:
Dynamic models built on known relations can do more. But the model is not perfect and there is a risk for something not foreseen (oil crises, war, failure of crops...).

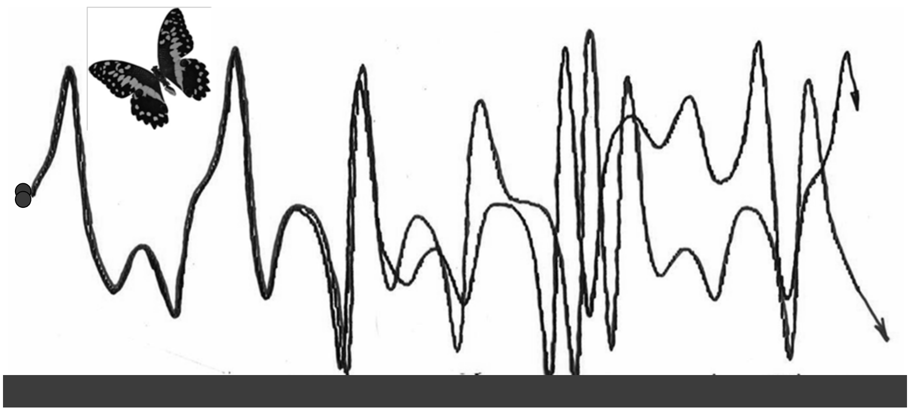


The precision decreases with the time span. E.g. Weather forecasts are often rather good only for a few days ahead.

Warning: *Wishful thinking easily replaces knowledge in the model!*

Since the model was never fitted and validated to future data - don't expect too much from its predictions of the future!

The butterfly effect
sensitivity to initial conditions



”The flaps of the wings of a butterfly in Amazonas may cause a blizzard in Uppsala”

Scenarios for GHG emissions from 2000 to 2100 (in the absence of additional climate policies) and projections of surface temperatures

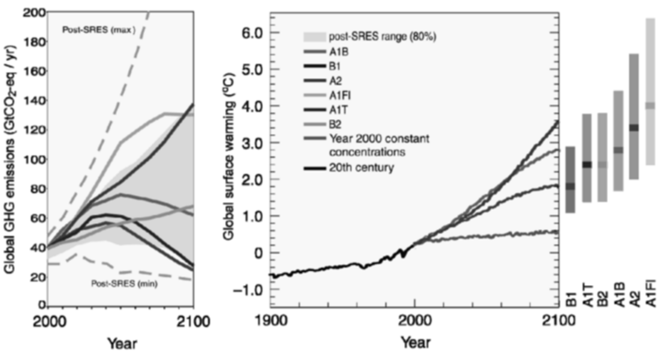


Figure SPM.5. Left Panel: Global GHG emissions (in CO_2-eq) in the absence of climate policies: six illustrative SRES marker scenarios (coloured lines) and the 80[th] percentile range of recent scenarios published since SRES (post-SRES) (gray shaded area). Dashed lines show the full range of post-SRES scenarios. The emissions cover CO_2, CH_4, N_2O, and F-gases. Right Panel: Solid lines are multi-model global averages of surface warming for scenarios A2, A1B and B1, shown as continuations of the 20[th]-century simulations. These projections also take into account emissions of short-lived GHGs and aerosols. The pink line is not a scenario, but is for Atmosphere-Ocean General Circulation Model (AOGCM) simulations where atmospheric concentrations are held constant at year 2000 values. The bars at the right of the figure indicate the best estimate (solid line within each bar) and the *likely* range assessed for the six SRES marker scenarios at 2090-2099. All temperatures are relative to the period 1980-1999. {Figures 3.1 and 3.2}

Predictions of human development

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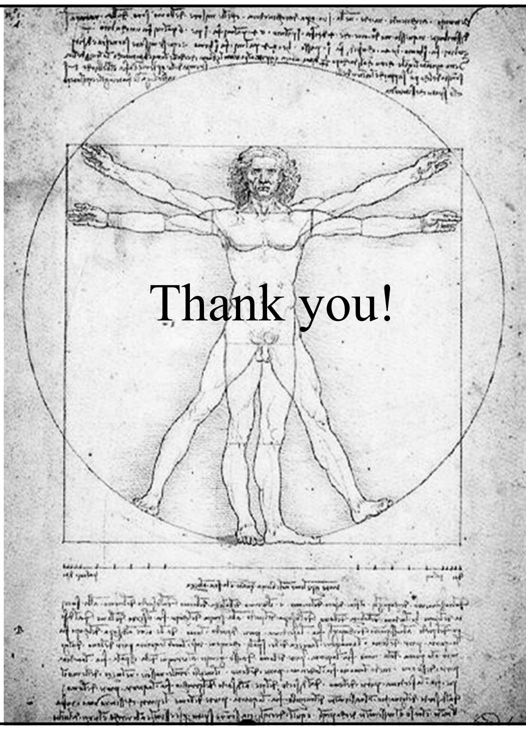

Thank you!