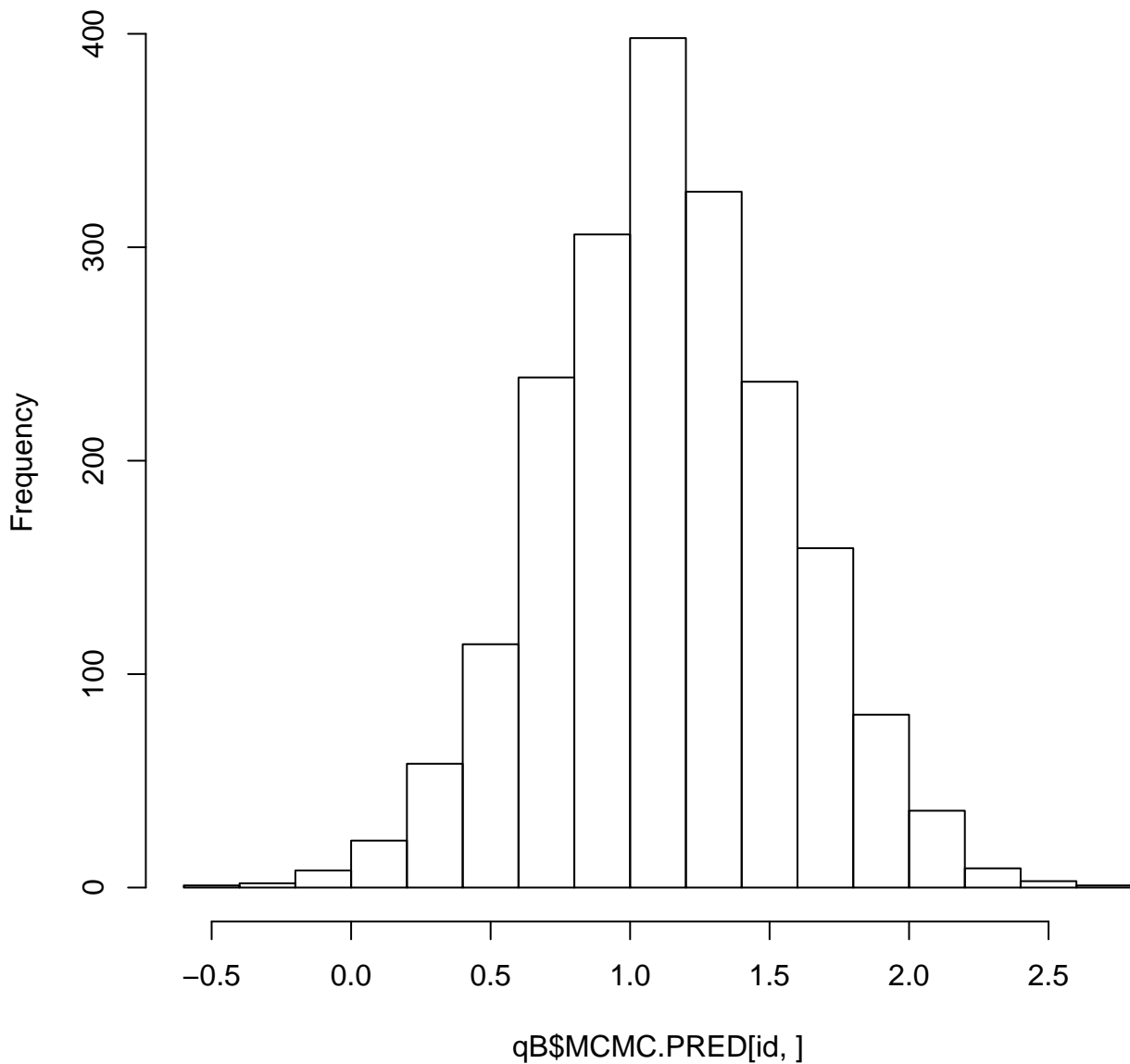
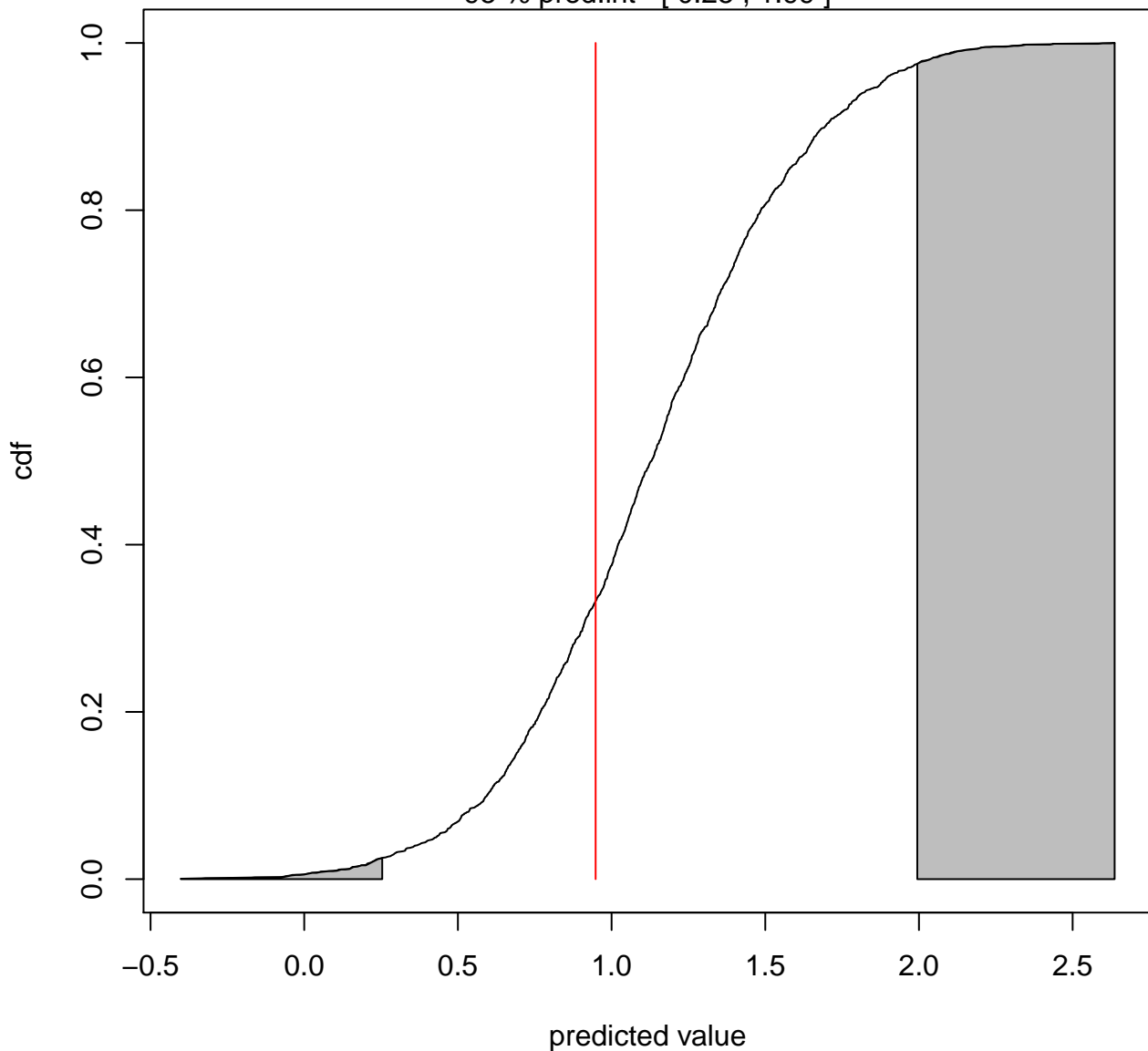


predictive distribution for compound 4

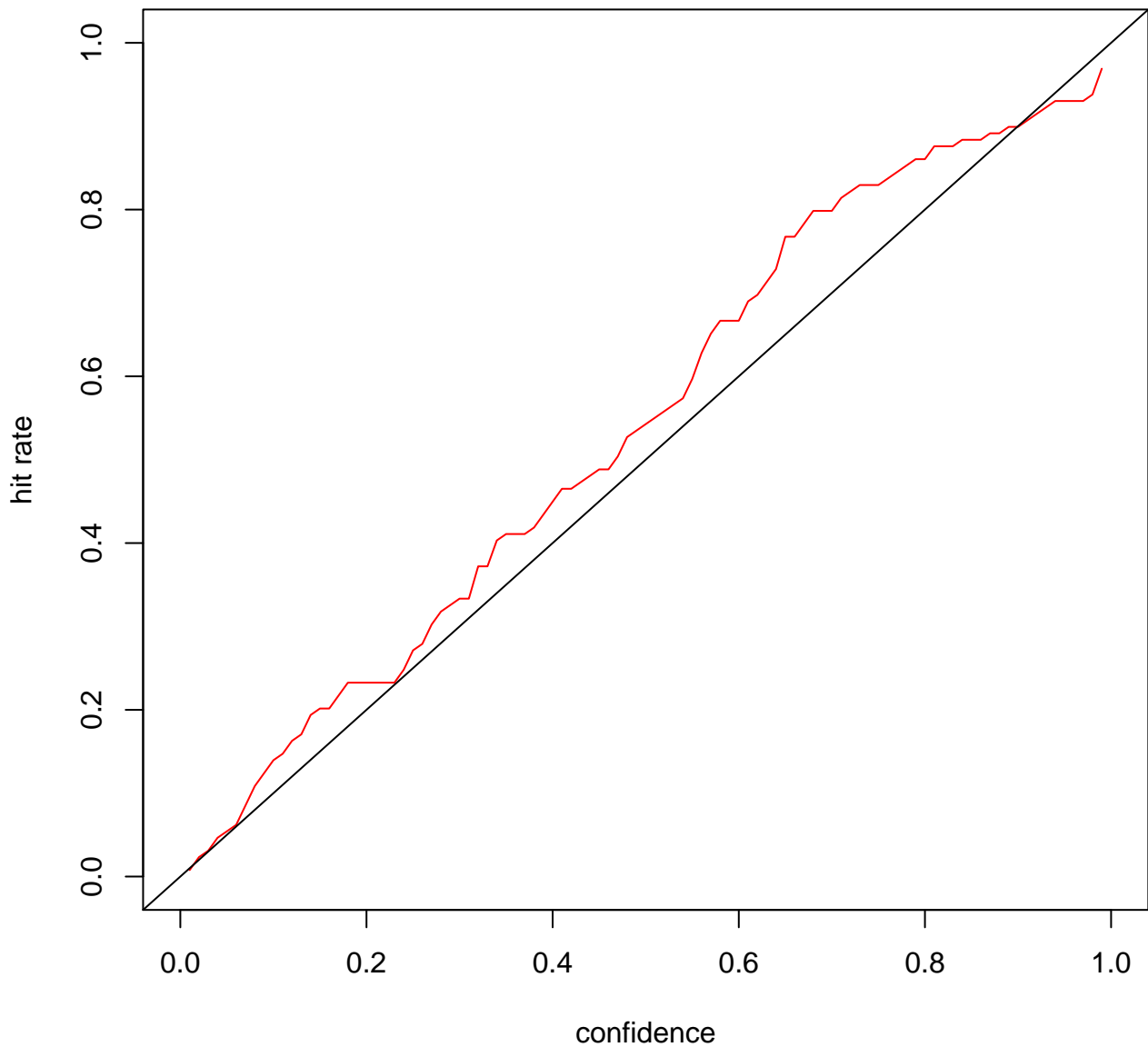


predictive distribution for compound 4

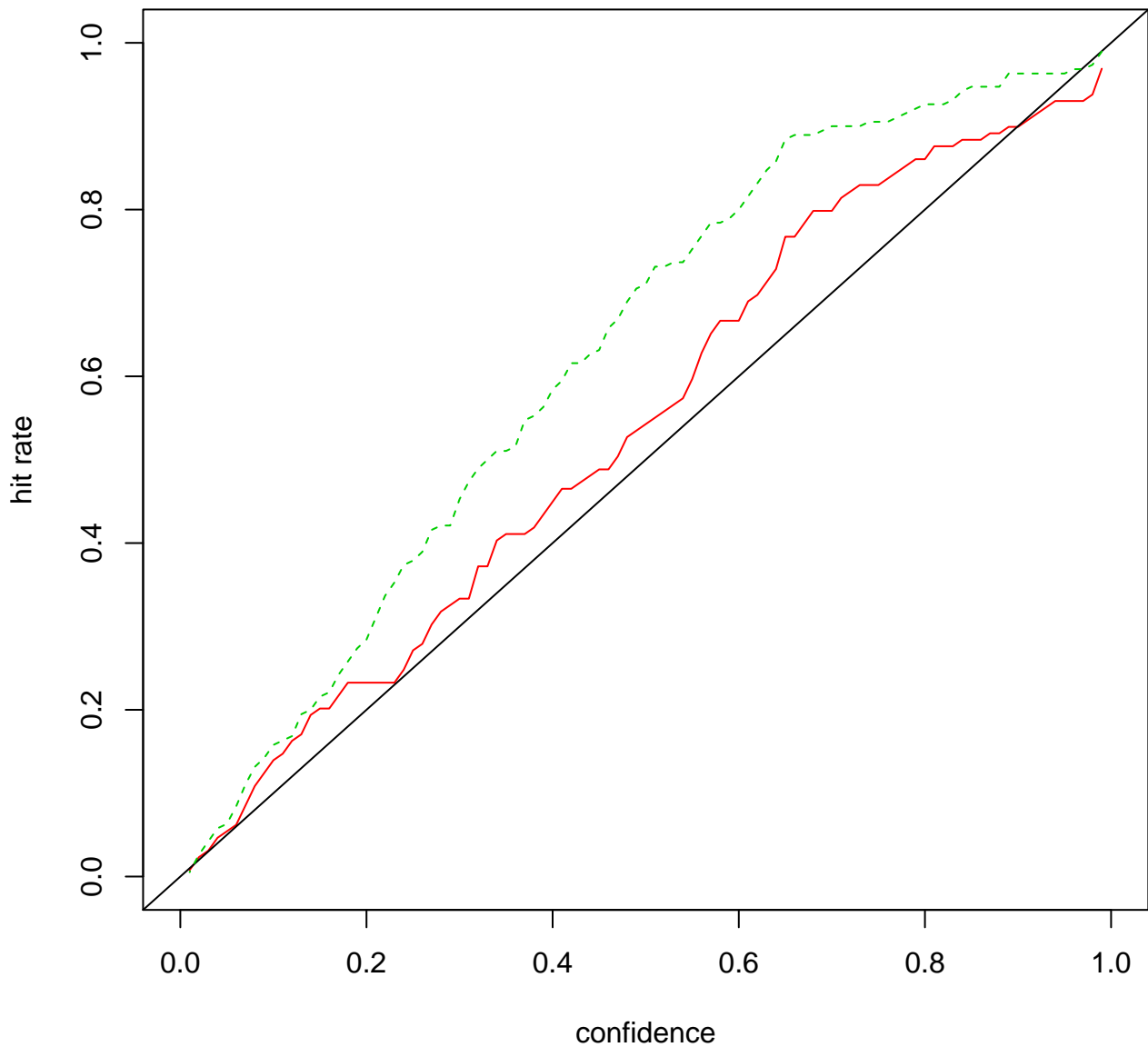
95 % pred.int= [0.25 , 1.99]



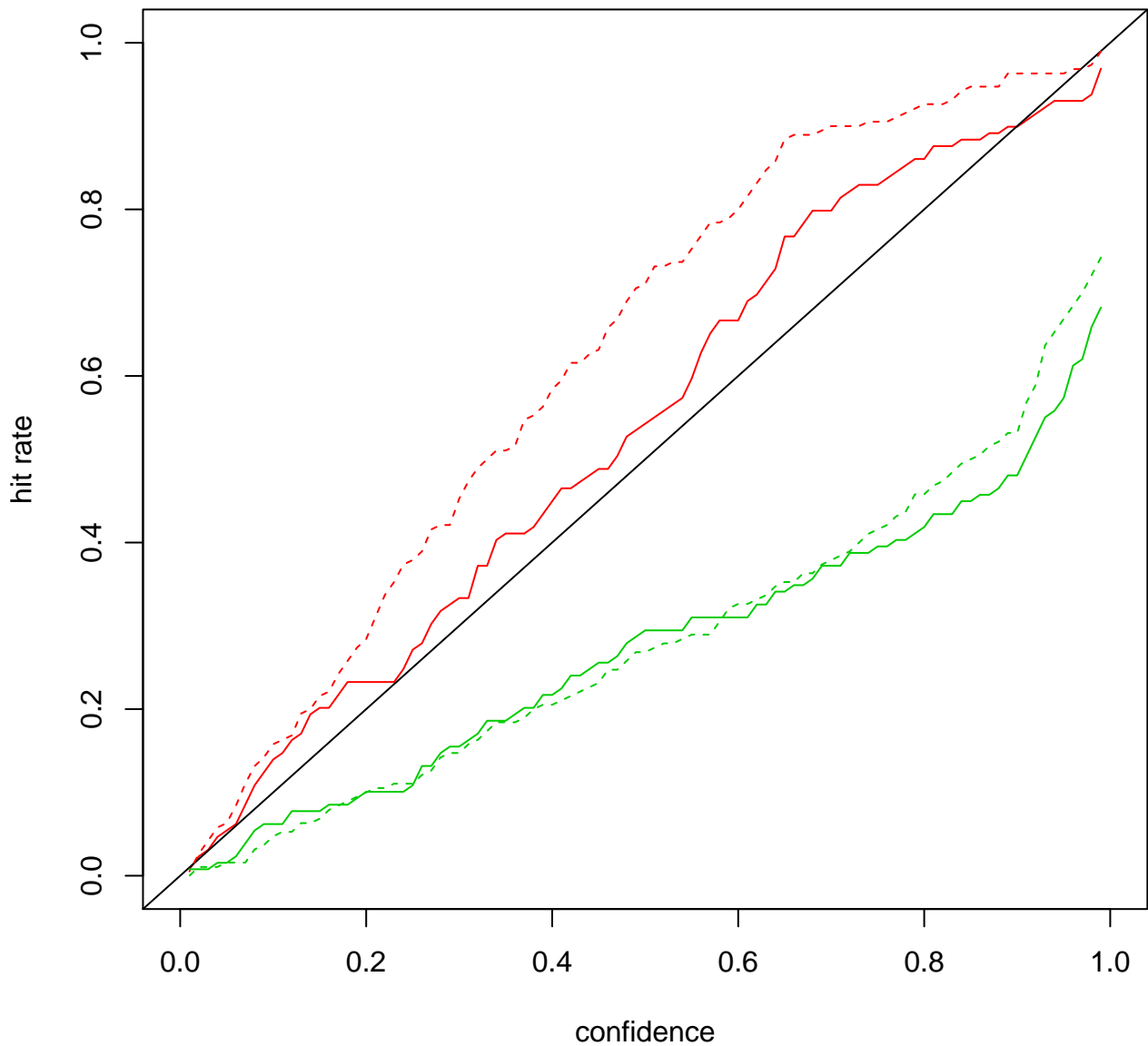
empirical coverage



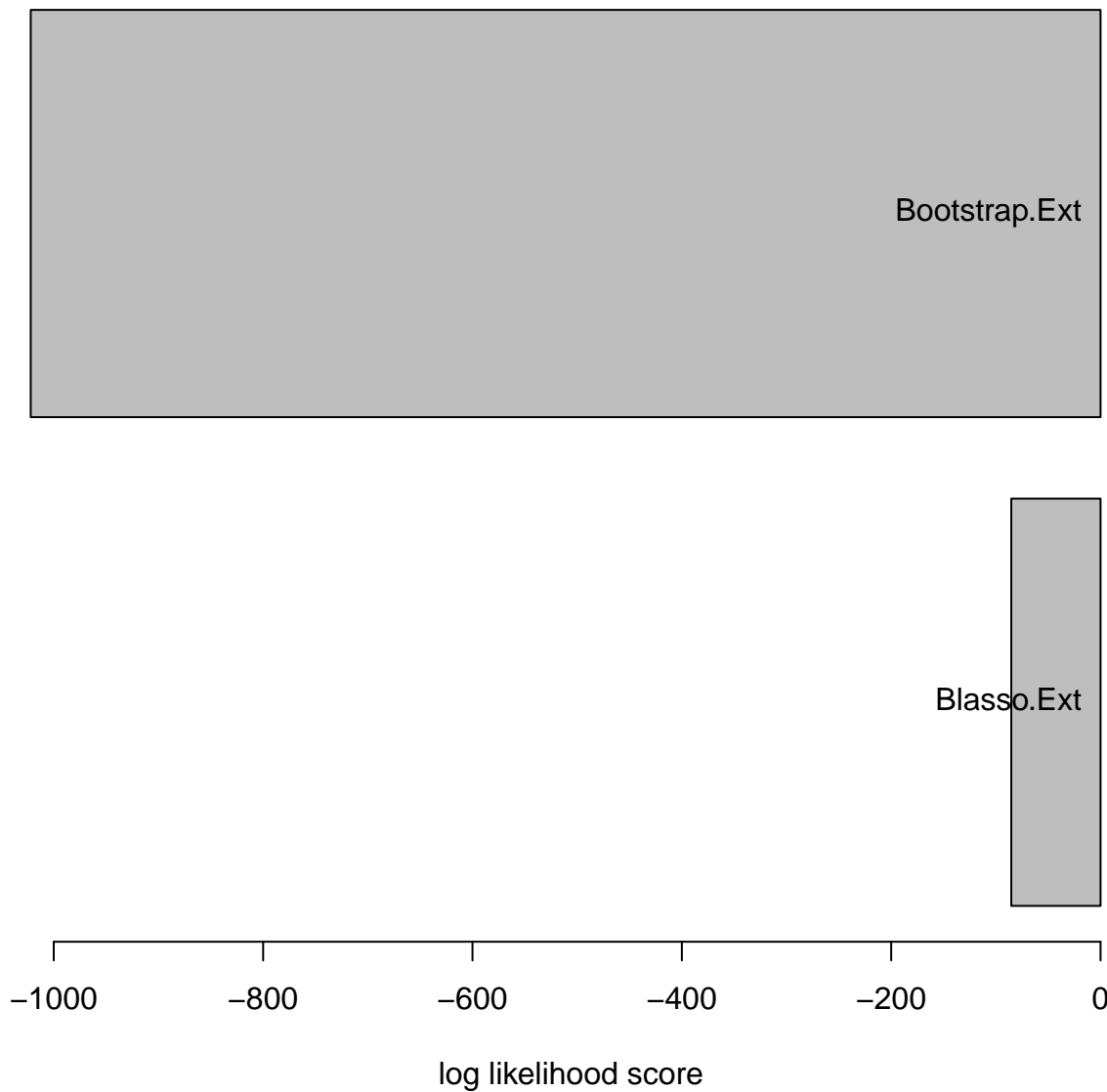
empirical coverage



empirical coverage

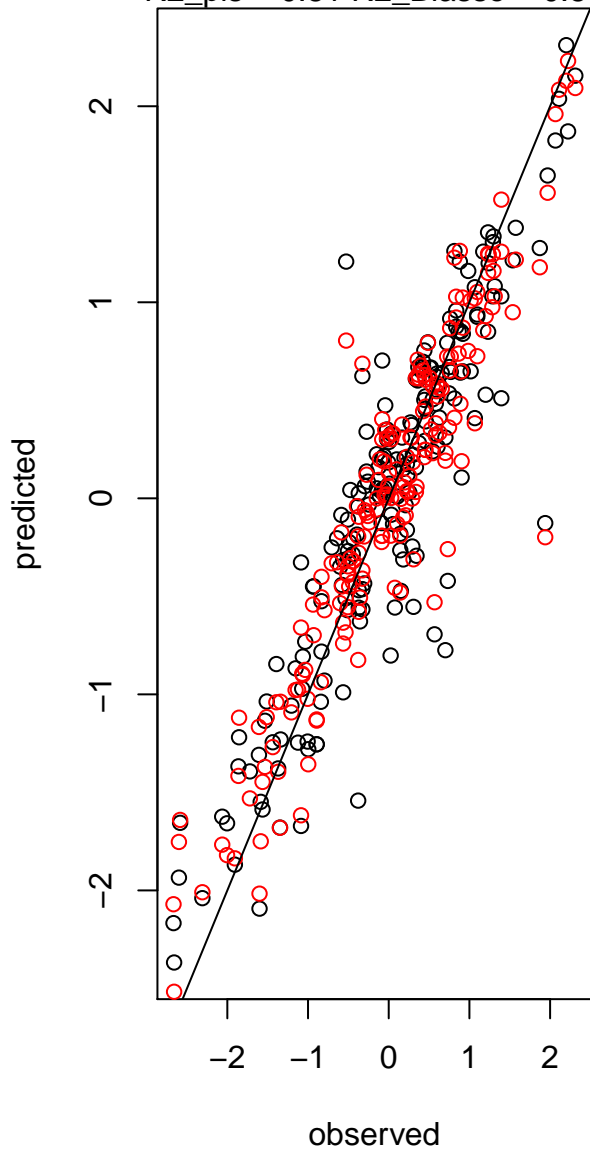


Assessment of predictive error



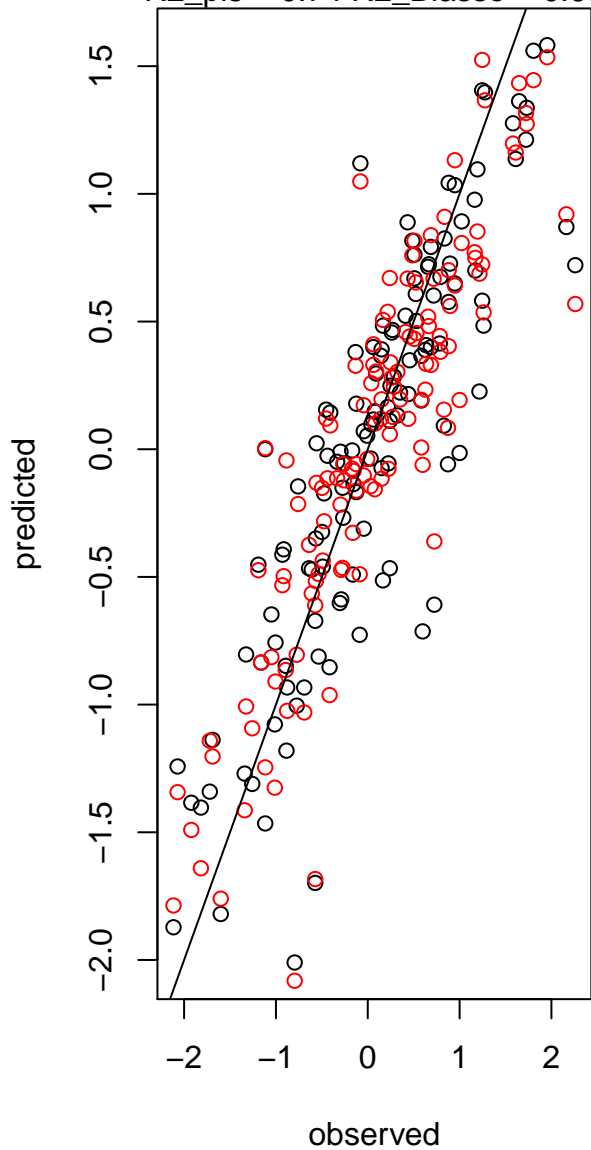
training data

R2_pls = 0.81 R2_Blasso = 0.87



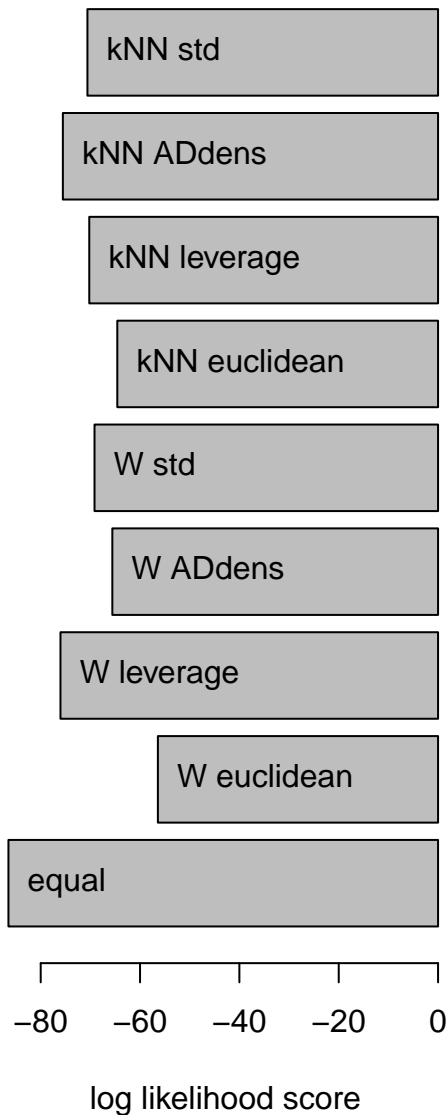
test data

R2_pls = 0.74 R2_Blasso = 0.69

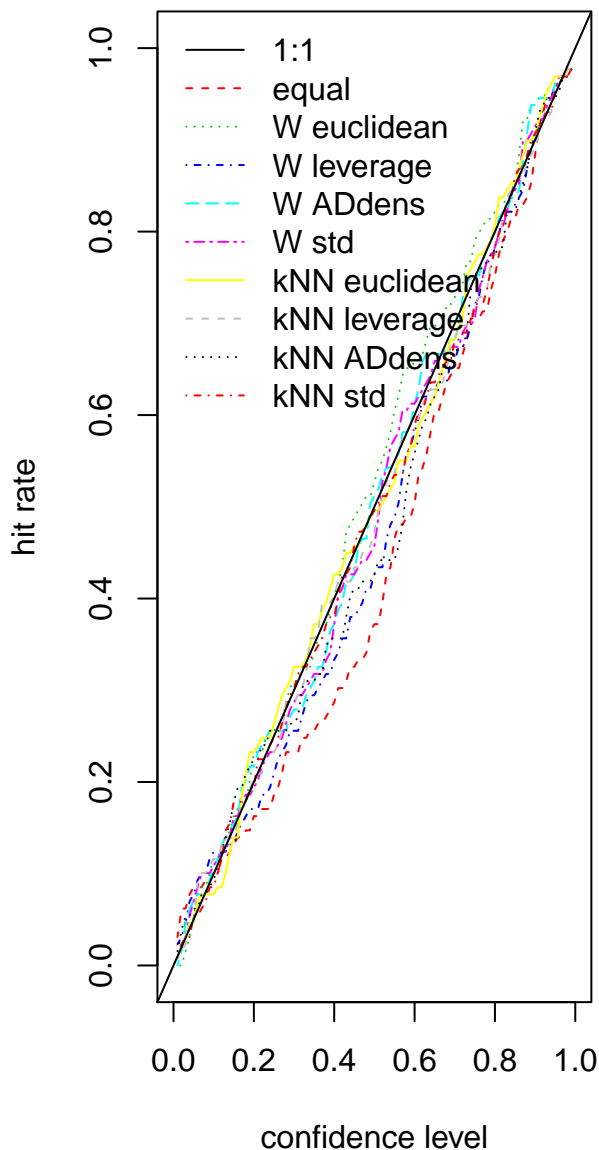


Evaluation on External data

Assessment of predictive error

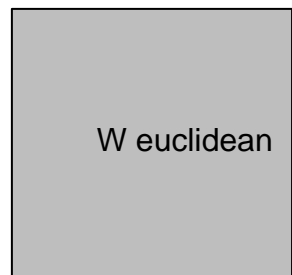
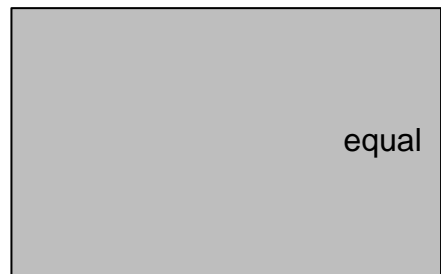


Empirical coverage (External data)



Relative comparison

Assessment of predictive error



-80 -60 -40 -20 0

log likelihood score