

Mutual Information of Dependent Random Variables

1 Probability Theory

In this section we give a quick recap of some important ideas from probability theory. We will be focusing on the discrete case.

1.1 Events and Random Variables

The first important point is to distinguish between an *event* in some sample space Ω and a *random variable* $X : \Omega \rightarrow \mathbb{R}$ which assigns real values to outcomes.

Let Ω denote the sample space of all possible outcomes of an experiment. An **event** is any subset of Ω . It represents a collection of outcomes about which we are interested.

For example, consider tossing a fair coin twice. The sample space is

$$\Omega = \{HH, HT, TH, TT\}.$$

The event $A = \{\text{exactly one head}\} = \{HT, TH\}$ is a subset of Ω . Since the coins are both fair, the probability of this event is:

$$P(A) = P(\{HT, TH\}) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}.$$

A **random variable** X is a function

$$X : \Omega \rightarrow \mathbb{R}$$

that assigns a numerical value to each outcome in the sample space. When we write $X = x$, we are referring to the *event* consisting of all outcomes $\omega \in \Omega$ for which $X(\omega) = x$:

$$\{\omega \in \Omega : X(\omega) = x\}.$$

For example, let $X = \# \text{heads in two tosses}$. Then

$$X(HH) = 2, \quad X(HT) = 1, \quad X(TH) = 1, \quad X(TT) = 0.$$

The statement $X = 1$ corresponds to the event

$$\{\omega \in \Omega : X(\omega) = 1\} = \{HT, TH\},$$

which is exactly the same event as A in the previous example. Thus, a random variable taking on a particular value is just a special kind of event.

We may use the notation:

$$P_X(1) = \frac{1}{2}$$

To summarize: An **event** is a subset of the sample space, representing outcomes of interest. A **random variable taking a value** defines an event consisting of all outcomes that map to that value.

1.2 Conditional Probability, Independence and Bayes Theorem

The **conditional probability** of A given B is defined as:

$$P(A | B) = \frac{P(A \cap B)}{P(B)}, \quad \text{for } P(B) > 0.$$

Equivalently,

$$P(B | A) = \frac{P(A \cap B)}{P(A)}, \quad \text{for } P(A) > 0.$$

Setting the two different expressions for $P(A \cap B)$ equal to each other in the above equations gives us **Bayes' theorem**:

$$P(A | B) = \frac{P(B | A) P(A)}{P(B)}, \quad \text{for } P(B) > 0$$

For random variables X and Y the notation for conditional probability looks like:

$$P_{X|Y}(x | y) = \frac{P_{X,Y}(x, y)}{P_Y(y)}, \quad P_Y(y) > 0.$$

In this case, $X = x$ and $Y = y$ are themselves events in Ω , and $P_{X|Y}(x | y)$ measures the probability that X takes value x given that Y takes value y .

In this notation Bayes' theorem looks like:

$$P_{X|Y}(x | y) = \frac{P_{Y|X}(y | x) P_X(x)}{P_Y(y)}$$

Two **events** A and B are *independent* if:

$$P(A \cap B) = P(A) P(B)$$

Otherwise, for dependent events, we have:

$$P(A \cap B) = P(A) P(B | A) = P(B) P(A | B)$$

Equivalently, A and B are independent if knowing one tells you nothing about the other:

$$P(B) = P(B | A) \quad \text{or equivalently} \quad P(A) = P(A | B)$$

1.3 Example of Dependent Events

Consider rolling two fair six-sided dice.

Define the events:

$$A = \{\text{sum of the dice is even}\}, \quad B = \{\text{sum of the dice is greater than 7}\}$$

There are 36 equally likely outcomes. The probabilities are calculated as follows:

- $P(A) = \frac{18}{36} = 0.5$
- $P(B) = \frac{15}{36} \approx 0.4167$
- $P(A \cap B) = \frac{9}{36} = 0.25$.

To check for independence, we compute the product:

$$P(A)P(B) = 0.5 \cdot \frac{15}{36} \approx 0.2083$$

Since $0.25 \neq 0.2083$, $P(A \cap B) \neq P(A)P(B)$, and the events A and B are **dependent**.

The conditional probability $P(A | B) = \frac{P(A \cap B)}{P(B)} = \frac{0.25}{0.4167} \approx 0.6$.

Since $P(A | B) > P(A)$, knowing that the sum is greater than 7 increases the probability that the sum is even, confirming dependence.

1.4 Another Example of Dependent Events

Define the events:

$$C = \{\text{at least one die shows 6}\}, \quad D = \{\text{sum of the dice is greater than 10}\}$$

The probabilities are:

- $P(C) = \frac{11}{36} \approx 0.3056$
- $P(D) = \frac{3}{36} \approx 0.0833$
- $P(C \cap D) = \frac{3}{36} \approx 0.0833$.

To check for independence, we compare $P(C \cap D)$ with $P(C)P(D)$:

$$P(C)P(D) = \frac{11}{36} \cdot \frac{3}{36} = \frac{33}{1296} \approx 0.0254$$

Since $0.0833 \neq 0.0254$, $P(C \cap D) \neq P(C)P(D)$, and the events C and D are **dependent**.

The conditional probability $P(D \mid C) = \frac{P(C \cap D)}{P(C)} = \frac{0.0833}{0.3056} \approx 0.2727$.

Since $P(D \mid C) > P(D)$, knowing that one die is a 6 significantly increases the probability of a sum greater than 10, demonstrating dependence.

2 Coin Tossing Experiment

We toss a fair coin **twice**. The four possible **elementary outcomes** (or *events*) are:

- **HH**: heads then heads
- **HT**: heads then tails
- **TH**: tails then heads
- **TT**: tails then tails

Each occurs with probability $\frac{1}{4}$, since the coin is fair and tosses are independent. From these raw outcomes, we define two **random variables**—that is, numerical summaries:

- Let X be the difference between the number of heads and tails:

$$X = (\text{\#heads}) - (\text{\#tails})$$

So:

- HH $\rightarrow X = 2 - 0 = +2$
- HT or TH $\rightarrow X = 1 - 1 = 0$
- TT $\rightarrow X = 0 - 2 = -2$
- Let Y indicate whether the two tosses **match**:

$$Y = \begin{cases} +1 & \text{if both tosses are the same (HH or TT)} \\ -1 & \text{if they differ (HT or TH)} \end{cases}$$

It is important not to confuse the *outcomes* and the *random variables*. The **underlying events** are HH, HT, TH, TT, the **random variables** X and Y assign numbers to the underlying events in such a way that multiple events can lead to the same (X, Y) pair.

Event	X	Y	Probability
HH	+2	+1	1/4
HT	0	-1	1/4
TH	0	-1	1/4
TT	-2	+1	1/4

Notice that **HT and TH both give** $(X = 0, Y = -1)$, so their probabilities add:

- $P(X = 0, Y = -1) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$
- $P(X = +2, Y = +1) = \frac{1}{4}$
- $P(X = -2, Y = +1) = \frac{1}{4}$

All other (x, y) pairs have probability 0.

We can now build the **joint probability distribution** $P_{X,Y}(x, y) = \mathbb{P}(X = x \text{ and } Y = y)$. After grouping outcomes that lead to the same (X, Y) pair, the joint probability distribution of the random variables is:

X	Y	$P(X, Y)$
+2	+1	1/4
0	-1	1/2
-2	+1	1/4

This will be useful later for calculating the conditional entropy later on.

Entropy

Information Content of a Single Outcome

For a random variable X with possible outcome x and probability $P_X(x)$, the **information content** (or *self-information*) of observing x is defined as:

$$I(x) = -\log_2 P_X(x)$$

Intuitively:

- Rare events (small $P_X(x)$) are more **surprising** and carry more information.
- Common events (large $P_X(x)$) are less surprising and carry less information.

Example 1: Fair Coin

A fair coin has:

$$P(\text{Heads}) = P(\text{Tails}) = 1/2$$

$$I(\text{Heads}) = I(\text{Tails}) = -\log_2(1/2) = 1 \text{ bit}$$

Each flip of a fair coin provides 1 bit of information on average.

Example 2: Biased Coin

Consider a biased coin with:

$$P(\text{Heads}) = 0.9, \quad P(\text{Tails}) = 0.1$$

Information content of each outcome:

$$I(\text{Heads}) = -\log_2 0.9 \approx 0.152 \text{ bits}, \quad I(\text{Tails}) = -\log_2 0.1 \approx 3.32 \text{ bits}$$

Observing **Heads** is unsurprising and carries very little information, while observing **Tails** is rare and highly informative.

Entropy: Average Information

The **entropy** of a random variable X measures the **average information content** over all outcomes:

$$H(X) = \mathbb{E}[I(X)] = - \sum_x P_X(x) \log_2 P_X(x)$$

Entropy quantifies the *expected surprise* or *uncertainty* before observing the outcome.

Fair Coin

$$H(X) = - \left(\frac{1}{2} \log_2 \frac{1}{2} + \frac{1}{2} \log_2 \frac{1}{2} \right) = 1 \text{ bit}$$

Biased Coin

$$H(X) = - (0.9 \log_2 0.9 + 0.1 \log_2 0.1) \approx 0.61 \text{ bits}$$

Because the biased coin outcome is more predictable, each flip provides less information on average than a fair coin.

Summary

- **Information** measures the surprise of a single outcome.
- **Entropy** measures the **average information** across all outcomes.
- High entropy = outcomes are uncertain (fair coin).
- Low entropy = outcomes are predictable (biased coin).

Additivity

Because of the logarithm, entropy is additive. If X and Y are independent then:

$$H(X, Y) = H(X) + H(Y)$$

The unit of entropy is the **bit**.

If we flip n independent fair coins X_1, X_2, \dots, X_n , the total entropy is additive:

$$H(X_1, X_2, \dots, X_n) = H(X_1) + H(X_2) + \dots + H(X_n) = n \text{ bits.}$$

Intuitively, additivity works because independent variables carry *separate, non-overlapping information*. If the variables are **not independent**, knowing one gives partial information about the other, so the joint entropy is less than the sum:

$$H(X, Y) < H(X) + H(Y) \quad \text{if } X \text{ and } Y \text{ are dependent.}$$

We will see concrete examples of this later.

Back to our example, for X , which takes values $-2, 0, +2$ with probabilities $\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$, we compute:

$$\begin{aligned} H(X) &= - \sum_x P_X(x) \log_2 P_X(x) \\ &= - \left[\frac{1}{4} \log_2 \frac{1}{4} + \frac{1}{2} \log_2 \frac{1}{2} + \frac{1}{4} \log_2 \frac{1}{4} \right] \\ &= - \left[\frac{1}{4}(-2) + \frac{1}{2}(-1) + \frac{1}{4}(-2) \right] = -[-1.5] = 1.5 \end{aligned}$$

So $H(X) = \frac{3}{2}$ **bits**.

Now let's calculate the entropy of Y

Y can take either of the values $+1$ or -1 , each with probability $\frac{1}{2}$, so:

$$H(Y) = - \left[\frac{1}{2} \log_2 \frac{1}{2} + \frac{1}{2} \log_2 \frac{1}{2} \right] = 1 \text{ bit}$$

Knowing nothing, it takes 1 bit to describe whether the tosses matched.

Conditional Entropy $H(X | Y)$

We are now working with **non-independent** random variables. Suppose we **first learn the value of Y** . How much uncertainty about X remains?

First, we define the **conditional entropy for a specific value of Y** :

$$H(X | Y = y) = - \sum_x P_{X|Y}(x | y) \log_2 P_{X|Y}(x | y),$$

where the **conditional probability** is

$$P_{X|Y}(x | y) = \frac{P_{X,Y}(x, y)}{P_Y(y)}, \quad \text{for } P_Y(y) > 0.$$

In words:

The conditional probability $P_{X|Y}(x | y)$ gives the probability that $X = x$ given that $Y = y$. It is computed by dividing the joint probability $P_{X,Y}(x, y)$ by the marginal probability $P_Y(y)$.

The **conditional entropy of X given Y** is then the *average* of $H(X | Y = y)$ over all possible values of Y , weighted by their probabilities:

$$H(X | Y) = \sum_y P_Y(y) H(X | Y = y).$$

This expresses that the conditional entropy is the **average remaining uncertainty about X** once we know Y .

We are working now with non-independent random variables. Suppose we **first learn the value of Y** . How much uncertainty about X remains?

Let us first define:

$$H(X | Y = y) = - \sum_x P_{X|Y}(x | y) \log_2 P_{X|Y}(x | y)$$

where:

$$P_{X|Y}(x | y) = \frac{P_{X,Y}(x, y)}{P_Y(y)}, \quad \text{for } P_Y(y) > 0$$

The conditional probability $P_{X|Y}(x | y)$ is the probability that $X = x$ given that $Y = y$.

We now have the definition:

$$H(X | Y) = \sum_y P_Y(y) \cdot H(X | Y = y)$$

This says that the conditional entropy is the average uncertainty remaining about X once we know Y averaged over all possible values that Y can take, weighted by their probabilities.”

When $Y = +1$ (tosses match \rightarrow HH or TT):

- This happens with probability $P_Y(+1) = \frac{1}{2}$
- Given this, $X = +2$ (HH) or $X = -2$ (TT), each with conditional probability:

$$P(X = +2 | Y = +1) = \frac{P(X = +2, Y = +1)}{P_Y(+1)} = \frac{1/4}{1/2} = \frac{1}{2}$$

(same for $X = -2$)

- So the conditional entropy is:

$$H(X | Y = +1) = - \left[\frac{1}{2} \log_2 \frac{1}{2} + \frac{1}{2} \log_2 \frac{1}{2} \right] = 1 \text{ bit}$$

When $Y = -1$ (tosses differ \rightarrow HT or TH):

- Probability $P_Y(-1) = \frac{1}{2}$

- Both HT and TH give $X = 0$, so:

$$P(X = 0 \mid Y = -1) = 1$$

- Thus:

$$H(X \mid Y = -1) = -[1 \cdot \log_2 1] = 0 \text{ bits}$$

Average over Y :

$$H(X \mid Y) = \frac{1}{2} \cdot 1 + \frac{1}{2} \cdot 0 = \frac{1}{2} \text{ bit}$$

On average, once we know whether the tosses matched, we only need **half a bit more** to pin down X .

Step 4 Mutual Information $I(X; Y)$

Mutual information answers: “How many bits of uncertainty about X are **removed** by knowing Y ?” Or equivalently: “How much do X and Y tell us about each other?”

Mathematically:

$$I(X; Y) = H(X) - H(X \mid Y)$$

Plugging in:

$$I(X; Y) = \frac{3}{2} - \frac{1}{2} = 1 \text{ bit}$$

We can **verify this another way**: check $H(Y \mid X)$.

- If $X = 0 \rightarrow$ must be HT or TH $\rightarrow Y = -1$ for sure
- If $X = +2 \rightarrow$ must be HH $\rightarrow Y = +1$
- If $X = -2 \rightarrow$ must be TT $\rightarrow Y = +1$

So **knowing X tells us Y exactly** $\rightarrow H(Y \mid X) = 0$

Thus:

$$I(X; Y) = H(Y) - H(Y \mid X) = 1 - 0 = 1 \text{ bit}$$

Both ways agree.

Interpretation: X and Y share **1 bit of information**. In fact, Y is a **function of X** (you can compute matching status from the head–tail difference), so all of Y ’s information is contained in X . But X has extra detail (sign of the difference) that Y doesn’t capture—which is why $H(X) > H(Y)$.

Final Results

Quantity	Value
$H(X)$	1.5 bits
$H(Y)$	1 bit
$H(X Y)$	0.5 bits
$H(Y X)$	0 bits
$I(X; Y)$	1 bit

Key Takeaway

Even though we started with **four equally likely physical outcomes** (HH, HT, TH, TT), the random variables X and Y **compress** this information in different ways.

- X distinguishes **three cases** ($++$, $+-/-+$, $-$)
- Y distinguishes **two cases** (same vs. different) Their **mutual information** quantifies exactly how much these summaries overlap—and in this case, **all of Y 's content is inside X** , but not vice versa.

This is the power of information theory: it lets us **measure shared knowledge** between any two descriptions of the same experiment—whether they're numbers, categories, or even words.

💡 What Is Conditional Entropy?

Conditional entropy $H(X | Y)$ quantifies the **average remaining uncertainty** in a random variable X after the value of another random variable Y has been observed. In other words, it answers:

“If I know Y , how much don't I still know about X —on average?”

It is always true that $H(X | Y) \leq H(X)$, with equality if and only if X and Y are statistically independent.

🔑 Joint Probability

Before defining conditional entropy, we need the **joint probability distribution** of X and Y :

$$P_{X,Y}(x, y) = \mathbb{P}(X = x \text{ and } Y = y)$$

This is the probability that **both** X takes the value x **and** Y takes the value y in the same trial of the experiment. The joint distribution fully describes how X and Y behave together.

From it, we obtain the **marginal distributions** by summing out the other variable:

$$P_X(x) = \sum_y P_{X,Y}(x, y), \quad P_Y(y) = \sum_x P_{X,Y}(x, y)$$

🔧 for Conditional Entropy

All three formulas below compute the **same quantity**—they are just different ways of writing the same idea.

1. Average of Conditional Entropies (Conceptual Form)

$$H(X | Y) = \sum_y P_Y(y) H(X | Y = y)$$

- Here, $H(X | Y = y)$ is the entropy of X **in the scenario where** $Y = y$ **is known**.
- This form emphasizes that conditional entropy is an **expectation over the possible values of** Y .

2. Expanded with Conditional Probabilities

$$H(X | Y) = - \sum_y P_Y(y) \sum_x P_{X|Y}(x | y) \log_2 P_{X|Y}(x | y)$$

- The **conditional probability** is defined (when $P_Y(y) > 0$) as:

$$P_{X|Y}(x | y) = \frac{P_{X,Y}(x, y)}{P_Y(y)}$$

- This expression simply substitutes the definition of entropy into the average from Form 1.
- It highlights that for each fixed y , we compute the entropy of the **conditional distribution** $P_{X|Y}(\cdot | y)$.

3. Joint-Probability Form (Computational Form)

$$H(X | Y) = - \sum_x \sum_y P_{X,Y}(x, y) \log_2 \left(\frac{P_{X,Y}(x, y)}{P_Y(y)} \right)$$

- This version uses **only the joint distribution** $P_{X,Y}(x, y)$ and the marginal $P_Y(y)$ —no explicit reference to conditional probabilities is needed in the notation.
- It is obtained by replacing $P_Y(y)P_{X|Y}(x | y)$ with $P_{X,Y}(x, y)$ in Form 2.
- This is often the most convenient form when working from a joint probability table or empirical data.



- **Form 1** tells you *what conditional entropy means*: an average of uncertainties.
- **Form 2** shows *how it's built*: using conditional probability distributions.
- **Form 3** shows *how to compute it*: directly from joint and marginal probabilities.

All three are mathematically identical and interchangeable—choose the one that best fits your context: understanding, derivation, or calculation.

Remember: Conditional entropy measures **residual uncertainty**, not shared information. The shared information is captured by **mutual information**:

$$I(X; Y) = H(X) - H(X | Y)$$

Mutual Information and Bayes' Theorem: Information Gain from Bayesian Updating

Mutual information and Bayes' theorem are deeply connected:

- **Bayes' theorem** tells you how to update a *single prior* $P(X)$ to a *posterior* $P(X | Y = y)$ after observing a specific outcome $Y = y$.
- **Mutual information** $I(X; Y)$ tells you the *expected reduction in uncertainty* about X *on average* over all possible outcomes y , weighted by their likelihood.

In short:

Mutual information = Expected information gain from Bayesian updating.

Formal Connection

1. Bayes' Theorem and Information Gain for a Single Observation

Given a prior distribution $P(X)$, observing $Y = y$ yields the posterior via Bayes' rule:

$$P(X | Y = y) = \frac{P(Y = y | X) P(X)}{P(Y = y)}.$$

The **information gained** from this observation is measured by the Kullback–Leibler (KL) divergence from the prior to the posterior:

$$D_{\text{KL}}(P(X | Y = y) \| P(X)) = \sum_x P(x | y) \log_2 \frac{P(x | y)}{P(x)}.$$

This quantifies how much the belief about X changed due to seeing $Y = y$.

2. Mutual Information as Expected KL Divergence

Mutual information is the expectation of this KL divergence over all possible outcomes y :

$$I(X; Y) = \mathbb{E}_Y [D_{\text{KL}}(P(X | Y) \| P(X))] = \sum_y P(y) \sum_x P(x | y) \log_2 \frac{P(x | y)}{P(x)}.$$

Using $P(x, y) = P(x | y)P(y)$, this is algebraically equivalent to the standard definition:

$$I(X; Y) = \sum_{x, y} P(x, y) \log_2 \left(\frac{P(x, y)}{P(x)P(y)} \right).$$

Thus, mutual information is precisely the **average information gain** from applying Bayes' rule.

Interpretation

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- **KL divergence** $D_{\text{KL}}(P(X|y) || P(X))$:
 “How many extra bits would I waste if I encoded X using the prior instead of the correct posterior?”
 -! This is the *information gained* from observing $Y = y$.
- **Mutual information** $I(X; Y)$:
 “On average, how many bits do I gain about X per observation of Y ?”
 -! This is the *expected information gain* from Bayesian updating.

Concrete Dice Example: Connecting Bayes + Mutual Information

Recall the setup:

- Roll two fair dice: D_1, D_2 .
- Let $X = D_1$ (first die), $Y = D_1 + D_2$ (sum).
- Prior: $P(X = x) = \frac{1}{6}$ for $x = 1, \dots, 6$.

Bayesian Updating for Specific Observations

1. Observe $Y = 2$:

Only possible if $D_1 = 1, D_2 = 1$.

Posterior: $P(X = 1 | Y = 2) = 1$, others 0.

Information gain:

$$D_{\text{KL}}(P(X|2) || P(X)) = \log_2 \frac{1}{1/6} = \log_2 6 \approx 2.585 \text{ bits.}$$

2. Observe $Y = 7$:

All pairs $(1, 6), (2, 5), \dots, (6, 1)$ equally likely.

Posterior: $P(X = x \mid Y = 7) = \frac{1}{6}$ for all x .

Information gain:

$$D_{\text{KL}}(P(X|7) \| P(X)) = \sum_{x=1}^6 \frac{1}{6} \log_2 \frac{1/6}{1/6} = 0 \text{ bits.}$$

Mutual Information as the Average Gain

Mutual information averages these gains over all possible sums:

$$I(X; Y) = \sum_{y=2}^{12} P(Y = y) \cdot D_{\text{KL}}(P(X \mid Y = y) \| P(X)).$$

Using the known distribution of Y :

y	2	3	4	5	6	7	8	9	10	11	12
$P(Y = y)$	$\frac{1}{36}$	$\frac{2}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{5}{36}$	$\frac{6}{36}$	$\frac{5}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{2}{36}$	$\frac{1}{36}$
n_y (support size)	1	2	3	4	5	6	5	4	3	2	1
D_{KL}	$\log_2 6$	$\log_2 3$	$\log_2 2$	$\log_2 \frac{4}{3}?$	\dots	0	\dots				

More precisely, since $P(X \mid Y = y)$ is uniform over n_y values,

$$D_{\text{KL}}(P(X \mid Y = y) \| P(X)) = \log_2 n_y - \log_2 6 = \log_2 \left(\frac{n_y}{6} \right) \quad (\text{but note: actually } = \log_2 n_y - \log_2 6)$$

Carrying out the full calculation (as in the earlier example) yields:

$$I(X; Y) \approx 0.6895 \text{ bits.}$$

This is exactly the **expected information gain** from observing the sum and applying Bayes' rule.

Why This Matters

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- **Bayesian inference:** Every Bayes update provides information; mutual information quantifies its average value.

- **Experimental design:** Choose observations Y that maximize $I(X;Y)$ to learn most about X .
- **Machine learning:** In variational inference, mutual information appears in bounds on model evidence.
- **Cognitive science:** Models perception as Bayesian updating, with mutual information measuring sensory informativeness.

Summary

Concept	Role
Bayes' theorem	Updates prior $P(X) \rightarrow$ posterior $P(X \mid Y = y)$ for
KL divergence $D_{\text{KL}}(P(X y) \ P(X))$	Information gained from that <i>specific</i> update.
Mutual information $I(X;Y)$	<i>Expected</i> information gain over all y .

Thus, mutual information provides an **information-theoretic foundation for Bayesian learning**: it measures how much an observation is expected to teach us about the world.