Hierarchical modeling solutions

A powerful decision-tree approach to multivariate modeling of complex data

- Make modeling of non-linear data more efficient and robust
- Join Classification and Prediction models using multi-level modeling
- Use Hierarchical Models on-line with instrument integration
When analyzing process or other complex data, it is often necessary to refine models based on the output of initial investigations. In most cases, this is done manually and in many steps, becoming a laborious and time consuming process which is prone to error.

Hierarchical Modeling (HM) is the joining of a number of multivariate models using logic statements in order to arrive at a single, unique result. This is the classic logic tree or decision tree approach to systematically solve problems, where the analysis in one step is guided by the previous step.

With most data, it is very difficult to make a global prediction or classification model that predicts well in every area. In many real-world applications non-linear models are needed to understand the data.

- Manually developing models with 3 or 4 levels is very time consuming, but with hierarchical models you only need to set it up once and validate once, then you can use the model as much as required in run time applications.

- Once set up, validated models can be applied across different sites and processes for use by non-experts, enabling efficient process management and technology transfer.

- Hierarchical models are ideal for at-line process analysis. They allow non-normal situations to be identified and alarmed so that third-party control systems can make quality decisions.

- In the example above, the material is first classified by the model, and then the correct prediction methods are assigned automatically. Alarms are shown by the red cells, where the model has detected that the samples are new or unknown.

Unscrambler® X Hierarchical Model Development Module & Hierarchical Model Engine

Hierarchical models address these issues by focusing, or ‘zooming in’, on smaller areas of a data set more precisely.

Hierarchical models are ideal for applications such as:
- Fermentation analysis of batches in biotech, food, brewing, wine
- Managing products with hard to control or unwanted additives
- Gasoline blending in petroleum refining
- Reaction monitoring in chemical manufacturing
- Classifying and characterizing pharmaceutical raw materials for better campaigning into batches
- Early stage development of drug formulations and manufacturing systems used to develop them
We offer a range of tools so you can use the power of hierarchical models on your data in the way that suits you.

- **Hierarchical Model Development Module:**
  Plug-in module for The Unscrambler® X software for off-line data analysis or to develop hierarchical models for on-line use.

- **Hierarchical Model Engine:**
  Apply hierarchical models in real-time by integrating them into scientific instruments or process equipment.

- **Full customization options:**
  Unscrambler® X Hierarchical Models can be integrated into process monitoring or control systems with customization as required.

Hierarchical models are very useful for complex classification problems such as raw material analysis. If a global classification model cannot uniquely identify all the groups, a hierarchical model can be developed to do the classification in a stepwise manner. This is a convenient way to join multivariate models into one versatile tool.

The example above shows a global model of different raw material spectra developed and plotted in The Unscrambler® X software. Hierarchical modeling is performed by joining together up to 10 levels of models in The Unscrambler® X.

Hierarchical models are useful if dealing with non-linear regression problems over large concentration ranges. The first predictor lets you define where you are, then the second model gives a more precise analysis of the area in question. In this manner a set of robust and locally validated models can replace highly non-linear models that are prone to over-fitting.

The example above shows how a non-linear response can be modeled by two linear models, each applied to different concentration ranges.

**Key features**

- Projection methods (PCA, PCR, PLSR)
- Classification methods (SIMCA, LDA, SVM)
- Regression methods (MLR, PCR, PLSR)
- Accepts data in wide range of formats
- Auto-pretreatment options for data
- Alarms and warnings can be set
- Output in tabular format with cell colours according to alarm state
- Can be integrated with 3rd party systems including OPC UA
Hierarchical models allow a number of multivariate models to be joined using logic statements in order to arrive at a single, unique result. Most of the powerful classification, prediction or projection methods in The Unscrambler® X can be used as the building blocks.

- The hierarchical model is built in a top-down manner, with a global model in level 1
- Conditional statements about the outcome at one level define the actions to be taken on the next level
- Outcomes such as classification, prediction, deviation, leverage, etc. can be tested
- Up to 10 levels can be defined
- Events and alarms are set up to highlight suspect samples or stop the hierarchy