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Sustainability Assessment of Coffee By-Product Valorization Using Explainable Neural Networks in Smallholder Food Systems

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Abstract

Coffee by-product valorization offers resource recovery opportunities, although implementation depends on smallholder capacities. This study developed a multidimensional assessment using a multitask neural network. Literature informed the conceptual framework, while the implementation generated 260 producer profiles and reference targets for 12 technologies. Sampling with replacement produced 3600 records containing 2120 distinct producer–technology pairs, rather than independent empirical observations. Environmental, economic, social, and technological scores were constructed through predefined rules, alongside suitability and generated adoption labels. Evaluation separated producer identifiers across partitions. Suitability predictions yielded MAE = 0.0492 and RMSE = 0.0628, equivalent to 4.92 and 6.28 points on a 0–100 scale. R^2 = 0.5538 indicated that predictions accounted for 55.38% of reference-score variation, rather than a 55.38% probability of correct prediction. Performance was moderate, leaving substantial variation unaccounted for. Adoption discrimination reached AUC = 0.7087. Technological feasibility was most strongly associated with reference suitability, partly reflecting target construction. For phenolic extraction, budget and technical skills jointly shaped predicted compatibility. These results support exploratory comparison within the computational setting; usefulness remains unverified. Future research should validate outcomes against independent producer records, compare simpler models, and incorporate producer priorities into weighting before using predictions to screen valorization pathways or inform investment decisions.

Keywords: coffee byproducts; sustainability assessment; explainable neural networks; waste valorization; smallholder food systems

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1. Introduction

Coffee production forms part of an extensive agri-food system in which environmental pressures, market conditions, and rural livelihoods remain closely intertwined. Its value chain extends from cultivation and primary processing to roasting, distribution, and consumption, with sustainability concerns emerging at almost every stage [1]. These concerns

are particularly significant in regions where coffee farming depends on small-scale production units whose economic stability is affected by price volatility, climate variability, limited infrastructure, and unequal participation in downstream markets. Recent analyses have therefore moved beyond productivity alone to examine the distribution of responsibilities, risks, and opportunities among coffee supply-chain actors [2]. Smallholder systems require particular attention because investment constraints, access to knowledge, and production scale influence their capacity to adopt environmental practices and processing technologies. Sustainability in this context concerns both ecological pressures and the ability of households and producer organizations to sustain their livelihoods and retain part of the value generated through innovation.

The processing of coffee cherries produces pulp, husk, mucilage, parchment, and other organic materials, while silverskin and spent coffee grounds arise during roasting and beverage preparation. Their characteristics vary with species, processing method, geographical setting, and production stage. Inadequate disposal may contribute to organic pollution, greenhouse gas emissions, and local sanitation problems; however, these materials also contain components that can be recovered as dietary fibre, phenolic compounds, pectin, energy carriers, and agricultural inputs [3,4]. Coffee pulp and husk have been explored in food ingredients, fermentation processes, biocomposites, and biological conversion [5]. The available literature therefore establishes that coffee by-products possess considerable recovery potential. What remains less clear is how this potential translates into sustainable and implementable alternatives under the unequal operating conditions of smallholder producers.

Valorization routes range from composting and mushroom cultivation to processes requiring extraction, purification, torrefaction, or advanced material production. Research in rural communities has demonstrated the use of coffee pulp in productive alternatives with local economic and food-system relevance [6], while other studies have examined coffee by-products in fermentation practices adapted to smallholder production [7]. Yet recovering a material does not necessarily produce a sustainable outcome. Waste reduction may be accompanied by greater energy demand, transportation requirements, or dependence on costly equipment. Comparative life-cycle evidence shows that the environmental advantages of reuse can change with processing conditions and the distance between residue-generation and valorization sites [8]. The analytical challenge is consequently to distinguish the technical potential of a pathway from its environmental consequences, economic viability, social implications, and compatibility with the resources available to producers.

These considerations require a multidimensional assessment with clearly differentiated criteria. Environmental performance concerns waste reduction, resource recovery, emissions, and water and energy demand. Economic performance addresses investment requirements, operating costs, revenue potential, profitability, and market access. Social performance encompasses employment opportunities, occupational conditions, skills development, participation, equity, and the distribution of local benefits. Technological performance refers to infrastructure requirements, process complexity, technical knowledge, operational readiness, maintenance, and scalability. Multidimensional assessments of coffee agribusiness indicate that favorable aggregate results can conceal weaknesses in individual dimensions [9]. Evidence from smallholder specialty-coffee systems also suggests that traceability, organizational practices, and value-chain coordination influence environmental, economic, and social outcomes [10]. Research on sustainable coffee pathways further documents context-dependent synergies and trade-offs [11]. These findings support retaining the four dimensions separately, even when an aggregate index is used for comparison.

Conventional sustainability indices and multicriteria procedures provide transparent structures for organizing indicators and expressing decision priorities. Their representation

of nonlinear relationships and interactions, however, depends on the aggregation rules and relationships specified by the analyst. A technology with favorable environmental characteristics may remain unsuitable for a producer lacking the necessary infrastructure or technical skills; economic promise may likewise fail to translate into adoption. Sustainability performance, producer–technology suitability, and documented adoption are therefore related but distinct outcomes. Modelling them independently may overlook information shared across tasks, whereas reducing them to a single score can obscure their differences. A multitask neural network offers a structure for addressing this problem: shared layers learn representations of producer conditions and technology attributes, while specialized outputs retain the distinct meanings of sustainability dimensions, suitability, and adoption. This architecture is relevant to the assessment challenge, although its usefulness must be evaluated rather than inferred from model complexity alone.

Explainability is equally necessary because predictive accuracy does not establish why an alternative receives a favorable assessment. Recent research has applied explainable machine learning to the thermal behaviour of oxidatively torrefied spent coffee grounds [12], environmental impacts in the agri-food sector [13], and the relationship between biomass composition and bioenergy potential [14]. These studies demonstrate the value of examining the information underlying predictions, but their emphasis on particular technical properties or environmental outcomes leaves a different question unresolved: how can several sustainability dimensions be assessed jointly while accounting for producer-specific suitability and adoption constraints? The proposed framework combines shared and task-specific neural representations with interpretation and uncertainty analyses to examine these relationships. Such analyses describe model behaviour and prediction sensitivity; they do not establish causal effects or independently verify the sustainability assumptions embedded in the assessment.

Despite these advances, the reviewed literature remains fragmented across by-product characterization, conversion technologies, sustainability evaluation, and computational prediction [4,11,12]. Limited integration among these areas makes it difficult to compare pathways while preserving both multidimensional performance and differences in smallholder implementation capacity. This study addresses that gap through four objectives: (i) to construct a traceable analytical dataset linking smallholder profiles with coffee by-product valorization alternatives; (ii) to assess environmental, economic, social, and technological performance through explicitly defined indicators and a reference weighting scheme; (iii) to develop and evaluate a multitask neural network that jointly estimates the four sustainability dimensions, technology suitability, and documented adoption probability; and (iv) to examine model behaviour, prediction uncertainty, and sensitivity to producer conditions in order to support context-specific comparison of valorization pathways. The contribution lies in connecting these outcomes within a common assessment framework while retaining their analytical differences, thereby supporting preliminary decision-making where technological promise may exceed local implementation capacity.

2. Theoretical Framework

2.1. Coffee By-Product Valorization and the Circular Bioeconomy

Coffee processing generates several organic materials whose characteristics depend on the production stage and processing method. Pulp, husk, mucilage and parchment mainly originate during primary processing near producing farms, whereas silverskin and spent coffee grounds emerge later during roasting and beverage preparation. These materials contain cellulose, hemicellulose, lignin, proteins, lipids, minerals and bioactive compounds in proportions that vary across origins and processing conditions [3–5]. Their heterogeneous composition permits different forms of utilization, including composting,

mushroom cultivation, animal feed, bioenergy production, extraction of functional ingredients and the manufacture of composite materials. Coffee pulp has already been used as a substrate for producing edible fungi in Colombian rural communities, illustrating that valorisation can relate to local food systems instead of being restricted to industrial biorefineries [6]. Recent reviews have nevertheless drawn attention to safety concerns, such as caffeine, tannins, microbial contamination and other compounds that may restrict food or feed applications when adequate processing controls are absent [15]. A distinction is therefore needed between the theoretical presence of valuable compounds and their safe, feasible recovery under actual production conditions.

Within a circular bioeconomy, valorisation involves more than diverting coffee residues from disposal. It requires the recovery of biological resources through processes capable of creating environmental, economic or social value while avoiding the transfer of impacts to another stage of the system. Biorefinery research has demonstrated that spent coffee grounds can support the production of biodiesel, bioethanol, solid fuels, adsorbents and other materials [16,17]. Yet many of these pathways require centralized facilities, stable feedstock volumes and specialized equipment, conditions that may not be immediately available in smallholder settings. Other alternatives, including the use of coffee residues in construction materials, reveal a different pattern: they may reduce the consumption of conventional raw materials, but their viability depends on collection, transportation, processing and local demand [18]. Consequently, a circular strategy should not be regarded as sustainable simply because it reuses a residue. Its performance must be examined through the quantity of by-product recovered, the resources required for transformation, the value created and the compatibility of the technology with the context in which it would be implemented [4,15–18].

Coffee by-products offer several potential routes toward food ingredients and product formulations, although their suitability depends on the material and processing conditions. Figure 1 illustrates twelve examples connecting coffee pulp, husk, mucilage, silverskin, spent coffee grounds, and derived extracts with transformation practices and possible applications. Drying and milling can support the preparation of flour-like ingredients for bread, crackers, and biscuits, whereas extraction and recovery processes can yield pectin, dietary fibre, and phenolic-rich ingredients. Other examples include cascara-based infusions, controlled fermentation for potential beverages, and substrate preparation for edible mushroom cultivation. Ingredient incorporation, stabilization, and encapsulation extend the illustration to fibre-enriched formulations, granola, and potential beverage ingredients. Their implementation requires appropriate processing, safety assessment, and consideration of technical capacity and market conditions, particularly within smallholder systems.

Coffee by-products have been investigated in food development through direct ingredient incorporation, extraction, fermentation, and biological conversion, with outcomes that depend on the formulation and processing conditions. In bakery products, isolated coffee cascara dietary fibre has been incorporated at 3% and 4.5% into gluten-free bread formulations, with evaluation of nutritional, physicochemical, and sensory properties [19]. Coffee silverskin has also been used to replace wheat flour at 2%, 4%, and 6% in vegan biscuits, with favorable consumer acceptance reported for the formulation containing 4% decaffeinated silverskin [20]. Spent coffee grounds have been incorporated into muffins to examine functional, microstructural, and sensory changes [21], and ingredients obtained from defatted grounds have been evaluated in cookies [22]. Applications extend beyond baking: coffee silverskin has been investigated in yogurt at three incorporation levels, assessing functional properties and bioaccessibility during storage [23], while yogurt formulations containing coffee cascara and silverskin extracts have been evaluated for consumer acceptance and other product characteristics [24].



Figure 1. Illustrative coffee by-product valorization pathways linking raw materials, transformation practices, and potential food applications.

Coffee silverskin flour has also been explored as a partial replacement for milk cream in ice cream; its incorporation altered nutritional and physicochemical properties, although increased bitterness and grittiness highlighted sensory trade-offs [25]. Coffee side-stream incorporation into granola has been examined through technological, qualitative, and environmental assessment [26], whereas spent-coffee-ground extracts have been used in

fresh pasta to investigate quality attributes, bioactive content, thermal properties, and in vitro phenolic bioaccessibility [27]. Fermentation provides another route: coffee cascara kombuchas have been developed and assessed through microbial and volatile profiles alongside consumer acceptance [28]. In Colombia, coffee pulp has been used as a substrate for producing the edible mushroom Pleurotus pulmonarius, linking residue recovery with food production in rural communities [29].

2.2. Multidimensional Sustainability in Smallholder Coffee Systems

Sustainability in coffee production has generally been discussed through environmental protection, economic continuity and social well-being, although recent approaches also recognize governance, technological capacity and value-chain coordination [1,2]. For smallholder producers, these dimensions are closely related. Limited income may restrict investment in water treatment or residue-processing equipment; weak organizational arrangements can reduce access to markets; and environmental shocks may affect both household livelihoods and the volume of material available for valorisation. Evidence from certified and non-certified coffee farms in Uganda indicates that sustainability performance varies across dimensions and cannot be inferred solely from participation in certification schemes [30]. Comparative assessments of coffee systems in Brazil and Ethiopia have reached a similar conclusion, showing that production models may perform favourably in some areas while retaining weaknesses in others [31]. A multidimensional perspective is thus needed to prevent one favourable result, such as waste reduction or additional revenue, from concealing adverse outcomes elsewhere in the system [7,9].

The smallholder context also introduces questions of technological accessibility, livelihood resilience and the distribution of benefits. Diversification can contribute to more sustainable coffee farming, although its results depend on the trajectory followed, available resources and connections with other productive activities [32]. Adaptation strategies adopted by smallholder households similarly reflect a combination of environmental pressures, economic needs and local capacities rather than a single decision criterion [33]. In the case of by-product valorisation, an alternative could be environmentally promising but remain inaccessible because of its capital requirements, technical complexity or dependence on external inputs. Traceability and coordination mechanisms may strengthen triple-bottom-line performance, yet their effects are mediated by organizational conditions and producers' ability to participate in the value chain [10]. Recent studies of sustainable coffee pathways have therefore emphasized trade-offs and context-dependent outcomes [11]. Under this perspective, sustainability refers to the capacity of a valorization pathway to remain environmentally sound, economically viable, socially beneficial and technologically manageable within the operating conditions of small-scale coffee systems [7,9–11,19–33].

Three constructs are distinguished within this framework. Sustainability performance describes the environmental, economic, social, and technological characteristics of a valorization pathway under specified operating conditions. Suitability expresses the compatibility between that pathway's requirements and the resources available to a particular smallholder profile. Technological performance therefore concerns process attributes, such as readiness, complexity, and maintenance requirements, whereas suitability concerns whether a producer can meet those requirements. Adoption refers to documented implementation, rather than technical potential, producer intention, or a sustainability score. Its predicted probability represents the likelihood of the adoption outcome encoded in the secondary dataset; it should not be interpreted as a directly measured willingness to adopt or as a forecast of future behavior without longitudinal validation. A pathway may consequently perform favorably on sustainability indicators while remaining unsuitable for a resource-constrained

producer, and a suitable pathway may still lack documented adoption. Moreover, absence of implementation information does not, by itself, establish non-adoption.

2.3. Sustainability Assessment, Indicators and Trade-Offs

Sustainability assessment translates broad principles into variables that can be observed and compared. In coffee by-product valorisation, the environmental dimension may include waste recovery, energy demand, water consumption, emissions, toxicity and the substitution of conventional resources. Economic performance can be represented through investment requirements, operating costs, potential revenue, profitability, payback conditions and market accessibility. Social indicators may cover employment, occupational conditions, inclusion, local participation and the distribution of benefits, while technological indicators can address process complexity, equipment availability, maintenance, scalability and required knowledge. Multidimensional coffee assessments demonstrate the usefulness of examining these categories separately before constructing an overall result [9]. This separation is important because environmental life-cycle studies have found considerable differences among alternative routes for spent coffee grounds, particularly when energy inputs, avoided products, transportation distances and system boundaries are modified [8,34]. Techno-economic studies also indicate that a pathway with an attractive conversion yield may still encounter economic restrictions associated with scale, process configuration and input costs [35].

Indicators do not operate independently. A change in one variable can improve one dimension while weakening another, and the direction of that effect may differ between locations. For instance, centralizing processing could improve technical efficiency but increase transport-related emissions and costs; a low-technology alternative may be easier to adopt but generate limited economic value. Dynamic modelling of circular coffee agroforestry has illustrated the importance of temporal relationships and feedback among productive, environmental and economic factors [36]. Life-cycle assessment of dietary-fibre extraction from spent coffee grounds has likewise shown that process optimization must consider environmental burdens alongside the value of the recovered product [37]. These findings support an assessment structure capable of preserving trade-offs instead of assuming that all indicators contribute equally or linearly to sustainability. Sensitivity to location [8], differences among valorisation routes [18,23], techno-economic restrictions [32] and changing system relationships [25,34] suggest that a fixed additive score may provide an incomplete account. A more flexible approach should identify interactions among indicators and determine whether their effects vary across technologies or production contexts [5,9,11].

The conceptual relationships underlying the assessment operate at the producer–technology level. By-product characteristics determine feedstock compatibility, while producer resources and technology requirements jointly condition implementation feasibility. Environmental, economic, social, and technological indicators describe different aspects of the resulting combination. Several relationships are expected to be conditional: increasing investment capacity may improve suitability only when technical skills and infrastructure are also sufficient; greater by-product availability may support processing scale without ensuring market access; and environmental benefits may coexist with unfavorable operating costs. Organizational participation and market connections may further condition whether suitable alternatives are implemented. These expectations motivate an analysis of interactions rather than an assumption that each predictor has a constant, independent contribution. The computational model is intended to represent associations consistent with these relationships, while sensitivity analysis examines its responses to changes in producer conditions. Neither predictive associations nor sensitivity responses establish causal mechanisms.

2.4. Artificial Neural Networks for Sustainability Assessment

Artificial neural networks are computational models composed of interconnected processing units that learn relationships between input variables and expected outputs. In a sustainability assessment, their inputs can consist of environmental, economic, social and technological indicators, whereas the output may represent a continuous sustainability score or a defined performance category. Their main analytical value lies in the ability to approximate nonlinear relationships and interactions that are difficult to specify in advance. Applications related to coffee and other agri-food systems have already used machine learning to predict material properties, biological risks and environmental outcomes. Experimental data and machine-learning methods, for example, have been combined to predict the mechanical properties of asphalt containing spent-coffee-ground ash [38]. Bayesian inference and supervised learning have also been used to model coffee-rust incidence among Kenyan smallholders [39], while data-driven approaches have estimated greenhouse gas emissions within livestock supply chains [40]. Although these studies address different outcomes, they demonstrate that heterogeneous technical, environmental and productive variables can be incorporated into predictive models relevant to agricultural decision-making [4,12,14,38–40].

The choice of a neural network in this study is motivated by the structure of the assessment problem rather than by nonlinearity alone. Producer conditions and technology attributes provide overlapping information for predicting four sustainability dimensions, suitability, and documented adoption. Estimating these outcomes through unrelated models would require separate representations of information that may be relevant across tasks. A multitask architecture instead permits shared feature learning while retaining distinct outputs and loss functions for continuous performance scores and the binary adoption outcome. Its suitability and adoption branches can also incorporate intermediate predictions, representing the proposed connection between sustainability performance, producer–technology compatibility, and implementation. This connection is a modelling assumption whose usefulness requires evaluation, not evidence that sustainability necessarily causes adoption.

Simpler models remain credible alternatives. Linear or regularized regression offers a transparent reference for continuous outcomes, logistic regression provides a baseline for adoption, and tree-based methods can represent nonlinear associations without the same shared neural architecture. The proposed network is therefore appropriate only insofar as its joint representation supports useful predictive performance, interpretable responses, and acceptable generalization relative to simpler approaches. Potential disadvantages include overfitting, negative transfer between tasks, and propagation of errors from intermediate predictions. Where sustainability targets are constructed from indicators and predefined weights, accurate prediction demonstrates approximation of those targets rather than independent validation of their underlying assumptions.

Model design must consequently consider the effective number of independent producer profiles, data quality, missingness, scaling, regularization, and separation between training and evaluation data. Interpretable domain adaptation in waste-based fermentation illustrates the importance of generalization across operating contexts [41], while machine-learning applications to spent-coffee-ground co-pyrolysis show how processing conditions can interact in determining technical outcomes [42]. Explainable prediction of coffee-residue combustion [12] and hybrid estimation of biomass energy potential [14] provide further methodological precedents. These studies support investigating the proposed architecture, but do not establish its superiority for the present task. Comparisons with simpler baselines and evaluation on previously unseen producer profiles are needed to assess whether the additional complexity is justified [12,14,27–42].

2.5. Explainable Artificial Intelligence and Sustainability-Oriented Decision Support

The use of neural networks creates an interpretive difficulty because model parameters do not immediately reveal how each indicator contributes to a prediction. Explainable artificial intelligence addresses this problem through methods that estimate the direction and magnitude of variable contributions at global and individual levels. Global explanations indicate which features are most influential across the complete dataset, whereas local explanations clarify why a specific case receives a particular result. In the coffee sector, explainable machine learning has been applied to climate-driven price forecasting [43], image-based coffee classification [44], quality detection in green beans [45] and the prediction of coffee traits from analytical measurements [46]. Other studies have extended interpretability to environmental impacts in the agri-food industry [13], biomass energy properties [14], waste-fermentation monitoring [41] and thermal behaviour of spent coffee grounds [12]. Together, these applications show that explainability can assist in examining complex predictions, although their substantive objectives differ from multidimensional sustainability assessment.

For sustainability-oriented decision support, explanations should reveal not only which variables improve predictive performance but also how they shape the evaluation of valorisation pathways. An environmental indicator may increase the predicted sustainability score while investment requirements or technological complexity reduce it. Methods based on feature attribution can make those competing contributions visible, allowing global patterns to be distinguished from conditions affecting specific technologies or smallholder systems [12–14]. Nevertheless, explainability does not establish causality. A variable identified as influential describes the behaviour learned by the model and may also reflect correlations, measurement choices or unequal representation within the underlying data. Explanations must therefore be interpreted alongside life-cycle evidence [8,23], multidimensional sustainability findings [9,11] and the practical constraints of smallholder production [19,31,32]. When this distinction is maintained, explainable neural networks can function as a transparent analytical instrument: they can compare valorization alternatives, identify influential sustainability indicators and expose trade-offs without presenting the model as an autonomous replacement for contextual judgement [38,40,42–46].

Within the proposed conceptual model, smallholder conditions and coffee by-product characteristics are linked to the requirements of valorization technologies. Production scale, investment capacity, infrastructure, technical skills, and market access describe the producer context, while feedstock compatibility, resource demand, process complexity, and technological readiness characterize the alternatives. Their interaction informs environmental, economic, social, and technological performance, which is represented through dimension-specific indicators and a weighted sustainability index. Suitability expresses whether a technology's requirements match the resources of a particular producer, whereas adoption concerns documented implementation and remains a distinct outcome. These relationships need not be linear: additional financial resources may improve suitability only when technical capacity is sufficient, and favorable sustainability performance may coexist with limited adoption. The multitask network represents these related outcomes through shared features and specialized prediction branches. Feature attribution, sensitivity analysis, and uncertainty estimates support interpretation of the resulting predictions and comparison of alternatives.

2.6. Conceptual Model Linking Smallholder Conditions, Sustainability, Suitability, and Adoption

The proposed conceptual model connects smallholder conditions and by-product characteristics with the requirements of valorization technologies. Producer conditions include production scale, investment capacity, resource access, technical skills, organizational partic-

ipation, and market connections (Figure 2). By-product characteristics identify the available material and its compatibility with a processing route. Technology attributes describe feedstock requirements, resource demand, readiness, and operational complexity. At their intersection, environmental, economic, social, and technological indicators characterize the producer–technology combination rather than the technology in isolation.

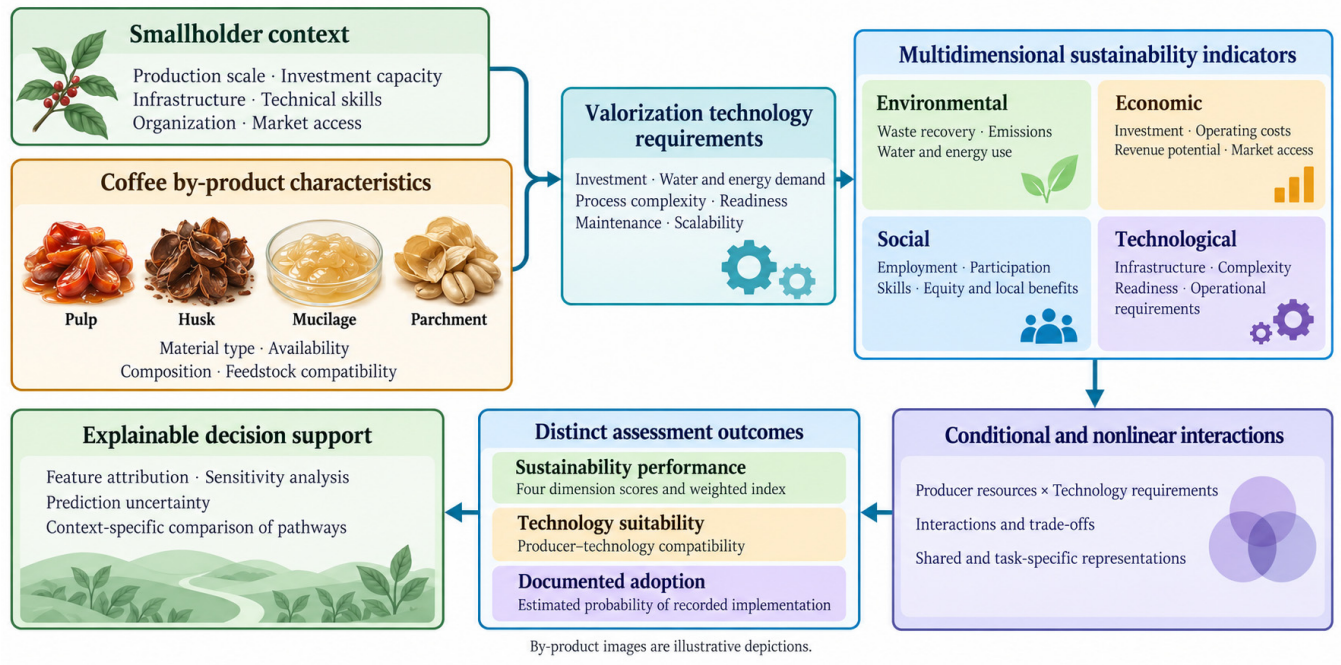


Figure 2. Conceptual framework linking smallholder context, coffee by-product characteristics, valorization technology requirements, multidimensional sustainability indicators, nonlinear interactions, sustainability performance, technology suitability, and documented adoption with explainable decision support.

The four dimensions provide a differentiated account of sustainability performance, while their weighted aggregation yields a reference sustainability index. Suitability represents compatibility with the producer's operating conditions, and documented adoption constitutes a separate implementation outcome. The multitask network is intended to learn shared and outcome-specific associations among these constructs, including conditional relationships that additive aggregation alone may not capture. Explanations, sensitivity responses, and uncertainty estimates then inform the interpretation of predictions and the comparison of alternatives. The conceptual pathway therefore links context, material characteristics, technology requirements, multidimensional performance, and implementation outcomes to decision support. Its connections express analytical relationships to be represented and examined; they do not constitute a validated causal sequence.

3. Materials and Methods

3.1. Study Design and Analytical Framework

The study followed a quantitative, non-experimental and data-driven design intended to assess the sustainability of coffee by-product valorization pathways in smallholder food systems. The analytical unit was the documented pairing between a smallholder production profile i and a valorization technology j. The consolidated database comprised 3600 real observations obtained from web-accessible documents and databases, representing 260 small-scale producer profiles and 12 valorization technologies. Because several technologies could be associated with the same profile, observations were not treated as

entirely independent; the producer profile was retained as the grouping unit throughout model development and evaluation.

The technological catalogue covered composting, anaerobic digestion, biochar production, mushroom cultivation, coffee flour, phenolic extraction, pectin extraction, dietary-fibre production, fermented beverages, animal feed, biodegradable packaging and wastewater biotreatment. The selected routes involved coffee pulp, husk, mucilage, parchment, silver skin, spent coffee grounds and processing wastewater. Environmental and economic variables were informed by life cycle and techno-economic assessments of spent coffee-ground conversion [47], together with cradle-to-grave evaluations of coffee processing and waste valorization [48]. Evidence concerning coffee-silver skin management supported the definition of system boundaries [49], while commercialization studies indicated that technical recovery potential should be distinguished from economic feasibility [50].

The methodological sequence comprised web-based evidence acquisition, source screening, data harmonization, multidimensional sustainability measurement, grouped predictive modelling, independent evaluation, explainability and technology ranking (Figure 3). It can be summarized as

$$\mathcal{D}_{raw} \overset{screening}{\rightarrow} \mathcal{D}_{eligible} \overset{harmonization}{\rightarrow} \mathbf{X} \overset{grouped\ learning}{\rightarrow} f_{\boldsymbol{\theta}}(\mathbf{X}) \overset{SHAP}{\rightarrow} \left\{\hat{\mathbf{s}}_{ij}, \hat{R}_{ij}, \hat{A}_{ij}, \boldsymbol{\Phi}_{ij}\right\}, \quad (1)$$

where $\mathcal{D}_{raw}$ denotes the initially retrieved evidence, $\mathcal{D}_{eligible}$ contains the accepted records, $\mathbf{X}$ is the processed feature matrix, $\hat{\mathbf{s}}_{ij}$ contains the predicted sustainability dimensions, $\hat{R}_{ij}$ is producer-technology suitability, $\hat{A}_{ij}$ is the probability of documented adoption and $\boldsymbol{\Phi}_{ij}$ contains the feature contributions.

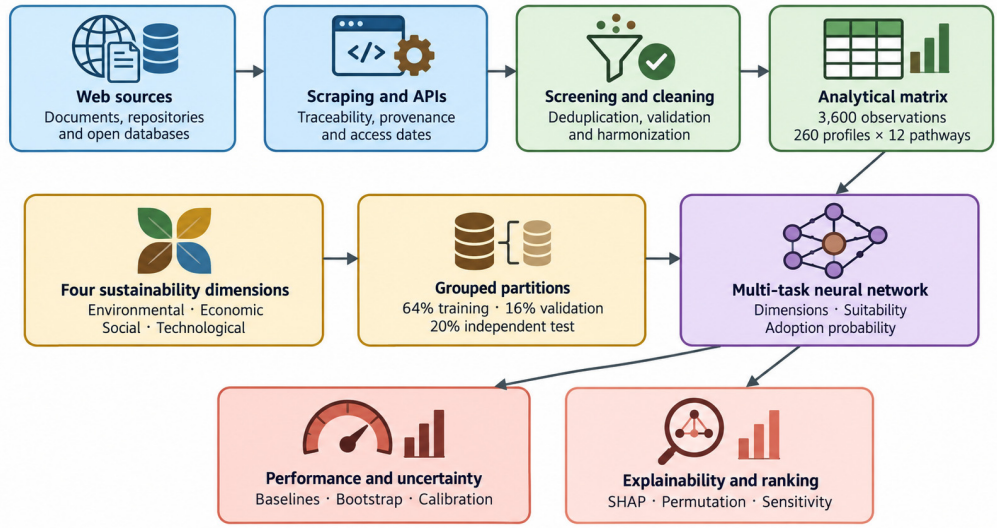


Figure 3. Methodological design for the web-based sustainability assessment and explainable neural-network model.

A methodological Jupyter notebook is provided in the Supplementary Materials to illustrate data preprocessing, multitask neural-network training, performance evaluation, sensitivity analysis, and uncertainty estimation using synthetic data. The notebook documents the computational workflow and supports examination of the modelling procedures and assumptions.

3.2. Web-Based Data Acquisition and Dataset Construction

Data were compiled from publicly accessible scientific publications, institutional repositories, government databases, international agricultural databases, technical reports, and open statistical resources. The selection process focused on evidence describing smallholder

production conditions, coffee by-product availability, and the requirements or performance of valorization technologies. Search terms combined coffee, smallholder production, farm size, production volume, by-product generation, resource access, valorization, investment, operating requirements, environmental impacts, market conditions, and technological readiness. Records were eligible when they provided an identifiable source, geographical context, production-profile information, and coffee-related data relevant to the analytical variables. Authentication-restricted pages, unverifiable commercial material, duplicate observations, and records lacking essential analytical fields were excluded. Structured information was retrieved from downloadable files and application programming interfaces, whereas HTML tables and text-based records were processed through web-scraping procedures.

Data integration distinguished producer-profile characteristics, technology attributes, and producer–technology observations. These components were assembled into a common analytical matrix while preserving the provenance of the underlying evidence. Each observation retained a source identifier, URL or persistent identifier, access date, publication year, geographical coverage, original measurement unit, transformed unit, and evidence-quality score. Incompatible units were converted into a common measurement system without overwriting the original values. Documents referring to the same production profile and technology were linked through a composite key, and overlapping information was reconciled according to source date, methodological transparency, and completeness. Duplicate candidates were identified using location, production-profile identifier, technology, and reference year, and matching keys were reviewed before consolidation.

Data reliability was addressed through source traceability, exclusion of unverifiable records, preservation of original values, unit harmonization, and review of overlapping evidence. These procedures supported the consistency and auditability of the integrated dataset, although they did not constitute independent field verification of every reported value. The analytical matrix therefore represents a secondary-data assessment whose interpretation remains subject to differences in the methods, geographical coverage, and reporting periods of the original sources. Technical fields were refined using evidence on industrial recycling configurations [51], multi-product coffee biorefineries [52], enzyme production from coffee husk [53], and energy recovery through biogas and biomethane [54].

The record balance was defined as

$$N_{final} = N_{raw} - N_{duplicate} - N_{ineligible} - N_{unverifiable} - N_{incomplete} = 3600. \quad (2)$$

Duplicate candidates were detected through

$$K_r = \text{hash}\,[\text{norm}(c_r), \text{norm}(g_r), \text{norm}(t_r), y_r], \quad (3)$$

where c_r represents country or location, g_r the production-profile identifier, t_r the technology and y_r the reference year. Matching keys were reviewed before consolidation. The resulting matrix contained 3600 observations, 260 distinct producer profiles and 12 technologies. The average number of technology observations per profile was

$$\bar{n} = \frac{3600}{260} = 13.85, \quad (4)$$

The analytical structure distinguishes producer profiles from producer–technology records. A profile contains production and resource characteristics associated with a producer configuration, whereas a record pairs that profile with one valorization technology. The dataset contains 3600 records associated with 260 profile identifiers and 12 technologies (Table 1). In the supplied computational implementation, pairs were sampled with replacement, yielding 2120 distinct profile–technology combinations and 1480 additional occurrences of already represented combinations. The file does not contain measurement dates or reporting periods that would identify these occurrences as longitudinal observations.

Table 1. Composition of the analytical dataset.

Component	Final Quantity	Analytical Role
Producer profiles	260	Independent grouping unit
Valorization technologies	12	Alternatives evaluated
Producer-technology observations	3600	Rows in the modelling matrix
Conceptual predictors	34	Inputs before categorical encoding
Sustainability outputs	4	Environmental, economic, social and technological
Additional outputs	2	Suitability and documented adoption

The Colombian geographical distribution supplied by the authors comprises 183 profiles from the Andean region, 26 from the Caribbean region, 32 from the Pacific region, 12 from Orinoquía, and seven from the Amazon region. This distribution is reported separately from the regional labels generated in the supplied code. Table 1 identifies the provenance of the geographical counts and the numerical summaries. Producer attributes are summarized once per distinct profile, while technology representation is summarized through record counts and the number of profiles represented. Annual coffee production is not included in the supplied dataset and is therefore reported as unavailable rather than estimated.

Table 2 complements the dataset composition by describing geographical coverage, farm size, by-product types, resource availability, technology representation, and records per profile. It distinguishes the regional counts supplied by the authors from the numerical summaries reconstructed from the computational implementation. Annual coffee production is reported as unavailable in the supplied dataset.

Table 2. Author-supplied geographical distribution and characteristics reconstructed from the computational dataset.

Characteristic	Description and Results
Geographical distribution—author supplied	Andean: 183 profiles (70.38%); Caribbean: 26 (10.00%); Pacific: 32 (12.31%); Orinoquía: 12 (4.62%); Amazon: 7 (2.69%). Total: 260.
Farm size—reconstructed from code	Median: 1.86 ha; Q1–Q3: 1.10–2.77 ha; minimum–maximum: 0.30–12.00 ha.
Annual coffee production	Not available in the supplied dataset; not used as a predictor.
Principal by-product—reconstructed from code	Pulp: 85 profiles (32.69%); mucilage: 58 (22.31%); husk: 32 (12.31%); parchment: 32 (12.31%); spent coffee grounds: 12 (4.62%); wastewater: 41 (15.77%).
Annual by-product availability—reconstructed from code	Median: 1.28 tonnes/year; Q1–Q3: 0.79–2.24; minimum–maximum: 0.15–7.95.
Investment capacity—reconstructed from code	Median: USD 3126.57; Q1–Q3: USD 2054.65–4837.85; minimum–maximum: USD 611.80–16,107.03.
Resource availability—reconstructed from code	Energy access, water access, technical skills, market access, and labour availability: median 3; Q1–Q3 2–4; range 1–5 for each variable.
Association membership—reconstructed from code	Members: 127 profiles (48.85%); non-members: 133 (51.15%).

Table 2. *Cont.*

Characteristic	Description and Results
Technology representation—records/ distinct profiles	Composting: 265/165; anaerobic digestion: 316/177; biochar production: 277/174; mushroom cultivation: 293/179; coffee flour: 279/177; phenolic extraction: 295/175; pectin extraction: 307/171; dietary fiber ingredient: 315/177; fermented beverage: 323/183; animal feed: 297/184; biodegradable packaging: 318/185; wastewater bio-treatment: 315/173.
Records per profile—reconstructed from code	Mean: 13.85; median: 14; Q1–Q3: 12–16.25; minimum–maximum: 3–23.

3.3. Variables and Multidimensional Sustainability Measurement

The 34 conceptual predictors described producer conditions, technology requirements and their compatibility. Producer-profile fields included geographical region, farm size, annual coffee production, main by-product, by-product availability, investment capacity, energy and water access, technical capacity, market access, labour availability, organizational participation, income diversification and innovation readiness. Technology fields covered technology family, required feedstock, investment level, energy and water demand, skill requirements, readiness, circularity potential, evidence quality and food or nutrition relevance. Sustainability and livelihood research supported the inclusion of production capacity and resource-access indicators [55]. Documented implementation was coded as adoption rather than interpreted as a response obtained directly from producers; organizational and environmental adoption determinants were considered in accordance with interpretable technology-adoption research [56]. Agricultural-waste optimization studies informed the integration of material and operating characteristics [57], while farm-level coffee-pulp characterization supported variables related to biomass and energy suitability [58].

In the supplied implementation, the four sustainability targets were calculated from predefined combinations of technology attributes and producer-resource compatibility terms, with Gaussian perturbations and clipping to $[0, 1]$. The perturbation standard deviations were 0.05 for environmental and technological scores and 0.06 for economic and social scores. The sustainability index was defined as $S = 0.35E + 0.25Ec + 0.20So + 0.20T$. Suitability was calculated as $R = \mathrm{clip}(0.70S + 0.12SK + 0.08B + 0.06M + 0.04MA)$, where SK denotes skill compatibility, B budget compatibility, M feedstock matching, and MA market compatibility. Adoption probability was obtained as $p = 1/[1 + \exp(-(R - 0.61)/0.08)]$, and binary adoption labels were sampled from a Bernoulli distribution with probability p. These labels are therefore generated outcomes in the supplied implementation, not independently documented producer decisions. Predictive performance must be interpreted in relation to this target-construction procedure.

Indicators were assigned to environmental, economic, social and technological dimensions. Benefit indicators were normalized as

$$z_{ijk}^{+} = \frac{x_{ijk} - \min(x_k)}{\max(x_k) - \min(x_k)}, \tag{5}$$

whereas cost indicators were transformed as

$$z_{ijk}^{-} = \frac{\max(x_k) - x_{ijk}}{\max(x_k) - \min(x_k)}. \tag{6}$$

For dimension d, performance was calculated through

$$D_{ij}^{(d)} = 100 \sum_{k \in \mathcal{K}_d} \omega_{kd} z_{ijk}, \tag{7}$$

$$\sum_{k \in \mathcal{K}_d} \omega_{kd} = 1. \tag{8}$$

The multidimensional index followed the reference configuration implemented in the analytical notebook:

$$S_{ij} = 0.35E_{ij} + 0.25Ec_{ij} + 0.20So_{ij} + 0.20T_{ij}. \tag{9}$$

The weighting scheme was specified as a reference scenario reflecting the analytical priorities of the study. The environmental dimension received the largest weight (0.35) because the assessment focuses on coffee by-product valorization as a means of addressing residual-material management and associated environmental pressures. Economic performance received a weight of 0.25 to recognize that implementation in smallholder systems also depends on investment requirements, operating costs, and opportunities for value creation. Social and technological performance each received a weight of 0.20, retaining their contribution through indicators of employment, inclusion, collective benefit, technical capacity, and operational feasibility. The four sustainability dimensions, their representative indicators, and the direction of their contribution to the assessment are summarized in Table 3.

Table 3. Sustainability dimensions and representative indicators.

Dimension	Representative Indicators	Direction
Environmental	Waste diversion, water and energy demand, avoided emissions, nutrient recovery	Positive/negative
Economic	Investment, operating cost, revenue, payback, market access	Positive/negative
Social	Employment, safety, inclusion, collective benefit, local value retention	Positive
Technological	Readiness, compatibility, skills, maintenance and scalability	Positive/negative

These coefficients express the relative emphasis adopted for the aggregate index; they should not be interpreted as empirically estimated contributions or universally applicable priorities. The lower weights assigned to social and technological performance do not imply that these dimensions are dispensable. Their scores remain separate assessment outputs, while suitability and adoption are also evaluated through dedicated model branches. Nevertheless, weighted aggregation permits compensation between dimensions, meaning that a favorable overall index may coexist with weaknesses in a particular domain.

To examine dependence on these choices, the reference vector (0.35, 0.25, 0.20, 0.20) was assessed against an equal-weight scenario (0.25, 0.25, 0.25, 0.25) and dimension-priority scenarios. This sensitivity analysis was intended to identify whether the comparison of valorization alternatives changed when different sustainability priorities were adopted.

The weighting vector was assessed against a balanced scenario (0.25,0.25,0.25,0.25) and dimension-priority scenarios. Compatibility between available resource a_{iq} and technological requirement r_{jq}, both measured on a 1–5 scale, was defined as

$$C_{ij}^{(q)} = 1 - \frac{\left|a_{iq} - r_{jq}\right|}{4}, \tag{10}$$

$$C_{ij}^{(q)} \in [0, 1]. \tag{11}$$

By-product matching was represented by

$$C_{ij}^{(b)} = \begin{cases} 1, & b_i = b_j, \\ 0, & b_i \neq b_j. \end{cases} \tag{12}$$

3.4. Data Preprocessing and Neural-Network Architecture

All computational analyses were performed using Python, with TensorFlow and Keras for neural-network implementation, scikit-learn for preprocessing and baseline models, SHAP for model explainability, and NumPy, pandas, SciPy, and statsmodels for numerical computation and statistical analysis. The latest versions available at the time of the analyses were used. A random seed of 2026 was used.

Missingness was quantified for each predictor using

$$M_k = \frac{1}{N}\sum_{n=1}^{N} \mathbb{I}(x_{nk} \text{ is missing}) \times 100. \quad (13)$$

Outcome variables were not imputed. Numerical predictors were imputed with training-set medians when required, while categorical missingness was represented through an explicit unknown category. All preprocessing parameters were fitted exclusively on the training data. Continuous variables were standardized as

$$x^*_{nk} = \frac{x_{nk} - \mu_{k,train}}{\sigma_{k,train}}, \quad (14)$$

and categorical variables were one-hot encoded. The input vector for profile i and technology j was

$$\mathbf{x}_{ij} = [\mathbf{p}_i, \mathbf{t}_j, \mathbf{c}_{ij}], \quad (15)$$

where $\mathbf{p}_i$ contains producer-profile variables, $\mathbf{t}_j$ technology attributes and $\mathbf{c}_{ij}$ compatibility terms.

A multi-task neural network was selected because the assessment involves related but distinct outcomes: environmental, economic, social, and technological performance, technology suitability, and documented adoption. These outcomes draw on overlapping information about producer resources and technology requirements, but they should not be treated as interchangeable. The shared layers learn representations that can inform several outcomes, while task-specific branches preserve their different analytical meanings. This structure also avoids fitting an entirely separate model for each outcome and allows potentially useful information to be shared across tasks. However, such sharing does not necessarily improve every prediction, particularly when the relationships between tasks are weak or conflicting.

Traditional weighted indices and multicriteria methods remain useful because their aggregation rules are explicit and relatively easy to communicate. Their ability to represent nonlinear relationships and context-dependent interactions, however, depends on how those relationships are specified. In coffee by-product valorization, the contribution of a technological attribute may vary with farm scale, investment capacity, infrastructure, and technical skills. The neural network provides a flexible means of learning these associations rather than requiring all interactions to be defined beforehand. Its role therefore complements the indicator framework and weighting rules.

The methodological advantage sought was the joint estimation of several outcomes while retaining sensitivity to differences among producer profiles. Explainability and uncertainty analyses were incorporated to support interpretation of this more complex model. Nevertheless, neural predictions remain dependent on data quality and target construction; learning indicator-derived scores does not independently validate their sustainability assumptions. Comparisons with simpler predictive baselines were therefore included to assess whether the additional model complexity was justified, rather than if a neural approach would necessarily outperform traditional assessment methods.

The multi-task network received 54 input features after preprocessing and categorical encoding, with shared and task-specific layers arranged as illustrated in Figure 4. The shared

representation comprised a dense layer with 128 neurons and Swish activation, followed by batch normalization and dropout at a rate of 0.20. A second dense layer with 64 neurons and Swish activation was followed by a 24-component sustainability embedding, also using Swish. This embedding supplied a sigmoid output layer that jointly estimated the four sustainability dimensions.

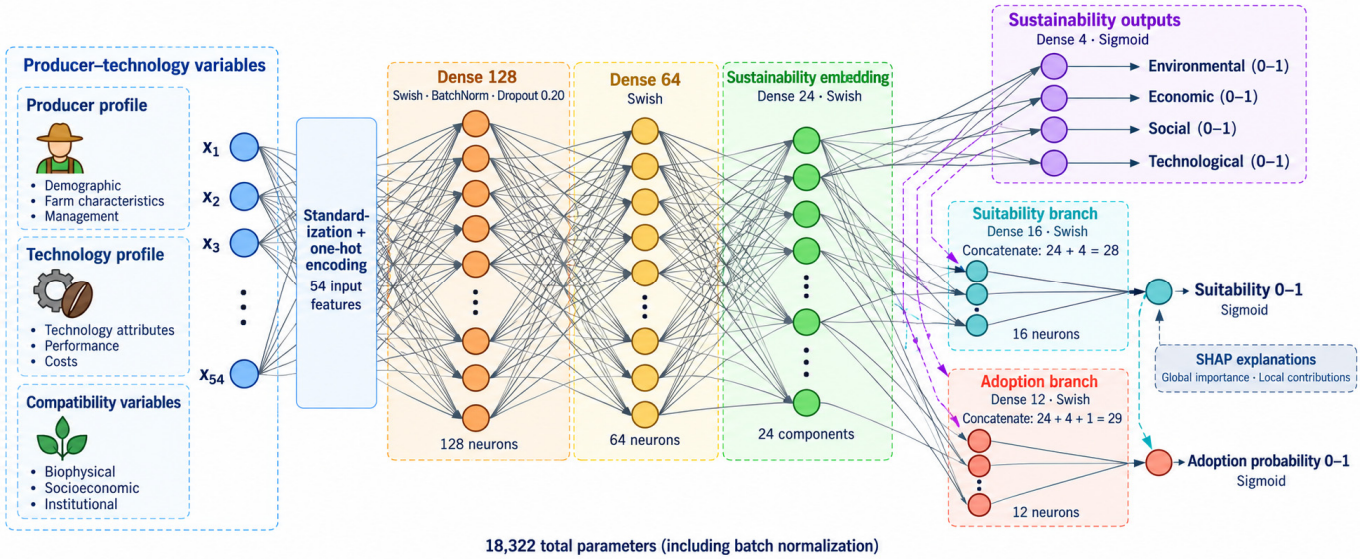


Figure 4. Shared and task-specific layers of the explainable multi-task neural network.

The suitability branch concatenated the 24 embedding components with the four predicted sustainability scores, producing a 28-component input. A 16-neuron hidden layer with Swish activation then supplied a single sigmoid suitability output. The adoption branch concatenated the embedding, the four sustainability predictions, and the predicted suitability score, producing a 29-component input. This branch contained a 12-neuron hidden layer with Swish activation and a single sigmoid adoption output. The resulting architecture contained 18,322 parameters, including those associated with batch normalization.

$$\mathbf{h}^{(l)} = \mathrm{Swish}(\mathbf{W}^{(l)}\mathbf{h}^{(l-1)} + \mathbf{b}^{(l)}) \tag{16}$$

$$\mathrm{Swish}(u) = u\,\sigma(u) = \frac{u}{1+\exp(-u)}, \tag{17}$$

and bounded outputs used

$$\sigma(u) = \frac{1}{1+\exp(-u)}. \tag{18}$$

The network produced

$$\hat{\mathbf{s}}_{ij} = \left(\hat{E}_{ij}, \hat{Ec}_{ij}, \hat{So}_{ij}, \hat{T}_{ij}\right), \tag{19}$$

$$\hat{R}_{ij} \in [0,1], \tag{20}$$

$$\hat{A}_{ij} = P\left(A_{ij} = 1 \mid \mathbf{x}_{ij}\right). \tag{21}$$

The joint loss was

$$\mathcal{L}(\boldsymbol{\theta}) = \mathcal{L}_D + \mathcal{L}_R + 0.50\mathcal{L}_A + 10^{-4} \parallel \boldsymbol{\theta} \parallel_2^2 . \tag{22}$$

Huber loss with $\delta = 0.10$ was applied to the dimension and suitability outputs:

$$L_\delta(e) = \begin{cases} 1/2e^2, & |e| \le \delta, \\ \delta(|e| - 1/2\delta), & |e| > \delta, \end{cases} \qquad e = y - \hat{y}, \tag{23}$$

whereas adoption used binary cross-entropy:

$$\mathcal{L}_A = -\frac{1}{N}\sum_{n=1}^{N}[y_n \log(\hat{p}_n) + (1 - y_n)\log(1 - \hat{p}_n)]. \quad (24)$$

3.5. Training, Validation and Performance Evaluation

All observations belonging to the same producer profile remained in one partition. Grouped splitting reserved approximately 64% of profiles for training, 16% for validation and 20% for independent testing, subject to preservation of complete groups. Leakage prevention required.

Grouped partitioning retained all records sharing a producer identifier within one partition. Training comprised 166 profiles and 2314 records, validation comprised 42 profiles and 562 records, and testing comprised 52 profiles and 724 records. This prevented overlap of generated profile identifiers across partitions, including repeated profile–technology combinations. However, all partitions originated from the same generation mechanism and technology catalogue. The procedure evaluates performance on unseen generated profiles and does not, by itself, demonstrate generalization to independently observed Colombian farms.

$$G_{train} \cap G_{validation} = G_{train} \cap G_{test} = G_{validation} \cap G_{test} = \varnothing. \quad (25)$$

The neural-network architecture and its main configuration parameters are summarized in Table 4. The network was optimized with Adam at an initial learning rate of 5×10^{-4} for a maximum of 300 epochs. Early stopping monitored validation loss with a patience of 20 epochs and restored the best weights. The learning rate was reduced by 50% after eight epochs without improvement, with a minimum of 10^{-6}. Class weights for adoption were

$$w_c = \frac{N}{2N_c}. \quad (26)$$

Table 4. Neural-network configuration.

Component	Specification
Encoded input features	54
Shared dense layers	128 and 64 neurons; Swish activation
Regularization	Batch normalization; dropout rate 0.20
Sustainability embedding	24 components; Swish activation
Sustainability output	Four sigmoid outputs
Suitability branch	28-component concatenation; 16-neuron hidden layer; one sigmoid output
Adoption branch	29-component concatenation; 12-neuron hidden layer; one sigmoid output
Total parameters	18,322, including batch-normalization parameters
Component	Specification
Encoded input features	54
Shared dense layers	128 and 64 neurons; Swish activation

Continuous outcomes were evaluated using

$$MAE = \frac{1}{N}\sum_{n=1}^{N}|y_n - \hat{y}_n|, \quad (27)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}_n)^2}, \quad (28)$$

and

$$R^2 = 1 - \frac{\sum_{n=1}^{N}(y_n - \hat{y}_n)^2}{\sum_{n=1}^{N}(y_n - \bar{y})^2}. \tag{29}$$

Adoption performance was assessed using ROC AUC, precision-recall AUC, accuracy, precision, recall, F_1 and the Brier score. The classification threshold was selected only on validation data by maximizing

$$F_1 = 2\frac{Precision \times Recall}{Precision + Recall}, \tag{30}$$

while calibration was evaluated through

$$BS = \frac{1}{N}\sum_{n=1}^{N}(\hat{p}_n - y_n)^2. \tag{31}$$

Ridge regression and random-forest regression served as suitability baselines; regularized logistic regression and random-forest classification were used for adoption. Identical partitions and preprocessing were retained for every comparison.

3.6. Explainability, Uncertainty and Recommendation Analysis

SHAP was applied to the neural suitability output. A training background of up to 40 observations defined the reference expectation, and up to 60 test observations were explained. The additive representation was

$$f(\mathbf{x}_{ij}) = \phi_0 + \sum_{m=1}^{M}\phi_{m,ij}, \tag{32}$$

where ϕ_0 is the expected output and $\phi_{m,ij}$ is the contribution of feature m. Global importance was

$$I_m = \frac{1}{N_{explain}}\sum_{n=1}^{N_{explain}}|\phi_{mn}|. \tag{33}$$

Permutation importance from the random-forest baseline was calculated as

$$PI_m = \mathcal{E}\left[y, \hat{f}(\mathbf{X}^{\pi_m})\right] - \mathcal{E}\left[y, \hat{f}(\mathbf{X})\right]. \tag{34}$$

Prediction uncertainty was estimated through 100 Monte Carlo-dropout passes. For prediction b,

$$\hat{y}_{ij}^{(b)} = f_{\boldsymbol{\theta}}^{(b)}(\mathbf{x}_{ij}), \qquad b = 1, \ldots, 100, \tag{35}$$

with

$$\bar{y}_{ij} = \frac{1}{B}\sum_{b=1}^{B}\hat{y}_{ij}^{(b)}, \tag{36}$$

$$s_{ij} = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}\left(\hat{y}_{ij}^{(b)} - \bar{y}_{ij}\right)^2}. \tag{37}$$

Confidence intervals for primary metrics were calculated from 1000 bootstrap samples drawn at producer-profile level. The final recommendation score was

$$Q_{ij} = 0.45\hat{S}_{ij} + 0.40\hat{R}_{ij} + 0.15\left(100\hat{A}_{ij}\right). \tag{38}$$

Its stability was examined under balanced, environmental-priority, economic-priority and social-priority weights. Ranking quality was summarized through

$$DCG@K = \sum_{r=1}^{K}\frac{2^{rel_r} - 1}{\log_2(r+1)}, \tag{39}$$

$$NDCG@K = \frac{DCG@K}{IDCG@K}. \tag{40}$$

Robustness checks included grouped cross-validation, exclusion of low-quality sources, baseline comparisons, weighting sensitivity, and analyses by region, by-product, and technology family. The robustness and uncertainty analyses, their purposes, and their main outputs are summarized in Table 5. SHAP values were interpreted as explanations of model behaviour rather than causal effects. The analyses were performed using Python 3.15.1, TensorFlow 2.21.0, Keras 3.15.1, scikit-learn 1.9.1, SHAP 0.54.1, NumPy 2.5.4, pandas 3.1.0, SciPy 1.18.1, and statsmodels 0.15.0. A random seed of 2026 was used.

Table 5. Robustness and uncertainty analyses.

Analysis	Purpose	Main Output
Grouped holdout	Generalization to unseen profiles	Independent test metrics
Grouped cross-validation	Stability between profile groups	Mean and dispersion
Cluster bootstrap	Sampling uncertainty	95% confidence intervals
Alternative weights	Dependence on sustainability priorities	Ranking changes
Baseline comparison	Justification of neural complexity	MAE, RMSE, R^2 and AUC
SHAP and permutation	Explanation robustness	Leading predictor comparison
Monte Carlo dropout	Case-level predictive uncertainty	Prediction intervals

4. Results and Discussion

The results are presented according to three categories: empirical and documentary findings, derived indicators, and model-generated predictions. Documentary findings refer to information directly supported by the reviewed sources, whereas derived indicators correspond to scores calculated using predefined assessment rules. Model-generated predictions comprise the outputs estimated by the neural network and their evaluation against the reference targets. Computationally generated inputs and targets are identified separately within this organization, since they do not constitute documentary findings.

4.1. Documentary Findings and Conceptual Synthesis

This subsection presents a qualitative synthesis of the reviewed literature. The thematic and conceptual maps summarize relationships identified across the cited studies; they do not represent measured sustainability outcomes, observed adoption rates, or neural-network predictions.

The conceptual thematic map synthesizes the coffee by-product valorization literature discussed in the manuscript, including studies published through 2026. Its organization reflects a qualitative interpretation of thematic relevance to the assessment framework and development within the reviewed literature, rather than calculated bibliometric centrality or density. Environmental sustainability, economic viability, social sustainability, and technological feasibility are grouped as core assessment themes alongside circular bioeconomy, explainable multi-task neural networks, life-cycle assessment, techno-economic assessment, and resource efficiency and waste reduction. This grouping brings the four sustainability dimensions into direct relation with the approaches used to evaluate valorization alternatives and interpret their potential benefits and constraints. Specialized themes include phenolic extraction, pectin recovery, dietary-fibre production, coffee flour, fermented beverages, animal feed, and biodegradable packaging. These pathways represent distinct applications whose relevance to smallholder systems depends on processing requirements, product safety, available resources, and commercialization conditions.

The foundational themes connect coffee by-products and smallholder food systems with technology suitability and adoption, resources and infrastructure, market access, and collective benefits. Composting, anaerobic digestion, biochar production, mushroom culti-

vation, and wastewater biotreatment are included in this quadrant to relate the assessment to practical transformation and treatment pathways. A separate group identifies themes requiring further integration: smallholder digital readiness, gender-responsive adoption, blockchain traceability, food and feed safety, uncertainty quantification, external validation, and technology ranking and trade-offs. Their placement highlights questions that warrant closer examination within the proposed framework; it does not establish that these topics are declining or uniformly underdeveloped across the wider literature. The map therefore connects contemporary technological applications with sustainability criteria, implementation conditions, and methodological challenges. Its positions and bubble sizes serve a conceptual purpose and should not be interpreted as measurements of publication frequency, research impact, or temporal evolution (Figure 5).

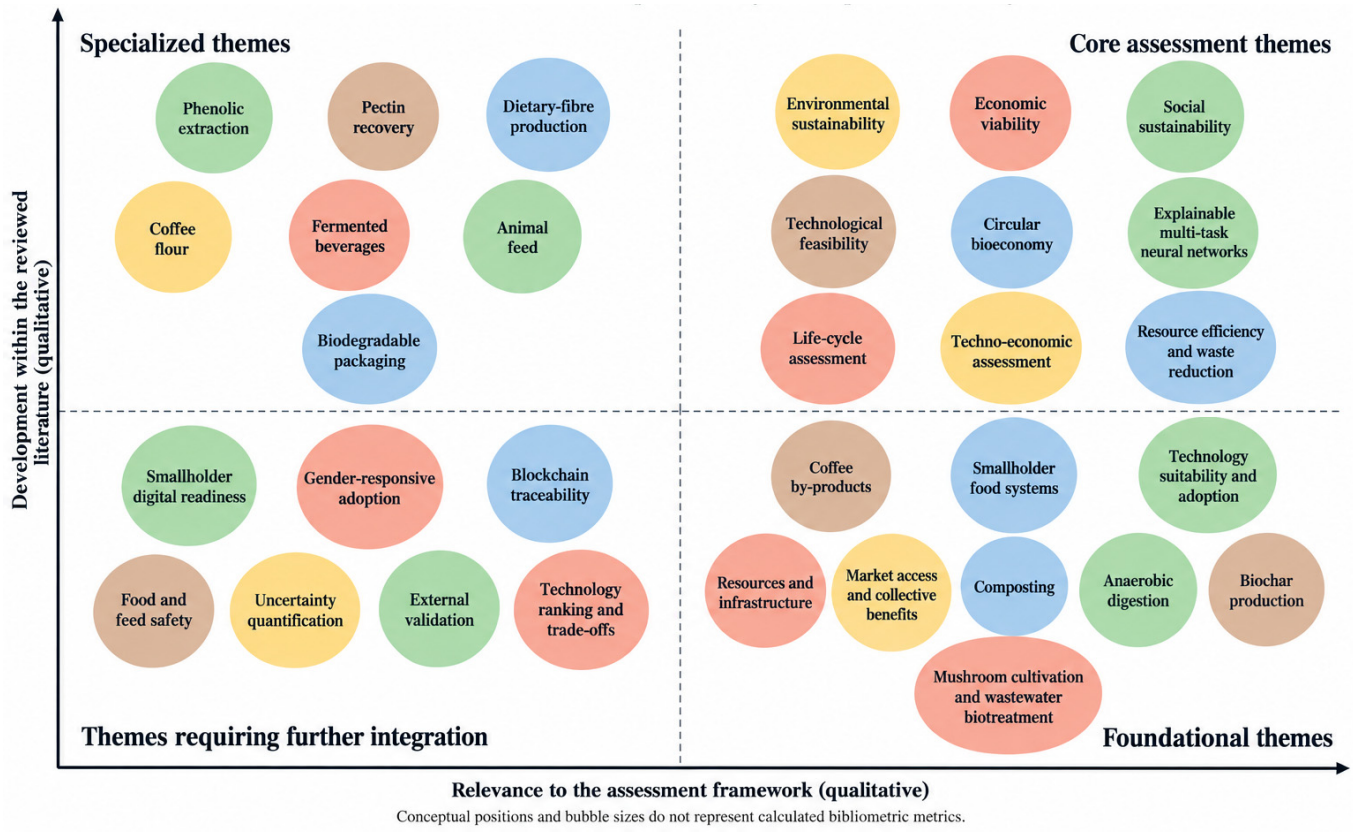


Figure 5. Conceptual synthesis of coffee by-product valorization research discussed in the manuscript, including studies published through 2026. Themes encompass sustainability dimensions, valorization pathways, smallholder conditions, and methodological challenges. Their placement is qualitative; positions and bubble sizes do not represent calculated bibliometric centrality, density, or frequency.

Figure 6 presents the conceptual flow connecting documentary sources, coffee by-products, producer conditions, sustainability indicators, and predictive outputs. It describes how these components are intended to contribute to decision support. The diagram should therefore be read as an analytical framework rather than evidence that every illustrated procedure was implemented or that the resulting recommendations were validated in producer settings. The resulting variables support the assessment of environmental performance, economic viability, social sustainability, technological feasibility, resource efficiency, waste reduction, energy demand, implementation costs, income potential, adoption readiness, operational complexity, and scalability. In the final stage, the explainable neural-network architecture integrates these dimensions to estimate sustainability scores, technology suitability, and adoption probability, while SHAP values, permutation impor-

tance, and uncertainty estimates clarify the factors influencing each prediction. This process ultimately produces a ranked set of valorization pathways intended to support smallholder decisions and strengthen the circular bioeconomy.

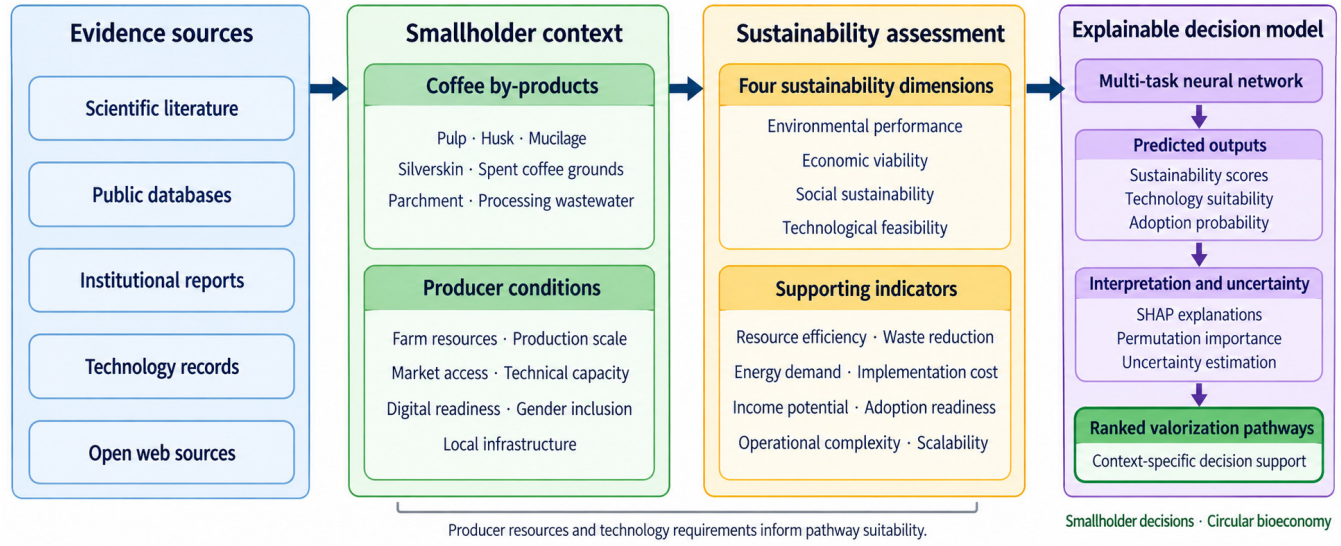


Figure 6. Conceptual flow linking web-based evidence sources, coffee by-products, smallholder production conditions, sustainability dimensions, and explainable neural-network outputs.

The conceptual structure map indicates that the research field is organized around three closely related areas. The largest cluster integrates coffee residues, valorization alternatives, resource recovery, circular bioeconomy, and the environmental, economic, social, and technological dimensions of sustainability. This concentration suggests that the selection of a valorization pathway depends on several interacting criteria rather than on technical efficiency alone. Another cluster brings together processes such as composting, anaerobic digestion, biochar production, fermentation, extraction, and wastewater treatment, reflecting the technological diversity available for transforming coffee residues. The third cluster connects the conditions of smallholder producers, including farm resources, market access, infrastructure, financial capacity, digital readiness, and gender inclusion, with explainable neural networks, prediction of adoption, uncertainty analysis, and technology ranking. The proximity among these concepts supports the premise that sustainability performance, interpretability, and implementation feasibility should be assessed jointly when identifying appropriate valorization alternatives for smallholder food systems (Figure 7).

4.2. Analytical Dataset and Input Characteristics

The analytical matrix comprised 3600 observations representing combinations between 260 smallholder producer profiles and 12 coffee byproduct valorization technologies. Each observation contained 33 variables describing the geographical and productive context, the availability of coffee residues, farm resources, technological requirements, expected sustainability performance, suitability, and adoption. The definitions, analytical roles, measurement scales, and interpretations of the input and output variables are provided in Table 6. The producer profiles covered the Andean region, Central America, East Africa, and Southeast Asia, while the principal residual materials included coffee pulp, mucilage, husk, parchment, spent coffee grounds, and wastewater. Rather than treating a producer or a technology as an isolated unit, the matrix represented their possible compatibility under different resource and operating conditions. This structure made it possible to examine why the same valorization alternative may produce different results when applied to farms

with unequal production scales, investment capacities, infrastructure, technical skills, and market access.

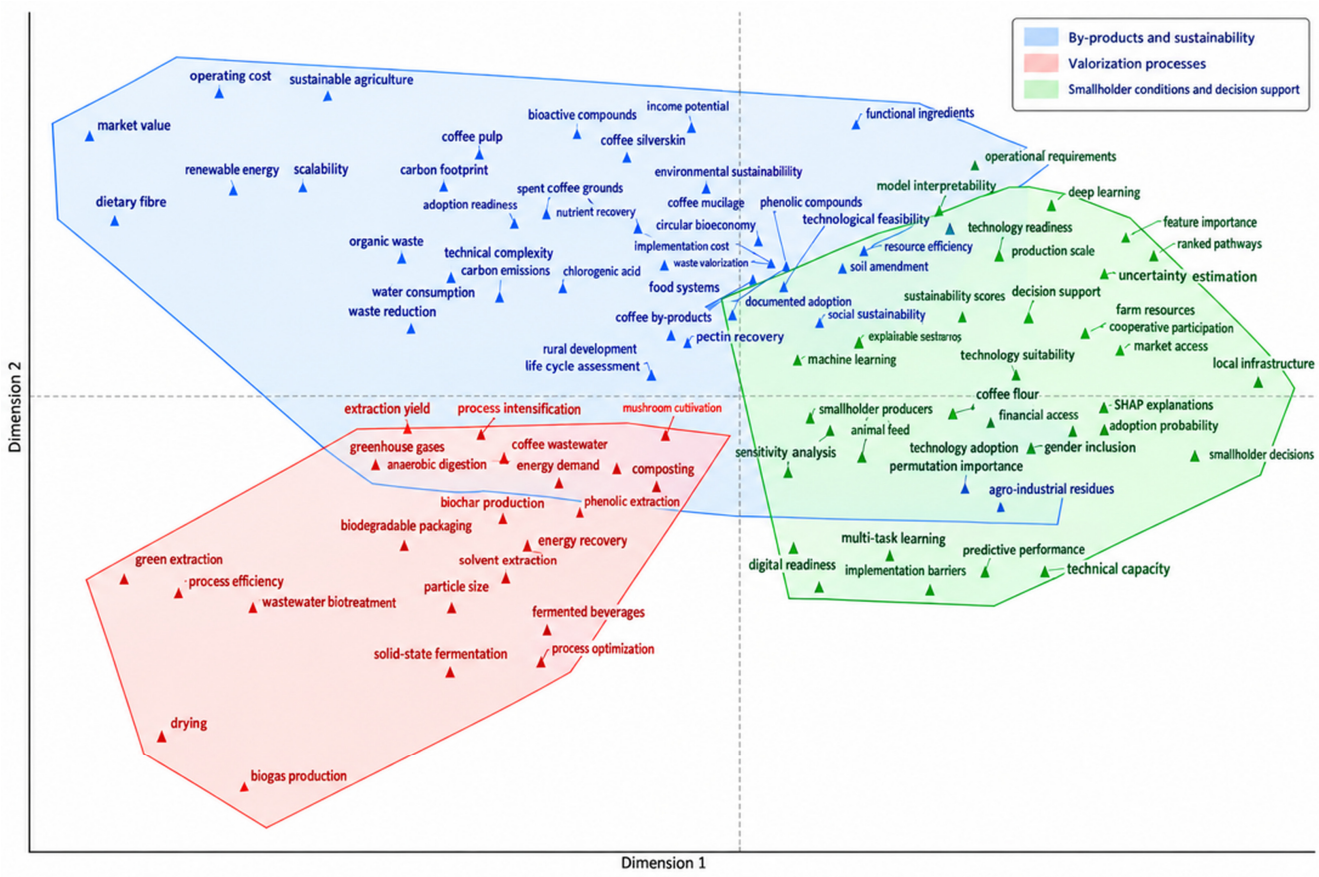


Figure 7. Conceptual structure map of coffee by-products, valorization technologies, sustainability dimensions, smallholder production conditions, and explainable neural-network components.

Table 6. Definition, role, measurement scale, and interpretation of the input and output variables used in the neural network.

Variable	Role	Measurement Scale	Interpretation
region	Producer input	Nominal categorical	Regional category assigned to the producer profile.
main_byproduct	Producer input	Nominal categorical	Principal coffee by-product assigned to the producer profile.
farm_size_ha	Producer input	Continuous, hectares	Farm area represented in the producer profile.
byproduct_tons	Producer input	Continuous, tonnes per year	Annual quantity of coffee by-product represented as available for valorization.
budget_usd	Producer input	Continuous, USD	Investment capacity represented as available for technology implementation.
energy_access	Producer input	Ordinal, 1–5: very low to very high energy access	Higher values represent greater availability and reliability of energy infrastructure.
water_access	Producer input	Ordinal, 1–5: very low to very high water access	Higher values represent greater water availability for processing and cleaning.

Table 6. *Cont.*

Variable	Role	Measurement Scale	Interpretation
technical_skill	Producer input	Ordinal, 1–5: very low to very high technical capability	Higher values represent greater capability to operate and maintain a technology.
market_access	Producer input	Ordinal, 1–5: very low to very high market access	Higher values represent greater access to potential buyers and commercialization channels.
labor_access	Producer input	Ordinal, 1–5: very low to very high labour availability	Higher values represent greater availability of labour for the valorization process.
association_member	Producer input	Binary: 0 = non-member; 1 = member	Association or cooperative membership assigned to the producer profile.
technology	Technology input	Nominal categorical	Specific coffee by-product valorization alternative.
family	Technology input	Nominal categorical	Technological family assigned to the valorization alternative.
target_byproduct	Technology input	Nominal categorical	Target feedstock specified for the technology in the computational catalogue.
investment	Technology input	Ordinal, 1–5: very low to very high investment requirement	Higher values indicate greater relative investment requirements.
energy_demand	Technology input	Ordinal, 1–5: very low to very high energy demand	Higher values indicate greater relative energy requirements.
water_demand	Technology input	Ordinal, 1–5: very low to very high water demand	Higher values indicate greater relative water requirements.
readiness	Technology input	Ordinal, 1–5: very low to very high technological readiness	Higher values indicate greater assigned technological maturity and operational readiness.
skill_required	Technology input	Ordinal, 1–5: very low to very high technical skill requirement	Higher values indicate greater technical knowledge required to operate the technology.
circularity	Technology input	Ordinal, 1–5: very low to very high circularity potential	Higher values indicate greater assigned potential for residue recovery and circular resource use.
environmental_ potential	Technology input	Ordinal, 1–5: very low to very high environmental potential	Higher values indicate greater assigned potential to reduce environmental pressures or provide environmental benefits.
revenue_potential	Technology input	Ordinal, 1–5: very low to very high revenue potential	Higher values indicate greater assigned revenue-generation potential, without establishing realized profitability.
employment_ potential	Technology input	Ordinal, 1–5: very low to very high employment potential	Higher values indicate greater assigned potential to generate employment.
environmental_ score	Reference target and corresponding neural-network prediction	Continuous, 0–1; multiplied by 100 for reporting	Rule-based environmental reference score and its corresponding model estimate, reported separately.

Table 6. *Cont.*

Variable	Role	Measurement Scale	Interpretation
economic_score	Reference target and corresponding neural-network prediction	Continuous, 0–1; multiplied by 100 for reporting	Rule-based economic reference score and its corresponding model estimate, reported separately.
social_score	Reference target and corresponding neural-network prediction	Continuous, 0–1; multiplied by 100 for reporting	Rule-based social reference score and its corresponding model estimate, reported separately.
technical_score	Reference target and corresponding neural-network prediction	Continuous, 0–1; multiplied by 100 for reporting	Rule-based technological reference score and its corresponding model estimate, reported separately.
sustainability_index	Derived aggregate indicator	Continuous, 0–1; multiplied by 100 for reporting	Weighted combination of the four sustainability dimensions: 0.35 environmental, 0.25 economic, 0.20 social, and 0.20 technological. Aggregation of reference scores is distinguished from aggregation of predicted scores.
suitability	Reference target and corresponding neural-network prediction	Continuous, 0–1; multiplied by 100 for reporting	Rule-based compatibility score linking producer resources and technology requirements, and its corresponding neural-network estimate.
adoption_ probability	Target-generation probability or neural-network probability output, distinguished by context	Continuous, 0–1	The target-generation probability determines Bernoulli sampling of adoption labels; the neural-network output estimates the probability of a positive generated label. Neither establishes empirically validated adoption likelihood.
adoption	Generated binary reference target; predicted class when a threshold is applied	Binary: 0 = negative label; 1 = positive label	Computationally generated adoption label. A predicted class is obtained separately by thresholding the neural-network probability. These labels do not represent independently documented implementation decisions.

Note: For all ordinal variables, 1 = very low, 2 = low, 3 = moderate, 4 = high, and 5 = very high. Higher producer-resource scores indicate greater access, availability, or capability. Higher investment, energy demand, water demand, and skill requirements indicate greater implementation demands; higher readiness and potential scores indicate greater maturity or higher assigned potential. Thus, a higher value is not uniformly more favourable. The categories denote ordered relative levels rather than standardized physical quantities. Although the computational formulas apply numerical transformations to these codes, equal substantive differences between adjacent levels have not been empirically established. Producer-profile attributes were computationally generated, while technology ratings were predefined in the catalogue. Reference targets, neural-network predictions, and aggregates calculated from either are distinguished throughout the analysis.

The input variables captured the main conditions that could influence the implementation of a valorization pathway. Farm size and annual byproduct availability represented the productive scale, while budget reflected the approximate investment capacity of each producer profile. Energy access, water access, technical skill, market access, labor availability, and association membership described the enabling or limiting conditions surrounding

implementation. Categorical variables, including geographical region, principal byproduct, technology family, and target material, were transformed using one hot encoding. Numerical variables were standardized using the mean and standard deviation estimated exclusively from the training partition:

$$z_{ik} = \frac{x_{ik} - \mu_k}{\sigma_k} \tag{41}$$

where x_{ik} denotes the original value of variable k for observation i, μ_k is the mean of the variable in the training set, and σ_k is its corresponding standard deviation. This transformation placed variables measured on different scales within a comparable numerical range and prevented variables such as investment capacity or farm size from dominating the learning process because of their original units.

The twelve technologies represented biological, thermochemical, food based, bioenergy, biomaterial, and environmental valorization pathways. The characteristics, operational requirements, and sustainability potential assigned to each technology in the catalogue are summarized in Table 7. Composting, mushroom cultivation, coffee flour, fermented beverages, and animal feed were characterized by comparatively moderate investment and technical requirements. Anaerobic digestion and biochar production required more demanding infrastructure, although they presented substantial environmental and circularity potential. Phenolic extraction, pectin recovery, dietary fibre production, and biodegradable packaging offered opportunities for obtaining higher value products, but their implementation depended more heavily on specialized knowledge, market access, process control, and investment capacity. Wastewater biotreatment addressed a different component of the coffee processing system by reducing the environmental burden associated with liquid effluents. The technological catalogue therefore did not assume that the most advanced alternative would necessarily be the most appropriate for every producer. Its purpose was to represent the tradeoffs between expected benefits and the resources required for implementation.

4.3. Derived Sustainability and Suitability Indicators

The model generated four sustainability outcomes corresponding to environmental performance, economic viability, social contribution, and technological feasibility. These outputs remained within the interval from 0 to 1 during model training and were converted to a scale from 0 to 100 for interpretation. A weighted sustainability index was subsequently calculated by assigning a weight of 0.35 to the environmental dimension, 0.25 to the economic dimension, and 0.20 to both the social and technological dimensions. Suitability was maintained as a separate output because overall sustainability does not necessarily imply compatibility with the actual conditions of a smallholder producer. Adoption was treated as a binary outcome, while adoption probability represented the estimated likelihood that a producer and technology combination would lead to implementation.

The distribution of the multidimensional sustainability index was concentrated mainly between 50 and 65 points, with the highest frequency located around the upper part of the 50 point range. Fewer observations appeared at the lowest and highest ends of the distribution, although a moderate extension toward scores above 70 was evident. This pattern suggests that most combinations offered intermediate sustainability performance rather than uniformly favorable or unfavorable outcomes. It also indicates that the analytical matrix retained sufficient variability to distinguish among producer conditions and technological alternatives. The absence of an excessive concentration near zero or 100 was relevant for model training because it reduced the likelihood of predictions being driven principally by extreme cases.

Table 7. Characteristics, operational requirements, and sustainability potential of the twelve coffee byproduct valorization technologies.

Technology	Family	Target Byproduct	Investment	Energy Demand	Water Demand	Readiness	Skill Required	Circularity	Environmental Potential	Revenue Potential	Employment Potential
Composting	Biological	Pulp	1	1	2	5	1	4	4	2	3
Anaerobic digestion	Bioenergy	Mucilage	3	2	2	4	3	5	5	3	3
Biochar production	Thermochemical	Husk	3	4	1	4	3	5	5	3	3
Mushroom cultivation	Food	Pulp	2	2	3	4	3	5	4	4	5
Coffee flour	Food	Pulp	2	2	2	3	3	5	4	4	4
Phenolic extraction	Food ingredient	Pulp	5	4	4	3	5	5	4	5	3
Pectin extraction	Food ingredient	Pulp	4	3	4	3	4	5	4	5	4
Dietary fiber ingredient	Food ingredient	Spent coffee grounds	3	3	2	3	4	5	4	5	4
Fermented beverage	Food	Mucilage	2	2	3	3	3	5	3	4	4
Animal feed	Feed	Pulp	2	2	2	4	3	4	3	3	3
Biodegradable packaging	Biomaterial	Parchment	5	4	3	2	5	5	5	5	4
Wastewater biotreatment	Environmental	Wastewater	3	2	3	4	3	5	5	2	3

The correlation analysis revealed positive relationships among all four sustainability dimensions and technology suitability, although their magnitude varied considerably (Figure 8). Technological feasibility exhibited the strongest association with suitability, reaching $r = 0.83$. This result indicates that compatibility was closely linked to whether a producer possessed the infrastructure, skills, energy, water, and productive capacity required by a particular technology. Social performance showed the second strongest relationship with suitability, with $r = 0.60$, followed by environmental performance at $r = 0.48$ and economic viability at $r = 0.37$. The comparatively weaker relationship between economic and technological performance, $r = 0.094$, suggests that economic potential did not automatically correspond to ease of implementation. A technology could offer attractive revenue prospects while remaining difficult to operate under restricted technical or infrastructural conditions.

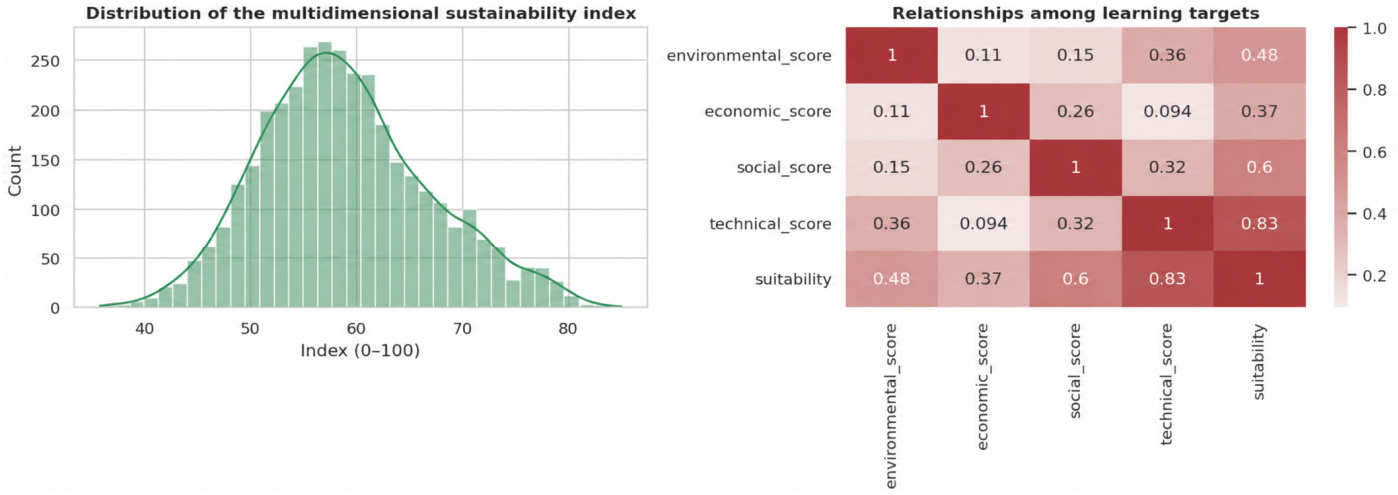


Figure 8. Distribution of the multidimensional sustainability index and correlation structure among environmental, economic, social, technological, and suitability outcomes.

Relationships among the sustainability dimensions were generally low or moderate. Environmental and technological performance reached a correlation of $r = 0.36$, while social and technological performance were associated at $r = 0.32$. Economic and social outcomes presented a correlation of $r = 0.26$. Lower values were observed between environmental and social performance, $r = 0.15$, and between environmental and economic performance, $r = 0.11$. These results support the use of a multidimensional framework, since none of the dimensions could adequately substitute for the others. Environmental advantages, income opportunities, social contributions, and technological feasibility captured different characteristics of each producer and technology combination. Reducing them prematurely to a single indicator would have concealed tensions that are particularly relevant in smallholder food systems.

The descriptive analysis identifies relationships among the constructed reference scores. Technological feasibility showed the strongest correlation with suitability, although this association must be interpreted considering the equations used to calculate both indicators. These correlations do not independently demonstrate which factors determine suitability in producer settings, nor do they establish the superiority of a multitask neural network over simpler models. They describe the target relationships that the predictive model subsequently attempts to reproduce.

The four sustainability dimensions were integrated through a weighted aggregation procedure that preserved their individual contributions while providing a common measure

for comparing producer and technology combinations. The resulting sustainability index for observation *i*was calculated as:

$$S_i = 0.35E_i + 0.25Ec_i + 0.20So_i + 0.20Te_i \quad (42)$$

where S_i represents the multidimensional sustainability index, E_i denotes environmental performance, Ec_i represents economic viability, So_i corresponds to social contribution, and Te_i expresses technological feasibility. Environmental performance received a weight of 0.35, economic viability received 0.25, and the social and technological dimensions were each assigned a weight of 0.20. As the weights summed to one, the aggregated result remained within the same bounded interval as the four component scores. Values were retained between 0 and 1 during model estimation and converted to a scale from 0 to 100 for reporting and comparison.

The calculation was verified for a selected combination of producer conditions and valorization technology (Table 8). The environmental score reached 0.7397 and contributed 0.2589 to the aggregated result. Economic viability was estimated at 0.5602, producing a weighted contribution of 0.1401. The social and technological scores were 0.5855 and 0.7329, with contributions of 0.1171 and 0.1466, respectively. Their sum produced a multidimensional sustainability index of 0.6626, equivalent to 66.26 points on a scale from 0 to 100. This value coincided with the sustainability index stored in the analytical matrix, confirming the internal consistency of the aggregation procedure.

Table 8. Verification of the weighted multidimensional sustainability index for a selected producer and technology combination.

Sustainability Dimensión	Reference Score	Weight	Weighted Contribution
Environmental	0.7397	0.35	0.2589
Economic	0.5602	0.25	0.1401
Social	0.5855	0.20	0.1171
Technological	0.7329	0.20	0.1466
Multidimensional sustainability index		1.00	0.6626

Note: The aggregated value of 0.6626 corresponds to a sustainability score of 66.26 on a scale from 0 to 100.

Although the environmental dimension made the largest contribution in this example, the result was not determined by a single component. Economic and social performance moderated the comparatively high environmental and technological scores. The calculation therefore illustrates the purpose of the multidimensional formulation: an alternative with substantial environmental potential may still obtain an intermediate overall result when its economic or social contribution is more limited. The index was used as an integrated reference measure, while the four component scores were retained as separate outputs of the neural network.

4.4. Neural-Network Training and Learning Diagnostics

The analytical matrix was subsequently divided at the producer level. This decision prevented observations associated with the same smallholder profile from being included in more than one partition. Of the 3600 producer and technology combinations, 2314 observations were assigned to training, 562 to validation, and 724 to independent testing. These groups contained 166, 42, and 52 unique producer profiles, respectively. The resulting distribution allocated 64.28% of the observations to training, 15.61% to validation, and 20.11% to testing (Table 9).

Table 9. Distribution of observations and unique smallholder producers across the training, validation, and test partitions.

Partition	Observations	Percentage of Observations	Unique Producers	Percentage of Producers
Training	2314	64.28%	166	63.85%
Validation	562	15.61%	42	16.15%
Test	724	20.11%	52	20.00%
Total	3600	100.00%	260	100.00%

Note: Observations associated with the same producer were retained within a single partition. The processed input matrix contained 54 encoded features.

The grouped partition provided a stricter evaluation than a random separation at the observation level. Because every producer could be paired with several technologies, an unrestricted random partition could place combinations belonging to the same producer in both training and testing. Such a configuration would allow the model to recognize characteristics already encountered during estimation and would produce an overly favorable assessment of predictive performance. Keeping producer profiles separate required the network to generalize its predictions to production contexts that had not been observed during training.

Following preprocessing, the model received an input vector containing 54 features. This expansion resulted mainly from transforming categorical predictors through one hot encoding, while the numerical variables retained one standardized component each. The preprocessing transformation was fitted only with the training partition. The same estimated means, standard deviations, and categorical levels were then applied to the validation and test observations without recalculation, reducing the possibility of information from the evaluation partitions influencing model estimation.

The multitask neural network combined a shared representation with specialized prediction branches. The input vector was initially processed by a dense layer of 128 neurons using the Swish activation function. Batch normalization and dropout were then applied to stabilize training and reduce dependence on particular neural units. A second dense layer transformed the representation into 64 components, followed by a 24 component sustainability embedding. From this common representation, the model generated four bounded scores corresponding to environmental, economic, social, and technological performance.

The suitability branch concatenated the 24 latent components with the four predicted sustainability dimensions, resulting in a representation of 28 elements. This information passed through a hidden layer of 16 neurons before producing a suitability score between 0 and 1. The adoption branch incorporated the sustainability embedding, the four dimensional predictions, and the estimated suitability. Its 29 element representation was processed through a hidden layer of 12 neurons before generating adoption probability. In this manner, the network treated sustainability, suitability, and adoption as related but distinct outcomes. The layer structure, output dimensions, and parameter counts of the multitask neural network are detailed in Table 10.

The shared architecture contained 18,322 parameters. Most were concentrated in the first and second dense layers, which jointly accounted for 15,296 parameters. This concentration was consistent with their function of extracting nonlinear relationships from the producer and technology variables before constructing the lower dimensional sustainability representation. The specialized branches were considerably smaller, which limited their capacity to override the information learned by the common structure.

Table 10. Layer structure, output dimensions, and parameters of the multitask neural network.

Layer	Type	Output Shape	Parameters
Producer and technology vector	Input	54	0
Dense layer 1	Dense, Swish	128	7040
Batch normalization 1	Batch normalization	128	512
Dropout 1	Dropout, 0.20	128	0
Dense layer 2	Dense, Swish	64	8256
Sustainability embedding	Dense, Swish	24	1560
Sustainability dimensions	Dense, sigmoid	4	100
Suitability information	Concatenation	28	0
Suitability hidden layer	Dense, Swish	16	464
Suitability output	Dense, sigmoid	1	17
Adoption information	Concatenation	29	0
Adoption hidden layer	Dense, Swish	12	360
Adoption output	Dense, sigmoid	1	13
Total			18,322

Note: The four dimensional output corresponds to environmental, economic, social, and technological performance. The reported parameter count includes the parameters associated with batch normalization.

Model optimization combined three prediction tasks within a single objective function:

$$\mathcal{L} = L_D + 1.2L_S + 0.5L_A + \lambda \parallel \theta \parallel_2^2 \quad (43)$$

where L_D represents Huber loss for the four sustainability dimensions, L_S denotes Huber loss for suitability, L_A corresponds to binary cross entropy for adoption, and $\lambda \parallel \theta \parallel_2^2$ represents regularization of the neural parameters. Suitability received a weight of 1.2 because compatibility between producer conditions and technological requirements constituted the principal recommendation outcome. The adoption component received a weight of 0.5, limiting the influence of the binary task on the shared sustainability representation.

The parameters were updated through backpropagation according to:

$$\theta_{t+1} = \theta_t - \eta \frac{\partial \mathcal{L}}{\partial \theta_t} \quad (44)$$

where θ_t denotes the parameter value at iteration t, η represents the learning rate, and $\partial \mathcal{L} / \partial \theta_t$ is the gradient of the total loss. The explicit gradient calculation confirmed that the kernel, bias, gamma, and beta parameters received nonzero updates. Kernel parameters showed the largest gradient magnitude, followed by biases and the normalization parameters (Figure 9). This result indicated that the main transformations learned by the dense layers accounted for most of the adjustment during the evaluated optimization step.

The training process was monitored through the total multitask loss, the individual task losses, and the AUC associated with adoption. Training loss decreased steadily from approximately 0.35 to below 0.24. Validation loss also declined during the initial epochs and reached its lowest level near epoch 10 but subsequently increased as training continued. A comparable divergence was observed for adoption. Training AUC rose progressively to approximately 0.86, whereas validation AUC stabilized near 0.70 after its initial improvement.

The separation between training and validation trajectories indicated that the model began to adapt too closely to the training observations after the first part of the optimization process (Figure 10). The increase in validation loss, despite the continuing reduction in training loss, provided evidence of overfitting. For this reason, early stopping restored the parameter configuration associated with the lowest validation loss rather than retaining the weights from the final epoch. The validation AUC also suggests that adoption was more difficult to generalize than the continuous sustainability and suitability outcomes, perhaps

because adoption depends on contextual factors that are not completely represented by the available predictor set.

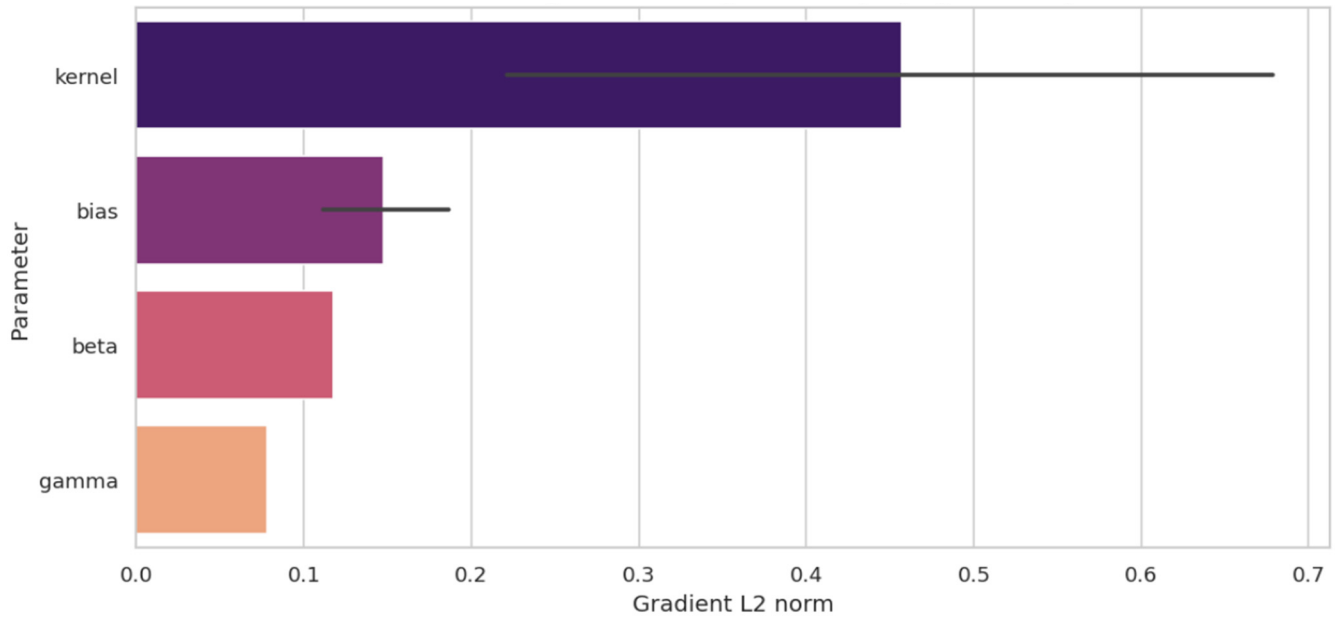


Figure 9. Gradient magnitudes of the principal trainable parameters during an explicit backpropagation step.

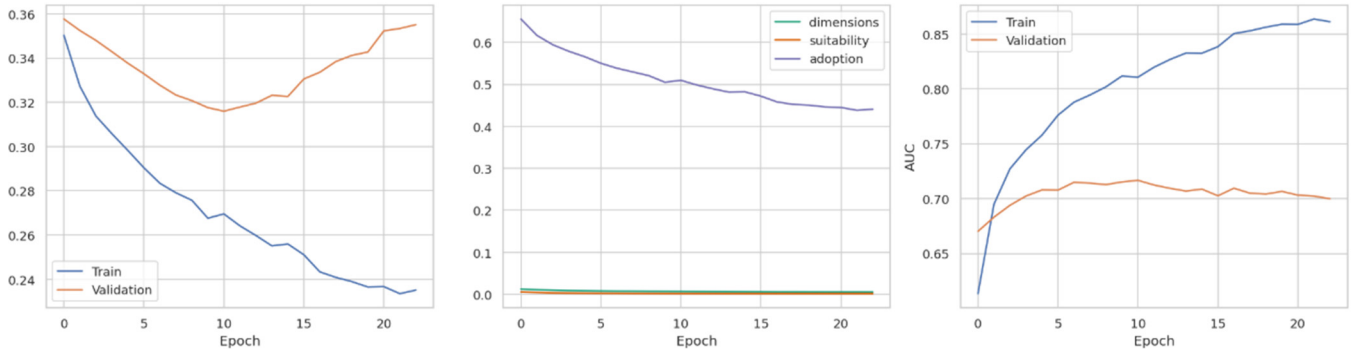


Figure 10. Training and validation trajectories for total multitask loss, task specific losses, and adoption AUC.

Overall, the results show that the network learned a compact shared representation capable of supporting the three related prediction tasks. The agreement between the manually calculated and stored sustainability indices verified the aggregation procedure, while the producer level partition established a more credible basis for evaluating generalization. Nevertheless, the divergence between training and validation performance indicates that the independent test results and uncertainty estimates remain necessary before drawing conclusions about the reliability of the technology recommendations.

4.5. Model-Generated Predictions, Predictive Performance, and Uncertainty

Model-generated predictions were evaluated using the 724 records in the held-out test partition. Predicted suitability was compared with the rule-based suitability target, while predicted adoption probabilities were evaluated against the computationally generated binary labels. The reported metrics therefore quantify agreement with the reference targets within the evaluated dataset; they do not measure agreement with independently observed producer decisions.

Predictive performance was evaluated with the 724 observations assigned to the independent test partition. The assessment considered the continuous suitability output and the binary adoption output separately because they represented different aspects of the recommendation problem. Suitability measured the compatibility between producer conditions and technological requirements, whereas adoption probability estimated whether that compatibility could translate into implementation. For suitability, the mean absolute error, root mean squared error, and coefficient of determination were calculated as follows:

$$MAE = \frac{1}{n}\sum_{i=1}^{n} | y_i - \hat{y}_i | \quad (45)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2} \quad (46)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \overline{y})^2} \quad (47)$$

where y_i denotes the observed suitability, $\hat{y}_i$ represents the corresponding neural prediction, $\overline{y}$ is the mean observed suitability, and n is the number of observations in the test partition. Adoption performance was assessed using the area under the receiver operating characteristic curve because this measure considers the capacity of the model to discriminate between adopted and nonadopted alternatives across multiple probability thresholds.

The model obtained a suitability MAE of 0.0492 and an RMSE of 0.0628 (Table 11). When expressed on the reporting scale, these values corresponded to average absolute and quadratic errors of approximately 4.92 and 6.28 points, respectively. The coefficient of determination reached 0.5538, indicating that the model explained 55.38% of the variability in technology suitability among producer and technology combinations not included during training. Predictive capacity was therefore moderate rather than complete. The adoption branch achieved an AUC of 0.7087, indicating discrimination between positive and negative reference labels in the test partition. This result concerns the generated adoption task and should not be interpreted as validation against documented technology uptake.

Table 11. Predictive performance of the multitask neural network in the independent test partition.

Prediction Task	Performance Metric	Value	Interpretation
Technology suitability	MAE	0.0492	Mean absolute deviation equivalent to 4.92 points on the reporting scale
Technology suitability	RMSE	0.0628	Quadratic prediction error equivalent to 6.28 points
Technology suitability	R^2	0.5538	The model explained 55.38% of test suitability variance
Technology adoption	AUC	0.7087	Acceptable discrimination between adoption and nonadoption cases

Note: MAE and RMSE were calculated on the original interval from 0 to 1. Multiplying these values by 100 provides their equivalent interpretation on the reporting scale.

The comparison between observed and predicted suitability revealed a clear positive relationship, although the neural estimates occupied a narrower range than the observed values (Figure 11). Predictions were concentrated primarily between approximately 45 and 74 points, while the observed suitability values extended from nearly 30 to more than 80. This compression toward intermediate values indicates a tendency to overestimate some low suitability combinations and underestimate alternatives located at the upper end of the observed distribution. Such behavior is consistent with regression toward the mean and partly explains why R^2 remained moderate despite relatively low absolute error.

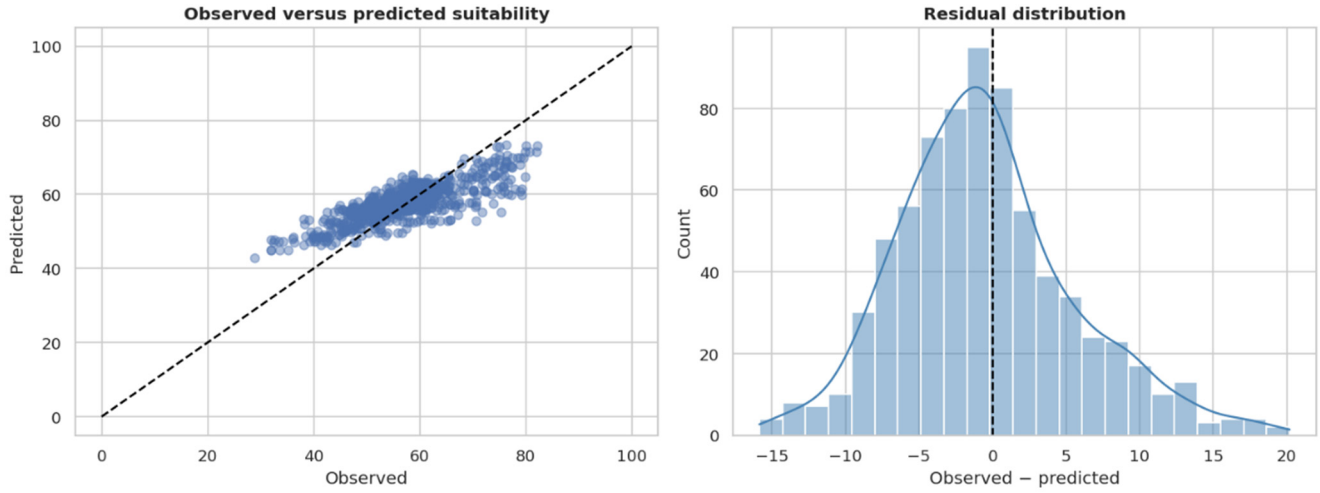


Figure 11. Reference and predicted technology suitability and residual distribution in the held-out test partition.

Residuals were concentrated near zero, which indicates that most test predictions did not differ substantially from their corresponding observed values. Nevertheless, the distribution was slightly asymmetric and extended farther toward positive residuals. Since residuals were defined as observed minus predicted suitability, positive values represented underestimation by the model, whereas negative values indicated overestimation. A small number of cases produced errors greater than ten points in either direction. These observations may correspond to producer and technology combinations with uncommon resource profiles or technological requirements that were insufficiently represented during training.

The internal activations provided a more detailed view of how the network transformed the encoded inputs (Figure 12). The first hidden layer showed a relatively broad activation pattern, with numerous neurons responding to the same producer and technology configurations. This behavior was expected because the initial layer received all 54 encoded characteristics and was responsible for extracting elementary combinations among resource availability, geographical context, byproduct type, and technological requirements. Several neurons remained weakly activated across most observations, while others displayed higher responses for cases.

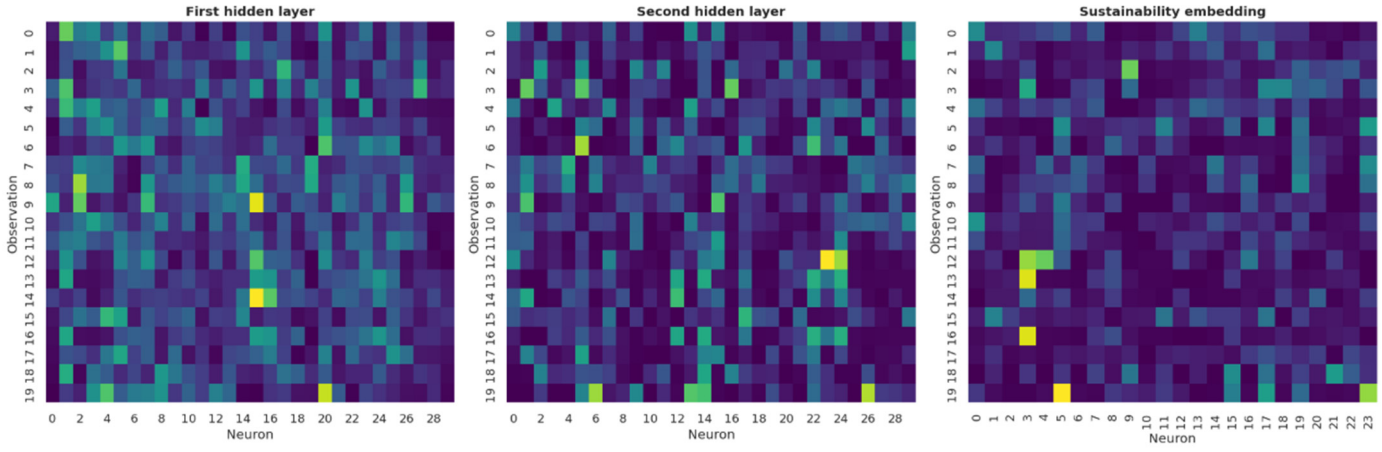


Figure 12. Activation patterns in the first hidden layer, second hidden layer, and shared sustainability embedding.

The second hidden layer produced a more selective pattern. High activation values were concentrated in fewer neurons and observations, suggesting that the model progressively compressed the broad input representation into more specific nonlinear configurations. This selectivity became more visible in the 24 component sustainability embedding, where a limited number of latent units presented strong responses for individual observations. The embedding therefore did not operate as a simple reproduction of the original variables. It represented combinations of producer and technology attributes that contributed jointly to environmental, economic, social, and technological predictions.

The activation maps should not be interpreted as direct measures of variable importance. A highly activated neuron may respond to several inputs simultaneously, and its substantive meaning cannot be established only from the intensity of the heat map. Their value lies instead in showing that the internal representation was neither constant nor homogeneous across observations. Different combinations of producer resources and technological demands generated distinguishable activation profiles, which provided the shared basis for estimating sustainability, suitability, and adoption.

The distributions of learned weights were generally centered near zero, although their dispersion differed across layers (Figure 13). Weights associated with the shared dense layers and sustainability embedding were comparatively concentrated, reflecting the regularized transformation of the 54 encoded inputs into the common latent representation. The output layers displayed different degrees of dispersion, particularly in the adoption branch, where a wider range of values was required to separate the two adoption classes. No dominant displacement of all weights toward highly positive or negative values was evident, which suggests that the network avoided complete parameter saturation.

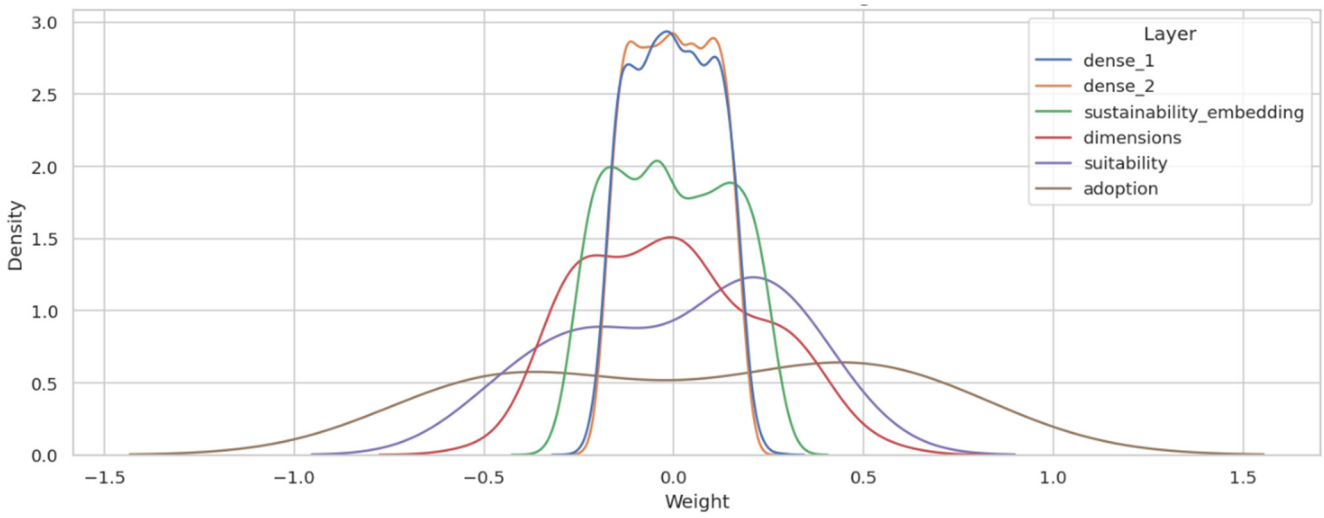


Figure 13. Distribution of the weights learned by the shared, sustainability, suitability, and adoption layers of the multitask neural network.

Weight distributions provide a general diagnostic of model stability, but they do not independently establish which original variables influenced a prediction. Each parameter operates within a sequence of nonlinear transformations and cannot be interpreted in isolation. Consequently, these distributions were considered an internal diagnostic and not a substitute for feature attribution methods. The explanation of individual and global predictions would require SHAP values or permutation importance applied to the final model outputs.

The 24 component sustainability embedding was projected onto two principal components to examine whether the learned representation separated the technologies according

to their technological families (Figure 14). The first two components retained approximately 38.1% of the variance in the latent representation. Observations occupied a relatively continuous space rather than forming completely separated technological clusters. Food, biological, environmental, bioenergy, biomaterial, and food ingredient alternatives overlapped throughout the central region, although some families extended toward more distant areas of the projection.

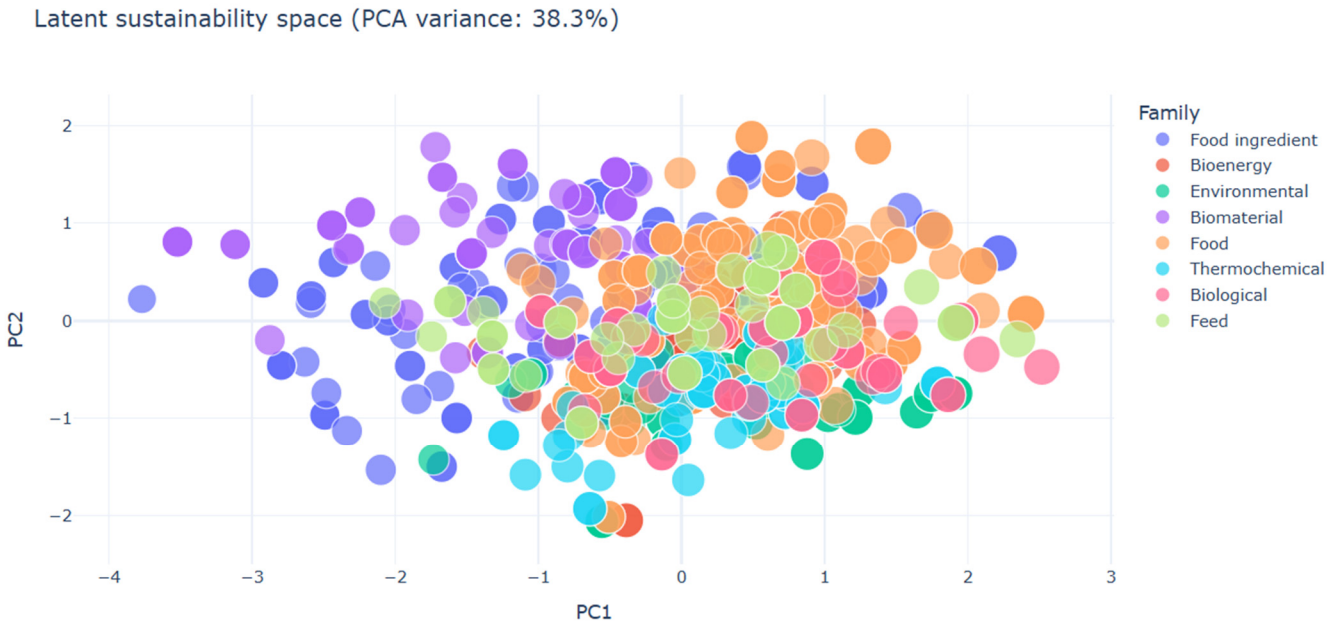


Figure 14. Latent sustainability space projected through principal component analysis according to technology family and predicted suitability.

The overlap suggests that the network did not organize the observations solely according to the nominal family assigned to each technology. Producer conditions and suitability also affected their position in the latent space. Two observations belonging to the same technological family could therefore appear in different regions when their budget, biomass availability, infrastructure, technical capacity, or market access differed. Conversely, alternatives from different families could occupy nearby positions when they exhibited comparable sustainability and implementation profiles. This pattern is relevant for smallholder food systems because it indicates that technological classification alone is insufficient for identifying the most appropriate valorization pathway.

A complete prediction was examined for a combination involving phenolic extraction and producer profile 200 (Table 12). The neural network generated separate scores for the environmental, economic, social, and technological dimensions. After applying the sustainability weights, the predicted multidimensional index reached 0.5357, equivalent to 53.57 points. The suitability branch produced a higher value of 0.5647, or 56.47 points, whereas the estimated adoption probability was 0.4033, equivalent to 40.33%.

The difference among these three results illustrates why sustainability, suitability, and adoption were modeled separately. Phenolic extraction achieved an intermediate sustainability assessment and a slightly higher compatibility score, but its adoption probability remained below 0.50. In practical terms, an alternative may provide recognizable environmental or economic benefits without becoming immediately adoptable. The remaining difference may reflect the high investment, energy demand, water demand, and technical skills associated with phenolic extraction. This distinction prevents the recommendation

system from equating an attractive sustainability profile with automatic feasibility for a smallholder producer.

Table 12. Sustainability, suitability, and adoption results for the selected phenolic extraction case.

Result	Predicted Value	Reporting Scale
Weighted multidimensional sustainability	0.5357	53.57 out of 100
Technology suitability	0.5647	56.47 out of 100
Adoption probability	0.4033	40.33%
Predicted adoption at a 0.50 threshold	0	Nonadoption

Note: The selected observation corresponded to phenolic extraction and producer profile 200. The adoption classification was obtained by applying a probability threshold of 0.50.

A sensitivity surface was constructed for the same phenolic extraction configuration by varying investment capacity between USD 500 and USD 30,000 and technical skill between levels 1 and 5 (Figure 15). All remaining producer and technology variables were held constant. Predicted suitability increased as both technical capacity and available budget improved, although the response was not linear. Technical skill produced a particularly visible change across the surface, while the marginal effect of additional budget varied according to the producer's skill level.

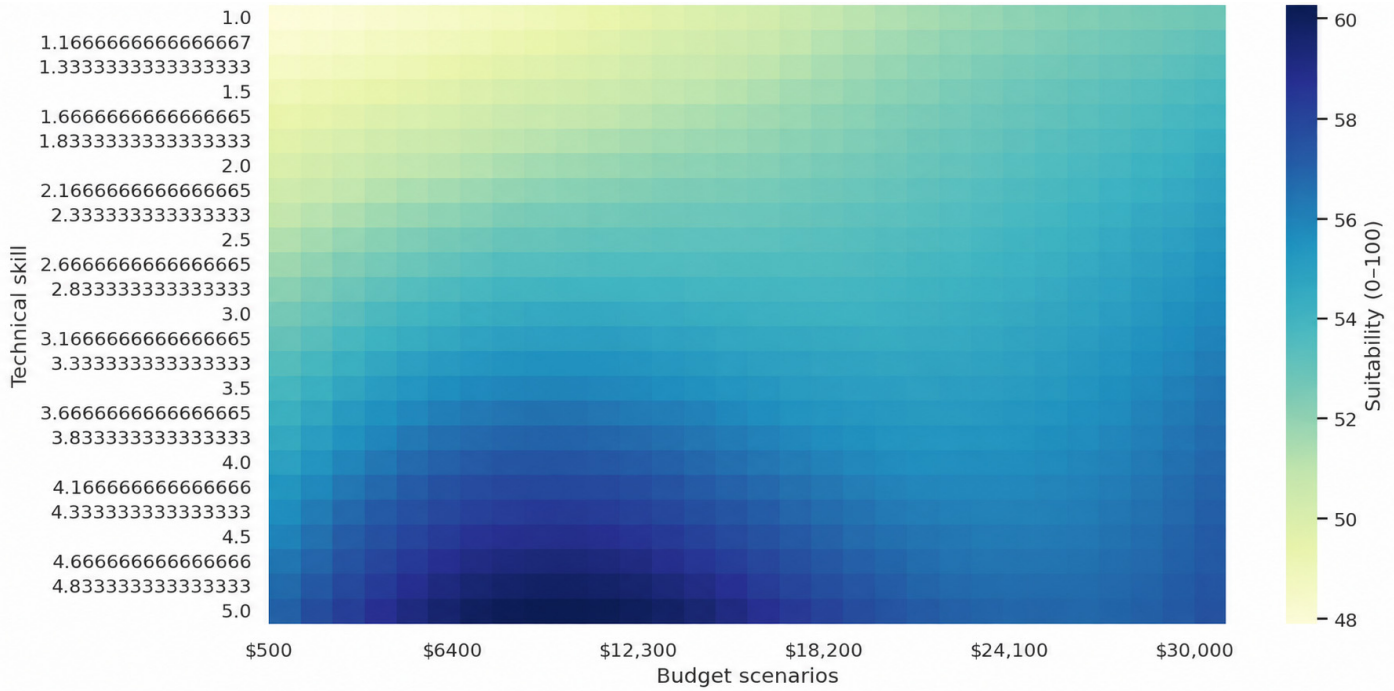


Figure 15. Neural response surface for phenolic extraction across investment capacity and producer technical skill.

The surface should not be interpreted as evidence of a causal relationship. It represents the response of the fitted neural model when two predictors are modified, and the remaining inputs are held constant. Its main contribution lies in identifying combinations under which a technology becomes compatible with smallholder conditions. For phenolic extraction, financial capacity alone did not guarantee high suitability. Improved technical skill was also required, which suggests that financing and technical assistance may need to be considered jointly when promoting more specialized valorization alternatives.

Prediction uncertainty was evaluated using 100 forward passes with dropout activated. For each observation, the procedure produced a distribution of suitability estimates from which the mean, standard deviation, and empirical 95% interval were calculated. The results varied across technologies and producer configurations (Table 13). For example, the first phenolic extraction case obtained a mean suitability of 52.56 points, with a standard deviation of 2.83 and an interval from 47.24 to 58.15. The anaerobic digestion case achieved a higher mean of 74.74 points but also presented a wider interval, ranging from 67.95 to 81.05.

Table 13. Illustrative uncertainty estimates obtained through Monte Carlo dropout.

Technology	Mean Suitability	Standard Deviation	Lower 95% Limit	Upper 95% Limit
Phenolic extraction	52.56	2.83	47.24	58.15
Dietary fiber ingredient	51.99	1.69	48.70	55.16
Anaerobic digestion	74.74	3.52	67.95	81.05
Wastewater biotreatment	56.56	2.92	51.56	61.45
Phenolic extraction	49.23	2.81	43.26	54.02

Note: Estimates were calculated from 100 predictions with dropout active. The repeated appearance of a technology represents different producer and technology combinations rather than duplicate observations.

The variation between the two phenolic extraction cases confirms that uncertainty was associated with the complete producer and technology configuration rather than with the technology name alone. Some recommendations remained relatively stable, while others crossed interpretive thresholds depending on the sampled neural configuration (Figure 16). For this reason, the mean predicted suitability should not be reported without its corresponding uncertainty range. Cases with wider intervals require more cautious interpretation and may justify additional technical evidence before a recommendation is communicated.

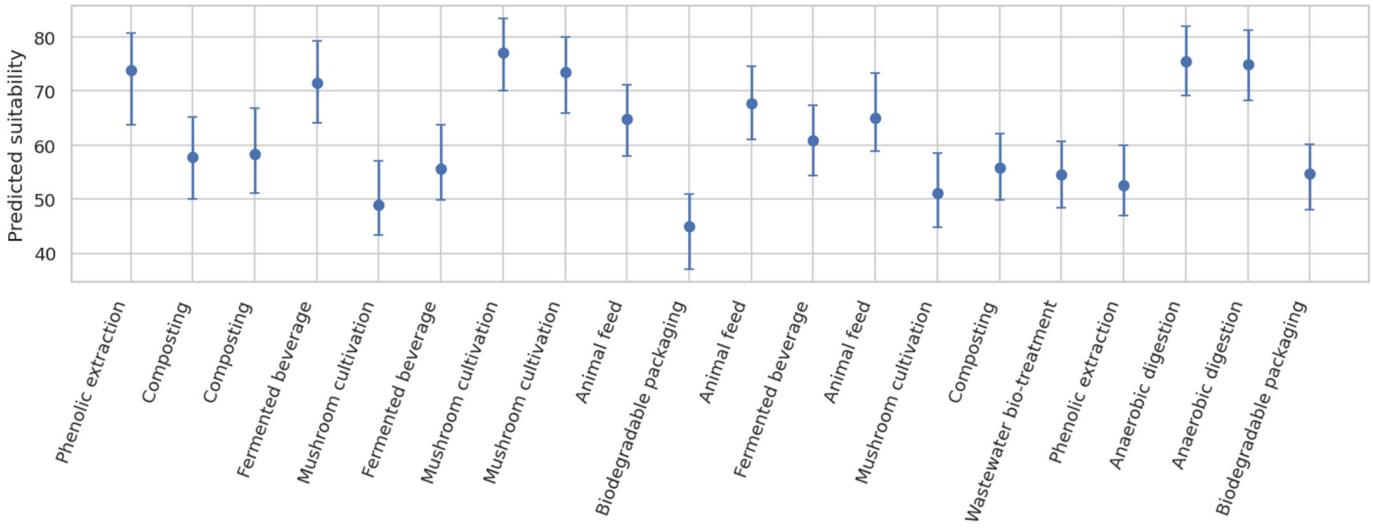


Figure 16. Uncertainty intervals for neural suitability recommendations obtained through Monte Carlo dropout.

Taken together, the results indicate that the neural network achieved moderate explanatory capacity for technology suitability and acceptable discrimination for adoption. The internal representations captured heterogeneous patterns that were not determined exclusively by technological family, while sensitivity analysis demonstrated that the compatibility

of specialized alternatives depended on combinations of financial and technical capacity. Uncertainty estimates added a necessary qualification to the rankings because apparently similar mean predictions did not always possess the same level of stability. The model therefore provides a basis for comparative decision support, although its recommendations should be interpreted as conditional estimates rather than definitive prescriptions.

5. Conclusions

5.1. Main Findings and Contributions

The findings indicate that coffee byproduct valorization cannot be assessed as a uniform technological problem detached from the conditions under which production occurs. The analytical matrix contained 3600 records sampled with replacement from 260 producer profiles and 12 technologies. Although these totals allow 3120 possible distinct profile–technology pairs, the dataset contained 2120 distinct pairs and 1480 additional occurrences of those pairs. The record count therefore does not represent 3600 unique combinations or documented repeated measurements. The multidimensional assessment further showed that environmental performance, economic viability, social contribution, and technological feasibility captured related but noninterchangeable aspects of sustainability. Such a distinction is consistent with recent research that recognizes coffee processing residues as heterogeneous resources whose potential depends on the conversion route, territorial setting, and broader development objectives [59]. Spent coffee grounds and other coffee residues offer several opportunities within bioenergy and circular economy systems [60], while their incorporation into food and feed products introduces additional questions concerning processing, safety, accessibility, and value creation [61].

Within the constructed reference indicators, technological feasibility showed the strongest association with suitability. This relationship partly reflects the target-construction rules and should not be interpreted as independent evidence of the determinants of technology implementation. Relatively accessible processes, such as composting, may be compatible with restricted infrastructure and investment capacity, although their performance depends on operating conditions and adequate control of the transformation process [62]. Anaerobic digestion presents considerable resource recovery and energy potential, but pretreatment requirements and process stability remain relevant constraints [63]. More specialized alternatives, including oligosaccharide extraction from spent coffee grounds, can generate higher value products, yet their technical demands may exceed the capabilities available in decentralized production environments [64]. The principal contribution therefore lies in evaluating valorization as a relationship between technology performance and producer capacity rather than as an intrinsic property of the technology alone.

5.2. Contributions to Multidimensional Sustainability Assessment and Explainable Modelling

The study developed an integrated assessment structure in which the four sustainability dimensions were predicted jointly and subsequently connected with technology suitability and adoption probability. The shared neural representation avoided estimating these outcomes through unrelated models, while the specialized branches preserved their distinct analytical meaning. The illustrative phenolic extraction case produced different sustainability, suitability, and adoption outputs. This separation demonstrates the architecture's treatment of distinct prediction tasks, rather than confirming the feasibility or adoption of that technology in an actual producer setting. Recent applications based on upcycled coffee grounds show that technically advanced materials can deliver additional environmental or energy functions [65], while integrated biorefinery approaches increasingly combine biofuels, bioplastics, and bioactive compounds within a common valorization system [66]. Nevertheless, the diversity of conversion pathways and sustainability challenges

surrounding carbonaceous products confirms that technological potential should not be interpreted independently of resource demand and implementation context [67].

The neural network achieved a mean absolute error of 0.0492, an RMSE of 0.0628, and an R^2 of 0.5538 for suitability in the independent test partition. Adoption discrimination reached an AUC of 0.7087. These metrics describe agreement with the constructed reference targets in held-out profiles; they do not establish predictive validity for independently observed farms or documented adoption decisions. Still, internal activations and weight distributions do not by themselves provide a complete explanation of the original predictors. Recent coffee research combining convolutional models with SHAP demonstrates how feature attribution can reveal the information supporting individual predictions [68]. Digital twins applied to organic waste valorization similarly suggest that data driven models become more useful when their outputs remain connected with operational conditions and clearly defined decision contexts [69]. The architecture developed here consequently provides a basis for explainability, although global and local SHAP analyses should be completed before the model is presented as a fully interpretable decision system.

5.3. Practical Implications for Coffee Byproduct Valorization

The practical value of the assessment lies in its ability to distinguish between general sustainability performance and compatibility with the circumstances of a particular producer. The twelve technologies differed in investment requirements, energy and water demand, technological readiness, circularity, environmental potential, revenue generation, and employment potential. These differences mean that no pathway can be recommended universally. Composting, animal feed, coffee flour, mushroom cultivation, and fermented beverages may offer relatively accessible entry points where capital and infrastructure are limited. Conversely, phenolic extraction, pectin recovery, biodegradable packaging, and other specialized processes may require collective arrangements, technical support, quality control, and stable market connections. Comparative research on biochar production has likewise shown that feedstock characteristics and processing conditions influence the properties and potential uses of the resulting material [70].

Sensitivity analysis provided a more concrete interpretation of these differences. For phenolic extraction, predicted suitability increased when investment capacity and technical skill improved, but financial resources alone did not produce the highest compatibility levels. This pattern suggests that credit or equipment provision may have limited effects when it is not accompanied by training, technical assistance, and market development. Coffee side streams incorporated into food products also require joint consideration of technological quality and environmental performance [71]. Reviews of food applications emphasize that functional ingredients and packaging materials derived from coffee residues must satisfy processing, safety, and quality requirements before their circular potential can be realized [72]. Accordingly, support programs should avoid promoting advanced technologies solely because they offer high theoretical value. Their selection should consider the producer's available biomass, capacity to operate the process, commercial opportunities, and ability to maintain the technology over time.

Following external validation, the model could contribute to preliminary screening through dimension-specific predictions, suitability estimates, and uncertainty information. Composting offers a pathway for returning organic material to agricultural production, while edible mushroom cultivation deserves consideration when coffee pulp is available and producers can maintain appropriate substrate preparation, hygiene, and marketing conditions. Among food-oriented alternatives, cascara infusions and flour-like ingredients may be worth screening before more demanding extraction processes, provided that drying, storage, food safety, and consumer acceptance can be adequately addressed. The reviewed

studies also identify opportunities involving silverskin-enriched bakery products, yogurt, granola, and other formulations, although successful experimental incorporation does not establish commercial viability. Pectin, dietary-fibre, and phenolic extraction may be more appropriate for producer associations or partnerships with specialized processors capable of supporting equipment, purification, quality control, and consistent feedstock supply. Anaerobic digestion and biochar production provide additional options where energy recovery or agricultural applications better match local needs. A practical starting point is therefore to characterize the available material, identify a realistic outlet for the resulting product, and compare processing requirements with existing resources. The model can support this screening through dimension-specific scores, suitability estimates, and prediction uncertainty. The main coffee by-product valorization options and their implementation requirements for smallholder systems are summarized in Figure 17.



Figure 17. Coffee by-product valorization options and implementation requirements for smallholder systems.

5.4. Implications for Smallholder Food Systems and Decision Support

The reviewed literature provides a conceptual basis for considering coffee by-product management within strategies to strengthen smallholder food systems; the present computational analysis does not demonstrate improvements in those systems. Residues generated during primary processing are often located close to farms, while some alternatives depend on aggregation, transport, or centralized transformation. This spatial and organizational distinction affects who can participate in valorization and how the resulting benefits are distributed. Smallholder suitability therefore depends not only on individual farm resources but also on associations, shared infrastructure, technical services, and access to downstream markets. The model reflects this tension by treating association membership,

market access, labor availability, and technical capacity as part of the producer profile rather than as external considerations.

The uncertainty analysis showed that similar mean predictions could have different ranges of variability. These ranges describe variation across stochastic model evaluations, rather than verified uncertainty about field outcomes, and should accompany any preliminary interpretation of the predictions. Recent evidence concerning the environmental footprints of spent coffee ground valorization indicates that impacts can change substantially across waste management, fuel production, and material applications [73]. In this sense, the model should be used to identify plausible and contextually compatible alternatives, while final investment decisions remain subject to technical verification, local prices, environmental regulation, and the actual organization of each producer system.

5.5. Limitations and Future Research Directions

The principal limitation concerns the provenance of the modelling records. Although documentary sources informed the assessment framework, the supplied computational implementation generated producer attributes and reference targets. Correspondence with independently documented producer records remains unresolved. Grouped splitting prevents overlap of profile identifiers, but all partitions originate from the same generation mechanism and technology catalogue. The results therefore support evaluation within this computational setting rather than empirical validation for Colombian smallholders. The predefined sustainability weights also represent an analytical reference rather than an established expression of producer priorities.

The model showed signs of overfitting after the first part of training, as validation loss increased while training loss continued to decline. Early stopping limited overfitting, although the remaining prediction errors cannot establish which contextual factors are missing from the assessment. Future work should incorporate repeated grouped cross validation, comparisons with simpler baseline models, external validation using independent regions, and systematic analysis of alternative sustainability weights. Global and local SHAP values, permutation importance, calibration analysis, and counterfactual explanations should also be added to clarify how each predictor affects sustainability, suitability, and adoption. Longitudinal evidence would allow the model to move beyond static compatibility and examine whether recommended technologies remain viable after implementation. Advancing in these directions could produce a more transparent decision support framework capable of connecting circular bioeconomy opportunities with the actual operating constraints of smallholder coffee systems.

Supplementary Materials: A methodological Jupyter notebook illustrating data preprocessing, multitask neural-network training, evaluation, sensitivity analysis, and uncertainty estimation using synthetic data is available at https://github.com/coffeebyproducts-hue (accessed on 19 October 2026).

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