

# CROSS-VALIDATION IN TMVA UPDATE

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AGNI BETHANI\*, ADRIAN BEVAN, RODRIGO GAMBOA GONI,  
JON HAYS, TOM STEVENSON

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\* NOW AT LPSC, GRENOBLE

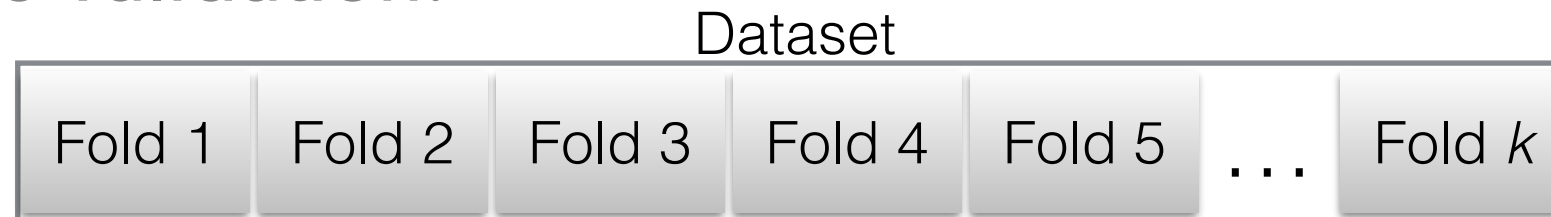
# OUTLINE

- ▶ *k*-fold cross-validation:
  - ▶ Performance estimation:
    - ▶ Overview
    - ▶ Status
  - ▶ Hyper-Parameter optimisation:
    - ▶ Overview
    - ▶ Status

## K-FOLD CROSS-VALIDATION

- ▶ [Previous talk](#)

- ▶ k-fold cross-validation:



- ▶ Split the dataset into  $k$  randomly sampled independent subsets (folds).
- ▶ Train classifier with  $k-1$  folds and test with remaining fold.
- ▶ Repeat  $k$  times.

- ▶ Advantage of using the whole dataset for testing and training.

## PERFORMANCE ESTIMATION

- ▶ Metrics estimated using average
  - ▶ e.g. error rate for  $k$  folds

$$E = \frac{1}{k} \sum_{i=1}^k E_i.$$

- ▶ Current status:
  - ▶ Basic implementation completed and in github version of ROOT.
  - ▶ Currently just outputs average ROCIntegral, in the process of adding more metrics.

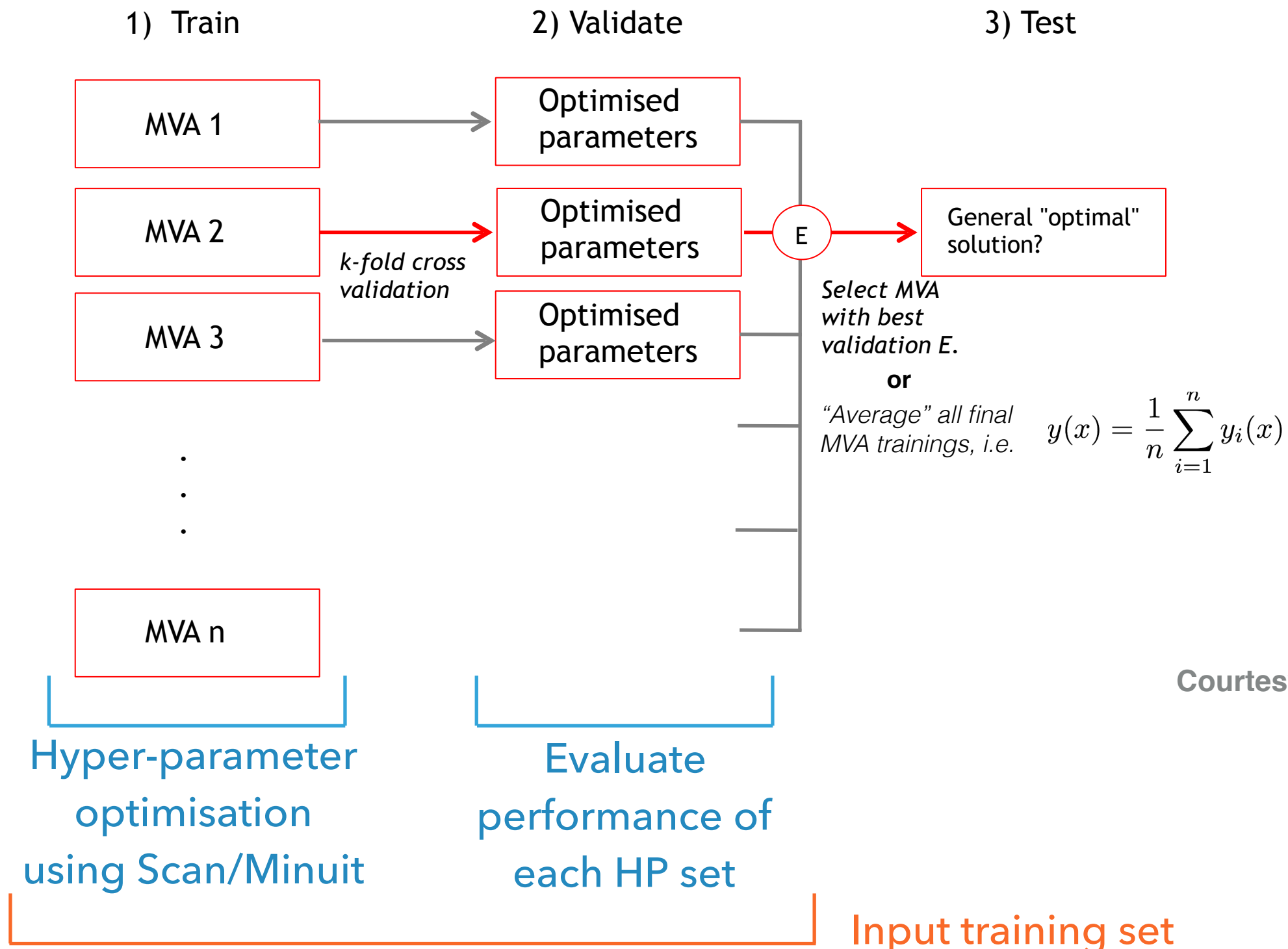
```
Fold 1 ROCIntegral: 0.818641
Fold 2 ROCIntegral: 0.835983
Fold 3 ROCIntegral: 0.83611
Fold 4 ROCIntegral: 0.818627
Fold 5 ROCIntegral: 0.818756
Average ROCIntegral: 0.825623
```

- ▶ Used with:

```
factory->CrossValidate(dataLoader, TMVA::Types::kSVM, "SVM", "VarTransform=Norm",
/*optimise hyper-parameters*/ false, /*Number of folds*/ 5);
```

# HYPER-PARAMETER OPTIMISATION

- ▶ Ideally 3 statistically independent datasets.



Courtesy of Adrian Bevan

## HYPER-PARAMETER OPTIMISATION

- ▶ Current status:
  - ▶ Only for MVAs with implementations for "OptimizeTuningParameters".
  - ▶ No splitting of the input training set yet.
  - ▶ Basic implementation started:
    - ▶ Outputs hyper-parameter sets with ROCIntegral.
  - ▶ Used with:

```
factory->CrossValidate(dataLoader, TMVA::Types::kSVM, "SVM", "VarTransform=Norm",  
/*optimise hyper-parameters*/ true, /*Number of folds*/ 5);
```

## SUMMARY

- ▶ Basic implementation for cross-validation in TMVA started.
- ▶ Next steps:
  - ▶ Splitting training set.
  - ▶ Adding more metrics.
- ▶ More details found in [previous talk](#).

**BACKUP**