Optimization Modulo Theory: A Tutorial Using Z3 and Practical Case Studies

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Outline

Motivation

Part 1: Optimization Modulo Theory - background and examples

Part 2: Optimization Modulo Theory - Case Study

- Problem Specification
- Problem Formalization
  - Model-driven approach: Formulation of the Satisfiability/Optimization Modulo Theory Problem
  - Data-driven approach: Graph Neural Network Formulation
- Solution
  - Dataset generation
  - Training a GNN model for edge classification
  - Integrated GNN and Exact Techniques: Experimental Results
- Future Work

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Z3 solver online to be used during the tutorial

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Files used in this presentation

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  - incorporate domain-specific reasoning, e.g: arithmetic, equality, data structures (arrays, lists, stacks, ...) and valid combinations

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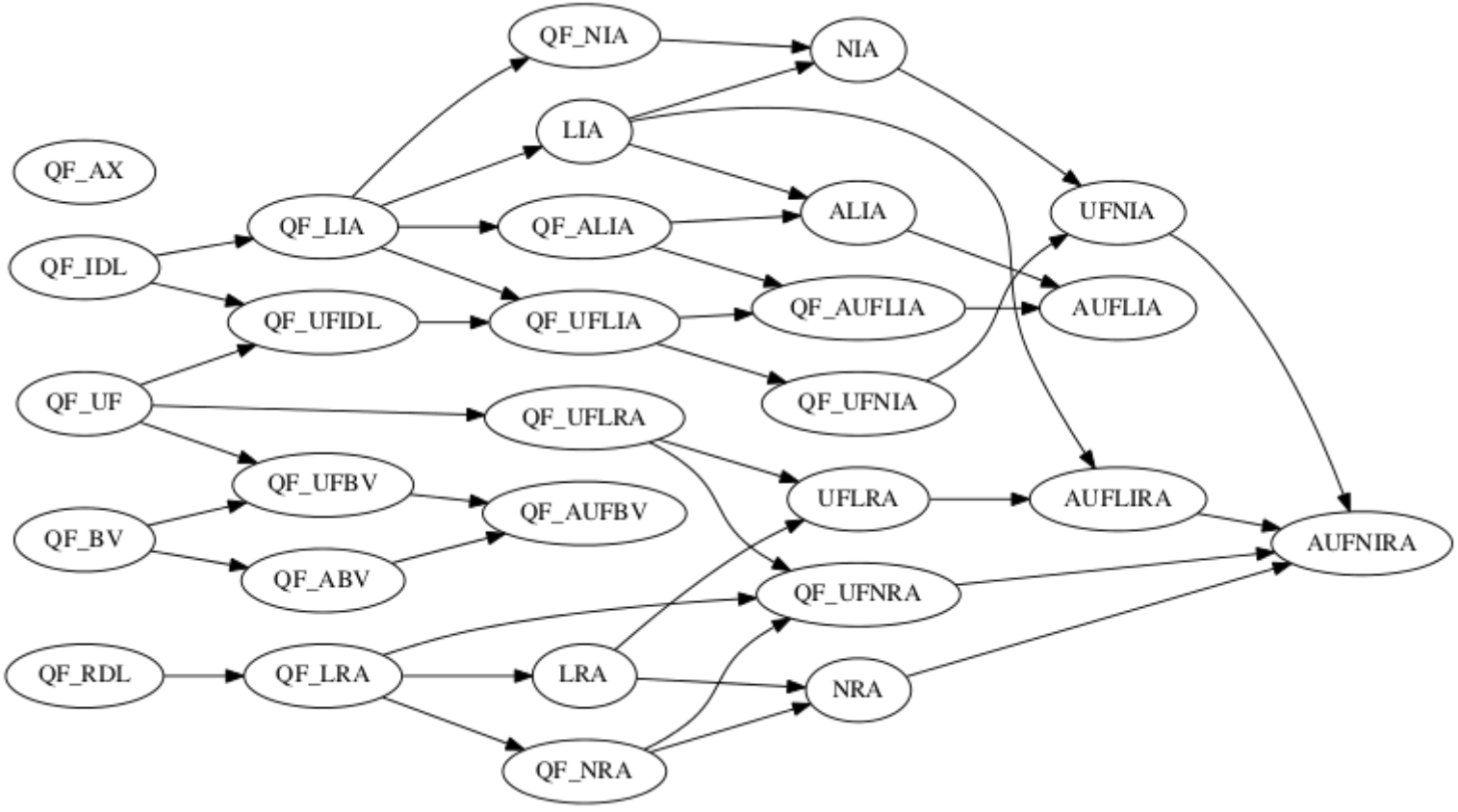
- Some SMT solvers offer optimization features $\rightsquigarrow$ optimization modulo theory (OMT): Z3 [4], OptiMathSAT [18]; Symba [13], HAZEL [14], MAXHS-MSAT [10], PULI [11], CEGIO [2], BCLT [12].

SMT Theories



Source: `http://smtlib.cs.uiowa.edu/logics.shtml`

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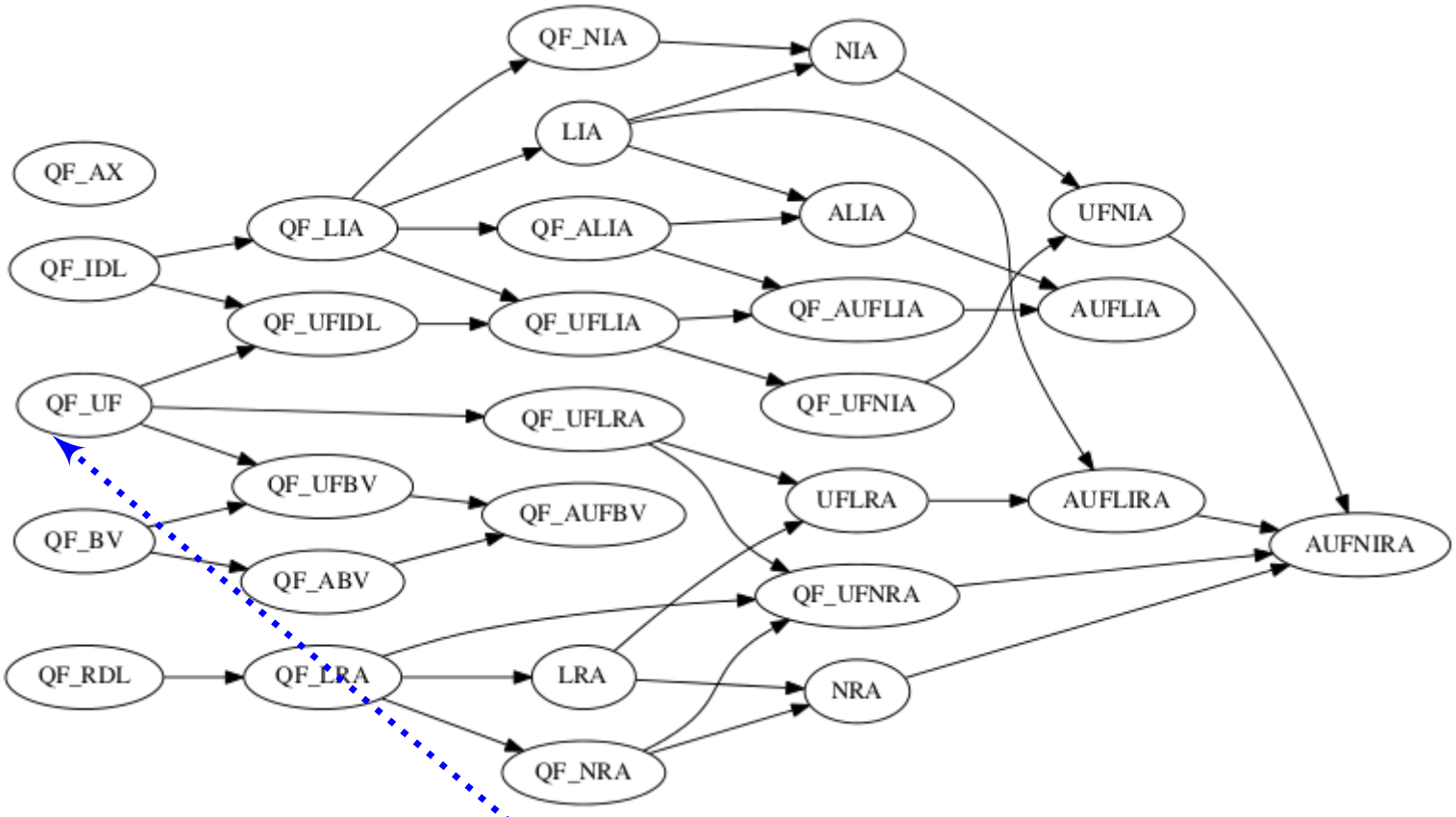

Quantifier-free equality logic with uninterpreted functions

$$(a = c \wedge b = d) \rightarrow f(a, b) = f(c, d)$$

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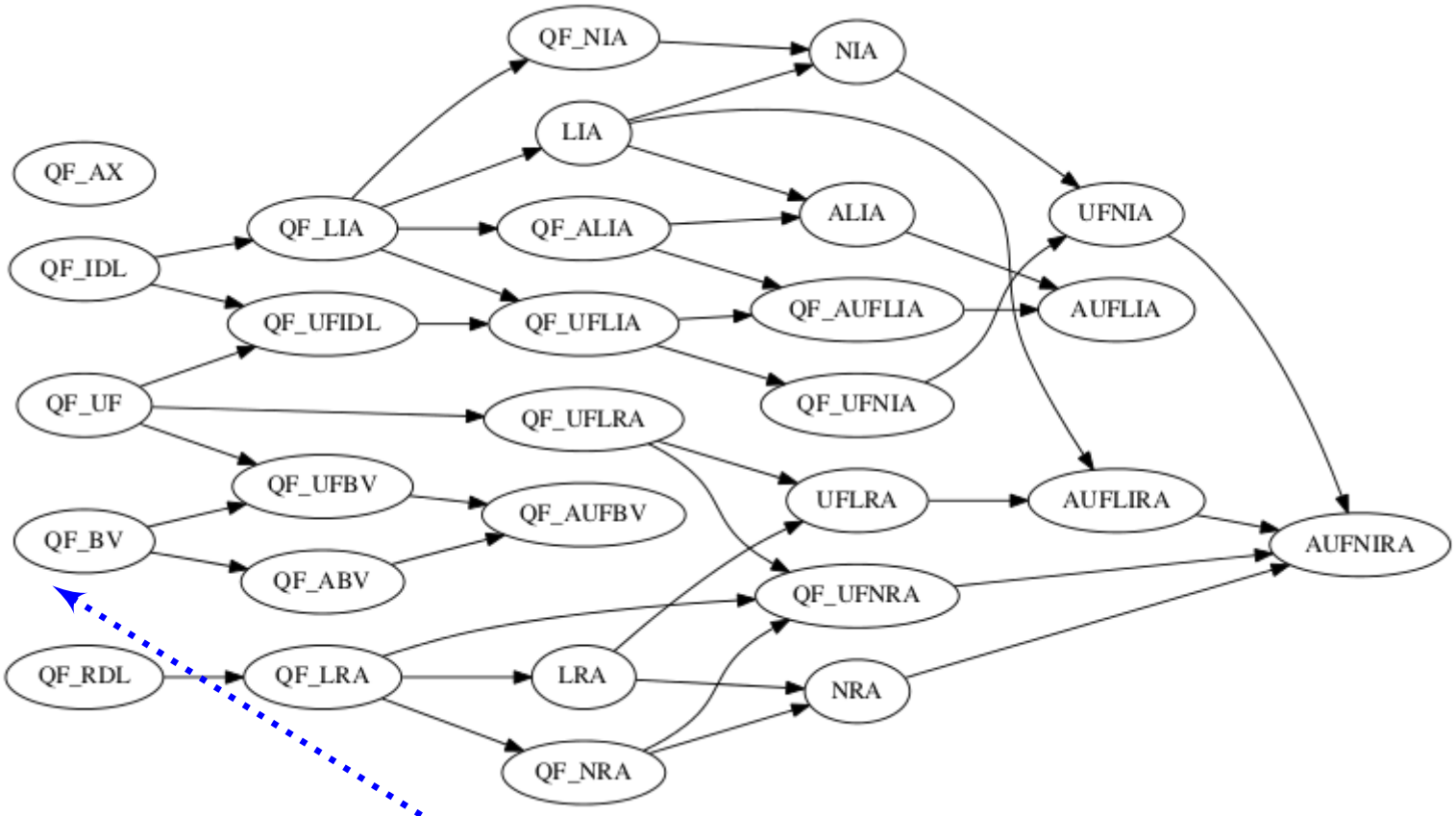

Quantifier-free bit-vector arithmetic

$a + b \geq 0 \wedge (a|b) \leq (a\&b)$

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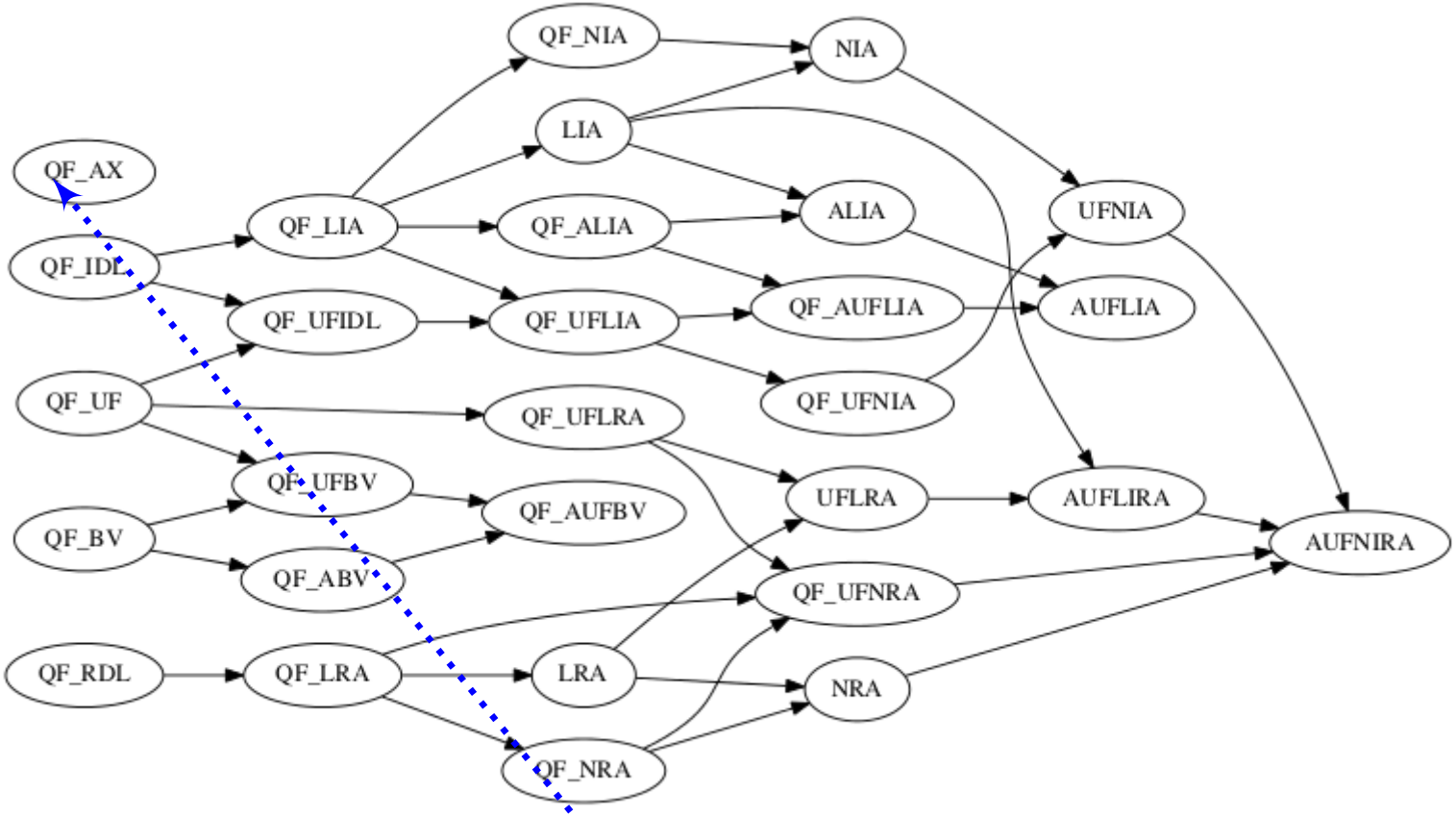

Quantifier-free array theory

$i = j \rightarrow read(write(a, i, v), j) = v$

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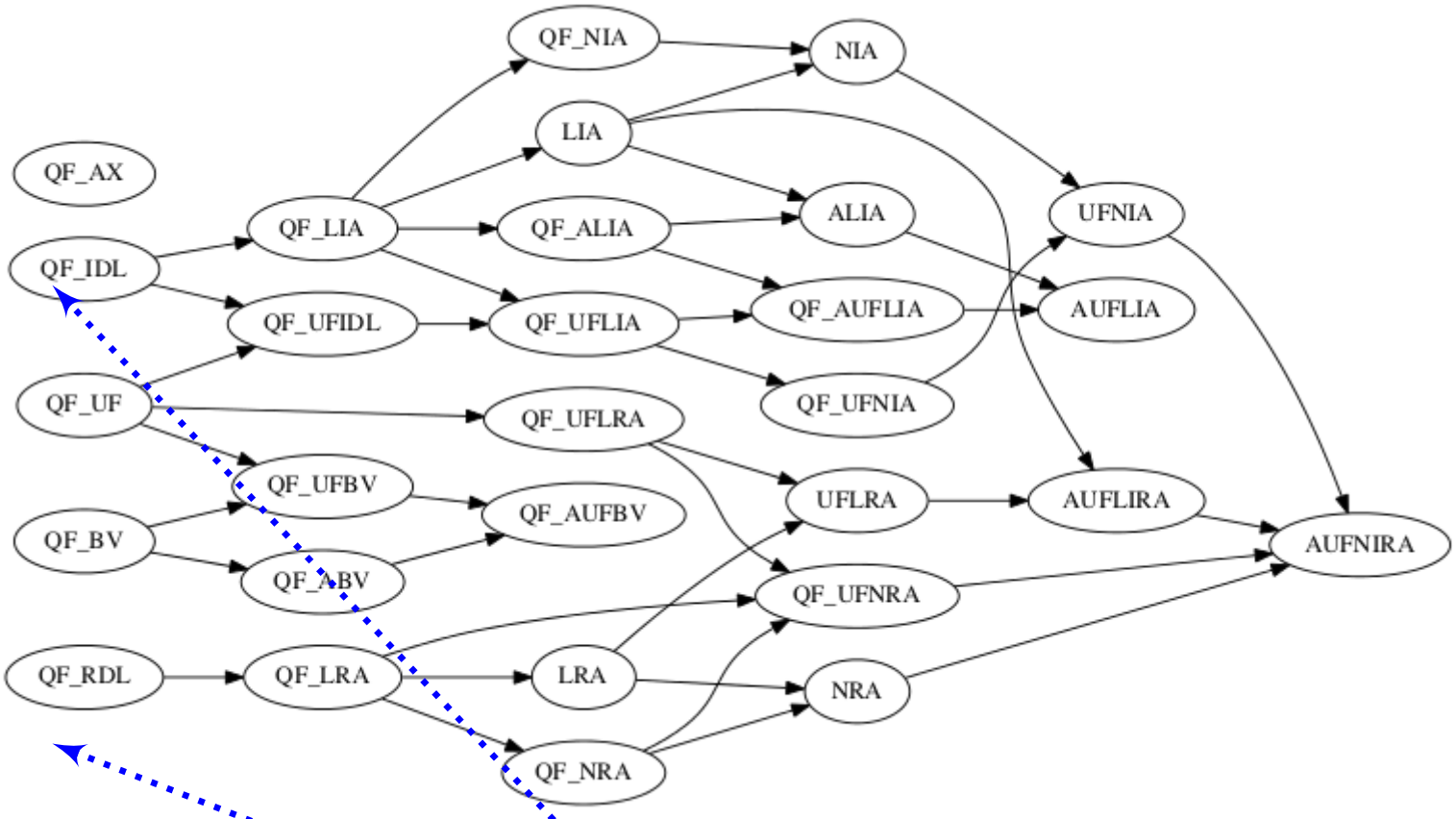

Quantifier-free integer/rational difference logic

$x - y \geq 0 \vee x - z < 0$

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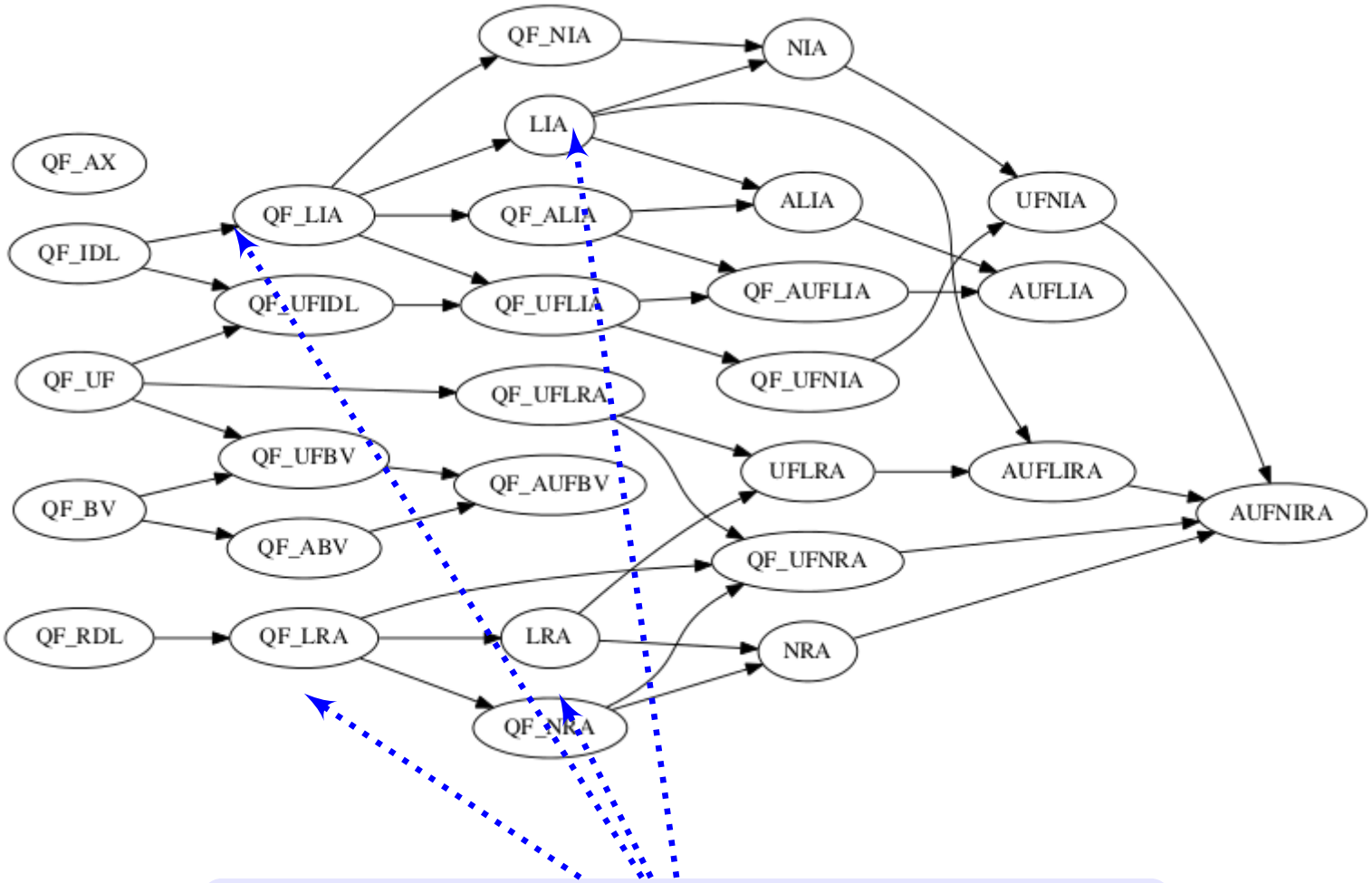

(Quantifier-free) real/integer linear arithmetic

$$4x + 7y = 8 \wedge (y = 0 \vee x > y)$$

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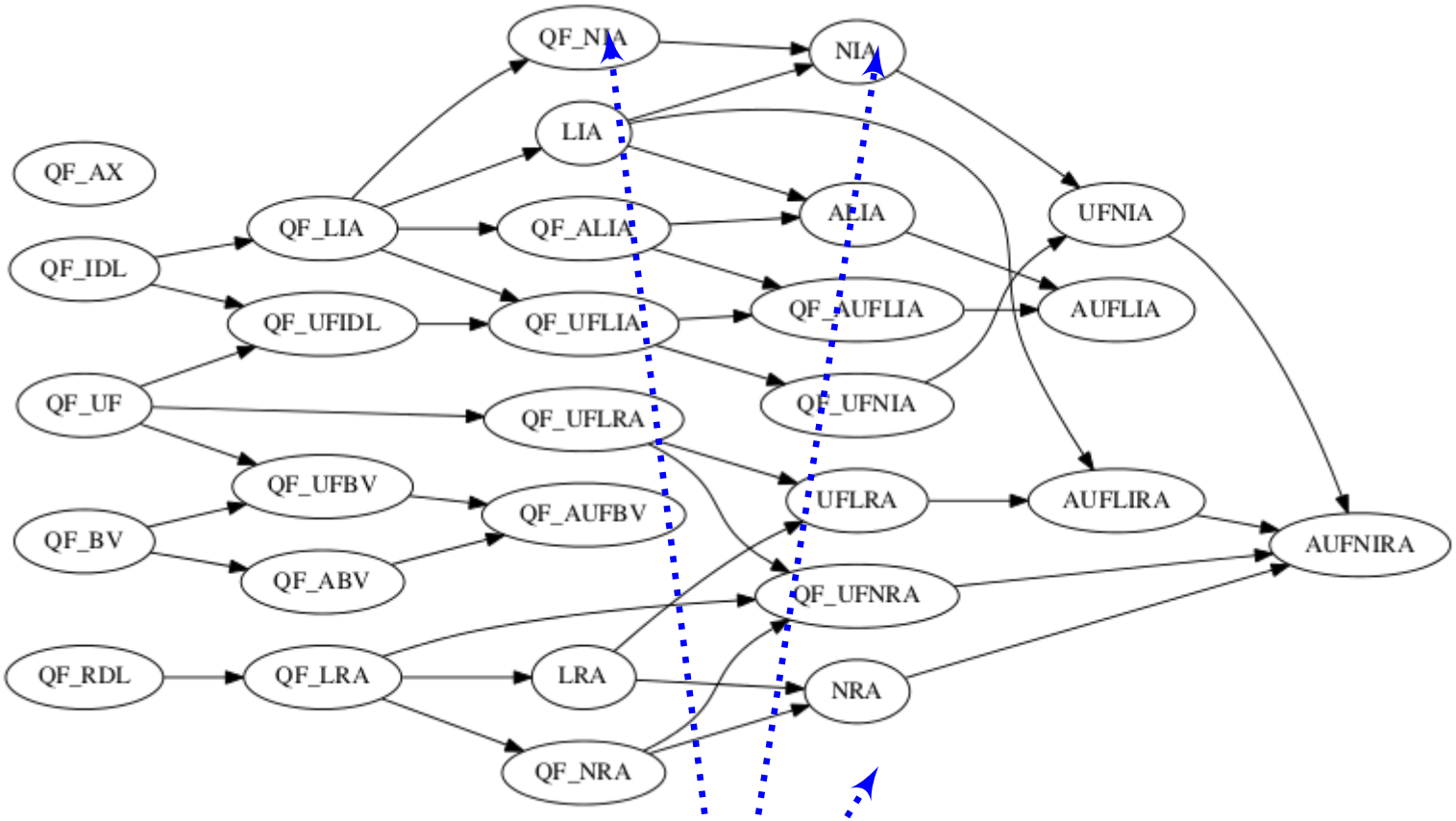

(Quantifier-free) real/integer non-linear arithmetic

$x^2 + 2xy + y^2 > 0 \vee (x \geq 1 \wedge xz + yz^2 = 0)$

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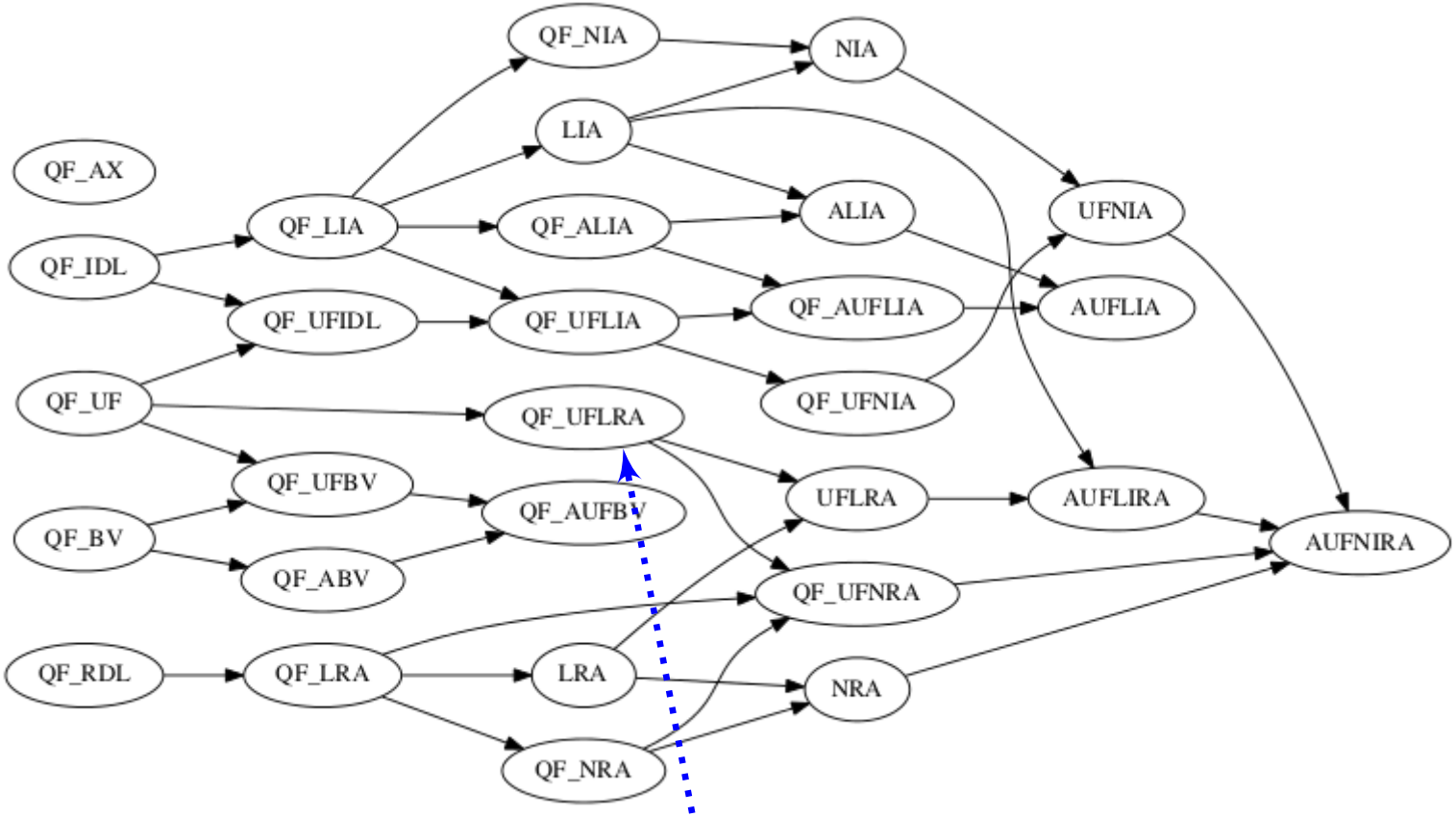

Combined theories

$2f(x) + 5y > 0 \wedge \neg(f(x) = y \vee x + 2y = 0)$

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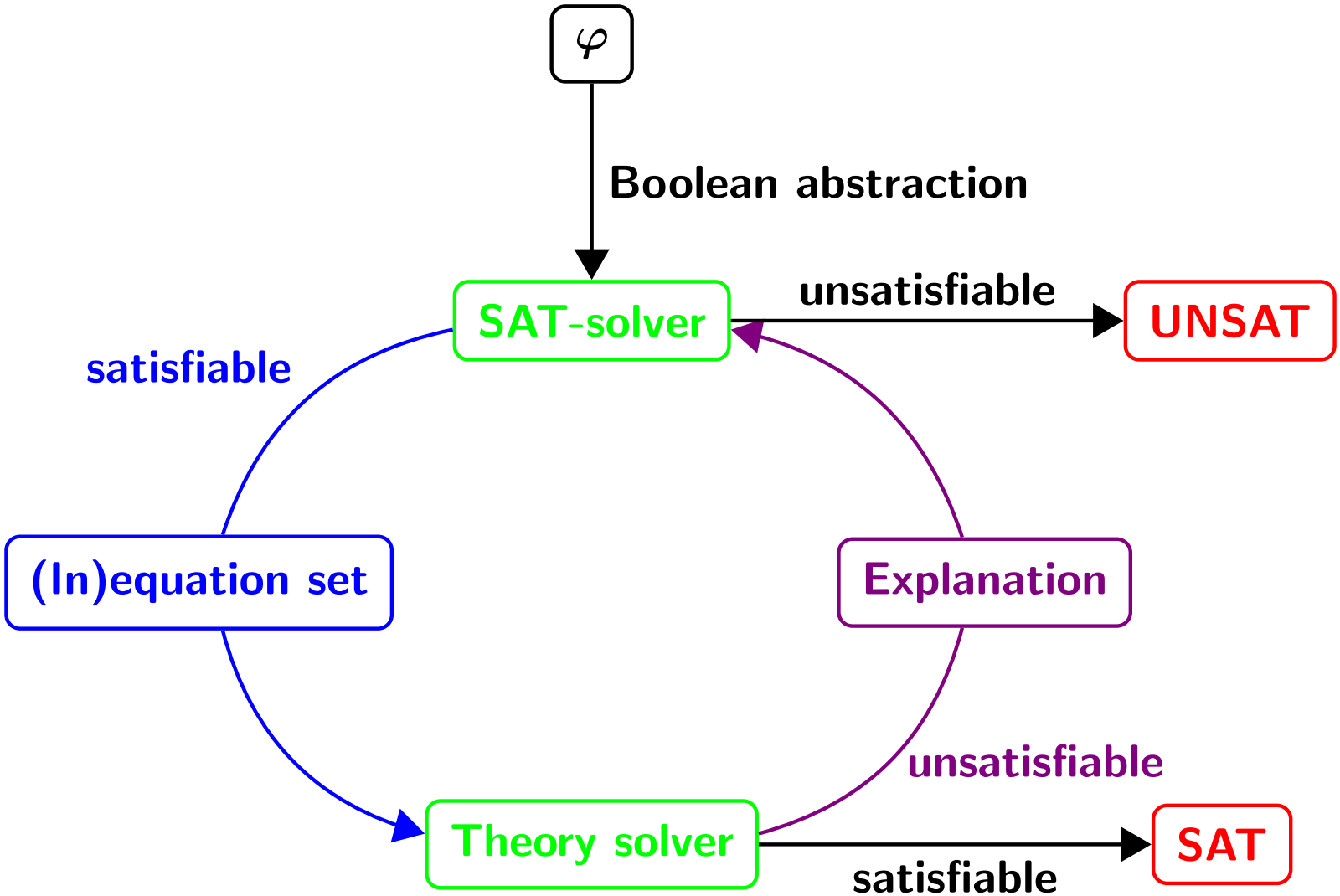
How an extension to SMT solving looks like?

There are basically two different approaches:

- Eager SMT solving transforms logical formulas over some theories into satisfiability-equivalent propositional logic formulas and applies SAT solving. ("Eager" means theory first)
- Lazy SMT solving uses a SAT solver to find solutions for the Boolean skeleton of the formula, and a theory solver to check satisfiability in the underlying theory. ("Lazy" means theory later)

Lazy SMT solving



Running Example

Assume that we have three virtual machines (VMs) which require 100, 50 and 15 GB hard disk respectively. There are three servers with capabilities 100, 75 and 200 GB in that order. Find out a way to place VMs into servers in order to:

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Formalization. Let x_{ij} denote that VM i is placed on the server j and y_j denote that server j is in use.

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Solution. Choosing the suitable underlying theory is determined by the principles of the formalization: $x_{ij}, y_j \in \{0, 1\}$

- linear constraints with integer variables with 0,1 restriction
- linear constraints with real variables with 0,1 restriction
- linear constraints boolean variables

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$$x_{ij} = 0 \vee x_{ij} = 1, \quad \forall i, j = \overline{1,3}$$

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Assume the case: linear constraints with integer variables with 0,1 restriction

- Implicit constraints
  - Variables are integers:

$$x_{ij}, y_j \in \mathbb{Z}, \quad \forall i, j = \overline{1,3}$$

  - Variables have only 0,1 value:

$$x_{ij} = 0 \vee x_{ij} = 1, \quad \forall i, j = \overline{1,3}$$

  - A VM is on exactly one server:

$$x_{i1} + x_{i2} + x_{i3} = 1, \quad \forall i = \overline{1,3}$$

Running Example (cont'd)

Assume that we have three virtual machines (VMs) which require 100, 50 and 15 GB hard disk respectively. There are three servers with capabilities 100, 75 and 200 GB in that order. Find out a way to place VMs into servers in order to:

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  - A used server has at least a VM on it:

$$(y_j \geq x_{1j}) \wedge (y_j \geq x_{2j}) \wedge (y_j \geq x_{3j}), \quad j = \overline{1,3}$$

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- Explicit constraints
  - Capacity constraints:
    $100x_{11} + 50x_{21} + 15x_{31} \leq 100y_1$
    $100x_{12} + 50x_{22} + 15x_{32} \leq 75y_2$
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  - $y_1 + y_2 + y_3$

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Solution approaches.

1. Formalization in SMT-LIB2 format: useful for toy examples, some SMT tools are available online to try their capabilities.

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Is the order of the optimization functions important?

Types of optimization (in Z3)

Single-criteria optimization:
$OMT(\mathcal{LIRA} \cup \mathcal{T})$, $OMT(\mathcal{BV} \cup \mathcal{T})$, $OMT(\mathcal{PB} \cup \mathcal{T})$ and MAXSMT solving [19].

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To the best of our knowledge, in the SMT solver Z3, there are three ways to combine objective functions.

1. lexicographic combinations (by default) variant-int.smt2

Algorithm 3 Sequential algorithm for general objectives

1: **for** $t = 1$ to n **do**
2: Solve the single-objective problem:

$$\begin{aligned} \max \quad & f_t(x) \\ \text{subject to} \quad & x \in X, \\ & f_k(x) \geq z_k \text{ for all } k \in 1, \ldots, t-1. \end{aligned}$$

3: **if** the problem is infeasible or unbounded **then**
4: print "no solution"
5: **else**
6: Add as additional constraints the values of the decision variables x and $f_k(x) = z_t$
7: **end if**
8: **end for**

Types of optimization (in Z3) (cont'd)

2. Boxes are used to specify independent optima subject to given constraints: variant-int-box.smt2

Types of optimization (in Z3) (cont'd)

2. Boxes are used to specify independent optima subject to given constraints: variant-int-box.smt2
3. Pareto optimization involves more than one objective function to be optimized simultaneously. variant-int-pareto.smt2

Programming Z3 (Python API)

- variant-int.py

Programming Z3 (Python API)

- variant-int.py
- variant-bool.py

Feedback Part 1

Please fill out the form!

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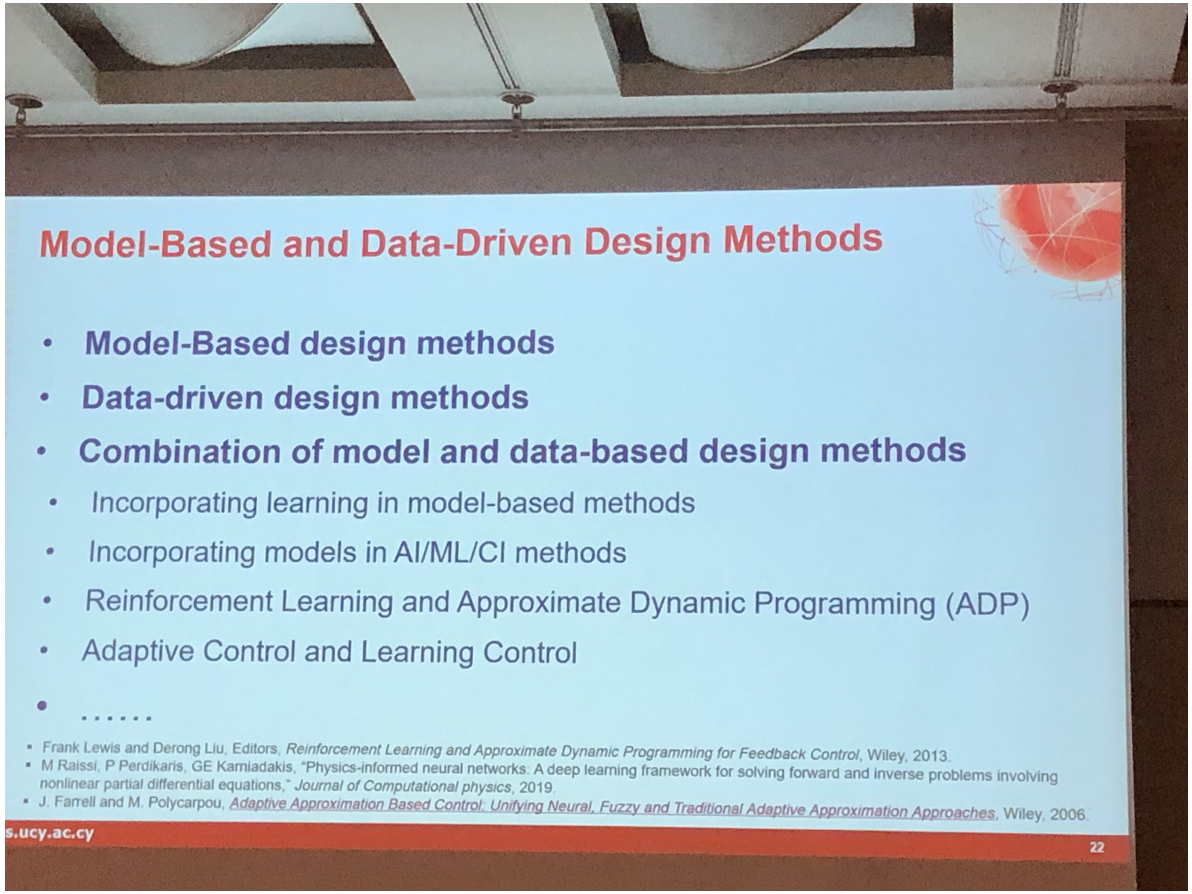

- The data-driven approach focuses on using data to drive the development and improvement of AI systems.
- The model-based approach focuses on developing a mathematical model of the system or process being studied.

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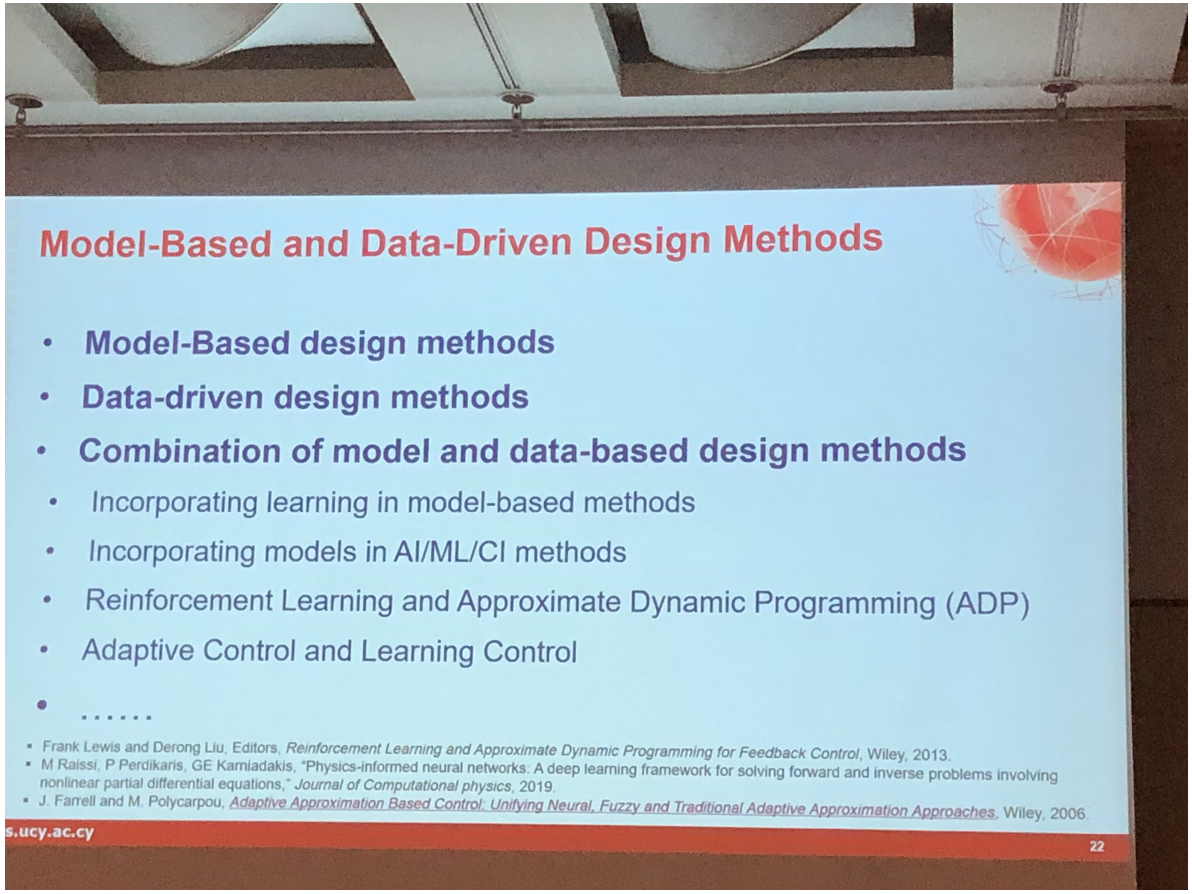
From Marios M. Polycarpou talk



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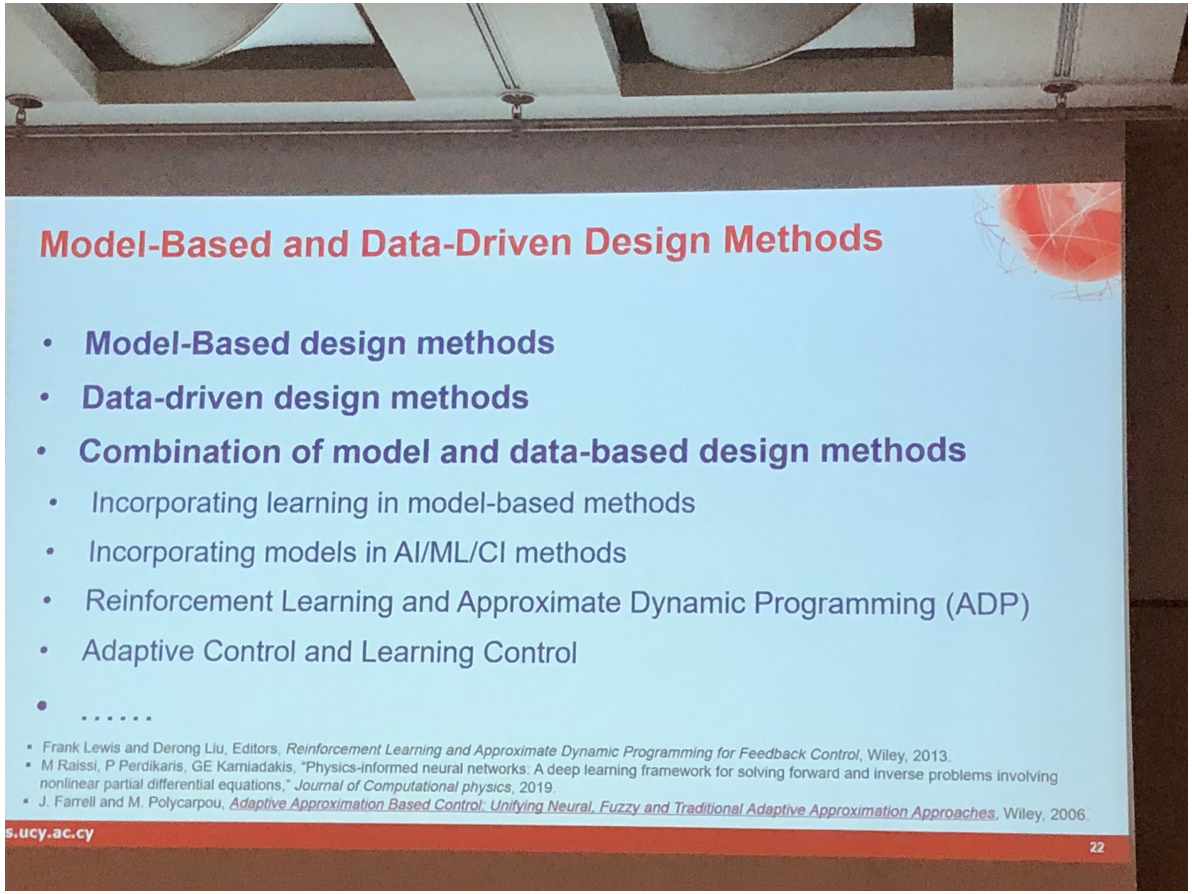

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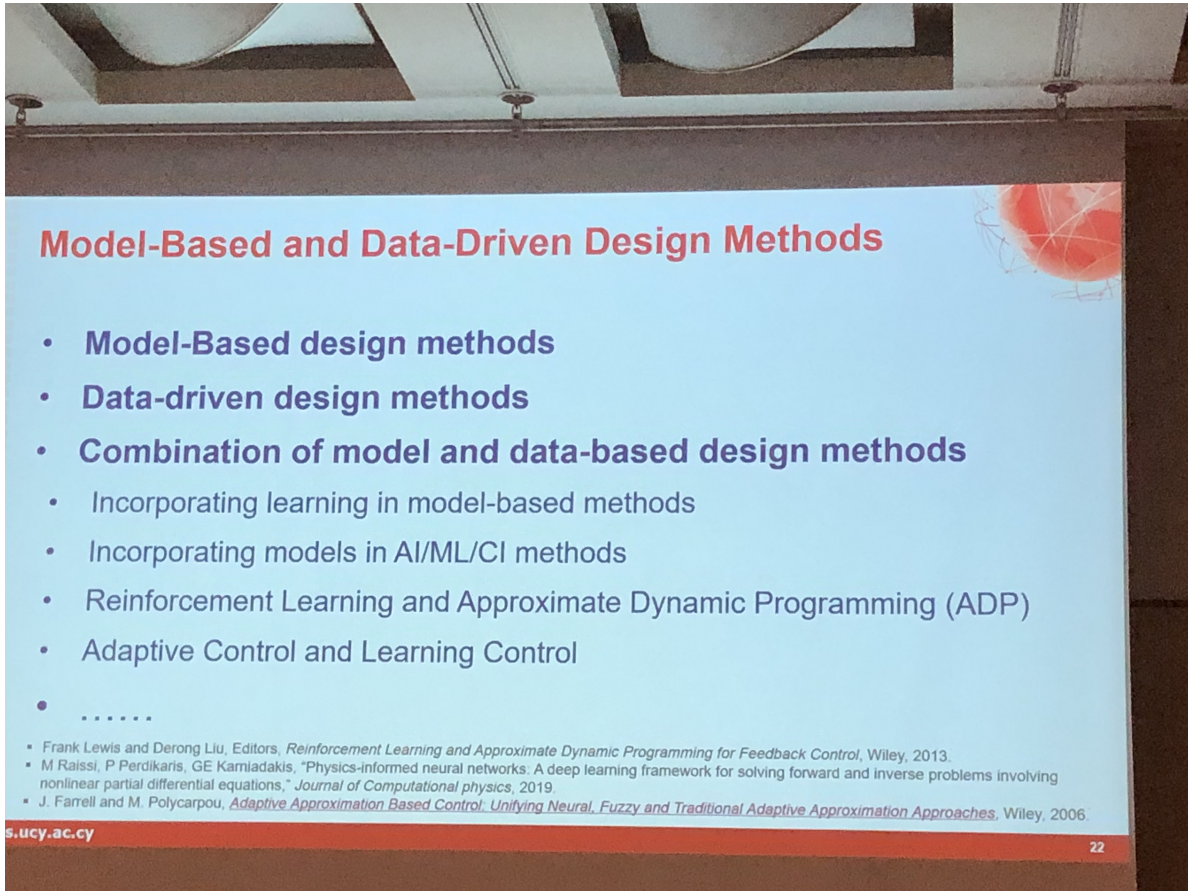

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Motivation (cont'd)

Advent of Cloud computing $\rightsquigarrow$ loosely-coupled architecture $\rightsquigarrow$ DevOps paradigm $\rightsquigarrow$ application modeling $\rightsquigarrow$ optimal deployment

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Automated deployment of component-based applications in the Cloud consists of:

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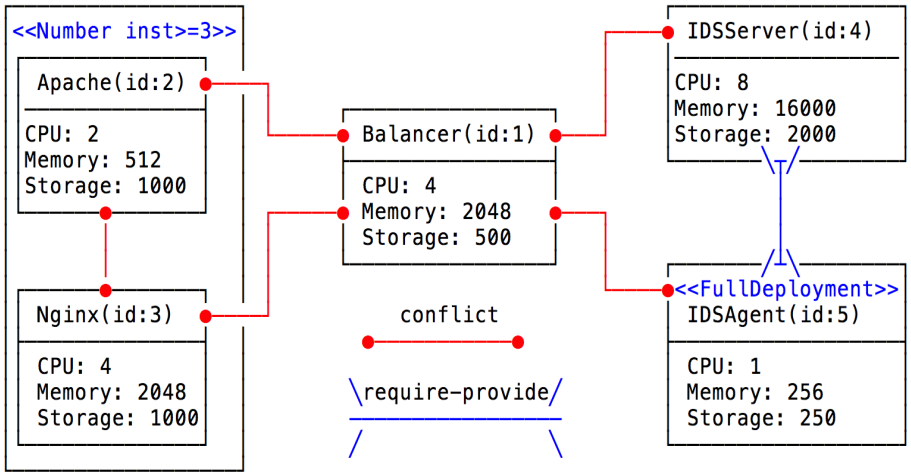
Motivating Example

Problem: finding the best offer for a Secure Web Container



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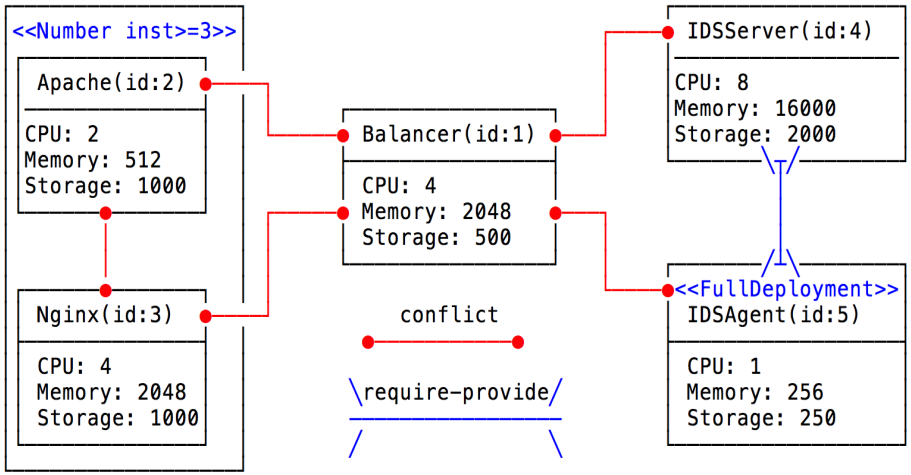

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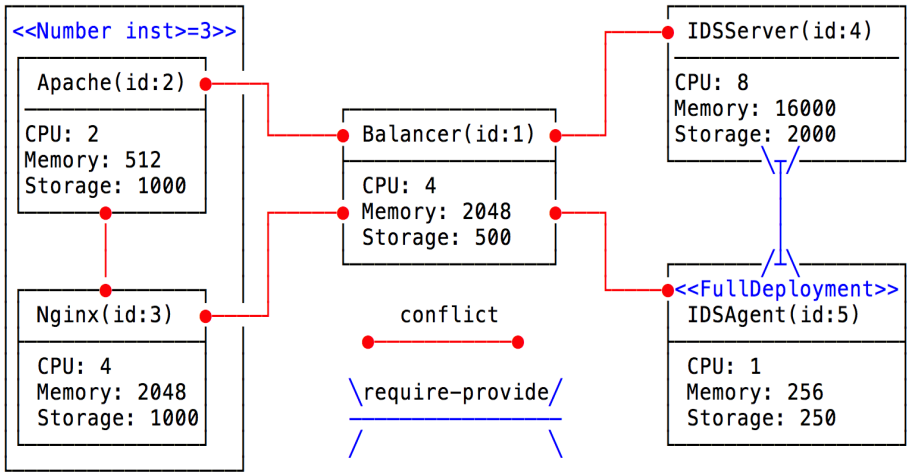

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Motivating Example (cont'd)

Spot Instance Prices

Spot Instances | Defined Duration for Linux | Defined Duration for Windows

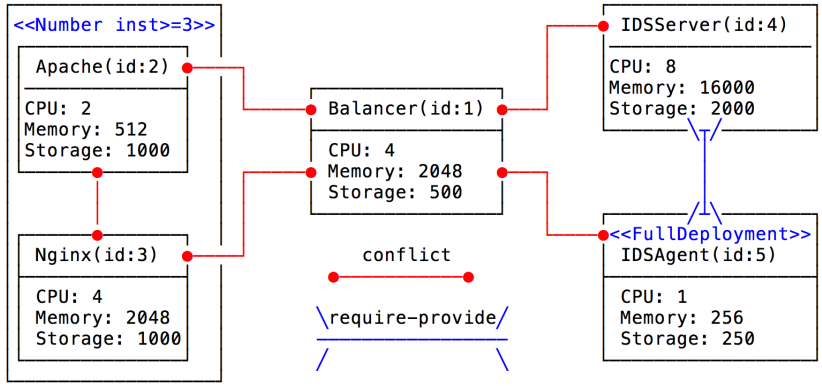
Region: EU (Ireland)

	Linux/UNIX Usage	Windows Usage
General Purpose - Current Generation		
t2.micro	$0.0038 per Hour	$0.0084 per Hour
t2.small	$0.0075 per Hour	$0.0165 per Hour
t2.medium	$0.015 per Hour	$0.033 per Hour
t2.large	$0.0302 per Hour	$0.0582 per Hour
t2.xlarge	$0.0605 per Hour	$0.1015 per Hour
t2.2xlarge	$0.121 per Hour	$0.183 per Hour
m3.medium	$0.0073 per Hour	$0.0633 per Hour
m3.large	$0.0306 per Hour	$0.1226 per Hour
m3.xlarge	$0.0612 per Hour	$0.2452 per Hour

Model	vCPU	CPU Credits / hour	Mem (GiB)	Storage
t2.nano	1	3	0.5	EBS-Only
t2.micro	1	6	1	EBS-Only
t2.small	1	12	2	EBS-Only
t2.medium	2	24	4	EBS-Only
t2.large	2	36	8	EBS-Only
t2.xlarge	4	54	16	EBS-Only
t2.2xlarge	8	81	32	EBS-Only

Remark: [snapshot from https://aws.amazon.com/ec2/] tens of thousands of price offers corresponding to different configurations and zones

Motivating Example (cont'd)



Example solution

- VM_1 (CPU:8, RAM: 15 GB, Storage: 2000 GB, Price: 0.0526 \$/hour): Nginx + IDS Agent
- VM_2 (CPU:4, RAM: 7.5 GB, Storage: 2000 GB, Price: 0.0283 \$/hour): Balancer
- VM_3 (CPU:4, RAM: 30 GB, Storage: 2000 GB, Price: 0.0644 \$/hour): IDSServer
- VM_4 (CPU:4, RAM: 7.5 GB, Storage: 2000 GB, Price: 0.0283 \$/hour): Apache + IDS Agent
- VM_5 (CPU:4, RAM: 7.5 GB, Storage: 2000 GB, Price: 0.0283 \$/hour): Apache + IDS Agent

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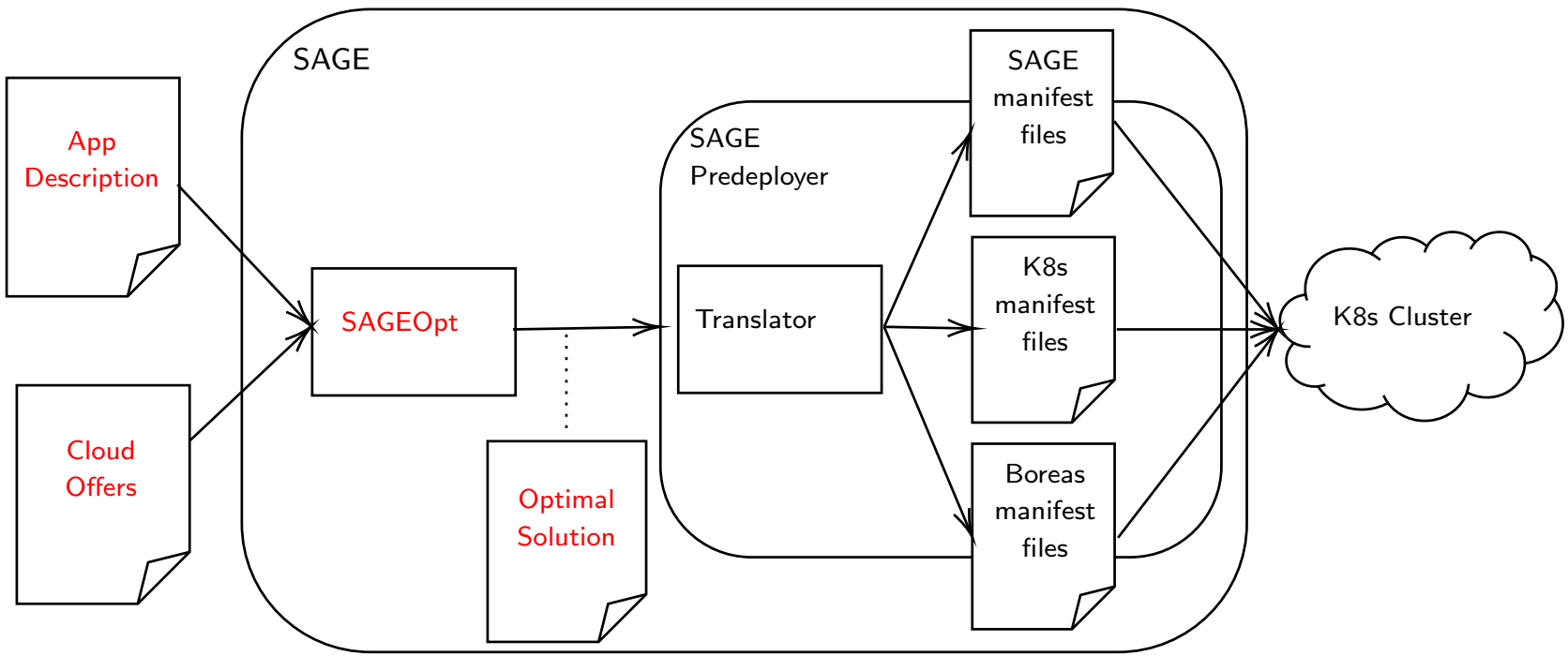

Figure: SAGE General Architecture

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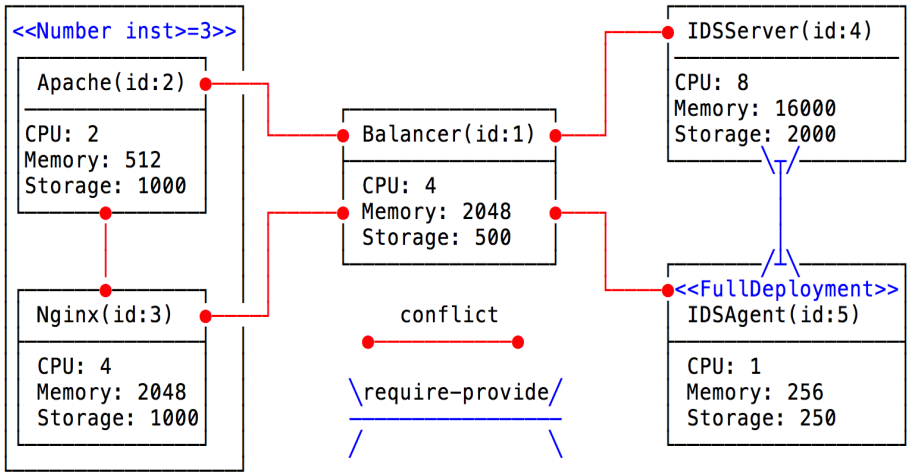

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Model-driven approach: Formulation of the Satisfiability/Optimization Modulo Theory Problem

General constraints

$$
\begin{array}{rll}
\textit{Basic allocation} & \sum_{k=1}^{M} a_{ik} \geq 1 & \forall i = \overline{1, N} \\
\textit{Occupancy} & \sum_{i=1}^{N} a_{ik} \geq 1 \Rightarrow v_k = 1 & \forall k = \overline{1, M} \\
\textit{Capacity} & \sum_{i=1}^{N} a_{ik} \cdot R_i^h \leq F_{t_k}^h & \forall k = \overline{1, M}, \forall h = \overline{1, H} \\
\textit{Link} & v_k{=}1 \wedge t_k{=}o \Rightarrow \bigwedge_{h=1}^{H} \left(r_k^h{=}F_{t_k}^h\right) \wedge p_k{=}P_{t_k} & \forall o = \overline{1, O},\ O \in \mathbb{N}^* \\
 & \sum_{i=1}^{N} a_{ik} = 0 \Rightarrow t_k = 0 & \forall k = \overline{1, M}
\end{array}
$$

where:

- $R_i^h \in \mathbb{N}^*$ is the hardware requirement of type h of the component i;
- $F_{t_k}^h \in \mathbb{N}^*$ is the hardware characteristic h of the VM of type t_k.

Problem Formalization (cont'd)

Application-specific constraints

Conflicts $a_{ik} + a_{jk} \leq 1$ $\quad \forall k = \overline{1, M},\ \forall (i,j)\ \mathcal{R}_{ij} = 1$

Co-location $a_{ik} = a_{jk}$ $\quad \forall k = \overline{1, M},\ \forall (i,j)\ \mathcal{D}_{ij} = 1$

Exclusive deployment

$$\mathcal{H}\left(\sum_{k=1}^{M} a_{i_1 k}\right) + \ldots + \mathcal{H}\left(\sum_{k=1}^{M} a_{i_q k}\right) = 1 \quad \text{for fixed } q \in \{1, \ldots, N\}$$

$$\mathcal{H}(u) = \begin{cases} 1 & u > 0 \\ 0 & u = 0 \end{cases}$$

Require-Provide

$$n_{ij} \sum_{k=1}^{M} a_{ik} \leq m_{ij} \sum_{k=1}^{M} a_{jk} \qquad \forall (i,j) \mathcal{Q}_{ij}(n_{ij}, m_{ij}) = 1$$

$$0 \leq n \sum_{k=1}^{M} a_{jk} - \sum_{k=1}^{M} a_{ik} < n \qquad n, n_{ij}, m_{ij} \in \mathbb{N}^*$$

where:

- $\mathcal{R}_{ij} = 1$ if components i and j are in conflict (can not be placed in the same VM);
- $\mathcal{D}_{ij} = 1$ if components i and j must be co-located (must be placed in the same VM);
- $\mathcal{Q}_{ij}(n, m)$=1 if C_i requires at least n instances of C_j and C_j can serve at most m instances of C_i

Problem Formalization (cont'd)

Application-specific constraints

$$\textit{Full deployment} \quad \sum_{k=1}^{M} \left(a_{ik} + \mathcal{H} \left(\sum_{j, \mathcal{R}_{ij}=1} a_{jk} \right) \right) = \sum_{k=1}^{M} v_k$$

Deployment with *bounded number of instances*

$$\sum_{i \in \overline{C}} \sum_{k=1}^{M} a_{ik} \langle \text{op} \rangle n \qquad |\overline{C}| \leq N,\ \langle \text{op} \rangle \in \{=, \leq, \geq\},\ n \in \mathbb{N}$$

Find:

- assignment matrix a with binary entries $a_{ik} \in \{0, 1\}$ for $i = \overline{1, N}$, $k = \overline{1, M}$, which are interpreted as follows:

$$a_{ik} = \begin{cases} 1 & \text{if } C_i \text{ is assigned to } V_k \\ 0 & \text{if } C_i \text{ is not assigned to } V_k. \end{cases}$$

- the type selection vector t with integer entries t_k for $k = \overline{1, M}$, representing the type (from a predefined set) of each VM leased.

Such that: the leasing price is minimal $\sum_{k=1}^{M} v_k \cdot p_k$

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The first step in solving the edge classification problem is to model it as graph data.

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- to $[0, 1]$ is needed in order to prevent one feature from dominating while preserving min-max relationships, crucial for prediction algorithms
- is needed for the hardware specifications/requirements and the VM price.

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Edge classification

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The task is to implement a GNN model in order to predict the type (linked/unlinked) for all the edges.

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1. Generate the dataset which is used to train a GNN model of the application to be deployed. This dataset, representing optimal deployment plans, is obtained by multiple runs of the exact solver previously developed by us.

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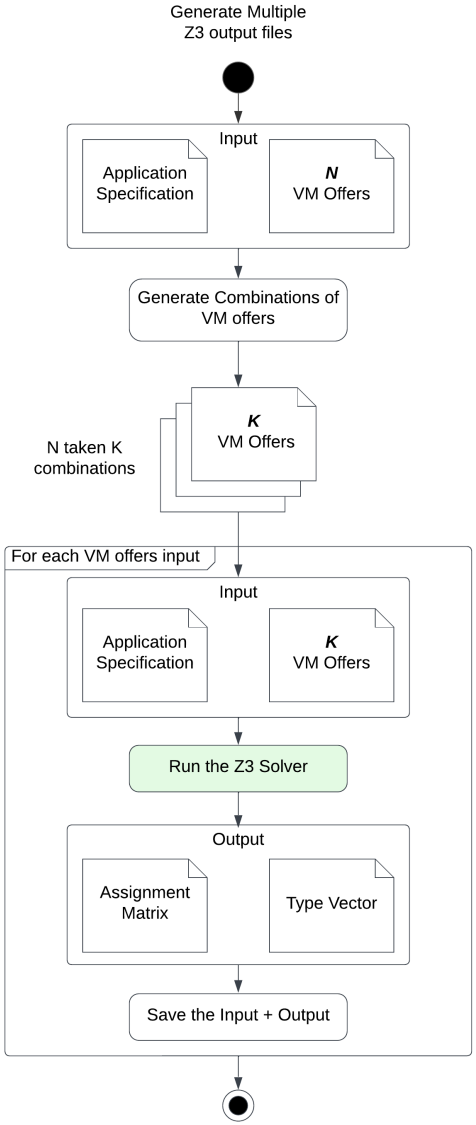
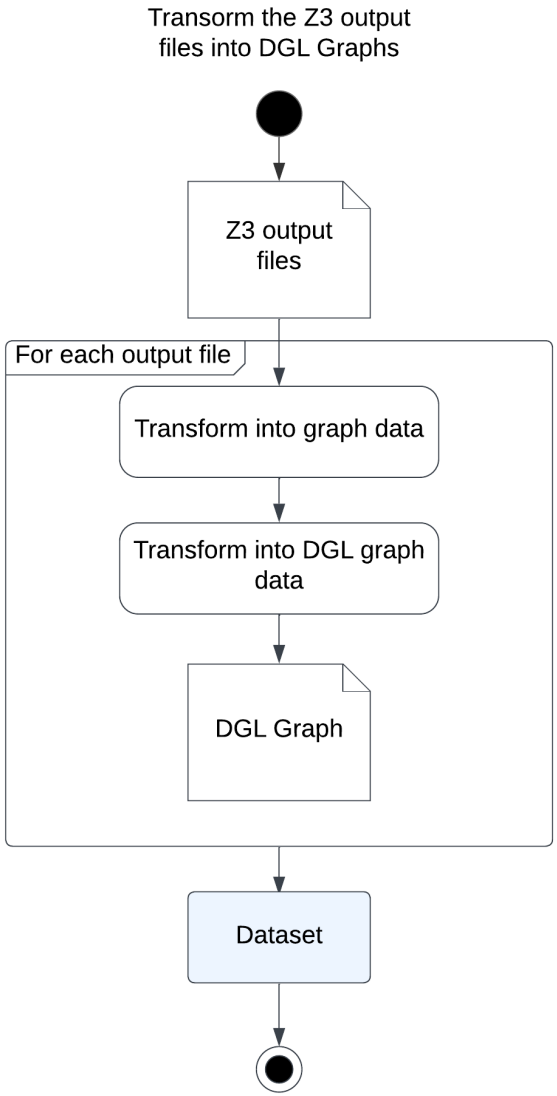
Solution

1. Generate the dataset which is used to train a GNN model of the application to be deployed. This dataset, representing optimal deployment plans, is obtained by multiple runs of the exact solver previously developed by us.
2. Train a GNN model which *predicts* the assignments of components to VMs as well as the VM Offers.
3. Transform the predictions into *soft constraints* to guide the search exploration of the Base solver towards an optimal solution.

Dataset generation

Large dataset to train the model $\binom{20}{15} \approx 15000$ different VM Offers inputs.





Training a GNN model for edge classification

Supervised GNN learning approach:

Training a GNN model for edge classification

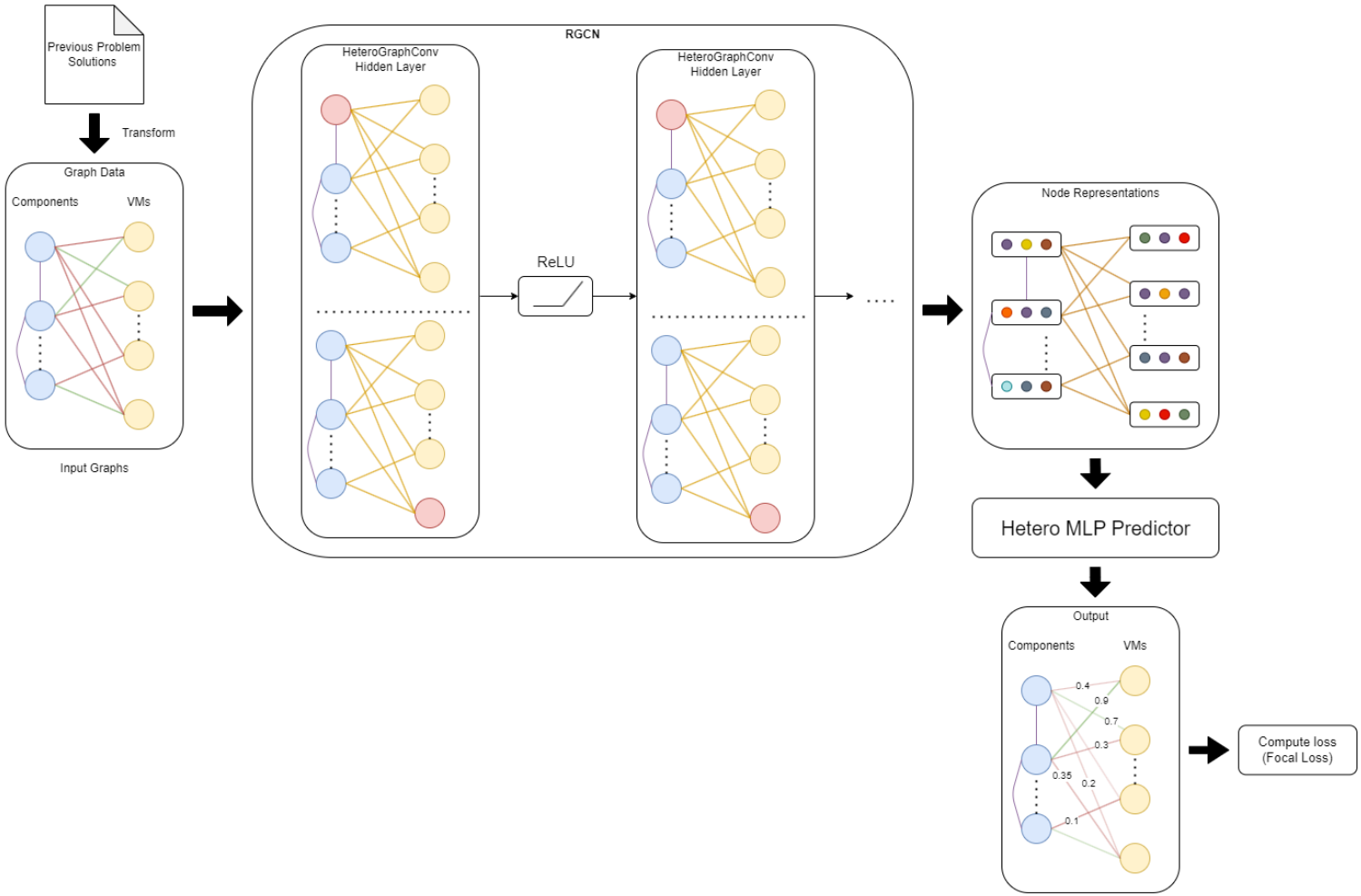
Supervised GNN learning approach:

1. Data Preparation: graph representation and nodes and edges feature extraction.
2. Graph Construction: application graph's structure (nodes, edges, and their relationships)

Training a GNN model for edge classification

Supervised GNN learning approach:

3. Choosing Model Architecture which allows heterogeneity modeling and edge classification.



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   - train, test, validation: $60\%, 20\%, 20\%$

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   - batch size $= 50$

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#	Sample Size	#Ep	Acc	Time	Pred. $\mathbb{T}$ Links	Pred. $\mathbb{F}$ Links	GT True Links
3	50	200	0.95	21.36	7	10	8
7	100	100	0.95	21.92	7	13	
11	100	400	0.95	87.92	8	13	

Integrated GNN and Exact Techniques: Experimental Results

- the scalability of the GNN approach for increasing number of VM offers, possibly previously unseen (see table), and

Integrated GNN and Exact Techniques: Experimental Results

- the scalability of the GNN approach for increasing number of VM offers, possibly previously unseen (see table), and
- the generalization of the GNN approach for applications characterized by similar constraints between components but with different hardware requirements (see the paper [9]).

Experimental Analysis (cont'd)

Explanation of the FV symmetry breaker

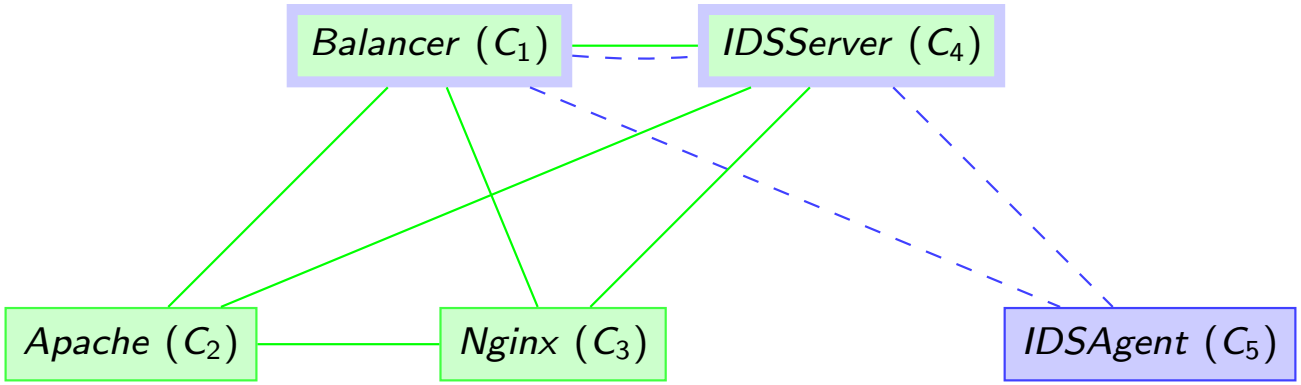


Figure: Secure Web Container conflict graph. The components with green background belong to the clique $\overline{G}$.

	VM_1	VM_2	VM_3	VM_4	VM_5	VM_6
C_1	1	0	0	0	0	0
C_2	0	0	1	0	1	0
C_3	0	0	0	1	0	0
C_4	0	1	0	0	0	0
C_5	0	0	1	1	1	0

Table: Effect of FV symmetry breaking strategy

Integrated GNN and Exact Techniques: Experimental Results

- the scalability of the GNN approach for increasing number of VM offers, possibly previously unseen (see table). Base = Z3

#o	Solver	Model#3	Model#7	Model#11	Opt. Price
20	Base		0.24		3.759
	Base+FVPR		0.11		
	Base+GNN	0.12	0.12	0.07	
	Base+FVPR+GNN	0.12	0.09	0.10	
40	Base		0.54		2.676
	Base+FVPR		0.27		
	Base+GNN	0.28	0.33	0.28	
	Base+FVPR+GNN	0.29	0.28	0.29	
250	Base		2.82		1.622
	Base+FVPR		0.98		
	Base+GNN	0.76	0.77	1	
	Base+FVPR+GNN	1.40	1.39	1.15	
500	Base		8.71		1.582
	Base+FVPR		2.42		
	Base+GNN	4.56	2.92	1.5	
	Base+FVPR+GNN	3.09	3	3.01	
27	Base		0.26		2.400
	Base+FVPR		0.09		
	Base+GNN	0.10	0.14	0.14	
	Base+FVPR+GNN	0.10	0.10	0.07	

Experimental Analysis (cont'd)

Using the GNN Prediction as Soft Constraints

Formalization of the assignment predictions as a binary 3D tensor *pred* with $pred_{iko} \in \{0, 1\}$ for $i = \overline{1, N}$, $k = \overline{1, M}$ and $o = \overline{1, O}$:

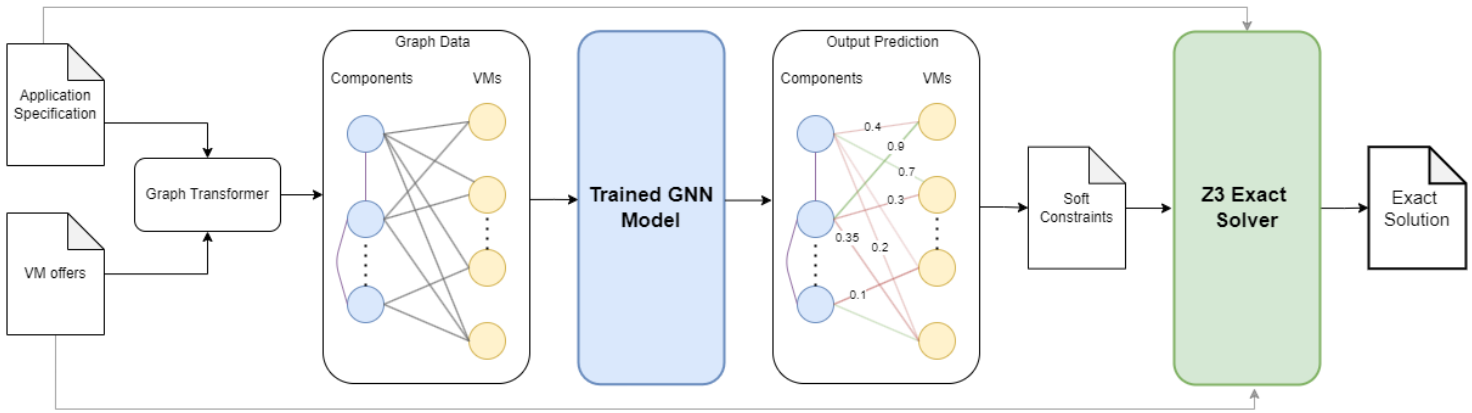
$$pred_{iko} = \begin{cases} 1 & \text{if } C_i \text{ is assigned to } V_j \text{ of type } O_o \\ 0 & \text{if } C_i \text{ is not assigned to } V_j \text{ of type } O_o \end{cases}$$

From tensors to soft constraints

$$\exists o \in \overline{1, O} \text{ s.t. } pred_{iko} = 1 \implies a_{ik} = 1 \wedge \bigwedge_{h=1}^{H} \left(r_k^h = F_o^h \right) \wedge p_k = P_o$$

$$\nexists o \in \overline{1, O} \text{ s.t. } pred_{iko} = 1 \implies a_{ik} = 0$$

Diagram describing the integration of the GNN model with the Base solver



Experimental Analysis (cont'd)

Using the GNN Prediction as Soft Constraints The *pred* tensor for the *first component* of the Secure Web Container application, generated from running the GNN model prediction on the case study application with 10 VM offers, looks like:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

where $M = 6$ rows and $O = 10$ columns.
The corresponding soft constraints are:

- for assignment matrix a:

```
(assert-soft (= a11 0))    (assert-soft (= a13 1))    (assert-soft (= a15 0))
(assert-soft (= a12 1))    (assert-soft (= a14 1))    (assert-soft (= a16 0))
```

- for type vector t:

```
(assert-soft (and (= PriceProv2 8.403)...))
(assert-soft (and (= PriceProv3 8.403)...))
(assert-soft (and (= PriceProv4 0.093)...))
```

where the predictions obtained for the VM offers type were $t_2 = 7$, $t_3 = 7$, $t_4 = 5$. For example, the VM Offer 5 has the specification $(1, 3750, 1000, 0.093)$.

Experimental Analysis (cont'd)

Implementation of soft constraints in Z3 optimization

Optimization in Z3:

1. If the soft constraints are added before the optimization function, then the solver tries to satisfy as many as possible and will use the intermediate results for the optimization function (multi-criterial optimization with lexicographic option by default). $\rightsquigarrow$ hence the soft constraints might destry the actual optimim

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Pseudo-Boolean constraint

A linear *pseudo-Boolean constraint* has the form: $\sum_j a_i l_j \triangleright b$ where a_i and b are integer constants, l_j are literals and $\triangleright$ is a relational operator.

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A *cardinality constraint* is a constraint on the number of literals which are true among a given set of literals.

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Cardinality Constraint

A *cardinality constraint* is a constraint on the number of literals which are true among a given set of literals.

In our case: `atmost(`k`,` $\{x_1, x_2, ..., x_n\}$`)` is true if and only if at most k literals among $x_1, x_2, ..., x_n$ are true.

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- Investigate better the timings of Base+GNN and Base+FV+GNN on this use case and others.
- Investigate the characteristics of the datasets.
- Improve the GNN model.
- New case studies, from different application domains.

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