SHOGUN-tutorial

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Chapter 2

Multiclass learning

In this chapter we describe multiclass learning algorithms available in the SHOGUN toolbox. Multiclass learning refers to the problem with the output space $\mathcal{Y} = \{1, \ldots, K\}$[1], where $K > 2$. Most of real world machine learning classification problems are naturally multiclass. Typical examples include document categorization, image classification, hand-written digit recognition, etc.

Generally, no assumption of any specific structure for the set $\mathcal{Y}$ are made in multiclass learning. When priori knowledge are available for a rich structure of $\mathcal{Y}$, *structured-output learning* algorithms are usually used instead.

Many algorithms, like K-Nearest Neighbors and Naive Bayes, handle both multiclass problems and binary problems naturally (and in an uniform way). Those are described in section 2.1. Section 2.2 describes reduction from multiclass problems into binary problems. Tree-styled classifiers are described in section 2.3.

Several standard datasets are used by examples in this chapter. We summarize them in Table 2.1. All of those datasets can be found in `http://mldata.org`.

2.1 Natural Multiclass Algorithms

2.1.1 K-Nearest Neighbors

K-Nearest Neighbors (KNN) is a very simple and effective algorithm. The learning step actually does nothing but memorizing all the training points and the associated labels. The prediction is carried out by finding the K nearest neighbors of the query point, and then voting. Here K is a hyper-parameter for the algorithm. Smaller K gives the model low bias but high variance; while larger K gives low variance but high bias.

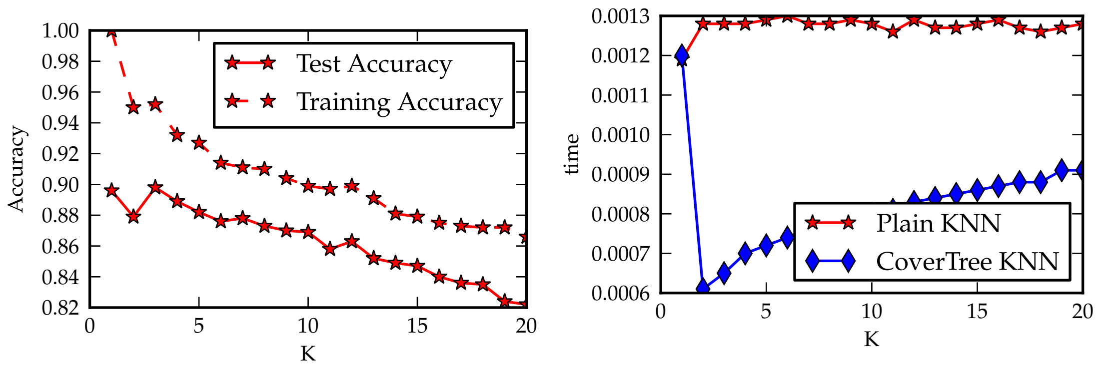
KNN has attracted focus from both industrial and academia ever since its conception. It is easy to implement, and can handle almost arbitrarily complex problem by adjusting one single parameter K. Besides, it also has many nice theoretical properties [Devroye et al., 1996].

In SHOGUN, you can use `CKNN` to perform KNN learning. To construct a KNN machine, you must choose the hyper-parameter K and a distance function. Usually, we simply use the `CEuclideanDistance`, but in general, any subclass of `CDistance` can be used. For demonstration, we select a random subset of 1000 samples from USPS, and run 2-fold cross validation of

[1] Note while we describe the class numbers as from 1 to K, the multiclass machines in SHOGUN expect the examples to be labeled with $0, \ldots, K-1$.

Name	# Classes	# Samples	# Attributes	Remarks
USPS	10	9298	256	Hand-written Digits

Table 2.1: Standard datasets for multiclass learning used in examples.



(a) KNN classification accuracy on USPS.

(b) Prediction time (per example) with and without CoverTree.

Figure 2.1: KNN classification on a random subset (1000 samples) of USPS.

KNN on it with varying K. The accuracy is shown in Fig. 2.1a.

In SHOGUN, you can also use *Cover Tree* [Beygelzimer et al., 2006] to speed up the nearest neighbor searching process in KNN. Just call `set_use_covertree` on the KNN machine to enable or disable this feature. The prediction time comparison for this experiment with and without Cover Tree are shown in Fig. 2.1b.

Although simple and elegant, KNN is generally very resource costly. Because all the training samples are to be memorized literally, the memory cost of KNN "learning" becomes prohibitive when the dataset is huge. Even though the memory is big enough to hold all the data, the prediction will be slow, since the distances between the query point and all the training points need to be computed and ranked. The situation becomes worse if in addition the data samples are all very high-dimensional.

2.1.2 Naive Bayes

Naive Bayes is a simple and fast algorithm for multiclass learning. Formally, it predict the class by computing the posterior probability of each class k after observing the input x:

$$P(Y = k|X = x) = \frac{P(X = x|Y = k)P(Y = k)}{P(X = x)}$$

The prediction is then made by

$$y = \arg\max_{k \in \{1,\ldots,K\}} P(Y = k|X = x)$$

Since $P(X = x)$ is a constant factor for all $P(Y = k|X = x)$, $k = 1, \ldots, K$, there is no need to compute it.

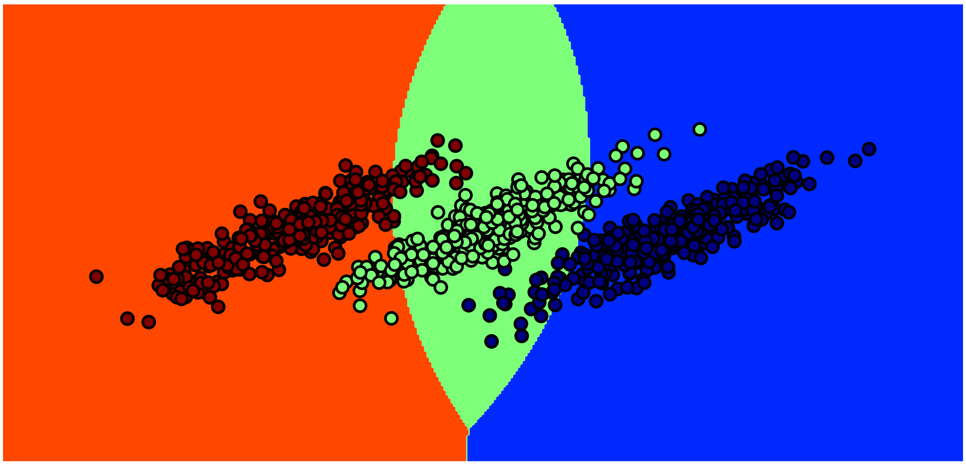


Figure 2.2: Gaussian Naive Bayes fails to learn on a simple 2D example with 3 linearly separable classes.

In SHOGUN, `CGaussianNaiveBayes` implements the Naive Bayes algorithm. It is prefixed with "Gaussian" because the probability model for $P(X = x|Y = k)$ for each k is taken to be a multi-variate Gaussian distribution. Furthermore, each dimension of the feature vector X is assumed to be independent. The "Naive" independence assumption enables us the learn the model by estimating the parameters for each feature dimension independently, thus the whole learning algorithm runs very quickly. And this is also the reason for its name. However, this assumption can be very restrictive. In Fig. 2.2, we show a simple 2D example. There are 3 linearly separable classes. The scattered points are training samples with colors indicating their labels. The filled area indicate the hypothesis learned by the `CGaussianNaiveBayes`. The training samples are actually generated from three Gaussian distributions. But since the covariance for those Gaussian distributions are not diagonal (i.e. there are "rotations"), the GNB algorithm cannot handle them properly.

Although the independent assumption is usually considered to be too optimistic in reality, Naive Bayes sometimes works very well in some applications. For example, in email spam filtering, Naive Bayes[2] is a very popular and widely used method.

This algorithm is closely related to the *Gaussian Mixture Model* (GMM) learning algorithm. However, while GMM is an unsupervised learning algorithm, Gaussian Naive Bayes is supervised learning. It uses the training labels to directly estimate the Gaussian parameters for each class, thus avoids the iterative *Expectation Maximization* procedures in GMM.

The merit of GNB is that both training and predicting are very fast, and it has no hyper-parameters.

[2]More specifically, the discrete Naive Bayes is generally used in this scenario. The main difference with Gaussian Naive Bayes is that a tabular instead of a parametric Gaussian distribution is used to describe the likelihood $P(X = x|K = k)$.

2.1.3 Logistic Regression

Although named logistic *regression*, it is actually a classification algorithm. Similar to *Naive Bayes*, logistic regression computes the posterior $P(Y = k|X = x)$ and makes prediction by

$$y = \arg\max_{k\in\{1,\ldots,K\}} P(Y = k|X = x)$$

However, Naive Bayes is a *generative model*, in which the distribution of the input variable X is also modeled (by a Gaussian distribution in this case). But logistic regression is a *discriminative model*, which doesn't care about the distribution of X, and models the posterior directly. Actually, the two algorithms are a *generative-discriminative pair* [Ng et al., 2001].

To be specific, logistic regression uses *linear* functions in X to model the posterior probabilities:

$$\log \frac{P(Y=1|X=x)}{P(Y=K|X=x)} = \beta_{10} + \beta_1^T x \tag{2.1}$$

$$\log \frac{P(Y=2|X=x)}{P(Y=K|X=x)} = \beta_{20} + \beta_2^T x \tag{2.2}$$

$$\vdots$$

$$\log \frac{P(Y=K-1|X=x)}{P(Y=K|X=x)} = \beta_{(K-1)0} + \beta_{K-1}^T x \tag{2.3}$$

The training of a logistic regression model is carried out via *maximum likelihood estimation* of the parameters $\boldsymbol{\beta} = \{\beta_{10}, \beta_1^T, \ldots, \beta_{(K-1)0}, \beta_{K-1}^T\}$. There is no closed form solution for the estimated parameters.

There is not independent implementation of logistic regression in SHOGUN, but the `CLibLinear` becomes a logistic regression model when constructed with the argument `L2R_LR`. This model also include a regularization term of the ℓ_2-norm of $\boldsymbol{\beta}$. If sparsity in $\boldsymbol{\beta}$ is needed, one can also use `L1R_LR`, which replaces the ℓ_2-norm regularizer with a ℓ_1-norm regularizer.

Unfortunately, the logistic regression in SHOGUN does not support multiclass problem yet.

2.2 Reduction to Binary Problems

Since binary classification problems are one of the most thoroughly studied problems in machine learning, it is very appealing to consider reducing multiclass problems to binary ones. Then many advanced learning and optimization techniques as well as generalization bound analysis for binary classification can be utilized.

In SHOGUN, the strategies of reducing a multiclass problem to binary classification problems are described by an instance of `CMulticlassStrategy`. A multiclass strategy describes

1. How to train the multiclass machine as a number of binary machines?
    - How many binary machines are needed?
    - For each binary machine, what subset of the training samples are used, and how are they colored[3]?

[3] In multiclass problems, we use *coloring* to refer partitioning the classes into two groups: $+1$ and -1, or black and white, or any other meaningful names.

Strategy	Training Time	Test Time	Accuracy
One-vs-Rest	1.72	2.25	92.05%
One-vs-One	2.14	4.45	93.75%

Table 2.2: Comparison of One-vs-Rest and One-vs-One multiclass reduction strategy on the USPS dataset.

2. How to combine the prediction results of binary machines into the final multiclass prediction?

The user can derive from the virtual class `CMulticlassStrategy` to implement a customized multiclass strategy. But usually the built-in strategies are enough for general problems. We will describe the built-in *One-vs-Rest*, *One-vs-One* and *Error-Correcting Output Codes* strategies in the following subsections.

The basic routine to use a multiclass machine with reduction to binary problems in shogun is to create a generic multiclass machine and then assign a particular multiclass strategy and a base binary machine.

2.2.1 One-vs-Rest and One-vs-One

The *One-vs-Rest* strategy is implemented in `CMulticlassOneVsRestStrategy`. As indicated by the name, this strategy reduce a K-class problem to K binary sub-problems. For the k-th problem, where $k \in \{1, \dots, K\}$, the samples from class k are colored as $+1$, and the samples from other classes are colored as -1. The multiclass prediction is given as

$$f(x) = \arg\max_{k \in \{1,\dots,K\}} f_k(x)$$

where $f_k(x)$ is the prediction of the k-th binary machines.

The One-vs-Rest strategy is easy to implement yet produces the good performance in many cases. One interesting paper [Rifkin and Klautau, 2004] shows that the One-vs-Rest strategy can be

> *as accurate as any other approach, assuming that the underlying binary classifiers are well-tuned regularized classifiers such as support vector machines.*

Implemented in `CMulticlassOneVsOneStrategy`, the *One-vs-One* strategy [Hastie and Tibshirani, 1997] is another simple and intuitive strategy: it basically produces one binary problem for each pair of classes. So there will be $\binom{K}{2}$ binary problems. At prediction time, the output of every binary classifiers are collected to do voting for the K classes. The class with the highest vote becomes the final prediction.

Compared with the One-vs-Rest strategy, the One-vs-One strategy is usually more costly to train and evaluate because more binary machines are used.

In the following, we demonstrate how to use SHOGUN's One-vs-Rest and One-vs-One multiclass learning strategy on the USPS dataset. For demonstration, we randomly 200 samples from each class for training and 200 samples from each class for testing.

How to organize and reference example code for tutorial?

The `CLibLinear` is used as the base binary classifier in a `CLinearMulticlassMachine`, with One-vs-Rest and One-vs-One strategies. The running time and performance is reported in Table 2.2.

2.2.2 Error-Correcting Output Codes

Error-Correcting Output Codes (ECOC) [Dietterich and Bakiri, 1995; Allwein et al., 2000] is a generalization of the One-vs-Rest and One-vs-One strategies. For example, we can represent the One-vs-Rest strategy with the following $K \times K$ coding matrix, or a codebook:

$$\begin{bmatrix} +1 & -1 & -1 & \dots & -1 & -1 \\ -1 & +1 & -1 & \dots & -1 & -1 \\ -1 & -1 & +1 & \dots & -1 & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & -1 & \dots & +1 & -1 \\ -1 & -1 & -1 & \dots & -1 & +1 \end{bmatrix}$$

Denote the codebook by B, there is one column of the codebook associated with each of the K classes. For example, the code for class 1 is $[+1, -1, -1, \dots, -1]$. Each row of the codebook corresponds to a binary coloring of all the K classes. For example, in the first row, the class 1 is colored as $+1$, while the rest of the classes are all colored as -1. Associated with each row, there is a binary classifier trained according to the coloring. For example, the binary classifier associated with the first row is trained by treating all the examples of class 1 as positive examples, and all the examples of the rest of the classes as negative examples.

In this special case, there are K rows in the codebook. The number of rows in the codebook is usually called the *code length*. As we can see, this codebook exactly describes how the One-vs-Rest strategy trains the binary sub-machines.

A further generalization is to allow 0-values in the codebook. A 0 for a class k in a row means we ignore (the examples of) class k when training the binary classifiers associated with this row. With this generalization, we can also easily describes the One-vs-One strategy with a $\binom{K}{2} \times K$ codebook:

$$\begin{bmatrix} +1 & -1 & 0 & \dots & 0 & 0 \\ +1 & 0 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & 0 \\ +1 & 0 & 0 & \dots & -1 & 0 \\ 0 & +1 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & +1 & -1 \end{bmatrix}$$

Here each of the $\binom{K}{2}$ rows describes a binary classifier trained with a pair of classes. The resultant binary classifiers will be identical as those described by a One-vs-One strategy.

Since 0 is allowed in the codebook to ignore some classes, this kind of codebooks are usually called *sparse codebook*s, while the codebooks with only $+1$ and -1 are usually called *dense codebook*.

In general case, we can specify any code length and fill the codebook arbitrarily. However, some rules should be followed:

1. Each row must describe a *valid* binary coloring. In other words, both $+1$ and -1 should appear at least once in each row. Or else a binary classifier cannot be obtained for this row.

2. It is good to avoid duplicated rows. There is generally no harm to have duplicated rows, but the resultant binary classifiers are completely identical provided the training algorithm for the binary classifiers are deterministic. So this can be a waste of computational resource.

3. Negative rows are also duplicated. Simply inversing the sign of a code row does not produce a "new" code row. Because the resultant binary classifier will simply be the negative classifier associated with the original row.

Though you can certainly generate your own codebook, it is usually easier to use the SHOGUN built-in procedures to generate codebook automatically. There are various codebook generators (called *encoders*) in SHOGUN. However, before describing those encoders in details, let us notice that a codebook only describes how the sub-machines are trained. But we still need a way to specify how the binary classification results of the sub-machines can be combined to get a multiclass classification result.

Review the codebook again: corresponding to each class, there is a column. We call the codebook column the (binary) *code* for that class. For a new sample x, by applying the binary classifiers associated with each row successively, we get a prediction vector of the same length as the *code*s. Deciding the multiclass label from the prediction vector (called *decoding*) can be done by minimizing the *distance* between the codes and the prediction vector. Different *decoders* define different choices of distance functions. For this reason, it is usually good to make the mutual distance between codes of different classes large. In this way, even though several binary classifiers make wrong predictions, the distance of the resultant prediction vector to the code of the *true* class is likely to be still smaller than the distance to other classes. So correct results can still be obtained even when some of the binary classifiers make mistakes. This is the reason for the name *Error-Correcting Output Codes*.

In SHOGUN, encoding schemes are described by subclasses of `CECOCEncoder`, while decoding schemes are described by subclasses of `CECOCDecoder`. Theoretically, any combinations of encoder-decoder pairs can be used. Here we will introduce several common encoder/decoders in shogun.

- `CECOCRandomDenseEncoder`: This encoder generate random dense ($+1/-1$) codebooks and choose the one with the largest *minimum mutual distance* among the classes. The recommended code length for this encoder is $10 \log K$ [Allwein et al., 2000].

- `CECOCRandomSparseEncoder`: This is similar to the random dense encoder, except that sparse ($+1/-1/0$) codebooks are generated. The recommended code length for this encoder is $15 \log K$ [Escalera et al., 2009].

- `CECOCOVREncoder`, `CECOCOVOEncoder`: These two encoders mimic the One-vs-Rest and One-vs-One strategies respectively. They are implemented mainly for demonstrative purpose. When suitable decoders are used, the results will be equivalent to the corresponding strategies, respectively.

- `CECOCDiscriminantEncoder`

- `CECOCForestEncoder`

Describe the name ECOC here, and describe the SHOGUN ECOC encoding/decoding pairs.

2.3 Tree-style Algorithms

Chapter 3

Statistical Testing

This chapter describes SHOGUN's framework for statistical hypothesis testing. We begin by giving a brief outline of the problem setting in section 3.1. Then, we describe methods for two-sample testing for independence testing.

Methods for two-sample testing currently consist of tests based on the *Maximum Mean Discrepancy*, section 3.2. There are two types of tests available, a quadratic time test, which is described in section 3.2.1; and a linear time test, which is described in section 3.2.2. Both come in various flavours.

Independence testing is currently based in the *Hilbert Schmidt Independence Criterion*, which is described in section 3.3 along with a test using it.

3.1 Statistical Hypothesis Testing

To set the context, we here briefly describe statistical hypothesis testing. Informally, one defines a hypothesis on a certain domain and then uses a statistical test to check whether this hypothesis is true. Formally, the goal is to reject a so-called *null-hypothesis* H_0, which is the complement of an *alternative-hypothesis* H_A.

To distinguish the hypothesises, a test statistic is computed on sample data. Since sample data is finite, this corresponds to sampling the true distribution of the test statistic. There are two different distributions of the test statistic – one for each hypothesis. The *null-distribution* corresponds to test statistic samples under the model that H_0 holds; the *alternative-distribution* corresponds to test statistic samples under the model that H_A holds.

In practice, one tries to compute the quantile of the test statistic in the null-distribution. In case the test statistic is in a high quantile, i.e. it is unlikely that the null-distribution has generated the test statistic – the null-hypothesis H_0 is rejected.

There are two different kinds of errors in hypothesis testing:

- A *type I error* is made when $H_0 : p = q$ is wrongly rejected. That is, the tests says that the samples are from different distributions when they are not.

- A *type II error* is made when $H_A : p = q$ is wrongly accepted. That is, the tests says that the samples are from same distributions when they are from the same.

A so called *consistent* test achieves zero type 2 error for a fixed type 1 error.

To decide whether to reject H_0, one could set a threshold, say at the 95% quantile of the null-distribution, and reject H_0 when the test statistic lies below that threshold. This means that the chance that the samples were generated under H_0 are 5%. We call this number the test power α (in this case $\alpha = 0.05$). It is an upper bound on the probability for a type 1 error. An alternative way is simply to compute the quantile of the test statistic in the null-distribution, the so-called *p-value*, and to compare the p-value against a desired test power, say $\alpha = 0.05$, by hand. The advantage of the second method is that one not only gets a binary answer, but also an upper bound on the type 1 error.

In order to construct a two-sample test, the null-distribution of the test statistic has to be approximated. One way of doing this for any two-sample test is called *bootstrapping*:

Algorithm 3.1 Bootstrapping a null-distribution.

Inputs are:

- X, Y, sets of samples from p, q of size m, n respectively

Output is:

- One sample from null-distribution. Simply repeat for more samples.

$Z \leftarrow \{X, Y\}$
$\hat{Z} = \{\hat{z}_1, ..., \hat{z}_{m+n}\} \leftarrow \text{randperm}(Z)$ (generate a random ordering)
$\hat{X} \leftarrow \{\hat{z}_1, ...\hat{z}_m\}$
$\hat{Y} \leftarrow \{\hat{z}_{m+1}, ...\hat{z}_{m+n}\}$
return Test statistic for $\hat{X}, \hat{Y}$

Bootstrapping is a useful technique to create ground-truth samples for a null-distribution. However, it is rather costly because the statistic has to be re-computed for every sample.

SHOGUN implements statistical testing in the abstract class `CTestStatistic`.

- Test statistics can be computed with `compute_statistic`.
- P-values for a given statistic can be computed via `compute_p_value`. Results depend on method that is set for approximating null-distribution.
- Statistic thresholds for a given p-value can be computed via `compute_threshold`. Results depend on method that is set for approximating null-distribution.
- A number of samples can be drawn from the null-distribution using bootstrapping via `bootstrap_null`.

An important class of hypothesis tests are the *two-sample-tests*, which will be defined in the following.

3.2 Two-Sample-Testing with the Maximum Mean Discrepancy

In two-sample testing, one tries to find out whether to sets of samples come from different distributions. Given two probability distributions p, q and i.i.d. samples $X = \{x_i\}_{i=1}^m \subseteq \mathbb{R}^d \sim p$ and $Y = \{y_i\}_{i=1}^n \subseteq \mathbb{R}^d \sim p$, the two sample test distinguishes the hypotheses

$$H_0 : p = q$$
$$H_A : p \neq q$$

In order to solve this problem, it is desirable to have a criterion than takes a positive unique value if $p \neq q$, and zero if and only if $p = q$. The so called *Maximum Mean Discrepancy* (MMD), has this property and allows to distinguish any two probability distributions, if used in a *reproducing kernel Hilbert space* (RKHS). It is the distance of the mean embeddings μ_p, μ_q of the distributions p, q in such a RKHS $\mathcal{F}$ – which can also be expressed in terms of expectation of kernel functions, i.e.

$$\begin{aligned}\text{MMD}[\mathcal{F}, p, q] &= ||\mu_p - \mu_q||^2_{\mathcal{F}} \\ &= \mathbf{E}_{x,x'}\left[k(x,x')\right] - 2\mathbf{E}_{x,y}\left[k(x,y)\right] + \mathbf{E}_{y,y'}\left[k(y,y')\right]\end{aligned} \tag{3.1}$$

See [Gretton et al., 2012a, Section 2] for details. We here only describe how to use the MMD for two-sample testing. SHOGUN offers two types of test statistic based on the MMD, one with quadratic costs both in time and space, and on with linear time and constant space costs. Both come in different versions and with different methods how to approximate the null-distribution in order to construct a two-sample test.

3.2.1 Quadratic Time MMD Statistic

We now describe the quadratic time MMD, as described in [Gretton et al., 2012a, Lemma 6], which is implemented in SHOGUN. All methods in this section are implemented in `CQuadraticTimeMMD`.

An unbiased estimate for expression 3.1 can be obtained by estimating expected values with sample means

$$\begin{aligned}\text{MMD}_u^2[\mathcal{F}, X, Y] =& \frac{1}{m(m-1)} \sum_{i=1}^m \sum_{j\neq i}^m k(x_i, x_j) + \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j\neq i}^n k(y_i, y_j) \\ &- \frac{2}{mn} \sum_{i=1}^m \sum_{j\neq i}^n k(x_i, y_j)\end{aligned}$$

A biased estimate would be

$$\begin{aligned}\text{MMD}_b^2[\mathcal{F}, X, Y] =& \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m k(x_i, x_j) + \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(y_i, y_j) \\ &- \frac{2}{mn} \sum_{i=1}^m \sum_{j\neq i}^n k(x_i, y_j)\end{aligned}$$

To compute statistic, use `compute_statistic`. To decide which statistic to use, use `set_statistic_type` with arguments `BIASED` or `UNBIASED` to activate this statistic type. Note that some methods for approximating the null-distribution only work with one of both types. Both statistics' computational costs are quadratic both in time and space. Note that the method returns $m\,\text{MMD}_b^2[\mathcal{F}, X, Y]$ since null distribution approximations work on m times null distribution.

Bootstrapping

As for any two-sample test in SHOGUN, bootstrapping can be used to approximate the null-distribution with both types of quadratic MMD statistic. This results in a consistent, but slow test. Note that for each sample, the quadratic time estimate has to be recomputed. The number of samples to take is the only parameter. As a rule of thumb, use at least 250 samples. See `bootstrap_null` in `CTwoDistributionsTestStatistic` and `CKernelTwoSampleTestStatistic`. Strongly consider using pre-computed kernel matrices as described in section 3.2.3.

Spectrum Approximation

Approximates the null-distribution using the Eigen-Spectrum of the kernel matrix of the joint samples. Was described in [Gretton et al., 2012b]. This is a fast and consistent test. Effectively, the null-distribution of the biased statistic is sampled, but in a more efficient way than the bootstrapping approach. The converges as

$$m\,\mathrm{MMD}_b^2 \to \sum_{l=1}^{\infty} \lambda_l z_l^2 \tag{3.2}$$

where $z_l \sim \mathcal{N}(0,2)$ are i.i.d. normal samples and λ_l Eigenvalues of expression 2 in [Gretton et al., 2012b], which can be empirically estimated by $\hat{\lambda}_l = \frac{1}{m}\nu_l$ where ν_l are the Eigenvalues of the centred kernel matrix of the joint samples X and Y. The distribution in expression 3.2 can be easily sampled. SHOGUN's implementation has two parameters:

- Number of samples from null-distribution. The more, the more accurate. As a rule of thumb, use 250.
- Number of Eigenvalues of the Eigen-decomposition of the kernel matrix to use. The more, the better the results get; however, the Eigen-spectrum of the joint gram matrix usually decreases very fast. See [Gretton et al., 2012b] for details.

If the kernel matrices are diagonal dominant, this method is likely to fail. For that and more details, see the original paper. Computational costs are much lower than bootstrapping, which is the only consistent alternative. Since Eigenvalues of the gram matrix has to be computed, costs are in $\mathcal{O}(m^3)$.

To get a number of samples, use `sample_null_spectrum`; to use that method for testing, use `set_null_approximation_method(MMD2_SPECTRUM)`. Both methods are to be found in `CQuadraticTimeMMD`. Important: This method only works with the biased statistic.

Gamma Approximation

Another method for approximating the null-distribution is by matching the first two moments of a gamma-distribution and then use that. This is not consistent, but usually also gives good results while being very fast. However, there are distributions where the method fails; therefore, the type I error should always be monitored. Described in [Gretton et al., 2012b]. It uses

$$m\,\mathrm{MMD}_b(Z) \sim \frac{x^{\alpha-1}\exp(-\frac{x}{\beta})}{\beta^{\alpha}\Gamma(\alpha)} \tag{3.3}$$

where

$$\alpha = \frac{(\mathbf{E}(\mathrm{MMD}_b(Z)))^2}{\mathrm{var}(\mathrm{MMD}_b(Z))} \qquad \text{and} \qquad \beta = \frac{m\,\mathrm{var}(\mathrm{MMD}_b(Z))}{(\mathbf{E}(\mathrm{MMD}_b(Z)))^2}$$

Then, any threshold and p-value can be computed using the gamma distribution in expression 3.3. Computational costs are in $\mathcal{O}(m^2)$.

To use that method for testing, use `set_null_approximation_method(MMD2_GAMMA)`, to be found in `CQuadraticTimeMMD`. Important: This method only works with the biased statistic.

3.2.2 Linear Time MMD Statistic

We now describe the linear time MMD, as described in [Gretton et al., 2012a, Section 6], which is implemented in SHOGUN. All methods in this section are implemented in CLinearTimeMMD.

An fast, unbiased estimate for expression 3.1 which still uses all available data can be obtained by dividing data into two parts and then compute

$$\mathrm{MMD}_l^2[\mathcal{F}, X, Y] = \frac{1}{m_2}\sum_{i=1}^{m_2} k(x_{2i}, x_{2i+1}) + k(y_{2i}, y_{2i+1}) - k(x_{2i}, y_{2i+1}) - k(x_{2i+1}, y_{2i})$$

where $m_2 = \lfloor \frac{m}{2} \rfloor$. This statistic is interesting for large scale tests since its computational costs are linear in the number of samples; and the space costs are constant – it is therefore very suitable for large amounts of streaming data. To compute statistic, use `compute_statistic`.

Bootstrapping

As for any two-sample test in SHOGUN, bootstrapping can be used to approximate the null distribution. This results in a consistent, but slow test. The number of samples to take is the only parameter. As a rule of thumb, use at least 250 samples. See `bootstrap_null` in CTwoSampleTestStatistic. Note that this method is not really necessary since with the Gaussian approximation, a fast and consistent estimate of the null-distribution is available for the linear time MMD.

Gaussian Approximation

Since both the null- and the alternative distribution are Gaussians with equal variance (and different mean), it is possible to approximate the null-distribution by using a linear time estimate for this variance. An unbiased, linear time estimator for

$$\mathrm{var}[\mathrm{MMD}_l^2[\mathcal{F}, X, Y]]$$

can simply be computed by computing the empirical variance of

$$k(x_{2i}, x_{2i+1}) + k(y_{2i}, y_{2i+1}) - k(x_{2i}, y_{2i+1}) - k(x_{2i+1}, y_{2i}) \qquad (1 \leq i \leq m_2)$$

A normal distribution with this variance and zero mean can then be used as an approximation for the null-distribution. This results in a consistent test and is very fast. The approximation gets accurate from about $m = 1000$.

To use that method for testing, use `set_null_approximation_method(MMD1_GAUSSIAN)`, to be found in CLinearTimeMMD.

3.2.3 Precomputed Kernel Matrices for Quadratic Time MMD

For all MMD-based two-sample-tests, elements of kernel matrices of sample data have to be used. By default, all computations are done *in-place* when possible, which means that the underlying kernel is evaluated on the fly (There are exceptions, when the matrix has to be stored, for example in order so solve Eigenvalue problems). However, for the quadratic time MMD, this may be inefficient when statistics are computed multiple times – as in bootstrapping. Therefore, it is possible to initialize CQuadraticTimeMMD with a pre-computed CCusotmKernel.

This kernel may be computed from any other kernel by simply passing the latter to the constructor of `CCusotmKernel`. This should be done whenever the kernel matrix fits into memory; it greatly improves performance. In bootstrapping, the kernel matrix only has to be permuted instead of being re-computed in every iteration. But there is also a (small) advantage for all other methods since SHOGUN computes kernel matrices in multiple threads.

In contrast, `CLinearTimeMMD` should not be used with `CCusotmKernel`s since it does not even need all elements – so pointless computations would be made. Also, `CLinearTimeMMD` might be c

Kernel Selection

Kernel selection for MMD-based two-sample tests is an ongoing subject of research. In the near future, recent results on this topic will be implemented into SHOGUN. In the meantime, a good heuristic to start with, when using a Gaussian kernel as implemented in `CGaussianKernel`, is to use the median distance in the underlying data as kernel bandwidth. This way, the kernel captures at least the scaling of underlying data. In many cases, this leads to usable first results, however, the method may badly fail if signal is hidden at another length scale than the one of the overall data. The method is mentioned in [Gretton et al., 2012a, Appendix C].

In order to do this, note that SHOGUN's Gaussian kernel implementation uses a different parametrization as most other literature:

$$k(x, x') = \exp\left(\frac{||x - x'||_2^2}{\tau}\right)$$

where τ is the width that is passed to the constructor of `CGaussianKernel`. In order to translate a median distance d to this kernel, simply pass $\tau = d^2$.

SHOGUN implements classes that can compute median distances. Create an instance of the class `CEulideanDistance`, call the method `distance_matrix` to compute all pairwise distances of passed data. Then, use the method `matrix_median` of `CStatistics` in order to compute the median of all elements in the matrix. Store this distance and pass it to the Gaussian kernel as described above.

Note that the median is a very stable statistic, therefore, it is not necessary to compute all pairwise distances. A subset of a few hundred points is sufficient. This can be done via setting a subset to the instance of `CFeatures` that holds the data. To do so, create a random index permutation via calling method `randperm_vec` of class `CMath`, and only keep the n first indices where n is the number of distances that should be computed. Call `add_subset` on the instance of `CFeatures` that holds the data and give the indices as parameter. Then, this instance can be passed to `CEulideanDistance` as described above. Distances will only be computed for specified indices. Once the distance matrix is computed, call `remove_subset` to reset the original state of the data.

The whole procedure is included in all python examples, including the graphical ones.

Examples

There are graphical python examples which plot example data, alternative and null-distributions. See figures 3.2 and 3.1 for a screenshot for quadratic and linear time MMD respectively.

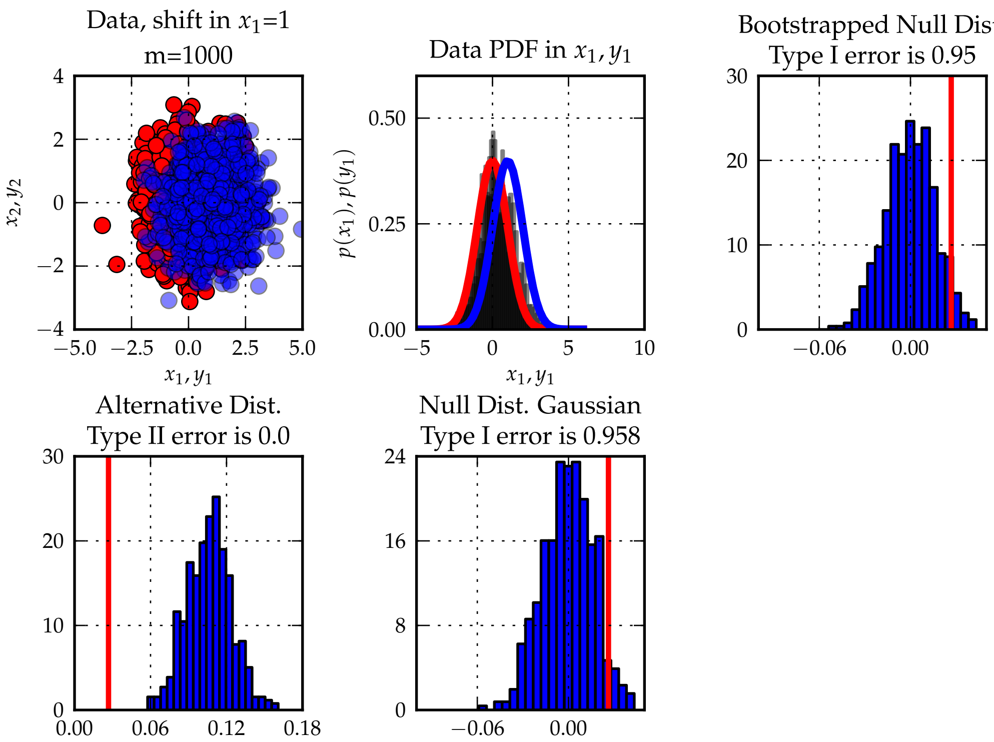


Figure 3.1: Screenshot of graphical python example for linear time MMD.

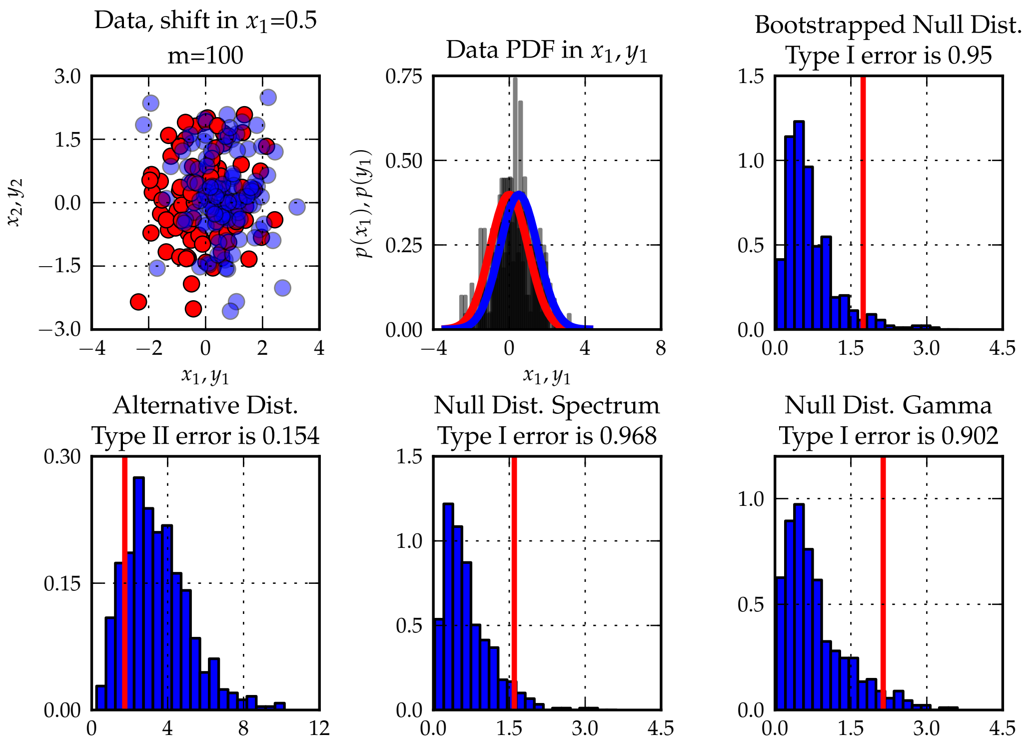


Figure 3.2: Screenshot of graphical python example for quadratic time MMD.

3.3 Independence Testing with the HSIC Statistic

Independence testing tries to solve the following problem (taken from [Gretton et al., 2008]): Let $\mathbf{P}_{xy}$ be a Borel probability measure defined on a domain $\mathcal{X} \times \mathcal{Y}$, and let $\mathbf{P}_x$ and $\mathbf{P}_y$ be the respective marginal distributions on $\mathcal{X}$ and $\mathcal{Y}$. Given samples $Z = (X, Y) = \{(x_1, y_1), ..., (x_m, y_m)\}$ of size m drawn independently and identically distributed according to $\mathbf{P}_{xy}$, does $\mathbf{P}_{xy}$ factorise as $\mathbf{P}_{xy} = \mathbf{P}_x\mathbf{P}_y$? This corresponds to the question: Are $\mathbf{P}_x$ and $\mathbf{P}_y$ statistically independent? An independence test will distinguish between the hypothesises

$$H_0 : \mathbf{P}_{xy} = \mathbf{P}_x\mathbf{P}_y$$
$$H_1 : \mathbf{P}_{xy} \neq \mathbf{P}_x\mathbf{P}_y$$

As for two-sample-testing, it is desirable to have a statistic that is zero if and only if $\mathbf{P}_x$ and $\mathbf{P}_y$ are independent. The so-called *Hilbert Schmidt Independence Criterion* has this property. It is the squared Hilbert-Schmidt norm of the cross-covariance operator. We will now briefly describe where it comes from.

Let $\mathcal{F}$ be a RKHS with continuous feature mapping $\phi : \mathcal{X} \to \mathcal{F}$ and kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that $\langle \phi(x)\phi(x') \rangle_{\mathcal{F}} = k(x, x')$; let $\mathcal{G}$ be another RKHS with continuous feature mapping $\psi : \mathcal{X} \to \mathcal{G}$ and kernel $l : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ such that $\langle \psi(y)\psi(y') \rangle_{\mathcal{G}} = k(y, y')$. The cross-covariance operator $C_{xy} : \mathcal{G} \to \mathcal{F}$ is defined such that for all $f \in \mathcal{F}$ and $g \in \mathcal{G}$

$$\langle f, C_{xy}g \rangle_{\mathcal{F}} = \mathbf{E}_{xy}([f(x) - \mathbf{E}_x(f(x))][g(y) - \mathbf{E}_y(g(y))]$$

The operator itself can be written as

$$C_{xy} = \mathbf{E}_{xy}(\phi(x) - \mu_x) \otimes (\psi(y) - \mu_y)]$$

where $\otimes$ is the tensor product. This is the generalisation of the cross-covariance matrix between random vectors in a RKHS. When $\mathcal{F}$ and $\mathcal{G}$ are *universal*, then $||C_{xy}||$ is z is zero if and only if $H_0 : \mathbf{P}_{xy} = \mathbf{P}_x\mathbf{P}_y$ holds. Collecting everything gives the population expression for the HSIC. Let x', y' be independent copies of the random variables x, y respectively.

$$\begin{aligned} \text{HSIC}[\mathbf{P}_{xy}, \mathcal{F}, \mathcal{G}] = \mathbf{E}_{xx'yy'}[k(x, x')l(y, y')] + \mathbf{E}_{xx'}[k(x, x')]\mathbf{E}_{yy'}[l(y, y')] \\ - 2\mathbf{E}_{xy}[\mathbf{E}_{x'}[k(x, x')]\mathbf{E}_{y'}[l(y, y')] \end{aligned} \tag{3.4}$$

See [Gretton et al., 2008] for details. SHOGUN implements a biased estimator of the HSIC along with various methods to approximate its null distribution.

3.3.1 Estimate of HSIC

We now describe the method to estimate the HSIC that is implemented in SHOGUN, as described in [Gretton et al., 2008, Equation 4]. All methods are implemented in `CHSIC`. The HSIC statistic has quadratic time and space costs, since it involves computing full kernel matrices and centring them.

A biased estimator for expression 3.4 is given by

$$\text{HSIC}_b[(X, Y), \mathcal{F}, \mathcal{G}] = \frac{1}{m^2}\text{trace}(\mathbf{KHLH})$$

where $\mathbf{K}, \mathbf{L}$ are the full kernel matrices of kernels k, l respectively and $\mathbf{H} = \mathbf{I} - \frac{1}{m}\mathbf{1}\mathbf{1}^T$ is a centring matrix with $\mathbf{1}$ being a $m \times m$ matrix of ones. In SHOGUN, this expression is not evaluated using matrix multiplication, but the centring is done by hand. Call `compute_statistic` in order to compute the estimate. Note that the method returns $m\,\mathrm{HSIC}_b[(X,Y),\mathcal{F},\mathcal{G}]$ since null distribution approximations work on m times null distribution.

Bootstrapping

As for any independence test in SHOGUN, bootstrapping can be used to approximate the null-distribution with any type of statistic. This results in a consistent, but slow test. Note that for each sample, the HSIC estimate has to be re-computed. The number of samples to take is the only parameter. As a rule of thumb, use at least 250 samples. See `bootstrap_null` in `CTwoDistributionsTestStatistic`, `CKernelIndependenceTestStatistic`, and `CHSIC`. Note that since the full kernel matrices have to be stored anyway when computing the HSIC estimate, in `bootstrap_null`, these are pre-computed automatically for the current bootstrapping instance. Bootstrapping is the only consistent HSIC test that is implemented in SHOGUN.

Gamma

Another, fast but heuristic method for approximating the null distribution for the HSIC is by matching the first two moments of a gamma distribution to it [Gretton et al., 2008, Equation 9]. This is not consistent but usually gives good results in practice. However, there are distributions which break the gamma test. Therefore, the type I error should always be monitored.

It uses

$$m\,\mathrm{HSIC}_b(Z) \sim \frac{x^{\alpha-1}\exp(-\frac{x}{\beta})}{\beta^\alpha\Gamma(\alpha)} \tag{3.5}$$

where

$$\alpha = \frac{(\mathbf{E}(\mathrm{HSIC}_b(Z)))^2}{\mathrm{var}(\mathrm{HSIC}_b(Z))} \qquad \text{and} \qquad \beta = \frac{m\,\mathrm{var}(\mathrm{HSIC}_b(Z))}{(\mathbf{E}(\mathrm{HSIC}_b(Z)))^2}$$

Then, any threshold and p-value can be computed using the gamma distribution in expression 3.5. Computational costs are in $\mathcal{O}(m^2)$, similar for space.

To use that method for testing, use `set_null_approximation_method(HSIC_GAMMA)`, to be found in `CHSIC`.

Kernel Selection

See section 3.2.3. The same principle may be applied for HSIC-based tests. Note that since there is a kernel for each distribution, two kernel parameters have to be selected. Using the described median heuristic also leads to good results in some cases, as mentioned in [Gretton et al., 2008].

Example

There is a graphical python example which plots example data, alternative and null-distributions. See figure 3.3.

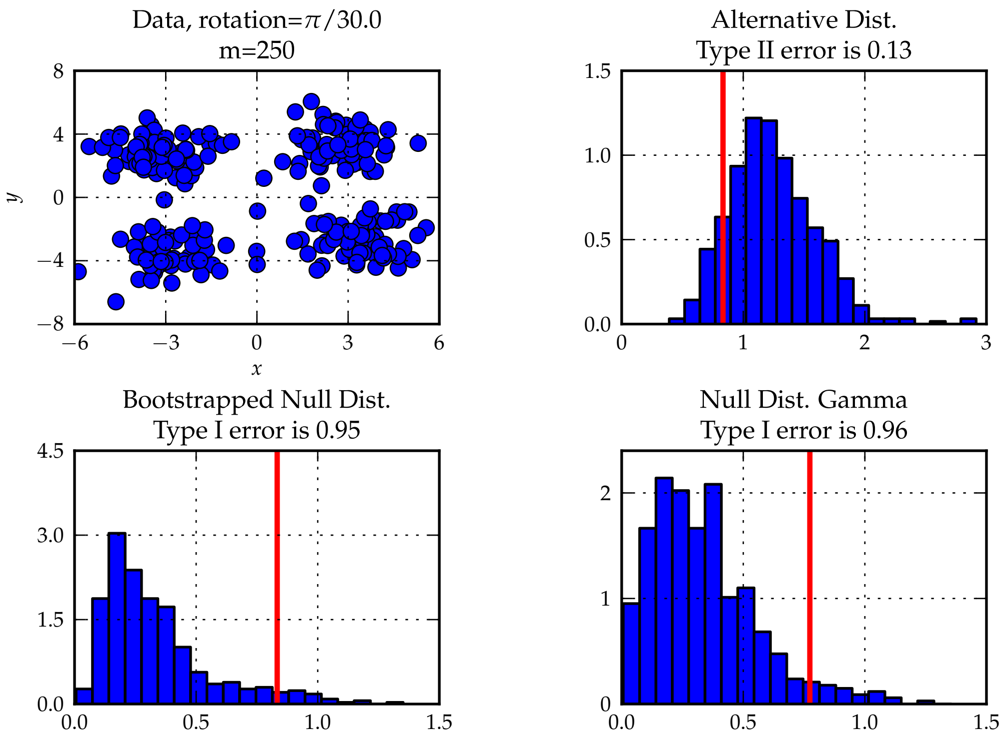


Figure 3.3: Screenshot of graphical python example for HSIC.

Chapter 4

Multitask learning

In this chapter we describe multitask learning algorithms available in the SHOGUN toolbox. In the toolbox we include descriptions of some multitask learning algorithms ported from two packages: SLEP (the Sparse LEarning Package) and the MALSAR (Multi-tAsk Learning via StructurAl Regularization) package.

4.1 L_1/L_q-norm regularized multitask learning

One of the simplest approaches to learn linear classification and regression models in the multitask environment is to come with regularization based on L_1/L_q norm of the common w hyperparameter

$$\|w\|_{1/q} = \sum_{t=1}^{T} \|w\|_q.$$

That kind of regularization in the same time pulls corresponding weights of hyperparameters w_t to be similar and pulls non-relevant feature weights to be zero.

4.1.1 Least squares linear regression

The algorithm learns a multitask linear least squares regression model of regression

$$f_t(x) = \langle w_t, x \rangle + b_t, \quad t = 1, \dots, T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_w \sum_{t=1}^{T} \sum_{i \in G_t} (\langle w_t, x_i \rangle + b_t - y_i)^2 + \lambda \|w\|_{1/q},$$

where $G = \{G_1, \dots, G_T\}$ is a set of tasks' non-overlapping indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \mathbb{R}$ are labels.

The algoritm is implemented in `CMultitaskLeastSquaresRegression`.

4.1.2 Logistic regression

The algorithm learns a multitask linear logistic model of classification

$$f_t(x) = sign(\langle w_t, x\rangle + b_t), \quad t = 1, \dots, T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_{w} \sum_{t=1}^{T} \sum_{i \in G_t} \frac{1}{|G_t|} \log(1 + \exp\left(-y_i(\langle w_t, x_i\rangle + b_t)\right) + \lambda \|w\|_{1/q},$$

where $G = \{G_1, \dots, G_T\}$ is a set of tasks' non-overlapping indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \{-1, 1\}$ are labels.

The algorithm is implemented in `CMultitaskLogisticRegression`.

4.2 Tree structured group lasso multitask learning

In some cases relations between tasks can be described via tree structure.

4.2.1 Least squares linear regression

The algorithm learns a multitask linear least squares regression model of regression

$$f_t(x) = \langle w_t, x\rangle + b_t, \quad t = 1, \dots, T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_{w} \sum_{t=1}^{T} \sum_{i \in G_t} \left(\langle w_t, x_i\rangle + b_t - y_i\right)^2 + \lambda \|w\|_{1/q},$$

where $G = \{G_0, \dots, G_T\}$ is a set of tasks' tree indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \mathbb{R}$ are labels.

The algorithm is implemented in `CMultitaskLeastSquaresRegression`.

4.2.2 Logistic regression

The algorithm learns a multitask linear logistic model of classification

$$f_t(x) = sign(\langle w_t, x\rangle + b_t), \quad t = 1, \dots, T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_{w,c} \sum_{t=1}^{T} \sum_{i \in G_t} \frac{1}{|G_t|} \log(1 + \exp\left(-y_i(\langle w_t, x_i\rangle + b_t)\right) + \lambda \|w\|_{1/q},$$

where $G = \{G_0, \dots, G_T\}$ is a set of tasks' tree indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \{-1, 1\}$ are labels.

The algorithm is implemented in `CMultitaskLogisticRegression`.

4.3 Low rank approximations

Tasks relationship can be constrained with models based on shared low-dimensional subspace. That can be done via solving the following optimization problem:

$$\min_{W=[w_1,\ldots,w_T]} L(W) + \lambda \operatorname{rank}(W),$$

where L is a pre-defined loss function. It is known that the problem is NP-hard which makes it infeasible to solve in real applications. In practice similar problem is

$$\min_{W=[w_1,\ldots,w_T]} L(W) + \lambda \|W\|_*,$$

where the sum of the singular values $\|W\|_* = \sum_i \sigma_i(W)$ is the trace norm.

4.3.1 Least squares linear regression

The algorithm learns a multitask linear least squares regression model of regression

$$f_t(x) = \langle w_t, x\rangle + b_t, \quad t = 1, \ldots, T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_{W=[w_1,\ldots,w_T]} \sum_{t=1}^{T} \sum_{i \in G_t} (\langle w_t, x_i\rangle + b_t - y_i)^2 + \sum_i \sigma_i(W),$$

where $G = \{G_1, \ldots, G_T\}$ is a set of tasks' non-overlapping indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \mathbb{R}$ are labels.

4.3.2 Logistic regression

The algorithm learns a multitask linear logistic model of classification

$$f_t(x) = sign(\langle w_t, x\rangle + b_t), \quad t = 1, \ldots, T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_{W=[w_1,\ldots,w_T]} \sum_{t=1}^{T} \sum_{i \in G_t} \frac{1}{|G_t|} \log(1 + \exp\left(-y_i(\langle w_t, x_i\rangle + b_t)\right) + \sum_i \sigma_i(W),$$

where $G = \{G_1, \ldots, G_T\}$ is a set of tasks' non-overlapping indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \{-1, 1\}$ are labels.

The algorithm is implemented in `CMultitaskTraceLogisticRegression`.

4.4 Clustered multitask learning

Other approach assuming tasks may exhibit k-cluster structure. That kind of structure makes learned models of similar tasks (i.e. tasks of one cluster) to be closer to each other than to other tasks. The approach can be formalized to the following optimization problem

$$\min_{W=[w_1,\ldots,w_T]} L(W) + \alpha(\operatorname{tr} W^T W - \operatorname{tr} F^T W^T W F) + \beta \operatorname{tr} W^T W,$$

where L is a pre-defined loss function. The problem can be also relaxed to be convex:

$$\min_{W=[w_1,\ldots,w_T]} L(W) + \rho_1\eta(1+\eta)(\mathrm{tr}(W(\eta I + M)^{-1}W^T)$$

subject to $\mathrm{tr}\, M = k$, $M \preceq I$, $\eta = \frac{\rho_2}{\rho_1}$.

4.4.1 Least squares linear regression

The algorithm learns a multitask linear least squares regression model of regression

$$f_t(x) = \langle w_t, x\rangle + b_t, \quad t = 1,\ldots,T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_{W=[w_1,\ldots,w_T]} \sum_{t=1}^{T}\sum_{i\in G_t} \left(\langle w_t, x_i\rangle + b_t - y_i\right)^2 + \rho_1\eta(1+\eta)(\mathrm{tr}(W(\eta I + M)^{-1}W^T),$$

subject to $\mathrm{tr}\, M = k$, $M \preceq I$, $\eta = \frac{\rho_2}{\rho_1}$; where $G = \{G_1,\ldots,G_T\}$ is a set of tasks' non-overlapping indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \mathbb{R}$ are labels.

4.4.2 Logistic regression

The algorithm learns a multitask linear logistic model of classification

$$f_t(x) = sign(\langle w_t, x\rangle + b_t), \quad t = 1,\ldots,T,$$

where T is a number of tasks, from the solution of the following optimization problem:

$$\min_{W=[w_1,\ldots,w_T]} \sum_{t=1}^{T}\sum_{i\in G_t} \frac{1}{|G_t|}\log(1+\exp\left(-y_i(\langle w_t, x_i\rangle + b_t)\right) + \rho_1\eta(1+\eta)(\mathrm{tr}(W(\eta I + M)^{-1}W^T),$$

subject to $\mathrm{tr}\, M = k$, $M \preceq I$, $\eta = \frac{\rho_2}{\rho_1}$; where $G = \{G_1,\ldots,G_T\}$ is a set of tasks' non-overlapping indices, $\forall_i x_i$ are feature vectors and $\forall_i y_i \in \{-1,1\}$ are labels.

The algorithm is implemented in `CMultitaskClusteredLogisticRegression`.

Appendix A

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