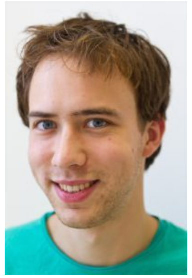
Deep Learning for Combinatorial Optimization

Count your flops and make them count!

Wouter Kool



Herke van Hoof

Joaquim Gromicho

Max Welling

University of Amsterdam

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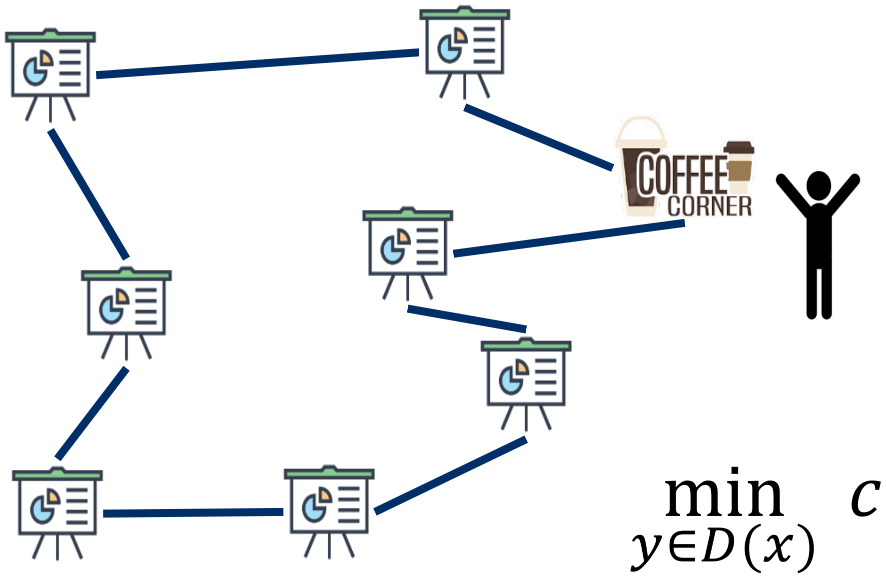
Machine Learning Lab

What we’re talking about?

$$y = \sigma\left(\sum_i x_i \theta_i\right)$$

for

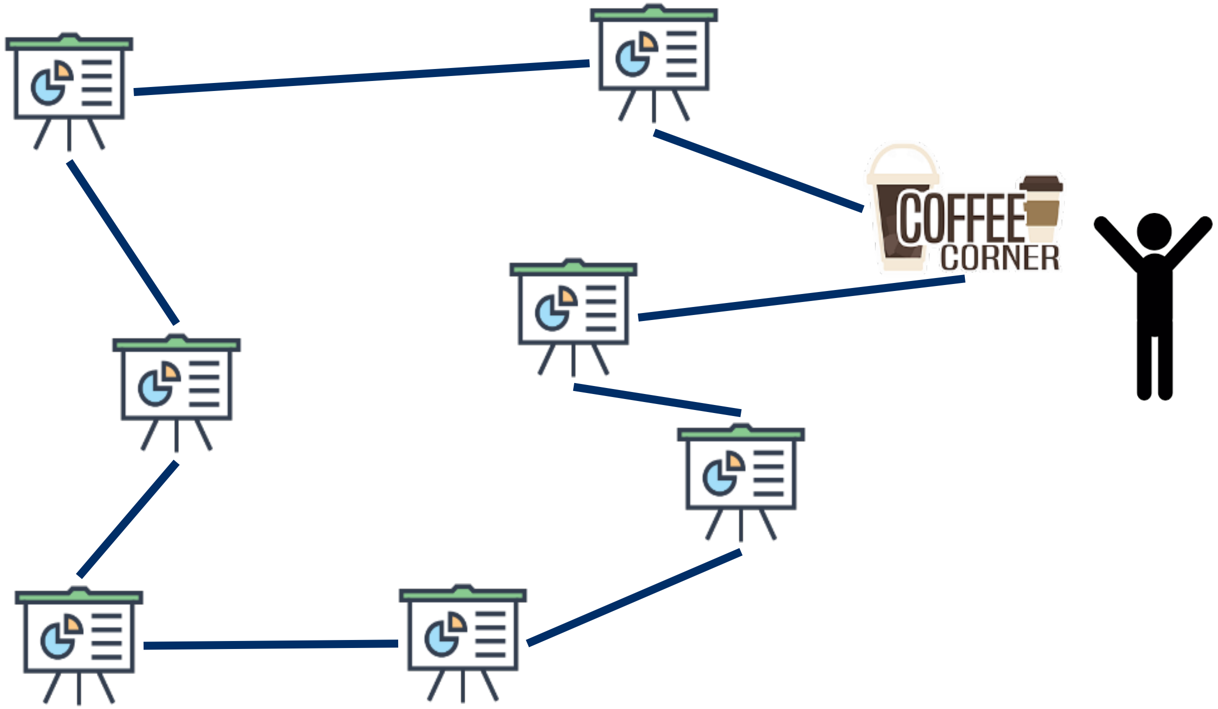


$$\min_{y \in D(x)} c(x, y)$$

Deep Learning

Combinatorial Optimization

Travelling Scientist Problem (TSP)



Kool et al., 2019

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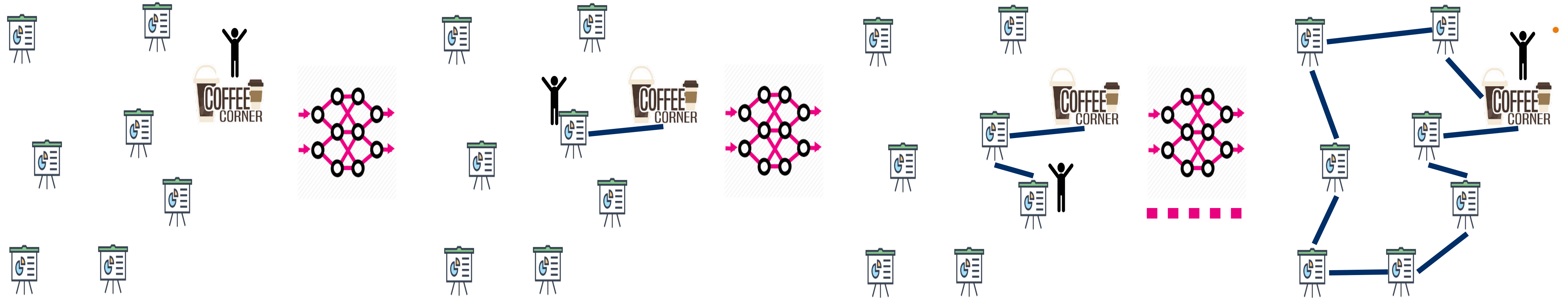
Travelling Scientist Problem (TSP)



Vinyals et al., 2015
Bello et al., 2016
Kool et al., 2019

Neural Information Processing Systems Conference

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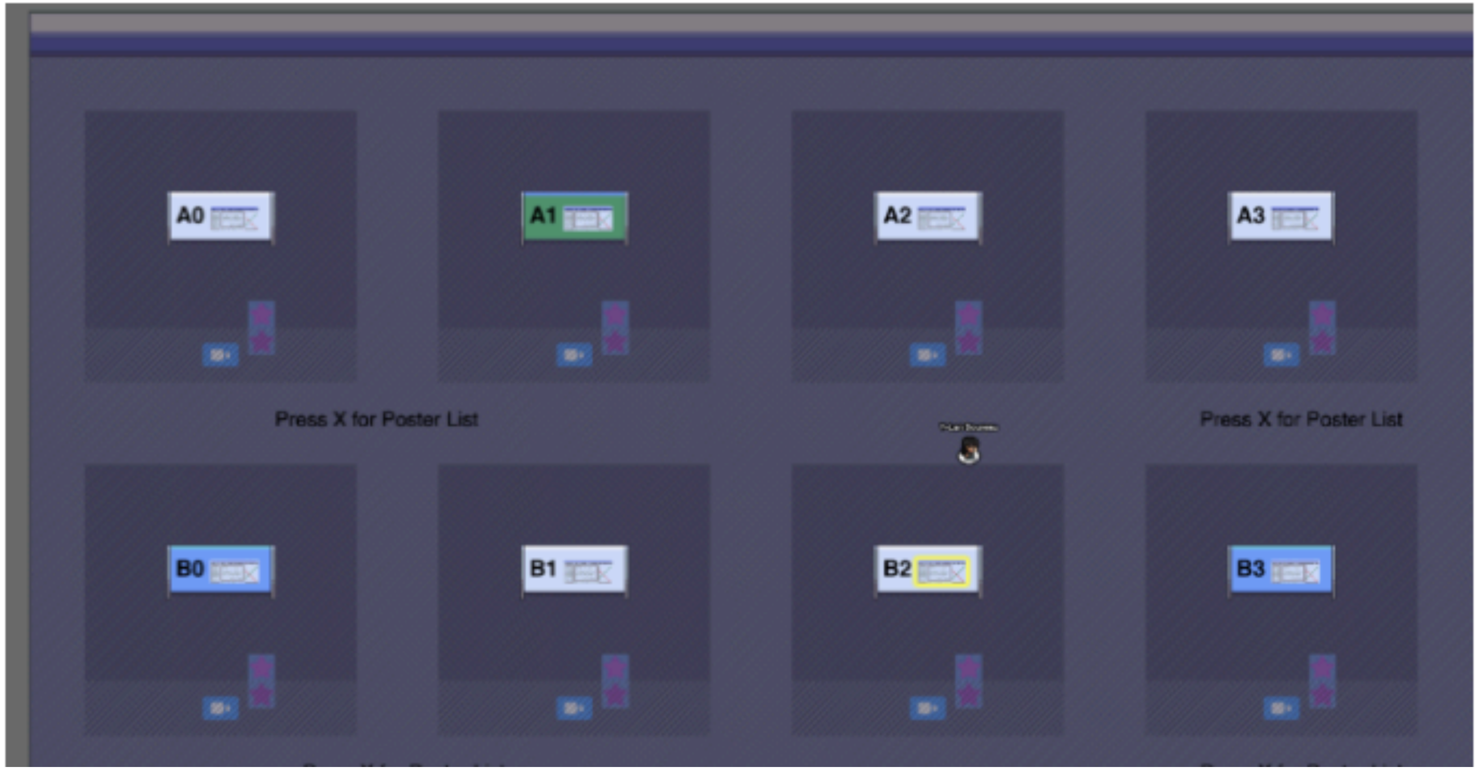
simply wandering; each poster had a clearly marked presenter spot to easily spot the presenter; people could teleport directly to the poster of their choice from the NeurIPS website, and a coordinate systems allowed people to locate a poster of interest once they were in a room.

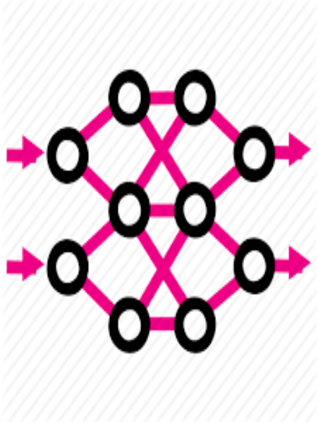


https://neuripsconf.medium.com/neurips-2020-online-experiments-gather-town-poster-sessions-and-mementor-ac1573d61c8a

‘Predicting’ translations

Neural
Machine
Translation

Sentence



Translation

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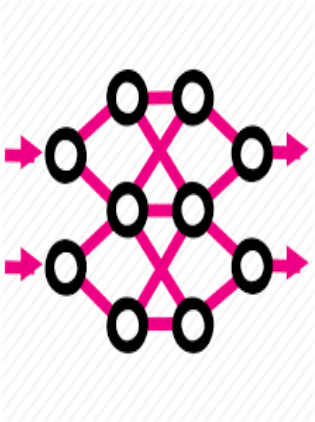
‘Predicting’ solutions

Neural Combinatorial Optimization

Problem



Solution

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It’s not the same!

Machine Translation $\neq$ Combinatorial Optimization

It’s not the same!

Machine Translation $\neq$ Combinatorial Optimization

Learning problem

Scoring translations (learning a model)

Finding a good translation (inference)

No problem

Scoring solution (objective function)

Finding a good solution (optimization)

Computational problem

Stahlberg & Byrne, 2019

It’s not the same!

Machine Translation	$\neq$	Combinatorial Optimization
Maximize quality		Minimize cost
(computation is 2nd)		with minimum computation

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It’s not the same!

Machine Translation ≠ Combinatorial Optimization

Maximize quality

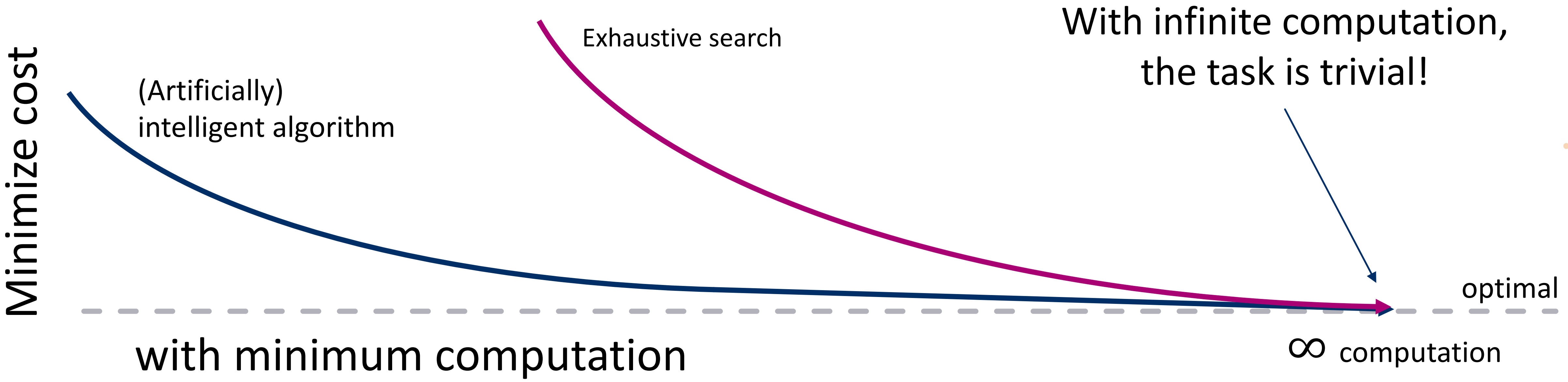
(computation is 2nd)

Minimize cost

with minimum computation

If we have infinite computation…

Combinatorial Optimization



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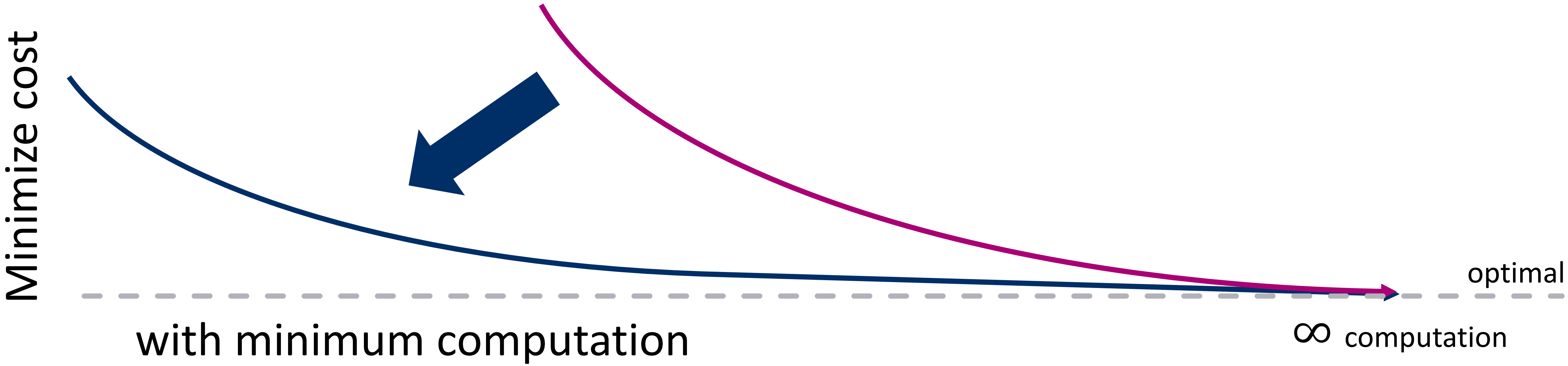
The goal

To find better solutions

...with less computation!



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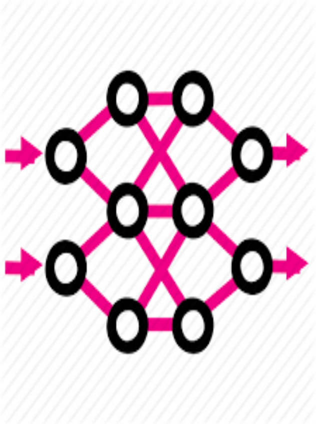
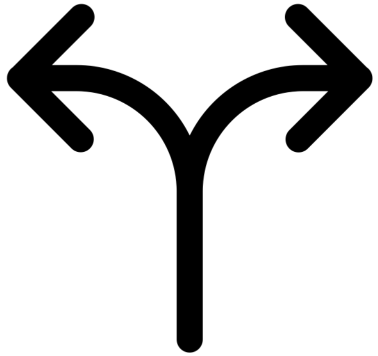
How?



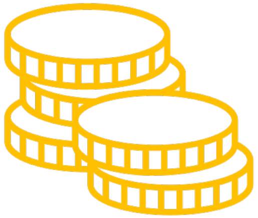


Using neural networks…

…to make better (heuristic) decisions!

Adding computation…

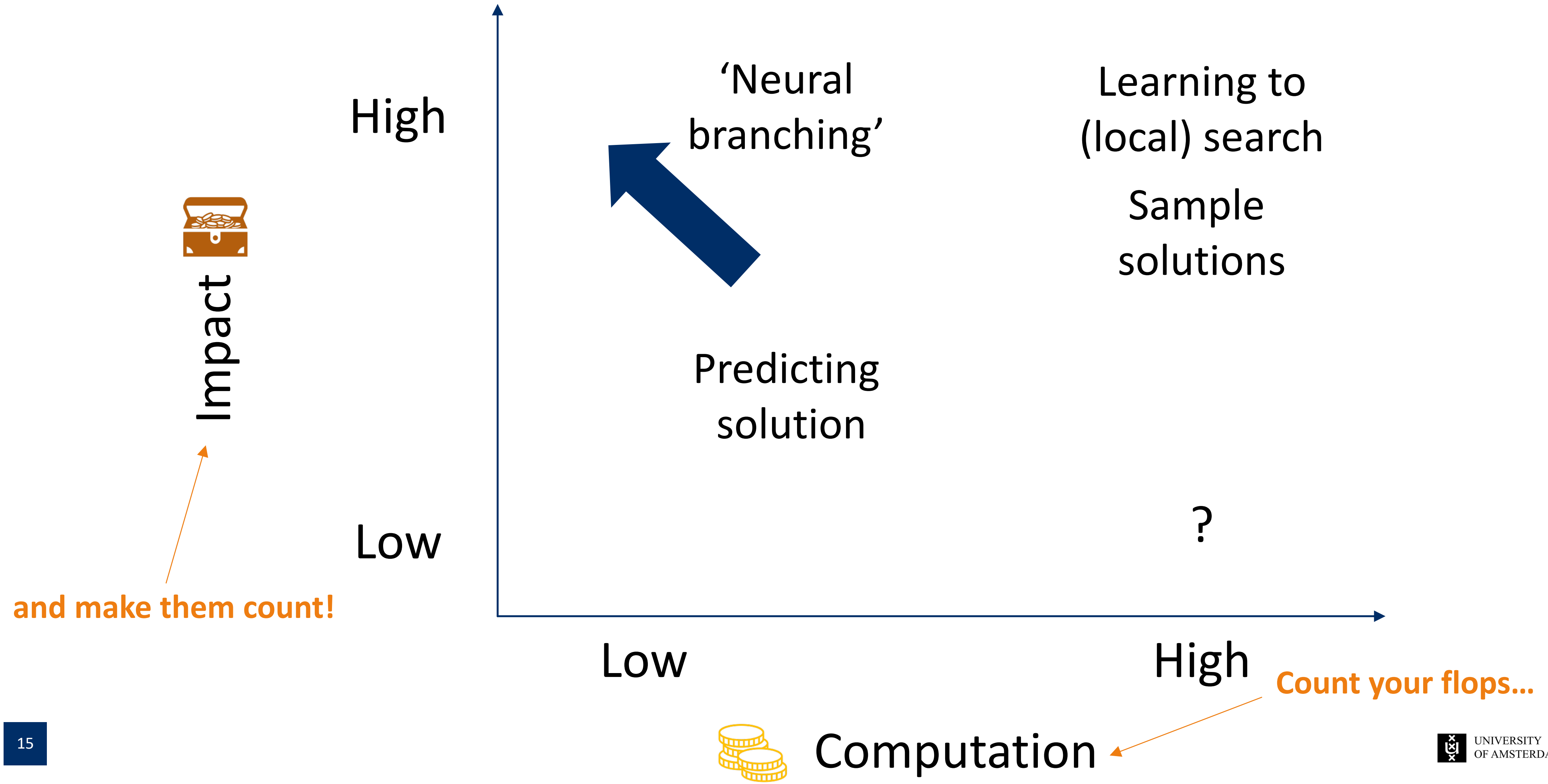
…to reduce computation!



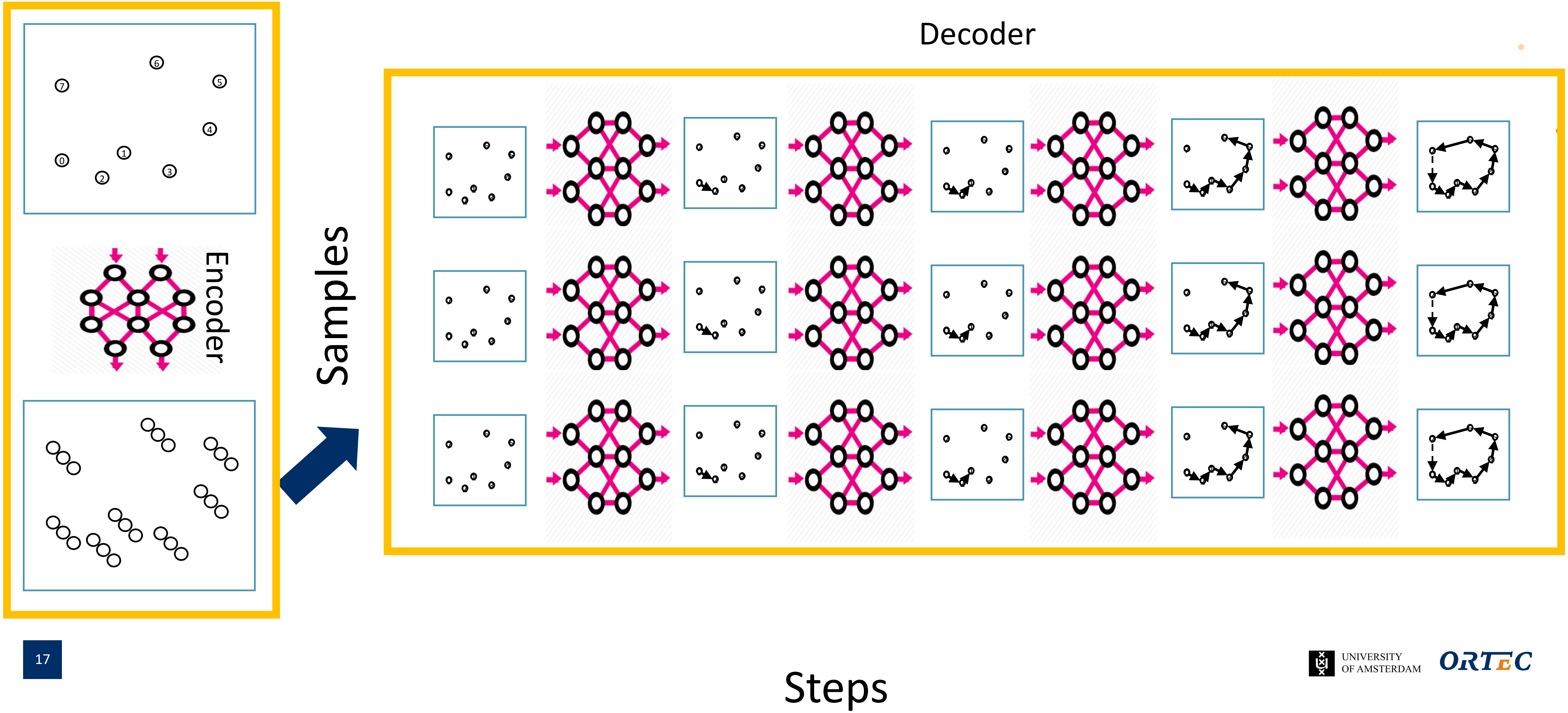
Investment

Pay-off

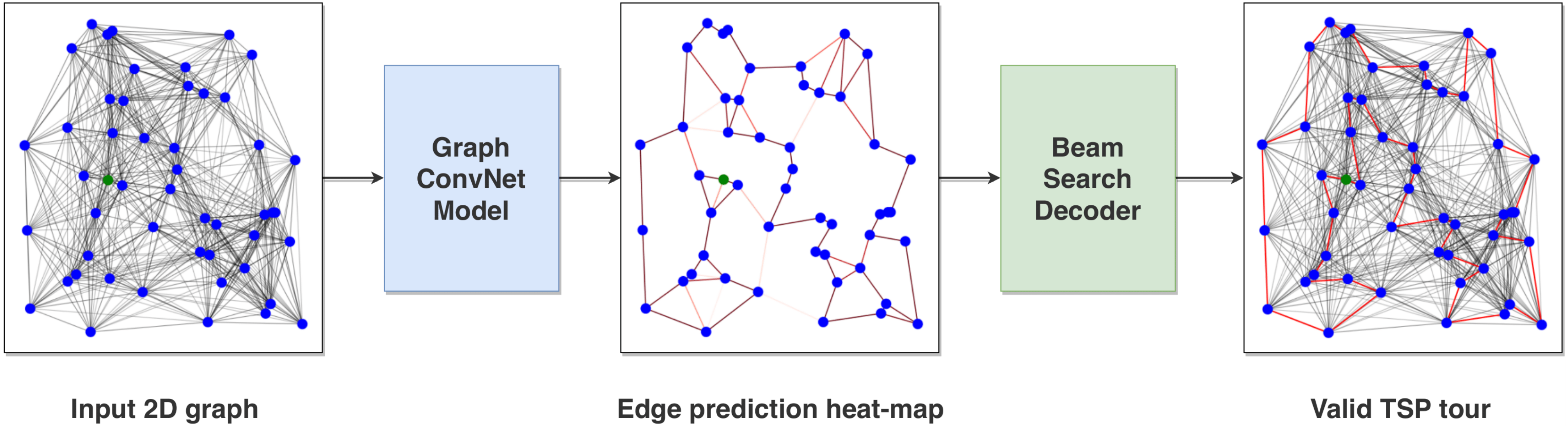
Impact vs. computation (of your neural network)



Example: sampling using Attention Model (Kool et al., 2019)

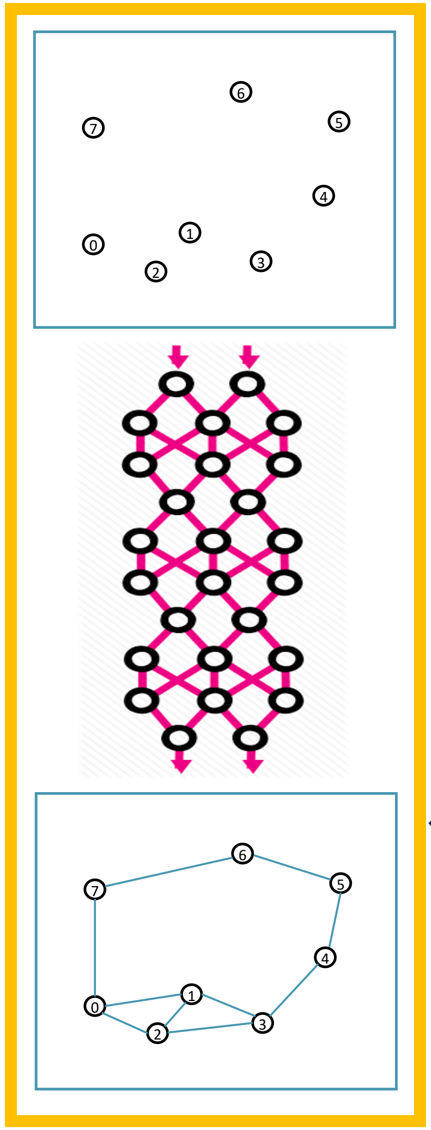


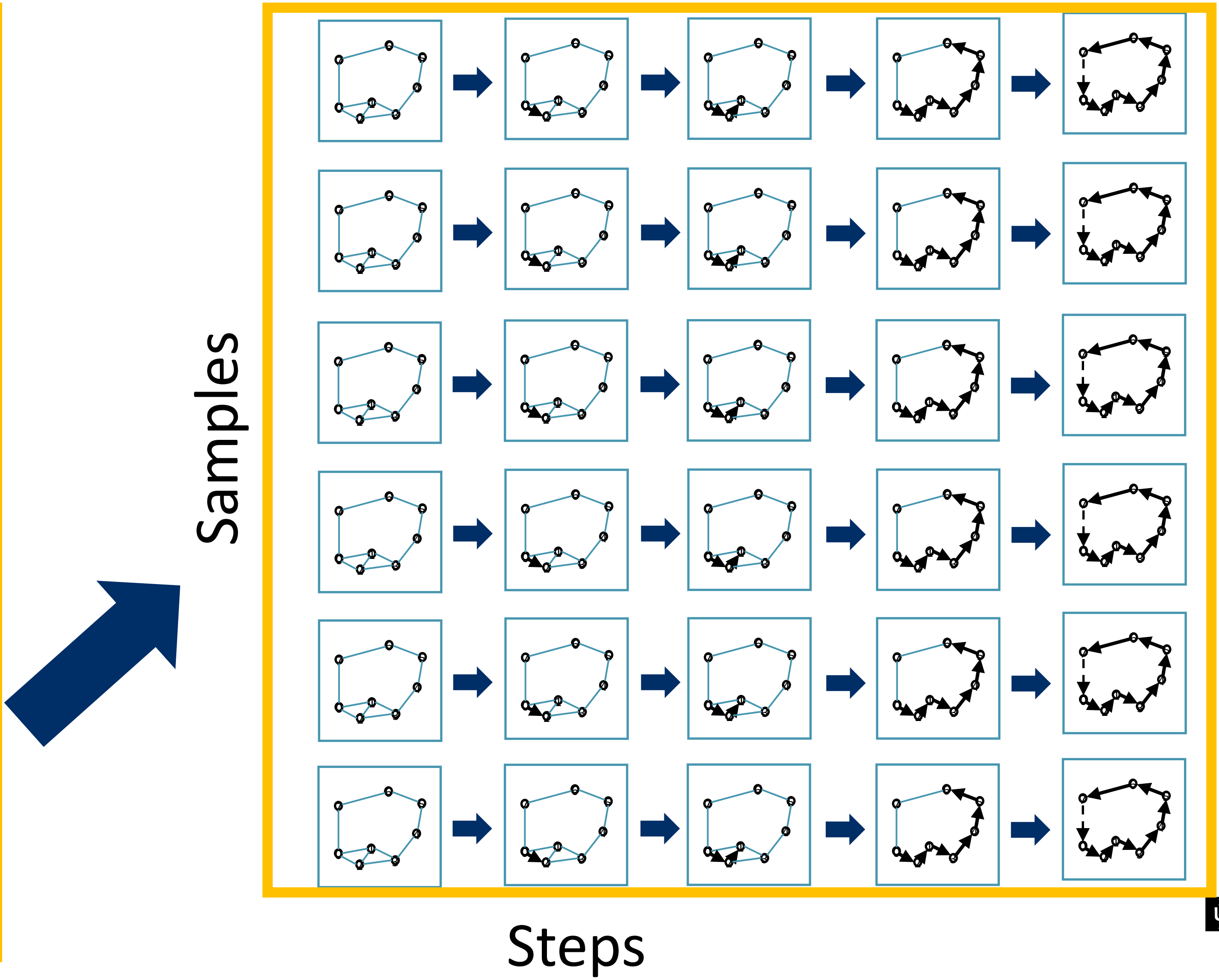
Example: sampling/BS using Heatmap Model (Joshi et al., 2019)



Picture by Joshi et al., 2019

Example: sampling/BS using Heatmap Model (Joshi et al., 2019)





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Dynamic Programming

Held-Karp DP for TSP (Held & Karp, 1962; Bellman, 1962)

$$\underbrace{C(S, i)}_{\text{DP state}} = \min_{j \in S \setminus \{i\}} C(S \setminus \{i\}, j) + c_{ji}$$

Minimum cost to go from 0 to i visiting all nodes in S

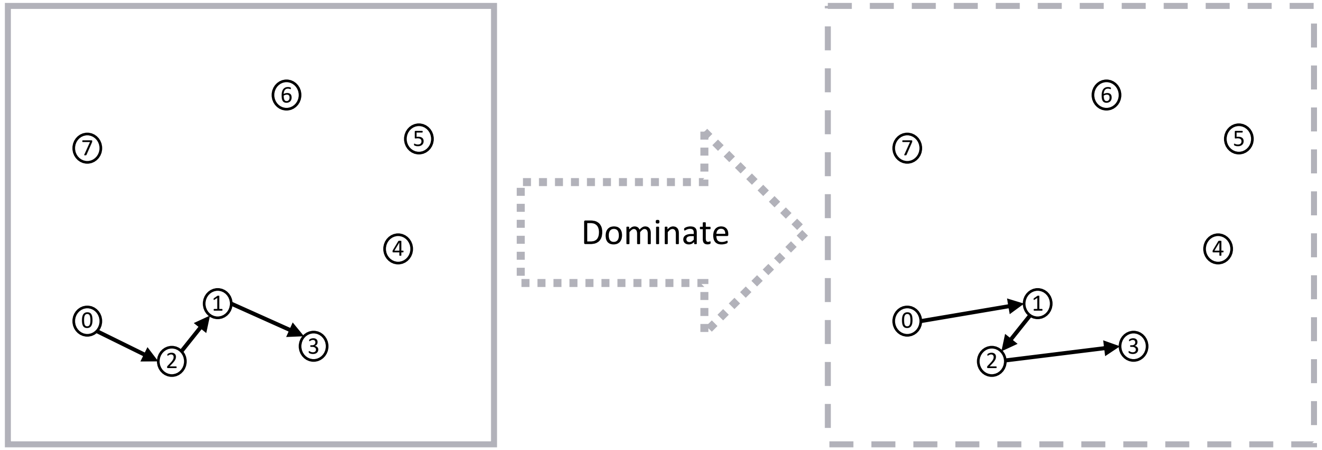
Set of visited nodes

Current node

DP state

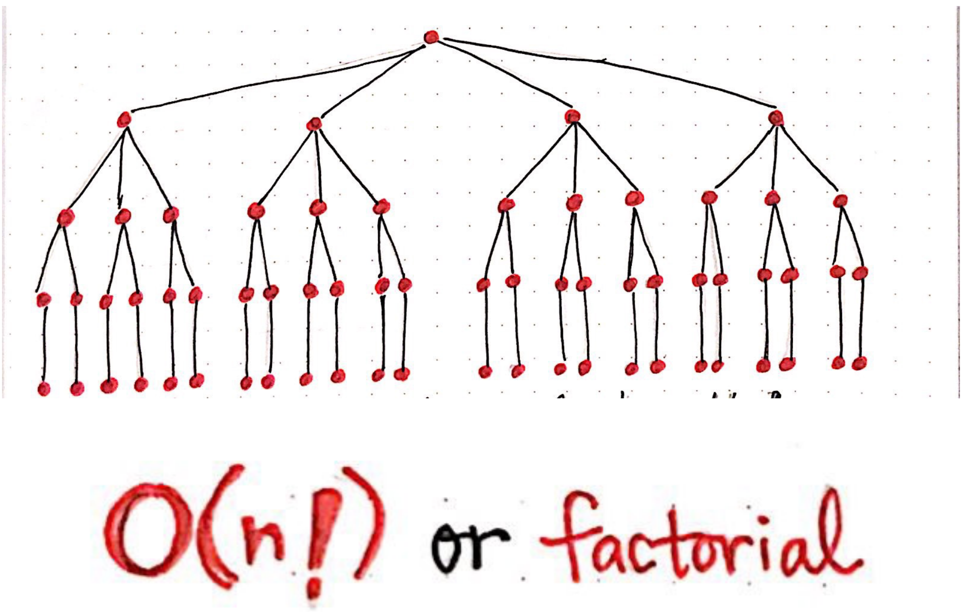
Cost/distance from j to i

Find best solution for each DP state

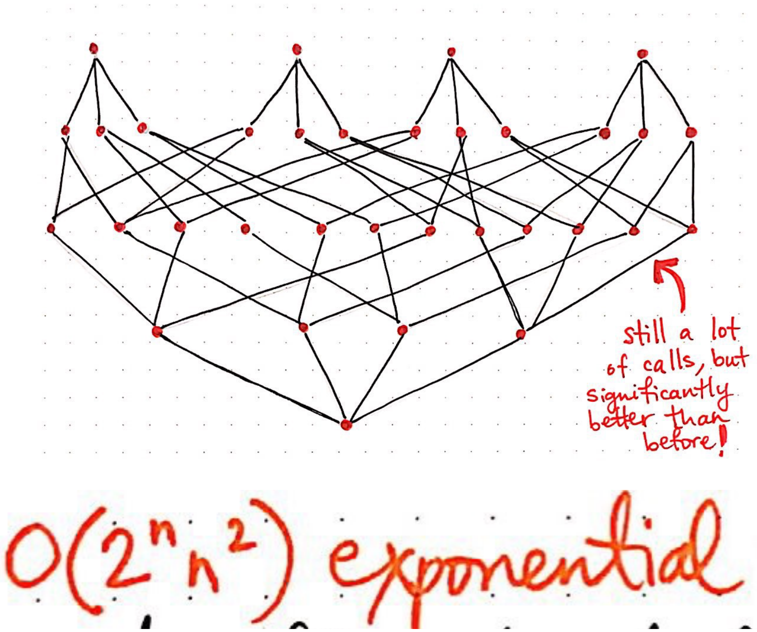


Held-Karp DP for TSP (Held & Karp, 1962; Bellman, 1962)

Brute-force (forward view)



DP (top-down or backward view)

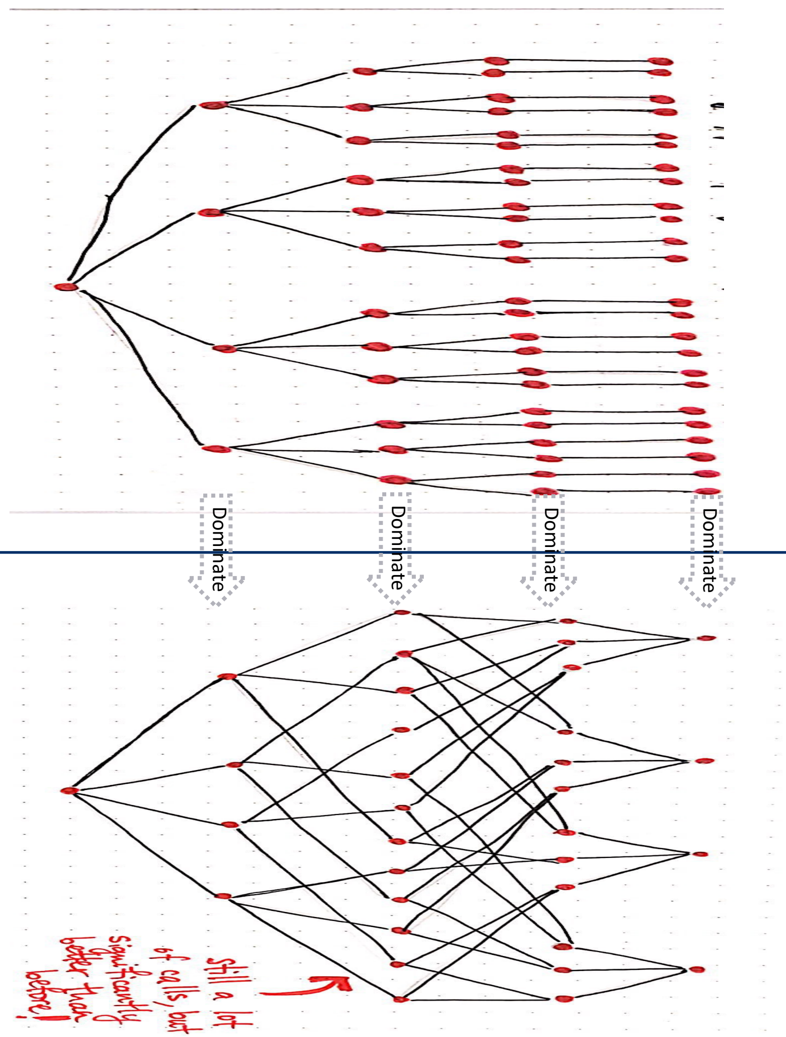


Artwork by Vaidehi Joshi, https://medium.com/basecs/speeding-up-the-traveling-salesman-using-dynamic-programming-b76d7552e8dd

Held-Karp DP for TSP (Held & Karp, 1962; Bellman, 1962)

Brute-force

$O(n!)$ or factorial



Forward view

Still impractical!

DP

$O(2^n n^2)$ exponential

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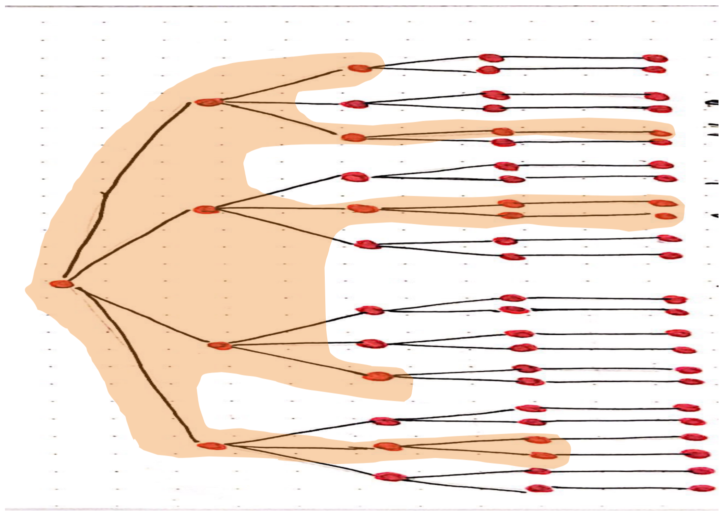
Held-Karp DP for TSP (Held & Karp, 1962; Bellman, 1962)

Beam search

$O(Bn)$ or *linear*

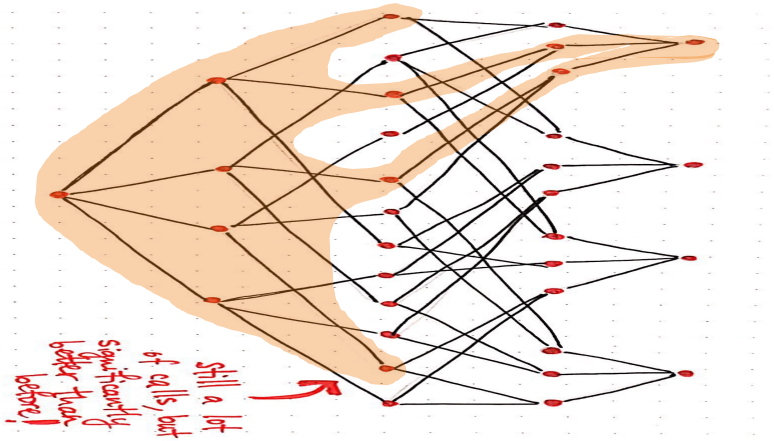


We need a *good policy* to restrict the search space!

Forward view

Restricted DP

$O(Bn)$ or *linear*



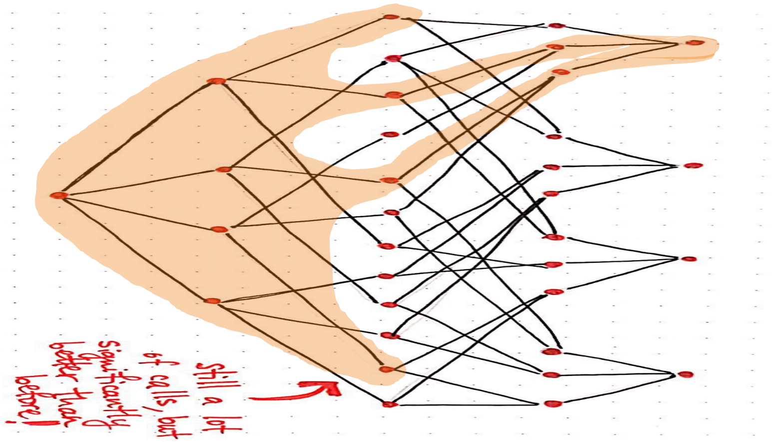
Malandraki & Dial, 1996
Gromicho et al., 2012

Deep Policy Dynamic Programming (DPDP)

https://arxiv.org/abs/2102.11756

DPDP

$O(Bn)$ or linear



For each iteration
- Expand solutions
- Remove dominated solutions
- Select top B according to *policy*
- Repeat

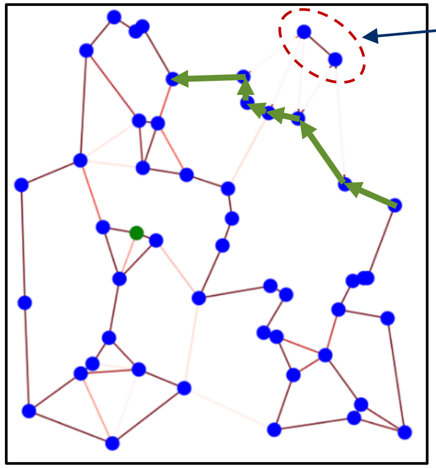
Forward view

Policy: select top B solutions that maximize the score.

$$\text{SCORE} = \text{HEAT} + \text{POTENTIAL}$$

Heat of edges in solution

Estimate for unvisited nodes
based on remaining edges



Potential avoids 'skipped nodes'

Heat
$h_{ij} \in (0,1)$

Picture by Joshi et al., 2019

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Deep Policy Dynamic Programming (DPDP)

https://arxiv.org/abs/2102.11756

- DP is flexible framework for many VRP variants e.g. time windows
- Suitable for GPU implementation
- Natural trade-off compute vs. performance -> asymptotically optimal
- Supervised training based on example solutions
- Test time: only evaluate NN once!

I hear you thinking…

Show me the pay-off!

Results

Travelling Salesman Problem

Table 1. Main results for TSP with 100 nodes.

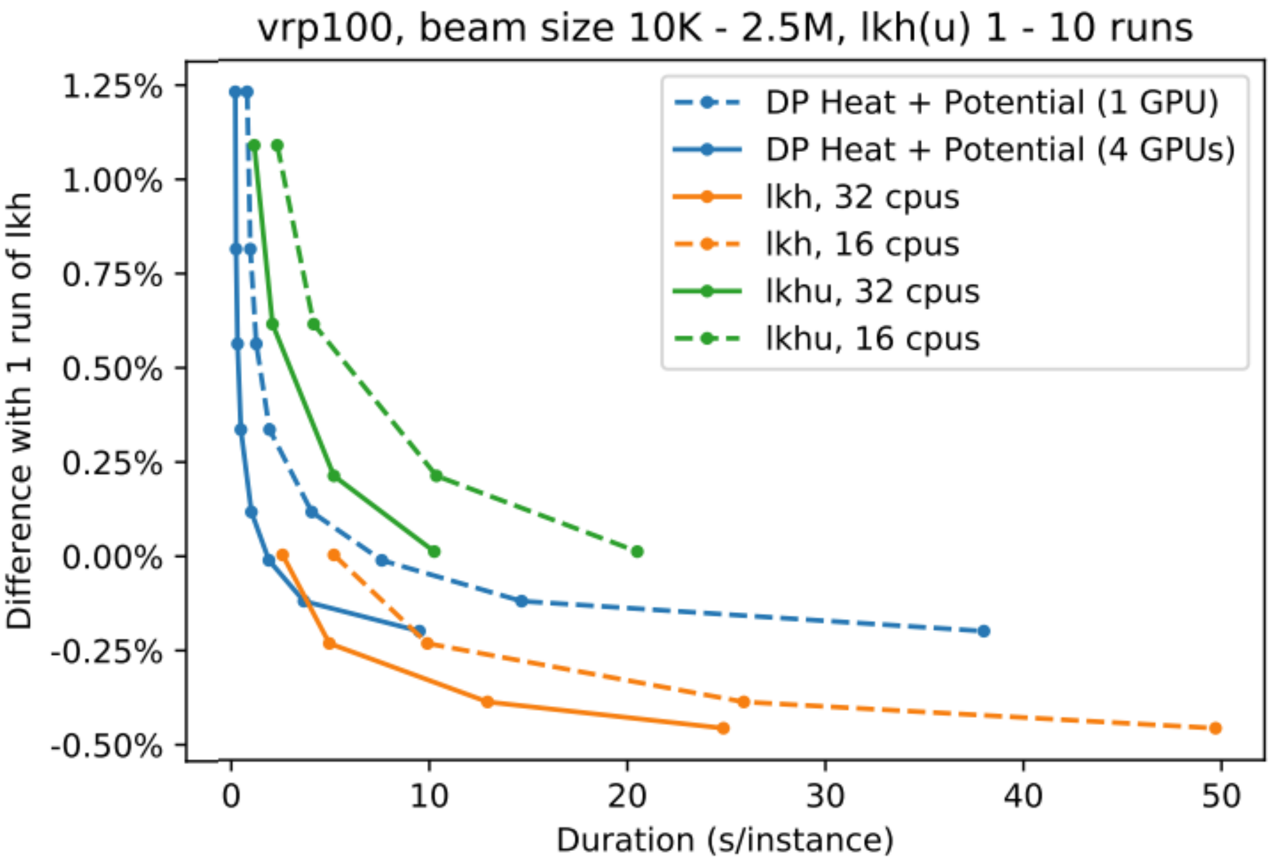
METHOD	COST	GAP	TIME
CONCORDE	7.765	0.000 %	6M
LKH	7.765	0.000 %	42M
GUROBI	7.776	0.15 %	31M
KOOL ET AL. (2019)	7.94	2.26 %	1H
JOSHI ET AL. (2019A)	7.87	1.39 %	40M
DA COSTA ET AL. (2020)	7.83	0.87 %	41M
FU ET AL. (2020)	7.764*	0.04 %	4M + 11M
DPDP 10K	7.765	0.009 %	10M + 1H06M
DPDP 100K	7.765	0.004 %	10M + 2H35M

Vehicle Routing Problem

Table 2. Main results for VRP with 100 nodes.

METHOD	COST	GAP	TIME
LKH	15.647	0.000 %	12H59M
XIN ET AL. (2020)	16.49	4.99 %	39S
KOOL ET AL. (2019)	16.23	3.72 %	2H
CHEN & TIAN (2019)	16.10	2.90 %	1H
PENG ET AL. (2019)	16.27	3.96 %	6H
WU ET AL. (2019)	16.03	2.47 %	5H
HOTTUNG & TIERNEY (2019)	15.99	1.02 %	1H
LU ET AL. (2020)	15.57*	-	4000H
DPDP 10K	15.832	1.183 %	10M + 2H24M
DPDP 100K	15.694	0.305 %	10M + 5H48M
DPDP 1M	15.627	- 0.127 %	10M + 48H27M

Quality vs. computation



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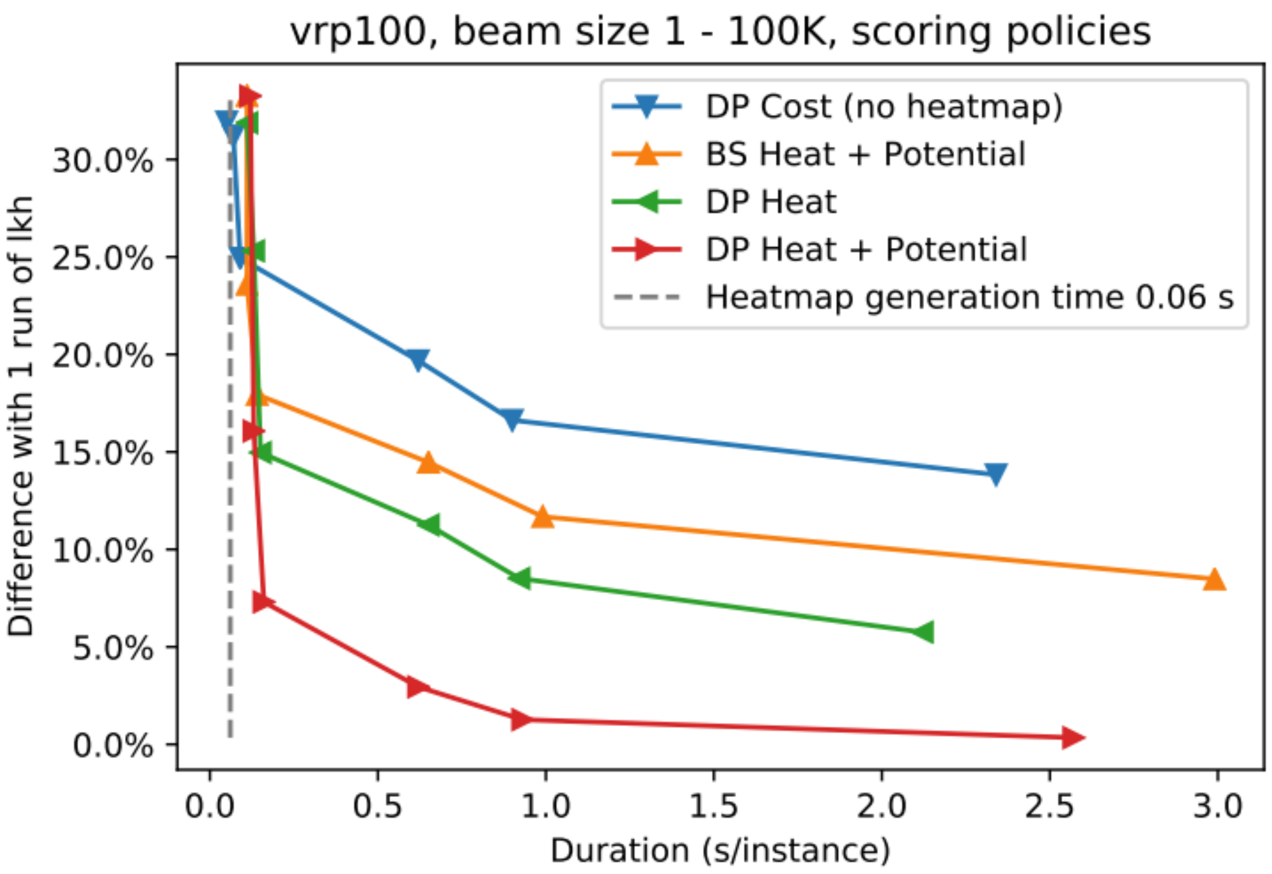
Ablations



vrp100, beam size 1 - 100K, scoring policies
DP Cost (no heatmap)
BS Heat + Potential
DP Heat
DP Heat + Potential
Heatmap generation time 0.06 s
30.0%
25.0%
20.0%
15.0%
10.0%
5.0%
0.0%
Difference with 1 run of lkh
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Duration (s/instance)

That’s it! So remember…

Count your flops…

and make them count!