## Generalisation in theory and practice

Christos Dimitrakakis

September 30, 2025

## Outline

#### Quality metrics

Supervised machine learning problems

#### Generalisation

### Estimating quality

Methodology

#### Learning and generalisation

Introduction
Bias and variance
Generalisation

#### **PAC Learning**

The realisable setting

#### Quality metrics

Supervised machine learning problems

#### Generalisation

## Estimating quality

Methodology

#### Learning and generalisation

Introduction Bias and variance

#### PAC Learning

The realisable setting

### Classification

#### The classifier as a decision rule

A decision rule  $\pi(a|x)$  generates a decision  $a \in [m]$ . It is the conditional probability of a given x.

## Classification

#### The classifier as a decision rule

A decision rule  $\pi(a|x)$  generates a decision  $a \in [m]$ . It is the conditional probability of a given x.

Deterministic predictions given a model P(y|x)

Here, we pick the most likely class:

$$\pi(a|x_t) = \mathbb{I}\left\{a = \operatorname*{max}_y P(y|x_t)\right\}$$

## Classification

#### The classifier as a decision rule

A decision rule  $\pi(a|x)$  generates a decision  $a \in [m]$ . It is the conditional probability of a given x.

## Deterministic predictions given a model P(y|x)

Here, we pick the most likely class:

$$\pi(a|x_t) = \mathbb{I}\left\{a = \operatorname*{max}_{y} P(y|x_t)\right\}$$

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

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

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

The accuracy of a single decision

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

The accuracy of a single decision

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

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

The accuracy of a single decision

$$U(a_t, y_t) = \mathbb{I}\left\{a_t = y_t\right\} = egin{cases} 1, & ext{if } a_t = y_t \\ 0, & ext{otherwise} \end{cases}$$

### 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

If  $(x, y) \sim P$ , the accuracy U of a stochastic decision rule  $\pi$  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 $U: \mathcal{Y} \times \mathcal{A} \to \mathbb{R}$

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
- ightharpoonup A utility U(y, a) for each class and action combination

## The optimal decision

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

## Expected utility

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.

## The optimal decision

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

## Expected utility

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.

### 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  $\mathcal{X} \to \mathcal{A}$ , which is the Bayes-optimal decision rule.



## The optimal decision rule

- ightharpoonup A model P(y|x) of class probabilities
- ightharpoonup 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

## The optimal decision rule

- ightharpoonup A model P(y|x) of class probabilities
- ightharpoonup 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

## Expected utility over a dataset.

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

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

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.

## The optimal decision rule

- ightharpoonup A model P(y|x) of class probabilities
- ightharpoonup 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

### Expected utility over a dataset.

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

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

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.

## Expected utility over P

We can marginalise over possible datasets D

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

## 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  $\pi$  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  $\pi: \mathcal{X} \to \mathbb{R}$  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  $\pi$  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.

#### Quality metrics

Supervised machine learning problems

#### Generalisation

# Estimating quality Methodology

Learning and generalisation

Introduction
Bias and variance
Generalisation

#### PAC Learning

The realisable setting

## Training data

- $\triangleright D = ((x_t, y_t) : t = 1, ..., T).$
- $ightharpoonup x_t \in \mathcal{X}, \ y_t \in \mathcal{Y}.$

## Training data

- $\triangleright D = ((x_t, y_t) : t = 1, ..., T).$
- $ightharpoonup x_t \in \mathcal{X}, \ y_t \in \mathcal{Y}.$

## Assumption: The data is generated i.i.d.

- ▶  $(x_t, y_t) \sim P$  for all t (identical)
- ▶  $D \sim P^T$  (independent)

## Training data

- $\triangleright D = ((x_t, y_t) : t = 1, ..., T).$
- $ightharpoonup x_t \in \mathcal{X}, y_t \in \mathcal{Y}.$

## Assumption: The data is generated i.i.d.

- $ightharpoonup (x_t, y_t) \sim P$  for all t (identical)
- ▶  $D \sim P^T$  (independent)

## 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.

## Training data

- $\triangleright D = ((x_t, y_t) : t = 1, ..., T).$
- $ightharpoonup x_t \in \mathcal{X}, \ y_t \in \mathcal{Y}.$

## Assumption: The data is generated i.i.d.

- $ightharpoonup (x_t, y_t) \sim P$  for all t (identical)
- ▶  $D \sim P^T$  (independent)

## 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.

## 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  $\lambda: \mathcal{D} \to \Pi$
- ▶ If  $\pi = \lambda(D)$ , then we instead measure  $U(\lambda(D), D)$ .
- ▶ However  $\mathbb{E}_P[U(\lambda(D), D)] \ge U(\pi, P) \ \forall \pi$  (biased estimator)

### Generalisation

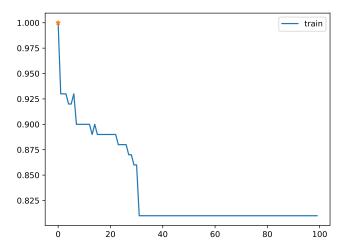
## The fundamental problem

- 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  $\lambda: \mathcal{D} \to \Pi$
- ▶ If  $\pi = \lambda(D)$ , then we instead measure  $U(\lambda(D), D)$ .
- ▶ However  $\mathbb{E}_P[U(\lambda(D), D)] \ge U(\pi, P) \ \forall \pi \ (biased \ estimator)$

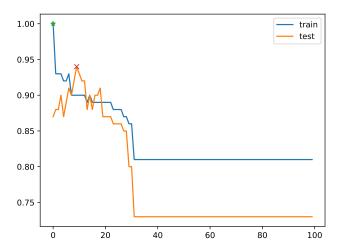
### Training and testing

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

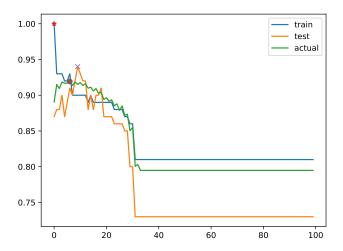
## kNN Classifier Accuracy on a single dataset



## kNN Classifier Accuracy on a single dataset

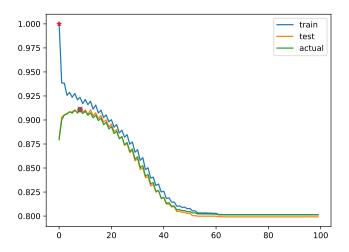


## kNN Classifier Accuracy on a single dataset



## Expected kNN Classifier Accuracy

Expectation approximated over 100 datasets D sampled from P.



### Quality metrics

Supervised machine learning problems

#### Generalisation

# Estimating quality Methodology

## Learning and generalisation

Bias and variance

#### PAC Learning

The realisable setting

## 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
                                        4D > 4B > 4B > 4B > 900
```

# Bootstrapping

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

# Bootstrapping

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

## BootstrapSample(D)

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

# Bootstrapping

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

## BootstrapSample(D)

```
input Data D = (z_1, \ldots, z_T), of size T for t \in \{1, \ldots, T\} do

Select i uniformly in [T]

Add the i-th point to D_b

end for

return D_b
```

## BootstrapEstimate( $D, \lambda, N$ )

```
input Data D \in \mathcal{D}, algorithm \lambda : \mathcal{D} \to \Theta, N > 0 number of samples for n \in \{1, \dots, N\} do \theta_n = \lambda(\operatorname{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  $k = 1, 2, \ldots, K$
- 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

#### Quality metrics

Supervised machine learning problems

#### Generalisation

# Estimating quality Methodology

#### Learning and generalisation Introduction Bias and variance Generalisation

#### PAC Learning

The realisable setting

## Learning and generalisation

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  $f: \mathcal{D} \to \Theta$ , where  $\Theta$  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  $\theta$  and corresponding distribution  $P(D|\theta)$ :

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

## Example (Sample mean estimator)

Consider  $D=(x_1,\ldots,x_T)$  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  $\pi$  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  $\pi'$

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

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

$$\geq \int_{D} dP(D)U(\pi', D) \tag{3}$$

$$=U(\pi',P) \tag{4}$$

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  $y = f(x) + \epsilon$
- $ightharpoonup \mathbb{E} \epsilon = 0$  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  $D = y_1, ..., y_T$  with  $\mathbb{E}[y_t] = \mu$ .
- ▶ Goal: estimate  $\mu$  with some estimator  $f_D$  to minimise
- ► MSE:  $\mathbb{E}[(y f_D)^2]$ , the expected square difference between new samples our guess.

## Optimal estimate

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

### Empirical mean estimator:

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

### Laplace mean estimator:

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



# A proof of the bias/variance trade-off

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

$$\mathbb{E}[(f_{D} - y_{t})^{2}] = \mathbb{E}[f_{D}^{2}] - 2 \mathbb{E}[f_{D}y_{t}] + \mathbb{E}[y_{t}^{2}]$$

$$= \mathbb{V}[f_{D}] + \mathbb{E}[f_{D}]^{2} - 2 \mathbb{E}[f_{D}y_{t}] + \mathbb{E}[y_{t}^{2}]$$

$$= \mathbb{V}[f_{D}] + \mathbb{E}[f_{D}]^{2} - 2 \mathbb{E}[f_{D}] \mathbb{E}[y_{t}] + \mathbb{E}[y_{t}^{2}]$$

$$= \mathbb{V}[f_{D}] + \mathbb{E}[f_{D}]^{2} - 2 \mathbb{E}[f_{D}]\mu + \mathbb{E}[y_{t}^{2}]$$

$$= \mathbb{V}[f_{D}] + \mathbb{E}[f_{D}]^{2} - 2 \mathbb{E}[f_{D}]\mu + \mathbb{E}[(\mu + \epsilon_{t})^{2}]$$

$$= \mathbb{V}[f_{D}] + \mathbb{E}[f_{D}]^{2} - 2 \mathbb{E}[f_{D}]\mu + \mathbb{E}[\mu^{2} + 2\mu\epsilon_{t} + \epsilon_{t}^{2}]$$

$$= \mathbb{V}[f_{D}] + \mathbb{E}[f_{D}]^{2} - 2 \mathbb{E}[f_{D}]\mu + \mu^{2} + \sigma^{2}$$

$$= \mathbb{V}[f_{D}] + (\mathbb{E}[f_{D}] - \mu)^{2} + \sigma^{2}$$

$$= \mathbb{V}(f_{D}) + \mathbb{B}(f_{D})^{2} + \sigma^{2}$$

#### Generalisation error

## Regret decomposition

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

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

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:

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

The gap can be characterised in some cases.

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

- Assume  $U(\pi, P)$  is a Lipschitz function of  $\pi$  for all P, i.e.  $|U(\pi, P) U(\pi', P)| \le Ld(\pi, \pi')$  for some metric d.
- Let  $\hat{\Pi}$  be an  $\epsilon$ -net on  $\Pi$ , 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  $f,g:S\to\mathbb{R}$ . 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

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

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

### Corollary

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

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

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



# Bounding the estimation error

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

$$P^{T}(|U(\pi,D)-U(\pi,P)| \ge \epsilon) \le 2\exp(-2T\epsilon^{2}).$$

This is a direct application of Hoeffding's inequality  $^1$ . Taking the union bound over the set  $\hat{H}$  gives:

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

Setting the right side equal to  $\delta$  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: $\epsilon$ -net.

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

# 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  $1-\delta$ 

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

$$U(\pi^*, P) - U(\hat{\pi}, P) \le \Delta + \sqrt{2\ln(2|\hat{H}|/\delta)/T}$$
(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  $\Pi$  of deterministic rules  $\pi: \mathcal{X} \to \{0,1\}$ .

## Shattering

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

#### The VC dimension

This is the largest-size set S that  $\Pi$  can shatter.

## Example: Perceptrons on $\mathbb{R}^2$

This class has VC dimension 3 on the plane.

#### Quality metrics

Supervised machine learning problems

#### Generalisation

# Estimating quality Methodology

#### Learning and generalisation

Introduction Bias and variance Congression

# PAC Learning The realisable setting

# Binary classification

## Learning algorithm $\lambda$

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

#### The loss of a rule $\pi$ .

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

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

#### Realisable PAC learner

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

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

