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Applications of Artificial Intelligence and Machine Learning in Engineering Optimization

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Abstract: *Engineering optimization seeks the best feasible design or operating condition under competing objectives, physical laws, resource limits, and uncertainty. Conventional approaches including gradient-based methods, evolutionary algorithms, and simulation-driven search remain valuable, but can become computationally expensive when the design space is nonlinear, high-dimensional, noisy, or dependent on costly simulations. This review examines how artificial intelligence and machine learning are being integrated into engineering optimization, with emphasis on surrogate modelling, deep learning, Bayesian optimization, reinforcement learning, and hybrid physics-informed approaches. The literature indicates that ML can learn approximate relationships between design variables and performance, reduce the number of expensive simulations, identify promising regions of a design space, and support adaptive control of complex systems.*

Keywords: Artificial Intelligence, Reinforcement Learning, Multi-Objective Optimization, Physics-Informed Learning, Digital Twins

I. INTRODUCTION

Engineering optimization can be expressed as the systematic selection of decision variables to minimize or maximize a performance measure while satisfying constraints. Typical goals include reducing mass, cost, energy consumption, emissions, or production time while improving strength, reliability, throughput, or efficiency. In many practical systems, these goals conflict: a lighter component may be more expensive to manufacture, and a highly efficient operating point may reduce durability or increase risk. Optimization is therefore not simply the search for a single best value; it is a structured process for comparing feasible alternatives under explicit assumptions.

Classical numerical methods are effective when objective functions are smooth, derivatives are available, and the number of variables is manageable. Yet engineering analyses often rely on computational fluid dynamics, finite-element analysis, multiphysics simulation, or physical testing. Repeatedly evaluating such models can dominate the total optimization cost. ML offers an additional layer: it learns a mapping from design inputs to predicted outputs and can be incorporated into the search process. Ramu et al. (2022) survey ML methods across structural and multidisciplinary optimization, including structural design, materials, fluid mechanics, aerodynamics, and heat transfer. Recent reviews also emphasize the role of AI in mechanical engineering design, predictive maintenance, structural monitoring, and energy optimization (Artificial intelligence and machine learning in mechanical engineering, 2025).

This is a narrative review of representative methods and application patterns rather than a statistical meta-analysis. It focuses on the ways AI/ML can support optimization, the engineering settings in which the methods are useful, and the practical limitations that affect deployment. The central distinction is between using AI to predict system behaviour and using AI to improve the optimization process itself. In the first case, a model approximates an objective or constraint; in the second, it helps select new evaluations, generate candidate designs, or adapt control decisions. Strong engineering practice combines both roles with independent verification.

A general constrained optimization problem can be written as:

minimize $f(x)$ subject to $g_i(x) \le 0,\ i = 1,\ldots,m;\ \ h_j(x) = 0,\ j = 1,\ldots,p;\ \ x \in \Omega$

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Here, x is the vector of design or operating variables, f(x) is the objective function, $g_i(x)$ represents inequality constraints, $h_j(x)$ represents equality constraints, and Ω defines the allowable design space. In AI-assisted optimization, an ML model may estimate f(x), constraint functions, or the response of an expensive simulator. The approximation must be accurate enough in the region where decisions are made not merely across the average training dataset.

AI AND MACHINE LEARNING METHODS WITH KEY EQUATIONS

Surrogate modelling is among the most established connections between ML and engineering optimization. A surrogate is a computationally cheaper approximation of a high-fidelity simulation or experiment. Common choices include polynomial response surfaces, Gaussian processes, support vector regression, random forests, and neural networks. The optimization algorithm queries the surrogate to screen many candidates and then evaluates selected candidates with the original solver. Khatouri et al. (2022) describe metamodeling, multi-fidelity methods, reduced-order models, and design-of-experiments enrichment as strategies for managing expensive simulation budgets. Surrogates are particularly useful when each finite-element or fluid-dynamics run requires substantial computation.

A basic supervised learning model estimates the response as $\hat{y} = f_\theta(x)$, where θ denotes learned parameters. For regression, the mean squared error objective is:

$$MSE(\theta) = (1/N) \Sigma_{i=1}^{N} [y_i - f_\theta(x_i)]^2$$

Minimizing prediction error is necessary but not sufficient for optimization. A model with low average error can still be inaccurate near a constraint boundary or around the optimum. Engineering validation should therefore assess errors in critical operating regions, check extrapolation risk, and compare surrogate predictions with independent simulations or experiments.

Bayesian optimization is valuable when evaluations are expensive and gradients are unavailable. It uses a probabilistic surrogate to balance exploitation testing designs predicted to perform well and exploration testing uncertain areas that may contain better solutions. A common acquisition rule is expected improvement:

$$EI(x) = E[\max(0, f_best - f(x))]$$

For minimization, the expectation is computed under the predictive distribution of the surrogate; practical formulations account for uncertainty and the current best feasible result. The next design is chosen by maximizing the acquisition function, evaluated using the real simulator, and then added to the training set. This sequential process can reduce the number of expensive evaluations, although its benefit depends on the problem dimension, noise level, and surrogate quality.

Deep learning can represent complicated nonlinear relations between geometry, material properties, operating conditions, and performance. Convolutional networks can process images or spatial fields; graph neural networks can represent connected structures and meshes; and generative models can propose new candidate geometries.

Their main advantage is expressive capacity, but they may require substantial training data and can be difficult to interpret. Physics-informed neural networks and hybrid models introduce governing equations or physical constraints into training, helping discourage predictions that violate known relationships. In optimization, these approaches are promising where simulation data are available but costly, or where physical consistency is essential.

Reinforcement learning frames sequential decision-making as an interaction between an agent and an environment. It can be applied to process control, energy scheduling, robotics, and adaptive operation. A policy selects an action based on the current state, and the reward encodes performance and penalties. A standard objective is:

$$J(\pi) = E\pi [\Sigma\square_{=0}^{T} \gamma^t r\square]$$

Here, π is the policy, $r\square$ is the reward at time t, and γ is a discount factor. RL can discover operating strategies that are difficult to specify with fixed rules, but unsafe exploration, simulation-to-reality mismatch, and reward design remain major concerns. For safety-critical engineering, training should occur in validated simulations and candidate policies should be constrained and tested before live deployment.

Many engineering tasks involve more than one objective. For example, a design may need to minimize cost and mass while maximizing efficiency and reliability. A weighted-sum formulation is:

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$$F(x) = \Sigma_{k=1}^{K} w_k f_k(x), \quad \text{where } w_k \geq 0 \text{ and } \Sigma_k w_k = 1$$

Weighted sums are simple, but a single set of weights may hide trade-offs and may not recover every point on a non-convex Pareto front. Multi-objective evolutionary algorithms and ML-assisted Pareto search can instead identify a set of non-dominated alternatives. Engineers and stakeholders can then select a solution based on safety, cost, sustainability, and operational priorities. Houssein et al. (2024) review metaheuristics for global and engineering optimization and highlight continuing issues involving evaluation cost, parameter settings, and reliable comparisons.

ENGINEERING APPLICATIONS, LIMITATIONS, AND FUTURE DIRECTIONS

In mechanical and structural engineering, AI-assisted optimization supports lightweight component design, topology optimization, fatigue and vibration control, and the selection of structural parameters. Surrogate models can approximate finite-element responses, while deep learning can rapidly predict candidate performance. These methods are attractive when many design iterations are required, but numerical feasibility does not automatically guarantee manufacturability. Minimum feature size, material behaviour, assembly requirements, and manufacturing tolerances should be included in the formulation and checked after optimization. Ramu et al. (2022) identify structural and multidisciplinary design as important areas for ML-assisted optimization.

In fluid mechanics and thermal engineering, AI models can approximate pressure drop, heat transfer, aerodynamic forces, and flow-field behaviour. Optimization may seek improved aerodynamic efficiency, reduced drag, uniform temperature, or lower pumping power. The potential benefit is greatest when each high-fidelity computational fluid dynamics evaluation is costly. Nevertheless, the training data must cover relevant geometries and boundary conditions. A surrogate trained on one regime should not be assumed reliable for a substantially different Reynolds number, material, or operating condition without additional validation.

In energy systems, ML-assisted optimization can coordinate renewable generation, storage, building energy use, and industrial demand. Forecasting models estimate loads or renewable output, while optimization algorithms schedule equipment under operational constraints. In manufacturing, AI can support process parameter selection, production scheduling, quality improvement, and predictive maintenance. In civil engineering, data-driven approaches can help optimize building energy performance and structural design.

A recent review of data-driven AI in building structures similarly describes the potential to improve optimization design while noting challenges with implicit constraints and computational efficiency (Leveraging data-driven artificial intelligence in optimization design for building structures, 2025). Across these applications, gains should be reported against a clear baseline and should include computational cost, constraint violations, and robustness not only predictive accuracy.

Several cross-cutting limitations require attention.

First, data quality and coverage determine whether a learned model can represent the real system. Engineering datasets may be small, expensive, imbalanced, or generated under idealized simulation conditions. Second, model uncertainty must be quantified because an apparently optimal prediction may be unreliable. Third, interpretability matters where engineers need to explain why a design was selected or demonstrate compliance. Fourth, optimization can exploit model errors: a search algorithm may discover a candidate that looks excellent to the surrogate but performs poorly in the original simulator. This is often addressed through iterative validation, uncertainty-aware sampling, and periodic high-fidelity evaluations.

Fifth, deployment introduces operational and organizational constraints. Real systems can change over time, sensors may drift, and operating conditions can move beyond the training distribution. A responsible workflow therefore needs monitoring, version control, documented assumptions, human review, and a process for retraining or reverting a model. AI recommendations should not replace certified engineering analysis where safety standards, regulatory approval, or physical testing are required. The most credible approach is human-in-the-loop optimization: AI accelerates search, while engineers define objectives, impose constraints, assess uncertainty, and approve final designs.

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Future research should develop benchmark datasets that combine simulation, experiments, and operational measurements; improve uncertainty calibration; and test model transfer across related engineering problems. Multi-fidelity learning can combine cheap approximate models with a smaller number of expensive evaluations. Physics-informed and differentiable models may improve physical consistency, while digital twins can connect optimization to live operational data. Researchers should also report reproducible settings, computational budgets, feasibility rates, and comparisons with strong conventional baselines. The overall aim should be dependable engineering decisions, not merely a lower objective value on a single benchmark.

II. CONCLUSION

Artificial intelligence and machine learning are expanding the capabilities of engineering optimization by learning complex input–output relationships, accelerating expensive simulations, supporting sequential experimentation, and enabling adaptive decision-making. Surrogate models and Bayesian optimization are particularly useful when objective evaluations are costly; deep learning can represent high-dimensional nonlinear behaviour; reinforcement learning can optimize sequential control; and multi-objective methods can clarify trade-offs among competing engineering goals. Applications across mechanical design, structures, fluid and thermal systems, energy, manufacturing, and civil engineering show that these methods can complement conventional numerical analysis.

However, AI does not guarantee a globally optimal, physically valid, or deployable solution. Model bias, limited training data, uncertainty, poor generalization, and hidden constraint violations can undermine apparently strong results. Successful use therefore requires carefully defined objectives, domain-relevant datasets, transparent evaluation, physical and safety constraints, and independent verification using trusted solvers or experiments. The most promising direction is hybrid engineering optimization in which AI improves search efficiency while physical models and engineering expertise provide validation and accountability. With reproducible benchmarks and uncertainty-aware workflows, AI/ML can become a reliable component of engineering design and operation.

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