Modelling data

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Key concepts

Non-technical introduction to terminology in modelling in machine learning:

- purpose of models
- central concepts
  - data
  - parameters
  - latent variables
- prediction and probabilistic predictions
- role of assumptions
- training and testing

Purpose of models

Mathematical models are useful for many purposes, including

- making predictions. For example, in a time series model, we may want to predict the future from the past. Often predictions are inherently uncertain. In *probabilistic models* probabilities express the confidence of predictions
- generalize from observations in the training set to new test cases (interpolation and extrapolation)
- understanding and interpreting statistical relationships in the data
- evaluating the relative probability of hypothesis about the data
- compressing or summarising data
- generating more data, from a similar distribution as the training set

Different tasks require different models. Useful models focus on some aspects and neglect others, to *trade off accuracy with simplicity and interpretability*.

Origin of a model

Models may originate from different sources, such as

- **first principles** For example, Newtonian mechanics is a model of planetary motion with a high degree of accuracy
- **observations, data** For example the annual production of timber per hectare of forrest, and its dependency on geographical and climatic factors may be modelled based on *data*.

Most practical models lie somewhere within the above spectrum, involving both first principles and data.

Machine learning is a broad term which covers the theory and practise of mathematical models which to a significant degree rely on data.

Knowledge, assumptions and simplifying assumptions

Every model relies on (explicit or implicit) assumptions, such as

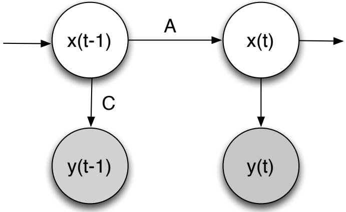
- **knowledge** For example, we know that a variable which measures the distance between two points must be non-negative.
- **assumptions** It could be assumed that income is independent of gender given age and profession. This assumption may be either true or false.
- **simplifying assumptions** We might assume that the response to a drug depends linearly on the dosage within some range. We don't believe that such an assumption is necessarily literally true, but rather that it is *good enough*, not to distort the uses we have of the model too much.

Probabilistic models may use *priors* to express knowlege (or beliefs) about aspects of the model.

Simplifying assumptions often facilitate use of the model. But, the conclusions drawn from a model are conditional on the assumptions being valid.

Practical modelling is therefore always a trade off between model expressivity and computational simplicity.

Observations, parameters and latent variables



This time series model is imagined repeated for $t = 1, \ldots, T$. It has *observations* y (shaded) for each time point and also *unobserved* or *hidden* or *latent variables* x and two sets of *parameters* A (for transitions) and C (for emissions).

To use the model we must decide what to do with all unobserved quantities. This is broadly known as *learning* or *training* a model. Options include *inference*, *estimation*, *sampling* and *marginalisation*.

Note, that the difference between *latent variables* and *parameters* is that the number latent variables grow with the number of observations (in this case, one for each time point), whereas the number of parameters remains constant.

Practical modelling

The specification of a model includes the complete structure as well as all assumptions (and priors) used as well as any pre-specified parameters.
In practise, we need to be able to do the following tasks

- treat the unobserved quantities (training), including
  - the latent variables
  - the parameters
  - possibly some aspects of the structure of the model
- make predictions on test cases
- interpret the trained model, what insights is the model providing?
- evaluate the accuracy of model
  - note: accuracy on the training and test sets may differ systematically
- do model selection and model criticism: chose between different models, or between different variants of a model, what are limitations of the model?

All these tasks need to be solved either exactly or approximately, on a given budget of computation and memory.

A common misunderstanding

The role of a model is to make predictions and provide insight into certain aspects of the data.

The role of a model is *not* to be a complete description of all aspects of the data (only the data itself does this).

From this perspective, it is clear that terms such as *true model* or *correct model* are *meaningless* in the context of machine learning.

Essentially, all models are wrong, but some are useful.

— George E. T. Box