

Hyperspace benchmarks for ver. 1.2.1

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1 Introduction

The three benchmark setups are:

- §2.1 „Donut” — described in the original paper [1, Fig. 6(a)&(b)];
- §2.2 „Double Donut” — described in the original paper [1, Fig. 6(c)&(d)];
- §2.3 „Wurst” — see the code for all details (`Tests/AllTest>testIntegrateWurst` and `Tests/+hstest/+wurst/initRandWurst.m`).

Important All benchmarks were run using default values for all internal parameters of the methods. There was no method fine-tuning per a test case.

Note Additionally, I've benchmarked few sample size splits among the three integration steps: 1. adaptive out-of-equilibrium MCMC exploration; 2. ellipsoids cover expansions, and 3. MC ellipsoids cover-based sampling (for volume estimation and cost integration). The best one over all case-studies is shown here.

1.1 How to reproduce

Run:

```
runtests('AllTest');
```

with the following adjustments in the `Tests/AllTest.m` file:

```
function tests = AllTest()
    ...
    tests = functiontests({@setupOnce, @teardownOnce, @setup, @teardown, ...
        @testIntegrateDonut, @testIntegrateDoubleDonut, @testIntegrateWurst});
    ...
end
...
function setupOnce(testCase)
```

```

...
% bulk integration: benchmarking setup
s.dim_vec = [2 5 10 15];
s.nfeval_vec = [5e4 1e5 2e5 5e5];
s.volRelErrTol = 0;
s.nrep = 4;
s.saveMat = true;
s.parallelize = true;
s.nfevalProportionsArray = [...  

    4 5 1;...  

    3 5 2;...  

    3 6 1;...  

    2 7 1;  

]; % function evaluations proportions for MCexp, ELexp and Volint  

testCase.TestData.bulk = s;  

...
end

```

1.2 Setup

Tests results presented here were run overnight in 4 parallel MATLAB pool threads in the following setup:

```

Name: 'Intel(R) Core(TM) i7-3615QM CPU @ 2.30GHz'
Clock: '2300 MHz'
Cache: '256 KB'
NumProcessors: 4
OSType: 'Mac OS/X'
OSVersion: '10.10.5'
MATLABVersion: '8.3.0.532 (R2014a)'

```

Note Plots were done using MATLAB R2015b.

2 Benchmark results

2.1 Donut

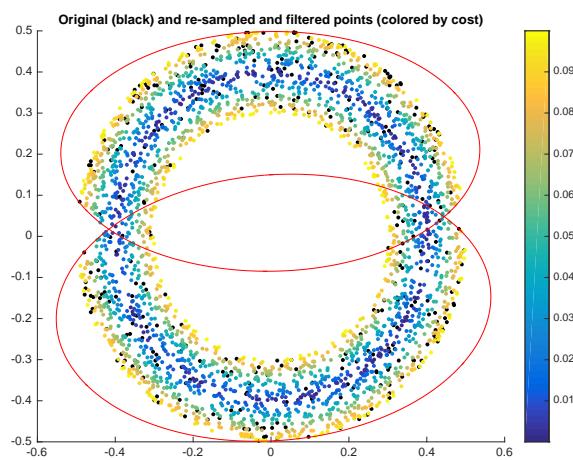


Figure 2.1.1: 2-D „Donut” sample and ellipsoid cover after running OEAMC+MEBS+Volint.

Sample proportions (OEAMC+MEBS+Volint): 40%+50%+10%

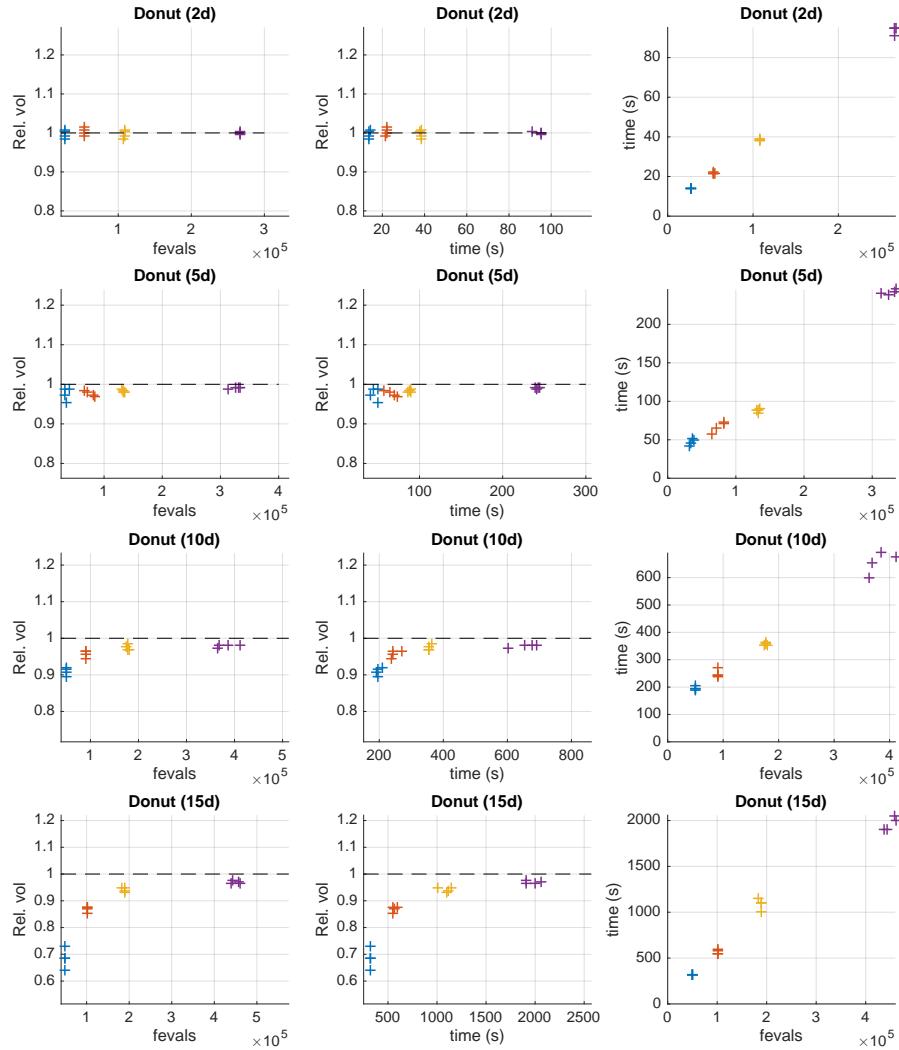


Figure 2.1.2: „Donut” benchmark results for different dimensions and sample sizes after running `OEAMC+MEBS+Volint`, with given sample split proportions.

2.2 Double Donut

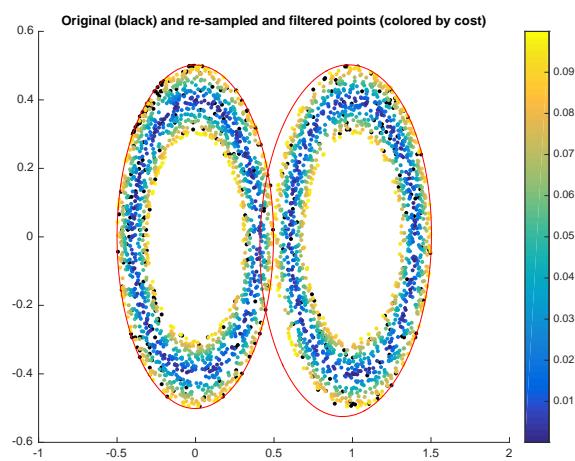


Figure 2.2.1: 2-D „Double Donut” sample and ellipsoid cover after running OEAMC+MEBS+Volint.

Sample proportions (OEAMC+MEBS+Volint): 40%+50%+10%

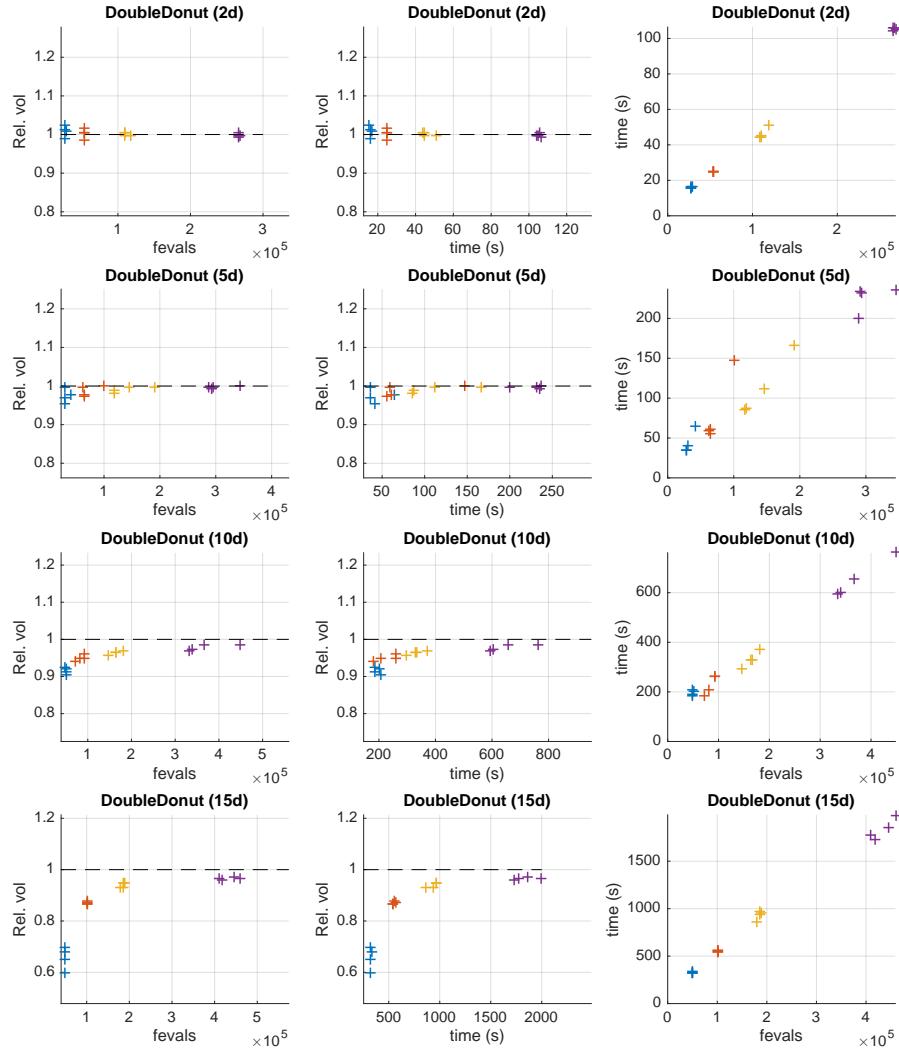


Figure 2.2.2: „Double Donut” benchmark results for different dimensions and sample sizes after running `OEAMC+MEBS+Volint`, with given sample split proportions.

2.3 Wurst

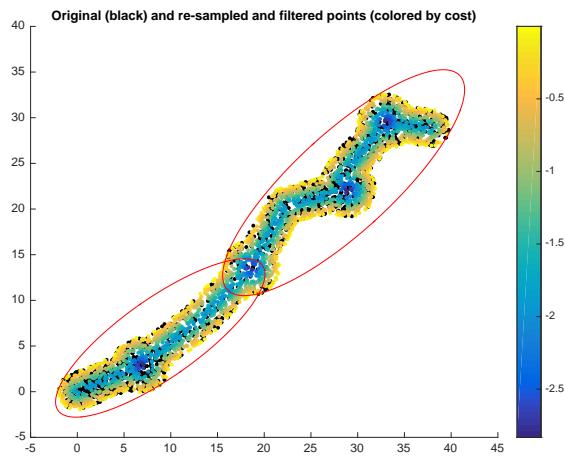


Figure 2.3.1: 2-D „Wurst” sample and ellipsoid cover after running OEAMC+MEBS+Volint.

Sample proportions (OEAMC+MEBS+Volint): 40%+50%+10%

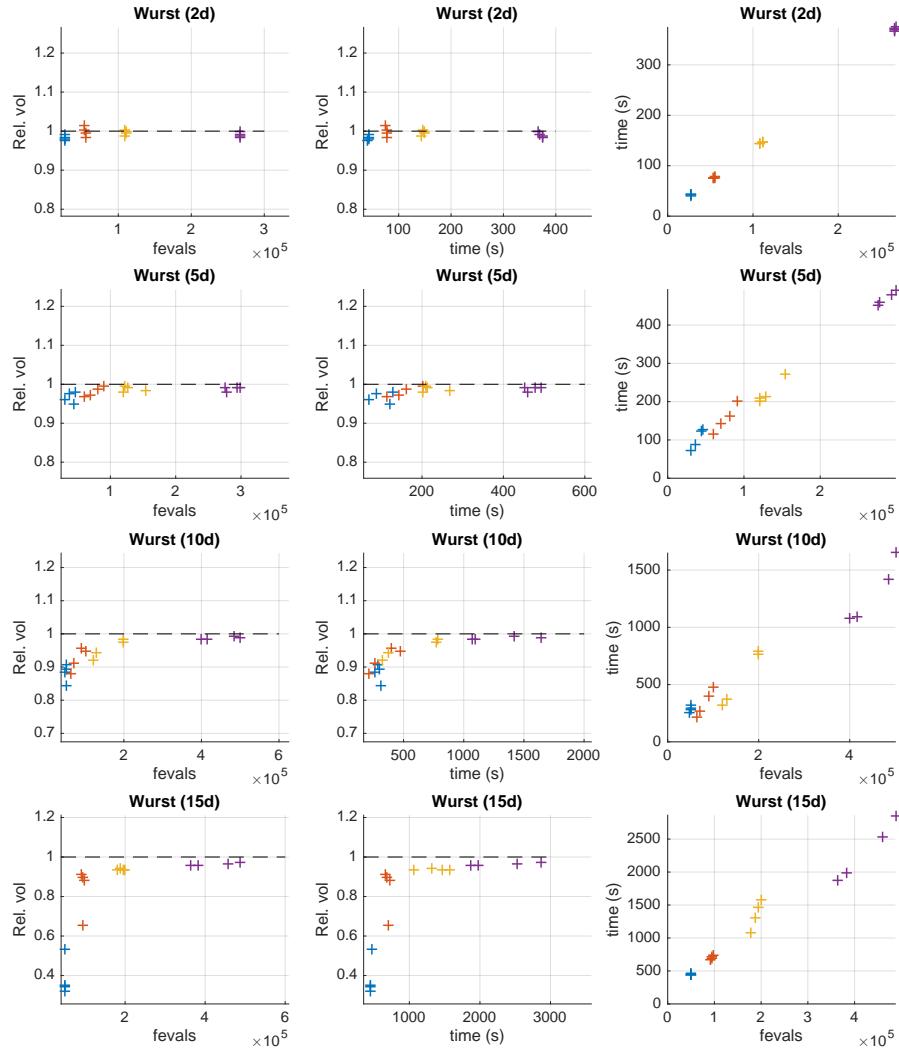


Figure 2.3.2: „Wurst” benchmark results for different dimensions and sample sizes after running `OEAMC+MEBS+Volint`, with given sample split proportions.

3 Conclusions

Hyperspace package does well, recovering even the 15-D „Wurst”. Running time of less than 1h, although not spectacular, is sufficiently small with respect to what would be a time of evaluation of relatively fast cost function which would run in ca. 0.1 sec, for a complex enough viable space (with more than $2 \cdot 10^5$ evaluations it is over 5.5h net total time of just cost function evaluations).

The more complex the viable space shape the more MCMC (OEAMC) samples are needed to get good seeds for the ellipsoids expansion via sampling (MEBS). Once, the ellipsoids fill well the viable volume, integration can be done with relatively few samples (min. tested: 10%). In particular, for the „Donut” case-study, the 40-50-10 % sample split was not the best, but it was good-enough and the best for the most complex „Wurst” case-study.

References

- [1] Elías Zamora-Sillero, Marc Hafner, Ariane Ibig, Joerg Stelling, and Andreas Wagner. Efficient characterization of high-dimensional parameter spaces for systems biology. *BMC Systems Biology*, 5:142, 2011.