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Advancing Decision Science: Lessons from Machine Learning

Bridge on Constraint Programming and Machine Learning



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skadio.github.io



BROWN

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 solutions
- 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.

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.



**MACHINE
LEARNING**

**DECISION
SCIENCE**

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, OR-Tools, PyOptInt, ALNS, PyVRP, PyJobShop, DIDPpy, ...

Seq2Pat

Sequence to
Pattern generation
for constrained
pattern mining

Discover frequent
sequential
patterns in large
sequence
databases with
constraints

Collaboration with CMU
Kadioğlu et. al. ([AI Magazine'23](#))

```
# Example to show how to find frequent sequential patterns
# from a given sequence database subject to constraints
from sequential.seq2pat import Seq2Pat, Attribute

# Seq2Pat over 3 sequences
seq2pat = Seq2Pat(sequences=[["A", "A", "B", "A", "D"],
                             ["C", "B", "A"],
                             ["C", "A", "C", "D"]])

# Price attribute corresponding to each item
price = Attribute(values=[[5, 5, 3, 8, 2],
                          [1, 3, 3],
                          [4, 5, 2, 1]])

# Average price constraint
seq2pat.add_constraint(3 <= price.average() <= 4)

# Patterns that occur at least twice (A-D)
patterns = seq2pat.get_patterns(min_frequency=2)
```

pip install seq2pat
35K+ 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.

③ 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 \approx 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, Ner4Opt, Text2Zinc, ChatOpt, 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 AI** development.



Model Registry & DecisionOps

- 1 Version Control**
Keeps track of different **versions of models**, allowing management of updates and changes over time.
- 2 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.

3 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

Integrate with existing systems



Monitor

Continuous eval and improve



Hugging Face

Hugging Face & Community



Transformers Library

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



Model Hub

Platform for sharing and discovering pre-trained models.



Datasets

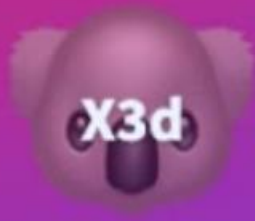
Offers a wide range of **datasets** for machine learning tasks.

Ex: Ner4Opt 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 🙌
Rastion



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.

Ner4Opt

Named entity
recognition for
optimization

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

Kadioğlu et. al. (Constraints'24)

Cautious Asset Investment has a total of \$150,000 to manage and decides to invest it in money market fund, which yields a 2% return as well as in foreign bonds, which gives an average rate of return of 10.2%. Internal policies require PAI to diversify the asset allocation so that the minimum investment in money market fund is 40% of the total investment. Due to the risk of default of foreign countries, no more than 40% of the total investment should be allocated to foreign bonds. How much should the Cautious Asset Investment allocate in each asset so as to maximize its average return?

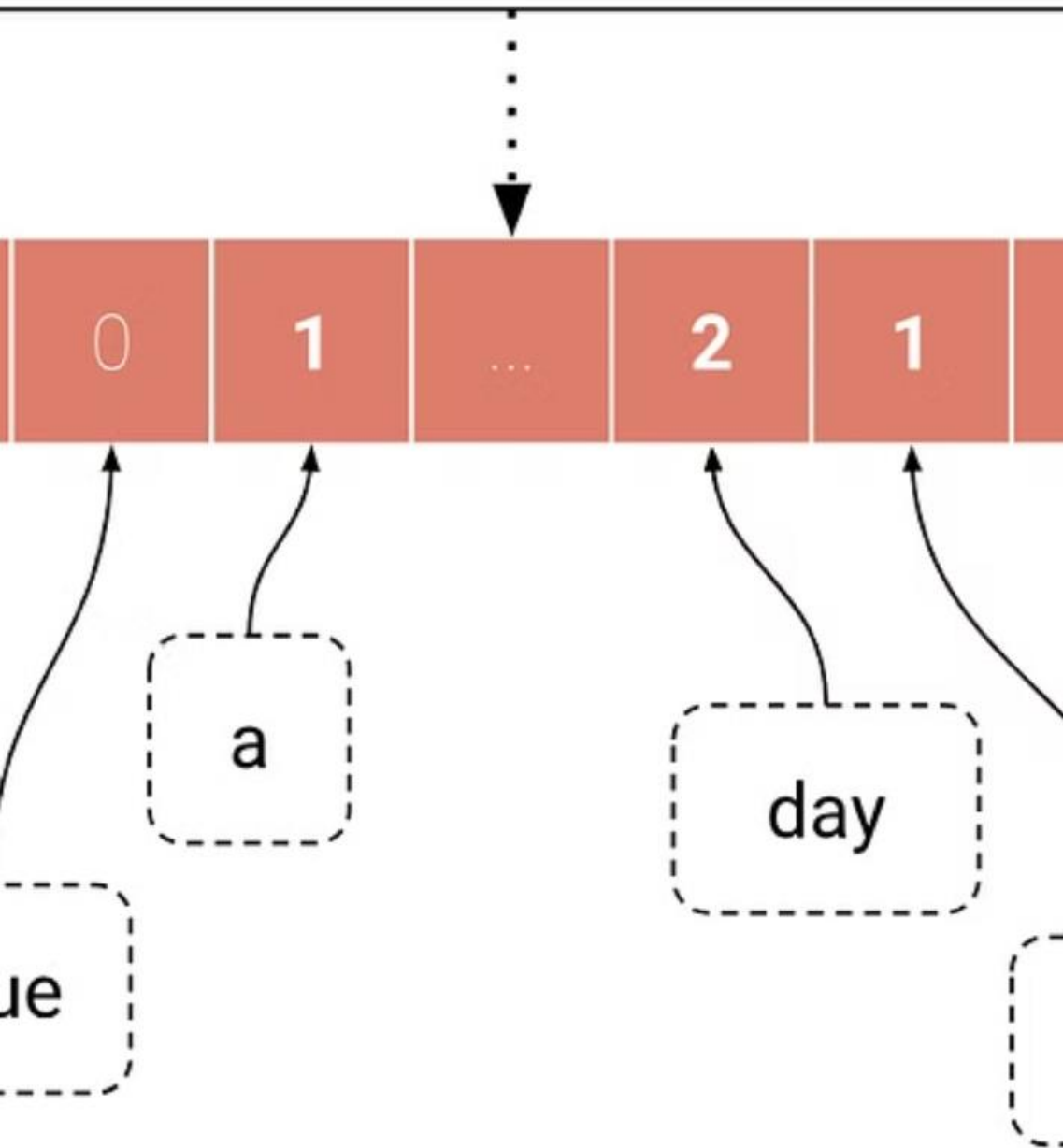
Named Entities

Cautious Asset Investment has a **total** **CONST_DIR** of \$ **150,000** **LIMIT** to manage and decides to invest it in **money market fund** **VAR**, which yields a **2 %** **PARAM** **return** **OBJ_NAME** as well as in **foreign bonds** **VAR**, which gives an average rate of **return** **OBJ_NAME** of **10.2 %** **PARAM**. Internal policies require PAI to diversify the asset allocation so that the **minimum** **CONST_DIR** investment in **money market fund** **VAR** is **40 %** **LIMIT** of the total investment. Due to the risk of default of foreign countries, **no more than** **CONST_DIR** **40 %** **LIMIT** of the total investment should be allocated to **foreign bonds** **VAR**. How much should the Cautious Asset Investment allocate in each asset so as to **maximize** **OBJ_DIR** its **average return** **OBJ_NAME** ?

pip install ner4opt

[Ner4Opt Named Entity Recognition for Optimization Demo](#)

This day was a good day



Pre-Trained Embeddings

1 Sentence Transformers

Framework for generating **dense vector representations** for sentences, paragraphs, and images.

2 Key Features

Pre-trained models, custom training, similarity computation, and multilingual support.

3 Applications

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



OpenML

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

2

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

1

Community-Driven Development

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

2

Benchmarking & Leaderboards

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

3

Educational Resources

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

[The CP-SAT Primer](#) [LP Primer](#)

[Text2Zinc Cross-Domain Dataset & Leaderboard for LLM Modeling](#)



Advanced Features and Integration

Explainability

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

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.

Accessibility

Low code/no code environments and modeling assistants.

Constraint Model Registry

Hosting base constraint models for common applications.

Pre-trained Embeddings

Latent instance representations for CP, MIP, SAT.

Cloud Services and APIs

Online services, API integration, and emergence of DecisionOps.

Community-Driven Development

Collaborative development, events, mentorship, and certification programs.

Datasets and Leaderboards

Publicly accessible datasets and benchmarks for decision science problems.

Educational Resources

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

Successful Applications

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



**MACHINE
LEARNING**

**DECISION
SCIENCE**

Call to Action

1

Contribute

Participate in open-source development of decision science tools.

2

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.