TECHNISCHE UNIVERSITÄT
KAISERSLAUTERN

8.2 LOOCV

Machine Learning 1: Foundations

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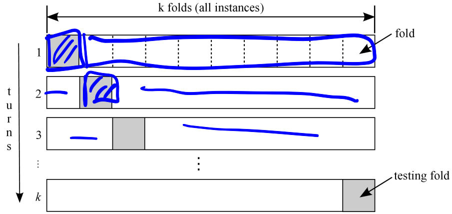

1: split data into $k \overset{\text{e.g.}}{=} 10$ equally-sized chunks (called “folds”)
2: **for** $i = 1, \ldots, k$ and $C \overset{\text{e.g.}}{\in} \{0.01, 0.1, 1, 10, 100\}$ **do**
3: use ith fold as **test set** and union of all others as **training set**
4: train learner on training set (using C) and test on test set
5: **end for**
6: output learner with lowest average error

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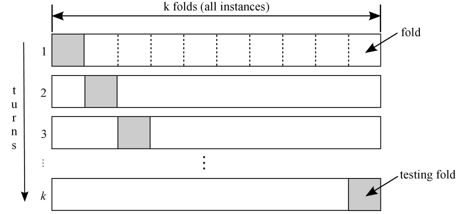

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end for
output learner with lowest average error

Similarly, can select constants in other learning methods, e.g.:

- RBF-kernel width in SVM, learning rate in ANNs, etc.

But What Does **Error** Mean in Regression?

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The common error measure in regression is:

Definition

Let $\{(\mathbf{x}_1, y_1), \ldots (\mathbf{x}_n, y_n)\}$ be a test set, and let f be a learned regression function. The **root mean squared error (RMSE)** of f is:

$$\text{RSME}(f) := \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\underline{f(\mathbf{x}_i)} - \underline{y_i})^2}$$

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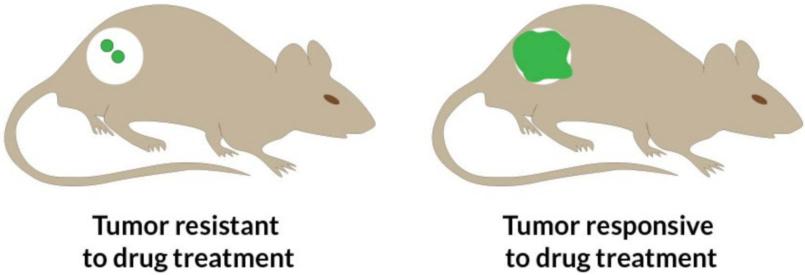

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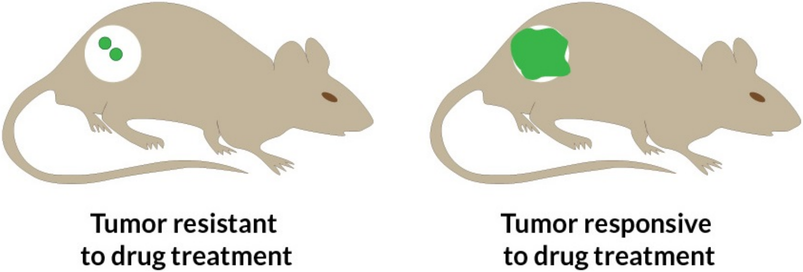

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How can we use **as much data as possible**
in cross-validation?

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But what could be a problem with LOOCV?

LOOCV is Usually Super Slow

Involves a loop over all data points: $O(n)$

- In each iteration, train learner with $n-1$ data points:
  - is $O(d^3)$ for RR

Total LOOCV (for RR): $O(d^3 n)$

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can we do ~~the~~ LOOCV faster?

- for ridge regression: yes!
- for classification: no!

even for other error measures

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Question here!

Can we get rid of the loop over all data points?

LOOCV Trick for RR

The LOOCV error is:

$$\mathrm{RSME}_{\mathrm{loocv}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{x}_i^\top \mathbf{w}_i - y_i\right)^2}$$

where:

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Thus: $$\mathbf{w}_i = \left(XX^\top \boxed{-\mathbf{x}_i\mathbf{x}_i^\top} + \frac{1}{2C}I\right)^{-1}\left(Xy \boxed{-\mathbf{x}_i y_i}\right)$$

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- Need to invert the matrix occuring in $\mathbf{w}_i$ for all $i = 1, \ldots, n$
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How does this trick work?

Skipping the Matrix Inversion—Here's the Trick:

Write: $$\mathbf{w}_i = (\underbrace{XX^\top + \frac{1}{2C}I}_{=:A} - \underbrace{\mathbf{x}_i\mathbf{x}_i^\top}_{\mathbf{u}\mathbf{u}^\top})^{-1}(Xy - \mathbf{x}_i y_i)$$

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Apply the following theorem:

Theorem (Sherman-Morrison formula)

Let $A \in \mathbb{R}^{d\times d}$ be an invertible matrix, and let $\mathbf{u} \in \mathbb{R}^d$.
If $\mathbf{u}^\top A^{-1}\mathbf{u} \neq 1$, then:

$$(A - \mathbf{u}\mathbf{u}^\top)^{-1} = A^{-1} + \frac{A^{-1}\mathbf{u}\mathbf{u}^\top A^{-1}}{1 - \mathbf{u}^\top A^{-1}\mathbf{u}}$$

Full rank

rank 1

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The LOOCV-RMSE of ridge regression can be computed in $O(d^3)$ through:

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where $A := XX^\top + \frac{1}{2C} I.$

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Order of computation:

- first compute A^{-1}, then $\mathbf{w}_{\mathrm{RR}}$, and last $\mathrm{RSME}_{\mathrm{loocv}}$

Proof

Recalling $\mathbf{w}_{\text{RR}} = A^{-1}Xy$ and denoting $\beta_i := \mathbf{x}_i^\top A^{-1}\mathbf{x}_i$, it is:

$\text{RSME}_{\text{loocv}}$

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