Fast k-Nearest Neighbor Classifier

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Fast KNN with shrinkage estimator for the class membership probabilities

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:

```r
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:

```
## 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 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.

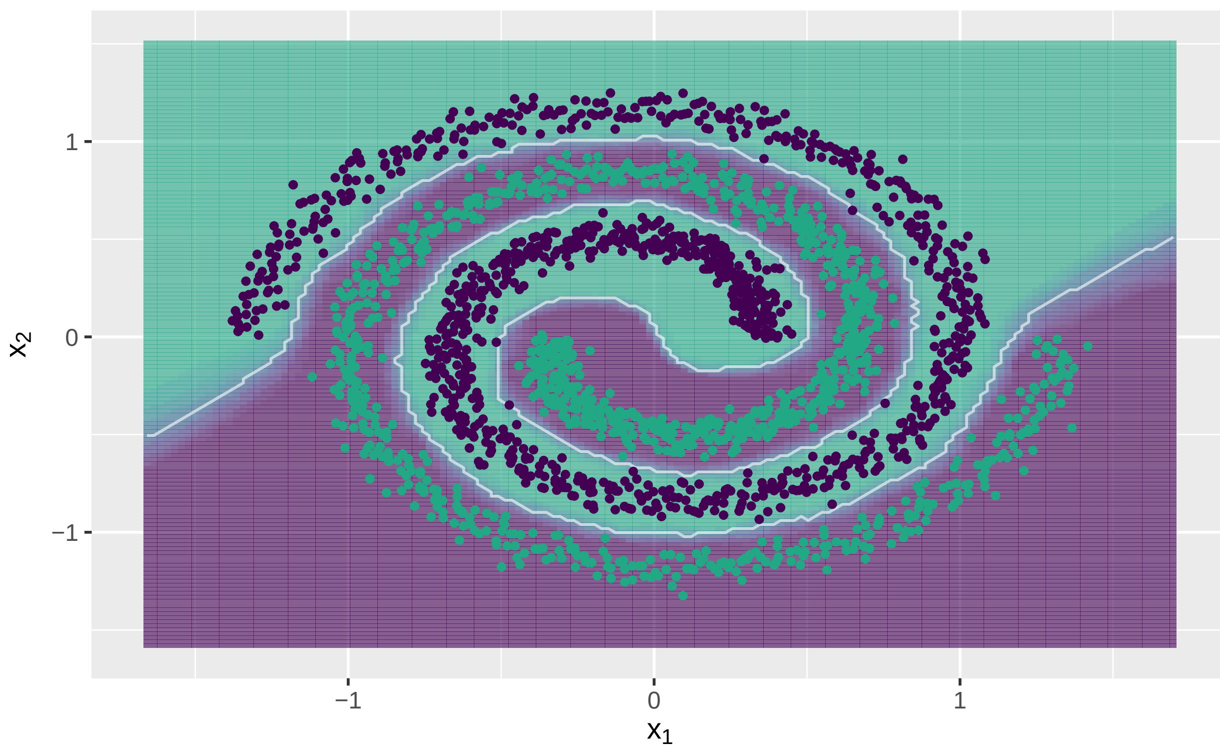
Plot Classification Decision Boundary

Two-class Problem

```r
## 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)
```



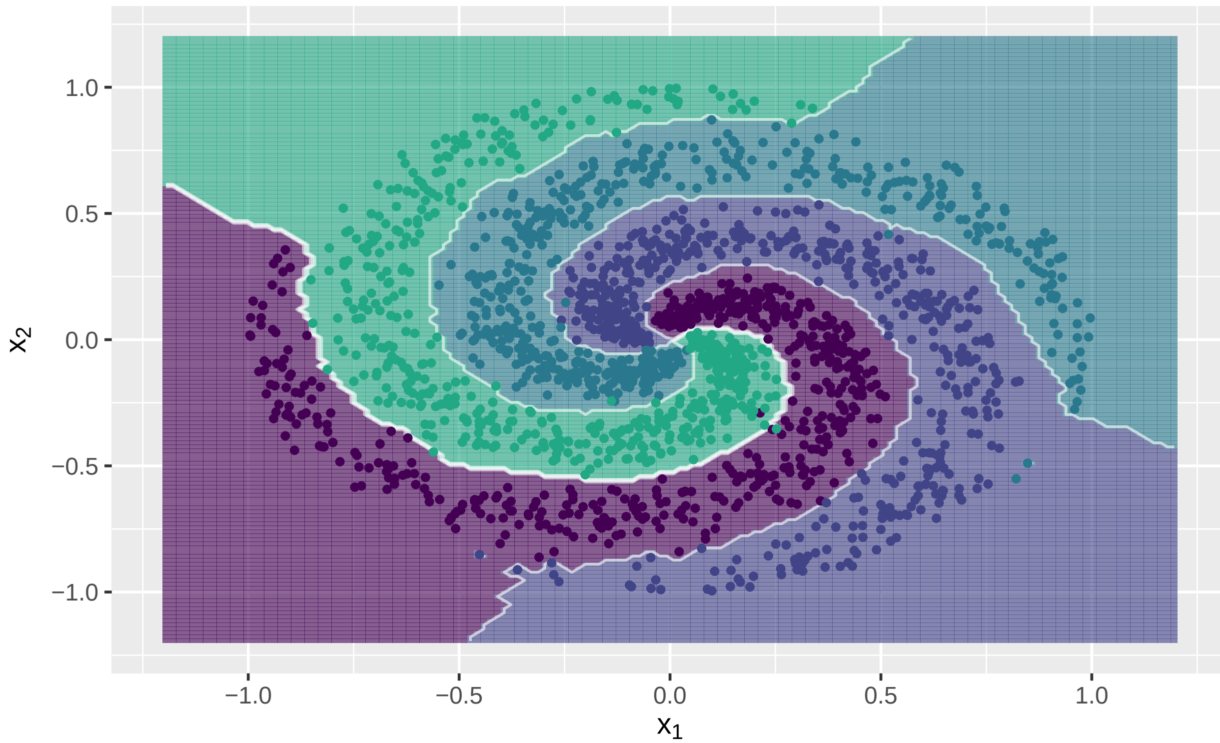
Multi-class Problem

```r
## 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)
```



Benchmark