A Practical & Unified Notation for Information-Theoretic Quantities in ML

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Abstract
A practical notation conveys valuable intuitions and concisely expresses new ideas. The currently employed notation in information theory, however, can be ambiguous for more complex expressions found in applied settings and often deviates between published works because researchers are from different backgrounds such as statistics, computer science, information engineering, which all use information theory. For example, \( H(X, Y) \) is sometimes used to denote the cross-entropy between \( X \) and \( Y \), which conflicts with common notation of the joint entropy \( H(X, Y) \) for \( X \) and \( Y \), or it is not clarified that \( H(X \mid Y) \) as conditional entropy of \( X \) given \( Y \) is an expectation over \( Y \). We present a disambiguated and consistent notation while striving to stay close to known notation when possible.

In addition, we show that an extension of information-theoretic quantities to relations between observed outcomes (events) and random variables can be of great use in machine learning. Commonly, the mutual information \( I(X; Y) \) is only defined for random variables \( X, Y \), while in natural language processing the point-wise information (Church and Hanks, 1990) has been introduced for two outcomes. This follows earlier work in information theory by Fano (1962), which also considers a natural extension to the mutual information between an outcome \( x \) and a random variable \( Y \), referred to as ‘conditional average of the [point-wise] mutual information’. Variants of this have been used more recently in the cognitive sciences and neuroscience as ‘(response-)specific information’ and ‘specific surprise’ (DeWeese and Meister, 1999; Williams, 2011), but they might not be well-known outside of neuroscience and the cognitive sciences. Our consistent extension also unifies these two previously separate quantities.

As an application for information quantities on observed outcomes, we present a different and intuitive derivation of Stirling’s approximation for binomial coefficients. The original deduction is found in MacKay (2003) on page 2. Furthermore, we show this allows for a simple analysis of the approximation error.

As another application of the notation, we derive the evidence lower bound (ELBO) from Kingma and Welling (2014) in a single (relatively long) line.

And, finally, as an application for mutual information terms that include observed outcomes, we examine the core-set problem.

1. Introduction
Information theory has provided insights for deep learning: information bottlenecks explain objectives both for supervised and unsupervised learning of high-dimensional data (Shwartz-Ziv and Tishby, 2017; Kirsch et al., 2020; Jónsson et al., 2020); similarly, information theory has inspired Bayesian experiment design, Bayesian optimization, and active learning as well as provided inspiration for research into submodularity in general (Lindley, 1956; Foster et al., 2019; Kirsch et al., 2019).

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problem which consists of selecting the most informative samples of a training set given the labels and provide new results. We also rederive the evidence-lower-bound inequality for variational inference of approximate Bayesian neural networks using our proposed notation.

The goal of this is to illustrate that our proposed notation is useful and show that it allows for more concise expression of important ideas.

Concretely, for the last example, we examine BALD (Bayesian Active Learning by Disagreement), an acquisition function in Bayesian active learning (Gal et al., 2017; Houlsby et al., 2011), and extend it to the core-set problem. In pool-based active learning, we have access to a huge reservoir of unlabelled data in a pool set and iteratively select samples from this pool set to be labeled by an oracle (e.g., human experts) to increase the model performance as quickly as possible. Acquisition functions are used to score all pool samples and the highest scorer is acquired. The goal of an acquisition function is to score the most “informative” samples the highest. BALD maximizes the expected information gain $I[Ω; Y \mid x]$ of the model parameters $Ω$ given the prediction variable $Y$ for a candidate sample $x$ from the pool set. It is equivalent to the concept of reduction in posterior uncertainty known from Bayesian optimal experimental design (Lindley, 1956). The core-set problem on the other hand consists of identifying the most informative samples given the labels, the core set, such that training a model on this core set will perform as well as a model trained on the whole dataset. We examine the connection between BALD and information gain in a case where the information gain equals the information-theoretic surprise, which we define later. As such, we introduce Core-Set by Disagreement (CSD), which maximizes the information gain of the model parameters given the true label $y$ of a sample $x$ in the dataset.

2. A Practical & Unified Notation

For a general introduction to information theory, we refer to Cover and Thomas (2006); Yeung (2008). In the following section, we introduce our practical and unified notation. We start with notation that is explicit about the probability distribution $p(\cdot)$.

**Definition 2.1.** Let Shannon’s information content $h(\cdot)$, cross-entropy $H(\cdot \mid \cdot)$, entropy $H(\cdot)$, and KL divergence $D_{KL}(\cdot \mid \cdot)$ (Kullback-Leibler divergence) be defined for a probability distribution $p$ and non-negative function $q$ for a random variable $X$ and non-negative real number $\rho$ as:

$$h(\rho) := -\ln \rho \tag{1}$$
$$H(p(X) \mid q(X)) := \mathbb{E}_{p(x)} h(q(x)) \tag{2}$$
$$H(p(X)) := H(p(X) \mid p(X)) \tag{3}$$
$$D_{KL}(p(X) \mid q(X)) := H(p(X)) - H(p(X) \mid q(X)) \tag{4}$$

Shannon (1948) introduced the information content as negative logarithm due to its additivity for independent messages: $h(p(x, y)) = h(p(x)) + h(p(x, y))$ for independent random variables $X$ and $Y$.

**Proposition 2.2.** For a random variable $X$ with probability distributions $p$, $p_1$, and $p_2$, and non-negative functions $q$, $q_1$, and $q_2$ and $\alpha \in [0, 1]$:

$$H(p \parallel \alpha q) = H(p \parallel q) + h(\alpha), \tag{5}$$
$$H(p \parallel q^\alpha) = \alpha H(p \parallel q), \tag{6}$$
$$H(p \parallel q_1 q_2) = H(p \parallel q_1) + H(p \parallel q_2), \tag{7}$$
$$H(\alpha p_1 + (1 - \alpha) p_2 \parallel q) = \alpha H(p_1 \parallel q) + (1 - \alpha) H(p_2 \parallel q) \tag{8}$$
$$= \alpha H(p_1 \parallel q^\alpha) + H(p_2 \parallel q^{1-\alpha}), \tag{9}$$

where we have left out “$(X)$” everywhere for brevity.

**Proof.** The statements follows from the linearity of the expectation and the additivity of the logarithm for products.

This can be extended to show that cross-entropies are linear in their left-hand argument and log-linear in their right-hand argument.

When we want to emphasize that we approximate the true distribution $p$ using a different distribution $q$ and the true probability distribution $p$ is understood, we use the notation $H_q(\cdot)$ for $H(p(\cdot) \mid q(\cdot))$ following notation in Kirsch et al. (2020); Xu et al. (2020):

**Definition 2.3.** When the true probability distribution $p$ is understood from context, we will use the following short-hands:

$$H[X] := H(p(X)) \tag{11}$$
$$H_q[X] := H(p(X) \mid q(X)). \tag{12}$$
When we have a parameterized distribution \( q_\theta \) with parameters \( \theta \), we will write \( H_{\theta} (\cdot) \) instead of \( H_{q_\theta} (\cdot) \) when the context is clear.

Approximating a possibly intractable distribution with a parameterized one is common when performing variational inference, that is. The main motivation for this notation is that when \( q = p \), we have \( H_{\theta} (\cdot) \geq H (\cdot) \) with equality when \( q = p \). Thus, we have the following useful identities:

**Proposition 2.4.** We have the following lower-bounds for the cross-entropy and KL, with \( Z_q := \int q(x) \, dx \):

\[
\begin{align*}
H(p(X) \parallel q(X)) &\geq H(p(X)) + h(Z_q), \\
D_{\text{KL}}(p(X) \parallel q(X)) &\geq h(Z_q),
\end{align*}
\]

with equality exactly when \( q/Z_q = p \) for \( Z_q := \int q(x) \, dx \).

**Proof.** The statements follow from Jensen’s inequality and the convexity of \( h(\cdot) \).

This also implies the non-negativity of the KL for densities when we substitute \( Z_q = 1 \) in above statements. We repeat the result as it is often used:

**Corollary 2.5.** When \( q \) is a probability distribution, we have:

\[
\begin{align*}
H(p(X) \parallel q(X)) &\geq H(p(X)), \\
D_{\text{KL}}(p(X) \parallel q(X)) &\geq 0,
\end{align*}
\]

with equality exactly when \( q = p \).

Note that for continuous distributions, above equality \( p = q \) only has to hold almost everywhere.

Above definitions are trivially extended to joints of random variables by substituting the random variable of the product space. Similarly, the conditional entropy is defined by taking the expectation over both \( X \) and \( Y \). For example:

**Proposition 2.6.** Given random variables \( X \) and \( Y \), we have:

\[
\begin{align*}
H[X, Y] &= \mathbb{E}_{p(x,y)} h(p(x,y)); \\
H[X \mid Y] &= \mathbb{E}_{p(x,y)} h(p(x \mid y)).
\end{align*}
\]

In particular, note that \( H[X \mid Y] \) is an expectation over \( X \) and \( Y \).

For cross-entropies and KL divergences, we expand the definitions similarly. In particular, we have the following equality for cross-entropies, which follows from these definitions:

\[
H(p(X \mid Y) \parallel q(X \mid Y)) = \mathbb{E}_{p(x,y)} h(q(x \mid y)) = H(p(X, Y) \parallel q(X \mid Y)).
\]

The last idiosyncrasy only applies to cross-entropies. Indeed, for KL divergences, we have:

\[
\begin{align*}
D_{\text{KL}}(p(X \mid Y) \parallel q(X \mid Y)) &= H(p(X, Y) \parallel q(X \mid Y)) - H(p(X \mid Y)) \\
D_{\text{KL}}(p(X, Y) \parallel q(X \mid Y)) &= H(p(X, Y) \parallel q(X \mid Y)) - H(p(X, Y)).
\end{align*}
\]

Note, that the second terms are usually not equal \( H(p(X \mid Y)) \neq H(p(X, Y)) \), and the two terms are thus different.

The reader might wonder when we are interested in \( D_{\text{KL}}(p(X, Y) \parallel q(X \mid Y)) \). It can arise when performing symbolic manipulations, so we mention it explicitly here.

MacKay (2003) has an elegant visualizations for information quantities, which we reproduce in Figure 1. Yeung (1991) introduces I-diagrams which provide another useful intuitive approach, but they do not scale as easily to what we introduce next.

**Observed outcomes.** So far, we have introduced well-known information-theoretic quantities using a more consistent notation. Now, we further canonically extend the definitions to tie random variables to specific observed outcomes, e.g. \( X = x \). We refer to \( X \) when we have \( X = x \) in an expression as tied random variable as it is tied to an outcome. If we mix (untied) random variables and tied random variables, we define \( H[\cdot \mid \cdot] \) as an operator which takes an expectation of Shannon’s information content for the given expression over the (untied) random variables conditioned on the tied outcomes. For example, \( H[X, Y = y \mid Z, W = w] = \mathbb{E}_{p(x,z,y,w)} h(p(x, y \mid z, w)) \) following this notation. We generally shorten \( Y = y \) to \( y \) when the connection is clear from context. Similarly, we have \( H(p(X \mid y) \parallel q(X \mid y)) = \mathbb{E}_{p(x \mid y)} h(q(x \mid y)) \). Importantly, all of the above maintain the identities \( H[X, Y] = \mathbb{E}_{p(x,y)} H[x, y] = \mathbb{E}_{p(y)} H[X, y] \), which is the motivation behind these extensions. Figure 2 provides an overview over the quantities for two random variables \( X \) and \( Y \) when \( Y = y \) is observed. We define everything in detail below and provide intuitions.

**Definition 2.7.** Given random variables \( X \) and \( Y \) and outcome \( y \), we define:

\[
\begin{align*}
H[y] &:= h(p(y)) \\
H[X, y] &:= \mathbb{E}_{p(x,y)} H[x, y] = \mathbb{E}_{p(x|y)} h(p(x \mid y)) \\
H[X \mid y] &:= \mathbb{E}_{p(x|y)} H[x \mid y] = \mathbb{E}_{p(x|y)} h(p(x \mid y)) \\
H[y \mid X] &:= \mathbb{E}_{p(x|y)} H[y \mid x] = \mathbb{E}_{p(x|y)} h(p(y \mid x)),
\end{align*}
\]

where we have shortened \( Y = y \) to \( y \).

Note \( H[y], H[X, y] \), and so on are shorthands for \( H(p(y)) \), \( H(p(X, y)) \), and so on. Shannon’s information content
The mutual information and point-wise mutual information (Fano, 1962; Church and Hanks, 1990) are defined as:

**Definition 2.9.** For random variables $X$ and $Y$ and outcomes $x$ and $y$ respectively, the point-wise mutual information $I[x; y]$ and the mutual information $I[X; Y]$ are:

\[
I[x; y] := H[x] - H[x | y] = h\left(\frac{p(x)p(y)}{p(x)}\right) \\
I[X; Y] := H[X] - H[X | Y] = E_{p(x,y)} I[x; y].
\]

This is similarly extended to $I[X; Y | Z] = H[X | Z] - H[X | Y, Z]$ or $I[X_1, X_2; Y] = H[X_1, X_2] - H[X_1, X_2 | Y]$ and so on.

There are two common, sensible quantities we can define when we want to consider the information overlap between an random variable and an outcome: the information gain, also known as specific information and the surprise (DeWeese and Meister, 1999; Butts, 2003). These two quantities are usually defined separately in the cognitive sciences and neuroscience (Williams, 2011); however, we can unify them after relaxing the symmetry of the mutual information as done above:

**Definition 2.10.** Given random variables $X$ and $Y$ and outcome $y$ for $Y$, we define the information gain $I[X; y]$ and the surprise $I[y; X]$ as:

\[
I[x; y] := H[X] - H[X | y] \\
I[y; X] := H[y] - H[y | X].
\]

This unifying definition is novel to the best of our knowledge. It works by breaking the symmetry that otherwise exists for the regular and point-wise mutual information.

Note that the surprise can also be expressed as $I[y; X] = D_{KL}(p(X | y) \parallel p(Y))$. For example, this is done in Bellemare et al. (2016)—even though the paper mistakenly calls this surprise an information gain when it is not.

We enumerate a few equivalent ways of writing the mutual information and surprise—the information gain has no such equivalences. This can be helpful to spot these quantities in the wild.

**Proposition 2.11.** We have

\[
I[X; Y] = D_{KL}(p(X, Y) \parallel p(X)p(Y)) \\
I[y; X] = E_{p(x|y)} I[y; x] \\
= E_{p(x|y)} [H[x] | y] \\
= D_{KL}(p(X | y) \parallel p(Y)).
\]

The information gain $I[X; y]$ for $X$ given $y$ measures the reduction in uncertainty about $H[X]$ when we observe $y$. 

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**Figure 2.** The relationship between between joint entropy $H[X, y]$, entropies $H[X], H[y], \text{conditional entropies } H[X | y], H[y | X], \text{information gain } I[X; y] \text{ and surprise } I[y; X] \text{ when } Y = y \text{ is observed. We include } E_{p(x|y)} H[x] \text{ to visualize Proposition 2.8. The figure follows Figure 8.1 in MacKay (2003).}

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The intuition from information theory behind these definitions is that, e.g., $H[X, y]$ measures the average length of transmitting $X$ and $Y$ together when $Y = y$ is unknown to the sender and receiver, and $H[y | X]$ measures how much additional information needs to be transferred on average for the receiver to learn $y$ when it already knows $X | y$.

As a memory hook for the reader, lower-case letters are always used for tied random variables and upper-case letters for (untied) random variables over which we take an expectation. This makes it easy to differentiate between the two cases and write down the actual expressions.

From above definition, we also have $H[x, y] = h(p(x, y))$ and $H[x | y] = h(p(x | y))$. Beware, however, that while we have $H[X | y] = H[X, y] - H[y]$, for $H[y | X]$, there is no such equality for $H[y | X]$:

**Proposition 2.8.** Given random variables $X$ and $Y$ and outcome $y$, we generally have:

\[
H[X | y] = H[X, y] - H[y] \\
H[y | X] = H[X, y] - E_{p(x|y)} H[x] \\
\neq H[X, y] - H[X].
\]

**Proof.** $H[X | y] = H[X, y] - H[y]$ follows immediately from the definitions. $H[y | X] \neq H[X, y] - H[X]$ follows because, generally, $E_{p(x|y)} H[x] \neq H[X]$ when $p(x | y) \neq p(x)$. E.g., for $X$ and $Y$ only taking binary values, 0 or 1, let $p(x, y) = \frac{1}{3} \mathbb{1}_{x=y=0} + \frac{2}{3} \mathbb{1}_{x=y=1}$, then $E_{p(x|y)} H[x] = \log \left(\frac{3}{2}\right) \neq \log \left(\frac{3}{2}^2\right) = H[X]$. \hfill \Box
H[X] is the uncertainty about the true \( X \) that we want to learn as then entropy quantifies the amount of additional information that we need to transmit to fix \( X \), and similarly \( H[X \mid y] \) quantifies the additional information we need to transmit to fix \( X \) once \( y \) is known (Lindley, 1956). On the other hand, the surprise \( I[y; X] \) of \( y \) for \( X \) measures how much the posterior \( X \mid y \) lies in areas where \( p(x) \) was small before observing \( y \) (DeWeese and Meister, 1999).

An important difference between the two is that the information gain can be chained while the surprise cannot:

**Proposition 2.12.** Given random variables \( X, Y_1, \) and \( Y_2 \) and outcomes \( y_1 \) and \( y_2 \) for \( Y_1 \) and \( Y_2 \), respectively, we have:

\[
I[X; y_1, y_2] = I[X; y_1] + I[X; y_2 \mid y_1] \quad (38)
\]
\[
I[y_1, y_2; X] \neq I[y_1; X] + I[y_2; X \mid y_1]. \quad (39)
\]

**Proof.** We have

\[
I[X; y_1, y_2] = H[X] - H[X \mid y_1, y_2]
\]
\[
= H[X] - H[X \mid y_1] + H[X \mid y_1] - H[X \mid y_1, y_2]
\]
\[
= I[X; y_1] + I[X; y_2 \mid y_1],
\]

while

\[
I[y_1, y_2; X] = \mathbb{E}_{p(x|y_1, y_2)} I[y_1, y_2; x]
\]
\[
= \mathbb{E}_{p(x|y_1, y_2)} I[y_1; x] + \mathbb{E}_{p(x|y_1, y_2)} I[y_2; x \mid y_1].
\]

That is, generally, \( \mathbb{E}_{p(x|y_1, y_2)} I[y_1; x] \neq I[y_1; X] \). To conclude the proof, we instantiate \( p(x \mid y_1, y_2) \neq p(x \mid y_1) \): for \( X, Y_1, \) and \( Y_2 \) taking binary values 0, 1 only, let \( p(y_1) = \frac{1}{2}, p(x, y_2) = 0 \Rightarrow \frac{1}{4}, p(x \mid y_2 = 0, y_1 = 1) = \frac{3}{4}, p(x = 0 \mid y_2 = 1, y_1 = 1) = \frac{1}{4}. \) Then

\[
\mathbb{E}_{p(x|y_1, y_2)} I[y_1; x] = \log \left( \frac{\frac{1}{4}}{\frac{3}{4}} \right) = \log \left( \frac{6}{5} \right) = I[y_1; X]
\]

for \( y_1 = 1, y_2 = 1 \) as the reader can easily verify.

However, both quantities do chain in their (untied) random variables:

**Proposition 2.13.** Given random variables \( X_1, X_2, Y, \) and outcome \( y \) for \( Y \):

\[
I[X_1, X_2; y] = I[X_1; y] + I[X_2; y \mid X_1] \quad (40)
\]
\[
I[y; X_1, X_2] = I[y; X_1] + I[y; X_2 \mid X_1]. \quad (41)
\]

**Proof.** We have

\[
I[X_1; y] + I[X_2; y \mid X_1] = \]

\[
= H[X_1] - H[X_1 \mid y] + H[X_2 \mid X_1] + H[X_2 \mid X_1, y]
\]
\[
= H[X_1] + H[X_2 \mid X_1] - (H[X_1 \mid y] + H[X_2 \mid X_1, y])
\]
\[
= H[X_1, X_2] - (H[X_1, X_2 \mid y] - H[X_1, X_2])
\]
\[
= I[X_1, X_2; y].
\]

Similarly, we have

\[
I[y; X_1] + I[y; X_2 \mid X_1] = \]
\[
= H[y] - H[y \mid X_1] + H[y \mid X_1] - H[y \mid X_1, X_2]
\]
\[
= H[y] - H[y \mid X_1, X_2]
\]
\[
= I[y; X_1, X_2].
\]

These extensions of the mutual information are canonical as they permute with taking expectations over tied variables to obtain the regular (untied) quantities:

**Proposition 2.14.** For random variables \( X \) and \( Y \):

\[
I[X; Y] = \mathbb{E}_{p(y)} I[X; y] = \mathbb{E}_{p(y)} I[y; X] = \mathbb{E}_{p(x, y)} I[x, y]. \quad (42)
\]

**Proof.** Follows immediately from substituting the definitions.

Likewise, when all random variables are tied to a specific outcome, the quantities behaves as expected:

**Proposition 2.15.** For random variables \( X, Y, Y_1 \) and \( Y_2 \):

\[
I[X; Y] = I[X; Y], \text{ and}
\]
\[
I[x; y] = I[y; x]; \quad (44)
\]
\[
I[X; Y_1, Y_2] = I[X; Y_1] + I[X; Y_2], \text{ and}
\]
\[
I[x; y_1, y_2] = I[x; y_1] + I[x; y_2 \mid y_1]. \quad (46)
\]

**Proof.** The only interesting equality is \( I[x; y_1, y_2] = I[x; y_1] + I[x; y_2 \mid y_1] \):

\[
I[x; y_1] + I[x; y_2 \mid y_1] = \]
\[
= h_p(x) p(y_1) p(x, y_1) p(y_2 | y_1) p(y_2) - h_p(x) p(y_2 | y_1) p(y_2)
\]
\[
= h_p(x) p(y_2 | y_1) p(y_2)
\]
\[
= I[x; y_1, y_2].
\]

We can extend this to triple mutual information terms by adopting the extension \( I[X; Y; Z] = I[X; Y] - I[X; Y \mid Z] \) (Yeung, 2008) for outcomes as well: \( I[X; Y; z] = I[X; Y] - I[X; Y \mid z] \), which also works for higher-order terms.
Overall, for the reader, there will be little surprise when working with the fully point-wise information-theoretic quantities, that is, when all random variables are observed. But the mixed ones require more care. We refer the reader back to Figure 2 to recall the relationships which also provide intuitions for the inequalities we will examine next.

**Inequalities.** We review some well-known inequalities first:

**Proposition 2.16.** For random variables $X$ and $Y$, we have:

\[
I[X; Y] \geq 0 \quad \text{(48)}
\]

\[
H[X] \geq H[X \mid Y], \quad \text{(49)}
\]

and if $X$ is a discrete random variables, we also have:

\[
H[X] \geq 0 \quad \text{(50)}
\]

\[
I[X; Y] \leq H[X]. \quad \text{(51)}
\]

**Proof.** The first two statements follow from:

\[
H[X] - H[X \mid Y] = I[X; Y] = D_{KL}(p(X, Y) \parallel p(X) p(Y)) \geq 0. \quad \text{(52)}
\]

The third statement follows from the monotony of the expectation and $p(x) \leq 1$ for all $x$. □

Following Kirsch et al. (2020), if we assume that we add independent zero-entropy noise $\epsilon_0 \sim N(0, \frac{1}{2\pi\epsilon^2})$ to continuous random variables as observation noise, we can also force their continuous entropy to be non-negative: we have $H[X + \epsilon_0] \geq 0$ and also $I[X + \epsilon_0; Y] \leq H[X + \epsilon_0]$ as $I[X + \epsilon_0; Y] = H[X + \epsilon_0] - H[X + \epsilon_0 \mid Y]$ and $H[X + \epsilon_0 \mid Y] \geq 0$, too. We say, we inject zero-entropy noise when we assume that zero-entropy noise has already been added to a continuous random variable.

**Corollary 2.17.** For continuous random variables $X$ and $Y$ where we inject zero-entropy noise into $X$, we have:

\[
H[X] \geq 0 \quad \text{(53)}
\]

\[
I[X; Y] \leq H[X]. \quad \text{(54)}
\]

For mixed outcomes we find similar inequalities:

**Proposition 2.18.** For random variables $X$ and $Y$ with outcome $y$, we have:

\[
I[y; X] \geq 0 \quad \text{(55)}
\]

\[
H[y] \geq H[y \mid X] \quad \text{(56)}
\]

\[
\mathbb{E}_{p(x \mid y) H[x]} \geq H[X \mid y], \quad \text{(57)}
\]

and if $Y$ is a discrete random variable (or we inject zero-entropy noise), we also have:

\[
H[y \mid X], H[y] \geq 0 \quad \text{(58)}
\]

\[
I[y; X] \leq H[y], \quad \text{(59)}
\]

**Proof.** Again, the first two statements follow from:

\[
H[y] - H[y \mid X] = I[y; X] = \mathbb{E}_{p(x \mid y)} I[y; x] = \mathbb{E}_{p(x \mid y)} [H[x] - H[x \mid y]] = D_{KL}(p(X \mid y) \parallel p(X)) \geq 0. \quad \text{(62)}
\]

The third statement follows from eq. (61) above as $0 \leq \mathbb{E}_{p(x \mid y)} [H[x] - H[x \mid y]] = \mathbb{E}_{p(x \mid y)} H[x] - H[X \mid y]$. The fourth statement follows from $p(y \mid x) \leq 1$ when $Y$ is a discrete random variable, and thus $H[y \mid X] \geq 0$ due to the monotony of the expectation. When we inject zero-entropy noise, we similarly have $p(y \mid x) \leq 1$ for almost all $y$ as otherwise $H[X] \leq 0$ in contradiction to eq. (53). The fifth statement follows from the fourth statement and $I[y; X] = H[y] - H[y \mid X] \leq H[y]$. Finally, if $X$ is a discrete random variable as well, we also have $H[X \mid y] \geq 0$, and thus

\[
I[y; X] = \mathbb{E}_{p(x \mid y)} [H[x] - H[X \mid y]] \leq \mathbb{E}_{p(x \mid y)} H[x].
\]

Similarly, when we inject zero-entropy noise into $X$, we also $H[X \mid y] \geq 0$ following eq. (53) as the noise is assumed to be independent. □

Note that there are no such general bound for $I[X; y]$, $H[X \mid y]$ and $H[y \mid X]$.

**Corollary 2.19.** We have $I[y; X] = 0$ exactly when $p(x \mid y) = p(x)$ for all $x$ for given $y$.

**Proof.** This follows from $0 = I[y; X] = D_{KL}(p(x \mid y) \parallel p(x))$ exactly when $p(x \mid y) = p(x)$. □

In particular, there is a misleading intuition that the information gain $I[X; y] = H[X] - H[X \mid y]$ ought to be non-negative for any $y$. This is not true. This intuition may exist because in many cases when we look at posterior distributions, we only model the mean and assume a fixed variance of these distributions. The uncertainty around the mean does indeed reduce with additional observations; however, the uncertainty around the variance might not. The reader is invited to experiment with a normal distribution
Figure 3. The relationship between between the information quantities used in §3. $B$ is the joint of the binomial random variables, $R$ is the number of successes in $B$ with observed outcome $r$. The arrow below $H[r]$ symbolizes that we minimize $H[r]$ by optimizing the success probability $\rho$ to close the gap between $E_{p(b|r)} H[b]$ and $H[B | r]$.

with known mean and compute the information gain on the variance depending on new observations.

In a sense, the information-theoretic surprise is much better behaved than the information gain because we can bound it in various ways, which does not seem possible for the information gain. The information gain is a more useful quantity though for active learning and Bayesian optimal experimental design. As such it is useful to have a unified notation that includes both quantities.

3. Example Application: Stirling’s Approximation for Binomial Coefficients

In MacKay (2003) on page 2, the following simple approximation for a binomial coefficient is introduced:

$$ \log \binom{N}{r} \simeq (N - r) \log \frac{N}{N - r} + r \log \frac{N}{r}. \quad (63) $$

We will derive this result using the proposed extension to observed outcomes as it allows for an intuitive deduction. Moreover, we will see that this allows us to use other tools from probability theory to estimate the approximation error.

**Setup.** Let $B_1, \ldots, B_N$ be $N$ Bernoulli random variables with success probability $p$, and let $B$ be the joint of these random variables.

Further, let $R$ be the random variable that counts the number of successes in $B$. $R$ follows a Binomial distribution with success probability $\rho$ and $N$ trials.

**Main Idea.** For a given outcome $r$ of $R$, we have:

$$ H[B, r] = H[B | r] + H[r] \geq H[B | r], \quad (64) $$
as $H[\cdot]$ is non-negative for discrete random variables. We will examine this inequality to obtain the approximation in eq. (63).

Note that $H[B | r]$ is the additional number of bits needed to encode $B$ when the number of successes is already known.

Similarly, $H[B, r]$ is the number of bits needed to encode both $B$ and $R$ under the circumstance that $R = r$.

**Determining** $H[B, r]$. $R$ is fully determined by $B$, and thus we have $H[B, R] = H[B]$ and hence:

$$ H[B, r] = E_{p(b|r)} H[b]. \quad (65) $$

$E_{p(b|r)} H[b]$ is the expected number of bits needed to transmit the outcome $b$ of $B$ when $r$ is given. When we encode $B$, we do not know $r$ upfront, so we need to transmit $N$ Bernoulli outcomes. Hence, we need to transmit $r$ successes and $N - r$ failures. Given the success probability $\rho$, the optimal message length for this is:

$$ E_{p(b|r)} H[b] = r \log \rho + (N - r) \log (1 - \rho) \quad (66) $$

$$ = -r \log \rho - (N - r) \log (1 - \rho). \quad (67) $$

All this is visualized in Figure 3.

**Alternative Argument.** We can also look at the terms $H[B | r] + H[r]$ separately. We have

$$ H[r] = -\log p(r) = -\log \left( \binom{N}{r} \rho^r (1 - \rho)^{N-r} \right), \quad (68) $$

and

$$ H[B | r] = -E_{p(b|r)} \log p(b | r) = \log \binom{N}{r}. \quad (69) $$

The former follows from $R$ being binomially distributed. For the latter, we observe that we need to encode $B$ while knowing $r$ already. Given $r$, $p(b | r) = \text{const}$ for all valid $b$. There are $\binom{N}{r}$ possible $b$ for fixed $r$. Hence, we can simply create a table with all possible configurations with $r$ successes. There are $\binom{N}{r}$ many. We then encode the index into this table.

Each configuration with $r$ successes has an equal probability of happening, so we have a uniform discrete distribution with entropy $\log \binom{N}{r}$ and obtain the same result.

**Determining $\rho$.** We already have

$$ H[B | r] + H[r] = -r \log \rho - (N - r) \log (1 - \rho) \geq \log \binom{N}{r} = H[B | r]. \quad (70) $$

How do we make this inequality as tight as possible?

We need to minimize the gap $H[r]$ which creates the inequality in the first place, and $H[r] = -\log p(r)$ is minimized exactly when $p(r)$ becomes maximal. Hence, we choose the success probability $\rho$ to do so: the maximum likelihood solution $\arg \max_\rho p(r | \rho)$ is $\rho = \frac{r}{N}$.

---

This also follows immediately from $H[R | B] = 0 \Rightarrow \forall r : H[r | B] = 0.$
The Binomial distribution of $R$ then has its mode, mean, and median at $r$.

Altogether, after substituting $\rho = \frac{r}{N}$ and rearranging, we see that the wanted approximation is actually an inequality:

$$\log \left( \frac{N}{r} \right) \leq -r \log \rho - (N - r) \log (1 - \rho)$$

(71)

$$= r \log \frac{N}{r} + (N - r) \log \frac{N}{N - r}.$$  

(72)

**Approximation Error** $H[r]$. The approximation error is just $H[r]$ as we can read off from eq. (70). We can easily upper-bound it with $H[r] \leq \log N$: First, $H[R] \leq \log N$ as the uniform distribution with entropy $\log N$ is the maximum entropy distribution in this case (discrete random variable with finite support). Second, $H[R]$ is the expectation over different $H[R = r']$. We have chosen $\rho = \frac{r}{N}$ such that $r$ is the mean of binominal distribution and has maximal information content. Hence $H[r] = \log N$ by contraposition as otherwise $\log N < H[r] \leq H[R]$.

4. Example Application: ELBO of a Variational Auto-Encoder

The specific evidence lower bound inequality (ELBO) developed in Kingma and Welling (2014) is a useful tool. The derivation in the paper has been described as hard to follow, however. We can elegantly derive the relevant inequality at a high level using our practical notation and Bayes’ theorem.

**Variational Auto-Encoder.** We have a probabilistic model $p(x, z) := p_\theta(z)p_\theta(x \mid z)$ of observed $X$ given some hidden latent variable $Z$ with parameters $\theta$. Usually $p_\theta(z)$ is fixed as $p(z)$ and follows a simple distribution: a unit Gaussian, for example. We desire to learn a variational approximation $q_\phi(z \mid x)$ with parameters $\phi$ of $p_\theta(z \mid x)$, where the latter might be intractable. $p(x)$ is only available implicitly through the available training data, which means that we can sample from it but not compute the density directly. This is where the ELBO comes in.

**ELBO.** Following Kingma and Welling (2014), we minimize a forward KL divergence as variational objective: when $D_{KL}(q_\phi(Z \mid X) \| p(Z \mid X)) = 0$, we also have $q_\phi(z \mid x) = p(z \mid x)$. In this case, we have found a consistent variational approximation. But in general this does not hold. Depending on the quality of the approximation, we can draw approximate samples of $p(x)$ by first sampling $z \sim p_\theta(z)$ and then sampling $x \sim p_\theta(x \mid z)$.

**Proposition 4.1.** Minimizing the forward KL divergence $D_{KL}(q_\phi(Z \mid X) \| p(Z \mid X)) \geq 0$ is equivalent to maximizing (the left-hand side in) the evidence lower bound $E_{p(x)} q_\phi(z \mid x) \left[ \log p_\theta(x \mid z) \right] - D_{KL}(q_\phi(Z \mid X) \| p_\theta(Z)) \leq E_{p(x)} \log p(x)$.

**Proof.** We begin with an information-theoretic deduction which is straightforward using Bayes’ theorem and the rules in Proposition 2.2:

$$0 \leq D_{KL}(q_\phi(Z \mid X) \| p(Z \mid X))$$

$$= H(q_\phi(Z \mid X) \| p(Z \mid X)) - H(q_\phi(Z \mid X) \| p_\theta(Z))$$

$$= \log p_\theta(X) - H(q_\phi(Z \mid X))$$

$$+ D_{KL}(q_\phi(Z \mid X) \| p_\theta(Z)) - H(p(X))$$

Finally, we can rearrange and expand the definitions to obtain the ELBO:

$$H(p(X)) \leq E_{p(x)} q_\phi(z \mid x) \left[ \log p_\theta(x \mid z) \right]$$

$$+ D_{KL}(q_\phi(Z \mid X) \| p_\theta(Z))$$

$$\Leftrightarrow E_{p(x)} \log p(x) \geq E_{p(x)} E_{q_\phi(z \mid x)} \left[ \log p_\theta(x \mid z) \right]$$

$$- D_{KL}(q_\phi(Z \mid X) \| p_\theta(Z)).$$

From an information-theoretic perspective, the ELBO is actually an upper-bound on the entropy of the inputs:

$$H[X] \leq H(q_\phi(Z \mid X) \| p_\theta(X \mid Z))$$

$$+ D_{KL}(q_\phi(Z \mid X) \| p_\theta(Z))$$.

Note that in comparison to Kingma and Welling (2014), we take an expectation over $x$ right away. The non-expected version would be

$$H[x] \leq H(q_\phi(Z \mid x) \| p_\theta(x \mid Z))$$

(73)

$$+ D_{KL}(q_\phi(Z \mid x) \| p_\theta(Z))$$.

(74)

5. Example Application: Variational Inference, Active Learning, and Core-Set Methods

We start by briefly revisiting Bayesian deep learning, variational inference, and the evidence-lower-bound inequality, before introducing active learning and defining the Core-Set by Disagreement acquisition function.

**Probabilistic Model.** The model parameters are treated as a random variable $\Omega$ with prior distribution $p(\Omega)$. We denote the training set $D_{\text{train}} = \{(x_i^{\text{train}}, y_i^{\text{train}})\}_{i=1,...,n}$, where $\{x_i^{\text{train}}\}_{i=1,...,n}$ are the input samples and $\{y_i^{\text{train}}\}_{i=1,...,n}$ the labels or targets.
The probabilistic model is as follows:

\[ p(y, x, \omega) = p(y \mid x, \omega) \cdot p(\omega) \cdot p(x), \quad (75) \]

where \( x, y, \) and \( \omega \) are outcomes for the random variables \( X, Y, \) and \( \Omega \) denoting the input, label, and model parameters, respectively.

To include multiple labels and inputs, we expand the model to joints of random variables \( \{x_i\}_{i \in I} \) and \( \{y_i\}_{i \in I} \) obtaining

\[ p(\{y_i\}_i, \{x_i\}_i, \omega) = \prod_{i \in I} p(y_i \mid x_i, \omega) \cdot p(x_i) \cdot p(\omega). \quad (76) \]

We are only interested in discriminative models and thus do not explicitly model \( p(x) \).

The posterior parameter distribution \( p(\omega \mid D_{\text{train}}) \) is determined via Bayesian inference. We obtain \( p(\omega \mid D_{\text{train}}) \) using Bayes’ theorem:

\[ p(\omega \mid D_{\text{train}}) \propto p(\{y_i^{\text{train}}\}_i \mid \{x_i^{\text{train}}\}_i, \omega) \cdot p(\omega). \quad (77) \]

which allows for predictions by marginalizing over \( \omega \):

\[ p(y \mid x, D_{\text{train}}) = \mathbb{E}_{\omega \sim p(\omega \mid D_{\text{train}})} [p(y \mid x, \omega)]. \quad (78) \]

**Variational Inference & ELBO.** Exact Bayesian inference is intractable for complex models, and we use variational inference for approximate inference using a variational distribution \( q(\omega) \). We can determine \( q(\omega) \) by minimizing the following KL divergence:

\[
\begin{align*}
D_{\text{KL}}(q(\omega) \parallel p(\omega \mid D_{\text{train}})) &= \\
&= \underbrace{\text{likelihood}}_{\sum_i \mathbb{E}_{\omega} \log p(y_i^{\text{train}} \mid x_i^{\text{train}}, \omega)} - \underbrace{D_{\text{KL}}(q(\omega) \parallel p(\omega))}_{\text{prior regularization}} + \underbrace{\text{model evidence}}_{\log p(D_{\text{train}}) \geq 0}, (79)
\end{align*}
\]

where we used Bayes’ theorem. We proof this using the notation from this paper as an application:

**Proposition 5.1.** Minimizing the forward KL divergence \( D_{\text{KL}}(q(\omega) \parallel p(\omega \mid D_{\text{train}})) \) is equivalent to maximizing the evidence lower-bound (ELBO) \( \sum_i \mathbb{E}_{\omega} \log p(y_i^{\text{train}} \mid x_i^{\text{train}}, \omega) - D_{\text{KL}}(q(\omega) \parallel p(\omega)). \)

**Proof.** We start with the information-theoretic deduction which is straightforward using Bayes’ theorem and the rules in Proposition 2.2:

\[
\begin{align*}
0 &\leq D_{\text{KL}}(q(\omega) \parallel p(\omega \mid D_{\text{train}})) \\
&= H(q(\omega) \mid p(\omega \mid D_{\text{train}})) - H(q(\omega)) \\
&= H(q(\omega) \mid p(\{y_i^{\text{train}}\}_i \mid \{x_i^{\text{train}}\}_i, \omega) \cdot p(\omega)) - H(q(\omega)) \\
&= H(q(\omega) \mid p(\{y_i^{\text{train}}\}_i \mid \{x_i^{\text{train}}\}_i, \omega)) + H(q(\omega)) - H(q(\omega)) - H(q(\omega)) - H(p(D_{\text{train}})) \\
&= H(q(\omega) \mid p(\{y_i^{\text{train}}\}_i \mid \{x_i^{\text{train}}\}_i, \omega)) \\
&\quad + D_{\text{KL}}(q(\omega) \parallel p(\omega)) + h(p(D_{\text{train}})).
\end{align*}
\]

It thus follows:

\[ h(p(D_{\text{train}})) \leq H(q(\omega) \parallel p(\{y_i^{\text{train}}\}_i \mid \{x_i^{\text{train}}\}_i, \omega)) + D_{\text{KL}}(q(\omega) \parallel p(\omega)). \]

Expanding the definitions, we obtain

\[ -\log p(D_{\text{train}}) \leq \mathbb{E}_{\omega} \left[ -\log \prod_i p(y_i^{\text{train}} \mid x_i^{\text{train}}, \omega) \right] + D_{\text{KL}}(q(\omega) \parallel p(\omega)), \]

and after some rearranging, the ELBO surfaces:

\[ \log p(D_{\text{train}}) \geq \mathbb{E}_{\omega} \left[ \log p(y_i^{\text{train}} \mid x_i^{\text{train}}, \omega) \right] - D_{\text{KL}}(q(\omega) \parallel p(\omega)), \]

with equality exactly when \( q(\omega) = p(\omega \mid D_{\text{train}}) \). \( \square \)

For Bayesian deep learning models, we can use the local reparameterization trick or Monte-Carlo dropout for \( q(\omega) \) (Kingma et al., 2015; Gal and Ghahramani, 2016).

**Active Learning.** In active learning, we have access to an unlabelled pool set \( D_{\text{pool}} = \{x_i^{\text{pool}}\}_{i \in \{1, \ldots, |D_{\text{pool}}|\}} \). We iteratively acquire batches of samples \( \{x_i^{\text{acq}}\}_i \) from the pool set into the training set by acquiring labels for them through an oracle and retrain our model. We repeat these steps until the model satisfies our performance requirements.

To determine which samples to select for acquisition, we score candidate acquisition batches \( \{x_i^{\text{acq}}\}_i \), with the acquisition batch size \( b \) using an acquisition function \( a(\{x_i^{\text{acq}}\}_i, p(\Omega \mid D_{\text{train}})) \) and pick the highest scoring one:

\[ \arg \max_{\{x_i^{\text{acq}}\}_i \in \{1, \ldots, b\} \subseteq D_{\text{pool}}} a(\{x_i^{\text{acq}}\}_i, p(\Omega \mid D_{\text{train}})) \]

\[ \text{BALD was originally introduced as a one-sample acquisition function of the expected information gain between the prediction } Y_i^{\text{acq}} \text{ for a candidate input } x_i^{\text{acq}} \text{ and the model parameters } \Omega; I[\Omega; Y_i^{\text{acq}} \mid x_i^{\text{acq}}, D_{\text{train}}]. \text{ In BatchBALD (Kirsch et al., 2019), this one-sample case was canonically extended to the batch acquisition case using the expected information gain between the joint of the predictions } \{Y_i^{\text{acq}}\}_i \text{ for the batch candidates } \{x_i^{\text{acq}}\}_i \text{ and the model parameters } \Omega: \]

\[
 q_{\text{BALD}}(\{x_i^{\text{acq}}\}_i, p(\Omega \mid D_{\text{train}})) := I[\Omega; \{Y_i^{\text{acq}}\}_i \mid \{x_i^{\text{acq}}\}_i, D_{\text{train}}] \quad (81)
\]
Notation. Instead of \( \{ Y_i^{\text{eval}} \}, \{ x_i^{\text{eval}} \} \), we will write \( Y^{\text{eval}}, x^{\text{eval}} \) and so on to to cut down on notation. Like above, all terms can be canonically extended to sets by substituting the joint. Lower-case variables like \( y^{\text{eval}} \) are outcomes of random variables while upper-case variables like \( Y^{\text{eval}} \) are random variables. The datasets \( D^{\text{pool}}, D^{\text{train}} \) are sets of outcomes.

5.1. BALD → Core-Set by Disagreement

We examine BALD through the lens of our new notation and develop CSD as information gain. First, we note that BALD does not optimize the loss of the test distribution to become minimal. It does not try to pick labels which minimize the generalization loss.

BALD maximizes the expected information gain: \( I[\Omega; Y^{\text{acq}} | \omega^{\text{acq}}, D^{\text{train}}] = H[\Omega] - H[\Omega | Y^{\text{acq}}, \omega^{\text{acq}}, D^{\text{train}}] \). We assume that our Bayesian model contains the true generating model parameters and by selecting samples that minimize the uncertainty \( H[\Omega | Y^{\text{acq}}, \omega^{\text{acq}}, D^{\text{train}}] \), the model parameters will converge towards these true parameters as \( H[\Omega | D^{\text{train}}] \rightarrow 0 \).

BALD as an Approximation. BALD as the expected information gain is the expectation of the information gain over the current model’s predictions for \( x \):

\[
I[\Omega; y | x, D^{\text{train}}] = \mathbb{E}_{\omega \sim p(\omega | x, \Omega, D^{\text{train}})}[I[\Omega; y | x, D^{\text{train}}]]. \tag{82}
\]

Using the definition, we have:

\[
I[\Omega; y | x, D^{\text{train}}] = H[\Omega | D^{\text{train}}] - H[\Omega | y, x, D^{\text{train}}]. \tag{83}
\]

That is, we can view BALD as weighting the information gains \( I[\Omega; y | x, D^{\text{train}}] \) for different \( y \) by the current model’s belief that \( y \) is correct. If we had access to the labels or a better surrogate distribution for the labels, we could improve on this. This could in particular help with the cold starting problem in active learning when one starts training with no initial training set and the model predictions are not trustworthy at all. When we have access to the labels, we can directly use the information gain \( I[\Omega; y^{\text{true}} | x, D^{\text{train}}] \) and select the samples using a Core-Set by Disagreement acquisition function:

\[
\alpha_{\text{CSD}}(y^{\text{acq}}, \omega^{\text{acq}}, p(\Omega | D^{\text{train}})) := I[\Omega; y^{\text{acq}} | \omega^{\text{acq}}, D^{\text{train}}] \tag{84}
\]

Evaluating the Information Gain. We show how to compute the information for the special case of an MC dropout model with dropout rate \( \frac{1}{2} \) to obtain a variational model distribution \( q(\omega) \), we have \( q(\omega) = \text{const} \), and we can approximate (83) as:

\[
\mathbb{E}_{\omega \sim p(\omega | D^{\text{train}})}[H(\omega | D^{\text{train}}) - H(\omega | y, x, D^{\text{train}})] = H(\omega) - H(\omega | y, x, D^{\text{train}}).
\]

Finally, if we use Monte-Carlo dropout with dropout rate \( \frac{1}{2} \) to obtain a variational model distribution \( q(\omega) \), we have \( q(\omega) = \text{const} \), and we can approximate (83) as:

\[
\mathbb{E}_{\omega \sim p(\omega | D^{\text{train}})}[H(\omega | D^{\text{train}}) - H(\omega | y, x, D^{\text{train}})] = H(\omega) - H(\omega | y, x, D^{\text{train}}).
\]

As an example, Figure 4 shows that CSD strongly outperforms BALD on MNIST in this setup. This approximation is brittle, however. We study this in experiments in §A in the appendix.
Figure 4. CSD vs BALD vs uniform acquisition on MNIST after ambiguous and mislabeled training samples have been removed from the training set. CSD requires only 58 samples to reach 90% accuracy compared to 91 samples for BALD. 5 trials each. Dashed horizontal lines at 90% and 95% accuracy.

6. Conclusion

We have introduced a unified notation for information-theoretic quantities for both random variables and outcomes. We have also unified information gain and surprise by defining the mutual information appropriately. Finally, we have examined applications of our notation which show potential avenues for future research. This shows that our notation allows for new perspectives on well-known problems that simplify thinking about them—a strong signal that it is a useful abstraction.

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A. On CoreSet-by-Disagreement

A.1. Experiments

MNIST. We implement CSD and evaluate it on MNIST to show that it can identify a core-set of training samples that achieves high accuracy and low loss.

CSD is very sensitive to mislabeled samples because we compute the information gain using the provided labels: if a sample is mislabeled and the model has high confidence for the true label already, it will necessarily have a very high information gain and the model will acquire this mislabeled sample.

To avoid this, we train a LeNet ensemble with 5 models on MNIST and discard all training samples with predictive entropy $> 0.01$ nats and whose labels do not match the predictions. This removes about 5678 samples from the training set.

We use a LeNet model (LeCun et al., 1998) with MC dropout (dropout rate $\frac{1}{2}$) in the core-set setting where we have access to labels but otherwise use an active learning setup. We use individual acquisition and compare to BALD, which does not make use of label information, and which we use as a sanity baseline. The training regime follows the one described in Kirsch et al. (2019).

Figure 4 shows that CSD strongly outperforms BALD on MNIST (both with individual acquisitions). Indeed, only 58 samples are required to reach 90% accuracy on average and 111 samples for 95% accuracy compared to BALD which needs about 30 samples more in each case; see also Table 1.

In Figure 5, we show an ablation of using CSD without removing mislabeled or ambiguous samples from the training set. Here, BALD (without label information) outperforms CSD, which shows that CSD suffers from mislabeled examples.

CIFAR-10. However, we cannot produce the same results on cleaned CIFAR-10 (similar like MNIST described above) with ResNet18 models and MC dropout. BALD performs much better than CSD, even when cold starting. The accuracy plot is depicted in Figure 6. This indicates that something is wrong. We have not been able to identify the issue yet.

BatchCSD. Finally, we examine an extension of CSD to the batch case following Kirsch et al. (2019) and compute $I[\Omega; y^{\text{acq}} | x^{\text{acq}}]$ using the approximation $I[y^{\text{acq}}; \Omega | x^{\text{acq}}]$. This approximation does not work well in the batch case, however, even for a batch acquisition size of 5, as depicted in fig. 7 (on MNIST). BatchCSD performs worse than Uniform for $\approx 70$ samples and worse than BALD for 150 samples.

A reason for this could be that the information gain and thus CSD are not submodular. This means that the sequential selection of acquisition (batch) samples has no optimality guarantee, unlike with BALD (Kirsch et al., 2019).

| Acquisition Function | 90% Acc | 95% Acc |
|----------------------|---------|---------|
| Uniform              | 125/130/150 | —   |
| BALD                 | 88/91/99  | 130/145/167 |
| CSD (ours)           | 55/58/58  | 105/111/115 |

Table 1. 25%/50%/75% quantiles for reaching 90% and 95% accuracy on MNIST. 5 trials each.
A.2. Limitations of our Implementation & Approach

We have used our proposed notation to reinterpret BALD as the expected information gain and found an approximation for the information gain which allowed use to introduce CSD and show that it works on MNIST. But we have not been able to provide good results for CIFAR-10 or successfully extend our approximation to the batch case. Moreover, the approximation we have used only works for MC dropout with dropout rate $\frac{1}{2}$. Our approach requires an explicit model, otherwise. Importantly, unlike BALD, the information gain in CSD does also not seem to be submodular, and we cannot infer a $1 - \frac{1}{2}$ optimality that way (Kirsch et al., 2019)—although BALD’s submodularity and optimality is not tied to the generalization loss anyway.