AI / ML @GOKUL
(Global Optimization and Knowledge Unearthing Lab)

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Recent improvements in state-of-the-art experimental and computational infrastructures, affordability, automation, ubiquitous connectivity through IoT, a global push towards meeting environmental constraints to ensure safety and sustainability resulted into generation, processing and management of enormous amounts of heterogeneous data in the domain of Process Systems Engineering (PSE). PSE, which deals with the process design for the purpose of converting raw goods to usable end products, focuses on the design, operation, control, optimization and intensification of chemical, physical, and biological processes. Our aim @ GOKUL is to develop state-of-the-art data tools that can cater to the special needs for vast amounts of highly complex data generated by the PSE community.

We target potential areas in PSE and investigate how the applications of deep supervised/unsupervised learning methods based on artificial neural networks (ANN) can be made useful there. Exploiting the novel multi-objective evolutionary Neural Architectural Search technique developed @GOKUL, TRANSFORM, we could successfully show how (i) optimization of computationally expensive models can be improved multiple folds using surrogate models (ANN), (ii) accurate system identification and data-based model predictive control of extremely nonlinear industrial processes can be performed (RNN, LSTM), (iii) image-based sensing can be improved for better optimization of the process (CNN, AE, VAE), (iv) the uncertainty quantifications for nonlinear models using analytical derivations can be obtained through Sobol indices and global sensitivity analysis (PUNNs), (v) the ideas of approximation of control vector using ANNs can be utilized to solve complex single and multi-objective optimal control problems efficiently, (vi) fuzzy clustering performance can be improved by neural networks based reformulation for identification of global optimum and (vii) generative modelling can be utilized to accurately solve the industrial nonlinear multi-objective optimization problems in uncertain framework (GAN, VAE). Our targeted applications include wind farm layout optimization, new alloy discovery by enhanced computational materials science calculations, monitoring environmental parameters due to climate change, smart sensing of particulate matter, fast-charging protocols in Li+ battery management, bio-fuel supply chain optimization, systems biology (cell classification based on Ca+ oscillations in neurons), chemical engineering (polymerization reactors), metallurgical engineering (steel making processes etc.), mineral processing (grinding and flotation) and mechanical engineering (uncertainty analysis in supersonic flow of tactical missiles, surrogate optimization using CFD models) applications. Apart from the desired tangible benefits, some of these results brought laurels to GOKUL as they were bestowed with the best paper award in the international platforms (e.g. ACODS in 2020) and highlighted as works which can open up new opportunities to explore new designs in future (e.g. BATTERY 2030+, a long-term roadmap for forward-looking battery research in Europe, prepared by the EU Horizon 2020 initiative mentions our work in the Li+ Battery space).

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