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机器学习算法在高光谱感知作物信息中的应用及展望*

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摘要：机器学习作为一种统计学与计算机科学相结合的新兴技术，近年来在作物信息获取任务中得到广泛应用。传统的作物信息获取方式主要依靠化学检测法，测定过程耗时、耗力。基于机器学习算法和高光谱遥感技术能够通过无损的方式，快速感知作物外观及内部理化参数，具有明显的应用优势和发展前景。本文对国内外作物信息高光谱遥感相关研究进行系统性梳理。总结了不同机器学习算法在高光谱感知作物信息中的应用及优缺点，归纳了机器学习算法建模的不确定性，指出高光谱感知作物信息的未来发展趋势为，通过多源遥感协同观测实现作物信息获取方式互补，发展高光谱遥感与作物模型同化技术、高光谱遥感与人工智能深度融合技术，从而实现面向作物全生育期的关键信息智能化获取与决策。
关键词：机器学习；深度学习；偏最小二乘法；农作物；高光谱遥感

Hyperspectral Remote Sensing of Crop Information Based on Machine Learning Algorithm: State of the Art and Beyond

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Abstract: Machine learning, as a new technique combining statistics and computer science, has been widely used in crop information acquisition tasks in recent years. Traditional methods for obtaining crop information mainly rely on chemical detection methods, which is time-consuming and labor-intensive. Based on machine learning algorithms and hyperspectral remote sensing techniques, crop appearance and internal physical and chemical parameters can be quickly sensed in a non-destructive way, which has obvious application advantages and development prospects. First, the researches related to the hyperspectral remote sensing of crop information were systematically reviewed in this paper. Second, the application, advantages and disadvantages and uncertainties of different machine learning algorithms in hyperspectral sensing crop information were summarized. Finally, it was pointed out that the future development trends of hyperspectral sensing crop information were as follows: (1) complementary crop information acquisition methods could be realized through multi-source remote sensing collaborative observations. (2) The assimilation technologies of hyperspectral remote sensing and crop model as well as the deep integration technologies of hyperspectral remote sensing and artificial intelligence could be developed.

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(3) The intelligent acquisition of key information oriented to the whole growth period of crops and decision-making could be realized.

Key words: Machine learning; Deep learning; Partial least squares; Crops; Hyperspectral remote sensing

人类健康主要依赖于来自农作物丰富而有营养的食物供应[1]。快速、准确地掌握作物关键信息，对作物长势监测、水肥管理、品质提升具有重要参考价值。传统的作物信息获取方式主要采用化学检测法，测定过程耗时长、复杂。光谱分析是科学研究和工业行业使用最广泛的分析工具之一[2]。与传统方法相比，高光谱技术具有快速、无损等明显优势。将高光谱技术应用于获取植物叶片理化参数的研究最早可追溯到 20 世纪 60、70 年代[3]。半个多世纪以来，随着化学计量学的发展，高光谱技术呈现出多谱段、多模态、多平台的发展态势。基于机器学习算法和高光谱技术感知作物信息成为国内外的研究热点。

机器学习算法具备强大的处理高维数据与冗余数据的能力，能够有效抵抗高维数据中的噪声，实现对数据有效信息的提取[4]。作物信息高光谱遥感中使用的机器学习算法主要包括回归和分类两种。经典算法如逐步回归法（SR）、偏最小二乘法（PLS）相对成熟，所建模型可解释性较强。传统机器学习算法如支持向量机（SVM）、梯度提升树（XGBoost）以及集合多个单一学习器优势的 Stacking 集成学习算法在处理非线性问题方面优势明显。深度学习是机器学习领域的一个新方向，利用数据增强技术能够在一定程度上解决作物信息实测数据有限的小样本问题，同时具备强大的特征挖掘能力，在田间复杂场景建模方面具有独特优势。

尽管基于机器学习算法和高光谱技术在感知作物水分[5−6]、叶绿素[7]、营养成分[8−9]、品种[10]、产量[11]、成熟度[12−13]、病虫害[14]、盐胁迫[15]、水分胁迫[16−17]方面取得不错的进展，然而，距离实现真正的作物信息智能感知还有一定距离。本文以 Web of Science 核心库和中国知识基础设施工程（CNKI）中文库近年来发表的作物信息高光谱遥感相关文献为主要参考，对其中采用的机器学习算法进行系统性梳理，按照光源条件、观测平台、光谱数据预处理方法、敏感波段提取方法和化学检测方法 5 方面总结归纳机器学习算法建模的不确定性，并对未来发展趋势进行展望，旨在为作物信息智能感知技术的发展提供科学参考。

1 高光谱感知作物信息中的回归任务

1.1 传统线性回归算法建模

最小二乘法（OLS）是一种数学优化技术，通过最小化误差的平方和寻找数据的最佳函数匹配。在作物高光谱研究中，OLS 常用来拟合基于最优光谱指数的一元线性回归[16]、二次多项式[18]、指数函数[19]、幂函数[20]模型，间接获取作物色素、氮含量、水分含量、冠层结构、产量等关键信息。其优势在于所建模型简单、可解释性强，但模型泛化性能一般。主要表现在对单一生育期的建模效果较好，但对全生育期的建模效果不理想[9,21]。

逐步回归法是一种减少自变量之间相关性的常见方法，通过调节引入和删除变量的置信度[22]，可以获得在给定显著性水平下的“最优”回归方程，常用于识别传感器谱带中与叶片或冠层不同化合物相关性最强的波段[23]。基于该算法构建的模型对大豆[22]、草莓叶绿素含量的反演效果较好[24]。

偏最小二乘法是一种建立高光谱反射率与特征间联系的常用方法[25]。与其他需要大量训练样本数据的机器学习算法不同，PLS 仅需少量训练数据，尤其适用于因变量数少于自变量数的场景。PLS 建模的关键是确定最优潜在变量数（ONLVs）。比如以相对均方根误差最小的原则选取 5～8 个 ONLVs 建模，可评估臭氧升高对 5 种基因型大豆叶片矿质养分（Ca、Cu、Fe、K、Mg、Mn）含量的影响[26]。采用 10 折交叉检验法选取 2～18 个 ONLVs 建模，可估测大豆不同生长阶段关键参数[27]。

然而，当自变量含有较多干扰信息时，PLS 并非总能获得最佳效果。在 PLS 基础上提出的区间 PLS（iPLS）[28]，能够提取敏感波段，对水稻冠层氮含量的估测效果比 PLS 更好[29]。稀疏 PLS（SPLS）是一种基于 PLS 原理并应用稀疏解[30]来选择敏感波段的方法，对大量营养素浓度的估测准确性更高[31]。

1.2 传统机器学习算法在回归任务中的应用

支持向量机是一种有监督的统计学习算法。与 PLS 相比，SVM 对于豆类作物和牧草的氮含量、粗蛋白含量、干物质量的估测精度更高[32]。将 5 折交

叉检验法与SVM相结合构建的支持向量机联合回归算法(C-SVR)能够准确估测苹果树冠层叶绿素含量，比 PLS 和支持向量回归（SVR）精度提高 3.8%～4.0%[33]。基于最小二乘支持向量机（LSSVM）构建的不同光照强度下生菜叶绿素含量估测模型，能够获得比 PLS 更好的效果[34]。

集成学习可以通过优化数据分布和模型组合，提高模型泛化性能和预测精度[35]。代表性算法有随机森林（RF）、XGBoost 和 Stacking 等。基于 RF 算法建立的棉花地上部生物量反演模型能够获得比多数机器学习算法，如人工神经网络（ANN）、回归树（RT）、袋装树（BaT）、增强树（BoT）、SVM 和高斯过程回归（GPR）更高的精度[36]。而 XGBoost 在训练过程中参考了随机森林的思想，每次迭代过程中有选择地采取部分样本的部分特征进行训练，对冬小麦氮含量的反演效果更好[37]。Stacking 算法通过元学习器对基学习器的输出结果再次训练，从而将不同模型解析数据的能力进行结合，通常能得到比单一算法更高的估测精度[38]。

极限学习机（ELM）是一类具有随机初始化输入权重和偏差的单隐藏层前馈神经网络，其输出权重是通过网络解析确定[39]，具有易实现、学习速度快和泛化性能好的优势。但由于 ELM 的目标是最小化训练集误差，因此可能导致模型过拟合[40]。而正则极限学习机（RELM）通过引入正则化参数缓解了这个问题[41]。加权正则极限学习机（WRELM）能够进一步削弱异常值的影响[42]。激活函数是加权输入信号和偏置的非线性转换[43]，能够将输入数据转换至非线性特征空间，改进激活函数可以提高模型精度。比如将激活函数 ReLU 的正值部分与 Tanh 的负值部分结合，构建新的激活函数 TanhRe，能有效提高 WRELM 模型对葡萄浆果产量和品质的估测精度[11]。

1.3　深度学习算法在回归任务中的应用

高光谱感知作物信息的回归任务研究成果如表 1 所示。总体上，传统线性回归算法和机器学习算法在估测作物叶绿素含量、氮含量、产量方面均表现出不错的效果。

表 1　高光谱感知作物信息的回归任务研究成果

Table 1　Research on regression task of hyperspectral sensing crop information

作物种类 Crop type	方法 Method	作物信息 Crop information	技术特点 Technical characteristic	精度 Precision(%)	文献 Reference
葡萄 Grape	OLS	叶片气孔导度 Stomatal conductance	以归一化差异光谱指数 NDSI(R_{603},R_{558})建立的一元线性回归模型比 PLS 精度提高 5.88%The precision of unary linear regression model established with normalized difference spectral index NDSI(R_{603}, R_{558}) was 5.88% higher than that of PLS	72	[16]
水稻 Rice	OLS	产量 Yield	以比值光谱指数RSI(R_{920},R_{690})建立的二次多项式模型在稻纵卷叶螟为害下精度最优 The quadratic polynomial model based on the ratio spectral index RSI(R_{920}, R_{690}) had the best precision under the damage of *Cnaphalocrocis medinalis*	77.8~89.3	[18]
水稻 Rice	OLS	叶绿素含量 Chlorophyll	以 NDSI(R_{790},R_{630})建立的指数模型在稻纵卷叶螟为害下精度优于多元逐步回归模型 The precision of index model based on NDSI(R_{790}, R_{630}) was better than that of multiple stepwise regression model under the damage of *Cnaphalocrocis medinalis*	72	[19]
冬小麦 Winter wheat	OLS	叶绿素含量 Chlorophyll	以 D_{694} 建立的幂函数模型在低温胁迫下精度最优 The precision of the power function model established by D_{694} was the best under low temperature stress	69.4	[20]
大豆 Soybean	SR	叶绿素含量 Chlorophyll	融合光谱和空间信息的模型精度比仅使用光谱特征的模型提高 30%～45%The precision of the model combining spectral and spatial information was 30%−45% higher than that of the model using only spectral features	91	[22]
草莓 Strawberry	SR	叶绿素含量 Chlorophyll	以 R_{747}、R_{800}、D_{716}、D_{906} 为敏感波段建立的模型在苗期高温条件下精度最优 The model with R_{747}, R_{800}, D_{716} and D_{906} as sensitive bands had the best precision under high temperature stress in seedling stage	84.3	[24]

（续表）

作物种类 Crop type	方法 Method	作物信息 Crop information	技术特点 Technical characteristic	精度 Precision(%)	文献 Reference
马铃薯 Potato	PLS	叶柄 NO_3-N、叶片全氮、植株全氮、块茎产量 Petiole NO_3-N, leaf total nitrogen, plant total nitrogen, tuber yield	相较于 OLS 算法,PLS 算法在航空高光谱的全谱段、可见−近红外、短波红外波段区间均表现出更稳定的效果 Compared with OLS, PLS showed more stable effect in the full-range, visible-near infrared and short wave infrared bands of aircraft hyperspectral imagery	68~82	[9]
春小麦 Spring wheat	PLS	叶绿素含量 Chlorophyll	以叶绿素指数 CI(R_{849},R_{850})、CI(R_{539},R_{553})、CI(R_{540},R_{553})和 CI(R_{536},R_{553})的建模精度最高 The CI(R_{849}, R_{850}), CI(R_{539}, R_{553}), CI(R_{540}, R_{553}), and CI(R_{536}, R_{553}) had the highest modeling precision	74	[44]
玉米 Maize	PLS	叶绿素含量、氮含量、光合速率 Chlorophyll, nitrogen, photosynthetic rate	以航空高光谱数据为驱动建立的作物关键参数反演模型,精度优于传统辐射传输模型 The precision of crop key parameters inversion model driven by airborne hyperspectral data was better than that of traditional radiation transfer model	69~83	[45]
马铃薯 Potato	PLS	叶绿素含量 Chlorophyll	利用无人机高光谱敏感波段和 PLS 建立的模型在芽期和块茎增长期的精度优于 SR、SVM、RF 算法 The precision of the model established by using the UAV hyperspectral sensitive bands and PLS was better than that of SR, SVM and RF in bud stage and tuber growth stage	69~85	[46]
水稻 Rice	BRR	产量 Yield	相较于支持向量回归(SVR)和 PLS，贝叶斯岭回归(BRR)算法的效果更好 Compared with support vector regression (SVR) and PLS, Bayesian ridge regression (BRR) had better effect	94	[47]
葡萄 Grape	GBM	叶水势 Leaf water potential	以 NDSI(R_{561},R_{554})、RSI(R_{900},R_{970})、RSI(D_{730},D_{706})为特征变量,对比多元自适应回归样条(B-MARS)、广义相加模型(GAM)、广义提升回归模型(GBM)、贝叶斯正则化神经网络(BRNN)、Cubist 回归、广义线性模型(GLM)、RF、SVM、PLS 算法建模效果,其中以 GBM 最优 Using NDSI(R_{561}, R_{554}), RSI(R_{900}, R_{970}), and RSI(D_{730}, D_{706}) as variables, the bagged multivariate adaptive regression splines (B-MARS), generalized additive models (GAM), generalized boosted models (GBM), bayesian regularized neural networks (BRNN), cubist regression, generalized linear models (GLM), RF, SVM, and PLS were compared, and GBM was the best	80	[48]
冬小麦 Winter wheat	XGBoost	植株全氮 Plant total nitrogen	采用贝叶斯优化算法对 XGBoost 算法进行超参数调优,构建基于无人机高光谱的不同土壤肥力条件下田块尺度全氮含量反演模型 The Bayesian optimization algorithm was used to optimize the hyperparameters of XGBoost, and the inversion model of total nitrogen content at field scale under different soil fertility conditions was constructed based on UAV hyperspectral data	76	[37]
冬小麦 Winter wheat	Stacking	产量 Yield	以 ANN、GPR、多元线性回归(MLR)、RF、岭回归(RR)和 SVM 为基学习器，以 MLR 为元学习器建立的集成学习模型能够获得比单一算法更高的精度 Based on ANN, GPR, multiple linear regression (MLR), RF, ridge regression (RR) and SVM, the integrated learning model established with MLR as the meta-learner could obtain higher precision than single algorithm	43.3~67.5	[38]
冬小麦 Winter wheat	KNN	叶面积指数 Leaf area index	基于三波段光谱指数(D_{714}-D_{400})/(D_{400}-D_{1001})与 K 近邻算法(KNN)的建模精度优于 ANN 和 SVR 算法 Modeling precision based on three-band spectral index (D_{714}-D_{400})/(D_{400}-D_{1001}) and k-nearest neighbor (KNN) was superior to ANN and SVR	89	[49]

（续表）

作物种类 Crop type	方法 Method	作物信息 Crop information	技术特点 Technical characteristic	精度 Precision(%)	文献 Reference
水稻 Rice	DF	叶片氮含量 Leaf nitrogen	基于少量全光谱反射率的一阶导数建立的一种新的深度森林(DF)模型，精度优于多层感知器(MLP)、RF 和 SVM 算法 A novel deep forest (DF) model based on the first derivative of a small amount of full-range spectral reflectance was developed with better precision than the multi-layer perceptron (MLP), RF and SVM	91.9	[50]
柑橘 Citrus	CNN	叶片含水率 Leaf moisture	利用敏感波段结合卷积神经网络算法(CNN)的建模精度比 SVR、PLS、RF 提高 10.36%～54.59%Compared with SVR, PLS and RF, the modeling precision of sensitive bands combined with convolutional neural networks (CNN) was improved by 10.36%−54.59%	94.7	[51]

注：精度=决定系数×100；归一化差异光谱指数 NDSI(i, j) = (i–j)/(i+j)，比值光谱指数 RSI(i, j) = i/j，叶绿素指数 CI(i, j) = $(i^{-1}–j^{-1})j$，其中 i、j 表示波长，单位为 nm；R 表示原始光谱反射率，D 表示原始光谱反射率的一阶导数，下角的数字表示波长。

Note: The precision means that the coefficient of determination (R^2) is expanded by 100 times. The normalized difference spectral index NDSI(i, j) = (i–j)/(i+j), the ratio spectral index RSI(i, j) = i/j, and the chlorophyll index CI(i, j) = $(i^{-1}–j^{-1})$ j, where i and j represent the wavelength, and the unit is nm. R represents the original spectral reflectance, D represents the first derivative of the original spectral reflectance, and the subscript with number represents the wavelength.

近年来，深度学习技术在农业领域得到快速发展。相较于传统算法，深度学习算法精度高，模型泛化能力强，与传统算法的优缺点对比如表 2 所示。长短时记忆网络（LSTM）和卷积神经网络（CNN）是作物高光谱遥感领域的研究热点[52]。三维卷积神经网络（3D–CNN）能够同时获取高光谱图像的空间特征和光谱特征。但当模型增加新的维度时，参数量会呈指数增加，容易导致模型过拟合和计算负载过高。为解决这个问题，Torres-Tello 等[5]首先通过 1×1 逐点卷积对高光谱数据降维，采用预训练的 VGG-16 网络提取图像空间特征，再采用双向长短时记忆网络（BiLSTM）挖掘光谱数据的前、后向关系，最后通过线性加权集成法将多种特征融合实现油菜和小麦水分含量的有效估测。

表 2　深度学习回归算法与传统算法对比

Table 2　Comparison between deep learning and traditional algorithm in regression task

	深度学习算法 Deep learning algorithm	传统算法 Traditional algorithm
优势 Advantage	1.模型估测精度高,泛化能力强,有较好的可迁移性 The model has higher accuracy, stronger generalization ability and better portability 2.不需要人工设计特征,具备自动挖掘光谱特征和图像空间特征的能力 Without manual feature design, it has the ability to automatically mine spectral features and image spatial features 3.模型满足实时性检测的要求 The model meets the requirement of real-time detection	1.模型特征变量较少,可解释性强 The model has fewer characteristic variables and stronger interpretability 2.敏感波段对作物理化参数有较好的指示作用 Sensitive bands can indicate the physical and chemical parameters of crops 3.对于作物理化参数实测值较少的场景建模效果较好 The model is better for the situation with few measured physical and chemical parameters
不足 Disadvantage	1.需要大量的训练样本 A large number of training samples are required 2.模型训练阶段对计算机硬件有较高要求 The model training stage has higher requirements for computer hardware 3.缺乏针对作物理化参数等小样本数据集的数据增强技术 Lack of data enhancement techniques for small sample datasets such as physical and chemical parameters 4.模型调参复杂 The model parameters are complex	1.处理具有共线性问题的数据时,效果欠佳,因为多数模型假设变量之间是相互独立的 Dealing with data with collinearity problems is not effective because most models assume that variables are independent of each other 2.多数模型仅使用像元的光谱信息,未包含空间细节,而空间上下文信息是光谱特征的重要补充,对建模同样重要 Most models only use spectral information of pixels without spatial details, while spatial context information is an important supplement to spectral features and is also important for modeling

多任务学习（MTL）是一种前沿的机器学习技术，通过发现任务之间的潜在相关性来联合学习多个任务提高模型泛化性能，在深度学习中应用广泛。由于每个任务都作为额外任务的归纳偏差，使得模型能够有效忽略噪声，稳健性更强。同时，在学习相关任务中通过发现额外信息可实现数据增强[53]。Feng 等[54]利用多时相无人机高光谱数据，将基于 LSTM 的普通层与 ANN 的任务特定层结合提出了一种新的多任务学习模型，实现了对紫花苜蓿品质的准确评价。

2 高光谱感知作物信息中的分类任务

2.1 传统线性分类算法建模

线性判别分析（LDA）模型使用特征的线性组合作为分类标准，将数据从高维空间投影到低维空间，同时确保投影后每个类的类内方差较小、类间方差较大，尤其适用于样本和特征数较少的线性分类。作物感染病害，会引起电磁波谱响应特征变化，进而可借助机器学习算法构建鉴别模型，实现对不同严重度分级[55]。比如玉米矮花叶病识别[56]、大豆锈病严重度分级[55]等。

偏最小二乘法判别分析（PLS-LDA）是一种通过响应变量和预测变量投影潜在变量来区分类别的高维数据统计方法，能够降低数据维数并最大限度地提高预测精度[15]，在处理小样本和多重共线性问题方面具有优势[57]。基于该算法通过融合光谱和纹理特征可实现小麦白粉病早期诊断[58−59]。

2.2 传统机器学习算法在分类任务中的应用

SVM 是核变换技术的代表性算法之一，在解决小样本、非线性和高维数据等问题上具有优势。SVM 建模的关键是挑选合适的核函数。常用的核函数有线性核函数、径向基核函数（RBF）、多项式核函数和 Sigmoid 核函数。其中，基于 RBF 核函数的 SVM 算法模型在烟叶成熟度[60]、柑橘病虫害识别[61]方面效果更好。

RF 是以决策树为基学习器的集成学习算法，具有分类准确度高、不易过拟合等优势。XGBoost 与 RF 的区别在于新生长的树依赖于先前树提供的反馈信息[62]，从而可以减少后续迭代中产生的错误，具有高效、灵活和可移植性优势。而 Stacking 集成学习算法能够获得比单一分类器更好的训练效果。比如以 RF 为基础开发的集成学习模型可识别冬油菜养分亏缺水平，与仅使用 RF、SVM、ANN 的模型相比，精度分别提高 16.55%、18.43%和 35.74%[63]。

BP 神经网络（BPNN）是一种应用广泛的机器学习算法，由许多高度互连的神经元组成，这些神经元被分为 3 部分，即输入层、隐藏层和输出层。在训练过程，网络可以根据分类误差调整连接权重生成输入与输出模式之间的目标映射。基于该算法可实现白萝卜空心度分级[64]、葡萄衰枯病和黄叶病准确识别[65]。激活函数的选取以及隐藏层结构的设计是 BPNN 建模的关键。

2.3 深度学习算法在分类任务中的应用

高光谱感知作物信息的分类任务研究成果如表 3 所示。总体上，传统线性分类算法和机器学习算法在作物病虫害识别方面均取得不错效果。

在作物信息高光谱遥感分类任务中，应用最广、最具代表性的深度学习算法是 CNN。CNN 是为模拟生物感知机制而开发的深度神经网络，能够自动提取数据中浅层和深层的敏感特征，与传统算法在分类任务中的优缺点对比如表 4 所示。AlexNet 和残差网络（ResNet）是 CNN 的典型代表。2012 年 AlexNet 一经提出便掀起了深度学习的应用热潮，比如基于 AlexNet 与 1467.38nm 波长处高光谱图像建模，可实现东北和非东北大米产地的快速、无损检测[73]。ResNet 是由一系列残差块（直接映射部分和残差部分）组成。残差块的作用是更好地提取数据特征，防止网络退化。在 ResNet 的基础上通过向网络中添加批标准化层（BN）和随机失活层（Dropout）提出的一种新的一维深度卷积神经网络（1DCNN）可实现水稻叶瘟病的有效识别，比传统机器学习算法（SVM、ELM）精度提高 3.04%～6.91%[74]。相较于传统 SVM 算法，多尺度三维卷积神经网络（MS-3DCNN）对高光谱图像的特征挖掘能力更强，基于该算法可实现小麦种子品种鉴别[75]。将 CNN 与多层感知器（MLP）相结合提出的一种多输入深度学习模型，可实现香蕉出口质量准确分级，比单一特征或传统机器学习算法（逻辑回归、决策树、K 近邻、高斯朴素贝叶斯、SVM、RF）建模精度提高 9.58%～71.62%[76]。

表 3　高光谱感知作物信息的分类任务研究成果

Table 3　Research on classification task of hyperspectral sensing crop information

作物种类 Crop type	方法 Method	作物信息 Crop information	技术特点 Technical characteristic	精度 Precision(%)	文献 Reference
大豆 Soybean	LDA	叶片锈病 Leaf rust	采用第一、二主成分对原始光谱数据压缩,再采用逐步回归选取敏感波段建模 The first and second principal components were used to compress the original spectral data, and then the sensitive bands were selected by stepwise regression to establish the model	82.51	[55]
玉米 Maize	LDA, SVM	矮花叶病 Dwarf mosaic	利用最优植被指数结合 LDA 或 SVM 算法建模精度更高 The model based on the optimal vegetation index combined with LDA or SVM algorithm had higher precision	100	[56]
小麦 Wheat	PLS-LDA	白粉病 Powdery mildew	基于小波特征和纹理特征建模精度更高 The model based on wavelet and texture features had higher precision	81.17	[66]
石榴 Pomegranate	PLS-LDA	品种、盐胁迫 Variety, salt stress	当训练集与验证集比例为 80%和 20%时,模型精度最优 When the ratio of training set to validation set was 80% and 20%, the precision of the model was optimal	79~89	[15]
小麦 Wheat	PLS-LDA	白粉病 Powdery mildew	采用第一、二、三主成分压缩原始光谱数据,再使用融合敏感波段和纹理特征的数据建模 The first, second and third principal components were used to compress the original spectral data, and then the data fused with sensitive bands and texture features was used for modeling	91.4	[59]
烟叶 Tobacco leaf	SVM	成熟度 Maturity	基于遗传算法(GA)提取敏感波段结合 SVM 建模,比 BPNN 精度提高 3.35%Based on genetic algorithm (GA) extraction of sensitive bands combined with SVM modeling, the precision was 3.35% higher than BPNN	95.28	[60]
柑橘 Citrus	SVM	溃疡病、除草剂、红蜘蛛、煤烟病 Canker, herbicide, starscream, soot	利用全光谱波段的一阶导数,基于 RBF 核函数的 SVM 建模,比 RF 精度提高 4.99%Using the first derivative of the full-range band, SVM modeling based on RBF kernel function improved the precision by 4.99% compared with RF	95.98	[61]
葡萄 Grape	RF, XGBoost	水分胁迫 Water stress	基于 XGBoost 的增益和 RF 的平均精度下降(MDA)提取敏感波段建模比全光谱波段模型精度提高 1.7%～5.5%The precision of sensitive bands modeling based on XGBoost gain and RF mean decrease accuracy (MDA) was 1.7%-5.5% higher than that of full-range band model	80.0~83.3	[17]
柑橘 Citrus	XGBoost	黄龙病 Huanglongbing	提出一种基于典型成分分析(ECA)的敏感波段优选方法,并对比逻辑回归(LR)、SVM、RF、引导聚类算法(Bagging)、迭代算法(Adaboost)、XGBoost 建模效果，其中 XGBoost 的稳定性最好,可用于研制低成本病害检测多光谱仪 A sensitive band optimization method based on exemplar component analysis (ECA) was proposed, and the precision of logistic regression (LR), SVM, RF, Bagging, Adaboost and XGBoost were compared. Among them, XGBoost had the best stability and could be used to develop low cost multi-spectrometer for disease detection	95	[67]
库尔勒香梨 Korla pear	Stacking	黑斑病 Black spot	以 KNN、LSSVM 和 RF 为基学习器,LSSVM 为元学习器,建立的 Stacking 集成学习模型,比单一分类器精度提高 5.18%With KNN, LSSVM, and RF as the base learner and LSSVM as the meta-learner, the integrated learning model of Stacking was established with a precision of 5.18% higher than that of a single classifier	98.28	[68]
白萝卜 White radish	BPNN	空心度 Hollowness	将双曲正切函数和 softmax 函数分别作为 BPNN 算法输入层和隐藏层以及隐藏层和输出层之间的激活函数建模,比 PLS-LDA 精度提高 2.19%The hyperbolic tangent function and softmax function were modeled as the activation function between the input layer and the hidden layer and between the hidden layer and the output layer of BPNN, respectively. The precision was improved by 2.19% compared with that of the PLS-LDA	98	[64]

（续表）

作物种类 Crop type	方法 Method	作物信息 Crop information	技术特点 Technical characteristic	精度 Precision(%)	文献 Reference
葡萄 Grape	BPNN	衰枯病、黄叶病 Esca, Yellowness	将高光谱数据提取的植物理化参数与RGB图像提取的纹理参数相结合,采用包含 10 个神经元隐藏层的 BPNN 算法建模精度更高 Combining phytochemical parameters extracted from hyperspectral data with texture parameters extracted from RGB images, BPNN algorithm containing 10 neurons of hidden layers had higher precision	99.37~99.54	[65]
咖啡豆 Coffee bean	CNN	质量缺陷 Quality defect	采用 2D-3D 融合卷积神经网络创建了一种多模式实时检测算法(RT-CBDIA),比仅使用2D或3D卷积核的模型精度提高0.41%～4.78%A real-time coffee-bean defect inspection algorithm (RT-CBDIA) was created by 2D, 3D convolution neural networks, which improved the precision by 0.41%−4.78% compared with the models using only 2D or 3D convolution kernel	98.6	[69]
大米 Rice	CNN	产地 Origin	基于光谱、形态特征和CNN算法建模,比KNN和RF精度提高41.12%～6.12%The precision of the model based on spectral, morphological features and CNN was 41.12%−6.12% higher than KNN and RF	94.55	[70]
白菜 Chinese cabbage	CNN	农药残留 Pesticide residue	采用离散小波变换(DWT)和CNN算法建模,比MLP、SVM、KNN精度提高 0.8%～24.8%Discrete wavelet transform (DWT) and CNN were used for modeling, which improved the precision by 0.8%−24.8% compared with MLP, SVM and KNN	91.2	[71]
玉米 Maize	CNN	种子品种 Seed variety	利用主成分分析法(PCA)对原始光谱数据压缩,基于像素级光谱信息和CNN 建模,精度优于 SVM 和 KNN 算法 Principal component analysis (PCA) was used to compress the original spectral data, and the precision was better than SVM and KNN based on pixel-level spectral information and CNN modeling	100	[72]

注：精度表示分类的准确率或总体精度。

Note: The precision represents the accuracy or overall accuracy of the classification.

表 4　深度学习分类算法与传统算法对比

Table 4　Comparison between deep learning and traditional algorithm in classification task

	深度学习算法 Deep learning algorithm	传统算法 Traditional algorithm
优势 Advantage	1.自动挖掘高光谱图像上下文特征,实现逐像素分类 Automatic mining of hyperspectral image context features to achieve pixel by pixel classification 2.算法精度满足田间复杂环境下的实时性要求 The accuracy of the algorithm meets the real-time requirement in the complex field environment 3.模型泛化能力强,鲁棒性高 The model has stronger generalization ability and higher robustness 4.数据增强技术相对成熟 Data enhancement technology is relatively mature	1.分类特征对模型的重要性明确 The importance of classification features is clear 2.通过人工筛选敏感波段,可以压缩数据量,避免数据冗余和多重共线性等问题 By manually screening the sensitive bands, the data volume can be compressed to avoid data redundancy and multicollinearity 3.模型训练时间成本低,调参相对容易 The model training time cost is lower and the parameter adjustment is relatively easier
不足 Disadvantage	1.模型参数复杂,可解释性不足 The parameters of the model are complex and the interpretability is insufficient 2.缺乏面向深度学习分类任务的作物高光谱公开数据集 Lack of open crop hyperspectral data sets for deep learning classification tasks 3.样本标注成本较高 The cost of sample labeling is higher 4.模型训练对计算机硬件有较高要求 Model training stage has higher requirements on computer hardware	1.人工筛选特征过程繁琐 The process of manually selecting features is cumbersome 2.模型精度受样本数据集丰富度、训练集与验证集比例的影响较大 The model accuracy is greatly affected by the richness of data set and the ratio of training set to validation set 3.特征提取局限于光谱与纹理特征,对于更深层信息的挖掘能力不足 Feature extraction is limited to spectral and texture features, and the ability to mine deeper information is insufficient

3　机器学习算法建模的不确定性

3.1　光源条件的不确定性

高光谱传感器对光源条件极其敏感。光源灯材质、强度、角度差异会影响光通量，给建模带来不确定性。许多在实验室暗环境下进行的研究[58,74,77]，是依托卤钨光源灯实现。此时，由于光照强度、角度可控，模型一般能获得较高的稳健性。尽管如此，多数室内模型仍难以满足田间复杂环境下的实时监测要求。在自然光照条件下，薄云、烟尘等气溶胶是影响机器学习模型稳健性的主要因素。尽管高光谱野外试验设计的原则是在晴空条件下进行，但由于田块尺度上天气预报技术实现难度较大，以及野外观测任务繁重，研究者往往希望在电池续航能力有限的情况下获取足够多的数据。因此，即使试验过程存在一些近地面气溶胶污染对太阳辐射传输的影响，这些误差通常也会被忽略，进而对所建模型的真实性提出考验。

3.2　观测平台的不确定性

高光谱观测平台主要分为地面、无人机、卫星。传感器的空间分辨率、探测谱段、天顶角差异直接影响了机器学习模型的精度。目前，地面上常用的非成像光谱仪有美国产 ASD[10,63]、PSR-3500[11,16]和 SR-3500[78−79]等。探测波段为 350−2500nm，光谱分辨率可达 1nm。地面光谱仪有着探测距离近、光谱分辨率高的优势，获得的试验数据更准确，建模精度较高。但关于传感器通量对建模的影响仍有待深入研究。值得关注的是，随着物联网、计算机视觉技术的快速发展，地面成像高光谱其“图谱合一”的优势为作物信息在线检测创造了条件[69]，成为近些年的研究热点[8,12]。无人机和卫星遥感更适用于较大空间尺度，如田块或区域的作物信息监测[46,80]。为提高建模精度，通常需要配合同步进行地面高光谱观测试验。在这个过程，所选样区是否具有代表性以及不同卫星源光谱响应函数的区域适用性差异，为建模增加了不确定性。

3.3　光谱数据预处理方法的不确定性

光谱测量仪器在使用过程会受到许多干扰因素的影响，使得原始光谱曲线不仅包含了被测作物的特征光谱，还包含了仪器本身的高频随机噪声、基线漂移等噪声数据。因此，使用前需要对原始光谱数据进行预处理，以降低或消除噪声对模型的影响。大量研究表明[81−83]，原始光谱数据经过平滑和散射校正后，光谱曲线上的这些“毛刺”能够得到有效剔除，光散射引起的光谱变化能够得到抑制，更好地还原作物本身光谱特征。常用的预处理方法有 SG 平滑、导数变换、多元散射校正（MSC）和标准正态变换（SNV）等。但目前尚缺少一种通用的预处理模式。原则上，以模型测试集精度最高的预处理组合为最优方法。但由于预处理方法众多，实现对不同组合的逐一测试相对困难。因此，目前亟需发展一种不需要对高光谱数据预处理的稳健的机器学习建模算法，避免因预处理不充分给建模带来的不确定性。

3.4　敏感波段提取的不确定性

敏感波段提取能够解决处理高维数据时遇到的维数灾难问题[84]，是高光谱建模的一个重要过程。相关性分析法常用来获取逐波段反射率与作物信息的相关系数，从中提取通过显著性检验的波段作为敏感波段。逐步回归法[22,55]是将波段逐个引入回归方程，剔除不显著的波段，从而避免多重共线性问题。赤池信息量准则（AIC）是一种评估模型拟合效果的方法，以 AIC 值最低为标准提取敏感波段，可实现谷物氮吸收量的准确估测[85]。基于 PLS 变量投影重要性（VIP）提取的敏感波段，可实现玉米冠层垂直分布中氮利用效率的有效估测[86]。连续投影算法（SPA）是一种使矢量空间共线性最小化的前向变量选择算法，提取的敏感波段可用于小麦白粉病早期识别[58−59]、马铃薯叶绿素含量[46]和枸杞营养成分含量估测[79]。此外，SHAP 算法[5]、JM 距离[10]、竞争自适应重加权采样法[6]、随机森林的 Gini 指数[63]、β 系数[77]也常用于高光谱敏感波段提取。综合来看，敏感波段提取对减少数据冗余、增强模型鲁棒性至关重要，但由于目前关于光谱敏感波段与作物理化参数之间响应机制的研究较少，它们之间的关系并不明确，这给面向快速检测的轻量级模型构建及低成本专用仪器开发增加了不确定性。

3.5　化学检测方法的不确定性

作物理化参数作为高光谱遥感建模的因变量，其测定结果直接关系到机器学习建模精度。由于相同理化参数的化学测定方法不止一种（如全氮的测定有凯氏定氮法[87]、同位素比值质谱法[77]），使用的测定仪器存在差别（如叶绿素测定使用的分光光度计 Shimadzu UV-1700[88]和 UV-1800[7]对吸光度波长要求不同），以及检测过程不可避免产生的系统误

差。这些因素都会使不同研究者获得相同参数“真值”的可比性和可重复性降低，进而给机器学习建模增加了不确定性。

4　研究展望

高光谱技术是推进精确农业发展和解决粮食安全问题的关键技术[89]。在当前全球粮食安全面临挑战的背景下，充分利用高光谱无损获取作物信息的优势，发展天空地一体化协同观测技术，实现物理模型与数据驱动模型的有效结合，将集成学习、迁移学习等机器学习算法与深度学习融合，从而推动作物信息高光谱遥感技术从“感知”到“认知”的智能化转变是未来的发展趋势。

（1）高光谱遥感信息感知方式的转变。随着高光谱遥感技术在农业领域的广泛应用，观测平台逐渐由传统的地基遥感向近地面无人机、航空飞机以及卫星遥感平台拓展。针对海量遥感数据，充分利用谷歌地球引擎（GEE）、亚马逊网络服务云（AWS）、中科院先导地球大数据挖掘分析系统（EDM）等遥感云计算平台的数据处理优势，充分发挥机载激光雷达（LiDAR）获取作物表型信息的优势、星载合成孔径雷达（SAR）全天候对地观测优势以及将高分辨率光学卫星与高光谱卫星数据进行时空谱融合，实现地基、空基、天基遥感信息优势互补，研发面向地区特色经济作物的多源遥感信息协同反演技术，是未来作物信息高光谱感知方式的发展方向。

（2）高光谱遥感与作物模型同化。将高光谱反演的作物表型和生理参数引入作物模型已成为作物生长监测与模拟研究的有效工具和潜在方法[90]。比如将高光谱反演的冬小麦叶面积指数和氮含量作为同化变量校正 DSSAT-CERES 作物模型，可提高小麦籽粒产量和蛋白质含量的估测精度[90]。基于航空高光谱数据量化叶片叶绿素和叶面积指数，结合 SCOPE 模型的光辐射传输模块，能更好地估测玉米籽粒产量[45]。未来，高光谱遥感与作物模型的结合仍然是作物长势监测、估产的研究热点。而如何实现高光谱观测频次与作物生长过程的同步，是建立面向全生育期作物信息高光谱感知模型的关键。

（3）高光谱遥感与人工智能技术的深度融合。随着人工智能技术的广泛应用和计算机 GPU 显卡性能的大幅提升，利用非线性模型解决回归和分类问题的优势越发明显，进而促进了人工神经网络模型由浅层结构不断向深层结构提升。与传统机器学习算法相比，深度学习技术充分利用了高光谱图像“图谱合一”的优势，提高了作物信息感知的自动化、精细化程度。但尽管如此，在处理实测数据较少的小样本问题方面，经典算法如偏最小二乘法与化学计量学相结合仍广泛应用于作物水分含量估测、营养成分反演及病虫害识别。将集成学习、多任务学习、多输入特征融入深度学习，研发针对作物理化参数、土壤环境参数等有限实测样本数据集的数据增强技术和迁移学习模型，实现面向生产的低成本多光谱仪开发与应用是未来需要重点关注的研究方向。

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