# The Impact of Computational Drug Discovery on Society

GREETINGS and welcome to the fifth issue of IEEE TRANSACTIONS ON COMPUTATIONAL SOCIAL SYSTEMS (TCSS) for 2023. This edition presents a collection of 55 diverse regular articles that illuminate various facets of the interaction between computer technology and society.

In this release, we are excited to introduce the Special Issue on Social Studies, Human Factors, and Applications in Metaverse. Comprising five articles, this special issue delves into the intricacies of the metaverse—an evolving digital realm entwined with our lives. We extend our gratitude to the authors, reviewers, and guest editors for their valuable contributions to this exploration.

Moreover, we seize this moment to share some of our opinions and perspectives on "The Impact of Computational Drug Discovery on Society." This topic underscores the convergence of computational methodologies and biology.

Our appreciation goes to the dedicated authors, reviewers, and editorial board members who drive TCSS forward.

## I. SCANNING THE ISSUE

In [A1], a local spatial-temporal synchronous network (LSTSN) for skeleton-based dynamic gesture recognition is proposed. Specifically, a coupled position embedding and a three-neighbor local spatial-temporal graph (LSTG) are constructed. An adaptive threshold method is designed to describe the joint connections of LSTG, and then, an attention mechanism is used to efficiently capture complex local spatial-temporal correlations. Meanwhile, multiple spatial–temporal attention modules of different periods are designed to effectively capture the LSTG's heterogeneity. Besides, from the data aspect, a hand motion vector (HMV) is also introduced into the model to express subtle finger motions.

The authors in [A2] develop three new visualization methods for collective idea generation and innovation processes and applied them to data from online social network experiments. The first visualization is the Idea Cloud, which helps monitor collective idea-posting activity. The second is the Idea Geography, which helps understand how the idea space and its utility landscape are structured and how collaboration was performed. The third is the Idea Network, which connects idea dynamics with the social structure, displaying how social influence may have affected collaborative activities and where innovative ideas arose and spread.

In [A3], the authors propose a confidence-based opinion adoption model, which considers the opinion and confidence according to the traditional linear threshold model. Based on this model, they propose the directed graph convolutional network method to select the k most influential positive cascade nodes to suppress the propagation of rumors. The experimental results show that the method can sufficiently suppress the propagation of rumors and obtain a smaller number of rumor nodes than the baseline algorithms.

To explore recommendation-specific auxiliary tasks, the authors in [A4] first quantitatively analyze the heterogeneous interaction data and find a strong positive correlation between the interactions and the number of users. Based on the findings, they design two auxiliary tasks that are tightly coupled with the target task toward connecting recommendation with the self-supervision signals hiding in the positive correlation. Finally, a model-agnostic dual-auxiliary learning framework, which unifies the self-supervised learning and recommendation tasks, is developed.

In [A5], the authors propose an interaction recommendation model that is based on enhanced graph convolution and fuses review properties (PGIR), which incorporates property information into text modeling by different activations and matches useful property feature interaction pairs for review text in a self-supervised manner. They design an enhanced graph convolution method to capture the collaborative signals between users and items and model the dynamic features on this basis. The results show that the PGIR model achieves a substantial improvement over existing state-of-the-art models in terms of rating prediction, and the superiority property activation method, which further improves the rating prediction performance of the PGIR model.

In [A6], the authors propose a biased-random-walk-based community detection (BRWCD) algorithm to capture the intricate relationships between nodes. First, a topology-weighted degree is designed to enhance the random walk at the boundary of and inside a community to extract communities precisely. Second, they design an attribute to node influence index and an attribute-weighted degree to distinguish different attributes' influence on node transition to obtain communities with high internal cohesion. Comprehensive experiments on the real-world and synthetic networks demonstrate that BRWCD achieves nearly 10% higher accuracy at most than the state-of-the-art algorithms.

In [A7], the authors propose an agent-based framework equipped with a population-mixing algorithm, and stochastic disease transmission and evolutionary dynamics. The disease

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model characterizes the health condition of agents using three crucial traits of the disease: 1) infection status; 2) severity; and 3) awareness, endowed with age-dependent probabilities for transmission, progress, and recovery of the disease. Together with different mobility patterns, they demonstrate the impact of migratory measures, such as social distancing, vaccination, testing, isolation, and containment zones, on the spread of disease. The results indicate that enhanced mobility of agents facilitates contagion, and a combination of mitigation strategies needs to be adopted to combat the spread of the disease effectively.

Brain–computer interface (BCI) has been widely used in medical diagnosis, rehabilitation, education, entertainment, and so on. To protect privacy in BCIs, the authors in [A8] fill this gap, by describing potential privacy threats and protection strategies in BCIs. They also point out several challenges and future research directions in developing privacy-preserving BCIs.

In [A9], the authors present a Reddit health mention dataset (RHMD), a new dataset of multidomain Reddit data for the HMC. RHMD is composed of 10015 manually annotated Reddit posts that include 15 common disease or symptom terms and are labeled with four labels: personal health mentions (HMs), nonperson HMs, figurative HMs, and hyperbolic HMs.

In [A10], the authors propose a new methodology framework, the semiparallel service system (SPSS) framework, following the CPSS architecture and artificial societies, computational experiments, and parallel execution methodologies emerging in complex system modeling. They design two decomposition-then-aggregation loops to reduce the complexity of service systems innovation. Following this framework, it can design prototypes, perform experiments, and run the hybrid service system. They use two cases, an Internet hospital platform design and a new service design in a customs-bonded warehouse, to demonstrate the advantages and potential of the proposed methodology.

The authors in [A11] propose a social network rumor detection method combining a dual attention mechanism and graph convolutional network (GCN) (dual-attention GCN, DA-GCN). First, build an event propagation graph, the anti-interference propagation structure features are extracted from the propagation graph. Second, make use of the attention mechanism to fuse source microblog (tweet) with the comment-retweet information and extract interactive semantic features from it. Finally, the above two features are fused to generate a new event representation. The experimental results show that the proposed DA-GCN has an accuracy of 94.4%, 90.5%, and 90.2% on the Weibo dataset, the Twitter15 dataset, and the Twitter16 dataset, respectively, which proves that the proposed method is reasonable and effective.

In [A12], the authors propose a method to predict election results via Twitter. They develop four different counting methods for prediction tasks. They evaluate the proposed methods with the data collected for the presidential election of Turkey held in 2018. The extensive evaluation shows that utilizing domain-specific information and location-based weighted counting is effective in reducing bias.

In [A13], Rising Business Managers are classified by exploring features of Co-Business Managers, rather than their own work history. The dataset is classified into two different evaluation set-ups. One is Average Revenue and the other one is Average Relative Increase in Revenue- class labels. All instances for both labels are randomly sorted into multisize (10, 20, 30, to 100) datasets. Later on, these datasets are explored through machine learning classifiers using 5-fold cross-validation. In terms of precision, recall, and f-measure, feature, category, and model-based experimental results show that the generative models, particularly Bayesian Networks produce better results for an average revenue-based dataset.

The authors in [A14] propose a novel search space reduction strategy-based progressive evolutionary algorithm (SSR-PEA) for solving Influence maximization (IM) problems effectively and efficiently. A novel search space reduction strategy is designed to reduce the computational overheads, which eliminates a great deal of less influential nodes in a sensible way. They propose a progressive evolutionary framework based on SSR, where the $k$-element individual is optimized on the basis of the ($k$-1)-element individual to speed up the optimal solution search process. The experimental results on ten real-world networks demonstrate that the proposed algorithm SSR-PEA can achieve 98% of the influence spread achieved by cost-effective lazy forward on average, and its running time is two or even three orders of magnitude shorter.

In [A15], the authors develop an extended model to simulate the evacuation process involving nondisabled, visual-disabled, acoustic-disabled, and physically disabled pedestrians. Numerical simulations indicate that this model achieves a more realistic mixed crowd evacuation in the library scene and reproduces the escape movement of multitype disabled pedestrians. Moreover, several management strategies are provided to guide the evacuation of disabled pedestrians, and the appropriate strategy can be determined by comprehensively considering multiple factors such as efficiency, safety, and cost.

A new code hybrid corpus called BullySentEmo is created in [A16], annotated with bully, sentiment, and emotion labels. The author solved the problem of considering the emotions and emotional tag information of tweets when identifying online bullies. A multitasking and multimodal framework based on end-to-end dyadic attention mechanism (DAM), called multitask multimodal cyberbully detection (MM-CBD), is proposed for emotion and emotion-assisted network bullying detection. The experimental results demonstrate that the MM-CBD framework has significant advantages over all single-task and single-peak models.

In [A17], the authors propose two unsupervised learning algorithms that belong to a special class of graph convolution networks (GCNs): 1) clustering as feature embedding (CAFE) and 2) Sphere. It has been proven that CAFE and Sphere can also be used to solve dimensionality reduction problems and obtain approximations of the eigenvectors from principal component analysis (PCA). A multilayer CAFE algorithm was also proposed to output multiresolution embedding vectors for sampling images. Various experiments were conducted to evaluate the algorithm and demonstrate that the proposed algorithm outperforms several baseline methods.

In [A18], the authors propose a hybrid deep neural network for multimodal personalized label recommendation, namely multimoDal pErSonalIzed hashtaG recommeNdation, which can solve label recommendation tasks by jointly developing multilabel classification and sequence generation problems. The method proposed in the article predicts suitable tags for posts by mining information from text and visual patterns. Word-level attention is used in text mode, and then a parallel co-attention mechanism is used to simulate the interaction between text and visual modes. The experimental results show that this method achieves superior performance compared to existing methods.

In [A19], the authors design a controlled indecisive weighted voting system (WVS) with unknown inputs (UIs). In order to monitor the decision-making process, feedforward control is applied to eliminate interference and generate fast output in WVS. To stabilize the system, feedback control is used to create a closed-loop system. The input is provided by the unknown input observer (UIO) system. Two unresolved issues were briefly introduced, namely the observer selection criteria for UIO systems and the overall system stability of nonlinear WVS. Finally, the difficulties of future research were pointed out.

In [A20], the authors design a condition-dependent inspection and maintenance strategy with imperfect preventive maintenance and applies it to the performance and cost modeling of safety monitoring systems with competitive failure modes and degradation processes. The expected long-run cost rate (ELCR) of minimizing the system is used as an evaluation indicator for the system. An improved Nelder–Mead downhill simplex method is proposed to find the optimal inspection strategy for minimizing ELCR. The modeling process and results of this article can be applied to security monitoring systems in many fields.

In [A21], the authors construct a zero-sample hate to nonhate text style conversion system. This system effectively converts unsupervised hatred to nonhatred without using any hate domain text for training. The author also proposes a decoding technique based on lexical constraints on a zero sample style transmission system and defines additional steps to introduce lexical constraints when decoding the output generated by the system to better preserve content. Detailed empirical evaluation shows that the method outperforms traditional unsupervised style transfer methods for a given task.

In [A22], the authors propose a new indexing technique called global structure influence (GSI) to identify the dynamics of disease transmission in heterogeneous networks. Due to its consideration of the local and global impacts of network nodes, the proposed GSI is more robust. This method can collect information from multiple levels of the neighborhood and use susceptible-infected-recovered (SIR) evaluation metrics as a traditional benchmark to determine the probability of infectious transmission in the network. The method was evaluated by considering different types of networks, and the results showed that the GSI method outperformed the baseline indexing technique in the SIR benchmark ranking.

In [A23], the authors propose a summary and conclusion of the research progress and future research directions of social manufacturing (SM). Covering the definition and basic theory of SM, it also discusses the SM ecosystem and business model, value chain design and analysis, and the transformation model towards SM. In addition, key supporting technologies that can be used to implement SM, such as blockchain, 3-D printing, and big data, were also introduced. Then, examples were provided to illustrate the application of SM in various product production processes. Finally, the future trends of SM ecosystem development were briefly discussed.

The authors in [A24] propose a new target label adversarial attack for graph embedding methods to generate effective perturbations with minimal impact on prediction confidence, namely Graphfool. It utilizes the classification boundaries and gradient information in the target graph embedding method to generate adversarial graphs to attack the graph embedding method. Graphfool can take any differentiable graph classifier as an attack model, and construct a decision boundary according to its classification results, thus generating the minimum distance perturbation that allows target instances to cross the specified classification boundary. Experiments have shown that Graphfool achieves state-of-the-art attack performance in a more covert manner.

The authors in [A25] propose a multimodal cooperative guidance (MMCG) system framework that considers three guidance modes for crowd evacuation command in emergency situations. A double-layer MMCG optimization problem was established to determine the optimal allocation scheme, namely the number and initial position of multimodal guidance. The MMCG scheme is designed by minimizing the cost function. An extended social force model is proposed for the problem of crowd evacuation dynamics under multimodal guidance. The experimental results indicate that the system improves the efficiency of crowd evacuation and the utilization of exits.

In [A26], the authors propose an effective supervised deep neural network, called the human action attention network (HAANet), which can be used for action recognition to capture long-term dependencies in videos. HAANet effectively distinguishes fuzzy action classes based on emotions and gestures. A new shallow backbone network is designed, in which lateral connections are used to learn the spatio-temporal features with rich details. The article also proposes a temporal attention pooling that combines class-aware attention pools to capture discriminative semantic features. The effectiveness of HAANet was validated on five benchmark datasets.

In [A27], the authors develop a novel graph-based model, which is named graph-aware deep fusion networks (GDFNs). It uses information from relevant metadata and relational data to capture the semantic information from their complex heterogeneous interactions via graph convolutional networks (GCNs). Besides, the authors also use the fusion mechanism to obtain the inherent relationship among users, reviews, and items. Extensive experiments on publicly available datasets show that the model proposed in this article is effective and outperforms several strong state-of-the-art baselines.

In [A28], the authors propose an online clustering approach utilizing the autoencoder. The training is performed by considering the multiple views of articles and posing the topic

modeling (TM) problem as a multiview (MV) clustering problem. Besides, the authors employ an evolutionary-based approach to the latent representation of data to automatically determine the number of clusters. The model simultaneously optimizes the reconstruction loss and clustering loss in an MV framework. The superiority of the proposed method in generating clusters as well as in determining scope is shown by comparing the results with many existing and baseline methods.

In [A29], the authors developed and tested a scoring system to estimate the risk of low bone density (LBD) in women aged 50 years or older. Five variables about the body were obtained and used to construct the system mentioned earlier. The results suggested that the performance of the proposed scoring system on the evaluation of LBD is encouraging. This proposed scoring system, based on very basic check-up items, is of great practical use for mass screening for LBD in older women post-body examination.

In [A30], the authors propose a trust-aware detection framework to detect malicious users based on different kinds of data from a real dating site. Particularly, the authors develop a user trust model to distinguish between malicious and legitimate users. Furthermore, the authors propose a novel data-balancing method to improve the recall rate of malicious user detection. The results of extensive experiments over real-world datasets show that the proposed approach yields a precision of up to 59.16% and a recall rate of up to 73%, which is significantly higher than other baseline algorithms.

In [A31], the authors define a simple yet effective network generation mechanism. It can learn model parameters efficiently and produces simulated networks having structural properties close to a given input real-world signed social network. In the proposed model, a characteristic function is defined that controls its dynamics and its link formation process corresponding to each node. Besides, two layers are modeled independently, and further superimposition of layers is applied to get the final simulated signed network. Apart from that, the experimental results manifest that the proposed model performs better for structural reconstruction compared to the considered state-of-the-art network models.

The authors in [A32] present an ensemble model based on recurrent neural networks (RNNs) for financial market prediction via news disclosures. Sentiment analysis and the sliding window method are applied to extract the most representative features from financial news and historical data. This greatly reduces the number of dimensions compared to traditional preprocessing strategies that extract tens of thousands of features. With the extracted features, an ensemble approach of RNNs is applied for stock market prediction, and the results demonstrate that the ensemble model outperforms the other state-of-the-art models under comparison.

The authors [A33] propose a problem about maximizing the positive influence in signed networks within a limited time; furthermore, they utilize the influence path to calculate the influence probability and propose an algorithm that is based on forwarding index and inverted index. In the proposed algorithm, the authors first select candidate seed nodes by combining two effective heuristic methods. Then, they design an algorithm to get the activation probability between node pairs in social networks. At last, they devise a method that combines the forward index and the inverted index with the idea of cost delay.

In [A34], the authors build a four-layer mining pool evaluation model. The model contains three first-level indicators and nine second-level indicators, covering various aspects of the performance of the mining pool. Miner address extraction provides basic data for the calculation of these indicators. By utilizing the model proposed, the authors evaluate and rank eight mainstream mining pools. Through comparative analysis of evaluation results, the authors find that the 65% decline in mining power in June did not pose a threat to the stability of the Bitcoin system. In addition, they also reveal the reasons for various fluctuations.

In [A35], the authors propose a diffusion method for online rumors based on three messages: rumor, anti-rumor, and motivation-rumor. First, the authors decide to use the representation learning method to the diversity and complexity of the content and structure feature space. Second, they construct a new network topology using cooperative and competitive relationships based on the evolutionary game theory. Finally, considering the ability of graph convolutional network (GCN) to convolute non-Euclidean structure data such as social network, and in view of the time effectiveness of topic evolution, this study proposes a dynamic and game-GCN (evolutionary game theory GCN)-based rumor diffusion model.

In [A36], the authors propose the Adversarial Heterogeneous Graph Neural Network for RECommendation (AHGNNRec). This is a neural framework that learns user and item embedding by exploring the different contributions of various types of interactions between users and items using a hierarchical heterogeneous graph neural network (HGNN). In order to improve robustness, the authors adopt the adversarial training (AT) method to optimize the HGNN layer. Finally, a large number of experiments are conducted on two real datasets, and the results prove the effectiveness of AHGNNRec.

The authors in [A37] use the content data and communication relationship structure data of multinews rumor topic transmission space in social networks to construct a rumor topic forwarding prediction model, which can predict the rumor and anti-rumor forwarding situation in the next period. The authors design presentation learning to fully represent various features of communication space and integrate the influence of multiple messages on the communication relationship structure. Finally, they predict the behaviors of potential users and discretize the active time of topics to get the development trend of rumor topics.

In [A38], the authors propose an information-enhanced hierarchical self-attention network. The self-attention mechanism performs well in capturing long-term dependency; however, it does not efficiently capture the local context in the sequence and relies heavily on position embeddings. Therefore, they propose adding local and syntactic information to the word-level encoder and adding the dialog structure information to the utterance-level encoder to improve the hierarchical self-attention mechanism's contextual information

modeling ability. Finally, the correlation between context and reply is calculated and used in further decoding.

In [A39], the authors creatively propose an aboosting-truth blocking-rumor cascade model. Second, based on it, they propose a positive boosting-truth blocking-rumor cascade model. They design a multihop neighbor boosting algorithm that considers influence probability, hops of truth spreads, and the number of out-neighbors of nodes. They design a multihop neighbor boosting algorithm, which can get effective results with a data-parameter-dependent approximation ratio. Based on the above model, they also propose a positive boosting-truth blocking-rumor cascade model and design a connected multihop neighbor boosting algorithm to solve the connected positive boosting rumor controlling problem that requires a seed set to be connected under this model.

In [A40], in order to extract events from academic we-media blogs into the academic knowledge graph, the authors propose a framework construct-SCHOLAT knowledge graph to complete event extraction that integrates the academic social attributes of the scholar. The framework mainly includes two parts: data preprocessing and event extraction. In the data preprocessing, they propose a knowledge graph embedding method to represent scholars' academic social features. In the event extraction, they concatenate the preprocessed scholar vector with academic we-media blog text into the extraction model based on BiLSTM-CRF fused with an attention mechanism.

In [A41], the authors address the challenges of using call detail record (CDR) data to study migration. Repurposing CDR data for this task has many advantages, including the lower costs of data collection and the potential for contemporaneous analysis. The authors present a framework for the repurposing and analysis of CDR data. They identify the home location of a subscriber, with corresponding confidence measures, and determine if the subscriber is a definite migrant, likely migrant, likely nonmigrant, or definite nonmigrant. A predictive model then uses mobility and social network features, extracted from the CDR data, to predict the individual decision to migrate.

In [A42], the authors propose a multiview deep matrix factorization model to learn a shared compact representation from multiview data. The proposed method represents each view through a uniform representation matrix, which makes full use of the information of weights and relationships across all views. The encoding of the representation matrix is restricted so that the learned low-dimensional subspace can preserve the discriminative components for downstream tasks. The proposed model also improves the pertinence of the information and the performance of the subsequent tasks. And it is easily built and trained end-to-end for the output of a clustering indicator.

In [A43], authors obtain data from up to 135 000 000 blocks of EOSIO and conduct a data-driven decentralization analysis. Specifically, they characterize the decentralization evolution of the two phases in Delegated Proof-of-Stake (DPoS), namely, block producer election and block production. Some suspected voting manipulation phenomena are revealed in their analysis. Besides, they discuss the root cause of the oligopoly trend and the mechanisms for enhancing the decentralization of EOSIO according to the analysis results, which can also provide a reference for other DPoS-based blockchain systems.

In [A44], the authors develop a multimodal Siamese-based architecture, which uses attention between the text and emoji parts of the tweet for generating a combined representation of the tweet. Using a weighted attention-based mechanism, their proposed system filters out the relevant information generated from two modalities. After that, the filtered features are fed to the softmax layer for the final prediction. The effect of the attention module is shown through different examples, which proves the importance of the proposed attention-based system. It is demonstrated that the attention module is able to filter out relevant features from emojis and tweets.

In [A45], the authors propose a hybrid social evolution mechanism based on Q-learning. The evolution of social relations is realized from the perspective of individual, group, and global situations to improve the success rate and comprehensive effectiveness of task allocation in the system while reducing the communication cost during task execution. In addition, the hybrid evolution mechanism considers the balance of interests between the global and the individual, which can guarantee the rationality of task benefit distribution while improving global effectiveness.

In [A46], the authors follow a qualitative approach. The data analysis approach considered is an axial coding technique as part of the grounded theory, which includes open coding, axial coding, and selective coding stages. The results reveal that the time factor, trust in Insta shops distrust, and the associated risks can impact users' behaviors toward Insta shopping. Also, the study classifies participants' viewpoints and experiences' themes into advantages, disadvantages, and issues that are associated with Insta shopping.

In [A47], the authors construct a novel end-to-end model that hierarchically learns discriminative features for accurate depression detection. After that, they design a hierarchical multifeature fusion framework, in which the intraresponse fusion facilitates the aggregation of multiple acoustic features from the original audio signals, while the interresponse fusion enables the in-depth aggregation of multiple response segments. The stages of intraresponse fusion and interresponse fusion facilitate the extraction and aggregation of automatic depression detection (ADD)-specific information from multiple kinds of acoustic features. In this way, they obtain the compact feature representation that is able to accurately differentiate the depression state from the normal state.

In [A48], the authors conduct research on automatic depression detection based on the visual cues recorded in the interviewing process. They first construct a temporal dilated convolutional network (TDCN), in which multiple dilated convolution blocks are designed and stacked, to learn the long-range temporal information from sequences. Then, the feature-wise attention module is adopted to fuse different features extracted from TDCNs. The module learns to assign weights for the feature channels, aiming to better incorporate different kinds of visual features and further enhance the detection accuracy.

The authors in [A49] present the predictive lethality analysis of terrorist organization (PLATO) algorithm to measure the lethality of terrorist networks. PLATO algorithm merges machine learning with techniques from graph theory and social network analysis. This article shows that the most significant macrofeatures for predicting Al Qaeda (AQ)'s lethality are related to their public communications (PCs) and logistical subnetworks, while the leadership and operational subnetworks are most impactful for predicting ISISs lethality. PLATO is highly accurate on two novel datasets, which cover AQ and the Islamic State.

The authors in [A50] propose an inductive representation learning model (IRLM) for location recommendation to address the problems in the current enhancement of point of interest (POI) recommendation based on auxiliary geographical information. IRLM contains two parts, namely geographic feature extraction and inductive representation learning. This article first extracts the geographical features by taking all check-in data into account. Then, it learns the user and POI embeddings with an attention convolutional network by considering the aggregation of vertex neighbors.

In [A51], the authors propose a dynamic model of information dissemination based on the user's own awareness and evolutionary game. The proposed model comprehensively considers the impact of differences in user awareness on information dissemination and the mutual game between different awareness messages. In addition, considering that a trend may gradually fade away over time with the emergence of new trends, the authors introduce a time-slicing mechanism to analyze the information dissemination trend under different heats and verify it using a public dataset, and the results show that the model can more realistically describe the information dissemination trend in social networks.

The authors in [A52] examine adversarial robustness problems on deep hashing models designed for similarity retrieval. By theoretically analyzing the designing principle of deep hashing models, they present an approximately inferred method to produce effective adversarial perturbations for attacking well-trained retrieval models. They retrain several state-of-the-art deep hashing models to evaluate the effectiveness of our perturbation generation method, and find that existing deep hashing models designed for image text retrieval and large-scale image-retrieval tasks are all vulnerable against small attacks. By adding human-unrecognized attacks on image samples, the retrieval accuracy of well-crafted deep hashing models can be decreased sharply.

In [A53], the authors investigate the persistent divergence and consensus of opinion dynamics on the issue sequence. The issue-sequence-based opinion dynamics model is proposed to reproduce the social phenomenon of cognitive freezing. In addition, the evolution of opinions under the bounded confidence issue sequence is studied, proving that private opinions and public opinions can reach a consensus. Simulation analysis shows that the convergence speed of individuals is inversely proportional to the social power of individuals, and the number of consensus-reached issue sequences is directly proportional to the number of individuals and inversely proportional to the confidence threshold.

In [A54], the authors address the problem of modeling and orchestrating the interactions between a museum and its visitors, viewing the system as a cyber-physical-social system (CPSS). Following the principles of labor economics, an optimization problem between a museum and visitors is formulated and solved. Based on the results obtained, the authors conclude that a visitor's high cost to provide evaluation results in low levels of engagement with the museum touring and knowledge sharing, and more.

Recently, the social network DeGroot (SNDG) model has been widely used in opinion dynamics. Based on this, the authors in [A55] study how agents' high self-confidence levels affect the consensus convergence speed in the SNDG model. Using theoretical analysis, the authors prove that: 1) the speed of consensus reaching is subject to the largest self-confidence level of opinion followers and 2) the speed of consensus reaching is also subject to the top two self-confidence levels of opinion leaders. Furthermore, through extensive simulation, they find that the theoretical results are robust to the topological structure and the size of social networks.

## II. The Impact of Computational Drug Discovery on Society

The development of pharmaceuticals is intricately linked to individuals' health conditions and the burden of diseases, profoundly shaping patients' lives and impacting overall societal well-being. Precision targeting in drug development achieves accurate disease treatment. Take imatinib as an example, it is a targeted therapy for chronic myeloid leukemia that significantly elevates patients' survival rates and quality of life by inhibiting the BCR-ABL fusion protein [1]. Similarly, drug repositioning injects vitality into pharmaceutical research. Thalidomide, initially introduced in the 1950s as a sedative and analgesic for relieving preg-nancy-induced nausea in women, was later found to cause severe fetal abnormalities, leading to its prohibition. However, through extensive investigation, Thalidomide exhibited remarkable efficacy in treating various leprosy reactions. The successful application of Thalidomide yielded significant societal benefits, notably improving patients' quality of life [2]. Furthermore, breakthroughs in small molecule drugs have been achieved in other fields. For instance, in 2013, the FDA approved the first direct-acting antiviral drugs (DAAs) for the treatment of Hepatitis C, including sofosbuvir and daclatasvir. Statistics reveal that the combined therapy of these drugs achieves a treatment success rate of over 90%, significantly reducing the risks of severe complications like cirrhosis and liver cancer [3].

However, as diseases continually evolve, the demand for drug development becomes more pressing. Despite technological advancements and a deeper understanding of human diseases, the translation of these advantages into therapeutic progress has been far slower than expected. Recent estimates suggest that introducing a novel medication to the market demands around 13 years and an investment of roughly US$1.8 billion [4]. This cost includes both the creation of the approved pharmaceutical and the inclusion of expenses related to compounds that did not reach market fruition. Unfortunately, failures can occur at various stages of the

drug discovery process, especially in the advanced phases of development. Common reasons for this high attrition rate include lack of clinical efficacy of the potential drug (approximately 30%), unexpected toxicities (>20%) [5]. Therefore, minimizing expenses and the time needed for each distinct stage within the drug discovery pipeline is crucial for improved pharmaceuticals.

The identification of drug-target interactions (DTIs) is a crucial step in drug discovery and development [6]. It involves the identification and validation of specific proteins (e.g., Enzymes, Receptors, Ion Channels) or molecules within the body that are associated with a disease or condition and can be targeted by drugs to treat or alleviate the condition. Historically, the traditional approach to detecting DTIs primarily relied on pre-clinical experiments, encompassing in vitro and in vivo studies, conducted prior to clinical trials, which is known for the large amount of funds and time it consumes. In contrast, contemporary advances in computer technology have facilitated the integration of computer-assisted methods, including the prediction of DTIs. These methods utilize machine learning to mine known information about drug molecules, target proteins, and DTIs from large amounts of biological, chemical, and medical data and to predict potential DTIs. It is important to note that computer-aided DTI prediction does not replace essential experiments in the drug development process. Instead, this approach can guide researchers to conduct targeted drug experiments during the development process, thereby reducing the costs associated with the experimental process [7]. In addition, computer-aided DTI prediction methods can provide clinical guidance, offering medication recommendations and risk prevention measures to healthcare professionals. Compared to traditional methods, computer-assisted techniques dramatically speed up DTI identification, reduce equipment-related losses, and lower costs associated with drug development.

However, target-based drug discovery approaches are difficult to work especially when emerging diseases are poorly understood or targets for diseases are difficult to identify. To this end, drug repositioning is regarded as the potential to increase the efficiency of the drug discovery process. Theoretically, drug repositioning could decrease drug development costs, increase drug approval rates, and decrease attrition rates while maximizing the clinical utility of the repurposed molecule. Repositioned drugs, in which the clinical and safety profiles in humans have already been evaluated, enable a faster, cheaper, and more efficient translation into the clinic [8]. Examples include the repurposing of sildenafil citrate for erectile dysfunction and thalidomide for erythema nodosum leprosum and multiple myeloma. More recently, rapidly developing sin-gle-cell sequencing analyses produce more comprehensive profiles of the genomic, transcriptomic, and epigenomic heterogeneity of tumor subpopulations [9]. This provides a new direction for the development of drug repositioning.

In the process of drug discovery, obtaining biologically active compounds is consistently a highly challenging endeavor. It is estimated that there are approximately 1060 compounds conforming to Lipinski's Rule of Five [10]. Within this vast chemical space, identifying molecules with specific biological activity presents an exceptionally formidable task. Furthermore, even upon identifying hit compounds, further optimization is needed for properties such as absorption, distribution, metabolism, excretion, and toxicity, to identify candidate drug molecules for pre-clinical studies. This entire process can be likened to searching for a needle in a vast ocean. Traditional methods of candidate drug discovery encompass approaches like uncovering potential active molecules from natural sources, employing design strategies by medicinal chemists, and utilizing high-throughput screening (HTS) techniques. However, these methods not only demand a substantial investment of resources but also face challenges of low efficiency and high costs in the pursuit of candidate drugs.

### A. Bioinformatics in Drug Discovery

Bioinformatics techniques are used to assess whether a target is 'druggable'. Conducting such assessments during the phases of drug discovery, it is possible to reduce the risk of project failure later on in the discovery proces [11], [12]. In this section, we will introduce the application of bioinformatics in drug discovery in three parts, e.g., drug-target, drug repositioning, and drug molecule generation and optimization.

Original methods for DTI prediction can be broadly categorized into structure-based and ligand-based approaches. Structure-based approaches rely on the availability of accurate 3-D structures of target proteins and require a large amount of computational resources. They are not applicable when such structures are unknown or challenging to obtain. Ligand-based approaches heavily rely on historical bioactivity data. They have limited predictive power when there is insufficient or no bioactivity data available for specific ligands or targets. With the advancement of computational power, deep learning has surged forward. In recent years, its application has gained prominence in various domains due to its potent learning and representation capabilities. In the realm of DTI prediction, deep learning models have demonstrated success in improving accuracy and interpretability. For instance, Li et al. [13] developed a multiobjective neural network, called MONN, to predict both non covalent interactions and binding affinities between compounds and proteins. Bai et al. [14] presented Drug-BAN, a deep bilinear attention network (BAN) framework with domain adaptation to explicitly learn pairwise local interactions between drugs and targets, and adapt in response to out-of-distribution data. In recent years, knowledge graph technology has garnered attention from researchers. As a structured data representation, knowledge graphs have found extensive use in fields like natural language processing, intelligent question-answering, recommendation systems, and DTI prediction. For example, Ye et al. [15] developed a unified framework, called KGE_NFM, to integrate diverse information from different sources to predict novel DTI by combining knowledge graph (KG) and recommendation system. In addition, further exploration of the mechanism of action between drugs and targets can provide a new perspective for drug discovery. Zhang et al. [16] proposed a multiview deep-

learning model, called DrugAI, to predict activating/inhibiting mechanisms between drugs and targets.

By now, many methods have been developed for drug repositioning. The machine learning-based method utilizes publicly available databases and bioinformatics tools to systematically identify interactions among drugs, diseases, and genes or proteins. For instance, Napolitano et al. [17] utilized known drug-related data including gene expression, chemical structure, and target information to predict therapeutic classes. Li et al. [18] developed a novel simi-larity-based method to identify new indications of an existing drug through its similar drugs. With the development of high throughput technology and continuously updating databases, there are other types of biological entities frequently involved in drug-disease prediction, such as proteins, diseases, genes, and side effects. Therefore, network-based methods have been widely adopted. Wang et al. [19] presented a novel scoring algorithm to repurpose drugs, which integrates chemical structures, drug-target interactions, pathways, and disease-gene associations. Recently, graph convolutional networks have achieved promising results in various tasks by utilizing both node features and graph topology. A few GCNs-based methods have been proposed for drug-disease association prediction. For instance, Yu et al. [20] designed layer-attention GCNs to capture structural information from the heterogeneous network to predict new drug-disease associations. Cellular heterogeneity inferred from single-cell data can greatly facilitate the accurate prediction of drug sensitivity and help drug repositioning. Although still a relatively new technology, researchers are using single-cell technologies with an increasing frequency to study heterogeneous disorders. For example, gene subnetworks identified from scRNA-seq profiles can be highly correlated with a patient's survival and drug response to cancer [21].

Deep generation models, due to their ability to capture associations between known active molecules and target entities within chemical libraries, have found widespread application in rational design candidate drugs with desired properties. It is shown that the new drug development pipeline based on artificial intelligence and computational biology can complete preclinical drug research in an average of 1–2 years [22]. This holds great potential to significantly accelerate drug development, reduce costs, enhance efficiency, and provide more reliable support for preclinical drug research.

Currently, deep generation models can be broadly categorized into two main types in drug design [23]. The first category involves deep learning techniques used for de novo molecule design. These methods can be classified into those reliant on variational autoencoders, those using autoregressive models, those based on generative adversarial networks, and those flow models. For instance, the GRNN [24] employs a CRU-RNN model based on the SMILES representation to train on the ChEMBL database. It then employs transfer learning to migrate the learned patterns onto 18 small-scale databases, aiming to capture specific molecular features for generating compounds with particular properties. The SyntaLinker [25] is a transformer-based approach for molecule generation. Rooted in the concept of molecular fragments, it retains interacting fragments while ingeniously designing and enhancing the interlinking fragments. The second category comprises molecular optimization models based on reinforcement learning. For instance, the MCMG [26] employs a conditional transformer to generate molecules and subsequently refines the model through reinforcement learning using small-scale datasets. This fine-tuning aims to enable the model to generate biologically active molecules tailored to different target entities. DeepLigBuilder [27], on the other hand, utilizes an L-Net to train the generation of effective 3-D structures for molecules. The approach introduces target-based information into the model to yield molecules with predicted high binding affinity.

### B. Summary

Network pharmacology and deep learning-based approaches have significantly advanced the field of drug discovery. With the improved prediction accuracy on drug targets, a logical next step would be the modeling of the complexity of human biology to understand the heterogeneity of drug response across individual patients and suggest novel treatment options for non responders. To ensure the successful translation of the computer-aided models into drug development and treatment decision-making, it is imperative to refine our models to predict drug-target interactions within specific disease contexts and ultimately to personalize these predictions for each patient.

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## APPENDIX: RELATED ARTICLES

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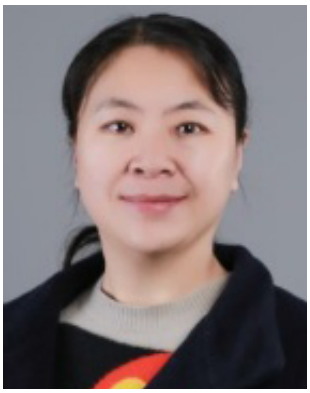

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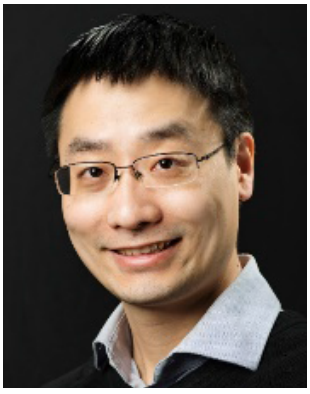

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