Open science software development

Tim Head

28 September 2017

Tim Head
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@betatim

Personal

Pragmatic

Problematic

Code for your latest paper

IMPROVING *GAIA* PARALLAX PRECISION WITH A DATA-DRIVEN MODEL OF STARS

LAUREN ANDERSON,[1] DAVID W. HOGG,[1,2,3,4] BORIS LEISTEDT,[2,5]
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[8] *Alfred P. Sloan Fellow*

ABSTRACT

Converting a noisy parallax measurement into a posterior belief over distance requires inference with a prior. Usually this prior represents beliefs about the stellar density distribution of the Milky Way. However, multi-band photometry exists for a large fraction of the *Gaia TGAS* Catalog and is incredibly informative about stellar distances. Here we use *2MASS* colors for 1.4 million *TGAS* stars to build a noise-deconvolved

data-driven photometric parallaxes, built with Gaia and 2MASS

143 commits | 1 branch | 0 releases | 4 contributors

Branch: master | New pull request | Create new file | Upload files | Find file | Clone or download

davidwhogg tweaks — Latest commit 4a8d72e 28 days ago

paper	arxiver	3 months ago
presentation	tweaks	28 days ago
toy	paper figure updates	4 months ago
README.md	readme	4 months ago
comparePrior.py	plot tweaks;	4 months ago
demo_plots.py	tweaks	4 months ago
drawEllipse.py	splitting directories	4 months ago
dustDiff.py	splitting directories	4 months ago
plots.py	last tweaks	4 months ago
stellarTwins.py	added stellar twins	4 months ago
testXD.py	paper figure updates	4 months ago
tightPosterior.py	tweaks	4 months ago

README.md

photoParallax

Capitalizing on the simplicity of stars for *good*.

authors

- **Lauren Anderson** (Flatiron)

splatlab / cqf

Watch 7 | Star 29 | Fork 3

Code | Issues 0 | Pull requests 0 | Projects 0 | Wiki | Insights

A General-Purpose Counting Filter: Counting Quotient Filter

7 commits | 1 branch | 0 releases | 1 contributor | BSD-3-Clause

Branch: master | New pull request | Create new file | Upload files | Find file | Clone or download

prashantpandey Merge branch 'master' of github.com:splatlab/cqf — Latest commit 0f937c7 on Apr 12

LICENSE	Initial commit	8 months ago
Makefile	Added an alternate implementation of select on machine words to work ...	6 months ago
README.md	Update README.	6 months ago
gqf.c	Fixing a small assertion bug in the CQF.	6 months ago
gqf.h	Adding code for the CQF.	8 months ago
main.c	Adding code for the CQF.	8 months ago

README.md

cqf

A General-Purpose Counting Filter: Counting Quotient Filter (CQF)

Overview

The CQF supports approximate membership testing and counting the occurrences of items in a data set. This general-purpose AMQ is small and fast, has good locality of reference, scales out of RAM to SSD, and supports deletions, counting (even on skewed data sets), resizing, merging, and highly concurrent access.

API

- 'qf_insert(item, count)': insert an item to the filter

Why do it?

- Making source code available helps your ideas spread faster
- More people will understand what you did
- Sharing your code will raise your profile
- Basically free, no promise of support or further development

Recent uploads

August 30, 2017 (v2) | Working paper | Open Access

View

Introducing Parsl: A Python Parallel Scripting Library

Babuji, Yadu; Brizius, Alison; Chard, Kyle; Foster, Ian; Katz, Daniel S.; Wilde, Michael; Wozniak, Justin

Researchers frequently rely on large-scale and domain-specific workflows to conduct their science. These workflows may integrate a variety of independent software functions and external applications. However, developing and executing such workflows can be difficult, requiring complex...

Uploaded on September 15, 2017

1 more version(s) exist for this record

September 6, 2017 (v4) | Software | Open Access

View

geodynamics/pylith: PyLith v2.2.1

Brad Aagaard; Charles Williams; Matthew Knepley; Eric Heien

Added new examples. examples/3d/subduction: New suite of examples for a 3-D subduction zone. This intermediate level suite of examples illustrates a wide range of PyLith features for quasi-static simulations. examples/2d/subduction: Added quasi-static spontaneous rupture earthquake cycle...

Uploaded on September 6, 2017

3 more version(s) exist for this record

August 31, 2017 (v1) | Figure | Open Access

View

Fig. 1 in Vanmanenia orcicampus ı a new species of loach from the Plain of Jarsı Laos (Teleostei: Gastromyzontidae)

Maurice Kottelat

generation	move and update conversion script	5 months ago
models	default to better path and only one file	5 months ago
.gitignore	add 3d viz + move notebooks to analysis/	5 months ago
LICENSE	Create LICENSE	3 months ago
README.md	Update README.md	a month ago

README.md

CaloGAN

Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks.

This repository contains what you'll need to reproduce M. Paganini (@mickypaganini), L. de Oliveira (@lukedeo), B. Nachman (@bnachman), *CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks* [arXiv:1705.02355].

You are more than welcome to use the open data and open-source software provided here for any of your projects, but we kindly ask you that you please cite them using the DOIs provided below:

Asset	Location
Training Data (GEANT4 showers, ⊥ to center)	DOI 10.17632/pvn3xc3wy5.1
Source Code (this repo!)	DOI 10.5281/zenodo.584155

For any use of paper ideas and results, please cite

```
@article{paganini_calogan,
      author         = "Paganini, Michela and de Oliveira, Luke and Nachman,
                        Benjamin",
      title          = "{CaloGAN: Simulating 3D High Energy Particle Showers in
                        Multi-Layer Electromagnetic Calorimeters with Generative
                        Adversarial Networks}",
      year           = "2017",
      eprint         = "1705.02355"
```

Please destroy this software after publication. kthxbye.

tl;dr? A while back I wrote that there are three uses of research software: replication, reproduction, and reuse. The world of computational science would be better off if people clearly delineated whether or not they wanted anyone else to reuse their software, and I think it's a massive mistake to expect that everyone's software should be reusable.

Fri 17 April 2015
By C. Titus Brown
In science.
tags: software sustainability

A few months back, I reviewed a pretty exciting paper - one I will probably highlight on my blog, when it comes out. The paper outlined a fairly simple concept for comparing sequences and then used that to develop some new ultra-scalable functionality. The theory seemed novel, the computational results were pretty good, and I recommended acceptance (or minor revisions). This was in spite of the fact that the authors stated quite clearly that they had produced largely unusable software.

Other reviewers were not quite so forgiving, however -- one reviewer declined to review the paper until they could run the software on their own data.

What does successful software look like?

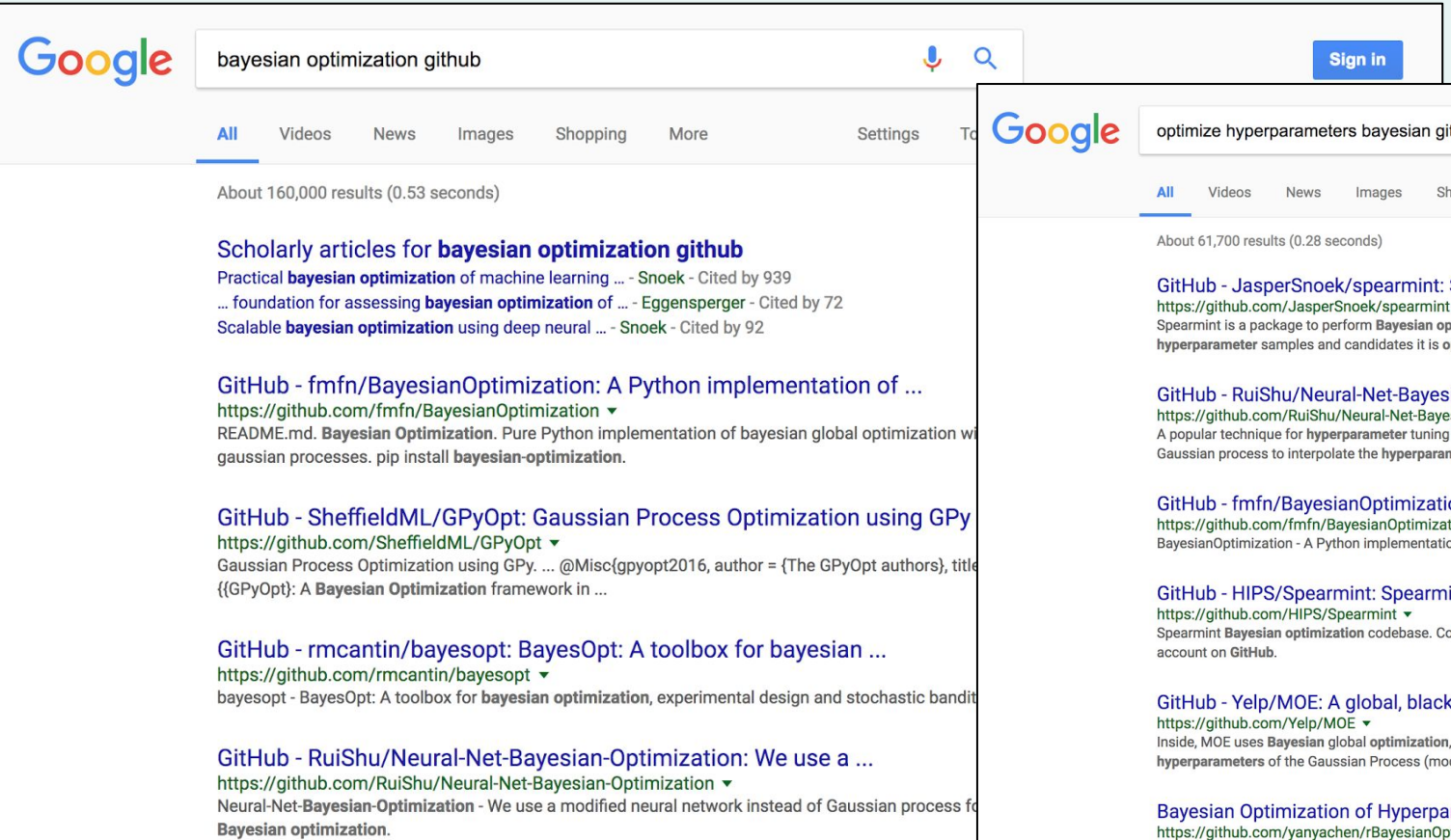
Plan A - join someone else

How to find existing projects?

- Ask a friend
- Ask google
- Specialist websites like libraries.io

Ask a friend

How to find other projects?

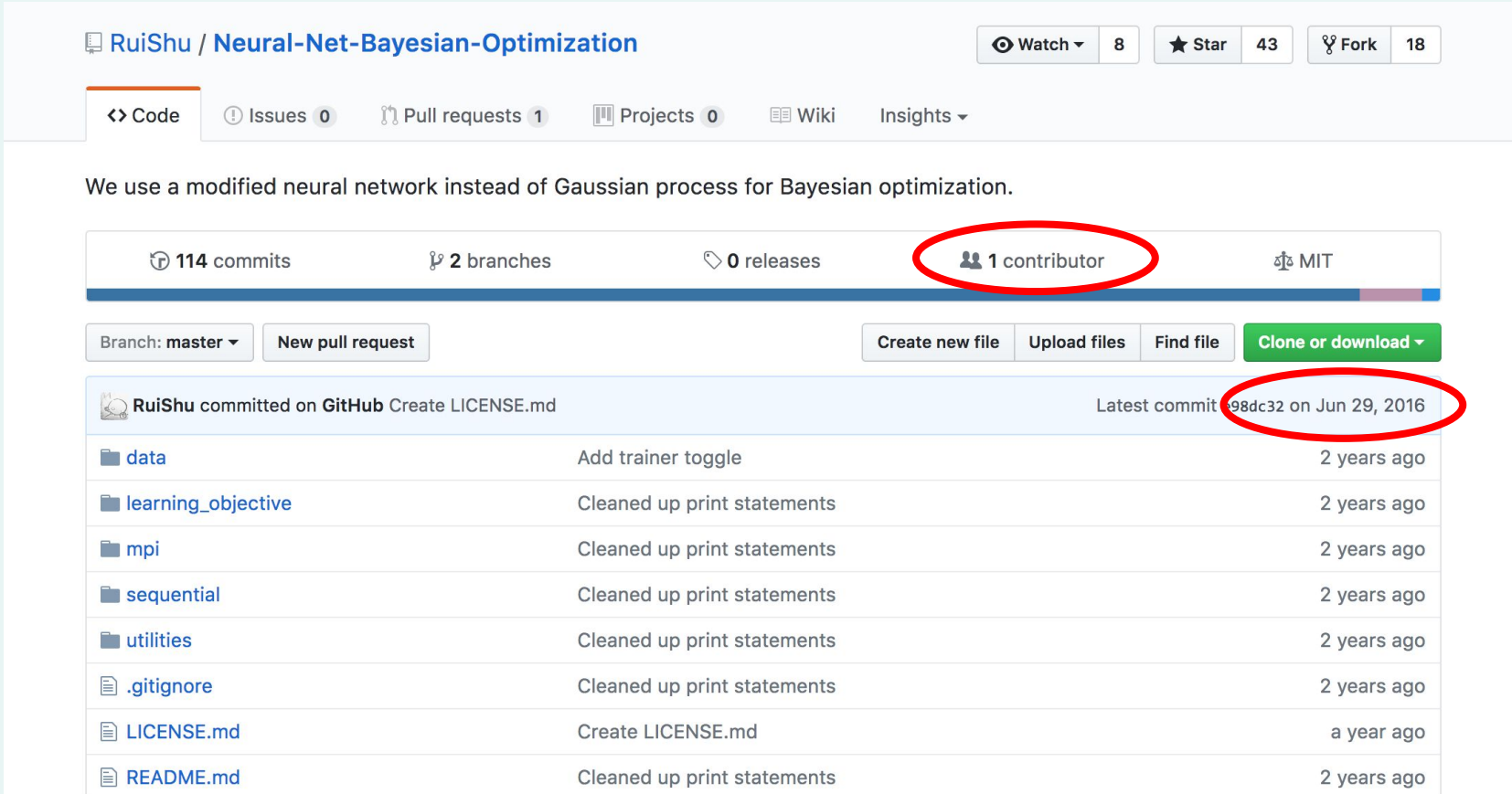


How to choose?

How to choose between all the options?

- Do I know someone else who is using it?
- Works well with what I already have?
- Can I modify it?
- Does it look “good”?
- Documentation and examples?
- How can I get help?
- Is the project still alive?

How to choose between the options?



RuiShu / Neural-Net-Bayesian-Optimization

Watch 8 | Star 43 | Fork 18

Code | Issues 0 | Pull requests 1 | Projects 0 | Wiki | Insights

We use a modified neural network instead of Gaussian process for Bayesian optimization.

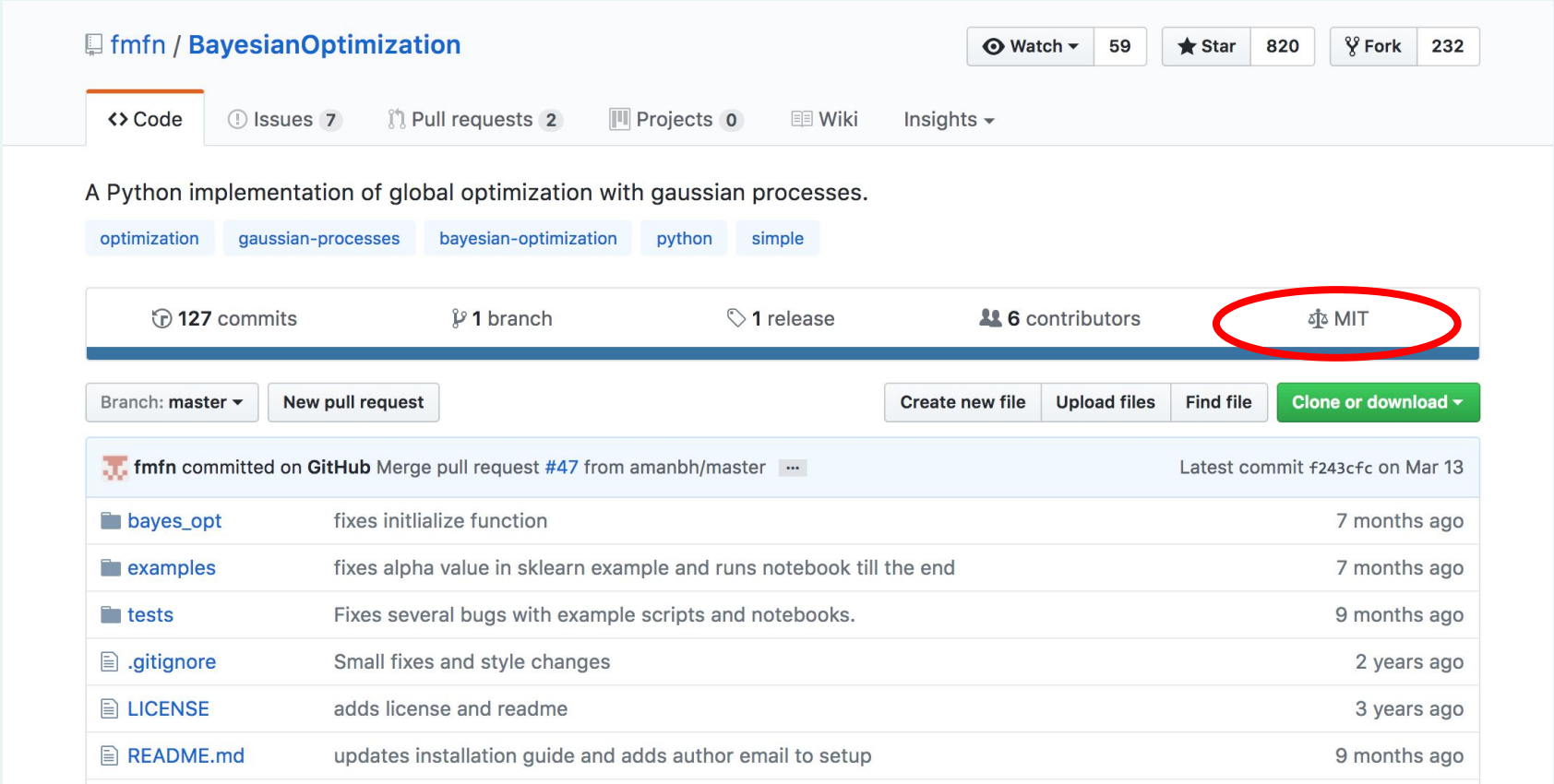
114 commits | 2 branches | 0 releases | 1 contributor | MIT

Branch: master | New pull request | Create new file | Upload files | Find file | Clone or download

RuiShu committed on GitHub Create LICENSE.md — Latest commit 98dc32 on Jun 29, 2016

data	Add trainer toggle	2 years ago
learning_objective	Cleaned up print statements	2 years ago
mpi	Cleaned up print statements	2 years ago
sequential	Cleaned up print statements	2 years ago
utilities	Cleaned up print statements	2 years ago
.gitignore	Cleaned up print statements	2 years ago
LICENSE.md	Create LICENSE.md	a year ago
README.md	Cleaned up print statements	2 years ago

How to choose between the options?



How to choose between the options?

README.md

Bayesian Optimization

Pure Python implementation of bayesian global optimization with gaussian processes.

```
pip install bayesian-optimization
```

This is a constrained global optimization package built upon bayesian inference and gaussian process, that attempts to find the maximum value of an unknown function in as few iterations as possible. This technique is particularly suited for optimization of high cost functions, situations where the balance between exploration and exploitation is important.

Quick Start

In the examples folder you can get a grip of how the method and this package work by:

- Checking out this notebook with a step by step visualization of how this method works.

How to choose between the options?

####Setting up Spearmint

STEP 1: Installation

1. Install python, numpy, scipy, pymongo. For academic users, the anaconda distribution is great. Use numpy 1.8 or higher. We use python 2.7.
2. Download/clone the spearmint code
3. Install the spearmint package using pip: `pip install -e \</path/to/spearmint/root\>` (the -e means changes will be reflected automatically)
4. Download and install MongoDB: https://www.mongodb.org/
5. Install the pymongo package using e.g., pip `pip install pymongo` or anaconda `conda install pymongo`

STEP 2: Setting up your experiment

1. Create a callable objective function. See `./examples/simple/branin.py` as an example
2. Create a config file. There are 3 example config files in the ../examples directory. Note 1: There are more parameters that can be set in the config files than what is shown in the examples, but these parameters all have default values. Note 2: By default Spearmint assumes your function is noisy (non-deterministic). If it is noise-free, you should set this explicitly as in the ../examples/simple/config.json file.

STEP 3: Running spearmint

1. Start up a MongoDB daemon instance:
   `mongod --fork --logpath <path/to/logfile\> --dbpath <path/to/dbfolder\>`
2. Run spearmint: `python main.py \</path/to/experiment/directory\>`

STEP 4: Looking at your results

Spearmint will output results to standard out / standard err. You can also load the results from the database and manipulate them directly.

How to get unstuck?

How to get help?

- In general people love to help.
- Show that you tried to help yourself.
- People are volunteering their time, respect it.
- Grammar and spelling, srsly.
- Make a simple example https://stackoverflow.com/help/mcve

People like helping,

...

How to get help?

jupyter nbviewer

JUPYTER FAQ

GPyOpt / manual

GPyOpt: armed bandits optimiza

Written by Javier Gonzalez, University of Sheffi

Last updated Monday, 14 March 2016.

In this notebook we will see how to do armed bandits optimizati
use data of weather forecasts at weather stations across more t
United States. The project OpenWeatherMap project provides a
information and at that dataset it is possible to find the weather
this notebook we will use the file target_day_20140422.dat that
for each station in the United States for the April 22, 2014. The l
stations is available as well as the forecasts for the next 7 days.

We start by loading the packages that we will need in out analys

In [1]:
```
%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
import numpy as np
```

scikit learn

Home Installation Documentation Examples Google Custom Search

Previous 7. Computatio... Next Plotting Cros...

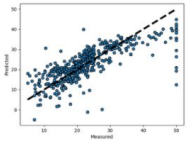
scikit-learn v0.19.0
Other versions

Please cite us if you use the software.

- General examples
- Examples based on real world datasets
- Biclustering
- Calibration
- Classification
- Clustering
- Covariance estimation
- Cross decomposition
- Dataset examples
- Decomposition
- Ensemble methods
- Tutorial exercises
- Feature Selection
- Gaussian Process for Machine Learning
- Generalized Linear Models
- Manifold learning

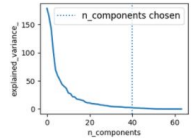
General examples

General-purpose and introductory examples for the scikit.

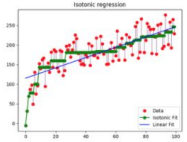


Plotting Cross-Validated Predictions

Concatenating multiple feature extraction methods



Pipelining: chaining a PCA and a logistic regression

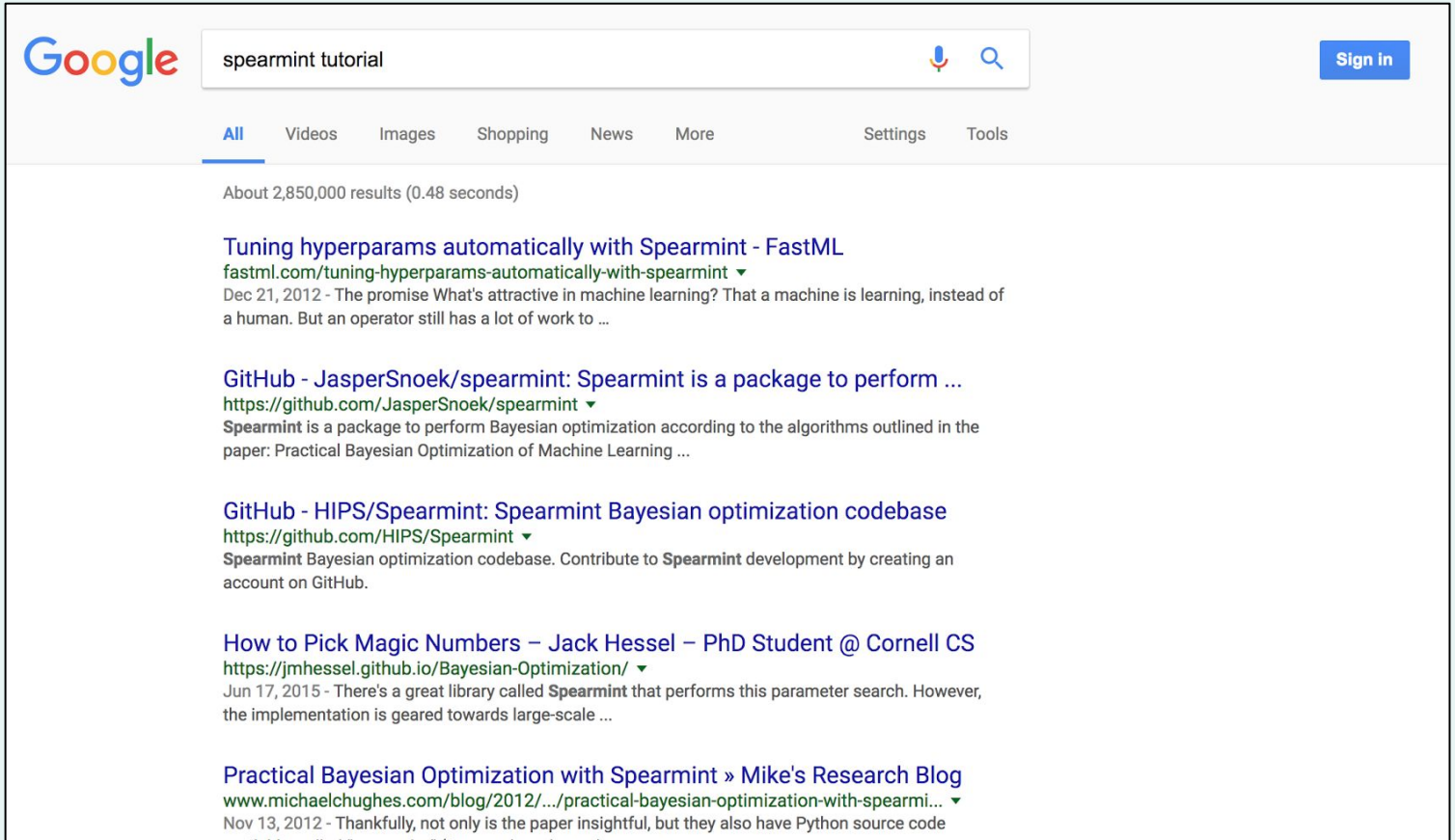


Isotonic Regression

Imputing missing values

Face completion with a

How to get help?



Don’t ask for help when you are angry.

Grammur and Speeling. Srsly.

Contribute back?

How to contribute?

- Learn the mechanics of working in a team
- Make your changes official so you don’t have to keep modifying code
- Get reputation and credit for your work
- Mentorship from (world) experts on the topic
- Meet interesting people

I am too busy ...

scikit-learn / scikit-learn

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Code Issues 901 Pull requests 578 Projects 5 Wiki Insights

[MRG+1] Document oob estimates of RandomForest* and Bagging* #4489

Edit

Merged **glouppe** merged 2 commits into `scikit-learn:master` from `betatim:rf-oob-docs` on Apr 2, 2015

Conversation 4 Commits 2 Files changed 1 +6 −1

betatim commented on Apr 2, 2015 Contributor

Added a sentence each to the RandomForest* and Bagging* sections of the narrative documentation mentioning how to enable out-of-bag estimates of the generalisation error. This is meant to fix #4290

betatim added some commits on Apr 2, 2015

- Mention oob_score in narrative documentation of RandomForest* `fd3c630`
- Mention oob_score in the narrative docs for Bagging* `88811be`

glouppe changed the title from **Document oob estimates of RandomForest* and Bagging*** to **[MRG+1] Document oob estimates of RandomForest* and Bagging*** on Apr 2, 2015

glouppe commented on Apr 2, 2015 Owner

Reviewers
No reviews

Assignees
No one assigned

Labels
None yet

Projects
None yet

Milestone
No milestone

scikit-learn / scikit-learn

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Code Issues 901 Pull requests 578 Projects 5 Wiki Insights

[MRG+1] Document oob estimates of RandomForest* and Bagging* #4489

Edit

Merged glouppe merged 2 commits into `scikit-learn:master` from `betatim:rf-oob-docs` on Apr 2, 2015

Conversation 4 Commits 2 Files changed 1

Changes from all commits Jump to... +6 −1 Unified Split Review changes

7 doc/modules/ensemble.rst No coverage View

```
@@ -65,7 +65,9 @@ taking as input a user-specified base estimator along with parameters
 specifying the strategy to draw random subsets. In particular, ``max_samples``
 and ``max_features`` control the size of the subsets (in terms of samples and
 features), while ``bootstrap`` and ``bootstrap_features`` control whether
-samples and features are drawn with or without replacement. As an example, the
+samples and features are drawn with or without replacement. When using a subset
+of the available samples the generalization error can be estimated with the
+out-of-bag samples by setting ``oob_score=True``. As an example, the
 snippet below illustrates how to instantiate a bagging ensemble of
 :class:`KNeighborsClassifier` base estimators, each built on random subsets of
```

scikit-learn / scikit-learn

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Code | Issues 901 | Pull requests 578 | Projects 5 | Wiki | Insights

[MRG + 2] Rename scorers like `mse` to `neg_mse` #7261

Edit

Merged **GaelVaroquaux** merged 15 commits into `scikit-learn:master` from `betatim:negative-scorers` on Sep 8, 2016

Conversation 99 | Commits 15 | Files changed 9 | +112 −45

betatim commented on Aug 27, 2016 • edited — Contributor

Reference Issue

Fixes #2439

What does this implement/fix? Explain your changes.

Renaming scorers for which smaller is better (like MSE) to `neg_mse` so that they fit the idea of "bigger is better".

Reviewers

No reviews

Assignees

No one assigned

Labels

Blocker

Creating software is a craft,
be an apprentice.

nilearn - examples are reproducible science

http://nilearn.github.io/auto_examples/02_decoding/plot_miyawaki_reconstruction.html

Plan B - write your own

Choices and preliminary things

- Make it extremely focussed, one small part of your PhD thesis, that lots of people want
- What is the mission of your project?
- Persuade a friend to join you

scikit-optimize:

- *easy to install*
- *good documentation*
- *expensive, black-box functions*

Manoj, Gilles and Tim

Getting started, from zero to one

Keep it simple.
Very simple.

Simple
code base

Quality is free

style.py

```
1  import sys, random
2  import os
3  print('one'); print('two')
4
5  x = 3
6  y = 3.141
7  if x == 1: print('one')
8
9  if abs(x) > 3 and y % 2 == 0:
10     print('woah!')
11 def myfunc():
12     rando = random.random()
13     return random.randint(0,100)
14
15 def multiply  (x,y) :
16     return x *  y
17
18 print(multiply(myfunc(), myfunc()))
19
```

E231 — missing whitespace after ','

Discuss code changes with someone

From one to ten

Get users!

How do others choose between all the options?

- Do I know someone else who is using it?
- Works well with what I already have?
- Can I modify it?
- Does it look “good”?
- Documentation and examples?
- How can I get help?
- Is the project still alive?

How do others profit when they contribute?

How do others get help?

Read the Docs v: latest

Welcome to Sphinx-Gallery's documentation!

A Sphinx extension that builds an HTML gallery of examples from any set of Python scripts.

It is extracted from the scikit-learn project and aims to be an independent general purpose extension.

The code of the project is on Github: Sphinx-Gallery

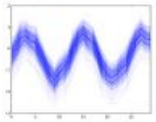
Why Sphinx-Gallery?

- Simple examples that run out of the box are the best way to learn a library
- Pleasing, organized, visual layouts
- Links, searching, backlinks throughout examples and documentation

What does it look like?

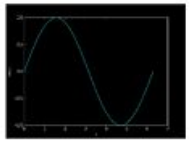
Here is an example gallery generated from a few Python scripts.

Examples using `numpy.sin`



Seaborn example

Plotting simple sin function



Plotting simple sin function on a black background

Here we put only the examples of our gallery that use a specific function. This display granularity

Automate things

About pytest

pytest is a mature full-featured Python testing tool that helps you write better programs.

Table Of Contents

pytest: helps you write better programs

The `pytest` framework makes it easy to write small tests, yet scales to support complex functional testing for applications and libraries.

An example of a simple test:

```
# content of test_sample.py
def inc(x):
    return x + 1

def test_answer():
    assert inc(3) == 5
```

To execute it:

```
$ pytest
======= test session starts ========
platform linux -- Python 3.x.y, pytest-3.x.y, py-1.x.y, pluggy-0.x.y
rootdir: $REGENDOC_TMPDIR, inifile:
collected 1 item

test_sample.py F

======= FAILURES ========
_______ test_answer ________

    def test_answer():
>       assert inc(3) == 5
E       assert 4 == 5
E        +  where 4 = inc(3)

test_sample.py:5: AssertionError
------- 1 failed in 0.12 seconds --------
```

From ten to infinity

What if you left now?

Distributed leadership: Mozilla Open Leadership Training

Summary

Don’t maintain code

Join an existing project

This is a long term investment

??!?

Tim Head
tim@wildtreetech.com
@betatim

More reading

- https://opensource.guide/
- https://mozilla.github.io/leadership-training/
- Can I modify it?
- Does it look “good”?
- Documentation and examples?
- How can I get help?
- Is the project still alive?

Tim Head
tim@wildtreetech.com
@betatim