Optimization of antioxidant extraction through artificial neural network

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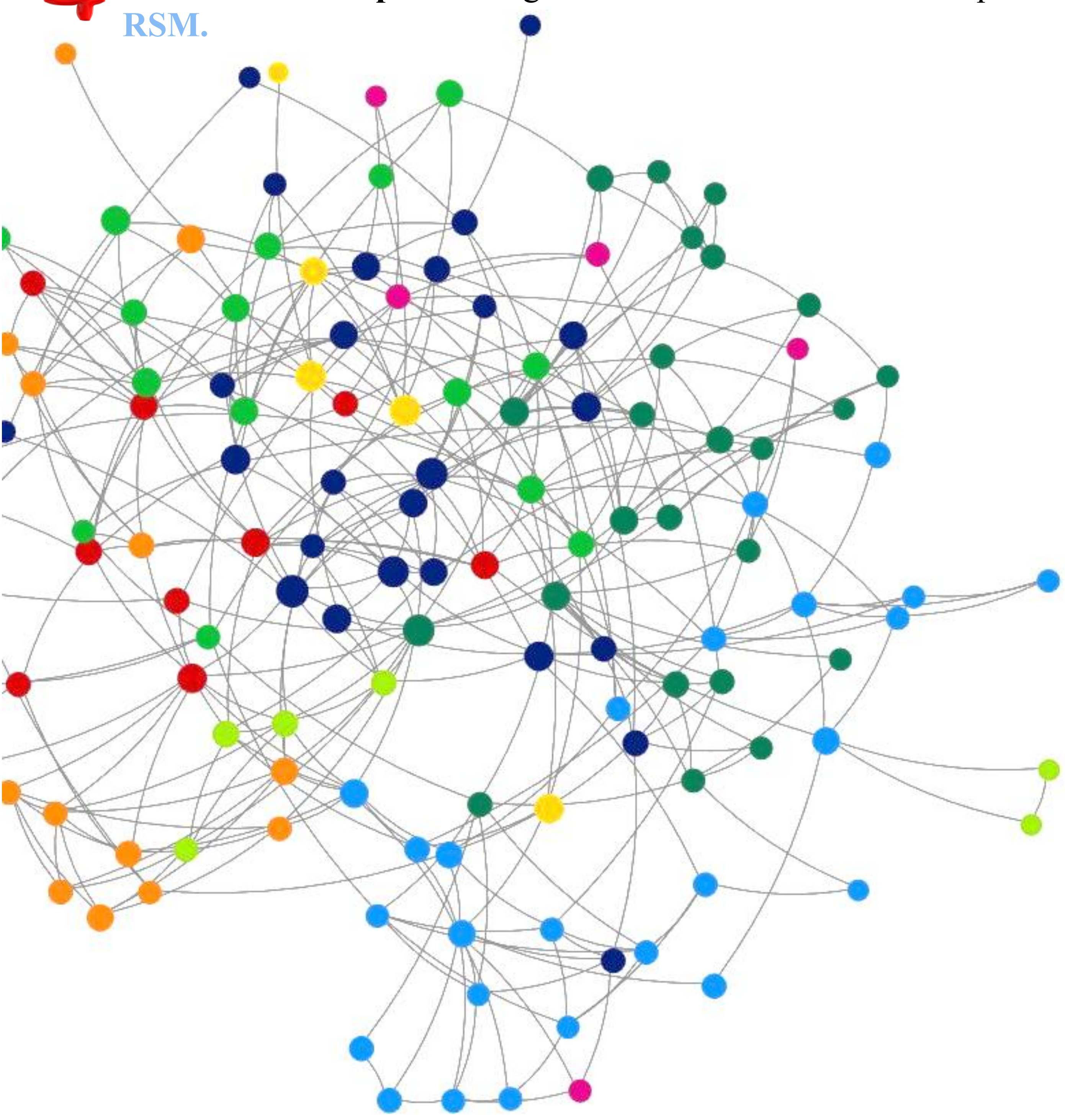
Introduction

The increasing demand in modern society for natural sources of bioactive compounds with potential applications in preventive medicine has driven the development of **innovative approaches** to optimize extraction processes. While Response Surface Methodology (RSM) has been extensively utilized for **prediction** and **optimization** in extraction studies, Artificial Neural Networks (ANNs) offer a **powerful** alternative by enabling the **development** of **non-linear computational** models based on Deep Learning (DL).

These models are capable of **self-learning** and **training to address practical challenges**, without relying on **pre-defined mathematical equations**, by mimicking the **structure** and **functionality** of **biological neural networks**. The application of ANNs offers numerous **advantages**, including the ability to **interpret complex datasets**, and **scale results through optimization.** Furthermore, ANNs allow handling large datasets and generalizing across systems, **all without the limitations of predefined models or specific experimental designs.**

Objectives

1. Explore the impact of ANNs on enhancing sustainable and green extraction technologies.
2. Explore the **applicability of** ANNs in **designing industrial processes for incorporating natural antioxidants.**
3. Compile real studies on ANN application in optimizing antioxidant extraction from **natural matrices**
4. Offer **novel insights** into improving **extraction efficiency** and **resource consumption** using ANNs over traditional techniques like RSM.



Results

What exactly are ANNs? Are they useful?

ANNs are AI **models** inspired by the human brain, consisting of **interconnected** nodes. They are used solve **complex problems** such as **prediction, classification,** and optimization by learning from data.

ANNs in antioxidant extraction processes

1 Advanced modeling: ANNs surpass RSM by effectively handling complex, **non-linear relationships** in antioxidant extraction optimization.

2 Adaptive learning: Multilayer Perceptron-based ANNs process data, **recognize patterns**, and **optimize parameters** for **improved efficiency.**

3 Improved accuracy: GAs refine ANN models to increase **accuracy**, reduce **resource consumption**, and **promote sustainability.**

Optimized antioxidant extraction workflow

① **Parameter Selection:**
- **Solvent mixture components:** , , and .
- **Process parameters:** Extraction 00:00, solid-to-liquid (S/M) ratio, and .

② **Experimental Design:**
- **RSM:** Optimize extraction 00:00, concentration, and to enhance antioxidant yield.
- **Mixture design:** Optimize solvent mixtures (e.g., -) for extraction based on properties.
- **Optimal Mixture Process Design (OMPD):** Combine **RSM** and **Mixture Design** to optimize both
- conditions and composition, using **D-optimality** to select the design for a of experimental trials.

③ **Mathematical Model:**
- **Mixture model:** Combines non-linear effects and second-order process variables effects for .
- **Process model:** Evaluates main effects, , and second-order effects of process variables like and S/M ratio.

④ **Modeling with ANNs:**
- **ANNs** to predict antioxidant yields by analyzing complex . The model uses **inputs** with **outputs** representing antioxidant activity (**yield, TPC, DPPH IC_{50}, TAC, FRAP EC_{50}**).
- Validation through **k-fold cross-validation (K=4)** with 75% of the data used for and 25% for validation.
- Evaluate significance using **R²**, Root Mean Square Error (**RMSE**), and Mean Absolute Difference (**MAD**).
- **Generic Algorithms (GAs) optimization:** Enhances ANN optimization via **selection**, **crossover**, and .

⑤ **Evaluation and Validation:**
- Validate ANN predictions by the optimal conditions to ensure improve antioxidant from samples.

Applications of ANNs in antioxidant extraction

Luangsakul et al., (2025) optimized the **ultrasound-assisted extraction (UAE)** of flavonoids from *Gnaphalium affine* D. Don (chewcut) using the **Box-Behnken design**. They compared ANN and RSM, with ANN providing more accurate predictions. Optimal conditions **(65.92°C, 58.22% ultrasound power, 37.95 min)** achieved **high yields of antioxidants**, suggesting the potential of chewcut as a **natural, functional ingredient** for health-oriented foods.

Harkat-Madouri, et al., (2025) applied RSM and ANNs to optimize microwave-assisted extraction (MAE) of total phenolic compounds from almond skins. ANNs (R^2 = 0.99) outperformed RSM (R^2 = 0.97) in predicting optimal conditions: **562 W microwave power, 30 s extraction time, and 53% EtOH, yielding 560.79 mg GAEs/100g.** The extract showed **strong antioxidant and antihyperglycemic activities**, including **α-amylase** inhibition **(IC_{50} = 27.87 µg/mL).**

Acknoledgments

The research leading to these results was supported by the Xunta de Galicia with the pre-doctoral grant of P. Barciela (ED481A-2024-230). The authors are also grateful to the National Funding by FCT, Foundation for Science and Technology, through the research grant of A.O.S. Jorge (2023.00981.BD).

Final remarks and outstanding questions

ANNs improve antioxidant extraction by efficiently managing complexity, predictive accuracy and resource utilization. However, challenges such as **data quality, model interpretability, and scalability** of ANN models for large-scale industrial use remain critical obstacles.

1. How to scale ANNs for industrial applications without compromising **yield** or **cost**?
2. Can DL combined with traditional methods **outperform resource optimizing?**
3. How **well** can ANNs predictions **be generalized** across different food matrices?
4. Can AI-powered optimization help energy **efficiency** and sustainable mining at scale?