The SHOGUN Machine Learning Toolbox

(let's get started)

Sören Sonnenburg

(for the SHOGUN Team)

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Who Am I?

About Me

- 1997-2002 studied Computer Science
- 2002-2009 doing ML & Bioinformatics research at Fraunhofer Institute FIRST and Max Planck Society
- 2008 PhD: Machine Learning for Genomic Sequence Analysis
- 2009-2011 Researcher at Berlin Institute of Technology
- 2011- TomTom R&D

Open Source Involvement

- Debian Developer `http://www.debian.org`
- Machine Learning OSS `http://mloss.org`
- Machine Learning Data `http://mldata.org`
- **Initiator of SHOGUN - this talk**

More about me `http://sonnenburgs.de/soeren`

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What is Machine Learning and what can it do for you?

What is ML?

AIM: Learning from empirical data!

Applications

- speech and handwriting recognition
- search engines, natural language processing
- medical diagnosis, bioinformatics, chemoinformatics
- detecting credit card fraud
- computer vision, object recognition
- stock market analysis
- network security, intrusion detection
- brain-machine interfaces

...

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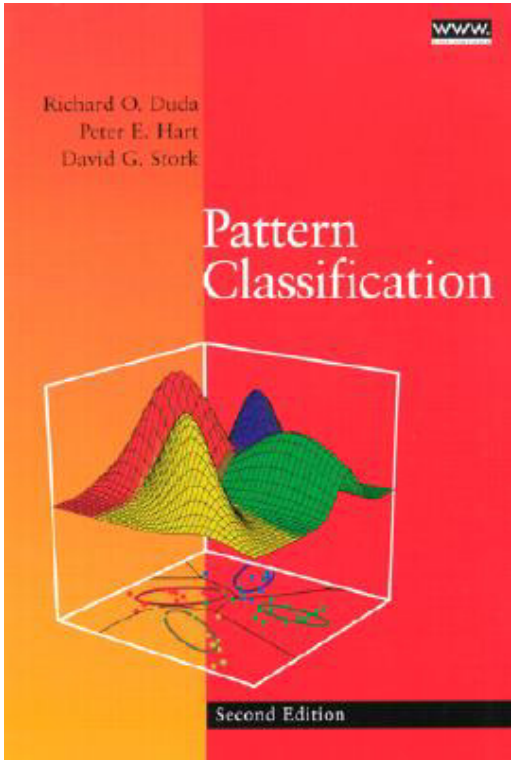
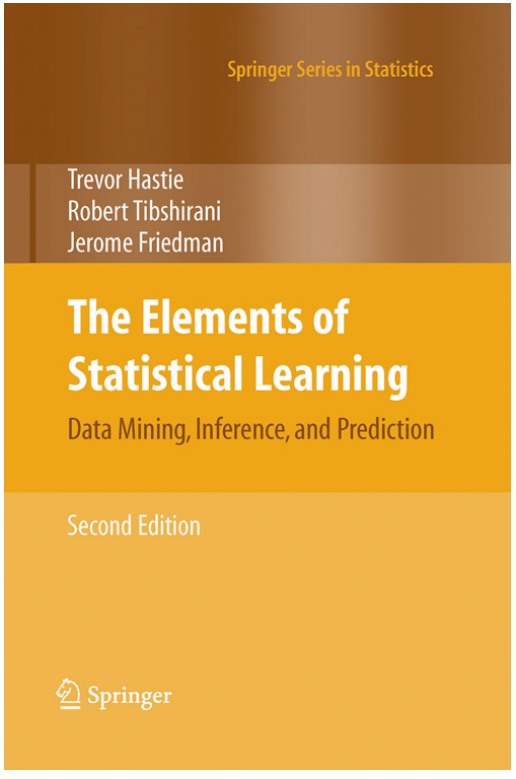
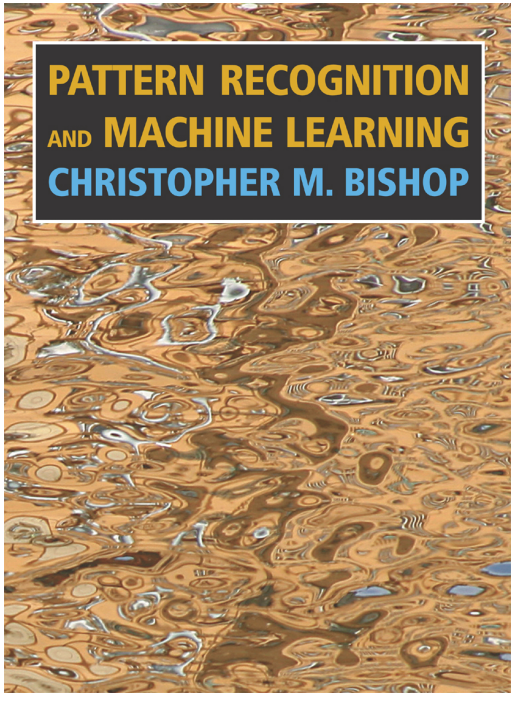
Books on Machine Learning







. . . **and many more** . . .

SHOGUN Machine Learning Toolbox History

History

1999	Roots in my student research project *Hidden Markov Model for Genome Analysis*
2001	Framework for Kernels, and SVMs (with G. Rätsch) architectures linux, solaris, ospf1 alpha cluster first interface (cmdline)
2002-2005	Developed at Fraunhofer FIRST under the name **gf**
2006	First public release (June) under (SHOGUN) based on the initators first names S. Sonnenburg and G. Rätsch
2008	used in 3rd party code (PyVMPA)
2011-2013	Part of Google Summer of Code

Current Core Developers

Core Developers

- Fernando Iglesias (since GSoC 2012)
- Heiko Strathmann (since GSoC 2011)
- Sergey Lisitsyn (since GSoC 2011)
- Sören Sonnenburg
- Viktor Gal (since GSoC 2012)

By now

- $> 20,000$ commits
- $> 240,000$ lines of code
- over 1100 examples
- from 96 contributors

SHOGUN Main Features and Focus

Machine Learning Methods Overview

- Regression
- Distributions
- Dimension Reduction
- Performance Measures
- Clustering
- Classification
- Structured Output Learning
- Transfer Learning
- Model Selection

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Focus

Unified (large-scale) learning for various feature types and settings

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SHOGUN Machine Learning Toolbox

Implementation and Interfaces

- Implemented in C++
- **Interfaces:** libshogun, python, octave, R, matlab, cmdline, lua, ruby, java, csharp
- **Over 1100 examples**
- Doxygen documentation
- Inline python documentation (e.g. `help(GaussianKernel)`)
- **Testsuite** ensuring that obvious bugs do not slip through

Continuity

Due to being GPLv3'd it survived policy changes at the authors institute and job changes.

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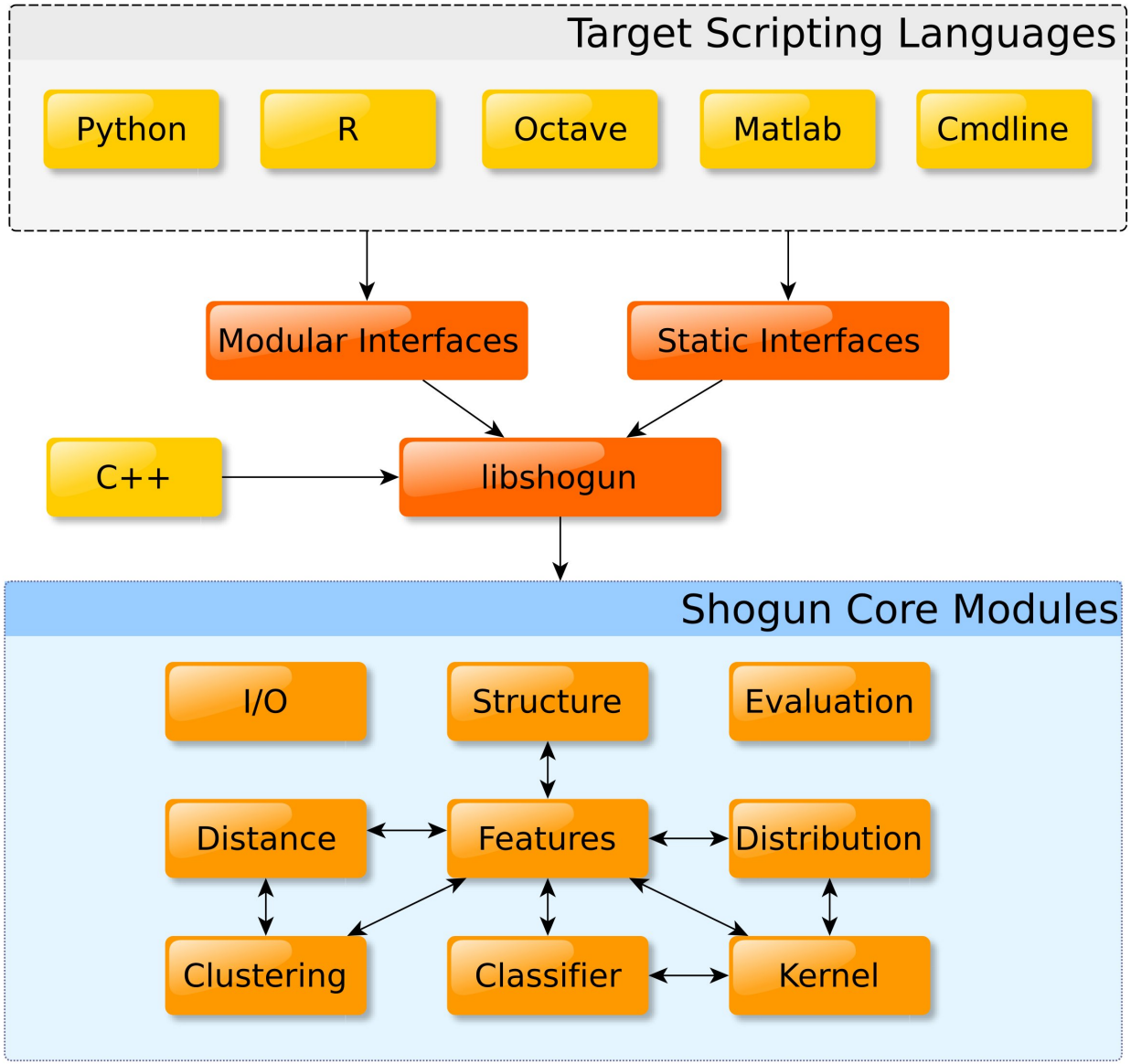
Architecture



Installing SHOGUN

Steps to Install SHOGUN from Source

- `$ git clone \`
  `https://github.com/shogun-toolbox/shogun.git`
- `($ cd shogun && git submodule update --init)`
- `$ cd shogun/src`
- `$ ./configure --interface=` (for libshogun)
- `$ ./configure --interface=python_modular` (for python)
- `$ make && sudo make install`

Don't

- Don't use a static interface if you can avoid it.
- Don't compile for all interfaces (it takes loooong).

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First Steps

A) Generate Toy Data

```
from numpy import concatenate as con
from numpy import ones,mean,sign
from numpy.random import randn

num=1000; dist=1; width=2.1; C=1.0

traindata=con((randn(2,num)-dist,
                    randn(2,num)+dist), axis=1)
testdata=con((randn(2,num)-dist,
                   randn(2,num)+dist), axis=1)
trainlab=con((-ones(num), ones(num)))
testlab=con((-ones(num), ones(num)))
```

Simple code example: SVM Training

B) Train and Apply SVM with SHOGUN

```
from shogun.Features import BinaryLabels,RealFeatures
from shogun.Kernel import GaussianKernel
from shogun.Classifier import LibSVM

feats_train=RealFeatures(traindata)
kernel=GaussianKernel(feats_train, feats_train, width)
labels=BinaryLabels(trainlab)
svm=LibSVM(C, kernel, labels)
svm.train()

out=svm.apply(RealFeatures(testdata)).get_labels()
testerr=mean(out!=testlab)
print testerr
```

Shogun Development Process

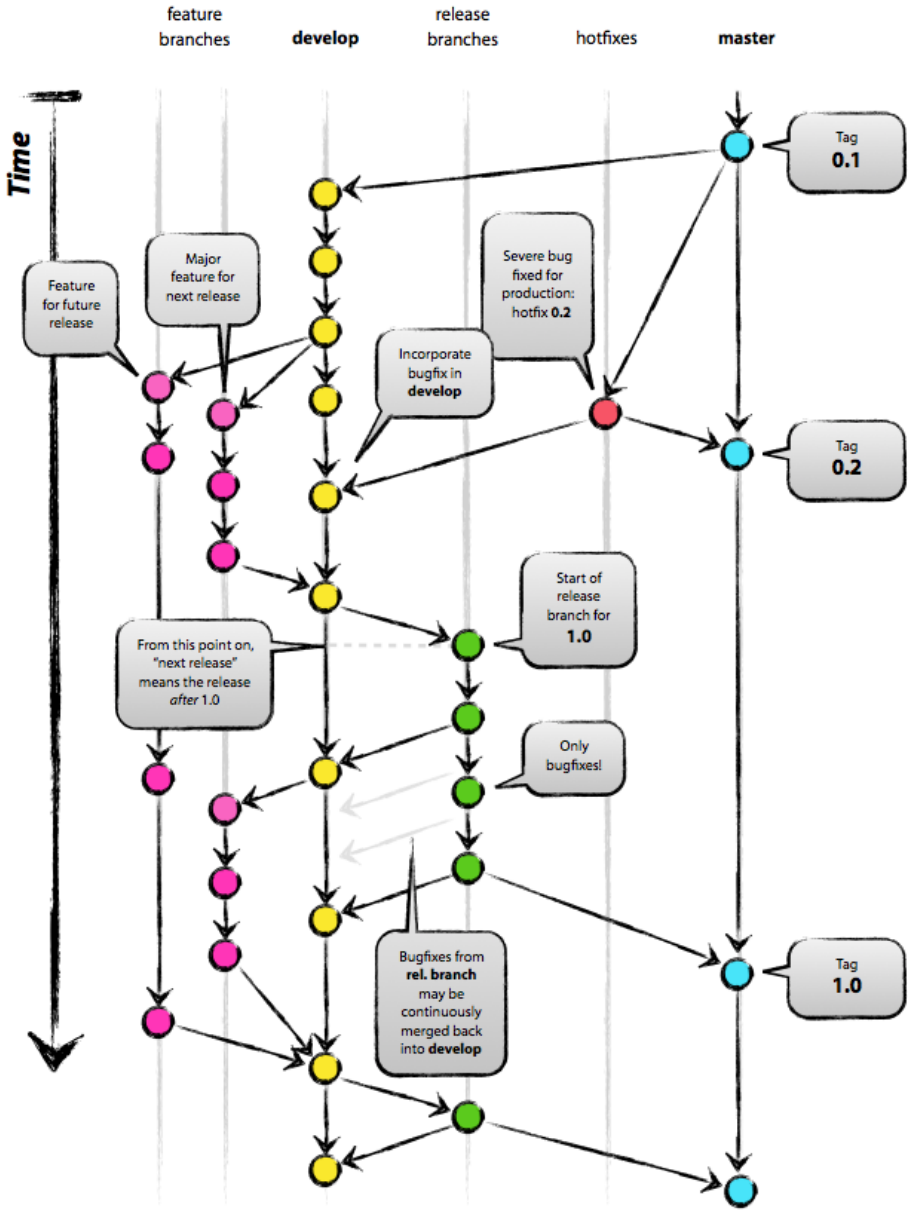
We use git & github

- shogun at github `https://github.com/shogun-toolbox`
- workflow is
  1. fork the project
  2. create a development branch with your changes
  3. do a pull request against the development branch
  4. we will do a code review
  5. eventually merged
- `https://help.github.com/articles/using-pull-requests`

Benefits

- Collaborative code review
- Unit and integration tests help to keep things stable.

git flow model



In a nutshell

- development happens on feature branches
- when a feature is ready it is merged to the development branch
- when we do a release we merge into master and tag the release

`http://nvie.com/posts/a-successful-git-branching-model/`

Developing an Algorithm

Flow to get an algorithm into shogun

- Follow `http://www.shogun-toolbox.org/doc/en/current/developer_tutorial.html` outside of shogun
- write a unit test (shogun uses gtest/gmock), write an example
- move file under the `src/shogun` hierarchy and get interface support

Efficient Native Data Representations

Input Features

- Dense Vectors/Matrices (DenseFeatures)
  - `uint8_t`
  - ⋮
  - float64_t
- Sparse Vectors/Matrices (SparseFeatures)
  - `uint8_t`
  - ⋮
  - float64_t
- Variable Length Vectors/Matrices (String-,MatrixFeatures)
  - `uint8_t`
  - ⋮
  - float64_t

Interfaces (legacy static interface)

Interface Types

- (legacy) Static Interfaces (single object of each type only)
- Modular Interfaces (really object oriented, SWIG based)

Support for all Feature Types

- Dense, Sparse, Strings
- Possible by defining generic get/set functions, e.g.

```
void set_int(int32_t scalar);
void set_real(float64_t scalar);
void set_bool(bool scalar);
void set_vector(float64_t* vector, int32_t len);
void set_matrix(float64_t* m, int32_t rws, int32_t cls);
...
```

$\Rightarrow$ set/get functions for access from python, R, octave, matlab

The Eierlegendewollmilchsau™ Interface

Embed Interface A from Interface B

- possible to run python code from octave
- possible to run octave code from python
- possible to run r code from python
- ...

Demo: Use matplotlib to plot functions from octave.

Modular Python SWIG based Interface

⇒ typemaps for numpy,scipy.sparse,files,lists of strings defined

Wrapping a C++ Object with swig (Kernel)

```
%{
#include <shogun/kernel/GaussianKernel.h>
%}
%rename(GaussianKernel) CGaussianKernel;
%include <shogun/kernel/GaussianKernel.h>
```

Wrapping a C++ Object with swig (Classifier)

```
%{
#include <shogun/classifier/svm/LibSVM.h>
%}
%rename(LibSVM) CLibSVM;
%include <shogun/classifier/svm/LibSVM.h>
```

Unique Features of SHOGUN I

Input Features

- efficient feature representation
- possible to stack together features of arbitrary types (sparse, dense, string) via CombinedFeatures and DotFeatures
- chains of "preprocessors" (e.g. substracting the mean) can be attached to each feature object (on-the-fly pre-processing)

Kernels

- working with custom pre-computed kernels.
- possible to stack together kernels via CombinedKernel (weighted linear combination of a number of sub-kernels, not necessarily working on the same domain)
- kernel weighting can be learned using MKL
- Methods (e.g., SVMs) can be trained using unified interface

Unique Features of SHOGUN II

Large Scale

- multiprocessor parallelization (training with up to 10 million examples and kernels)
- implements COFFIN framework (dynamic feature / example generation; training on 200,000,000 dimensions and 50,000,000 examples)
- streaming features for online methods

Unified Framework

- Interfaces to many languages available at **no coding cost.**
- Serialization - loading from other language possible
- Documentation available, many many examples
- There is a Debian Package, MacOSX
- IRC, Mailing-List, git repository & buildbot infrastructure

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Application

Genomic Signals

- Transcription Start (Sonnenburg et al., 2006)
- Acceptor Splice Site (Sonnenburg et al., 2007)
- Donor Splice Site (Sonnenburg et al., 2007)
- Alternative Splicing (Rätsch et al., 2005)
- Transsplicing (Schweikert et al., 2009)
- Translation Initiation (Sonnenburg et al., 2008)

Genefinding

- Splice form recognition - mSplicer (Rätsch et al. 2008)
- Genefinding - mGene (Schweikert et al., 2009)

Demo I

Support Vector Classification

- Task: separate 2 clouds of gaussian distributed points in 2D

Simple code example: SVM Training

```
lab = Labels(labels)
train = RealFeatures(features)
gk = GaussianKernel(train, train, width)
svm = LibSVM(10.0, gk, lab)
svm.train()
```

Demo II

Support Vector Regression

- Task: learn a sine function

Simple code example: Support Vector Regression

```
lab = Labels(labels)
train = RealFeatures(features)
gk = GaussianKernel(train, train, width)
svm = LibSVR(10.0, gk, lab)
svm.train()
```

Demo III

Clustering

- Task: find clustering of 3 clouds of gaussian distributed points in 2D

Many more available

- dimension reduction
- EM density estimation

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Check them out

- see `examples/<interface>/*`
- see `examples/<interface>/graphical/*`

Summary

SHOGUN Machine Learning Toolbox

- Unified framework, for various interfaces
- Applicable to huge datasets
- Various Algorithms

Documentation, Examples, Source Code

- Implementation `http://www.shogun-toolbox.org`
- Documentation `http://www.shogun-toolbox.org/doc`
- More machine learning software `http://mloss.org`
- Machine Learning Data `http://mldata.org`

We need you!

- Documentation, Examples, Testing, Extensions

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