The Application of Artificial Intelligence in Magnetic Hyperthermia

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Magnetic hyperthermia (MHT) is more commonly used in various biomedical applications. Magnetic hyperthermia (MH), a clinical alternative to tumor treatments, also became a powerful tool for cancer treatment by exposing tumor tissue to elevated temperatures to achieve a therapeutic effect. It has been successfully applied to the treatment of different types of cancer including the brain, spine, lung, prostate, breast, and pancreas. It is also a promising alternative to traditional cancer therapies, particularly in the case of aggressive brain cancer like glioblastoma. MHT's huge advantages are connected with biosafety, deep tissue penetration, and a focused place of action. The development of nanomedicine involves complex nanomaterial research involving magnetic nanomaterials and their use in magnetic hyperthermia. The selection of the optimal treatment strategies is time-consuming, expensive, unpredictable, and not consistently effective. Delivering personalized therapy that obtains maximal efficiency and minimal side effects is highly important. Thus, Artificial Intelligence (AI) based algorithms provide the opportunity to overcome these crucial issues.

artificial intelligence | magnetic hyperthermia | drug

1. Introduction

Artificial Intelligence (AI), including Machine Learning (ML), can be used to solve various issues of information processing, including pattern recognition, classification, clustering, dimensionality reduction, image recognition, natural language processing, and predictive analysis [1]. AI-based algorithms can be applied to solve complex problems [2][3][4]. Recent algorithm development enables its application in many areas of everyday life, such as industry, medicine, and nanomedicine; including nanomaterials with magnetic properties [5]. Consequently, a new opportunity to predict drug influence and responsiveness based on retrospective databases became available [6]. It may contribute to the development of optimized healthcare [7].

An important direction in developing medicine is to provide an effective method of dealing with various neoplastic diseases. The heterogeneous nature of tumors contributes to the problems in selecting effective treatment mechanisms. It is crucial to deliver drugs directly to the tumor core, the area most active in proliferation but less vascularized and hypoxic. Thus, the critical challenge in choosing the optimal therapy is determining the synergy of the drug depending on its dose, administration timing, and current treatment process. The latest development in nanotechnology enables the design of nanocarriers for targeted drug delivery, improving medicine release and beating cancer cells. In turn, manufacturing the nanoparticles, which can be loaded with drugs or other agents (stabilizers, compounds for diagnostics), is a time and financial outlays-consuming process. Thus, the AI-based prediction of the effect of nanoparticles with drugs on living tissues enables the development of targeted nanomedicine [8][9].

2. Artificial Intelligence and Machine Learning as Support for Magnetic Hyperthermia-Based Research and Prediction Properties of Nanoparticles

Since each subject is different, and drug synergy gives a different output in an individual case, transforming Artificial Intelligence (AI) to nanomedicine enables the analysis of large data sets and the effective selection of the optimal therapy [10][11]. It is essential in cancer therapy, particularly in the application of magnetic hyperthermia, to predict the optimal parameters of the process. AI includes various algorithms; researchers reviewed the existing solutions in the area of research, which involve the use of magnetic hyperthermia, taking into account their effectiveness, type and size of data sets, input and output parameters, and application fields. In [12], ANN was applied to predict the size of $AgNO_3$ particles. It turned out that the most sensitive parameters are both $AgNO_3$ concentration and reaction temperature. As the $AgNO_3$ suspension has no relation with magnetic hyperthermia, the literature shows the successful use of ANN in the prediction of particular properties of nanomaterials. In [13], the ANN was proposed to predict the shape and size of TiO_2 nanoparticles. In **Table 1**, the algorithms for the evaluation of the nanoparticle size were compared. It turned out that neural networks, in particular networks based on multilayer perceptrons, enable the prediction of the size of nanoparticles with high accuracy, i.e., 0.97 based on the experimental data.

Table 1. The comparison of the algorithm's performance takes account of the prediction of the optimal size of the nanoparticles.

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: Artificial Neural Network				
0.94	experimental data	- polymer concentration - drug - solvent ratio - mixing rate	- size	[14]
0.97	experimental data	- polymer molecular weight-number of blocks in the copolymer used - ratio of polymer to drug	- size	[15]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: multilayer perceptron				
0.97	745 experimental data from the literature	- inherent viscosity - molecular weight - lactide-co-glycolide ratio - inner/outer phase Polyvinyl alcohol (PVA) - concentration - PVA molecular weight - inner phase volume - encapsulation rate - mean particle size - concentration - dissolution pH - number of dissolution additives - dissolution additive concentration - production method - dissolution time	- size	[16]
0.99	experimental data	- particle concentration - reaction temperature - UV-visible wavelength - montmorillonite d-	- size	[12]

... spherical, ellipsoidal, clubbed, and sheet), has been made in [17]. It turned out that AI-based prediction can substantially

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
		- spacing		

e thermal

vity.

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: cascade-forward neural network				
0.93	1273 data collected from the literature	- temperature-solid volume fraction-solid volume fraction	- effective thermal conductivity	[18]
0.99	80 dataset experimental data and 389 data collected from the literature	- temperature concentration - shape factor - thermal conductivity	- relative thermal conductivity	[17]
Algorithm Type: Artificial Neural Network				
0.99	776 experimental data set	- average diameter - volume fraction - temperature	- the ratio of thermal conductivity	[19]
Algorithm Type: multilayer perceptron, radial basis function neural network generalized regression, Least-Squares Support Vector Machines				
0.97	80 dataset experimental data and 389 data collected from the literature	- temperature concentration - shape factor - thermal conductivity	- relative thermal conductivity	[17]
Algorithm Type: radial basis function neural network				
0.95	80 dataset experimental data and 389 data collected from the literature	- temperature concentration - shape factor	- relative thermal conductivity	[17]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
		- thermal conductivity		
Algorithm Type: Adaptive neuro-fuzzy inference system				
0.96	80 dataset experimental data and 389 data collected from the literature	- temperature concentration - shape factor - thermal conductivity	- relative thermal conductivity	[17]

[18] [20] [21] [22] model for tibacterial evaluate toxicity of the nanoparticle was compiled. So far, the ANN can also be used to predict specific parameters for magnetic nanoparticles, see **Table 4**.

Table 3. The comparison of the algorithms for prediction of the nanoparticle toxicity.

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: Artificial Neural Networks				
0.97	260 datasets from the literature	- average values of the - descriptors for nontoxic - toxic cases with the specific value of the descriptor of each toxic or nontoxic	- toxicity	[22]
Algorithm Type: Least Absolute Shrinkage Selection Operator Regression, Ridge Regression Elastic Net Regression, Support Vector Machine				
0.78	datasets from literature	- specific surface - area - hydrodynamic size - zeta potential - core size - exposure dose	- core size - exposure dose - species of bacterium	[21]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
		- duration - shape - type - coating - bacterium - aggregation Available online: https://github.com/mahsa-mirzaei/RFR_ABA/commits?author=mahsa-mirzaei (accessed on 24 November 2022).		
Algorithm Type: Random Forest				
0.78	datasets from literature	- specific surface - area - hydrodynamic size - zeta potential - core size - exposure dose - duration - shape - type - coating - bacterium - aggregation	- core size - exposure dose - species of bacterium	[21]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
		Available online: https://github.com/mahsa-mirzaei/RFR_ABA/commits?author=mahsa-mirzaei (accessed on 24 November 2022).		
0.98		- dose - duration - nanoparticle type - nanoparticle shape - zeta potential - surface area	- cell viability	[23]

rmance.

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: Artificial Neural Network				
0.93 (for Young's modulus) 0.96 (ultimate tensile strength)	153 datasets from the literature	- weight percent - - particle size	- Young's modulus - ultimate tensile strength	[24]
0.97	3404 experimental dataset	- wavelength - peak intensity - full width at half-maximum - peak area of the main peak	- particle size - reaction yield - quantum yield	[25]
0.98	experimental data sets	- extraction time - temperature - pressure -	- extraction yield of essential oils	[26]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
		modifier volume		
0.99	experimental data sets	- composition	- specific absorption rate	[27]
0.99	420 experimental data sets	- particle concentration - alternating magnetic field strength - temperature - time	- optimal parameters	[28]
Algorithm Type: Random Forest				
0.75	652 datasets from the literature	- nanoparticle type - nanoparticle core - surface modification - modification type-size - zeta potential - polydispersity index - corona formation - corona isolation	- optimal composition	[29]
Algorithm Type: multilayer perceptron				
0.94 (compressive strength) 0.97 (porosity)	data collected from the literature	- elastic modulus -	- compressive strength	[26]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
[26]	[24]	fracture toughness diopside - hardystonite - bredigite	- porosity	

particles, containing ble 5, the ion of the ceramics- een made s (GA) in predicting Young's modulus and ultimate tensile strength of nanocomposites, particularly polyethylene composites with multiple nanoparticles.

Table 5. The comparison of the algorithm's performance takes into account the prediction of power losses of magnetic particles.

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: Neural Network				
0.90	3963 records of simulated records	- temperature - vertex field - nanoparticles diameter - magnetic anisotropy - saturation magnetization - the identity of nanoparticles	- coercive field - magnetic remanence - hysteresis loop area	[5]
Algorithm Type: Random Forrest				
0.90	3963 records of simulated records	- temperature - vertex field - nanoparticles diameter - magnetic anisotropy -	- coercive field - magnetic remanence - hysteresis loop area	[5]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
[27]		saturation magnetization - the identity of nanoparticles		

...sed in the ...imize the ...ential and ...Bupropion hydrochloride loaded agar nanospheres. In turn, [28] the closed-loop optimization of the release process of the Poly (lactic-co-glycolic acid) (PLGA) biodegradable particles with ANN and genetic algorithms was described. As input data, particle size, and initial burst percent at the desired levels were chosen. It was postulated that the proposed algorithm can predict drug delivery.

In [29], the ANN was used to predict the optimal composition of two-dimensional graphene–Fe_3O_4 nanohybrids, which are dedicated to magnetic hyperthermia. It enables the prediction of the composition of the optimal nanohybrid, which can be applied to magnetic hypothermia in low dosage. The optimization based on multilayer perceptron neural networks of the experimental conditions of nanoparticles was described in [30]. The influence on nanoparticle characteristics factors like environmental conditions and type of precipitating agent was investigated. In turn, the mathematical framework for the magnetic drug delivery taking into account the ferrofluid flow was shown in [31].

Another critical issue in the manufacturing of nanoparticles is the synthesis process [32][33]. It should maintain precisely controlled characteristics. Since the synthesis of nanoparticles is a long-term and cost-consuming process due to the involvement of multiple chemical substances, the AI-based algorithm provides the opportunity to develop efficient experimental protocols. The following research describes the application of AI to the synthesis of semiconductor, metal, carbon-based and polymeric nanoparticles [34]. In [25], based on ultraviolet-visible (UV-vis) and PL spectrum data, the prediction of the optimal parameters of the synthesis of combinatorial CdSe nanoparticles was proposed. Thus, the heuristic and Bayesian optimization can be applied to the evaluation of the synthesis of the nanoparticles. Such an example is far from the magnetic hyperthermia application, while AI support can improve the experimental work also in the magnetic nanoparticles and magnetic hyperthermia field. In [35] the genetics algorithm particle swarm optimization (PSO) was used to predict the magnetic field generation. In [35], GA was used to optimize the Specific Absorption Rate in the case of hyperthermia treatment of the human head.

Recently, attempts were made to apply AI-based algorithms in the research of hydrogels. In reference [36], the Artificial Neural Network and Least Square Support Vector Machine were used to evaluate the swelling degree in the hydrogel, namely poly(NIPAAm-co-AAc) IPN. It turned out that Artificial Intelligence-based algorithms can, successfully and with high accuracy, predict the influence of pH and temperature on hydrogel deswelling behaviors. At the same time, the ANN model has higher computational efficiencies than the LS-SVM approach while maintaining this similar accuracy. Thus, in [37], ANN was used to evaluate the deswelling and heating behavior of the field-sensitive hydrogels, like poly(NIPAAm-co-VSA)/Fe_3O_4 IPN. The comparison of the algorithms for predicting deswelling behaviors is made in **Table 6**. It turned out that ANN achieved the highest efficiency in predicting deswelling degrees.

Table 6. The comparison of the algorithms for the prediction of deswelling behavior.

Accuracy	Application Field Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: Artificial Neural Network				
0.99	1638 experimental data set	- time - temperature - pH	- swelling degree	[36]
0.99	438 experimental data set	- alternating magnetic field strength - time - temperature	- swelling degree - temperature	[37]
Algorithm Type: Least Square Support Vector Machine				
0.98	1638 experimental data set	- time - temperature - pH	- swelling degree	[36]

Magnetic nanoparticles are also used to remove various types of substances. The efficiency of the approach is strictly connected with the percent of compounds adsorbed onto modified magnetic nanoparticles [37][38][39]. Thus, AI-based algorithms can be applied to predict removal efficiency. In [39] the application of the Artificial Neural Network and adaptive neuro-fuzzy inference system for the prediction of the chromium removal efficiency was shown. In **Table 7**, the comparison of algorithms for the evaluation of the removal efficiency is presented. It turned out that the combination of the Artificial Neural Network with an adaptive neuro-fuzzy inference system provides higher prediction efficiency.

Table 7. The comparison of the algorithms for prediction of the removal efficiency.

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
Algorithm Type: Artificial Neural Network				
0.88	29 experimental data set	- initial dye concentration - initial pH - contact time - temperature	- maximum removal efficiency	[38]
0.97	experimental data set	- temperature - stirring rate - initial ethyl benzene - xylene (BTEX) concentration - contact time - pH - adsorbent dose	- removal efficiency	[40]
0.98	18 experimental datasets from the literature	- pH - adsorbent dose - initial coupons concentration	- removal efficiency	[41]
0.98	experimental dataset	- pH - initial heptachlor concentration - contact time	- heptachlor removal efficiency	[42]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
		- stirring rate - adsorbent dose		
0.99	experimental dataset	- dose of photocatalyst - the power of visible light - initial concentration of tetracycline - radiation time - oxidant concentration	- removal percentage of tetracycline	[4]
Algorithm Type: genetic algorithm				
0.86	29 experimental data set	- initial dye concentration - initial pH - contact time - temperature	- maximum removal efficiency	[38]
Algorithm Type: adaptive neuro-fuzzy inference system				
0.94	18 experimental datasets from the literature	- pH - adsorbent dose - initial coupons concentration	- removal efficiency	[41]
0.98	experimental dataset	- pH -	- heptachlor removal efficiency	[42]

Accuracy	Database (Type and Size if Available)	Input Parameters	Output Parameters	Reference
		initial heptachlor concentration - contact time - stirring rate - adsorbent dose		
0.99	experimental data	- dose of photocatalyst - the power of visible light - initial concentration of tetracycline - radiation time - oxidant concentration	- removal percentage of tetracycline	[4]

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