

人工智能与中药领域融合的应用与挑战

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[摘要] 中医(TCM)作为一种传统的治疗手段,在慢性病、传染病等疾病的治疗显现出独特的潜力,日益受到全球关注。随着人工智能技术在多领域兴起,其在中药产业的应用研究已收获显著进展。然而人工智能对中药产业发展也存在局限性,涵盖药理学研究深度不足、数据库质量参差、人机交互挑战等问题。尽管存在上述瓶颈,人工智能仍为中医现代化开辟了全新机遇与创新路径。通过推动人工智能技术在中药产业全链条的深度融合应用,有望攻克产业发展的核心难题,加速中药产业现代化进程。本文从新药发现、药物靶点确定及药物活性检测等维度,梳理了人工智能融入中药产业进程和挑战。

[关键词] 中医药; 人工智能; 深度学习

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Challenges and Development of the Integration of Artificial Intelligence and Traditional Chinese Medicine

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[Abstract] Traditional Chinese Medicine (TCM), as a traditional treatment method, has shown unique potential in the treatment of chronic diseases, infectious diseases and other diseases, and is increasingly receiving global attention. With the rise of artificial intelligence technology in multiple fields, significant progress has been made in its application research in the traditional Chinese medicine industry. Artificial intelligence has limitations in the development of the traditional Chinese medicine industry, including insufficient depth of pharmacological research, uneven database quality, and challenges in human-computer interaction. Despite the aforementioned bottlenecks, artificial intelligence has opened up new opportunities and innovative paths for the modernization of traditional Chinese medicine. By promoting the deep integration and application of artificial intelligence technology throughout the entire chain of the traditional Chinese medicine industry, it is expected to overcome the core challenges of industrial development and accelerate the modernization process of the traditional Chinese medicine industry. This article systematically reviews the process and challenges of integrating artificial intelligence into the traditional Chinese medicine industry from the dimensions of new drug discovery, drug target determination and drug activity detection.

[Key words] Traditional Chinese Medicine; artificial intelligence; Deep learning

中医(TCM)是中华民族在长期医学实践中形成的独特药理学体系,以中药方剂为核心,拥有丰富的医疗资源和悠久的疾病防治历史^[1]。研究表明,TCM在增强抗肿瘤效果及治疗多种疾病方面具有一定疗效^[2],其部分成分对慢性疾病的治疗与缓解作用尤为显著^[3]。因来源于天然植物且副作用相对较低,TCM相较于现代化学合成药物更受医疗卫生工作者关注^[4]。尽管其药理活性广泛、具备深入探索价值,但其配伍机制仍缺乏现代科学阐释^[5],且标准化质量体系尚未建立,这些仍是当前TCM研究面临的核心问题与挑战。

人工智能(AI)作为快速发展的新兴技术科学,其理论与方法已拓展至多个领域。近几十年来,AI在金融、交通、电气自动化、医疗及生物医学研究等领域均取得重大突破^[6],尤其在TCM产业中的应用日益广泛^[7]。AI通过支持向量机(SVM)、随机森林(RF)、卷积神经网络(CNN)等算法开展机器学习与深度学习^[8],显著提升了诊断、靶点筛选及新药研究的可靠性与准确性,引发学者广泛关注,AI药学亦成为学术界热点研究方向^[9]。例如,Lam等运用关联规则挖掘技术,探究了中医药在儿童癌症护理中的应用模式^[10]。AI推动中医药领域的发展与创新,有着许多应用与挑战(如图1)。

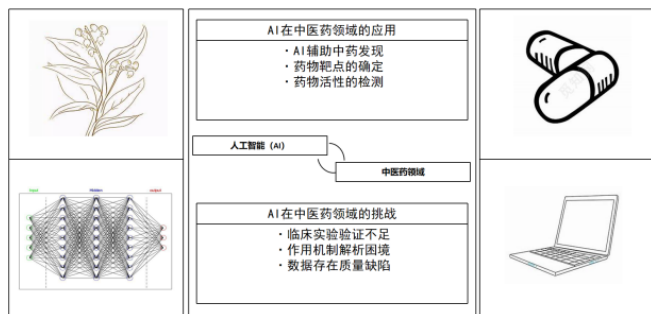


图1 AI在中医药领域的应用与挑战

1 AI在中医药领域的融合应用

1.1 AI辅助中药发现

中药新药的研发需历经临床前研究与临床研究方能获批,且中药成分与生物作用网络极为复杂,处方数量庞大^[11]。传统研发模式依赖临床经验处方与长期人体实践,存在效率低下、资源消耗大、作用机制模糊等瓶颈,亟待新方法突破。大数据与AI技术的兴起,为中药发现提供了全新路径。通过机器学习、深度学习及自然语言处理等AI技术,可对中药文献、临床病例及数据库进行深度挖掘,显著提升信息处理效率,精准识别潜在活性成分与作用机制,大幅提高中药发现的效率与准确性。^[12]

1.2 药物靶点的确定

基于高效的数据处理能力,大数据在中药靶点识别中应用广泛。AI驱动的机器学习技术可通过挖掘生物医学数据库,识别并验证与疾病病理相关的靶蛋白,在新药发现初期发挥关键作用。例如,He等人^[13]利用多层感知器(MLP)、支持向量回归(SVR)等算法构建多靶点药理学预测模型(mTPP),成功预测出20种抗药物性肝损伤(DILI)的潜在候选药物,其中2种通过实验验证,该模型为探索多靶点效应与药物整体疗效的关联提供了工具。Pun^[14]等人借助AI靶点发现平台PandaOmics,分析中枢神经系统(CNS)样本及肌萎缩侧索硬化症(ALS)相关运动神经元的表达图谱,鉴定出28个ALS潜在治疗靶点,其中8个为未报道基因。这些AI方法显著加速了靶点发现进程,有效缩小了下游实验的候选筛选范围。

1.3 药物活性的检测

要明确中药是否具有活性,需要先通过初筛获得具有基础活性的命中化合物,再从中确定活性更优的先导化合物。这类化合物可来源于动植物、海洋生物等天然物质或已知化合物^[15]。AI在此过程中展现双重价值:一方面,借助算法从植物、微生物等天然资源中挖掘药理活性先导化合物,精准解析中药复杂成分。例如,Xu等^[16]运用关联规则挖掘技术(ARM),从中药公共数据库中筛选出74种辅助治疗胃癌的活性物质及2128首方剂,并通过网络药理学及体内实验验证了处方对肿瘤进展的抑制作用,证实了机器学习的准确性。另一方面,通过虚拟筛选模拟靶标与候选分子的相互作用,高效搜索已知活性化合物。Singh等^[17]构建深度学习模型DeepDocking,基于300万种化合物对接数据筛选出两种新型腺苷受体拮抗剂,经体外实验验证有效;Lin

等^[18]通过结构虚拟筛选鉴定出三种肾谷氨酰胺酶抑制剂,其抑制作用在酶学及细胞实验中得到进一步证实。上述研究凸显了AI在中药成分挖掘与活性预测中的关键作用与潜力。

2 AI在中医药领域的局限性和挑战

当前AI驱动的中药发现研究仍存在显著局限:(1)临床验证不足:尽管AI可辅助计算机模拟设计中药分子,但其在目标疾病中的有效性仍需临床实验验证。部分研究仅提供计算机预测结果,缺乏对筛选候选药物的实验验证。(2)作用机制解析困境:中药以整体治疗为核心,其分子机制研究尚不深入,难以与AI技术形成有效协同,成为技术应用的关键瓶颈。(3)数据库质量缺陷:中药数据库存在数据质量参差不齐、管理不规范等问题,可能导致网络分析出现假阳性结果^[19]。高质量、全覆盖的中草药及配方数据库缺失,严重制约AI模型的训练与验证效果。

3 结论与展望

3.1 结论

AI与中医药现代化的融合是极具前景的前沿方向,在中药产业各环节均展现出巨大潜力。AI凭借强大的计算与学习能力,可显著提升新药发现效率:通过数据挖掘技术对中医药古籍进行数字化处理,有助于分析中药化合物的配伍规律、预测核心药对;借助AI云平台可实现中药饮片的统一资源管理与在线监管,推动质量标准化进程;基于AI驱动的大数据平台整合患者多维数据,能构建覆盖诊断、治疗及健康管理的精准医疗服务体系。上述结论凸显了AI作为中医药现代化驱动力的重要价值,为行业发展带来突破性机遇。

然而,AI在中药产业中的应用仍面临多重挑战:中药处方的药理学机制研究滞后、数据库质量参差不齐等问题,直接影响AI算法的准确性与可靠性;而实现AI系统与中医药从业者的高效协同,是技术落地的关键环节;此外,AI应用可能导致医患沟通场景减少,因此人机交互设计与用户体验优化亦需重点关注。

3.2 展望

未来,需通过强化药理学基础研究、构建标准化高质量数据库,突破技术应用瓶颈,同时深化跨领域协作,推动AI与中医药的深度融合,为中医药现代化开辟更广阔的发展路径。

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