## Fast pairwise redundancy calculation

For the purpose of visualization in FEXUM, we require a redundancy score of every feature pair. To avoid running our correlation measure for each pair and thus reduce runtime, we use a heuristic to estimate the score. Given the circumstance that our contrast measure (see [2] in paper) is defined between a set and a feature, we can extrapolate redundancy for each feature from random subsets.

Given a feature set  $F = \{f_1, ..., f_d\}$  in a d-dimensional dataset and  $k \in \mathbb{N}$  where k is the number of iterations to run, we can define the following algorithm:

```
function FastPairwiseRedundancy (F, k)

redundancies \leftarrow empty dictionary

for k do

S \leftarrow pickRandomSubset(F)

f \leftarrow pickRandomFeature(F \setminus S)

score \leftarrow contrast(S, f)

for i \in S do

redundancies[\{f, i\}] = min(score, redundancies[\{f, i\}])

end for

end for

return redundancies
end function
```

We pick a random subset  $S \subseteq F$  and a random feature f out of the remaining set  $F \setminus S$ , and calculate contrast. For each pair i, j with  $i \in S$  and j = f, we save the minimum of our current score and previous calculations.

For all tuples (S, f) given features i, j with  $i \in S$ , j = f, it is true that  $contrast(\{i\}, j) \leq contrast(S, f)$ , because contrast is a measure and as such must be monotonic. As a result, our algorithm will converge toward the correct result, slightly overestimating redundancy until convergence. To be more specific, the score for the aforementioned pair i, j will be correct once there is an iteration with a set  $S' = S \setminus \{i\}$  where each element of S' is either completely redundant to i or irredundant to j. Therefore, the time to achieve an optimal solution will depend on the individual dataset, although an approximation running for a predetermined amount of iterations k will be sufficient in most cases.

To give an example let us consider  $F_1 = \{f_1, f_2, f_3, f_4\}$ , where we would like to determine the redundancy of  $f_1$  to  $f_2$ . We assume that the iterations of  $contrast(S, f_1)$  used the subsets  $S_1 = \{f_2, f_3\}$ ,  $S_2 = \{f_2, f_4\}$ , and that  $f_3$  is redundant to  $f_1$  but irredundant to  $f_2$ , while  $f_4$  is irredundant to  $f_1$ . Scoring  $(S_1, f_1)$  will overestimate redundancy of  $\{f_1, f_2\}$ , as  $f_3$  supplies additional information about  $f_1$  compared to  $f_2$  alone. Scoring  $(S_2, f_1)$  will exactly equal the redundancy of  $\{f_1, f_2\}$ , as  $f_4$  does not contain any information pertaining to  $f_1$ .