
Algorithm 5.1 The k -fold cross-validation algorithm. It can be used to estimate generalization error of a learning algorithm A when the given dataset \mathbb{D} is too small for a simple train/test or train/valid split to yield accurate estimation of generalization error, because the mean of a loss L on a small test set may have too high variance. The dataset \mathbb{D} contains as elements the abstract examples $\mathbf{z}^{(i)}$ (for the i -th example), which could stand for an (input,target) pair $\mathbf{z}^{(i)} = (\mathbf{x}^{(i)}, y^{(i)})$ in the case of supervised learning, or for just an input $\mathbf{z}^{(i)} = \mathbf{x}^{(i)}$ in the case of unsupervised learning. The algorithm returns the vector of errors \mathbf{e} for each example in \mathbb{D} , whose mean is the estimated generalization error. The errors on individual examples can be used to compute a confidence interval around the mean (equation 5.47). While these confidence intervals are not well-justified after the use of cross-validation, it is still common practice to use them to declare that algorithm A is better than algorithm B only if the confidence interval of the error of algorithm A lies below and does not intersect the confidence interval of algorithm B .

Define $\text{KFoldXV}(\mathbb{D}, A, L, k)$:

Require: \mathbb{D} , the given dataset, with elements $\mathbf{z}^{(i)}$

Require: A , the learning algorithm, seen as a function that takes a dataset as input and outputs a learned function

Require: L , the loss function, seen as a function from a learned function f and an example $\mathbf{z}^{(i)} \in \mathbb{D}$ to a scalar $\in \mathbb{R}$

Require: k , the number of folds

Split \mathbb{D} into k mutually exclusive subsets \mathbb{D}_i , whose union is \mathbb{D} .

for i from 1 to k **do**

$f_i = A(\mathbb{D} \setminus \mathbb{D}_i)$

for $\mathbf{z}^{(j)}$ in \mathbb{D}_i **do**

$e_j = L(f_i, \mathbf{z}^{(j)})$

end for

end for

Return \mathbf{e}
