The caret Package: A Unified Interface for Predictive Models

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The **caret** package, short for **C**lassification **And RE**gression **T**raining, contains numerous tools for developing predictive models using the rich set of techniques available in R. The package focuses on simplifying model training and tuning across a wide variety of models. It also includes methods for pre-processing training data, calculating variable importance, feature selection and model visualization. An example from computational chemistry is used to illustrate the functionality on a real data set.