The Future Potential of Computer-Based Empirical Modeling

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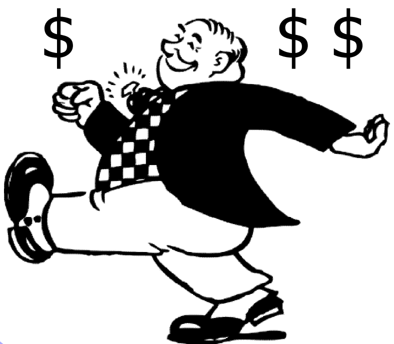
What if we could foresee the future?

- …then we would know, for example, when to alter things to avoid foreseen undesirable outcomes.

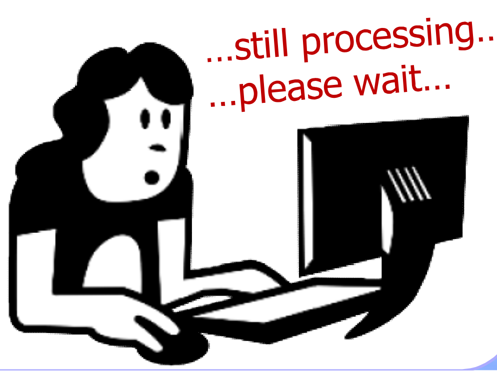
and what if we could predict the effect on the future of altering things?

- …then we could determine an optimal future for ourselves.



We are developing this ability, not using a crystal ball of course:

- …but using computer-based mathematical modelling!



Of course, computer modelling is not the only way to predict the future:

- …but it is the most pervasive and powerful such tool
  - from assisting decision-making
  - to automated systems control
- …and importantly it has a tremendous untapped potential
  - the main subject of this presentation (later)

and it is not just used for predicting the future; other applications include:

- …evaluating the past (eg: legal claims, what happened?)
- …evaluating the present (eg: locating fatigue cracks in structures)
- …pattern recognition
- …teaching and training (simulators)…

SOME BACKGROUND:

What is a mathematical model?

- abstraction of a system (real or otherwise) using the language of some branch of mathematics:
  - logic, statistics, algebra, algorithms, etc…
- uses include:
  - experimentation (to investigate a system)
  - prediction (for decision-making, automated control, etc…)
  - evaluation (for pattern recognition, classification, etc…)
- greatly facilitated by modern digital computing

Common dichotomy of mathematical modelling:

- theoretically derived models

versus

- empirically derived models

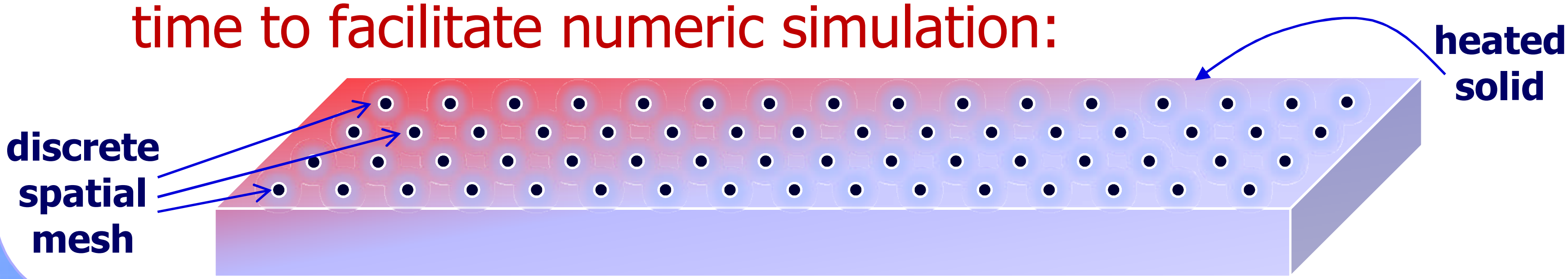
What is a **theoretically** derived model?

- …one developed from the fundamental laws or principles that govern the response of the real system
- eg: a model of **heat dissipation** in a non-translucent solid would be based on the following:

$$\partial T/\partial t = k \cdot (\partial^2 T/\partial x^2 + \partial^2 T/\partial y^2 + \partial^2 T/\partial z^2)$$

T = temperature
t = time
k = thermal diffusivity of solid
x, y, z = spatial dimensions

- which would usually be discretized across space and time to facilitate numeric simulation:

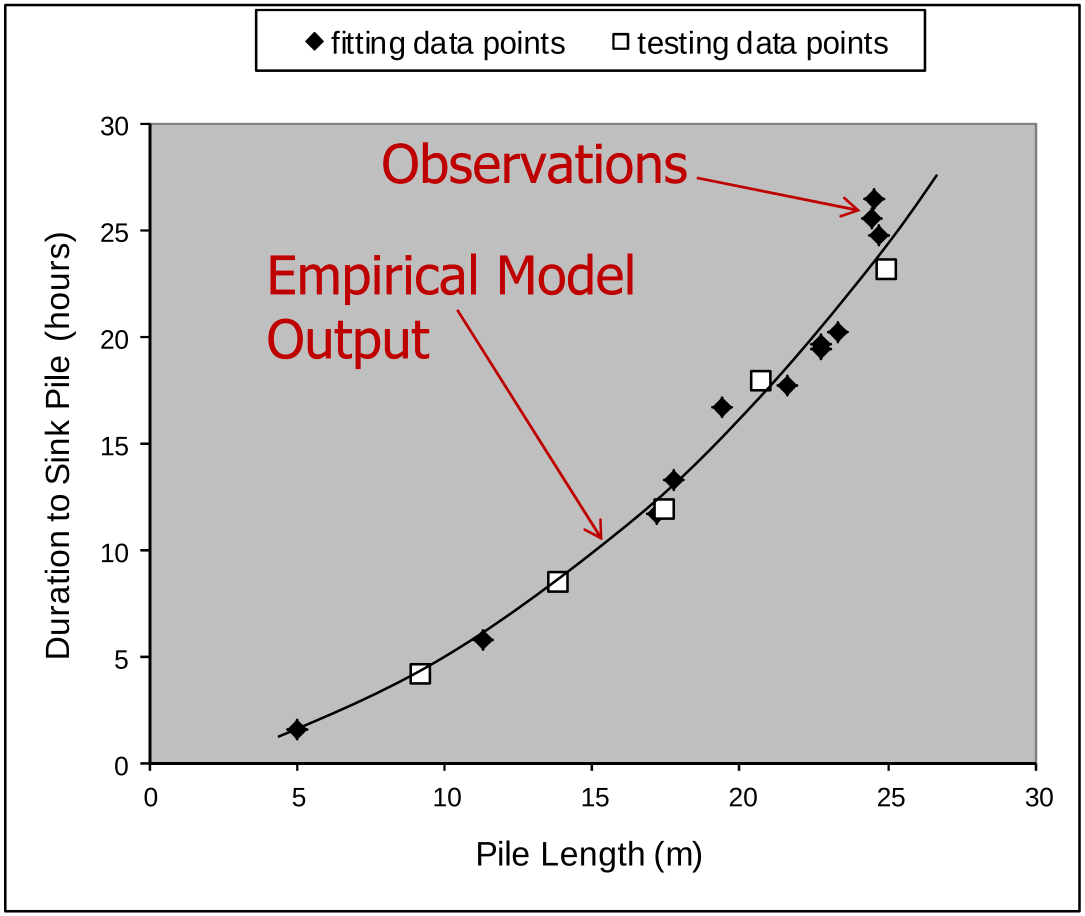


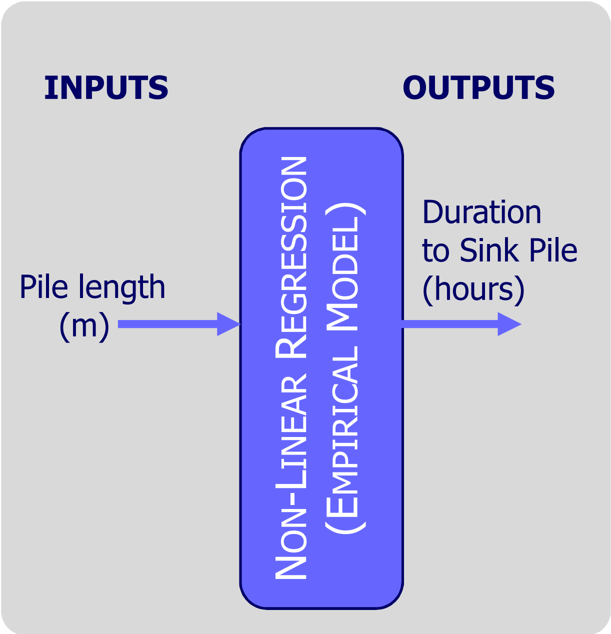
Disadvantage of theory based modelling:

- if the theory is not known then cannot develop the model
  …the theory is often not known (or only partially known)!
- and so we must resort to empirically based modelling
  …or if possible a hybrid of theoretical and empirical

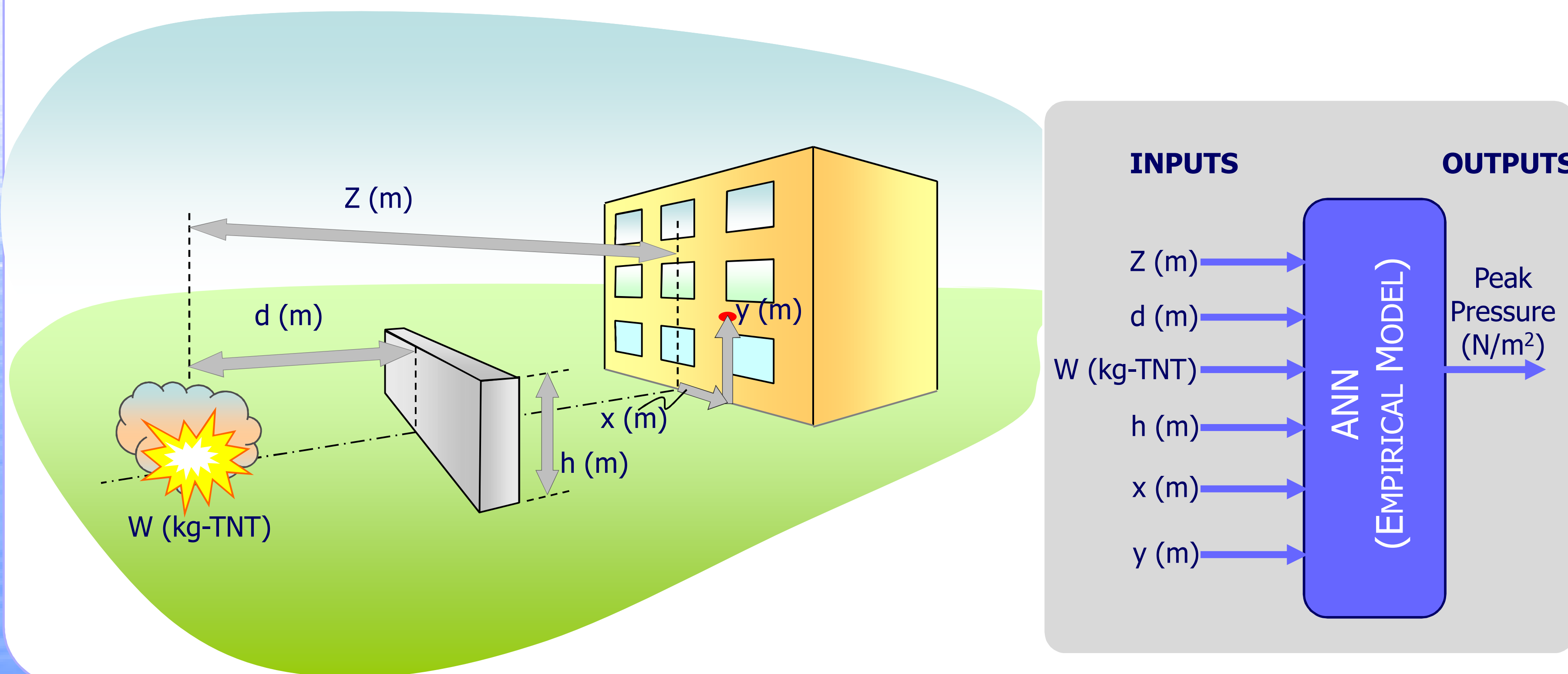
What is an **empirical** model?[1]

- one developed from observations of the type of system under investigation
  - based on some measure of the quality of its output (replication, utility)
- simple example:

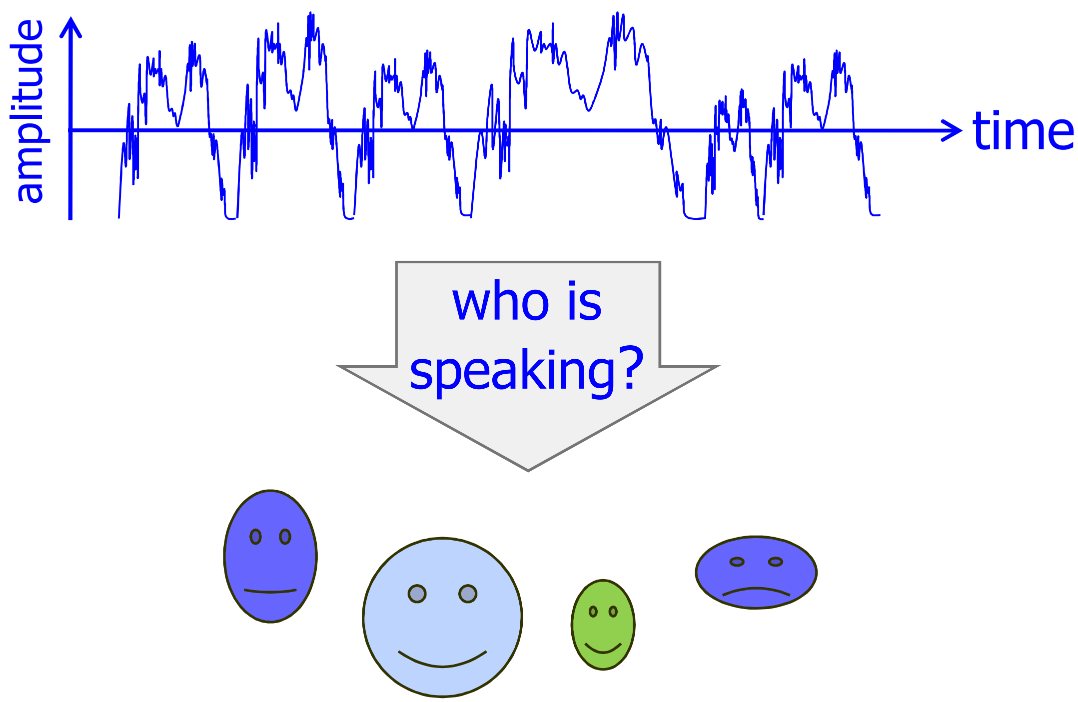


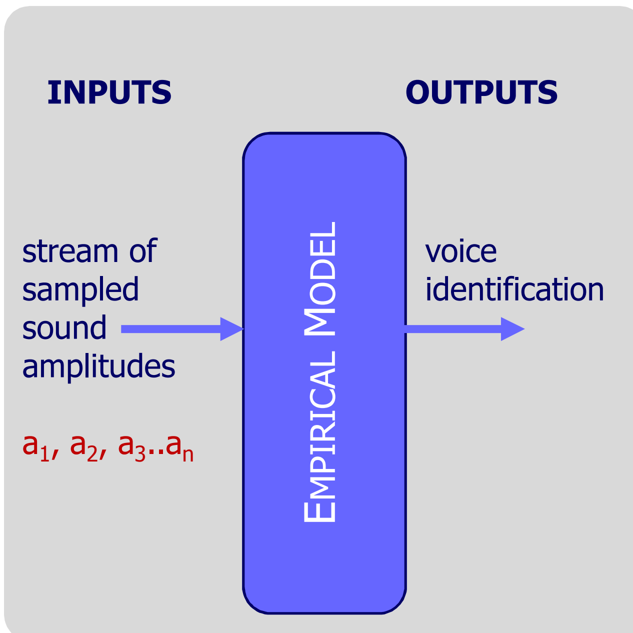


- …**or** one developed from observations of an **analog** of the system under investigation (a model of a model):
  - eg: neural net (ANN) for predicting bomb blast pressures on a structure … since the simulation model was too slow for use by engineers.[2]
  - used the simulation model to generate training patterns for the ANN …since detonating explosives near real buildings was too expensive!

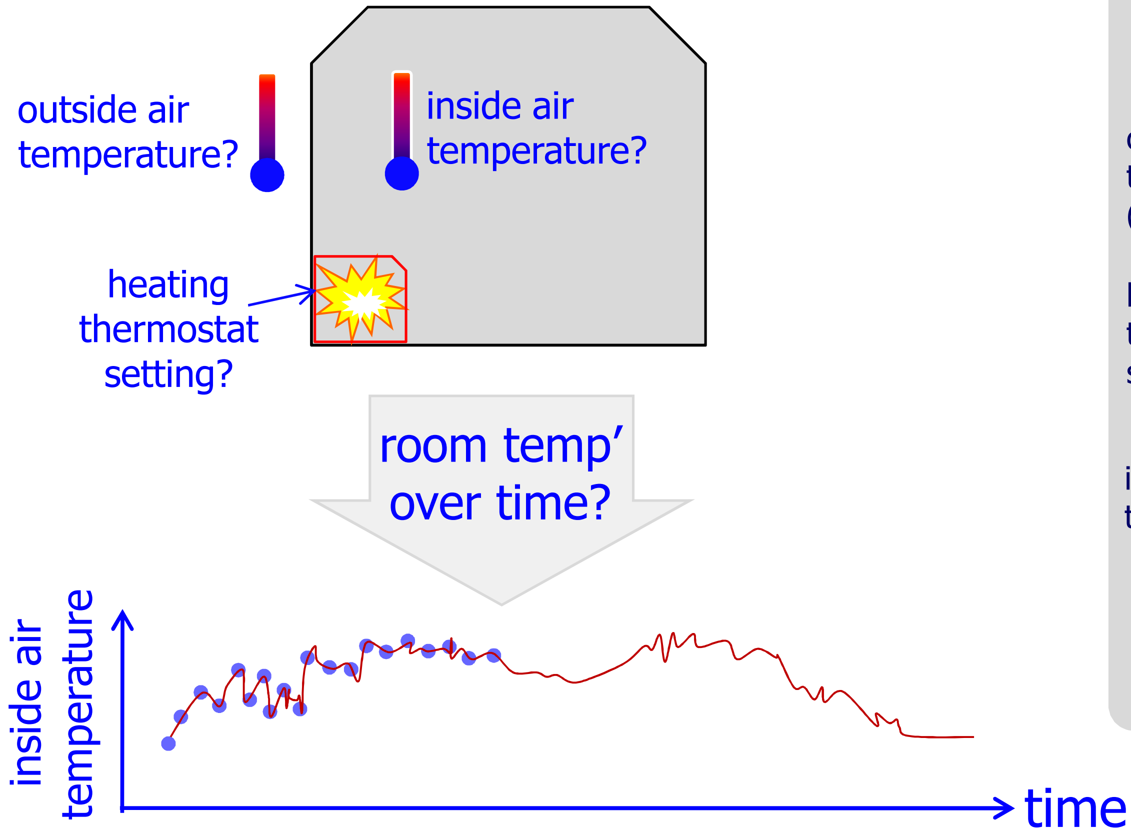


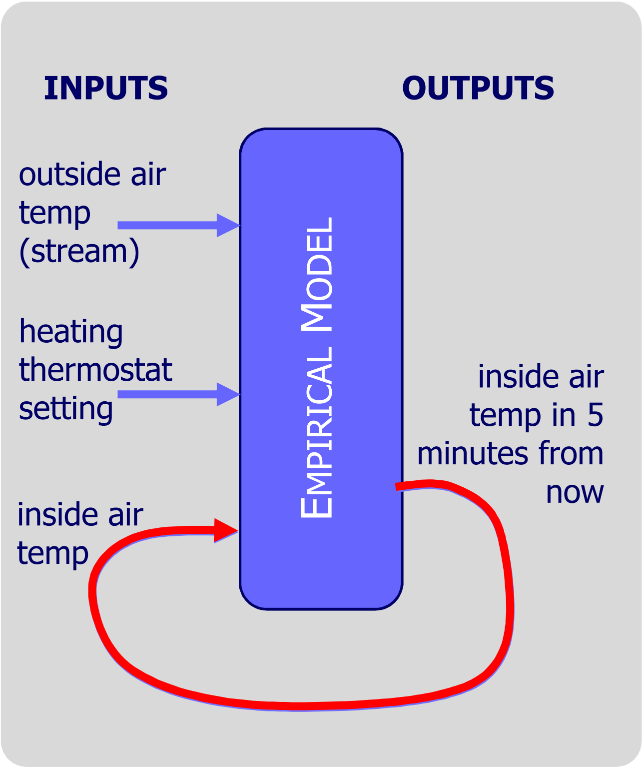
- …can receive **streams** of input (time-wise input)
- …and/or generate streams of outputs:
  - eg: for voice identification, a stream of inputs representing sound amplitude are integrated by the model to generate a single conclusion:



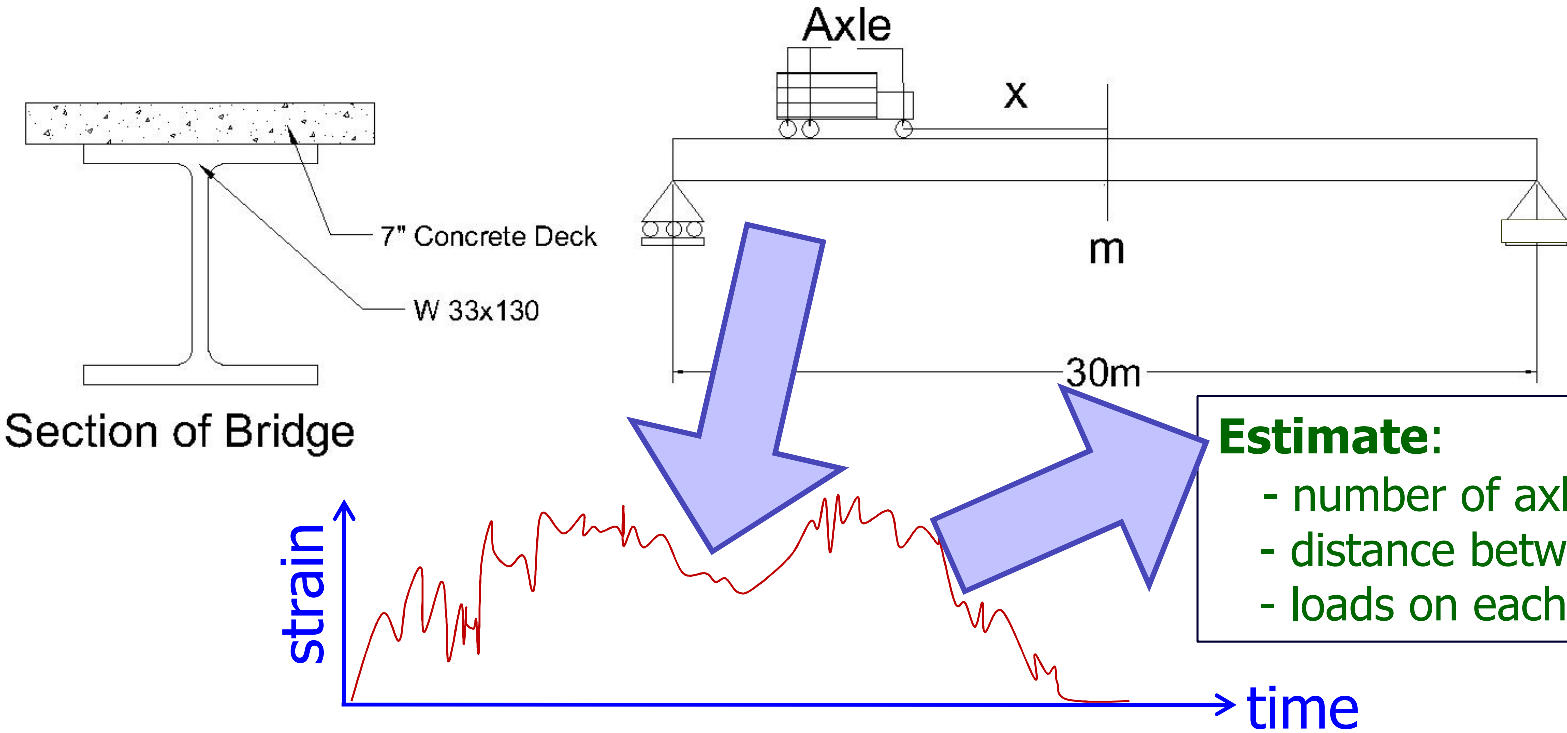


- …can operate **recursively** (self-feedback), a special case of streaming input and streaming output:
  - eg: predicting room temperature over time:



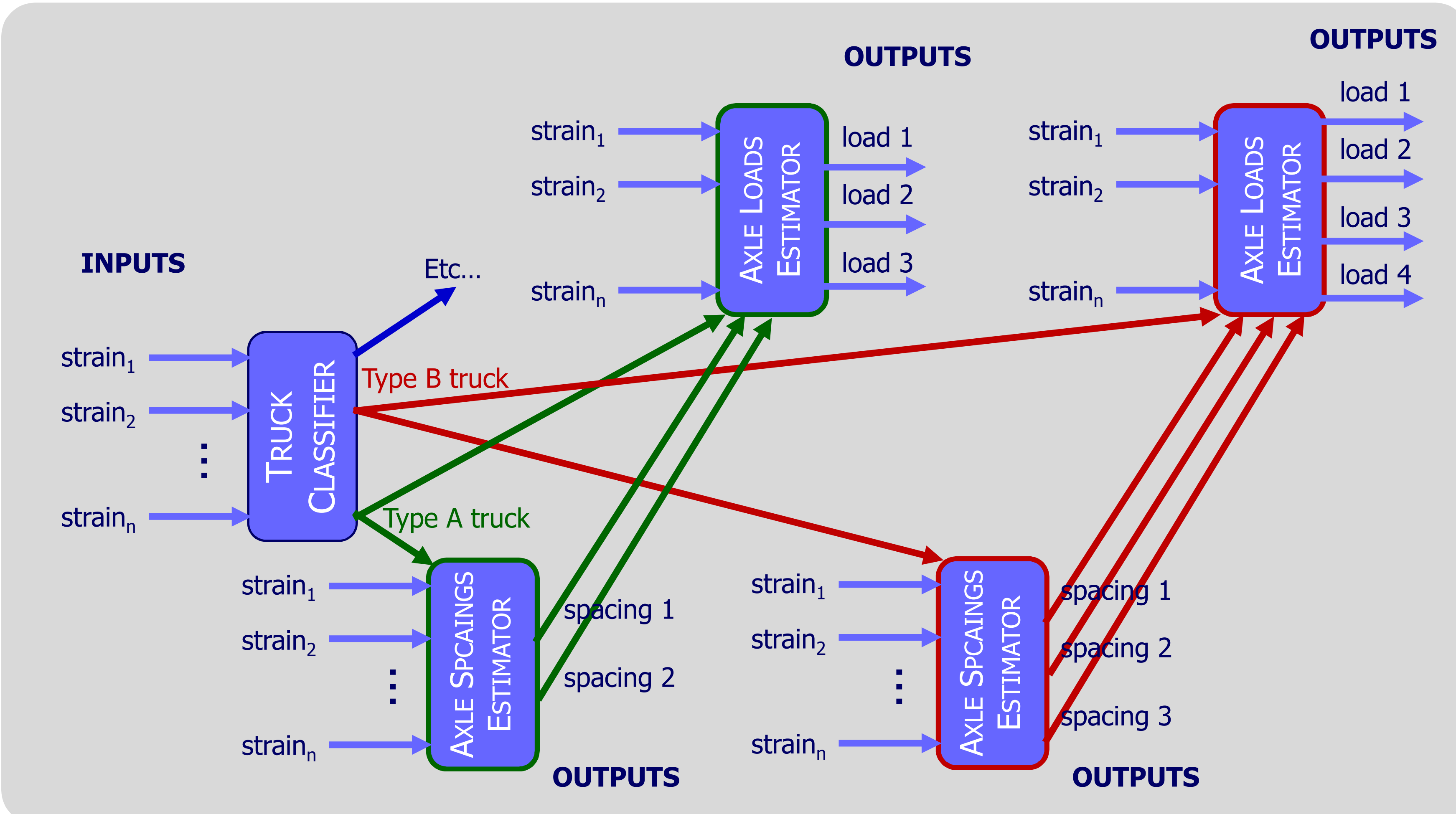


- …can have a rich **internal structure**:
  - maybe developed directly by the modeler (handcrafted & modular)
  - …or developed automatically (such as by a genetic algorithm)
  - eg: determining truck attributes from the strain they induce on a bridge



Estimate:
- number of axles,
- distance between axles
- loads on each axle.

– the model may be crafted as follows comprising a set of modules performing predefined functions (sequential and concurrent ordering)[3]:

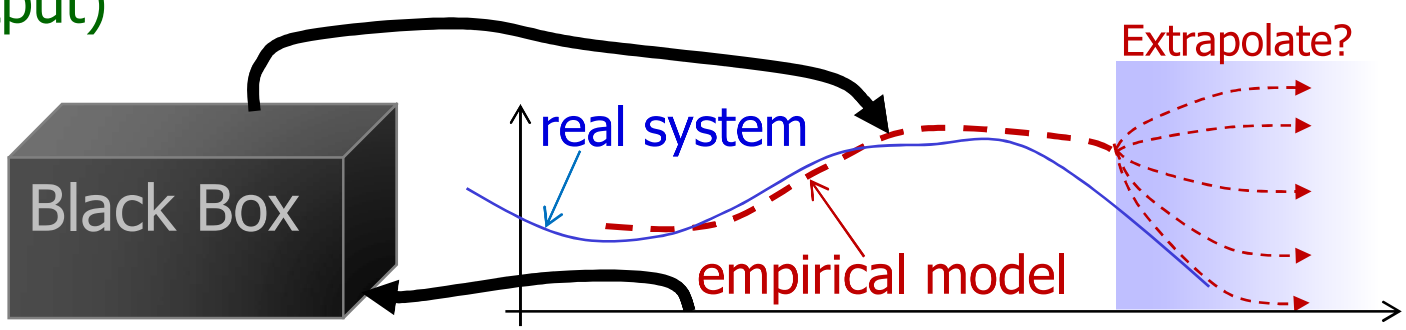


Disadvantages of empirical modeling:

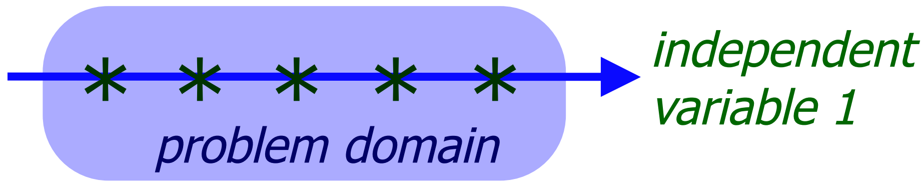
- many disadvantages are cited…
- …however, these are not absolute limitations but rather **challenges** that we are attempting to overcome:

Challenges:

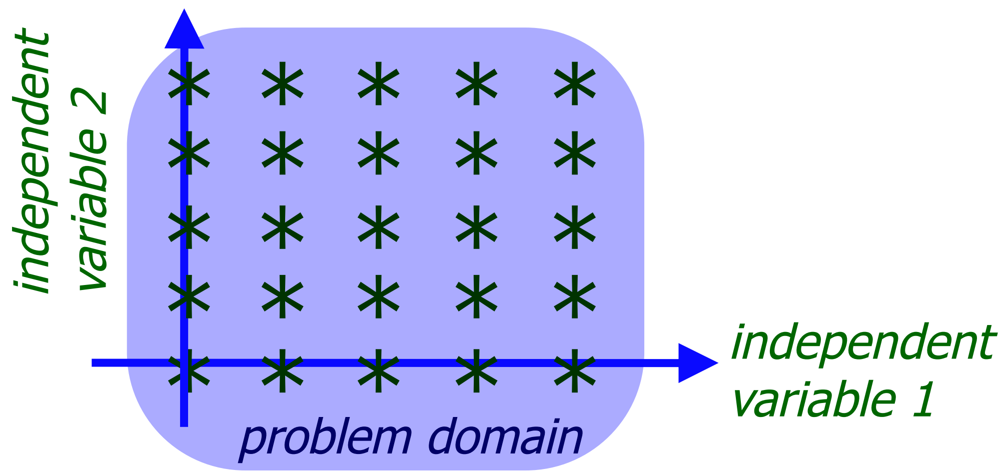
- can interpolate but less accurate than theoretical models (in truth is often more accurate than theoretical modelling)
- limited ability to extrapolate (beyond the set of solutions used in their development)
- are *black box* devices (providing no explanation of their output)



- the number of observations required increases geometrically with the number of independent variables:
  - say we need a density of **5** training examples across the range of an independent variable:



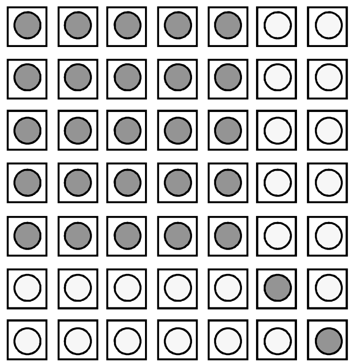
  - with two independent variables this increases to 5^2=**25** examples:



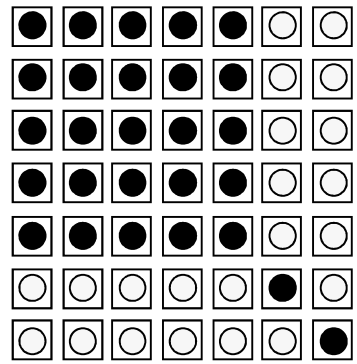
  - for ANN's a practical limit is typically **5 or 6** independent variables, say 5^6=**15,625** observations, otherwise training is too slow.

# independent variables:	1	2	3	4	5	6	7	8	9
# observations (5/variable):	5	25	125	625	3,125	15,625	78,125	390,625	1,953,125

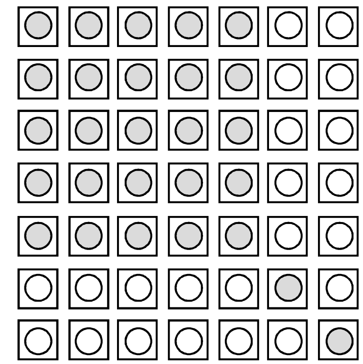
- a need to handle various types of variance, such as:
  - value/amplitude variance for spatially distributed inputs:



Base values (amplitudes)

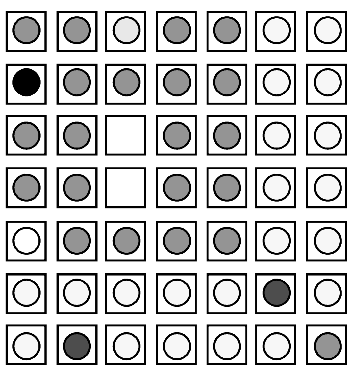


Values (amplitudes) increased



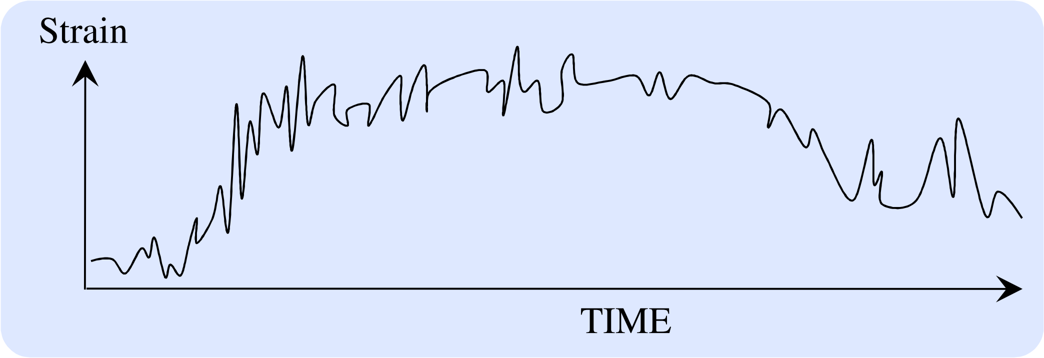
Values (amplitudes) decreased

  - stochastic variance and error for spatially distributed inputs:

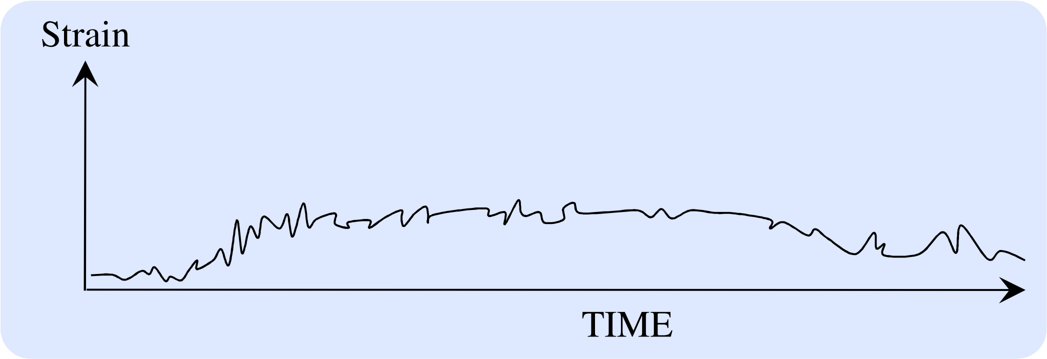


Noisy and missing values

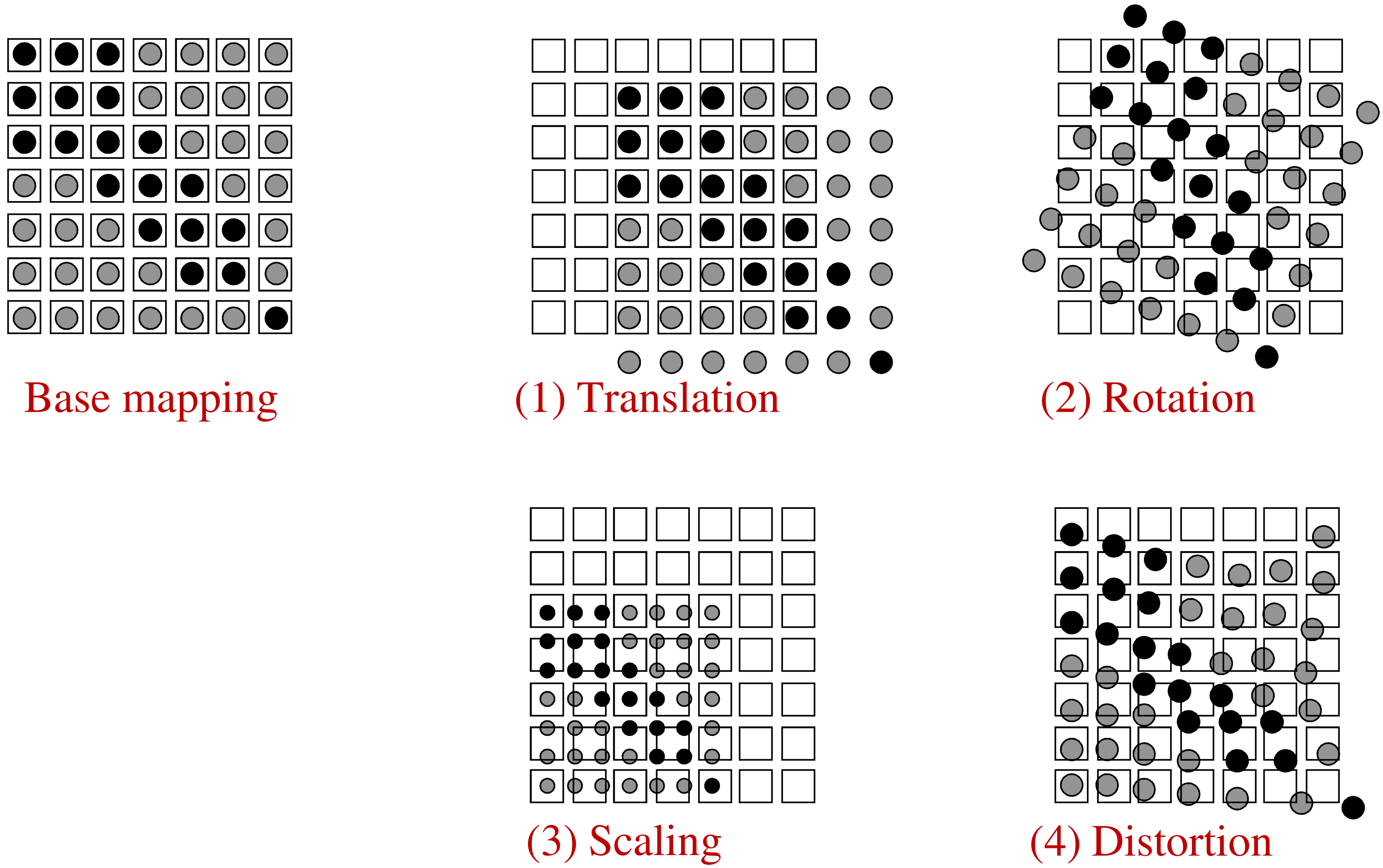
- value/amplitude variance for streams of input
- eg: strain in girder induced by truck crossing bridge



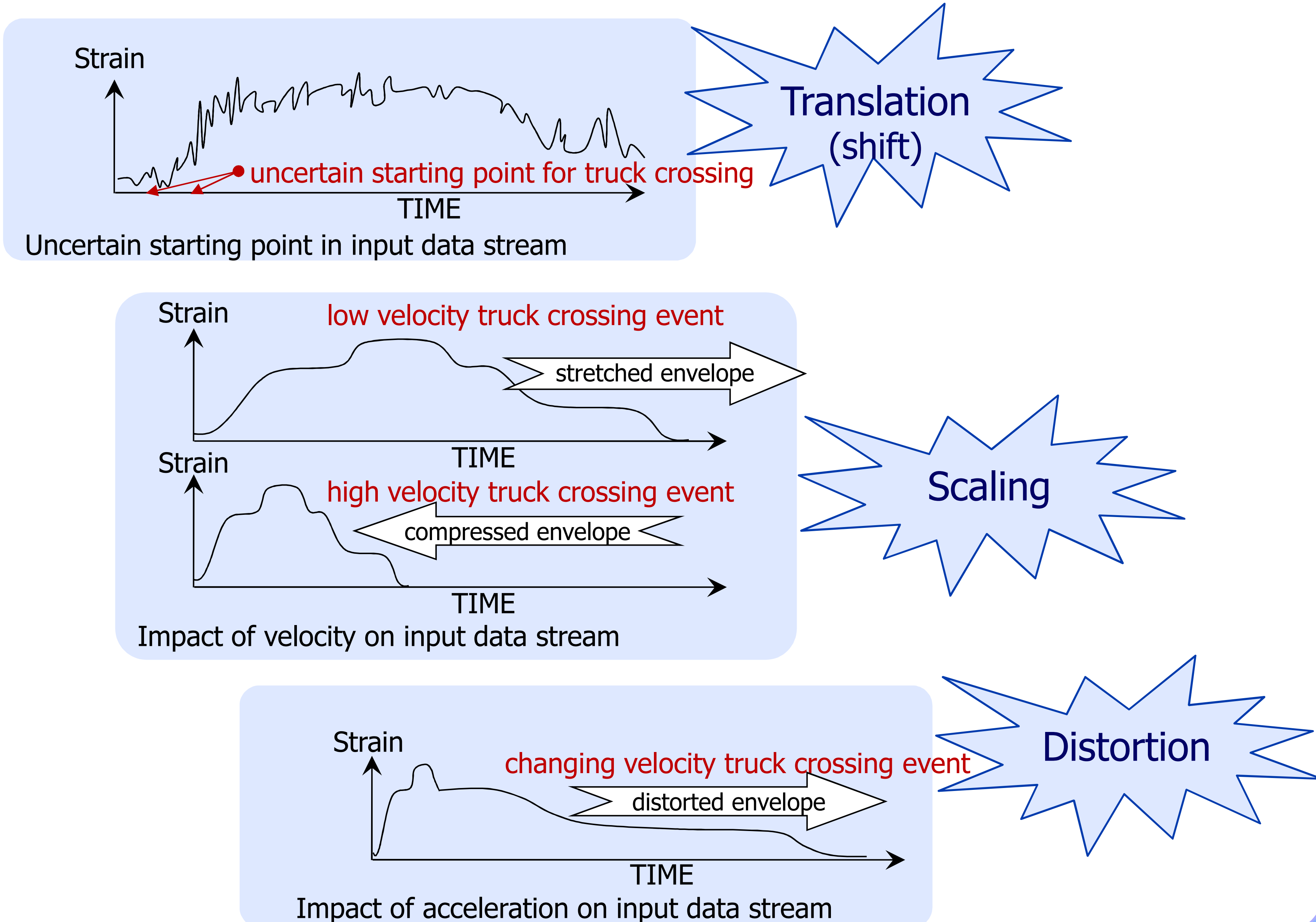
lower amplitude could be due to lighter loads
OR due to truck travelling in adjacent lane
- ambiguous



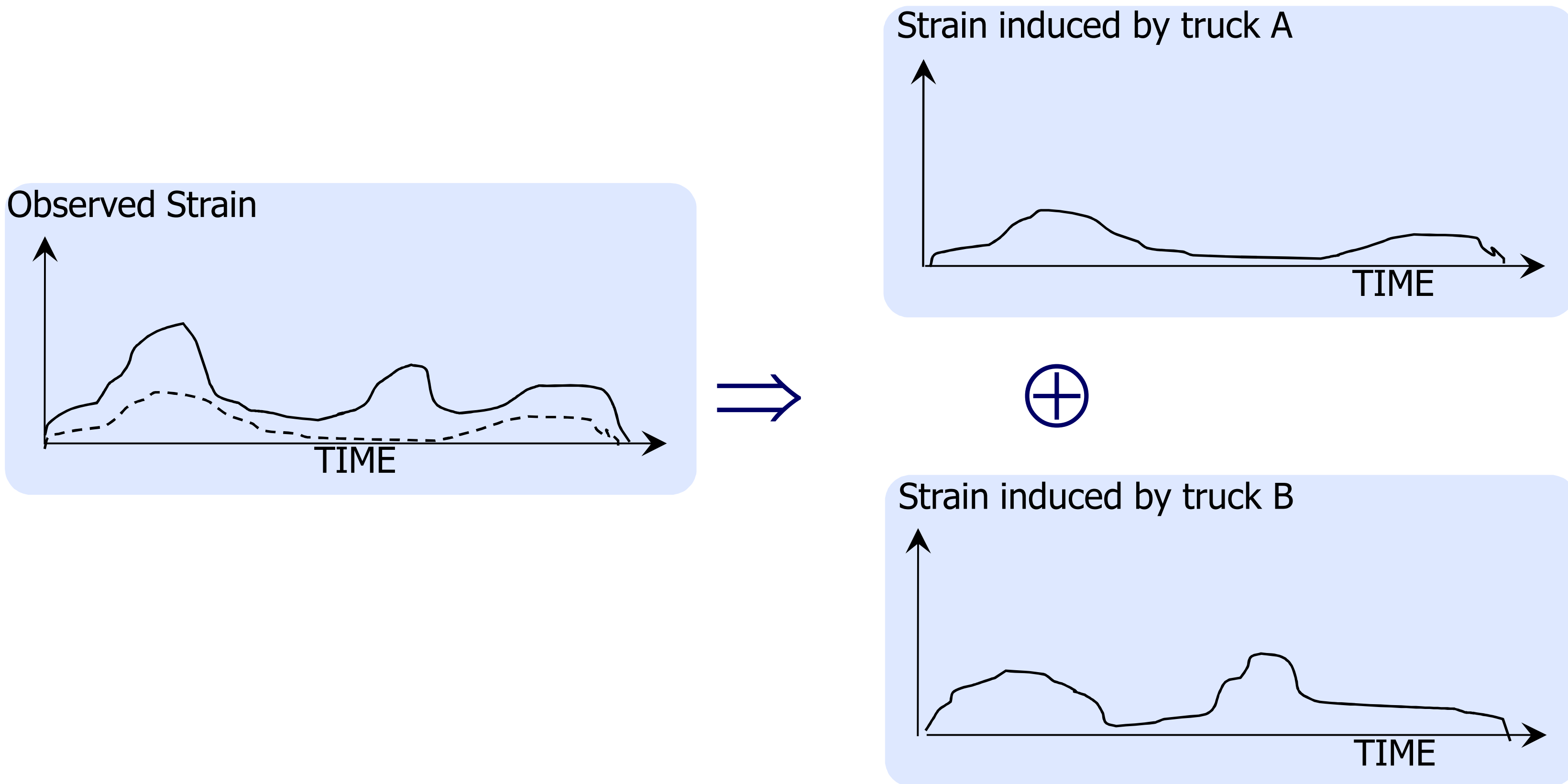
- a need for flexibility in the input format:
  - empirical models usually restricted to a fixed layout of the input values
  - …yet many problems require variation in the presentation of the inputs
  - variation may be for spatially distributed inputs:



- …or variation may be for streams of inputs
- eg: strain in girder induced by truck crossing bridge

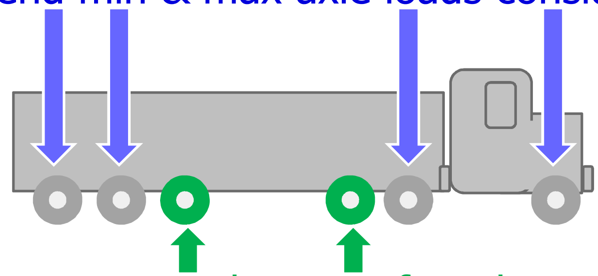


- uncoupling data sets:
  - many data sets/streams comprise two or more **overlapping** (or partially overlapping) data sets/streams
  - …we often need to **uncouple** them to handle them separately
  - eg: strain induced in girder by 2 trucks crossing bridge simultaneously



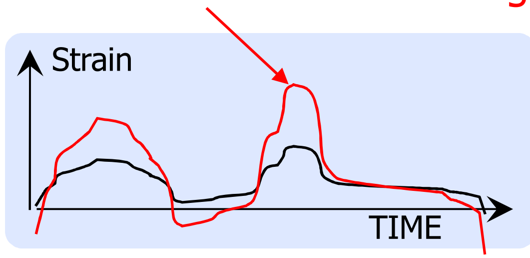
- extendibility of a model:
  - empirical models are developed to solve a class of problems
  - …often there is a need to **extend** the class of problems solved (increase the functionality of the model)
  - …eg: determining truck attributes from bridge strain data:

extend min & max axle loads considered (extend values of dependent variables)



extend range of truck types considered
(extend model internal structure, extend number of dependent variables)

extend range of values for strain readings considered (extend values of independent variables)



Others:
extend bridge lengths considered,
extend number of lanes, etc…

  - extension should be achievable without the model-user having to rebuild the existing model

APPROACH TO THESE CHALLENGES:

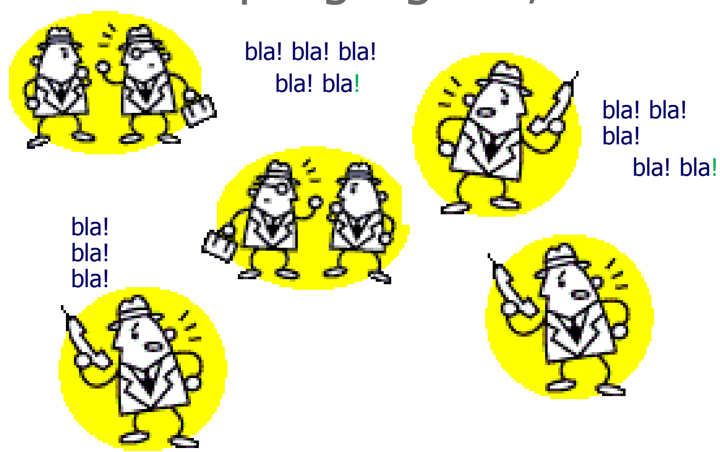
Two key considerations in empirical modelling:

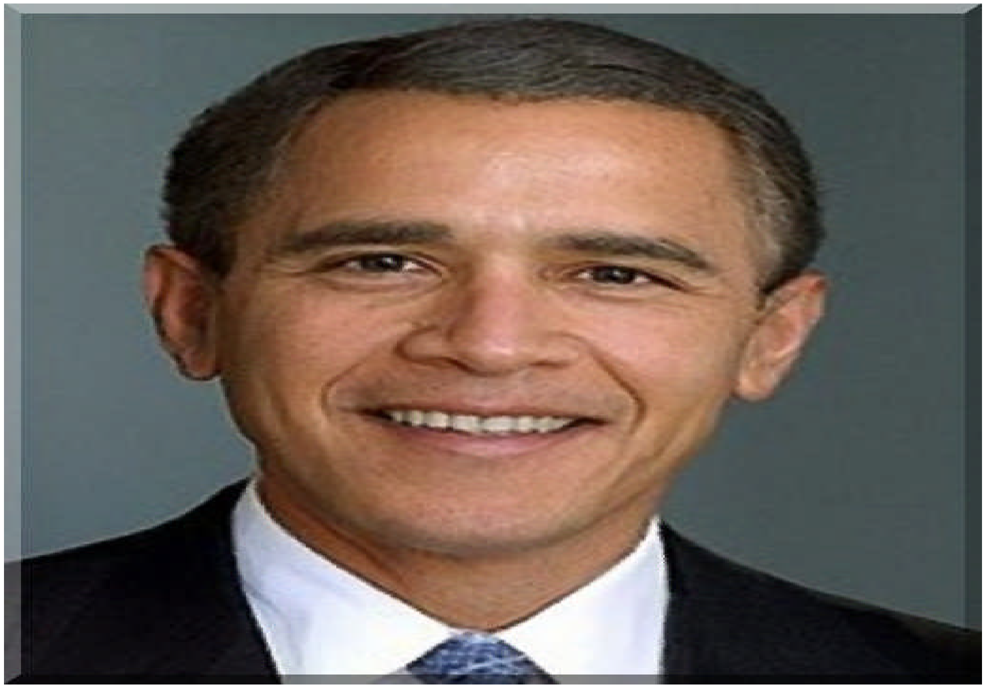
- (1) the structure and operation of the model
  - eg: feedforward ANN with sigmoidal activation functions
- (2) the method of developing the model
  - eg: backpropagation training to develop the weights in an ANN

…any approach to empirical modeling must consider both these aspects

A rich future source of inspiration for empirical modelling is **the brain**:

- provides effective **empirically derived** solutions to many complex problems
- overcomes many of the challenges identified earlier:
  - eg: face recognition: spatial interpolation, translation, rotation, scaling, distortion, amplitude, noise:
  - eg: following a single conversation amongst a chattering crowd: uncoupling signals, etc…





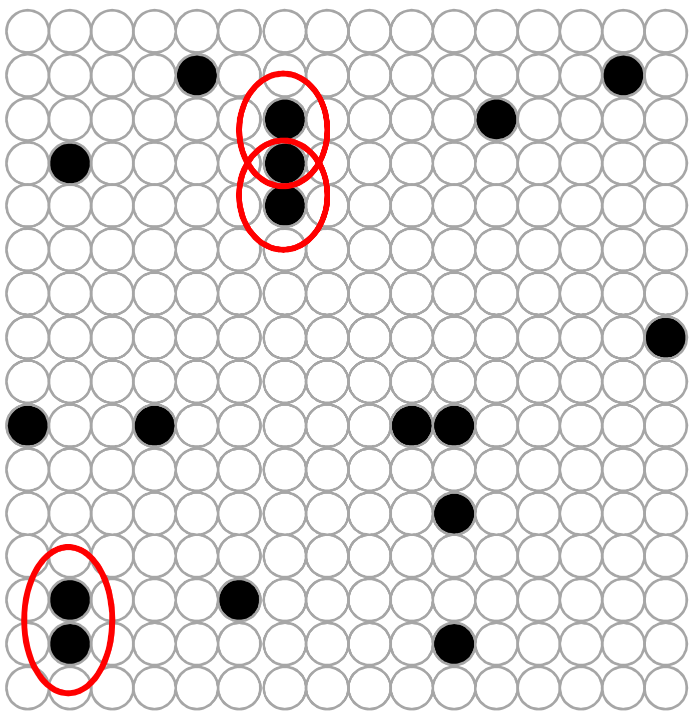
Which US president(s) do you recognize?

Image: Adapted from Washington's Blog March 2013

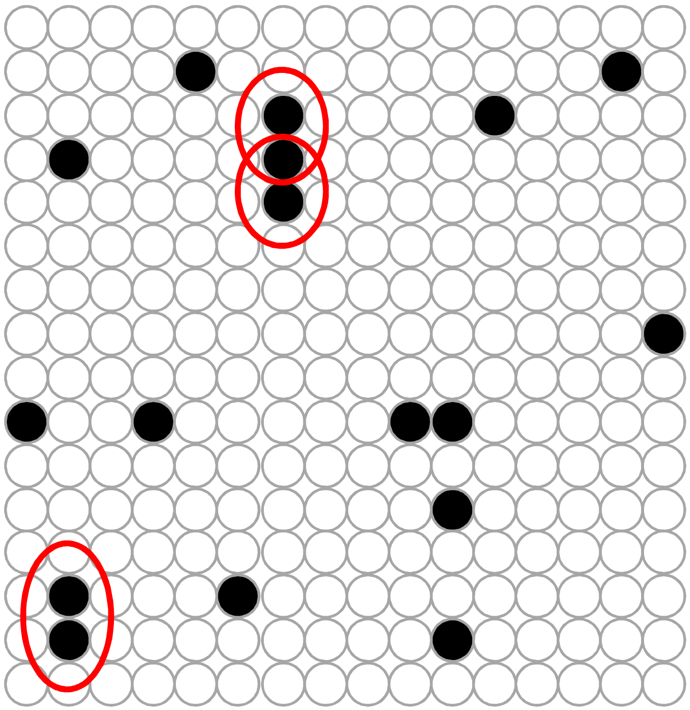
- arguably **the brain** is the ultimate black box

  …but as we start to analyze its organization and operation we are discovering:
  - parts of the brain, at least, model the world as a set of **meaningful** features within a rich **hierarchical** structure
  - **lowest level in the visual system hierarchy** comprises detectors tuned to local features in an image such as orientation, spatial frequency, direction of movement, speed…
  - **second level in the visual system** integrates lowest level output with more specialized detectors tuned to features such as contours
  - **ultimately within the hierarchy** there are detectors tuned to very high level tasks such as recognition of a face (a US president)
- similarly other brain systems, such as the auditory system, are based on a hierarchy of tuned feature detectors
  - …(although there are many other sub-systems in the brain for which we currently have little or no understanding)
- so, empirical models do not have to be black boxes
  - they can develop **richly structured models** of the world
  - …where the internal structure is an **insightful analog** of the internal structure of the problem represented

- what about exponential explosion in number of observations required?
  - richly structured models can resolve (or help resolve) this challenge
  - consider the simple problem of identifying vertical lines of two adjacent dots on a receptive matrix:



matrix size	total # of possible observations	# of 2 dot features that are vertical and adjacent
2 x 2	$4^2 = 16$	2
3 x 3	$9^2 = 512$	6
4 x 4	$16^2 = 65,536$	12
5 x 5	$25^2 = 3.36 \times 10^7$	20
…		
16 x 16	$256^2 = 1.16 \times 10^{77}$	240



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…		
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- a direct mapping model (mapping directly from input to output) would require a # of example observations proportional to column 2

  …the model would also be proportional in complexity to this

  …currently, most empirical models are implemented as direct maps
- a structured model (in this case with local feature detectors) would be proportional in complexity to column 3
- this is a simple example, but the argument extends to more complex patterns (if use a hierarchy of feature detectors)

- what about extendibility?
  - structured models are highly conducive to extension due to their inherent modularity
  - …extending the size of the receptive field (previous example) would just require an extension in the number of feature detectors
  - example is the coarse-grain modelling approach for the simulation of blast wave propagation around complex geometries:[4]
    - the spatial matrix through which the wave propagates is composed of empirically derived sub-models

      …allows model to be configured from a course mesh (1 m vs. 2 cm)

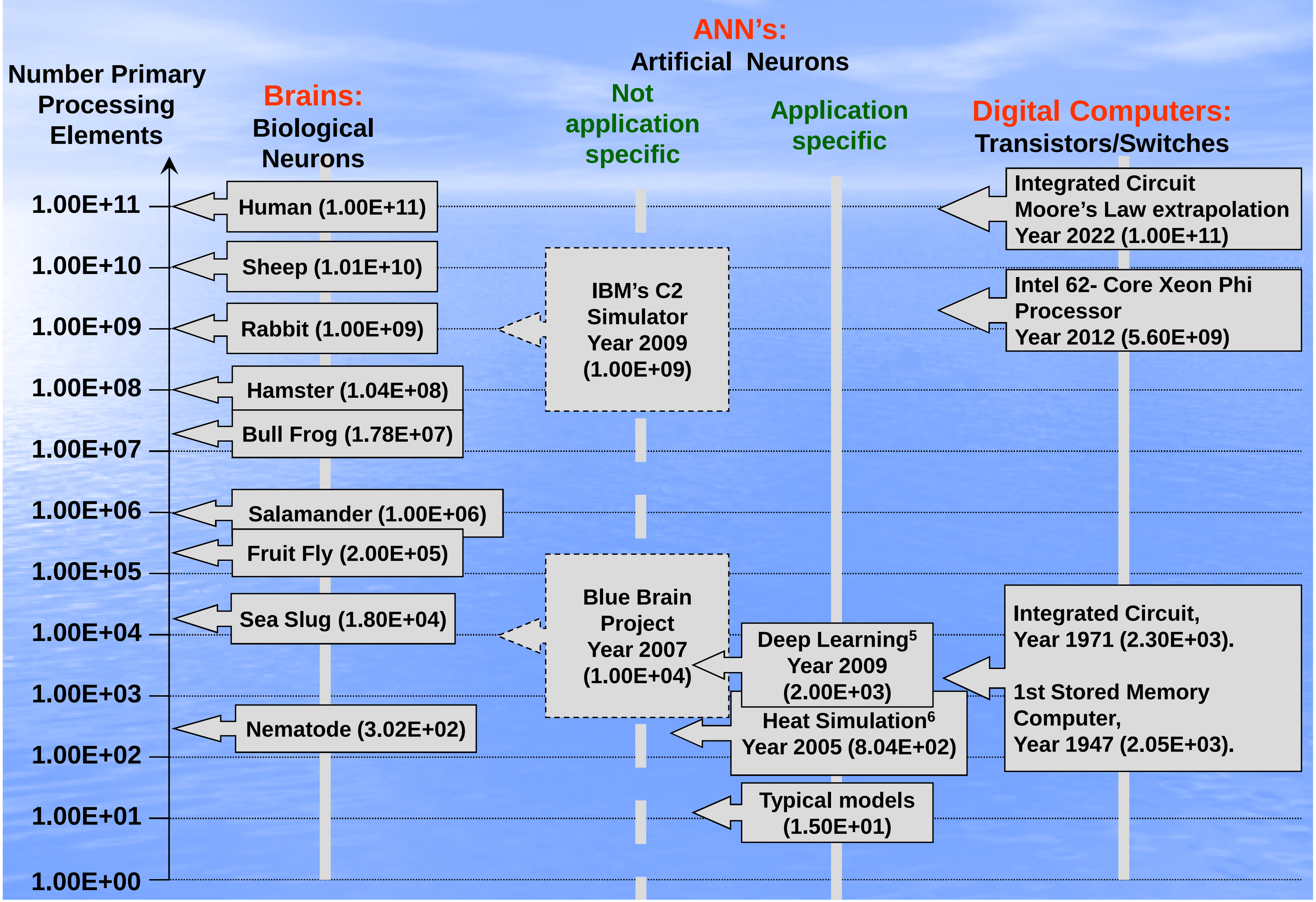
      …yet retains accuracy of conventional simulation

- indeed, the brain has provided modelling inspiration for 60/70 years in the fields of:
  - artificial intelligence (emulate intelligence at a high level)
  - …and in particular ANN's (intelligence is an emergent property)

- …however, progress has been frustratingly slow
  - our knowledge of how the brain interprets, represents, and processes different types of information is still **rudimentary**
  - **practical applications** have similarly been limited in terms of the complexity of the problems solved

- compare the progress of ANNs with other devices:
  - **digital computing** has developed exponentially
  - can now build **massive ANNs** comparable in size to small mammalian brains (although operationally simplified)
  - …but not been able to exploit this in **practical applications**
  - biological model indicates a far **greater potential**

Compare progress: ANNs versus General Purpose Digital Computer



- then there is the question how to develop richly structured models:
  - need to learn their own **internal structure** and **representations**

    …these are not an explicit part of the observation data
  - for the brain:
    - parts of a model that are common to a broad range of problems may be developed through **evolution**
    - more novel aspects of a problem developed through direct experience (training)

    …how to apply either of these processes effectively within a computing environment is not clear

    …especially true for very large models (comprising say millions of neurons)
    - simulated evolution and other training methods are slow to converge for large models
- **Deep Learning** (Hinton et al.) is one of several attempts at developing models with rich internal structures
  - however, applications have been fairly limited (character recognition for example).

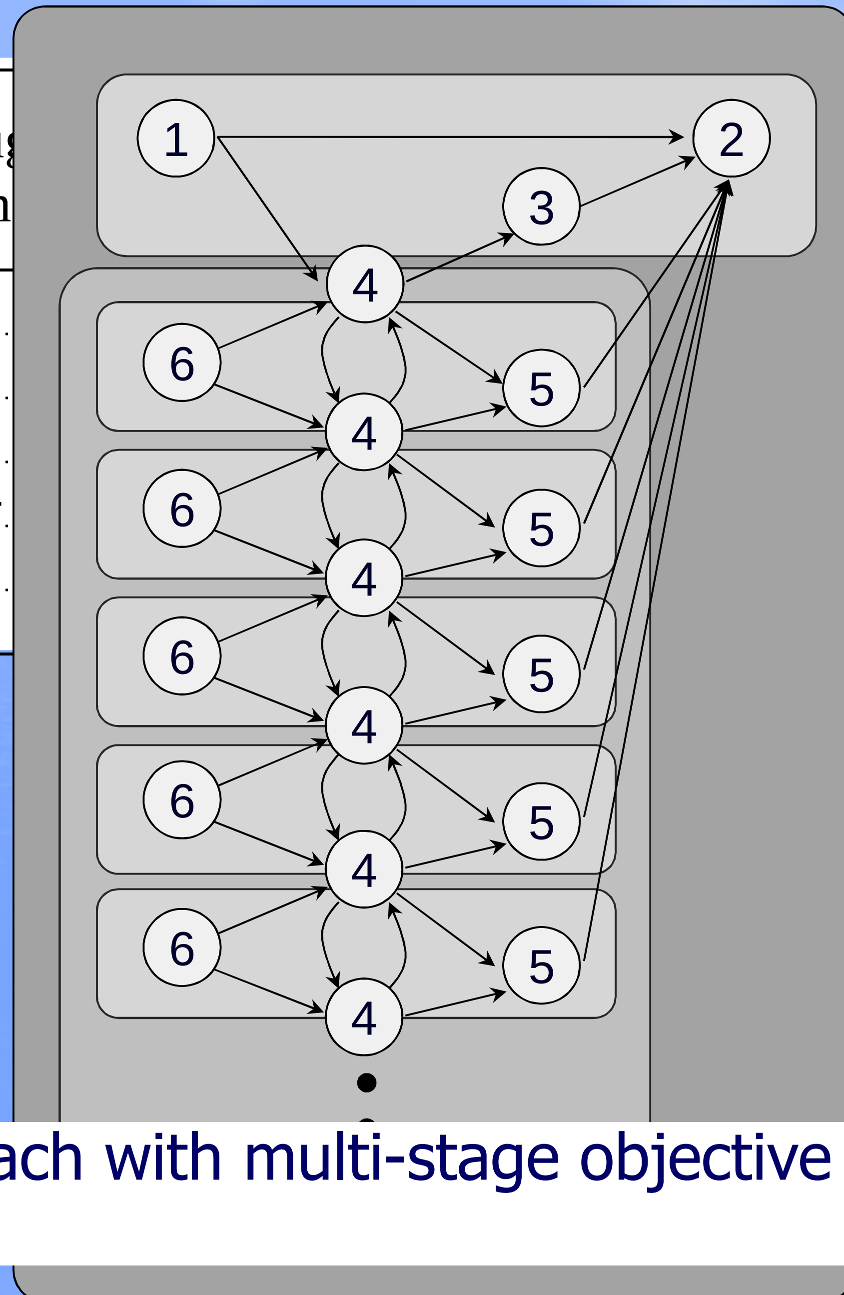
- an alternative approach for developing massive very complex model structures is **artificial embryogenesis** (growth algorithms)
  - simulated evolution would be applied to a **genotype**
  - the genotype is NOT the end model but rather a **code** used to direct the growth of the model
  - possibly well suited to structures that have a lot of **repetition**

    …only one version of the repeated element would have to be learned

- Consider the following simple growth table:

Neuron type:		1^{st} daug neuron	er pe
1	$\Rightarrow$	2	
2	$\Rightarrow$		
3	$\Rightarrow$	5	
4	$\Rightarrow$	4	
5	$\Rightarrow$	5	
6	$\Rightarrow$		

...continue this process:



- could enhance this approach with multi-stage objective functions

SUMMARY AND CONCLUSIONS:

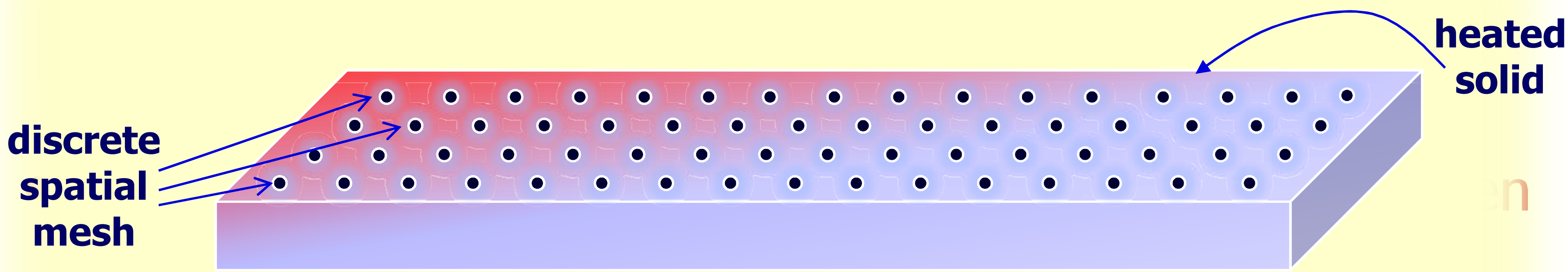
Empirical modeling:

- a very powerful means of modelling
  …but its potential has been largely untapped
- current models tend to be direct mapping devices:
  - no significant internal structure
  - provide no analog of the internal workings of the system under consideration
  - consequently restricted by issues such as:
    - **black box** devices
    - **number of observations** required for development = geometric function of number of independent variables
    - limited ability to handle **variance** in the presentation of a problem
    - limited ability to **extrapolate** and extend to new versions of a problem
- approach to overcoming these challenges:
  - inspiration from biology:
    - structure, operation, evolution, development, and learning in the brain

Ultimately, all mathematical models (theory based or otherwise) are derived empirically

- reconsider modelling heat dissipation in solids:

$$\partial T/\partial t = k \cdot (\partial^2 T/\partial x^2 + \partial^2 T/\partial y^2 + \partial^2 T/\partial z^2)$$



- the equation will have to be discretized in time and space to account for the geometry of the solid:
  - an appropriate size of the discrete elements and time steps would have to be determined by **trial and error**

  …to find a trade off between processing speed and accuracy.

Equally, we can claim the opposite:

- empirically derived models provide a theory describing a system
- …just that some theories provided are stronger than others
- …strength of the theory provided by an empirically derived model can be measured by its utility:
  - how accurately does it map from input to output
  - how well it extrapolates beyond the examples used to develop it
  - how well it extends to new versions of the problem
  - how well it helps us understand the pertinent aspects of the system it represents
- the idea is that: if the model has an internal structure that is analogous to that of the internal structure of the system represented:
  - …then it may provide a stronger theory
  - but it must capture the pertinent aspects of the system's structure.

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