apsis

Automated Hyperparameter Optimization Using Bayesian Optimization

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March 10, 2015

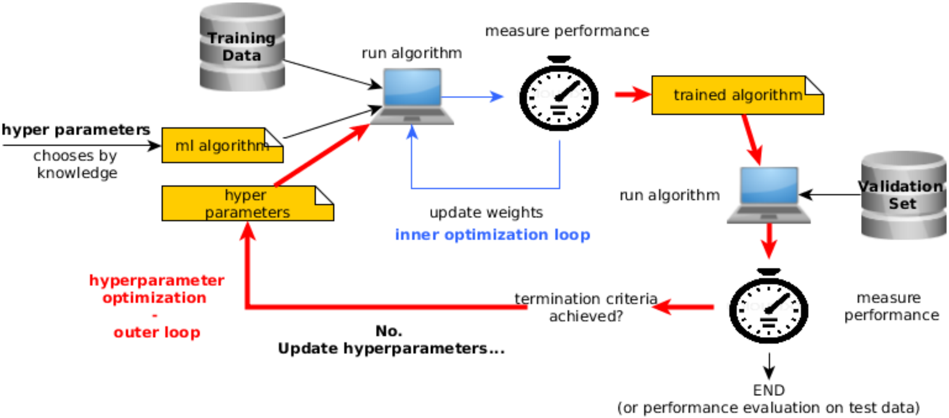
AGENDA

MOTIVATION

Why Hyperparameter Optimization and why automating it?

- hyperparameter tuning often leads to huge performance gain
- "more of an art than a science"
- reproducibility of published results
- automatic methods might be better than humans
- provide ml algorithms to non-expert users

ML PROCESS OVERVIEW



FORMAL PROBLEM DESCRIPTION

$$
\begin{aligned}
\lambda &: \text{hyperparameter vector } \lambda = (\lambda^{(1)}, ..., \lambda^{(n)}) \\
L(X, f) &: \text{loss function evaluated for model } f \text{ and dataset } x \\
A_\lambda(X) &: \text{learning algorithm with hyperparameter vector } \lambda \\
& \text{ learning on dataset } X \\
X_{\text{train}} &: \text{training data, } X_{\text{valid}} : \text{validation data, } X_{\text{test}} : \text{ test data} \\
\Psi(\lambda) &: \text{hyperparameter response function/surface}
\end{aligned}
$$

Hyperparameter Optimization Problem

$$
\hat{\lambda} \approx \underset{\lambda \epsilon \Lambda}{\operatorname{argmin}} \underbrace{\left(\underset{X_i \in X_{\text{valid}}}{\text{mean}} \left(L(x_i, A_\lambda(X_{\text{train}})) \right) \right)}_{\Psi(\lambda)} \tag{1}
$$

$$
= \underset{\lambda \epsilon \Lambda}{\operatorname{argmin}} \left(\Psi(\lambda) \right) \tag{2}
$$

KEY PROBLEM PROPERTIES

- unknown, probably non-convex response surface Ψ
- no derivative-based optimization possible

- every evaluation of Ψ is expensive
- evaluation time of Ψ depends on individual value of λ

- low effective dimensionality of Ψ
- which dimensions are important is dataset dependent

- tree-structured configuration space[1]

[1] not addressed in *apsis* yet

State of the Art

- optimization still manual in many projects
- grid search most common method
  - often the only provided method by many ml frameworks
- random search
- bayesian optimization
  - code of Jasper Snoek et. al. Harvard/Toronto
  - whetlab - bay opt in the cloud

Bayesian Optimization

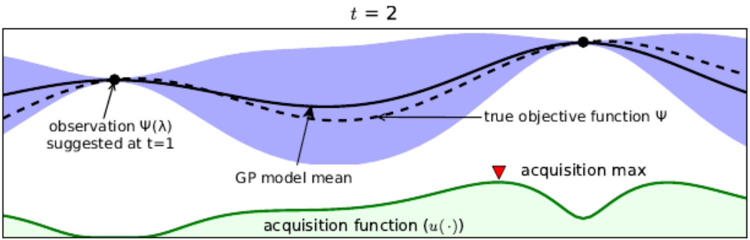
- approximate $\Psi(\lambda)$ by a *surrogate* function $M(\lambda) = y$
- surrogate function cheaper to evaluate than Ψ
- interpret model to find minimization candidates for Ψ
- evaluate Ψ for promising candidates

Bayesian Optimization Fundamentals

We need two design choices

- Surrogate Modelling Function - Gaussian Processes
  - universal approximation
  - very flexible and have many useful properties
  - closed under sampling
- Acquisition Function
  - Probability of Improvement
  - Expected Improvement

ACQUISITION FUNCTION u



- measures the expected utility of evaluating the objective function at a point λ_{next}
- exploitation vs. exploration trade-off

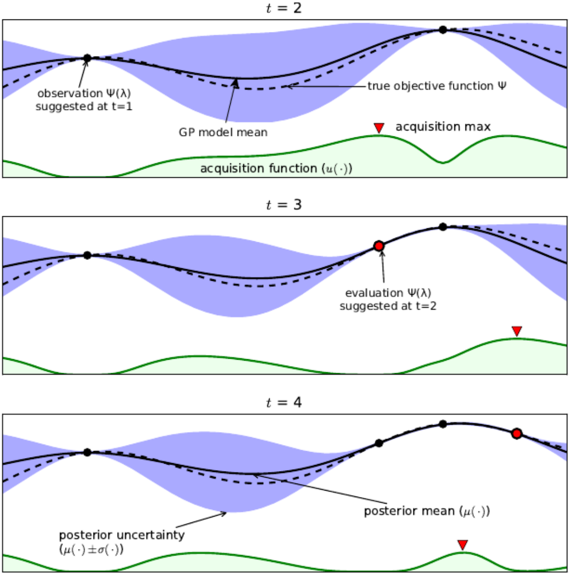
(picture adopted from [1])

Optimization - successively updating the GP

1. find

$$\max_{\lambda}(u(\lambda)) = \lambda_{\text{next}}$$

   max of acquisition
2. Evaluate M at λ_{next}
3. Update the GP



(picture adopted from [1])

Fitting the GP to the problem

by tuning the covariance!

- Squared Exponential Kernel

$$K_{SE}(\lambda, \lambda') = \exp\left(-\frac{1}{2l^2} \cdot \sum_{1..\dim(D)} (\lambda_d - \lambda'_d)^2\right)$$

- use Automatic Relevance Determination (ARD)

$$K_{SE}(\lambda, \lambda') = \theta_0 \cdot \exp\left(-\frac{1}{2} \cdot \sum_{1..\dim(D)} \left(\frac{1}{{\theta_d}^2}(\lambda_d - \lambda'_d)^2\right)\right)$$

with ARD vector $\boldsymbol{\theta}$

$$\theta = (\underbrace{\theta_0}_{\text{bias}}, \underbrace{\theta_1, \ldots, \theta_d}_{\text{dimension weights}})$$

How do acquisition functions look like?

Expected Improvement (EI)

$$u_{\mathrm{EI}}(\lambda) = \int_{-\infty}^{\infty} max(\Psi(\lambda^*) - y, 0) \cdot p_M(y|\lambda)\, dy$$

- closed form solution for GPs available

$$u_{\mathrm{EI}}(\lambda|M_t) = \sigma(\lambda) \cdot \left(\frac{f(\lambda^*) - \mu(\lambda)}{\sigma(\lambda)} \cdot \Phi(\lambda) + \phi(\lambda) \right)$$

- gradient analytically derived in *apsis* for more effective optimization

THE *apsis* TOOLKIT

Automated Hyperparameter Optimization Framework for

- random search
- bayesian optimization

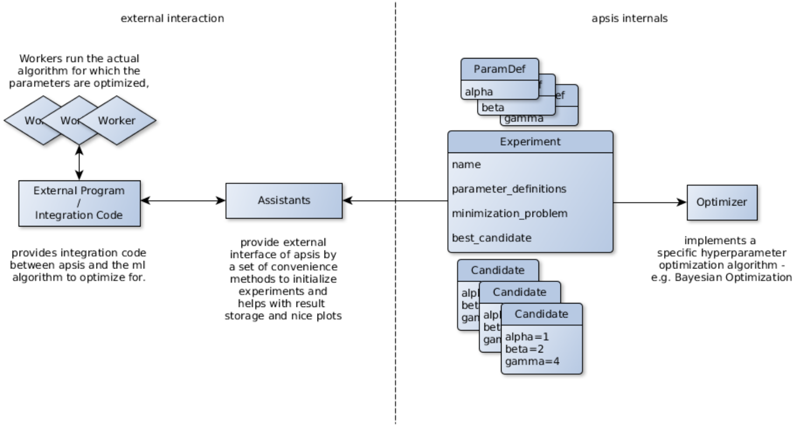
as an open source framework featuring

- flexible architecture, ready to be extended for more optimizers
- ready for use with scikit-learn and theano
- implemented in Python

Project Objectives

- open source implementation of state of the art research in bayesian optimization
- extendible project to encourage collaboration with other researchers
- easy integration with existing machine learning frameworks
- multi core support

apsis Architecture Overview



apsis Core Model Components

Parameter Definitions

- define the meta information for each hyperparameter

Candidates

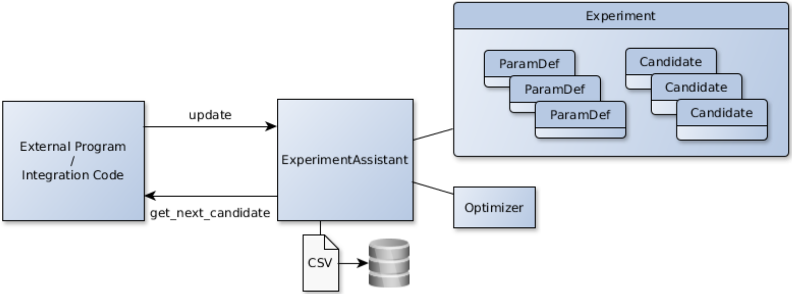
- represent a specific hyperparameter vector and its value
- holds function value if available

Experiments

- represent an optimization object
- keeps track of finished and unfinished Candidates

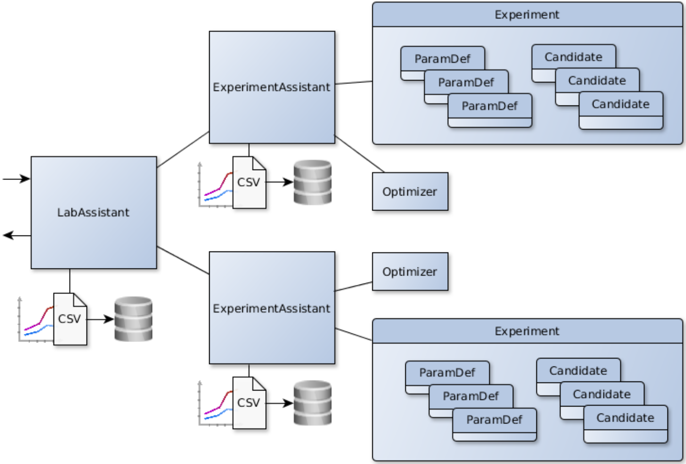
USING *apsis* - EXPERIMENT ASSISTANTS

- single experiment interaction interface
- provides plots and result bookkeeping



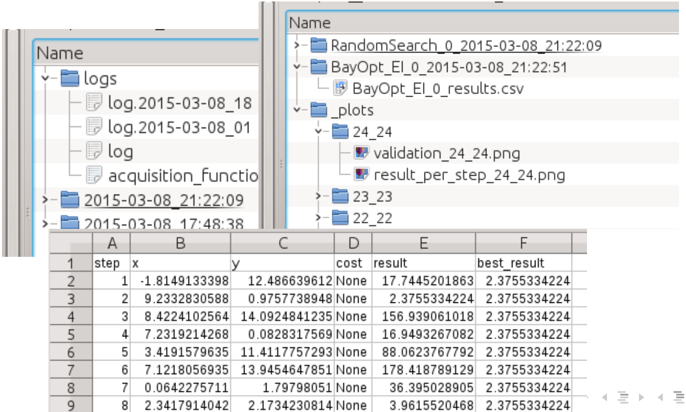
USING *apsis* - LAB ASSISTANTS

- multiple experiments to compare different optimization techniques
- cross validation



Extensive Experiment Tracking

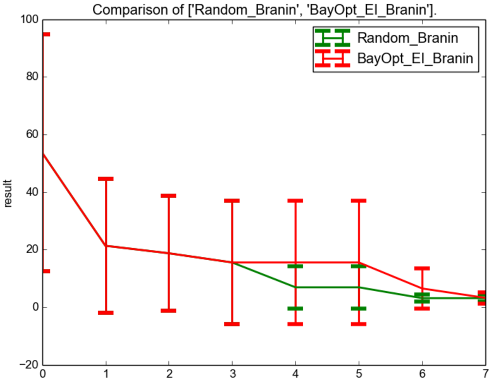
- automated plot writing
- automated results writing
- write out information at every step



	A	B	C	D	E	F
1	step	x	y	cost	result	best_result
2	1	-1.8149133398	12.486639612	None	17.7445201863	2.3755334224
3	2	9.2332830588	0.9757738948	None	2.3755334224	2.3755334224
4	3	8.4224102564	14.0924841235	None	156.939061018	2.3755334224
5	4	7.2319214268	0.0828317569	None	16.9493267082	2.3755334224
6	5	3.4191579635	11.4117757293	None	88.0623767792	2.3755334224
7	6	7.1218056935	13.9454647851	None	178.418789129	2.3755334224
8	7	0.0642275711	1.79798051	None	36.395028905	2.3755334224
9	8	2.3417914042	2.1734230814	None	3.9615520468	2.3755334224

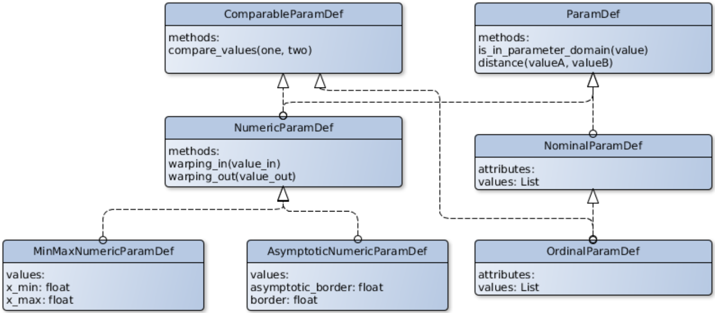
Automated Plotting

- plot function evaluations and best results
- plot confidence bars when using cross validation
- write out plots at every step



PARAMETER REPRESENTATION IN *apsis*

- different representation by parameter type
- various nominal and numeric types



NUMERIC PARAMETERS IN *apsis*

Warping Mechanism

- parameters are warped into $[0, 1]$ interval
- optimization core can assume a uniform and equal distribution in $[0, 1]$ space
- warping can be user defined

Provided Warpings for

- normalization of arbitrary intervals $[a, b]$ into $[0, 1]$ space.
- asymptotic parameters, e.g. learning rate asymptotic at 0

Nominal Parameters in *apsis*

- generally supported in *apsis*
- no support in Bayesian Optimization
- GP kernels based on distance metrics between parameters

- interesting topic for further research
- no publications on this topic so far
- whetlab pretends to deal well with them - but doesn't say how

Expected Improvement Optimization

- gradient analytically derived[2]
- 1000 Steps Random Search for Initialization
- Several iterative optimization methods integrated
  - L-BFGS-B Bounded Low Memory Quasi Newton Method
  - BFGS Quasi Newton Method
  - Nelder-Mead
  - Inexact Newton with Conjugate Gradient Solver
  - ...

[2] See our paper for derivation.

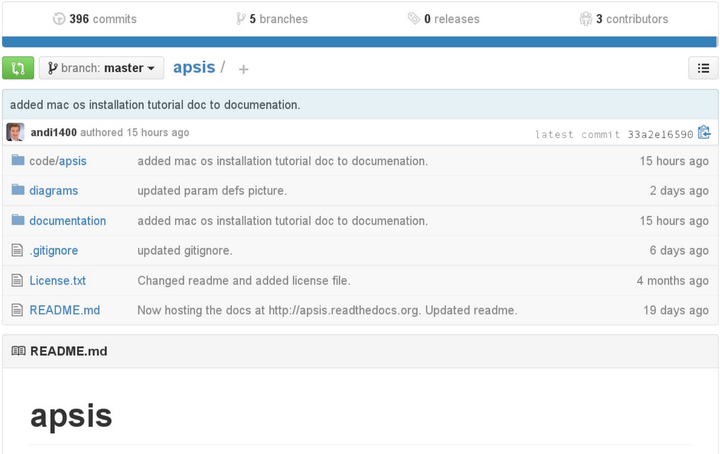
Dealing with GP Hyperparameters

- the GP surrogate model introduces new hyperparameter
  - not subject of optimization $\Rightarrow$ hyper-hyperparameters
- optimization by maximum likelihood method
- integrating over these parameters in the acquisition function using Hybrid Monte Carlo sampling

apsis Project Set Up

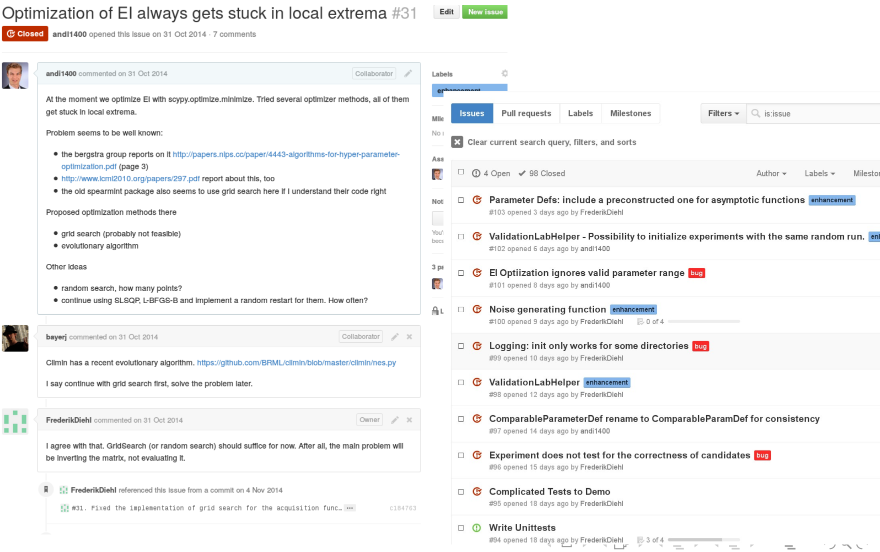
- Open-Source project from the beginning
- MIT-License
- active issue tracking
- PEP-8 code styling convention
- Fully automated sphinx documentation build on every commit
- 90% test coverage
- clear commit messages

apsis GITHUB REPOSITORY



Check out `http://github.com/FrederikDiehl/apsis`!

Issue Tracking and Discussion



UNIT TESTS

```
[fred@fred-W540 apsis]$ nosetests --with-coverage --cover-package apsis
/usr/lib/python2.7/site-packages/GPy/util/linalg.py:48: UserWarning: warning: caught this exception:'module' object has no attribute '_dotblas'
  warnings.warn("warning: caught this exception:" + str(e))
..................................
Name                                              Stmts   Miss  Cover   Missing
-------------------------------------------------------------------------------
apsis                                                 0      0   100%
apsis.assistants                                      0      0   100%
apsis.assistants.experiment_assistant               114      3    97%   199, 283, 354
apsis.assistants.lab_assistant                      230     30    87%   268, 424-444, 490-491, 535, 576, 597-601, 622-625, 750-762
apsis.demos                                           1      0   100%
apsis.demos.demo_MNIST                               56     19    66%   40, 43-47, 50, 70, 85, 93-96, 99, 110, 118, 120-133, 136
apsis.demos.demo_MNIST_MCMC                          19      4    79%   34, 36-38, 41
apsis.models                                          0      0   100%
apsis.models.candidate                               51      0   100%
apsis.models.experiment                             126      3    98%   357-359, 405
apsis.models.parameter_definition                   171     22    87%   34, 41-42, 81, 337, 346-350, 448-453, 474, 476, 483-488
apsis.optimizers                                      0      0   100%
apsis.optimizers.bayesian                             1      0   100%
apsis.optimizers.bayesian.acquisition_functions     201     15    93%   59, 74-75, 131-137, 295, 393-395, 460-461, 484, 494, 509, 542
apsis.optimizers.bayesian_optimization               87      1    99%   223
apsis.optimizers.optimizer                           21     11    48%   26, 45, 63-66, 82-87
apsis.optimizers.random_search                       28      0   100%
apsis.utilities                                       0      0   100%
apsis.utilities.file_utils                            4      0   100%
apsis.utilities.import_utils                          9      3    67%   24-27
apsis.utilities.logging_utils                        28      0   100%
apsis.utilities.optimizer_utils                      12      2    83%   36-37
apsis.utilities.plot_utils                           69     12    83%   62, 65, 104-107, 177, 224, 246, 257, 262, 266
apsis.utilities.randomization                        12      2    83%   20, 23
-------------------------------------------------------------------------------
TOTAL                                              1240    127    90%
----------------------------------------------------------------------
Ran 34 tests in 70.357s

OK
```

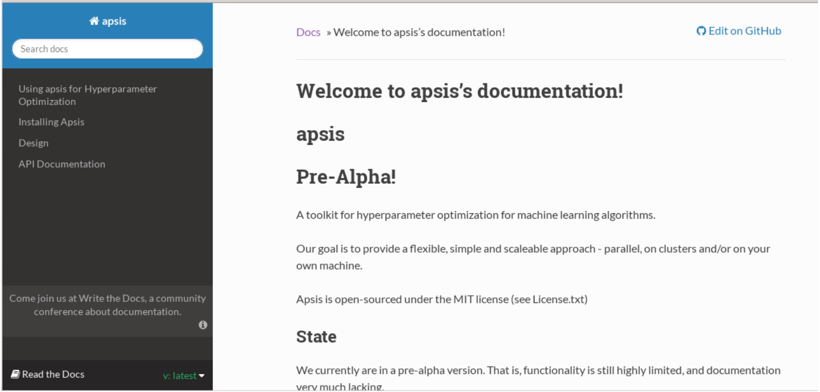
- 90% overall test coverage
- 100% in most core components

Good Code Documentation

```
http://cloc.sourceforge.net v 1.62  T=0.16 s (224.5 files/s, 33127.1 lines/s)
-------------------------------------------------------------------------------
Language                     files          blank        comment           code
-------------------------------------------------------------------------------
Python                          36            865           2039           2408
-------------------------------------------------------------------------------
SUM:                            36            865           2039           2408
-------------------------------------------------------------------------------
```

- almost 50:50 ratio of code vs. doc
- documented according to sphinx standard

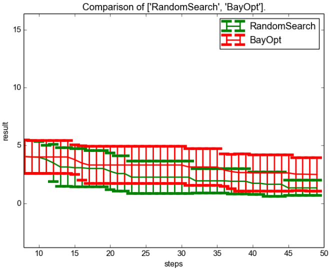
Fully automated documentation build



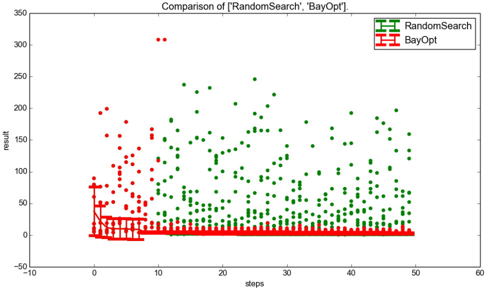
- builds on every commit

Visit `http://apsis.readthedocs.org` !

Branin Hoo Optimization



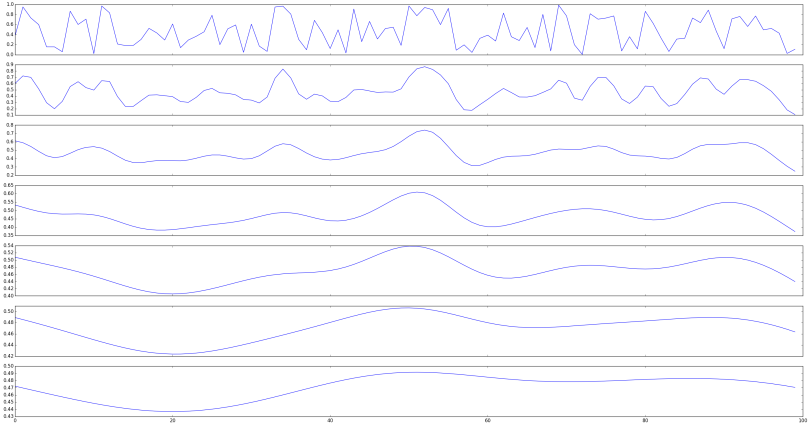
Best Value by Optimizer



Values by Optimizer

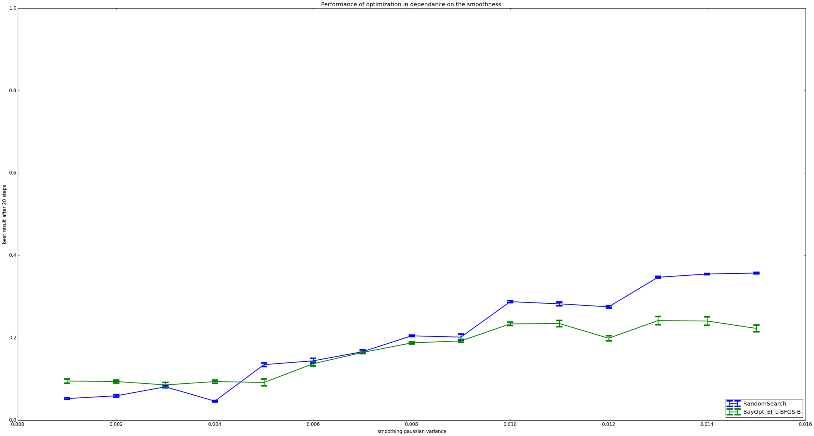
- random search finds better end result but bay opt is more stable
- similar performance as in other bay opt literature
- no other group publishes comparison to random search

Optimizing Artificial Noise Function



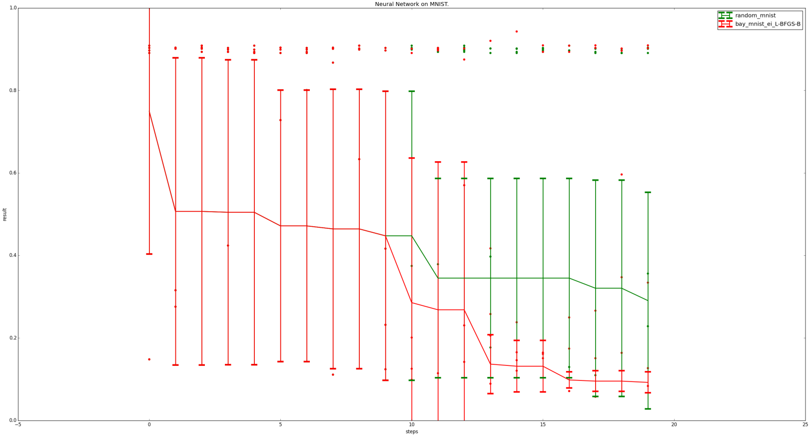
One dimensional noise function with several smoothing variances

Optimizing Artificial Noise Function



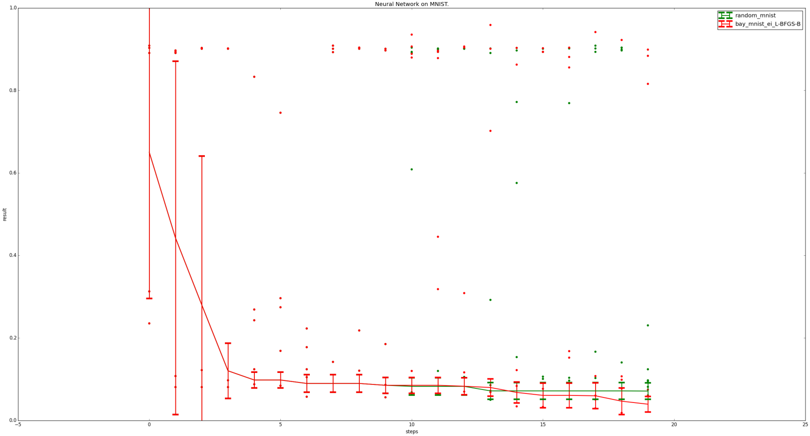
Minimization result on 3d noise by smoothing factor.

BREZE MNIST NEURAL NETWORK



Neural Network on MNIST using uniform parameters

BREZE MNIST NEURAL NETWORK (2)



Neural Network on MNIST using asymptotic parameters for learning rate and learning rate decay

Taking the project to the next Level - Program

- implement full multicore support
- implement a REST web-service to offer interoperability with any language
- improve integration of matplotlib

Taking the project to the next Level - Bayesian Optimization

- deal with nominal parameters
- try replacing GPs with Student-t processes
- try to take tree structured configuration space into account
- account for evaluation cost depending on hyperparameter setting
- implement freeze-thaw optimization idea [3]
- automated learning of input warping [2]

Thank You!

References I

Eric Brochu, Vlad M. Cora, and Nando de Freitas.
A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning.
IEEE Transactions on Reliability, abs/1012.2, 2010.

Jasper Snoek, Kevin Swersky, Richard S Zemel, and Ryan P Adams.
Input warping for bayesian optimization of non-stationary functions.
arXiv preprint arXiv:1402.0929, 2014.

Kevin Swersky, Jasper Snoek, and Ryan Prescott Adams.
Freeze-thaw bayesian optimization.
arXiv preprint arXiv:1406.3896, 2014.

References II