Methods and results

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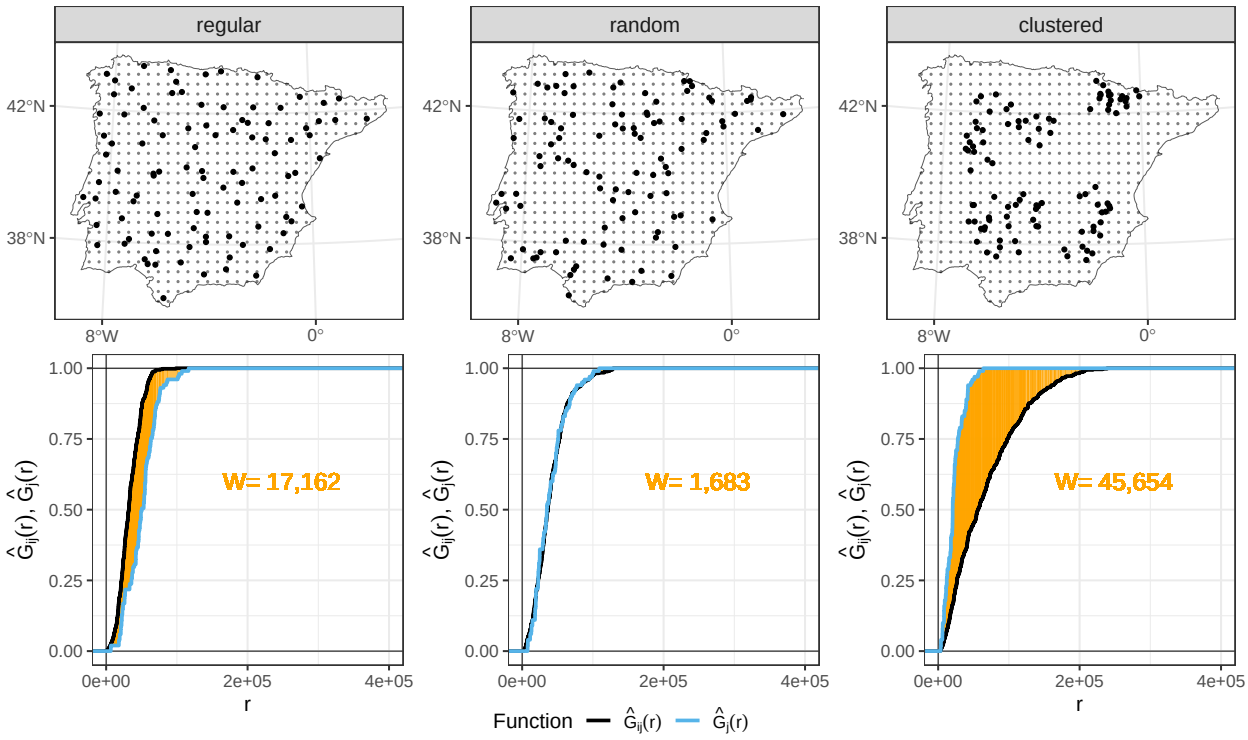
This file contains the code to reproduce figures 1, 3, 5, 6 & 7 of the paper "kNNDM: k-fold Nearest Neighbour Distance Matching Cross-Validation for map accuracy estimation" by J Linnenbrink, C Milà, M Ludwig & H Meyer.

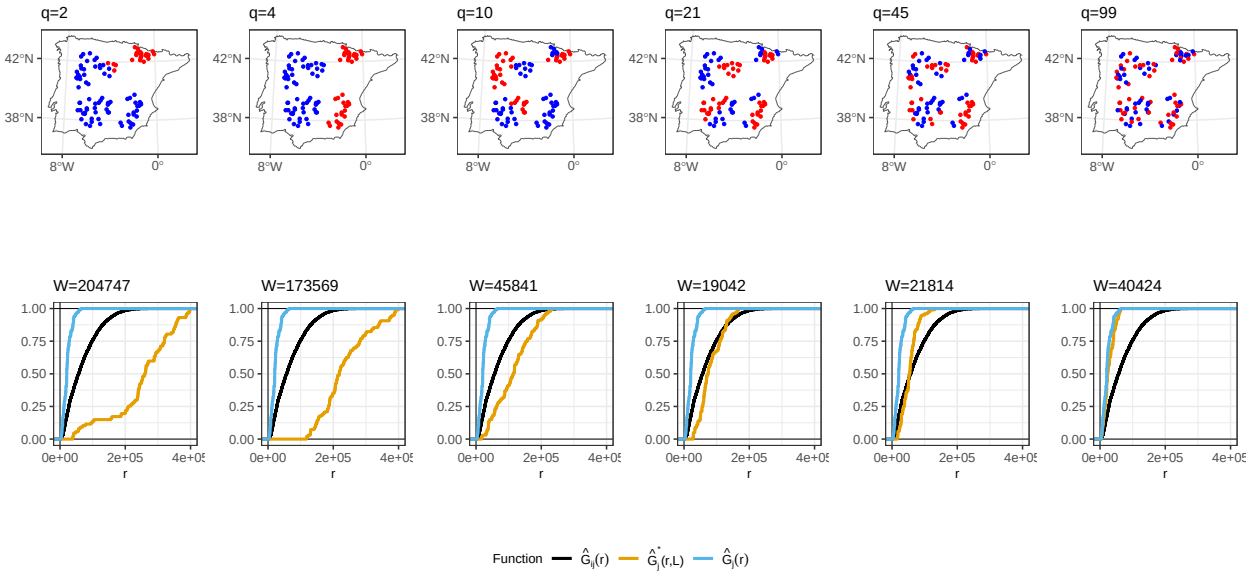
Example: different clustering, NND ECDFs and W statistics

This code reproduces figure 1, where different configurations of training samples and their corresponding nearest neighbour distance (NND) empirical cumulative distribution functions (ECDF) are shown. Also, the Wasserstein statistic is shown in orange.



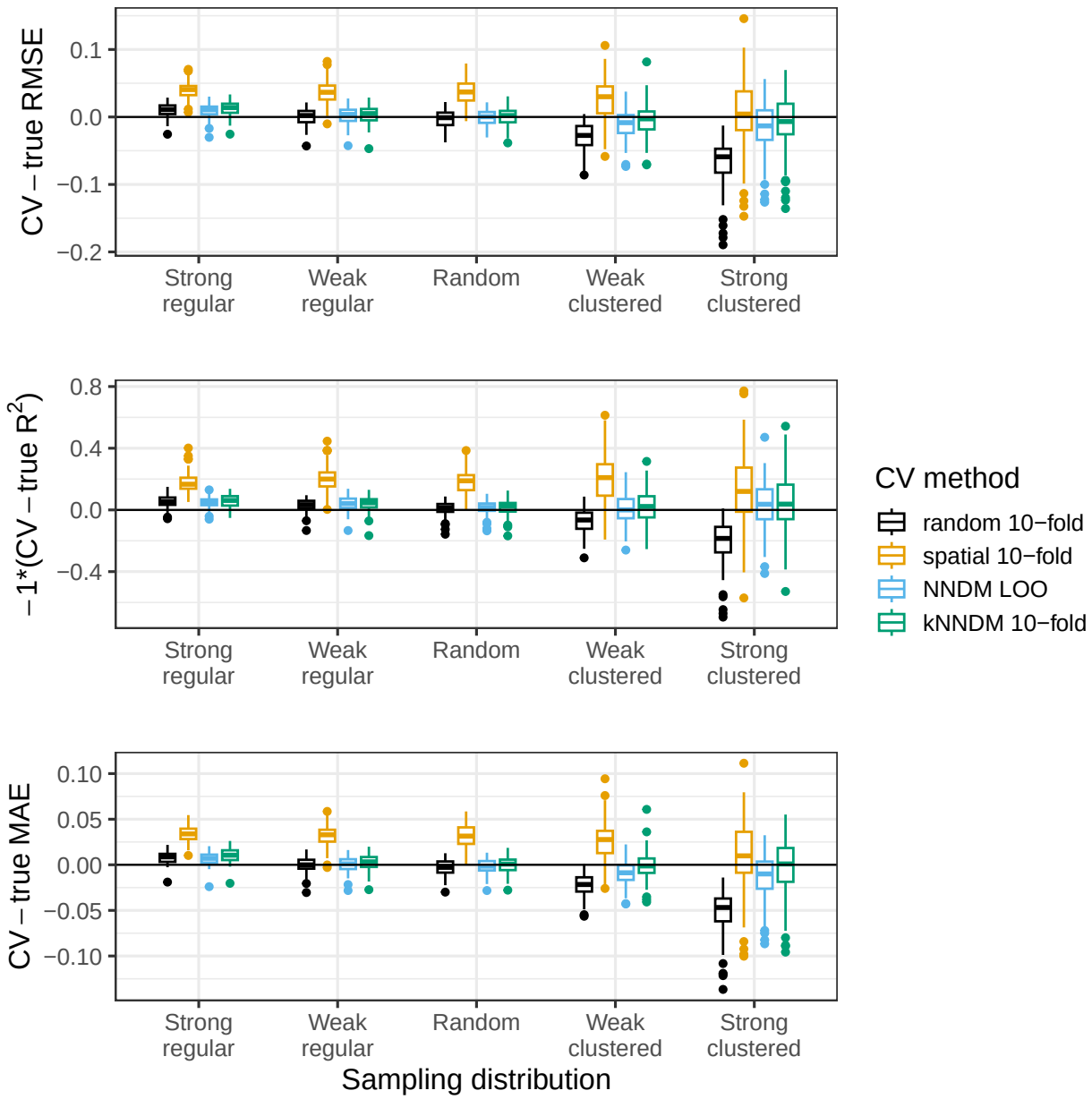
kNNDM workflow

This code reproduces the kNNDM workflow shown in figure 3. Several numbers of clusters q are compared regarding their W statistic (bottom row).



Simulation results

The following code reproduces figure 5, and shows the differences between cross-validated and true RMSE, R^2 and MAE for different sampling distributions.

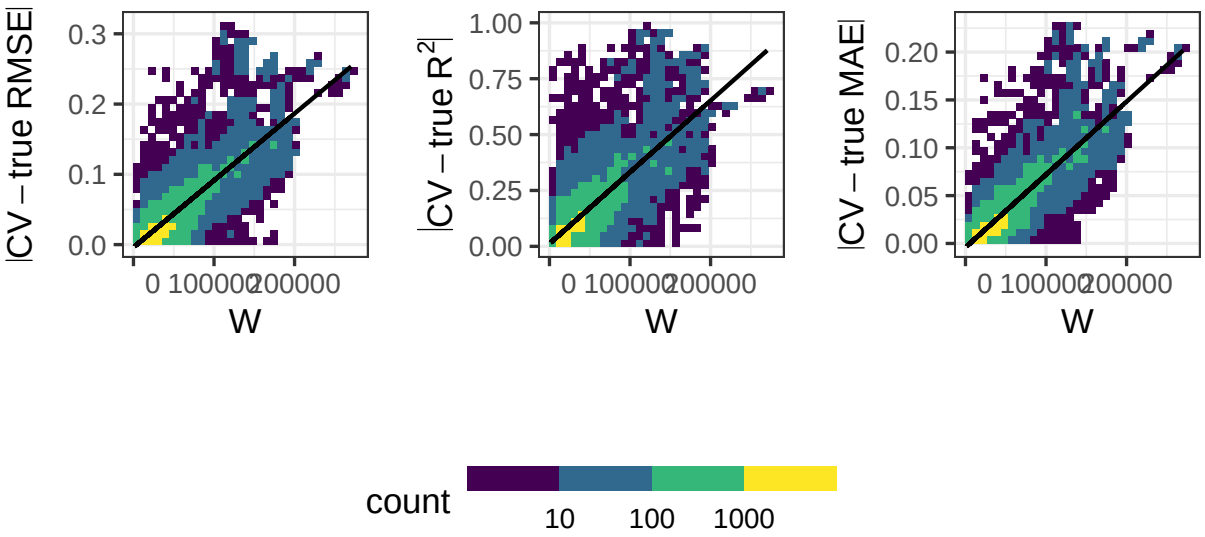



```
## # A tibble: 4 x 4
## # Groups:   name [4]
##   name      dsample     mean     sd
##   <chr>     <chr>      <dbl>  <dbl>
## 1 mae_kndm  sclust  -0.00310 0.0307
## 2 mae_nndm  sclust  -0.0126  0.0257
## 3 rmse_kndm sclust  -0.00837 0.0425
## 4 rmse_nndm sclust  -0.0146  0.0377
```

Association CV - True error and W statistic

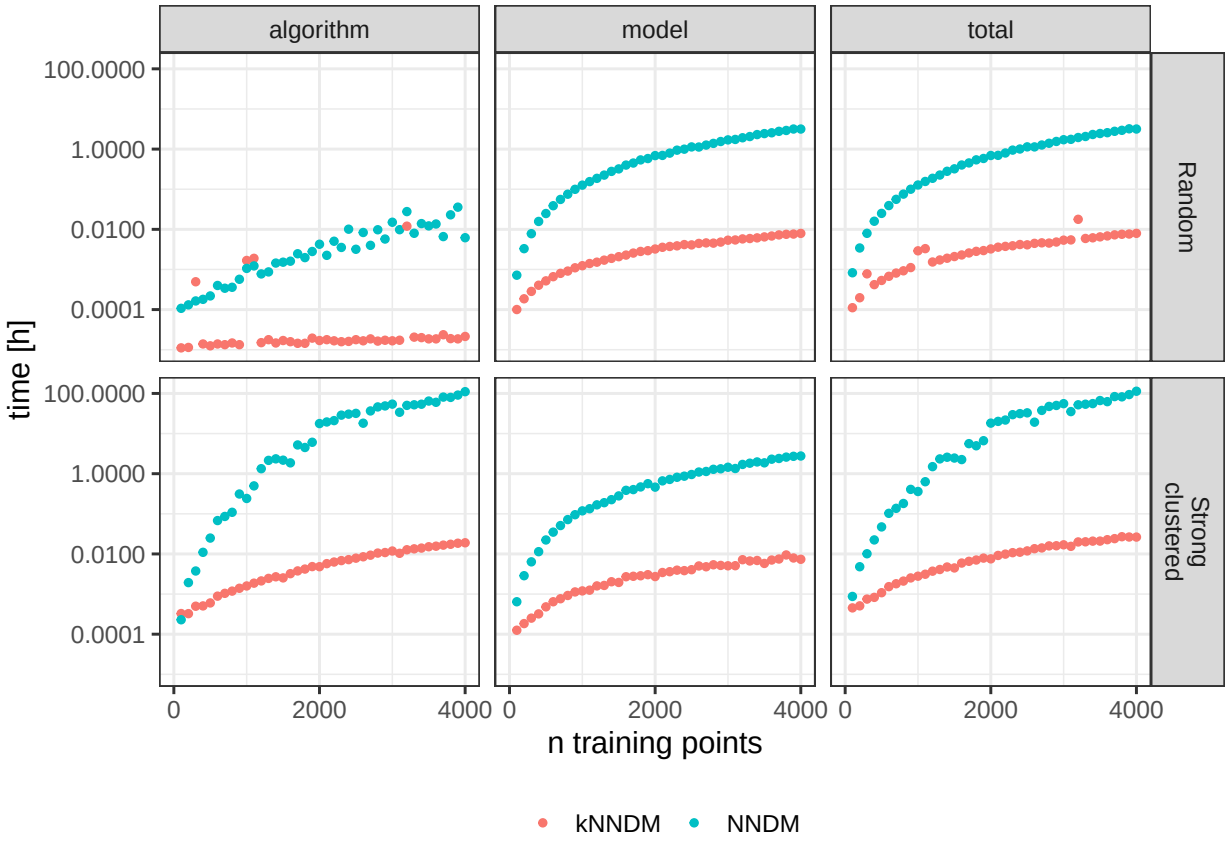
The following code reproduces figure 6, which shows the association between the absolute value difference between the CV and true map accuracy statistics and W statistic.

```
## [1] "Rsquared for Rsquared: 0.6 ; Rsquared for MAE: 0.73 ; Rsquared for RMSE: 0.66"
```



Computational time

The following code reproduces figure 7, which compares NNDM LOOCV and kNNDM CV regarding their computational time requirements.


algorithm
model
total
Random
Strong clustered
time [h]
100.0000
1.0000
0.0100
0.0001
0
2000
4000
n training points
kNNDM
NNDM