

机器学习在大气气溶胶卫星遥感中的应用和挑战

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摘要: 大气气溶胶作为影响大气环境、气候变化和人类健康的关键因子, 在过去五十年间引起了广泛关注。随着遥感技术的不断发展, 卫星观测已成为获取全球尺度气溶胶特性的重要手段。传统查找表方法在一定程度上简化了气溶胶卫星遥感的流程, 但仍难以满足反演精度和空间信息实时处理的需求。近年来, 人工智能的发展为气溶胶遥感领域带来了重大变革, 机器学习算法不仅可以显著提升反演效率, 还具备解决传统物理方法遥感反演难题的潜力(例如长期困扰研究者的地气解耦合等问题), 有助于推动卫星气溶胶反演进入智能化发展阶段。本文针对这一趋势梳理了气溶胶卫星遥感反演方法的发展脉络, 分析了现有机器学习方法在气溶胶领域应用的主要优劣势以及局限性, 并进一步探讨了人工智能在气溶胶遥感领域的未来发展方向, 为气溶胶遥感研究者提供参考。

关键词: 气溶胶, 大气遥感, 机器学习, 人工智能, 反演算法

中图分类号: TP701/P4

引用格式: 李正强, 冀哲, 张子晗, 阎晓曦, 顾浩然, 李智宇, 姚前, 王舜之, 王家耀. 2025. 机器学习在大气气溶胶卫星遥感中的应用和挑战. 遥感学报, 29(6): 1788-1803

Li Z Q, Ji Z, Zhang Z H, Yan X X, Gu H R, Li Z Y, Yao Q, Wang S Z and Wang J Y. 2025. Application and challenge of machine learning in the satellite remote sensing of atmospheric aerosols. National Remote Sensing Bulletin, 29(6):1788-1803[DOI:10.11834/jrs.20255214]

1 引言

大气气溶胶主要由悬浮在大气中的固态或液态微粒组成(Rabha和Saikia, 2020)。其形成机制复杂, 随着气溶胶粒子的沉降、凝聚以及与云的相互作用, 其粒径分布和化学成分会持续发生变化(Seinfeld和Pandis, 2016)。根据来源特征, 气溶胶可分为直接源和间接源两大类: 直接源指通过自然或人为过程直接向大气排放气溶胶颗粒, 如海洋喷雾气溶胶和沙尘气溶胶; 间接源则是由气态前体物(如NO₂、SO₂、NH₃、挥发性有机化合物等)经过气相或液相化学反应转化而成。此外, 由于气溶胶寿命较短(通常为数小时至数天), 其复杂的形成机制和多样化的源排放导致气溶胶颗粒的理化特性在时空上表现出显著的异质

性(Prospero等, 1983)。

随着温室效应的加剧, 地球和大气的辐射强迫问题受到了更多的关注。政府间气候变化专门委员会IPCC(Intergovernmental Panel on Climate Change)最新评估报告指出: 气溶胶是辐射强迫估计中最大的不确定性来源之一(Lee等, 2024)。尽管卫星遥感产品已成为评估气溶胶影响的重要数据来源(Kaufman等, 2002), 但目前通过卫星观测反演的气溶胶参数精度仍难以满足气候变化某些特定应用的需求(Bender, 2020)。同时, 气溶胶对人类健康也构成严重威胁, 由森林火灾或工业活动产生的细颗粒物被人体吸入后可能引发严重的肺部疾病(Lelieveld等, 2020)。此外, 研究还表明, 大气气溶胶的存在显著影响陆地、海洋参量以及温室气体浓度等参数的遥感反演精度

收稿日期: 2025-05-19; 预印本: 2025-05-29

基金项目: 国家自然科学基金(编号:42305151); 国家重点研发计划(编号:2023YFB3907405)

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(Huang等, 2020), 气溶胶效应的大气校正已经成为定量遥感的关键环节。因此, 为满足日益增长的地球环境监测需求, 开发更高精度的卫星气溶胶产品势在必行。

星载气溶胶反演研究始于20世纪70年代, 其观测技术经历了从单角度到多角度、从多光谱到高光谱、从强度到偏振的演进过程, 已用于大气气溶胶遥感的代表性卫星传感器如表1所示。

表 1 全球气溶胶观测的主要卫星平台和传感器

Table 1 The main satellite platforms and sensors for global aerosol observations.

传感器(全名)	卫星平台	开始年份	最大幅宽/km	最高空间分辨率/km
AATSR Advanced Along-Track Scanning Radiometer	Envisat-1	2002	500	1.0
AGRI Advanced Geostationary Radiation Imager	FY-4A, -4B	2016	7000	0.5
AHI Advanced Himawari Imager	Himawari-8, -9	2014	8000	0.5
ATSR-2 Along-Track Scanning Radiometer	ERS-2	1995	500	1.0
AVHRR Advanced Very High Resolution Radiometer	NOAA-7, -9, -11, -14, -L, Metop-1	1978	2800	1.1
CAPI Cloud and Aerosol Polarization Imager	TANSAT	2016	200	0.25
DPC-1, -2, -3, -4 Directional Polarimetric Camera	GF-5, -5(02), DQ-1, TECIS-1	2018	2400	3.3
GLI Global Imager	ADEOS II	2003	1600	0.25
GOME, -2 Global Ozone Monitoring Experiment	ERS-2, Metop-A, -B, -C	1995	1920	40.0
HARP2 Hyper-Angular Rainbow Polarimeter-2	PACE	2024	1556	2.6
MERIS Medium Resolution Imaging Spectro radiometer	Envisat-1	2002	1150	0.3
MERSI-1, -2, -3 Medium Resolution Spectral Imager	FY-3A, -3B, -3D, -3F	2008	2800	0.25
MISR Multi-angle Imaging Spectroradiometer	Terra	2000	380	0.25
MODIS Moderate Resolution Imaging Spectro radiometer	Terra, Aqua	1999	2230	0.25
OCTS Ocean Color and Temperature Scanner	ADEOS	1996	1400	0.7
OMI Ozone Monitoring Instrument	Aura	2004	2600	13
POLDER-1, -2, -3 Polarization and Directionality of the Earth's Reflectances	ADEOS, ADEOS II, PARASOL	1996	2400	6.5
POSP-1, -2 Particulate observing scanning polarimeter	GF-5(02), DQ-1	2021	1850	6.4
PSAC Polarized Scanning Atmospheric Corrector	HJ-2A/2B	2020	800	6.0
SCIAMACHY Scanning Imaging Absorption Spectrometer for Atmospheric Cartography	Envisat	2002	960	30
SeaWiFS Sea-viewing Wide Field-of-view Sensor	OrbView-2	1997	2800	1.1
SLSTR Sea and Land Surface Temperature Radiometer	Sentinel-3A, 3B	2016	1400	0.5
SMAC Synchronization Monitoring Atmospheric Corrector	GFDM	2020	15	7.0
SPEXone Spectro-polarimeter for Planetary Exploration one	PACE	2024	100	4.6
TOMS Total Ozone Mapping Spectrometer	Nimbus-7, Meteor-3, ADEOS, Earth Probe,	1978	3000	50.0
TROPOMI Tropospheric Monitoring Instrument	Sentinel-5p	2017	2600	7.0
VIIRS Visual/Infrared Imager Radiometer Suite	Suomi-NPP, NOAA-20, -21	2011	3000	0.375

早期的代表性传感器包括美国 AVHRR (Advanced Very High Resolution Radiometer), 以及 21 世纪初发射的 MODIS (MODerate-resolution Imaging Spectroradiometer) 等。这些传感器的初始设计目标并非专门针对气溶胶监测。以欧洲 ATSR (Along-Track Scanning Radiometer) 系列传感器为例, 尽管其主要设计目标是获取海面温度和植被指数, 但它在气溶胶研究中也发挥了重要作用 (Holben, 1986), 也是最早实现陆地上空气溶胶光学厚度反演的传感器之一 (Veefkind 等, 1998)。此后, MODIS 的运行标志着气溶胶遥感技术的重要突破。该传感器分别于 1999 年和 2002 年搭载在美国 Terra 和 Aqua 卫星上发射, 其 36 个光谱波段和 0.25—1 km 的空间分辨率显著提升了气溶胶遥感产品的应用水平 (Remer 等, 2005)。

除上述单角度传感器外, 多角度观测的重要性也逐渐被气溶胶研究领域所关注, 与 MODIS 同平台搭载的 MISR (Multi-angle Imaging SpectroRadiometer) 以其独特的多角度观测能力为气溶胶研究提供了新的维度 (Martonchik 等, 2002)。此外, Mishchenko 和 Travis 等人的研究表明, 相较于标量观测, 偏振观测在气溶胶反演, 特别是气溶胶微物理特性反演方面具有显著优势 (Mishchenko 和 Travis, 1997)。这一发现促使 POLDER 系列 (Polarization and Directionality of the Earth's Reflectances) 的诞生, 其作为全球首个兼具偏振和多角度观测能力的气溶胶探测传感器为大气气溶胶研究带来了前所未有的革新 (Deschamps 等, 1994)。此后, 随着 POLDER-1、POLDER-2、POLDER-3 的成功发射, 多角度联合偏振观测逐渐成为大气气溶胶监测的重要发展方向 (Dubovik 等, 2019)。

随着大气观测技术的不断革新, 我国在偏振卫星载荷研制方面取得了显著进展。其中, 2016 年 9 月发射的 MAI (Multi-Angle polarization Imager) (Jiang 等, 2019) 和同年 12 月搭载中国 TanSat 卫星发射的 CAPI (Cloud and Aerosol Polarization Imager) (Chen 等, 2017) 是我国探索偏振气溶胶卫星遥感的重要尝试; 此后, 2018 年 5 月随高分五号 (GF-5) 发射的 DPC (Directional Polarimetric Camera) 是我国首台实现业务化运行的多角度偏振星载气溶胶遥感传感器 (Li 等, 2018); 2020 年 7 月, 高分多模 (GFDM) 卫星搭载的 SMAC

(Synchronization Monitoring Atmospheric Corrector) 成功发射 (Li 等, 2022c; 余婧等, 2022); 同年 9 月, 环境二号 A/B (HJ-2A/B) 两颗卫星搭载的 PSAC (Polarized Scanning Atmospheric Corrector) 发射升空 (Li 等, 2022a), 标志着我国偏振气溶胶卫星遥感进入国际先进行列。2021 年 9 月, 高分五号 02 卫星首次搭载了以突破 $PM_{2.5}$ 等大气环境关键参数监测瓶颈为目标的偏振交火 (Polarization Crossfire) 载荷组件, 同时包含了 POSP (Particulate Observing Scanning Polarimeter) 和 DPC (Li 等, 2022b), 实现了国际领先的气溶胶在轨综合观测能力。随后, 中国又陆续发射了搭载偏振交火传感器的大气环境监测卫星 (DQ-1) (李正强等, 2022)、新一代 DPC 载荷的陆地生态系统碳监测卫星 (TECIS) (Du 等, 2022) 等, 代表着中国在偏振遥感卫星领域进入国际先进行列。

国际上, 考虑到偏振观测的独特优势, 欧美国家同样致力于加快大气、海洋偏振遥感卫星的研发。2024 年 2 月 8 日, 美国国家航空航天局的 PACE (Plankton, Aerosol, Cloud, ocean Ecosystem) 卫星成功发射, 搭载了 SPEXone (Spectro-polarimeter for Planetary Exploration one) 和 HARP2 (Hyper-Angular Rainbow Polarimeter 2) 两种先进的偏振成像光谱仪。这两种仪器的协同观测可为全球气溶胶研究提供高精度数据支持 (Werdell 等, 2019)。

回顾大气气溶胶的卫星遥感研究历程可以发现, 早期的观测手段相对单一, 且受限于计算能力与观测数据量的限制, 在平衡反演精度与算法可行性的前提下主要采用查找表等方法 (Levy 等, 2013)。随着卫星观测手段的进步, 气溶胶反演算法也在持续演进。在拥有海量卫星观测数据的当下, 如何进一步挖掘大数据中潜藏的大气信息是卫星遥感气溶胶领域的核心问题。近十年来, 基于统计最优化的算法成为最有可能的解决方案之一 (Dubovik 等, 2011; Lu 等, 2022; 郑逢勋等, 2022), 作为基于物理过程的反演算法, 其核心是通过拟合辐射传输前向模拟值与卫星观测真值来实现大气气溶胶参数反演。然而, 最优化算法具有很高的计算成本, 使得基于海量数据的实时卫星产品生产面临巨大挑战, 亟需新的技术突破。

人工智能技术的出现为解决这一难题提供了

新的思路。该技术起源于20世纪40年代McCulloch和Pitts提出的人工神经元模型(McCulloch等, 1943)。21世纪20年代以来, 随着GPT (Floridi等, 2020)、Gemini (Gemini Team Google, 2023)、Llama 2/3 (Touvron等, 2023)以及DeepSeek (Guo等, 2024)等通用人工智能的相继问世, 机器学习技术得到了广泛应用。在此背景下, 人工智能与气溶胶遥感的深度融合是重要发展趋势之一 (Remer等, 2024)。本文结合这一趋势, 阐述并分析人工智能方法在大气气溶胶遥感反演领域的应用现状与挑战。

2 大气气溶胶遥感领域文献分析

2.1 发表数据检索

在本研究中, 采用Web of Science作为主要文献分析平台。通过其高级检索功能, 共检索到543条相关记录。经过筛选, 最终纳入471篇发表于

2000年—2024年间的文献进行后续分析。

2.2 统计分析

2.2.1 按发表时间统计的分析结果

图1展示了2000年—2024年间气溶胶遥感领域相关论文的发表数量情况(柱状图表示气溶胶遥感相关文章数量, 折线图表示机器学习相关论文占比)。整体来看, 气溶胶反演相关研究呈持续增长态势, 尤其自2010年起增速明显, 在2022年达到高峰, 年发表量近400篇。与此同时, 机器学习方法在气溶胶遥感领域受到的关注迅速上升, 其占比从2015年前的不足5%上升至2024年的近40%。这一快速增长期与大规模语言模型的出现时间相吻合(2019年—2020年)。此后, 数据驱动方法快速取代传统物理模型, 成为气溶胶遥感研究的重要发展方向。这一趋势反映出遥感数据获取能力提升、算法更新以及计算资源增强对研究范式变革的深刻推动。

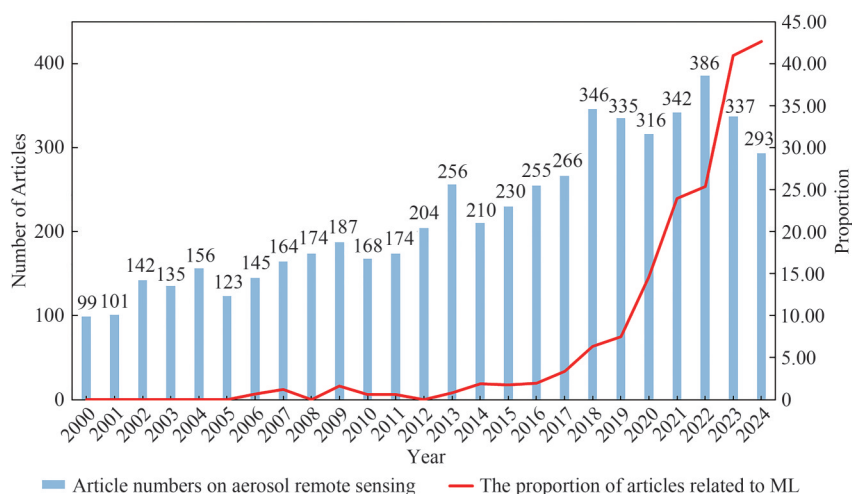


图1 气溶胶遥感领域发表文章数量及机器学习相关论文数量的逐年变化

Fig. 1 Number of published articles year by year in the field of aerosol remote sensing and those related to machine learning

2.2.2 按国家和期刊统计的分析结果

图2展示了各国在气溶胶遥感领域的论文发表占比情况。统计分析显示, 主要论文发表国(相关论文发表数位于前10)的发表量占全球总量的80%, 构成了该领域的研究主体。其中, 中国在该领域的贡献最为突出, 论文发表数量占比接近50%; 美国发表量仅次于中国, 占比为14.8%, 位列第二; 英国、印度、韩国等发文量位于第三梯队。

2.2.3 按文献关键词的统计分析

图3展示了气溶胶遥感与机器学习相关的论文中出现关键词的分布情况, 其中圆圈的大小与关键词的出现频率正相关。从研究对象来看, 气溶胶、细颗粒物($PM_{2.5}$)、云和沙尘是主要的研究关注点。此外, 中国作为研究区域, 出现频率同样较高。综合上述文献分析结果表明, 中国不仅是大气气溶胶研究领域的主要贡献国家, 同时也是大气气溶胶的主要研究区域, 这揭示了我国在全球大气气溶胶遥感领域的体量和重要地位。

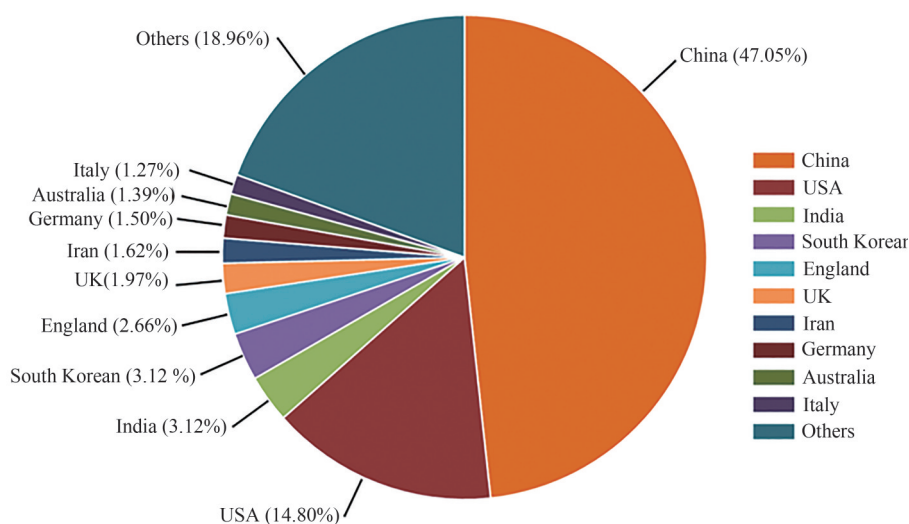


图2 与机器学习相关的气溶胶遥感领域2000年—2024年间发表文章数量的各国占比

Fig. 2 Proportion of published article numbers by different countries in the field of machine learning related aerosol remote sensing from 2000 to 2024

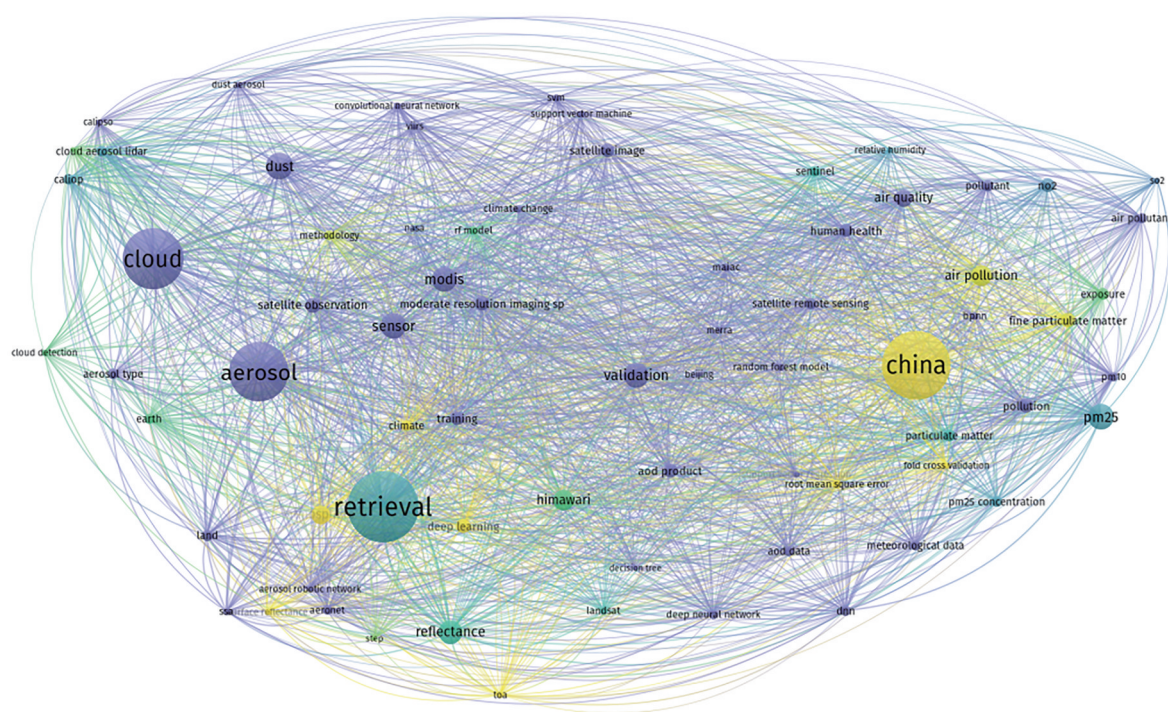


图3 与机器学习相关的气溶胶遥感领域文献关键词共现网络图

Fig. 3 A visualization of the keyword co-occurrence network for machine learning related aerosol remote sensing articles

3 机器学习与大气气溶胶反演

气溶胶遥感难题的根本在于悬浮在大气中的气溶胶颗粒物具有复杂多变的形状、尺寸和组成(即化学成分),用于表征和需要反演的气溶胶参数复杂且数量众多。同时,卫星对地观测时,探测器信号中气溶胶信息和地表信息耦合在一起,存在地气解耦合的挑战。为了梳理气溶胶遥感的发展以及机器学习方法的应用,本文尝试从气溶

胶遥感参数增加导致的反演难度增加这一角度入手,将机器学习方法在大气气溶胶定量遥感中的应用分为3个方向进行分析,分别是气溶胶光学物理参数反演(气溶胶光学厚度、Ångström指数、单次散射反照率等)、气溶胶化学成分反演、以及细颗粒物质量估算。表2列出了按这3个方向分类的机器学习方法在大气气溶胶定量遥感中应用的典型文献。

表 2 机器学习方法在大气气溶胶定量遥感反演中应用的典型方法

Table 2 Methodological literature on quantitative remote sensing inversion of atmospheric aerosols using machine learning methods

类别	传感器	方法	现有研究文献
气溶胶光学厚度(AOD)	MODIS/Terra	人工神经网络	Chen 等(2020)
	MODIS/Aqua		
	MODIS/Terra	随机森林	Liang 等(2021)
	MODIS/Aqua		
	MSI/Sentinel-2	卷积神经网络	Jiang 等(2023)
	MODIS/Terra	生成对抗网络	Fan 等(2024)
Ångström 指数(AE)	AHI/Himawari-8	Transformer	She 等(2024)
	SeaWiFS/OrbView-2	神经网络	Jamet 等(2004)
	AHI/Himawari-8	随机森林	Bao 等(2023)
	ASI	LightGBM	Logothetis 等(2023)
	MODIS/Terra	随机森林	Cao 等(2023)
	MODIS/Aqua	极端梯度提升 LightGBM	
单次散射反照率(SSA)	MODIS/Terra	神经网络	Taylor 等(2014)
	OMI/Aura		
气溶胶化学成分	MODIS/Terra	人工神经网络	Qi 等(2022)
	仿真数据	图形神经网络	Lamb 和 Gentine(2023)
	POSP/GF-5(02)	Transformer	Li 等(2024)
细颗粒物质量(PM _{2.5})	MODIS/Terra	bootstrap 聚合	Li(2020)
	MODIS/Aqua		
	MODIS/Terra	图卷积网络	Chen 等(2023)
	MODIS/Aqua		
	MODIS/Terra	极度随机树	Wei 等(2023b)
	再分析数据	极端梯度提升	Chen 等(2024)

3.1 气溶胶光学物理参数反演

在早期研究阶段，机器学习方法往往依赖地基遥感观测数据作为卫星遥感数据的真实值进行机器学习驱动，因此主要应用于反演地基遥感观测站点（例如全球 AErosol RObotic NETwork 和中国 Sun-sky radiometer Observation NETwork 观测网的站点）获取的气溶胶参数类型，包括气溶胶光学厚度 AOD（Aerosol Optical Depth）、Ångström 指数 AE（Ångström Exponent）、细模态比例 FMF（Fine Mode Fraction）、细模态气溶胶光学厚度 FAOD（Fine-mode Aerosol Optical Depth）和单次散射反照率 SSA（Single Scattering Albedo）等（李正强等，2015）。

Jia 等（2022）通过辐射传输方程构建训练样本，开发了一种不依赖地表参数输入的神经网络模型，并将其应用于 MODIS 卫星数据的反演，生

成了 1 km 空间分辨率的 AOD 产品。Mauceri 等（2019）则基于 MODTRAN 前向模拟，生成了硫酸盐、沙尘和黑碳气溶胶的高光谱仿真数据作为训练样本，进而训练模型用于 AVIRIS-NG（Airborne Visible/Infrared Imaging Spectrometer Next Generation）高光谱数据的气溶胶反演，获得了不同成分气溶胶粒子的 AOD 分布。She 等（2020）利用神经网络模型，通过 AHI（Advanced Himawari Imager）卫星数据与 AERONET 的 AOD 地基观测数据进行匹配构建训练集，开发了针对 AOD 的快速反演模型，并通过对比实验证明了神经网络方法的性能优势。Jamet 等（2004）利用神经网络替代传统查找表方法，结合 SeaWiFS（Sea-viewing Wide Field-of-view Sensor）数据的红光和近红外波段观测，实现了 AOD 和 AE 的同时反演。Shi 等（2025）基于 POSP 观测数据，选用集成神经网络

模型 ENN (Ensemble Neural Networks), 以更低的不确定性实现了 FMF 参数的反演。

传统的机器学习模型在从卫星观测数据反演多种气溶胶参数时存在显著局限性, 主要在于其难以捕捉不同大气条件下卫星观测数据的细微差异。为应对解决该问题并进一步提升反演精度, 研究者们提出了新的反演策略, 以更好地适应大气气溶胶动态变化的时空特性。Shi 等 (2022) 提出了一种分步反演方法, 首先利用辐射传输模型进行正向计算, 生成 PSAC 偏振卫星载荷观测数据的模拟数据集, 随后分别训练气溶胶类型识别和 AOD 反演的神经网络模型, 通过“先识别气溶胶类型, 再反演 AOD”的策略, 实现了高精度的 AOD 反演。Cao 等 (2023) 则开发了一种两阶段机器学习算法, 该方法基于 AERONET 地基观测数据与 MODIS 卫星数据, 构建了神经网络模型用于反演陆地上的 AOD、AE、FMF 以及 FAOD, 通过划分低值和高值样本分别训练专用模型, 采用权重插值方法将三个独立模型整合为一个统一的反演系统, 有效提升了反演精度和适用性。Tao 等 (2023) 基于多角度偏振仪 MAP (Multi-Angle Polarimeter) 观测数据, 开发了一种灵活的气溶胶反演算法, 充分利用 MAP 观测在获取气溶胶光学和微物理特性方面的优势, 采用物理引导深度学习 PDL (Physics-informed Deep Learning), 提升了其在气溶胶遥感领域的应用潜力。

与传统机器学习方法相比, Transformer 模型采用了创新的自注意力机制和前馈神经网络架构, 显著提升了训练并行效率和对长距离依赖关系的建模能力 (Vaswani 等, 2017)。在气溶胶遥感领域, She 等 (2024) 基于 AHI 静止卫星传感器观测数据构建训练数据集, 利用 Transformer 模型中的掩蔽机制, 有效消除了云污染等因素导致的数据空缺对时间序列反演的干扰, 实现了 AOD 和 AE 的静止卫星高频次、高精度反演。此外, Wei 等 (2024) 同样采用 Transformer 模型, 实现了高空间分辨率 AOD 产品的生成, 进一步验证了该模型在气溶胶遥感领域的应用潜力。

随着气溶胶遥感技术的不断进步, 单纯反演气溶胶光学参数已难以满足对大气气溶胶特性深入认知的需求。近年来, 研究重点逐渐转向利用遥感手段获取气溶胶的微物理特性, 包括气溶胶粒子谱分布、体积浓度以及复折射指数等关键参

数, 以更全面地揭示气溶胶的理化特性及其环境效应。Taylor 等 (2014) 基于 NN 模型, 结合 MODIS 卫星数据, 实现了撒哈拉沙漠地区强沙尘天气条件下气溶胶光学特性与微物理参数的反演。由于不同区域的气溶胶特性存在极大的差异, 进一步获取全球范围的气溶胶微物理参数卫星反演结果更为困难, 目前仅有少数算法尝试了全球范围内的气溶胶微物理参数反演。Zhang 等 (2024) 提出了一种名为 S2STM 的端到端气溶胶多参数通用机器学习反演算法, 在融合偏振卫星观测数据、气象数据、大气模式数据以及地表特征等多源信息的基础上, 引入符合物理机理的损失函数, 应用于国产偏振卫星传感器 POSP 的全球观测数据, 实现了气溶胶光学特性与微物理参数的同步反演。

以上所述基于机器学习方法的气溶胶参数反演研究主要依赖于卫星观测与地基站点数据的匹配, 导致大量无法与地基站点匹配的卫星观测数据未能有效参与模型训练。为解决这一问题, Yan 等 (2024) 采用了预训练模型策略, 通过将模型暴露于大量未标记数据中以提取对反演有益的特征信息, 构建了 DLFE-satellite 模型, 显著提升了数据利用效率。与传统的训练方法相比, 该方法在缺乏地基观测数据的区域表现出更高的反演精度, 这一改进已通过原位测量结果得到验证。此外, 还有研究人员通过将辐射传输计算替换为机器学习模型, 该方法同样被证明可以有效提高计算效率。例如, Fan 等 (2019) 采用神经网络 NN (Neural Networks) 模型替代了传统的海洋生物光学模型, NN 模型的应用显著提升了计算效率, 还大幅降低了存储需求, 成功实现了海洋上空气溶胶参数的高效反演。Di Noia 等 (2017) 则通过神经网络反演为 Phillips-Tikhonov 正则化迭代提供初始值, 显著提升了反演效率。

3.2 气溶胶化学成分反演

不同气溶胶成分的辐射特性差异显著, 其不确定性直接影响气溶胶辐射强迫的准确评估 (李正强等, 2019)。根据光学吸收特性的差异, 气溶胶成分可分为吸光性和非吸光性两大类。吸光性成分主要包括黑碳 BC (Black Carbon)、棕色碳 BrC (Brown Carbon) 以及氧化铁构成的沙尘 Du (Dust) 等; 非吸光性成分则以铵盐 AS (Ammonium Sulfate)、海盐 SS (Sea Salt) 和非吸光性有机碳

OC (Organic Carbon) 为主 (Benedetti 等, 2009; Morcrette 等, 2009)。其中, 黑碳作为大气中吸光能力最强的气溶胶组分, 是煤烟的主要成分, 主要来源于化石燃料和生物质燃烧 (Andreae 和 Gelencsér, 2006)。与黑碳不同, 棕色碳的光学吸收特性随波长增加而显著减弱 (Feng 等, 2013)。棕色碳同样来源于燃烧过程, 但通常在低温燃烧条件下生成, 其成分中含有具有吸收特性的有机物, 在近紫外和蓝光波段表现出强吸收特性。此外, 沙尘气溶胶中的铁氧化物也具有一定的吸光性, 但其吸收特性因来源和区域差异而表现出显著的空间异质性 (Koven 和 Fung, 2006)。

传统上, 全球尺度气溶胶化学成分信息主要来源于再分析资料和大气化学模式产品, 这些产品通常存在空间分辨率较低、依赖排放清单以及数据获取时间滞后等局限性 (Randles 等, 2017)。近年研究表明, 卫星观测具备反演全球气溶胶类型的潜力 (Chen 等, 2019a, 2018; Dubovik 等, 2008)。早期研究主要基于已反演得到的光学参数进行气溶胶类型识别, 其中 Zhang 等在前向模型中引入多源溶液混合机制来描述复折射指数, 并通过拟合不同典型气溶胶的复折射指数实现了气溶胶类型的识别 (Zhang 等, 2020, 2018, 2017)。Bahadur 等 (2012) 则基于 AERONET 观测的吸收 Ångström 指数 AAE (Absorption Ångström Exponent) 和 SSA 值, 量化了 Dust、OC 和元素碳 EC (Elemental Carbon) 的相对比例。Wang 等 (2013) 基于 SSA 的光谱变化特征, 区分 BrC 和 Dust 等吸光性成分。然而, 上述方法依赖地基观测结果, 其时空覆盖范围有限。为解决这一问题, Li 等 (2019) 开发了一种从卫星观测辐射量反演气溶胶化学成分的算法, 该算法不依赖于反演得到的光学特性或预设的气溶胶模型, 在可靠性方面具有优势。为克服传统物理模型计算成本高的问题, 研究人员开始探索利用机器学习方法开发新型反演技术, 以期在提升效率的同时保持或提高反演精度。Wei 等 (2023a) 结合地基观测网络的 $PM_{2.5}$ 浓度测量、卫星 $PM_{2.5}$ 浓度反演数据以及大气再分析产品, 采用四维-时空深度森林 (4D-STDF) 模型, 获取了中国区域 1 km 空间分辨率的细颗粒物化学成分数据。

为了获取更全面的全球气溶胶化学成分, Li 等 (2024) 提出了基于跨层自适应融合的 Transformer 模型, 该模型通过跨层信息交互、注意力机制增

强和自适应特征融合, 克服了传统 Transformer 在高维特征学习中的局限性。残差分析表明, 该模型在气溶胶化学成分的反演中表现出良好的泛化能力, 有助于基于卫星观测捕捉野火、沙尘暴和颗粒物污染等典型环境污染事件。

3.3 细颗粒物质量估算

大气颗粒物的粒径分布范围广泛, 从 10^{-3} 到 10^2 微米不等, 其中空气动力学等效直径小于 2.5 微米和 10 微米的颗粒物分别被定义为 $PM_{2.5}$ 和 PM_{10} 。作为气溶胶的重要组成部分, $PM_{2.5}$ 和 PM_{10} 因能够深入人体呼吸系统并引发严重的健康危害而受到广泛关注 (张莹 等, 2022)。卫星观测虽然具有监测大范围近地表气溶胶颗粒物的潜力, 但正如 Hoff 和 Christopher (2009) 的研究所表明的那样, 关联近地表气溶胶颗粒物浓度与整层大气气溶胶消光特性的物理模型尚不完善。因此, 传统上, 全球或区域尺度 PM_x 浓度的获取主要依赖于半经验算法 (Zhang 和 Li, 2015; 张莹 等, 2013; 李正强 等, 2013) 或大气化学传输模型模拟 (Van Donkelaar 等, 2010)。

近地表颗粒物质量浓度估算研究发展早期受限于观测数据的匮乏, 主要采用简单的比例因子法, 通过建立整层大气柱 AOD 与近地表 $PM_{2.5}$ 浓度之间的线性关系进行估算 (Liu 等, 2004; Van Donkelaar 等, 2006)。随着研究的深入, 将物理过程耦合到反演中的半经验方法被提出 (Koelemeijer 等, 2006; Zhang 和 Li, 2015; Lin 等, 2015)。随着地基观测站点和卫星遥感数据的不断积累, 统计模型逐渐成为主流研究方法, 如多元线性回归、广义加性模型等, 这些方法通过引入气象参数、地理因子等辅助变量, 显著提高了估算精度和效率 (Liu 等, 2005; Pelletier 等, 2007)。近年来, 人工智能技术的快速发展推动了机器学习方法在该领域的广泛应用 (包括随机森林、支持向量机、神经网络等算法), 这些方法能够更好地捕捉整层大气柱 AOD 与近地表 $PM_{2.5}$ 浓度之间的非线性关系, 进一步提升估算精度。Sun 和 Sun (2017) 提出了一种基于主成分分析 PCA (Principal Component Analysis) 的新型混合模型, 通过 PCA 降维提取特征后, 利用最小二乘支持向量机进行每日 $PM_{2.5}$ 浓度预测。Hu 等 (2017) 采用随机森林模型, 整合气溶胶光学厚度数据、气象场和土地利用变量,

实现了美国近地表 $PM_{2.5}$ 浓度的预测。Shao等(2020)开发的模型有效捕捉了预测因子间的非线性相互作用,并解释了近地表 $PM_{2.5}$ 浓度的时空依赖性,其性能优于传统随机森林模型。Elangasinghe等(2014)将NN方法与k均值聚类相结合,通过融合风速、风向、太阳辐射等气象参数,实现了特定地点污染物扩散机制的提取。Chen等(2019b)将非线性暴露滞后响应模型与极端梯度增强模型相结合,并开发了一种两步插值方法(混合效应模型和逆距离加权方法)来替换AOD中的缺失值,以解决AOD反演结果缺失的问题。Chen等(2024)提出了一种时空插值的图卷积网络模型,该模型对高分辨率图像处理以提取影像特征,随后结合气象因子和AOD,实现了在城市功能区尺度上的近地表 $PM_{2.5}$ 浓度反演。

尽管上述机器学习模型相比传统统计方法具有显著优势,但仍存在单一模型的局限。为充分发挥各模型的优势,集成学习方法应运而生,通过组合多个模型提升了预测性能,具有更强的泛化能力、更高的准确率和更好的稳定性。此外,随着计算能力的显著提升和大规模数据的持续积累,深度学习技术在气溶胶遥感领域逐渐崭露头角。Zhu和Lu(2016)提出了一种基于自回归滑动平均和改进反向传播神经网络的混合模型用于近地表 $PM_{2.5}$ 浓度预测。Li等(2017a)将地理相关信息引入深度置信网络,并通过逐层预训练技术实现了中国区域高精度 $PM_{2.5}$ 浓度的卫星遥感反演。Shen等(2018)基于时空深度置信网络对武汉城市群近地面 $PM_{2.5}$ 浓度进行了预测,通过与地基点观测数据的交叉验证,证明了该模型的预测精度。Zang等(2019)结合主成分分析(PCA)方法,提出了改进的广义回归神经网络模型以反演近地表 $PM_{2.5}$ 浓度。Chen等(2024)提出了一种基于极端梯度提升的两阶段模型,其中一阶段模型通过改进时间编码和引入地形分类因素增强了时序信息的表达。二阶段模型则通过融合观测和估计值增强了空间相关性,最终实现了不依赖AOD产品的全覆盖、高精度的逐日 $PM_{2.5}$ 反演。鉴于大气遥感数据普遍具有时间序列特性,长短时记忆网络LSTM(Long Short-Term Memory)受到研究者关注。Li等(2017b)对LSTM模型进行了改进,充分考虑了空气污染物浓度的时空相关性,该模型利用LSTM从历史空气污染物数据中提取初级特

征,将气象等辅助数据整合到已建立的LSTM模型中以提高性能,具有更高的估计精度。Wei等(2019a)基于1 km分辨率的MODIS MAIAC气溶胶产品,结合地基 $PM_{2.5}$ 观测值和气象等辅助变量,通过集成统计回归模型,生成了中国大陆1 km空间分辨率的卫星 $PM_{2.5}$ 产品。Wei等(2019b)通过扩充 $PM_{2.5}$ 影响因子集和改进时空特征提取方法,开发了“时空一极端随机树”模型,进一步提升了预测精度。随后,为提高全球尺度 $PM_{2.5}$ 产品的精度,Wei等(2023b)在原有模型框架基础上引入欧氏球面空间结构与三角螺旋时间建模方法,实现了全球陆地区域逐日、1 km空间分辨率的长时间序列 $PM_{2.5}$ 数据集的构建,提升了产品的时空连续性表现。

4 讨论

机器学习方法在气溶胶卫星遥感领域的研究方法大致可归纳为两大类:一是利用机器学习方法直接构建卫星观测数据与目标参数之间的统计关系;二是采用机器学习方法替代反演过程中复杂的物理模型计算,以达到提高运算速度和精度的效果。第一类方法通过机器学习直接建立卫星观测与目标参数之间的映射关系,能够有效规避传统物理模型中的难点问题,例如气溶胶遥感中经典的地气解耦合难题(Hsu等,2004)以及近地表 $PM_{2.5}$ 浓度与气溶胶光学特性间的复杂物理机制(Zhang等,2021)。然而,这类数据驱动的方法需要大量高质量的训练数据才能实现准确预测。同时,这种端到端的学习方法受限于地基观测提供的真值数据,对于缺乏原位观测的关键气溶胶参数,其应用受到显著限制。另外,由于不同传感器在光谱响应函数和波段设计等方面的差异,基于单一传感器数据训练的机器学习模型往往难以迁移到其他传感器上并保持相同的精度水平,仍需开展大量深入研究,以量化不同传感器间观测精度差异对机器学习反演结果的影响。第二类方法则聚焦于利用机器学习替代反演过程中的物理模型计算。尽管当前气溶胶遥感领域已发展出能够反演多种气溶胶参数的高精度统计最优化算法(Dubovik等,2011; Fu等,2025),但这些算法依赖的高精度辐射传输计算往往需要巨大的计算资源,难以满足近实时反演的需求。机器学习方法在这一方向展现出独特优势,能够替代计算密集

型的物理过程。

需要指出的是, 当前气溶胶定量遥感反演仍处于快速发展阶段, 某些复杂参数的理化和遥感机理尚未完全解析, 机器学习方法虽然能够在一定程度上规避这一问题, 但并未从根本上解决。由此可见, 机器学习方法作为一种重要的技术手段, 未来研究可着重探索机器学习方法与物理模型的深度融合, 以推动气溶胶遥感领域的进一步发展。

5 结 语

由于气溶胶对自然环境和人类健康的重要影响, 近实时、精确的大气气溶胶卫星遥感数据产品具有重要的科学意义和应用价值。机器学习作为一种新兴的技术手段, 在气溶胶遥感领域展现出巨大潜力, 但仍旧存在一定的局限性 (例如模型训练中的过拟合或欠拟合现象、模型结果的可解释性不足以及适用性受限等)。因此, 在气溶胶遥感领域, 机器学习方法目前尚无法完全取代物理方法, 但具有巨大的发展前景。针对气溶胶光学参数, 相关研究的重点主要集中在提升反演精度和计算效率方面; 对于气溶胶微物理参数和化学成分含量, 当前的机器学习反演技术仍处于探索阶段, 需要未来更多的研究投入; 在近地表细颗粒物浓度反演方面, 机器学习方法已能够在气象数据的支持下构建卫星观测与反演参数之间的统计模型, 但仍需完善相关的物理和遥感机制, 为了进一步提高反演效能, 将机器学习方法与物理方法深度融合是未来重要的研究方向。本研究详细分析了机器学习在卫星遥感大气气溶胶领域的研究进展、面临的挑战以及未来前景, 可以为机器学习方法在气溶胶遥感领域的改进与优化提供参考。

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Application and challenge of machine learning in the satellite remote sensing of atmospheric aerosols

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Abstract: Atmospheric aerosols play a crucial role in the atmospheric environment, impacting climate change and human health, gathering significant attention over the last fifty years. With the continuous development of satellite remote sensing technologies, satellite-based

aerosol observation has become one of the most important and effective means of acquiring large-scale, long-term aerosol data. The advancement of satellite sensor technologies has also played a critical role in enabling highly accurate aerosol retrieval. Moreover, with the successful launch of POLDER (Polarization and Directionality of the Earth's Reflectances), multi-angle joint polarization observation has become a key development direction for atmospheric aerosol monitoring. China has made significant progress in satellite-borne polarimeters, including DPC (Directional Polarimetric Camera) on GF-5 in 2018, SMAC (Synchronization Monitoring Atmospheric Corrector) on GFDM in 2020, PSAC (Polarized Scanning Atmospheric Corrector) on HJ-2A/B in 2020, and the PCF (Polarization Crossfire Payload) on GF-5(02) in 2021. Subsequently, China launched a series of atmospheric environment monitoring satellites equipped with PCF suits. Internationally, NASA launched the PACE satellite in 2024, equipped with SPEXone and HARP2 polarimeters. A review of the development of satellite remote sensing for atmospheric aerosols reveals that early observation methods were limited. Constrained by computational capacity and the few satellite data, early retrieval algorithms primarily relied on lookup table (LUT) approaches to strike a balance between retrieval accuracy and algorithmic feasibility. With advancements in satellite observation technologies, aerosol retrieval algorithms have continued to evolve. In the current era of massive satellite datasets, a central challenge in aerosol remote sensing is how to effectively extract meaningful atmospheric information from these vast data resources. Over the past decade, statistically optimized algorithms have emerged as one of the most promising solutions. These physically based inversion methods aim to retrieve aerosol parameters by fitting satellite observations with forward radiative transfer simulations. However, the high computational cost of optimization algorithms poses a significant barrier to the real-time generation of satellite aerosol products on a large scale, highlighting the urgent need for innovative technological breakthroughs.

Recently, the evolution of Artificial Intelligence (AI) has introduced transformative changes to aerosol remote sensing. Machine Learning (ML) techniques have shown notable enhancements in retrieval efficiency and the capability to tackle persistent issues that traditional physical methods face, such as separating signals from the surface and atmosphere. ML technologies are propelling satellite aerosol retrieval into an era of intelligent development. This paper presents a comprehensive review of the latest advancements in satellite-based aerosol retrieval algorithms using ML methods. It evaluates the strengths and limitations of mainstream ML techniques in different retrieval contexts. Overall, ML methods show great potential in aerosol remote sensing but still face limitations. It cannot yet fully replace physical models, but it offers promising prospects. Current research focuses on improving retrieval accuracy and efficiency for aerosol optical properties, while retrieval of microphysical and chemical properties remains exploratory. For near-surface Particulate Matter (PM) concentrations, ML methods can build statistical models supported by meteorological data, yet underlying physical mechanisms need refinement. Integrating ML with physical models is a key future direction to enhance the accuracy and robustness of aerosol retrieval. This review aims to offer useful insights for researchers and developers working on next-generation aerosol retrieval systems.

Key words: aerosol, atmospheric remote sensing, machine learning, artificial intelligence, retrieval algorithms

Supported by National Natural Science Foundation of China (No. 42305151); National Key Research and Development Program of China (No. 2023YFB3907405)