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- Neural Reasoning Machines
- Data Storage and Machine Learning
- Implications of Extant Literature
- Productivity with Foundation Models

Discovering Thoughts, Inventing Future

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Neural Reasoning Machine for Recommendation

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Abstract- Most of the existing recommendation models are designed based on the principles of learning and matching: by learning the user and item embeddings and using learned or designed functions as matching models, they try to explore the similarity pattern between users and items for recommendation. However, recommendation is not only a perceptual matching task, but also a cognitive reasoning task because user behaviors are not merely based on item similarity but also based on users' careful reasoning about what they need and what they want.

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NEURALREASONINGMACHINESFORRECOMMENDATION

Neural Reasoning Machine for Recommendation

Jianchao Ji [α], Zelong Li [σ] & Yongfeng Zhang [ρ]

Abstract- Most of the existing recommendation models are designed based on the principles of learning and matching: by learning the user and item embeddings and using learned or designed functions as matching models, they try to explore the similarity pattern between users and items for recommendation. However, recommendation is not only a perceptual matching task, but also a cognitive reasoning task because user behaviors are not merely based on item similarity but also based on users' careful reasoning about what they need and what they want.

In this paper, we propose a Neural Reasoning Machine (NRM) for recommendation. NRM is a neural-symbolic reasoning architecture that can construct different neural networks based on different input logical expressions. Distinct from the continuous prediction values in differentiable machine learning models, the output in symbolic logical reasoning space is binary (true or false). Therefore, an important challenge is to seamlessly integrate symbolic reasoning and continuous learning. To solve the problem, we offer a modularized reasoning architecture NRM. The architecture is designed to acquire symbolic operations like AND, OR, and NOT through neural modules. This allows logical reasoning expressions to be represented as neural networks. By using these neural-symbolic operations, we are able to model complex feature interactions in a latent reasoning space, which is beneficial for tasks such as prediction and recommendation. We test our approach by constructing the feature-based recommendation task as a logical reasoning problem. Experiments show that our neural reasoning machine is significantly better than state-of-the-art (neural or linear) factorization machines in terms of the Top-K recommendation task, and case studies also show the importance of reasoning beyond learning for intelligent decision making tasks such as recommendation.

Keywords: neural-symbolic learning and reasoning; neural logic reasoning; machine reasoning; factorization machines; recommendation.

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I. Introduction

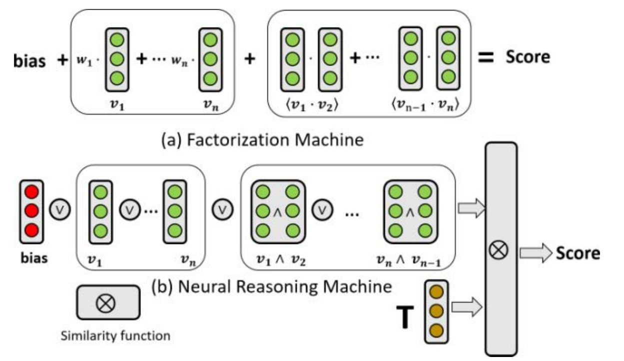

Figure 1: An overview of the fundamental structure of (a) Factorization Machine and (b) Neural Reasoning Machine. As we can see, FM has three components: bias term, first-order features and second-order feature interactions, and it adds up the scores from the three components to calculate the final ranking score, while NRM considers first-order and second-order logical interactions between features, which enables the model to learn the compositional relationships between features for recommendation.

Recommender Systems (RS) play an important role on the modern web as well as in many intelligent information systems. They connect users and information by predicting the potential interest of users and proactively provide relevant information to users [1–3]. Many of the existing recommendation methods are designed based on the fundamental idea of similarity matching [4–13]. For example, some early Collaborative Filtering (CF) models [4, 5, 7]— which predict a user's future preferences based on their previous records—use manually designed similarity functions such as cosine similarity [4], Pearson correlation [5] or vector inner product [7] to calculate the user-item similarities. More recently, researchers have considered learning-based similarity functions such as neural networks to match users and items [6, 8] based on the user and item embeddings that are learned from various types of information sources such as text [14, 15], image [16] and knowledge graphs [17–19].

Factorization Machine (FM) [20–23]—as a type of matching- based model that integrates the power of feature-level and user- item-level similarity—unifies the advantages of different matching- based models and achieves better performance in many recommendation tasks. As illustrated in Figure 1(a), FM considers both 1-order and 2-order feature interactions to predict the user-item preference. Researchers further explored FM under the framework of neural similarity matching. One approach is to increase the neural network depth of the feature similarity matching model, such as Deep Factorization Machine (DeepFM) [21] and eXtremely Deep Factorization Machine (xDeepFM) [22], which provided better recommendation accuracy than the original shallow Factorization Machine (FM) model [20]. Other researchers tried to augment the second-order feature interaction from inner-product to neural networks, such as Neural Factorization Machines (NFM) [23], which overcomes the difficulty that FM model cannot learn feature interactions that did not appear in the training set.

Due to the generally good performance and the flexibility to incorporate various features, similarity matching-based Factorization Machine models have been widely used in real-world applications [22, 24, 25]. However, as a cognition rather than a perception intelligent task, recommendation not only requires the ability of pattern recognition and matching from data, but also the ability of concrete reasoning in data [26]. This is because users do not make decisions simply based on similar users or items, but they make concrete reasoning about the item features and their relationships to decide the next steps. For example, if a user has already purchased a USB hub, then he or she might purchase a USB drive or an external hard drive instead of purchasing another USB hub in the next step, even though the two USB hubs can be very similar. As a result, if we merely rely on similarity-based models for recommendation, the system might recommend similar products to what the user has already purchased even though the user may not need it any more. In this paper, we propose Neural Reasoning Machine (NRM), which is a neural logical reasoning model for recommendation. NRM is able to learn the conjunction and disjunction relationships between features and items so as to model the compositional nature of the recommendation problem. For example, if a user has already purchased a USB hub, then it's unlikely for the user to purchase another one since the two items are substitutive, which can be represented as a low probability between the conjunction of the two items. Technically, we learn the basic logical operations such as AND (∧), OR (∨) and NOT (¬) as neural modules, which are regularized by logical rules to guarantee their logical behavior, and then we represent the feature set of each user-item pair as a logical expression to predict the preference score for the user-item pair, where the logical expression models the logical conjunction and disjunction relationship among the features. For example, if there are two relevant features v_1 and v_2 for a user-item pair, then the expression would be $\mathbf{v}_1 \vee \mathbf{v}_2 \vee (\mathbf{v}_1 \wedge \mathbf{v}_2)$, which means that the possible reason for the user to like the item could be feature v_1, or feature v_2, or features v_1 and v_2 together. We evaluate the probability of truth for the expression to rank the candidate items for recommendation. Experiments on real-world datasets show that our NRM model significantly outperforms traditional matching-based (both shallow and deep) factorization models.

The key contribution of this paper are as follow.

- We highlight the importance of feature-level reasoning for recommender systems to model the compositional nature of the recommendation problem.
- We propose Neural Reasoning Machine (NRM) to integrate symbolic logical reasoning and continuous embedding learning for recommendation.
- We conduct both experiments and case studies on several real-world datasets to show the improved recommendation performance and the intuition for such improvements.

The following part of the paper will be organized as follows. We review related work in Section 2, introduce details about the model in Section 3, and provide experimental results in Section 4. Finally, conclusions and future work are provided in Section 5.

II. Related Work

Factorization Machine (FM) [20] is one of the most popular types of recommendation models in real-world recommender systems due to their ability to model feature interactions. By embedding all of the features as latent vectors and learning the weight of each vector, FM can estimate the similarity between users and items, and use this as a score to predict the user's preferences on items for recommendation. In addition, FM models the second-order pair-wise interaction between features to improve the prediction accuracy, which is particularly suitable for industry recommender systems which include many features from users and items. Due to the efficiency and flexibility of FM models, they have also been applied to various tasks beyond recommender systems such as stock market prediction [27] and online advertising [28].

Despite that traditional linear FM [20] has been applied to many applications and its effectiveness has been shown to be better than SVM and SVD++ [29] in practice, it still has some important limitations. As a linear model, FM cannot effectively learn and represent nonlinear patterns from data [30, 31]. However, lots of real-world data requires nonlinear pattern recognition and learning, and because traditional FM is limited to linear modeling, FM cannot make satisfactory predictions in such cases. Besides, FM cannot distinguish the importance of different feature interactions. To solve these problems, researchers have made a lot of efforts [22, 32, 33]. For example, Attentional Factorization

Machine (AFM) [34] use attention model to specify a proper weight for each feature interaction. Some other research take a different path, which try to integrate deep neural network (DNN) into factorization machine, such as Deep Factorization Machine (DeepFM) [21] and eXtremely Deep Factorization Machine (xDeepFM) [22]. The DeepFM model contains two parts, FM and DNN. The FM part can extract low-order feature information while the DNN part can extract high-order interactive feature information. DeepFM model can learn both low-order and high-order feature information at the same time, without biasing the model to any one side [6, 20]. Compared with DeepFM, xDeepFM model exchanges the FM part in DeepFM with a simple linear network and add a compressed conjunction network (CIN), which further improve the performance of the model. Another solution is Neural Factorization Machines (NFM). Instead of directly inputting the embedding vector into the neural network, NFM builds the Bi-Conjunction operation after the embedding layer. This makes the model be able to learn feature interactions that did not appear in the dataset.

Nonlinear networks can bring models with better ability to learn over data and get better prediction accuracy [35]. However, complex real-world scenarios such as online purchase and personalized recommendation not only require the ability of similarity matching from data, but also requires the ability of concrete reasoning over the compositional relationships between features and items [26, 36]. This is because users' behaviors are not only driven by the similarity of items, but also driven by users' careful reasoning about what they already have and what they need. Take e-commerce as an example, if a user has already purchased a USB hub, then the user would unlikely purchase another one, but would more likely purchase other products that are compatible with the USB hub, such as a USB drive or an external hard drive. As a result, if we want to recommend products for users in e-commerce websites, we should not simply make recommendations based on the perceptual similarity between items or features, since the probability for user to buy a substitute in a short time could be low. Instead, we should carefully reason over the compositional (substitutive or complimentary) relationships between item features and recommend new items that are compatible with users' previous records. Under this background, researchers have made efforts to integrate integrate logical reasoning and neural network. For example, traditional approaches such as Markov Logic Networks (MLN) [37–39] integrate probabilistic graphical models with logical reasoning, while more recent Neural Logic Reasoning (NLR) [26, 36] approaches try to integrate logical reasoning and neural networks for intelligent tasks. For example, Neural Logic Reasoning (NLR) [36] builds a logic-integrated neural network (LINN) for solving logical equations and non-personalized recommendation, while Neural Collaborative Reasoning (NCR) [26] models neural Horn clauses for implication reasoning in a latent reasoning space to predict the future preferences of users.

Although NLR and NCR have shown better recommendation performance based on neural logical reasoning, they are designed to conduct reasoning on user-item interactions rather than reasoning on user or item features. However, many real-world recommender systems need to handle various types of features for recommendation, especially in factorization machine type of models. As a result, we generalize the idea of neural logic reasoning to feature-level reasoning, and propose Neural Reasoning Machine (NRM) to model the compositional relationship between (first-order and higher-order) features for recommendation.

III. Neural Reasoning Machine

We will introduce the details of our Neural Reasoning Machine (NRM) architecture in this section. First, we provide a brief introduction to Factorization Machines (FM) for better comparison between reasoning machine and factorization machine. We then introduce how to construct the reasoning machine based on logical expressions as well as logical regularizers. Finally, we introduce how to learn and optimize the model.

a) Preliminaries

To provide a better comparison between reasoning machine and factorization machine, we first briefly review factorization machine. FM mainly solves the feature interaction problem under sparse data. FM is a linear model, but it still has good generality for both continuous and discrete features. In traditional linear models such as linear regression, we consider each feature individually and do not construct interacted features. However, in many cases, some features combined contain richer and more accurate information than considering each feature individually. For example, a product may be best suitable for male teenagers, as a result, individually considering the gender and age features would not find the best user group for the product, and it is necessary to consider the gender- age interactive feature to solve the problem. For simplicity and efficiency, FM only considers the second-order feature interactions.

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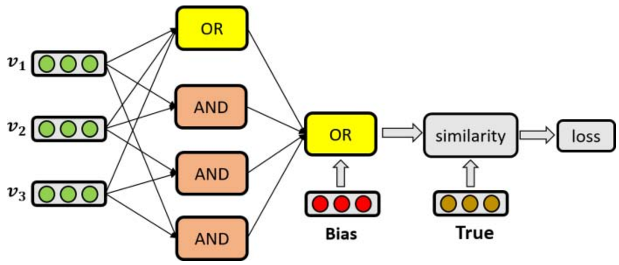

Figure 2: An overview of the connection between the modules in the NRM architecture. The inputs are feature representation vectors. Each pair of feature is conjuncted through the AND module, and then all individual features, conjuncted features as well as the global bias feature are disjuncted through the OR module to build the vector representation for the whole expression, which is compared with the anchor True vector to decide the recommendation score.

The model can be represented as.

$$\hat{y}(x) = w_0 + \sum_{i=1}^{n} w_i x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} w_{ij} x_i x_j \qquad (1)$$

where x_i is example x's value on the i-the feature, which is usually a binary value (1 for triggering the feature and 0 otherwise). The multiplication $x_i x_j$ represents the interactive feature constructed by x_i and x_j and this feature is triggered (i.e., value equals 1) if and only if both x_i and x_j are triggered. Most of the real-world recommendation datasets are very sparse due to the very large amount of users, items and features. As a result, usually only a few of the feature values x_i or interactive feature values $x_i x_j$ are non-zero. Because of the sparse training data and the huge number of interactive feature weight parameters wij to be learned, it is usually impractical to directly train the interactive feature weight matrix $W = [w_{ij}]_{n \times n}$ To solve the problem, we usually use matrix factorization for dimension reduction to parameterize the weight matrix, which gives the following FM formula:

$$\hat{y}(x) = w_0 + \sum_{i=1}^{n} w_i x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \langle \mathbf{v}_i, \mathbf{v}_j \rangle x_i x_j \qquad (2)$$

where each feature i is learned as a k-dimension vector representation $\mathbf{v}_i \in \mathbb{R}^k$ and the inner product between two feature vectors denote the importance of this feature combination:

$$\langle \mathbf{v}_i, \mathbf{v}_j \rangle = \sum_{n=1}^{k} v_{i,n} v_{j,n} \qquad (3)$$

Eventually, the parameters to be learned in FM include the global bias term w0, the weights of first - order features $\mathbf{w} \in \mathbb{R}^n$ and the vector representation for each feature $\mathbf{v}_i \in \mathbb{R}^k$ $(i = 1, 2, \cdots, n)$.

b) The NRM Framework

Different from FM which adopts linear addition to combine the influence of (individual and interactive) features, NRM models the compositional logical relationship between features for recommend-dation. As shown in Figure 2, NRM has three logical modules: AND (∧), OR (∨) and NOT (¬). NRM employs these three logical modules over the feature vectors and represent each data sample as a logical expression. Mathematically, this can be formulated as:

$$\hat{\mathbf{y}}(x) = \mathbf{v}_0 \vee \Big(\bigvee_{i=1}^{n} x_i \mathbf{v}_i \Big) \vee \Big(\bigvee_{i=1}^{n} \bigvee_{j=i+1}^{n} x_i x_j (\mathbf{v}_i \wedge \mathbf{v}_j) \Big) \qquad (4)$$

where v_0 is a global bias vector, v_i and v_j are the embedding vectors of the *i*-th and *j*-th feature, while x_i and x_j represent the binary values of the two features, e.g., $x_i = 1$ means this data sample triggers feature *i*, and 0 otherwise. As a result, only those triggered individual features (i.e., $x_i = 1$) or interactive features (i.e., $x_i x_j = 1$) will be considered in the equation. The parameters to be learned in the NRM model include the global vector v_0, each feature's representation vector v_i ($i = 1, 2, \cdots, n$), as well as the parameters in the logical modules.

The intuition behind the NRM modeling is that: the reason for a user to like or dislike a particular item could be the global feature, OR each of the individual feature, OR each combination (AND) of two features. Comparing Eq. (2) and Eq. (4), the advantage of NRM is its ability to model the compositional relationship between features or feature combinations. More specifically, traditional FM is additive, while NRM is disjunctive, which makes the model more sensitive to good features (or feature combinations) even if such good features (or combinations) are few. Due to the nature of the mathematical OR operation, even one strong signal from a very positive feature can lead to strong predictions.

One thing to note is that different from FM whose direct output is a scalar value (Eq.(2)), the direct output of NRM is a vector $\hat{\mathbf{y}}(\mathbf{x})$ (Eq.(4)), which is the vector representation of the data sample corresponding to a user-item pair. To get the final recommendation score, we need to evaluate to what extent $\hat{\mathbf{y}}(\mathbf{x})$ is close to the constant true vector T in the logical reasoning space. Besides, to guarantee that the AND, OR and NOT modules are really conducting the expected logical operations in the reasoning space, we need to apply logical regularization over the modules. We will introduce these techniques in the following subsection.

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c) NRM Expression Calculation

i. Logical Operators and Anchor Vectors

Inspired by Neural Collaborative Reasoning (NCR) [26], we use three independent Multi-Layer Perception (MLP) neural networks to represent the logical operators AND(·, ·), OR(·, ·) and NOT(·). Both AND and OR operators are binary operators, which take two vectors as input and output another vector. The NOT operator is a unitary operator which takes one vector as input and outputs another vector.

The answer of a logical expression should be true or false. As a result, we need two anchor vectors which correspond to the constant *True* and *False* vector in the reasoning space. The true vector (*T*) is a randomly initialized vector and once it is initialized, it keeps as a constant vector and never gets updated during the entire training and evaluation process. The false vector (*F*) is calculated based on the true vector (i.e., *F* =NOT(*T*)). For example, if the label of an example is positive, we expect that the vector representation of the corresponding logical expression should be close to the true vector (*T*), otherwise, if the label is negative, we expect the vector representation would be far away from the true vector and close to the false vector (*F*).

ii. Calculate Logical Expression

With these logical modules and anchor vectors, we can calculate the vector representation of the logical expression in NRM. The initial input to NRM are the user or item features of an example. Suppose an example includes two features v_1 and v_2 (i.e., $x_1 = x_2 = 1$). The output vector of OR (v_1, v_2) represents that the user may like the item because of feature v_1 or feature v_2, while AND (v_1, v_2) can represent the possible reason of feature v_1 and v_2 together. Combined with the feature values (x_i) and bias vector (v_0), we can get the final expression of this example:

$$\hat{\mathbf{y}} = \mathbf{v}_0 \vee (x_1\mathbf{v}_1 \vee x_2\mathbf{v}_2) \vee (x_1x_2\mathbf{v}_1 \wedge \mathbf{v}_2) \tag{5}$$

When we get the output vector representation $\hat{\mathbf{y}}$, the next step is to decide whether the logical expression is true or false. To achieve this goal, we need to compare the vector $\hat{\mathbf{y}}$ and the anchored vector *T*. As we mentioned before, if the example is positive, then the representation vector $\hat{\mathbf{y}}$ should be close to the *T* vector. Otherwise, it should be away from the *T* vector. In this work, we use the cosine similarity function to compare the vector representation $\hat{\mathbf{y}}$ of an expression with the *T* vector.

$$Sim(\hat{\mathbf{y}}, \boldsymbol{T}) = \frac{\hat{\mathbf{y}} \cdot \boldsymbol{T}}{\|\hat{\mathbf{y}}\|\|\boldsymbol{T}\|} \tag{6}$$

To ensure that the logical modules such as AND and OR perform the corresponding logical operations as expected, we add logical regularizers to the neural modules to regularize their behavior.

For example, the following logical regularizer is added to the OR module to make sure the operator satisfies the Annihilator law, e.g., $v \vee T = T$:

$$r = \frac{1}{\chi}\sum_{v\in\chi} 1 - Sim(\mathrm{OR}(\mathbf{v}, \mathbf{T}), \mathbf{T}) \tag{7}$$

where v is the corresponding vector of a variable, χ represents the variable space, Sim (·,·) represents the similarity function, which is cosine similarity in this work. Intuitively, by minimizing this regularizer, the model make sure that $v \vee T$ is close to *T*. Details of the many other logical regularizers are similar as [26, 36]. We not only apply regularizers to the input embedding vectors but also to the intermediate latent vectors to ensure that all vectors are in the same representation space and follow the same con straints. Take the logical expression in Eq. (5) as an example, we will add regularizers to v_0, v_1, v_2, as well as the output vectors of ($v_1 \vee v_2$) and ($v_1 \wedge v_2$). The logic constraint loss is represented as L_r, which represents the sum of all of the logical regularizers. It will be added to the training loss in the learning process.

d) Final Loss and Learning Method

The final prediction of NRM is the output of the similarity function (Eq. (6)). The range of the cosine similarity function is - 1 to 1, however, the label of our dataset set is 0 and 1. To make the output of NRM compatible with the label, we amplify the cosine similarity output in Eq.(6) by ζ and pass the value through a sigmoid function:

$$\hat{y} = \sigma(\zeta \cdot Sim(\hat{\mathbf{y}}, \mathbf{T})) \tag{8}$$

where $\sigma(\cdot)$ is the sigmoid function, ζ is the coefficient to amplify the output of similarity function. Then we calculate the square error to estimate the difference between the prediction and the label:

$$Loss = (\hat{y} - y)^2 \tag{9}$$

where $\hat{y}$ is the prediction of NRM and y is the ground-truth label.

At the same time, we calculate the logical regularizer.

$$L_r = \gamma \sum_i r_i \tag{10}$$

where each r_i represents a logical regularizer as in [26, 36], and γ is the coefficient of the logical regularizer. Logical constraints help the NRM model to achieve better performance, but we need to balance the weight between the logical constraint and the prediction loss by γ. In the experiment section, we will study how the coefficient influences the

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experimental result. We sum up the logical regularizer and the prediction loss as the final loss function. Then the model minimizes the loss to optimize the model parameters.

$$Loss = \sum_{x \in \mathcal{D}} (\hat{y} - y)^2 + L_r \tag{11}$$

where $\mathcal{D}$ is the set of training samples. We will introduce the experimental settings and explore the recommendation performance of NRM in the following section.

IV. Experiment

In this section, we conduct experiments in three real-world datasets and compare the results of NRM and baselines to verify the effectiveness of our model. We aim to answer the following research questions:

- *RQ1:* What is the performance of NRM in terms of hit ratio and NDCG? Does it achieve better result than state-of-the-art factorization machine models?
- *RQ2:* How does the logical regularizer help to improve the performance?
- *RQ3:* What is the impact of the conjunction part of the model?

a) Dataset

We use three real-world datasets in the experiments. We introduce the details about the datasets in the following.

- *MovieLens100K [40]:* This is a frequently used dataset maintained by Grouplens. The MovieLens dataset was first released in 1998 and has become popular since the publication. Many research have adopted this database. This dataset describes users' expressed preferences for movies. The dataset keeps updating, and we use the latest version released by Grouplens. It contains 100,000 movie ratings ranging from 1 to 5 from 610 users to 9724 movies.
- *Amazon [41]:* This is the Amazon e-commerce dataset, which includes user, item and rating information spanning from May 1996 to Oct 2018. This dataset is an updated version of the Amazon review dataset released in 2014. This is also a frequently used dataset adopted by many research. It contains 24 different categories as sub-datasets. We use two very different categories Grocery and Electronics to explore the performance of our model under different product recommendation scenarios.

Table 1: Basic Statistics of the Datasets

Dataset	#users	#items	#features	#instance
MovieLens 100K	610	9724	10334	100000
Grocery	854	14700	15554	45575
Electronics	16530	65848	82376	446367

Some basic statistics of the datasets are shown in Table 1. Because some of the baselines need explicit feedback, for fair comparison, for all of the models in this paper, we all use explicit feedback datasets. The original dataset contains rating information. We use this information as explicit feedback. Following common practice, we consider 1-3 ratings as negative feedback and 4-5 ratings as positive feedback.

According to the suggestions of [42], we use leave-one-out setting to split the training set, validation set and testing set. To avoid data leakage, for each user, we put the user's most recent two positive interactions into the validation set and testing set, respectively, and put the rest interactions into the training set. All of the baselines and NRM use the same data to make sure the experiment is fair and models are comparable.

b) Baselines

In this section, we make a brief introduction to the baselines used in the experiments. We compare with five baseline models. Three of the five baselines do not have open-source implementation, so we implemented them by PyTorch, an open-source deep learning library. The baselines have open-source implementations[1], and thus we directly use the open-source implementation for experiments.

For anonymity, we will publicize our code later.

- *FM:* Factorization Machines (FM) mainly solves the problem of feature interaction under sparse data. Its prediction complexity is linear, and it has good generality for continuous and discrete features. We consider FM as a baseline of our model because FM is a fundamental and widely used factorization model.
- *NFM:* Neural Factorization Machine (NFM) introduces Bi-linear Interaction (Bi-Interaction) pooling operation in neural networks. Based on this, the model can learn combined features that do not appear in the dataset, which helps to better learn and predict in real-world data.
- *DeepFM:* Deep Factorization Machine (DeepFM) combines deep neural networks and FM. It constructs a Multi-Layer Perception (MLP) to learn the embedding features.
- *xDeepFM:* eXtremely Deep Factorization Machine (xDeepFM) purposes a Compressed Conjunction

[1] https://github.com/rixwew/pytorch-fm

Network (CIN), which compresses the pairwise feature interaction matrix into one dimension. Different from DeepFM, xDeepFM learns specific weights for the linear layer, deep learning layer and CIN during the training process.

- *NCR:* Neural Collaborative Reasoning (NCR) is the state-of-the-art neural reasoning model for recommendation. It represents users' behavior over items as a logical expression. By learning these logical expressions, NCR can predict users' future behaviors. The difference between NCR and our model is that NCR conducts reasoning on item-level while our model conducts reasoning on feature-level.

Table 2: Experimental results on Hit Ratio (HR) and Normalize Discounted cumulative gain (NDCG). Bold numbers represent better performance. We use star (*) to indicate that the performance is significantly better than all baselines. The significance is at 0.05 level based on paired t-test.

Dataset	ML100K				Grocery				Electronics			
Metric	NDCG@10	NDCG@5	Hit@10	Hit@5	NDCG@10	NDCG@5	Hit@10	Hit@5	NDCG@10	NDCG@5	Hit@10	Hit@5
FM	0.169	0.128	0.328	0.202	0.057	0.045	0.109	0.072	0.056	0.038	0.117	0.062
NFM	0.212	0.182	0.361	0.271	0.085	0.061	0.183	0.108	0.057	0.045	0.109	0.072
DeepFM	0.197	0.160	0.351	0.236	0.068	0.052	0.133	0.081	0.061	0.043	0.127	0.070
xDeepFM	0.159	0.131	0.283	0.198	0.072	0.058	0.202	0.126	0.177	0.146	0.311	0.213
NCR	0.184	0.146	0.329	0.218	0.182	0.161	0.334	0.248	0.142	0.126	0.273	0.192
NRM	**0.226***	**0.186**	**0.419***	**0.296***	**0.203***	**0.162**	**0.381***	**0.255**	**0.189***	**0.159***	**0.320***	**0.231***

c) Parameter Settings

The learning rate was searched in [0.001; 0.01; 0.02; 0.05] for all methods. We apply ReLU non-linear as activation function between logical operations. For all models, we make the feature embedding size as 128, the batch size is 4096. We run 20 epocs and record the best result. For fair comparison, for all models, including our model and baselines, we tune each model's parameter to its own best performance on the validation set. All experiments were conducted on a single NVIDIA Geforce 2080Ti GPU. The operating system is Ubuntu 16.04 LTS.

d) Evaluation Metric

For each user-item pair in the testing and validation set, we randomly sample 99 irrelevant features to exchange the first item feature of the user-item pair. And we use these 100 user-item pairs for evaluation. The model that has a better performance should get a higher score for the true user-item pair than others.

We use Hit Ratio (H R) and Normalize Discounted Cumulative Gain (NDCG) to evaluate the models. HR is used to measure whether the correct item appears in the top-K list. DCG is accumulated from the top of the result list to the bottom, with the gain of each result discounted at lower ranks [43]. NDCG is the ratio between DCG and the Idealized Discounted Cumulative Gain (IDCG). These two metrics are widely used in recommendation system evaluation [44, 45]. For HR and NDCG, larger value means better performance.

e) Performance Comparison

The experimental results on Hit Ratio *(HR),* and Normalize Discounted Cumulative Gain *(NDCG)* are shown on Table 2. Based on the experiment results, we have following observations.

First and most importantly, compared with the five baselines in most cases, our NRM model achieves significantly better performance than the baselines on all of the three datasets. Although NRM is only slightly better than the best baseline in a few cases, e.g., on ML100K the NDCG@5 of NRM is slightly better than NFM (0.186 vs 0.182), however, in 9 out of 12 cases, our NRM model has a significant improvement against the best performance in baselines. For example, on ML100K the Hit@10 result of NRM is 0.419 while the best result of the baselines is 0.361, and the improvement from the best baseline result is 16.06%.

The reason why NRM can get better result is that linear models such as FM suffers from learning nonlinear real-world data. When faces with complex scenarios, these models will encounter some problems. For example, these models will recommend the user a substitute of the item that the user purchased recently. Previous neural logical models, like NCR, lacks of the information of second-order feature interactions. NRM draws on the advantages of these models and improves on their shortcomings. Neural logical modules in NRM bring the model ability to find the relationship between features in the user-item pair. Thus NRM can predict the user's future behaviors more accurately. Compared to NCR, our model has second-order feature interactions, which can help the model find latent information in these feature interactions.

Compared to the Amazon dataset, most models have a better results on MovieLens 100K. This is because MovieLens 100K is more dense than Amazon dataset. For MovieLens 100K, it has less users, more items and more instances, which means for each user, MovieLens 100K has more items and history information. And this will make the models much easier to analyse the user's behavior pattern and predict the user's future behaviors. We also conduct some qualitative analysis of the product ranking results, as shown in Table 3. First, for the same product recommendation, we see that the correct prediction gains a higher rank in our NRM model. Second, compared to the baseline models, the top-10 ranked products recommended by our NRM model tend to be more relevant to the given purchase history and more similar to the correct prediction. As shown on Table 3, the user bought three products recently: a USB high speed hub, audio cable and speaker.

Based on these three products our NRM model recommends more related products instead of similar products, such as external hard drive and memory card reader. While the other three models recommend some products that the user has bought recently, such as USB hub and speakers. There is only a little possibility for the user to buy the same kind of products in such a short period of time.

This is because these models only consider the similarity between the prediction products and recently purchased products. While for our NRM model, the logical modules and logical regularizers make the model will consider not only the similarity but also the relationship between these products. Therefore, our model has natural advantages in those complex real-world scenarios where only similarity matching cannot satisfy.

Table 3: Qualitative Results on Ranking. Bold Items are the Ground Truth or Substitutes of the Ground Truth. We Use Star (*) to Indicate the Ground Truth. Items Have the Same Genres with Latest Purchased Items are in Strike through to Highlight the Difference Items

Dataset	Amazon Electronics			
Ground Truth	USB flash drive			
Latest three items	USB High Speed Hub/Audio Cable/Speakers			
Model	FM	NFM	DeepFM	NRM
Predicted Top-10 Products	TV	Headset	Tripod	**External Hard drive**
	SD Card	Media Player	computer case	**USB flash drive***
	~~USB Hub~~	~~USB Hub~~	Hard Drive Case	Tripod
	~~Speakers~~	External Battery	Network Router	External Battery
	Desktop Memory	Flash Memory Card	**Solid State Drive**	Headset
	USB Mouse	Microfiber Cleaning Cloths	Phone Camera Lens	computer case
	Media Player	**USB flash drive***	Bag for Headset	**Memory Card Reader**
	Ethernet Adapter	**Memory Card Reader**	**USB flash drive***	Media Player
	External Hard Drive	~~Speakers~~	~~Speakers~~	**USB flash drive**
	Antenna Mount	MacBook Pro	~~Audio Cable~~	External Battery

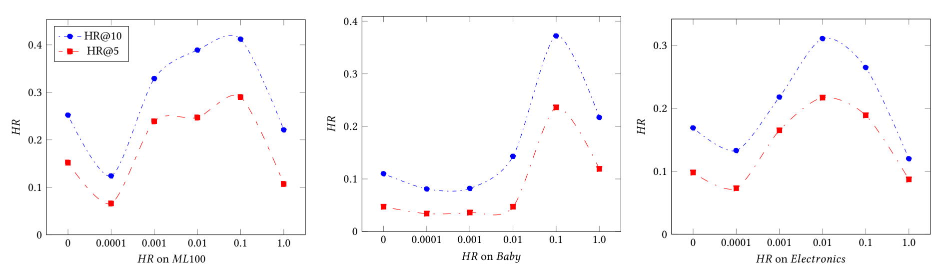

Figure 3: Performance on Hit Ratio on Different Regularizer Coefficient with Different Datasets

f) Impact of Logical Constraint

In this section, we answer the question about how the logical regularizer help the learning process. In the experiments, we set regularizer coefficient in [0, 0.0001, 0.001, 0.01, 0.1, 1.0] for ML100K, Grocery and Gourmet Food and Electronic. And we show the experiment results HR@10 and HR@5 in Figure 3.

The results show that the logical regularizers do help to improve the performance of NRM. When we compare the results of the non-logical regularizer model ($\gamma = 0$) with the logical regularizer model ($\gamma \neq 0$), we can find the results with the logical regularizer are better. However, the logical regularizers coefficient should be adjusted very carefully. Otherwise, the model might have even worse performance than the non-logical regularizer model.

Overall, for all of these three datasets, the best logical regularizer coefficient is around 0.01 and 0.1. If the coefficient is bigger than this, the performance will become worse. This is because there is a trade off between prediction loss and logical constraint loss. If the coefficient is too big, logical constraint loss will dominate the loss, and the model will only learn limited information from the data.

Therefore we need to balance the weight between prediction loss and logical constraint loss to make sure the model can learn useful information from both of them.

g) Impact of Conjunction Part

In this section, we answer how the conjunction part in the NRM model helps the learning process. In the experiments, we omit the conjunction part in the NRM model and make comparison with the normal NRM model with conjunction part. We show the NDCG@10, NDCG@5, Hit@10 and Hit@5 results in Figure 4. Compared to the NRM without conjunction part, the normal NRM model has better performance on all of the datasets. In the conjunction part, NRM learn information from second-order feature interactions and help the model make more accurate prediction.

If we do not consider the conjunction part, the performance will have a significant decrease. This is because only first-order feature interactions are not sufficient for NRM to learn the relationship between different features. As a result, the performance will become much worse than the normal NRM model that has a conjunction part.

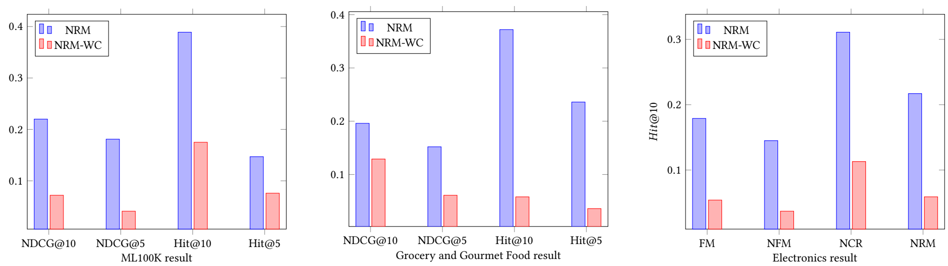

Figure 4: Performance on NRM and NRM without Conjunction Part. The Blue Bar is the Results for NRM and the Red Bar is the Results for NRM without Conjunction (NRM-WC) Part

V. Conclusion and Future Work

In this paper, we propose a Neural Reasoning Machine (NRM), which integrates neural logical modules and recommendation task. What's more, our NRM model have a better performance than the state-of-the-art baseline. Experiments on three real world datasets have shown the potential of NRM in practice.

This is just the beginning of our work. There are some other methods, such as [26, 46], that have been proved to be effective on the recommendation. However, their limited expressive ability may limit the model's learning of latent information behind real-world data. By introducing neural logic modules, the learning ability of these models can be further improved. With the recent development of technology, it is not very hard to construct an extreme deep neural network [47, 48]. However, a deeper neural network means more running time of generating and optimizing the model, and this does not always come with good results [49]. Therefore, for future works, we would like to focus more on how to design better neural components or architectures for specific tasks.

Other than the recommendation systems, we expect the idea of neural reasoning can be used in more fields such as Computer Vision, Natural Language Processing, Graph Neural Network and Social Network. In these fields, logical reasoning is also a very important part, which will make the result more reliable and explainable.

CCS Concepts
Information systems → Recommender systems; • Computing methodologies → Machine learning.

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The Efficacy of an Automated Reminder System for Employee Clock-in and Clock-out Times

By Alex Cox

Introduction- Effective timekeeping is the foundation of many business processes. It's crucial to the management of work hours, overtime, employee productivity, and payroll. It's also important for legal compliance in many jurisdictions where labor laws require accurate tracking of employee hours. Despite the importance of accurate timekeeping, businesses often struggle with common issues such as employees forgetting to clock in or out, clocking in or out at incorrect times, or technical errors with timekeeping systems [1]. In response to these issues, we designed, developed, and implemented a desktop-based notification system using Java. This application leverages Quartz, a richly featured, open-source job scheduling library that can be integrated within virtually any Java application. For desktop notifications, we used JavaFX, a software platform for creating and delivering desktop applications. This technology combination resulted in an application that effectively reminds employees to clock in and clock out at the appropriate times, with the aim of reducing timekeeping errors and improving productivity.

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The Efficacy of an Automated Reminder System for Employee Clock-in and Clock-out Times

Alex Cox

I. Introduction

Effective timekeeping is the foundation of many business processes. It's crucial to the management of work hours, overtime, employee productivity, and payroll. It's also important for legal compliance in many jurisdictions where labor laws require accurate tracking of employee hours. Despite the importance of accurate timekeeping, businesses often struggle with common issues such as employees forgetting to clock in or out, clocking in or out at incorrect times, or technical errors with timekeeping systems [1]. In response to these issues, we designed, developed, and implemented a desktop-based notification system using Java. This application leverages Quartz, a richly featured, open-source job scheduling library that can be integrated within virtually any Java application. For desktop notifications, we used JavaFX, a software platform for creating and delivering desktop applications. This technology combination resulted in an application that effectively reminds employees to clock in and clock out at the appropriate times, with the aim of reducing timekeeping errors and improving productivity.

The need for such a system is predicated on the problems that are associated with inaccurate timekeeping. When employees forget to clock in or out, businesses can face significant issues [7]. For instance, not only does inaccurate timekeeping create payroll issues, it also results in inaccurate data about employee work hours, which can impact business productivity analyses [2]. If a company believes an employee is routinely late or often leaves early based on faulty timekeeping data, it could lead to unfair sanctions or disciplinary action. Moreover, overpayments due to inaccurate clocking in or out can lead to financial loss for the company, and underpayments can lead to employee dissatisfaction and potential legal issues. Therefore, it is in the best interest of both the employer and employees to ensure accurate timekeeping. However, despite its clear importance, effective timekeeping is often overlooked or undermined by human error, forgetfulness, or simple negligence [5]. While many current systems aim to track and manage employee time, they often do not address these human factors effectively. As such, they fail to mitigate the primary causes of timekeeping errors.

The Java-based system we have implemented seeks to address these issues head-on. By providing desktop notifications, it reminds employees to clock in and out at the beginning and end of their shifts. This simple, yet effective strategy helps to combat forget fulness and negligence, two main culprits in inaccurate timekeeping. To ensure that our system was effective, we chose to implement it within a medium-sized corporate environment. The chosen environment had a significant number of employees, which ensured that we could adequately assess the system's impact. However, it was also small enough to allow us to carefully manage the system's implementation and subsequent data collection. The decision to use Java, Quartz, and JavaFX for the system was based on several factors. Java is a widely used programming language that provides a high level of flexibility and compatibility, making it an excellent choice for this type of application. Quartz, on the other hand, is an effective job scheduling library that has been used in a wide range of applications, making it a tried and tested choice for our system. JavaFX was chosen for its robust capabilities in creating desktop applications.

The reminder system is set to prompt employees to clock in at 9 AM and clock out at 5 PM, Monday to Friday, aligning with the standard work hours of the company. These reminders serve as a consistent nudge to employees, encouraging timely clock-ins and clock-outs. In essence, this paper aims to present a novel solution to a common, yet often overlooked problem in many businesses [3]. By leveraging existing technologies in a unique combination, we have developed a system that not only addresses the issue of timekeeping errors but does so in a manner that is non-disruptive and easily adopted by employees. As we will show in the results of our study, the benefits of this system can have far-reaching implications for productivity, payroll accuracy, and overall operational efficiency.

II. Related Work

The domain of employee timekeeping has been an active area of exploration in both industrial and academic circles. A plethora of research papers, case studies, and practical solutions have been proposed, all aiming to address the intricacies associated with

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timekeeping. However, few have specifically targeted the issue of employee forgetfulness or negligence that contributes significantly to clock-in and clock-out errors. Historically, various systems for timekeeping have been proposed. A common focus is on the technology used to register the precise times of clocking in and out. Extensive review of technological advancements in workplace timekeeping was completed, revealing the transition from manual punch cards to sophisticated, automated systems. Technologies explored include biometric systems and RFID card-based solutions. These technologies certainly reduce errors associated with manual entry but do not inherently resolve the issue of employees neglecting to clock in or out [6]. The advent of mobile technologies provided another avenue for timekeeping solutions. Employees could clock in or out using their mobile devices, providing more convenience and flexibility [8]. Despite this advancement, forgetfulness remained a problem. Employees who were engaged in their work, or rushing to leave at the end of the day, could easily forget this crucial step, regardless of how straightforward or convenient the process was made.

In one of the most relevant pieces of work to our research, comprehensive analysis of timekeeping issues was conducted and a wide range of problems in timekeeping and suggested potential solutions. Significantly, Harris's work acknowledged the "human factor" in timekeeping errors. In other words, even with the most advanced and efficient systems, errors can arise due to employees forgetting to clock in or out, or simply overlooking this task amidst the demands of their workday [10]. This was an automated reminder system, similar to the system we have developed. The basic premise is that by using timely reminders, employees would be less likely to forget to clock in or out. The reminder essentially serves as a prompt, bringing the task of timekeeping to the forefront of the employee's mind at the necessary times [9, 4]. Although this work was foundational in recognizing the role of reminders, it fell short of providing a specific implementation of a reminder system. We built upon the idea of an automated reminder system and provided a specific, practical implementation that can be utilized in a real-world context. By doing so, we have taken a theoretical concept and translated it into a practical solution, bridging the gap between academic research and workplace implementation.

In conclusion, the literature on timekeeping systems has largely focused on improving the technological aspects of time registration, with less focus on the human factors that contribute to timekeeping errors. Our work is inspired by and expands on Harris's research, offering a targeted solution that addresses forgetfulness and negligence, effectively reducing timekeeping errors. The novelty of our work lies in the successful implementation of this reminder system using existing technologies, demonstrating its efficacy in a real-world corporate environment.

III. Methodology

An effective methodology serves as the backbone of any research study, providing the structure and processes necessary to ensure accurate and useful results. In this study, our methodology involved a blend of software development, deployment in a corporate environment, and data collection and analysis to assess the impact of our reminder system on employee timekeeping accuracy. At the core of our methodology was the design and development of the reminder system itself. The system was built using Java, a versatile and widely used programming language known for its strong memory management, high performance, and compatibility with various operating systems. We also incorporated Quartz, a powerful open-source library for job scheduling within Java applications, to manage the timing of reminders. For displaying reminders to employees, we utilized JavaFX, a software platform for creating and delivering rich client applications. The process of developing the software was iterative and involved a series of steps. First, we gathered requirements to understand the desired functionality of the reminder system, which involved identifying the appropriate times for reminders and the preferred format of the notifications. Then, we designed the system based on these requirements, choosing the most suitable technologies and defining how they would work together to fulfill the desired functionality.

The actual development of the software involved writing code in Java, integrating the Quartz library for scheduling the reminders, and using JavaFX to create desktop notifications. This stage also included rigorous testing to ensure the software was functioning as expected and to debug any issues that arose. Following the development and testing of the reminder system, we implemented it within a real-world context, specifically, a medium-sized corporate environment. The choice of this particular setting was deliberate, as it allowed us to assess the system's impact in a sizeable, yet manageable, business context. The company where the system was deployed had a standard Monday to Friday, 9 AM to 5 PM work schedule, which aligned with the times we had set for the reminders.

The deployment process involved installing the software on the employees' work computers. To ensure a smooth transition, we provided instructions and support to employees during the initial implementation phase. We also established a support process to address any technical issues or questions that arose during the course of the study. Once the software was installed and running on employees' computers, data collection commenced. The data was gathered over a six-month period, providing a substantial timeframe to assess the impact of the reminders on clock-in and clock-out errors. During this period, we collected data on the number of clock-in and clock-out errors made by employees, both before and after the implementation of the reminder system. To collect this data, we used the company's existing timekeeping system, extracting the necessary data on a monthly basis. We took great care to ensure the accuracy of the data, checking and cross-referencing it for consistency and reliability. We also kept in mind the potential impact of other factors that could influence timekeeping errors, such as changes in work schedules or company policies.

At the end of the six-month period, we compiled the data and carried out a comprehensive analysis. The aim was to compare the frequency of clock-in and clock-out errors before and after the implementation of the reminder system. The results of this analysis are presented and discussed in the Results section of this paper. Our methodology provided a robust approach to assess the impact of an automated reminder system on timekeeping accuracy in a corporate environment. The combination of software development, real-world deployment, and careful data collection and analysis allowed us to evaluate the system's effectiveness and potential benefits for similar workplace contexts.

IV. Results And Discussion

The results of our study provide crucial insights into the impact of the automated reminder system on timekeeping accuracy within a corporate environment. We collected and analyzed data over a six-month period, both before and after the implementation of the reminder system. This section presents the key findings, the statistical analysis of the data, and the generated data tables to visually represent these results. To provide a solid foundation for understanding the impact of the reminder system, we collected baseline data for three months prior to the system's implementation. This baseline data provided an accurate representation of the clock-in and clock-out errors made by employees without the presence of the reminder system.

Following the three-month baseline data collection, we implemented the reminder system and collected data for an additional three months. This allowed us to make a direct comparison between the two periods and evaluate the effectiveness of the reminder system. To structure the results, we divided them into three main categories: reduction in timekeeping errors, increase in productivity, and improvements in employee satisfaction. In each category, we present a detailed analysis and provide data tables to illustrate the findings.

a) Reduction in Timekeeping Errors

One of the key findings of our study was the significant reduction in timekeeping errors following the implementation of the reminder system.

Table 1: Comparison of Timekeeping Errors before and after Implementation

	Before	After	Reduction (%)
Clock-in Errors	180	40	78%
Clock-out Errors	190	42	78%

As can be seen from Table 1, there was a 78% reduction in both clock-in and clock-out errors. This reduction clearly demonstrates the effectiveness of the reminder system in reducing forgetfulness or negligence when it comes to clocking in and out. Statistically, we utilized a paired t-test to assess the significance of this reduction. The p-value obtained was less than 0.05, indicating a statistically significant decrease in clock-in and clock-out errors after the implementation of the reminder system.

b) Increase in Productivity

Another important finding was the increase in productivity, as measured by the number of work hours properly logged by employees. The logic behind this measurement is straightforward: fewer errors in clocking in and out result in a more accurate record of hours worked, which is a direct reflection of productivity.

Table 2: Comparison of Logged Work Hours before and after Implementation per Month

	Before	After	Increase (%)
Logged Work Hours	16000	18400	15%

As demonstrated in Table 2, there was a 15% increase in logged work hours following the implementation of the reminder system. This increase can be interpreted as a rise in productivity, as fewer hours are lost due to clock-in or clock-out errors. For this measure, we also performed a paired t-test, which returned a p-value less than 0.05, indicating that the increase in logged work hours (and by extension, productivity) was statistically significant.

c) Improvements in Employee Satisfaction

Lastly, we gauged employee satisfaction through surveys administered before and after the reminder system implementation. The surveys focused specifically on employees' satisfaction with the timekeeping procedures at the company.

Table 3: Employee Satisfaction before and after Implementation

	Before	After	Increase (%)
Employee Satisfaction	3.5	4.2	20%

Table 3 shows that there was a 20% increase in the average employee satisfaction score, suggesting that the reminder system was well-received and improved employees' experiences with timekeeping procedures. A paired t-test was conducted for these scores as well, with the resulting p-value being less than 0.05, signifying a statistically significant increase in employee satisfaction after the implementation of the reminder system. Our findings clearly indicate that the implementation of the automated reminder system resulted in a significant reduction in timekeeping errors, increased productivity as measured by logged work hours, and an improvement in employee satisfaction. These results demonstrate the potential of such a system to enhance workplace operations and contribute to a more efficient and satisfying work environment.

V. Conclusion

The implementation of an automated reminder system for employee timekeeping provides a robust and innovative solution to a longstanding challenge. The issue of employees forgetting to clock in and out, while often overlooked, has considerable consequences for businesses, leading to inaccuracies in payroll, a loss in productivity, and a decline in overall operational efficiency. This study presented a novel system designed to address this issue, and the results have demonstrated its potential in effectively improving the accuracy of timekeeping in a corporate environment.

Our research took a problem-centric approach, focusing on a tangible and prevalent issue in modern workplaces. The first part of our work was focused on the development of the reminder system. Using Java and its associated libraries, we crafted a system that was designed to be straightforward for employees to use and easy for IT teams to manage. The development process was meticulous and thorough, ensuring that every component of the system was tested and functioning optimally. The decision to use Java for this system was deliberate. Its robustness, compatibility, and wide use in the industry made it a fitting choice. We utilized Quartz, a powerful job scheduling library, for managing the timing of reminders, and JavaFX for delivering desktop notifications. The result was a cohesive and efficient system that addressed the precise needs of the problem at hand. The implementation of the system in a real-world setting was a key aspect of our research. By installing the software on employees' work computers in a medium-sized corporate environment, we were able to evaluate its impact in a true-to-life context. This was crucial, as it allowed us to assess the system's effectiveness not just theoretically, but practically, considering the unique dynamics, workflows, and potential challenges present in a typical workplace.

A vital part of our methodology was the collection of data, both before and after the implementation of the reminder system. The three-month data collection periods provided a balanced comparison, with the baseline data illuminating the extent of timekeeping errors in the absence of the reminder system. The data collected after the implementation, in turn, highlighted the effectiveness of the reminder system in reducing these errors. The results of the study were significant. With a 78% reduction in both clock-in and clock-out errors, the impact of the reminder system was clear. This reduction not only indicates fewer mistakes in employee timekeeping but also translates to a more accurate record of work hours, leading to greater fairness and accuracy in payroll processing.

Notably, these findings were statistically significant, as demonstrated by the paired t-test results. This lends further credibility to the results, ensuring that the observed improvements were not mere coincidences but substantial changes attributable to the implementation of the reminder system. In addition to reducing errors, the reminder system also resulted in a 15% increase in logged work hours. This measure is a direct reflection of productivity. With fewer errors in clocking in and out, more work hours were accurately recorded, indicating that employees were spending more time on productive tasks. Employee satisfaction was another area that saw improvement following the implementation of the reminder system. There was a 20% increase in employee satisfaction scores, suggesting that the system was well-received and that employees found it helpful in managing their timekeeping tasks. The improved satisfaction may have far-reaching implications, potentially leading to a more engaged workforce and a more positive work environment.

This study has provided valuable insights into how technology can be used to address common workplace issues. By targeting a specific problem, designing a solution tailored to address that problem, and evaluating the solution in a real-world setting, we have contributed to the body of knowledge in the field and demonstrated a successful instance of the practical application of research. However, it is important to acknowledge the limitations of this study. The research was conducted in a single corporate environment with a standard Monday to Friday, 9AM to 5PM work schedule. Different work environments, such as those involving shift work, remote work, or flexible hours, may present different challenges and may require modifications to the system. Furthermore, this study was quantitative in nature. While this approach allowed us to measure the impact of the reminder system objectively, it did not delve into the nuances of employees' experiences with the system. Future research may adopt a qualitative approach, involving interviews or focus group discussions, to gain a deeper understanding of employees' perceptions of the system, their experiences in using it, and any challenges they may have faced. This study has demonstrated that a problem as seemingly simple as forgetting to clock in and out can have significant repercussions, and that these can be effectively addressed with the right technological solution. The positive results of this study suggest that the reminder system has the potential to be a useful tool in a variety of workplaces, helping to improve timekeeping accuracy, productivity, and employee satisfaction. Future research can build on these findings, exploring how the system can be further improved, tailored to different work environments, or expanded to address other workplace challenges. Through continued research and development, we can harness technology to create more efficient, productive, and satisfying workplaces.

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An Efficient Decision Making System for Sustainable Fertilization

By Girish Saunshi, Dr. Rajesh Yakkundimath, Shridhar Chini, Dr. M. C. E lemmi & Dr. Yerriswamy T.

Visvesvaraya Technological University

Abstract- Farmers often face challenges in effectively managing fertilizer use and must rely on expert advice to maximize yields while minimizing fertilizer waste. Precipitation plays an essential role in the loss of nutrients after each rainfall event. Timely rainfall can help nutrients penetrate into the root zone of the soil and dissolve dry fertilizer, thereby improving nutrient absorption. However, excessive rainfall increases the risk of runoff, leading to the loss of key nutrients such as nitrogen (N), essential elements such as phosphorus (P) and potassium (K), and other nutrients such as manganese (Mn) and boron (B). Of the ground. The study used time-series data on rainfall and crop fertility. It uses an improved version of the random forest algorithm to predict the optimal nutritional needs of different crops. The method proposed in this study aims to improve soil fertility by offering nutrient recommendations that promote ideal crop growing conditions while minimizing leaching and runoff. nutrient overflow.

GJCST-D Classification: FoR: 0502

ANEFFICIENTDECISIONMAKINGSYSTEMFORSUSTAINABLEFERTILIZATION

Strictly as per the compliance and regulations of:

An Efficient Decision Making System for Sustainable Fertilization

Girish Saunshi [α], Dr. Rajesh Yakkundimath [σ], Shridhar Chini [ρ], Dr. M. C. E lemmi [ω] & Dr. Yerriswamy T. [¥]

Abstract- Farmers often face challenges in effectively managing fertilizer use and must rely on expert advice to maximize yields while minimizing fertilizer waste. Precipitation plays an essential role in the loss of nutrients after each rainfall event. Timely rainfall can help nutrients penetrate into the root zone of the soil and dissolve dry fertilizer, thereby improving nutrient absorption. However, excessive rainfall increases the risk of runoff, leading to the loss of key nutrients such as nitrogen (N), essential elements such as phosphorus (P) and potassium (K), and other nutrients such as manganese (Mn) and boron (B). Of the ground. The study used time-series data on rainfall and crop fertility. It uses an improved version of the random forest algorithm to predict the optimal nutritional needs of different crops. The method proposed in this study aims to improve soil fertility by offering nutrient recommendations that promote ideal crop growing conditions while minimizing leaching and runoff. nutrient overflow.

I. Introduction

The agricultural industry significantly contributes to the overall economic advancement, especially in India, which contributes about 17-18% of GDP and ranks second in the world in agricultural production. Fertilizers play an vital role in maintaining plant growth by supplementing essential nutrients absorbed by plants from the topsoil. Inadequate use of fertilizers can significantly damage crop yields. However, precise fertilization is important, taking into account factors such as rainfall and the specific nutritional needs of the crop.

To solve this issue, machine learning technology provides a potential solution by leveraging data related to crop fertility and rainfall. Providing farmers with comprehensive insights into their crops can lead to substantial benefits. The proposed model utilizes a machine learning algorithm, specifically the random forest regression algorithm with k-fold cross-validation technique. It requires two key inputs from users: the crop type and the location of cultivation.

Once the algorithm is applied, the model generates predictions regarding the optimal quantity of nutrients required for the selected crop, as well as the ideal timing for fertilizer application. To make this resource accessible to a wide range of users, a website has been developed using the Flask Python web framework. This web-based platform ensures compatibility across various devices and allows for easy sharing among farmers and stakeholders, facilitating informed decisions and improved agricultural practices.

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II. Related Works

A thorough examination of available literature reveals a collection of prior studies aimed at addressing the issue of fertilizer usage. For instance, predicting fertilizer usage can help farmers achieve proper yields while minimizing waste by reducing plant toxicity and deficiency to some extent (Krutika Hampannavar et.al., [1]) Fuzzy logic systems that can reduce fertilizer usage, resulting in increased crop productivity (G. Prabakaran et.al., [2].) The study conducted to evaluate fertilizer consumption in Agro Climatic Zones (ACZ) through comprehensive data collection, which included daily field measurements and laboratory analysis spanning a three-year period. The primary objective was to precisely determine the specific fertilizer requirements for individual parcels of land within these zones.

The enhanced fertilizer efficiency alone is insufficient in preventing issues caused by soil compaction (A. Hussein et.al.[10]).The study delved into the agronomic performance and economic viability of cultivating grain sorghum under two different soil conditions: compacted soils, which simulate non-CTF (Controlled Traffic Farming) systems, and non-compacted soils, representing CTF systems.

To establish a quantifiable relationship between N and P for fertilizer usage in terms of agricultural yield, nitrogen need, and nitrate remnant level, (Zujiao Shi et.al. [11]). This is further supported by Yulong Yin et.al. [4], which provides a comprehensive measure for estimating nutrient requirements and the role of soil chemical properties.

Due to the stochastic nature of rainfall patterns and temperature variation, determining crop yield is a challenging task. Various data mining techniques, (Shital Bhojani [3]), can be applied to predict crop yield.

The intensification of rainfall may cause enhance the leaching of nitrogen into groundwater (Laura J.T. Hess et al. [5]), which can have impacts on both the economy and the environment. Implementing no-till management techniques could act as a safeguard by reducing the effects of this intensification, on loss.

A novel metric for soil quality and health (Tony Yang et. al. [7]), which includes soil refinement. Also suggested the creation of policies and strategies that has the potential to guarantee the preservation of fertile soils – a vital aspect for fostering sustainable growth, in ecosystems and promoting the overall welfare of agricultural systems and human society.

The changes in the creation and elements of soil populaces and capabilities resulting from the interaction between long-term treatment and precipitation variations (János Kátai [8]), to determine if preparation history affects soil microorganisms' water-obstruction. The study says the impacts of NPK (nitrogen, phosphorus and potassium) fertilization and variations, in rainfall, affect maize monoculture. The objective is to comprehend how the previously used fertilizers might affect the soil microbes to withstand water stress.

Predicting agricultural yield as a function of rainfall by providing a general summary of how production will be affected by rainfall and how much a given crop can yield (Benny Antony [13]). The suggested method of evaluation, which examines all regression procedures, is superior to other existing methods of evaluation.

A unique method to predict the yield of various crops grown in India (Potnuru Sai Nishant et.al [6]). With the use of simple criteria such as the state, district, and area, the user can forecast crop yields accurately for any year.

A proposed transfer learning approach to create a pre-trained model that can detect patterns in the dataset (Janmejay Pant et.al. [12]). This model is then utilized to predict crop yields with great accuracy.

The use of supervised algorithms, (Akash Manish Lad et.al. [14]) has proven to be an effective way of boosting crop yields while minimizing the human labor, time, and energy spent on various agricultural tasks. Moreover, this technique also offers plant suggestions based on specific soil parameters, which helps in predicting crop sustainability.

Machine learning models have demonstrated significant potential in interpreting and evaluating results related to the long-term usage of fertilizers. These models offer several advantages in the context of optimizing fertilizer application and assessing its impact over time (Saheed Garnaik et.al. [16]).

Development of a decision-based system that uses climatic, crop, and insecticide/pesticide data to predict crop yields (Rubby Aworka et. al. [17]). This method is incredibly useful in creating a comprehensive understanding of crop sustainability and offers valuable insights that can be employed in other long- term experiments.

An integrated solution to Pre- Cultivation activities, which aims to assist small farms in achieving high production at a low cost (Senthil Kumar Swami Durai et.al.[18]). This study also helps in estimating the total growth expenses and aids in planning for the future. The Pre-Cultivation activities suggested in this paper offer an integrated solution that can significantly improve the efficiency of agriculture.

An innovative solution to soil nutrient classification problems using a rapid learning classification technique called Extreme Learning Machine (ELM) with various activation functions (M.S. Suchitra and Maya L. Pai [19]). This method provides an efficient way of classifying soil nutrients, which is crucial for achieving high crop yields. By utilizing this technique, farmers can develop a comprehensive understanding of the nutrient levels in their soil, which allows them to take necessary measures to improve soil fertility and crop production.

Crop illnesses have a significant impact on the total crop output, according to study. In the Kashmir Valley, a study [15] was conducted using an IoT system to propose an apple disease prediction model using data analysis and machine learning. This article examines the challenges of combining modern technology with traditional agricultural methods.

III. The Proposed Model

In the study, a model to predict the crop nutrient requirements has been created using the RF method. The model is implemented as the RF regression with k-fold cross-validation, demonstrating satisfactory accuracy in predicting nutrient requirements. The fundamental approach in this research involves user input, including factors such as place of the crop and type of crop, as essential components of the system.

- The Weather API receives the location and provides specific weather attributes in response. And also receives information such as temperature, humidity and rainfall.
- The user will receive warning message when there's a potential heavy rainfall.
- The best possible time to fertilize using fetched weather data will be predicted.
- The NPK module estimate the required ratio of NPK (Nitrogen, Phosphorus and Potassium) content displayed on the website

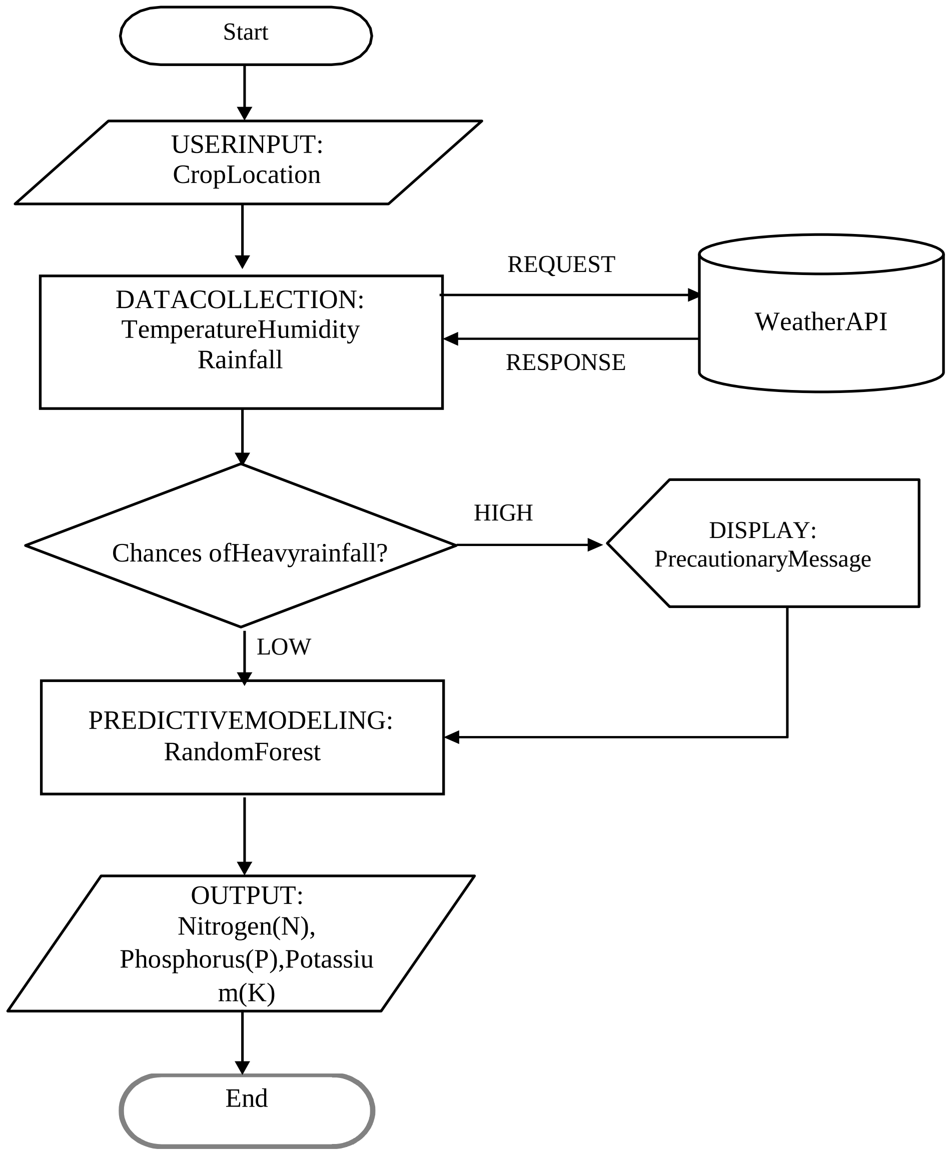

Fig. 1: Flow Diagram to Depict Overall Application

Random Forest Algorithm

This research involves the use of a random forest (RF), which consists of decision trees trained using different data subsets and different hyper-parameters. The input to the RF model is crop type and location, which will allow us to anticipate the values of N, P, K. The data set is split into training data sets and testing data sets, which Training data is 80% and the remaining 20% for testing. Three random forests with 50 decision trees each for N, P, K and produce a class average as a prediction for all trees.

Input Features

- Crop
- Location: State, City
- Weather Details: From weather API

Output Features

- Label N: *Amount of Nitrogen*
- Label P: *Amount of Phosphorous*
- Label K: *Amount of Potassium*

Data Preparation

The Crop Recommendation Dataset, which is last accessed on November 16th, 2022, has many features which includes features such as N, P, K, temperature, humidity, ph, rainfall and many more. However, not all of these features are relevant for the model being proposed. To address this, the technique of feature selection is used to reduce the dimensionality of the dataset, resulting in seven features that were then evaluated.

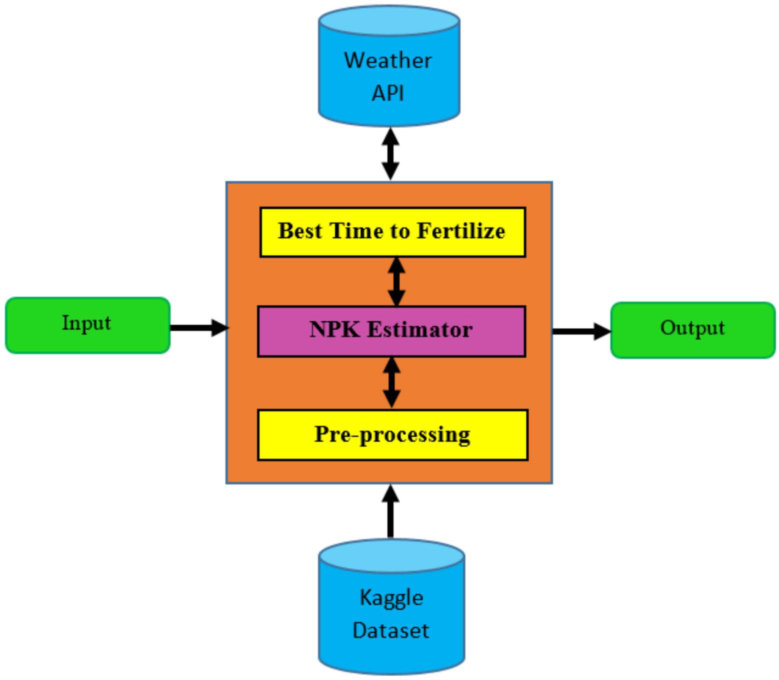

Fig. 2: Architectural Overview

Algorithm: The RF Algorithm

Begin:

Step 1: The initial dataset, consisting of 2,200 entries. The dataset is divided into two subsets: a training dataset comprising 80% of the data, equivalent to 1,760 entries, and a test dataset containing the remaining 20%, totaling 240 entries.

Step 2: Utilizing random forest regression, the N, P, and K values undergo analysis with the assistance of 50 decision trees.

Step 3: Within the training dataset, the N Label, P Label, and K Label are trained based on the dependent variable. Specifically, the variable is designated as N for N Label, P for P Label, and K for K Label.

Step 4: For each labels of N, P, K generates 50 decision trees as output during the training process using the training dataset.

End

IV. Results

Eco Fertilizer, has been developed as a website that recommends the appropriate timing and quantity of nutrients required for a selected crop. It is also introduced with a warning system that predicts heavy rainfall.

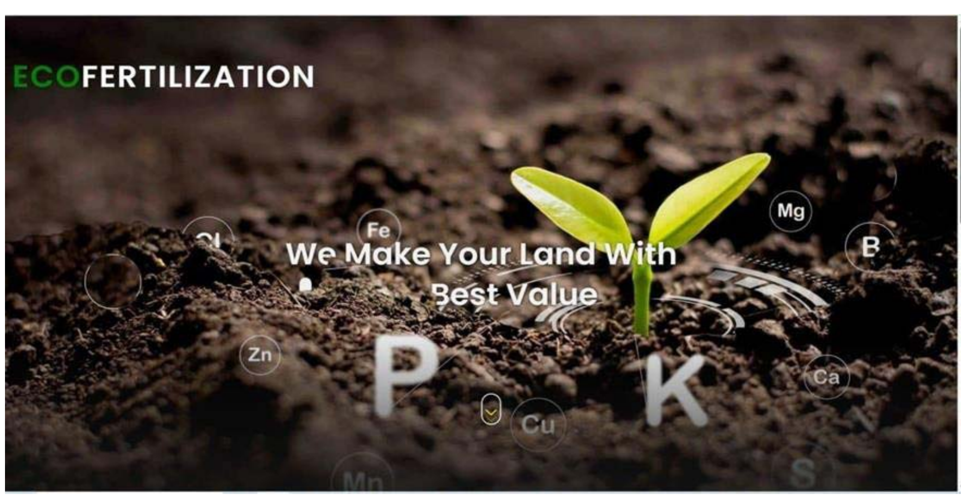

Fig.3: Landing Page of Eco-Fertilization

Fig. 4: Input Form

Fig. 5 Updated Details

Fig. 6: Applying Algorithm for the input details

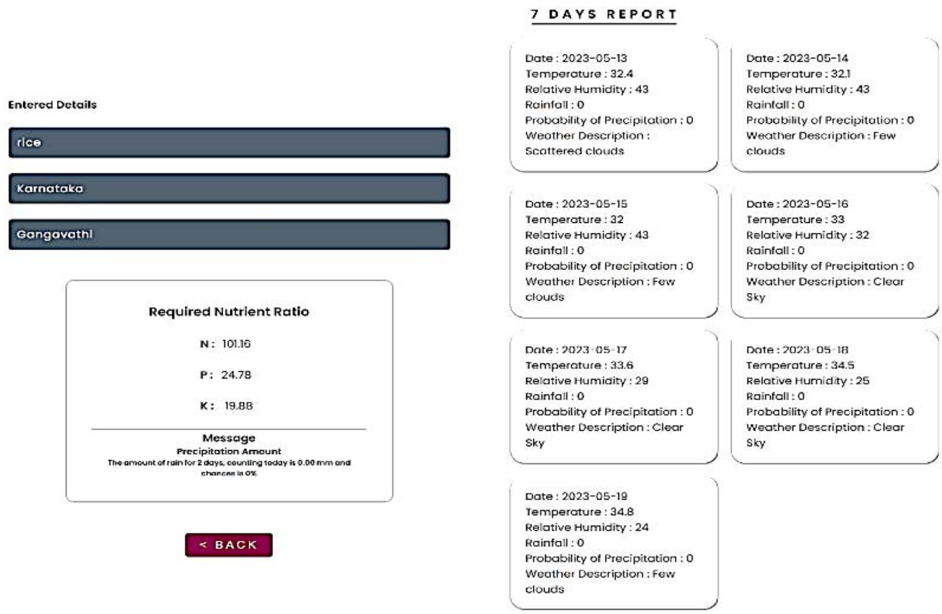

Fig. 7: Seven Days Report of Weather Forecasts & Alerts/Messages

V. Conclusion

The purpose of this study is to determine the quantity of nutrients and fertilizer required for effective growth and yield taking into account climatic conditions. Provides weather alerts and notifications. If bad weather, a warning displayed as output.

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Leveraging Foundation Models for Scientific Research Productivity

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LEVERAGINGFOUNDATIONMODELSFORSCIENTIFICRESEARCHPRODUCTIVITY

Strictly as per the compliance and regulations of:

Leveraging Foundation Models for Scientific Research Productivity

Ross Gruetzemacher

Abstract- The objective of this work was to elucidate paths for expediting and enhancing scientific research productivity from the emerging AI paradigm of foundation models (e.g., ChatGPT). Faster scientific progress can benefit mankind by speeding up progress toward solutions to shared human problems like cancer, aging, climate change, or water scarcity. Challenges to foundation model adoption in science threaten to slow progress in such research areas. This study attempted to survey decision support systems and expert system literature to provide insights regarding these challenges. We first reviewed extant literature on these topics to try to identify adoption patterns that would be useful for this purpose. However, this attempt, using a bibliometric approach and a very high level traditional literature review, was unsuccessful due to the overly broad scope of the study. We then surveyed the existing scientific software domain, finding there to be a huge breadth in what constitutes scientific software. However, we do glean some lessons from previous patterns of adoption of scientific software by simply looking at historical examples (e.g., the electronic spreadsheet). Ultimately all of these were unable to provide the degree of guidance that the study had aspired to, which could be used to assist in expediting the adoption of these systems, but our analysis of the speed of progress in these domains points to the likelihood of the future impact of large language models on science being more closely tied to augmenting or automating the creative tasks of hypothesis and experiment generation. In the discussion we explore the implications of these findings that suggest future work on this topic could benefit from focusing on empirical methods to better understand the natural roles of large language models in augmenting and automating scientific tasks.

I. Introduction

Technological progress is widely considered the key driver of economic growth (Moykr et al. 2015), and it is the result of knowledge creation from scientific research and development. Over the past fifty years, software has played an increasingly important role in scientific research and development, and it is poised to play an even greater role in accelerating technological progress in the future as artificial intelligence (AI) becomes widely used for productivity and creativity enhancement applications[1] (Gruetzemacher 2022).

AI technologies have continued to make incredible progress for more than a decade (Krizhevsky et al. 2012, Mnih et al. 2015, Silver et al. 2016, Brown et al. 2020, Reed et al. 2022). While this progress hasn't translated to practice as dramatically as some have anticipated (Brynjolfsson et al. 2018), it is unlikely that we are at the onset of a third AI winter[2]. In fact, the latest family of AI models appears to be ready to live up to the growing AI hype of the past decade, with many describing these models as a general purpose technology (Bommasani et al. 2021; Eloundou et al. 2023).

This recent progress has been driven by advances initially in the AI subdomain of natural language processing (NLP). These advances have most commonly been associated with language models, which are statistical models of human language that are essentially trained to be able to predict the next word in a sentence. To be certain, this is an oversimplification, but more detail is beyond the scope of this study[3]. However, the progress in NLP is now bleeding over to other subdomains of AI such as computer vision and robotics (Reed et al. 2022). This progress is in an emerging research area that is known as foundation models (Bommasani et al. 2021).

Language models are one type of foundation model, but they are only trained on language data. However, foundation models can be trained on different types of data, for example on image data or video data, in a semi-supervised fashion like language models (Bommasani et al 2021); they can even be trained on multiple data types in what can be described as multimodal models. An example of this is DALL·E 2 (Ramesh et al. 2022), a multimodal model that can take text as input and generate images as output. A version of GPT-4 (OpenAI 2023) integrated into ChatGPT (OpenAI 2022) was used to generate Figure 1 (see Figure caption for more detail), and is now being marketed by OpenAI for creative design tasks. An even more powerful multimodal model was used to create a generalist agent capable of interacting with the real world through robotics and natural language, and

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[1] Google's DeepMind AI research lab has a goal of "solving intelligence to advance science and humanity" (Hassabis 2022).

[2] AI has historically gone through two previous hype cycles that have been followed by periods of reduced interest and funding. The periods of reduced interest and funding are commonly described as AI winters.

[3] Interested readers can refer to Gruetzemacher and Paradice (2022).

capable of outperforming humans at video games [4] (Reed et al. 2022).

Figure 1: An Image Generated from a Text Prompt: “Create a Photorealistic Image of a Scientist Putting herself out of work by using an AI System to Generate Hypotheses and to Propose Experiments that her Research Assistants can conduct in her Laboratory.” This Image was Created Using GPT-4 (Openai 2023) Via Chatgpt Plus

Given the tremendous potential for capabilities such as those demonstrated by DALL·E 2, foundation models are expected to lead to a new generation of AI-driven software tools for enhancing creativity and productivity (Gruetzemacher 2022). Foundation models are actually thought to be a general purpose technology (GPT; Bommasani et al. 2021), with the potential to transform society in a manner similar to previous GPTs like electricity or the internal combustion engine (Lipsey et al. 2005). It is difficult to imagine how an emerging technology with such tremendous transformative potential will come to be used in society, much like it would be difficult to anticipate the impact that electricity would later have in 1882 when electricity generation began to first be used to light streets at night. We are

[4] This agent, Gato (Reed et al. 2022), was very impressive with respect to the breadth of its capabilities, and interested readers are encouraged to visit https://www.deepmind.com/publications/a-generalist -agent.

particularly interested in how foundation models, or other powerful AI tools of the future, might enhance creativity and productivity for research and experimental design, particularly as it relates to advancing science, as this appears to have the greatest potential for positive- and negative-impact to humanity.

There has been a significant amount of discussion regarding the use of AI for scientific discovery or as a driver of scientific progress. Google DeepMind's mission is to "solve intelligence to advance science and humanity" (Hassabis 2022), and Lila Ibrahim, their COO, recently explained that for scientific research the "ability to use a more generalized intelligence to augment human knowledge-to have some of these breakthroughs-is really going to be quite spectacular" (Kopytoff et al. 2022). While DeepMind may ultimately seek to automate scientific progress, augmenting human knowledge is the direction that current AI models are moving toward most rapidly. Software that uses AI, like foundation models, to augment human knowledge and enhance scientific research productivity and creativity is the focus of this study.

While we are more interested in AI technologies that can augment human intelligence to enhance scientific research productivity and creativity, it is important to point out other ways in which AI is being used to progress science. DeepMind's use of AI in science is already a game changer (Service 2020) because they have effectively solved the problem of protein folding with AlphaFold (Jumper et al. 2021) and created a comprehensive open source database of over two hundred million protein structure predictions [5]. Previously, AI software took the form of expert systems, which contained encoded expert knowledge but were limited to preprogrammed solutions. However, DeepMind is applying machine learning which enables learning generalizable solutions from first principles. DeepMind has also made progress in other scientific areas, such as nuclear fusion (Degrave 2022).

What is common about DeepMind's AI systems for the protein folding problem and for nuclear fusion is that they are systems developed to excel at a single well-defined task (i.e., predicting protein structures or maintaining stability in a high-energy plasma). The promise of foundation models, and tools that can be used to augment human intelligence, lies not in their ability to do one task well, but in the ability of these tools to adapt to whatever task humans require of them. In machine learning, this adaptability is known as the ability of a model to generalize.

While foundation models offer great potential for transforming the scientific landscape, they are also anticipated to create challenges. Applications of language models for science will involve the creation of academic work used for peer review, as well as more general productivity and creativity tools. Because language models are trained on data from the internet, they can come to exhibit biases or flawed data, which could make their use as an aid in peer review more difficult as scientists will not want to trust them (Okerlund et al. 2022). Moreover, because the models require a large amount of data for training, they will likely reinforce Anglo-American dominance in science.

a) Spreadsheets, The First "Killer Application"

In 1978, Dan Bricklin, a student at Harvard Business School, noticed a pattern in the errors his professor made when completing rows and columns of a table for a business case during a lecture (Castelluccio 2019). Dan noticed that the errors would propagate through the table; one error often required replacing multiple entries in the table to correct for it. Personal computers were emerging at the time, and Dan came up with the idea for a program that could act as a visual calculator for operations organized in tabular form. This idea is what we now think of as a spreadsheet, and while it was not entirely new, Dan's program VisiCalc became the first electronic spreadsheet and the first "killer application" for the personal computer (Zynda 2013).

The power of the electronic spreadsheet lay in its ability to do general computing tasks without requiring users to know how to program (Zynda 2013). Moreover, the application was designed with user experience in mind so as to be straightforward and easy to use for non-programmers. This led to many users purchasing personal computers solely for VisiCalc. Bricklin and his business partner Bob Frankston were urged not to pursue a patent for the software, which would have been difficult to get for software at that time. This left VisiCalc vulnerable to competition, and over the following years Lotus-1-2-3 overtook VisiCalc's market share (Sachs 2007).

In the decades since, electronic spreadsheets have grown to be used nearly ubiquitously for a variety of analytics-related tasks while changing very little from the initial versions. Looking at the history of spreadsheets, we see a pattern of development centered on creating a standardized product, one that looks, functions and feels like all other spreadsheets (Campbell-Kelly 2003). This may be the case because spreadsheets are functional as they are, and adding to it is not necessarily desirable (Sachs 2007). Microsoft Excel is now dominant in the market, but competitors are also widely used, such as Google Sheets, a cloud spreadsheet alternative.

The ability to complete a broad range of computing tasks without the need to know how to program was a game changer in 1979, and it meant that spreadsheets were software that had a great ability to

[5] AlphaFold is the system that was used for this, and the database can be found at: https://alphafold.ebi.ac.uk/.

generalize to a wide variety of problems. Due to their ability to generalize to a wide variety of tasks, they are a useful example to study when considering the next generation of software that AI will lead to—the next generation of AI is going to help create tools with this ability to generalize[6]. Perhaps foundation models are going to lead to a new 'killer app' similar to the spreadsheet, and in this study we will more carefully analyze what it means to be generalizable software. In fact, the generalizability of software is key to what we consider productivity and creativity enhancing software, the focus of this study that we will define in the following subsection.

b) This Study

Spreadsheets were one of the earliest decision support systems to become widely popular. To understand the significance of spreadsheets and other technologies relevant to this study, we can look at how frequently these technologies have been mentioned over time. In Figure 2 we use this approach to track the significance of six technologies-spreadsheets, expert systems, decision support systems, natural language processing, machine learning, and artificial intelligence-over the past 50 years. AI, spreadsheets and expert systems all gained a lot of interest in the 1980s. Interest in expert systems quickly diminished. Interest in AI and spreadsheets diminished also; significantly for AI, although substantial interest continued steadily; interest for spreadsheets diminished slightly, and stayed steady for some time, although it seems to have started to diminish more.

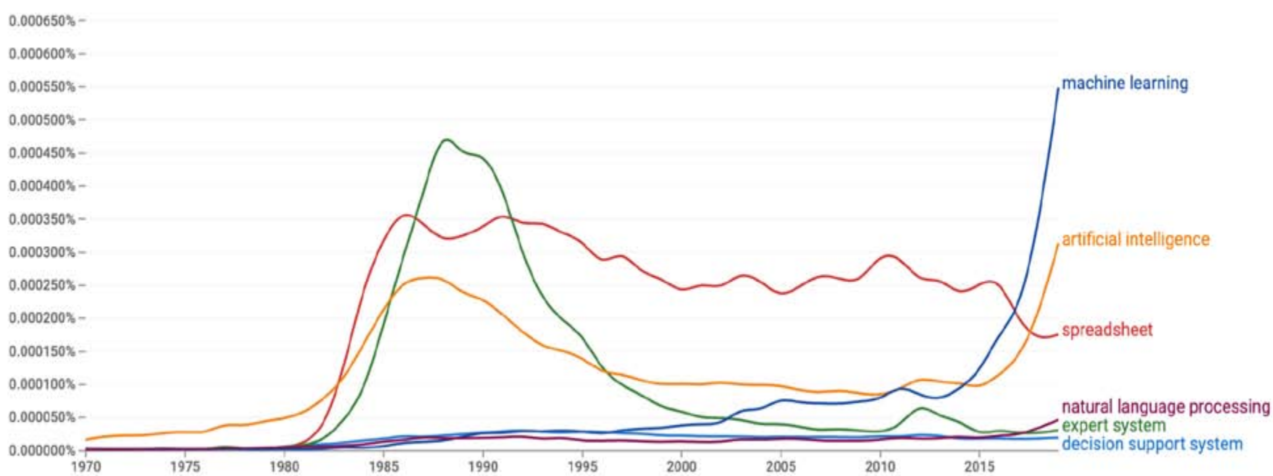

Figure 2: The Frequency of Select Words and Phrases in the Google Books Corpus Since 1970[7].

Lately, interest in machine learning and AI have begun to explode. Interest in natural language processing is also increasing, but it is unclear how significant this increase will become (i.e., will it increase dramatically like machine learning and AI). Natural language processing aside, it is important to note that AI is used more frequently now than ever, and that machine learning is used twice as often as AI was used during the last AI summer in the 1980s. This time it is unlikely that AI is as overhyped as it was four decades ago, and it is more likely that we will begin to see profound applications of foundation models-the new general purpose technology-across a wide variety of economically valuable applications.

We know that spreadsheets were the first 'killer app' for the personal computer, but it is an open question as to what is going to be the first 'killer app' for foundation models, the latest general purpose technology? Will the characteristics of spreadsheets that made them useful for a broad range of applications-their ability to generalize to a variety of tasks-lead to a new AI-driven app that transforms business? We do not know the answers to these questions, but in this study we attempt reviewing the existing literature to provide a lens through which to view these questions. Specifically, we review literature related to the development of software, scientific software, decision support systems, expert systems, etc. in order to identify insights that can improve the development and adoption of next-generation, AI-driven (i.e., foundation model-driven) software, thereby contributing to the progress of science.

We begin in the next section by identifying definitions of research and experimental development, science, scientific software, etc. We identify criteria for making classifications among different types of scientific software, resulting in a critical distinction between specialized scientific software, like what DeepMind is using for protein folding and nuclear fusion, and more generalizable scientific software, such as tools like spreadsheets which are not always strictly limited to

[6] Tools like Elicit, from ought, are already attempting to become the next 'killer app': https://www.elicit.org.
[7] https://books.google.com/ngrams/

scientific applications. In the following section we review relevant bodies of literature, ranging from software development, to scientific software, to earlier AI-based software like expert systems. We follow this with a discussion and synthesis of the literature, before finally making concluding remarks.

II. Background

Scientific software has been a topic of research since the early 1970s (Hatton 1970; Madison et al. 1970), although it was not heavily studied in academia until over a decade later. While not scientific software per se, electronic spreadsheets were initially developed in the late 1970s and have been widely used in scientific research. In this study, we are interested in both scientific software and more generally useful applications such as electronic spreadsheets. The latter can be used for a wider variety of applications but that also significantly enhance productivity and creativity with respect to scientific research and are our primary concern. However, before diving more deeply into the literature concerning the development of these tools, we first must define what is meant by terms such as scientific software or productivity and creativity enhancement software.

a) *Definitions*

We consider scientific research to encapsulate all research driving technological progress, be it in the social sciences, engineering, the hard sciences, etc. Thus, we define science broadly as a communal and systematic enterprise that builds and organizes knowledge through the process of research and experimental development (Wilson 1999; National Academies of Science 2019). The final portion of this definition-research and experimental development-is key to this study because this is the process through which scientific knowledge is created.

The Frascati Manual[8] is widely thought to be the authoritative source of metrics for evaluating scientific progress, especially for economic purposes (OECD 2015). The Frascati Manual is not directly concerned with scientific research, but focuses entirely on research and experimental development-referred to in the manual simply as R & D-and its components as measurement of such activity is of principal concern to economists. The Frascati Manual defines research and experimental development as creative and systematic work conducted to advance the body of knowledge, including knowledge of humanity, culture and society, and to generate new applications of available knowledge.

The Frascati Manual makes a critical distinction of the three components of R & D: 1) basic research, 2) applied research and 3) experimental development (OECD 2015). Basic research is experimental or theoretical work undertaken primarily to acquire new knowledge without a specific aim or application. Such research is often undertaken by academics or governments. Applied research refers to investigations that seek to generate new knowledge, but that have a specific, practical aim at the outset. Often applied research attempts to determine uses for theory or knowledge generated in basic research, and it is often conducted by organizations as the results are intended for practical applications to products, operations, methods and systems. Finally, experimental development draws on knowledge from research and practice to produce additional knowledge in the attempt to create novel products or processes, or to improve existing products or processes. Experimental development should not be confused with product development, as it is not concerned with commercialization of a product-it is only a single stage in the product development cycle.

Kanewala and Bieman (2014) define scientific software simply as “software used for scientific purposes”. In other prominent literature on scientific software, little effort has been made to define scientific software (Hannay et al. 2009; Joppa et al. 2013). We defer to Kanewala and Bieman’s definition for this study, and we point out that this would include software such as electronic spreadsheets if they are used for scientific purposes. This is appropriate for this study, as we are interested in generally capable software that can have a wide range of applications in science and R & D. However, the broad definition is not implicit in much of the prominent literature on the topic. Consequently, we will clarify this distinction between what is traditionally considered scientific software and the more general software that we also consider to be relevant in this study.

The use of the term scientific software in the existing literature is varied. A significant amount of previous work involving scientific software is tied to scientific computing and computational science. In these cases, scientific software refers to software designed to run in a distributed environment such as for high performance computing (i.e., supercomputing; Grannan et al. 2020). Other work refers to a scientific software ecosystem comprised of scientists developing custom software for specific domains, commercial scientific software developers and administrators of platforms for high performance computing (Howison et al. 2015). This broader vision of the scientific software ecosystem better captures the intent of our broad definition of scientific software.

We define specialized scientific software as software that is developed for a specific class of problems in a single domain or closely related domains which doesn’t have utility to those working on other problems or outside the domain(s). This could be a

[8] The first edition was published in 1963, and the current edition, published in 2015, is the 7th edition of the manual.

commercial program run on individual workstations, such as Pointwise for generating grids for computational engineering; it could be a proprietary program like DeepMind's AlphaFold that is run using distributed computing; or it could be an custom application for controlling physical actuators such as the software DeepMind created for steadying superheated plasma in nuclear fusion or software used in robotics. Specialized systems such as control systems, decision support systems and expert systems, when used for scientific applications, would also be considered specialized scientific software.

We define generalizable scientific software as software that is capable of tasks that are very general and which are useful for a wide variety of applications, with science and R&D being common applications. Generalizable scientific software is often software designed at enhancing creativity and productivity. Excel could be considered as part of this group. Other examples and a more granular discussion of generalizable scientific software are included in the next section.

b) *Categories of Scientific Software*

Above we have key terms such as science and research and experimental development (R & D; OECD 2015). We further made a distinction between specialized scientific software and generalizable scientific software. Here, we build on this dichotomy and again draw from the Frascati Manual to develop a set of criteria that we can use for mapping the space of scientific software.

As discussed in the previous subsection, the Frascati Manual proposes distinctions between three different categories of research and experimental development: 1) basic research, 2) applied research and 3) experimental development. The manual further lays out five criteria that are to be used when determining whether an activity constitutes an R&D activity. Specifically, the manual requires that activities be:

- Novel-the activity should be aimed at generating new knowledge.
- Creative-the activity should involve concepts that are original and not obvious.
- Uncertain-there should be substantial uncertainty about the outcome *a priori.*
- Systematic-the activity should be fastidiously planned and conducted systematically.
- Transferable and/or reproducible-it should lead to results that are reproducible.

Anything assisting in the criteria above can be considered to assist in the development of scientific software. However, we also need to understand the common activities that comprise scientific R & D. Below we propose lists of common activities for both basic and applied research.

There is a large amount of software that could be construed as scientific software, and in order to map the space of scientific software we must identify categories of software based on the activities or tasks that they assist scientists with. We have already described two broad categories—specialized scientific software and generalizable scientific software—and we discuss these further below. However, we also need to categorize further specialized scientific software so that we are able to create the map we desire.

First, we might identify software that can be used for scientific research but that is not relevant to the objective of our study. For one, we feel that project management software and its adoption lies outside the scope of this work[9].

Another categorization that may be useful is that of 'click-and-run' software and 'syntax-driven platforms'; 'click-and-run' refers to software with polished user interfaces whereas 'syntax-driven' refers to either application programming interfaces (APIs) or software navigated via command line interfaces (CLIs). In a survey conducted by Joppa et. al. (2013) scientific software users were split between those who preferred 'click-and-run' programs and those who preferred 'syntax-driven' programs.

Software that doesn't seem to fit nicely into one of the two categories provided poses challenges to the proposed definitions. An example might be computer-aided design software that enables designers, engineers and researchers to design parts, products and experimental apparati might be an example of something that doesn't fall clearly into one of the two categories. This would be the case because the task is very specific, to simply create a 3D object digitally. Objects can vary so much that there is often software specific to different domains, but some of the most generic applications can be useful to a wide range of domains. Because it is unclear how to classify such software, we further specify that in such cases of ambiguity, consider the task the software performs or the problem that it solves, and whether or not this is general or specialized.

III. Review of Literature

a) *Scientific Software Literature*

Increasingly, the generation of new knowledge in science and engineering is heavily dependent on software, and this trend is pervasive through all domains (Joppa et al. 2013).

A substantial amount of extant work in the literature on scientific software relates to the use of high performance computing (HPC) in the computational sciences (Basili et al. 2008; Joppa et al. 2013; Grannan

[9] For more on this topic, interested readers can see Romano et al. (2002) or Liberatore and Pollack Johnson (2003).

et al. 2020). While this may not seem relevant, there are some things that might be valuable from this literature. Consider that AI systems like foundation models require large amounts of computation to process language (Sevilla et al. 2022; Kaplan et al. 2020; Amodei and Hernandez 2018). And, another term for NLP is computational linguistics, and it is a subdiscipline of computer science that is effectively a computational science.

Many of the problems described in the HPC scientific software literature involve the portability of this software from one system architecture to another system architecture (Joppa et al. 2013). This can be particularly challenging, and may be relevant to the proliferation of AI scientific software. Particularly, two things may be impacted: large, open source foundation models and regulatory testing and evaluation of large foundation models.

The problems of parallelization of large distributed systems, even for the most simple of tasks, were so tremendous that the first real solution didn't emerge until the demands of the growing search market in the early 2000s led to Google's MepReduce programing paradigm, first reported in 2004 (Dean and Ghemawat 2004). Hadoop was created as an open source version of Google's MapReduce in 2007 (Borthakur 2007; Shvachko et al. 2010). Spark (Zaharia et al. 2012), built on top of the Hadoop distributed file system similarly works well for parallelizing general problems, but both Hadoop and Spark still are insufficient for scientific computing, even if still very useful for analysis of data generated in scientific computing applications. The only similar software enabling large scale distributed computing on compute clusters with various architectures might be Google's Tensorflow (Abadi et al. 2016) and Meta's Pytorch (Paske et al. 2019). These platforms are used specifically for deep learning applications, which would most likely be for scientific computing—specialized scientific software or generalizable scientific software—but would not necessarily be.

We describe the examples of MapReduce (Dean and Ghemawat 2004), Hadoop (Borthakur 2007), Spark (Zaharia et al. 2012), Tensorflow (Abadi et al. 2016), and Pytorch (Paske et al. 2019) to illustrate the limited number of platforms able to support automate parallelization on large-scale distributed compute clusters. This is important because HPC software is typically written for specific system architectures due to the need for parallelization under specific system constraints. While Tensorflow and Pytorch are written specifically to be able to be applied to a broad range of tasks, parallelization on very large models again encounters the challenges traditionally found in scientific computing (Basili et al. 2008; Joppa et al. 2013; Grannan et al. 2020). Challenges of parallelization on the proliferation and use of foundation models for all applications, including for scientific applications, is something that companies appear to be increasingly cautious of publishing publicly. One recent exception to this would be Google's description of their Pathways program (Barham et al. 2022). This architecture was used to train Google's largest model to date, PALM 2 (Anil et al. 2023), which is referenced in the acronym PALM is derived from Pathways Language Model (Chowdhery et al. 2022). Pathways is able to scale beyond the limitations of the TPU v4's 3d torus network topology (Jouppi et al. 2023), although the scalability is unclear beyond two TPU Pods. In the future, if proprietary systems for distributed inference are required, this could be problematic for sharing of open source systems or testing and evaluation of systems if a single architecture is not adopted. The architecture that is likely to be adopted will be that dictated by the market leader, Nvidia, with their Superpod architecture used in HPC systems like Nvidia's Selene compute cluster, number 13 on the Top 500[10] as of November 2023. It is likely that cloud providers will continue to use this architecture, and even possible that Nvidia provides a parallelization process for models that require more than a single pod to run inference or train on.

b) Technology Acceptance

Substantial work has been conducted on the topic of technology acceptance, and the Technology Acceptance Model (TAM), first proposed by Davis (1986), is the most commonly employed and influential theory related to an individual's acceptance of information technology (IT; Lee et al. 2003). TAM enables researchers to understand how users will respond when interacting with a new technology. It builds on Ajzen and Fishbein's (1980) theory of reasoned action, and it assumes that an individual's acceptance of IT is determined by two primary variables: perceived usefulness and perceived ease of use. It is very versatile, being able to be applied to various technologies in various situations with different control factors and with different subjects.

When discussing the results of prior research utilizing TAM, Lee et al. (2003) identify four categories of target IT systems: communications systems, general-purpose systems, office systems and specialized business systems. The issue with TAM is that it is specifically intended to analyze case studies in business applications, and is intended largely to provide theoretical contributions. It is intended to have implications for practitioners, but this is not the case in practice. Moreover, it is thought by researchers in information systems research to be a topic that academics should avoid because it is devoid of valuable contribution, and, in a period of what might seem to be a Kuhnian "mopping-up" period, or even a post "mopping-up" period (Kuhn 1962).

[10] https://www.top500.org/lists/top500/2023/11/

c) AI-Based Software

We conducted literature reviews of expert systems' and decision support systems' literature, first identifying existing surveys to provide an overview, and then using a bibliometric approach. For the bibliometric approach we used very generic search terms, and it was clear from the start that, for both decision support systems and expert systems, we would be unable to get useful results for a review so broad in scope.

For both topics we queried the database Scopus database, which allowed for querying large numbers of abstracts. We conducted our queries in May of 2022. Given our interest in enhancing scientific research productivity with foundation models, we focused broadly on decision support systems and expert systems to try to understand broad adoption trends.

d) Decision Support Systems

i. Existing Surveys

Prior to our bibliometric analysis of decision support systems literature, but using the results from our Scopus query, we reviewed extant literature reviews on decision support systems. After filtering the articles with 100 citations or more from the "decision support system" query, we identified those that were either surveys or literature reviews. There were several well-cited and broad literature reviews on the topic. The most significant of these involves a series of three surveys covering different spans of time: from 1971 to 1988 (Eom and Lee 1990), from 1988 to 1994 (Eom et al. 1998), and from 1995 to 2001 (Eom and Kim 2006). We summarize these literature reviews below:

- The first literature review in this group covering the earliest period-from 1971 to 1988 (Eom and Lee 1990)-concludes that Alter's proposed taxonomy for information systems (Alter 1977) was not suitable for decision support systems and proposed that integrating the separate decision-support systems that coexist in an organization was the next task in the future.
- The second literature review of this series covers the middle period-from 1988 to 1994 (Eom et al. 1998). In this survey, the authors proposed that: 1) supporting strategic decisions and the application of decision support systems to global management decision making should be the focal point of decision support system research, 2) the production and operations management and management information systems areas have become the two predominant fields of decision support systems research between the 1980s and the first half of the 1990s, and 3) graphics, visual interactive modeling, artificial intelligence techniques, fuzzy sets, and genetic algorithms had become widely used as decision support system tools.
- The third installment of this series, covering the final time frame-between 1995 and 2001 (Eom and Kim 2006)-concludes that during this time there were several important changes in decision support system application development including the development of negotiation support systems, organizational decision support systems, inter-organizational decision support systems, intelligent decision support systems, and web-based decision support systems.

We identified one other decision support systems literature review worth mentioning. Hosack et al. (2012) conducted a literature review to assess the future of decision support systems research. This study came to three valuable conclusions:

1. The paper suggested using the term decision support within a work system.
2. For research to continue to produce meaningful ideas for organizations, researchers of the future must strive to integrate technology evolution into the concept of organizational decision support while understanding that technology, decision-making processes, and organizational support are different foci of the research.
3. They predicted that knowledge management-based decision support systems and data warehousing, social media decision support, mobile computing, negotiation support would drive future trends in decision support systems research.

Clearly, these surveys did not illuminate any extant research relevant to the adoption of decision support systems for scientific applications. The technology acceptance model (TAM) remained the only robust body of relevant literature on technology acceptance (Davis 1989), but was insufficient for providing the guidance desired in this study related to adoption of new AI tools for scientific applications and expediting scientific progress.

Moreover, our literature review discovered that there were many, many more surveys of decision support system literature related to specific types of decision support systems. For example, reviews on a broad range of topics from agricultural decision support systems (Zhai et al. 2020), to manufacturing decision support systems (Kasie et al. 2017), to agent-based decision support systems for clinical management and research (Foster et al. 2005), to knowledge-based decision support systems in financial management (Zopounidis et al. 1997), to decision support systems' use in dental practices (Goh et al. 2016). A very large number of literature reviews focus on clinical decision support systems (Wright et al. 2016[11]; Kawamoto et al. 2005; Ahmadian et al. 2011; Kaushal et al. 2003; Sittig et al. 2006; Robinson et al. 2010). There is even a review related specifically to AI in clinical decision support systems (Montani et al. 2019). There are even numerous surveys on the use of machine learning in decision support systems alone (Hogenboom et al. 2016; Merkert et al. 2015; Ngai et al. 2011). There are many more domain-specific literature reviews, but we feel that those cited here demonstrate the breadth and volume of literature reviews on domain-specific topics as opposed to those more broadly on decision support systems research as a whole.

ii. *Bibliometric Analysis*

On the topic of decision support systems, we collected 120,019 abstracts using the search term "decision support systems". We used latent Dirichlet allocation (LDA; Blei et al. 2002), a statistical natural language processing technique widely used for topic modeling to identify the salient topics in the corpus. Based on the criterion of perplexity, commonly used as an evaluation metric when using LDA, it was determined that 23 topics was an optimal number of topics. We used 1-gram analysis with a default set of stop words and a default search for hyperparameters.

Figure 3: Above is a word cloud generated from the results of the LDA topic modeling for decision support systems. The trend noticed in the extant literature reviews of a large focus on clinical decision support systems can be seen to some degree with the terms clinical, patients, diagnosis, and health appearing in descending relevance. However, largely there is little with respect to structure in the clusters that is often associated with the use of LDA. We additionally had difficulty labeling the topics due to their poor quality.

Again, extensive effort was not placed on bibliometric analysis because 1) this study was not initially intended to utilize bibliometrics or scientometrics and 2) previous work had not had significant success with bibliometrics. Bibliometrics and scientometrics are more often used for identifying trends and predicting progress in technological development (Daim et al. 2016). Use of large language models may provide better results. However, given the findings of other elements of this literature review, we do not feel that further analysis of the data would have proven very valuable.

We concluded from these results, and their poor quality, that the breadth of the topic was too great to identify the types of trends we sought for providing a guide to enhancing scientific research productivity using foundation models. Foundation models are a novel, emerging technology, with emergent capabilities themselves (Bommasnie et al. 2021) that are difficult to predict (Wei et al. 2022). Thus, there are inherent challenges in finding insights that apply to our target topic, beyond just the challenges in the overly ambitious aims of our study.

e) *Expert Systems*

i. *Existing Surveys*

As depicted in Figure 2, the use of the term "expert systems" in literature exploded in the 1980s but had largely subsided by the end of the 1990s. Expert

[11] This was actually uncovered in a search and filtering, but not listed with the general literature reviews described above. In both expert systems and decision support systems Scopus searches, it was the only result in the contents filtered by citation that was not a review on the topics more broadly.

systems are a form of AI system that encode expert knowledge for retrieval and use in specific context to support the activities of professionals in a variety of jobs where extensive expertise is required. It could be thought that expert systems use AI techniques for information retrieval to the behavior or judgment of an organization, a human expert, or a group of human experts with exemplary expertise in a specific field.

As with decision support systems, we began by exploring the extant literature reviews on the topic. Again, we attempted to draw literature reviews from the bibliometric search we conducted of the Scopus database, after filtering out articles having less than 100 citations. Doing so, we found one highly cited literature review on the topic. Thus, we expanded our search slightly to try to identify more work.

The most widely cited reviews in this domain was that of Liao (2005) covering work done on expert systems in the decade from 1995 to 2004. This was the period during which interest in the topic was subsiding, at least based on the Google Books Corpus, as depicted in Figure 2. This review reported that, over this period: 1) expert systems methodologies were tending to develop towards expertise orientation and expert systems applications development was a problem-oriented domain; 2) that different social science methodologies, such as psychology, cognitive science, and human behavior could implement expert systems as another kind of methodology; and 3) that the ability to continually change and obtain new understanding is the driving power of expert systems methodologies, and should be the expert systems application of future works.

A text mining or bibliometric analysis of the topic was conducted and published relatively recently by Cortez et al. (2018). This paper talked significantly about authors' national affiliations, and worked used the results to propose a taxonomy which they compared with others, including not only a specialized expert systems taxonomy (Sahin et al., 2013) but also the two general library classification systems: the Dewey Decimal Classifications (DDC; Scott, 1998), and the Library of Congress Classifications (LCC; Chan, 1995). The EXSY journal recently (from 2018) adopted their taxonomy system.

Similar to what we found in decision support systems, there were numerous narrower reviews on specific types of expert systems. For example, we identified reviews on a breadth of subtopics including explanation in expert systems (Moore and Swartout 1998), expert systems in production planning and scheduling (Metaxiotis et al. 2002), expert systems evaluation techniques (Grogono et al. 1993), expert systems for fault detection (), and

Interestingly, expert systems showed up as topics in literature reviews focused on artificial intelligence techniques, as well (Bharammirzaee 2010; Horvitz et al. 1988).

ii. *Bibliometric Analysis*

On the topic of expert systems, we collected 65,551 abstracts using the search term "expert systems". We again used latent Dirichlet allocation (LDA; Blei et al. 2002) for our topic modeling. Based on the criterion of perplexity, it was determined that 16 topics was an optimal number of topics. Similar to the LDA analysis of the decision support systems corpus, we used 1-gram analysis with a default set of stop words and a default search for hyperparameters.

Figure 4: Above is a word cloud generated from the results of the LDA analysis. This illustrates the lack of value in the topics that were identified. It was difficult labeling the clusters in any meaningful way with the results from this process.

Overall, our perception of the expert systems literature was—just like the decision support system literature—that the scope was too broad to produce meaningful results. There were more general literature reviews than with decision support systems, but, in inspecting these studies we were unable to identify insights of substantive value to our goal of enhancing scientific productivity from foundation models. Much may lie in the fact that expert systems, like decision support systems, are more often used in business applications and not for advancing science. We see that much of the time neither decision support systems or expert systems would be categorized as specialized scientific software or generalizable scientific software as we define these terms in this study.

IV. Discussion

a) *Scientific Software Development*

There seem to be lessons that can be learnt from HPC-specific scientific software. One thing that we're not encountering yet is the need to port large language models or foundation models to different HPC compute clusters. However, as the need to test and evaluate increasingly generalizable systems grows, it will likely be necessary to have generic HPC architectures that large language models and foundation models can easily be ported to-at least for inference tasks-in order to test and evaluate them, particularly in the case of final pre-deployment system evaluations.

Particularly, the sensitivity of large AI models/systems to the coprocessor architecture, the system topology, and the interconnect bandwidth, will become an increasingly significant factor to porting large models to other systems. However, it is also critical that large models be deployed in very secure environments with near military levels of information security (Patel 2023). Therefore, any government facilities that are designed to test or evaluate such systems need to be very secure, and possibly even air-gapped or classified. The challenges of porting HPC software described by others are things that must be avoided for such testing and evaluation protocols to work, and these protocols must be enacted in legislation quickly due to the rapid pace of tech progress and the pace with which legislation is going to need to keep up (e.g., the NIST AI Safety Institute, the Federal AI Risk Management Act of 2023).

b) *Emerging AI Software Tools*

Some of the most valuable lessons from the literature regarding the development and adoption of novel software tools might be those taken from the case of the electronic spreadsheet. VisiCalc was novel, and brought new capabilities to non-programmers because it made general computing tasks possible without having to know a programming language or how to write a program. It is also significant to remember how important the user interface and user experience was-particularly the ease of use. We also note that Lotus 1-2-3 was able to overtake VisiCalc because it targeted IBM PCs, which were more widely adopted by businesses due to the reputation of IBM.

Other relevant lessons for enhancing scientific productivity from foundation models may involve the open sourcing of such models, but, there are inherent risks in open sourcing such powerful models. Additionally, lessons relevant to this were described in the previous subsection, being drawn from literature on software design in HPC.

For more complex software the users' need for trust increases, as they are not able to independently validate the results provided (Joppa et al. 2013). This is in contrast to previous generalizable scientific software that has been more transparent, with operations that are able to be verified with a calculator. Insights about emerging AI software tools was the inspiration for this study, and this proved to be a very difficult topic to glean insights on. However, we feel there is much greater potential in the automation of science described in the following subsection.

c) *Beyond Scientific Software Tools*

AI-powered NLP tools like ChatGPT (OpenAI 2022) have tremendous abilities, including abilities for foresight and creativity (Gruetzemacher 2022), and it would not be prudent to underestimate the transformative potential of AI driven by the capabilities of future systems (Gruetzemacher and Whittlestone 2022).

Moving beyond the notion of simply using foundation model-powered scientific software as a tool for discovery of new proteins (Jumper et al. 2021; Ferruz et al. 2023) or for accelerating human-supervised literature review (Gruetzemacher 2022; Manning et al. 2023; Haman and Skolnik 2023), it is possible to consider the use of increasingly powerful systems to automate literature review to the point where systems are able to 1) identify gaps in the existing literature and 2) to propose experiments and hypotheses to contribute to the body of knowledge in a field or domain. Perhaps this might be useful for scientific progress, albeit the mundane, or what Kuhn (1962) refers to as the "mopping-up".

Science has been thought to fundamentally be a process of conjectures and refutations (Popper 1963), and while at present much of experimentation seems likely to require human involvement, it is easy to expect that conjectures could be made by powerful foundation models in the near future. Moreover, conjectures that involve hypotheses testable by computational experiments might either avoid falsification or be refuted without human involvement. This is why Shevlane et al. (2023) foresee automation of AI research as an extreme risk. Ignoring that this is considered a risk, it is obvious that hypotheses beyond just machine learning or computer science can also be falsified computationally. Thus, we could see automation of such scientific areas in the future, first with "mopping-up" (Kuhn 1962) types of research, and later with novel or profound work.

Given the pace of recent progress in AI (Sevilla et al. 2022), and that progress is likely to continue[12] (Gruetzemacher et al. 2020) with continued scaling of model's training compute and dataset size (Amodei and Hernandez 2018; Kaplan et al. 2020), we must be cautious to not ignore these seemingly science fiction possibilities. Thus, this has significant potential for future work. In fact, we feel that a complete research agenda on the topic of automation of science is merited, but we outline some specific starting points for future work below.

i. *Future work*

One obvious starting point is to start experimentally trying to determine what hypothesis generation capabilities exist in today's cutting edge frontier models like GPT-4 (OpenAI 2023). Simple experiments could begin to uncover this, and we foresee a large range of potential experiments that could demonstrate different abilities of this phenomena. For example, simply identifying ten papers from a research group that could be confirmed to not be in the training data for a model, and then prompting the model-assuming a large enough context window, such as that with Claude 2 (Anthropic 2023) of 100,000 tokens-with the papers, asking it to propose new experiments and hypotheses. The results from this could simply be compared to the research group's actual plans for new experiments, or those that are published in the following six to twelve months.

Many variations of the above experiment could be conducted, and this could be done over a variety of domains. It might be useful to identify strengths and weaknesses of early systems, even if current systems are not practically useful, so as to anticipate weaknesses in future systems, and how we might go about addressing such deficiencies to expedite scientific progress.

Beyond just exploring the proof-of-concept, work could be done on the other half of the automation of science; i.e., for domains where experiments can be conclusively decided computationally. Research could be conducted to evaluate how well systems were able to take existing code from previous experiments in computational fluid dynamics or computational biology, and extend or adapt that code accurately and precisely enough to conduct an experiment testing a different hypothesis. These experiments need not begin with hypotheses generated from the systems, but rather, with very basic hypotheses simply extending the previous computational experiment. The key to this would be to understand the limitations of current foundation models at coding for scientific computing applications. It would be interesting to work on predicting whether the bottleneck for automating computational research disciplines will lie in the rigorous and robust 1) hypothesis creation, 2) design of experiments, or 3) execution of experiments.

Research along these lines could pave the way for a new pseudo-discipline of automated science. Previous work has described automated science for decades (King et al. 2009; Lenat 1979), but foundation models have unprecedented potential for this process. Further work should attempt to better understand how this might impact the economy and society, ensuring that rapid progress on this type of research does not wind up disproportionately benefitting the wealthiest of nations and ignoring the impacts to the Global South.

V. Conclusion

This paper has described an extensive effort to use literature review to identify potential paths for enhancing scientific research productivity through the use of foundation models. The initial plan, to review decision support systems and expert systems literature did not reveal much of value because the survey was overly ambitious. This was evidenced by previous literature reviews on these topics, which largely focused on reviews specific subtopics of the content in these broad topics. A review of the development of scientific software, such as literature on HPC software, as well as a review of applications often not considered scientific software, like the electronic spreadsheet, offered some useful insights, but none of the magnitude that we had sought.

During the course of the study, tremendous changes occurred in the field of artificial intelligence research, particularly the release of ChatGPT (OpenAI 2022) and the addition of GPT-4 (OpenAI 2023) into ChatGPT Plus. This has changed AI research dramatically, leading to governments taking seriously the transformative potential of AI for society more broadly (Gruetzemacher and Whittlestone 2022; Lazar and Nelson 2023). In the final subsection of the discussion we discussed some salient activities for future work to explore involving the use of advanced AI for driving and expediting scientific progress. We are particularly keen on the idea of using foundation models for automating scientific research, and encourage future work in this direction. Pursuing such research may avoid the limitations encountered by this study by looking forward to anticipate enhancing scientific software research productivity instead of looking backward.

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[12] Albeit possibly not as quickly as in the past five years (Gruetzemacher et al. 2020).

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9. Produce good diagrams of your own: Always try to include good charts or diagrams in your paper to improve quality. Using several unnecessary diagrams will degrade the quality of your paper by creating a hodgepodge. So always try to include diagrams which were made by you to improve the readability of your paper. Use of direct quotes: When you do research relevant to literature, history, or current affairs, then use of quotes becomes essential, but if the study is relevant to science, use of quotes is not preferable.

10.Use proper verb tense: Use proper verb tenses in your paper. Use past tense to present those events that have happened. Use present tense to indicate events that are going on. Use future tense to indicate events that will happen in the future. Use of wrong tenses will confuse the evaluator. Avoid sentences that are incomplete.

11. Pick a good study spot: Always try to pick a spot for your research which is quiet. Not every spot is good for studying.

12. Know what you know: Always try to know what you know by making objectives, otherwise you will be confused and unable to achieve your target.

13. Use good grammar: Always use good grammar and words that will have a positive impact on the evaluator; use of good vocabulary does not mean using tough words which the evaluator has to find in a dictionary. Do not fragment sentences. Eliminate one-word sentences. Do not ever use a big word when a smaller one would suffice.

Verbs have to be in agreement with their subjects. In a research paper, do not start sentences with conjunctions or finish them with prepositions. When writing formally, it is advisable to never split an infinitive because someone will (wrongly) complain. Avoid clichés like a disease. Always shun irritating alliteration. Use language which is simple and straightforward. Put together a neat summary.

14. Arrangement of information: Each section of the main body should start with an opening sentence, and there should be a changeover at the end of the section. Give only valid and powerful arguments for your topic. You may also maintain your arguments with records.

15. Never start at the last minute: Always allow enough time for research work. Leaving everything to the last minute will degrade your paper and spoil your work.

16. Multitasking in research is not good: Doing several things at the same time is a bad habit in the case of research activity. Research is an area where everything has a particular time slot. Divide your research work into parts, and do a particular part in a particular time slot.

17. Never copy others' work: Never copy others' work and give it your name because if the evaluator has seen it anywhere, you will be in trouble. Take proper rest and food: No matter how many hours you spend on your research activity, if you are not taking care of your health, then all your efforts will have been in vain. For quality research, take proper rest and food.

18. Go to seminars: Attend seminars if the topic is relevant to your research area. Utilize all your resources.

19. Refresh your mind after intervals: Try to give your mind a rest by listening to soft music or sleeping in intervals. This will also improve your memory. Acquire colleagues: Always try to acquire colleagues. No matter how sharp you are, if you acquire colleagues, they can give you ideas which will be helpful to your research.

20. Think technically: Always think technically. If anything happens, search for its reasons, benefits, and demerits. Think and then print: When you go to print your paper, check that tables are not split, headings are not detached from their descriptions, and page sequence is maintained.

21. Adding unnecessary information: Do not add unnecessary information like "I have used MS Excel to draw graphs." Irrelevant and inappropriate material is superfluous. Foreign terminology and phrases are not apropos. One should never take a broad view. Analogy is like feathers on a snake. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Never oversimplify: When adding material to your research paper, never go for oversimplification; this will definitely irritate the evaluator. Be specific. Never use rhythmic redundancies. Contractions shouldn't be used in a research paper. Comparisons are as terrible as clichés. Give up ampersands, abbreviations, and so on. Remove commas that are not necessary. Parenthetical words should be between brackets or commas. Understatement is always the best way to put forward earth-shaking thoughts. Give a detailed literary review.

22. Report concluded results: Use concluded results. From raw data, filter the results, and then conclude your studies based on measurements and observations taken. An appropriate number of decimal places should be used. Parenthetical remarks are prohibited here. Proofread carefully at the final stage. At the end, give an outline to your arguments. Spot perspectives of further study of the subject. Justify your conclusion at the bottom sufficiently, which will probably include examples.

23. Upon conclusion: Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium though which your research is going to be in print for the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects of your research.

Informal Guidelines of Research Paper Writing

Key points to remember:

- Submit all work in its final form.
- Write your paper in the form which is presented in the guidelines using the template.
- Please note the criteria peer reviewers will use for grading the final paper.

Final points:

One purpose of organizing a research paper is to let people interpret your efforts selectively. The journal requires the following sections, submitted in the order listed, with each section starting on a new page:

The introduction: This will be compiled from reference matter and reflect the design processes or outline of basis that directed you to make a study. As you carry out the process of study, the method and process section will be constructed like that. The results segment will show related statistics in nearly sequential order and direct reviewers to similar intellectual paths throughout the data that you gathered to carry out your study.

The discussion section:

This will provide understanding of the data and projections as to the implications of the results. The use of good quality references throughout the paper will give the effort trustworthiness by representing an alertness to prior workings.

Writing a research paper is not an easy job, no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record-keeping are the only means to make straightforward progression.

General style:

Specific editorial column necessities for compliance of a manuscript will always take over from directions in these general guidelines.

To make a paper clear: Adhere to recommended page limits.

Mistakes to avoid:

- Insertion of a title at the foot of a page with subsequent text on the next page.
- Separating a table, chart, or figure—confine each to a single page.
- Submitting a manuscript with pages out of sequence.
- In every section of your document, use standard writing style, including articles ("a" and "the").
- Keep paying attention to the topic of the paper.
- Use paragraphs to split each significant point (excluding the abstract).
- Align the primary line of each section.
- Present your points in sound order.
- Use present tense to report well-accepted matters.
- Use past tense to describe specific results.
- Do not use familiar wording; don't address the reviewer directly. Don't use slang or superlatives.
- Avoid use of extra pictures—include only those figures essential to presenting results.

Title page:

Choose a revealing title. It should be short and include the name(s) and address(es) of all authors. It should not have acronyms or abbreviations or exceed two printed lines.

Abstract: This summary should be two hundred words or less. It should clearly and briefly explain the key findings reported in the manuscript and must have precise statistics. It should not have acronyms or abbreviations. It should be logical in itself. Do not cite references at this point.

An abstract is a brief, distinct paragraph summary of finished work or work in development. In a minute or less, a reviewer can be taught the foundation behind the study, common approaches to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Use comprehensive sentences, and do not sacrifice readability for brevity; you can maintain it succinctly by phrasing sentences so that they provide more than a lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study with the subsequent elements in any summary. Try to limit the initial two items to no more than one line each.

Reason for writing the article—theory, overall issue, purpose.

- Fundamental goal.
- To-the-point depiction of the research.
- Consequences, including definite statistics—if the consequences are quantitative in nature, account for this; results of any numerical analysis should be reported. Significant conclusions or questions that emerge from the research.

Approach:

- o Single section and succinct.
- o An outline of the job done is always written in past tense.
- o Concentrate on shortening results—limit background information to a verdict or two.
- o Exact spelling, clarity of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else.

Introduction:

The introduction should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable of comprehending and calculating the purpose of your study without having to refer to other works. The basis for the study should be offered. Give the most important references, but avoid making a comprehensive appraisal of the topic. Describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will give no attention to your results. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here.

The following approach can create a valuable beginning:

- Explain the value (significance) of the study.
- Defend the model—why did you employ this particular system or method? What is its compensation? Remark upon its appropriateness from an abstract point of view as well as pointing out sensible reasons for using it.
- Present a justification. State your particular theory(-ies) or aim(s), and describe the logic that led you to choose them.
- Briefly explain the study's tentative purpose and how it meets the declared objectives.

Approach:

Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done. Sort out your thoughts; manufacture one key point for every section. If you make the four points listed above, you will need at least four paragraphs. Present surrounding information only when it is necessary to support a situation. The reviewer does not desire to read everything you know about a topic. Shape the theory specifically—do not take a broad view.

As always, give awareness to spelling, simplicity, and correctness of sentences and phrases.

Procedures (methods and materials):

This part is supposed to be the easiest to carve if you have good skills. A soundly written procedures segment allows a capable scientist to replicate your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order, but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt to give the least amount of information that would permit another capable scientist to replicate your outcome, but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section.

When a technique is used that has been well-described in another section, mention the specific item describing the way, but draw the basic principle while stating the situation. The purpose is to show all particular resources and broad procedures so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step-by-step report of the whole thing you did, nor is a methods section a set of orders.

Materials:

Materials may be reported in part of a section or else they may be recognized along with your measures.

Methods:

- Report the method and not the particulars of each process that engaged the same methodology.
- Describe the method entirely.
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures.
- Simplify—detail how procedures were completed, not how they were performed on a particular day.
- If well-known procedures were used, account for the procedure by name, possibly with a reference, and that's all.

Approach:

It is embarrassing to use vigorous voice when documenting methods without using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result, when writing up the methods, most authors use third person passive voice.

Use standard style in this and every other part of the paper—avoid familiar lists, and use full sentences.

What to keep away from:

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings—save it for the argument.
- Leave out information that is immaterial to a third party.

Results:

The principle of a results segment is to present and demonstrate your conclusion. Create this part as entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Use statistics and tables, if suitable, to present consequences most efficiently.

You must clearly differentiate material which would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matters should not be submitted at all except if requested by the instructor.

Content:

- Sum up your conclusions in text and demonstrate them, if suitable, with figures and tables.
- In the manuscript, explain each of your consequences, and point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation of an exacting study.
- Explain results of control experiments and give remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or manuscript.

What to stay away from:

- Do not discuss or infer your outcome, report surrounding information, or try to explain anything.
- Do not include raw data or intermediate calculations in a research manuscript.
- Do not present similar data more than once.
- A manuscript should complement any figures or tables, not duplicate information.
- Never confuse figures with tables—there is a difference.

Approach:

As always, use past tense when you submit your results, and put the whole thing in a reasonable order.

Put figures and tables, appropriately numbered, in order at the end of the report.

If you desire, you may place your figures and tables properly within the text of your results section.

Figures and tables:

If you put figures and tables at the end of some details, make certain that they are visibly distinguished from any attached appendix materials, such as raw facts. Whatever the position, each table must be titled, numbered one after the other, and include a heading. All figures and tables must be divided from the text.

Discussion:

The discussion is expected to be the trickiest segment to write. A lot of papers submitted to the journal are discarded based on problems with the discussion. There is no rule for how long an argument should be.

Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implications of the study. The purpose here is to offer an understanding of your results and support all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of results should be fully described.

Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact, you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved the prospect, and let it drop at that. Make a decision as to whether each premise is supported or discarded or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."

Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work.

- o You may propose future guidelines, such as how an experiment might be personalized to accomplish a new idea.
- o Give details of all of your remarks as much as possible, focusing on mechanisms.
- o Make a decision as to whether the tentative design sufficiently addressed the theory and whether or not it was correctly restricted. Try to present substitute explanations if they are sensible alternatives.
- o One piece of research will not counter an overall question, so maintain the large picture in mind. Where do you go next? The best studies unlock new avenues of study. What questions remain?
- o Recommendations for detailed papers will offer supplementary suggestions.

Approach:

When you refer to information, differentiate data generated by your own studies from other available information. Present work done by specific persons (including you) in past tense.

Describe generally acknowledged facts and main beliefs in present tense.

The Administration Rules

Administration Rules to Be Strictly Followed before Submitting Your Research Paper to Global Journals Inc.

Please read the following rules and regulations carefully before submitting your research paper to Global Journals Inc. to avoid rejection.

Segment draft and final research paper: You have to strictly follow the template of a research paper, failing which your paper may get rejected. You are expected to write each part of the paper wholly on your own. The peer reviewers need to identify your own perspective of the concepts in your own terms. Please do not extract straight from any other source, and do not rephrase someone else's analysis. Do not allow anyone else to proofread your manuscript.

Written material: You may discuss this with your guides and key sources. Do not copy anyone else's paper, even if this is only imitation, otherwise it will be rejected on the grounds of plagiarism, which is illegal. Various methods to avoid plagiarism are strictly applied by us to every paper, and, if found guilty, you may be blacklisted, which could affect your career adversely. To guard yourself and others from possible illegal use, please do not permit anyone to use or even read your paper and file.

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Topics	Grades		
	A-B	C-D	E-F
Abstract	Clear and concise with appropriate content, Correct format. 200 words or below	Unclear summary and no specific data, Incorrect form Above 200 words	No specific data with ambiguous information Above 250 words
Introduction	Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited	Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter	Out of place depth and content, hazy format
Methods and Procedures	Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads	Difficult to comprehend with embarrassed text, too much explanation but completed	Incorrect and unorganized structure with hazy meaning
Result	Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake	Complete and embarrassed text, difficult to comprehend	Irregular format with wrong facts and figures
Discussion	Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited	Wordy, unclear conclusion, spurious	Conclusion is not cited, unorganized, difficult to comprehend
References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring

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