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PTML: Perturbation-Theory Machine Learning notes

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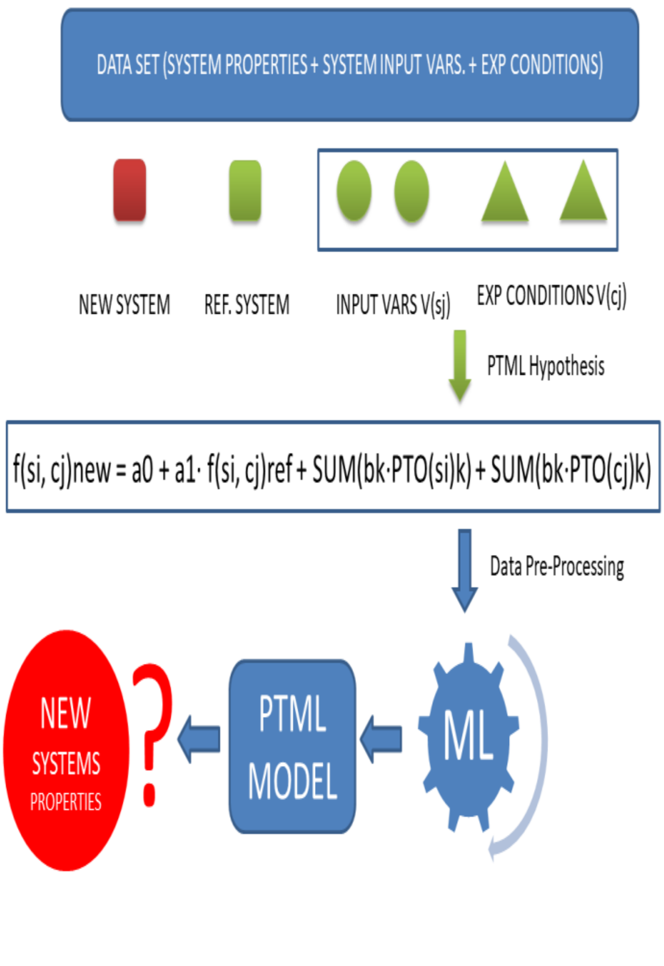
Graphical Abstract



Abstract. PTML: Perturbation-Theory Machine Learning methods have been developed by H. Gonzalez-Diaz et al [0] to seek models able to predict multiple properties f(si, cj)k of type k of a system (si) at the same time (multi-output and multi-objective) taking into consideration variations (perturbations) in multiple experimental conditions cj = (c0, c1, c2, ... cn) at the same time with respect to a value of reference or expected. PTML-like models have been applied for different authors to study drugs, proteins, nanoparticles, complex networks, social systems, etc. [1-17]. In the particular case of a PTML linear models we can fit an equation with the general form f(si, cj)new = a0 + a1· f(si, cj)ref + SUM(bk·PTO(cj)k). In this model PTO(cj)k are PT operators measuring the perturbations in the new system si with respect to the system of reference sr with observed or expected property f(si, cj)ref. First, we need to calculate the values of the PTOs in the data pre-processing step. This PTOs allow us to perform an Information Fusion process with variables and conditions from different sources. Moving Averages (MA), Multi-condition MA (MMAs), Double MAs, Co-variance Operators, etc. are some examples of useful PTOs. After that, we can use Multiple Linear Regression (MLR), Linear Discriminant Analysis (LDA), or other linear ML techniques to seek the PTML model. In the non-linear cases, we can fit the PTML models using Artificial Neural Networks (ANN), Support Vector Machines (SVM), Classification Trees, and other ML methods.

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