

Advancing Decision Science: Lessons from Machine Learning

Bridge on Constraint Programming and Machine Learning



Serdar Kadıoğlu

- ¹ Dept. of Computer Science, Brown University
- ² Al Center of Excellence, Fidelity Investments



skadio.github.io



Learning & Reasoning

Data Science: ML/DL/LLMs/etc.

Focuses on machine learning using historical data to identify patterns and make predictions. Excels at pattern recognition, classification, and forecasting.

System 1 - Predictive Models

- Learning from historical data patterns
- Probabilistic predictions and insights
- Ideal for unstructured problems
- Applications include recommendation systems, image recognition, and natural language processing

Decision Science: SAT/CP/MP/LS/etc.

Focuses on **combinatorial satisfaction and optimization** using logical and mathematical models. Provides provable optimality and explicit reasoning.

System 2 - Prescriptive Models

- Mathematical and logical formulations
- Provably optimal for deterministic environments
- Perfect for structured problems
- Applications include verification, planning, scheduling, routing, and resource allocation

The Software Gap in Decision Science

Success of Data Science

The Learning community has benefited tremendously from **open-source software** such as PyTorch, and TensorFlow, along with established **packages** like NumPy, SciPy, and scikit-learn.

Closed source/weight general-purpose models exist along with open-source alternatives.

The **performance gap** is narrowing.

Opportunity for Decision Science

The Reasoning community trails behind in establishing a similar software ecosystem, hindering widespread adoption and collaboration of reasoning solvers & software, limiting its potential and impact.

Commercial high-performance general-purpose solvers exist along with open-source alternatives.

The **performance gap** is wider.



Bridging the Gap

Let's explore **concrete examples** from the ML & Data Science community and consider their equivalents or similar versions for the Decision Science community.

1 Ease of Use and Accessibility

2 Integrated Environments

3 Community Driven Development

4 Showcase Success

Bridging the Gap: Ease of Use



One-Click Installation

Simple **pip install**command for all decision
science tools



No Dependency Hassles

Eliminate complex

dependency management

and version conflicts



Quick Start Experience

Making it easier for **new users** while supporting experienced developers

Ex: CPMPy, Pyomo, PySAT, SCIP, Seeker, OR-Tools, PyOptInt, ALNS, PyVRP, PyJobShop, DIDPpy, ...

Sequence to
Pattern generation
for constrained
pattern mining

Seq2Pat

Discover frequent sequential patterns in large sequence databases with constraints

Collaboration with CMU (Blog post)

Efficient C++ MDD solver backend with high-level declarative Python API Kadıoğlu et. al. (Al Magazine'23)

pip install seq2pat 40K+ downloads

Bridging the Gap: Ease of Use



Ready-to-Run Environments

Docker containers come fully configured with all necessary dependencies installed and ready to use



Instant Setup

Start solving problems
immediately without
dealing with complex
installation processes



Cross-Platform Consistency

Ensure **consistent behavior**across different platforms
and operating systems



Built-in Resources

Access **pre-loaded** example problems and documentation right out of the box

Ex: Dockerized SCIP for Teaching

Bridging the Gap: Ease of Use

1 Standardized Interfaces

Common APIs for solvers and models that provide a unified experience across different tools.

Reduce the learning curve when switching between solvers and enables easier integration with existing codebases and flows. 2 Interactive Documentation

Create comprehensive, interactive tutorials and documentation with real-time examples and **notebooks**.

Users understand concepts quickly and provides practical implementation guidance for common use cases.

Automated Model Validation

Built-in tools for **model**validation and debugging help
users identify common modeling
errors.

Reduce friction of working with complex constraint models and speeds up development time.

fit + predict ≈ model + solve

Bridging the Gap: Accessibility

1 Low Code/No Code Environments Intuitive drag-and-drop interfaces for model building that enable optimization models without writing code.

Visual model validation, pre-built components for common constraints, and the ability to import data directly from business databases.

Ex: AIMMS Modeling Environment, IBM Decision Studio, etc.

2 Modeling Assistants

Modeling Co-Pilots to suggest model improvements, identify potential issues, and help translate business requirements into mathematical constraints.

Learn from existing models to recommend best practices, detect common modeling patterns, and generate initial structures based on natural language.

Ex: Holy Grail 2.0, Ner40pt, Text2Zinc, Chat0pt, OptiGuide, OptiMUS, MeetMate, MCPSolver, etc.

Integrated Data & Model Cards

1 Purpose

Increase **transparency**and accountability in
dataset use by providing
detailed documentation.

2 Content

Includes dataset overview, collection methods, intended use, ethical considerations, and limitations.

Includes model details, intended use, performance metrics, ethical considerations, and limitations.

3 Benefits

Promotes transparency, accountability, and **Responsible Al** development.



Model Registry & DecisionOps

1 Version Control

Keeps track of different versions of models, allowing management of updates and changes over time.

Model Observability

Stores important
information about each
model, such as
parameters, training
data, and performance
metrics.

3 Collaboration

Facilitates collaboration among data scientists and engineers by providing a shared space to access and manage models.

Ex: NextMv, etc.

Decision Science as a Service

1 Cloud-based Tools

Provide scalable
infrastructure for
building and deploying
optimization models.

2 API Integration

Enable seamless

API integration with existing systems and workflows.

Managed Services

Maintenance and updates for decision science tools.

Ex: TimeFold Planning AI, Probabl, Google Routing API, MathOpt API

Prototype
Develop initial models

Scale
Adapt for large-scale data

Deploy

Monitor

Integrate with existing systems

Continuous eval and improve

3



Hugging Face & Community





Popular library for natural language processing with **pre-trained models.**



Model Hub

Platform for sharing and discovering pre-trained models.



Datasets

Offers a wide range of **datasets** for machine learning tasks.

Ex: Ner40pt fine-tuned transformer models on optimization corpora

Is there a Hugging Face for Decision Science?

1 Model Hub

Create a repository for sharing pre-built constraint models

2

Collaborative Platform

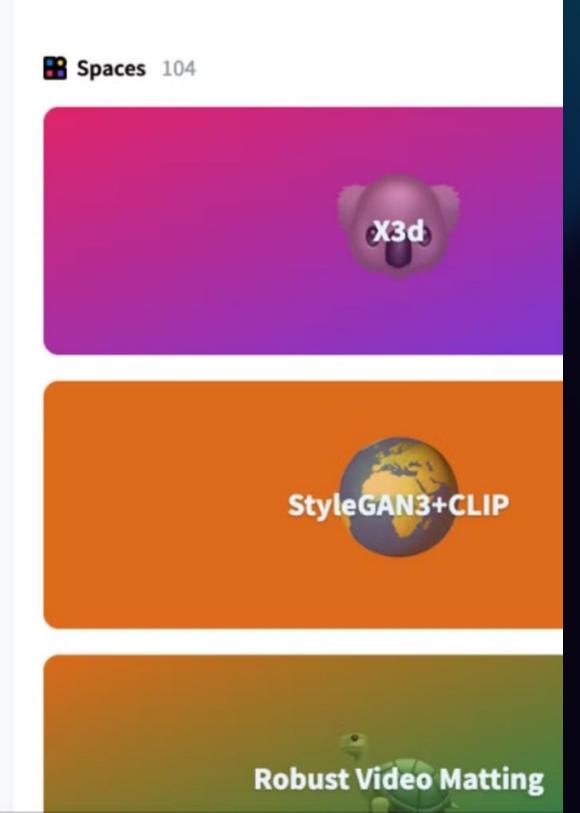
Foster community-driven development of decision science tools

3

Easy Deployment

Provide **infrastructure** for deploying decision models as web services

Ex: CoinOR founded in 2000 Santa Rastion , NextMv



Demo Spaces

1 Interactive ML Apps

Supports building applications using

Streamlit, Gradio,
Docker, or static HTML.

2 Hosting and Deployment

Provides easy

deployment options with

various hardware

choices.

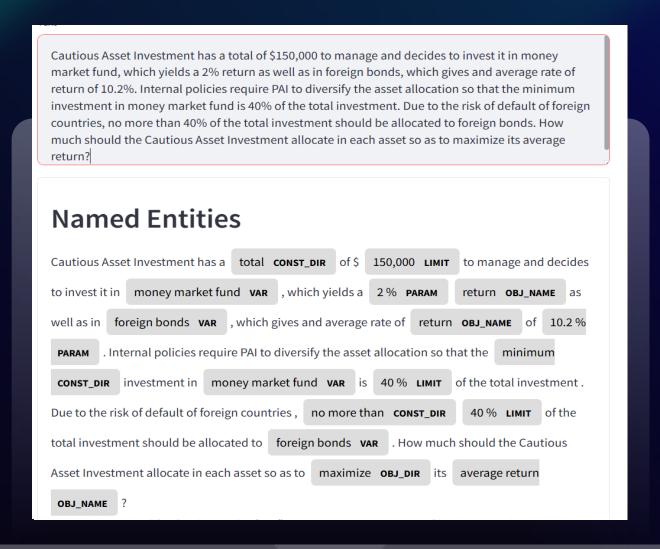
(3) Collaboration and Sharing

Enables **sharing ML projects** with the community and Git integration for version control.

Named entity recognition for optimization

Ner40pt

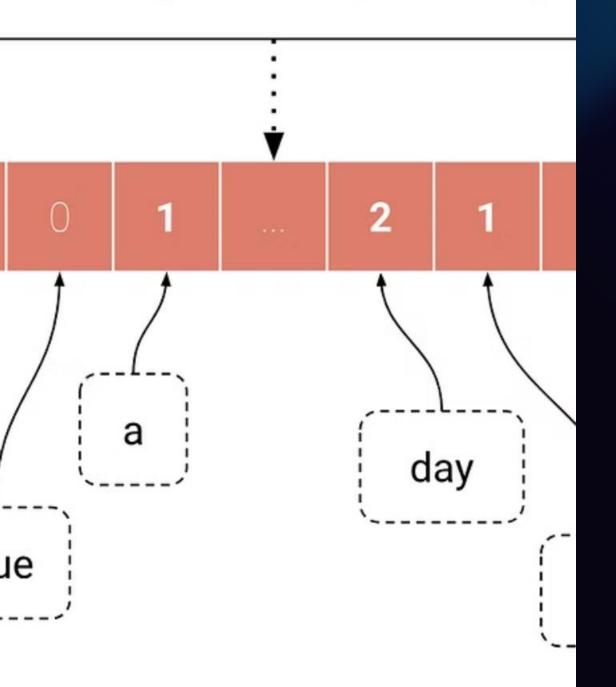
Extract variables, objective, parameters, and constraints from natural text



pip install ner4opt

Ner4Opt Named Entity Recognition for Optimization Demo

This day was a good day



Pre-Trained Embeddings

1 Sentence Transformers

2

Key Features

Framework for generating custor dense vector representations compu

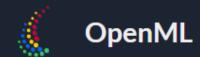
dense vector representations for sentences, paragraphs, and images.

Pre-trained models,

custom training, similarity computation, and multilingual support.

3 Applications

Semantic search, paraphrase mining, clustering, and textual similarity.



Search

Datasets 6.1k
Tasks 262.7k
Flows 22.8k

Runs 10.1M

Collections 218

Benchmarks

Task Types 8

Measures 230

Learn

■ Documentation [©]

👤 Discussions 🗹

OpenML

1 Datasets

Hosts a variety of
uniformly formatted
datasets with rich,
consistent metadata.

3 Experiments

Records exact datasets, algorithms, and library versions ensuring **reproducibility**.

Ex: MIPLIBing, DIMACS, CNF

<u>Text2Zinc Cross-Domain Dataset</u>

7 Tasks

Defines **standardized tasks** for benchmarking and comparing different algorithms and models.

```
import openml

# List all datasets and their properties
openml.datasets.list_datasets(output_format="dataframe")

# Get dataset by ID
dataset = openml.datasets.get_dataset(61)

# Get dataset by name
dataset = openml.datasets.get_dataset('Fashion-MNIST')

# Get the data itself as a dataframe (or otherwise)
X, y, _, _ = dataset.get_data(dataset_format="dataframe")
```

Resources and Tools

Community-Driven Development

Collaborative development, maintenance, and events including hackathons and competitions. Mentorship and certification programs to validate skills

Benchmarking & Leaderboards

Publicly accessible datasets with data cards, models with model cards, **benchmarks**, **leaderboards**, evals.

Educational Resources

Publicly available **educational material** including interactive tutorials, blog posts, and online courses.

<u>The CP-SAT Primer</u> <u>LP Primer</u> <u>Text2Zinc Cross-Domain Leaderboard for LLM Modeling</u>



Advanced Features and Integration

Explainability

Tools providing insights into optimization model decisions, similar to **Explainable Al** techniques.

Hybrid Software

Integrated tools for combining **learning and reasoning** models.



Interactive Dashboards

Visualize and interact with optimization models and results in real-time.

Automated Tuning

Hyperparameter optimization for best performance in optimization models.

<u>Ecole Library Extensible Combinatorial Optimization Learning Environments</u>

<u>DSPy: Declarative Self-Programming for LLM Prompting</u>

Showcasing Successful Applications

The Art of Possible

Demos and proof-of-concept application spaces to communicate the potential of decision science, similar to HuggingFace Spaces.

Industry Applications

Showcase successful industry applications with practical impact addressing unique needs of sectors such as healthcare, finance, and manufacturing.

Real-World Impact

Highlight how decision science solutions have improved efficiency, reduced costs, or solved complex problems in various industries.

Ex: INFORMS Prizes Constraint Applications Blog IAAI - Innovative Applications of AI

Opportunities to Advance Decision Science

Ease of Use

Easy installation, ready-to-run environments, and standardized interfaces.

Pre-trained Embeddings

Latent instance representations for CP, MIP, SAT.

Datasets and Leaderboards

Publicly accessible datasets and benchmarks for decision science problems.

Accessibility

Low code/no code environments and modeling assistants.

Cloud Services and APIs

Online services, API integration, and emergence of DecisionOps.

Educational Resources

Interactive tutorials, blog posts, and online courses on decision science topics.

Constraint Model Registry

Hosting base constraint models for common applications.

Community-Driven Development

Collaborative development, events, mentorship, and certification programs.

Successful Applications

Interactive tutorials, blog posts, and online courses on decision science topics.



Call to Action

1 Contribute

Participate in open-source development of decision science tools.

Collaborate

Build a robust ecosystem to share and collaborate.

3 Improve Tech Stack & Innovate

Enhance standards and user experience to attract new participants and foster collaboration.

skadio.github.io