National Ph.D. Program in *Artificial Intelligence for Society*

Statistics for Machine Learning

Lesson 07 - Statistical decision theory.

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The classification/concept learning problem

- $X = (W, C)$ where W are predictive features and C class, with $support(C) = \{0, 1, \ldots, n_C - 1\}$
- $x_1, \ldots, x_n$ are observations (*training set*), with $x_i = (w_i, c_i)$ for $i = 1, \ldots, n$
- $\theta \in \Theta$ with Θ hypothesis space (parameters of ML model) with f_θ joint density of W, C

Classification/concept learning: which hypothesis is the most probable given the observed data?

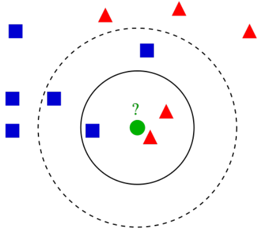
- $\theta_{MLE} = arg\ \max_\theta \ell(\theta) = arg\ \min_\theta -\ell(\theta) = arg\ \min_\theta \sum_{i=1}^{n} - \log f_\theta(x_i)$
- $f_\theta(x_i) = f_\theta(w_i, c_i) = f_\theta(c_i|w_i) f_\theta(w_i)$
- $\theta_{MLE} = arg\ \min_\theta \sum_{i=1}^{n} - \log f_\theta(c_i|w_i) - \sum_{i=1}^{n} \log f_\theta(w_i)$
- Assuming $\theta \perp\!\!\!\perp W$, we have $f_{\theta_1}(w_i) = f_{\theta_2}(w_i)$, and then:

$$\theta_{MLE} = arg\ \min_\theta \sum_{i=1}^{n} - \log f_\theta(c_i|w_i)$$

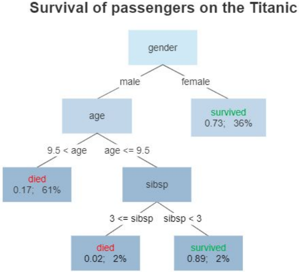
- How to compute θ_{MLE}? Closed form, brute force enumeration of $\theta \in \Theta$, heuristic search, ...

- $f_\theta(c|w) = P(C = c|W = w, \theta)$ is called a **probabilistic classifier** learned/trained from $x_1, \ldots, x_n$

Probabilistic classifiers: examples



- Logistic regression
- k-Nearest Neighbors (k-NN)
- Decision trees
- Neural networks
- Naive Bayes $P(C = c_0|W = w) = P(C = c_0)\prod_i P(W_i = w_i|C = c_0)/P(W = w)$ assuming $P(W = w|C = c_0) = \prod_i P(W_i = w_i|C = c_0)$
- Ensembles
- Gradient boosting
- ...
- More classifiers at the Machine Learning and Data Mining courses



MLE and KL divergence/Cross-Entropy

$$\theta_{MLE} = arg \min_{\theta} \sum_{i=1}^{n} - \log f_{\theta}(c_i|w_i)$$

- Assume data is generated from $f_{\theta_{TRUE}}$, i.e., $(W, C) \sim f_{\theta_{TRUE}}$
- We compute:

$$\theta_{MLE} = arg \min_{\theta} \sum_{i=1}^{n} (- \log f_{\theta}(c_i|w_i) + \log f_{\theta_{TRUE}}(c_i|w_i)) = arg \min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \log \frac{f_{\theta_{TRUE}}(c_i|w_i)}{f_{\theta}(c_i|w_i)}$$

$$\xrightarrow{n \to \infty}_{LLN} arg \min_{\theta} E_{(W,C)\sim f_{\theta_{TRUE}}} [log \frac{f_{\theta_{TRUE}}(C|W)}{f_{\theta}(C|W)}] = arg \min_{\theta} D_{KL}(\theta_{TRUE} \parallel \theta) = arg \min_{\theta} H(\theta_{TRUE}; \theta)$$

- Asymptotically: ML maximization = KL divergence minimization = Cross-entropy minimization

The classification/concept prediction problem

Question: which is the most probable class value given w and θ?

- **Problem**: given $\theta \in \Theta$ and $W = w$, what is the most probable $C = c$? i.e.:

$$arg\max_c P(C = c, W = w|\theta)$$

which is equivalent, assuming $\theta \perp\!\!\!\perp W$, to:

$$arg\max_c P(C = c|W = w, \theta) \cdot P(W = w|\theta) = arg\max_c f_\theta(c|w)$$

- **Bayes decision rule** $y^*_\theta(w) = arg\max_c f_\theta(c|w)$ *[or simply, y^*]*

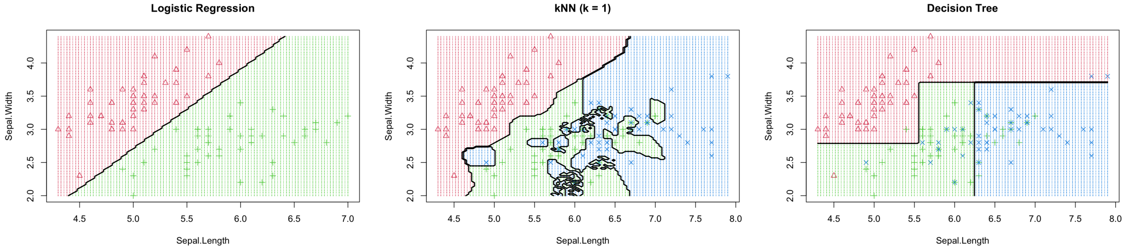
Theorem (Bayes decision rule is optimal)

Fix $\theta \in \Theta$. For any decision rule $y^+_\theta : \mathbb{R}^{|W|} \to \{0, \dots, n_C - 1\}$:

$$P(y^*_\theta(W) \neq C) \leq P(y^+_\theta(W) \neq C)$$

Proof. $P(y^*_\theta(W) = C) = E[\mathbb{1}_{y^*_\theta(W)=C}] = E[E_C[\mathbb{1}_{y^*_\theta(W)=C}|W = w]] \geq$
$\geq E[E_C[\mathbb{1}_{y^+_\theta(W)=C}|W = w]] = E[\mathbb{1}_{y^+_\theta(W)=C}] = P(y^+_\theta(W) = C)$ □

Decision boundary



- A decision boundary for a decision rule $y^+_\theta()$ is the region $w \in \mathbb{R}^{|W|}$ such that $y^+_\theta(w)$ could admit as possible answers two or more classes
- For y^*_θ, it is the region $w \in \mathbb{R}^{|W|}$ such that $arg\max_c f_\theta(c|w)$ is not unique.
- For y^*_θ and $n_C = 2$, it is the region $w \in \mathbb{R}^{|W|}$ such that $f_\theta(1|w) = 0.5$.

Bayes optimal predictions

Question: which is the most probable class value given w only (i.e., without fixing the parameters)?

- Possible answer: the prediction of the most probable model, i.e., $arg\max_c P(C = c|W = w, \theta_{MAP})$
- No, we can do better
  - Let $\Theta = \{\theta_1, \theta_2, \theta_3\}$ and
    - $P(\theta_1|X_1 = x_1, \ldots, X_n = x_n) = 0.4$
    - $P(\theta_2|X_1 = x_1, \ldots, X_n = x_n) = P(\theta_3|X_1 = x_1, \ldots, X_n = x_n) = 0.3$
  - Hence $\theta_{MAP} = \theta_1$
  - Assume $f_{\theta_1}(1|w) = 1$ and $f_{\theta_2}(0|w) = f_{\theta_3}(0|w) = 1$
  - Hence, class 0 has the largest probability (over the hypothesis space), whilst θ_{MAP} predicts 1
- **Problem**: given $W = w$, what is the most probable $C = c$? i.e.:

$$arg\max_c P(C = c|W = w, X_1 = x_1, \ldots, X_n = x_n)$$

Bayes optimal prediction

$$arg\max_c \sum_{\theta \in \Theta} f_\theta(c|w) P(\theta|X_1 = x_1, \ldots, X_n = x_n)$$

No-Free-Lunch theorem

- A **learner** $\mathcal{A}$ is a computable function that maps a training set $x_1, \ldots, x_n$ into a decision rule $y_\theta()$

  Question: Is there a learner $\mathcal{A}$ that always maps a training set into a decision rule with zero error?

No-Free-Lunch theorem (Wolpert, 1996)

Consider binary classification, i.e., $n_C = 2$, and a finite domain $dom(W) < \infty$. For any learner $\mathcal{A}$, there exists a distribution F with $(W, C) \sim F$ such that:

- for at least $1/7$ of the training sets $x_1, \ldots, x_n$ (realizations of F^n) with $n < |dom(W)|/2$, the decision rule y_θ^+ in output by $\mathcal{A}$ has an error of at least $1/8$, i.e.:

$$P_F(y_\theta^+(W) \neq C) \geq 1/8$$

- and there exists an error-free decision rule $y_\theta^\star$ s.t. $P_F(y_\theta^\star(W) \neq C) = 0$.

See here for an accessible proof

- A universal learner does no exist! No learner can succeed on all learning tasks: every learner has tasks on which it fails whereas other learners succeed.
- The learnt y_θ^+ is likely to have a large error for F, whereas there exists another learner that will output a decision rule $y_\theta^\star$ with no error.

Probabilistic classifiers

- Probabilistic classifier: $f_\theta(c|w) \in [0,1]$ with $\sum_c f_\theta(c|w) = 1$:
  - learned from $x_1, \ldots, x_n$
  - predicted probabilities $(p_0, \ldots, p_{n_C-1})$ with $p_i = f_\theta(i|w)$
  - most probable class $y^*_\theta = arg\max_c f_\theta(c|w)$
  - confidence (of most probable class) $p^*_\theta = \max_c f_\theta(c|w)$
- Unnormalized classifier: $uc_\theta(c|w) \in \mathbb{R}$
  - unnormalized values $(v_0, \ldots, v_{n_C-1})$ with $v_i = uc_\theta(i|w)$
  - normalization using **softmax**:

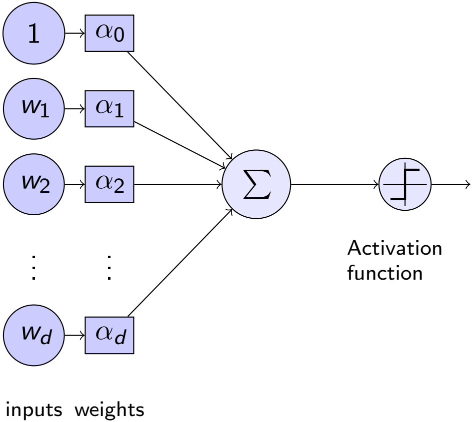
$$softmax((v_0, \ldots, v_{n_C-1})) = (\frac{e^{v_0}}{\sum_i e^{v_i}}, \ldots, \frac{e^{v_{n_C-1}}}{\sum_i e^{v_i}})$$

  - binary classes $(v_0 = 0, v_1)$:

$$softmax((0, v_1)) = (1 - z, z) \qquad \text{where } z = sigmoid(v_1) = inv.logit(v_1) = \frac{1}{1 + e^{-v_1}}$$

  - $softmax(\mathbf{v} + c) = softmax(\mathbf{v})$
  - $\frac{d}{d\mathbf{v}} softmax(\mathbf{v}) = softmax(\mathbf{v})(1 - softmax(\mathbf{v}))$

Example: Perceptron with sigmoid activation



$$\theta = (\alpha_0, \alpha_1, \dots, \alpha_d)$$

$$w = (w_1, \dots, w_d)$$

$$z = sigmoid(\theta \cdot (1, w)^T) = sigmoid(\alpha_0 + \sum_{i=1}^{d} \alpha_i \cdot w_i)$$

$$y_\theta^* = arg\max(1 - z, z)$$

- Difference with logistic regression?
  - Weights calculated differently (MLE vs gradient descent)
  - Perceptron is parametric to **activation functions**
  - Perceptron with sigmoid activation = Logistic regression

Binary classification/concept learning

- $X = (W, C)$ where W are predictive features and C class, with $support(C) = \{0, 1\}$
- $x_1, \ldots, x_n$ are observations (training set), with $x_i = (w_i, c_i)$
- **Definition.** Score function: $s_\theta(w) = f_\theta(1|w) = P(C = 1|W = w, \theta)$
  - predicted probabilities $(1 - s_\theta(w), s_\theta(w))$
  - confidence (of most probable class): $\max\{1 - s_\theta(w), s_\theta(w)\}$
  - $f_\theta(c_i|w_i) = s_\theta(w_i)^{c_i}(1 - s_\theta(w_i))^{(1-c_i)}$
- MLE estimation

$$\theta_{MLE} = arg\,\min_\theta \sum_{i=1}^{n} -\log f_\theta(c_i|w_i) = arg\,\min_\theta \frac{1}{n} \sum_{i=1}^{n} -c_i \log s_\theta(w_i) - (1 - c_i) \log (1 - s_\theta(w_i))$$

- Cross-entropy loss or log-loss:

$$\ell_\theta(c, w) = \begin{cases} -\log s_\theta(w) & \text{if } c = 1 \\ -\log (1 - s_\theta(w)) & \text{if } c = 0 \end{cases}$$

- MLE maximization = Log-loss minimization

$$\theta_{MLE} = arg\,\min_\theta \frac{1}{n} \sum_{i=1}^{n} \ell_\theta(c_i, w_i)$$

MLE and ERM for classification/concept learning

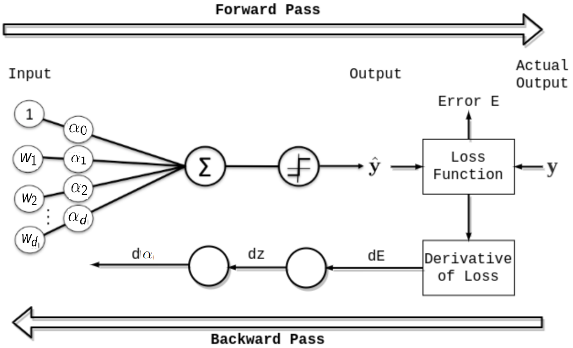
Empirical risk minimization

Let $\ell_\theta : \{0, \dots, n_C - 1\} \times \mathbb{R}^{|W|} \to \mathbb{R}_{\geq 0}$ be a loss function.

$$\theta_{ERM} = arg \min_\theta \frac{1}{n} \sum_{i=1}^{n} \ell_\theta(c_i, w_i)$$

- MLE is ERM with Log-loss $\ell_\theta(c, w) = -\log f_\theta(c|w) = \log \frac{1}{P(c|w,\theta)}$
- 0-1 loss $\ell_\theta(c, w) = \mathbb{1}_{y_\theta^+(w) \neq c}$ where $y_\theta^+(w) \in \{0, \dots, n_C - 1\}$ is a decision rule
  - not convex, not differentiable, optimization problem is NP-hard
- L_p error loss for binary classifiers $\ell_\theta(c, w) = |s_\theta(w) - c|^p$
  - absolute error loss or L_1: $|s_\theta(w) - c|$
  - squared error loss or L_2 or Brier score: $(s_\theta(w) - c)^2$

Loss functions and classifiers



- Gradient of loss function determines updates of weights $\alpha_0, \ldots, \alpha_d$ in the direction of improving the loss (Backpropagation)
- Similar idea in ensemble of decision trees, where each one improves on the error of the previous one (Gradient boosting trees)

MSE and the bias-variance trade-off

- Squared error loss $\theta_{ERM} = arg\min_\theta MSE$, where the Mean Squared Error is:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(s_\theta(w_i) - c_i)^2$$

  - Why named MSE? Because $MSE \xrightarrow{n\to\infty}_{LLN} E_{(W,C)\sim f_{\theta_{TRUE}}}[(s_\theta(W) - C)^2]$
  - MSE approximates the Mean Squared-Error over the population
  - Notice: in MSE for estimators C was a constant (parameter) *[See Lesson 18]*
- Assumes that $C = D + \epsilon$, where $E[\epsilon] = 0$
  - Observed class labels c_i include some noise w.r.t. true labels, i.e., $c_i = d_i + \epsilon_i$
- Decomposition of MSE:

$$E_{(W,C)\sim f_{\theta_{TRUE}}}[(s_\theta(W) - C)^2] = Var(s_\theta(W)) + E[s_\theta(W) - C]^2 + Var(\epsilon)$$

  - $Var(\epsilon)$ irreducible error (would require better curated class values in the training set)
  - $E[s_\theta(W) - C]^2$ is $Bias^2$. Minimized by interpolating training data, but with high variance.
  - $Var(s_\theta(W))$ variance of the scores. Minimized by a constant score, but with high bias.

See R script

Loss functions and risk

Squared error loss minimization on training set generalizes to the population:

$$\theta_{ERM} = arg\min_{\theta} \frac{1}{n}\sum_{i=1}^{n}(s_\theta(w) - c_i)^2 \xrightarrow{n\to\infty}_{LLN} arg\min_{\theta} E_{(W,C)\sim f_{\theta_{TRUE}}}[(s_\theta(W) - C)^2]$$

Risk (or Expected Prediction Error EPE)

The risk w.r.t. a loss function ℓ_θ is $R(\theta_{TRUE}, \theta) = E_{(W,C)\sim f_{\theta_{TRUE}}}[\ell_\theta(C, W)]$.

Definition. A loss function is a *proper scoring rule* if:

$$\theta_{TRUE} = arg\min_{\theta} R(\theta_{TRUE}, \theta)$$

- For log-loss, $R(\theta_{TRUE}, \theta) = D_{KL}(\theta_{TRUE} \parallel \theta) \geq 0$ and $D_{KL}(\theta_{TRUE} \parallel \theta) = 0$ iff $\theta = \theta_{TRUE}$
- Log-loss, squared error (L_2) and 0-1 loss are proper scoring rules, whilst L_1 is not
  - For proper scoring rules, $\theta_{ERM} \xrightarrow{n\to\infty} \theta_{TRUE}$ – recall we assume such $(W, C) \sim f_{\theta_{TRUE}}$ exists
  - Still, 0-1 loss is discontinuous and **can be harmful!**

Best classifier for 0-1 loss

Question: what is the decision rule with the smallest 0-1 risk? I.e., *arg* $\min_{y_\theta^+} E_{(W,C)\sim f_{\theta_{TRUE}}}[\mathbb{1}_{y_\theta^+(W)\neq C}]$?

Binary class *Bayes optimal classifier* (or *Bayes rule*):

$$y^*_{\theta_{TRUE}}(w) = \begin{cases} 1 & \text{if } \eta(w) \geq 1/2 \\ 0 & \text{if } \eta(w) < 1/2 \end{cases}$$

where $\eta(w) = P_{\theta_{TRUE}}(C = 1|W = w)$.

$$\begin{aligned} E_{(W,C)\sim f_{\theta_{TRUE}}}[\mathbb{1}_{y_\theta^+(W)\neq C}] &= E_W[E_C[\mathbb{1}_{y_\theta^+(W)\neq C}|W]] \\ &= E_W[P(C = 1|W) \cdot \mathbb{1}_{y_\theta^+(W)\neq 1} + P(C = 0|W) \cdot \mathbb{1}_{y_\theta^+(W)\neq 0}] \\ &= E_W[\eta(W) \cdot \mathbb{1}_{y_\theta^+(W)=0} + (1-\eta(W)) \cdot \mathbb{1}_{y_\theta^+(W)=1}] \\ &\geq E_W[\min\{\eta(W), 1-\eta(W)\}] \\ &= E_W[\eta(W) \cdot \mathbb{1}_{y^*_{\theta_{TRUE}}(W)=0} + (1-\eta(W)) \cdot \mathbb{1}_{y^*_{\theta_{TRUE}}(W)=1}] \\ &= E_{(W,C)\sim f_{\theta_{TRUE}}}[\mathbb{1}_{y^*_{\theta_{TRUE}}(W)\neq C}] \qquad \textit{Bayes error rate} \end{aligned}$$

Bayes optimal classifier

$$\eta(w) = P_{\theta_{TRUE}}(C = 1|W = w)$$

- $\eta()$ is unknown! (unless we are controlling data generation)
- **Plug-in rule:** use $\hat{\eta}(w) = f_\theta(c|w) = P_\theta(C = 1|W = w)$ as an estimate of $\eta(w)$
- Naive Bayes $P(C = c_0|W = w) = P(C = c_0)\prod_i P(W_i = w_i|C = c_0)/P(W = w)$ assuming $P(W = w|C = c_0) = \prod_i P(W_i = w_i|C = c_0)$
  - Naive Bayes estimates $\eta(w)$ from empirical distribution of $x_1, \ldots, x_n$
  - and assuming independence of features
- 1-NN asymptotically converges ($|\theta| \to \infty$) to risk: [**Cover and Hart (1967)**]

$$r \leq E_{(W,C)\sim f_{\theta_{TRUE}}}[\mathbb{1}_{y_\theta^{1\text{-}NN}(W)\neq C}] \leq 2r(1-r) \leq 2r$$

  where r is the Bayes error rate.
- Bayes optimal classifier is optimal also for squared loss
  - Squared loss is convex and differentiable (good for optimization solving)

Loss functions and margin

- Binary classes $C = \{-1, 1\}$, unnormalized scores $s_\theta(w) \in \mathbb{R}$
  - Bayes decision rule becomes: $y^*_\theta = sgn(s_\theta(w))$
- Margin for (w, c) defined as

$$m = c \cdot s_\theta(w)$$

  - Margin > 0 if prediction is correct (i..e, $s_\theta(w) \geq 0$ and $c = 1$, or if $s_\theta(w) < 0$ and $c = -1$)
  - Loss minimization equivalent to margin maximization
- *Margin-based loss*: Loss function $\ell_\theta(c, w)$ that can be written as $\phi(m)$:
  - 0-1 loss: $\phi(m) = \mathbb{1}_{m \leq 0}$
  - Logistic log-loss: $\phi(m) = \log_2(1 + e^{-m})$
  - L_2 loss: $\phi(m) = (1 - m)^2$
  - SVM/Hinge loss: $\phi(m) = \max\{0, 1 - m\}$
  - AdaBoost/Exponential loss: $\phi(m) = e^{-m}$
- Methods for margin maximization exists for a convex margin-based loss
  - that also provide bounds on 0-1 loss
  - that encode regularizations in the margin-based loss

See R script

Reject option in binary classification

$$\eta(w) = P_{\theta_{TRUE}}(C = 1 | W = w)$$

Bayes optimal classifier (or **Bayes rule**):

$$y^*_{\theta_{TRUE}}(w) = \begin{cases} 1 & \text{if } \eta(w) \geq 1/2 \\ 0 & \text{if } \eta(w) < 1/2 \end{cases}$$

- If $\eta(w) \approx 1/2$, we might just as well toss a coin to make a decision
- This motivates the introduction of a reject option for classifiers
  - reject, or abstain, expressing doubt or uncertainty in decisions
  - relevant in practice (e.g., to understand the cases where a classifier performs poorly),
  - relevant ethically for socially sensitive decision tasks (e.g., credit scoring, disease prediction, CV screeening, etc.)

Reject option in binary classification

$$\eta(w) = P_{\theta_{TRUE}}(C = 1 | W = w)$$

Bayes optimal classifier (with reject option):

$$y^{*,d}_{\theta_{TRUE}}(w) = \begin{cases} 1 & \text{if } \eta(w) > 1 - d \\ 0 & \text{if } \eta(w) < d \\ abstain & \text{otherwise, i.e., } d \leq \min\{\eta(w), 1 - \eta(w)\} \end{cases}$$

where $d \in [0, 1/2]$ is the reject cost.

- If $y^{*,d}_{\theta_{TRUE}}(w) \neq abstain$ *[d upper bound on misclassification error]*

$$d > \min\{\eta(w), 1 - \eta(w)\} = P_{\theta_{TRUE}}(y^*_\theta(w) \neq C) \qquad \textit{[error of Bayes optimal]}$$

Theorem (Chow 1970).

$$\arg\min_{y^+_\theta} E_{(W,C)\sim f_{\theta_{TRUE}}}[d\mathbb{1}_{y^+_\theta(W)=abstain} + \mathbb{1}_{y^+_\theta(W)\neq C, y^+_\theta(W)\neq abstain}] = y^{*,d}_{\theta_{TRUE}}$$

Selective binary classification

A *selective binary classifier* (score) is a pair (s_θ, g_θ), where $s_\theta()$ is a classifier (score) and $g_\theta : \mathbb{R}^{|W|} \to \{0,1\}$ is a *selection function*, which determines when to accept/abstain from using s_θ:

$$(s_\theta, g_\theta)(w) = \begin{cases} s_\theta(w) & \text{if } g_\theta(w) = 1 \\ \textit{abstain} & \text{otherwise} \end{cases}$$

Support and Risk

The *coverage* of a selective classifier is $\phi(g_\theta) = E_{(W,C)\sim f_{\theta_{TRUE}}}[g_\theta(W)]$, i.e., the expected probability of the accepted region.
The risk w.r.t. a loss function ℓ_θ is $R(s_\theta, g_\theta) = E_{(W,C)\sim f_{\theta_{TRUE}}}[\ell_\theta(C, W) g_\theta(W)]/\phi(g_\theta)$.

- Empirical coverage and empirical selective risk:

$$\hat{\phi}(g_\theta) = \frac{\sum_{i=1}^n g_\theta(w_i)}{n} \qquad \hat{r}(s_\theta, g_\theta) = \frac{\frac{1}{n}\sum_{i=1}^n \ell_\theta(c_i, w_i) g_\theta(w_i)}{\hat{\phi}(g_\theta)}$$

- *Selective classification problem*: minimize risk while guaranteeing a minimum support c

$$\textit{arg} \min_\theta R(s_\theta, g_\theta) \quad \text{s.t.} \quad \phi(g_\theta) \geq c$$

Soft selective binary classification

A *soft selective binary classifier*:
$$(s_\theta, g_\theta)(w) = \begin{cases} s_\theta(w) & \text{if } k_\theta(w) \geq \tau \\ \textit{abstain} & \text{otherwise} \end{cases}$$

- $k_\theta(w)$ is called the *confidence function*
  - A good confidence function should rank instances based on descending loss, i.e., if $k(w) \leq k(w')$ then $E[\ell_\theta(C, w)] \geq E[\ell_\theta(C, w')]$.
- Confidence of the classifier (see slide 9) and $\tau \in [1/2, 1]$:
$$k_\theta(w) = \max\{s_\theta(w), 1 - s_\theta(w)\}$$
- The inherent trade-off between risk and coverage is summarized by the *risk-coverage curve*