

# No-free-lunch theorem for machine learning

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## Abstract

This entry is a formalization of the no-free-lunch theorem for machine learning following Section 5.1 of the book *Understanding Machine Learning: From Theory to Algorithms* [1] by Shai Shalev-Shwartz and Shai Ben-David. The theorem states that for binary classification prediction tasks, there is no universal learner, meaning that for every learning algorithms, there exists a distribution on which it fails.

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## 1 No-Free-Lunch Theorem for ML

```
theory No-Free-Lunch-ML
imports
  HOL-Probability.Probability
begin
```

### 1.1 Preliminaries

```
lemma sum-le-card-Max-of-nat:finite A
   $\implies \text{sum } f \ A \leq (\text{of-nat} :: - \Rightarrow - :: \{\text{semiring-1}, \text{ordered-comm-monoid-add}\}) (\text{card } A) * \text{Max } (f \text{ ` } A)$ 
  using sum-bounded-above[of A f Max (f ` A)] by simp

lemma card-Min-le-sum-of-nat: finite A
   $\implies (\text{of-nat} :: - \Rightarrow - :: \{\text{semiring-1}, \text{ordered-comm-monoid-add}\}) (\text{card } A) * \text{Min } (f \text{ ` } A) \leq \text{sum } f \ A$ 
  using sum-bounded-below[of A Min (f ` A) f] by simp
```

The following lemma is used to show the last equation of the proof of the no-free-lunch theorem in the book [1].

Let  $A$  be a finite set. If  $A$  is divided into the pairs  $(x_1, y_1), \dots, (x_n, y_n)$  such that  $f(x_i) + f(y_i) = k$  for all  $i = 1, \dots, n$ . Then, we have  $\sum_{x \in A} f(x) = k * |A|/2$ .

```

lemma sum-of-const-pairs:
  fixes  $k :: \text{real}$ 
  assumes  $A:\text{finite } A$ 
    and  $\text{fst} \, ' B \cup \text{snd} \, ' B = A$   $\text{fst} \, ' B \cap \text{snd} \, ' B = \{\}$ 
    and  $\text{inj-on } \text{fst } B \text{ inj-on } \text{snd } B$ 
    and  $\text{sum}: \bigwedge x y. (x,y) \in B \implies f \, x + f \, y = k$ 
  shows  $(\sum_{x \in A}. f \, x) = k * \text{real } (\text{card } A) / 2$ 
  using assms
proof(induction A arbitrary: B rule: finite-psubset-induct)
  case  $\text{ih}:(\text{psubset } A)$ 
  show ?case
  proof(cases A = \{\})
    assume  $A \neq \{\}$ 
    then obtain  $x$  where  $x:x \in A$ 
    by blast
    then obtain  $y$  where  $xy:(x,y) \in B \vee (y,x) \in B$ 
    using  $\text{ih}(3)$  by fastforce
    then have  $xy':x \neq y$ 
    by (metis emptyE fst-eqD ih(4) imageI mem-simps(4) snd-eqD)
    have  $y:y \in A$ 
    using  $\text{ih}(3)$   $xy$  by force
    have  $*$ : $(\sum_{a \in A - \{x,y\}}. f \, a) = k * \text{real } (\text{card } (A - \{x,y\})) / 2$ 
    proof -
      consider  $(x,y) \in B \mid (y,x) \in B$ 
      using  $xy$  by blast
      then show ?thesis
      proof cases
        assume  $xy:(x,y) \in B$ 
        show ?thesis
        proof(intro ih(2))
          have  $*$ : $\text{fst} \, ' (B - \{(x, y)\}) = \text{fst} \, ' B - \{x\}$ 
          by(subst inj-on-image-set-diff[of fst B]) (use ih(5) xy in auto)
          have  $**$ :  $\text{snd} \, ' (B - \{(x, y)\}) = \text{snd} \, ' B - \{y\}$ 
          by(subst inj-on-image-set-diff[of snd B]) (use ih(6) xy in auto)
          have  $x \notin \text{snd} \, ' B$   $y \notin \text{fst} \, ' B$ 
          using  $\text{ih}(4)$   $xy$  by(force simp: disjoint-iff)+
          thus  $\text{fst} \, ' (B - \{(x,y)\}) \cup \text{snd} \, ' (B - \{(x,y)\}) = A - \{x,y\}$ 
          using  $\text{ih}(3)$  by(auto simp: * **)
          qed(use x ih(4) in auto intro!: inj-on-diff ih(5,6,7))
        next
          assume  $xy:(y,x) \in B$ 
          show ?thesis
          proof(intro ih(2))
            have  $*$ : $\text{fst} \, ' (B - \{(y, x)\}) = \text{fst} \, ' B - \{y\}$ 
            by(subst inj-on-image-set-diff[of fst B]) (use ih(5) xy in auto)
            have  $**$ :  $\text{snd} \, ' (B - \{(y, x)\}) = \text{snd} \, ' B - \{x\}$ 

```

```

    by(subst inj-on-image-set-diff[of snd B]) (use ih(6) xy in auto)
  have  $y \notin \text{snd } B \implies x \notin \text{fst } B$ 
    using ih(4) xy by(force simp: disjoint-iff)+
  thus  $\text{fst } (B - \{(y,x)\}) \cup \text{snd } (B - \{(y,x)\}) = A - \{x,y\}$ 
    using ih(3) by(auto simp: ***)
qed(use x ih(4) in auto intro!: inj-on-diff ih(5,6,7))
qed
qed
have  $(\sum_{a \in A} f a) = (\sum_{a \in A - \{x,y\}} f a) + (f x + f y)$ 
  using x y xy' by (simp add: ih(1) sum-diff)
also have  $\dots = k * \text{real } (\text{card } (A - \{x,y\})) / 2 + (f x + f y)$ 
  by(simp add: *)
also have  $\dots = k * \text{real } (\text{card } (A - \{x,y\})) / 2 + k$ 
  using xy ih(7) by fastforce
also have  $\dots = k * \text{real } (\text{card } A) / 2$ 
  using x y xy' by(subst card-Diff-subset)
  (auto simp: of-nat-diff-if card-le-Suc0-iff-eq[OF ih(1)] not-less-eq-eq right-diff-distrib)
finally show ?thesis .
qed simp
qed

```

```

lemma(in prob-space) Markov-inequality-measure-minus:
  assumes  $u \in \text{borel-measurable } M$  and  $\text{AE } x \text{ in } M. 0 \leq u x \text{ AE } x \text{ in } M. 1 \geq u x$ 
    and [arith]:  $0 < (a::\text{real})$ 
  shows  $\mathcal{P}(x \text{ in } M. u x > 1 - a) \geq ((\int x. u x \partial M) - (1 - a)) / a$ 
proof -
  have [measurable,simp]:integrable  $M u$ 
    using assms by(auto intro!: integrable-const-bound[where B=1])
  have  $\text{measure } M \{x \in \text{space } M. u x \leq 1 - a\} = \text{measure } M \{x \in \text{space } M. a \leq 1 - u x\}$ 
  by(rule arg-cong[where f=measure M]) auto
  also have  $\dots \leq (\int x. 1 - u x \partial M) / a$ 
    using assms by(intro integral-Markov-inequality-measure) auto
  finally have  $*:\text{measure } M \{x \in \text{space } M. u x \leq 1 - a\} \leq (\int x. 1 - u x \partial M) / a$  .
  have  $((\int x. u x \partial M) - (1 - a)) / a = 1 - (\int x. 1 - u x \partial M) / a$ 
    by (auto simp : prob-space diff-divide-distrib)
  also have  $\dots \leq 1 - \text{measure } M \{x \in \text{space } M. u x \leq 1 - a\}$ 
    using * by simp
  also have  $\dots = \text{measure } M \{x \in \text{space } M. \neg u x \leq 1 - a\}$ 
    by(intro prob-neg[symmetric]) simp
  also have  $\dots = \text{measure } M \{x \in \text{space } M. u x > 1 - a\}$ 
    by(rule arg-cong[where f=measure M]) auto
  finally show ?thesis .
qed

```

## 1.2 No-Free-Lunch Theorem

In our implementation, a learning algorithm of binary clasification is represented as a function  $A : nat \Rightarrow (nat \Rightarrow 'a \times bool) \Rightarrow 'a \Rightarrow bool$  where the first argument is the number of training data, the second argument is the training data ( $S\ n = (x_n, y_n)$  denotes the  $n$ th data for a training data  $S$ ), and  $A\ m\ S$  is a predictor. The first argument, which denotes the number of training data, is normally used to specify the number of loop executions in learning algorithm. In this formalization, we omit the first argument because we do not need the concrete definitions of learning algorithms.

Let  $X$  be the domain set. In order to analyze the error of predictors, we assume that each data  $(x, y)$  is obtained from a distribution  $\mathcal{D}$  on  $X \times \mathbb{B}$ . The error of a predictor  $f$  with respect to  $\mathcal{D}$  is defined as follows.

$$\begin{aligned}\mathcal{L}_{\mathcal{D}}(f) &\stackrel{\text{def}}{=} \text{P}_{(x,y) \sim \mathcal{D}} (f(x) \neq y) \\ &= \mathcal{D}(\{(x, y) \in X \times \mathbb{B} \mid f(x) \neq y\})\end{aligned}$$

In these settings, the no-free-lunch theorem states that for any learning algorithm  $A$  and  $m < |X|/2$ , there exists a distribution  $\mathcal{D}$  on  $X \times \mathbb{B}$  and a predictor  $f$  such that

- $\mathcal{L}_{\mathcal{D}}(f) = 0$ , and
- $\text{P}_{S \sim \mathcal{D}^m} \left( \mathcal{L}_{\mathcal{D}}(A(S)) > \frac{1}{8} \right) \geq \frac{1}{7}$ .

**theorem** *no-free-lunch-ML:*

**fixes**  $X :: 'a\ \text{measure}$  **and**  $m :: nat$   
**and**  $A :: (nat \Rightarrow 'a \times bool) \Rightarrow 'a \Rightarrow bool$   
**assumes**  $X1:finite\ (space\ X) \implies 2 * m < card\ (space\ X)$   
**and**  $X2[measurable]: \bigwedge x. x \in space\ X \implies \{x\} \in sets\ X$   
**and**  $m[arith]: 0 < m$   
**and**  $A[measurable]: (\lambda(s,x). A\ s\ x) \in (PiM\ \{..<m\}\ (\lambda i. X \otimes_M count\ space\ (UNIV :: bool\ set)))) \otimes_M X$   
 $\rightarrow_M count\ space\ (UNIV :: bool\ set)$   
**shows**  $\exists \mathcal{D} :: ('a \times bool)\ \text{measure. sets}\ \mathcal{D} = sets\ (X \otimes_M count\ space\ (UNIV :: bool\ set)) \wedge$   
 $prob\ space\ \mathcal{D} \wedge$   
 $(\exists f. f \in X \rightarrow_M count\ space\ (UNIV :: bool\ set) \wedge \mathcal{P}((x, y) \text{ in } \mathcal{D}. f\ x \neq y) = 0) \wedge$   
 $\mathcal{P}(s \text{ in } PiM\ \{..<m\}\ (\lambda i. \mathcal{D}). \mathcal{P}((x, y) \text{ in } \mathcal{D}. A\ s\ x \neq y) > 1 / 8) \geq 1 / 7$   
**proof** –  
**let**  $?B = count\ space\ (UNIV :: bool\ set)$   
**let**  $?B' = UNIV :: bool\ set$   
**let**  $?L = \lambda D\ f. \mathcal{P}((x, y) \text{ in } D. f\ x = (\neg y))$

**have**  $XB[\text{measurable}]$ :  $xy \in \text{space } (X \otimes_M ?B) \implies \{xy\} \in \text{sets } (X \otimes_M ?B)$   
**for**  $xy$   
**by** (*auto simp: space-pair-measure sets-Pair*)  
**have**  $\text{space } X \neq \{\}$   
**using**  $X1$  **by** *force*  
**have**  $\exists C \subseteq \text{space } X. \text{finite } C \wedge \text{card } C = 2 * m$   
**by** (*meson X1 infinite-arbitrarily-large obtain-subset-with-card-n order-less-le*)  
**then obtain**  $C$  **where**  $C: C \subseteq \text{space } X \text{ finite } C \text{ card } C = 2 * m$   
**by** *blast*  
**have**  $C\text{-ne}: C \neq \{\}$   
**using**  $C$  *assms* **by** *force*  
**have**  $C\text{-sets}[\text{measurable}]: C \in \text{sets } X$   
**using**  $C$  **by** (*auto intro!: sets.countable[OF X2 countable-finite]*)  
**have**  $\text{meas}[\text{measurable}]: \{(x, y). (x, y) \in \text{space } (X \otimes_M ?B) \wedge g\ x = (\neg y)\} \in$   
 $\text{sets } (X \otimes_M ?B)$   
**if**  $g[\text{measurable}]: g \in X \rightarrow_M ?B$  **for**  $g$   
**proof** –  
**have**  $\{(x, y). (x, y) \in \text{space } (X \otimes_M ?B) \wedge g\ x = (\neg y)\}$   
 $= (g - \{ \text{True} \} \cap \text{space } X) \times \{ \text{False} \} \cup (g - \{ \text{False} \} \cap \text{space } X) \times$   
 $\{ \text{True} \}$   
**by** (*auto simp: space-pair-measure*)  
**also have**  $\dots \in \text{sets } (X \otimes_M ?B)$   
**by** *simp*  
**finally show**  $?thesis$  .  
**qed**

**define**  $fn$  **where**  $fn \equiv \text{from-nat-into } (C \rightarrow_E (UNIV :: \text{bool set}))$   
**define**  $Dn$  **where**  $Dn \equiv (\lambda n. \text{measure-of } (\text{space } (X \otimes_M ?B)) (\text{sets } (X \otimes_M ?B)))$   
 $(\lambda U. \text{real } (\text{card } ((\text{SIGMA } x:C. \{fn\ n\ x\}) \cap U)) /$   
 $\text{real } (\text{card } C)))$

**have**  $fn\text{-}PiE: n < \text{card } (C \rightarrow_E ?B') \implies fn\ n \in C \rightarrow_E ?B'$  **for**  $n$   
**by** (*simp add: PiE-eq-empty-iff fn-def from-nat-into*)  
**have**  $ex\text{-}n: f \in C \rightarrow_E ?B' \implies \exists n < \text{card } (C \rightarrow_E ?B'). f = fn\ n$  **for**  $f$   
**using** *bij-betw-from-nat-into-finite[OF finite-PiE[OF C(2), of  $\lambda i. ?B'$ ]]*  
**by** (*auto simp: bij-betw-def fn-def*)  
**have**  $fn\text{-}inj: n < \text{card } (C \rightarrow_E ?B') \implies n' < \text{card } (C \rightarrow_E ?B') \implies (\bigwedge x. x \in C$   
 $\implies fn\ n\ x = fn\ n'\ x) \implies n = n'$  **for**  $n\ n'$   
**using** *bij-betw-from-nat-into-finite[OF finite-PiE[OF C(2), of  $\lambda i. ?B'$ ]] PiE-ext[OF fn-PiE[of  $n$ ] fn-PiE[of  $n'$ ]]*  
**by** (*auto simp: bij-betw-def fn-def inj-on-def*)

**have**  $fn\text{-}meas[\text{measurable}]: fn\ n \in X \rightarrow_M ?B$  **for**  $n$   
**proof** –  
**have**  $\text{countable } (C \rightarrow_E (UNIV :: \text{bool set}))$   
**using**  $C$  **by** (*auto intro!: countable-PiE*)  
**hence**  $fn\ n \in C \rightarrow_E (UNIV :: \text{bool set})$   
**by** (*simp add: PiE-eq-empty-iff fn-def from-nat-into*)

```

hence fn n = (λx. if x ∈ C then fn n x else undefined)
  by auto
also have ... ∈ X →M ?B
proof(subst measurable-restrict-space-iff[symmetric])
  have sets (restrict-space X C) = Pow C
  using X2 C by(intro sets-eq-countable) (auto simp: countable-finite sets-restrict-space-iff)
  thus fn n ∈ restrict-space X C →M ?B
    by (simp add: Measurable.pred-def assms(1))
qed auto
finally show ?thesis .
qed

have sets-Dn[measurable-cong]: ∧n. sets (Dn n) = sets (X ⊗M ?B)
  and space-Dn: ∧n. space (Dn n) = space (X ⊗M ?B)
  by(simp-all add: Dn-def)
have emeasure-Dn: emeasure (Dn n) U = ennreal (real (card ((SIGMA x:C. {fn
n x}) ∩ U)) / real (card C))
  (is - = ennreal (?μ U))
  if U[measurable]: U ∈ X ⊗M ?B for U n
proof(rule emeasure-measure-of[where Ω=space (X ⊗M ?B) and A=sets (X
⊗M ?B)])
  let ?μ' = λU. ennreal (?μ U)
  show countably-additive (sets (Dn n)) ?μ'
    unfolding countably-additive-def
  proof safe
    fix Ui :: nat ⇒ - set
    assume Ui: range Ui ⊆ sets (Dn n) disjoint-family Ui
    have fin: finite {i. (SIGMA x:C. {fn n x}) ∩ Ui i ≠ {}} (is finite ?I)
    proof(rule ccontr)
      assume infinite {i. (SIGMA x:C. {fn n x}) ∩ Ui i ≠ {}}
      with Ui(2)
      have infinite (⋃ ((λi. (SIGMA x:C. {fn n x}) ∩ Ui i) ‘ {i. (SIGMA x:C.
{fn n x}) ∩ Ui i ≠ {}}))
        (is infinite ?U)
      by(intro infinite-disjoint-family-imp-infinite-UNION) (auto simp: dis-
joint-family-on-def)
      moreover have ?U ⊆ (SIGMA x:C. {fn n x})
        by blast
      ultimately have infinite (SIGMA x:C. {fn n x})
        by fastforce
      with C(2) show False
        by blast
    qed
  hence sum: summable (λi. ?μ (Ui i))
    by(intro summable-finite[where N={i. (SIGMA x:C. {fn n x}) ∩ Ui i ≠
{}}]) auto
  have (∑ i. ?μ' (Ui i)) = ennreal (∑ i. ?μ (Ui i))
    by(intro sum suminf-ennreal2) auto
  also have ... = (∑ i∈?I. ?μ (Ui i))

```

```

    by(subst suminf-finite[OF fn]) auto
  also have ... = ?μ' (⋃ (range Ui))
  proof -
    have *: (∑ i ∈ ?I. real (card ((SIGMA x:C. {fn n x}) ∩ Ui i))) = real
      (∑ i ∈ ?I. (card ((SIGMA x:C. {fn n x}) ∩ Ui i)))
    by simp
    also have ... = real (card (⋃ ((λ i. (SIGMA x:C. {fn n x}) ∩ Ui i) ' ?I)))
    using C Ui fn unfolding disjoint-family-on-def
    by(subst card-UN-disjoint) blast+
    also have ... = real (card ((SIGMA x:C. {fn n x}) ∩ ⋃ (range Ui)))
    by(rule arg-cong[where f=λx. real (card x)]) blast
    finally show ?thesis
    by(simp add: sum-divide-distrib[symmetric])
  qed
  finally show (∑ i. ?μ' (Ui i)) = ?μ' (⋃ (range Ui)) .
  qed
  qed(auto simp: Dn-def positive-def intro!:sets.sets-into-space)
  interpret Dn: prob-space Dn n for n
  proof
    have [simp]: (SIGMA x:C. {fn n x}) ∩ space (X ⊗M ?B) = (SIGMA x:C.
      {fn n x})
    using measurable-space[OF fn-meas] C(1) space-pair-measure by blast
    show emeasure (Dn n) (space (Dn n)) = 1
    using C-ne C by(simp add: emeasure-Dn space-Dn)
  qed
  interpret fp: finite-product-prob-space λi. Dn n {..M ?B for U n
  using emeasure-Dn[OF U] by(simp add: Dn.emeasure-eq-measure)
  have measure-Dn': measure (Dn n) U = (∑ x ∈ C. of_bool ((x, fn n x) ∈ U)) /
    real (card C)
  if U[measurable]: U ∈ X ⊗M ?B for U n
  proof -
    have *: (SIGMA x:C. {fn n x}) ∩ U = (SIGMA x:C. {y. y = fn n x ∧ (x, y)
      ∈ U})
    by blast
    have (x, fn n x) ∈ U ⟹ {y. y = fn n x ∧ (x, y) ∈ U} = {fn n x}
    and (x, fn n x) ∉ U ⟹ {y. y = fn n x ∧ (x, y) ∈ U} = {} for x
    by blast+
    hence **: real (card {y. y = fn n x ∧ (x, y) ∈ U}) = of_bool ((x, fn n x) ∈ U)
  for x
  by auto
  show ?thesis
  by(auto simp: measure-Dn * card-SigmaI[OF C(2)])
  qed

  let ?LossA = λn s. ?L (Dn n) (A s)

```

**have**  $[measurable]: (\lambda s. ?LossA\ n\ s) \in \text{borel-measurable } (PiM\ \{..<m\})\ (\lambda i. X \otimes_M ?B))$  **for**  $n$   
**by**  $measurable\ (auto\ simp\ add: space-Dn)$   
**have**  $Dn\text{-}fn\text{-}0: \mathcal{P}((x, y) \text{ in } Dn\ n. fn\ n\ x \neq y) = 0$  **for**  $n$   
**proof** –  
**have**  $(SIGMA\ x:C. \{fn\ n\ x\}) \cap \{(x, y). (x, y) \in space\ (X \otimes_M count\text{-}space\ UNIV) \wedge fn\ n\ x = (\neg y)\} = \{\}$   
**by**  $auto$   
**thus**  $?thesis$   
**by**  $(simp\ add: measure\text{-}Dn\ space\text{-}Dn)$   
**qed**

**have**  $[measurable]: (SIGMA\ x:C. \{fn\ n\ x\}) \in sets\ (X \otimes_M count\text{-}space\ UNIV)$   
**for**  $n$   
**by**  $(rule\ sets.countable)\ (use\ C\ \text{in}\ auto\ intro!: sets\text{-}Pair\ X2\ C(1)\ countable\text{-}finite)$   
**have**  $integ[simp]: integrable\ (PiM\ \{..<m\})\ (\lambda i. Dn\ n))\ (\lambda s. ?LossA\ n\ s)$  **for**  $n$   
**by**  $(auto\ intro!: fp.P.integrable\text{-}const\text{-}bound[\text{where } B=1])$

**have**  $[measurable]: \{xn\} \in sets\ (PiM\ \{..<m\})\ (\lambda i. X \otimes_M ?B))$   
**and**  $fp\text{-}prob: fp.prob\ n\ \{xn\} = 1 / \text{real } (card\ C) ^ m$   
**if**  $h: xn \in \{..<m\} \rightarrow_E (SIGMA\ x:C. \{fn\ n\ x\})$  **for**  $xn\ n$   
**proof** –  
**have**  $[simp]: i < m \implies xn\ i \in space\ (X \otimes_M ?B)$  **for**  $i$   
**using**  $h\ C(1)$  **by**  $(fastforce\ simp: PiE\text{-}def\ space\text{-}pair\text{-}measure\ Pi\text{-}def)$   
**have**  $*: \{xn\} = (\Pi_E\ i \in \{..<m\}. \{xn\ i\})$   
**proof**  $safe$   
**show**  $\bigwedge x. x \in (\Pi_E\ i \in \{..<m\}. \{xn\ i\}) \implies x = xn$   
**by**  $standard\ (metis\ PiE\text{-}E\ singletonD\ h)$   
**qed**  $(use\ h\ \text{in}\ auto)$   
**also** **have**  $\dots \in sets\ (PiM\ \{..<m\})\ (\lambda i. X \otimes_M ?B))$   
**by**  $measurable$   
**finally** **show**  $\{xn\} \in sets\ (PiM\ \{..<m\})\ (\lambda i. X \otimes_M ?B))$  .  
**have**  $fp.prob\ n\ (\Pi_E\ i \in \{..<m\}. \{xn\ i\}) = (\prod i < m. Dn.prob\ n\ \{xn\ i\})$   
**using**  $h$  **by**  $(intro\ fp.finite\text{-}measure\text{-}PiM\text{-}emb)\ simp$   
**also** **have**  $\dots = (1 / \text{real } (card\ C) ^ m)$   
**proof** –  
**have**  $\bigwedge i. i < m \implies ((SIGMA\ x:C. \{fn\ n\ x\}) \cap \{xn\ i\}) = \{xn\ i\}$   
**using**  $h$  **by**  $blast$   
**thus**  $?thesis$   
**by**  $(simp\ add: measure\text{-}Dn\ power\text{-}one\text{-}over)$   
**qed**  
**finally** **show**  $fp.prob\ n\ \{xn\} = 1 / \text{real } (card\ C) ^ m$   
**using**  $*$  **by**  $simp$   
**qed**

**have**  $exp\text{-}eq: (\int s. ?LossA\ n\ s\ \partial(PiM\ \{..<m\})\ (\lambda i. Dn\ n))) = (\sum s \in \{..<m\} \rightarrow_E C. ?LossA\ n\ (\lambda i \in \{..<m\}. (s\ i, fn\ n\ (s\ i)))) / \text{real } (card\ C) ^ m$  **for**  $n$   
**proof** –



**have**  $(\int s. ?LossA\ n\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n)))$   
 $= (\int s. ?LossA\ n\ s * indicat-real\ (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s$   
 $+ ?LossA\ n\ s * indicat-real\ (space\ (PiM\ \{..<m\}\ (\lambda i. Dn\ n)) - (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n)))$   
**by**(*auto intro!:* *Bochner-Integration.integral-cong simp: indicator-def*)  
**also have**  $... = (\int s. ?LossA\ n\ s * indicat-real\ (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n)))$   
 $+ (\int s. ?LossA\ n\ s * indicat-real\ (space\ (PiM\ \{..<m\}\ (\lambda i. Dn\ n)) - (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n)))$   
**by**(*rule Bochner-Integration.integral-add*)  
 $(auto\ intro!:\ fp.P.integrable-const-bound[where\ B=1]\ simp: mult-le-one)$   
**also have**  $... = (\int s. ?LossA\ n\ s * indicat-real\ (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n)))$   
**proof**  $-$   
**have**  $*(\int s. ?LossA\ n\ s * indicat-real\ (space\ (PiM\ \{..<m\}\ (\lambda i. Dn\ n)) - (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n))) \geq 0$   
**by** *simp*  
**have**  $(\int s. ?LossA\ n\ s * indicat-real\ (space\ (PiM\ \{..<m\}\ (\lambda i. Dn\ n)) - (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n)))$   
 $\leq (\int s. indicat-real\ (space\ (PiM\ \{..<m\}\ (\lambda i. Dn\ n)) - (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\}))))\ s\ \partial(PiM\ \{..<m\}\ (\lambda i. Dn\ n)))$   
**by**(*intro integral-mono*) (*auto intro!:* *fp.P.integrable-const-bound[where B=1] simp: mult-le-one indicator-def*)  
**also have**  $... = 1 - fp.prob\ n\ (PiE\ \{..<m\}\ (\lambda i. (SIGMA\ x:C. \{fn\ n\ x\})))$   
**by**(*simp add: fp.P.prob-compl*)  
**also have**  $... = 0$   
**using** *C* **by**(*simp add: fp.finite-measure-PiM-emb measure-Dn*)  
**finally show** *?thesis*  
**using**  $*$  **by** *simp*  
**qed**  
**also have**  $... = (\sum s \in \{..<m\} \rightarrow_E (SIGMA\ x:C. \{fn\ n\ x\}). ?LossA\ n\ s * fp.prob\ n\ \{s\})$   
**using** *C* **by**(*auto intro!:* *integral-indicator-finite-real finite-PiE le-neq-trans*)  
**also have**  $... = (\sum s \in \{..<m\} \rightarrow_E (SIGMA\ x:C. \{fn\ n\ x\}). ?LossA\ n\ s) / real\ (card\ C) ^ m$   
**by**(*simp add: fp-prob sum-divide-distrib*)  
**also have**  $... = (\sum s \in \{..<m\} \rightarrow_E C. ?LossA\ n\ (\lambda i \in \{..<m\}. (s\ i, fn\ n\ (s\ i)))) / real\ (card\ C) ^ m$   
**proof**  $-$   
**have**  $*(\{..<m\} \rightarrow_E (SIGMA\ x:C. \{fn\ n\ x\}) = (\lambda s. \lambda i \in \{..<m\}. (s\ i, fn\ n\ (s\ i)))) '(\{..<m\} \rightarrow_E C)$   
**unfolding** *set-eq-iff*  
**proof** *safe*  
**show**  $s \in \{..<m\} \rightarrow_E (SIGMA\ x:C. \{fn\ n\ x\}) \implies s \in (\lambda s. \lambda i \in \{..<m\}. (s\ i, fn\ n\ (s\ i))) '(\{..<m\} \rightarrow_E C)$  **for**  $s$   
**by**(*intro rev-image-eqI[where b=s and x=λi∈{..<m}. fst (s i)] (force simp: PiE-def Pi-def extensional-def)+*)  
**qed** *auto*

```

have **:inj-on ( $\lambda s. \lambda i \in \{..<m\}. (s\ i, fn\ n\ (s\ i))$ ) ( $\{..<m\} \rightarrow_E C$ )
by(intro inj-onI) (metis (mono-tags, lifting) PiE-ext prod.simps(1) re-
strict-apply1)
show ?thesis
by(subst sum.reindex[where  $A = \{..<m\} \rightarrow_E C$  and  $h = \lambda s. \lambda i \in \{..<m\}. (s\ i, fn\ n\ (s\ i))$ ],simplified,symmetric])
(use * ** in auto)
qed
finally show ?thesis .
qed

```

```

have eqL: ?L (Dn n) h = ( $\sum x \in C. of\_bool\ (h\ x = (\neg\ fn\ n\ x))$ ) / real (card C) if
h[measurable]: h  $\in X \rightarrow_M ?B$  for n h
proof -
have ?L (Dn n) h = ( $\sum x \in C. of\_bool\ ((x, fn\ n\ x) \in space\ (X \otimes_M ?B) \wedge h\ x = (\neg\ fn\ n\ x))$ ) / real (card C)
by(simp add: space-Dn measure-Dn1)
also have ... = ( $\sum x \in C. of\_bool\ (h\ x = (\neg\ fn\ n\ x))$ ) / real (card C)
using C by(auto simp: space-pair-measure Collect-conj-eq Int-assoc[symmetric])
finally show ?thesis .
qed

```

```

have nz1[arith]: real (card (C  $\rightarrow_E ?B'$ )) > 0 real (card C) > 0 0 < real (card
( $\{..<m\} \rightarrow_E C$ ))
using C(2) C-ne by(simp-all add: card-funcsetE card-gt-0-iff)

```

```

have ne:finite (( $\lambda n. fp.expectation\ n$ 
( $\lambda s. Dn.prob\ n\ \{(x, y). (x, y) \in space\ (Dn\ n) \wedge A\ s\ x = (\neg\ y)\}$ )) '
 $\{..<card\ (C \rightarrow_E ?B')\}$ )
( $\lambda n. fp.expectation\ n$ 
( $\lambda s. Dn.prob\ n\ \{(x, y). (x, y) \in space\ (Dn\ n) \wedge A\ s\ x = (\neg\ y)\}$ )) '
 $\{..<card\ (C \rightarrow_E ?B')\}$ )  $\neq \{\}$  (is ?ne)
proof -
have 0 < card (C  $\rightarrow_E ?B'$ )
using C-ne C(2) by(auto simp: card-gt-0-iff finite-PiE)
thus ?ne
by blast
qed simp

```

```

have max-geq-q:( $MAX\ n \in \{..<card\ (C \rightarrow_E ?B')\}. (\int s. ?LossA\ n\ s\ \partial(PiM\ \{..<m\} (\lambda i. Dn\ n)))) \geq 1 / 4$  (is -  $\leq ?Max$ )
proof -

```

```

have (MIN  $s \in \{..<m\} \rightarrow_E C. (\sum n < card\ (C \rightarrow_E ?B'). ?LossA\ n\ (\lambda i \in \{..<m\}. (s\ i, fn\ n\ (s\ i))))$ ) / real (card (C  $\rightarrow_E ?B'$ ))
 $\leq ?Max$  (is ?Min1  $\leq -$ )
proof -
have ?Min1

```

```

≤ (∑ s∈{.. $m$ } →E C.
  (∑ n<card (C →E ?B').
    ?LossA n (λi∈{.. $m$ }. (s i, fn n (s i)))) / real (card (C →E
?B')) / real (card ({.. $m$ } →E C))
proof(subst pos-le-divide-eq)
  show ?Min1 * real (card ({.. $m$ } →E C))
    ≤ (∑ s∈{.. $m$ } →E C. (∑ n<card (C →E ?B'). ?LossA n (λi∈{.. $m$ }.
(s i, fn n (s i)))) / real (card (C →E ?B'))
  using C by(simp add: mult.commute) (auto intro!: finite-PiE card-Min-le-sum-of-nat)
qed fact
also have ...
  = (∑ s∈{.. $m$ } →E C.
    (∑ n<card (C →E ?B').
      ?LossA n (λi∈{.. $m$ }. (s i, fn n (s i)))) / real (card (C →E
?B')) / real (card C) ^ m
  by(simp add: card-PiE)
also have ...
  = (∑ n<card (C →E ?B').
    (∑ s∈{.. $m$ } →E C.
      ?LossA n (λi∈{.. $m$ }. (s i, fn n (s i)))) / real (card C) ^ m) /
real (card (C →E ?B'))
  unfolding sum-divide-distrib[symmetric] by(subst sum.swap) simp
also have ... ≤ ?Max
proof -
  have real (card (C →E ?B')) * ?Max
    = real (card (C →E ?B'))
      * (MAX n∈{.. $m$ }. (∑ s∈{.. $m$ } →E C. ?LossA n
(λi∈{.. $m$ }. (s i, fn n (s i)))) / real (card C) ^ m)
  by (simp add: exp-eq)
  also have ... ≥ (∑ n<card (C →E ?B'). (∑ s∈{.. $m$ } →E C. ?LossA n
(λi∈{.. $m$ }. (s i, fn n (s i)))) / real (card C) ^ m)
  using sum-le-card-Max-of-nat[of {.. $m$ }. (C →E ?B')] finite-PiE[OF
C(2)] by auto
  finally show ?thesis
    by(subst pos-divide-le-eq) (simp, argo)
qed
finally show ?thesis .
qed

```

```

have 1 / 4 ≤ ?Min1
proof(safe intro!: Min-ge-iff[THEN iffD2])
  fix s
  assume s: s ∈ {.. $m$ } →E C
  hence [measurable]: (λi∈{.. $m$ }. (s i, fn n (s i))) ∈ space (PiM {.. $m$ } (λi.
X ⊗M ?B)) for n
  using C by(auto simp: space-PiM space-pair-measure)
  let ?V = C - (s ‘ {.. $m$ })
  have fin-V:finite ?V

```

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    using C by blast
  have cardV: card ?V ≥ m
proof -
  have card (s ' {.. $m$ }) ≤ m
    by (metis card-image-le card-lessThan finite-lessThan)
  hence m ≤ card C - card (s ' {.. $m$ })
    using C(3) by simp
  also have card C - card (s ' {.. $m$ }) ≤ card ?V
    by (rule diff-card-le-card-Diff) simp
  finally show ?thesis .
qed
hence V-ne: ?V ≠ {} card ?V > 0
  using m by force+
have (1 / 2) * (1 / 2)
  = (1 / 2)
  * (MIN v ∈ ?V. (∑ n < card (C →E ?B'). of-bool (A (λi ∈ {.. $m$ }. (s i, fn
n (s i))) v = (¬ fn n v))) / real (card (C →E ?B'))))
proof (rule arg-cong[where f=(*) (1 / 2)])
  have (∑ n < card (C →E ?B'). of-bool (A (λi ∈ {.. $m$ }. (s i, fn n (s i))) v
= (¬ fn n v))) / real (card (C →E ?B')) = 1 / 2
    if v: v ∈ ?V for v
  proof -
    define B where B ≡ {(n, n') | n n'. n < card (C →E ?B') ∧ fn n v =
False ∧ n' < card (C →E ?B')
    ∧ fn n' v = True ∧ (∀ x ∈ C - {v}. fn n x =
fn n' x)}
    have B1: fst ' B ∪ snd ' B = {.. $\text{card } (C \rightarrow_E ?B')$ }
    proof -
      have n ∈ fst ' B ∪ snd ' B if n: n < card (C →E ?B') for n
      proof (cases fn n v = True)
        assume h: fn n v = True
        let ?fn' = λx. if x = v then False else fn n x
        have fn': ∧ x. x ≠ v ⇒ fn n x = ?fn' x ?fn' v = False
          by auto
        hence fn'1: ?fn' ∈ C →E ?B'
          using fn-PiE[OF n] v by auto
        then obtain n' where n': n' < card (C →E ?B') fn n' = ?fn'
          using ex-n by (metis (lifting))
        hence (n', n) ∈ B
          using n' fn'1 fn-PiE[OF n] n h fn' by (auto simp: B-def)
        thus ?thesis
          by force
      next
        assume h: fn n v ≠ True
        let ?fn' = λx. if x = v then True else fn n x
        have fn': ∧ x. x ≠ v ⇒ fn n x = ?fn' x ?fn' v = True
          by auto
        hence fn'1: ?fn' ∈ C →E ?B'
          using fn-PiE[OF n] v by auto

```

then obtain  $n'$  where  $n': n' < \text{card } (C \rightarrow_E ?B')$   $\text{fn } n' = ?\text{fn}'$   
 using  $\text{ex-}n$  by  $(\text{metis } (\text{lifting}))$   
 hence  $(n, n') \in B$   
 using  $n' \text{ fn}' 1 \text{ fn-PiE}[OF \ n] \ n \ h \ \text{fn}'$  by  $(\text{auto simp: } B\text{-def})$   
 thus  $?thesis$   
 by force  
 qed  
 moreover have  $\bigwedge n. n \in \text{fst } 'B \cup \text{snd } 'B \implies n < \text{card } (C \rightarrow_E ?B')$   
 by  $(\text{auto simp: } B\text{-def})$   
 ultimately show  $?thesis$   
 by blast  
 qed  
 have  $B2: \text{fst } 'B \cap \text{snd } 'B = \{\}$   
 by  $(\text{auto simp: } B\text{-def})$   
 have  $B3: \text{inj-on } \text{fst } B$   
 by  $(\text{auto intro!: } \text{fn-inj } \text{inj-onI } \text{simp: } B\text{-def})$   
 have  $B4: \text{inj-on } \text{snd } B$   
 by  $(\text{fastforce intro!: } \text{fn-inj } \text{inj-onI } \text{simp: } B\text{-def})$   
 have  $B5: \text{of-bool } (A \ (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v$   
 $= (\neg \text{fn } n \ v) + \text{of-bool } (A \ (\lambda i \in \{..<m\}. (s \ i, \text{fn } n' \ (s \ i)))) \ v = (\neg$   
 $\text{fn } n' \ v)) = (1 :: \text{real})$   
 if  $nn': (n, n') \in B$  for  $n \ n'$   
 proof -  
 have  $(\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i))) = (\lambda i \in \{..<m\}. (s \ i, \text{fn } n' \ (s \ i)))$   
 by  $\text{standard } (\text{use } s \ nn' \ v \ \text{in } \text{auto simp: } B\text{-def})$   
 thus  $?thesis$   
 using  $nn'$  by  $(\text{auto simp: } B\text{-def})$   
 qed  
 have  $(\sum n < \text{card } (C \rightarrow_E ?B'). \text{of-bool } (A \ (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v$   
 $= (\neg \text{fn } n \ v)))$   
 $= 1 * \text{real } (\text{card } \{..<\text{card } (C \rightarrow_E ?B')\}) / 2$   
 by  $(\text{intro sum-of-const-pairs}[\text{where } B=B] \ B1 \ B2 \ B3 \ B4 \ B5) \ \text{simp}$   
 thus  $?thesis$   
 by  $\text{simp}$   
 qed  
 thus  $1 / 2 = (\text{MIN } v \in ?V. (\sum n < \text{card } (C \rightarrow_E ?B'). \text{of-bool } (A \ (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v = (\neg \text{fn } n \ v))) / \text{real } (\text{card } (C \rightarrow_E ?B'))$   
 by  $(\text{metis } (\text{mono-tags, lifting}) \ V\text{-ne}(1) \ \text{fin-}V \ \text{obtains-MIN})$   
 qed  
 also have ...  
 $\leq (1 / 2)$   
 $* ((\sum v \in ?V. (\sum n < \text{card } (C \rightarrow_E ?B'). \text{of-bool } (A \ (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v = (\neg \text{fn } n \ v)))$   
 $/ \text{real } (\text{card } (C \rightarrow_E ?B'))$   
 $/ \text{real } (\text{card } ?V))$   
 using  $V\text{-ne}$  by  $(\text{intro mult-le-cancel-left-pos}[\text{THEN } \text{iffD2}] \ \text{pos-le-divide-eq}[\text{THEN } \text{iffD2}])$   
 $(\text{simp-all add: Groups.mult-ac}(2) \ \text{card-Min-le-sum-of-nat fin-}V)$   
 also have ...

$$= (\sum n < \text{card } (C \rightarrow_E ?B')). ((\sum v \in ?V. \text{ of\_bool } (A (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v = (\neg \text{fn } n \ v)))$$

$$/ (2 * \text{real } (\text{card } ?V))) / \text{real } (\text{card } (C \rightarrow_E ?B'))$$
**unfolding** *sum-divide-distrib[symmetric]* **by** (*subst sum.swap*) *simp*  
**also have** ...  $\leq (\sum n < \text{card } (C \rightarrow_E ?B')). ?\text{LossA } n (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i))) / \text{real } (\text{card } (C \rightarrow_E ?B'))$   
**proof** (*safe intro!: sum-mono divide-right-mono*)  
**fix** *n*  
**have**  $(\sum v \in ?V. \text{ of\_bool } (A (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v = (\neg \text{fn } n \ v))$   

$$/ (2 * \text{real } (\text{card } ?V))$$

$$\leq (\sum v \in ?V. \text{ of\_bool } (A (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v = (\neg \text{fn } n \ v))$$

$$/ \text{real } (\text{card } C)$$
**using** *cardV* **by** (*auto simp: C(3) intro!: divide-left-mono sum-nonneg*)  
**also have** ...  $\leq (\sum x \in C. \text{ of\_bool } (A (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ x = (\neg \text{fn } n \ x)) / \text{real } (\text{card } C)$   
**using** *C* **by** (*intro sum-mono2 divide-right-mono*) *auto*  
**also have** ...  $= ?\text{LossA } n (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))$   
**by** (*simp add: eqL*)  
**finally show**  $(\sum v \in ?V. \text{ of\_bool } (A (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) \ v = (\neg \text{fn } n \ v)) / (2 * \text{real } (\text{card } ?V))$   

$$\leq ?\text{LossA } n (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i))) .$$
**qed** *simp*  
**finally show**  $1 / 4 \leq (\sum n < \text{card } (C \rightarrow_E ?B'). ?\text{LossA } n (\lambda i \in \{..<m\}. (s \ i, \text{fn } n \ (s \ i)))) / \text{real } (\text{card } (C \rightarrow_E ?B'))$   
**by** (*simp add: sum-divide-distrib*)  
**qed** (*use m C in auto intro!: finite-PiE simp: PiE-eq-empty-iff*)  
**also have** ...  $\leq ?\text{Max}$   
**by** *fact*  
**finally show** *?thesis* .  
**qed**

**hence**  $\exists n. n < \text{card } (C \rightarrow_E ?B') \wedge (\int s. ?\text{LossA } n \ s \ \partial(\text{PiM } \{..<m\} (\lambda i. Dn \ n))) \geq 1 / 4$   
**using** *Max-ge-iff[OF ne]* **by** *blast*  
**then obtain** *n* **where**  $n : n < \text{card } (C \rightarrow_E ?B') (\int s. ?\text{LossA } n \ s \ \partial(\text{PiM } \{..<m\} (\lambda i. Dn \ n))) \geq 1 / 4$   
**by** *blast*

**have**  $1 / 7 \leq ((\int s. ?\text{LossA } n \ s \ \partial(\text{PiM } \{..<m\} (\lambda i. Dn \ n))) - (1 - 7 / 8)) / (7 / 8)$   
**using** *n* **by** *argo*  
**also have** ...  $\leq \mathcal{P}(s \text{ in } \text{Pi}_M \{..<m\} (\lambda i. Dn \ n). \mathcal{P}((x, y) \text{ in } Dn \ n. A \ s \ x = (\neg y))) > 1 - 7 / 8$   
**by** (*intro fp.Markov-inequality-measure-minus*) *auto*  
**also have** ...  $= \mathcal{P}(s \text{ in } \text{Pi}_M \{..<m\} (\lambda i. Dn \ n). \mathcal{P}((x, y) \text{ in } Dn \ n. A \ s \ x = (\neg y))) > 1 / 8$   
**by** *simp*  
**finally have**  $1 / 7 \leq \mathcal{P}(s \text{ in } \text{Pi}_M \{..<m\} (\lambda i. Dn \ n). \mathcal{P}((x, y) \text{ in } Dn \ n. A \ s \ x = (\neg y))) > 1 / 8$  .

```

thus ?thesis
  using Dn-fn-0[of n]
  by(auto intro!: exI[where x=Dn n] exI[where x=fn n] simp: sets-Dn Dn.prob-space-axioms)
qed

end

```

## References

- [1] S. Shalev-Shwartz and S. Ben-David. *Understanding Machine Learning: From Theory to Algorithms*. Cambridge University Press, 2014.