Ethical and Sustainability Considerations for Knowledge Graph based Machine Learning

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Abstract. Artificial Intelligence (AI) and Machine Learning (ML) are becoming common in our daily lives. The AI-driven processes significantly affect us as individuals and as a society, spanning across ethical dimensions like discrimination, misinformation, and fraud. Several of these AI & ML approaches rely on Knowledge Graph (KG) data. Due to the large volume and complexity of today's KG-driven approaches, enormous resources are spent to utilize the complex AI approaches. Efficient usage of the resources like hardware and power consumption is essential for sustainable KG-based ML technologies. This paper introduces the ethical and sustainability considerations, challenges, and optimizations in the context of KG-based ML. We have grouped the ethical and sustainability aspects according to the typical Research & Development (R&D) lifecycle: an initial investigation of AI approach's responsibility dimensions; technical system setup; central KG data analytics and curating; model selection, training, and evaluation; and final technology deployment. We also describe significant trade-offs and alternative options for dedicated scenarios, enriched through existing and reported ethical and sustainability issues in AI-driven approaches and research. These include, e.g., efficient hardware usage guidelines; or the trade-off between transparency and accessibility compared to the risk of manipulability and privacy-related data disclosure. In addition, we propose how biased data and barely explainable AI can result in discriminating ML predictions. This work supports researchers and developers in reflecting, evaluating, and optimizing dedicated KG-based ML approaches in the dimensions of ethics and sustainability.

Keywords: Semantic Processing · Knowledge Graphs · Machine Learning · Ethical AI · Sustainable Machine Learning · Explainable AI · RDF

1 Introduction

Artificial Intelligence (AI) implemented through Machine Learning (ML) driven processes increasingly impacts our daily lives. Those reach from how we: buy products, consume streaming content, preselect CVs in job applications, and interact with customer service over chatbots. A significant share of these scenarios relies on Knowledge Graph (KG) data [29]. The Semantic Web [7] project describes the joint effort to integrate various internet data sources into a relation-centric linked Big Data structure. Out of this concept, several open KGs have emerged (DBpedia [26], YAGO [38], Freebase [8], Wikidata [44]) as well as big tech companies implemented enterprise KGs for their products (Meta, Google, Linked-In, eBay, IBM) [29]. The KG-based ML models have already substantially impacted individuals and overall society. Based on already reported problems and challenges with AI-driven approaches [46, 17, 3, 42, 31, 15], we see a need to investigate KG-based ML. Due to the complexity of the applied Machine Learning models and the enormous underlying training data, the investigation and optimization of respective processes are challenging. So we need best practice guidelines to offer Data Scientists and Machine Learning Engineers a starting point for improved and more holistic KG ML R&D.

Contributions Within this work, we provide a set of novel contributions:

- Introduction of a novel Ethical AI perspective on KG-based ML.
- Sustainability considerations on the KG-based ML R&D lifecycle.
- Presentation of interwoven ethical and sustainability dimensions along the Downstream Pipeline, including Responsible Approach, Technical Setup, Data Insights, Machine Learning & Deployment.
- Ethical and Sustainable KG-based ML pipeline components, each structured by Definition, Challenges, Examples, Research Questions, and Recommendations.

Structure In Section 2 we introduce the major terms: Ethical AI, Sustainable AI, Knowledge Graphs, AI/ML, and KG based ML. In Section 3 we introduce the dimensions of Ethical and Sustainability considerations for KG based ML. Those are grouped by an initial Responsible AI Approach Check (3.1), followed by the Technical Environment Setup (3.2), the KG Data Insights (3.3), Machine Learning (3.4) and finally the overall Deployment (3.5). Within the Conclusion in Section 4 we summarize our work and provide future work directions.

2 Preliminaries

This section introduces the fundamental concepts interwoven within this work: Knowledge Graphs, Artificial Intelligence, Machine Learning, Ethical AI, and Sustainable AI.
Knowledge Graphs: Knowledge Graphs (KGs) are linked data representations of information. Entities and values are associated with directed relations. A KG corresponds to a directed labeled multi-graph. A central concept is that entities, despite different naming or nicknames, are associated with one unique identifier (IRI, URI) or a dedicated node in the graph [11]. Example: The words Apple, Apple, and the Big Apple can correspond to a fruit, a tech company, or a US city, while New York and the big apple primarily refer to the same entity. In social media graphs, multiple persons can have *friendOf* relations to each other and

like relations to, e.g., music genres. Also, values can be related to entities like the date of birth of a person or the number of inhabitants of a city. With the power of these data structures, knowledge databases, e-commerce shop items, social media graphs, or streaming on-demand content can be represented.

Artificial Intelligence (AI), Machine Learning (ML): Artificial intelligence is the theory and development of computer systems able to perform tasks usually requiring human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages [12]. One option to reach and implement AI is Machine Learning (ML). Machine Learning is the capacity of computers to learn and adapt without following explicit instructions by using algorithms and statistical models to analyze and infer from patterns in data [13]. Despite the conceptual differences, AI and ML are often used synonymously.

KG Based ML: In several approaches, KGs are the key element of ML pipelines. On the one hand, ML approaches can perform knowledge retrieval to enrich a KG database. In those cases, information is extracted from multi-modal data sources like natural language texts, images, tables, audio, and video. Also, existing KG can be further enriched over Link Prediction, Entity Resolution, Entity Matching, and Inference. On the other hand, KG can be used as a source for downstream ML pipelines. Those pipelines can implement Classification, Regression, or Recommendation Systems. The ML model uses stored values inside the KG and uses the graph structure. As the structure can be arbitrary complex, and common ML models need fixed-length numeric feature tensors across all samples, KG-based ML uses latent embeddings reach through, e.g., Knowledge Graph Embeddings (KGE).

Ethical AI: Ethical AI describes the efforts to investigate ethical and moral aspects of AI-driven processes [21, 31]. As AI-driven processes can impact our daily lives and might perform autonomous decisions based on pre-trained models, those can lead to unethical, discriminating situations [31]. Bad AI behavior can be due to various reasons like data bias or model failure. Especial complex neural networks are perceived as black-box systems. Through the effort of Explainable AI, the models are leveraged to create reasonable and explainable results[31, 17]. A typical example of Ethical AI comes from the already known trolley dilemma. In this dilemma, a lore or a train can no longer be stopped, and a decision is to be made, which group of people the train will hit and damage. The scenarios describe one vs. five people, one child vs. two seniors. These extreme situations should establish moral awareness, which might also be made [21], e.g., in self-driving cars in a brake failure accident situation. This car will be driven by an AI and thus need guidance for those edge case decision-making processes. Besides the self-driving car scenario, many existing and foreseeable situations might involve AI in ethics-related processing [20, 47] also based on KG data.

Sustainable AI: Sustainable AI includes optimizations of AI/ML methods that minimize the resource consumption of ml algorithms and, if necessary, also justify it concerning the purpose [46, 17, 1]. In contrast to Sustainable AI, AI for

Sustainability are approaches that use AI to drive processes that lead to a more sustainable world [46].

3 Ethical and Sustainability considerations for Knowledge Graph based Machine Learning

This section introduces ethical and sustainability considerations of Knowledge Graph-based Machine Learning. AI and ML-driven approaches mostly follow a classical schema of the Research & Development (R&D) life cycle [17]. This section introduces concepts to optimize each step according to this lifecycle and downstream pipeline development. The classical life cycle consists of the initial Responsible AI check, followed by the technical environment setup, data insights, machine learning, and deployment. Figure 1 introduces an overview of this classical scheme according to key questions the development team has to answer when improving the ethical and sustainability dimensions of the KG-driven ML approach. Each paragraph provides first the *Definition & Challenges* followed by *Examples* and finally presents *Research Questions & Recommendations*.

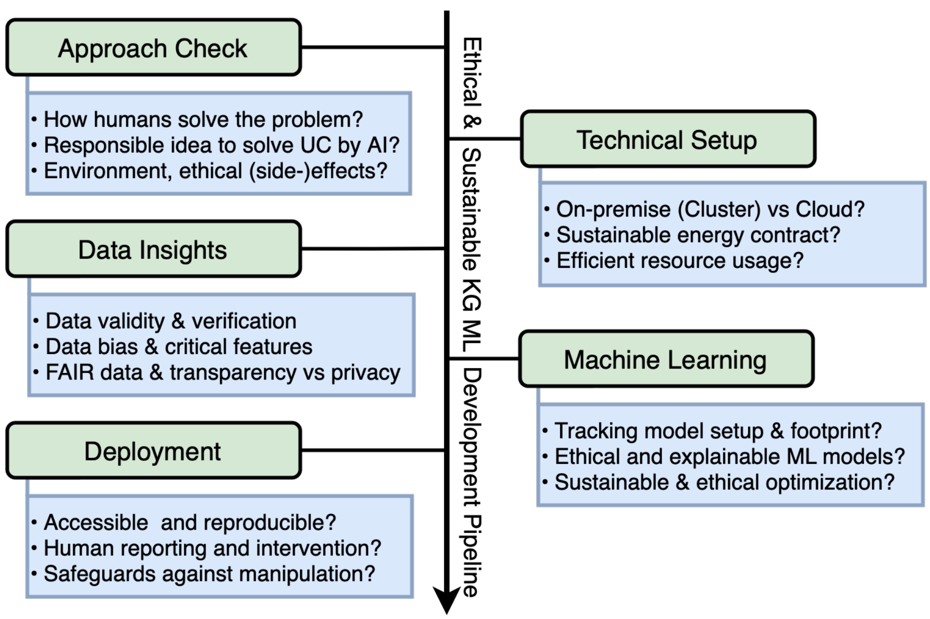


Fig. 1: Ethical and Sustainable KG based ML pipeline with key questions

3.1 Responsible AI Approach

***Definition*:** Applying AI, in particular, to KG data has ethical and sustainability implications. These lie in the social implications of the applications and the consumption of resources. [31, 17, 46] ***Challenges*:** The consideration of whether a KG-based AI approach should be implemented depends on many factors. It is impossible to draw conclusions about all different effects directly from the initial application and resource consumption. In basic research, complex models are trained and evaluated using illustrative examples, which can then be applied to more socially relevant topics. ***Examples*:** (1) Chatbots handle customer service centers for e-commerce products. However, chatbots do not handle emergency calls, although both implement dialog-based conversational AI systems to ask for help and solve problems [21]. (2) The AI Alpha Go Zero, which is optimized to play a well-known board game GO, generated 96 tons of CO2 in 40 days of research training, equivalent to 1000h of air travel or 23 American households [46]. ***Research Questions*:** Have the social and ethical implications of the specific KG-driven AI been evaluated and allow for responsible research and development of this technology? Are the resources used worth consuming? ***Recommendations*:** The ethical and sustainability implications should be assessed and justified as an initial step. The stakeholders concerned can initiate a multi-layered evaluation in multidisciplinary teams. It can reflect how it was solved in the past by humans or classical imperative programs and if the use case should be solved autonomously at all [21].

3.2 Sustainable Technical Environment Setup

***Definition*:** KG-based AI R&D lifecycle is performed on computers. The necessary resources have a sustainability footprint. This consists of the acquisition and production of the hardware, the power consumption, and the expected longevity [24, 46, 3]. ***Challenges*:** The hardware capabilities of KG-based ML can be immense as KGE correlate to large language model training that is processing power and memory intensive [19]. The selection of hardware involves trade-offs between reusing existing hardware or accumulating multiple nodes in a cluster to make the necessary processing power available. New hardware may still be necessary as requirements increase because it has more power or features and is more power-efficient [24]. In addition, specific applications require dedicated hardware and software platforms. With on-premise system architecture, more individual decisions can be made than with cloud computation systems [24], and underutilization less justifies the initial hardware costs [9]. ***Examples*:** The European CO2 footprint of electricity production differs significantly due to a different share of renewable energies, nuclear power, and fossil fuels[22]. Because of weather and solar radiation, the CO2 footprint is also dependent on the time of day (Figs. 2 & 4). ***Research Questions*:** How can the hardware resources be used, reused, and utilized as efficiently as possible? How can the resource carbon footprint be minimized? ***Recommendations*:** The hardware used should be based on CO2-neutral energy sources [24]. Hardware should be deployed and efficiently utilized either as a cloud solution or alternatively as a crowd-shared on-premise architecture. As part of the setup, tracking [3] and documentation of the effectively used resources and emissions footprint create transparency. Software abstraction layers and containerization should contribute to hardware-independent R&D and comfortable deployment.

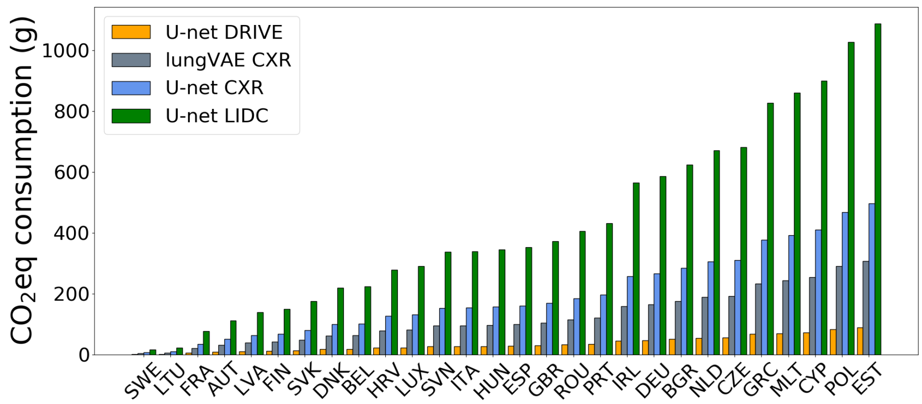


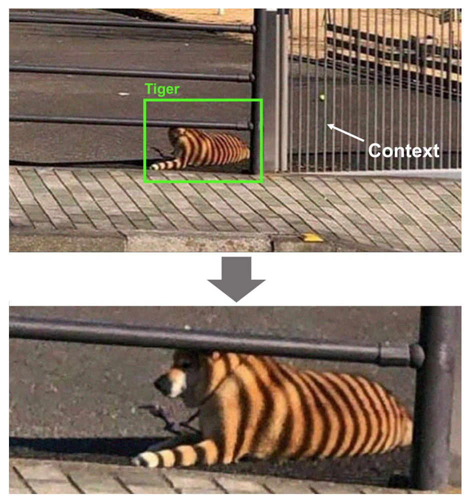
Fig. 2: Evaluation plot of estimated CO2 emissions of Carbon Tracker experiment [3]

3.3 Data Insights

The KG data specifics play an extraordinary role in the performance and behavior of KG-based AI processes [35]. The initial data selection decides which sources of information and data are accessible to the process. Existing KGs can be selected, merged, or further enriched by non-KG data.

KG Data Reliability Verification - ***Definition*** Knowledge Graphs are created and enriched by a variety of processes. Incorrect or inaccurate information can be mapped through the source data and process. Also, the concept of open-world assumption (OWA) is part of KG data. OWA states that information can be correct even if this data is not in KG. ***Challenges*****:** The sources of false information are complex and sometimes difficult to trace. False data is not always apparent at first sight. ***Examples*****:** (1) Automatic retrieval of KG data from texts or other multi-modal data can create inaccurate knowledge data as those techniques do not work perfectly [48]. (2) The Open World Assumption (OWA) is a central element in KG data, which implies that information can also exist if they are not stored in the KG. This OWA idea implies the causality if a KG does not contain specific data; this information can still be accurate, which can lead by chance to problems in the negative sampling in KGEs. (3) Also, fraud and manipulation can happen as, e.g., DBpedia extracts its information from Wikipedia, but public figures and institutions try to influence how they are perceived and presented on the internet [17]. (4) Not only bad intention but also humor or sarcasm can lead to incorrect data as facts about pop culture people, e.g., Chuck Norris (see Fig. 3a) [42]. (5) As facts change, knowledge graph data could also be not up to date [28]. ***Research Questions*:** What is the data quality, especially to which extent is the stored information reliable? With which intent, by whom, and through which processes has this data been created? ***Recommendations*:** Quality, noise, and incorrect data are identified through data analytics and should be documented and published through transparent FAIR principles.

(a) Google Search Knowledge Graph result about actor and pop-figure "Chuck Norris", see what is stated as **Fact**, Example taken from Vang et. al. [42]



(b) Sample Image [33] motivating context in data for accurate ML predictions

Fig. 3: Validity of KG data (a) and need for context AI data (b)

Bias and Critical Features - *Definition*: KG ML training is based on structural and value features. The distribution of the values may not represent the accurate distribution of the values [21]. Also, special features are associated with discrimination, so handling these features poses particular challenges [36, 23]. ***Challenges*:** The simple omission/deletion of features can still lead to discrimination because, in these cases, meta-data may still allow unintended feature reconstruction [15]. ***Examples*:** Features associated with discrimination include age, gender, heritage, skin color, political orientation, sexual orientation, and religion [17]. ***Research Questions*:** Which features associated with discrimination are present in the KG? In which dimensions is there a bias, and why? Can features be aggregated, pseudonymized, or re-balanced to reduce the bias? ***Recommendations*:** Identify the presence of critical features. Describe bias distributions in these features. Aggregate, pseudonymize or remove critical features in a transparent process. Evaluate whether removed features can be reconstructed through metadata. Optimize labeling and curation procedures to minimize bias [28, 5].

Transparency and Privacy in KGs - *Definition*: KGs have great potential to combine many data sources and make them accessible to humans and machines. More context can support AI-driven predictions (see Fig. 3b). For trustworthy AI, underlying transparent and FAIR training data and metadata are essential. ***Challenges*:** However, a high level of transparency of fully integrated data can also be exploited and used for ethical purposes [23]. Therefore, there is a trade-off in data accessibility between high transparency and the need-to-know principle [10]. The model can be more challenging to reproduce and validate with reduced transparency by independent institutions. ***Examples*:** In some countries, personal relationships or research in specific subject areas can lead to discrimination, persecution, or prison [23]. ***Research Questions*:** For what ethical purposes can transparent data be used? How can data be made both sufficiently transparent for validation and securely accessible? Which training and metadata should be made accessible to humans and machines? ***Recommendations*:** Take a clear position in the trade-off between the need-to-know and transparency. Enable independent validation of technologies to justify why the transparently available data is likely safe [31, 17].

3.4 Machine Learning

Tracking Pipeline - *Definition*: For the application, validation, and further development of KG-based AI, accessibility, and reproducibility are fundamentally important. In addition to the technical details, resource consumption can also be tracked [46, 3]. ***Challenges*:** Throughout the ML pipeline, there are many (hyper-)parameters and resource-consuming instances necessary for holistic tracking. At the same time, the carbon footprint is not traceable at all times since not every phase transparently breaks down the used resources. ***Examples*:** The tool Carbontracker supports the automated evaluation of CO2 footprints [24, 46, 3, 37]. ***Research Questions*:** Which resources were used throughout the KG ML lifecycle, and how can they be tracked automatically? Which (hyper-)parameters and configuration information are necessary to use, reproduce, validate and further develop the entire KG AI [46, 31]? ***Recommendations*:** Existing AI CO2 tracking systems can be used to add resource consumption to documentation automatically (see Fig. 1) [24, 46, 3, 37]. The use of standardized ontologies like MEX and MLschema allows a human and machine-readable tracking and documentation of the AI setup [16, 32].

Sustainable Training - *Definition*: Training KG-based ML requires considerable resources since both latent embeddings and (Graph-)Neural Networks

Roundtrip flight b/w NY and SF (one passenger)	1,984
Human life (avg. one year)	11,023
American life (avg. one year)	36,156
US car including fuel (avg. one lifetime)	126,000
Transformer (213M parameters) W/ neural architecture search	626,155

Table 1: Carbon Footprint Large Language Model [39, 37]

have significant training efforts [49, 27, 3]. During the initial exploration of the models, the optimal configuration of the hyper-parameters must be found. ***Challenges*:** Since KGE are optimized from random vectors and represent exact KG entities, these models cannot handle out-of-sample entities by default. Models that support out-of-sample handling or inductive link prediction require further adjustments to minimize re-training from scratch [19]. Additionally the search within the hyper-parameter grid requires recurrent training of the same model. ***Examples*:** The training of latent embeddings KGE exceeds the already vast complexity of large language models [19, 49] which already produced huge carbon emissions [39, 37] (see Table 1). ***Research Questions*:** How does KG-based AI deal with samples not yet seen? How can transfer learning and update ability be implemented in the approaches so that it is not necessary to train from scratch with changing KG data or novel entities [19]? ***Recommendations*:** Evaluate the KG data volatility. Use KG-based AI models that allow out-of-sample learning [2], inductive link prediction, and transfer learning. Reduce the hyper-parameter space to a minimum in a grid search and use early stopping to minimize both overfitting and unnecessary training cycles [24, 3]. Further optimization in data and model compression can further minimize the necessary resources [34].

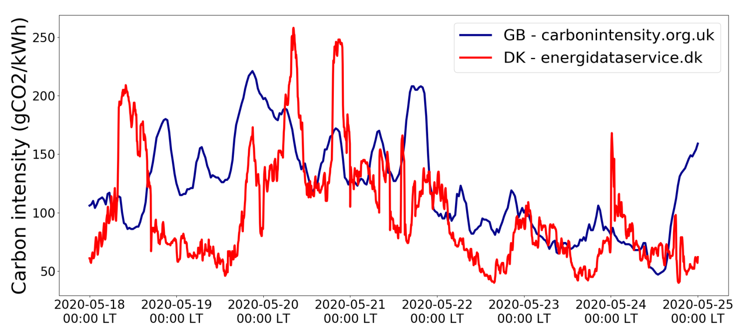


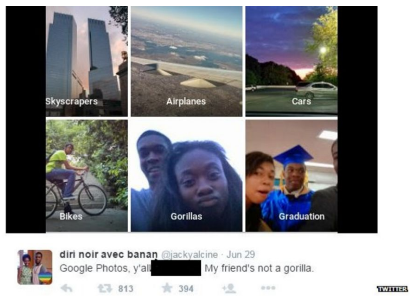
Fig. 4: Real-time carbon intensity (gCO 2eq/kWh) for Denmark (DK) and Great Britain (GB) from 2020-05-18 to 2020-05-25 shown in local time from Carbon Tracker analytics [3]

Ethical & Explainable ML for KGs - ***Definition*****:** KG-based ML models and the corresponding latent embeddings are multidimensional parameters and feature spaces encoding properties and processes of the AI. Accessibility, reproducibility, reusability, and explainability are essential for ethical AI [21, 31, 45]. ***Challenges*****:** Since the data and features in KG are arbitrarily complex for each sample and standard ML models assume fixed numeric feature vectors, latent embeddings like KGE are necessary [49, 27, 19]. Especially the high-performance neural network models and latent embeddings significantly complicate explainability and lead to AI often being perceived as a black box [25, 30, 4]. ***Examples*****:** (1) The approach distilling neural networks transforms complex neural network ML models into more explainable decision forest models [18]. (2) Explainable AI approaches can also describe the features or embedding components that were most influential [17] for a dedicated prediction. ***Research Questions*****:** Can the models produce explainable predictions? Does KG-based ML's complexity also allow less powerful hardware to use the new technology? ***Recommendations*****:** Use existing benchmarks to fit already developed models instead of developing new ones [22]. Use KG-based ML models that focus on explainability. With conversational AI and result semantification, the results become intuitively more accessible [40, 17]. Use scalable models for KG-based AI [41, 34, 14] also working on distributed systems [27, 49].

Non-discriminating Evaluation - ***Definition*****:** ML models are trained by minimizing the error of predicted results compared to the actual annotated true label. The performance of a model is measured by performance over unseen samples. ***Challenges*****:** If the test and validation data are biased or do not contain sufficient data about possibly discriminated entities, they will not be present in overall precision or recall measures [31]. ***Examples*****:** (1) ML-based image grouping within Google Photos led to a hurtful, racist classification of people of colour [6]. (2) The Microsoft chatbot Tay was influenced by Twitter users to state offending and hate speech texts (See Fig. 5a & Fig. 5b) [43]. ***Research Questions*****:** Are the test and validation set biased? Are opportunities available to live annotated in production KG AI predictions? ***Recommendations*****:** A definition of critical samples and tests of dedicated edge cases should be performed. Users or affected humans should have the option to report problematic predictions in live systems as it is already typical for bug and issue reports in open source projects [17, 28]. The model should be tested before deploying and afterward to ensure that the initially made claims still suit outside world scenarios [17]. As part of evaluation dissemination, the performance across all samples and subset performances should be accessible. Additionally, the performance across critical features should be validated [15].

3.5 Accessible Deployment

Definition**:** A well-performed deployment is a fundamental part of building AI trust and justifying the spent resources. The deployment includes an open-source



(a) BBC article [6] about hurtful/racism ML annotated Google Photos image category

(b) Twitter BlogPost from the Verge article [43] about manipulated Chatbot AI stating offending and hate speech texts

Fig. 5: Hurtful and offending real world AI predictions

publication of code and data sets. Through precise and well usable documentation, details can be described [45]. ***Challenges*:** A holistic, accessible deployment requires a variety of technical and documentation deployments across multiple channels. ***Examples*:** Blog posts over known channels like: Towards Data Science, Reddit, or Stackoverflow[3], for informal discussion and exchange of ideas, can be used to further motivate developments through appealing examples (See Fig. 3b). ***Research Questions*:** Is every component available open-source to fully use, reproduce, validate, and further develop the provided resource? ***Recommendations*:** Third-party researchers can comment on the methodology and technology efforts within scientific review and publication processes. Access to the technology can be improved by containerized versions of the tool, handy notebook sample pipelines, or AI as a service approaches (AIaaS, PaaS). The usage and try-out options can be supported by handy notebooks like Jupyter, Google Colab, Apache Zeppelin, and Databricks[4] [31]. The use of the tool within own developments can be improved through package management like pip or maven[5]. Ongoing testing should be performed through unit tests and integration tests but also through benchmarking of changing and relevant datasets [17].

4 Conclusion

The opportunities for ethical and sustainability optimizations for knowledge graph-based machine learning are manifold. This work introduced the most prominent ethical concerns raised by the large-scale deployment of KG-based ML applications. We show how sustainability, ethics, knowledge graphs, and

[3] stackoverflow.com, towardsdatascience.com, reddit.com
[4] jupyter.org, colab.research.google.com, zeppelin.apache.org, databricks.com
[5] maven.org, pypi.org/project/pip/

ML are interwoven across the entire approach life cycle. The possibilities range from an initial reflective check on how far use cases should be automated by AIs, taking into account potential side effects and edge cases. Even during the initial setup of the processing environment, foreseeable resource utilization can be optimized and technical reproducibility improved. The data in KG-based ML pipelines also significantly affect the process and should be evaluated regarding reliability, bias, and fairness. In addition, careful handling of special features is essential, including the trade-off between sufficient data context and data privacy principles. The development of ML models can also be optimized technically in pipeline development through more sustainable training and ethical models with the help of explainable AI, fair evaluation, and accessible deployment. The deployed models should fulfill a broad range of interaction options with humans to report problems, handle unseen samples, and be used in transfer learning tasks. Through the work presented here, we introduce the application of Ethical AI and Sustainable AI to the Knowledge Graph-based Machine Learning domain. The work presented here is not intended to be complete as the field is broad. However, it is a starting point for KG-based AI R&D teams interested in optimizing technology under ethical and sustainability concerns. The findings are presented by a transfer of ethical, sustainable, and novel introduced considerations, including examples of past problems and suggestions for hands-on optimizations and solutions.

Future Work The concepts presented here are mostly part of every KG-based ML pipeline. We believe that through easy-to-use tools and integration into widely used libraries, assistance should be offered as already the first applications provide it [3]. We are committed to support the process of ethical and sustainable KG-based ML research and development with hands-on solutions to advance this field. Corresponding to the FAIR concept, this paper should introduce meta dimensions of good research and development for KG-based ML in dimensions of Ethics and Sustainability.

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