

S3 Text: Relationship between training and  
prediction RMSE for individual and ensemble  
models

Data-driven reverse engineering of signaling pathways using  
ensembles of dynamic models

David Henriques, Alejandro F. Villaverde, Miguel Rocha,  
Julio Saez-Rodriguez, Julio R. Banga

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# 1 Relationship between the training and prediction RMSE for individual and ensemble models

## 1.1 Case study 1a (MAPKp)

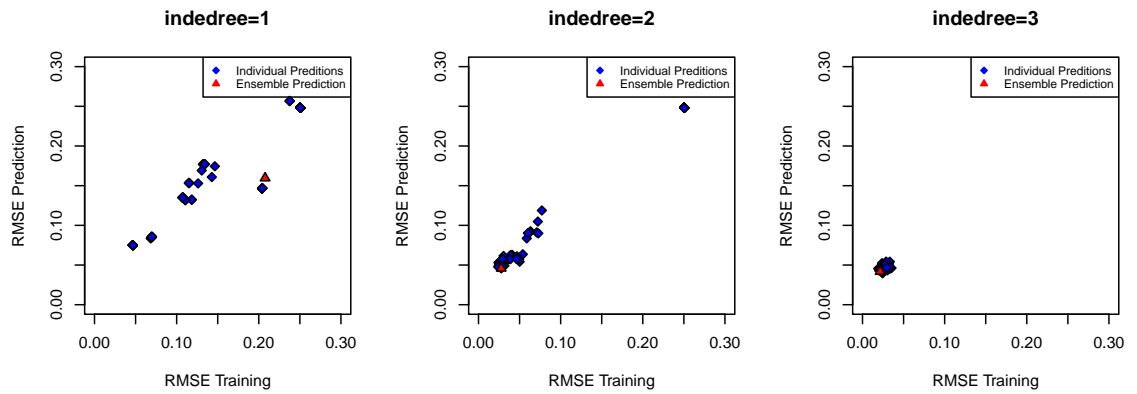


Figure 1: *Relationship between training and prediction RMSE for case study 1a (MAPFp).* The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red).

## 1.2 Case study 1b (MAPKf)

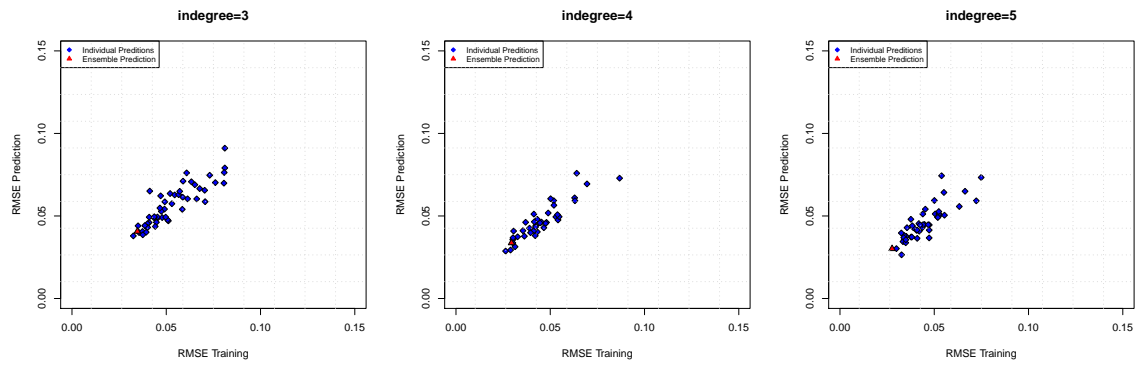


Figure 2: Relationship between training and prediction RMSE for case study 1b (MAPKf). The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red).

### 1.3 Case study 2 (SSP)

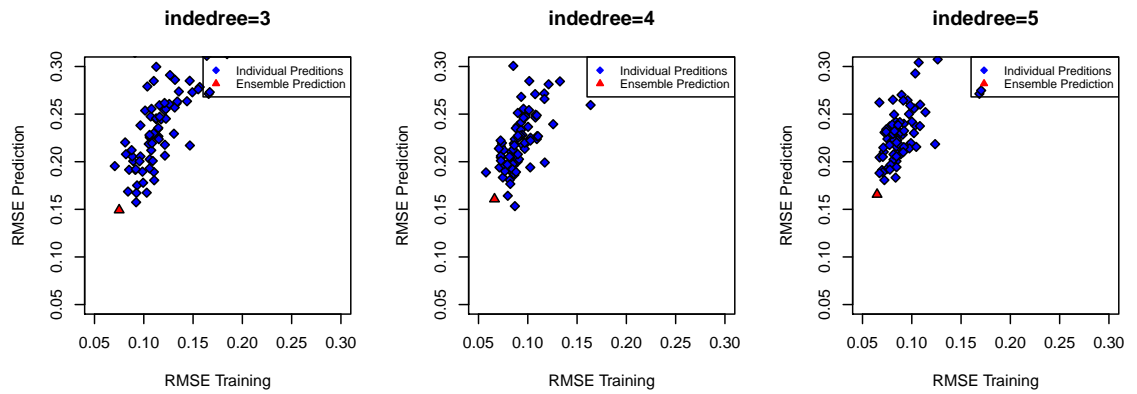


Figure 3: *Relationship between training and prediction RMSE for case study 2 (SSP).* The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red).

### 1.4 Case study 3 (DREAMiS)

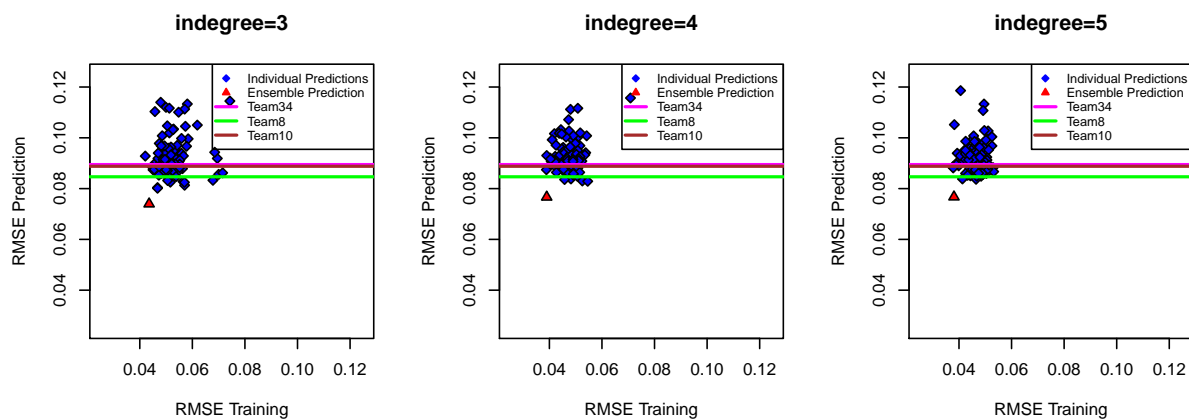


Figure 4: *Relationship between training and prediction RMSE for case study 3 (DREAMiS).* The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red). RMSE scores for the top 3 performing teams in the HPN-DREAM *in silico* time-course prediction sub-challenge (Team34, Team8 and Team10) are also shown colored lines.

## 1.5 Case study 4a (DREAMBT20)

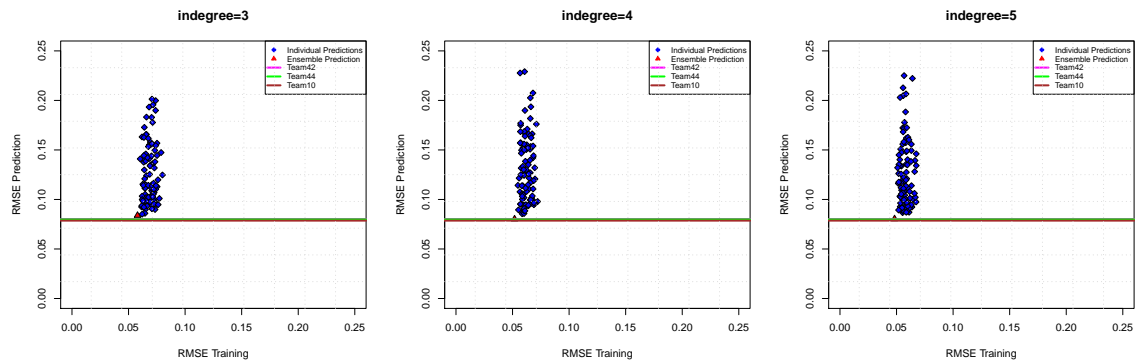


Figure 5: *Relationship between training and prediction RMSE for case study 4a (DREAMBT20).* The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red). RMSE scores for the top 3 performing teams in the HPN-DREAM experimental time-course prediction sub-challenge (Team44, Team42 and Team10) are also shown colored lines.

## 1.6 Case study 4b (DREAMBT549)

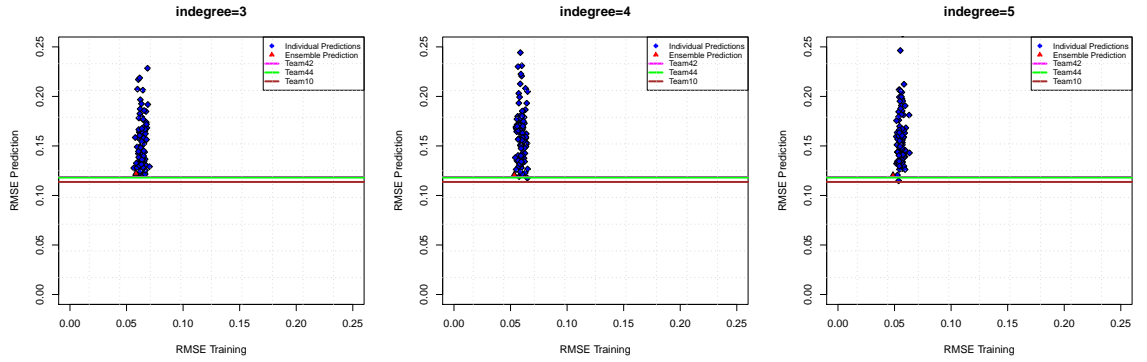


Figure 6: *Relationship between training and prediction RMSE for case study 4b (DREAMBT549).* The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red). RMSE scores for the top 3 performing teams in the HPN-DREAM experimental time-course prediction sub-challenge (Team44, Team42 and Team10) are also shown colored lines.



## 1.7 Case study 4c (DREAMMCF7)

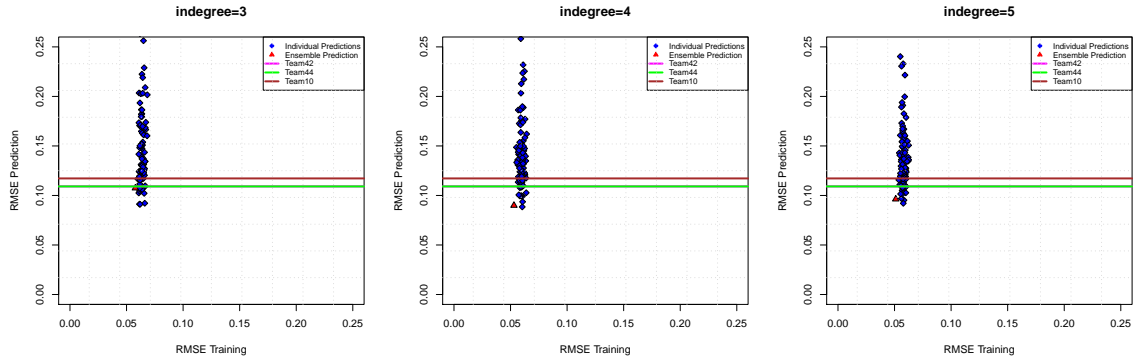


Figure 7: Relationship between training and prediction RMSE for case study 4c (DREAMMCF7). The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red). RMSE scores for the top 3 performing teams in the HPN-DREAM experimental time-course prediction sub-challenge (Team44, Team42 and Team10) are also shown colored lines.

## 1.8 Case study 4d (DREAMUACC812)

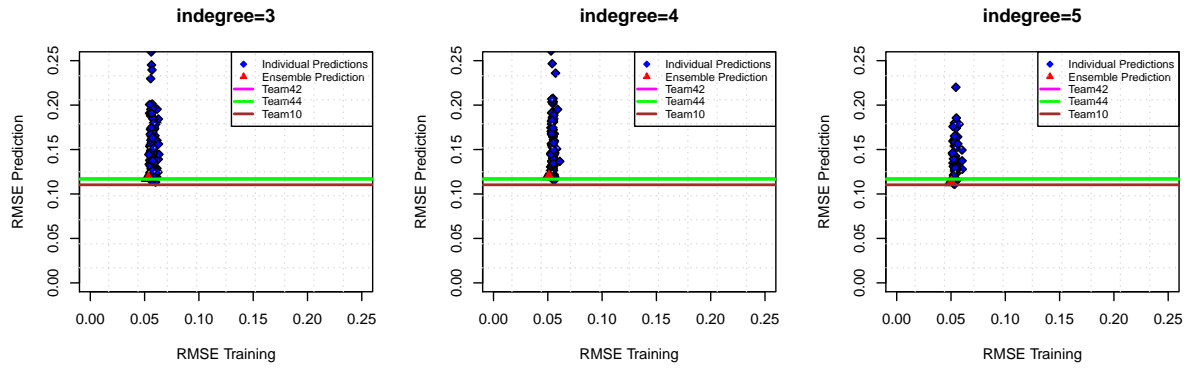


Figure 8: *Relationship between training and prediction RMSE for case study 4d (DREAMUACC812).* The prediction RMSE is plotted here against the training RMSE for each individual model (blue) and the ensemble (red). RMSE scores for the top 3 performing teams in the HPN-DREAM experimental time-course prediction sub-challenge (Team44, Team42 and Team10) are also shown colored lines.