Zekarias T. Kefato
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SUMMARY

I am a **Senior AI Scientist** specializing in **graph machine learning** and **generative AI**. With a PhD from the University of Trento and postdoctoral experience at KTH Royal Institute of Technology, I bridge the gap between advanced research and production-level ML systems. Currently leveraging expertise in Graph Machine Learning, including Graph Neural Networks (GNNs) and Knowledge Graph Embeddings, to advance drug discovery while integrating emerging technologies like Large Language Models (LLMs), agents, and MLOps principles.

CORE EXPERTISE

- **Machine Learning:** Graph Neural Networks (GNNs), Transformers, Self-Supervised Learning, Knowledge Graph Embeddings.
- **Generative AI:** Building ML Systems based on **LLMs and agents** to streamline drug discovery pipelines.
- **Engineering & MLOps:** Implementing MLOps principles for model deployment; proficient in PyTorch, TensorFlow, MLFlow, Databricks, CI/CD, and Docker.
- **Data Science:** Large-scale graph analytics, predictive modelling, and computer vision (trajectory forecasting).

EXPERIENCE

AstraZeneca, Cambridge, UK — Senior AI Scientist
Dec 2022 – Present

- **Graph Machine Learning:** Applying knowledge graph embeddings and GNNs to biological knowledge graphs to identify novel target genes for disease treatment.
- **MLOps Implementation:** Standardizing the deployment of predictive models by implementing MLOps principles to ensure scalability and reproducibility.
- **LLM Systems & Agents:** Architecting and building ML systems leveraging LLMs and autonomous agents to automate and streamline the drug discovery pipeline.

KTH Royal Institute of Technology, Stockholm, Sweden — Postdoctoral Researcher
June 2019 – Dec 2022

- Developed computational frameworks combining **GNNs and Transformer architectures** for complex graph analytics.
- Designed computer vision models for **pedestrian trajectory forecasting** in collaboration with **Scania** to enhance autonomous driving safety.
- Researched heterogeneous and contextual graph representation learning.

Ethiopian Information Network Security Agency (INSA) — Software Engineer
Sep 2009 – Aug 2011

- Architected a mission-critical **loan management subsystem** using Java and Hibernate ORM.
- Managed the full software development lifecycle (SDLC) from design to production deployment.
- Optimized system maintainability through the implementation of advanced software design patterns.

TECHNICAL SKILLS

Category	Tools & Languages
Languages	Python, R, SQL, Java, C++, Scala, JavaScript, Shell Scripting
ML & Ops	PyTorch, TensorFlow, MLFlow, Databricks, Docker, CI/CD, Apache Spark
Data Libraries	Pandas, NumPy, Scipy, Scikit-learn, NetworkX, Dplyr, Tidyverse
Visualization	Plotly, Matplotlib, Shiny, ggplot, Chart.js

EDUCATION

- PhD in Computer Science, University of Trento, Italy (2014 - 2019)
- MSc in Computer Science, University of Trento, Italy (2011 - 2013)
- BSc in Software Engineering, Microlink IT College, Ethiopia (2004 - 2007)

PUBLICATIONS

- Ahmed Yossef Ahmed, Zekarias T. Kefato, Sarunas Girdzijauskas. Leap: Inductive Link Prediction via Learnable Topology Augmentation. MLOD 2024.
- Ahmed Yossef Ahmed, Zekarias T. Kefato, Sarunas Girdzijauskas. Graph2Feat: Inductive Link Prediction via Knowledge Distillation. WWW 2023.
- Ahmed Yossef Ahmed, Zekarias T. Kefato, Sarunas Girdzijauskas. Data-Driven Self-Supervised Graph Representation Learning. ECAI 2023.
- Ahmed Yossef Ahmed, Lodovico Giaretta, Zekarias T. Kefato, and Sarunas Girdzijauskas. SchemaWalk: Schema Aware Random Walks for Heterogeneous Graph Embedding. WWW 2022.
- Zekarias T. Kefato, Sarunas Girdzijauskas, and Hannes Stärk. Self-Supervised GNN that Jointly Learns to Augment. NeurIPS 2021.
- Zekarias T. Kefato, Sarunas Girdzijauskas, Nasrullah Sheikh, and Alberto Montresor. Next Item Prediction using Contextualized Dynamic Embeddings. WWW 2021.
- Zekarias T. Kefato, Sarunas Girdzijauskas. SelfGNN: Self-supervised Graph Neural Networks without explicit negative sampling. WWW 2021.
- Zamboni, S., Kefato, Z.T., et al. Pedestrian Trajectory Prediction with Convolutional Neural Networks. Pattern Recognition Journal 2021.
- Zekarias T. Kefato, Sarunas Girdzijauskas. Gossip and Attend: Context-sensitive Graph Representation Learning. ICWSM 2020.
- Zekarias T. Kefato, Sarunas Girdzijauskas. Graph Neighborhood Attentive Pooling. ArXiv 2020.

- Zekarias T. Kefato, Nasrullah Sheikh, and Alberto Montresor. Which way? Direction-Aware Attributed Graph Embedding. GEM 2020.
- Sheikh, N., Kefato, Z.T., and Montresor, A. A simple approach to attributed graph embedding via enhanced autoencoder. Complex Networks 2019.
- Zekarias T. Kefato, et al. CAS2VEC: Network-Agnostic Cascade Prediction in Online Social Networks. IEEE SNAMS 2018 (Best Paper).
- Sheikh, N., Kefato, Z.T., and Montresor, A. Semi-Supervised Heterogeneous Information Network Embedding. SNAMS 2018.
- Zekarias T. Kefato, et al. REFINE: Representation Learning from Diffusion Events. MLOD 2018.
- Sheikh, N., Kefato, Z.T., and Montresor, A. GAT2VEC: Representation learning for attributed graphs. Computing Journal 2018.
- Zekarias T. Kefato, et al. Mineral: Multi-modal Network Representation Learning. MLOD 2017.
- Zekarias T. Kefato, et al. DeepInfer: Diffusion Network Inference through Representation Learning. MLG 2017.

SKILLS

- Languages: Python, R, SQL, Java, C++, Scala, JavaScript, Shell Scripting
- Frameworks: PyTorch, TensorFlow, MLFlow, Databricks, Spark, Docker, CI/CD

References

Upon Request