# An Introduction to Information Theory with Applications to Machine Learning

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#### Outline

- Motivating Information Entropy
  - lacksquare  $\alpha$ -weighted coins
  - Binary Trees
  - Encoding Coin Flips
  - Information Entropy
  - Computing Information Entropy
  - An Alternative Characterization
  - Ideas of Information Theory
  - Ideas of Information Theory
  - Ideas of Information Theory
- 2 Applications To Machine Learning
  - A Proof of the Comparison-Based Sorting Lower Bound
  - Entropy Decision Trees
  - Cross-Entropy as a Cost Function
  - Kernel Principle Component Analysis



#### $\alpha$ -weighted coins

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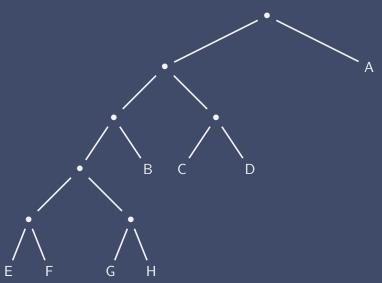
- Let  $lpha \in \mathbb{R}$  be a real paramater with  $0 \leq lpha \leq 1$
- We define an  $\alpha$ -weighted coin, or simply an  $\alpha$ -coin, to be a coin which lands heads (H) with probability  $\alpha$  and tails (T) with probability  $1-\alpha$
- We want to encode the result of this coin toss as information

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- a binary tree is a recursive graph-like data structure with parent nodes and leaves. Each parent node contains two children, starting with one node known as the root, and each leaf contains no children but a value

```
def __init__(self, is_leaf, left, right, val):
    if is_leaf:
        self.is_leaf = True
        self.left_child = None
        self.right_child = None
        self.val = val
        self.is_leaf = False
        self.left_child = left
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- "Normal" binary trees in most of CS (such as BSTs), can contain a value at all nodes, not just leaves. Why isn't that true for encoding binary information?
- Because to read that as an encoding, the encoder has to recognize at the end of the encoding string that it has ended. Thus, implicitly, saying some string has ended adds an extra termination bit of information at the end.

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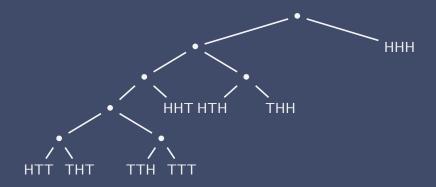
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- Maybe if you toss the coin once, T is not avoidable since  $\varepsilon$  is not neglible, but say you toss the coin 10 times.
- $\varepsilon^{10}$  will be pretty well negligible, so there ought to be at least effectively one less outcome (TTTTTTTTTT) than in the case of  $\alpha = \frac{1}{2}$ , when all strings are equally likely.

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- Thus, we might expect that we can somehow do better encoding 10 coin tosses than 1 coin toss.

Let's imagine encoding the result of 3 .9-coin flips in a binary tree, such that we minimize the expected length of the message.



Result	Encoding	Length	Probability	%
HHH	1	1	(.9)(.9)(.9)	72.9%
HHT	001	3	(.9)(.9)(.1)	8.1%
HTH	010	3	(.9)(.1)(.9)	8.1%
THH	011	3	(.1)(.9)(.9)	8.1%
HTT	00000	5	(.9)(.1)(.1)	0.9%
THT	00001	5	(.1)(.9)(.1)	0.9%
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So our expected length is (.729)(1) + (3)(.081)(3) + (3)(.009)(5) + (.001)(5) =**1.598** 

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Thus, there's not really a full bit of information in tossing a coin with  $\alpha=.9$ 

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- Somewhat miraculously, we have that the best average length approaches an actual limit.

#### Theorem (Shannon's Source Coding Theorem, Bernoulli Trial)

Let  $\mathbb{T}_n$  denote the set of all binary trees with  $2^n$  leaves, let  $C_n \in \{H, T\}^n$  be a random variable, the result of n iid  $\alpha$ -coin tosses, and let  $\operatorname{len}_{\tau}(C_n)$  for a binary tree  $\tau \in \mathbb{T}_n$  denote the length of encoding  $C_n$  within the binary tree  $\tau$ . Then

$$\lim_{n\to\infty} \min_{\tau\in\mathbb{T}_n} \frac{\mathbb{E}[\mathsf{len}_\tau(C_n)]}{n} = H$$

for some real constant  $H \ge 0$ 

*Proof.* The minimum expected length is monotone decreasing and bounded below by 0, the result follows trivially from the monotone convergence theorem

■ This limit *H* is called the *information entropy* of the coin toss, in units of bits (or Shannons).

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- We're going to consider a slightly less rigorous derivation.

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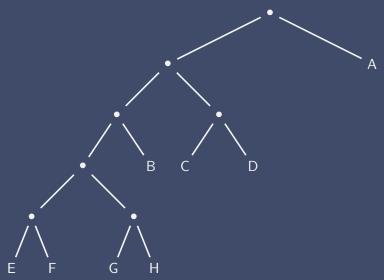
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- Besides the fact this length isn't technically defined, we also haven't shown that we can generate binary trees that create average lengths (pointwise) convergent, to some set of averages.
- Surely not any set of lengths will do. Which ones will?



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- There an infinite number of such invariant you could define based on the constant of proportionality, but the simplest is to sum simply 2<sup>-(depth)</sup> And considering the simplest binary tree, one with just a single node of depth zero, this sum may be one.

#### Theorem (Kraft-McMillan Inequality, Full Binary Trees)

Some tuple of number  $(\ell_1, \ell_2, \dots, \ell_n)$  can form the depth of nodes on some valid binary tree  $\tau$  if and only if

$$\sum_{k=1}^{n} 2^{-\ell_k} = 1$$

Proof (Necessity). We use strong induction on the maximum depth. The sum is invariant under bifurcation, so if we "combine" a pair of leaves into a lead of depth 1 lower, that leaves the sum unchanged. Do that for all nodes of maximum depth, and the depth is reduced. The base case is the trivial tree which clearly holds.

*Proof (Sufficiency).* Simply consider the binary tree that always has children up to some fixed maximum depth, larger than the maximum of  $\{\ell_k | k \in \mathbb{Z} \cap [1,n]\}$ . Then simply keep going left up to depth  $\ell_1$ , then go left as much as you can, only stopping if you already reach a terminal leaf to go right. This process will yield such a tree. (Exercise: prove it rigorously).

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- Consider average depths  $\ell_H$  and  $\ell_T$  that are suitable for binary trees (in the sense of satisfying Kraft's inequality).
- ullet Find the minimum average length among all such  $\ell_H$  and  $\ell_T$

Thus we have

$$H = \min_{(\ell_H, \ell_T) \in \{(\ell_H, \ell_T) \mid 2^{-\ell_H} + 2^{-\ell_T} = 1\}} (\alpha \ell_H + (1 - \alpha)\ell_T)$$

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 Thus our problem is reduced to the 1-dimensional minimization problem

$$\min_{\ell_H} \left( lpha \ell_H - (1 - lpha) \log_2 \left( 1 - 2^{-\ell_H} 
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■ We can do this with some elementary calculus

$$\begin{split} &\frac{\mathsf{d}}{\mathsf{d}\ell_H} \left(\alpha\ell_H - (1-\alpha)\log_2\left(1-2^{-\ell_H}\right)\right) \\ &= \alpha - (1-\alpha)\frac{\mathsf{d}}{\mathsf{d}\ell_H}\log_2\left(1-2^{-\ell_H}\right) \\ &= \alpha - \frac{1-\alpha}{2^{\ell_H}-1} \end{split}$$

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Setting this equal to 0 we get

$$\ell_H = -\log_2(\alpha)$$

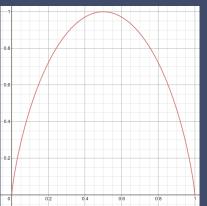
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- But in fact, it is easy to adapt this method to any random variable with a finite image (set of possible values it could take).
- Simply assign all values the RV could take with an average length, so that all the lengths satisfy Kraft's inequality, and then find the minimum expected length over all such values.

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We can solve this problem using the method of lagrange multipliers.



We define the Lagrangian function

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Setting that equal to zero gives

$$\ell_k = -\log_2\left(\frac{-p_k}{\lambda \ln(2)}\right)$$

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It follows that the optimizer is given simply by

$$\ell_k = -\log_2(p_k)$$

# Computing Information Entropy

Thus, we have that the information entropy of a random variable taking values  $x_1, x_2, \ldots, x_n$  with probabilities  $p_1, p_2, \ldots, p_n$  is simply

$$H = -\sum_{k=1}^{n} p_k \log_2(p_k)$$

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- So, now that we have this pinned down a bit, it's nice to have an alternative characterization of information entropy that is
  - 1 Easier to prove formally
  - 2 Coincident with our above result

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- The idea is quite intuitive. For simplicity, we again begin with the simple case of the  $\alpha$ -coin.
- In particular, consider the result of  $\ell$  iid  $\alpha$ -coin tosses. There are  $2^n$  possible strings, but many of those are very unlikely.
- Let's consider ℓ large, and think about asymptotically how many of these strings are possible?

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- By the strong law of large numbers (say), we know that we need to consider strings that have roughly  $\alpha\ell$  heads, those are the ones with non-negligible likelihood
- We can compute the number of those, with binomial coefficients.

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$$\binom{\ell}{h} = \frac{\ell!}{h!(\ell-h)!}$$

It follows pretty simply that our entropy ought to be asymptotically the number of bits needed to encompass all of the states with a number of heads equal to the mean as a ratio of  $\ell$ .

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We can use *Stirling's Approximation*, an asymptotic result about the factorial.

$$n! \sim \sqrt{2\pi n} \left(\frac{n}{\epsilon}\right)^n$$

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$$= \lim_{\ell \to \infty} \frac{\log_2\left(\frac{\sqrt{2\pi\ell\ell}e^{-\ell}}{\left(\sqrt{2\pi\alpha\ell}(\alpha\ell)^{\alpha\ell}e^{-\alpha\ell}\right)\left(\sqrt{2\pi(1-\alpha)\ell}((1-\alpha)\ell)^{(1-\alpha)\ell}e^{-(1-\alpha)\ell}\right)}\right)}{\ell}$$

$$= \lim_{\ell \to \infty} \frac{\log_2\left(\frac{1}{\sqrt{2\pi\alpha(1-\alpha)\ell}\alpha^{\alpha\ell}(1-\alpha)^{(1-\alpha)\ell}}\right)}{\ell}$$

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where 
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Imagine a random variable taking values  $x_1, x_2, ..., x_n$  with probabilities  $\alpha_1, \alpha_2, ..., \alpha_n$ . By the same logic

$$H = \lim_{\ell \to \infty} \frac{1}{\ell} \left( \log_2 \left( \binom{\ell}{\alpha_1 \ell, \alpha_2 \ell, \dots, \alpha_n \ell} \right) \right) \right)$$

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$$\begin{split} H &= \lim_{\ell \to \infty} \frac{1}{\ell} \left( \log_2 \left( \left( \frac{\ell}{\alpha_1 \ell, \alpha_2 \ell, \dots, \alpha_n \ell} \right) \right) \right) \\ &= \lim_{\ell \to \infty} \frac{1}{\ell} \log_2 \left( \frac{\ell!}{\prod_{k=1}^n (\alpha_k \ell)!} \right) \\ &= \lim_{\ell \to \infty} \frac{1}{\ell} \log_2 \left( \frac{\sqrt{2\pi \ell} \ell^\ell e^{-\ell}}{\prod_{k=1}^n \sqrt{2\pi \alpha_k \ell} (\alpha_k \ell)^{\alpha_k \ell} e^{-\alpha_k \ell}} \right) \end{split}$$

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 $\max_{1 \le k \le n} H(X_k) \le H(X_1, X_2, \dots, X_n) \le \sum_{k=1}^{n} H(X_k)$ 



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Gibb's inequality

$$H(P,Q) \geq H(P,P)$$

Yes, the notation is terrible

Mutual Information I(X; Y) = H(X) - H(X|Y). The amount of information Y carries on X.

- Mutual Information I(X; Y) = H(X) H(X|Y). The amount of information Y carries on X.
- Differential Entropy

$$H(x) = -\int_{\mathcal{X}} p(x) \log_2(p(x)) dx$$

### A Proof of the Comparison-Based Sorting Lower Bound

- Imagine a permutation  $\sigma$  chose uniformly at random from  $\mathcal{S}_{n}$ .
- A comparison-based sort makes Q queries of random variables C checking  $\sigma(i_1) < \sigma(i_2)$ , and  $H(C_1) = 1$
- lacksquare The entropy of  $\sigma$  is easily seen to be  $\log_2(n!)$
- lacksquare The joint entropy  $H(\sigma, \mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_Q) \geq H(\sigma) = \log_2(n!)$
- By the chain rule

$$H(\sigma, C_1, C_2, ..., C_Q) = H(\sigma | C_1, C_2, ..., C_Q)$$
  
  $+ H(C_Q | C_1, C_2, ..., C_{Q-1})$   
  $+ \cdots + H(C_1)$ 

Hence

$$H(\sigma, C_1, C_2, \ldots, C_Q) \ge \log_2(n!) - Q$$

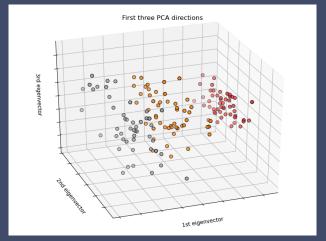


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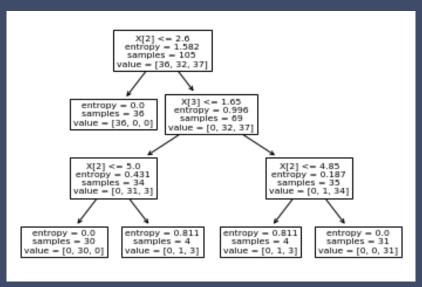
- Very old method in Machine Learning.
  - The idea: split data-set in half recursively in some meaningful way.
- How to determine this splitting? So that the information entropy of the children is minimized!

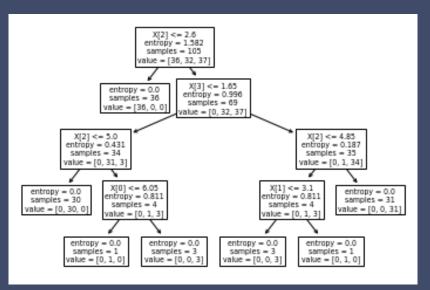
Iris dataset. Flower data.

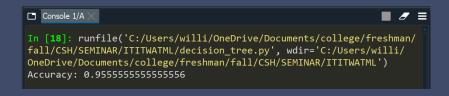


```
from sklearn.datasets import load iris
 2 from sklearn import tree
   from sklearn import metrics
    from sklearn.model selection import train test split
 7 X, y = load iris(return X y=True)
 8 \(\times X\) train, \(X\) test, \(y\) train, \(y\) test = train_test_split(\(X\), \(y\),
                                                           test size=0.3,
                                                           random state=1)
12 clf = tree.DecisionTreeClassifier(criterion="entropy", max depth=2)
13 clf = clf.fit(X train, y train)
   v pred = clf.predict(X test)
16 print("Accuracy:",metrics.accuracy score(y test, y pred))
17 tree.plot tree(clf)
```

```
X[3] \le 0.8
           entropy = 1.582
           samples = 105
         value = [36, 32, 37]
                       X[3] \le 1.65
 entropy = 0.0
                     entropy = 0.996
 samples = 36
                       samples = 69
value = [36, 0, 0]
                    value = [0, 32, 37]
           entropy = 0.431
                                entropy = 0.187
            samples = 34
                                 samples = 35
          value = [0, 31, 3]
                               value = [0, 1, 34]
```







Suppose we are attempting binary classification, with a logistic model

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$$-\sum_{k=1}^{N} y_k \log(p(x_k)) + (1-y_k) \log(1-p(x_k))$$

This is a result called logistic regression.

```
■ decision_tree.py*
   1 from sklearn.datasets import load iris
   2 from sklearn.linear model import LogisticRegression
   3 from sklearn.metrics import classification report
   4 from sklearn import metrics
     from sklearn.model selection import train test split
   8 X, y = load iris(return X y=True)
          y[i] = 1 if y[i] == 2 else 0
  13 ▼X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                           test size=0.3,
                                                           random state=17)
  17 mod = LogisticRegression()
      mod.fit(X train, y train)
     v pred = mod.predict(X test)
      print("Accuracy:",metrics.accuracy_score(y_test, y_pred))
      print(classification report(y test, y pred))
  23
```

```
In [29]: runfile('C:/Users/willi/OneDrive/Documents/college/freshman/
fall/CSH/SEMINAR/ITITWATML/decision tree.py', wdir='C:/Users/willi/
OneDrive/Documents/college/freshman/fall/CSH/SEMINAR/ITITWATML')
Accuracy: 0.977777777777777
             precision
                          recall f1-score support
                  0.97
                            1.00
                                      0.98
                  1.00
                            0.93
                                      0.96
                                                  14
                                      0.98
                                                  45
   accuracy
                                      0.97
   macro avg
                  0.98
                            0.96
weighted avg
                  0.98
                            0.98
                                      0.98
                                                  45
```

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- http://citeseerx.ist.psu.edu/ viewdoc/download?doi=10.1.1. 381.288rep=rep1type=pdf