



ChE-609

Seyed Mohamad Moosavi, Kevin Maik Jablonka & Berend Smit

Basics of machine learning for chemistry and materials science

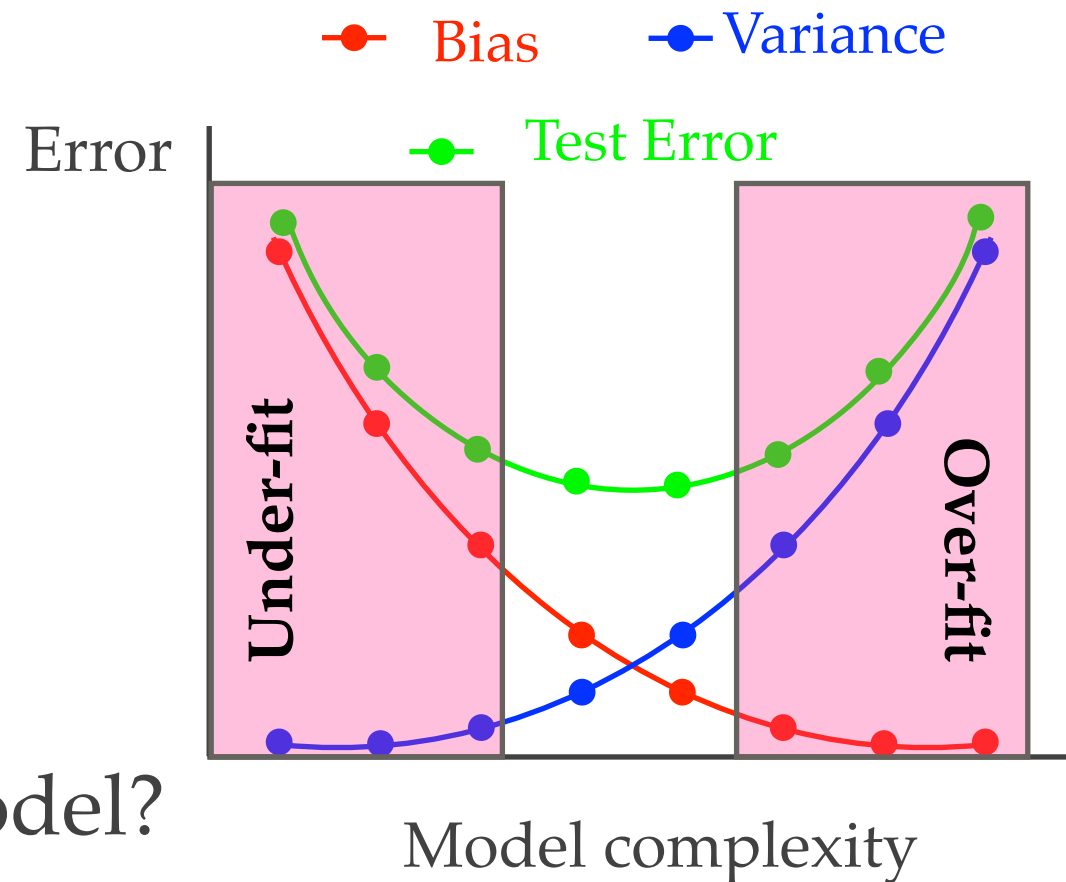
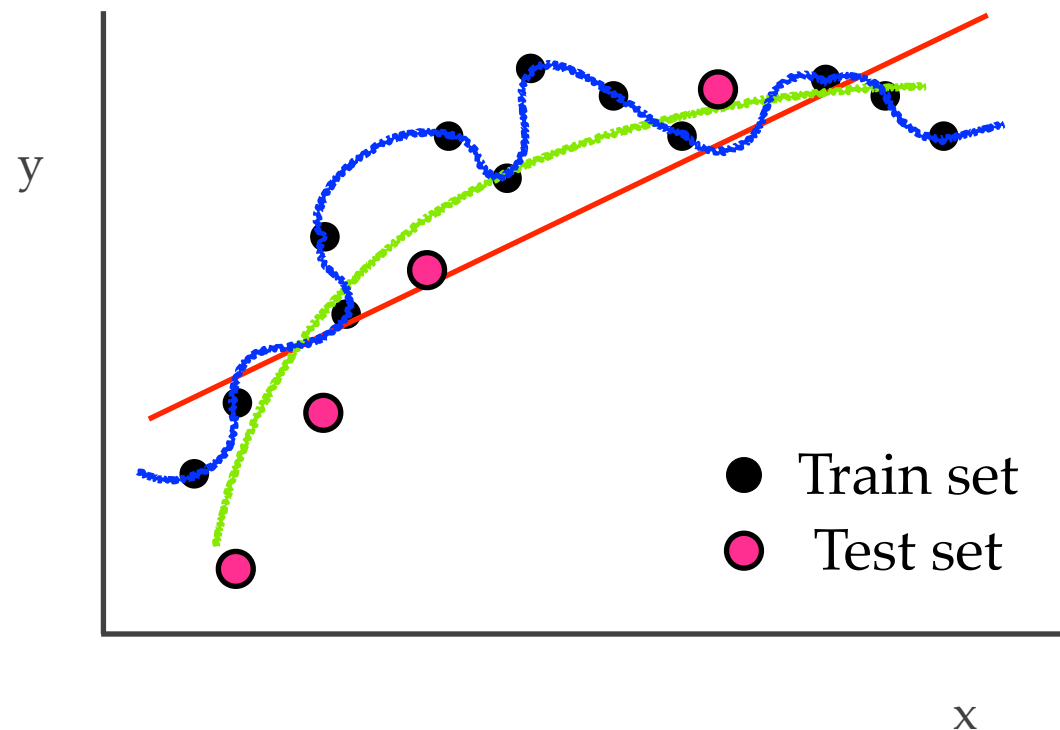


seyedmohamad.moosavi@epfl.ch



@SMohMoosavi

Bias –variance tradeoff: regularisation



How to include this in the model?

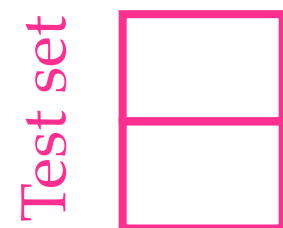
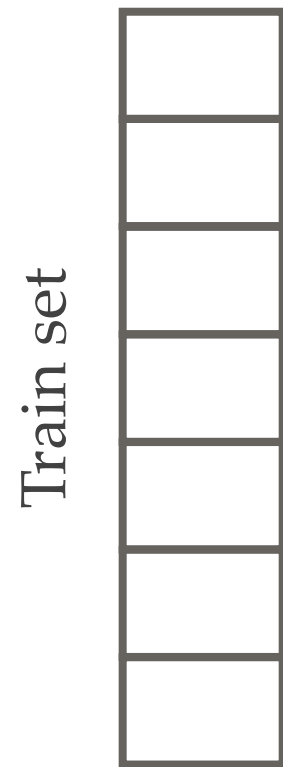
Regularise the loss function: $\mathcal{L} = \|\hat{y}_{ML} - y\|_2^2 + \lambda \|w\|_2^2$

Penalising the terms with large weight

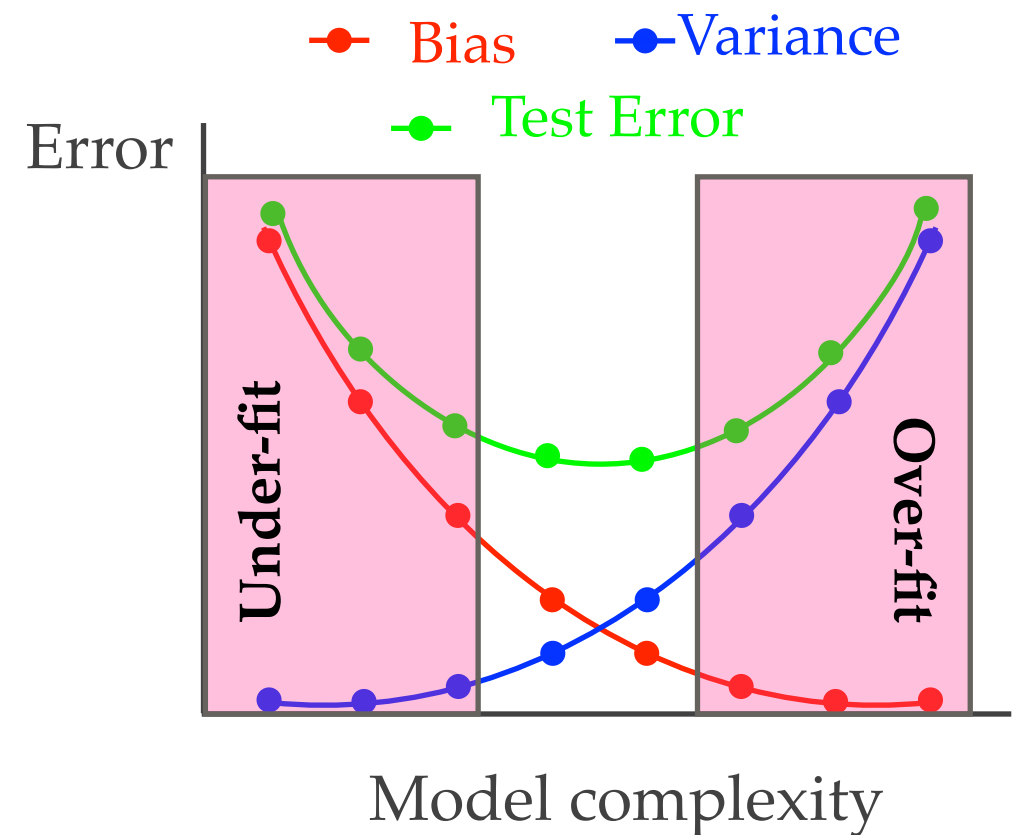
Hyperparameter optimisation

- We want a model that generalise $\rightarrow$ low test error
- $\rightarrow$ but we don't have access to the test error!
- $\rightarrow$ we need a way to assess model performance only from train data

$\rightarrow$ **Cross-validation**

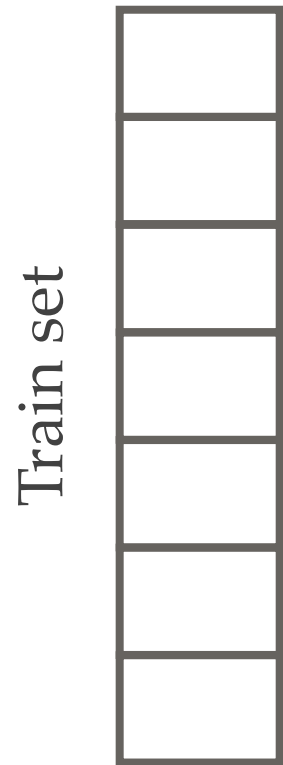


Model must not see
this before / while training



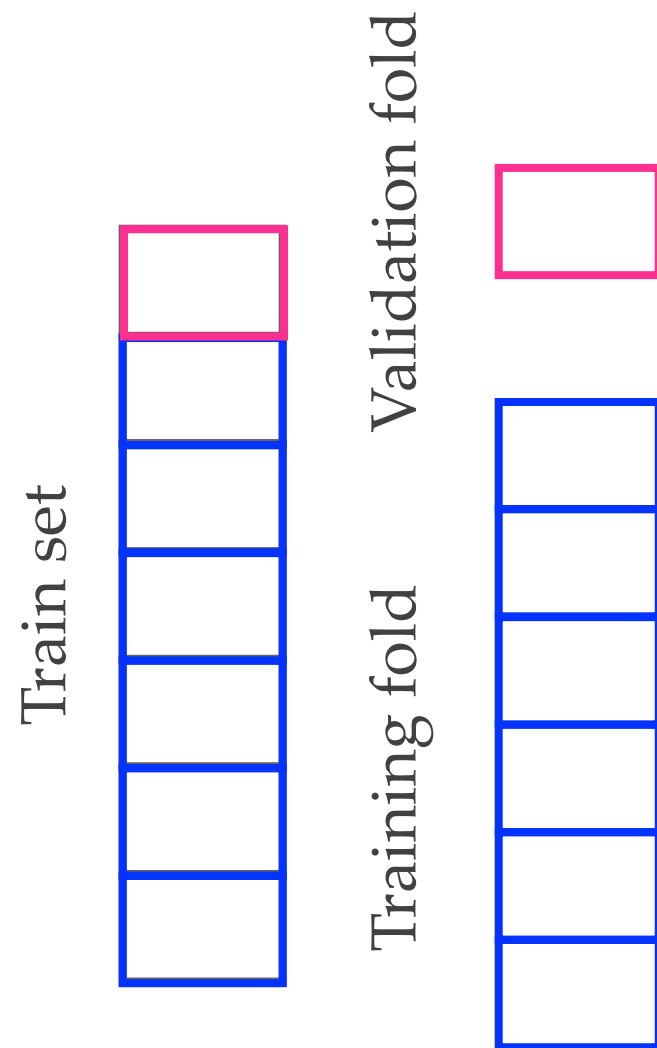
Hyperparameter optimisation: cross-validation

Split the train set into K folds $\rightarrow$ use one fold for validation



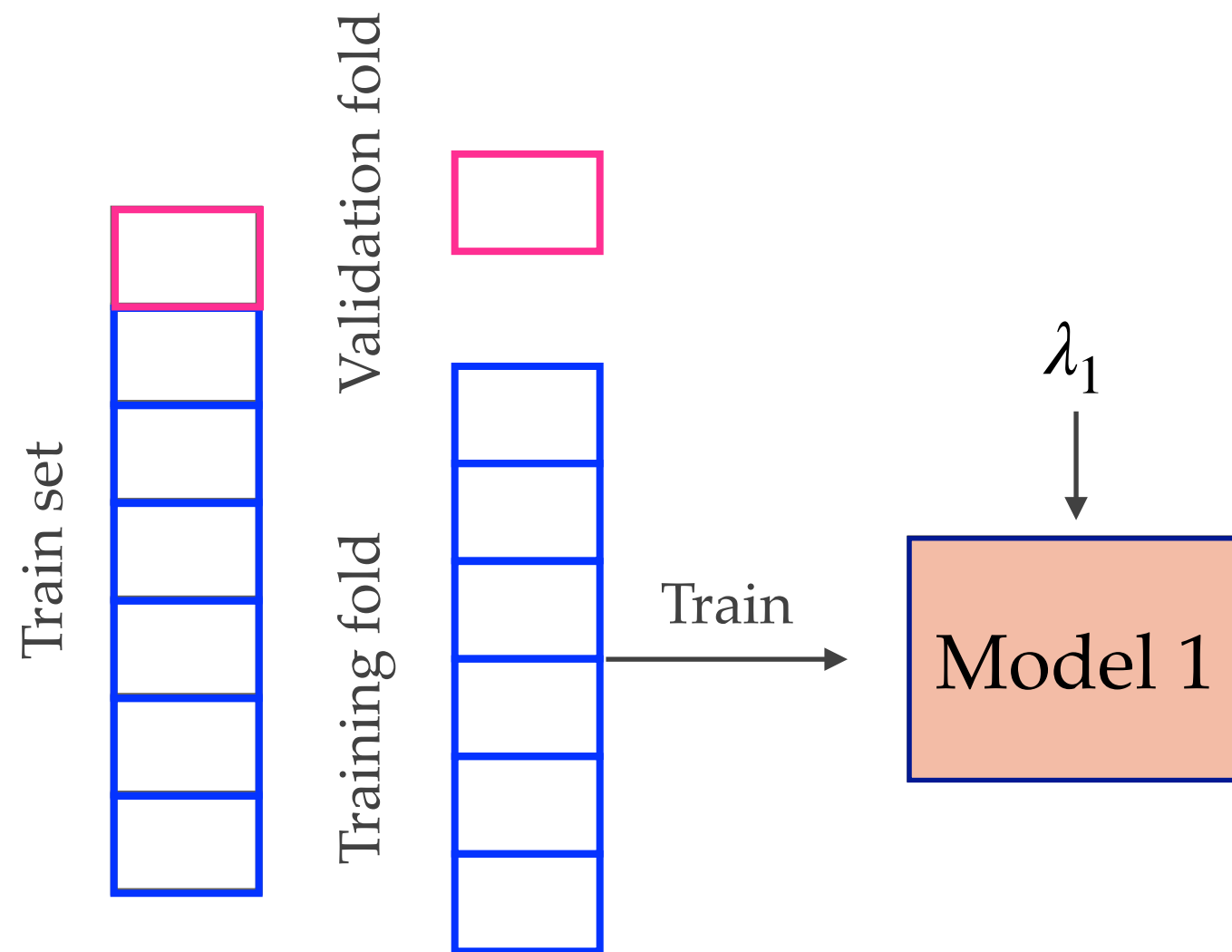
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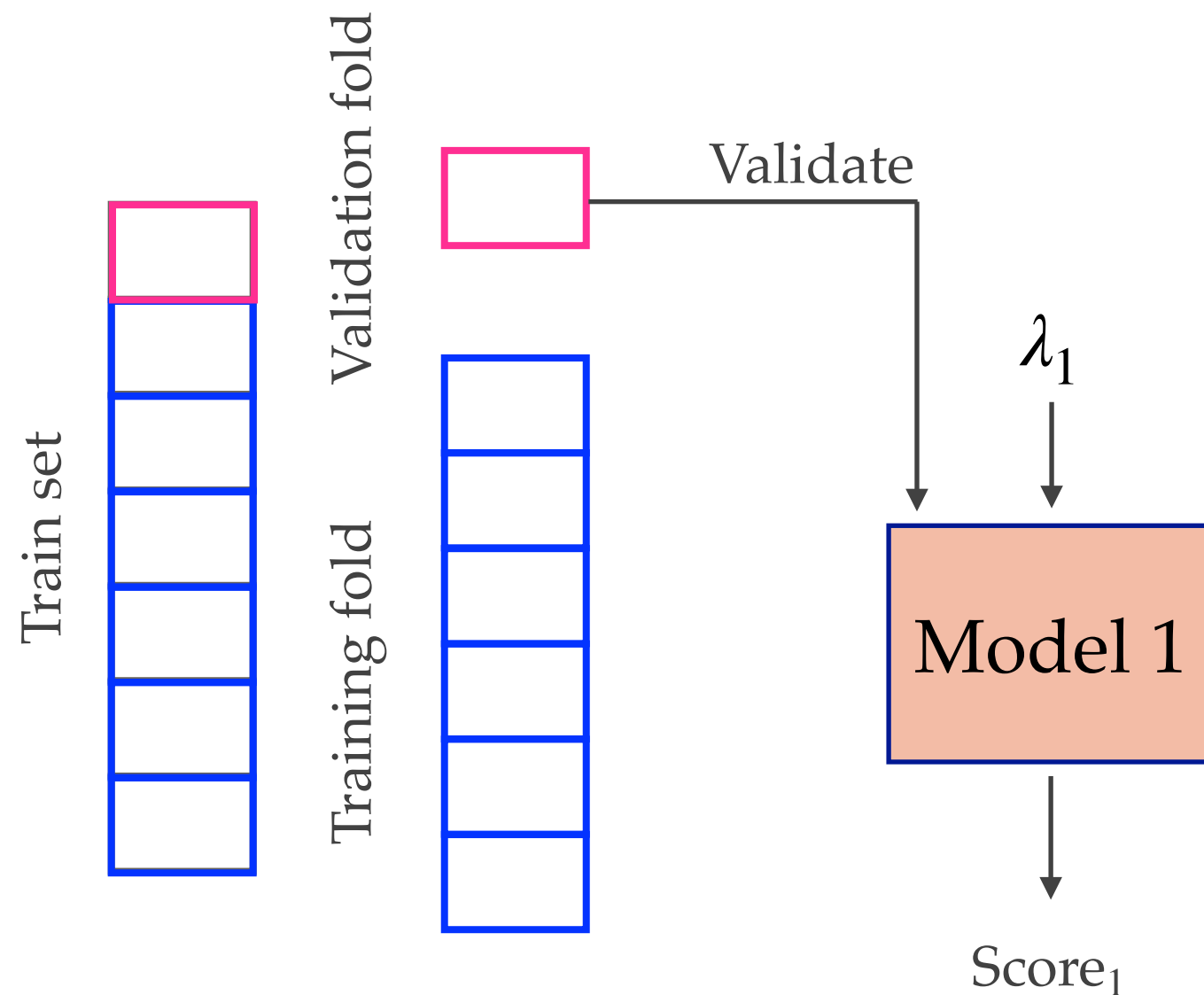
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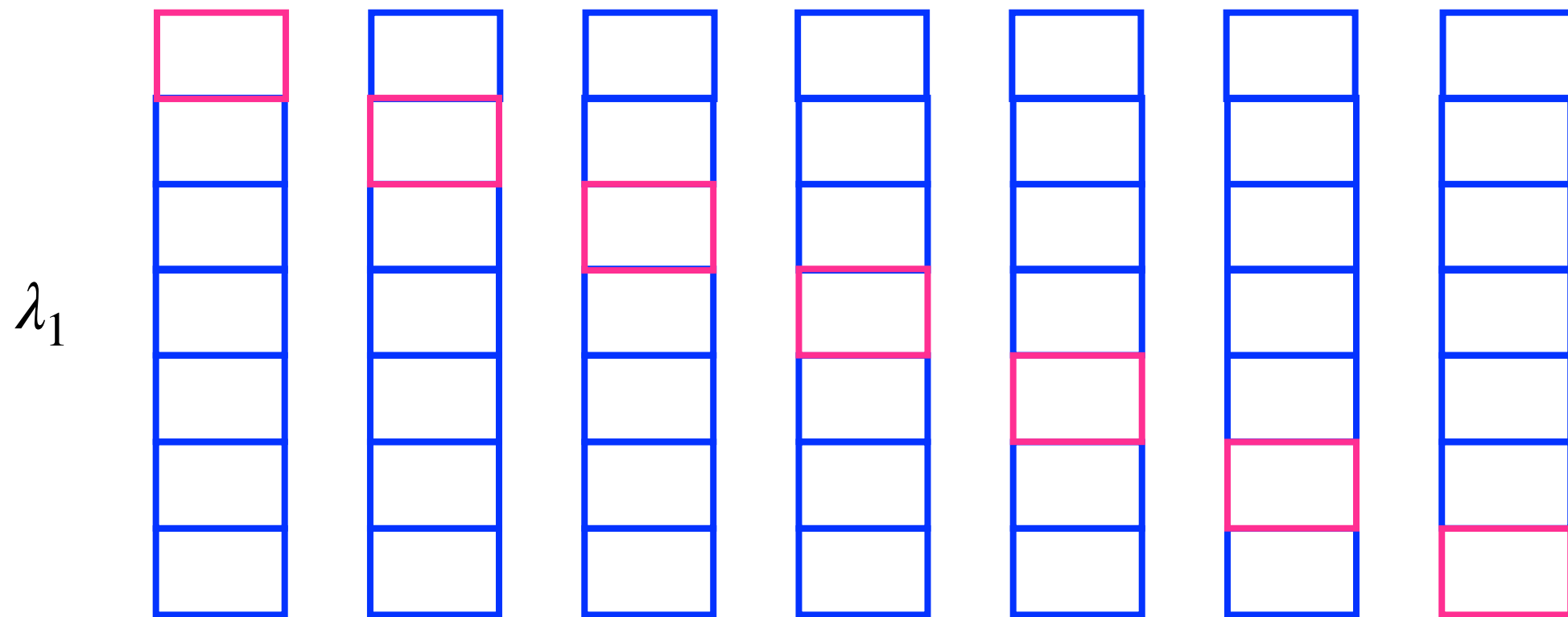
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Hyperparameter optimisation: cross-validation

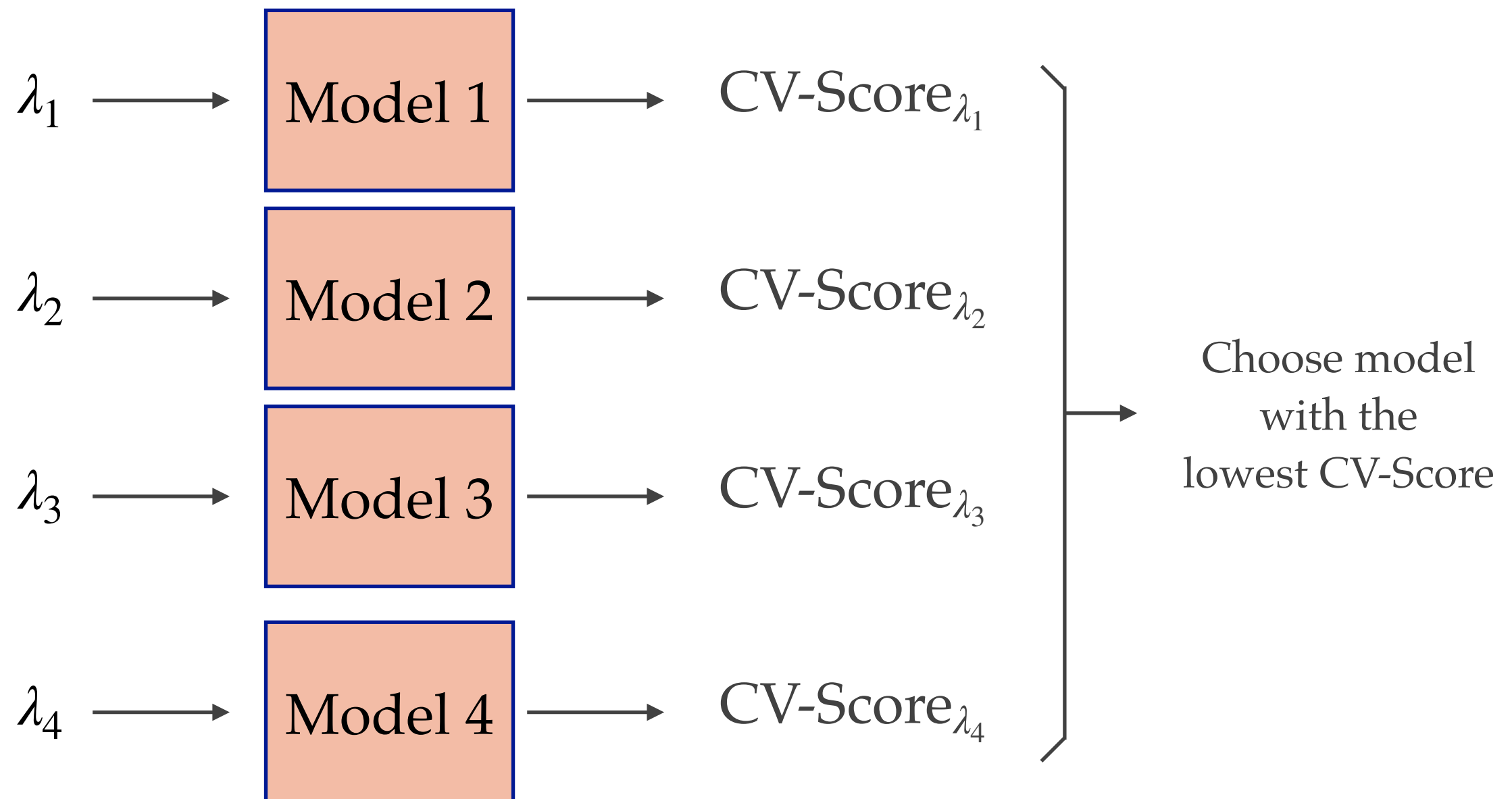
For each set of hyper parameters, we determine cross-validation score



$$\text{CV-Score}_{\lambda_1} = \frac{1}{K} \sum_{i=1}^K \text{Score}_{\lambda_1, i}$$

Hyperparameter optimisation: cross-validation

For each set of hyper parameters, we determine cross-validation score
This allows us to compare models



Summary of model training

- ❖ Split the data at first place to train-test sets, keep some for model evaluation
 - ☑ The model must not see test data before / during training
- ❖ Optimise loss function to find model parameters w
- ❖ Error on train set does not show anything about model generalisability
- ❖ Use cross validation to assign hyperparameters