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Booklet of Abstracts

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Content

Jakub Adamczyk, MSc. Eng. – 3rd Prize of the XVI Ed. PTIB Competition (2022)

APPLICATION OF GRAPH NEURAL NETWORKS AND GRAPH DESCRIPTORS FOR GRAPH CLASSIFICATION

Abstract: Graph classification is an important area in both modern research and industry. Multiple applications, especially in chemistry and novel drug discovery, encourage rapid development of machine learning models in this area. To keep up with the pace of new research, proper experimental design, fair evaluation, and independent benchmarks are essential. Design of strong baselines is an indispensable element of such works.

In this thesis, we explore multiple approaches to graph classification. We focus on Graph Neural Networks (GNNs), which emerged as a de facto standard deep learning technique for graph representation learning. Classical approaches, such as graph descriptors and molecular fingerprints, are also addressed. We design fair evaluation experimental protocol and choose proper datasets collection. This allows us to perform numerous experiments and rigorously analyze modern approaches. We arrive to many conclusions, which shed new light on performance and quality of novel algorithms.

We investigate application of Jumping Knowledge GNN architecture to graph classification, which proves to be an efficient tool for improving base graph neural network architectures. Multiple improvements to baseline models are also proposed and experimentally verified, which constitutes an important contribution to the field of fair model comparison.

Results of this thesis have been expanded into Local Topological Profile baseline method for graph classification [1] and published at ICCS 2023 conference [2].

References:

[1] Adamczyk, Jakub, and Wojciech Czech. "Strengthening structural baselines for graph classification using Local Topological Profile." arXiv preprint arXiv:2305.00724 (2023).

[2] Jakub Adamczyk and Wojciech Czech. 2023. Strengthening Structural Baselines for Graph Classification Using Local Topological Profile. In Computational Science – ICCS 2023: 23rd International Conference, Prague, Czech Republic, July 3–5, 2023, Proceedings, Part IV. Springer-Verlag, Berlin, Heidelberg, 597–611. https://doi.org/10.1007/978-3-031-36027-5_47

Karolina Knap, MSc. Eng. – 3rd Prize of the XV Ed. PTIB Competition (2021)

POLYMERIC DRUG MICROCARRIERS FOR THE TREATMENT OF RESPIRATORY INFECTIONS

Abstract: Nowadays, one of the significant health problems is bacterial recurrent lower respiratory tract infections. In my master's thesis, I worked on the development of a drug delivery system (DDS) for infected lungs by inhalation. In principle, such DDS has many advantages: large lung surface area, high doses delivered directly to the action place, the same therapeutic effect obtained with the use of the lower drug doses in comparison to oral or intravenous administration, decreased time between administration and the onset of action, reduced risk of drug inactivation and decreased systemic side effects. Such inhalable DDS must meet several requirements: the aerodynamic diameter in the range of 1 - 5 μm, matrix biocompatibility, high encapsulation efficiency, fast degradation rate, and antibacterial activity [1].

In my research, I used poly(sebacic acid) (PSA), which is a polyanhydride, which quickly degrades in an aqueous environment by surface erosion. The drug encapsulated in the PSA matrix was azithromycin, a macrolide antibiotic, which is used in the treatment of bacterial lung infections. The microparticles were manufactured using an oil-in-water emulsification with a solvent evaporation method. The morphology of the microparticles was characterized by scanning electron microscopy (SEM). All types of microparticles were smooth and spherical. On the basis of the SEM images, the microparticle geometric diameters were smaller than 2 μm. However, when the powder was measured by the dynamic light scattering (DLS) method, the microparticle size was in the range of 1 - 5 μm. It means that microparticles have a tendency to agglomerate. The encapsulation efficiency was determined by high-performance liquid chromatography, which showed encapsulation efficiency of up to 99.5%. The degradation study was evaluated in phosphate buffer saline and the morphology and mass of the microparticles, as well as the pH of a surrounding medium, were evaluated. The microparticles degraded very fast. After 24 h the mass of the microparticles decreased by around 50%, and after 96 hours by 70%. The pH decreased from 7.4 to 5.8. The cytocompatibility of empty and azithromycin-loaded microparticles was evaluated using the Alamarblue test and live/dead staining in contact with A549 and BEAS-2B lung epithelial cells. For both cell types, the concentration of 50 μg/ml was found to be non-toxic. The antibacterial activity of the microparticles was confirmed by an agar diffusion test against *Staphylococcus aureus* [2].

In summary, the microparticles were successfully manufactured using the emulsification method. They were characterized by a spherical shape, size suitable for inhalation, high encapsulation efficiency, and fast degradation allowing delivery of required doses to the infected place in the lungs. The microparticles were found to be not cytotoxic at a concentration of 50 μg/ml for both lung epithelial cells and have antibacterial properties.

References:

[1] K. Knap, K. Kwiecień, K. Reczyńska-Kolman, and E. Pamuła, "Inhalable microparticles as drug delivery systems to the lungs in a dry powder formulations," *Regen. Biomater.*, vol. 10, p. rbac099, Jan. 2023, doi: 10.1093/rb/rbac099.

[2] K. Knap *et al.*, "Poly(sebacic acid) microparticles loaded with azithromycin as potential pulmonary drug delivery system: Physicochemical properties, antibacterial behavior, and cytocompatibility studies," *Biomater. Adv.*, p. 213540, Jun. 2023, doi: 10.1016/j.bioadv.2023.213540.

Anna Maria Pawłowska, MSc. Eng. – 1st Prize of the XIV Ed. PTIB Competition (2020)

ASSESSMENT OF THE EFFECTIVENESS OF BREAST CANCER CHEMOTHERAPY USING ULTRASOUND DATA

Abstract: Breast cancer is the most commonly diagnosed cancer and the most common cancer-related cause of death in women in Poland [1]. Neoadjuvant chemotherapy (NAC) is one of the types of breast cancer treatment used before definitive surgical therapy. NAC treatment causes shrinkage of the tumor in size, thus facilitates resectability of inoperable tumors or enables breast-conserving surgery. After NAC and mastectomy, the number of remaining cancer cells is estimated in a histopathological examination to evaluate pathological response to treatment. The effectiveness of NAC is varying. The purpose of this work was to analyze the possibility of predicting tumor response for chemotherapy based on image quality indices from ultrasound data. Prediction of tumor response at an early course of NAC could guide further treatment. For responding patients, it could result in breast-conserving surgery and psychologically support patients. For non-responding patients, the NAC regimen could be stopped and switched to more appropriate therapy. In the presented study, image quality parameters were used as an impartial quantitative measure of changes in tumor tissue during NAC. The ultrasound data (which are available at the Institute of Fundamental Technological Research of the Polish Academy of Sciences) were collected from 38 breast tumors before the NAC therapy and after each of the six subsequent treatment cycles. Ten image quality parameters (mean square error, root-mean- square error, signal-to-noise ratio, peak signal-to-noise ratio, correlation coefficient, image quality index, structural similarity index, and Wu's, Wen's, Hsia's grey relational coefficients) were computed from log compressed envelope data. Four regions of interest were considered - three rectangular areas: inside the tumor, on the edge of the tumor, covering the tumor and the surrounding normal tissue, and the fourth region was represented by the mask indicated by the radiologist, i.e. the shape of the region depends on the shape of the tumor. Image quality indices were determined using sliding windows. The values of image quality indices were obtained for each chemotherapy cycle but the statistical analysis was carried out for the data derived from the images after the first cycle of chemotherapy (as the earliest prediction is needed). First, the differences among the group's means were assessed using the analysis of variance. Next, the ability to predict the effects of chemotherapy was evaluated based on the area under the ROC curve (AUC). As a final result of the work [2], the analysis showed that the algorithm determining the values of image quality parameters for breast ultrasound data allows to obtain an area under the ROC curve of 0.87 after the first cycle of NAC. The results indicate that the values of the GRC parameter may reflect the changes in tumor tissue structure during chemotherapy. Thus, it may support the physician in evaluating the effects of NAC and contribute to an increase in the number of breast-conserving procedures.

References:

[1] Nowotwory złośliwe w Polsce w 2018 roku. Krajowy Rejestr Nowotworów, Ministerstwo Zdrowia 2020

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