

Multivariate Analysis — PCA/PLS-DA & Model Validation — Hands-on

Turn high dimensional metabolomics tables into clear patterns and robust models. This module focuses on exploratory PCA, supervised PLS-DA, feature importance interpretation, and rigorous model validation so that you can distinguish real biological structure from noise, overfitting, and batch artifacts in LC-MS, GC-MS, and NMR metabolomics studies.

Multivariate Analysis — PCA/PLS-DA & Model Validation

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Session 1

Fee: Rs 8800 [Apply Now](#)

PCA Foundations & Exploratory Data Structure

Why multivariate analysis is essential in metabolomics

high dimensional feature spaces **correlated metabolites** **pattern discovery vs noise**

PCA concepts for metabolomics data matrices

scores and loadings **explained variance** **effect of scaling and centering**

Interpreting PCA plots for quality and biology (concepts)

outlier detection **QC vs study sample patterns** **group trends and confounders**

Session 2

Fee: Rs 11800 Apply Now

Supervised Models: PLS-DA & Classification

From unsupervised exploration to supervised discrimination

class labels and design **PCA vs PLS-DA roles** **risk of overfitting**

PLS-DA concepts and components in metabolomics context

latent variables **scores, loadings and weights** **VIP scores (concepts)**

Practical interpretation of PLS-DA score and loading plots

class separation and overlap **influential metabolites** **relating patterns back to biology**

Session 3

Fee: Rs 14800 Apply Now

Model Validation, Overfitting & Diagnostics

Why apparent separation can be misleading

overfitting in high dimensions **small n / large p issues** **data leakage concepts**

Cross validation and permutation tests (concepts)

k-fold and repeated CV **Q^2 and R^2 metrics** **class label permutation logic**

External test sets and practical diagnostic plots

training vs test performance **ROC/PR curve concepts**

confusion matrix thinking

Session 4

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Mini Capstone: PCA/PLS-DA Workflow & Report

Building a full PCA–PLS-DA pipeline on a metabolomics dataset

Theory + Practical

Summarising validation metrics and biological interpretation

PCA and PLS-DA plots **Q^2/R^2 and permutation**
summaries **top contributing metabolites list**

Deliverables: PCA/PLS-DA report & model diagnostics bundle

analysis report (PDF/HTML) **plots and metrics export**
feature importance table (CSV)