HYPERNOMAD: Hyperparameter optimization of deep neural networks using mesh adaptive direct search

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Presentation outline

Blackbox optimization

The MADS algorithm with categorical variables

Hyperparameters Optimization (HPO)

Computational experiments

Discussion
Blackbox optimization

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Discussion
Blackbox optimization (BBO) problems

- Optimization problem:

$$\min_{x \in \Omega} f(x)$$

- Evaluations of $f$ (the objective function) and of the functions defining $\Omega$ are usually the result of a computer code (a blackbox).

- Variables are typically continuous, but in this work, some of them are discrete – integers or categorical variables.
Blackbox optimization

We consider

$$\min_{x \in \Omega} f(x)$$

where the evaluations of $f$ and the functions defining $\Omega$ are the result of a computer simulation (a blackbox).

- Each call to the simulation may be expensive.
- The simulation can fail.
- Sometimes $f(x) \neq f(x')$.
- Derivatives are not available and cannot be approximated.

\[ x \in \mathbb{R}^n \quad \rightarrow \quad f(x) \quad \text{for} \quad i = 0; \quad i \leq \text{nc} ; \quad ++i \]
\[ \quad \quad \text{if} \quad (i \neq \text{hat}_i) \quad \{ \]
\[ \quad \quad \quad j = \text{rp.pickup}(); \]
\[ \quad \quad \text{if} \quad (j == \text{hat}_i) \]
\[ \quad \quad \quad j = \text{rp.pickup}(); \]
Blackbox optimization

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$$\min_{x \in \Omega} f(x)$$

where the evaluations of $f$ and the functions defining $\Omega$ are the result of a computer simulation (a blackbox).

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General framework

\[ f(x) \]

\( x \in \Omega \) ?

Algorithm

\( x \)
Mesh Adaptive Direct Search (MADS) in $\mathbb{R}^n$

- [Audet and Dennis, Jr., 2006].
- Iterative algorithm that evaluates the blackbox at some trial points on a spatial discretization called the mesh.
- One iteration = search and poll.
- The search allows trial points generated anywhere on the mesh.
- The poll consists in generating a list of trial points constructed from poll directions. These directions grow dense.
- At the end of the iteration, the mesh size is reduced if no new success point is found.
- Algorithm backed by a convergence analysis.
**[0] Initializations** \( (x_0, \Delta_0: \text{initial poll size}) \)

**[1] Iteration** \( k \)
- let \( \delta^k \leq \Delta^k \) be the mesh size parameter
- **Search**
  - test a finite number of mesh points
- **Poll** (if the Search failed)
  - construct set of directions \( D_k \)
  - test poll set \( P_k = \{ x_k + \delta^k d : d \in D_k \} \)
  - with \( \| \delta^k d \| \simeq \Delta_k \)

**[2] Updates**
- if success
  - \( x_{k+1} \leftarrow \text{success point} \)
  - increase \( \Delta^k \)
- else
  - \( x_{k+1} \leftarrow x_k \)
  - decrease \( \Delta^k \)
  - \( k \leftarrow k + 1 \), stop if \( \Delta^k \leq \Delta_{\text{min}} \) or go to **[1]**
Poll illustration (successive fails and mesh shrinks)

\[
\delta^k = 1 \\
\Delta^k = 1
\]

trial points\(=\)\(\{p_1, p_2, p_3\}\)
Poll illustration (successive fails and mesh shrinks)

\[
\delta^k = 1 \\
\Delta^k = 1
\]

\[
\delta^{k+1} = 1/4 \\
\Delta^{k+1} = 1/2
\]

trial points\(=\)\(\{p_1, p_2, p_3\}\)  \(=\) \(\{p_4, p_5, p_6\}\)
Poll illustration (successive fails and mesh shrinks)

\[ \delta^k = 1 \]
\[ \Delta^k = 1 \]

\[ \delta^{k+1} = 1/4 \]
\[ \Delta^{k+1} = 1/2 \]

\[ \delta^{k+2} = 1/16 \]
\[ \Delta^{k+2} = 1/4 \]

trial points = \{p_1, p_2, p_3\} = \{p_4, p_5, p_6\} = \{p_7, p_8, p_9\}
Types of variables in MADS

- MADS has been initially designed for continuous variables.

- Some theory exists for categorical variables [Audet and Dennis, Jr., 2001, Abramson, 2004, Abramson et al., 2009].

- (Other discrete variables now considered in MADS: Integer, binary, granular [Audet et al., 2019]).

- Two kinds of “categorical” variables:
  - Non-orderable and unrelaxable discrete variables.
  - An integer whose value changes the number of variables of the problem.
Example: A thermal insulation system

\[ \min_{\Delta x, T, n, M} \text{power}(\Delta x, T, n, M) \]

s.t.
\[ \Delta x \geq 0 \quad T_C \leq T \leq T_H \]
\[ n \in \mathbb{N} \quad M \in \text{Materials} \]
MADS with categorical variables

- [Abramson et al., 2009].

- The search is still a finite search on the mesh, free of any rules.

- The poll is the failsafe step that evaluates function values at mesh neighbors for the continuous variables, and in a user-defined set of neighbors $\mathcal{N}(x_k)$.

- This set of neighbors defines a notion of local optimality.
Extended poll

\[ y_k \quad \cdots \quad y^j_k \quad \cdots \quad z_k \]

\[ x_k \]

HYPERNOMAD: Hyperparameter optimization with MADS
Extended poll

\[
\begin{align*}
\hat{y} & \quad \cdots \quad y & \quad \cdots \quad \hat{z} \\
y_k+1 & \quad \cdots \quad y_k & \quad \cdots \quad z_{k+1} \\
y_{k-1} & \quad \cdots \quad y'_k & \quad \cdots \quad z_k \\
y_k & \quad \cdots \quad y'_k & \quad \cdots \quad z_{k-1} \\
\hat{x} & \quad \cdots \quad x_k & \quad \cdots \quad x_{k+1} \\
x_k & \quad \cdots \quad x_k & \quad \cdots \quad \hat{x}
\end{align*}
\]
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Hyperparameters Optimization (HPO)

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Discussion
HPO with HYPERNOMAD

- PhD project of Dounia Lakhmiri.
- We focus on the HPO of deep neural networks.
- Our advantages:
  - Blackbox optimization problem:
    
    \textit{One blackbox call = Training + validation + test, for a fixed set of hyperparameters.}
  - Presence of categorical variables \textit{(ex.: number of layers)}.
  - Existing methods are mostly heuristics
    \textit{(grid search, random search, GAs, etc.)}
- Based on the \textbf{NOMAD} implementation of MADS.
**Principle**

- **Initial parameters**
  - Dataset
  - Max number of evaluations

- **Construct the network**

- **Hyperparameters**
  - Number of conv layers,
  - learning rate,
  - batch size, etc.

- **Blackbox**
  - Training
  - Validation
  - Testing

- **NOMAD**
  - Look for a better point

- **New point**

- **Test accuracy**
HYPERNOMAD

- HYPERNOMAD is the interface between NOMAD and a deep learning platform.
- Based on the PyTorch library.
- Works with preexisting datasets such as MNIST or CIFAR-X, or on a custom data.
- Available at https://github.com/DouniaLakhmiri/HYPERNOMAD.

- We consider three types of hyperparameters:
  - Architecture of the neural network.
  - Optimizer.
  - Plus one for the size of mini-batches.

- Number of hyperparameters: \(5n_1 + n_2 + 10\).
Network architecture

A convolutional neural network is a deep neural network consisting of a succession of convolutional layers followed by fully connected layers:

Image from [Deshpande, 2019].
## Hyperparameters for the architecture \((5n_1 + n_2 + 4)\)

<table>
<thead>
<tr>
<th>Hyperparameter</th>
<th>Type</th>
<th>Scope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of convolutional layers ((n_1))</td>
<td>Categorical</td>
<td>[0, 20]</td>
</tr>
<tr>
<td>Number of output channels</td>
<td>Integer</td>
<td>[0, 50]</td>
</tr>
<tr>
<td>Kernel size</td>
<td>Integer</td>
<td>[0, 10]</td>
</tr>
<tr>
<td>Stride</td>
<td>Integer</td>
<td>[1, 3]</td>
</tr>
<tr>
<td>Padding</td>
<td>Integer</td>
<td>[0, 2]</td>
</tr>
<tr>
<td>Do a pooling</td>
<td>Boolean</td>
<td>0 or 1</td>
</tr>
<tr>
<td>Number of full layers ((n_2))</td>
<td>Categorical</td>
<td>[0, 30]</td>
</tr>
<tr>
<td>Size of the full layer</td>
<td>Integer</td>
<td>[0, 500]</td>
</tr>
<tr>
<td>Dropout rate</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td>Activation function</td>
<td>Categorical</td>
<td>ReLU, Sigmoid, Tanh</td>
</tr>
</tbody>
</table>
### Hyperparameters for the optimizer

<table>
<thead>
<tr>
<th>Optimizer</th>
<th>Hyperparameter</th>
<th>Type</th>
<th>Scope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stochastic Gradient Descent (SGD)</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Momentum</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Dampening</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td>Adam</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>$\beta_1$</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>$\beta_2$</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td>Adagrad</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Learning rate decay</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Initial accumulator</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td>RMSProp</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Momentum</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>$\alpha$</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0, 1]</td>
</tr>
</tbody>
</table>
Blocks of hyperparameters

- **Convolution block:** 2 convolutional layers with:
  - Number of output channels: 16, 7
  - Kernel size: 5, 3
  - Stride: 1, 1
  - Padding: 1, 1
  - Pooling: 0, 1

<table>
<thead>
<tr>
<th>Conv. 1</th>
<th>2</th>
<th>16</th>
<th>5</th>
<th>1</th>
<th>1</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conv. 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Fully connected block:** 3 fully connected layers with sizes of output = 1200, 512, 20:

<table>
<thead>
<tr>
<th>FC</th>
<th>3</th>
<th>1200</th>
<th>512</th>
<th>20</th>
</tr>
</thead>
</table>

- **Optimizer block:** SGD with learning rate = 0.1, momentum = 0.9, dampening = $1e^{-4}$, and weight decay = 0:

<table>
<thead>
<tr>
<th>Optimizer</th>
<th>1</th>
<th>0.1</th>
<th>0.9</th>
<th>$1e^{-4}$</th>
<th>0</th>
</tr>
</thead>
</table>
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The MADS algorithm with categorical variables

Hyperparameters Optimization (HPO)

Computational experiments

Discussion
## Average results on MNIST

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Avg accuracy on validation set</th>
<th>Avg accuracy on test set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rand. search [Bergstra and Bengio, 2012]</td>
<td>94.02</td>
<td>89.07</td>
</tr>
<tr>
<td>SMAC [Hutter et al., 2011]</td>
<td>95.48</td>
<td>97.54</td>
</tr>
<tr>
<td>RBFOpt [Diaz et al., 2017]</td>
<td>95.66</td>
<td>97.93</td>
</tr>
<tr>
<td>HYPERNOMAD</td>
<td><strong>97.54</strong></td>
<td><strong>97.95</strong></td>
</tr>
</tbody>
</table>

Best solution with HYPERNOMAD: 99.61%.
Results on CIFAR-10 (vs Hyperopt)

- Training with 40,000 images, validation/test on 10,000 images.
- One evaluation (training+test) \(\simeq\) 2 hours (i7-6700@3.4 GHz, GeForce GTX 1070).
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HYPERNOMAD: Library for the HPO problem.

Specialized for convolutional deep neural networks via the PyTorch library.

Key aspect: Optimize both the architecture and the optimization phase of a deep neural network.

Based on the blackbox optimization solver NOMAD and its ability to model categorical variables.

So far: Competitive results with state-of-the-art on the MNIST and CIFAR-10 datasets.

Future work: Expand the library to other types of problems than classification, provide interfaces to other libraries.

We thank G. Naniccini for his code and the NVIDIA GPU grant program.
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Algorithm 909: NOMAD: Nonlinear Optimization with the MADS algorithm.  