

机器学习方法用于水泥基材料的研究进展

张文生, 曹傅荔, 郅 晓, 叶家元, 任雪红

(中国建筑材料科学研究总院有限公司, 绿色建筑材料国家重点实验室, 北京 100024)

摘 要: 机器学习方法(ML)在解决数据高度非线性和大时滞问题上得到了关注, 为目标属性的预测及新材料的设计开辟了数据驱动的新模式。水泥基材料在组分、制备与其结构、性能的关系上存在时滞性和周期性长的问题。而机器学习方法在解决水泥基材料上述问题时具有积极作用和非常大的潜力。为此, 本文介绍了机器学习方法的特征及其应用过程, 综述了机器学习方法在预测水泥基材料微观结构、组分、力学性能和耐久性等方面的研究进展, 分析比较了几种用于水泥基材料研究模型的特点和优势, 并对所面临的问题和研究方向进行了展望分析, 以期促进机器学习方法的应用。

关键词: 机器学习方法; 水泥基材料; 微观结构和性能; 预测

中图分类号: TP181; TU528 文献标志码: A 文章编号: 0454-5648(2024)11-3617-14

网络出版时间: 2024-04-30



机器学习方法(ML)是一门介于计算机科学和统计学之间的交叉学科^[1-3]。它不需要知道各因素间潜在的作用机理, 只需要通过数据建立材料性能与成分、组织间“黑箱式”联系。ML 包括了从数据收集、性能预测到实验验证的完整循环过程, 建立了特征参量与目标性能之间的隐形映射关系, 推动了材料研发由“经验+试错”向“数据驱动”研发模式的转变, 更加容易建立材料成分-结构-组织-性能的构效关系, 实现材料多层次、多维度目标量的有效预测。在水泥基材料研究方面^[4-6], ML 能够从大量的实际生产或实验数据中学习模式和规律, 预测其抗压强度、抗碳化能力、微观结构形貌和力学参数等。ML 在解决水泥基材料组成、制备过程与性能、耐久性之间关系存在时滞性强和周期长等问题方面具有积极作用, 在提高水泥基材料研发、生产和应用的效率方面展现了广阔的应用前景。

本文介绍了 ML 的特征及其应用流程, 综述分析了近年来 ML 方法在预测水泥基材料的结构、组分和性能等方面的研究进展。结合其在水泥基材料方面的应用情况, 通过分析 ML 模型的特征参数、优化算法及模型评价指标等, 比较了不同模型算法的

特性及其优势, 以期 ML 在水泥基材料研究应用提供参考。

1 机器学习方法的特征及其应用流程

ML 与当前数据库、数学统计和知识发现等计算机科学热点问题有着密切的联系^[7](见图 1)。它通过评估数据集的训练样本, 从以前的经验中学习数据集背后的规律。这种方法在分类、回归等与高维数据相关的问题上的适用性强^[8]。ML 用于水泥基材料的研究流程主要包括数据收集、数据预处理、特征工程、模型构建和模型应用等 5 个关键步骤(见图 2)。

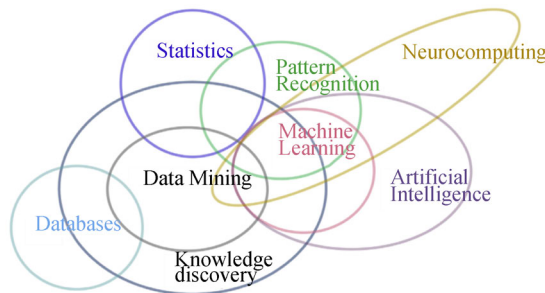


图 1 机器学习与当前计算机科学热点的关系^[7]

Fig. 1 Relationships among ML and current hot topics in computer science^[7]

收稿日期: 2023-11-30。 修订日期: 2023-12-18。

基金项目: 中国建材集团原创技术策源地“揭榜挂帅”任务-“水泥基材料数字化研发”项目(2021YCS01)。

第一作者: 张文生(1969—), 男, 博士, 教授。

Received date: 2023-11-30. Revised date: 2023-12-18.

First author: ZHANG Wensheng (1969—), male, Ph.D., Professor.

E-mail: wensheng_zhang01@163.com

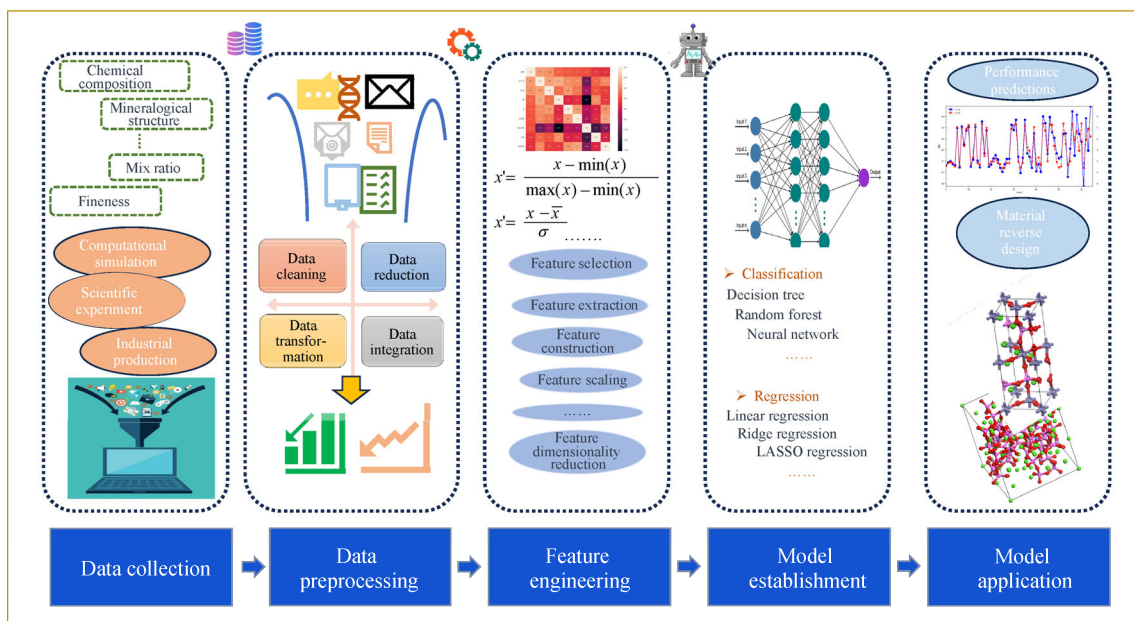


图2 机器学习在材料研究中的应用流程
Fig. 2 Processes for ML in materials research

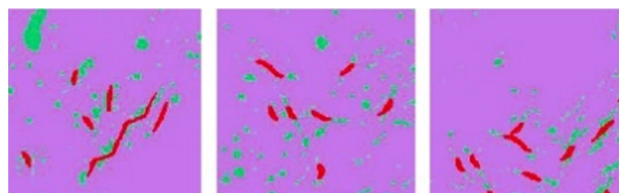
尽管水泥基材料通过多年的工业化生产和科学实验积累了大量的数据，但是这些数据通常是不完整的或是有噪声的。因此，从收集的原始数据中构建样本集时需进行数据预处理^[9]。数据预处理是 ML 和数据分析中关键一步，其中包含数据清洗、数据集成和数据变换等环节。所用方法根据具体的数据和分析目标而有所不同。但是正确的数据预处理对于建立有效的 ML 模型和深入的数据分析至关重要^[10]。特征工程则是最为复杂且关键的一步。它包括特征提取、特征选择、特征构造和特征缩放等步骤。其作用在于优化数据的表示方式，从而使 ML 模型更有效地学习，提高预测的准确性和模型的可解释性^[11]。模型构建本质上是应用一系列特定的线性或非线性函数，以实现从输入数据到输出数据的映射。水泥基材料数据的影响因素与目标属性之间常常存在复杂的相互作用，超出了传统分析方法的处理能力。ML 则可通过利用目标函数的样本来寻找一个映射函数，使得这个映射函数的系数尽可能地接近目标函数。这些算法被广泛的应用于揭示材料的组分-结构-性能间的关系，快速发现潜在的数据规律并做出准确的预测，以及材料的逆向设计^[12]。

2 机器学习在水泥基材料研究的应用

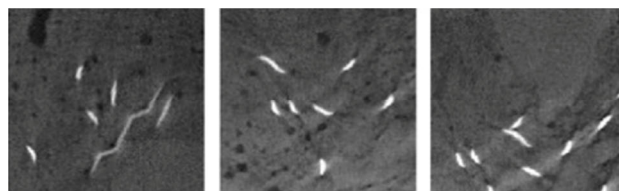
2.1 微观结构与组分预测

水泥基材料采用的传统分析方法往往存在耗时多、反应周期长等问题^[13–14]。近年来，材料表征技

术融入 ML 方法，显著提高了材料组分识别与微观结构分析的效率。刘芳玉等^[15]通过预处理混合纤维增强混凝土(HFRC)的 2DCT 图像，利用随机森林(RF)与 ANN 进行相位分割，为 HFRC-CT 图像的定量分析做准备。与手动分割相比，ML 方法更能从原始数据中发现检测或分类所需的特征值^[16](见图 3)。这提高了三维形态和统计分析的准确性和效率，能够更加具象的掌握纤维增强混凝土的微观结构。



(a) 2D CT images of preprocessed HFRC



(b) Segmented images using the Random Forest model

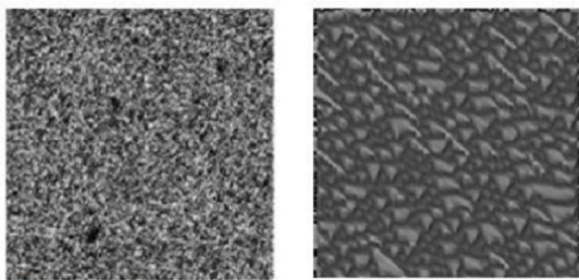
Purple region: matrix phase. Green region: pore phase. Red region: steel fiber phase.

图3 预处理 HFRC 的 2DCT 图像^[15]

Fig. 3 2D CT images of preprocessed HFRC^[15]

Wei 等^[17]提出了一种基于马尔夫随机场的合成算法，仅需要使用 1 个样本微区形貌作为输入特征，

从而合成水泥浆体的微观结构形貌。除此之外, 其合成速度也具有很大优势。范嘉薇等^[18]利用水泥浆体图像邻域像素和中心点像素的关系, 建立了前馈神经网络模型, 调整不同的参数以提高合成的水泥浆体微观结构的图像质量(见图 4)。相较于传统的基因表达式编程的方法, 这种方式更能反映水泥浆体微观结构物相组成。



(a) Gene expression programming (b) Feed-forward neural network

图 4 水泥浆体微观形貌图像的结果比较^[18]

Fig. 4 Comparison of microscopic morphology images of cement paste^[18]

ML 模型的集成提高了预测水泥基材料组分的准确性, 特别是在处理时序问题上和有限样本的情况下。张玉玲等^[19]结合多尺度时空特征提出了双向长短期记忆网络模型(MS-Bi-LSTM)和深度非负稀疏自编码网络(MS-DNSAE)模型, 实现了对熟料中游离氧化钙(f-CaO)含量的高精度实时预测, 其测试集的平均绝对误差(E_M)为 0.1651。Albert 等^[20]在样本有限的情况下, 利用 RF 和额外树算法预测了硬化胶凝体系的孔隙溶液中 OH^+ 、 Na^+ 和 K^+ 等离子含量, 预测的准确率高达 75%~90%。

不仅如此, ML 还能够实现逆向的晶体结构和成分预测^[9]。在逆向设计过程中, 相比于其他统计模型, 贝叶斯(Bayes)算法不仅重视全样本信息和单

个样本信息的利用, 还非常注重先验信息的收集、挖掘和处理。这使其在处理不确定性和融合各类信息方面显得更为高效和灵活^[21]。Ke 等^[22]提出了基于 Bayes 定理的材料分析和设计框架(见图 5), 通过 Gauss 过程模拟器, 实现了对特定高性能混凝土成分的逆向设计。然而, 在使用 ML 方法进行逆向设计的过程中, 数据收集仍然存在一些困难。这是由于制备数据库的高成本导致缺乏大规模且一致性的数据集, 降低了模型训练和预测效果。

2.2 宏观性能预测

2.2.1 力学性能预测 水泥 28 d 抗压强度是最重要的力学性能指标。ML 在快速准确预测水泥 28 d 抗压强度方面具有显著优势。裘国华等^[23]运用 ML 预测了煤矸石代替黏土后煅烧水泥的 28 d 抗压强度。研究选取了细度、比表面积、CaO 含量、1 d 抗折强度、3 d 抗折强度等 5 个特征值作为预测模型的输入参量, 将灰色预测模型 GM(1,N)和径向基函数(RBF)神经网络技术相结合, 提出了基于 GM-RBF 神经网络组合模型预测水泥强度的方法。该模型利用前期对累加生成运算和样本数据的预处理, 减少了由于训练样本的随机性对预测精度产生的影响, 平均相对误差(E_{MR})为 0.36%、均方根相对误差(E_{RRMS})为 0.47%(见图 6)。其预测精度与实际值具有较好的拟合性, 优于单个网络模型。Panagiotis 等^[24]针对掺有偏高岭土(MK)的水泥, 选用支持向量机(SVM)、决策树(DT)、RF、自适应增强(AdaBoost)和 k 最近邻(KNN)5 种模型预测分析了 28 d 抗压强度。其中, RF 和 AdaBoost 的模型预测获得的结果误差最小。其训练集的相关系数(R^2)分别为 0.976 8 和 0.996 5; 测试集的 R^2 分别为 0.943 9 和 0.947 3。图 7、图 8 分别是这 2 种模型的预测结果。

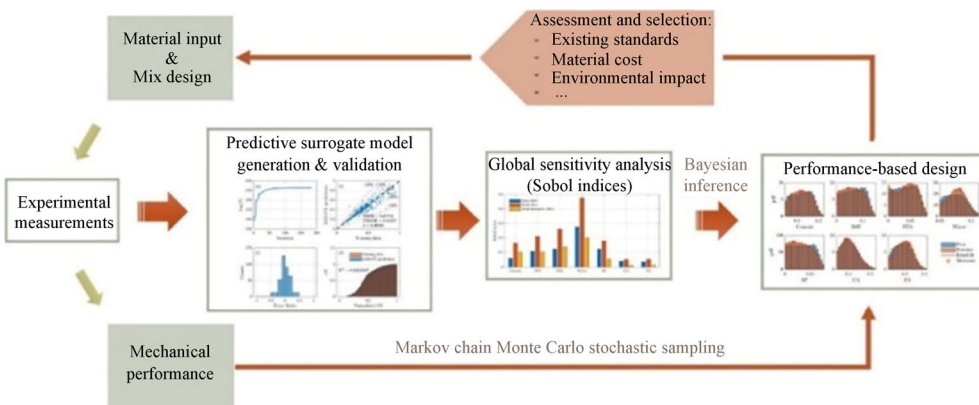
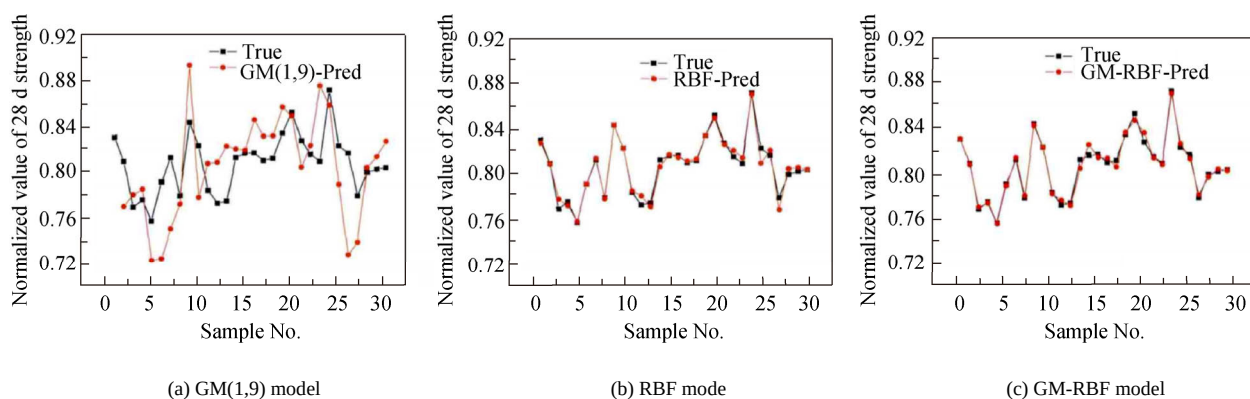


图 5 基于 Bayes 定理的材料分析和设计框架^[22]

Fig. 5 A framework for material analysis and design based on Bayes' theorem^[22]



Samples No. represents the number of training sessions.

图 6 基于 GM-RBF 神经网络组合模型与单一模型对比预测结果对比^[23]

Fig. 6 Comparison of prediction results based on the GM-RBF neural network combined model versus single models^[23]

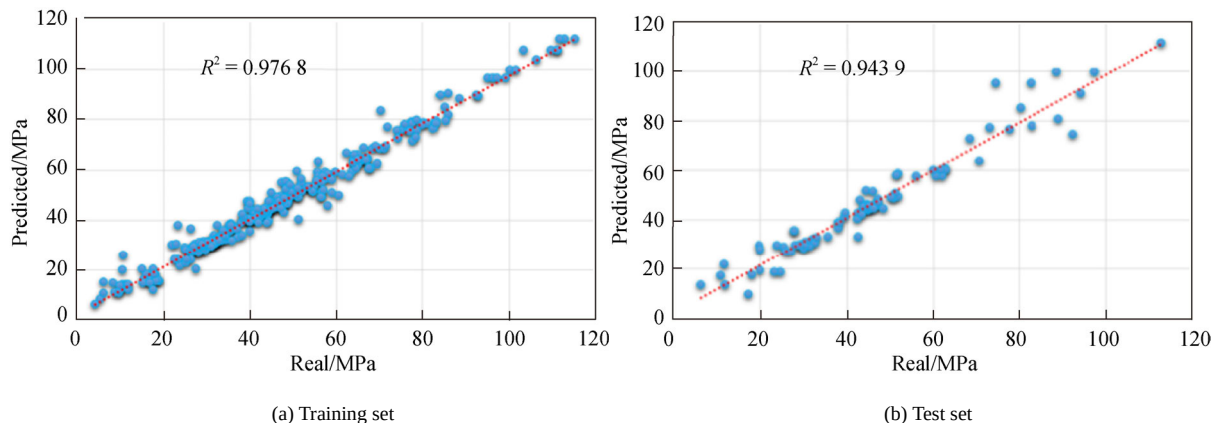


图 7 利用 RF 模型预测水泥-MK 砂浆的抗压强度^[24]

Fig. 7 Prediction of compressive strength of cement-MK mortar using the RF model^[24]

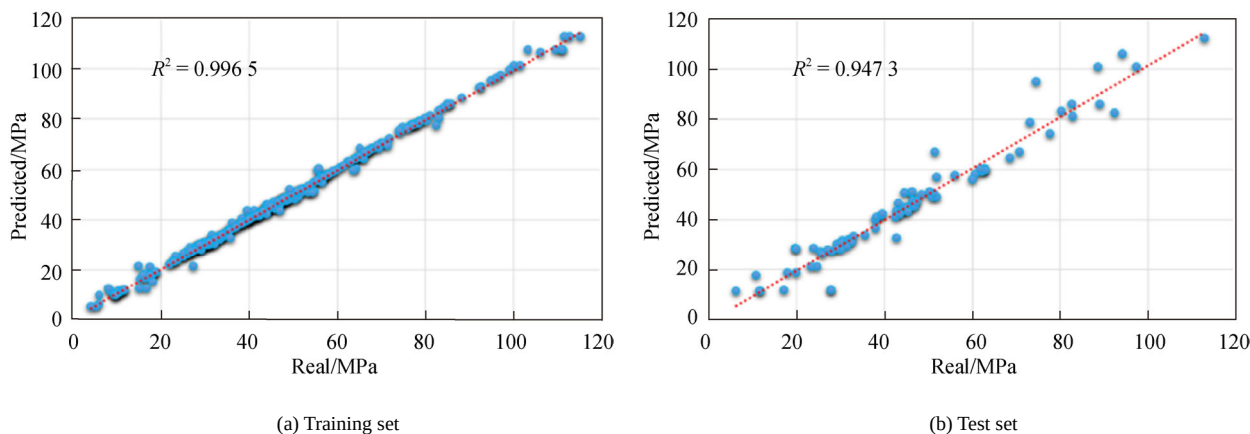


图 8 利用 AdaBoost 模型预测水泥-MK 砂浆的抗压强度^[24]

Fig. 8 Prediction of compressive strength of cement-MK mortar using the AdaBoost model^[24]

传统 ML 模型处理一些复杂的数据集或数据结构时, 由于对数据质量和数量的高度依赖, 以及其泛化能力的局限性, 会导致其模型性能显著受限^[25–28]。针对这一问题, 许多研究使用更为复杂的优化计算模型规避传统 ML 模型在预测期望输出时的局限性。例如: 粒子群优化(PSO)^[29–30]、差分进化(DE)^[31]、人工蜂群(ABC)^[32]、蚁群优化(ACO)^[33]

等计算模型。然而, 即使是经典的优化算法也容易陷入局部最小值的问题。为此, Hamidian 等^[34]提出了一种名为 ANN-PSOTD 的新方法, 用于优化 ANN 预测稻壳灰混凝土抗压强度时的权重和偏差。通过综合 PSO 和 DE 的优点, 提出了粒子群优化器(PSOTD)的混合算法。由图 9 模型泰勒图对比可知, ANN-PSOTD-LM 这一耦合模型的拟合程度更好,

预测精度更高。这种元启发式的混合算法在探索阶段具有很强的能力, 并且基于简单的 ANN 模型, 使得该模型在开发阶段就具有很大潜力^[35]。

此外, 多种传统 ML 模型的集成能够有效缓解单一模型因数据质量和数量限制, 以及泛化能力不足而存在的局限性, 从而提高模型的预测精度和拟合能力。Panagiotis 等^[36]以样本龄期、水胶比、粗骨料与细骨料的比例等特征参量作为参数预测混凝土

强度, 将多个单一传统 ML 的输出结果进行组合, 并使用 ANN 进行训练, 以构建混合集成模型 (HENSIM)。混合集成模型在训练和测试 2 个阶段, 其精度 R^2 (训练=0.988 8, 测试=0.889 4)、均方根误差 E_{RMS} (训练=0.070 1, 测试=0.220 0) 和平均绝对误差 E_{MA} (训练=0.010 4, 测试=0.049 0) 等都显著增加 (见图 10)。这种混合集成模型的预测能力比传统 ML 模型的更强, 拟合程度更好。

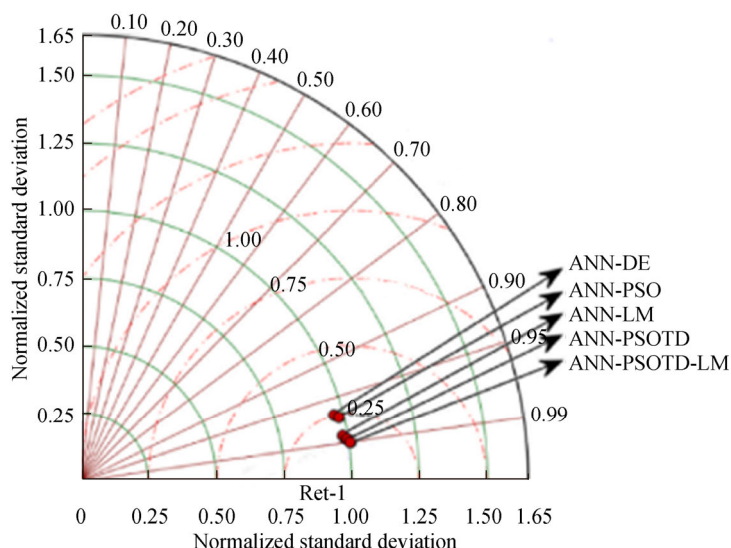
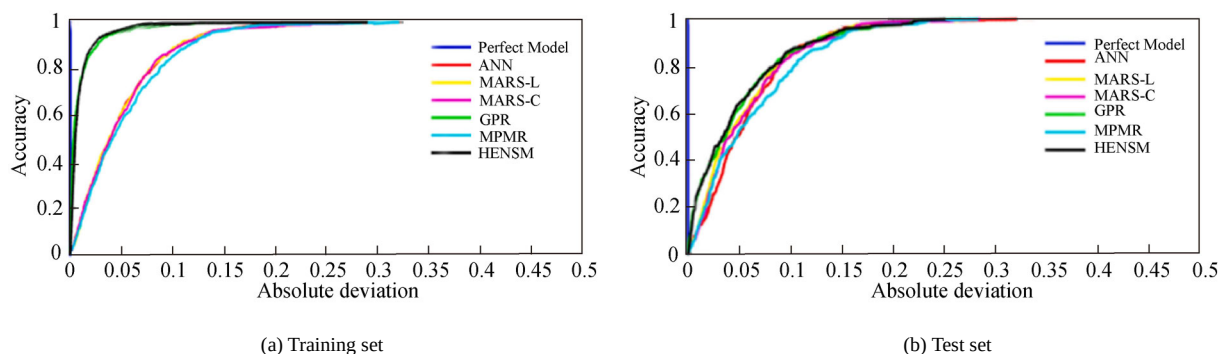


图 9 数据集 5 种模型泰勒图^[34]

Fig. 9 Taylor diagrams of the five models for the dataset^[34]



The horizontal axis represents the regression error tolerance ε , and the vertical axis represents the percentage of "correct classifications" within the tolerance.

图 10 回归误差特征曲线^[36]

Fig. 10 Regression error characteristic curves^[36]

混凝土中输入变量与目标输出之间呈现复杂的非线性关系, 且输入变量间互相关联。虽然传统的“黑盒”模型能够提供较为准确的预测结果, 但其结构的复杂性导致难以掌握输入与输出之间的准确关系。因此, 需要开发新的方法来解决这一问题, 以便准确掌握变量间的相互关系。近年来, 加法解释法 (SHAP)^[37-38] 因其优异的可解释性和广泛的适用性受到关注。Lyngdoh 等^[39]将 SHAP 与极端梯度

提升 (XGBoost) 集成, 并通过为每个输入变量分配权重值来解释输入特征的贡献比。图 11 为利用 XGBoost 模型预测混凝土抗压强度和抗拉强度的特征 SHAP 值的小提琴图, 其对应的 x 轴 (SHAP) 值则表示对输出性能的贡献值。对于输入参量水灰比, 右侧的蓝色点和左侧的红色值分别表示水灰比的低值和高值。通过可解释的 ML 算法和 SHAP 生成的可视化效果去评估特征的相对重要性, 提供

了一种对模型预测的可解释性方法, 进而通过不同特征间的相互作用揭示影响材料性能的内在机理。

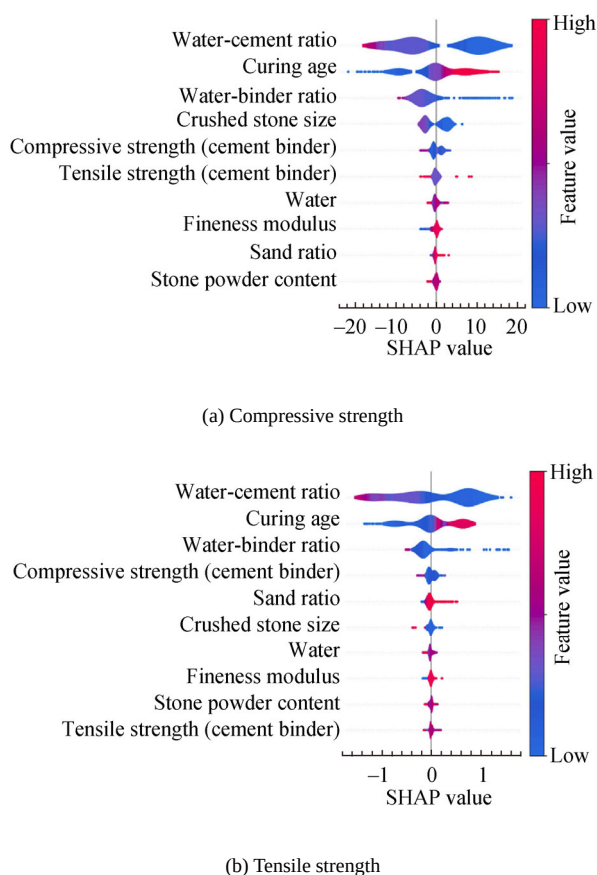
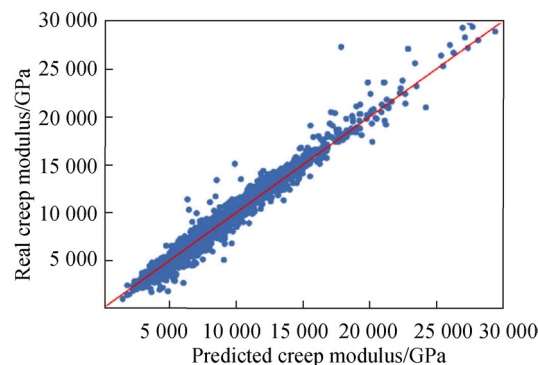


图 11 XGBoost 预测混凝土强度的 SHAP 小提琴图^[39]

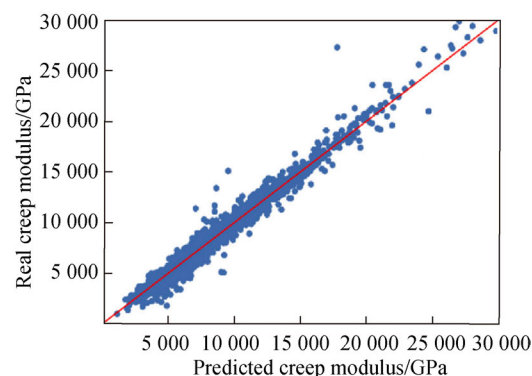
Fig. 11 SHAP violin plot for concrete characterization using XGBoost^[39]

ML 方法除了在预测水泥基材料的强度方面的研究较为广泛外, 在预测混凝土的徐变、蠕变和弹性模量等性能方面也得到了应用。Minfei Liang 等^[40]使用经过实验验证的短期徐变微尺度晶格模型, 建立了一个包含 18 920 个微结构及其相应徐变的数据集。以微结构为输入预测徐变模量, 建立具有不同连续卷积层数的深度卷积神经网络(DCNN), 通过对比深度卷积神经网络预测了徐变分布和晶格模型, 实现了徐变的高精度预测。预测结果如图 12 所示, 其 R^2 均高于 0.96, 且模型卷积层越多, 预测精度越高。Duan 等^[41]研究预测再生骨料混凝土的弹性模量。采用 ANN 模型的预测结果比传统相关方程更迅速、更精确。蠕变作为评价混凝土力学性能和长期行为的关键参数^[42], 不少学者用实验和数学统计的方法开展了研究^[43–46], 但这些方法在预测混凝土蠕变性能上仍存在局限, 效果并不理想。Feng 等^[47]利用最小二乘支持向量机(LSSVM)、反向传播神经网络(BPNN)、回归(RT)、RF 和 XGBoost 等 5

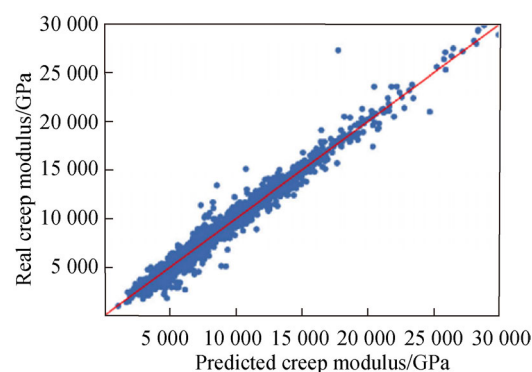
种典型 ML 算法, 在再生骨料混凝土_Creep_v1 数据库^[48]的训练下, 首次全面研究了再生骨料混凝土蠕变性能的预测模型。通过网格搜索算法和 5 折交叉验证, 找到了最佳的超参数, 进行了特征重要性分析和相关性分析, 以评估各种输入变量对结果的影响。研究表明, 荷载和龄期对再生骨料混凝土的蠕变性能影响最大。



(a) DCNN-1, $R^2 = 0.9678$, $E_{MS} = 0.00391$, $E_{MA} = 0.01285$



(b) DCNN-2, $R^2 = 0.9753$, $E_{MS} = 0.00300$, $E_{MA} = 0.01100$



(c) DCNN-3, $R^2 = 0.9757$, $E_{MS} = 0.00295$, $E_{MA} = 0.01080$

图 12 DCNN 模型对角线误差图^[40]

Fig. 12 Diagonal error plot for DCNN model^[40]

2.2.2 耐久性能预测 1) 抗碳化能力预测。尽管 ANN 模型相较于其他统计模型可以更好的预测混凝土碳化深度^[49–50], 但与其他经典优化算法一样,

ANN 模型中的参数极易陷入局部最优^[51]。而群智能算法能够进一步优化 ANN 模型的参数, 提高其预测模型的泛化能力。Liu 等^[52]开发了一种利用群智能算法的混合 ANN 模型(见图 13), 用于预测再生骨料混凝土的抗碳化性。该模型的输入参数包括再生骨料混凝土的固有特性和环境条件, 如含水量、水泥含量、再生骨料吸水率、再生骨料的体积置换率、温度、相对湿度、CO₂ 浓度、养护龄期和碳化时间等, 共涉及了 593 个样本量。采用了 PSO、鲸鱼优化算法(WO)和甲虫触角搜索算法(BAS)等群智能算法优化 ANN 模型。3 种混合 ANN 模型暨 PSOANN、WOANN 和 BASANN 的预测结果都优于独立模型。这些群智能算法对 ANN 的权重和偏差进行优化, 提高了模型的全局优化能力。

自动回归方法基于元启发式算法, 在预测精度和适应性方面与以往模型相比都有所突破。Seyed 等^[53]使用人工蜂群表达式编程模型, 在包含 655 个

样本的大型数据集上, 开发了多种人工蜂群表达式编程模型架构来预测再生骨料混凝土的碳化深度。通过比较证明了最佳架构人工蜂群表达式编程模型可以更加精确地预测再生骨料混凝土的碳化深度(E_{RMS} 为 3.33 mm)。当前预测算法模型的决策过程并不直观, 可解释性差^[54]。针对这一问题, Pearson 相关热力学图可以用来分析人工蜂群表达式编程模型输入和输出之间的相关性。Nunez 等^[55]通过使用 Pearson 相关系数分析, 研究了不同特征参数之间的相关性。研究发现混凝土的抗压强度和水胶比与碳化深度存在高度相关性, 而骨料、硅灰和粉煤灰含量与碳化深度呈现低相关性(见图 14)。利用随机搜索算法和交叉验证技术, 选择了梯度提升回归树模型的最佳超参数, 进一步预测再生骨料混凝土的抗碳化能力。结果表明, 所构建的梯度提升回归树模型具有稳定性, 并获得了较好的预测精度(E_{RMS} 为 1.5139, E_{MA} 为 0.948, R^2 为 0.9707)。

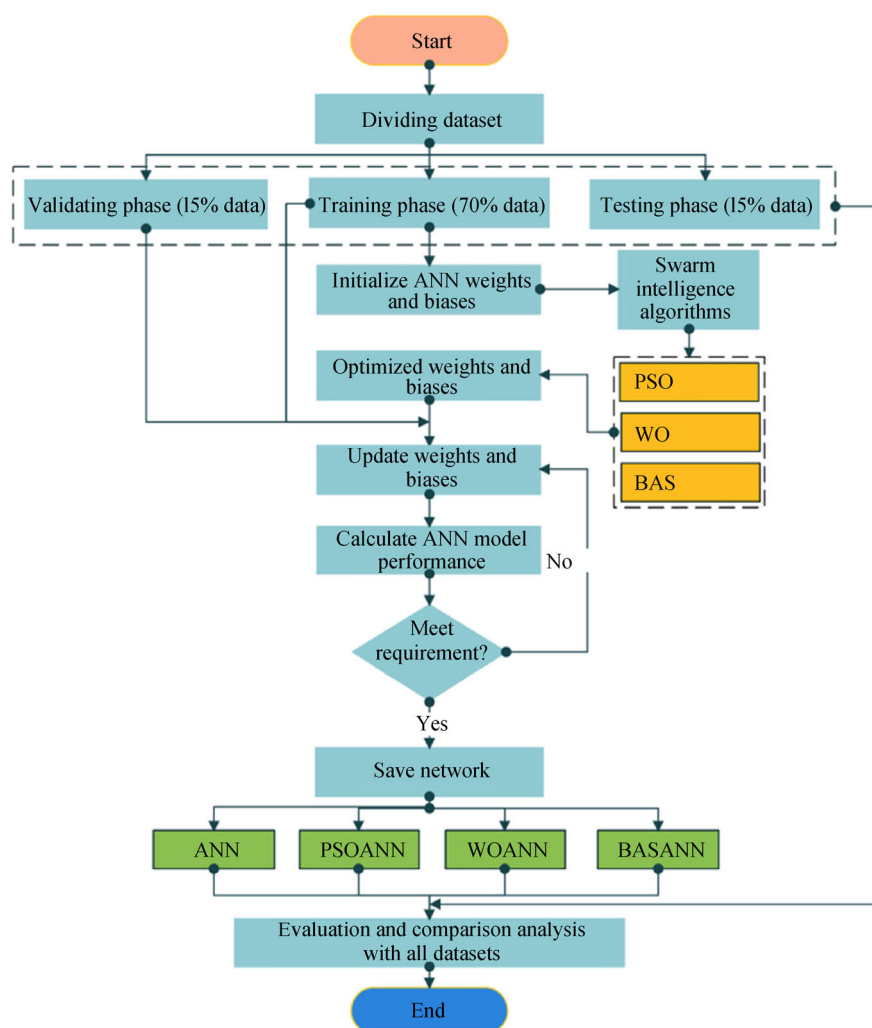
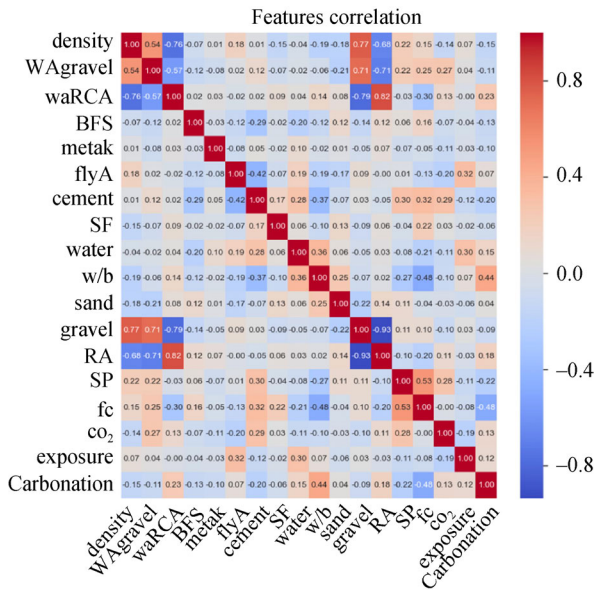


图 13 具有群体智能算法的混合 ANN 模型的流程图^[52]

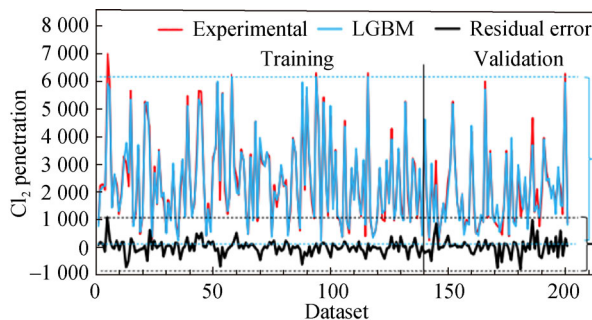
Fig. 13 Flowchart of the hybrid ANN model with swarm intelligence algorithms^[52]

图 14 数据集属性间的 Pearson 相关系数^[55]Fig. 14 Pearson correlation coefficients between attributes in the dataset^[55]

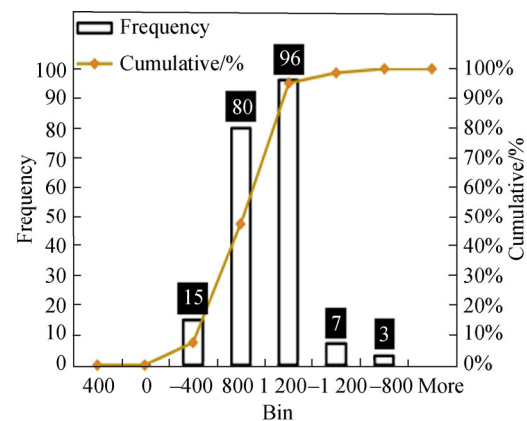
2) 抗氯离子渗透性预测。当前大多研究倾向于采用 ANN 模型来预测氯离子的扩散系数^[56–59]。

Liu 等^[57]基于 653 个数据样本, 构建了含矿粉、粉煤灰、硅灰等辅助胶凝材料的混凝土氯离子扩散系数 ANN 模型。然而模型尚未充分考虑 C_3A 含量、配合比设计(包括水泥、水和骨料的含量)等关键因素对氯离子扩散系数的影响。Van 等^[60]采用 SVM、极限学习机、KNN、轻量级梯度增强模型 (LightGBM)、XGBoost、RF、梯度提升 (GB) 和 AdaBoost 等 8 种经典 ML 算法, 选取 C_3A 含量、水灰比、粉煤灰掺量、硅灰掺量、粉煤灰比表面积等 9 个特征参数的数据库进行性能预测对比研究。结果表明, GB 模型预测效果最佳, E_{MA} 为 1.9997×10^{-12} 。

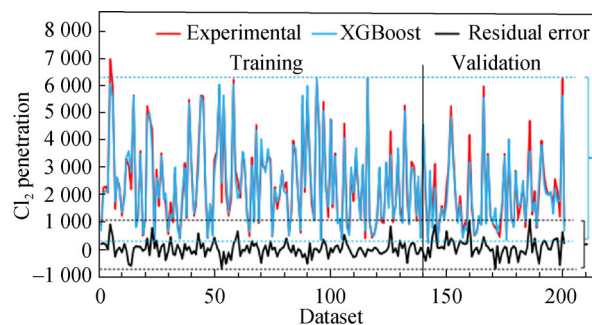
Anas 等^[61]研究了 LightGBM 和 XGBoost 这 2 种优化算法用于预测氯离子渗透。研究使用了 201 组实验数据, 将混凝土的老化、胶凝材料含量、水胶比、偏高岭土用量和粗细骨料的含量作为输入变量, 利用网格搜索优化训练模型, 优化参数以实现最佳性能。图 15 对比分析了所建立模型的误差结果。从图 15a 和图 15b 可见, LightGBM 和 XGBoost 模型预测结果与实验结果最为接近。误差直方图图 15c



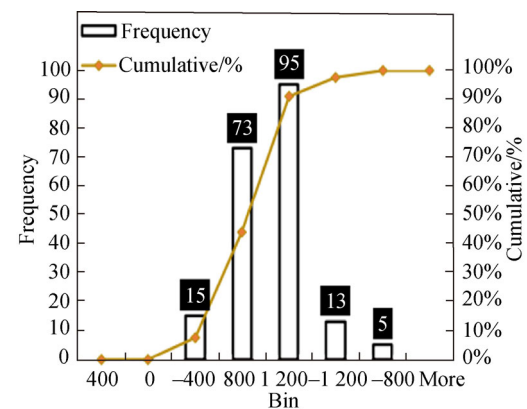
(a) Light GBM



(c) Light GBM



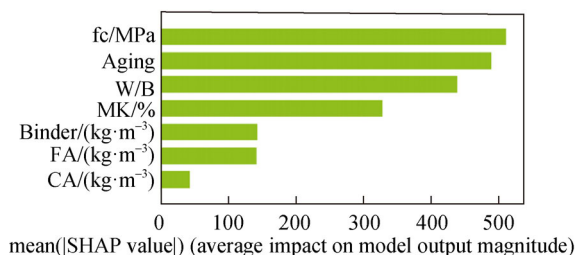
(b) XG Boost



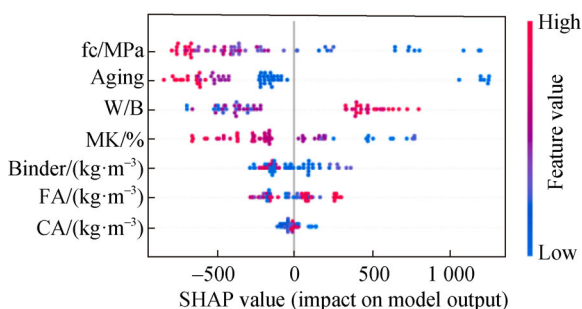
(d) XG Boost

图 15 Light GBM 和 XG Boost 模型的 Exp 预测趋势和误差分析^[61]Fig. 15 Prediction trends and error analysis for the Light GBM and XGBoost model with Exp^[61]

和图 15d 显示, 对于 LightGBM 模型, 95.02% 的数据点位于 -400 C 至 $1\ 200$ C 之间。通过比较模型评估参数性能指标(如 R^2 、 E_{RMS} 、 E_{MA} 、 E_{RS} 、 E_{RRMS} 、Nash-Sutcliffe 效率 E_{NS} 和性能指数 ρ)来看, LightGBM 的预测精度与鲁棒性均优于 XGBoost 算法。为深入探究模型的内在机制, 将 SHAP 理论集成当前最优模型来识别和量化特征参数的重要性^[62]。图 16a 是通过对整个数据集的 SHAP 值求平均得到的, 图 16b 是其所对应的蜂巢图。显然, 混凝土抗压强度(f_c)、老化时间(Aging)和水胶比(W/B)对抗氯离子渗透能力的预测具有重要作用。



(a) SHAP feature importance

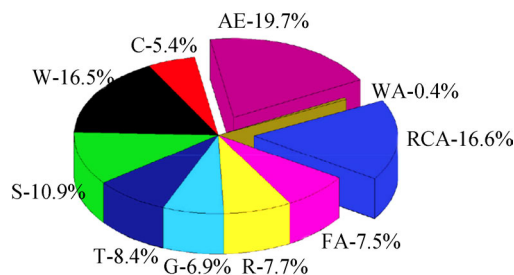


(b) SHAP summary plot

图 16 SHAP 值对 LightGBM 模型的全局解释^[61]Fig. 16 Global interpretation of the LightGBM model using SHAP values^[61]

3) 抗冻性预测。Liu 等^[63]采用 ANN、高斯过程回归和多元自适应回归样条等 3 种模型, 利用耐久性因子(Durability factor, DF)值对再生骨料混凝土的抗冻性能进行了建模预测。研究表明, ANN 模型表现出较高的预测精度, 优于高斯过程回归模型和多元自适应回归样条模型。此外, 通过余弦振幅法、米尔恩法和广义交叉验证法对实验数据的敏感性进行了分析, 并将其与建立的模型预测自由度值进行了对比, 分析了水(W)、水泥(C)、砂(S)、砾石(G)、再生粗骨料(RCA)、粉煤灰(FA)、RCA 替代率(R)、吸水率(WA)、RCA 处理方法(T)和引气剂(AE)等 10 个参数对 ANN 模型耐久性因子的影响(见图 17)。结果表明, 引气剂的影响因子最大(19.7%), 其次是再生粗骨料(16.6%)和水(16.5%), 而吸水率对耐久性因子

的影响最小(0.4%)。吴贤国等^[64]基于 LSSVM 的多目标优化算法模型, 结合遗传算法, 实现混凝土配合比的多目标优化设计, 以混凝土抗冻性和经济成本为目标, 实现了更加智能化和精确化的混凝土配合比多目标寻优。

图 17 输入参数对 ANN 模型 DF 值的影响^[63]Fig. 17 Impact of each input on the DF value of the ANN model^[63]

对比上述传统算法, 元启发式算法在混凝土耐久性预测方面显得更加灵活^[65-66]。Cemalgil 等^[67]以水泥的初凝时间和终凝时间、含气量、耐磨性、抗冻性等参数作为输入参量, 预测了钢纤维硅灰高强混凝土的抗冻性。以极限学习机(GRELM)模型为基准, 并参考元启发式算法中的 PSO 和灰狼优化算法(GWO)进行优化, 提出了 GRELM、GRELM-PSO、GRELM-GWO 和 GRELM-PSO-GWO 等 4 种模型。经过对比分析, 构建的 GRELM-PSO-GWO 模型在预测抗冻性方面具有最高的精度, 其中 E_{RMS} 小于 0.1。

需要说明的是, 本文涉及的水泥基材料耐久性预测仅仅着眼于材料物性。工程实践中的水泥基材料的耐久性与其建筑结构具有重要的关系, 其耐久性预测是另外一个更为复杂的体系。

2.3 水泥基材料常用预测模型的比较分析

随着 ML 的发展, 其预测模型也得到了不断的完善和拓展^[68-69], 例如, 决策树模型、SVM 模型、深度学习(DL)模型和集成学习(EL)模型等都在材料领域得到了广泛应用。不同的预测模型具有各自的特点和优势。表 1 分析比较了几种水泥基材料常用预测模型特点和优势^[70-77]。

上述模型中, DL 模型与其他 ML 模型存在本质上的区别。它不仅仅是 ML 算法的一个分支, 而是代表了一种更加复杂和高级的学习机制^[78]。DL 通过构建多层的神经网络结构, 能够自动学习数据中的高级特征和抽象表示, 这在传统 ML 模型中往往难以实现。因此, DL 被视为是实现更接近人类智能的关键步骤。为此, 表 2 详细比较了不同的 DL 模型^[79-85]。这些模型都有针对性强的数据类型和应用场景。

表 1 几种水泥基材料常用预测模型特点和优势^[70–77]Table 1 Features and Advantages of Commonly Used Prediction Models for Cement-based Materials^[70–77]

Model Types	Linear Regression(LR)	Support Vector Regression(SVR)	Artificial Neural Network(ANN)	Decision Tree(DT)	Deep Learning(DL)	Ensemble Learning(EL)
Characteristics	Few parameters, simple computation, easy to understand and apply	Suitable for predicting nonlinear data, effectively fitting multiple performance parameters	Used for predicting nonlinear data, effectively fitting multiple performance parameters	Has strong interpretability	It has strong adaptability, adjusting and optimizing itself based on different datasets and problems	Possesses strong generalization ability, can combine the advantages of different individual models, and enhance prediction accuracy
	The predicted results are highly interpretable, enabling a better understanding of the material's performance	It has strong robustness to noise and outliers, with the ability to filter out interference data	Highly adaptive, capable of self-adjusting and optimizing for different datasets and problems	Easy to Understand and Apply	Strong Nonlinear Fitting Ability: Effectively Captures Complex Features, Enhances Prediction Accuracy	Combining multiple individual models can reduce the influence of noise, improving the stability and accuracy of predictions
	Wide Application Range	Relatively high prediction accuracy, especially for small data sets	Has strong nonlinear fitting ability and can effectively capture complex features	The model can handle missing data.	Suitable for handling large-scale data, such as microscopic structure image analysis, and so on	Suitable for handling high variance, large-scale imbalanced data, and exhibits good scalability for evolving prediction problems
Advantages	Quickly accomplish data fitting and prediction, easy to adjust and improve	Applied to complex problems, such as predicting multiple performance parameters like compressive strength and elastic modulus	Can handle large-scale data. Learns and predicts through multiple layers of neurons	Applied to complex problems: has strong interpretability, enabling a better understanding of material performance	High prediction accuracy	Combining different individual models is more effective when dealing with a small sample size and high data noise
	Improve prediction accuracy by adjusting parameters.	Strong generalization ability	Applied to complex problems, such as multi-parameter performance prediction.	The model can handle missing data	Strong Generalization, Suitable for Multiple Data Types	Combining multiple individual models reduces noise impact, improving prediction stability and accuracy

表 2 常见深度学习模型比较^[79–85]Table 2 Comparison of common deep learning models^[79–85]

Model Types	Main Applications	Key Features
Convolutional Neural Network (CNN)	Image and video processing	Using convolutional layers to process grid data (such as images). suitable for feature extraction and pattern recognition in visual data.
Graph Neural Network (GNN)	Graph data analysis	Using spectral graph theory for data, suitable for graph-structured data analysis
Transformer	Natural language processing	Handling sequential data with self-attention mechanism, proficient in understanding context and dependencies in language and sequential data.
Recurrent Neural Network (RNN)	Sequential data processing	Handling time series data or sequences, suitable for context-sensitive tasks.
Autoencoder	Data compression, feature extraction	Efficient encoding for unsupervised learning, typically used for dimensionality reduction
Generative Adversarial Network (GAN)	Image generation	Comprised of a generator and discriminator, competing with each other, suitable for generating new data.

3 结论与展望

以 ML 为核心的新材料研发范式是当下研究热点。尽管 ML 方法在预测水泥基材料微观结构、性能方面取得了较大进展,但在数据质量与数量不平衡、ML 模型可解释性和泛化能力等方面仍然需要更多的工作:

1) 数据质量与数据数量不平衡问题:数据是驱动 ML 模型的基础。数据质量包括数据的准确性、完整性、一致性和时间敏感性。由于水泥流程及其性能发展的多时序关系,使得其组分-结构-性能数据链信息缺失甚至断点,数据质量和数据数量难以保证。这需建立全面的基础数据库,涵盖材料成分、结构、性能及其影响性能的环境因素,甚至化学反应过程的参数,以解决数据质量和数据数量不平衡的问题。

2) 模型可解释性不足:多数水泥基材料的预测模型因其高度复杂且非线性的特性而难以解释。这些模型涉及多个层次,其中参数通过复杂的关系相互影响,使得难以理解其模型的决策过程,从而使模型缺乏透明度和可解释性。模型可解释性的提升对于深入解析水泥基材料在多变环境和不同负载条件下的性能至关重要。利用高级后处理解释工具可有效揭示复杂预测模型中特征参数对水泥基材料力学性能、耐久性及化学反应动力学的具体影响。此外,将 ML 与精确的物理模型融合,能够增强模型预测的可解释性,并为准确预测水泥基材料性能的支持。

3) ML 模型泛化能力不足:水泥基材料的复杂性使得模型的训练数据难以涉及所有类别,导致模型在面对新数据时的预测性能下降。而元学习方法通过在一系列相关但不同的任务上训练模型,使其能够快速适应新的水泥基材料组合。未来的研究可深入探索元学习模型在更大范围内性能指标上的适用性,以及如何将元学习与其他先进的 ML 技术相结合,以进一步增强模型的预测能力和适应性。

人工智能的发展和算力的增强,为提升材料的研发效率提供了无限可能。例如,ChatGPT 的超大型生成式人工智能在各个领域展现出了显著的应用潜力^[86-87],水泥基材料的应用研究也不例外。这些模型的多维数据处理能力使其能够综合考虑影响目标性能的多种因素,从而预测不同条件下的水泥性能。随着模型自我学习和优化能力的提升,同时融合水泥基材料的分子动力学模拟、硬化浆体三维结

构模拟和组分间的反应动力学及热力学数据,实现其组分、结构和性能的精确预测,以及使水泥基材料的逆向设计成为可能。这必将有助于快速高效的开发新型水泥基材料。

参考文献:

- [1] CLAUDE S, GEOFFREY I W, Encyclopedia of machine learning[M]: Springer Science & Business Media, New York, US, 2011.
- [2] JORDAN M I, MITCHELL T M. Machine learning: Trends, perspectives, and prospects[J]. Science, 2015, 349(6245): 255-260.
- [3] TOM M M, Machine learning[M]: McGraw-Hill Science/Engineering/Math, New York, US, 1997.
- [4] KADRI E H, KENAI S, EZZIANE K, et al. Influence of metakaolin and silica fume on the heat of hydration and compressive strength development of mortar[J]. Appl Clay Sci, 2011, 53(4): 704-708.
- [5] LAWLER J S, ZAMPINI D, SHAH S P. Microfiber and macrofiber hybrid fiber-reinforced concrete[J]. J Mater Civ Eng, 2005, 17(5): 595-604.
- [6] 王云帆, 田原, 周玉美, 等. 主动学习辅助材料研发进展[J]. 硅酸盐学报, 2023, 51(2): 544-551.
- [7] WANG Yunfan, TIAN Yuan, ZHOU Yumei, et al. J Chin Ceram Soc, 2023, 51(2): 544-551.
- [7] On machine learning and the next wave of innovation[EB/OL]. (2020) [2023-12-05]. <http://www.linkedin.com/pulse/machine-learning-next-wave-innovation-eric-miley-mba>.
- [8] LIU Y, GUO B R, ZOU X X, et al. Machine learning assisted materials design and discovery for rechargeable batteries[J]. Energy Storage Mater, 2020, 31: 434-450.
- [9] LIU Y, ZHAO T L, JU W W, et al. Materials discovery and design using machine learning[J]. J Materomics, 2017, 3(3): 159-177.
- [10] BUTLER K T, DAVIES D W, CARTWRIGHT H, et al. Machine learning for molecular and materials science[J]. Nature, 2018, 559(7715): 547-555.
- [11] LIU Y, ZOU X X, MA S C, et al. Feature selection method reducing correlations among features by embedding domain knowledge[J]. Acta Mater, 2022, 238: 118195.
- [12] LIU Y, WANG S Y, YANG Z W, et al. Auto-MatRegressor: Liberating machine learning alchemists[J]. Sci Bull, 2023, 68(12): 1259-1270.
- [13] AZIMI S M, BRITZ D, ENGSTLER M, et al. Advanced steel microstructural classification by deep learning methods[J]. Sci Rep, 2018, 8: 2128.
- [14] SAHA S K, PRADHAN S, BARAI S V. Use of machine learning based technique to X-ray microtomographic images of concrete for phase segmentation at meso-scale[J]. Constr Build Mater, 2020, 249: 118744.
- [15] LIU F Y, XU K, DING W Q, et al. Microstructural characteristics and their impact on mechanical properties of steel-PVA fiber reinforced concrete[J]. Cem Concr Compos, 2021, 123: 104196.
- [16] LORENZONI R, CUROSU I, PACIORNIK S, et al. Semantic segmentation of the micro-structure of strain-hardening cement-based composites (SHCC) by applying deep learning on micro-computed tomography scans[J]. Cem Concr Compos, 2020, 108: 103551.
- [17] WEI L Y, LEVOY M. Fast texture synthesis using tree-structured vector quantization[C]//Proceedings of the 27th annual conference on Computer graphics and interactive techniques. ACM, 2000: 479-488.
- [18] 范嘉薇. 基于神经网络的水泥微结构快速建模及性能分析[D]. 济南: 济南大学, 2021.

- FAN Jiawei. Rapid modeling and performance analysis of cement microstructure based on neural network[D]. Jinan: University of Jinan, 2021.
- [19] 张玉玲. 基于数据驱动的水泥熟料游离氧化钙软测量方法研究[D]. 秦皇岛: 燕山大学, 2021.
- ZHANG Yuling. Research on soft-sensing method of free calcium oxide in cement clinker based on data drive[D]. Qinhuangdao: Yanshan University, 2021.
- [20] ALBERT C, ISGOR O B, ANGST U. Exploring machine learning to predict the pore solution composition of hardened cementitious systems[J]. *Cem Concr Res*, 2022, 162: 107001.
- [21] BOLSTAD W M. Introduction to Bayesian Statistics[M]. John Wiley & Sons, 2016: 428–595.
- [22] KE X Y, DUAN Y. A Bayesian machine learning approach for inverse prediction of high-performance concrete ingredients with targeted performance[J]. *Constr Build Mater*, 2021, 270: 121424.
- [23] 裘国华, 申屠南瑛, 施正伦. 基于 GM-RBF 神经网络组合模型的水泥强度预测方法[J]. *科技导报*, 2014, 32(3): 56–61.
- QIU Guohua, SHENTU Nanying, SHI Zhenglun. *Sci Tech Rev*, 2014, 32(03): 56–61.
- [24] ASTERIS P G, KOOPALIPOOR M, ARMAGHANI D J, et al. Prediction of cement-based mortars compressive strength using machine learning techniques[J]. *Neural Comput Appl*, 2021, 33(19): 13089–13121.
- [25] HABEEB G A, FAYYADH M M, Rice husk ash concrete: the effect of RHA average particle size on mechanical properties and drying shrinkage[J]. *Aust J Basic Appl Sci*, 2009, 3(3): 1616–1622.
- [26] JAIN A, PATEL H, NAGALAPATTI L, et al. Overview and importance of data quality for machine learning tasks[C]//Proceedings of the 26th ACM SIGKDD international conference on knowledge discovery & data mining. 2020: 3561–3562.
- [27] GUDIVADA V, APON A, DING J. Data quality considerations for big data and machine learning: Going beyond data cleaning and transformations[J]. *Int J Adv Softw*, 2017, 10(1): 1–20.
- [28] 刘悦, 马舒畅, 杨正伟, 等. 面向材料领域机器学习的数据质量治理[J]. *硅酸盐学报*, 2023, 51(2): 427–437.
- LIU Yue, MA Shuchang, YANG Zhengwei, et al. *J Chin Ceram Soc*, 2023, 51(2): 427–437.
- [29] EBERHART R, KENNEDY J. A new optimizer using particle swarm theory[C]//MHS'95. Proceedings of the Sixth International Symposium on Micro Machine and Human Science. Nagoya, Japan. IEEE, 1995: 39–43.
- [30] KENNEDY J, EBERHART R. Particle swarm optimization[C]//Proceedings of ICNN'95 - International Conference on Neural Networks. Perth, WA, Australia. IEEE, 1995: 1942–1948.
- [31] STORN R, PRICE K. Differential evolution—A simple and efficient heuristic for global optimization over continuous spaces[J]. *J Glob Optim*, 1997, 11(4): 341–359.
- [32] TEODOROVIC D, DELL'ORCO M, Bee colony optimization—a cooperative learning approach to complex transportation problems[J]. *Adv Or Ai*, 2005, 51: 60.
- [33] DORIGO M, MANIEZZO V, COLORNI A. Ant system: Optimization by a colony of cooperating agents[J]. *IEEE Trans Syst Man Cybern B Cybern*, 1996, 26(1): 29–41.
- [34] HAMIDIAN P, ALIDOUST P, GOLAFSHANI E M, et al. Introduction of a novel evolutionary neural network for evaluating the compressive strength of concretes: A case of rice husk ash concrete[J]. *J Build Eng*, 2022, 61: 105293.
- [35] GOLAFSHANI E M, BEHNOOD A, ARASHPOUR M. Predicting the compressive strength of normal and high-performance concretes using ANN and ANFIS hybridized with grey wolf optimizer[J]. *Constr Build Mater*, 2020, 232: 117266.
- [36] ASTERIS P G, SKENTOU A D, BARDHAN A, et al. Predicting concrete compressive strength using hybrid ensembling of surrogate machine learning models[J]. *Cem Concr Res*, 2021, 145: 106449.
- [37] LUNDBERG S M, NAIR B, VAVILALA M S, et al. Explainable machine-learning predictions for the prevention of hypoxaemia during surgery[J]. *Nat Biomed Eng*, 2018, 2(10): 749–760.
- [38] LAURITSEN S M, KRISTENSEN M, OLSEN M V, et al. Explainable artificial intelligence model to predict acute critical illness from electronic health records[J]. *Nat Commun*, 2020, 11(1): 3852.
- [39] LYNGDOH G A, ZAKI M, ANOOP KRISHNAN N M, et al. Prediction of concrete strengths enabled by missing data imputation and interpretable machine learning[J]. *Cem Concr Compos*, 2022, 128: 104414.
- [40] LIANG M F, GAN Y D, CHANG Z, et al. Microstructure-informed deep convolutional neural network for predicting short-term creep modulus of cement paste[J]. *Cem Concr Res*, 2022, 152: 106681.
- [41] DUAN Z H, KOU S C, POON C S. Using artificial neural networks for predicting the elastic modulus of recycled aggregate concrete[J]. *Constr Build Mater*, 2013, 44: 524–532.
- [42] LIANG M F, CHANG Z, WAN Z, et al. Interpretable Ensemble-Machine-Learning models for predicting creep behavior of concrete[J]. *Cem Concr Compos*, 2022, 125: 104295.
- [43] KHAN I, XU T F, CASTEL A, et al. Risk of early age cracking in geopolymer concrete due to restrained shrinkage[J]. *Constr Build Mater*, 2019, 229: 116840.
- [44] CASTEL A, FOSTER S J, NG T, et al. Creep and drying shrinkage of a blended slag and low calcium fly ash geopolymer concrete[J]. *Mater Struct*, 2016, 49(5): 1619–1628.
- [45] PACHECO-TORGAL F, DING Y N, JALALI S. Properties and durability of concrete containing polymeric wastes (tyre rubber and polyethylene terephthalate bottles): An overview[J]. *Constr Build Mater*, 2012, 30: 714–724.
- [46] SHEN L H, LI Q H, GE W, et al. The mechanical property and frost resistance of roller compacted concrete by mixing silica fume and limestone powder: Experimental study[J]. *Constr Build Mater*, 2020, 239: 117882.
- [47] FENG J P, ZHANG H W, GAO K, et al. Efficient creep prediction of recycled aggregate concrete via machine learning algorithms[J]. *Constr Build Mater*, 2022, 360: 129497.
- [48] TOŠIĆ N, DE LA FUENTE A, MARINKOVIĆ S. Creep of recycled aggregate concrete: Experimental database and creep prediction model according to the *fib* model code 2010[J]. *Constr Build Mater*, 2019, 195: 590–599.
- [49] PAUL S C, PANDA B, HUANG Y H, et al. An empirical model design for evaluation and estimation of carbonation depth in concrete[J]. *Measurement*, 2018, 124: 205–210.
- [50] KELLOUCHE Y, BOUKHATEM B, GHRICI M, et al. Exploring the major factors affecting fly-ash concrete carbonation using artificial neural network[J]. *Neural Comput Appl*, 2019, 31(2): 969–988.
- [51] CUNNINGHAM P, CARNEY J, JACOB S. Stability problems with artificial neural networks and the ensemble solution[J]. *Artif Intell Med*, 2000, 20(3): 217–225.
- [52] LIU K H, ALAM M S, ZHU J, et al. Prediction of carbonation depth for recycled aggregate concrete using ANN hybridized with swarm

- intelligence algorithms[J]. *Constr Build Mater*, 2021, 301: 124382.
- [53] MOGHADDAS S A, NEKOEI M, MOHAMMADI GOLAFSHANI E, et al. Modeling carbonation depth of recycled aggregate concrete using novel automatic regression technique[J]. *J Clean Prod*, 2022, 371: 133522.
- [54] STROBL C, BOULESTEIX A L, KNEIB T, et al. Conditional variable importance for random forests[J]. *BMC Bioinformatics*, 2008, 9: 307.
- [55] NUNEZ I, NEHDI M L. Machine learning prediction of carbonation depth in recycled aggregate concrete incorporating SCMs[J]. *Constr Build Mater*, 2021, 287: 123027.
- [56] BOĞA A R, ÖZTÜRK M, TOPÇU İ B. Using ANN and ANFIS to predict the mechanical and chloride permeability properties of concrete containing GGBFS and CNI[J]. *Compos Part B Eng*, 2013, 45(1): 688–696.
- [57] LIU Q, IQBAL M F, YANG J, et al. Prediction of chloride diffusivity in concrete using artificial neural network: Modelling and performance evaluation[J]. *Constr Build Mater*, 2021, 268: 121082.
- [58] INTHATA S, KOWTANAPANICH W, CHEERAROT R. Prediction of chloride permeability of concretes containing ground pozzolans by artificial neural networks[J]. *Mater Struct*, 2013, 46(10): 1707–1721.
- [59] SONG H W, KWON S J. Evaluation of chloride penetration in high performance concrete using neural network algorithm and micro pore structure[J]. *Cem Concr Res*, 2009, 39(9): 814–824.
- [60] VAN Q T. Machine learning approach for investigating chloride diffusion coefficient of concrete containing supplementary cementitious materials[J]. *Constr Build Mater*, 2022, 328: 127103.
- [61] ABDULALIM A A, IQBAL M, ZAHID M, et al. Prediction of rapid chloride penetration resistance of metakaolin based high strength concrete using light GBM and XGBoost models by incorporating SHAP analysis[J]. *Constr Build Mater*, 2022, 345: 128296.
- [62] LUNDBERG S M, LEE S I. A unified approach to interpreting model predictions[C]//*Proceedings of the 31st International Conference on Neural Information Processing Systems*. Long Beach, California, USA. ACM, 2017: 4768–4777.
- [63] LIU K H, ZOU C Y, ZHANG X C, et al. Innovative prediction models for the frost durability of recycled aggregate concrete using soft computing methods[J]. *J Build Eng*, 2021, 34: 101822.
- [64] 吴贤国, 刘茜, 王雷, 等. 基于 LSSVM 与 GA 的混凝土抗冻性多目标配对比优化研究[J]. *沈阳建筑大学学报(自然科学版)*, 2021, 37(3): 393–401.
WU Xianguo, LIU Xi, WANG Lei, et al. *J Shenyang Jianzhu Univ Nat Sci*, 2021, 37(3): 393–401.
- [65] Zhang J, Huang Y, Wang Y, et al. Multi-objective optimization of concrete mixture proportions using machine learning and metaheuristic algorithms[J]. *Constr Build Mater*, 2020, 253: 119208.
- [66] ZHANG J F, HUANG Y M, MA G W, et al. Mixture optimization for environmental, economical and mechanical objectives in silica fume concrete: A novel frame-work based on machine learning and a new meta-heuristic algorithm[J]. *Resour Conserv Recycl*, 2021, 167: 105395.
- [67] CEMALGIL S, GÜL E, ONAT O, et al. A novel prediction model for durability properties of concrete modified with steel fiber and Silica Fume by using Hybridized GRELM[J]. *Constr Build Mater*, 2022, 341: 127856.
- [68] ASTERIS P G, KOLOVOS K G, DOUVIKA M G, et al. Prediction of self-compacting concrete strength using artificial neural networks[J]. *Eur J Environ Civ Eng*, 2016, 20(s1): s102–s122.
- [69] RUTKOWSKA G, WICHOWSKI P, FRANUS M, et al. Modification of ordinary concrete using fly ash from combustion of municipal sewage sludge[J]. *Materials*, 2020, 13(2): 487.
- [70] SHEWA G A, UGWUOWO F I. A new hybrid estimator for linear regression model analysis: Computations and simulations[J]. *Sci Afr*, 2023, 19: e01441.
- [71] FAN C C, ZHENG Y X, WANG S Q, et al. Prediction of bond strength of reinforced concrete structures based on feature selection and GWO-SVR model[J]. *Constr Build Mater*, 2023, 400: 132602.
- [72] MOTLAGH S A T, NAGHIZADEHROKNI M. An extended multi-model regression approach for compressive strength prediction and optimization of a concrete mixture[J]. *Constr Build Mater*, 2022, 327: 126828.
- [73] ERDAL H I. Two-level and hybrid ensembles of decision trees for high performance concrete compressive strength prediction[J]. *Eng Appl Artif Intell*, 2013, 26(7): 1689–1697.
- [74] BELLO S A, OYEDELE L, OLAITAN O K, et al. A deep learning approach to concrete water-cement ratio prediction[J]. *Results Mater*, 2022, 15: 100300.
- [75] MIN C D, XIONG S, SHI Y, et al. Early-age compressive strength prediction of cemented phosphogypsum backfill using lab experiments and ensemble learning models[J]. *Case Stud Constr Mater*, 2023, 18: e02107.
- [76] WANG S Q, XIA P, CHEN K Y, et al. Prediction and optimization model of sustainable concrete properties using machine learning, deep learning and swarm intelligence: A review[J]. *J Build Eng*, 2023, 80: 108065.
- [77] PARUTHI S, HUSAIN A, ALAM P, et al. A review on material mix proportion and strength influence parameters of geopolymer concrete: Application of ANN model for GPC strength prediction[J]. *Constr Build Mater*, 2022, 356: 129253.
- [78] MOHTASHAM MOEIN M, SARADAR A, RAHMATI K, et al. Predictive models for concrete properties using machine learning and deep learning approaches: A review[J]. *J Build Eng*, 2023, 63: 105444.
- [79] LECUN Y, BENGIO Y, HINTON G. Deep learning[J]. *Nature*, 2015, 521: 436–444.
- [80] HEATON J. Ian Goodfellow, Yoshua Bengio, and Aaron Courville: Deep learning[J]. *Genet Program Evolvable Mach*, 2018, 19(1/2): 305–307.
- [81] EMMERT-STREIB F, YANG Z, FENG H, et al. An introductory review of deep learning for prediction models with big data[J]. *Front Artif Intell*, 2020, 3: 4.
- [82] ALZUBAIDI L, ZHANG J L, HUMAIDI A J, et al. Review of deep learning: Concepts, CNN architectures, challenges, applications, future directions[J]. *J Big Data*, 2021, 8(1): 53.
- [83] ZHOU J, CUI G Q, HU S D, et al. Graph neural networks: A review of methods and applications[J]. *AI Open*, 2020, 1: 57–81.
- [84] ISLAM S, ELMEKKI H, ELSEBAI A, et al. A comprehensive survey on applications of transformers for deep learning tasks[J]. *Expert Syst Appl*, 2024, 241: 122666.
- [85] YIN W P, KANN K, YU M, et al. Comparative study of CNN and RNN for natural language processing[EB/OL]. 2017: arXiv: 1702. 01923. <http://arxiv.org/abs/1702.01923.pdf>
- [86] LIU Y, YANG Z W, YU Z Y, et al. Generative artificial intelligence and its applications in materials science: Current situation and future perspectives[J]. *J Materiomics*, 2023, 9(4): 798–816.
- [87] YU J, WENG Y W, YU J T, et al. Generative AI for performance-based design of engineered cementitious composite[J]. *Compos Part B Eng*, 2023, 266: 110993.

Overview on Machine Learning Methods for Cement-Based Materials

ZHANG Wensheng, CAO Fuli, ZHI Xiao, YE Jiayuan, REN Xuehong

(State Key Laboratory of Green Building Materials, China Building Materials Academy, Beijing 100024, China)

Extended Abstract:

The integration of Machine Learning (ML) in material science, particularly in cement-based materials, is revolutionizing the field. This approach addresses challenges like high non-linearity and significant time-lags in data, which are prevalent in the complex interplay of composition, process, structure, and performance in these materials. ML's effectiveness in this context is not just in predictive accuracy, but also in its potential to significantly advance research and development.

ML operates at the intersection of computer science and statistics, functioning as a 'black-box' that links data without requiring an understanding of the underlying mechanisms. This enables a comprehensive cycle from data collection to performance prediction and experimental validation. By transitioning from a traditional 'experience plus trial-and-error' method to a data-driven approach, ML facilitates a deeper understanding of the cause-effect relationships aiming at material properties. This is particularly transformative in cement-based materials research, where ML's ability to predict various properties opens up new possibilities for enhancing the efficiency of their development and application.

This comprehensive article delves into the intricate characteristics and varied application processes of ML in the realm of material science, with a specific focus on cement-based materials. It provides a thorough review of the recent progress, showcasing how ML techniques have become instrumental in predicting key aspects such as microstructure, components, mechanical properties, and durability of these materials. The article not only illustrates the predictive power of ML, but also sheds light on its role in enhancing the understanding of complex material behaviors and properties. Additionally, the article examines the unique characteristics and structural intricacies of various ML models used in this context. It meticulously discusses and compares different model algorithms, dissecting their methodologies and computational approaches. By doing so, it offers a clear picture of the strengths and limitations of each algorithm, providing valuable insights into their practical applicability in predicting and understanding the behavior of cement-based materials. Moreover, the article reviews the evaluation metrics used to assess the performance of these ML models, emphasizing the importance of accuracy, reliability, and efficiency in material science research. This evaluation not only highlights the current state of ML applications in this field, but also suggests areas for future improvements and developments.

Despite the notable advancements in using ML for predicting the structure and performance of cement-based materials, significant challenges remain. Firstly, there is an issue of data quality and quantity imbalance due to the multi-temporal relationship between the cement process and the development of its properties, which necessitates the creation of a comprehensive database including diverse factors such as material components, structures, performance metrics, environmental influences, and chemical reaction parameters. Secondly, the highly complex and nonlinear nature of most predictive models for cement-based materials leads to insufficient model interpretability, that is, understanding of these models' decision-making processes is quite complicated. Enhancing interpretability is essential for a deeper comprehension of material performance under various conditions, which can be achieved through advanced post-processing tools and integrating ML with precise physical models. Lastly, the limited generalizability of ML models, due to the inherent complexity of cement-based materials, poses a challenge. Training data may not cover all categories, leading to diminished performance upon treating new data sets. To address this problem, it requires exploring meta-learning methods that can quickly adapt to new material combinations and combining these methods with other advanced ML techniques to improve the predictive power and adaptability of models.

The evolution of Artificial Intelligence and increased computational power, as exemplified by advanced generative AI models like ChatGPT, offer boundless potential in enhancing the efficiency of material research and development. Their multi-dimensional data processing capability allows for comprehensive consideration of various factors affecting target performance, predicting cement properties under different conditions. As these models evolve in self-learning and optimization, integrating molecular dynamics simulations of cement-based materials, three-dimensional simulations of hardened paste structures, and reaction kinetics and thermodynamics data becomes feasible. This integration could lead to precise predictions of composition, structure, and performance, and even the reverse engineering of cement-based materials, significantly accelerating the development of new cement-based materials.

Summary and prospects The integration with ML is a major advancement in the field of cement-based materials. ML is able to process and to learn from huge datasets to predict a range of material properties. This approach not only solves the complex problem of nonlinear regression of materials, but also marks a new era in materials research. However, to realize the full potential of machine learning in this area, challenges such as imbalances in data quality and quantity, insufficient model interpretability and limited model commonality need to be addressed. The research prospect of cement-based materials by integrating with artificial intelligence is promising. And, with the continuous improvement of AI capability and computational power, we can foresee that more complex models combined with more advanced algorithms will be able to predict and design cement-based materials more accurately. This progress will likely lead to the development of new materials with enhanced properties, contributing significantly to the field of construction and material science. This research area remains a hotspot, promisingly exciting developments and breakthroughs in the near future.

Keywords machine learning methods; cement-based materials; microstructure and properties; prediction