

The Role of Artificial Intelligence in Nutritional Biochemistry: A Review

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Abstract—Artificial Intelligence (AI), encompassing Machine Learning (ML) and Deep Learning (DL), is reshaping nutritional biochemistry and accelerating the transition from generalized dietary guidelines toward Precision Nutrition. The objective of this review was to synthesize current evidence on AI applications across the nutritional biochemistry pipeline, from dietary assessment to personalized intervention.

Literature published between 2015 and 2026 was retrieved from PubMed, Scopus, ScienceDirect, and Google Scholar using combinations of search terms relating to AI, machine learning, nutritional biochemistry, metabolomics, nutrigenomics, and the gut microbiome. The evidence shows that Computer Vision models, including Convolutional Neural Networks, now enable objective food recognition and portion estimation with volume errors as low as 10.5%, while Natural Language Processing and Large Language Models standardize unstructured dietary text with dietitian-level accuracy. ML algorithms support dynamic nutrient estimation beyond static food composition tables, discover dietary and disease biomarkers across metabolomics, lipidomics, and proteomics, and integrate multi-omics data to decipher gene–diet and diet–microbiome interactions, enabling metabotyping, prediction of individual nutrient requirements, and the design of personalized functional foods and probiotics. Significant challenges remain, including data privacy, algorithmic bias, limited model explainability, and inadequate representation of diverse populations, particularly in low-resource settings. We conclude that AI provides the computational foundation for individualized, biochemically informed dietary strategies capable of preventing and managing chronic diseases, provided that ethical, regulatory, and validation frameworks mature alongside the technology.

Index Terms—Artificial Intelligence; Nutritional Biochemistry; Precision Nutrition; Machine Learning; Metabolomics; Gut Microbiome

I. INTRODUCTION

1.1. Background

Artificial Intelligence (AI) describes computational systems designed to emulate human reasoning, learning, and decision-making (Junaid, 2025). The field is commonly divided into Narrow AI, built for specific functions such as image or speech recognition, and the still-theoretical General AI, which envisions human-like cognition across many tasks. Within AI, three subfields are of particular relevance to biochemical research.

Machine Learning (ML) develops algorithms that learn patterns from data and improve with experience rather than following explicit rules, spanning supervised learning (regression, classification), unsupervised learning (clustering, dimensionality reduction), and reinforcement learning (Junaid, 2025).

Deep Learning (DL) employs multi-layered artificial neural networks to detect intricate patterns in large datasets and has already transformed biochemistry through achievements such as protein structure prediction and molecular modeling (Junaid, 2025). Natural Language Processing (NLP) enables machines to interpret and generate human language, making it indispensable for mining scientific literature and unstructured health records (Junaid, 2025).

Rapid growth in computational power, data availability, and algorithmic sophistication has made AI a transformative force across the life sciences, exemplified by AlphaFold’s solution to the protein-folding problem and AI-accelerated drug discovery (Junaid, 2025; Quan et al., 2026).

1.2. Nutritional Biochemistry and the Limits of the One-Size-Fits-All Paradigm

Nutritional biochemistry investigates the molecular and metabolic interactions between dietary components and living organisms, encompassing digestion, absorption, transport, storage, and metabolism, and how these processes influence health, disease, and gene expression. Historically, the discipline has depended on population-based dietary guidelines and standard biochemical assays. These approaches, however, poorly capture the substantial inter-individual variability in metabolic responses to diet, which is shaped by genetics, gut microbiome composition, and lifestyle (Quan et al., 2026). Biochemical individuality, a concept first articulated by Roger Williams, has gained renewed scientific validation through high-throughput sequencing and metabolomics: individuals consuming identical meals can display markedly different glucose excursions, lipid profiles, and inflammatory markers (Zeevi et al., 2015; Quan et al., 2026). This variability is not random; it arises from complex, non-linear interactions between host biochemistry and the chemical complexity of food.

1.3. Rationale and Objectives

The advent of AI, particularly ML and DL, has introduced a paradigm shift. AI's capacity to process high-dimensional "big data" from multi-omics technologies (genomics, metabolomics, metagenomics) offers an unprecedented route toward Precision Nutrition (PN), which seeks to deliver personalized dietary advice by integrating complex biochemical data (Nongbet et al., 2026). Architectures such as Convolutional Neural Networks (CNNs) for image analysis and Recurrent Neural Networks (RNNs) for time-series metabolic data allow biological systems to be modeled holistically, uncovering hidden correlations between dietary patterns and metabolic outcomes that elude traditional linear statistics (Loganathan & Sinthiya, 2026). Traditional methodologies are further constrained by quantification errors in dietary assessment and by static food composition tables that ignore the influence of origin and processing on nutrient bioavailability, while the sheer volume of multi-omics data overwhelms conventional analysis (Hivre et al., 2025; Quan et al., 2026). By managing the "nutriome", the totality of an individual's nutritional status, AI enables

discovery of previously hidden diet–health associations and supports evidence-based personalized interventions (Quan et al., 2026).

The objective of this review is therefore to synthesize current evidence on the role of AI in nutritional biochemistry across three domains: (i) dietary assessment and nutrient estimation; (ii) metabolomics, lipidomics, and proteomics; and (iii) nutrigenomics and microbiome biochemistry. The review also examines emerging digital-health integrations, critical challenges, and future research directions.

II. METHODS

This work was conducted as a narrative literature review. Electronic searches were performed in PubMed/MEDLINE, Scopus, ScienceDirect, and Google Scholar for records published between January 2015 and 2026, with emphasis on literature from 2023 onwards to capture the most recent methodological advances. Search strings combined controlled vocabulary and free-text terms, including: "artificial intelligence" OR "machine learning" OR "deep learning" AND "nutritional biochemistry" OR "precision nutrition" OR "personalized nutrition" OR "dietary assessment" OR "metabolomics" OR "nutrigenomics" OR "gut microbiome" OR "biomarker discovery".

Records were eligible for inclusion if they (i) were peer-reviewed original research articles, reviews, or scholarly book chapters published in English; (ii) applied AI, ML, or DL methods to questions in nutrition, metabolism, or related omics sciences; and (iii) reported biochemically interpretable outcomes. Editorials, conference abstracts without full text, and studies applying AI outside nutritional or biochemical contexts were excluded. Reference lists of retrieved reviews were hand-searched to identify additional relevant publications. Because this is a narrative rather than a systematic review, no formal risk-of-bias assessment or meta-analysis was undertaken; instead, findings were synthesized thematically into the three domains outlined above.

III. RESULTS

3.1. AI-Driven Dietary Assessment and Nutrient Estimation

3.1.1 The Critical Need for Accurate Assessment

Accurate, objective assessment of dietary intake is the foundation of Precision Nutrition. Nutritional research has historically relied on self-reported instruments such as Food Frequency Questionnaires (FFQs) and 24-hour recalls, which are prone to recall bias, social desirability bias, and systematic under-reporting of energy-dense foods. AI technologies are transforming this process by automating data acquisition and enabling dynamic nutrient estimation (Quan et al., 2026; Zheng et al., 2024).

3.1.2 Computer Vision and Food Recognition

Computer Vision (CV) powered by DL architectures, particularly CNNs, automates the identification and quantification of food intake. Advanced models such as Faster R-CNN and EfficientNetB2 identify specific food items from smartphone photographs and isolate individual meal components (Quan et al., 2026).

The typical pipeline involves four stages: (1) image acquisition, in which users photograph meals with smartphones; (2) object detection and segmentation, in which trained models separate individual food items from the background, even in complex dishes; (3) food classification, which assigns each segmented item to a category and links it to nutritional databases; and (4) volume and portion-size estimation, the critical step for calculating nutrient intake.

Two volume-estimation strategies are prominent. Stereo vision and 3D reconstruction systems use dual images, or a single image with depth-estimation algorithms, to reconstruct a three-dimensional model of the food; such systems have achieved a Mean Absolute Percentage Error (MAPE) as low as 10.5% (Quan et al., 2026). RGB-D fusion networks combine standard color images with depth information to improve mass estimation and predict macronutrient content (calories, fat, protein) more precisely than single-modal approaches (Quan et al., 2026). The biochemical implication is profound: accurate identification and volumetry permit dietary intake to be linked to databases of polyphenol content, fatty acid profiles, and amino acid composition, enabling granular analysis of how specific bioactive compounds influence metabolic pathways and supporting reliable assessment of energy balance and substrate availability (Quan et al., 2026).

3.1.3 Natural Language Processing for Nutritional Data

A large share of nutritional information exists as unstructured text in food labels, receipts, and self-reports. NLP transforms such data into standardized, quantitative form. Large Language Models (LLMs) such as GPT-4o and Gemini are being fine-tuned for nutritional tasks, where they extract and standardize entities such as ingredients, serving sizes, and nutrient values and map them to food composition databases (Quan et al., 2026). LLMs can also contextualize vague or colloquial entries (for example, “ate a small salad”) and, when combined with image data, achieve dietitian-level performance in nutritional analysis (Sun et al., 2023). Beyond extraction, NLP captures the semantic dimension of nutrition, including cultural dietary patterns and the emotional context of eating, which can influence metabolic health through neuro-endocrine routes such as stress-induced cortisol elevation affecting glucose metabolism and fat storage.

3.1.4 Dynamic Nutrient Estimation: Transcending Static Tables

Static Food Composition Tables (FCTs) provide average nutrient values that ignore the dynamic factors shaping a food’s final biochemical profile. ML models such as Support Vector Regression (SVR) and Random Forest (RF) are trained on datasets that incorporate origin and seasonality (predicting variation in vitamin C or antioxidant content by harvest location and time) and processing and cooking methods (estimating vitamin degradation during boiling or the increased bioavailability of lycopene after cooking tomatoes) (Quan et al., 2026).

AI is also being integrated with non-destructive analytics: Hyperspectral Imaging (HSI) captures spatial and spectral information as a chemical fingerprint of food, and coupled with algorithms such as Principal Component Analysis (PCA) and Ridge Regression, HSI systems can non-destructively predict the nutritional value of complex food mixtures in real time (Quan et al., 2026). These developments extend “precision” from the individual to the specific food item, producing nutrient estimates that more faithfully reflect the biochemical components actually consumed.

3.2. AI in Metabolomics and Nutrient Metabolism

3.2.1 High-Throughput Metabolomics Data Analysis

Metabolomics, the large-scale study of small molecules in biological systems, provides a direct readout of biochemical activity: unlike the relatively static genome, the metabolome dynamically reflects recent dietary intake, environmental exposure, and disease state (Hivre et al., 2025). Platforms such as Liquid Chromatography–Mass Spectrometry (LC-MS) and Nuclear Magnetic Resonance (NMR) quantify thousands of metabolites per sample, yielding high-dimensional, noisy, inter-correlated data that defeat traditional statistics (Hivre et al., 2025). ML contributes at two levels. First, in data pre-processing and feature selection, algorithms normalize, scale, and reduce dimensionality, with PCA and Partial Least Squares-Discriminant Analysis (PLS-DA) identifying the most biochemically informative metabolites. Second, in pattern recognition, unsupervised methods (K-Means, hierarchical clustering, self-organizing maps) delineate distinct metabolic phenotypes, or “metabotypes”, within populations (Hivre et al., 2025). A metabotype characterized by elevated branched-chain amino acids (BCAAs) and particular lipid species, for instance, may signal incipient insulin resistance. Such distinctions allow genuinely personalized guidance: individuals with a “high-protein metabotype” may process amino acids efficiently, whereas “carbohydrate-sensitive” individuals may require stricter glycemic control.

3.2.2 Biomarker Discovery and Predictive Modeling

AI-driven metabolomics enables discovery of biomarkers, metabolites whose concentrations in biological fluids reliably reflect intake of a food or adherence to a dietary pattern, providing objective verification that bypasses self-report (Côté et al., 2025). ML models including RF and Support Vector Machines (SVM) have identified metabolic signatures (specific fatty acids, polyphenols, and their microbial co-metabolites) that predict adherence to the Mediterranean diet (Côté et al., 2025), while interpretable ML models precisely predict biomarkers of intermittent fasting, such as shifts in beta-hydroxybutyrate and amino acid profiles, permitting objective monitoring of fasting status (Hu et al., 2024). Ensemble algorithms such as Extreme Gradient Boosting (XGBoost) and RF excel at capturing non-linear variable interactions; they have linked nutrient

intake to chronic disease risk, identifying micronutrients such as potassium and vitamin E as significant predictors of cardiovascular health (Quan et al., 2026), and ML applied to metabolomic data has predicted incident type 2 diabetes mellitus (Leihner et al., 2024).

A useful mechanistic illustration is the folate cycle, which is central to one-carbon metabolism, DNA synthesis and repair, and methylation. The enzyme Methylene-tetrahydrofolate Reductase (MTHFR) catalyzes the irreversible reduction of 5,10-methylene-tetrahydrofolate to 5-methyl-tetrahydrofolate, the principal circulating folate and the methyl donor for conversion of homocysteine to methionine. Polymorphisms in MTHFR (C677T, A1298C) reduce enzyme activity, lowering 5-methyl-THF production and elevating homocysteine, with attendant risks of cardiovascular disease and neural tube defects. AI models now integrate genetic data, dietary folate intake, and metabolic markers to predict folate status and the impact of MTHFR variants on homocysteine, informing personalized recommendations to optimize folate metabolism (Mahdavi et al., 2024).

3.2.3 Lipidomics, Proteomics, and Metabolic Flux Analysis

In lipidomics, AI models decode the complete lipid profile of biological systems to clarify how dietary fats influence cell signaling, membrane integrity, and inflammation; ML algorithms identify lipid biomarkers of omega-3 fatty acid consumption and predict their cardiovascular impact (Naumova, 2025). In proteomics, DL models predict the bioactivity of food-derived peptides, including antihypertensive, antimicrobial, and antioxidant activities, directly from amino acid sequence and structure, bypassing costly laboratory screening and accelerating functional food design (Al Shareef et al., 2025).

Metabolic Flux Analysis (MFA) quantifies reaction rates within cells but is traditionally computation-heavy, relying on isotope labeling and stoichiometric models. DL-based MFA now maps isotope labeling patterns onto fluxes with high accuracy and speed, allowing real-time observation of pathway responses to nutrient challenges (Gonçalves et al., 2023). AI-enhanced MFA can identify rate-limiting enzymatic steps (for example, glycolytic or TCA-cycle bottlenecks contributing to insulin resistance), predict metabolic reprogramming under ketogenic or high-fat

diets, and model host–microbe metabolic exchange, such as the influence of microbial short-chain fatty acid production on host gluconeogenesis and lipogenesis (Gonçalves et al., 2023).

3.3. AI in Nutrigenomics and Microbiome Biochemistry

3.3.1 Gene–Diet Interactions

Nutrigenomics examines how nutrients influence gene expression and how genetic variation alters nutrient requirements; the combinatorial space of genes, dietary components, and their interactions demands AI-scale analysis (Loganathan & Sinthiya, 2026). ML analyses have probed interactions between dietary habits, such as carbonated sugar-sweetened beverage consumption, and single-nucleotide polymorphisms (SNPs) in glucose-metabolism genes to predict metabolic syndrome risk in large hospital-based cohorts (Park et al., 2024). Such models flag individuals genetically predisposed to adverse outcomes from particular dietary exposures, and related predictive frameworks estimate individual micronutrient requirements, for instance vitamin C, vitamin D, or vitamin B12, from SNPs affecting absorption, transport, and metabolism together with clinical markers (Mahdavi et al., 2024). Table 1 summarizes representative AI applications in nutrigenomics and microbiome biochemistry.

3.3.2 Gut Microbiome and Short-Chain Fatty Acid Synthesis

The gut microbiome, often termed a “virtual organ” for its immense metabolic capacity, ferments undigested dietary fiber into Short-Chain Fatty Acids (SCFAs), butyrate, propionate, and acetate, that modulate host energy metabolism, immunity, and, via the gut–brain axis, neurological function (Nathan et al., 2026). Butyrate deserves particular attention: it is the primary energy source for colonocytes and sustains gut barrier integrity, dampens inflammation, and influences gene expression. It is produced by anaerobic fermentation of fiber and resistant starch by bacteria such as *Faecalibacterium prausnitzii* and *Clostridium butyricum*, through lactate conversion or condensation of two acetyl-CoA molecules to acetoacetyl-CoA and stepwise reduction to butyryl-CoA (Sripada & Manjunath, 2026). AI models trained on metagenomic data predict the efficiency of these pathways, estimating a host’s capacity to generate

beneficial SCFAs from a given fiber source and thereby guiding targeted prebiotic interventions (Sripada & Manjunath, 2026). Multi-omics integration further uncovers biochemical links between gut microbes and neurodegenerative disease progression, informing precision therapy along the gut–brain axis (Zhu et al., 2025).

3.3.3 Personalized Functional Foods and Probiotics

By analyzing the genomes and metabolic pathways of candidate probiotic strains, AI accurately predicts functional traits such as SCFA synthesis capacity and antimicrobial peptide (AMP) production (Sripada & Manjunath, 2026). This supports two precision strategies: tailoring probiotic interventions by selecting strains biochemically matched to an individual’s metagenomic profile and metabolic deficiencies, and designing functional foods whose composition maximizes production of beneficial metabolites by the target microbial community, for example through choice of prebiotics or food matrices that enhance desired microbial pathways (Ashoka et al., 2026).

IV. DISCUSSION

4.1. Synthesis and Comparison with the Wider Literature

The evidence reviewed here indicates that AI has moved nutritional biochemistry from subjective, static, population-level practice toward an objective, dynamic, and personalized paradigm, a closed-loop framework spanning assessment, mechanistic insight, and intervention (Quan et al., 2026). This trajectory is consistent with landmark empirical work. Zeevi et al. (2015) demonstrated in 800 participants that postprandial glycemic responses to identical meals vary widely between individuals and that an ML model integrating dietary habits, anthropometrics, physical activity, and gut microbiota composition could accurately predict personalized glycemic responses and lower them through algorithm-designed diets. Scoping reviews similarly confirm that AI-based measurement of food and nutrient intake improves accuracy and reduces participant burden relative to self-report (Zheng et al., 2024), and bibliometric analyses show accelerating growth of AI-based precision nutrition research, with RF and gradient boosting among the most productive techniques,

particularly when microbiome data are incorporated (Ferreira et al., 2025; Mundt et al., 2025).

The scope of application is also widening beyond ambulatory wellness. Reinforcement learning systems now craft personalized meal plans with high user acceptance, adapting dynamically to preferences and goals (Amiri et al., 2024). Internet-of-Things (IoT) frameworks couple wearable sensors with ML to deliver continuous health assessment and dietary recommendations (Jagatheesaperumal et al., 2023), and the integration of continuous glucose monitors (CGMs) with AI enables real-time, feedback-driven dietary adjustment and even “digital twin” approaches to metabolic management. In clinical settings, AI-enabled precision nutrition is being explored for critically ill patients in intensive care, where metabolic demands shift hour by hour (Briassoulis et al., 2025). Importantly for regions such as sub-Saharan Africa, AI and precision nutrition approaches are increasingly proposed to strengthen maternal and child health in low-resource settings by enabling affordable, scalable nutritional assessment where dietitian coverage is sparse (Mehta et al., 2025).

4.2. Challenges and Limitations of AI in Nutritional Biochemistry

Despite this promise, several barriers temper enthusiasm. First, data privacy and governance: AI nutrition platforms process highly sensitive genomic, metabolomic, and behavioral data, and compliance with frameworks such as the GDPR and HIPAA, alongside robust consent and anonymization practices, remains inconsistent across commercial applications (Mundt et al., 2025). Second, algorithmic bias and equity: models trained predominantly on data from European-ancestry populations and Western food environments misclassify foods and mispredict nutrient requirements for under-represented groups, risking amplification of existing health disparities; training datasets that reflect African, Asian, and Indigenous diets and genomes are urgently needed (Mundt et al., 2025; Zheng et al., 2024). Third, explainability: many high-performing DL models operate as “black boxes”, limiting clinical trust and regulatory acceptance; explainable AI and interpretable model classes are prerequisites for adoption in dietetic practice (Ferreira et al., 2025). Fourth, validation and generalizability: much of the literature consists of proof-of-concept studies on small

or homogeneous cohorts, and long-term randomized evidence that AI-guided nutrition improves hard clinical endpoints is still scarce (Zheng et al., 2024). Finally, AI systems should augment rather than replace nutrition professionals, with clear guidelines, governance, and human oversight framing their deployment (Ferreira et al., 2025).

4.3. Limitations of This Review

As a narrative review, this work did not employ a registered protocol, formal quality scoring, or quantitative synthesis, and selection of illustrative studies involves inherent subjectivity. The field is evolving rapidly, and findings published after the search window may alter specific conclusions, though the broad trajectories identified here are expected to persist.

V. CONCLUSION

AI has initiated a profound shift toward precision-driven nutritional biochemistry. Computer Vision and NLP now provide objective dietary assessment; ML enables biomarker discovery across metabolomics, lipidomics, and proteomics; and multi-omics integration deciphers gene–diet and diet–microbiome interactions to support metabolotyping, individualized nutrient requirements, and personalized functional foods.

The capacity of AI to integrate vast heterogeneous datasets, from genetic predisposition to real-time metabolic response, affords a holistic view of the human nutriome and drives the field toward its ultimate goal: precise, individualized optimization of health through diet.

Future research should prioritize diverse and representative training data, explainable and clinically validated models, integration of wearable and CGM data streams into adaptive closed-loop interventions, and robust ethical and regulatory frameworks. With these foundations, the transition from generalized dietary guidelines to a truly personalized, biochemically informed approach to nutrition can be realized equitably, including in low-resource settings where its public health impact may be greatest.

CONFLICTS OF INTEREST

The authors declare no conflicts of interest.

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