Assessed Coursework #2: Profiling, Performance, & Parallelisation

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In this assessed coursework, I use profiling to identify inefficiencies in the `tune` function of the `e1071` package, particularly focusing on its application to tune support vector machines. Next, I work on several improvements to the function's efficiency, applying techniques such as `apply` functions and parallelisation. The coursework primarily focuses on profiling and parallel programming, as well as the use of vectorisation to improve performance.

Support vector machines

Support vector machines (SVMs) are a classification technique that works to find the optimal decision boundary between classes. To do so, they find the decision boundary with the thickest error margin possible. In situations where perfect classification accuracy on the training data is not possible, as with most real-world datasets, SVMs solve the soft margin problem to find the decision boundary $f(\mathbf{x}; \mathbf{w}) = 0$ in order to minimise

$$\|\mathbf{w}\|^2 + \sum_i \epsilon_i$$

subject to the constraints that, for all i,

$$y_i f(\mathbf{x}_i; \mathbf{w}) + \epsilon_i \geq 1, \epsilon_i \geq 0$$

Finding a solution to this constrained optimisation problem is difficult for high-dimensional datasets, and these constraints are relatively complex. The primal SVM problem can be reformulated into the dual problem using Lagrange multipliers. The dual problem simplifies the optimization process and allows for the computation of the support vectors without explicitly finding the high-dimensional vector $\mathbf{w}$ in the primal space. The dual problem also enables the use of kernel functions, allowing SVMs to handle non-linear separations efficiently. However, when solving the dual problem, SVMs are computationally expensive for datasets with large sample sizes.

SVM hyperparameters

SVMs rely on the use of several hyperparameters, depending on the use of kernel function. All SVMs use the cost hyperparameter C, which controls the trade-off between minimising errors on the training data and controlling the complexity of the model. This hyperparameter $C > 0$ comes into the primal problem such that the decision boundary minimises

$$\|\mathbf{w}\|^2 + C \sum_i \epsilon_i$$

SVMs can also use a variety of kernel functions, which can introduce additional hyperparameters. For instance, if using a radial basis kernel function

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\gamma |\mathbf{x}_i - \mathbf{x}_j|^2)$$

one must also specify the value of the bandwidth γ.

These hyperparameters should be tuned in order to find the values that yield the best performance. There are several methods for hyperparameter tuning, most notably cross-validation. Since cross-validation necessitates the creation of multiple SVMs, the computational burden increases, particularly for datasets with large sample sizes or situations where the number of folds selected for cross-validation is high.

e1071 package

The `e1071` R package is commonly used for implementing SVMs in R. Here is an example application on a dataset of penguin species. We use an SVM with a linear kernel ($C = 1$) to predict the penguin species using data about the bill length, bill depth, flipper length, and body mass:

```
library(tidyverse)
library(e1071) # svm package
library(palmerpenguins) # data package
library(caret) # ML package
library(here) # filepath package

# Filter to 2 penguin species for binary classification
adelie_gentoo <- penguins %>%
  filter(species %in% c("Adelie", "Gentoo")) %>%
  mutate(species = droplevels(species)) %>%
  filter(!is.na(bill_length_mm))

# Create training / test split
set.seed(999)
index <- createDataPartition(adelie_gentoo$species, p = 0.7, list = FALSE)
# Training data
penguin_training <- adelie_gentoo[index,] %>%
  select(species,
         ends_with("_mm"),
         body_mass_g)
penguin_testing <- adelie_gentoo[-index,] %>%
  select(species,
         ends_with("_mm"),
         body_mass_g)

# Train a Support Vector Machine (SVM) model
penguin_svm_model <- svm(species ~ ., data = penguin_training, kernel = "linear", cost = 1)

# Make predictions on the test set
penguin_svm_predictions <- predict(penguin_svm_model, newdata = penguin_testing)

# Evaluate the model performance
table(penguin_svm_predictions, penguin_testing$species)
```

```
##
## penguin_svm_predictions Adelie Gentoo
##                  Adelie     45      0
##                  Gentoo      0     36
```

We achieve 100% classification accuracy on the penguin dataset.

Let's try on a larger dataset of abalone data. This example predicts sex of abalones using some variables pertaining to the dimension of their shells. We now use an RBF kernel ($C = 1, \gamma = 0.2$):

```
library(AppliedPredictiveModeling)
data("abalone")
```

```r
mf_abalone <- abalone %>%
  select(-Rings) %>%
  filter(Type %in% c("M", "F")) %>%
  mutate(Type = droplevels(Type))

# Create training / test split
set.seed(999)
index <- createDataPartition(mf_abalone$Type, p = 0.7, list = FALSE)
# Training data
abalone_training <- mf_abalone[index,]
abalone_testing <- mf_abalone[-index,]

# Train a Support Vector Machine (SVM) model
abalone_svm_model <- svm(Type ~ .,
                         data = abalone_training,
                         kernel = "radial",
                         cost = 1,
                         gamma = 0.2)

# Make predictions on the test set
abalone_svm_predictions <- predict(abalone_svm_model, newdata = abalone_testing)

# Evaluate the model performance
abalone_conf_matrix <- table(abalone_svm_predictions, abalone_testing$Type)
abalone_accuracy <- sum(diag(abalone_conf_matrix)) / sum(abalone_conf_matrix)
cat("Accuracy:", abalone_accuracy, "\n")
```

```
## Accuracy: 0.5364706
```

```r
abalone_conf_matrix
```

```
##
## abalone_svm_predictions   F   M
##                       F 111 113
##                       M 281 345
```

We have poorer performance on this larger dataset. Let's see if tuning the hyperparameters using cross-validation helps.

Tuning in `e1071`

The `e1071` package has a `tune` function that tunes hyperparameters using a grid search. We can supply several values for the hyperparameters C and γ, and `tune` will yield the model with the hyperparameters that performed best, as measured by classification error:

```r
tictoc::tic()
abalone_tuned_svm <- tune(svm,
                          Type ~ .,
                          data = abalone_training,
                          kernel = "radial",
                          ranges = list(cost = c(0.5, 1, 1.5),
```

```
                                        gamma = c(0.02, 0.2, 2)),
                            tunecontrol = tune.control(sampling = "cross",
                                                       cross = 10))
tictoc::toc()
```

```
## 9.001 sec elapsed
```

Note that running `tune` on these 9 parameter combinations (3 values of C × 3 values of γ) was relatively slow. We will see why momentarily. We can now examine the parameters that gave the lowest classification error out of the combinations tried, and then test the best model on our testing data.

```
abalone_tuned_svm$best.parameters
```

```
##   cost gamma
## 9  1.5     2
```

```
# Make predictions on the test set
tuned_abalone_svm_predictions <- predict(abalone_tuned_svm$best.model,
                                         newdata = abalone_testing)

# Evaluate the model performance
tuned_abalone_conf_matrix <- table(tuned_abalone_svm_predictions, abalone_testing$Type)
tuned_abalone_accuracy <- sum(diag(tuned_abalone_conf_matrix)) / sum(tuned_abalone_conf_matrix)
cat("Accuracy:", tuned_abalone_accuracy, "\n")
```

```
## Accuracy: 0.54
```

```
tuned_abalone_conf_matrix
```

```
##
## tuned_abalone_svm_predictions   F   M
##                             F 158 157
##                             M 234 301
```

We have slightly improved accuracy on the new values of the hyperparameters, which use a higher bandwidth value, but performance is still poor. Trying more combinations of C and γ is incredibly slow and computationally intensive, however, because of the structure of the `tune` function.

Improving `tune` performance

Profiling

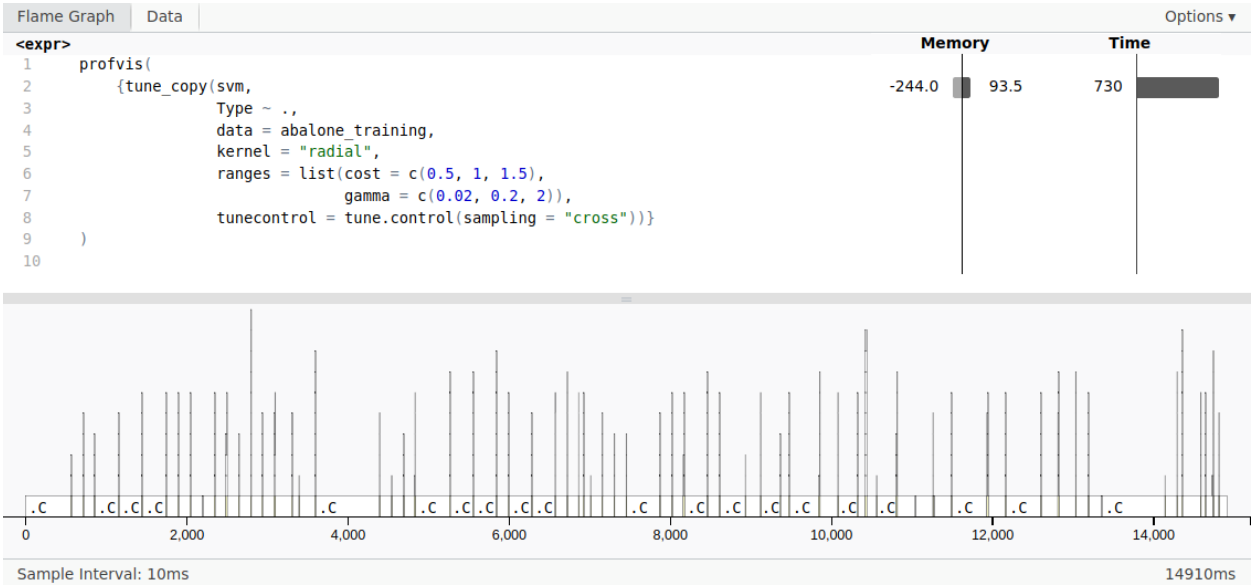
We can use profiling to determine what is causing the slow performance of `tune`. I copied the source code for `tune` from here into `e1071_tune_copy.R` to explore what's going on within the function:

```
library(profvis)

profvis(
  {tune_copy(svm,
```

```
            Type ~ .,
            data = abalone_training,
            kernel = "radial",
            ranges = list(cost = c(0.5, 1, 1.5),
                          gamma = c(0.02, 0.2, 2)),
            tunecontrol = tune.control(sampling = "cross",
                                       cross = 10))}
)
```

The profiling results look like this:



Flame Graph | Data | Options

Code	File	Memory (MB)		Time (ms)
.C		-312.0	460.4	14140
▼ tune_copy	<expr>	-244.0	93.5	730
▼ svm.formula		-132.5	80.8	530
▼ svm.default		-132.5	79.1	520
▶ data.frame		0	51.6	290
▶ predict.svm		-126.2	4.4	140
▶ scale_data_frame		0	17.4	50
t.default		-6.3	0	10
is.numeric		0	3.8	10
na.omit.default		0	0.1	10
▶ na.omit.data.frame		0	1.8	10
▶ predict.svm		0	2.6	70
[.data.frame		0	2.0	40
▶ model.frame.default		0	3.7	30
▶ resp		0	1.7	20
▶ table		0	1.8	20
tunecontrol$repeat.aggregate		0	0.9	10
▶ cbind		-111.5	0	10
is.pairlist		0	0.9	10
anyNA		0	2.1	10
.External2		0	0.5	10
as.integer		0	0.9	10

Sample Interval: 10ms 14910ms

Removing for-loops

By digging into the source code, we can see that `tune` contains 3 for loops nested within one another:

1. Looping over each parameter combination (9 in total in the example above)
2. Looping over each training sample (10 in the example since we performed 10-fold cross-validation)
3. Looping over the number of times training is repeated (1 in our example since `nrepeat = 1` by default)

We can eliminate the last loop by using the `replicate` function, which is a wrapper for `sapply`. I replaced the final loop with a use of `replicate` to create a new function, `tune_optimised`. Code for the `tune_optimised` function can be viewed here. We can compare how long `tune_optimised` takes as compared to the `e1071::tune` function:

```
source(here("R/tune_optimized.R"))
tictoc::tic()
abalone_tuned_svm_optimised <- tune_optimised(svm,
                                              Type ~ .,
                                              data = abalone_training,
                                              kernel = "radial",
                                              ranges = list(cost = c(0.5, 1, 1.5),
                                                            gamma = c(0.02, 0.2, 2)),
                                              tunecontrol = tune.control(sampling = "cross",
                                                                         cross = 10))
tictoc::toc()
```

```
## 9.023 sec elapsed
```

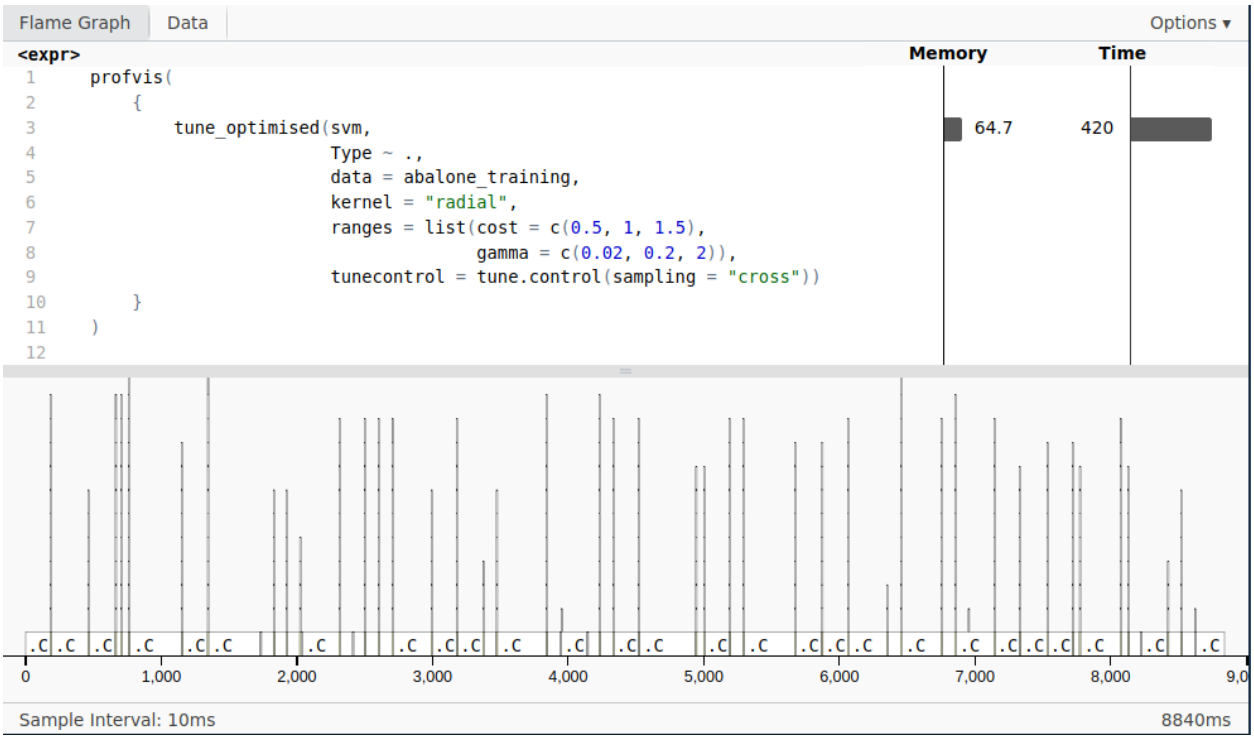
```
abalone_tuned_svm_optimised$best.parameters
```

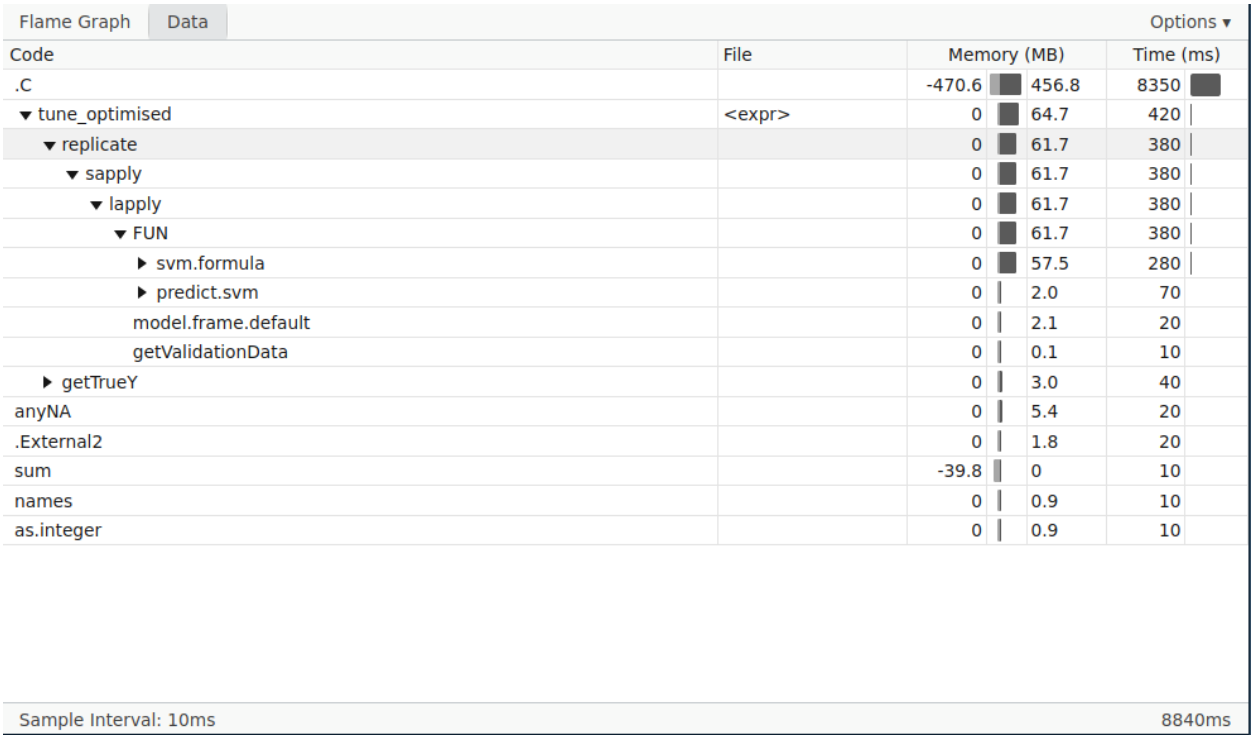
```
##   cost gamma
## 8    1     2
```

The results are slightly faster (depending on when it is run), but not by much (and they can be slightly slower as well). We can examine the profiling:

```
profvis(
  {
    tune_optimised(svm,
                   Type ~ .,
                   data = abalone_training,
                   kernel = "radial",
                   ranges = list(cost = c(0.5, 1, 1.5),
                                 gamma = c(0.02, 0.2, 2)),
                   tunecontrol = tune.control(sampling = "cross"))
  }
)
```

The profiling results with the new function look like this:





Code	File	Memory (MB)	Time (ms)
.C		-470.6 456.8	8350
▼ tune_optimised	<expr>	0 64.7	420
▼ replicate		0 61.7	380
▼ sapply		0 61.7	380
▼ lapply		0 61.7	380
▼ FUN		0 61.7	380
▶ svm.formula		0 57.5	280
▶ predict.svm		0 2.0	70
model.frame.default		0 2.1	20
getValidationData		0 0.1	10
▶ getTrueY		0 3.0	40
anyNA		0 5.4	20
.External2		0 1.8	20
sum		-39.8 0	10
names		0 0.9	10
as.integer		0 0.9	10

We appear to be spending a bit less time on .C, but the `apply` functions are still time-consuming.

Parallelization

To improve performance further, we can try using parallel programming to run the different iterations of cross-validation x parameter combinations in parallel, rather than sequentially via loops. I used the `foreach`

and `doParallel` packages to do so. I created a new function, `tune_parallel` (code available here), which uses 80% of the available cores. In my case, my laptop has 20 cores, so the function uses 16 of them. Rather than using the two loops followed by `replicate`, as in `tune_optimise`, the new function uses two `foreach` statements, with the inner `foreach` using `%dopar%` to execute the code in parallel.

```
library(foreach)
library(doParallel)
source(here("R/tune_parallel.R"))
tictoc::tic()
abalone_tuned_svm_parallel <- tune_parallel(svm,
                                            Type ~ .,
                                            data = abalone_training,
                                            kernel = "radial",
                                            ranges = list(cost = c(0.5, 1, 1.5),
                                                          gamma = c(0.02, 0.2, 2)),
                                            tunecontrol = tune.control(sampling = "cross"))
tictoc::toc()
```

```
## 1.718 sec elapsed
```

```
abalone_tuned_svm_parallel$best.parameters
```

```
##   cost gamma
## 8    1     2
```

We now see speed improvements of approximately 80%, an enormous improvement. Parallelisation makes the code far more efficient, enabling the possibility of searching far more values of the hyperparameters in tuning without undue computational burden.