Boosting Dynamic Programming with Neural Networks for Solving NP-hard Problems

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Outline

1. Revisiting Dynamic Programming
2. Approximating Dynamic Programming with Neural Networks
3. Application to Traveling Salesman Problem (TSP)
4. Experimental Results
5. Summary

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Dynamic Programming

- Dynamic programming is a powerful method for solving combinatorial optimization problems by utilizing the properties of
  - optimal substructures;
  - overlapping subproblems.

Problems	**Brute-force**	**DP**
chain matrix multiplication	Catalan number	$O(n^3)$
knapsack	$O(2^n)$	$O(cn)$
TSP	$O(n!)$	$O(2^n n^2)$

Dynamic Programming

- Multi-step decision-making problem: $s \to a \to \delta(s,a)$
  - s: the current state (subproblem)
  - a: a feasible decision under state s
  - $\delta(s,a)$: the set of subsequent sub-states
- Dynamic programming function: $f : S \to \mathbb{R}$
- Optimal substructures: $f(s) = \min_{a} \left\{ v(a) + \sum_{s' \in \delta(s,a)} f(s') \right\}$
  - $v(a)$ is the cost of making decision a
- Overlapping subproblems: tabular method
- Solution construction: $a = \arg\min_{a'} \left\{ v(a') + \sum_{s' \in \delta(s,a')} f(s') \right\}$

Challenges of DP for Solving NP-Hard Problems

- Exponential number of states
  - Exponential space complexity for tabular method
  - Exponential time to visit all states

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Some Related Work

- *Oriol Vinyals, Meire Fortunato, and Navdeep Jaitly*. **Pointer networks**. NIPS 2015
  - Sequence to sequence learning with RNN
  - Solving convex hull, Delaunay triangulation, and TSP
- *Anton Milan, S. Rezatofighi, Ravi Garg, Anthony Dick, and Ian Reid*. **Data-driven approximations to np-hard problems**. AAAI 2017
  - Introducing the original objects
  - Solving quadratic assignment problem and TSP
- . . .

- Prop.
  - End-to-end learning with powerful machine learning techniques;
  - The result model can be applied to different problem instances (with some limitations).
- Cons.
  - Did not utilize the intrinsic properties of the problems;
  - Cost to make label data;
  - Can only learn approximated solution.

Representing DP Functions with Neural Networks

Using a neural network to represent a function is much more flexible than the rigid tabular method.

- Extend a DP function to a continuous function;
- Universal approximation theorem;
- A DP function does not need to be absolutely precise;
- Not all states are equally useful;
- A suboptimal solution is adequate in practice.

But it is impractical to train a neural network with the idea of supervised learning for it is even difficult to compute a single label data.

Objective of Training the Network

$$\min J(\theta) = \sum_{s \in \mathcal{S}} \left(f(s;\theta) - \min_a \left\{ v(a) + \sum_{s' \in \delta(s,a)} f(s';\theta) \right\} \right)^2 .$$

Training the model with gradient descent

$$\begin{aligned} \nabla J = & 2 \sum_{s \in \mathcal{S}} \left(f(s;\theta) - \min_a \left\{ v(a) + \sum_{s' \in \delta(s,a)} f(s';\theta) \right\} \right) \\ & \left(\nabla f(s;\theta) - \nabla \min_a \left\{ v(a) + \sum_{s' \in \delta(s,a)} f(s';\theta) \right\} \right) . \end{aligned}$$

$$\theta_{t+1} = \theta_t - \eta_t \nabla J(\theta_t).$$

Training Algorithm

Algorithm 1 Training the neural network with solution reconstruction

Initialize neural network $f(s;\theta)$ with model parameter θ, maybe with pre-training on edge cases
Initialize data pool D
Initialize exploration parameter $\varepsilon_t = 1.0$ and learning rate η_t appropriately
for each iteration $t = 1, 2, \ldots$ **do**
    Initialize state list S, state scheduling data structure Q, and state visit-marking data structure V
    Add the state s_0 representing the original problem to Q and V
    while Q is not empty **do**
        $s =$ Q.pop()
        S.Add(s)
        With probability ε_t:
            select a random feasible decision a
        with probability $1 - \varepsilon_t$:
            select decision a according to equation (**??**)
        for each sub-state $s' \in \delta(s, a)$ **do**
            if cannot find s' in V **then**
                Add s' to Q and V
            end if
        end for
    end while
    Generate a mini-batch training data B=S+Sample(D)
    Preform a gradient descent step on data B to close the gap according to equations (**??**) and (**??**)
    Add S to D with a weight being the value of the solution
    Decay ε_t and η_t if necessary
end for

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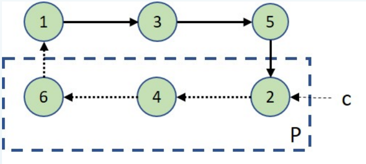
Application to TSP

Dynamic programming (Held-Karp algorithm) for solving TSP:

$$f(P, c) = \min_{c' \in P; c' \neq c} \{d(c, c') + f(P \backslash \{c\}, c')\}$$

$$c_{i+1} = \arg\min_{c \notin \{c_1, \ldots, c_i\}} \{d(c_i, c) + f([n] \backslash \{c_1, \ldots, c_i\}, c)\}$$

- $P \subseteq [n]$: vertices to be visited
- c: current starting point
- $f(P, c)$: the shortest length of paths visiting P, starting from c and returning to vertex 1



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Experimental Results

Table: Experimental results in TSPLIB[1]

Data	Opt.	NNDP		Held-Karp		Christofides		Greedy	
Gr17	2085	**2085**	**1**	**2085**	**1**	2287	1.1607	2178	1.0446
Bayg29	1610	**1610**	**1**	NA	NA	1737	1.0789	1935	1.2019
Dantzig42	699	**709**	**1.0143**	NA	NA	966	1.382	863	1.2346
HK48	11461	**11539**	**1.0068**	NA	NA	13182	1.1502	12137	1.059
Att48	10628	**10868**	**1.0226**	NA	NA	15321	1.4416	12012	1.1302
Eil76	538	**585**	**1.0874**	NA	NA	651	1.1128	598	1.1115
Rat99	1211	**1409**	**1.1635**	NA	NA	1665	1.3749	1443	1.1916
Br17	39	**39**	**1**	**39**	**1**	NA	NA	56	1.435
Ftv33	1286	**1324**	**1.0295**	NA	NA	NA	NA	1589	1.2002
Ft53	6905	**7343**	**1.0634**	NA	NA	NA	NA	8584	1.169

[1] The first 7 cases are symmetric TSP instances and the last 3 cases are asymmetric TSP instances. Each instance was run with 10000 iterations. The time complexity is $O(n^4)$ for each iteration, varying from 0.01 section to 0.1 sections for each iteration.

A Case Study

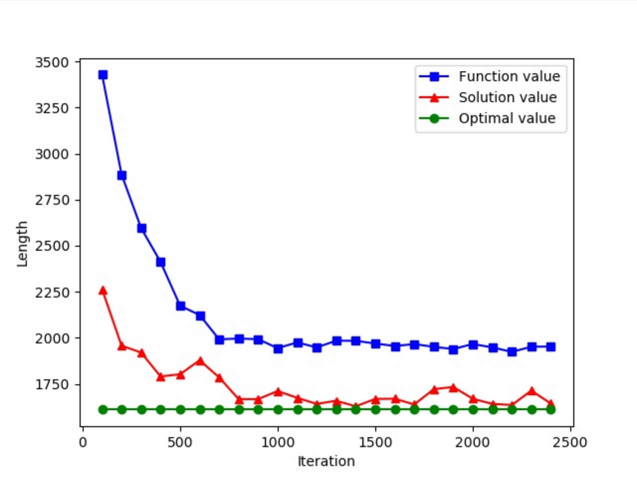

Figure: Convergence of the case Bayg29. The function values are the values the model outputs; the solution values are the exact values of the solutions constructed from the model.

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Summary

- An approach to boost the capability of dynamic programming with neural networks.
  - tabular method $\rightarrow$ neural network (polynomial size), approximately representing DP functions;
  - iterative training algorithm with data generated from a solution reconstruction process;
  - approximating ability and flexibility of neural networks + the advantage of dynamic programming;
  - significantly reduce the required space for some NP-hard problems, trading-off space, running time, and accuracy.
- Apply to the Held-Karp algorithm for TSP.
  - can handle larger problems that are intractable for the conventional DP;
  - outperform other well know approximation algorithms.

Thank You!