Reproducible and Efficient Benchmarks for Hyperparameter Optimization of Neural Machine Translation Systems

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Reproducible and Efficient Benchmarks for Hyperparameter Optimization of Neural Machine Translation Systems

Outline

1. Motivation

2. Introduction to Hyperparameter Optimization (HPO)

3. Contributions
   - a new HPO benchmark dataset (tabular dataset)
   - a new HPO algorithm (graph-based semi-supervised learning)

4. Summary
1. Motivation
Hyperparameter Search of NMT systems

Hyperparameters:
- preprocessing configurations: number of BPE symbols
- training settings: initial learning rate, warmup
- architecture designs: number of layers, embedding size,
  number of hidden units in each layer,
  number of self-attention heads

Objectives:
- training accuracy: BLEU, perplexity
- computational cost: decoding time, number of model parameters
Hyperparameter Search of NMT systems

--- Rewarded and Necessary
Challenges of HPO on NMT

- Large search space & high computational costs for NMT training

If we have 6 hyperparameters to tune, where we want to try 3 candidate values for each hyperparameter, and it takes 1 day to 1 week to train a model, then how long will it take for a grid search?

\[ 3^6 = 729 \text{ (days / weeks)} \]

HPO is expensive to run!
Challenges of HPO on NMT

- Large search space & high computational costs for NMT training
- Difficult to optimize multiple objectives

*Pareto-optimal system (There does not exist a system that outperforms it on both objectives.)*
Challenges of HPO on NMT

- Large search space & high computational costs for NMT training
- Difficult to optimize multiple objectives

HPO on NMT has been hardly studied.

It is prohibitively expensive to compare different HPO methods on NMT tasks in practice.
This work) **HPO Benchmark Dataset on NMT**

**Goal:** enable **reproducible** HPO research on NMT tasks

**Table-lookup benchmark procedure:**

1. train an extremely large number of NMT systems with diverse hyperparameter settings and record their performance.

   - a table of **(configuration, performance)** pairs

2. constrain HPO methods to sample from this finite set of models.
2. Intro to HPO
Let

\( \lambda \) be the hyperparameters of a ML algorithm with domain \( \Lambda \),
\( L(\lambda, D_{\text{train}}, D_{\text{valid}}) \) denote the loss of the ML algorithm, using
hyperparameters \( \lambda \) trained on \( D_{\text{train}} \) and evaluated on \( D_{\text{valid}} \).

The HPO problem is to find a configuration \( \lambda^* \) that minimizes this loss:

\[
\lambda^* \in \arg\min_{\lambda \in \Lambda} L(\lambda, D_{\text{train}}, D_{\text{valid}})
\]
HPO Methods

Model-Free Optimization Methods

- Grid Search
- Random Search
- Population-based methods
e.g. genetic algorithms, evolutionary algorithms --- CMA-ES

Sequential Model-Based Optimization Methods (SMBO)

- Bayesian Optimization (BO)
- Tree Parzen Estimator (TPE)
Sequential Model-Based Optimization (SMBO)

Acquisition Function

ML Algorithm

Surrogate Model

\( \lambda_1 \), \( \lambda_3 \), \( \lambda_4 \), \( \lambda_i \), \( \lambda_2 \)

(\( \lambda_1, \hat{f}(\lambda_1) \))
(\( \lambda_3, \hat{f}(\lambda_3) \))
(\( \lambda_i, \hat{f}(\lambda_i) \))
(\( \lambda_4, \hat{f}(\lambda_4) \))
(\( \lambda_2, \hat{f}(\lambda_2) \))

Sample

\( \lambda_p \)

Query

Fit (\( \lambda_p, f(\lambda_p) \))
Bayesian Optimization

1. Sample \( \lambda_p \) from the posterior distribution.
2. Query the ML Algorithm with \( \lambda_p \) and get \( f(\lambda_p) \).
3. Fit the Gaussian Process with \( \lambda_p, f(\lambda_p) \).
4. Calculate the Expected Improvement for \( \lambda_p \).
5. Repeat steps 1-4 with the next \( \lambda_i \) until termination.
3. Contributions

- a new HPO benchmark dataset (tabular dataset)
- a new HPO algorithm (graph-based semi-supervised learning)
One pitfall in the evaluation of HPO methods: The ranking between HPO methods varies between tasks. (Klein et al., 2019)

Solution:
Select HPO method based on its performance on various MT corpora.
HPO Method Selection

1. Evaluate MT Data c
2. Develop a robust HPO algorithm
3. Apply HPO B
   - Target MT Data
Table-Lookup HPO Datasets

6 MT Corpora:
- large resource (WMT2019 Robustness): ja-en, en-ja (4M lines)
- mid resource (TED Talks): zh-en, ru-en (170k lines)
- low resource: sw-en, so-en (24k lines)

Model: Transformers
Table-Lookup HPO Datasets

- **6 MT Corpora:**
  - large resource (WMT2019 Robustness): ja-en, en-ja (4M lines)
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  - low resource: sw-en, so-en (24k lines)

- **Model:** Transformers

- **Search Space:** 2245 Transformers (1547 GPU days)

<table>
<thead>
<tr>
<th>dataset</th>
<th>bpe (1k)</th>
<th>#layers</th>
<th>#embed</th>
<th>#hidden</th>
<th>#att_heads</th>
<th>init_lr ($10^{-4}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>zh, ru, ja, en</td>
<td>10, 30, 50</td>
<td>2, 4</td>
<td>256, 512, 1024</td>
<td>1024, 2048</td>
<td>8, 16</td>
<td>3, 6, 10</td>
</tr>
<tr>
<td>sw</td>
<td>1, 2, 4, 8, 16, 32</td>
<td>1, 2, 4, 6</td>
<td>256, 512, 1024</td>
<td>1024, 2048</td>
<td>8, 16</td>
<td>3, 6, 10</td>
</tr>
<tr>
<td>so</td>
<td>1, 2, 4, 8, 16, 32</td>
<td>1, 2, 4</td>
<td>256, 512, 1024</td>
<td>1024, 2048</td>
<td>8, 16</td>
<td>3, 6, 10</td>
</tr>
</tbody>
</table>

- **Objectives:** BLEU & perplexity; decoding time, #updates, GPU memory, #model parameters
Application I. HPO Method Comparison
Application I. HPO Method Comparison

fix the budget
Application I. HPO Method Comparison

fix the target performance
Application I. HPO Method Comparison

fix the target performance
Application II. Multiobjective Optimization

![Graph showing decoding time vs BLEU scores with various steps indicated.]
Hyperparameter Analyses

Hyperparameter Importance

top 1 vs. all NMT models

Top 1 Percentile (en-ja)

All (en-ja)
Application III. Hyperparameter Analyses

Hyperparameter Importance
en-ja vs. sw-en
Hyperparameter Ranking Correlation

- zh-en: 1.000
- ru-en: 0.688
- ja-en: 0.545
- en-ja: 0.529
- sw-en: 0.647
- so-en: 0.630

Correlation values represent the strength of the relationship between different language pairs.
3. Contributions

- a new HPO benchmark dataset (tabular dataset)
- a new HPO algorithm (graph-based semi-supervised learning)
Graph-Based SMBO

Expected Influence

ML Algorithm

Graph-Based Regression

(sample)

(query)

fit

(\lambda_1, \hat{f}(\lambda_1))
(\lambda_3, \hat{f}(\lambda_3))
(\lambda_i, \hat{f}(\lambda_i))
(\lambda_4, \hat{f}(\lambda_4))
(\lambda_2, \hat{f}(\lambda_2))

(\lambda_p, f(\lambda_p))
Let

- $G = (V, E)$ be a graph with nodes $V$, and edges $E$.
- $V = L \cup U$, $L$ denote the labeled nodes, $U$ the unlabeled.
- $W$ be the edge weights.
- $f$ be the soft labels of nodes.

Labels of $U$ can be predicted by minimizing the energy function:

$$E(f) = \frac{1}{2} \sum_{i,j} w_{i,j} (f(i) - f(j))^2,$$

with the constraint that $f(i), i \in L$ are true labels. (label propagation)
(this work) **Expected Influence** (Acquisition Function)

**Idea:**
To query a point such that, if its soft label $f$ is observed, has the highest potential to change $f(i)$ for all the node $i$ as we re-run label propagation through the graph.

**Results:**
It outperforms *expected improvement* significantly when combined with *graph-based regression*. 
(this work) **Expected Influence** (Acquisition Function)

- Scale $f$ to be within $[0, 1]$.

- If we were to query an unlabeled point $k$:
  - its label is $1$, with prob $f(k)$
  - its label is $0$, with prob $1 - f(k)$

- Include $k$ as a newly-added “labeled” point and re-run label propagation:
  - $k$ is added with label $1$, $f^+(\lambda_k, 1)(i)$ are the new predictions for points $i$
  - $k$ is added with label $0$, $f^+(\lambda_k, 0)(i)$ are the new predictions for points $i$

- If $k$ is an influencer,
  - added with label $1$, $f^+(\lambda_k, 1)(i)$ will be large for $i$
  - added with label $0$, $1 - f^+(\lambda_k, 0)(i)$ will be large for $i$
We want to seek a point that maximizes the expected influence score defined as the following:

$$a_{EIF}(\lambda_k) = (1 - f(k)) \sum_{i=1}^{n} (1 - f^{+(\lambda_k,0)}(i)) + f(k) \sum_{i=1}^{n} f^{+(\lambda_k,1)}(i)$$
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4. Summary
Li and Talwalkar (2019): “Of the 12 papers published since 2018 at NeurIPS, ICML, and ICLR that introduce novel Neural Architecture Search methods, none are exactly reproducible.”

Our benchmarks are reproducible.
- dataset: [https://github.com/Este1le/hpo_nmt](https://github.com/Este1le/hpo_nmt)
- code: [https://github.com/Este1le/gbopt](https://github.com/Este1le/gbopt)

Our benchmarks are efficient.
One can perform multiple random trials of the same algorithm to test robustness.

Our benchmarks are effective.
We cover various MT corpora and a reasonable search space.

We hope our dataset can facilitate reproducible research and rigorous evaluation of HPO for complex and expensive models.
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