Supplementary Figure 4

a

5-fold outer cross validation:

5-fold inner cross validation:

x 5 resampling repetitions
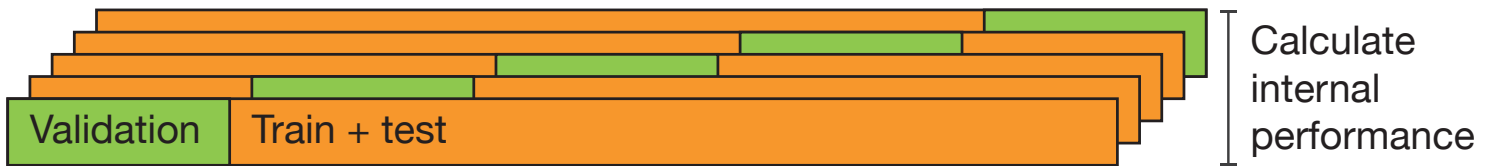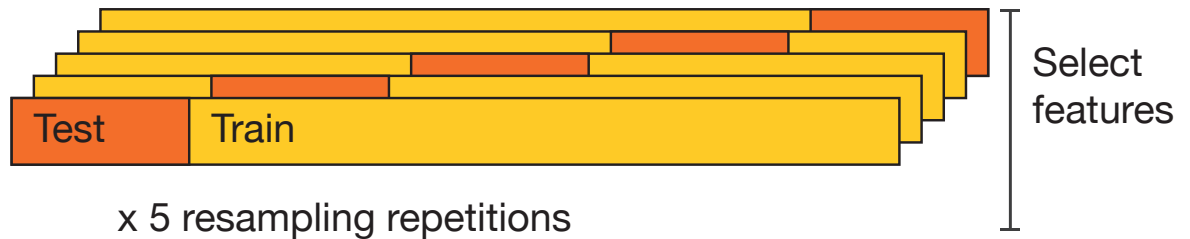
b

Select features:

for *each of the five outer cross-validation fold* **do**

    Partition original data into **(train+test)** and **validation** sets

    for *each of the five inner cross-validation fold and five resampling iteration* **do**

        Partition **(train+test) data** into **train** and **test** sets

        Standardise **train data**

        Standardise **test data** using standard deviation and mean of **train data**

        Forward feature selection by training neural network on **training data**, keep adding features as long as AUC on **test data** increase ≥ 0.01.

    end

end

Determine appropriate set of features: All features selected
  - at least once in each outer cross-validation fold, and
  - at least *X* times over all 125 cross-validation folds/resampling iterations

Calculate internal performance:

for *each of the five outer cross-validation fold* **do**

    Partition original data into **(train+test)** and **validation** sets

    Standardise **(train+test) data**

    Standardise **validation data** using standard deviation and mean of **(train+test) data**

    Train neural network model using **(train+test) data** and appropriate set of features

    Predict remission/non-remission for **validation** set

end

Calculate prediction performance for **validation** sets