

Generalisation in theory and practice

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Outline

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- Supervised machine learning problems

Generalisation

Estimating quality

- Methodology

Learning and generalisation

- Introduction

- Bias and variance

- Generalisation

PAC Learning

- The realisable setting

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Classification

The classifier as a decision rule

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Randomised predictions given a model $P(y|x)$

Here, we randomly select a class according to our model:

$$\pi(a|x_t) = P(y_t = a|x_t)$$

Accuracy as a classification metric

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The accuracy of a single decision

$$U(a_t, y_t) = \mathbb{I}\{a_t = y_t\} = \begin{cases} 1, & \text{if } a_t = y_t \\ 0, & \text{otherwise} \end{cases}$$

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The accuracy on a dataset

Let $D = \{(x_t, y_t) : t \in [T]\}$ be a dataset. We can measure the accuracy:

$$U(\pi, D) \triangleq \frac{1}{T} \sum_{t=1}^T \pi(y_t | x_t)$$

The expected accuracy of a decision rule

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The expected accuracy of a decision rule

If $(x, y) \sim P$, the accuracy U of a stochastic decision rule π under the distribution P is the probability it predicts correctly

$$U(\pi, P) \triangleq \int_{\mathcal{X}} dP(x) \sum_{y=1}^m P(y|x) \pi(y|x)$$

Beyond classification: Generalised decision rules

Consider a spam application, where the e-mail client can decide between different action for emails. Different actions being best for each type of e-mail. The quality of each action can be captured through a utility function.

Utility of the spam decision problem

What utility function would you use for the spam detection problem?

Utility	Pass	Flag	Trash
Normal			
Spam			
Virus			

The utility function $U : \mathcal{Y} \times \mathcal{A} \rightarrow \mathbb{R}$

The utility function $U(y, a)$ is a real-valued function so that, for a label y , we prefer taking action a to a' iff $U(y, a) > U(y, a')$.

The optimal decision

- ▶ A **model** $P(y|x)$ of class probabilities
- ▶ A **utility** $U(y, a)$ for each class and action combination

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We can calculate the expected utility of any decision

$$\mathbb{E}[U|a, x] = \sum_y P(y|x, a) U(y, a) = \sum_y P(y|x) U(y, a)$$

Here the first equality follows from the definition of conditional expectation and $P(y|x, a) = P(y|x)$ as the label does not depend on our actions.

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The optimal decision

For any observation x , and P , we take the action maximising expected utility:

$$a^* = \arg \max_a \mathbb{E}_P[U|a, x]$$

This defines a function $\mathcal{X} \rightarrow \mathcal{A}$, which is the Bayes-optimal decision rule.

The optimal decision rule

- ▶ A **model** $P(y|x)$ of class probabilities
- ▶ A **utility** $U(y, a)$ for each class and action combination
- ▶ A **decision rule** $\pi(a|x)$ assigning probability to action a for every possible input x

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Expected utility over a dataset.

We obtain the expected utility of the **decision rule** by marginalising over all actions

$$U(\pi, D) \triangleq \mathbb{E}[U|\pi, D] \stackrel{D=(x_t, y_t)_{t=1}^T}{=} \sum_{t=1}^T \mathbb{E}[U|\pi, x_t] = \sum_{t=1}^T \sum_{a \in \mathcal{A}} U(y_t, a) \pi(a|x_t)$$

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Expected utility over P

We can marginalise over possible datasets D

$$U(\pi, P) \triangleq \mathbb{E}_P^\pi[U] = \int_{\mathcal{D}} dP(D) U(\pi, D) \stackrel{\text{i.i.d.}}{=} \int_{\mathcal{X}} dP(x) \sum_{y \in \mathcal{Y}} P(y|x) \sum_{a \in \mathcal{A}} \pi(a|x) U(y, a)$$

Taking into account the probability

- ▶ For classification, it makes sense to look at the probability of the labels.
- ▶ If we are not very confident about our prediction, this should be taken into account:
- ▶ Define $P(y|x)$ to be our classifier's probability for label y , given features x . Then we can use two simple metrics:

Precision

The average probability of the actual class:

$$\sum_{t=1}^T P(y_t|x_t)/T$$

- ▶ If we always assign probability 1 to the correct label, this score is 1.
- ▶ If we always assign probability $1/m$ to all labels, the score is $1/m$.

Negative Log-Loss

Here we assign look at the **logarithm** of the probability. This really penalises bad guesses.

$$\sum_{t=1}^T \ln P(y_t|x_t) / T$$

- ▶ If we always assign probability 1 to the correct label, this score is 0.
- ▶ If we assign probability 0 to even a single label, the score is $-\infty$.

```
from sklearn.metrics import log_loss
```

in scikitlearn implements log-loss (**not** negative)

Regression

The regressor as a deterministic decision rule

A decision rule π generates a **decision** $a \in \mathbb{R}^m$.

- ▶ For **deterministic** rules $\pi(x)$ is the prediction for x .
- ▶ Since we can almost never guess correctly, we need to define the quality of our predictions somehow, either as a utility $U(y_t, a_t)$ or a loss function $\ell(y_t, a_t)$.

Mean-Squared Error Loss on a Dataset

This is the squared difference in predicted versus actual values:

$$\frac{1}{T} \sum_{t=1}^T [y_t - \pi(x_t)]^2$$

Expected MSE

If $(x, y) \sim P$, the expected MSE of a deterministic decision rule

$\pi : \mathcal{X} \rightarrow \mathbb{R}$ is

$$\int_{\mathcal{X}} \int_{\mathcal{Y}} dP(x, y) [y - \pi(x)]^2.$$

Probabilistic regression

The regressor as a stochastic decision rule

A decision rule π generates a **decision** $a \in \mathbb{R}^m$.

- ▶ For **stochastic** rules $\pi(a|x)$ defines a density over predictions.
- ▶ In this case it is natural to define $\pi(y_t, x_t)$ as our metric.

Likelihood on a Dataset

The mean-square error is simply the squared difference in predicted versus actual values:

$$\prod_{t=1}^T \pi(y_t | x_t)$$

We will later see a link between this metric, mean-square error and estimation.

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Training and overfitting

Training data

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The optimal decision rule for P

$$\max_{\pi} U(\pi, P) = \max_{\pi} \int_{\mathcal{X} \times \mathcal{Y}} dP(x, y) \sum_a \pi(a|x) U(a, y).$$

Here we measure performance for the data **distribution P** .

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The optimal decision rule for D

$$\max_{\pi} U(\pi, D) = \max_{\pi} \sum_{(x,y) \in D} \sum_a \pi(a|x) U(a, y).$$

Performance is measured over the **data D**

Generalisation

The fundamental problem

- ▶ We want to maximise $U(\pi, P)$, the **actual** performance.
- ▶ We can only measure $U(\pi, D)$, over **some data**.
- ▶ We have a **learning algorithm** $\lambda : \mathcal{D} \rightarrow \Pi$
- ▶ If $\pi = \lambda(D)$, then we instead measure $U(\lambda(D), D)$.
- ▶ However $\mathbb{E}_P[U(\lambda(D), D)] \geq U(\pi, P) \ \forall \pi$ (**biased** estimator)

Generalisation

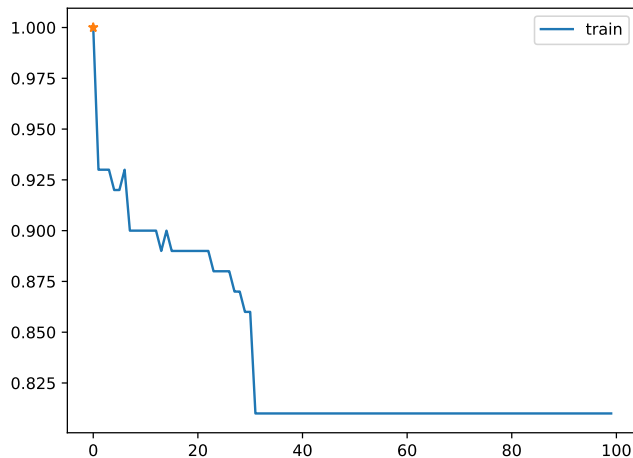
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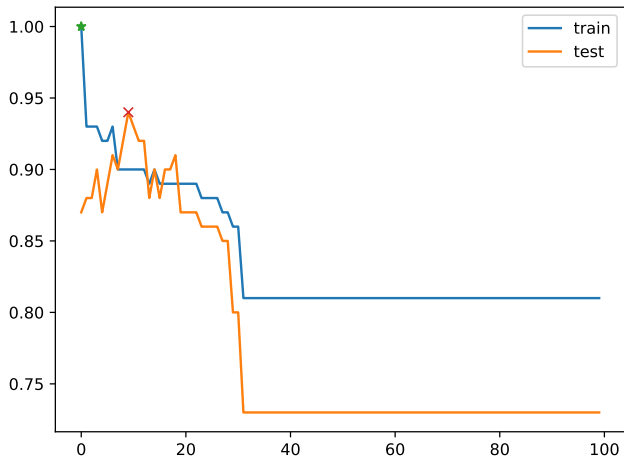
Training and testing

- ▶ Split D in $D_{\text{train}}, D_{\text{test}}$
- ▶ Obtain $\pi = \lambda(D_{\text{train}})$
- ▶ Calculate $U(\pi, D_{\text{test}})$
- ▶ $\mathbb{E}_P[U(\pi, D_{\text{test}})] = U(\pi, P)$ for any fixed π (unbiased estimator)
- ▶ $\mathbb{E}_P[U(\lambda(D_{\text{train}}), D_{\text{train}})] \geq U(\pi, P)$ (biased estimator)

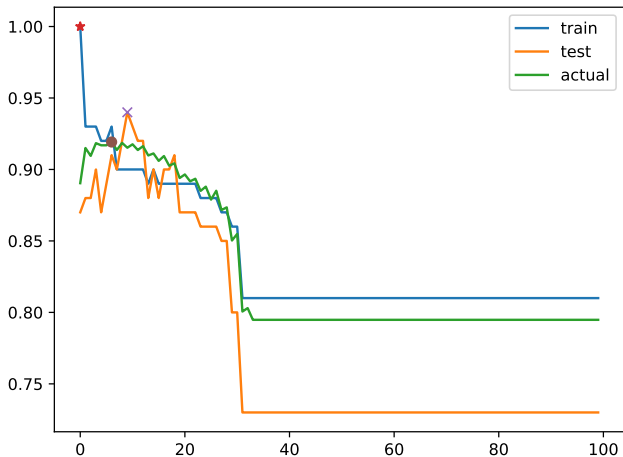
kNN Classifier Accuracy on a single dataset



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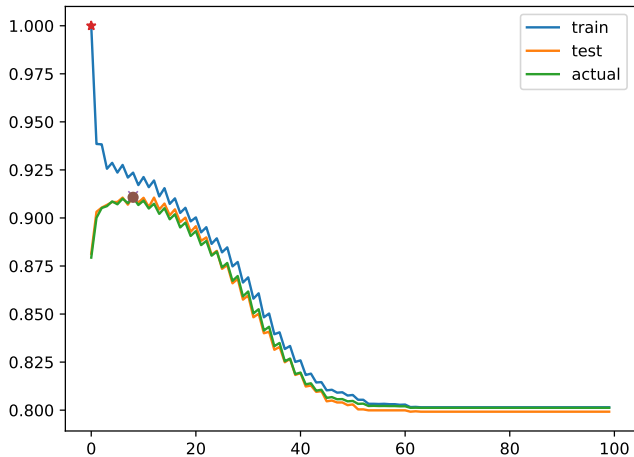


kNN Classifier Accuracy on a single dataset



Expected kNN Classifier Accuracy

Expectation approximated over 100 datasets D sampled from P .



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The Train/Validation/Test methodology

Main idea

Use each piece of data once to make decisions and measure

Training set

Use to decide low-level model parameters

Validation set

Use to decide between:

- ▶ different hyperparameters (e.g. K in nearest neighbours)
- ▶ model (e.g. neural networks versus kNN)

Test set

Use to measure the final quality of a model

Cross-validation (XV)

Idea

- ▶ Use XV to select hyperparameters instead of a single train/valid test.

Methodology

- ▶ Split training set D in k different subsets
- ▶ At iteration i
- ▶ Use the i -th subset for validation
- ▶ Use all the remaining $k - 1$ subsets for training
- ▶ Average results on validation sets

Cross-validation example: A mean estimate

Live coding in Python:

- ▶ Get a mean estimate
- ▶ Perform cross-validation

Hand-crafted

```
def xv_shuffler(x, estimator, scoring, n_folds):  
    rng = np.random.default_rng  
    # shuffle data  
    T = len(x)  
    indices = np.arange(T)  
    shuffle(indices)  
    fold_size = np.ceil(T / n_folds)  
    fold_start = np.zeros(n_folds)  
    fold_end = np.zeros(n_folds)  
    # create folds  
    for k in range(n_folds):  
        fold_start = k * fold_size  
        fold_end = np.min((k+1) * fold_size, T)  
    # for each fold:  
    # 1. Run estimator on k-1 folds
```

Bootstrapping

- ▶ Express uncertainty by resampling the data.
- ▶ Repeat your calculations for each resample

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BootstrapSample(D)

```
input Data  $D = (z_1, \dots, z_T)$ , of size  $T$   
for  $t \in \{1, \dots, T\}$  do  
    Select  $i$  uniformly in  $[T]$   
    Add the  $i$ -th point to  $D_b$   
end for  
return  $D_b$ 
```

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    Add the  $i$ -th point to  $D_b$   
end for  
return  $D_b$ 
```

BootstrapEstimate(D, λ, N)

```
input Data  $D \in \mathcal{D}$ , algorithm  $\lambda : \mathcal{D} \rightarrow \Theta$ ,  $N > 0$  number of samples  
for  $n \in \{1, \dots, N\}$  do  
     $\theta_n = \lambda(\text{BootstrapSample}(D))$   
end for  
return  $\{\theta_n : n \in [N]\}$ 
```


The wrong way to do XV for subset selection

1. Screen the predictors: find a subset of “good” predictors that show fairly strong (univariate) correlation with the class labels.
2. Using just this subset of predictors, build a multivariate classifier.
3. Use cross-validation to estimate the unknown tuning parameters and to estimate the prediction error of the final model.

Is this a correct application of cross-validation?

Consider a scenario with $N = 50$ samples in two equal-sized classes, and $p = 5000$ quantitative predictors (standard Gaussian) that are independent of the class labels. The true (test) error rate of any classifier is 50%.

The right way to do XV for feature selection

1. Divide the samples into K cross-validation folds (groups) at random.
2. For each fold $k = 1, 2, \dots, K$
3. Find a subset of “good” predictors that show fairly strong (univariate) correlation with the class labels, using all of the samples except those in fold k .
4. Using just this subset of predictors, build a multivariate classifier, using all of the samples except those in fold k .
5. Use the classifier to predict the class labels for the samples in fold k .

Lab

- ▶ scikitlearn KNN
- ▶ scikitlearn performance measures
- ▶ train/test/validate plot with increasing k
- ▶ XV plot with increasing k
- ▶ Scaling and other preprocessing
- ▶ Effect of outliers on preprocessing
- ▶ Optional: Bootstrap performance evaluation

===== end

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How well can decision rule perform?

Estimation theory view

- ▶ Bias: The expected difference between the estimated value and the unknown parameter
- ▶ Variance: The expected difference between the estimated value and the unknown parameter

Learning theory view

- ▶ Approximation ability: How well a class of rules can approximate the optimal one.
- ▶ Statistical error: How easy it is to choose the best rule in the class.

Unbiased estimators

Definition (Estimator)

An estimator is a function $f : \mathcal{D} \rightarrow \Theta$, where Θ is a set of parameters. For any given dataset $D \in \mathcal{D}$, it returns a single estimate $\hat{\theta} = f(D)$.

Definition (Unbiased estimator)

An estimator is **unbiased** if, for any θ and corresponding distribution $P(D|\theta)$:

$$\mathbb{E}[f \mid \theta] = \sum_D f(D)P(D|\theta) = \theta.$$

Example (Sample mean estimator)

Consider $D = (x_1, \dots, x_T)$ with $x_t \sim P$ being i.i.d samples with $\mathbb{E}[x_t] = \theta$. The sample mean estimator $f(D) = \sum_t x_t / T$ is unbiased, as :

$$\mathbb{E}[f] = \mathbb{E} \left[\sum_{t=1}^T x_t / T \right] = \frac{1}{T} \sum_{t=1}^T \mathbb{E}[x_t] = \frac{1}{T} \sum_{t=1}^T \theta = \theta.$$

Example of a biased and unbiased estimator: Training error

- ▶ $U(\pi, D)$ is the measured accuracy of a classifier π on D
- ▶ $U(\pi, P) = \mathbb{E}_{D \sim P}[U(\pi, D)]$ is the actual accuracy. So $U(\pi, D)$ is unbiased.
- ▶ $\lambda(D) = \arg \max_{\pi} U(\pi, D)$ is a learning algorithm picking the best classifier for a dataset D .
- ▶ Then $U(\lambda(D), D)$ is biased, as for any π'

$$\mathbb{E}_{D \sim P}[U(\lambda(D), D)] = \int_D dP(D) U(\lambda(D), D) \quad (1)$$

$$= \int_D dP(D) \max_{\pi} U(\pi, D) \quad (2)$$

$$\geq \int_D dP(D) U(\pi', D) \quad (3)$$

$$= U(\pi', P) \quad (4)$$

i.e. the expected value of the training accuracy is higher than the accuracy of **any** classifier.

The bias/variance trade-off

- ▶ Dataset $D \sim P$.
- ▶ Predictor $f_D(x)$
- ▶ Target function $y = f(x) + \epsilon$
- ▶ $\mathbb{E} \epsilon = 0$ zero-mean noise with variance $\sigma^2 = \mathbb{V}(\epsilon)$

MSE decomposition

$$\mathbb{E}[(f - f_D)^2] = \mathbb{V}(f_D) + \mathbb{B}(f_D)^2 + \sigma^2$$

Variance

How sensitive the estimator is to the data

$$\mathbb{V}(f_D) = \mathbb{E}[(f_D - \mathbb{E}(f_D))^2]$$

Bias

What is the expected deviation from the true function

$$\mathbb{B}(f_D) \triangleq \mathbb{E}[(f_D - f)]$$

Example: mean estimation

- ▶ Data $D = y_1, \dots, y_T$ with $\mathbb{E}[y_t] = \mu$.
- ▶ Goal: estimate μ with some estimator f_D to minimise
- ▶ MSE: $\mathbb{E}[(y - f_D)^2]$, the expected square difference between new samples and our guess.

Optimal estimate

To minimise the MSE, we use $f^* = \mu$. This gives us two ideas:

Empirical mean estimator:

- ▶ $f_D = \sum_{t=1}^T x_t / T$.
- ▶ $\mathbb{V}(f_D) = \mathbb{E}[f_D - \mu]^2 = 1/\sqrt{T}$
- ▶ $\mathbb{B}(f_D) = 0$. (unbiased estimator)

Laplace mean estimator:

- ▶ $f_D = \sum_{t=1}^T (\lambda + x_t) / T$.
- ▶ $\mathbb{V}(f_D) = \mathbb{E}[f_D - \mu]^2 = \frac{1}{1+\sqrt{T}}$
- ▶ $\mathbb{B}(f_D) = O(1/T)$.

A proof of the bias/variance trade-off

- ▶ RV's $y_t \sim P$, $\mathbb{E}[y_t] = \mu$, $y_t = \mu + \epsilon_t$.
- ▶ Estimator f_D , $D = y_1, \dots, y_{t-1}$.

$$\begin{aligned}\mathbb{E}[(f_D - y_t)^2] &= \mathbb{E}[f_D^2] - 2\mathbb{E}[f_D y_t] + \mathbb{E}[y_t^2] \\ &= \mathbb{V}[f_D] + \mathbb{E}[f_D]^2 - 2\mathbb{E}[f_D y_t] + \mathbb{E}[y_t^2] \\ &= \mathbb{V}[f_D] + \mathbb{E}[f_D]^2 - 2\mathbb{E}[f_D] \mathbb{E}[y_t] + \mathbb{E}[y_t^2] \\ &= \mathbb{V}[f_D] + \mathbb{E}[f_D]^2 - 2\mathbb{E}[f_D]\mu + \mathbb{E}[y_t^2] \\ &= \mathbb{V}[f_D] + \mathbb{E}[f_D]^2 - 2\mathbb{E}[f_D]\mu + \mathbb{E}[(\mu + \epsilon_t)^2] \\ &= \mathbb{V}[f_D] + \mathbb{E}[f_D]^2 - 2\mathbb{E}[f_D]\mu + \mathbb{E}[\mu^2 + 2\mu\epsilon_t + \epsilon_t^2] \\ &= \mathbb{V}[f_D] + \mathbb{E}[f_D]^2 - 2\mathbb{E}[f_D]\mu + \mu^2 + \sigma^2 \\ &= \mathbb{V}[f_D] + (\mathbb{E}[f_D] - \mu)^2 + \sigma^2 \\ &= \mathbb{V}(f_D) + \mathbb{B}(f_D)^2 + \sigma^2\end{aligned}$$

Generalisation error

Regret decomposition

Let the optimal rule be $\pi^* \in \Pi$, the best approximate rule be $\hat{\pi}^* \in \hat{\Pi}$ and our rule be $\hat{\pi} \in \hat{\Pi}$. We call the difference between the performance of π^* and $\hat{\pi}$ our **regret**:

$$\underbrace{U(\pi^*, P) - U(\hat{\pi}, P)}_{\text{regret}} = \underbrace{U(\pi^*, P) - U(\hat{\pi}^*, P)}_{\text{approximation error}} + \underbrace{U(\hat{\pi}^*, P) - U(\hat{\pi}, P)}_{\text{estimation error}}$$

We can bound the regret by bounding each term separately.

- ▶ The **approximation error** tells us how expressive our class of rules is, i.e. how much we lose by looking at a restricted class $\hat{\Pi}$ of rules. It is similar to estimator **bias**.
- ▶ The **statistical error** tells us how well the empirical performance on D approximates the true performance. It is similar to estimator **variance**.
- ▶ As a rule of thumb, the larger our class, the better the possible approximation but the higher the statistical error.

Approximation error

- ▶ Our model limits us to a set of decision rules $\hat{\Pi} \subset \Pi$.
- ▶ The most we could do is find the best rule in $\hat{\Pi}$.
- ▶ This still leaves a gap:

$$\Delta \triangleq \max_{\pi \in \Pi} U(\pi, P) - \max_{\hat{\pi} \in \hat{\Pi}} U(\hat{\pi}, P)$$

The gap can be characterised in some cases.

Example: ϵ -net on Lipschitz $U(\cdot, P)$.

- ▶ Assume $U(\pi, P)$ is a Lipschitz function of π for all P , i.e. $|U(\pi, P) - U(\pi', P)| \leq Ld(\pi, \pi')$ for some metric d .
- ▶ Let $\hat{\Pi}$ be an ϵ -net on Π , i.e. $\max_{\pi \in \Pi} \min_{\pi' \in \hat{\Pi}} d(\pi, \pi') = \epsilon$.
- ▶ Then $\Delta \leq L\epsilon$.

Estimation error

- ▶ First, let us bound $U(\hat{\pi}^*, P) - U(\hat{\pi}, P)$ by making an assumption.
- ▶ Then, we can prove that our assumption holds with high probability.

Lemma

Let $f, g : S \rightarrow \mathbb{R}$. If $\|f - g\|_{\infty} \leq \epsilon$ and $f(x) \geq f(z)$, while $g(y) \geq g(z)$, for all z , i.e. x, y maximise f, g respectively

$$f(x) - f(y) \leq 2\epsilon.$$

This holds as: $f(x) - f(y) \leq g(x) + \epsilon - f(y) \leq g(y) + \epsilon - f(y) \leq 2\epsilon$.

Corollary

If $|U(\pi, P) - U(\pi, D)| \leq \epsilon$ for all π then

$$U(\hat{\pi}^*, P) - U(\hat{\pi}, P) \leq 2\epsilon$$

- ▶ Let us now prove that, with high probability,
 $|U(\pi, P) - U(\pi, D)| \leq \epsilon$.

Bounding the estimation error

For any fixed rule $\pi \in \Pi$ and utility function $U : \Pi \times \mathcal{X}^T \rightarrow [0, 1]$,

$$P^T(|U(\pi, D) - U(\pi, P)| \geq \epsilon) \leq 2 \exp(-2T\epsilon^2).$$

This is a direct application of Hoeffding's inequality¹. Taking the union bound over the set $\hat{\Pi}$ gives:


$$P^T(\exists \pi \in \hat{\Pi} : |U(\pi, D) - U(\pi, P)| \geq \epsilon) \leq 2|\hat{\Pi}| \exp(-2T\epsilon^2).$$

Setting the right side equal to δ and re-arranging,

$$P^T\left(\max_{\pi \in \hat{\Pi}} |U(\pi, D) - U(\pi, P)| \geq \sqrt{\frac{\ln(2|\hat{\Pi}|/\delta)}{2T}}\right) \leq \delta.$$

Example: ϵ -net.

In a n dimensional space we require $|\hat{\Pi}| = O(\epsilon^{-n})$. This means that our statistical error is $O(\sqrt{n \ln(1/\epsilon\delta)}/T)$.

¹See Hoeffding's inequality in the confidence intervals presentation 

The finite hypothesis algorithm

- ▶ Input: a finite set of rules $\hat{\Pi}$, data D , utility U
- ▶ Return $\hat{\pi} \in \arg \max_{\pi \in \hat{\Pi}} U(\pi, D)$.

Regret of the finite hypothesis algorithm.

With probability $1 - \delta$

$$U(\hat{\pi}, P) \geq U(\hat{\pi}^*, P) - \sqrt{2 \ln(2|\hat{\Pi}|/\delta)/T} \quad (5)$$

$$U(\pi^*, P) - U(\hat{\pi}, P) \leq \Delta + \sqrt{2 \ln(2|\hat{\Pi}|/\delta)/T} \quad (6)$$

Examples

- ▶ ML estimation: $U(\beta, D) = P_{\beta}(D)$ is the data likelihood.
- ▶ Accuracy, etc: $U(\pi, D)$.

VC Dimension

Here we consider sets Π of deterministic rules $\pi : \mathcal{X} \rightarrow \{0, 1\}$.

Shattering

If a $S \subset \mathcal{X}$ can with $|S| = m$, can be assigned any labelling y_1, \dots, y_m by a $\pi \in \Pi$, then we say Π shatters S .

The VC dimension

This is the largest-size set S that Π can shatter.

Example: Perceptrons on \mathbb{R}^2

This class has VC dimension 3 on the plane.

Quality metrics

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Introduction

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Learning algorithm λ

- ▶ Takes data $D = \{(x_t, y_t)\}$ as input
- ▶ Generates deterministic decision rules $\pi : X \rightarrow \{0, 1\}$,

The loss of a rule π .

- ▶ Assume an existing concept class $\pi^* \in \Pi$
- ▶ Distribution $x_t \sim P$ is i.i.d. and $x_1, \dots, x_T \sim P^T$.
- ▶ The loss under distribution P is

$$L(\pi) = P(\{x : \pi(x) \neq \pi^*(x)\})$$

Realisable PAC learner

- ▶ $\lambda : (\mathcal{X} \times \mathcal{Y})^* \rightarrow \Pi$ is (ϵ, δ) -PAC, if for any P and $\epsilon, \delta > 0$, and any concept $\pi^* \in \Pi$, there is T such that

$$P^T(\{D : L[\lambda(D)] > \epsilon\}) < \delta, \quad D = (\{x_t, \pi^*(x_t)\}), x_t \sim P.$$