Fast k-Nearest Neighbor Classifier

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Fast Nearest Neighbor Searching

The `fastknn` method implements a k-Nearest Neighbor (KNN) classifier based on the ANN library. ANN is written in `C++` and is able to find the k nearest neighbors for every point in a given dataset in `O(N log N)` time. The package RANN provides an easy interface to use ANN library in `R`.

The FastKNN Classifier

The `fastknn` was developed to deal with very large datasets (> 100k rows) and is ideal to Kaggle competitions. It can be about 50x faster then the popular `knn` method from the `R` package class, for large datasets. Moreover, `fastknn` provides a shrinkage estimator to the class membership probabilities, based on the inverse distances of the nearest neighbors (**see the PDF version**):

$$P(x_i \in y_j) = \frac{\displaystyle\sum_{k=1}^{K} \left(\frac{1}{d_{ik}} \cdot (n_{ik} \in y_j) \right)}{\displaystyle\sum_{k=1}^{K} \left(\frac{1}{d_{ik}} \right)}$$

where x_i is the i^{th} test instance, y_j is the j^{th} unique class label, n_{ik} is the k^{th} nearest neighbor of x_i, and d_{ik} is the distance between x_i and n_{ik}. This estimator can be thought of as a weighted voting rule, where those neighbors that are more close to x_i will have more influence on predicting x_i's label.

In general, the weighted estimator provides more **calibrated probabilities** when compared with the traditional estimator based on the label proportions of the nearest neighbors, and reduces **logarithmic loss** (log-loss).

How to install `fastknn`?

The package `fastknn` is not on CRAN, so you need to install it directly from GitHub:

```
library("devtools")
install_github("davpinto/fastknn")
```

Required Packages

The base of `fastknn` is the `RANN` package, but other packages are required to make `fastknn` work properly. All of them are automatically installed when you install the `fastknn`.

- `RANN` for fast nearest neighbors searching,
- `magrittr` to use the pipe operator `%>%`,
- `pbapply` to show a progress bar during cross-validation,
- `Metrics` to measure classification performance,
- `ggplot2` to plot classification decision boundaries,
- `viridis` for modern color palletes.

Getting Started

Using `fastknn` is as simple as:

```r
## Load packages
library("fastknn")
library("caTools")

## Load toy data
data("chess", package = "fastknn")

## Split data for training and test
set.seed(123)
tr.idx <- caTools::sample.split(Y = chess$y, SplitRatio = 0.7)
x.tr   <- chess$x[tr.idx, ]
x.te   <- chess$x[-tr.idx, ]
y.tr   <- chess$y[tr.idx]
y.te   <- chess$y[-tr.idx]

## Fit KNN
yhat <- fastknn(x.tr, y.tr, x.te, k = 10)

## Evaluate model on test set
sprintf("Accuracy: %.2f", 100 * sum(yhat$class == y.te) / length(y.te))
```

```
## [1] "Accuracy: 99.30"
```

Find the Best k

The `fastknn` provides a interface to select the best `k` using n-fold cross-validation. There are 4 possible **loss functions**:

- Overall classification error rate: `eval.metric = "overall_error"`
- Mean in-class classification error rate: `eval.metric = "mean_error"`
- Mean in-class AUC: `eval.metric = "auc"`
- Cross-entropy / logarithmic loss: `eval.metric = "logloss"`

Cross-validation using the **voting** probability estimator:

```r
## Load dataset
library("mlbench")
data("Sonar", package = "mlbench")
x <- data.matrix(Sonar[, -61])
y <- Sonar$Class

## 5-fold CV using log-loss as evaluation metric
set.seed(123)
cv.out <- fastknnCV(x, y, k = 3:15, method = "vote", folds = 5, eval.metric = "logloss")
cv.out$cv_table
```

fold_1	fold_2	fold_3	fold_4	fold_5	mean	k
2.638	3.629	2.721	1.895	0.9809	2.373	3
1.139	2.079	2.789	1.104	0.2251	1.467	4
1.203	1.304	2.791	1.133	0.315	1.349	5
0.5285	1.333	2.011	1.198	0.358	1.086	6
0.5567	0.5874	2.031	1.244	0.3923	0.9622	7
0.5657	0.593	2.058	1.244	0.417	0.9755	8
0.5502	0.6228	1.286	0.4712	0.4478	0.6757	9
0.5864	0.6344	0.5025	0.4843	0.4854	0.5386	10
0.5975	0.6518	0.5116	0.4765	0.5134	0.5502	11
0.6059	0.6543	0.5022	0.4897	0.5383	0.5581	12
0.5996	0.6642	0.5212	0.5132	0.566	0.5728	13
0.6114	0.6572	0.5283	0.5242	0.5882	0.5819	14
0.6163	0.6416	0.5416	0.5449	0.5959	0.5881	15

Cross-validation using the **weighted voting** probability estimator:

```r
## 5-fold CV using log-loss as evaluation metric
set.seed(123)
cv.out <- fastknnCV(x, y, k = 3:15, method = "dist", folds = 5, eval.metric = "logloss")
cv.out$cv_table
```

fold_1	fold_2	fold_3	fold_4	fold_5	mean	k
2.626	3.608	2.707	1.891	0.9645	2.359	3
1.111	2.052	2.766	1.094	0.1965	1.444	4
1.15	1.263	2.766	1.112	0.2682	1.312	5
0.4569	1.288	1.987	1.165	0.2946	1.038	6
0.4715	0.5304	1.999	1.199	0.3192	0.9039	7
0.4786	0.5315	2.022	1.2	0.3391	0.9142	8
0.4628	0.5587	1.246	0.4257	0.3636	0.6114	9
0.4918	0.5664	0.4651	0.4357	0.3912	0.47	10
0.5002	0.5783	0.4686	0.427	0.415	0.4778	11
0.5101	0.5768	0.4625	0.4367	0.4386	0.485	12
0.503	0.5861	0.4765	0.4542	0.4626	0.4965	13
0.5116	0.5794	0.4826	0.4663	0.4836	0.5047	14
0.5194	0.5742	0.4938	0.4842	0.4926	0.5128	15

Note that the mean **log-loss** for the **weighted voting** estimator is lower for every `k` evaluated.

Plot Classification Decision Boundary

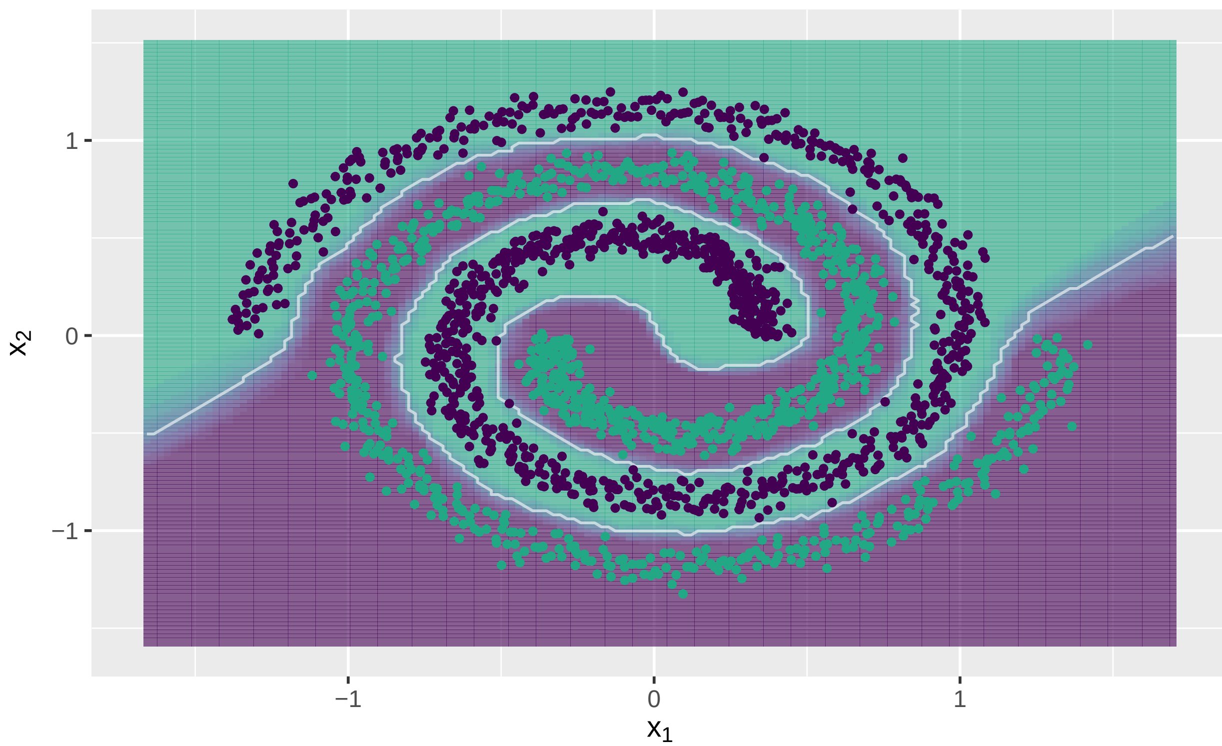
The `fastknn` provides a plotting function, based on `ggplot2`, to draw bi-dimensional decision boundaries. If your dataset has more than 3 variables, only the first two will be considered. In future versions of `fastknn` the most descriptive variables will be selected automatically beforehand, using a **feature ranking** tecnique.

Two-class Problem

```
## Load toy data
data("spirals", package = "fastknn")

## Split data for training and test
set.seed(123)
tr.idx <- caTools::sample.split(Y = spirals$y, SplitRatio = 0.7)
x.tr   <- spirals$x[tr.idx, ]
x.te   <- spirals$x[-tr.idx, ]
y.tr   <- spirals$y[tr.idx]
y.te   <- spirals$y[-tr.idx]

## Plot decision boundary
knnDecision(x.tr, y.tr, x.te, y.te, k = 15)
```

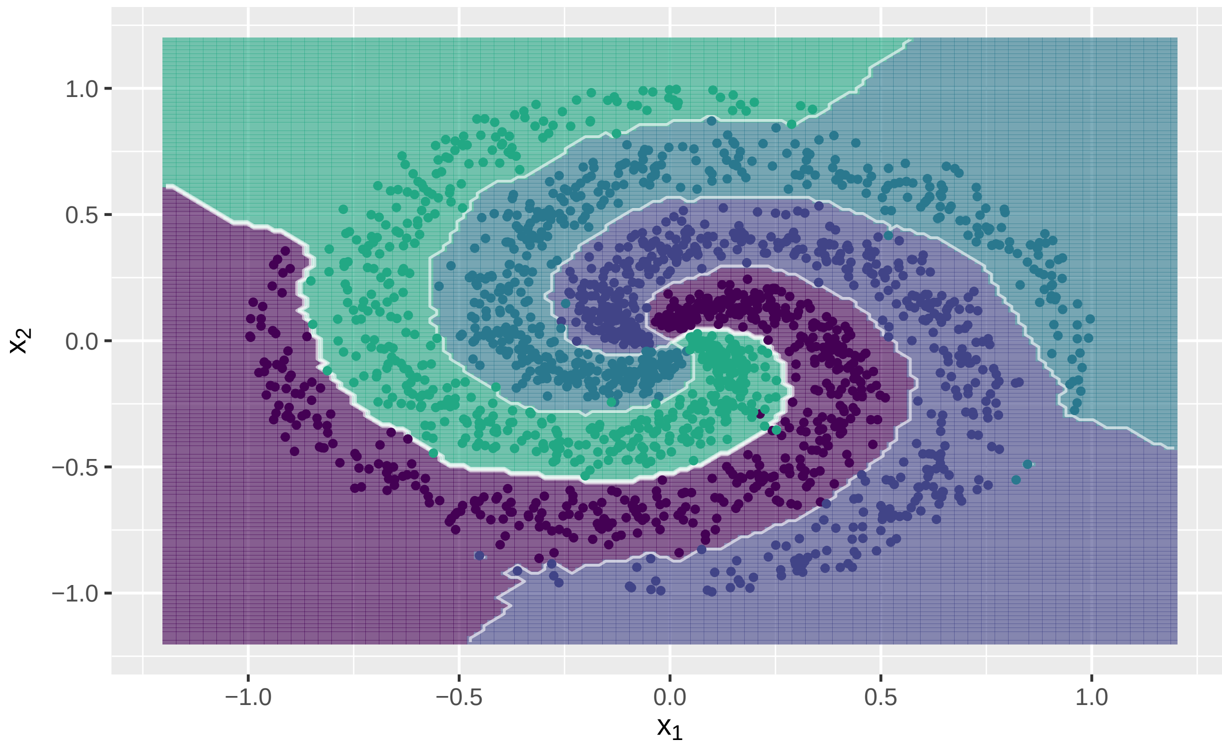


Multi-class Problem

```
## Load toy data
data("multi_spirals", package = "fastknn")
```

```
## Split data for training and test
set.seed(123)
tr.idx <- caTools::sample.split(Y = multi_spirals$y, SplitRatio = 0.7)
x.tr   <- multi_spirals$x[tr.idx, ]
x.te   <- multi_spirals$x[-tr.idx, ]
y.tr   <- multi_spirals$y[tr.idx]
y.te   <- multi_spirals$y[-tr.idx]

## Plot decision boundary
knnDecision(x.tr, y.tr, x.te, y.te, k = 15)
```



Performance Test

Here we test the performance of `fastknn` on the Covertype datset. It is hosted on UCI repository and has been already used in a **Kaggle** competition. The dataset contains 581012 observations on 54 numeric features, classified into 7 different categories.

All experiments were conducted on a **64-bit Ubuntu 16.04 with Intel Core i7-6700HQ 2.60GHz and 16GB RAM DDR4**.

Computing Time

Here `fastknn` is compared with the `knn` method from the package `class`. We had to use small samples from the Covertype data because `knn` takes too much time (> 1500s) to fit the entire dataset.

```
#### Load packages
library('class')
```

```r
library('fastknn')
library('readr')
library('caTools')

#### Load data
dtset <- read_csv('./data/covertype_sample.csv.gz')
dtset$Target <- as.factor(dtset$Target)

#### Test with different sample sizes
N <- nrow(dtset)
sample.frac <- c(10e3, 15e3, 20e3)/N
res <- lapply(sample.frac, function(frac, dt) {
   ## Reduce datset
   set.seed(123)
   sample.idx <- sample.split(dt$Target, SplitRatio = frac)
   x <- as.matrix(dt[sample.idx, -55])
   y <- dt$Target[sample.idx]

   ## Split data
   set.seed(123)
   tr.idx <- sample.split(y, SplitRatio = 0.7)
   x.tr   <- x[tr.idx, ]
   x.te   <- x[-tr.idx, ]
   y.tr   <- y[tr.idx]
   y.te   <- y[-tr.idx]

   ## Measure time
   t1 <- system.time({
      yhat1 <- knn(train = x.tr, test = x.te, cl = y.tr, k = 10, prob = TRUE)
   })
   t2 <- system.time({
      yhat2 <- fastknn(xtr = x.tr, ytr = y.tr, xte = x.te, k = 10, method = "dist")
   })

   ## Return
   list(
      method = c('knn', 'fastknn'),
      nobs = as.integer(rep(N*frac, 2)),
      time_sec = c(t1[3], t2[3]),
      accuracy = round(100 * c(sum(yhat1 == y.te), sum(yhat2$class == y.te)) / length(y.te), 2)
   )
}, dt = dtset)
res <- do.call('rbind.data.frame', res)
res
```

method	nobs	time_sec	accuracy
knn	10000	4.039	75.88
fastknn	10000	0.154	92.57
knn	15000	9.653	77.76
fastknn	15000	0.239	93.26
knn	20000	21.86	79.11
fastknn	20000	0.305	93.79

The `fastknn` takes **about 5s** to fit the entire dataset.

Probability Prediction

We compared the `voting` estimator with the `weighted voting` estimator:

Voting

```
#### Extract input variables and response variable
x <- as.matrix(dtset[, -55])
y <- dtset$Target

#### 5-fold cross-validation
res <- fastknnCV(x, y, k = 10, method = "vote", folds = 5, eval.metric = "logloss")
res$cv_table
```

fold_1	fold_2	fold_3	fold_4	fold_5	mean	k
0.5966	0.582	0.5655	0.5806	0.5863	0.5822	10

Weighted Voting

```
#### 5-fold cross-validation
res <- fastknnCV(x, y, k = 10, method = "dist", folds = 5, eval.metric = "logloss")
res$cv_table
```

fold_1	fold_2	fold_3	fold_4	fold_5	mean	k
0.5473	0.5417	0.5011	0.5558	0.5516	0.5395	10