# Statistical Data Mining and Machine Learning
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Slides and other materials available at:
http://www.stats.ox.ac.uk/~sejdinov/sdmml



# Performance Evaluation



## Example: Spam Dataset

A data set collected at Hewlett-Packard Labs, that classifies 4601 e-mails as spam or non-spam. 57 variables indicate the frequency of certain words and characters.

```
> library(kernlab)
> data(spam)
> dim(spam)
[1] 4601   58
> spam[1:2,]
  make address  all num3d  our over remove internet order mail receive will
1 0.00    0.64 0.64     0 0.32 0.00   0.00     0.00     0 0.00    0.00 0.64
2 0.21    0.28 0.50     0 0.14 0.28   0.21     0.07     0 0.94    0.21 0.79
  people report addresses free business email  you credit your font num000
1   0.00   0.00      0.00 0.32     0.00  1.29 1.93      0 0.96    0   0.00
2   0.65   0.21      0.14 0.14     0.07  0.28 3.47      0 1.59    0   0.43
  money hp hpl george num650 lab labs telnet num857 data num415 num85
1  0.00  0   0      0      0   0    0      0      0    0      0     0
2  0.43  0   0      0      0   0    0      0      0    0      0     0
  technology num1999 parts pm direct cs meeting original project re edu table
1          0    0.00     0  0      0  0       0        0       0  0   0 0
2          0    0.07     0  0      0  0       0        0       0  0   0 0
  conference charSemicolon charRoundbracket charSquarebracket charExclamation
1          0             0            0.000                 0           0.778
2          0             0            0.132                 0           0.372
  charDollar charHash capitalAve capitalLong capitalTotal type
1       0.00    0.000      3.756          61          278 spam
2       0.18    0.048      5.114         101         1028 spam
> str(spam$type)
 Factor w/ 2 levels "nonspam","spam": 2 2 2 2 2 2 2 2 2 2 ...
```



## Spam Dataset

Use logistic regression to predict spam/not spam.

```
## let Y=0 be non-spam and Y=1 be spam.
Y <- as.numeric(spam$type)-1
X <- spam[ ,-ncol(spam)]

gl <- glm(Y ~ ., data=X,family=binomial)
```

# Spam Dataset

How good is the classification?

```
> table(spam$type)
nonspam    spam
   2788    1813
> proba <- predict(gl,type="response")
> predicted_spam <- as.numeric( proba>0.5)
> table(predicted_spam,Y)
              Y
predicted_spam    0    1
             0 2666  194
             1  122 1619
> predicted_spam <- as.numeric( proba>0.95)
> table(predicted_spam,Y)
              Y
predicted_spam    0    1
             0 2766  810
             1   22 1003
```

Advantage of a probabilistic approach: predictive probabilities give interpretable confidence to predictions. Soft classification rules for other classifiers, e.g., support vector machines can be poorly calibrated if we are to interpret them as probabilities.



# Spam Dataset

- We are viewing the prediction error on the training set. Not necessarily representative of the generalization ability.
- Separate in training and test set 50/50.

```
n <- length(Y)
train <- sample( n, round(n/2) )
test<-(1:n)[-train]
```

- Fit only on training set and predict on both training and test set.

```
gl <- glm(Y[train] ~ ., data=X[train,],family=binomial)

proba_train <- predict(gl,newdata=X[train,],type="response")
proba_test  <- predict(gl,newdata=X[test,],type="response")
```



# Spam Dataset

Results for training and test set:

```
> predicted_spam_lr_train <- as.numeric(proba_train > 0.95)
> predicted_spam_lr_test  <- as.numeric(proba_test > 0.95)

> table(predicted_spam_lr_train, Y[train])
predicted_spam_lr_train    0    1
                      0 1401  358
                      1    8  533


> table(predicted_spam_lr_test, Y[test])
predicted_spam_lr_test    0    1
                     0 1357  392
                     1   22  530
```

Note: testing performance is worse than training performance.



# Spam Dataset

Compare with LDA.

```
library(MASS)
lda_res <- lda(x=X[train,],grouping=Y[train])

proba_lda_test <- predict(lda_res,newdata=X[test,])$posterior[,2]
predicted_spam_lda_test <- as.numeric(proba_lda_test > 0.95)

> table(predicted_spam_lr_test, Y[test])
predicted_spam_lr_test    0    1
                     0 1357  392
                     1   22  530

> table(predicted_spam_lda_test, Y[test])
predicted_spam_lda_test    0    1
                      0 1361  533
                      1   18  389
```

- LDA has a larger number of false positives but a smaller number of false negatives.
    - Above results are for a single threshold ($0.95$) - how to keep track of what happens across multiple thresholds?
    - More generally, how to compare the classifiers fairly when the number of positive and negative examples is very different?

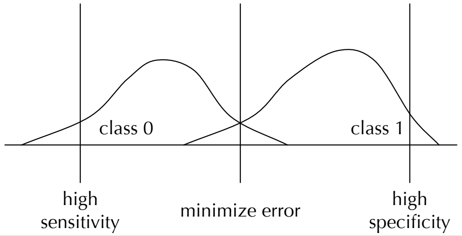
# Performance Measures

- **Confusion matrix**:

| True | state | 0 | 1 |
|---|---|---|---|
| Prediction | 0 | **# true negative** | **# false negative** |
| | 1 | **# false positive** | **# true positive** |

  - **Accuracy**: $(TP+TN)/(TP+TN+FP+FN)$.
  - **Error rate**: $(FP+FN)/(TP+TN+FP+FN)$.
  - **Sensitivity (true positive rate)**: $TP/(TP+FN)$.
  - **Specificity (true negative rate)**: $TN/(TN+FP)$.
  - **False positive rate** (1-Specificity): $FP/(TN+FP)$.
  - **Precision**: $TP/(TP+FP)$.
  - **Recall** (same as Sensitivity): $TP/(TP+FN)$.
  - **F1**: harmonic mean of precision and recall.

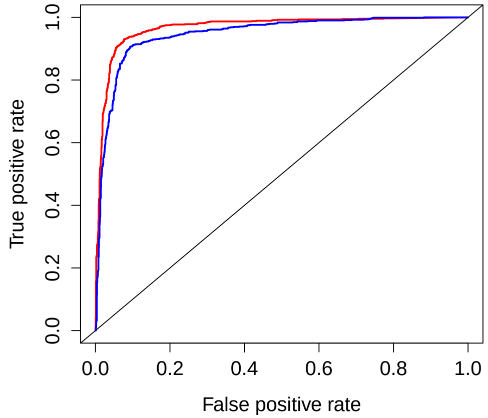
- As we vary the prediction threshold $c$ from 0 to 1:
  - Specificity varies from $0$ to $1$.
  - Sensitivity goes from $1$ to $0$.






# ROC (Receiver Operating Characteristic) Curves

ROC curve: plot TPR (sensitivity) vs FPR (1-specificity). LDA = blue; LR = red.




LR beats LDA on this dataset in terms of the **area under ROC (AUC): probability that the classifier will score a randomly drawn positive example higher than a randomly drawn negative example.** Also called Wilcoxon-Mann-Whitney statistic.



# ROC Curves

R library `ROCR` contains various performance measures, including AUC.

```
> library(ROCR)
> pred_lr <- prediction(proba_test,Y[test])
> perf <- performance(pred_lr, measure = "tpr", x.measure = "fpr")
> plot(perf,col='red',lwd=2)
> pred_lda <- prediction(proba_lda_test,Y[test])
> perf <- performance(pred_lda, measure = "tpr", x.measure = "fpr")
> plot(perf,col='blue',add=TRUE,lwd=2)
> abline(a=0,b=1)
> auc_lda <- as.numeric(performance(pred_lda,"auc")@y.values)
> auc_lda
[1] 0.9472542
> auc_lr <- as.numeric(performance(pred_lr,"auc")@y.values)
> auc_lr
[1] 0.9673279
```



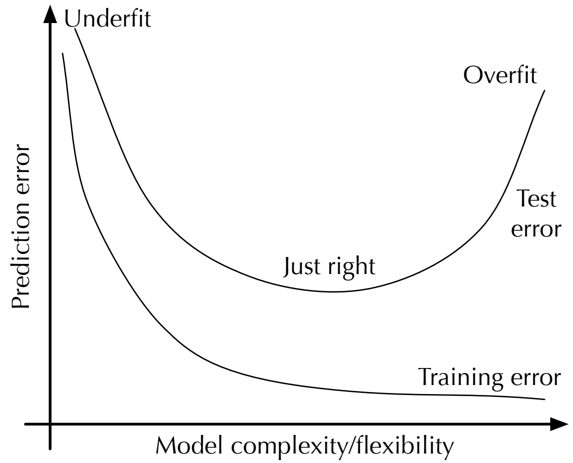
# Validation and Model Selection

# Generalization

- Generalization ability: what is the out-of-sample error of learner $f$?
- training error $\neq$ testing error.
- We learn $f$ by minimizing some variant of empirical risk $R^{\text{emp}}(f)$- what can we say about the true risk $R(f)$?
- Two important factors determining generalization ability:
  - Model complexity
  - Training data size



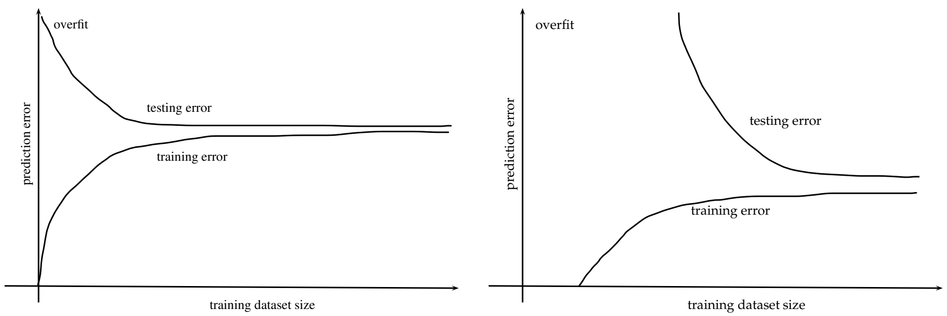
# Learning Curves




Fixed dataset size, varying model complexity.



# Learning Curves




Fixed model complexity, varying dataset size.
Two models: one simple, one complex. Which is which?



# Bias-Variance Tradeoff

- Where does the prediction error come from?
- Example: Squared loss in regression: $\mathcal{X} = \mathbb{R}^p$, $\mathcal{Y} = \mathbb{R}$,

$$L(Y, f(X)) = (Y - f(X))^2$$

- Optimal $f$ is the conditional mean:

$$f_*(x) = \mathbb{E}\left[Y|X = x\right]$$

- Follows from $R(f) = \mathbb{E}_X \mathbb{E}\left[ (Y - f(X))^2 \middle| X \right]$ and

$$\begin{aligned}
& \mathbb{E}\left[ (Y - f(X))^2 \middle| X = x \right] \\
= \; & \mathbb{E}\left[ Y^2 \middle| X = x \right] - 2f(x)\,\mathbb{E}\left[ Y \middle| X = x \right] + f(x)^2 \\
= \; & \text{Var}\left[ Y|X = x \right] + \left( \mathbb{E}\left[ Y \middle| X = x \right] - f(x) \right)^2 .
\end{aligned}$$

# Bias-Variance Tradeoff

- Optimal risk is the intrinsic conditional variability of $Y$ (noise):

$$R(f_*) = \mathbb{E}_X \left[\text{Var}\left[Y|X\right]\right]$$

- **Excess risk**:

$$R(f) - R(f_*) = \mathbb{E}_X \left[\left(f(X) - f_*(X)\right)^2\right]$$

- How does the excess risk behave **on average**?
- Consider a randomly selected dataset $\mathcal{D} = \{(X_i, Y_i)\}_{i=1}^n$ and $f^{(\mathcal{D})}$ trained on $\mathcal{D}$ using a model (hypothesis class) $\mathcal{H}$.

$$\begin{aligned}\mathbb{E}_\mathcal{D}\left[R(f^{(\mathcal{D})}) - R(f_*)\right] &= \mathbb{E}_\mathcal{D}\mathbb{E}_X\left[\left(f^{(\mathcal{D})}(X) - f_*(X)\right)^2\right] \\ &= \mathbb{E}_X\mathbb{E}_\mathcal{D}\left[\left(f^{(\mathcal{D})}(X) - f_*(X)\right)^2\right].\end{aligned}$$



# Bias-Variance Tradeoff

- Denote $\bar{f}(x) = \mathbb{E}_\mathcal{D} f^{(\mathcal{D})}(x)$ (average decision function over all possible datasets)

$$\mathbb{E}_\mathcal{D}\left[\left(f^{(\mathcal{D})}(X) - f_*(X)\right)^2\right] = \underbrace{\mathbb{E}_\mathcal{D}\left[\left(f^{(\mathcal{D})}(X) - \bar{f}(X)\right)^2\right]}_{\text{Var}_X(\mathcal{H},n)} + \underbrace{\left(\bar{f}(X) - f_*(X)\right)^2}_{\text{Bias}_X^2(\mathcal{H},n)}$$

Now,

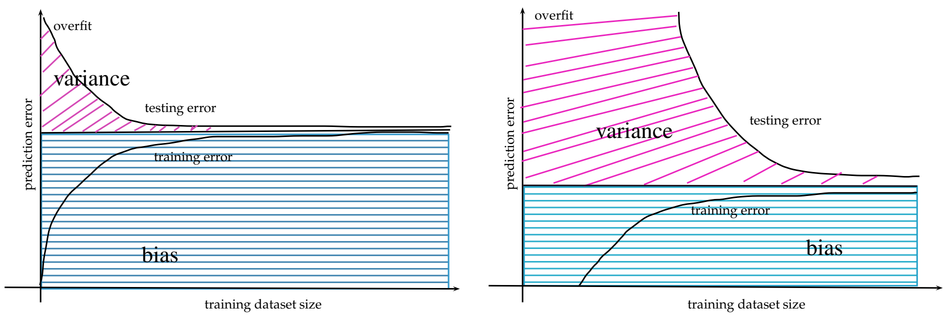
$$\mathbb{E}_\mathcal{D} R(f^{(\mathcal{D})}) = R(f_*) + \mathbb{E}_X \text{Var}_X(\mathcal{H}, n) + \mathbb{E}_X Bias_X^2(\mathcal{H}, n)$$

Where does the prediction error come from?

- **Noise**: Intrinsic difficulty of regression problem.
- **Bias**: How far away is the best learner in the model (average learner over all possible datasets) from the optimal one?
- **Variance**: How variable is our learning method if given different datasets?

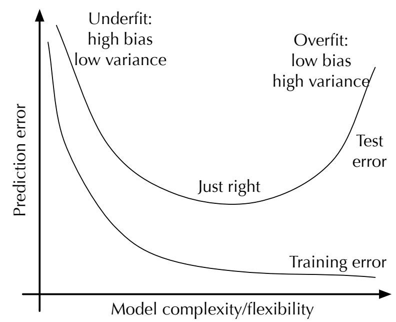


# Learning Curves






# Building models to trade bias with variance




- Building a machine learning model involves trading between its bias and variance.
  - Bias reduction at the expense of a variance increase: building more complex models, e.g. adding nonlinear features and additional parameters, increasing the number of hidden units in neural nets, using decision trees with larger depth.
  - Variance reduction at the expense of a bias increase: increasing the regularization parameter, early stopping, using k-nearest neighbours with larger k.

# Validation and Cross-Validation



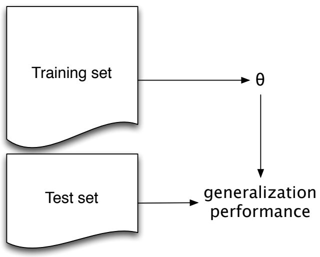
## Empirical vs True Risk

- In general,
$$R(f) = R^{\text{emp}}(f) + \text{overfit penalty}.$$
- Overfit penalty depends on the complexity of the model (**VC analysis**).
- Regularization: **approximate the overfit penalty**. More complex the model, larger the overfit penalty.
- (Cross-)Validation: try to **estimate** $R(f)$ **directly**.
- For any example not used in training:
$$\mathbb{E}\left[L\left(y_{\text{test}}, f\left(x_{\text{test}}\right)\right)\right] = R(f).$$
- But for examples used in training:
$$\mathbb{E}\left[L\left(y_{\text{train}}, f\left(x_{\text{train}}\right)\right)\right] \neq R(f).$$



## Optimizing Tuning Parameters

- How can we optimize generalization ability, via optimizing choice of tuning parameters, model size, and learning parameters?
- Suppose we have split data into training/test set.
- Test set can be used to determine generalization ability, and used to choose best setting of tuning parameters/model size/learning parameters with best generalization.
- Once these tuning parameters are chosen, still important to determine generalization ability, but cannot use performance on test set to gauge this anymore!
- Idea: split data into 3 sets: training set, test set, and **validation set**.

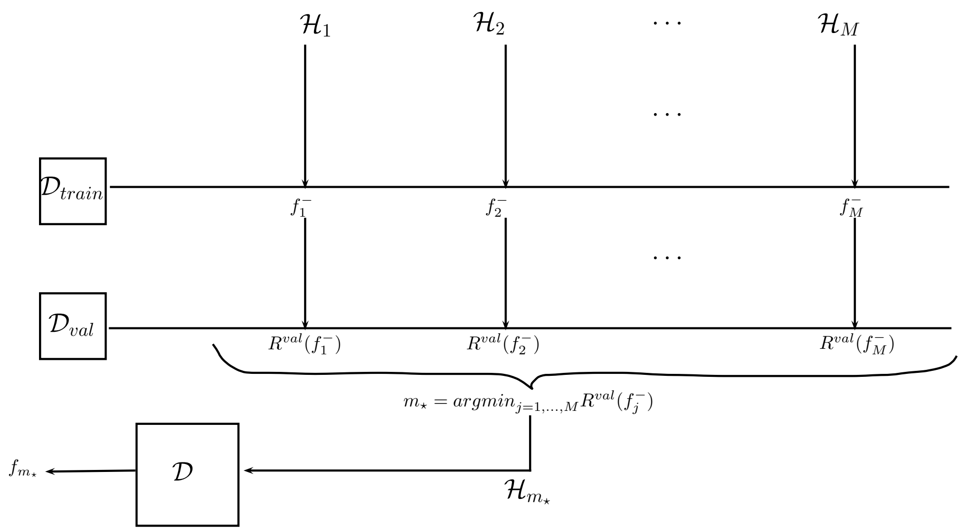





## Validation error

- **Out-of-sample average loss**. For a dataset $\{\tilde{x}_i, \tilde{y}_i\}_{i=1}^{v}$ unseen in training
$$R^{\text{val}}(f) = \frac{1}{v}\sum_{i=1}^{v} L\left(\tilde{y}_i, f\left(\tilde{x}_i\right)\right)$$
- $\mathbb{E}\left[R^{\text{val}}(f)\right] = R(f)$, Var $\left[R^{\text{val}}(f)\right] \asymp \frac{1}{v}$, i.e. $R^{\text{val}}(f) = R(f) \pm \mathcal{O}\left(\frac{1}{\sqrt{v}}\right)$
- Just like testing error so far.
- It becomes validation error only once it is used to **change our learning**.

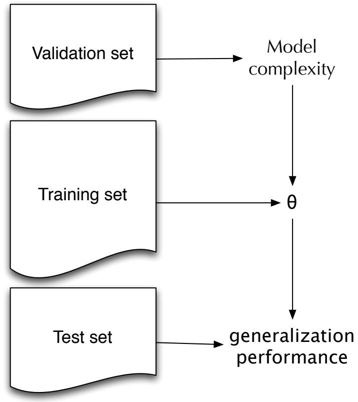
# Validation






# Validation

- For each combination of tuning parameters $\gamma$:
  - Train our model on the training set, fit parameters $\theta = \theta(\gamma)$, obtaining decision function $f_{\theta(\gamma)}$.
  - Evaluate $R^{\mathsf{val}}\left(f_{\theta(\gamma)}\right)$ average loss on a validation set.
- Pick $\gamma^*$ with best performance on validation set.
- Using $\gamma^*$, train on both training and validation set to obtain the optimal $\theta^*$.
- $R^{\mathsf{val}}(f_{\theta(\gamma^*)})$ is now a biased estimate of $R(f_{\theta(\gamma^*)})$ and can be overly optimistic!
- Evaluate model with $\gamma^*, \theta^*$ on test set, reporting generalization performance.






# Bias introduced by validation

- **Example**: Selecting between two equally bad classifiers $f_1$ and $f_2$:

$$R(f_1) = R(f_2) = 0.5.$$

- Assume that we have independent unbiased estimators $\mathsf{R}_1 = R^{\mathsf{val}}(f_1)$, $\mathsf{R}_2 = R^{\mathsf{val}}(f_2)$, both uniform on $[0, 1]$
- Learning rule $f_\star$ chosen to minimize $R^{\mathsf{val}}$ is either $f_1$ or $f_2$, so also equally bad.
- But $\mathbb{E} \min\{\mathsf{R}_1, \mathsf{R}_2\} = \frac{1}{3}$, so in terms of validation error it may appear that we are getting an improvement!



# Validation error and Generalization

How contaminated are different parts of data in terms of being able to tell us something about generalization ability?

- Training data: fully contaminated, used in learning - $R^{\mathsf{emp}}(f)$ is usually far from $R(f)$ (unless the model is too simple for the amount of data).
- Validation data: partly contaminated, used in model selection / meta-learning - $R^{\mathsf{val}}(f)$ is biased, but still useful, provided that:
  - we have a large enough validation set size $v$
  - we do not use it to select from a large number $M$ of models
- Test data: clean, not used for any part of learning.

Typically,

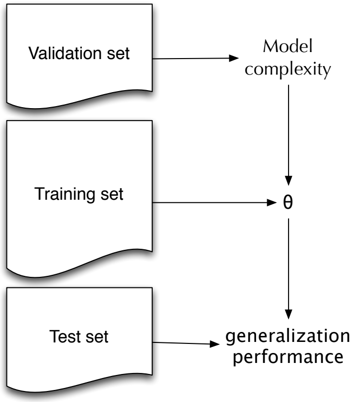
$$R(f) \leq R^{\mathsf{val}}(f) + \underbrace{\mathcal{O}\left(\sqrt{\frac{\log M}{v}}\right)}_{\text{overfit penalty of the meta-model}}$$

## Size of validation set?

- In practice, there is just one dataset! If $v$ is used for computing validation error, then only $n - v$ used for training.
  - Small $v$ : $R^{\text{val}}(f^-)$ is a bad estimate of $R(f^-)$
  - Large $v$ : $R^{\text{val}}(f^-)$ is a reliable estimate of a much worse risk ($f^-$ learned on much less data than $f$)!
- We are using:

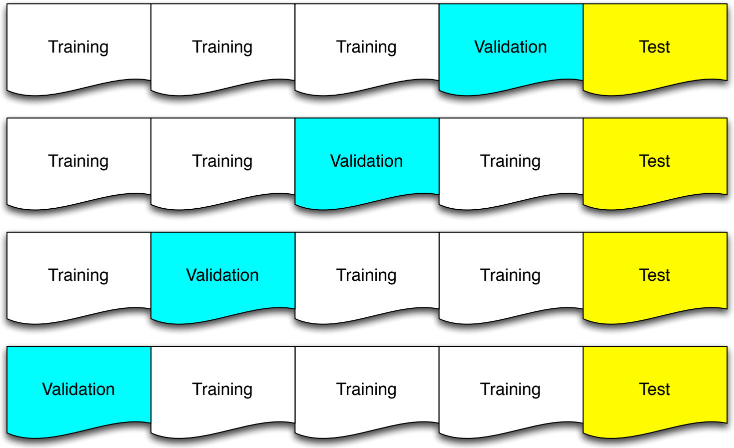
$$R(f) \underset{\text{(need small } v)}{\approx} R(f^-) \underset{\text{(need large } v)}{\approx} R^{\text{val}}(f^-)$$

- Wasteful to split into 3 subsets.
- Different approach: **cross-validation**.






## Cross-Validation






## Cross-Validation

- Basic approach:
  - Split training set into $T$ folds.
  - For each $\gamma$ and each $t = 1, \dots, T$:
    - Use fold $t$ as validation set and the rest to train the model parameters $\theta_t = \theta_t(\gamma)$, obtaining decision function $f^-_{t,\gamma}$.

$$R^{\text{val}}_t(f^-_{t,\gamma}) = \frac{1}{|\text{Fold}(t)|} \sum_{i \in \text{Fold}(t)} L(y_i, f^-_{t,\gamma}(x_i))$$

  - Choose $\gamma^*$ which minimizes validation error averaged over folds

$$\frac{1}{T} \sum_{t=1}^{T} R^{\text{val}}_t(f^-_{t,\gamma})$$

  - Train model with tuning parameter $\gamma^*$ on all training set to obtain $f_{\gamma^*}$.
  - Report generalization performance on test set.
- **Leave-One-Out (LOO)** cross validation: one data item per fold, i.e., $T = n$.

Cross-validation can be computationally expensive ($T\times$ increase in complexity).



## Leave-One-Out Cross-Validation

**Leave-one-out (LOO)** cross validation: one data item per fold, i.e., $T = n$.

- Since only one data item not used in training, $R(f^-_{t,\gamma})$ are all very close to $R(f_\gamma)$ (small $v$ benefit).
- Thus,

$$\frac{1}{n} \sum_{t=1}^{n} R^{\text{val}}_t(f^-_{t,\gamma}) = \frac{1}{n} \sum_{t=1}^{n} L(y_t, f^-_{t,\gamma}(x_t))$$

  has a small variance (large $v$ benefit).
- All examples for validation and all examples for training.
- summands are no longer independent