Software package for optical emission spectrometry with arc discharge (OES AD)

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Outline

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Direct analysis with visual interpretation

Direct analysis of optical emission spectrometry with arc discharge (OES AD)

Without physical modeling of samples (buffering, dilution etc).

- Fast.
- Cheap.

Direct analysis with visual interpretation

Visual interpretation

The visual interpretation of experienced analyst allows taking into account the spectral and other interferences. The analyst can make:

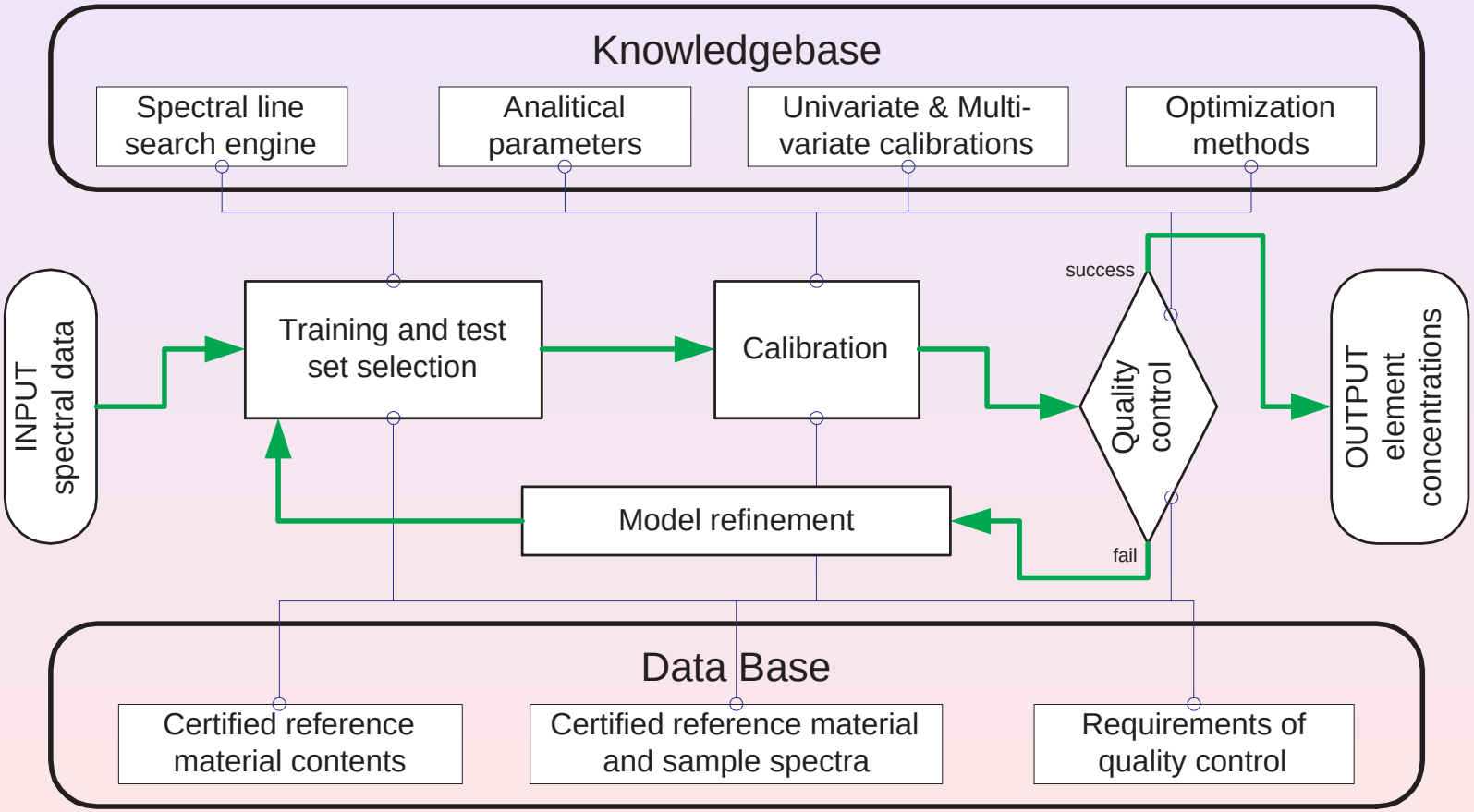
- qualitative analysis.
- semiquantitative analysis (more than 30% relative error).
- quantitative analysis using computer (more than 30% relative error).

Direct analysis with visual interpretation

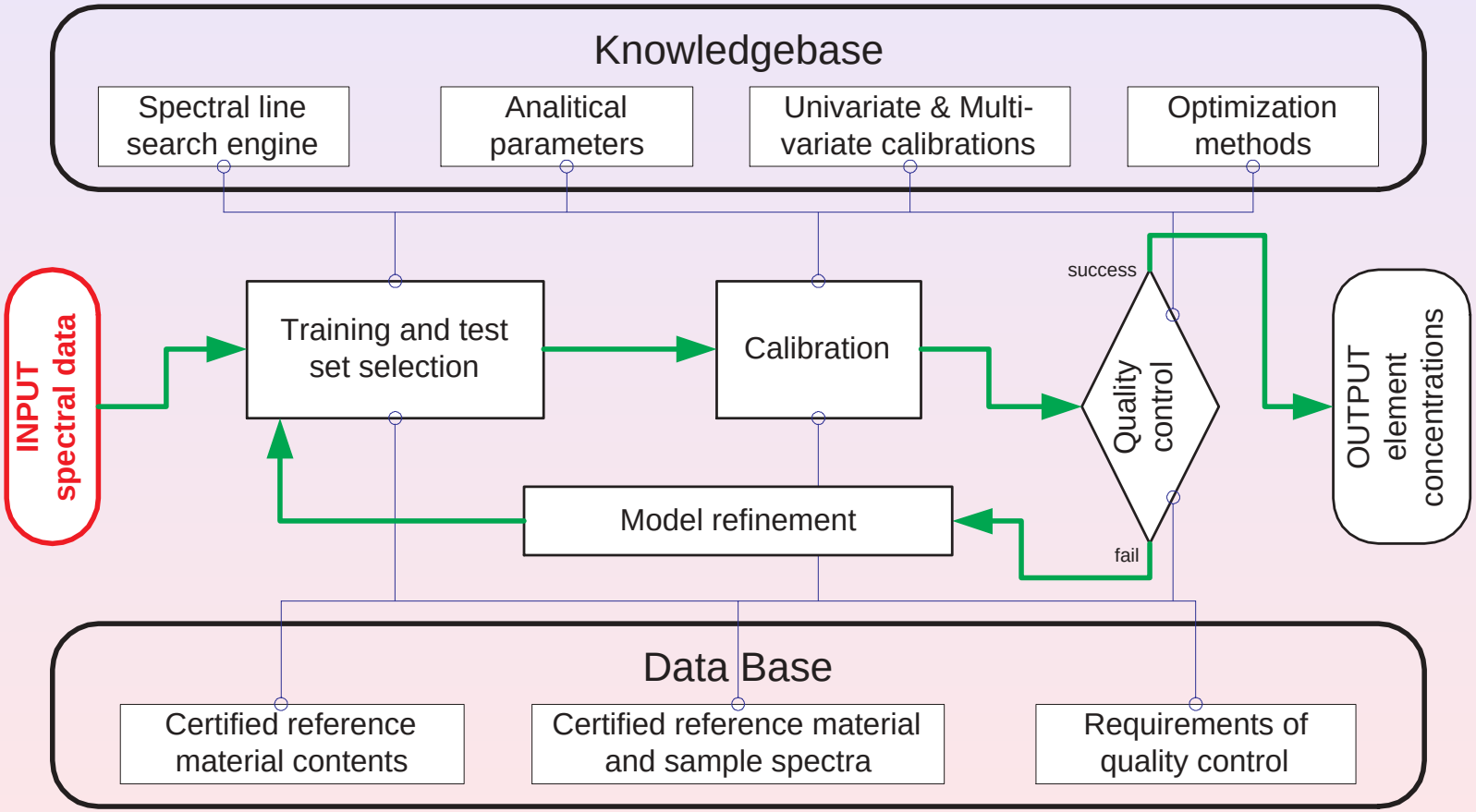
Expert system characteristics:

1. An analyst has to solve a lot of diagnostic problems arising in the sample classification.
2. The complete and adequate mathematical models have not been developed for the direct OES AD yet. Therefore, there is no a steady-state theory in this field.
3. Changing to the instrumental measurement leads that the small number of analysts remain able to make the visual analysis.
4. Noise pollution is a natural feature of the direct OES AD data since it operates with samples of variable composition.

OES AD software package



Input


Knowledgebase
Spectral line search engine
Analitical parameters
Univariate & Multi-variate calibrations
Optimization methods
INPUT spectral data
Training and test set selection
Calibration
success
Quality control
fail
OUTPUT element concentrations
Model refinement
Data Base
Certified reference material contents
Certified reference material and sample spectra
Requirements of quality control

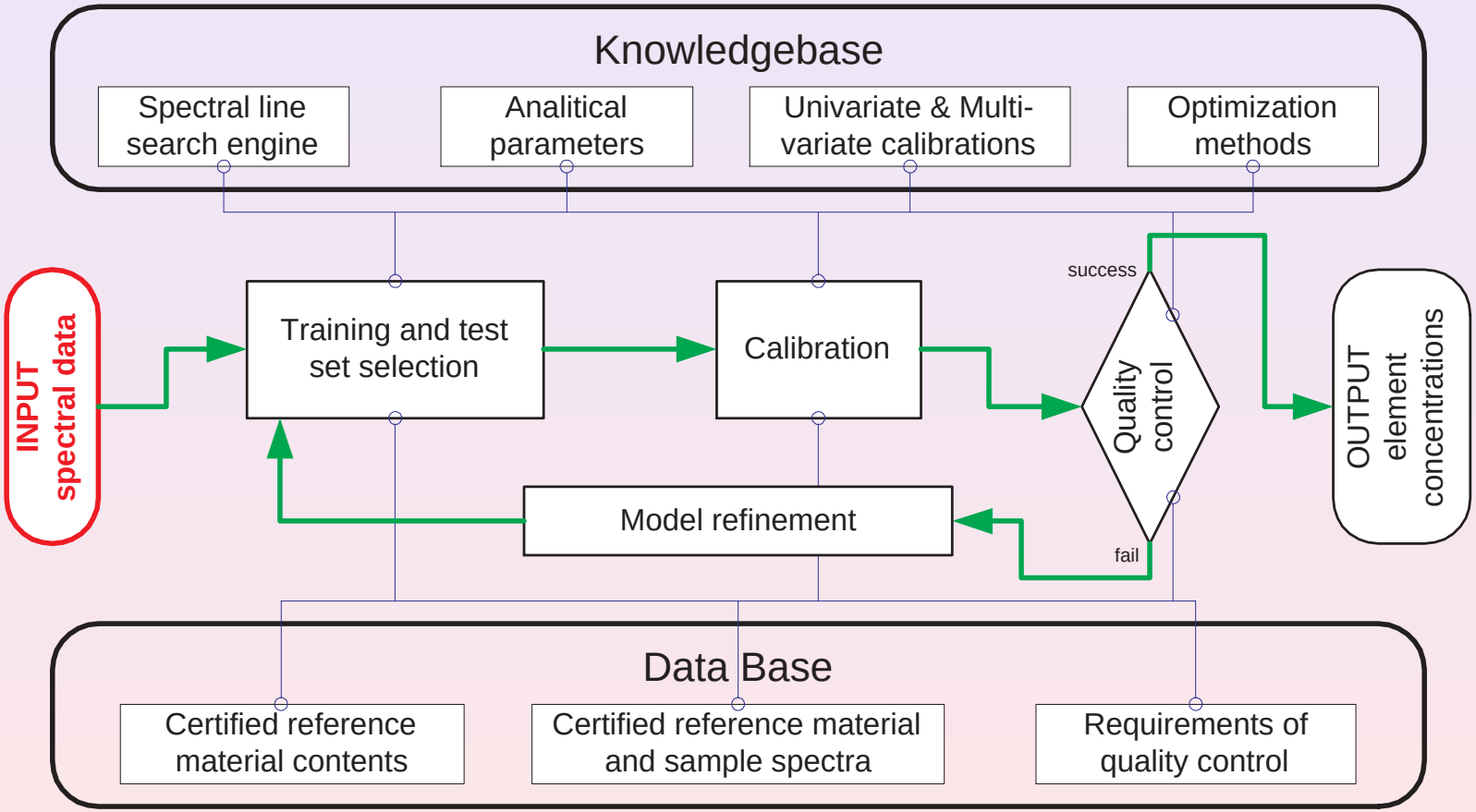
Input

Table of analytical parameters

Advantages:

- Provided by manufacturer's software.
- Universal way, can be adapted for another kind of analysis.

Input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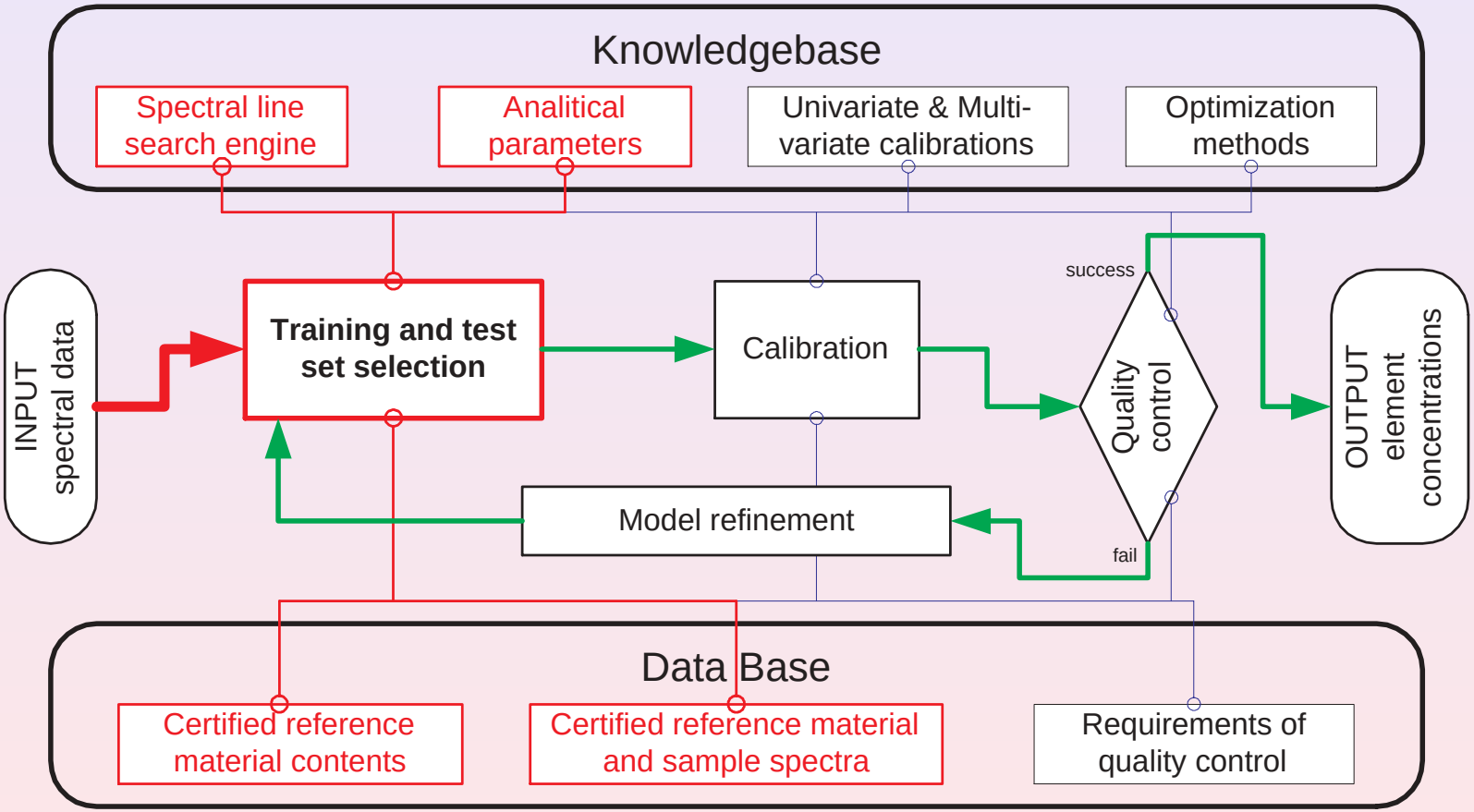
Training and test set selection



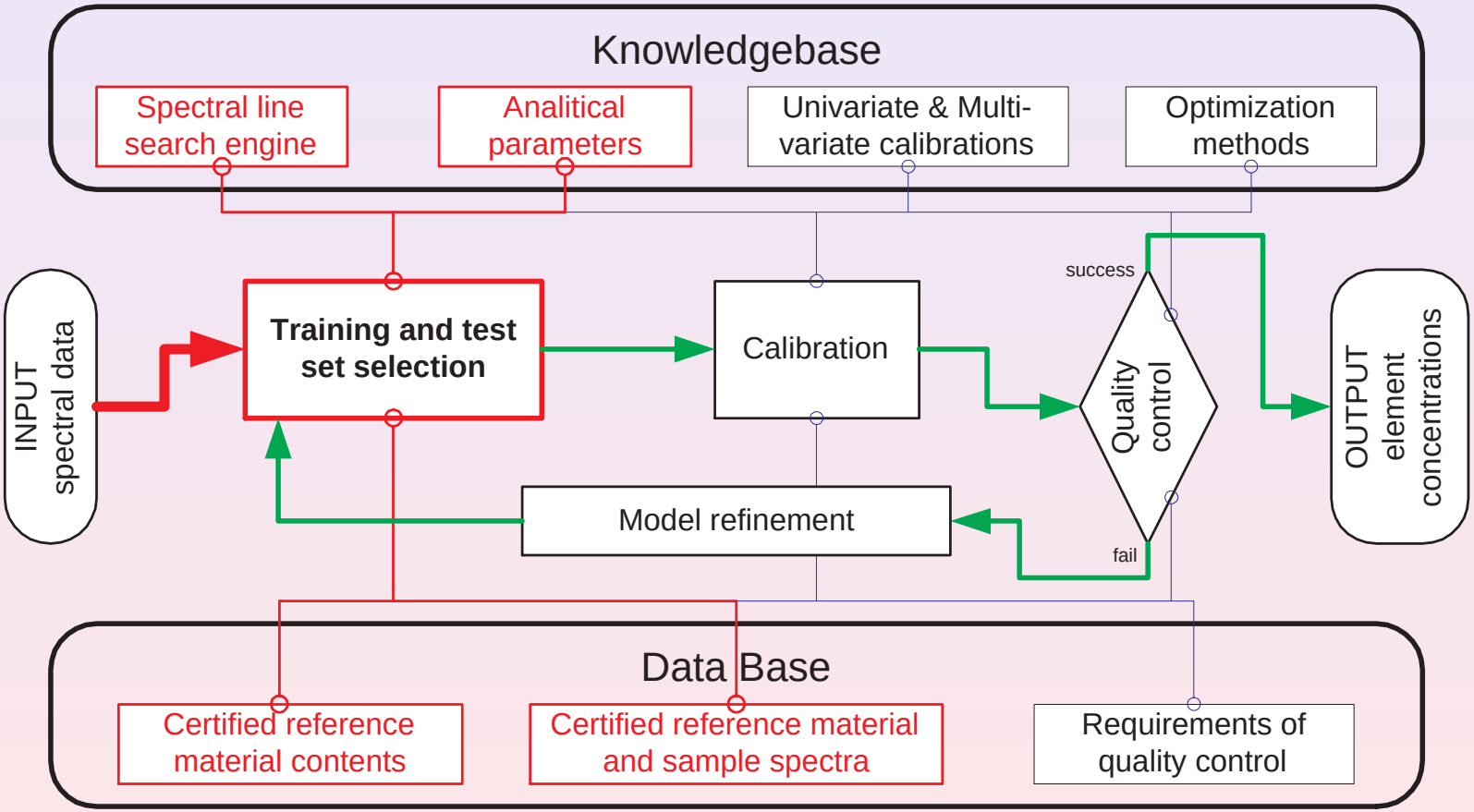
Training and test set selection

Classification problems

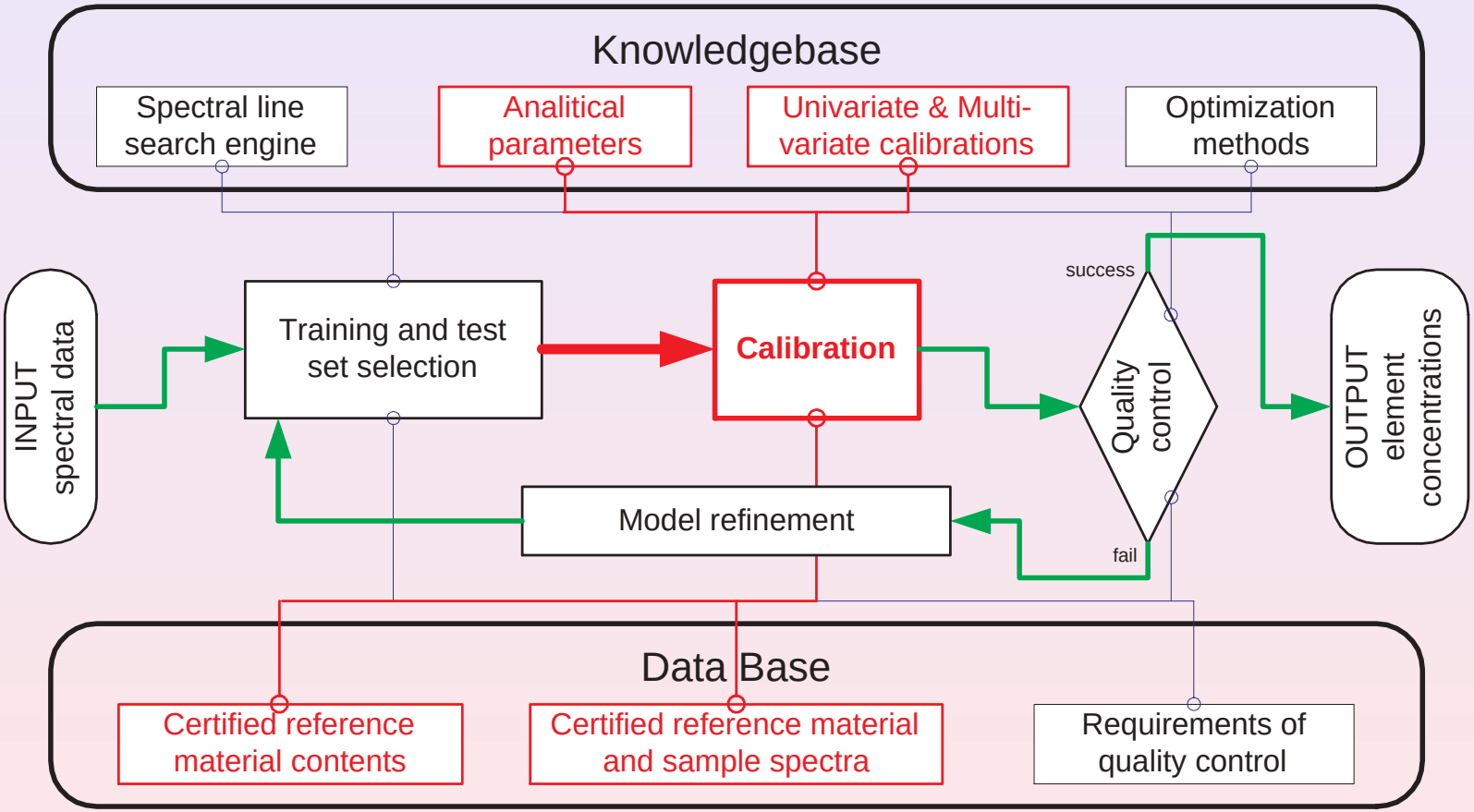
The sample spectra have to be classified to chose:

1. Training set of reference materials.
2. Test set of reference materials.
3. Set of analytical lines for each element and their type of analytical parameters.

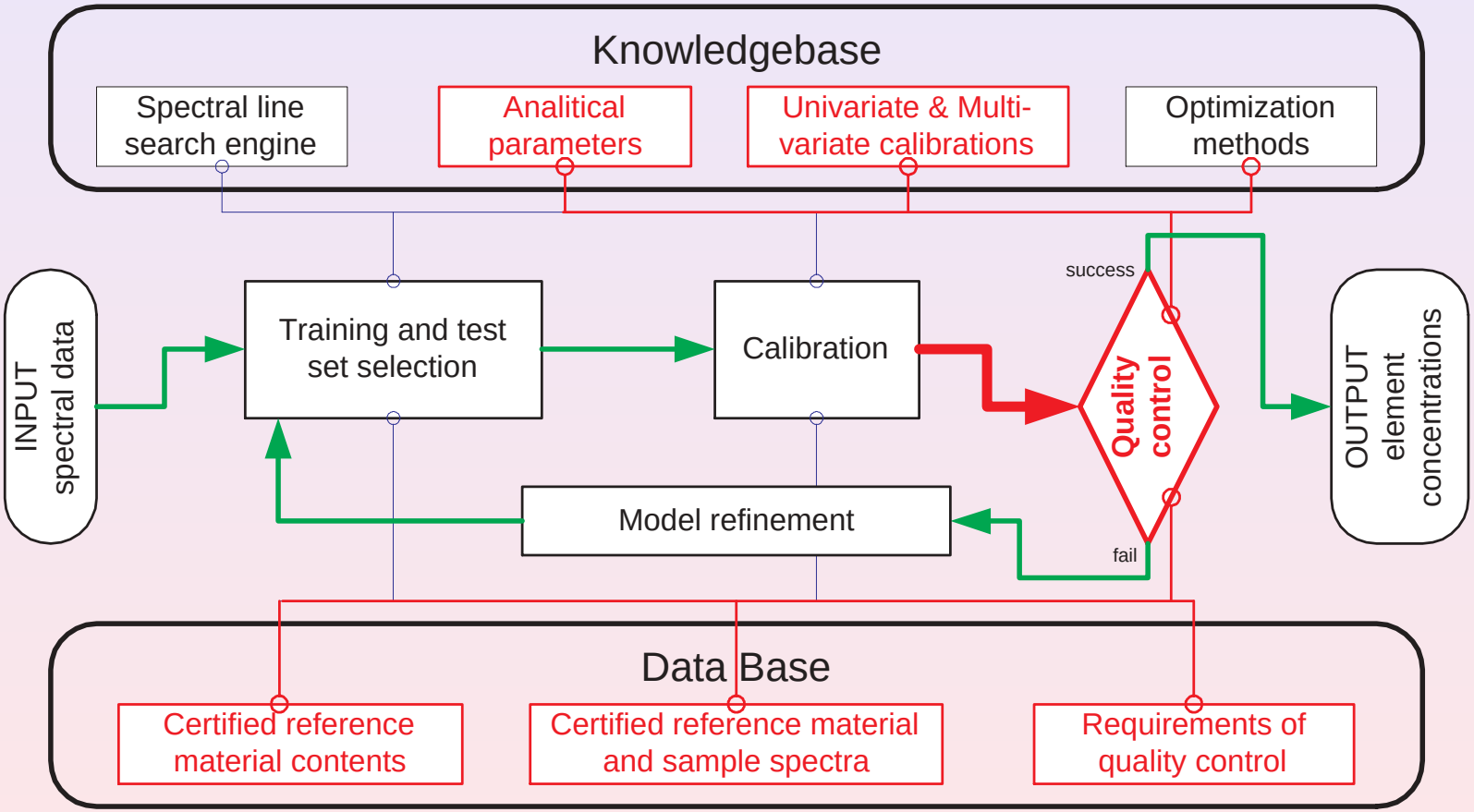
Training and test set selection



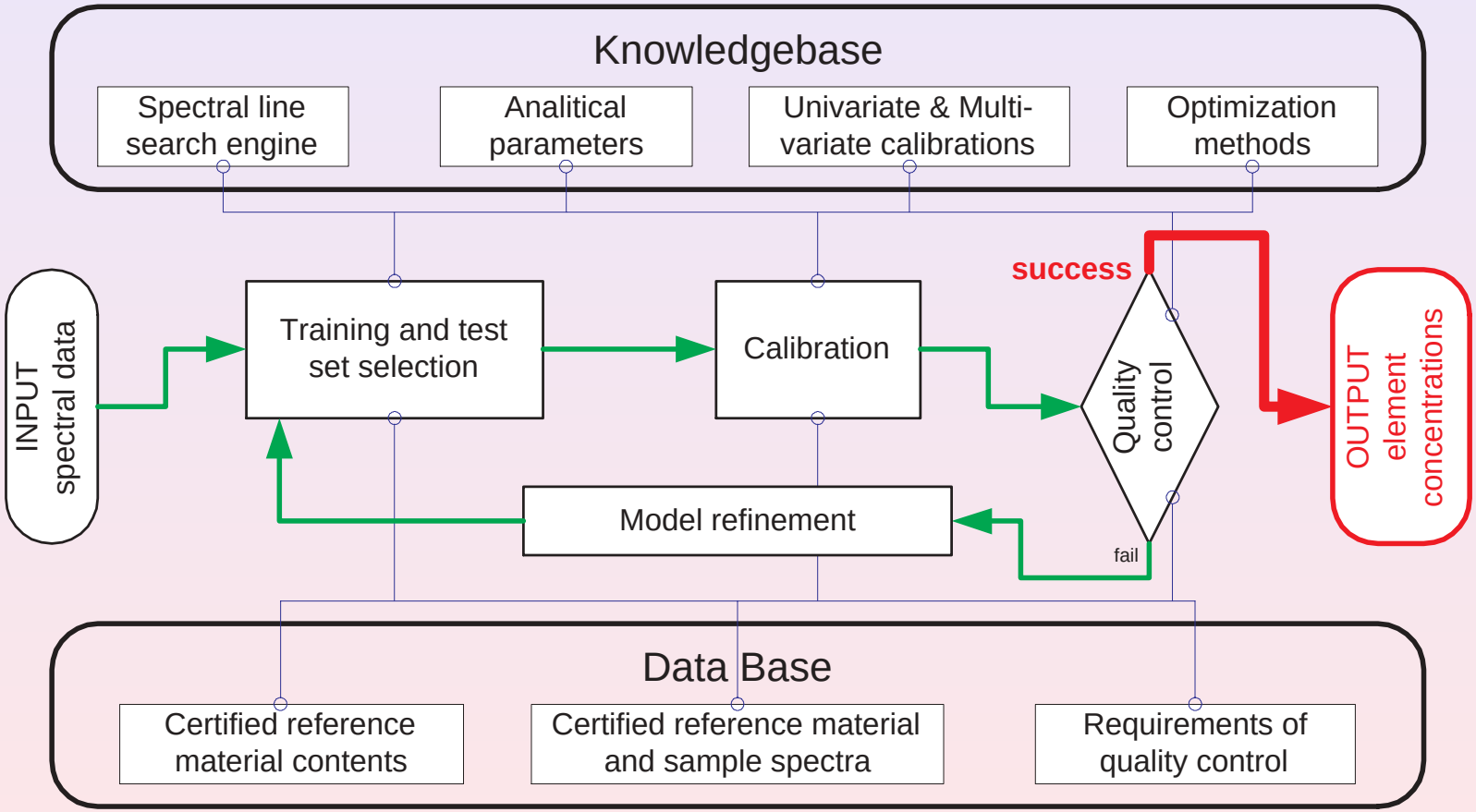
Calibration



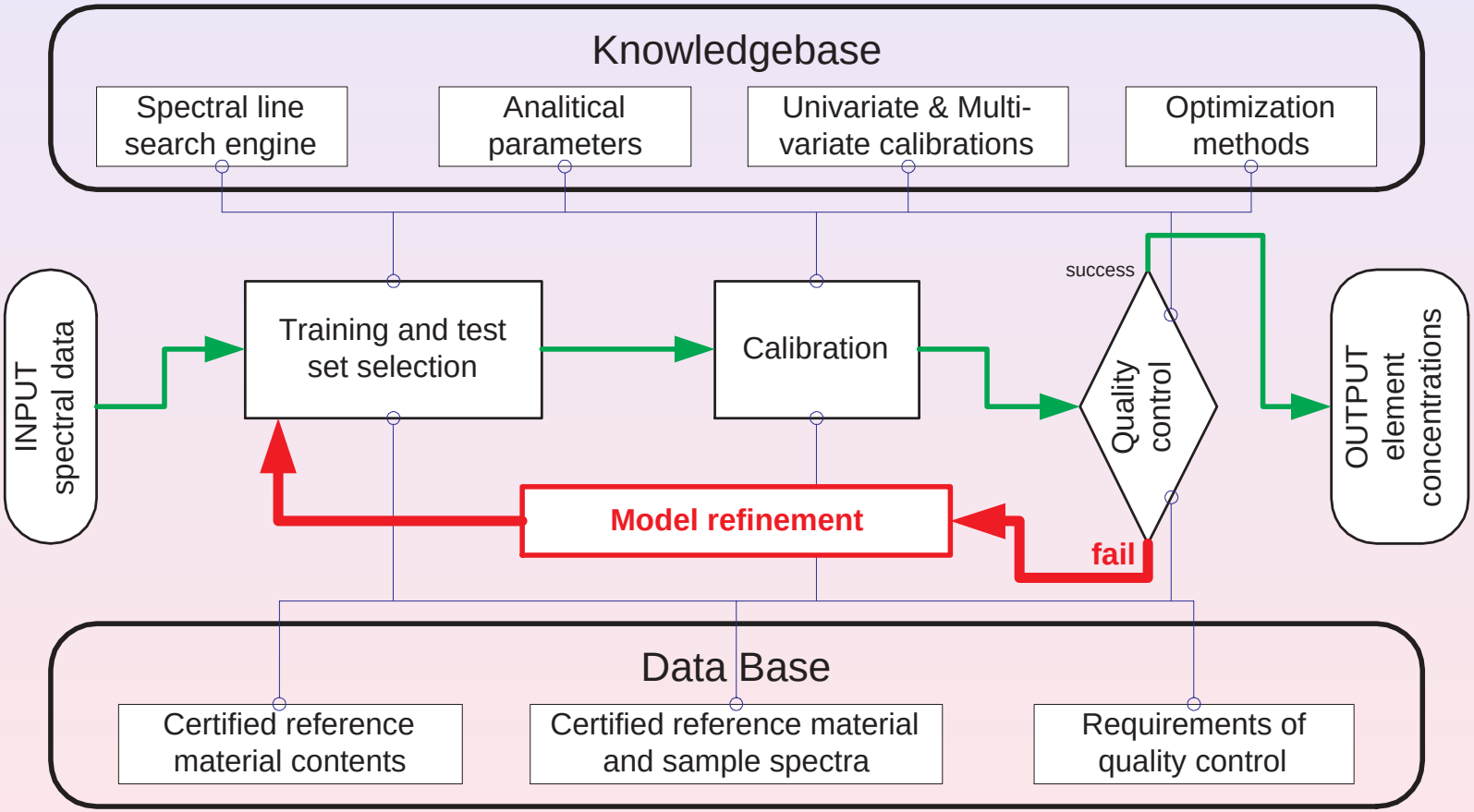
Quality control



Quality results



Model refinement



Multivariate calibration

Calibration

$$y = F(x)$$

y – concentration vector,
x - analytical parameter vector.

Training set

Y – concentration matrix.
X – analytical parameter matrix.

Two steps

1. Dimension reduction.
2. Regression.

Dimension reduction

Reduction

$$X \to X'$$

X' – less number of rows.

Projection

PCA – principal component analysis. Chose principal components according to the covariance (information) matrix $X^T X$.

Cluster analysis

Set of objects has to be parted into subsets of similar objects. One representative has to be picked for each subset (p-mean, p-median, p-center etc).

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Multivariate calibration

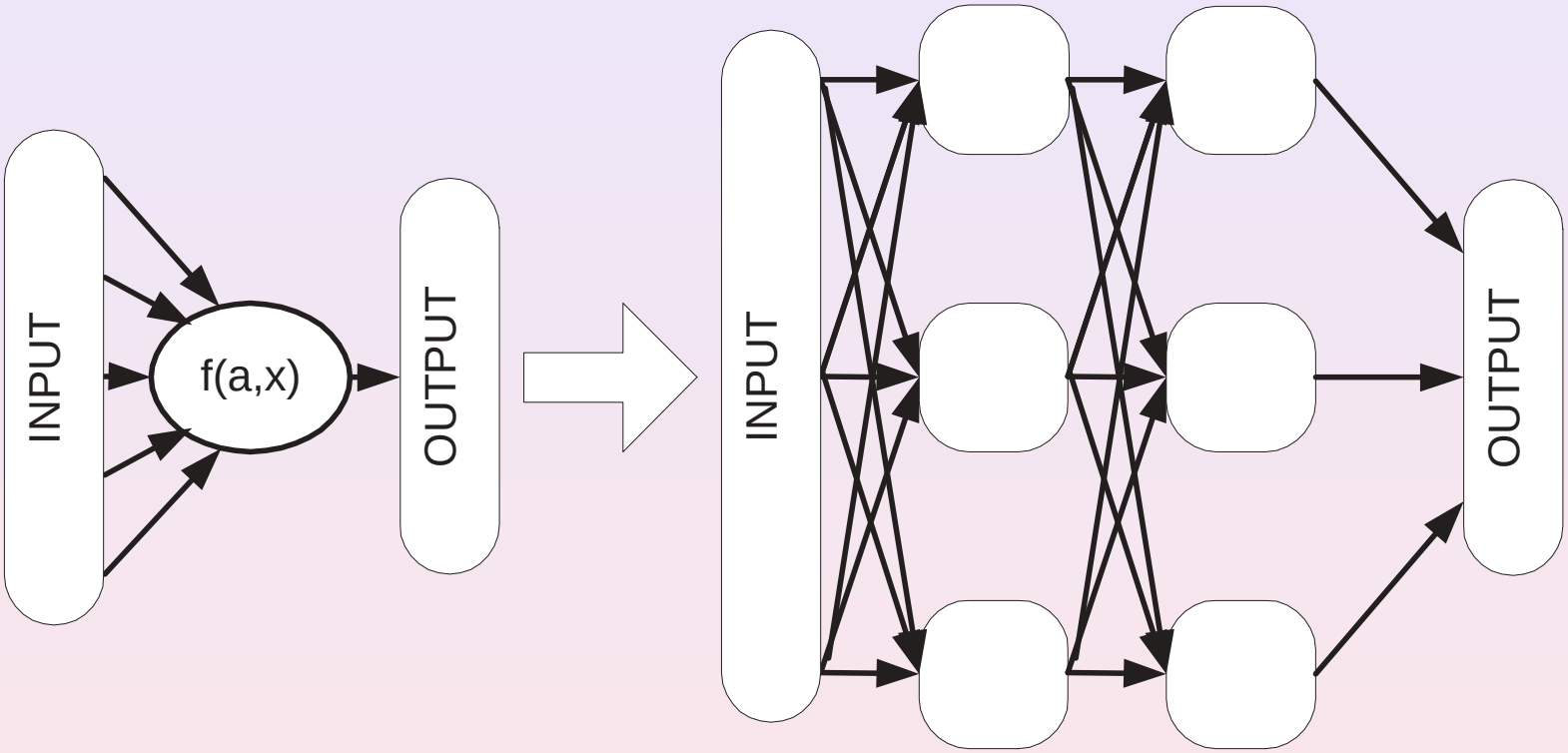
Least-squares method

Find matrix A and vector b

$$y = xA^T + b$$

minimizing the square of difference on training set.

Neural networks



$$f(a,x) = f\left(a_0 + \sum_{i=1}^{n} a_i x_i\right)$$

Neural networks

Implementation

Neuron $f(\cdot)$ – exponent, hyperbolic tangent, Fourier transformation etc.

Neural network – multilayered perceptron.

Learning – steepest descent method.

Conclusions

We are developing a software package for OES AD. It is an expert system simulating the direct analysis with visual interpretation.