Machine learning in Combinatorial Optimization

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Combinatorial Optimization problem

A combinatorial optimization problem A is a quadruple (I, f, m, g), where:

- I is a set of instances;
- given an instance $x \in I$, $f(x)$ is the finite set of feasible solutions;
- given an instance x and a feasible solution y of x, $m(x, y)$ denotes the measure of y, which is usually a positive real.
- g is the goal function, and is either $\min$ or $\max$.

The goal is then to find for some instance x an <u>optimal solution</u>, that is, a feasible solution y with

$$m(x, y) = g\{m(x, y') | y' \in f(x)\}$$

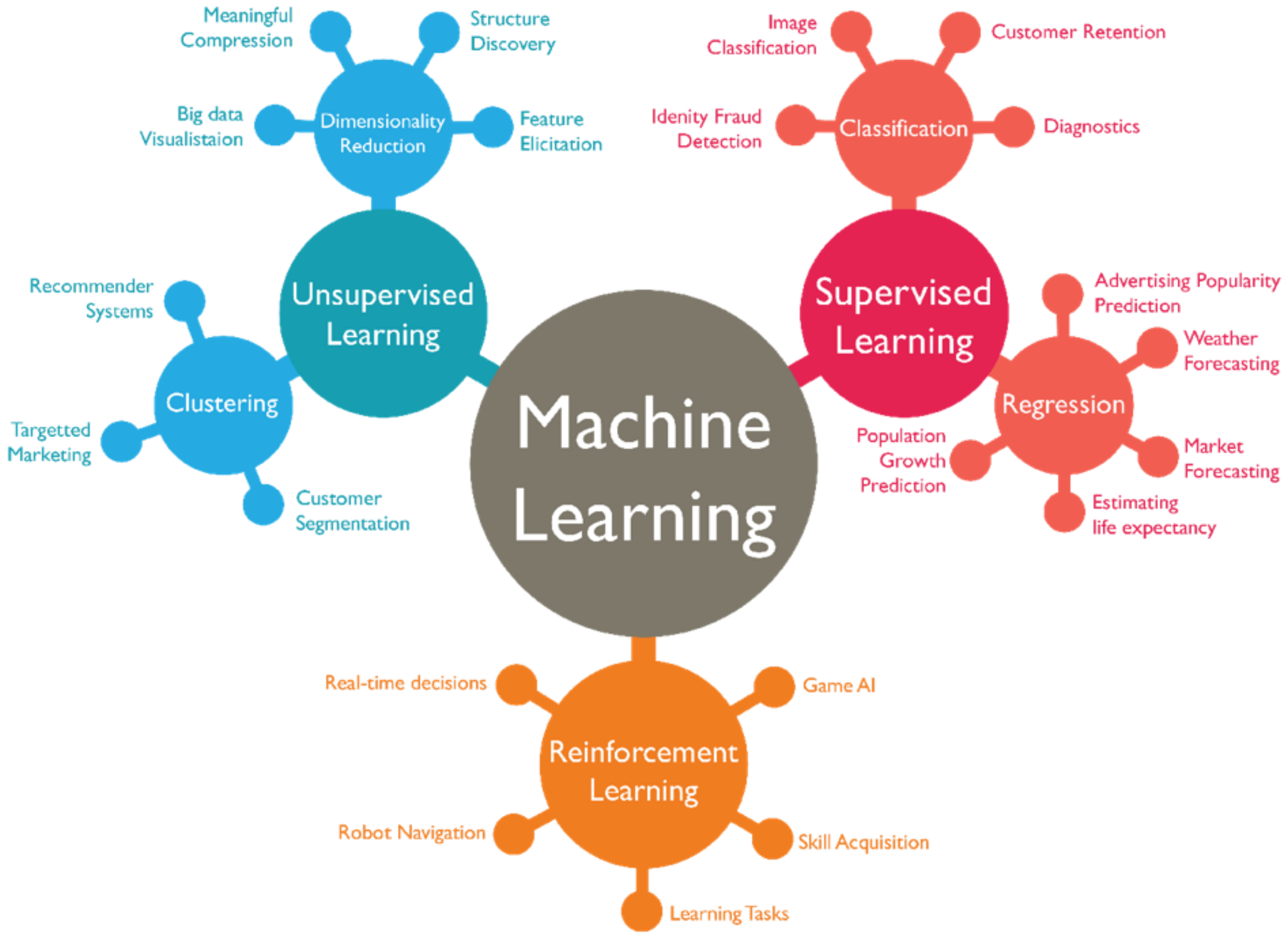
Without loss of generality, any CO problem can be formulated as a constrained min-optimization program.

Machine Learning

“Field of study that gives computers the ability to learn without being explicitly programmed.”
Machine learning definition by Arthur Samuel.

Machine learning approaches:

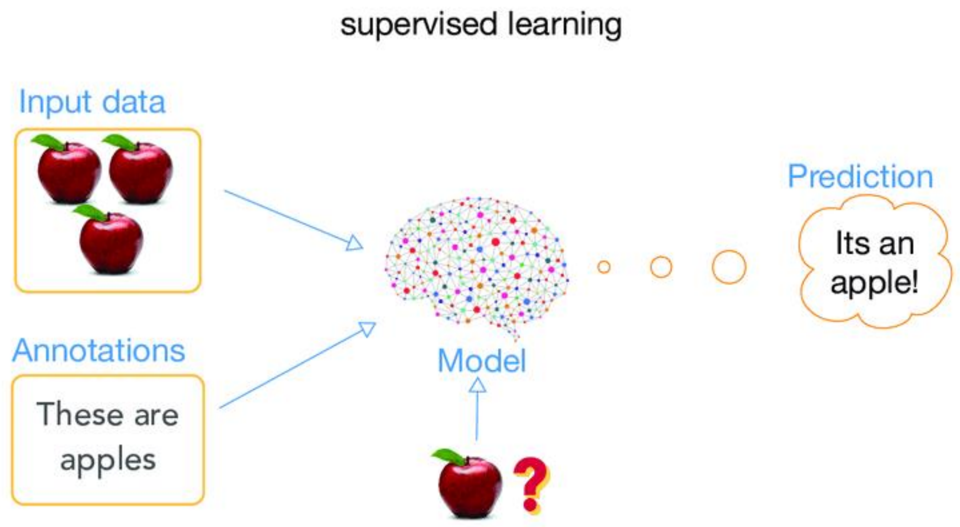
- Supervised learning
- Unsupervised learning
- Reinforcement learning



Supervised vs Unsupervised learning

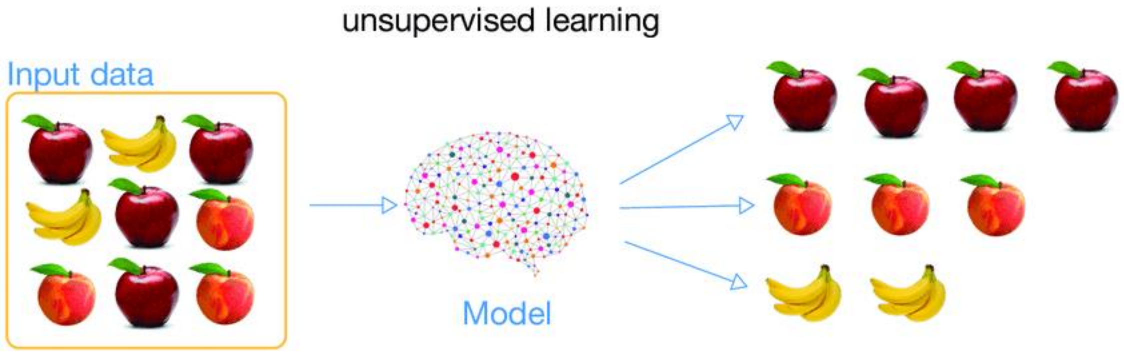
Supervised learning

a set of input (features) / target pairs is provided and the task is to find a function that for every input has a predicted output as close as possible to the provided target.



Unsupervised learning

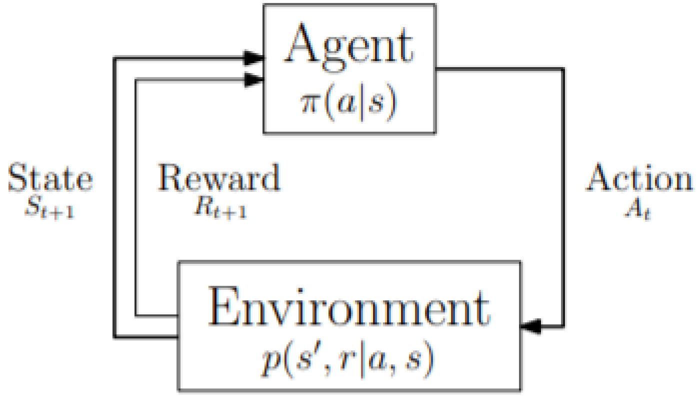
one does not have targets for the task one wants to solve, but rather tries to capture some characteristics of the joint distribution of the observed random variables.



Reinforcement learning

Reinforcement learning

an agent interacts with an environment through a Markov decision process (MDP) in order to maximize the notion of cumulative reward.



MDP

Discrete-time Markov chain

a sequence of random variables $X_1, X_2, X_3, \ldots$ with the Markov property:

$$\Pr(X_{n+1} = x | X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n) = \Pr(X_{n+1} = x | X_n = x_n)$$

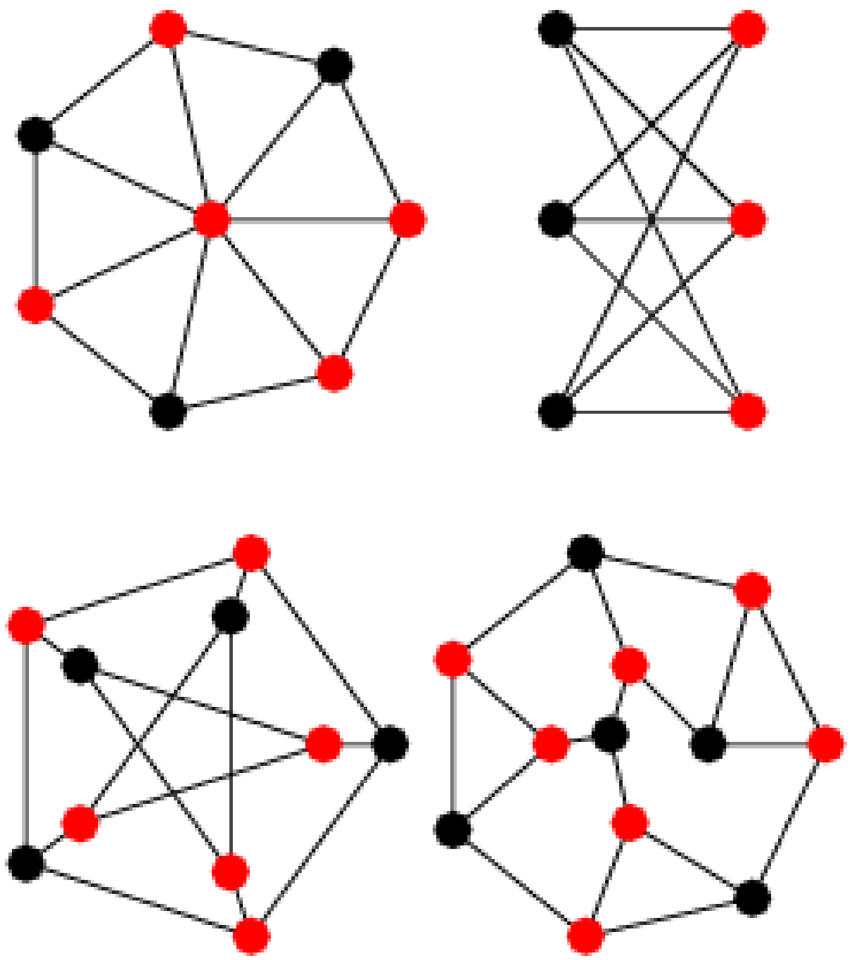
Heuristic

is any approach to problem solving or self-discovery that employs a practical method that is not guaranteed to be optimal, perfect, or rational, but is nevertheless sufficient for reaching an immediate, short-term goal or approximation. Where finding an optimal solution is impossible or impractical, heuristic methods can be used to speed up the process of finding a satisfactory solution.

Minimum Vertex Cover (MVC)

Minimum Vertex Cover

Given a graph G, find a subset of nodes $S \subseteq V$ such that every edge is covered, i.e. $(u, v) \in E \Leftrightarrow u \in S$ or $v \in S$, and $|S|$ is minimized.



MVCApprox iteratively selects an uncovered edge and adds both of its endpoints.
MVCApprox-Greedy, that greedily picks the uncovered edge with maximum sum of degrees of its endpoints.

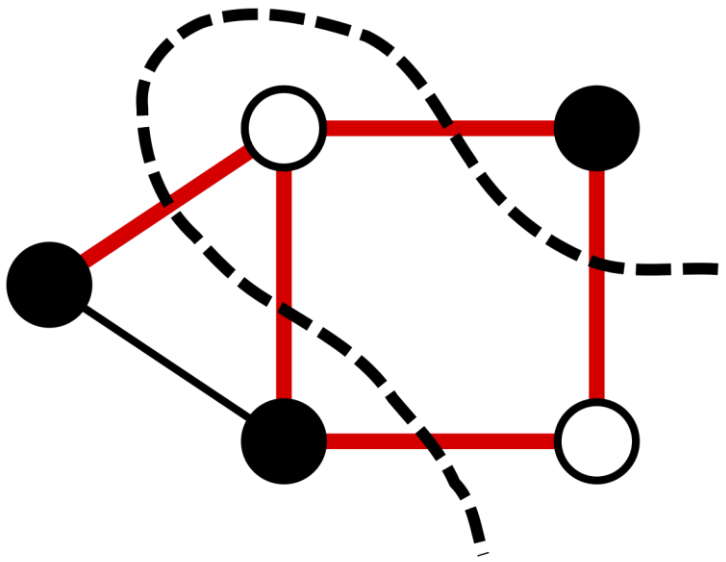
Instance	OPT	S2V-DQN	MVCApprox	MVCApprox-Greedy
full MemeTracker graph	473	**474**	666	578
Approx. ratio	1	**1.002**	1.408	1.222

Maximum Cut (MAXCUT)

Maximum Cut

Given a graph G, find a subset of nodes $S \subseteq V$ such that the weight of the cut-set $\sum_{(u,v)\in C} w(u,v)$ is maximized, where cut-set $C \subseteq E$ is the set of edges with one end in S and the other end in $V \backslash S$.

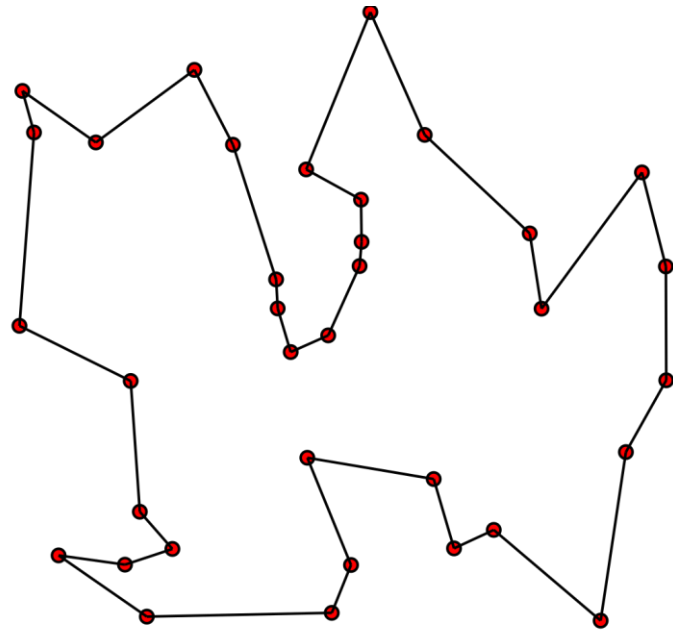
MaxcutApprox, which maintains the cut set $(S, V\backslash S)$ and moves a node from one side to the other side of the cut if that operation results in cut weight improvement. To make MaxcutApprox stronger, we greedily move the node that results in the largest improvement in cut weight.



Instance	OPT	S2V-DQN	MaxcutApprox	SDP
G54100	110	**108**	80	54
G54200	112	**108**	90	58
G54300	106	**104**	86	60
G54400	114	**108**	96	56
G54500	112	**112**	94	56
G54600	110	**110**	88	66
G54700	112	**108**	88	60
G54800	108	**108**	76	54
G54900	110	**108**	88	68
G5410000	112	**108**	80	54
Approx. ratio	1	**1.02**	1.28	1.90

Travelling Salesman Problem

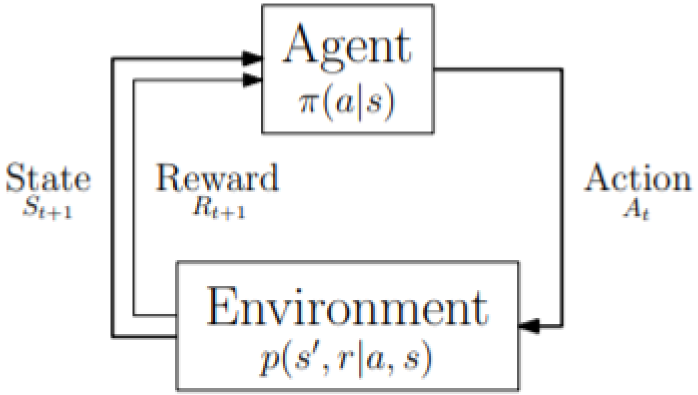
asks the following question: "Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?"



Instance	OPT	S2V-DQN	Farthest	2-opt	Cheapest	Christofides	Closest	Nearest	MST
eil51	426	**439**	467	446	494	527	488	511	614
berlin52	7,542	**7,542**	8,307	7,788	9,013	8,822	9,004	8,980	10,402
st70	675	**696**	712	753	776	836	814	801	858
eil76	538	**564**	583	591	607	646	615	705	743
pr76	108,159	**108,446**	119,692	115,460	125,935	137,258	128,381	153,462	133,471
rat99	1,211	**1,280**	1,314	1,390	1,473	1,399	1,465	1,558	1,665
kroA100	21,282	**21,897**	23,356	22,876	24,309	26,578	25,787	26,854	30,516
kroB100	22,141	**22,692**	23,222	23,496	25,582	25,714	26,875	29,158	28,807
kroC100	20,749	**21,074**	21,699	23,445	25,264	24,582	25,640	26,327	27,636
kroD100	21,294	22,102	**22,034**	23,967	25,204	27,863	25,213	26,947	28,599
kroE100	22,068	22,913	23,516	**22,800**	25,900	27,452	27,313	27,585	30,979
rd100	7,910	**8,159**	8,944	8,757	8,980	10,002	9,485	9,938	10,467
eil101	629	**659**	673	702	693	728	720	817	847
lin105	14,379	**15,023**	15,193	15,536	16,930	16,568	18,592	20,356	21,167
pr107	44,303	**45,113**	45,905	47,058	52,816	49,192	52,765	48,521	55,956
pr124	59,030	**61,623**	65,945	64,765	65,316	64,591	68,178	69,297	82,761
bier127	118,282	**121,576**	129,495	128,103	141,354	135,134	145,516	129,333	153,658
ch130	6,110	**6,270**	6,498	6,470	7,279	7,367	7,434	7,578	8,280
pr136	96,772	**99,474**	105,361	110,531	109,586	116,069	105,778	120,769	142,438
pr144	58,537	**59,436**	61,974	60,321	73,032	74,684	73,613	61,652	77,704
ch150	6,528	**6,985**	7,210	7,232	7,995	7,641	7,914	8,191	9,203
kroA150	26,524	**27,888**	28,658	29,666	29,963	32,631	31,341	33,612	38,763
kroB150	26,130	**27,209**	27,404	29,517	31,589	33,260	31,616	32,825	35,289
pr152	73,682	**75,283**	75,396	77,206	88,531	82,118	86,915	85,699	90,292
u159	42,080	**45,433**	46,789	47,664	49,986	48,908	52,009	53,641	54,399
rat195	2,323	**2,581**	2,609	2,605	2,806	2,906	2,935	2,753	3,163
d198	15,780	16,453	**16,138**	16,596	17,632	19,002	17,975	18,805	19,339
kroA200	29,368	**30,965**	31,949	32,760	35,340	37,487	36,025	35,794	40,234
kroB200	29,437	31,692	**31,522**	33,107	35,412	34,490	36,532	36,976	40,615
ts225	126,643	**136,302**	140,626	138,101	160,014	145,283	151,887	152,493	188,008
tsp225	3,916	**4,154**	4,280	4,278	4,470	4,733	4,780	4,749	5,344
pr226	80,369	**81,873**	84,130	89,262	91,023	98,101	100,118	94,389	114,373
gil262	2,378	**2,537**	2,623	2,597	2,800	2,963	2,908	3,211	3,336
pr264	49,135	**52,364**	54,462	54,547	57,602	55,955	65,819	58,635	66,400
a280	2,579	**2,867**	3,001	2,914	3,128	3,125	2,953	3,302	3,492
pr299	48,191	**51,895**	51,903	54,914	58,127	58,660	59,740	61,243	65,617
lin318	42,029	45,375	45,918	**45,263**	49,440	51,484	52,353	54,019	60,939
linhp318	41,345	45,444	45,918	**45,263**	49,440	51,484	52,353	54,019	60,939
Approx. ratio	1	**1.05**	1.08	1.09	1.18	1.2	1.21	1.24	1.37

CO Problem in RL language

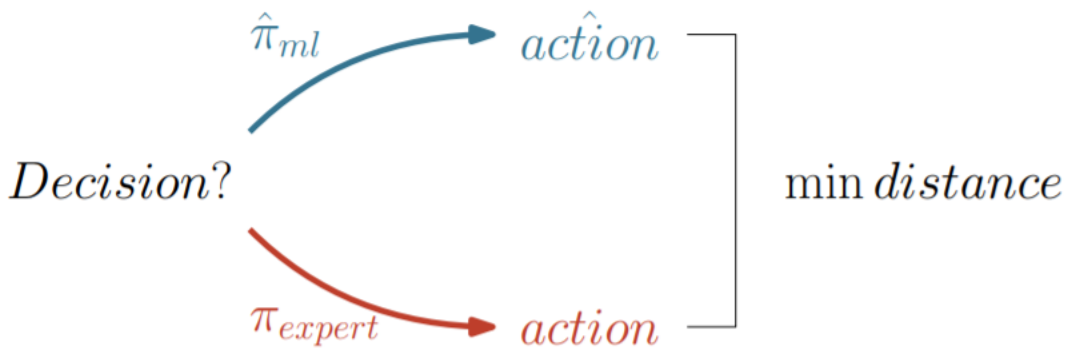
Problem	State	Action	Reward	Termination
MVC	subset of nodes selected so far	add node to subset	-1	all edges are covered
MAXCUT	subset of nodes selected so far	add node to subset	change in cut weight	cut weight cannot be improved
TSP	partial tour	grow tour by one node	change in tour cost	tour includes all nodes



RL: Learning methods

Demonstration

the policy is trained to reproduce the action of an expert policy by minimizing some discrepancy in the action space.



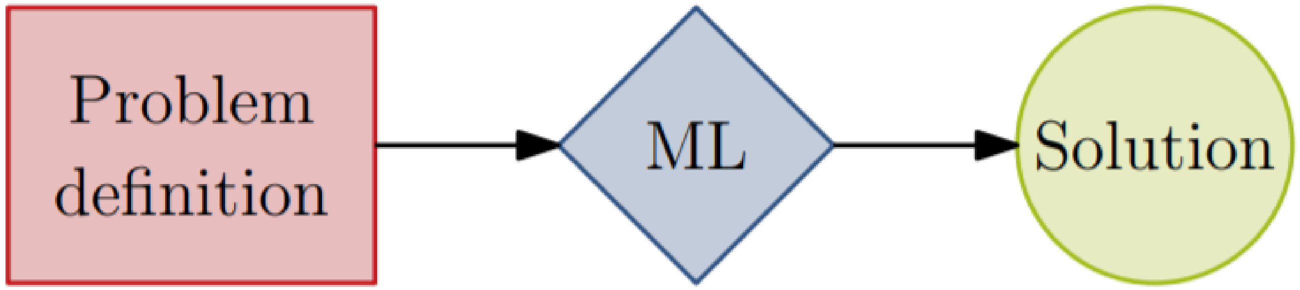
Experience

When learning through the experience, no expert is involved; only maximizing the expected sum of future rewards (the return) matters.

Ways of use: End to end

End to end learning

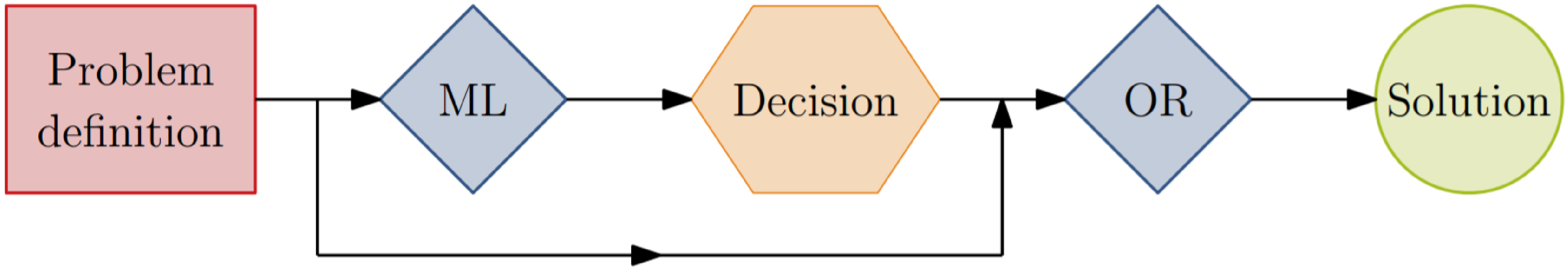
train the ML model to output solutions directly from the input instance.



Ways of use: Configure existing algorithm

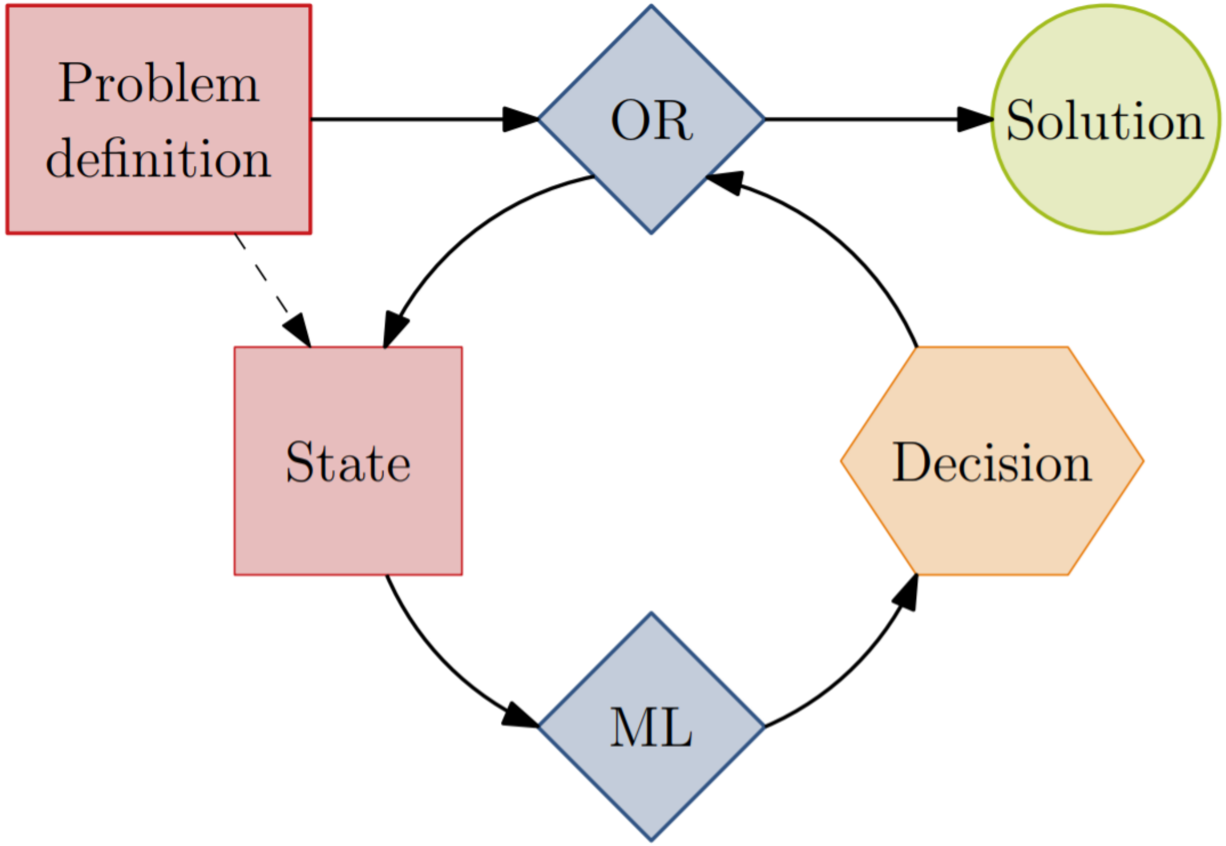
Learning to configure algorithms

ML is applied to provide additional pieces of information to a CO algorithm.



Alongside optimization algorithm

one can build CO algorithms that repeatedly call an ML model throughout their execution.



ML problems

- Feasibility
- Modelling
- Scaling
- Data generation

Thank you

Thank you!

Bibliography

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Images:

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