User Guide for autotune_nightly.py

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1 Program Description

- This script currently serves as part of the scripts that are running on a nightly basis for post-processing¹. Its primary purposes are to run an optimization algorithm, update an input file and record history so that the next nightly test will run a new iteration based on the updated input file. The corresponding outputs (timers, etc.) would be automatically extracted and recorded to the history file the next time calling this script, along with new input information for the next nightly test.
- This version utilizes random search in regards to the choice of parameters, i.e. each iteration is completely random from the previous ones.
- The current infrastructure focuses on tuning parameters from the ParameterList for two mySmoothers.
- Codes and relevant files are available at https://github.com/chkao831/ Autotuning/tree/main/autotune_nightly

2 Parameter Space

We currently focus on tuning parameters for two mySmoothers at a time. The input files are multiple-level nested YAML files, in which mySmoothers are represented in the form of

```
mySmoother1:

factory:

type: [TUNING FOCUS]

'smoother: pre or post':

ParameterList: [TUNING FOCUS]

mySmoother4:

factory:

type: [TUNING FOCUS]

'smoother: pre or post':

ParameterList: [TUNING FOCUS]
```

¹The real-time nightly tests produce a ctest json file that locates at either here: https://github.com/ikalash/ikalash.github.io/tree/master/ali/blake_nightly_data (CPU) or https://github.com/ikalash/ikalash.github.io/tree/master/ali/weaver_nightly_data (GPU)

The options that we enable for each smoothers are the following,

```
type: RELAXATION
   ParameterList:
3
       'relaxation: type': MT Gauss-Seidel
       'relaxation: sweeps': positive integer
       'relaxation: damping factor': positive real number
   type: RELAXATION
   ParameterList:
       'relaxation: type': Two-stage Gauss-Seidel
10
       'relaxation: sweeps': positive integer
11
       'relaxation: inner damping factor': positive real number
12
13
   type: CHEBYSHEV
14
   ParameterList:
15
       'chebyshev: degree': positive integer
16
       'chebyshev: ratio eigenvalue': positive real number
17
       'chebyshev: eigenvalue max iterations': positive integer
```

3 User Interface

The user would need to specify the input filename, the casename, the optimization algorithm, and the possible choices with ranges for each smoother in a file. A snapshot of a sample file called _properties.json follows,

```
"input": "input_albany_Velocity_MueLuKokkos_Wedge.yaml",
    "case": "humboldt-3-20km_vel_muk_wdg_tune_np1",
3
    "algorithm": "random_search",
    "mS1": {
5
        "type_options": ["Two-stage Gauss-Seidel", "MT Gauss-
            Seidel"], # CHEBYSHEV is disabled for mS1
        "relaxation: sweeps": {
6
            "inclusive_lower_bound": 1,
7
             "inclusive_upper_bound": 2
9
        "relaxation: damping factor": {
10
        # for MT Gauss-Seidel
11
                 "mean": 1,
12
                 "sd": 0.1,
13
                 "low": 0.8,
14
                 "upper": 1.2
        "relaxation: inner damping factor": {
17
        # for Two-stage Gauss-Seidel
18
                 "mean": 1,
19
                 "sd": 0.1,
20
                 "low": 0.8,
21
                 "upper": 1.2
22
23
24
        "chebyshev: degree": {
        \# since CHEBYSHEV is disabled for mS1, this is not used
                 "inclusive_lower_bound": 1,
```

```
"inclusive_upper_bound": 6
        },
28
        "chebyshev: ratio eigenvalue": {
29
        # not used
30
                 "inclusive_lower_bound": 10,
31
                 "inclusive_upper_bound": 50
32
33
        "chebyshev: eigenvalue max iterations": {
34
        # not used
35
                 "inclusive_lower_bound": 5,
36
                 "inclusive_upper_bound": 100
37
38
    }
39
    # "mS4" omitted due to the space constraint
40
```

Note that on line 5, only two types are listed – type: CHEBYSHEV is disabled for mySmoother1. Hence, the information from line 24-38 is not used (although they could still be listed). That being said, the user could also open up all three choices or simply enable only one choice.

If the specified type_options in the _properties.json file contains some string other than ["Two-stage Gauss-Seidel", "MT Gauss-Seidel", "CHEBYSHEV"], a ValueError("Type options are not defined by MT Gauss-Seidel, Two-stage Gauss-Seidel or CHEBYSHEV") would be raised.

In terms of the range, inclusive_lower_bound and inclusive_upper_bound define the range for integers within [inclusive_lower_bound, inclusive_upper_bound], inclusively.

In addition, mean, sd, low, and upper define the range for real numbers derived from that of a normally distributed continuous random variable, truncated to the range [low, upper], with distribution mean and standard deviation of mean and sd respectively.

4 Prerequisites

In addition to the properties file such as _properties.json, under the working directory, one needs

- An input yaml file that is listed in _properties.json
- ctest output files, starting from the second run
- to pip install pandas, ruamel.yaml, and scikit-learn

5 Command Line Usage

```
$ python3 autotune_nightly.py --help
usage: autotune_nightly.py [-h] properties_file
ctest_output_file
3
```

```
positional arguments:
properties_file parameter space definition (.json)
ctest_output_file ctest output filename (.json)

poptional arguments:
-h, --help show this help message and exit
```

For example, with

\$ python3 autotune_nightly.py _properties.json ctest-20210520.json, the 2nd argument _properties.json points to the properties file; the 3rd argument ctest-20210520.json specifies the output file from which the output information (such as timers) are extracted for evaluation.

However, for the first iteration of this script (#iter_id=0), the ctest argument is useless, as there's no nightly test run yet. In this case, the user could input any filename with .json extension to this required argument, but whatever it is, the argument would not be used.

If the specified case in the _properties.json file cannot be found from the ctest output file that is called in command line, a ValueError: The casename is not found in the ctest output file would be raised.

6 Simulation

For the first run (#iter_id=0), as there's no history file available, the script would simply update the input yaml file with a set of updated parameters by the optimization algorithm. By the end of this iteration, a history file [case]_hist.csv is created and the updated input parameters are written to file. Meanwhile, a copy of the input yaml file is saved, called [input]_0.yaml, where input corresponds to the yaml filename from _properties.json and 0 specifies the #iter_id. An example is as follows,

\$ python3 autotune_nightly.py _properties.json any_name.json

A dataframe is printed to the command line, as illustrated above. The last three entries, time_NOX, time_AlbanyTotal and passed, are temporarily set to None by the end of this iteration, since no nightly test is run yet.

 $\label{time_NOX} \textbf{ is defined as NOX Total Linear Solve + NOX Total Preconditioner Construction. time_AlbanyTotal is the Albany Total Time from the ctest output file.}$

Then, for the next-day iteration, given that the history file [case] hist.csv preexists, an output ctest json file should have been generated based on the previously-updated input file. As an example, let the output ctest file be ctest-20210520.json,

```
$ python3 autotune_nightly.py _properties.json ctest -20210520.json
```

From the first row of the dataframe, we could see that the timer data and a boolean that indicates test pass/fail of iteration 0 is extracted from ctest-20210520.json. At the same time, the updated input parameters are generated for the next round of nightly test.

This is repeated on a nightly basis.

7 Deliverables

7.1 [case]_hist.csv

Starting from the first run (#iter_id=0), a history file in csv format would be generated. The iteration id, updated input parameters, and corresponding output results are written to the file.

If the ctest does not pass for an experiment, the value of inf would be put to time_NOX and time_AlbanyTotal because not timer data is available for evaluation. In such cases, passed = FALSE.



Figure 1: (Example) humboldt-3-20km_vel_muk_wdg_tune_np1_hist.csv

7.2 [case]_hist_sorted.csv

Starting from the second run (#iter_id=1), a history file in csv format would be generated. It contains the same information as [case]_hist.csv does, except that it differs in row order – instead of ordering by #iter_id=0, 1, 2..., the experiments are sorted in ascending order by time_NOX.

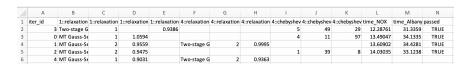


Figure 2: (Example) humboldt-3-20km_vel_muk_wdg_tune_np1_hist_sorted.csv

From here, we see that the experiment with #iter_id=3 achieves the best performance in terms of time_NOX(=12.28761).

7.3 [input]_Best.yaml

At every iteration, we have checked to see if the current iteration is better than all past iterations. If true, we update <code>[input]_Best.yaml</code> with the inputs from the current iteration.

To verify that the output matches,

diff input_albany_Velocity_MueLuKokkos_Wedge_3.yaml input_albany_Velocity_MueLuKokkos_Wedge_Best.yaml

This displays no difference in both files.

A Complete Command Line Sample