Knowledge-driven AutoML

...~A future current-trend in AI?~...

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= 10^{th} of May 2024 =

VUB

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- Outline

Outline

- AutoML - short introduction
- Knowledge-driven AutoML
  - The „Omina" project
  - Architecture & Motivation
  - Pipeline generation flow
- Open research challenges
  - mining & sharing experiments
  - wrapping ML-libs - inverting dependencies
  - optimization & evaluation

Auto ML

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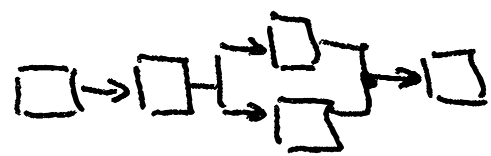
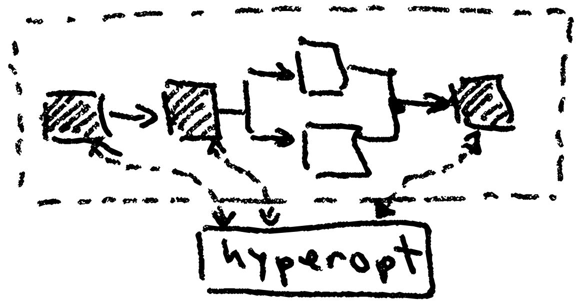
  1. pipe synthesis 

Auto ML

- The process of generating & tuning ML pipelines automatically

- Can be split into two parts:

  1. pipe synthesis
  2. hyperparameter optimization



Auto ML

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  trees → evolutionary

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- Sophisticated and flexible use of knowledge structures still not explored !

Auto ML

- Note: Neural-networks case i.e neural arch. search - not covered here :)

- More info on: https://automl.org/book

Knowledge-driven AutoML

Knowledge-driven AutoML

- Data-driven technique for AutoML
- Available at:
  * Experiments: https://github.com/zgornel/knowledge-driven-automl
  * Library: https://github.com/zgornel/Kdautoml.jl

The Omina project

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WHY?

- improve development quality
- adapt to limited data access
- scale: performance, use-cases etc.

The Omina project

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Knowledge

- data science: code, pipes etc.
- processes: how entities interrelate and generate data
- world: open data, knowledge bases, wiki's ...

Architecture & Motivation

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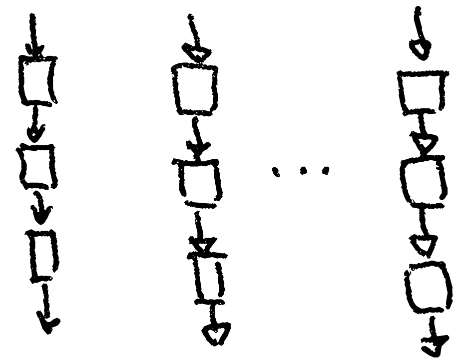
  - → generate complete pipelines first (a bunch of them, test, optimize, etc.)



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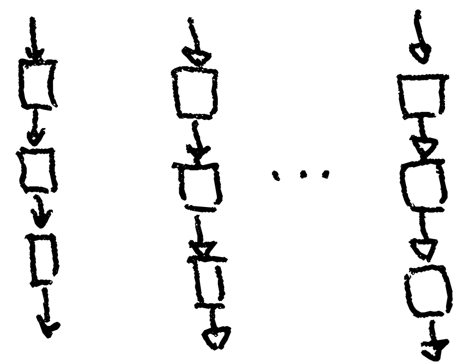
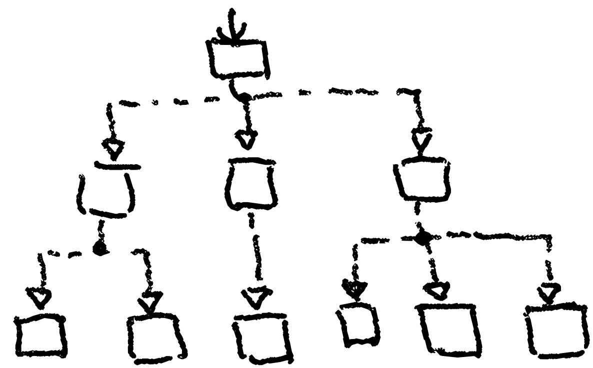


<u>Knowledge</u> used for:

- generating pipes
- post-process / combine them.
  i.e. optimization

Architecture & Motivation

- Two approaches become apparent:
  - → generate and execute dynamically pipes



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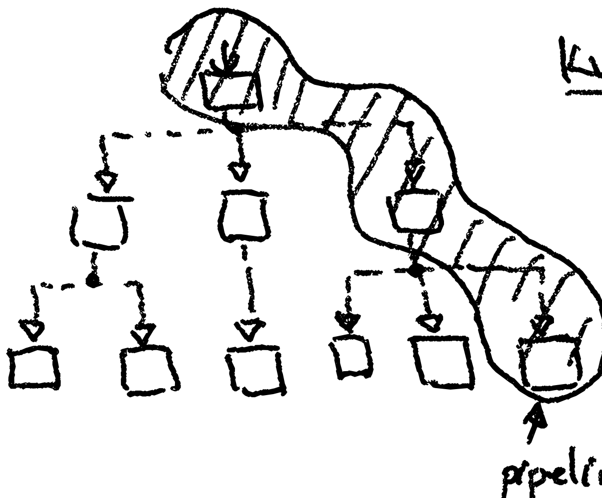

<u>Knowledge</u> used to

- decide what ops. are feasible based on:
  - → current operation
  - → partial pipe(s)
  - → execution results
  - → data science knowledge

Architecture & Motivation

- The latter „dynamic" approach chosen:
  - → better control over program space
    - → granularity in knowledge application
  - → more explanatory power
  - → allows for interactivity i.e. human intervention
    - → delays, partial execution etc.
  - → [potentially] more resource friendly
  - → the first one was already explored (by MIT)

Architecture & Motivation

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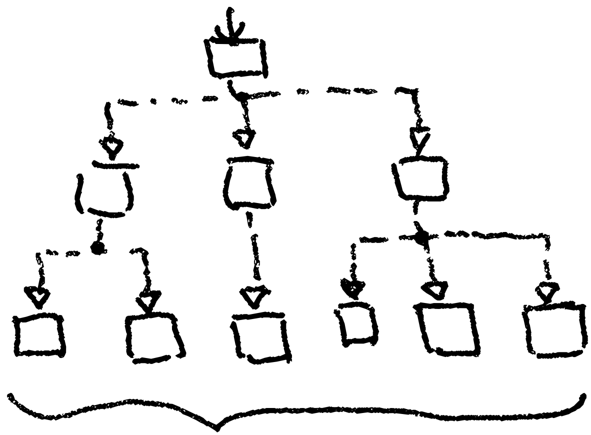
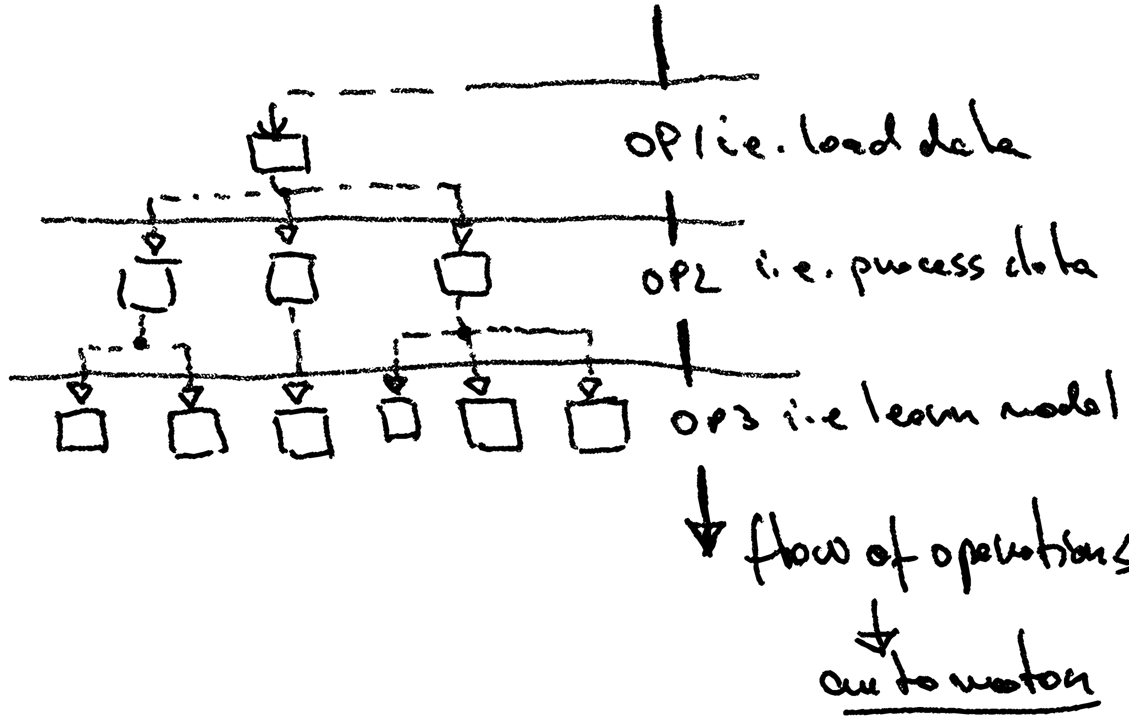


<u>program</u> <u>space</u> i.e all possible pipes

↓

<u>how</u> to construct it?

Architecture & Motivation



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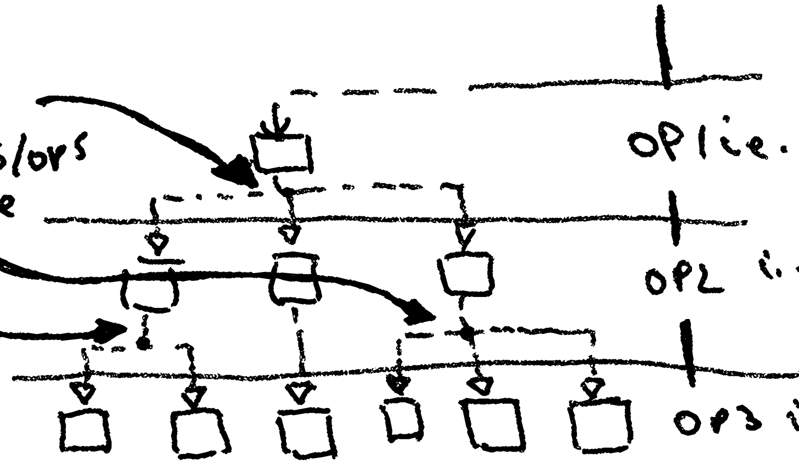


decisions on what blocks/ops are feasible

↓

Knowledge

↓

graph db

OP1 i.e. load data

OP2 i.e. process data

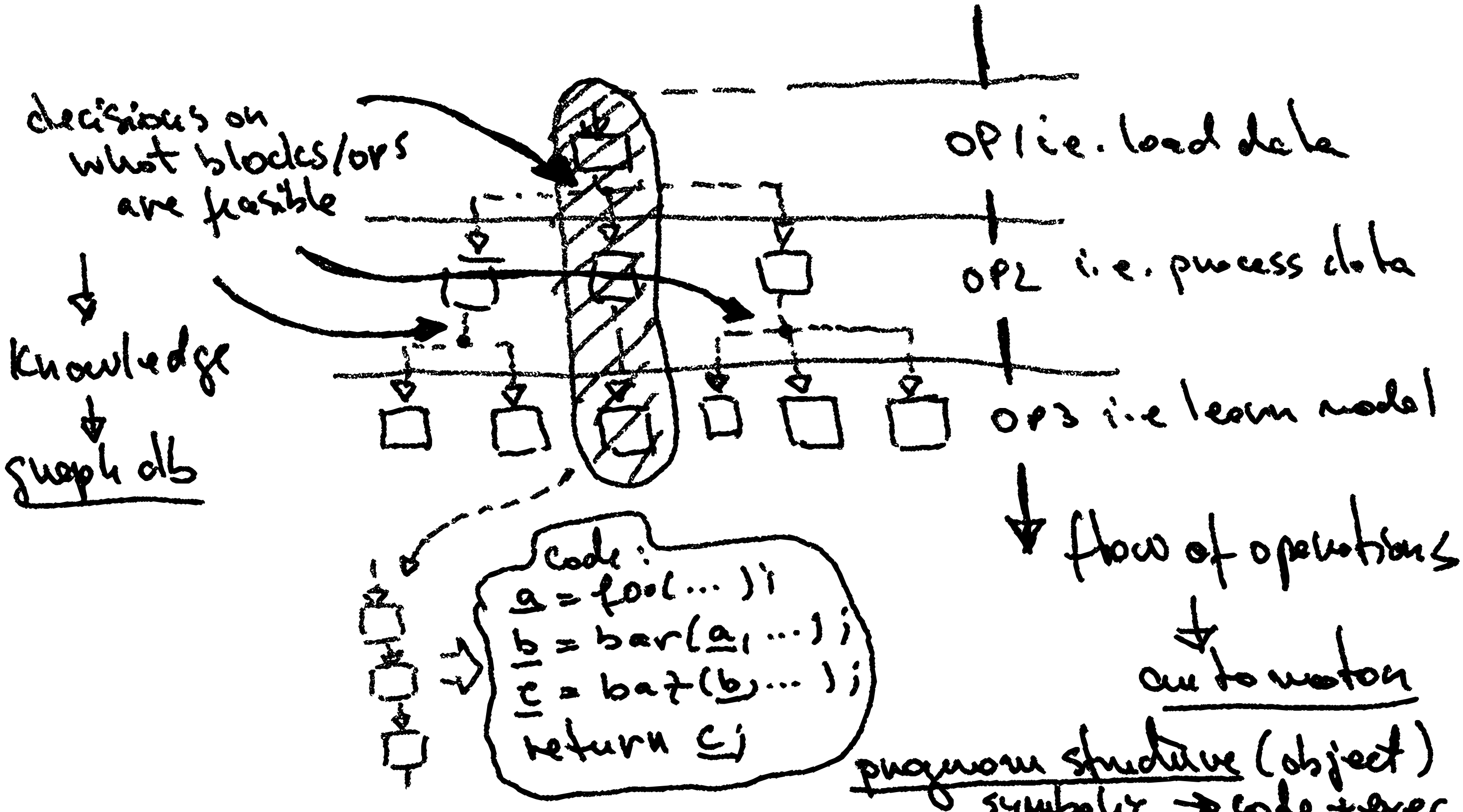
OP3 i.e. learn model

↓ flow of operations

↓

automaton

Architecture & Motivation



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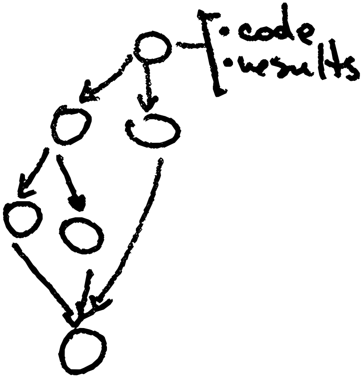

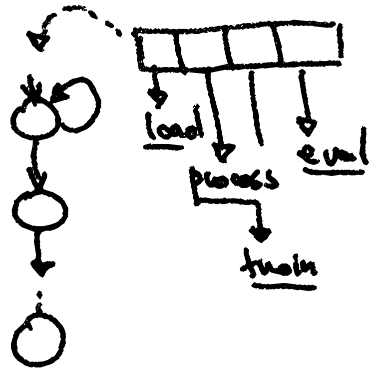

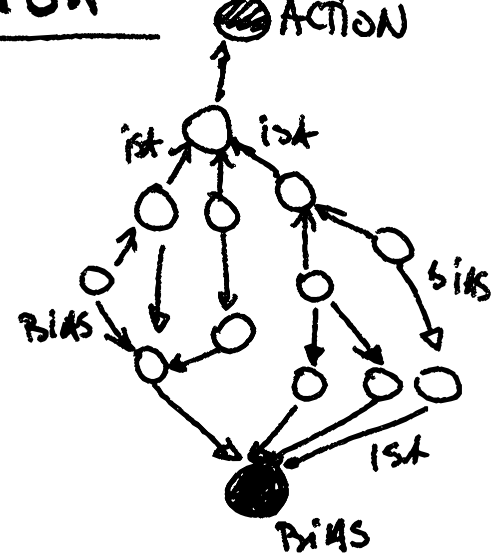

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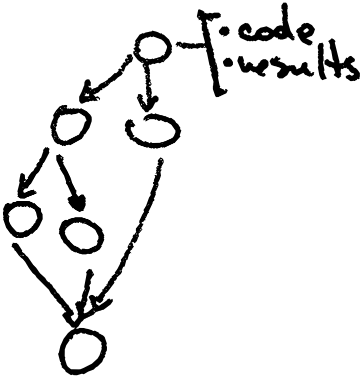
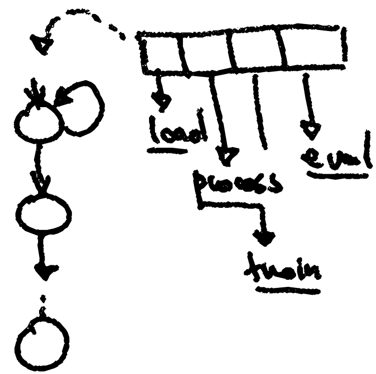
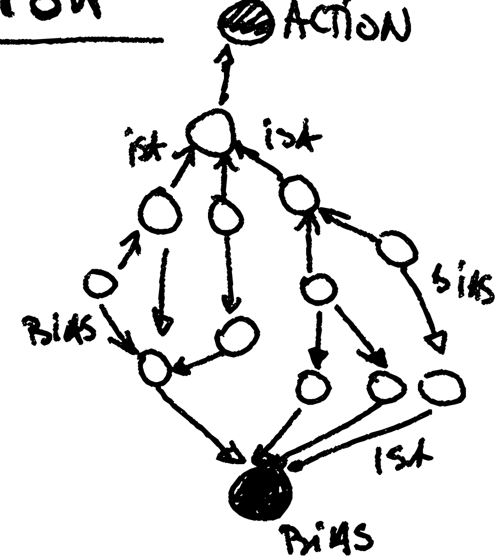


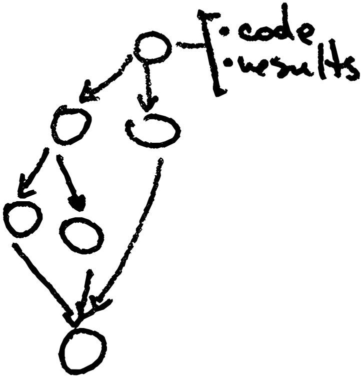


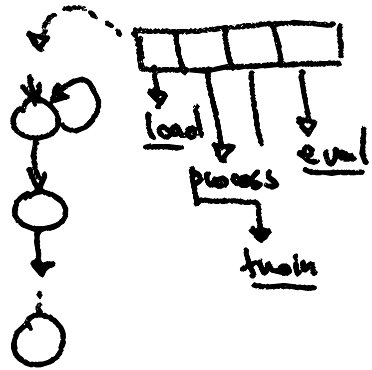


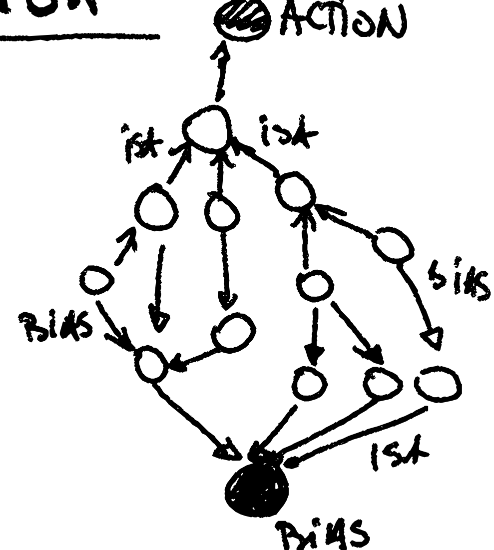
Automaton

- controls build flow
- communicates w. kb
- sends code / gets data from prep. structure

Architecture & Motivation







Automaton

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Kb

- stores code, actions hierarchy, * bias hierarchy, bias structure

*bias = condition over an action/block/op

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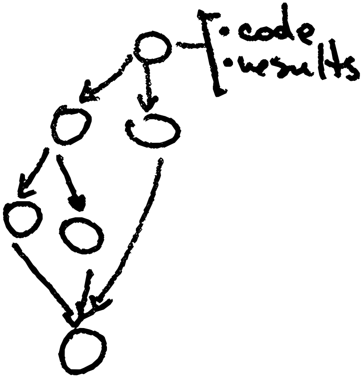
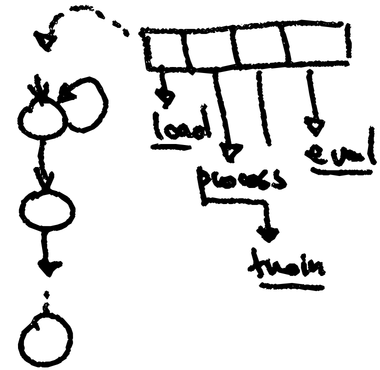
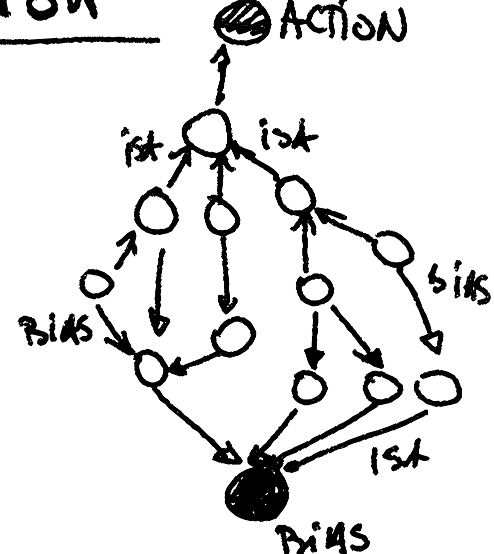
Architecture & Motivation







program struct.

- contains prog. space
- can build code
- can execute code
- holds data/results
- depends on programming language/library

Automaton

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- communicates w. kb
- sends code/gets data from prog. structure

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Pipeline generation flow

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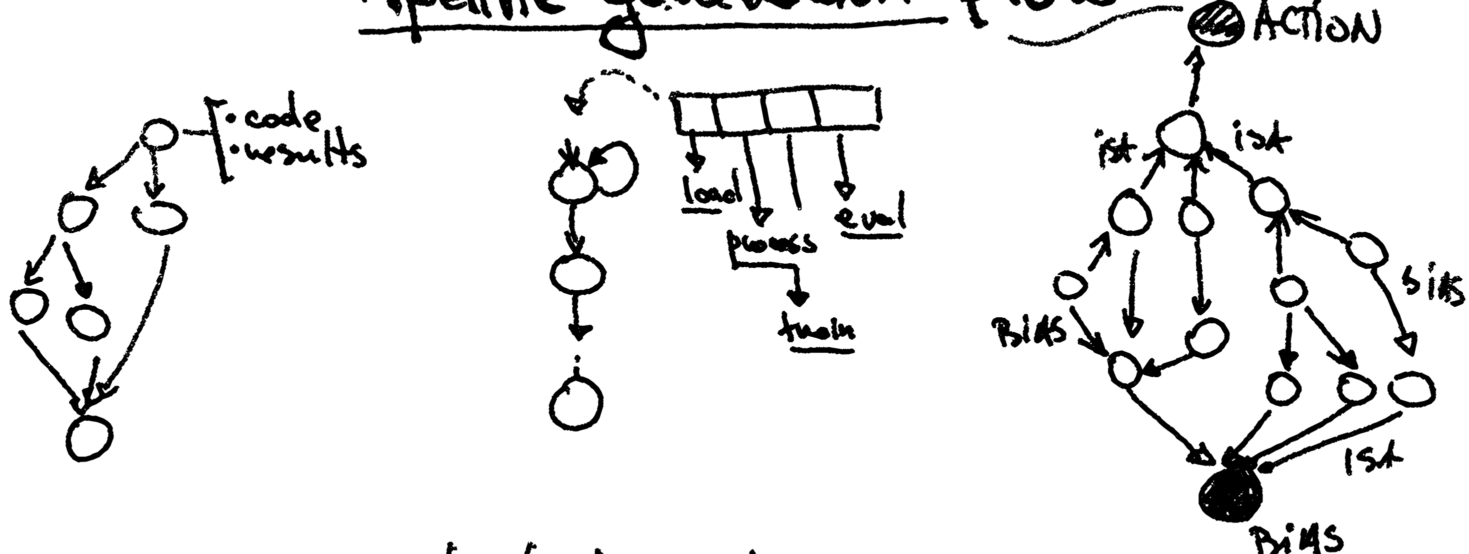
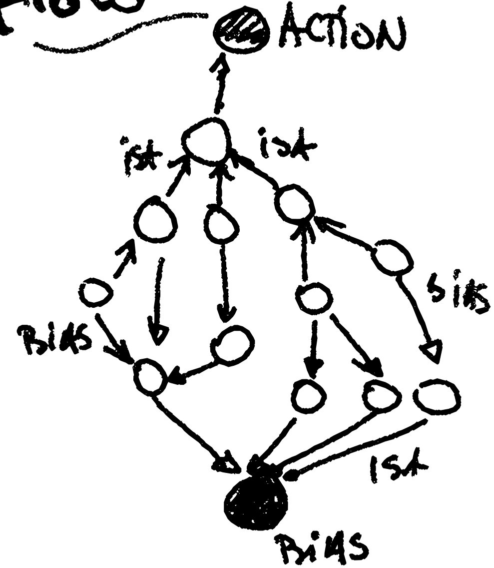


* Let's start from the beginning...

Pipeline generation flow

//no program.



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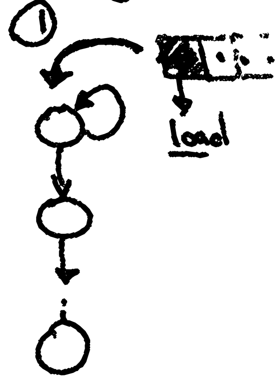
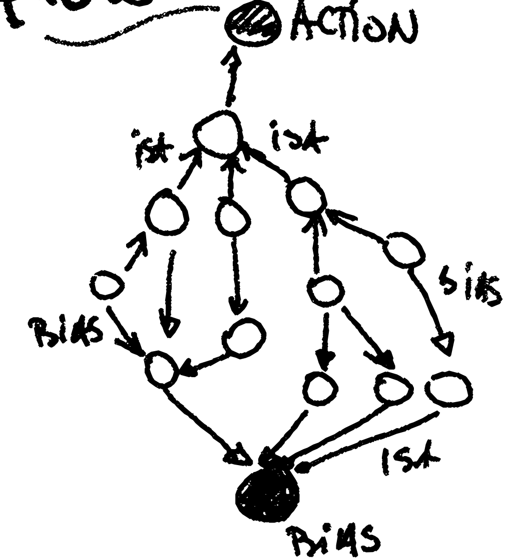
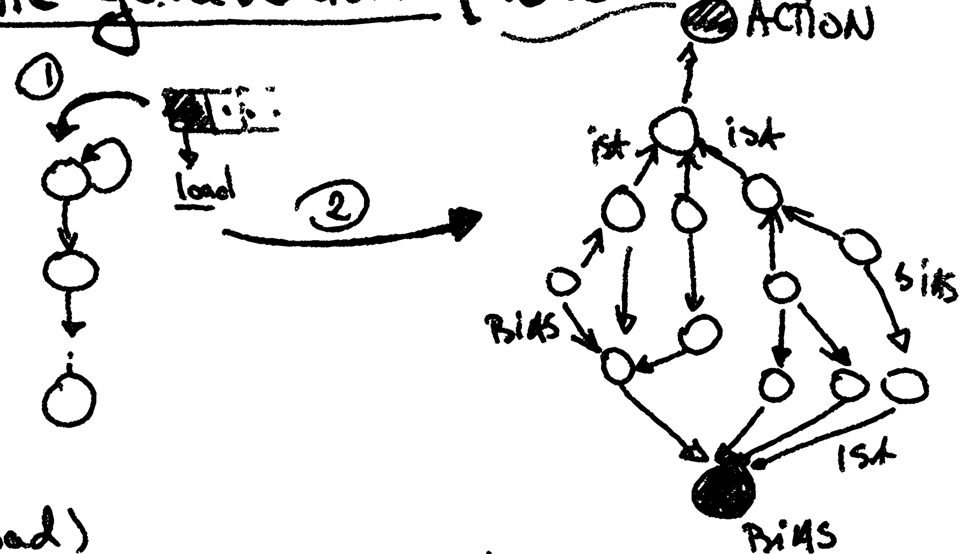




① Read first op (load)

Pipeline generation flow

//no programm.



1. Read first op (load)
2. Query KB what ops + biases are available

Pipeline generation flow

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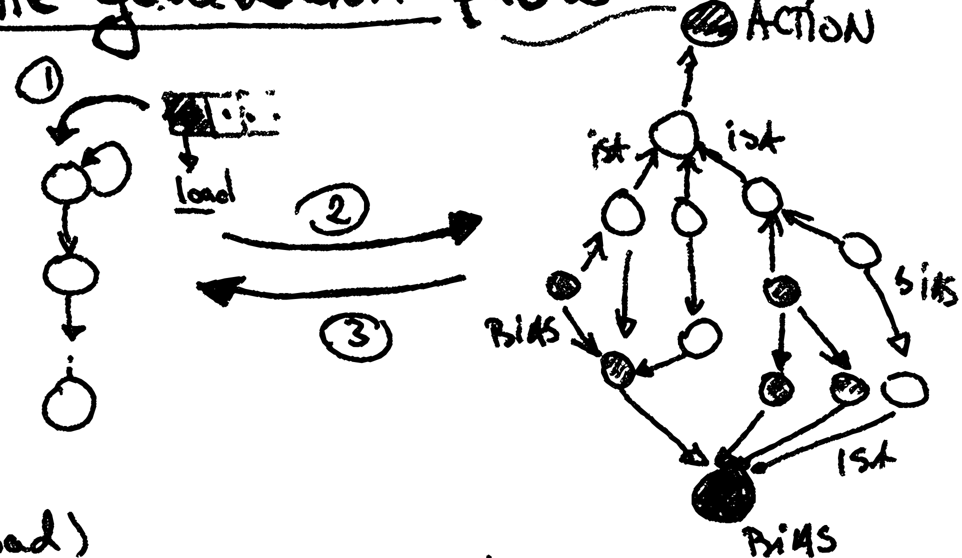

1. Read first op (load)
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3. Get list of (ops, biases)

Pipeline generation flow

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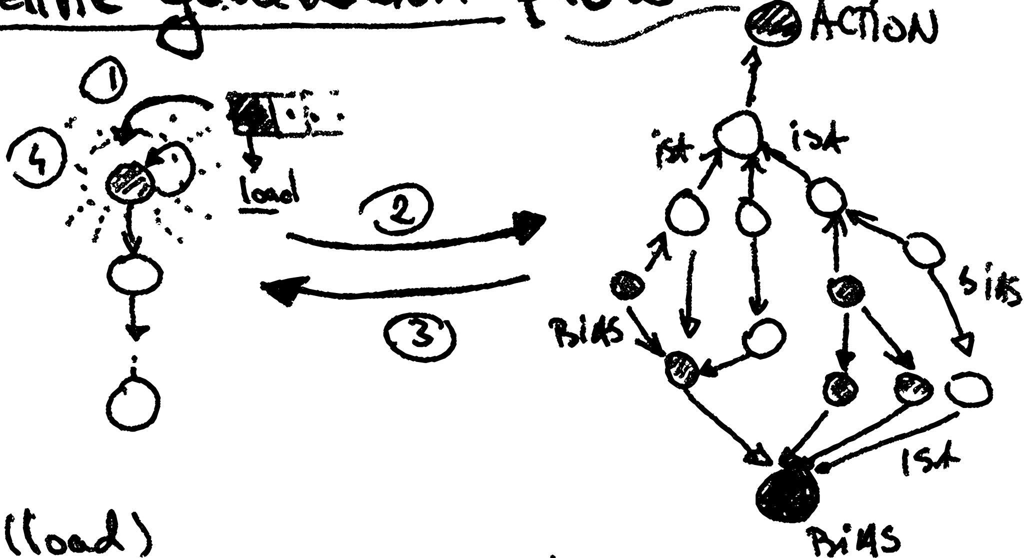

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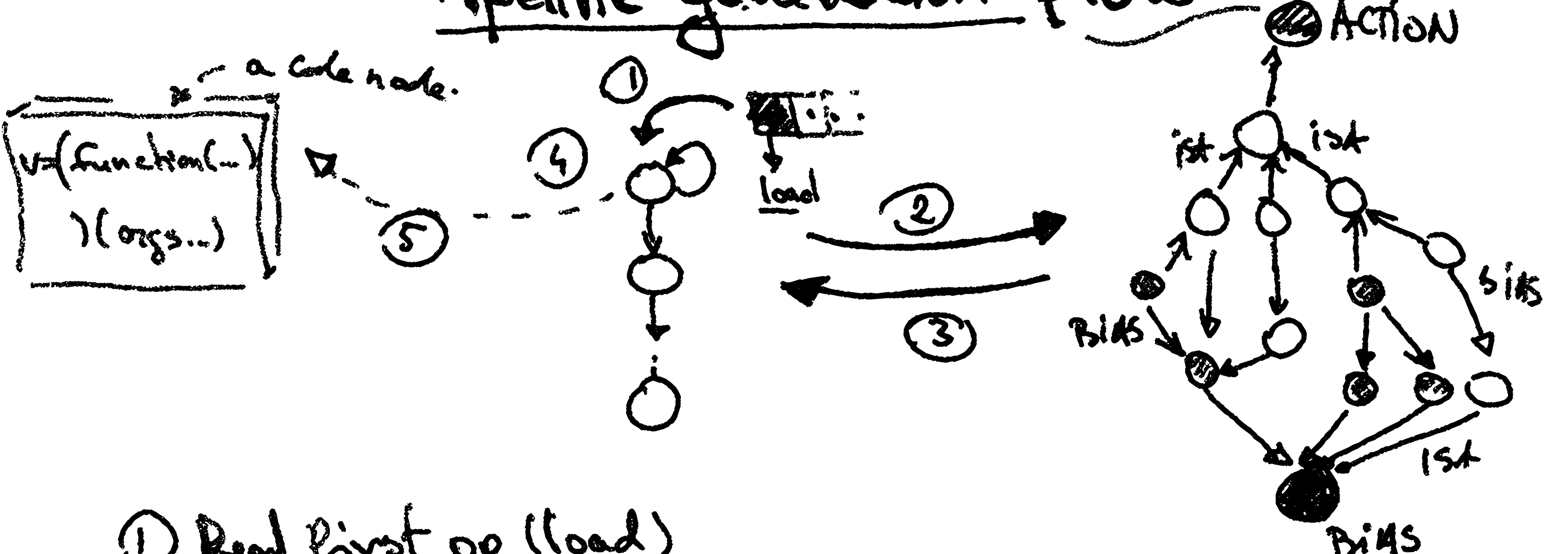
3. Got list of (ops, biases)
4. Execute bias functions, retain feasible ops

Pipeline generation flow



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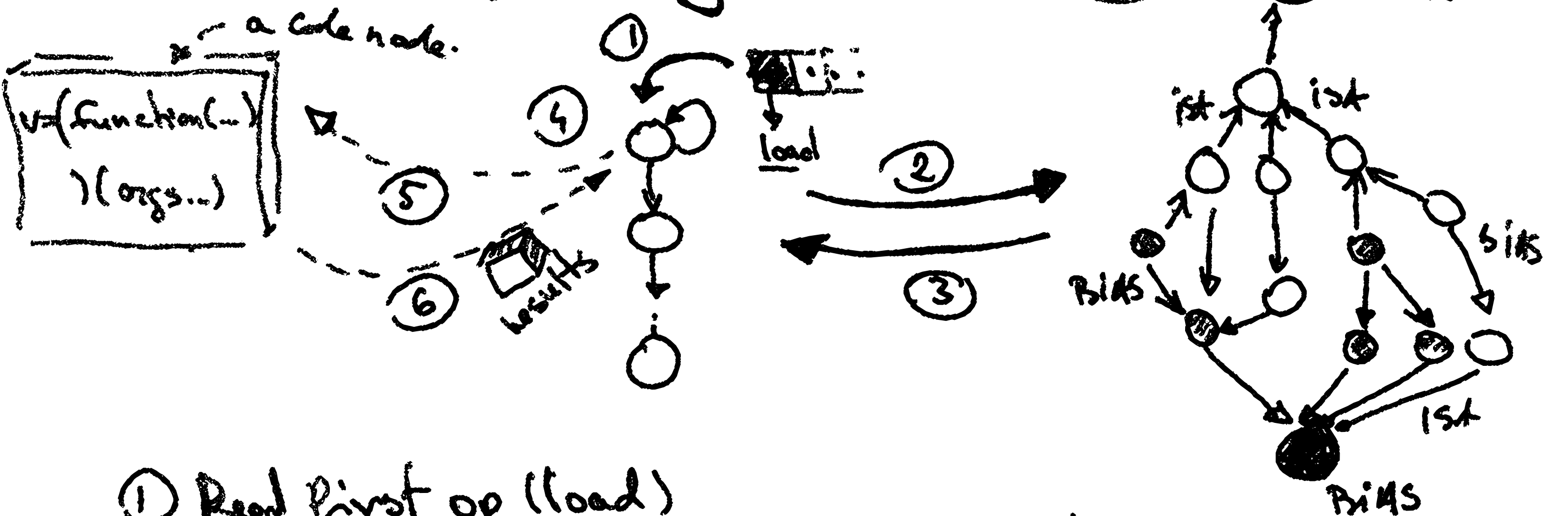
5. Construct code

Pipeline generation flow



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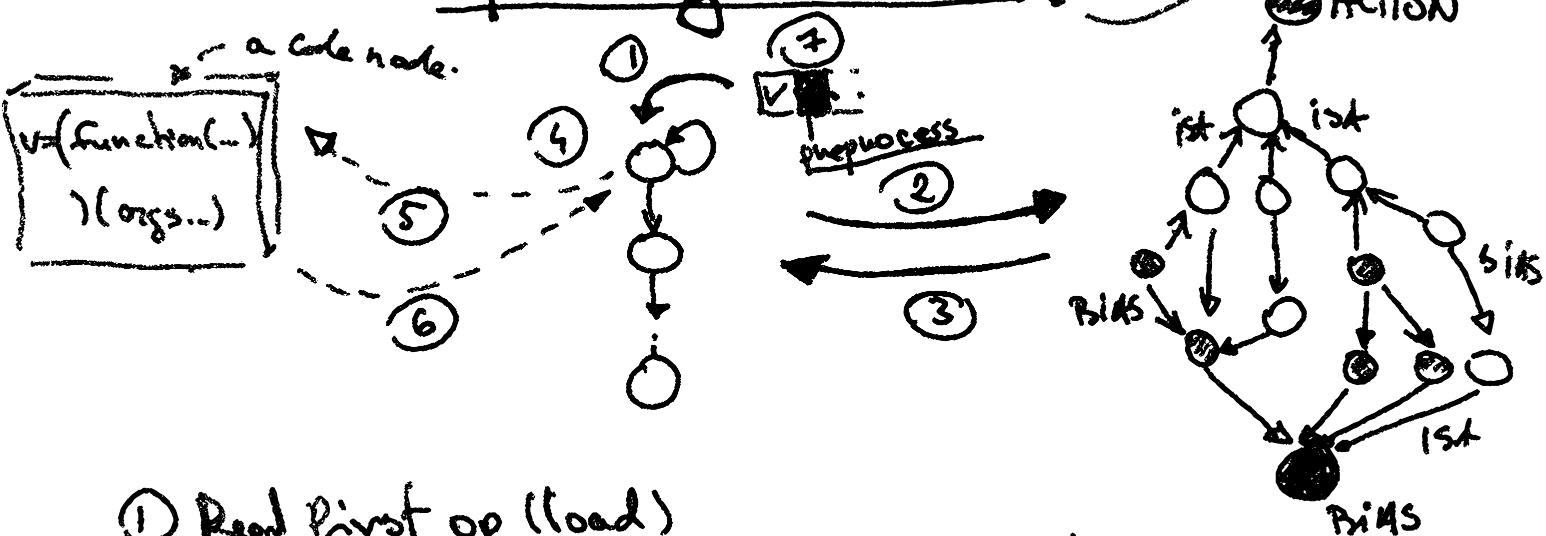
4. Execute bias functions, retain feasible ops
5. Construct code 6. Execute pipeline

Pipeline generation flow



1. Read first op (load)
2. Query KB what ops + biases are available
3. Got list of (ops, biases)
4. Execute bias functions, retain feasible ops
5. Construct code
6. Execute pipeline
7. next op

~ Open research challenges ~

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> Mining & sharing experiments

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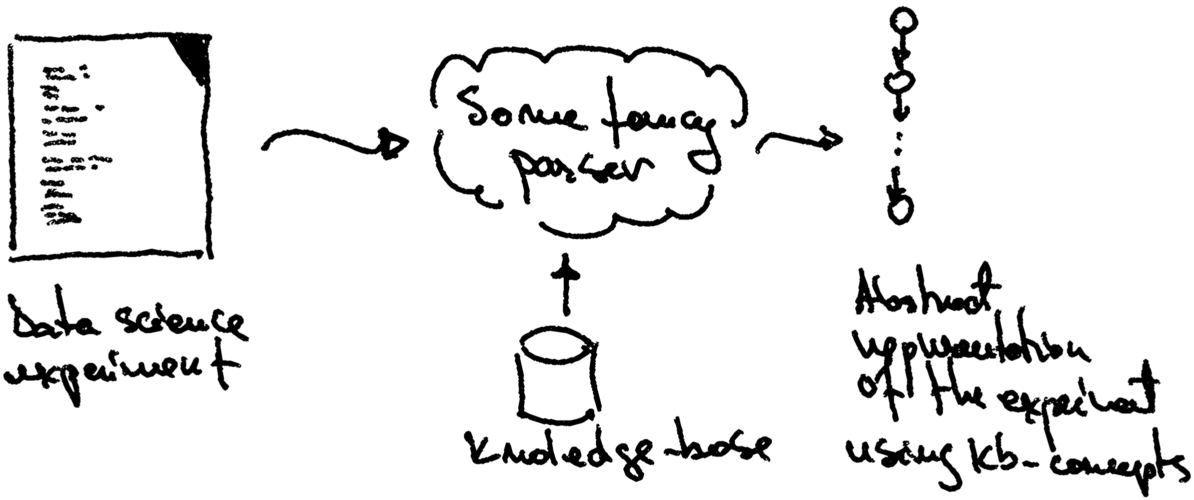

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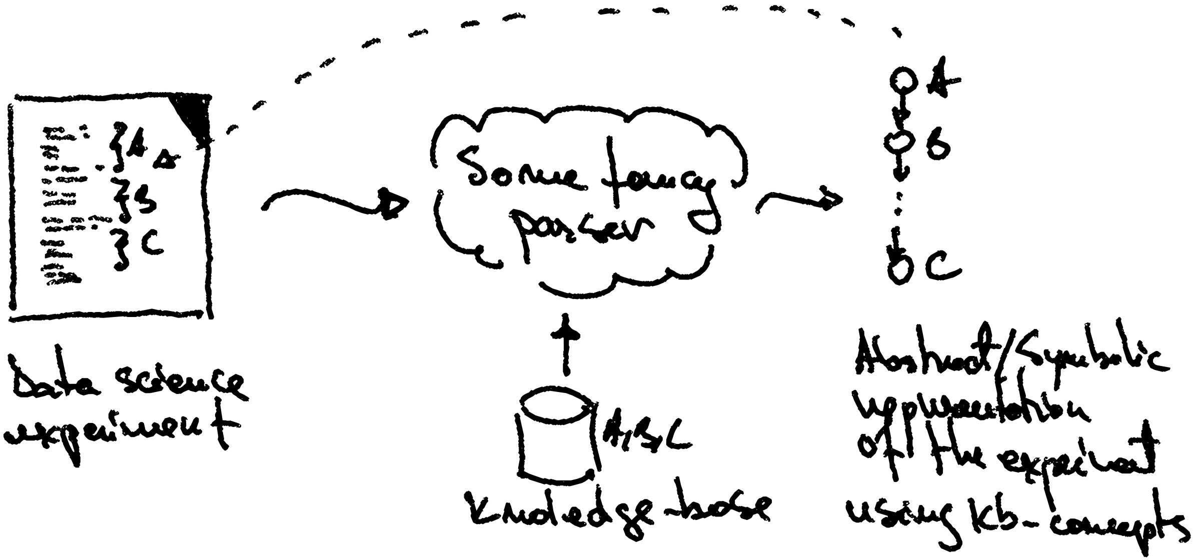

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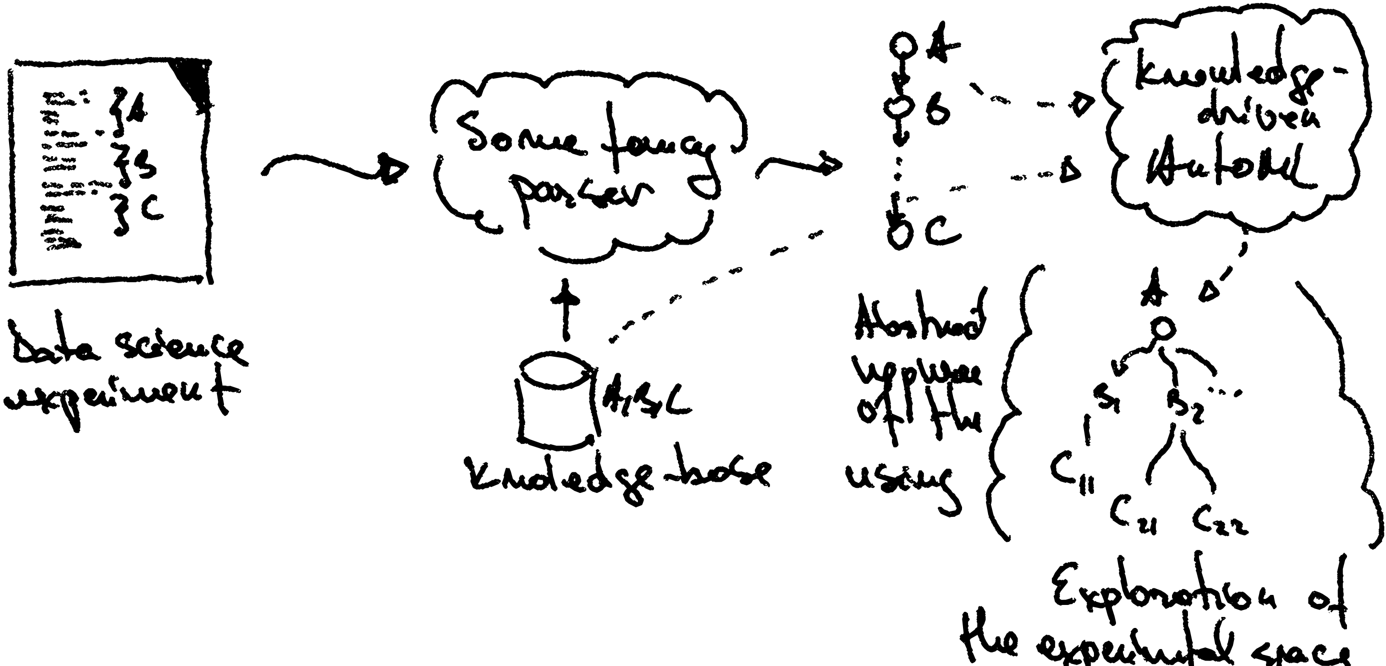

~ Open research challenges ~

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> wrapping ML libs

~ Open research challenges ~

> wrapping ML libs

> currently, each AutoML library depends on a <u>single</u> ML-library

$$
\begin{tikzcd}
\text{AutoML}_1 \arrow[d, "\text{DEPENDS}"] & & \text{AutoML}_2 \arrow[d, "\text{DEPENDS}"] & \dots & \text{AutoML}_n \arrow[d, "\text{DEPENDS}"] \\
\text{ML}_1 & \text{ML}_2 & \text{ML}_3 & \dots & \text{ML}_n
\end{tikzcd}
$$

> changes in ML (frequent) influence AutoML

~ Open research challenges ~

> wrapping ML libs

> what if a single AutoML library supports multiple ML libraries

AutoML$_1$

ML$_1$ ML$_2$ .. ML$_n$

~ Open research challenges ~

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$$\begin{array}{ccc} & AutoML_1 & \\ \nearrow & \uparrow & \nwarrow \\ ML_1 & ML_2 \,.. & ML_n \end{array}$$

Dependency inversion!

"Bob Martin – Clean Architecture"

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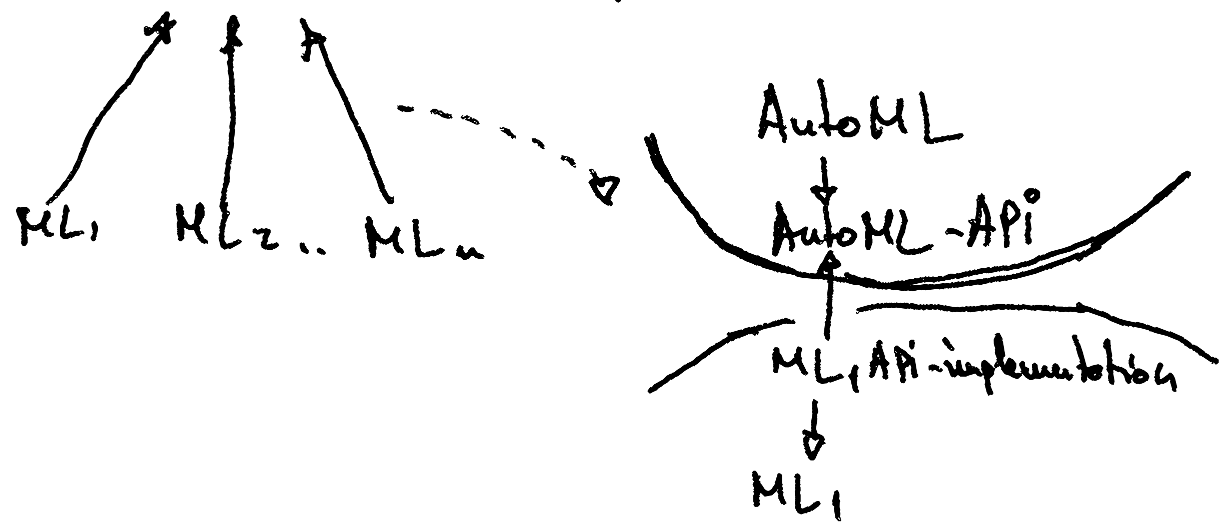
AutoML1



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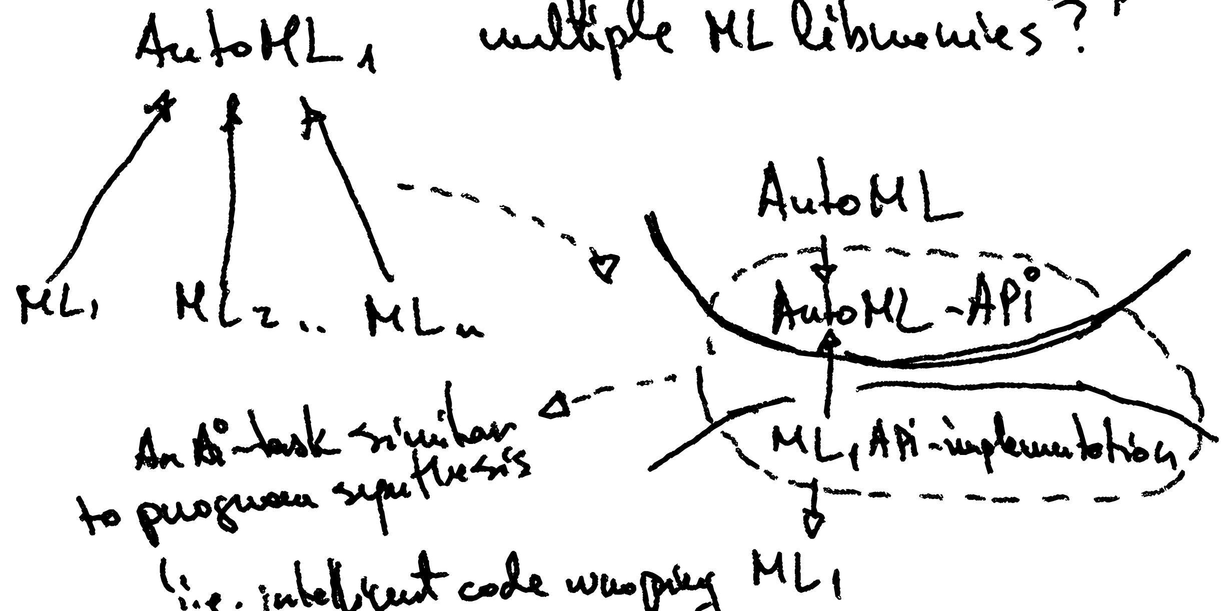

Open research challenges

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↓

Currently that's done using some form of metric involving accuracy & time/resources

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Interpretability?

Explainability?

Ease of use?

Scalability?

→ HOW TO BEST INTEGRATE THE QUALITATIVE?

Thank you.

Q & A Time ...