# Unifying Approaches in Data Subset Selection via Fisher Information and Information-Theoretic Quantities

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## Abstract

The mutual information between predictions and model parameters, also known as *expected information gain* or BALD in machine learning, measures informativeness. It is a popular acquisition function in Bayesian active learning. In data subset selection, that is, active learning and active sampling, several recent works use Fisher information, Hessians, similarity matrices based on the gradients, or simply the gradient lengths to compute the acquisition scores that guide sample selection. Are these different approaches connected, and if so, how? In this paper, we revisit the Fisher information and use it to show how several otherwise disparate methods are connected as approximations of information-theoretic quantities known from earlier works in Bayesian optimal experiment design.

## 1 Introduction

Label and training efficiency are the key to a wider deployment of deep learning. Deep learning generally requires a lot of data, most of which must be annotated. This is expensive and time-consuming. Together with semisupervised and unsupervised approaches, active learning helps increase label efficiency. Given access to unlabeled data, *active learning* (Atlas et al., 1990; Cohn et al., 1994) selects the most informative samples to label for a given model, thus decreasing the number of required annotations. In addition to label efficiency, training deep learning models is also expensive and time consuming, and *active sampling* improves training efficiency by filtering the training set to focus on the samples that will be the most informative for the model.

The acquisition functions used to select informative samples can be traced back to information-theoretic objectives that are known from Bayesian optimal experiment design (Lindley, 1956). The connection between contemporary acquisition functions and basic information-theoretic quantities (short: *information quantities*) is the topic of this work. Among them, we examine: for active learning, the *expected information gain (EIG)* (Lindley, 1956; Houlsby et al., 2011; Kirsch et al., 2019), the *(joint) expected predictive information gain (JEPIG or EPIG, respectively)* (Kirsch et al., 2021b; MacKay, 1992), and, for active sampling, the *information gain (IG)* (Sun et al., 2022) and *(joint) predictive information gain (JPIG or PIG, respectively)* (Mindermann et al., 2022).

We show that several contemporary methods can be seen as approximating information quantities with different trade-offs: BADGE (Ash et al., 2019), BAIT (Ash et al., 2021), PRISM[1](Kothawade et al., 2022), SIMILAR[1] (Kothawade et al., 2021), EGL (Settles et al., 2007), and GraNd (Paul et al., 2021). By examining how Fisher information and second-order posterior approximations (Gaussian approximations) can be used for estimating information quantities, we develop a unifying perspective on these existing approaches and relate them to information-theoretic approaches now used in Bayesian active learning: specifically, (Batch)BALD (Houlsby et al., 2011; Kirsch et al., 2019), and (J)EPIG (Kirsch et al., 2021b).

**Outline.** This paper is written in long-form, and we introduce and develop the theory before unifying approaches in the existing literature in data subset selection in §7: we look at second-order posterior approximations (Gaussian approximations) in §3, which we use to revisit Fisher information, its properties, specials case, and approximations in §4. Our contribution is to summarize results and provide a consistent notation that simplifies reasoning about information quantities, observed information, and Fisher information.

In §5, we approximate the information quantities mentioned above using observed information and Fisher information. We provide a comprehensive overview to understand the differences and similarities and make it easier to spot applications of the approximations in the literature. We pay special attention to the limitations: for example, we will see that approximations that use the trace of the Fisher information do not take redundancies between samples into account. They exhibit the same pathologies as other methods that, in essence, score points individually, also known as top-K batch acquisition (Kirsch et al., 2021a). In §6, we also connect these approximations to approximations that use similarity matrices of log-loss gradients. Our contributions are a comprehensive overview of the approximations and the connection to similarity matrices.

In §7, we show that (Batch-)BALD and EPIG on the one hand; and BADGE, BAIT, PRISM[1], and SIMILAR[1] on the other hand can be seen as optimizing the same objectives. The difference is that (Batch-)BALD (Houlsby et al., 2011; Kirsch et al., 2019) and EPIG (Kirsch et al., 2021b) operate in prediction space, while Fisher information-based methods operate in weight space: we show that an approximation of EPIG, a transductive active learning objective, using Fisher information, matches the BAIT objective (Ash et al., 2021); similarly, we show how BADGE (Ash et al., 2019) approximation of the EIG, using the connection between similarity matrices and EIG approximations; and we find that *submodularity*-based approaches (Iyer et al., 2021) such as SIMILAR (Kothawade et al., 2021) and PRISM (Kothawade et al., 2022), which report their best results using the log determinant of similarity matrices, approximate information quantities when they perform best. We also show that gradient-length-based methods like EGL (Settles et al., 2007) and GraNd (Paul et al., 2021) can be connected to information quantities.

**Limitations.** Although our results employ a hierarchy of approximations, we do not examine the error terms in detail. This is in line with how these approximations are used in deep learning, where they often only provide motivation for useful mechanisms. However, we try to identify where these approximations might break, enumerate their limitations, and raise several (empirical) research questions for future work.

**Summary.** Our work shows that various non-Bayesian approaches in data subset selection approximate information quantities from the Bayesian literature, going back to Lindley (1956) and MacKay (1992).

## 2 Background & Setting

This section introduces the relevant notation, concepts, and probabilistic model that we use in this paper.

**Information Theory.** We follow the practical notation of Kirsch and Gal (2021). In particular, for entropy, we use an implicit or explicit notation, $\mathrm{H}[X]$ or $\mathrm{H}(\mathrm{p}(X))$, while $\mathrm{H}(\mathrm{p} \parallel \mathrm{q})$ denotes the cross-entropy similar to the Kullback-Leibler divergence $\mathrm{D}_{\mathrm{KL}}(\mathrm{p} \parallel \mathrm{q})$, and $\mathrm{H}(\mathrm{p}(x))$ denotes Shannon's information content:

$$\mathrm{H}(\mathrm{p}(x)) := -\log \mathrm{p}(x), \tag{1}$$

$$\mathrm{H}[x] := \mathrm{H}(\mathrm{p}(x)), \tag{2}$$

$$\mathrm{H}(\mathrm{p}(X) \parallel \mathrm{q}(X)) := \mathbb{E}_{\mathrm{p}(x)}[\mathrm{H}(\mathrm{q}(x))], \tag{3}$$

$$\mathrm{H}[X] := \mathrm{H}(\mathrm{p}(X)) := \mathrm{H}(\mathrm{p}(X) \parallel \mathrm{p}(X)), \tag{4}$$

where p and q are probabilities distributions, $X$ is a random variable, and $x$ is an outcome. Conditional and joint entropies are defined as usual (note that we also take an expectation over $y$):

$$\mathrm{H}[X \mid Y] = \mathbb{E}_{\mathrm{p}(x,y)}[-\log \mathrm{p}(x \mid y)]. \tag{5}$$

The mutual information $\mathrm{I}[X; Y]$ for random variables $X$ and $Y$ is defined as:

$$\mathrm{I}[X; Y] := \mathrm{H}[X] - \mathrm{H}[X \mid Y], \tag{6}$$

and is also called expected uncertainty reduction or expected information gain (Lindley, 1956) because $\mathrm{H}[X]$ quantifies the uncertainty about $X$, and $\mathrm{H}[X \mid Y]$ about $X$ after observing $Y$ (in expectation).

Furthermore, when we mix random variables with realizations of random variables in (conditional) entropies, for example $\mathrm{H}[X, Y = y \mid Z]$, or short $\mathrm{H}[X, y \mid Z]$, we expand this to an expectation over the random variables

[1] using log determinant objectives

conditional on the realizations:

$$\mathrm{H}[X, y \mid Z] = \mathbb{E}_{\mathrm{p}(x,z|y)}[-\log \mathrm{p}(x, y \mid z)]. \tag{7}$$

**Probabilistic Model.** We assume a supervised setting: for inputs $X$, we have a Bayesian model with parameters $\Omega$ that makes predictions $Y$. What makes the model Bayesian is that the parameters follow a distribution $\mathrm{p}(\omega)$, and we have a probabilistic model:

$$\mathrm{p}(y, \omega \mid x) = \mathrm{p}(y \mid x, \omega)\ \mathrm{p}(\omega). \tag{8}$$

We extend this model to additional data $\mathcal{D} \coloneqq \{(x_i, y_i)\}$ as follows:

$$\mathrm{p}(\{y_i\}, \omega \mid \{x_i\}) = \mathrm{p}(\{y_i\} \mid \{x_i\}, \omega)\ \mathrm{p}(\omega) = \mathrm{p}(y_1, \ldots, y_n \mid x_1, \ldots, x_n, \omega)\ \mathrm{p}(\omega). \tag{9}$$

That is, we examine the common discriminative case where, unlike in the generative case, we do not model $\mathrm{p}(x)$. The corresponding marginal prediction of the model is $\mathrm{p}(y \mid x) = \mathbb{E}_{\mathrm{p}(\omega)}[\mathrm{p}(y \mid x, \omega)]$.

**Transductive Objectives.** When an objective uses (additional) data $\mathcal{D}^{\mathrm{eval}}$, unlabeled or labeled, to guide acquisitions, we refer to the objective as a *transductive* objective (Yu et al., 2006; Wang et al., 2020).

**Active Learning.** To increase label efficiency, instead of labeling data indiscriminately, active learning iteratively selects and acquires labels for the *most informative* unlabeled data from a *pool set* $\mathcal{D}^{\mathrm{pool}}$ to some underlying *acquisition function*. An acquisition function scores the informativeness of an unlabeled candidate sample $x^{\mathrm{acq}}$, and the sample that maximizes this score is selected for labeling. After each acquisition step, the model is retrained to take the newly labeled data into account. Labels can be acquired individually or in batches (*batch acquisition*, see below). The *expected information gain (EIG)*

$$\mathrm{I}[\Omega; Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}] \tag{EIG/BALD}$$

and *(joint) expected predictive information gain (JEPIG and EPIG, respectively)*

$$\mathrm{I}[\{Y_i^{\mathrm{eval}}\}; Y^{\mathrm{acq}} \mid \{x_i^{\mathrm{eval}}\}, x^{\mathrm{acq}}], \tag{JEPIG}$$

$$\mathrm{I}[Y^{\mathrm{eval}}; Y^{\mathrm{acq}} \mid X^{\mathrm{eval}}, x^{\mathrm{acq}}] \tag{EPIG}$$

are examples of such acquisition functions. EPIG and JEPIG are transductive acquisition functions as they depend on $X^{\mathrm{eval}}, \{x_i^{\mathrm{eval}}\}$, respectively.

**Active Sampling.** To increase training efficiency, instead of training with all samples, active sampling (sometimes also called *data pruning*) (Paul et al., 2021) selects the most informative sample $(x^{\mathrm{acq}}, y^{\mathrm{acq}})$ from the training set to train on next. This can be done statically before training the model, in which case this is also referred to as core-set selection, or dynamically, in which case it is also referred to as curriculum learning. The *information gain (IG)*

$$\mathrm{I}[\Omega; y^{\mathrm{acq}} \mid x^{\mathrm{acq}}], \tag{IG}$$

and *(joint) predictive information gain (JPIG or PIG, respectively)*

$$\mathrm{I}[\{y_i^{\mathrm{eval}}\}; y^{\mathrm{acq}} \mid \{x_i^{\mathrm{eval}}\}, x^{\mathrm{acq}}], \tag{JPIG}$$

$$\mathrm{I}[Y^{\mathrm{eval}}; y^{\mathrm{acq}} \mid X^{\mathrm{eval}}, x^{\mathrm{acq}}] \quad (= \mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}}, y^{\mathrm{eval}})}\, \mathrm{I}[y^{\mathrm{eval}}; y^{\mathrm{acq}} \mid x^{\mathrm{eval}}, x^{\mathrm{acq}}]) \tag{PIG}$$

are examples of such acquisition functions. PIG and JPIG are transductive acquisition functions.

**Batch Acquisition.** In batch active learning, the acquisition function is applied to a batch of candidates $\{{x^{\mathrm{acq}}}_i\}_{i=1}^B$ and the batch that maximizes the acquisition function is selected for labeling. Similarly, in batch active sampling, the acquisition function is applied to a batch of training samples $\{({x^{\mathrm{acq}}}_i, {y^{\mathrm{acq}}}_i)\}_{i=1}^B$ and the batch that maximizes the acquisition function is selected for training. For deep learning, batch acquisition is usually the only feasible option in both active learning and active sampling. We extend the above acquisition

Table 1: *Taxonomy of Information Quantities for Data Subset Selection.* In general, information quantities can be split into ones for active sampling or active learning, into non-transductive and transductive ones, and in the transductive case, into taking an expectation or the joint over (additional) evaluation samples. Here, we show the information quantities for individual acquisition. For batch acquisition, $\{Y_i^{\text{acq}}\}, \{y_i^{\text{acq}}\}, \{x_i^{\text{acq}}\}$ can be substituted.

| | | Active Learning | | Active Sampling | |
|---|---|---|---|---|---|
| Non-Transductive | | EIG/BALD | $\mathrm{I}[\Omega; Y^{\text{acq}} \mid x^{\text{acq}}]$ | IG | $\mathrm{I}[\Omega; y^{\text{acq}} \mid x^{\text{acq}}]$ |
| Transductive (using $\mathcal{D}^{\text{eval}}$) | Expectation | EPIG | $\mathbb{E}_{\hat{\mathrm{p}}(x^{\text{eval}})}\, \mathrm{I}[Y^{\text{eval}}; Y^{\text{acq}} \mid x^{\text{eval}}, x^{\text{acq}}]$ | PIG | $\mathbb{E}_{\hat{\mathrm{p}}(y^{\text{eval}}, x^{\text{eval}})}\, \mathrm{I}[y^{\text{eval}}; y^{\text{acq}} \mid x^{\text{eval}}, x^{\text{acq}}]$ |
| | Joint | JEPIG | $\mathrm{I}[\{Y_i^{\text{eval}}\}; Y^{\text{acq}} \mid \{x_i^{\text{eval}}\}, x^{\text{acq}}]$ | JPIG | $\mathrm{I}[\{y_i^{\text{eval}}\}; y^{\text{acq}} \mid \{x_i^{\text{eval}}\}, x^{\text{acq}}]$ |

functions to the batch case by substituting a set of samples in the definitions: $\{x_i^{\text{acq}}\}$ for $x^{\text{acq}}$, $\{Y_i^{\text{acq}}\}$ for $Y^{\text{acq}}$, and $\{y_i^{\text{acq}}\}$ for $y^{\text{acq}}$, respectively, and treating the sets as joint random variables (Kirsch et al., 2019).

**Submodular Acquisition Functions.** Choosing the subset $\{x_i^{\text{acq}}\}$ naively is intractable due to the exponential number of possible acquisition batches. Instead of maximizing the acquisition function on all possible batches, we can often make use of submodularity (Nemhauser et al., 1978): a set function $f$ is submodular when:

$$f(A \cup B) \leq f(A) + f(B) - f(A \cap B). \tag{submodular}$$

An acquisition batch $\{x_i^{\text{acq}}\}$ can be constructed greedily by selecting the samples that increase the acquisition function the most one-by-one. This greedy algorithm is guaranteed to find a $1 - \frac{1}{e}$-optimal acquisition batch for monotone submodular acquisition functions.

Although the EIG is (monotone) submodular, leading to efficient batch acquisition (Kirsch et al., 2019), the other information quantities are usually not submodular. Crucially, most information quantities (IG, EPIG, JEPIG, PIG) are not submodular (Kirsch et al., 2021b). We examine details of this and compare relevant literature in §7.

**Taxonomy of Information Quantities.** Table 1 shows the information quantities along three dimensions: active learning vs active sampling, non-transductive vs transductive, and taking the expectation vs the joint over evaluation samples for transductive information quantities.

**Log Loss.** While many active learning and active sampling methods are motivated independently of the underlying loss, we will focus on log losses, such as the common cross-entropy loss or squared error loss (Gaussian error), as these log losses can be viewed through an information-theoretic or probabilistic lens.

## 3 Second-Order Posterior Approximation

Laplace approximations are a common tool in Bayesian statistics and machine learning (Daxberger et al., 2021; Immer et al., 2020). In this section, we review the Laplace approximation and introduce it as a special case of a more flexible second-order posterior approximation, a *Gaussian approximation*. It is the central to approximating information quantities using observed information, defined in this section, and Fisher information, defined in §4.

Our goal is to approximate the posterior $\mathrm{p}(\omega \mid \mathcal{D}, \mathcal{D}^{\text{train}})$ using a (multivariate) Gaussian distribution, where $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ are additional (new) samples, and we start with $\mathrm{p}(\omega \mid \mathcal{D}^{\text{train}})$ as the "prior" distribution—we will drop $\mathcal{D}^{\text{train}}$ and use $\mathrm{p}(\omega)$ when possible, to shorten the notation.

To begin, we complete the square of a second-order Taylor approximation around the log-parameter likelihood for a fixed $\omega^*$:

$$\begin{aligned} \log \mathrm{p}(\omega) &\approx \log \mathrm{p}(\omega^*) + \nabla_\omega[\log \mathrm{p}(\omega^*)](\omega - \omega^*) + \frac{1}{2}(\omega - \omega^*)^T \nabla_\omega^2[\log \mathrm{p}(\omega^*)](\omega - \omega^*) \\ &= \frac{1}{2}(\omega - (\omega^* - \nabla_\omega^2[\log \mathrm{p}(\omega^*)]^{-1}\nabla_\omega[\log \mathrm{p}(\omega^*)])^T \nabla_\omega^2[\log \mathrm{p}(\omega^*)](\omega - (\omega^* - \nabla_\omega^2[\log \mathrm{p}(\omega^*)]^{-1}\nabla_\omega[\log \mathrm{p}(\omega^*)])) \end{aligned} \tag{10}$$

$$+ \dots . \tag{11}$$

Importantly, we can express this more concisely by extending the notation of $\mathrm{H}[\cdot]$ to its derivatives:

**Notation 3.1.** *We write* $\mathrm{H}'[\cdot]$ *for the Jacobian and* $\mathrm{H}''[\cdot]$ *for the Hessian of* $\mathrm{H}[\cdot]$*:*

$$\mathrm{H}'[\cdot] \coloneqq -\nabla_\omega \log \mathrm{p}(\cdot), \tag{12}$$

$$\mathrm{H}''[\cdot] \coloneqq -\nabla^2_\omega \log \mathrm{p}(\cdot). \tag{13}$$

This notation will be useful throughout this paper, as both observed information and Fisher information can be expressed in terms of the Hessian of the negative log-parameter likelihood.

Then, we have:

$$\mathrm{H}[\omega] \approx \mathrm{H}[\omega^*] + \mathrm{H}'[\omega^*](\omega - \omega^*) + \frac{1}{2}(\omega - \omega^*)^T \, \mathrm{H}''[\omega^*] \, (\omega - \omega^*) \tag{14}$$

$$= \frac{1}{2}(\omega - (\omega^* - \mathrm{H}''[\omega^*]^{-1} \, \mathrm{H}'[\omega^*])^T \, \mathrm{H}''[\omega^*] \, (\omega - (\omega^* - \mathrm{H}''[\omega^*]^{-1} \, \mathrm{H}'[\omega^*])) + \dots . \tag{15}$$

Comparing this to the information content of a multivariate Gaussian distribution:

$$\mathrm{H}[\mathcal{N}(w;\, \mu,\, \Sigma)] = \frac{1}{2}(\omega - \mu)^T \, \Sigma^{-1} \, (\omega - \mu) + \dots , \tag{16}$$

we obtain the Gaussian approximation, which we will apply throughout this paper:

**Proposition 3.2.** *The* Gaussian approximation *of the distribution* $\mathrm{p}(\omega)$ *of* $\Omega$ *around some* $\omega^*$ *is given by:*

$$\Omega \approxeq \mathcal{N}(\omega^* - \mathrm{H}''[\omega^*]^{-1} \, \mathrm{H}'[\omega^*],\, \mathrm{H}''[\omega^*]^{-1}), \tag{17}$$

*where* $\mathrm{H}''[\omega^*]$ *must be positive-definite. If* $\omega^*$ *is also a (global) minimizer of* $\mathrm{H}[\omega]$ *(that is,* $\mathrm{H}'[\omega^*] = 0$*), we obtain the* Laplace approximation*:*

$$\Omega \approxeq \mathcal{N}(\omega^*,\, \mathrm{H}''[\omega^*]^{-1}). \tag{18}$$

**Approximation Quality.** Obviously, this approximation can be arbitrarily bad depending on $\mathrm{p}(\omega)$ and $\omega^*$—however, given enough data, we expect that $\mathrm{p}(w)$ will concentrate around a maximum a posteriori (MAP) estimate, giving rise to the Laplace approximation. Obviously, insufficient data to reach concentration of parameters and multimodality in over-parameterized models (Long, 2021) can be issues for active learning and active sampling, in particular.

**Flat Minimum Intuition.** The information-geometric interpretation of the Hessian being positive definite is that the information content (pointwise entropy) is convex around $\omega^*$ and, equivalently, that the (log) posterior is concave around $\omega^*$. The latter provides an intuition for the Gaussian approximation: the Hessian measures curvature, and the "flatter" the Hessian, e.g., the smaller the largest eigenvalue or the smaller the determinant, the less the loss changes when $\omega^*$ is perturbed. This leads to the search for flat minima as a way to improve generalization (Hinton and Van Camp, 1993; Hochreiter and Schmidhuber, 1994).

**Notation 3.3.** *To further shorten the notation, we write* $\mathrm{H}''[\mathcal{D} \mid \omega^*]$ *instead of* $\mathrm{H}''[\{y_i\} \mid \{x_i\}, \omega^*]$.

**Posterior Approximation of $\Omega \mid \mathcal{D}$.** While the Laplace approximation is centered on a (global) minimizer, the approach above can be used for a (potentially low-quality) posterior approximation in general. We can expand $\mathrm{H}[\omega^* \mid \mathcal{D}]$ using Bayes' law and the additivity of the logarithm. That is, we have:

$$\mathrm{H}[\omega^* \mid \mathcal{D}] = \mathrm{H}[\mathcal{D} \mid \omega^*] + \mathrm{H}[\omega^*] - \mathrm{H}[\mathcal{D}], \tag{19}$$

and then, as $\mathrm{H}[\mathcal{D}]$ is independent of $\omega$:

$$\mathrm{H}'[\omega^* \mid \mathcal{D}] = \mathrm{H}'[\mathcal{D} \mid \omega^*] + \mathrm{H}'[\omega^*] + 0 = \mathrm{H}'[\mathcal{D} \mid \omega^*] + \mathrm{H}'[\omega^*], \tag{20}$$

$$\mathrm{H}''[\omega^* \mid \mathcal{D}] = \mathrm{H}''[\mathcal{D} \mid \omega^*] + \mathrm{H}''[\omega^*]. \tag{21}$$

**Proposition 3.4.** *The* observed information $\mathrm{H}''[\{y_i\} \mid \{x_i\}, \omega^*]$ *is additive:*

$$\mathrm{H}''[\{y_i\} \mid \{x_i\}, \omega^*] = \sum_i \mathrm{H}''[y_i \mid x_i, \omega^*] = \sum_i -\nabla^2_\omega \log \mathrm{p}(y_i \mid x_i, \omega^*). \tag{22}$$

We define the observed information with opposite sign compared to other works because it simplifies the exposition.

**Uninformative Prior.** For a typical Gaussian prior $\mathrm{p}(\omega) \sim \mathcal{N}(\mu, \Sigma)$, we have $\mathrm{H}''[\omega^*] = \Sigma^{-1}$ and $\mathrm{H}''[\omega^* \mid \mathcal{D}] = \mathrm{H}''[\mathcal{D} \mid \omega^*] + \Sigma^{-1}$. For an uninformative prior with "infinite prior variance" $\Sigma^{-1} \to 0$, we have $\mathrm{H}''[\omega^*] = 0$, and $\mathrm{H}''[\omega^* \mid \mathcal{D}] = \mathrm{H}''[\mathcal{D} \mid \omega^*]$.

**Proposition 3.5.** *The entropy of the second-order approximation of* $\mathrm{p}(\omega)$ *around* $\omega^*$ *is*

$$\mathrm{H}[\Omega] \approx -\tfrac{1}{2} \log \det \mathrm{H}''[\omega^*] + C_k, \tag{23}$$

*where* $C_k = \frac{k}{2} \log 2\pi e$ *is a constant (independent of* $\mathcal{D}$ *and* $\omega^*$*) and* $k$ *is the number of dimensions of* $\omega$*.*

While Proposition 3.5 is straightforward, it is the main result for this section as it will allow us to approximate all the mentioned information quantities in §5 and §6.

## 4 Fisher Information

Fisher information plays a central role in the approximations of information quantities because, unlike the observed information, it is always positive semidefinite. We use Fisher information to unify various acquisition functions in §7. The following section revisits Fisher information, its properties, special cases, and common approximations. All proofs are given in §A.

In particular, we look at two special cases with more favorable properties: following Kunstner et al. (2019), when we can write our model as $\mathrm{p}(y \mid \hat{z} = \hat{f}(x; \omega))$, where $\hat{f}(x; \omega)$ are the logits, and $\mathrm{p}(y \mid \hat{z})$ is a distribution from an exponential family, Fisher information is independent of $y$, which has useful consequences as we shall see; and following Chaudhuri et al. (2015), when we have a *Generalized Linear Model (GLM)*, the observed information is independent of $y$. The results for the GLM are also used as an approximation known as *Generalized Gauss-Newton approximation (GGN)*. Together with numerical approximations, such as using a diagonal approximation or low-rank factorizations, the observed information and Fisher information can be efficiently approximated for large deep neural networks (Daxberger et al., 2021).

**Definition 4.1.** *The* Fisher information $\mathrm{H}''[Y \mid x, \omega^*]$ *is the expectation over the observed information using the model's own predictions* $\mathrm{p}(y \mid x, \omega^*)$ *for given* $x$ *at* $\omega^*$*:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathbb{E}_{\mathrm{p}(y \mid x, \omega^*)}[\mathrm{H}''[y \mid x, \omega^*]]. \tag{24}$$

This notation of the Fisher information is consistent with the notation for information quantities from §2, introduced in Kirsch and Gal (2021), but extended to the observed information: the Fisher is but an expectation over the observed information, and the observed information is the Hessian of the negative log-likelihood.

**Proposition 4.2.** *Like the observed information, Fisher information is additive:*

$$\mathrm{H}''[\{Y_i\} \mid \{x_i\}, \omega^*] = \sum_i \mathrm{H}''[\{Y_i\} \mid x_i, \omega^*]. \tag{25}$$

There are two other equivalent definitions of Fisher information:

**Proposition 4.3.** *Fisher information is equivalent to:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathbb{E}_{\mathrm{p}(y \mid x, \omega^*)}[\mathrm{H}'[y \mid x, \omega^*]^T \, \mathrm{H}'[y \mid x, \omega^*]] = \mathrm{Cov}[\mathrm{H}'[Y \mid x, \omega^*]]. \tag{26}$$

**Special Case: Exponential Family.** Kunstner et al. (2019) show in their appendix that if we split a discriminative model into prelogits $\hat{f}(x;\omega)$ and a predictor $\mathrm{p}(y \mid \hat{z} = \hat{f}(x;\omega))$, the observed information does not depend on $y$ when $\mathrm{p}(y \mid \hat{z})$ is a distribution from an exponential family (independent of $\omega$). This covers a normal distribution for regression parameterized by mean and variance predictions or a categorical distribution via the softmax function. The following statements and proofs follow Kunstner et al. (2019):

**Proposition 4.4.** *The Fisher information* $\mathrm{H}''[Y \mid x, \omega^*]$ *for a model* $\mathrm{p}(y \mid \hat{z} = \hat{f}(x;\omega^*))$ *is equivalent to:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \nabla_\omega \hat{f}(x;\omega^*)^T \, \mathbb{E}_{\mathrm{p}(y|x,\omega^*)}[\nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x;\omega^*)]] \nabla_\omega \hat{f}(x;\omega^*), \tag{27}$$

*where* $\nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x;\omega^*)]$ *is short for* $\nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z}]\big|_{\hat{z}=\hat{f}(x;\omega^*)}$.

**Proposition 4.5.** *The Fisher information* $\mathrm{H}''[Y|x, \omega^*]$ *of a model of the form* $\mathrm{p}(y|\hat{z} = \hat{f}(x;\omega^*))$ *is independent of* $y$*, where* $\mathrm{p}(y \mid \hat{z})$ *is a distribution from an exponential family, i.e.,* $\log \mathrm{p}(y \mid \hat{z}) = \hat{z}^T T(y) - A(\hat{z}) + \log h(y)$*:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \nabla_\omega \hat{f}(x;\omega^*)^T \, \nabla^2_{\hat{z}} A(\hat{z} = \hat{f}(x;\omega^*)) \, \nabla_\omega \hat{f}(x;\omega^*). \tag{28}$$

*It is crucial that the exponential distribution not depend on* $\omega$*.* This simplifies computing the Fisher information: no expectation over $y$s is needed anymore. The full outer product may not be needed explicitly either.

As examples, we will consider two common parameteric distributions from the exponential family:

**Gaussian Distribution.** When $\mathrm{p}(y \mid \hat{z}) = \mathcal{N}(y;\, \hat{z},\, 1)$, we have $\mathrm{H}''[y \mid \hat{z}] = 1$ for all $y, \hat{z}$, and thus

$$\mathrm{H}''[Y \mid x, \omega^*] = \nabla_\omega \hat{f}(x;\omega^*)^T \, \nabla_\omega \hat{f}(x;\omega^*). \tag{29}$$

**Categorical Distribution.** When $\mathrm{p}(y \,|\, \hat{z}) = \mathrm{softmax}(\hat{z})_y$, we have $\mathrm{H}''[y \,|\, \hat{z}] = \mathrm{diag}(\pi) - \pi \, \pi^T$, with $\pi_y = \mathrm{p}(y \,|\, \hat{z})$, and thus:

$$\mathrm{H}''[Y \mid x, \omega^*] = \nabla_\omega \hat{f}(x;\omega^*)^T \, (\mathrm{diag}(\pi) - \pi \, \pi^T) \, \nabla_\omega \hat{f}(x;\omega^*). \tag{30}$$

**Special Case: Generalized Linear Models.** Chaudhuri et al. (2015) require that the observed information is independent of $y$, which we will also use later. This holds for Generalized Linear Models:

**Definition 4.6.** *A* generalized linear model (GLM) *is a model* $\mathrm{p}(y \mid \hat{z} = \hat{f}(x;\omega))$ *such that* $\log \mathrm{p}(y \mid \hat{z}) = \hat{z}^T T(y) - A(\hat{z}) + \log h(y)$ *is a distribution of the exponential family, independent of* $\omega$*, and* $\hat{f}(x;\omega) = \omega^T x$ *is linear in the parameters* $\omega$*.*

**Proposition 4.7.** *The observed information* $\mathrm{H}''[y \mid x, \omega^*]$ *of a GLM is independent of* $y$*.*

$$\mathrm{H}''[y \mid x, \omega^*] = \nabla_\omega \hat{f}(x;\omega^*)^T \, \nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x;\omega^*)] \, \nabla_\omega \hat{f}(x;\omega^*) \tag{31}$$

$$= \nabla_\omega \hat{f}(x;\omega^*)^T \, \nabla^2_{\hat{z}} A(w^T x) \, \nabla_\omega \hat{f}(x;\omega^*). \tag{32}$$

**Proposition 4.8.** *For a model such that the observed information* $\mathrm{H}''[y \mid x, \omega^*]$ *is independent of* $y$*, we have the following:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathrm{H}''[y^* \mid x, \omega^*] \tag{33}$$

*for any* $y^*$*, and also trivially:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathbb{E}_{\mathrm{p}(y|x)}[\mathrm{H}''[y \mid x, \omega^*]]. \tag{34}$$

Note that the expectation is over $\mathrm{p}(y \,|\, x)$ and not $\mathrm{p}(y \,|\, x, \omega^*)$, and $\mathbb{E}_{\mathrm{p}(\{y_i\}|\{x_i\})}[\mathrm{H}''[\{y_i\} \,|\, \{x_i\}, \omega^*]] = \mathrm{H}''[\{Y_i\} \,|\, \{x_i\}, \omega^*]$ is additive then.

**Proposition 4.9.** *For a GLM, when $\hat{f}(x;\omega) : \mathbb{R}^D \to \mathbb{R}^K$, where $K$ is the number of classes (outputs), $D$ is the number of input dimensions, $\omega \in \mathbb{R}^{D\times K}$, and assuming the parameters are flattened into a single vector for the Jacobian, we have $\nabla_\omega \hat{f}(x;\omega) = \mathrm{Id}_K \otimes x^T \in \mathbb{R}^{K\times(K\cdot D)}$, where $\otimes$ denotes the Kronecker product, and:*

$$\nabla_\omega \hat{f}(x;\omega^*)^T \, \nabla^2_{\hat{z}} A(\omega^T x) \, \nabla_\omega \hat{f}(x;\omega^*) = \nabla^2_{\hat{z}} A(w^T x) \otimes x \, x^T. \tag{35}$$

This property is useful for computing the Fisher information of a GLM in practice.

**$\mathrm{p}(y \mid x, \omega^*)$ vs $\mathrm{p}(y \mid x)$.** Having a GLM solves an important issue we will encounter in §5: approximating the EIG requires taking an expectation over $\mathrm{p}(y \mid x)$ and not $\mathrm{p}(y \mid x, \omega^*)$. One can approximate $\mathrm{p}(y \mid x) \approx \mathrm{p}(y \mid x, \omega^*)$, which can be justified in the limit, but this is probably not a good approximation in the cases interesting for active learning and active sampling. With a GLM, this is not a problem.

**Generalized Gauss-Newton Approximation.** In the case of an exponential family but not a GLM, the equality in Proposition 4.7 is often used as an approximation for the observed information—we simply use the Fisher information as an approximation of the observed information (via Proposition 4.5):

$$\mathrm{H}''[y \mid x, \omega^*] \approx \mathrm{H}''[Y \mid x, \omega^*] = \nabla_\omega \hat{f}(x;\omega^*)^T \, \nabla^2_{\hat{z}} A(w^T x) \, \nabla_\omega \hat{f}(x;\omega^*). \tag{36}$$

This is known as *Generalized Gauss-Newton (GGN) approximation* (Kunstner et al., 2019; Immer et al., 2020). This approximation has the advantage that it is always positive semidefinite unlike the true Hessian.

**Last-Layer Approaches.** GLMs are often used in deep active learning (Ash et al., 2019; 2021; Kothawade et al., 2022; 2021). If we split the model into $\mathrm{p}(y \mid x, \omega) = \mathrm{p}(y \mid z = \omega^T f(x))$, where $z = f(x)$ are the embeddings and treat the encoder $f(x)$ as fixed, we obtain a GLM that only uses the embeddings and weights of the last layer.

Armed with this knowledge, we can now derive approximations for the information quantities using the observed information and Fisher information and consider their properties. Both GGN approximation and last-layer approaches feature heavily in the literature to make computing these approximations more tractable as they reduce computational and memory requirements.

## 5 Approximating Information Quantities

We derive approximations and proxy objectives for information quantities. We base them on the observed information and Fisher information introduced in the previous sections. These approximations help us connect the information quantities to existing the literature in non-Bayesian data subset selection in §7.

In particular, we derive approximations for EIG and EPIG as they show the qualitative differences between transductive and non-transductive objectives, and compare the approximations of the IG and EIG: importantly, there is no difference between the two when we use a GLM or GGN approximation. This covers two of the three dimensions in Table 1. We examine JEPIG and the other quantities in the appendix in §B. In particular, we find that the trace approximations of the EPIG and JEPIG objective matches, suggesting that using the trace approximations might be too loose an approximation to capture important qualities of EPIG (Kirsch et al., 2021b). Additional derivations and details can also be found in §B. All this leads to Figure 1, which comprehensively relates the different approximations to each other and shows that they follow simple patterns.

### 5.1 Approximate Expected Information Gain

The expected information gain is a popular acquisition function in Bayesian optimal experimental design (Lindley, 1956) and in active learning, where it is also known as BALD (Houlsby et al., 2011; Gal et al., 2017).

We can approximate the EIG $\mathrm{I}[\Omega; \{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}]$ of acquisition candidates $\{x_i^{\mathrm{acq}}\}$ using Gaussian approximations:

$$\mathrm{I}[\Omega; \{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}] = \mathrm{H}[\Omega] - \mathrm{H}[\Omega \mid \{Y_i^{\mathrm{acq}}\}, \{x_i^{\mathrm{acq}}\}] \tag{37}$$

$$= \mathrm{H}[\Omega] - \mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\mathrm{H}[\Omega \mid \{y_i^{\mathrm{acq}}\}, \{x_i^{\mathrm{acq}}\}]] \tag{38}$$

$$\approx -\tfrac{1}{2}\log\det \mathrm{H}''[\omega^*] - \mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[-\tfrac{1}{2}\log\det \mathrm{H}''[\omega \mid \{y_i^{\mathrm{acq}}\}, \{x_i^{\mathrm{acq}}\}]] \tag{39}$$

$$= \tfrac{1}{2}\,\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\log\det\left((\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*] + \mathrm{H}''[\omega^*])\,\mathrm{H}''[\omega^*]^{-1}\right)] \tag{40}$$

$$= \tfrac{1}{2}\,\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\log\det\left(\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]\;\mathrm{H}''[\omega^*]^{-1} + Id\right)]. \tag{41}$$

using Proposition 3.5 twice, where the constant $C_k$ cancels out in eq. (39) as we subtract two entropy terms.

**Generalized Linear Model.** When we have a GLM, we can use Proposition 4.8 to obtain:

$$\mathrm{I}[\Omega; \{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}] \approx \ldots = \tfrac{1}{2}\,\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\log\det\left(\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]\;\mathrm{H}''[\omega^*]^{-1} + Id\right)] \tag{42}$$

$$= \tfrac{1}{2}\log\det\left(\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]\;\mathrm{H}''[\omega^*]^{-1} + Id\right). \tag{43}$$

We can upper-bound the log determinant and obtain:

$$\leq \tfrac{1}{2}\,\mathrm{tr}\left(\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]\;\mathrm{H}''[\omega^*]^{-1}\right) \tag{44}$$

$$= \tfrac{1}{2}\sum_i \mathrm{tr}\left(\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid {x^{\mathrm{acq}}}_i, \omega^*]\;\mathrm{H}''[\omega^*]^{-1}\right). \tag{45}$$

where we have used the following inequality (proof in §B.1):

**Lemma 5.1.** *For symmetric, positive semidefinite matrices $A$, we have (with equality iff $A = 0$):*

$$\log\det(A + Id) \leq \mathrm{tr}(A). \tag{46}$$

**General Case & Exponential Family.** For the general case, we need to make a strong approximation:

$$\mathrm{p}(\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}) \approx \mathrm{p}(\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*), \tag{47}$$

which probably holds for a mostly converged posterior, but might not in cases with little data. This turns the approximation into an upper bound. Alternatively, we could use the GGN approximation when we have an exponential family for the same result (but not an upper bound). See §B.1 for the derivation.

**Proposition 5.2** (EIG)**.** *The expected information gain can be approximately upper bounded via:*

$$\mathrm{I}[\Omega; \{Y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] \overset{\approx}{\leq} \tfrac{1}{2}\log\det\left(\sum_i \mathrm{H}''[{Y^{acq}}_i \mid {x^{acq}}_i, \omega^*]\;\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]^{-1} + Id\right) \tag{48}$$

$$\leq \tfrac{1}{2}\sum_i \mathrm{tr}\left(\mathrm{H}''[{Y^{acq}}_i \mid {x^{acq}}_i, \omega^*]\,\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]^{-1}\right). \tag{49}$$

*Furthermore, we have the following proxy objective:*

$$\arg\max_{\{x_i^{acq}\}} \mathrm{I}[\Omega; \{Y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] = \arg\max_{\{x_i^{acq}\}} -\mathrm{H}[\Omega \mid \{Y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}]\ ,\ \textit{and} \tag{50}$$

$$-\mathrm{H}[\Omega \mid \{Y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}] \overset{\approx}{\leq} \tfrac{1}{2}\log\det\left(\sum_i \mathrm{H}''[{Y^{acq}}_i \mid {x^{acq}}_i, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]\right) - C_k. \tag{51}$$

The second statement follows from Equation (37), since $\mathrm{H}[\Omega \,|\, \mathcal{D}^{\mathrm{train}}]$ is constant and provides a proxy objective when we are only interested in optimization of the EIG. In §7, we use it to show a connection to the expected gradient length approach in active learning and that an ablation in Ash et al. (2021) examines the wrong objective in ablation as alternative to BAIT.

**Batch Acquisition Pathologies.** Importantly, this approximation of the EIG using the trace is additive, whereas the one using the log determinant is not. This means that the trace approximation ignores the dependencies between the samples and can only lead to naive top-k batch acquisition; see Kirsch et al. (2019; 2021a) for details of the pathologies of top-k batch acquisition.

### 5.2 Approximate Information Gain

Following the same steps, we can also approximate the information gain, which is useful for active sampling:

**Proposition 5.3** (IG). *The* information gain $\mathrm{I}[\Omega; \{y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] = \mathrm{H}[\Omega \mid \mathcal{D}^{train}] - \mathrm{H}[\Omega \mid \{y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}]$ *can be approximately upper bounded via:*

$$\mathrm{I}[\Omega; \{y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] \approx \tfrac{1}{2} \log\det\left(\mathrm{H}''[\{y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*]\ \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]^{-1} + Id\right) \tag{52}$$

$$\leq \tfrac{1}{2} \sum_i \mathrm{tr}\left(\mathrm{H}''[{y^{acq}}_i \mid {x^{acq}}_i, \omega^*]\ \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]^{-1}\right). \tag{53}$$

*Furthermore, we have the following proxy objective:*

$$\arg\max_{\{x_i^{acq}\}} \mathrm{I}[\Omega; \{y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] = \arg\max_{\{x_i^{acq}\}} -\mathrm{H}[\Omega \mid \{y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}], \text{ and} \tag{54}$$

$$-\mathrm{H}[\Omega \mid \{y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}] \approx \tfrac{1}{2} \log\det\left(\mathrm{H}''[\{y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]\right) - C_k. \tag{55}$$

**Comparison to EIG.** Importantly, when we have a GLM or use the GGN approximation, this approximation of the IG is equal to the one of the EIG. This tells us that active learning on a GLM with the EIG approximation will work as well as if we had access to the labels. Equivalently, active sampling via IG with the GGN approximation will not work better than the respective active learning approach.

### 5.3 Approximate (Joint) Expected Predictive Information Gain

In transductive active learning, we have access to an (empirical) distribution $\hat{\mathrm{p}}(x^{\mathrm{eval}})$ (e.g., the pool set) and want to find the $\{x_i^{\mathrm{acq}}\}$ that maximizes the *expected predictive information gain (EPIG)* (Kirsch et al., 2021b). The approximations here will help us connect BAIT (Ash et al., 2021) to EPIG. For simplicity, we only consider the non-batch case. The batch case can be handled analogously. The EPIG objective is defined as:

$$\arg\max_{x^{\mathrm{acq}}} \mathrm{I}[Y^{\mathrm{eval}}; Y^{\mathrm{acq}} \mid X^{\mathrm{eval}}, x^{\mathrm{acq}}] = \arg\max_{x^{\mathrm{acq}}} \mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}})}\, \mathrm{I}[Y^{\mathrm{eval}}; Y^{\mathrm{acq}} \mid x^{\mathrm{eval}}, x^{\mathrm{acq}}], \tag{56}$$

We expand the objective as follows:

$$\mathrm{I}[Y^{\mathrm{eval}}; Y^{\mathrm{acq}} \mid X^{\mathrm{eval}}, x^{\mathrm{acq}}] = \mathrm{I}[\Omega; Y^{\mathrm{eval}} \mid X^{\mathrm{eval}}] - \mathrm{I}[\Omega; Y^{\mathrm{eval}} \mid X^{\mathrm{eval}}, Y^{\mathrm{acq}}, x^{\mathrm{acq}}], \tag{57}$$

where $\mathrm{I}[\Omega; Y^{\mathrm{eval}} \mid X^{\mathrm{eval}}]$ can be removed from the objective because it is independent of $x^{\mathrm{acq}}$. Thus, optimizing EPIG is equivalent to *minimizing* $\mathrm{I}[\Omega; Y^{\mathrm{eval}} \mid X^{\mathrm{eval}}, Y^{\mathrm{acq}}, x^{\mathrm{acq}}]$:

$$\arg\max_{x^{\mathrm{acq}}} \mathrm{I}[Y^{\mathrm{eval}}; Y^{\mathrm{acq}} \mid X^{\mathrm{eval}}, x^{\mathrm{acq}}] = \arg\min_{x^{\mathrm{acq}}} \mathrm{I}[\Omega; Y^{\mathrm{eval}} \mid X^{\mathrm{eval}}, Y^{\mathrm{acq}}, x^{\mathrm{acq}}]. \tag{58}$$

Following Proposition 5.2, this can be approximated by:

$$\begin{aligned} &\mathrm{I}[\Omega; Y^{\mathrm{eval}} \mid X^{\mathrm{eval}}, Y^{\mathrm{acq}}, x^{\mathrm{acq}}] \\ &\quad \approx \tfrac{1}{2}\, \mathbb{E}_{\mathrm{p}(y^{\mathrm{eval}}, y^{\mathrm{acq}} \mid x^{\mathrm{eval}}, x^{\mathrm{acq}})\, \hat{\mathrm{p}}(x^{\mathrm{eval}})} [\log\det\left(\mathrm{H}''[y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]\, (\mathrm{H}''[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\right)]. \end{aligned} \tag{59}$$

**Generalized Linear Model.** For a generalized linear model, we can drop the expectation and obtain:

$$\begin{aligned} &\mathrm{I}[\Omega; Y^{\mathrm{eval}} \mid X^{\mathrm{eval}}, Y^{\mathrm{acq}}, x^{\mathrm{acq}}] \\ &\quad \approx \tfrac{1}{2}\, \mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}})} [\log\det\left(\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]\, (\mathrm{H}''[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\right)] && (60) \\ &\quad \leq \tfrac{1}{2} \log\det\left(\mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}})} [\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]]\, (\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\right) && (61) \\ &\quad \leq \tfrac{1}{2} \mathrm{tr}\left(\mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}})} \left[\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]\right] (\mathrm{H}''[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1}\right), && (62) \end{aligned}$$

where we have used the concavity of the log determinant and Lemma 5.1. Alternatively, we could apply the trace approximation to eq. (60) and obtain:

$$\leq \tfrac{1}{2}\, \mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}})} [\mathrm{tr}\left(\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]\, (\mathrm{H}''[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1}\right)] \tag{63}$$

as a different upper bound.

**General Case & Exponential Family.** To our knowledge, there is no rigorous way to obtain a similar result in the general case as the Fisher information for an acquisition candidate now lies within an inverted term. Obviously, the GGN approximation can be applied when we have an exponential family, which leads to the GLM result above as an approximation. See §B.2 for more details.

**Proposition 5.4** (EPIG). *For a generalized linear model (or with the GGN approximation), we have:*

$$\arg\max_{\{x_i^{acq}\}} \mathrm{I}[Y^{eval}; \{Y_i^{acq}\} \mid X^{eval}, \{x_i^{acq}\}, \mathcal{D}^{train}] = \arg\min_{\{x_i^{acq}\}} \mathrm{I}[\Omega; Y^{eval} \mid X^{eval}, \{Y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}], \tag{64}$$

*with*

$$\begin{aligned}
&\mathrm{I}[\Omega; Y^{eval} \mid X^{eval}, \{Y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}] \\
&\quad \approx \mathbb{E}_{\hat{\mathrm{p}}(x^{eval})}[\log\det\left(\mathrm{H}''[Y^{eval} \mid x^{eval}, \omega^*]\,(\mathrm{H}''[Y^{acq} \mid x^{acq}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\right)] && (65)\\
&\quad \leq \tfrac{1}{2}\,\mathbb{E}_{\hat{\mathrm{p}}(x^{eval})}[\mathrm{tr}\left(\mathrm{H}''[Y^{eval} \mid x^{eval}, \omega^*]\,(\mathrm{H}''[Y^{acq} \mid x^{acq}, \omega^*] + \mathrm{H}''[\omega^*])^{-1}\right)], && (66)
\end{aligned}$$

*or as stronger approximation:*

$$\begin{aligned}
&\quad \leq \tfrac{1}{2}\log\det\left(\mathbb{E}_{\hat{\mathrm{p}}(x^{eval})}[\mathrm{H}''[Y^{eval} \mid x^{eval}, \omega^*]]\,(\mathrm{H}''[\{Y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1} + Id\right) && (67)\\
&\quad \leq \tfrac{1}{2}\mathrm{tr}\left(\mathbb{E}_{\hat{\mathrm{p}}(x^{eval})}\left[\mathrm{H}''[Y^{eval} \mid x^{eval}, \omega^*]\right]\,(\mathrm{H}''[\{Y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1}\right). && (68)
\end{aligned}$$

**Batch Acquisition Pathologies.** Unlike for the EIG, the trace approximation of EPIG is not additive in $\{x_i^{\mathrm{acq}}\}$, and we cannot conclude that it suffers from batch acquisition pathologies like the trace approximation of the EIG.

**Approximations for JEPIG, PIG and JPIG.** The same steps apply to JEPIG:

$$\begin{aligned}
&\mathrm{I}[\Omega; \{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, Y^{\mathrm{acq}}, x^{\mathrm{acq}}] && (69)\\
&\quad \approx \tfrac{1}{2}\log\det\Big(\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{eval}}\}, y^{\mathrm{acq}} \mid \{x_i^{\mathrm{eval}}\}, x^{\mathrm{acq}})}[\mathrm{H}''[\{y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \omega^*]]\,(\mathrm{H}''[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\Big).
\end{aligned}$$

Then, we can follow eq. (61), and devise similar approximations for JEPIG. PIG and JPIG follow the same pattern. Details can be found in §B.3 and §B.4. But how do all these approximations compare to each other?

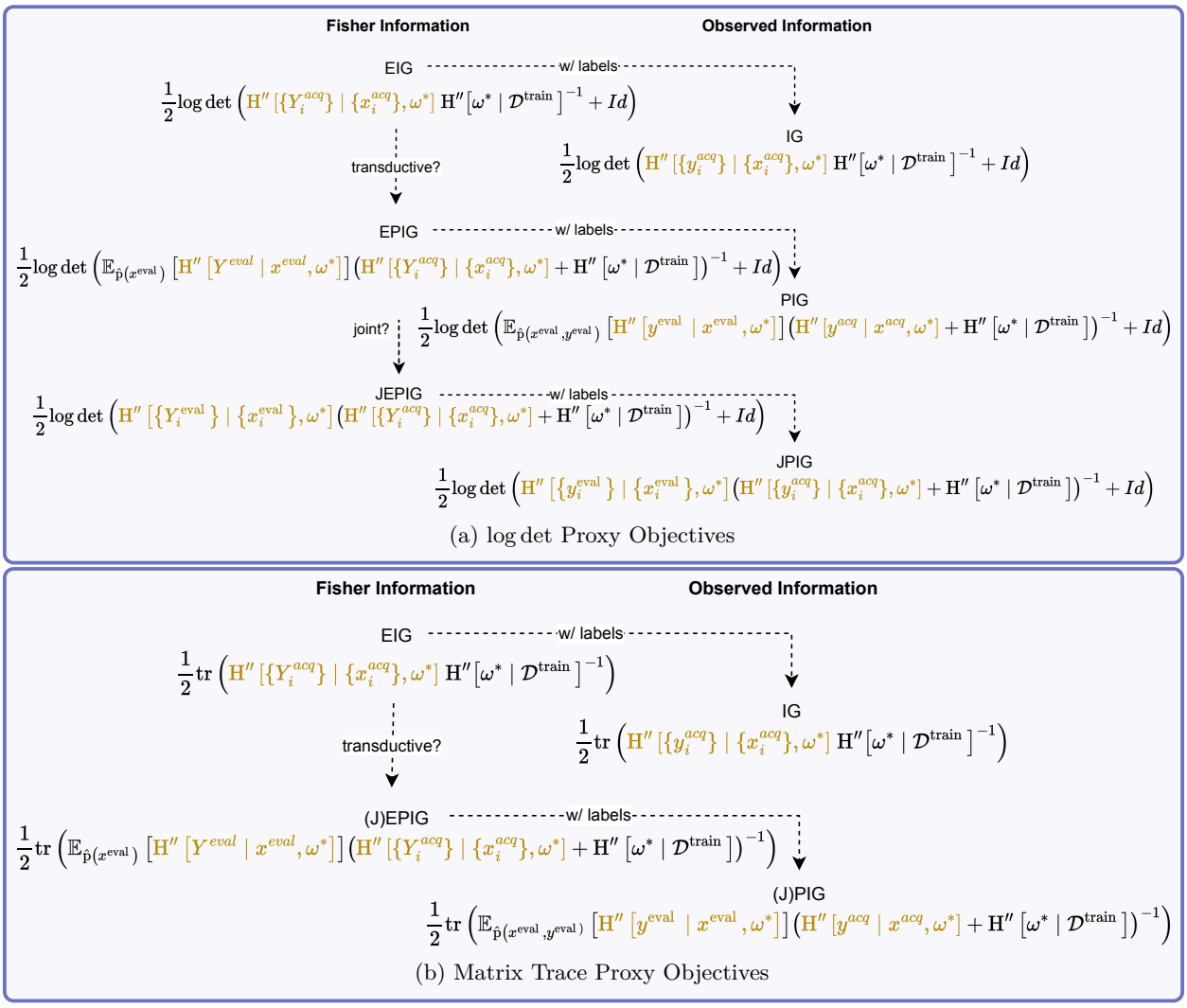
### 5.4 Comparison of the Different Information Quantity Approximations

Figure 1 compares the different information quantity approximations for both the log-determinant and trace approximations. Importantly, the trace approximations of (E)PIG match those of J(E)PIG up to a constant factor (unlike the log-determinant approximations), see §B.4 for details. Kirsch et al. (2021b) argue that JEPIG converges to BALD in the data limit for the evaluation set when there are no outliers in the pool set, while EPIG does not. The trace approximation is too strong to preserve this difference. Does this difference matter in practice? We leave this for future work.

Crucially, for GLMs or when using the GGN approximation, the respective active learning and active sampling objectives (EIG and IG, etc.) are equivalent as Fisher information and observed information are the same, while in the general case, the approximations for EPIG and JEPIG do not have a principled derivation.

## 6 Similarity Matrices and One-Sample Approximations of the Fisher Information

Many data subset selection methods (Iyer et al., 2021; Kothawade et al., 2022; 2021; Ash et al., 2019) use similarity matrices of the loss Jacobians $\mathrm{H}'[y^* \mid x]$, where $y^*$ is usually a hypothesized pseudolabel: usually the $\arg\max$ prediction of the model for $x$. Here, we connect such similarity matrices to the Fisher information and the approximations of information quantities from §5. The proofs are given in §C. Together with §5, this section provides a unified framework for understanding the approximations of information quantities using




(a) log det Proxy Objectives

(b) Matrix Trace Proxy Objectives

Figure 1: *Comparison of the Approximations/Proxy Objectives.* The difference between active learning and active sampling objectives is in using the Fisher information, which is label independent, or the observed information, which uses label information. JEPIG and EPIG have equivalent proxy objectives when using the matrix trace, see §B.4. The notation also makes obvious that in the GLM case, or when GGN approximation is used, active learning and active sampling approximations match as $\mathrm{H}''[y \mid x, \omega^*] \approx$ (resp. $=$) $\mathrm{H}''[Y \mid x, \omega^*]$.

Fisher information and lays the foundation for the next section, which will connect the cited works above to the approximations of information quantities.

**Connection to Fisher Information.** Crucially, given $\mathcal{D} = \{(y_i, x_i)_i\}$, if we let

$$\hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*] := \begin{pmatrix} \vdots \\ \mathrm{H}'[y_i \mid x_i, \omega^*] \\ \vdots \end{pmatrix} \tag{70}$$

be a "data matrix" of the Jacobians, then $\hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]\hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]^T$ gives the similarity matrix $S[\mathcal{D} \mid \omega^*]$ using the Euclidean inner product:

$$S[\mathcal{D} \mid \omega]_{ij} := \langle \mathrm{H}'[y_i \mid x_i, \omega^*], \mathrm{H}'[y_j \mid x_j, \omega^*] \rangle = \hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]\hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]^T. \tag{71}$$

Sampling $\{y_i\} \sim \mathrm{p}(\{y_i\} \mid \{x_i\}, \omega^*)$, the "flipped" product $\hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]^T \hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]$ yields a *one-sample estimate* of the Fisher information $\mathrm{H}''[\{Y_i\} \mid \{x_i\}, \omega^*]$:

$$\mathrm{H}''[\{Y_i\} \mid \{x_i\}, \omega^*] = \sum_i \mathrm{H}''[Y_i \mid x_i, \omega^*] = \mathbb{E}_{\mathrm{p}(\{y_i\} \mid \{x_i\}, \omega^*)} \sum_i \mathrm{H}'[y_i \mid x_i, \omega^*]^T \, \mathrm{H}'[y_i \mid x_i, \omega^*] \tag{72}$$

$$= \mathbb{E}_{\mathrm{p}(\{y_i\} \mid \{x_i\}, \omega^*)} \, \hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]^T \hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]. \tag{73}$$

**Hard Pseudo-Labels.** Importantly, using the arg max class for $y_i$, we only obtain a biased estimate (Kunstner et al., 2019, §B).

**True Labels.** Using the actual labels (e.g., in active sampling), we obtain an estimate of the respective observed information.

**Connection to the Expected Information Gain.** When we define an inner product $\langle \cdot, \cdot \rangle_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\text{train}}]}$ using the Hessian, we can connect the similarity matrix, which uses this inner product:

$$S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\text{train}}]}[\mathcal{D} \mid \omega^*] := \hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*] \, \mathrm{H}''[\omega^* \mid \mathcal{D}^{\text{train}}]^{-1} \hat{\mathrm{H}}'[\mathcal{D} \mid \omega^*]^T, \tag{74}$$

to our information gain approximations.

Specifically, we apply the matrix-determinant lemma $\det(AB + M) = \det M \det(Id + BM^{-1}B)$ to obtain:

**Proposition 6.1.** *Given $\mathcal{D}^{train}$, $\{x_i^{acq}\}$ and (sampled) $\{y_i^{acq}\}$, we have for the EIG:*

$$\mathrm{I}[\Omega; \{Y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] \overset{\approx}{\leq} \tfrac{1}{2} \log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]}[\mathcal{D}^{acq} \mid \omega^*] + Id\right) \tag{75}$$

$$\leq \tfrac{1}{2} \operatorname{tr} S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]}[\mathcal{D}^{acq} \mid \omega^*] \tag{76}$$

**Proposition 6.2.** *Assuming an uninformative posterior $\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}] = \lambda Id$ for $\lambda \to 0$, and given $\mathcal{D}^{train}$, $\{x_i^{acq}\}$, and (sampled) $\{y_i^{acq}\}$, we have for the EIG (before taking $\lambda \to 0$):*

$$\mathrm{I}[\Omega; \{Y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] \overset{\approx}{\leq} \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{acq} \mid \omega^*] + \lambda Id\right) - \tfrac{|\mathcal{D}^{acq}|}{2} \log \lambda. \tag{77}$$

*As the second term is independent of $\{x_i^{acq}\}$, we can use the following proxy objective in the limit:*

$$\frac{1}{2} \log\det\left(S[\mathcal{D}^{acq} \mid \omega^*]\right). \tag{78}$$

**Connection to Other Approximate Information Quantities.** Interestingly, we can use the above to obtain approximations of the predictive information gains (EPIG and JEPIG) because the terms that would go towards $-\infty$ cancel out; see §C for details. For EPIG, we have:

**Proposition 6.3.** *Given $\mathcal{D}^{eval}, \mathcal{D}^{train}$, $\{x_i^{acq}\}$ and (sampled) $\{y_i^{acq}\}$, we have for the EPIG:*

$$\mathrm{I}[Y^{eval}; \{Y_i^{acq}\} \mid X^{eval}, \{x_i^{acq}\}, \mathcal{D}^{train}]$$

$$\approx \tfrac{1}{2} \log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]}[\mathcal{D}^{eval} \mid \omega^*] + Id\right) - \tfrac{1}{2} \log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]}[\mathcal{D}^{acq}, \mathcal{D}^{eval} \mid \omega^*] + Id\right) \tag{79}$$

$$+ \tfrac{1}{2} \log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]}[\mathcal{D}^{acq} \mid \omega^*] + Id\right). \tag{80}$$

*For an uninformative prior, we have:*

$$\approx \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{eval} \mid \omega^*]\right) - \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{acq}, \mathcal{D}^{eval} \mid \omega^*]\right) + \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{acq} \mid \omega^*]\right). \tag{81}$$

*We can drop the terms that only depend on $\mathcal{D}^{eval}$ when we are only interested in proxy objectives for optimization.*

For similarity matrices using the true labels, we can see the statements above as approximating the IG, PIG, and JPIG, respectively.

These results help us connect the LogDet objective of PRISM and SIMILAR to the EIG and EPIG in the next section.

## 7 Connection to Other Acquisition Functions in the Literature

Now, we can connect approaches in non-Bayesian literature to information quantities. Additional proofs are given in §D.

### 7.1 BAIT in "Gone Fishing" (Ash et al., 2021), ActiveSetSelect in "Convergence Rates of Active Learning for Maximum Likelihood Estimation" (Chaudhuri et al., 2015), and EPIG (Kirsch et al., 2021b)

Ash et al. (2021) introduce the *BAIT* objective for deep active learning:

$$\arg\min_{\{x_i^{\text{acq}}\}} \operatorname{tr}\left(\left(\mathrm{H}''[\{Y_i^{\text{acq}}\} \mid \{x_i^{\text{acq}}\}, \omega^*] + \mathrm{H}''[Y^{\text{train}} \mid x^{\text{train}}, \omega^*] + \lambda I\right)^{-1} \mathrm{H}''[\{Y_i^{\text{eval}}\} \mid \{x_i^{\text{eval}}\}, \omega^*]\right), \tag{BAIT}$$

where $\lambda$ is a hyperparameter[2].

BAIT is based on a similar objective for GLMs from Chaudhuri et al. (2015). While Ash et al. (2021) apply this objective to DNNs, they only use the last layer to approximate Fisher information, and the last layer together with appropriate activation functions and losses also constitutes a GLM as we have seen in §4.

Following Proposition 5.4, we immediately see that Ash et al. (2021) performs transductive active learning (using the pool set as an evaluation set) and approximate a proxy objective for (J)EPIG:

**Proposition 7.1.** *Both Ash et al. (2021) and Chaudhuri et al. (2015) perform transductive active learning, approximating (J)EPIG (Kirsch et al., 2021b) using a last-layer approach (or GLM):*

$$\begin{aligned}&\arg\max_{x^{acq}} \mathrm{I}[Y^{eval}; \{Y_i^{acq}\} \mid X^{eval}, \{x_i^{acq}\}] \\ &\quad \approx \arg\min_{x^{acq}} \operatorname{tr}(\mathrm{H}''[\{Y_i^{eval}\} \mid \{x_i^{eval}\}, \omega^*] \left(\mathrm{H}''[Y^{acq} \mid x^{acq}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]\right)^{-1}),\end{aligned} \tag{82}$$

*with* $\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}] = \mathrm{H}''[\mathcal{D}^{train} \mid \omega^*] + \mathrm{H}''[\omega^*]$ *and* $\mathrm{H}''[\omega^*] = \lambda\, Id$.

*Proof.* This follows immediately for GLM (last-layer approaches) when we expand $\mathrm{H}''[\omega^* \mid \mathcal{D}^{\text{train}}]$. Chaudhuri et al. (2015) in particular uses an informative prior, that is $\lambda = 0$. Comparison of the resulting objectives yields the statement. □

Thus, Ash et al. (2021) and Kirsch et al. (2021b) employ the same underlying acquisition function, albeit using very different approaches: Ash et al. (2021) use a last-layer Fisher information matrix, whereas Kirsch et al. (2021b) use approximate BNNs and sample joint predictions in their implementation.

**Research Questions.** EPIG is not submodular, and the greedy selection of an acquisition batch does not come with optimality guarantees. While Kirsch et al. (2021b) ignore this, Ash et al. (2021) propose a heuristic that empirically performs better: They greedily select additional acquisition candidates in forward pass (twice the intended batch acquisition size) and then greedily remove the least informative samples from the batch in a backward pass. *Would this heuristic also prove beneficial for all the other information quantities that are not submodular?*

While Ash et al. (2021) state that they only use the last-layer approach for performance reasons, following §4, it does not seem that this approach translates beyond a last-layer approach for DNNs in a principled fashion (see §B.2). *Is there a principled approach for the general case that goes beyond last-layer active learning when using Fisher information without the GGN approximation?*

[2]This is the BAIT objective as computed in Algorithm 1 in Ash et al. (2021) and the published implementation https://github.com/JordanAsh/badge/blob/master/query_strategies/bait_sampling.py.

Ash et al. (2021) ablate trace and determinantal approaches, similar to comparing eq. (68) and eq. (67), yet they make a mistake: they do not include $+Id$ in the log determinant, which leads them to compute the negative EIG in their ablation:

$$\log\det(\mathrm{H}''[\{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \omega^*]\,(\sum_i \mathrm{H}''[{Y^{\mathrm{acq}}}_i \mid {x^{\mathrm{acq}}}_i, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}])^{-1})$$

$$= \log\det \mathrm{H}''[\{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \omega^*] - \log\det(\sum_i \mathrm{H}''[{Y^{\mathrm{acq}}}_i \mid {x^{\mathrm{acq}}}_i, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]) \tag{83}$$

$$= -\log\det(\sum_i \mathrm{H}''[{Y^{\mathrm{acq}}}_i \mid {x^{\mathrm{acq}}}_i, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]) + C, \tag{84}$$

and the last term matches the EIG in eq. (67) up to the negative sign (and constant terms independent of $\{x_i^{\mathrm{acq}}\}$). Thus, the ablation in Ash et al. (2021) actually only shows that minimizing instead of maximizing the log-determinant approximation of the EIG leads to bad performance. Intuitively, this is the opposite of what we want in any case and explains the results of the ablation in Ash et al. (2021). *Would comparing eq. (68) and eq. (67) provide more interesting results?*

### 7.2 BADGE (Ash et al., 2019) and BatchBALD (Kirsch et al., 2019)

BADGE performs batch acquisition using a similarity matrix: Using the concepts of §6, BADGE uses hard pseudo-labels $y^{\mathrm{acq}} = \arg\max_y \mathrm{p}(y \mid x^{\mathrm{acq}}, \omega^*)$ together with last-layer gradient embeddings for the similarity matrix $S[\mathcal{D}^{\mathrm{acq}} \mid \omega^*]$. The authors sample from a k-DPP (Kulesza and Taskar, 2011) based on this similarity matrix to select a diverse batch of samples for acquisition. However, to further speed up acquisitions, BADGE actually uses k-MEANS++ (Arthur and Vassilvitskii, 2006; Ostrovsky et al., 2013) instead of a k-DPP: it uses the Jacobians $\mathrm{H}'[y \mid x, \omega^*]$ of the data matrix directly and samples a diverse batch based on the Euclidean distance between these Jacobians. However, sampling from k-DPPs does not pick the most informative batch overall, and in fact the ablations in Ash et al. (2019) show that k-MEANS++ outperforms k-DPP. Finally, the paper only motivates using gradient embeddings with hard pseudo-labels through intuitions: the gradient length captures information about the model's uncertainty, and diverse update directions capture information about the model's diversity (Ash et al., 2019). No connection to information theory is made.

Following Proposition 6.1, since BADGE can be seen as using a last-layer approach for the similarity matrix $S[\mathcal{D}^{\mathrm{acq}} \mid \omega^*]$ with hard pseudo-labels, BADGE approximates $\mathrm{I}[\Omega; \{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \mathcal{D}^{\mathrm{train}}]$ with an uninformative posterior distribution:

**Proposition 7.2.** *BADGE maximizes an approximation of the EIG with an uninformative prior.*

**Comparison to BatchBALD.** Similarly, BatchBALD (Kirsch et al., 2019) approximates the EIG in the batch acquisition case, but by using prediction space samples, and BatchBALD uses a greedy approach to select batch candidates instead of sampling via k-DPP or k-MEANS++, respectively.

As the EIG as acquisition function is submodular, determining the acquisition batch is a submodular optimization problem and therefore can be solved by greedy selection with $1 - \frac{1}{e}$ optimality (Nemhauser et al., 1978).

**Research Questions.** Hard pseudo-labels lead to biased estimates. *Would one-sample estimates perform better? And could greedy batch selection work better than sampling via a k-DPP?* This would be closer to the batch acquisition strategy followed by BatchBALD.

### 7.3 SIMILAR (Kothawade et al., 2021) and PRISM (Kothawade et al., 2022)

Based on Iyer et al. (2021), Kothawade et al. (2021) and Kothawade et al. (2022) investigate *submodular active learning* for DNNs: they take an *information function* $f$, which is a non-negative, montone/non-decreasing, submodular function (and then is also subadditive as a consequence):

$$f(A) \geq 0, \qquad \text{(non-negative)}$$

$$f(A) \leq f(B) \text{ for } A \subseteq B, \tag{monotone}$$
$$f(A \cup B) \leq f(A) + f(B) - f(A \cap B), \tag{submodular}$$
$$f(A \cup B) \leq f(A) + f(B) \tag{subadditive}$$

for all $A, B \subseteq \mathcal{D}^{\text{pool}}$ and define a "*submodular conditional gain*" and an "*submodular (conditional) mutual information*" as

$$H_f(A \mid B) := f(A \cup B) - f(B) \tag{85}$$
$$I_f(A; B) := f(A \cup B) - f(A) - f(B). \tag{86}$$

For $f(\{x_i\}) = \mathrm{H}[\{Y_i\} \mid \{x_i\}]$, this simply yields the regular information quantities. Hence, Kothawade et al. (2021) and Kothawade et al. (2022) examine other information functions and submodular quantities in the context of active learning: amongst them set covers, graph cuts, facility location, and log determinants (LogDet) of similarity matrices. Like BADGE (Ash et al., 2019), the similarity matrix uses hard pseudo-labels and is biased. Like BatchBALD (Kirsch et al., 2019), they use a greedy approach to select a batch of samples for acquisition (Nemhauser et al., 1978).

Using our results, we immediately see that the LogDet objective $\log\det S[\mathcal{D}^{\text{acq}} \mid \omega^*]$ exactly matches the EIG approximation in §6.2; furthermore, in §D.1, we show that the LogDetMI objective matches an approximation of JEPIG (and similarly, derive the LogDetCMI objective as well):

The LogDet objective $\log\det S[\mathcal{D}^{\text{acq}} \mid \omega^*]$ is an approximation of the EIG and the LogDetMI objective

$$\log\det S[\mathcal{D}^{\text{acq}} \mid \omega^*] - \log\det(S[\mathcal{D}^{\text{acq}} \mid \omega^*] - S[\mathcal{D}^{\text{acq}}; \mathcal{D}^{\text{eval}} \mid \omega^*] S[\mathcal{D}^{\text{eval}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{eval}}; \mathcal{D}^{\text{acq}} \mid \omega^*]) \tag{87}$$

is an approximation of a proxy objective for EPIG, where we use $S[\mathcal{D}_1; \mathcal{D}_2 \mid \omega^*]$ to denote the non-symmetric similarity matrix between $\mathcal{D}_1$ and $\mathcal{D}_2$.

Importantly, the experimental results for the LogDet-based quantities are reported as among the best in Kothawade et al. (2021) and Kothawade et al. (2022). As such, since the LogDet quantities approximate Shannon's information quantities (which are not specifically examined in those works), the good experimental results compared to other submodular information functions support the hypothesis that approximating Shannon's information quantities works well in active learning and active sampling.

**Research Questions.** Similar to BADGE, the scores are biased by using hard pseudo-labels. *Could one-sample estimates perform better?* Furthermore, as LogDetMI is not submodular, *could the approach from BAIT of expanding and shrinking the acquisition batch in a forward and backward pass improve performance here as well?*

### 7.4 Expected Gradient Length

The *Expected Gradient Length (EGL)* (Settles et al., 2007; Settles, 2009) is an acquisition function in active learning and is usually defined for non-Bayesian models. Originally, it was an expectation over the gradient norm. In more recent literature (Huang et al., 2016), it is introduced using the squared gradient norm:

$$\mathbb{E}_{\mathrm{p}(y^{\text{acq}} \mid x^{\text{acq}}, \omega^*)} \left\| \mathrm{H}'[y^{\text{acq}} \mid x^{\text{acq}}, \omega^*] \right\|^2. \tag{EGL}$$

Using a diagonal approximation of Fisher information, we show in §D.2:

**Proposition 7.3.** *The EIG for a candidate sample $x^{acq}$ approximately lower-bounds the EGL:*

$$2\,\mathrm{I}[\Omega; Y^{acq} \mid x^{acq}] \overset{\approx}{\leq} \mathbb{E}_{\mathrm{p}(y^{acq} \mid x^{acq}, \omega^*)} \left\| \mathrm{H}'[y^{acq} \mid x^{acq}, \omega^*] \right\|^2 + \textit{const.} \tag{88}$$

### 7.5 Deep Learning on a Data Diet

In active sampling, Paul et al. (2021) use the gradient length of given labeled samples $x, y$ (averaged over multiple training runs) as an acquisition function to select the most informative samples from the training set for more speed-up training:

$$\mathbb{E}_{\mathrm{q}(\omega)} \left\| \mathrm{H}'[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega] \right\|^2, \tag{GraNd}$$

which they call the *gradient norm score (GraNd)*. The expectation is taken over the model parameters at initialization of after training for a few epochs—as this is not easily expressed using a posterior distribution, we use $\mathrm{q}(w)$ to denote the distribution.

**Proposition 7.4.** *The IG for a candidate sample $x^{acq}$ approximately lower-bounds the gradient norm score (GraNd) at $\omega^*$ up to a second-order term:*

$$2\,\mathrm{I}[\Omega; y^{acq} \mid x^{acq}] \overset{\approx}{\leq} \mathbb{E}_{\mathrm{q}(\omega)}[\left\| \mathrm{H}'[y^{acq} \mid x^{acq}, \omega] \right\|^2] - \mathbb{E}_{\mathrm{q}(\omega)}[\mathrm{tr}\left( \frac{\nabla^2_\omega \,\mathrm{p}(y \mid x, \omega)}{\mathrm{p}(y \mid x, \omega)} \right)] + \mathit{const.} \tag{89}$$

The second term might not be negligible. Hence, GraNd (the first term on the left) might deviate from the information gain. *How does the information gain compares to GraNd in practice?*

## 8 Conclusion & Outlook

We have examined Fisher information and Gaussian approximations and have derived weight-space approximations for various information quantities. This has allowed us to connect various information quantities to objectives already used in the literature. Moreover, we can make the following concluding points:

**Last-Layer Active Learning.** Methods that only use last-layer Fisher information or similar perform active learning on embeddings only, despite that feature learning is arguably the most important strength of deep neural networks. However, these approaches can find great use with large pre-trained models, which are only fine-tuned on new data domains (Tran et al., 2022).

**Bias in Hard Pseudo-Labels.** Several methods (BADGE, PRISM, SIMILAR) use hard pseudo-labels for computing the similarity matrices, leading to biased estimates. Is this an issue? Can one-sample estimates perform better? Do the equivalent approximations that do not make use of similarity matrices (and do not sample hard pseudo-labels) work better? We leave this comparison for future work.

**Trace vs $\log\det$ Approximations.** We have presented a hierarchy of approximations and bounds. Ablating these approximations along multiple dimensions, including whether to use the trace or $\log\det$ approximation and whether to use a GLM, the GGN approximation or the full Fisher information, could provide interesting insights into what is achievable. We leave this investigation for future work.

**Batch Acquisition Pathologies.** Approaches that use the matrix trace instead of the log determinant can end up being additive for batch candidates $\{x_i^{\mathrm{acq}}\}$ and therefore by definition cannot take redundancies between batch candidates into account, leading to failures detailed in Kirsch et al. (2019; 2021a). This is an issue for approximations of the (E)IG, not so much for (JE)PIG. Does (JE)PIG handle batch acquisition pathologies better? Similarly, most information quantities are not submodular, yet we use greedy acquisition strategies. Is the heuristic proposed by Ash et al. (2021) generally useful? Investigating these questions is an interesting direction for future work.

**Weight vs. Prediction Space.** BADGE, BAIT, and the LogDet objectives of PRISM and SIMILAR (Ash et al., 2019; 2021; Kothawade et al., 2021; 2022) approximate information quantities in weight space, while (Batch)BALD, (J)EPIG, and (J)PIG (Houlsby et al., 2011; Kirsch et al., 2019; 2021b; Mindermann et al., 2022) approximate the information quantities in prediction space. Both approaches have their limitations:

Weight-space approaches can suffer from the Gaussian approximation being of low quality: only the Laplace approximation captures the posterior well once the posterior distribution concentrates sufficiently. Yet, this is unlikely to happen in a low data regime.

Prediction-space approaches can suffer from a combinatorial explosion as the batch acquisition size increases because prediction configurations have to be enumerated or sampled to approximate the information quantities, and many parameter samples might be needed to obtain good estimates. Importantly, prediction space approaches also require drawing samples from the posterior distribution but do not estimate the information quantities using the posterior distribution unlike weight space approaches.

**Informativeness Scores.** Taking a step back, we have seen that a Bayesian perspective using information quantities connects seemingly disparate literature. Although Bayesian methods are often seen as separate from (non-Bayesian) active learning and active sampling, the sometimes fuzzy notion of "informativeness" expressed through various different objectives in non-Bayesian settings collapses to the same couple of information quantities, which were, in principle, already known by Lindley (1956) and MacKay (1992).

## References

David Arthur and Sergei Vassilvitskii. k-means++: The advantages of careful seeding. Technical report, 2006.

Jordan T. Ash, Chicheng Zhang, Akshay Krishnamurthy, John Langford, and Alekh Agarwal. Deep batch active learning by diverse, uncertain gradient lower bounds, 2019.

Jordan T. Ash, Surbhi Goel, Akshay Krishnamurthy, and Sham Kakade. Gone fishing: Neural active learning with fisher embeddings, 2021.

Les Atlas, David Cohn, and Richard Ladner. Training Connectionist Networks with Queries and Selective Sampling. *Neural Information Processing Systems*, 1990.

Kamalika Chaudhuri, Sham Kakade, Praneeth Netrapalli, and Sujay Sanghavi. Convergence rates of active learning for maximum likelihood estimation, 2015.

David Cohn, Les Atlas, and Richard Ladner. Improving generalization with active learning. *Machine learning*, 15(2):201–221, 1994.

Thomas M Cover and A Thomas. Determinant inequalities via information theory. *SIAM journal on Matrix Analysis and Applications*, 9(3):384–392, 1988.

Erik Daxberger, Agustinus Kristiadi, Alexander Immer, Runa Eschenhagen, Matthias Bauer, and Philipp Hennig. Laplace redux-effortless bayesian deep learning. *Advances in Neural Information Processing Systems*, 34:20089–20103, 2021.

Yarin Gal, Riashat Islam, and Zoubin Ghahramani. Deep bayesian active learning with image data. In *International Conference on Machine Learning*, pages 1183–1192. PMLR, 2017.

Geoffrey E Hinton and Drew Van Camp. Keeping the neural networks simple by minimizing the description length of the weights. In *Proceedings of the sixth annual conference on Computational learning theory*, pages 5–13, 1993.

Sepp Hochreiter and Jürgen Schmidhuber. Simplifying neural nets by discovering flat minima. *Advances in neural information processing systems*, 7, 1994.

Neil Houlsby, Ferenc Huszár, Zoubin Ghahramani, and Máté Lengyel. Bayesian active learning for classification and preference learning. *arXiv preprint arXiv:1112.5745*, 2011.

Jiaji Huang, Rewon Child, Vinay Rao, Hairong Liu, Sanjeev Satheesh, and Adam Coates. Active learning for speech recognition: the power of gradients, 2016.

Alexander Immer, Maciej Korzepa, and Matthias Bauer. Improving predictions of bayesian neural nets via local linearization, 2020.

Rishabh Iyer, Ninad Khargoankar, Jeff Bilmes, and Himanshu Asanani. Submodular combinatorial information measures with applications in machine learning. In *Algorithmic Learning Theory*, pages 722–754. PMLR, 2021.

Andreas Kirsch and Yarin Gal. A practical & unified notation for information-theoretic quantities in ml. *arXiv preprint arXiv:2106.12062*, 2021.

Andreas Kirsch, Joost van Amersfoort, and Yarin Gal. Batchbald: Efficient and diverse batch acquisition for deep bayesian active learning. In *Advances in Neural Information Processing Systems*, pages 7024–7035, 2019.

Andreas Kirsch, Sebastian Farquhar, Parmida Atighehchian, Andrew Jesson, Frederic Branchaud-Charron, and Yarin Gal. Stochastic batch acquisition for deep active learning, 2021a.

Andreas Kirsch, Tom Rainforth, and Yarin Gal. Test distribution-aware active learning: A principled approach against distribution shift and outliers, 2021b.

Suraj Kothawade, Nathan Beck, Krishnateja Killamsetty, and Rishabh Iyer. Similar: Submodular information measures based active learning in realistic scenarios. *Advances in Neural Information Processing Systems*, 34:18685–18697, 2021.

Suraj Kothawade, Vishal Kaushal, Ganesh Ramakrishnan, Jeff Bilmes, and Rishabh Iyer. Prism: A rich class of parameterized submodular information measures for guided data subset selection. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pages 10238–10246, 2022.

Alex Kulesza and Ben Taskar. k-dpps: Fixed-size determinantal point processes. In *ICML*, 2011.

Frederik Kunstner, Lukas Balles, and Philipp Hennig. Limitations of the empirical fisher approximation for natural gradient descent, 2019.

Dennis V Lindley. On a measure of the information provided by an experiment. *The Annals of Mathematical Statistics*, pages 986–1005, 1956.

Quan Long. Multimodal information gain in bayesian design of experiments, 2021.

David JC MacKay. Information-based objective functions for active data selection. *Neural computation*, 4(4): 590–604, 1992.

Sören Mindermann, Jan Brauner, Muhammed Razzak, Mrinank Sharma, Andreas Kirsch, Winnie Xu, Benedikt Höltgen, Aidan N. Gomez, Adrien Morisot, Sebastian Farquhar, and Yarin Gal. Prioritized training on points that are learnable, worth learning, and not yet learnt, 2022.

George L Nemhauser, Laurence A Wolsey, and Marshall L Fisher. An analysis of approximations for maximizing submodular set functions—i. *Mathematical programming*, 14(1):265–294, 1978.

Rafail Ostrovsky, Yuval Rabani, Leonard J Schulman, and Chaitanya Swamy. The effectiveness of lloyd-type methods for the k-means problem. *Journal of the ACM (JACM)*, 59(6):1–22, 2013.

Mansheej Paul, Surya Ganguli, and Gintare Karolina Dziugaite. Deep learning on a data diet: Finding important examples early in training, 2021.

Burr Settles. Active learning literature survey. 2009.

Burr Settles, Mark Craven, and Soumya Ray. Multiple-instance active learning. *Advances in neural information processing systems*, 20, 2007.

Shengyang Sun, Daniele Calandriello, Huiyi Hu, Ang Li, and Michalis Titsias. Information-theoretic online memory selection for continual learning, 2022.

Dustin Tran, Jeremiah Liu, Michael W Dusenberry, Du Phan, Mark Collier, Jie Ren, Kehang Han, Zi Wang, Zelda Mariet, Huiyi Hu, et al. Plex: Towards reliability using pretrained large model extensions. *arXiv preprint arXiv:2207.07411*, 2022.

Chaoqi Wang, Shengyang Sun, and Roger Grosse. Beyond marginal uncertainty: How accurately can bayesian regression models estimate posterior predictive correlations?, 2020.

Kai Yu, Jinbo Bi, and Volker Tresp. Active learning via transductive experimental design. In *Proceedings of the 23rd international conference on Machine learning*, pages 1081–1088, 2006.

## A Fisher Information: Additional Derivations & Proofs

**Proposition 4.2.** *Like the observed information, Fisher information is additive:*

$$\mathrm{H}''[\{Y_i\} \mid \{x_i\}, \omega^*] = \sum_i \mathrm{H}''[\{Y_i\} \mid x_i, \omega^*]. \tag{25}$$

*Proof.* This follows immediately from $Y_i \perp\!\!\!\perp Y_j \mid x_i, x_j, \omega^*$ for $i \neq j$ and the additivity of the observed information:

$$\mathrm{H}''[\{Y_i\} \mid \{x_i\}, \omega^*] = \mathbb{E}_{\mathrm{p}(\{y_i\}\mid\{x_i\},\omega^*)}[\mathrm{H}''[\{y_i\} \mid \{x_i\}, \omega^*]] = \mathbb{E}_{\mathrm{p}(\{y_i\}\mid\{x_i\},\omega^*)}[\sum_i \mathrm{H}''[y_i \mid x_i, \omega^*]] \tag{90}$$

$$= \sum_i \mathbb{E}_{\mathrm{p}(y_i\mid x_i,\omega^*)}[\mathrm{H}''[y_i \mid x_i, \omega^*]] = \sum_i \mathrm{H}''[y_i \mid x_i, \omega^*]. \tag{91}$$

□

**Proposition 4.3.** *Fisher information is equivalent to:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathbb{E}_{\mathrm{p}(y\mid x,\omega^*)}[\mathrm{H}'[y \mid x, \omega^*]^T \ \mathrm{H}'[y \mid x, \omega^*]] = \mathrm{Cov}[\mathrm{H}'[Y \mid x, \omega^*]]. \tag{26}$$

To prove Proposition 4.3, we use the two generally useful lemmas below:

**Lemma A.1.** *For the Jacobian* $\mathrm{H}'[y \mid x, \omega^*]$*, we have:*

$$\mathrm{H}'[y \mid x, \omega^*] = \nabla_\omega[-\log \mathrm{p}(y \mid x, \omega^*)] = -\frac{\nabla_\omega \mathrm{p}(y \mid x, \omega^*)}{\mathrm{p}(y \mid x, \omega^*)}, \tag{92}$$

*and for the Hessian* $\mathrm{H}''[y \mid x, \omega^*]$*, we have:*

$$\mathrm{H}''[y \mid x, \omega^*] = \mathrm{H}'[y \mid x, \omega^*]^T \ \mathrm{H}'[y \mid x, \omega^*] - \frac{\nabla^2_\omega \mathrm{p}(y \mid x, \omega^*)}{\mathrm{p}(y \mid x, \omega^*)}. \tag{93}$$

*Proof.* The result follows immediately from the application of the rules of multivariate calculus. □

**Lemma A.2.** *The following expectations over the model's own predictions vanish:*

$$\mathbb{E}_{\mathrm{p}(y\mid x,\omega^*)}[\mathrm{H}'[y \mid x, \omega^*]] = 0, \tag{94}$$

$$\mathbb{E}_{\mathrm{p}(y\mid x,\omega^*)}\left[\frac{\nabla^2_\omega \mathrm{p}(y \mid x, \omega^*)}{\mathrm{p}(y \mid x, \omega^*)}\right] = 0. \tag{95}$$

*Proof.* We use the previous equivalences and rewrite the expectations as integral; the results follows:

$$\mathbb{E}_{\mathrm{p}(y\mid x,\omega^*)}[\mathrm{H}'[y \mid x, \omega^*]] = \mathbb{E}_{\mathrm{p}(y\mid x,\omega^*)}[-\nabla_\omega \log \mathrm{p}(y \mid x, \omega^*)] = -\,\mathbb{E}_{\mathrm{p}(y\mid x,\omega^*)}\left[\frac{\nabla_\omega \mathrm{p}(y \mid x, \omega^*)}{\mathrm{p}(y \mid x, \omega^*)}\right] \tag{96}$$

$$= -\int \nabla_\omega \mathrm{p}(y \mid x, \omega^*)\, dy = -\nabla_\omega \int \mathrm{p}(y \mid x, \omega^*)\, dy = -\nabla_\omega 1 = 0, \tag{97}$$

$$\mathbb{E}_{\mathrm{p}(y\mid x,\omega^*)}\left[\frac{\nabla^2_\omega \mathrm{p}(y \mid x, \omega^*)}{\mathrm{p}(y \mid x, \omega^*)}\right] = \int \nabla^2_\omega \mathrm{p}(y \mid x, \omega^*)\, dy = \nabla^2_\omega \int \mathrm{p}(y \mid x, \omega^*)\, dy = \nabla^2_\omega 1 = 0. \tag{98}$$

□

*Proof of Proposition 4.3.* With the previous lemma, we have the following.

$$\mathrm{Cov}[\mathrm{H}'[Y \mid x, \omega^*]] = \mathbb{E}[\mathrm{H}'[Y \mid x, \omega^*]^T \ \mathrm{H}'[Y \mid x, \omega^*]] - \underbrace{\mathbb{E}[\mathrm{H}'[Y \mid x, \omega^*]^T]}_{=0} \underbrace{\mathbb{E}[\mathrm{H}'[Y \mid x, \omega^*]]}_{=0} \tag{99}$$

$$= \mathbb{E}[\mathrm{H}'[Y \mid x, \omega^*]^T \; \mathrm{H}'[Y \mid x, \omega^*]]. \tag{100}$$

For the expectation over the Hessian, we plug Lemma A.1 into Lemma A.2 and obtain:

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathbb{E}_{\mathrm{p}(y|x,\omega^*)}[\mathrm{H}''[y \mid x, \omega^*]] = \mathbb{E}_{\mathrm{p}(y|x,\omega^*)}\left[\mathrm{H}'[y \mid x, \omega^*]^T \; \mathrm{H}'[y \mid x, \omega^*] - \frac{\nabla^2_\omega \, \mathrm{p}(y \mid x, \omega^*)}{\mathrm{p}(y \mid x, \omega^*)}\right] \tag{101}$$

$$= \mathbb{E}_{\mathrm{p}(y|x,\omega^*)}[\mathrm{H}'[y \mid x, \omega^*]^T \; \mathrm{H}'[y \mid x, \omega^*]] - 0 = \mathrm{Cov}[\mathrm{H}'[Y \mid x, \omega^*]]. \tag{102}$$

□

### A.1 Special Case: Exponential Family

**Proposition 4.4.** *The Fisher information* $\mathrm{H}''[Y \mid x, \omega^*]$ *for a model* $\mathrm{p}(y \mid \hat{z} = \hat{f}(x; \omega^*))$ *is equivalent to:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \nabla_\omega \hat{f}(x; \omega^*)^T \, \mathbb{E}_{\mathrm{p}(y|x,\omega^*)}[\nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)]] \nabla_\omega \hat{f}(x; \omega^*), \tag{27}$$

*where* $\nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)]$ *is short for* $\nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z}]\big|_{\hat{z}=\hat{f}(x;\omega^*)}$.

*Proof.* We apply the second equivalence in Proposition 4.3 twice:

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathrm{Cov}[\mathrm{H}'[Y \mid x, \omega^*]] = \mathrm{Cov}[\nabla_\omega \hat{f}(x; \omega^*)^T \, \nabla_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)] \, \nabla_\omega \hat{f}(x; \omega^*)] \tag{103}$$

$$= \nabla_\omega \hat{f}(x; \omega^*)^T \, \mathrm{Cov}[\nabla_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)]] \, \nabla_\omega \hat{f}(x; \omega^*) \tag{104}$$

$$= \nabla_\omega \hat{f}(x; \omega^*)^T \, \mathbb{E}_{\mathrm{p}(y|x,\omega^*)}[\nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)]] \, \nabla_\omega \hat{f}(x; \omega^*) \tag{105}$$

□

### A.2 Special Case: Generalized Linear Models

**Proposition 4.7.** *The observed information* $\mathrm{H}''[y \mid x, \omega^*]$ *of a GLM is independent of* $y$.

$$\mathrm{H}''[y \mid x, \omega^*] = \nabla_\omega \hat{f}(x; \omega^*)^T \, \nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)] \, \nabla_\omega \hat{f}(x; \omega^*) \tag{31}$$

$$= \nabla_\omega \hat{f}(x; \omega^*)^T \, \nabla^2_{\hat{z}} A(w^T x) \, \nabla_\omega \hat{f}(x; \omega^*). \tag{32}$$

*Proof.*

$$\mathrm{H}''[y \mid x, \omega^*] \tag{106}$$

$$= \nabla_\omega [\mathrm{H}'[y \mid x, \omega^*]] \tag{107}$$

$$= \nabla_\omega [\nabla_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)] \, \nabla_\omega \hat{f}(x; \omega^*)] \tag{108}$$

$$= \nabla_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)] \, \underbrace{\nabla^2_\omega \hat{f}(x; \omega^*)}_{=\nabla^2_\omega [w^T x]=0} + \nabla_\omega \hat{f}(x; \omega^*)^T \, \nabla^2_{\hat{z}} \, \mathrm{H}[y \mid \hat{z} = \hat{f}(x; \omega^*)] \, \nabla_\omega \hat{f}(x; \omega^*) \tag{109}$$

$$= \nabla_\omega \hat{f}(x; \omega^*)^T \, \nabla^2_{\hat{z}} A(w^T x) \, \nabla_\omega \hat{f}(x; \omega^*). \tag{110}$$

□

**Proposition 4.9.** *For a GLM, when* $\hat{f}(x; \omega) : \mathbb{R}^D \to \mathbb{R}^K$*, where* $K$ *is the number of classes (outputs),* $D$ *is the number of input dimensions,* $\omega \in \mathbb{R}^{D \times K}$*, and assuming the parameters are flattened into a single vector for the Jacobian, we have* $\nabla_\omega \hat{f}(x; \omega) = \mathrm{Id}_K \otimes x^T \in \mathbb{R}^{K \times (K \cdot D)}$*, where* $\otimes$ *denotes the Kronecker product, and:*

$$\nabla_\omega \hat{f}(x; \omega^*)^T \, \nabla^2_{\hat{z}} A(\omega^T x) \, \nabla_\omega \hat{f}(x; \omega^*) = \nabla^2_{\hat{z}} A(w^T x) \otimes x \, x^T. \tag{35}$$

*Proof.* We begin with a few statements that lead to the conclusion step by step, where $x \in \mathbb{R}^D, A \in \mathbb{R}^{C\times C}, G \in \mathbb{R}^{C\times(C\cdot D)}$:

$$
\begin{aligned}
(x\,x^T)_{ij} &= x_i\,x_j && (111)\\
(Id_C \otimes x^T)_{c,d\,D+i} &= x_i \cdot \mathbb{1}\{c=d\} && (112)\\
(G^T\,A\,G)_{ij} &= \sum_{k,l} G_{ki}\,A_{kl}\,G_{lj} && (113)\\
(A \otimes x\,x^T)_{c\,D+i,d\,D+j} &= A_{cd}\,x_i\,x_j, && (114)\\
((Id_C \otimes x^T)^T\,A\,(Id_C \otimes x^T))_{c\,D+i,d\,D+j} &= \sum_{k,l} (Id_C \otimes x^T)_{k,c\,D+i}\,A_{kl}\,(Id_C \otimes x^T)_{l,d\,D+j} && (115)\\
&= \sum_{k,l} x_i \cdot \mathbb{1}\{k=c\}\,A_{kl}\,x_j \cdot \mathbb{1}\{l=d\} && (116)\\
&= x_i\,A_{cd}\,x_j && (117)\\
&= (A \otimes x\,x^T)_{c\,D+i,d\,D+j}. && (118)\\
\implies \nabla_\omega \hat{f}(x;\omega^*)^T\,\nabla^2_{\hat{z}} A(\omega^T x)\,\nabla_\omega \hat{f}(x;\omega^*) &= \nabla^2_{\hat{z}} A(w^T x) \otimes x\,x^T. && (119)
\end{aligned}
$$

□

**Proposition 4.8.** *For a model such that the observed information* $\mathrm{H}''[y \mid x, \omega^*]$ *is independent of* $y$*, we have the following:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathrm{H}''[y^* \mid x, \omega^*] \tag{33}$$

*for any* $y^*$*, and also trivially:*

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathbb{E}_{\mathrm{p}(y|x)}[\mathrm{H}''[y \mid x, \omega^*]]. \tag{34}$$

*Proof.* This follows directly from Proposition 4.5. In particular, we have:

$$\mathrm{H}''[Y \mid x, \omega^*] = \mathbb{E}_{\mathrm{p}(y|x,\omega^*)}[\mathrm{H}''[y \mid x, \omega^*]] = \mathrm{H}''[y^* \mid x, \omega^*], \tag{120}$$

where we have fixed $y^*$ to an arbitrary value. □

# B Approximating Information Quantities

## B.1 Approximate Expected Information Gain

**Lemma 5.1.** *For symmetric, positive semidefinite matrices* $A$*, we have (with equality iff* $A = 0$*):*

$$\log\det(A + Id) \leq \mathrm{tr}(A). \tag{46}$$

*Proof.* When $A$ is positive semidefinite and symmetric, its eigenvalues $(\lambda_i)_i$ are real and nonnegative. Moreover, $A + Id$ has eigenvalues $(\lambda_i + 1)_i$; $\det(A + Id) = \prod_i(\lambda_i + 1)$; and $\mathrm{tr}\,A = \sum_i \lambda_i$. These properties easily follow from the respective eigenvalue decomposition. Thus, we have:

$$\log\det(A + Id) \leq \log\prod_i(\lambda_i + 1) = \sum_i \log(\lambda_i + 1) \leq \sum_i \lambda_i = \mathrm{tr}(A), \tag{121}$$

where we have used $\log(x + 1) \leq x$ iff equality for $x = 0$. □

**General Case.** In the main text, we only skimmed the general case and mentioned the main assumption. Here, we look at the general case in detail.

For the general case, we need to make strong approximations to be able to pursue a similar derivation. First, we cannot drop the expectation; instead, we note that the log determinant is a concave function on the positive semidefinite symmetric cone (Cover and Thomas, 1988), and we can use Jensen's inequality on the log determinant term from Equation (41) as follows:

$$\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\log\det\left(\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]\ \mathrm{H}''[\omega^*]^{-1} + Id\right)] \tag{122}$$

$$\leq \log\det\left(\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]]\ \mathrm{H}''[\omega^*]^{-1} + Id\right). \tag{123}$$

Second, we need use the following approximation:

$$\mathrm{p}(\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}) \approx \mathrm{p}(\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*) \tag{124}$$

to obtain a Fisher information and use its additivity. That is, we obtain:

$$\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\},\omega^*)}[\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]] = \mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*] = \sum_i \mathrm{H}''[{y^{\mathrm{acq}}}_i \mid {x^{\mathrm{acq}}}_i, \omega^*]. \tag{125}$$

Plugging all of this together and applying Lemma 5.1, we obtain the same final approximation:

$$\mathrm{I}[\Omega; \{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}] = \ldots \approx \tfrac{1}{2}\,\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\log\det\left(\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]\ \mathrm{H}''[\omega^*]^{-1} + Id\right)] \tag{126}$$

$$\leq \tfrac{1}{2}\log\det\left(\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\})}[\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]]\ \mathrm{H}''[\omega^*]^{-1} + Id\right) \tag{127}$$

$$\approx \tfrac{1}{2}\log\det\left(\mathbb{E}_{\mathrm{p}(\{y_i^{\mathrm{acq}}\}|\{x_i^{\mathrm{acq}}\},\omega^*)}[\mathrm{H}''[\{y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]]\ \mathrm{H}''[\omega^*]^{-1} + Id\right) \tag{128}$$

$$= \tfrac{1}{2}\log\det\left(\sum_i \mathrm{H}''[{Y^{\mathrm{acq}}}_i \mid {x^{\mathrm{acq}}}_i, \omega^*]\ \mathrm{H}''[\omega^*]^{-1} + Id\right) \tag{129}$$

$$\leq \tfrac{1}{2}\sum_i \mathrm{tr}\left(\mathrm{H}''[{Y^{\mathrm{acq}}}_i \mid {x^{\mathrm{acq}}}_i, \omega^*]\ \mathrm{H}''[\omega^*]^{-1}\right). \tag{130}$$

Unlike in the case of generalized linear models, a stronger assumption was necessary to reach the same result. Alternatively, we could use the GGN approximation, which leads to the same result.

### B.2 Approximate Expected Predicted Information Gain

In the main text, we only briefly referred to not knowing a principled way to arrive at the same result of Proposition 5.4 for the general case. This is because unlike the expected information gain, the Fisher information for an acquisition candidate now lies within an matrix inversion. Even if we used the fact that $\log\det(Id + X\,Y^{-1})$ is concave in $X$ and convex in $Y$, we would end up with:

$$\ldots \tag{131}$$

$$\approx \tfrac{1}{2}\,\mathbb{E}_{\mathrm{p}(y^{\mathrm{eval}},y^{\mathrm{acq}}|x^{\mathrm{eval}},x^{\mathrm{acq}})\ \mathrm{p}(x^{\mathrm{eval}})}[\log\det\left(\mathrm{H}''[y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]\,(\mathrm{H}''[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\right)] \tag{132}$$

$$\leq \tfrac{1}{2}\,\mathbb{E}_{\mathrm{p}(y^{\mathrm{acq}}|x^{\mathrm{acq}})}[\log\det\left(\mathbb{E}_{\mathrm{p}(y^{\mathrm{eval}},x^{\mathrm{eval}})}[\mathrm{H}''[y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]]\,(\mathrm{H}''[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\right)] \tag{133}$$

$$\geq \tfrac{1}{2}\log\det\left(\mathbb{E}_{\mathrm{p}(y^{\mathrm{eval}},x^{\mathrm{eval}})}[\mathrm{H}''[y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]]\,(\mathbb{E}_{\mathrm{p}(y^{\mathrm{acq}}|x^{\mathrm{acq}})}[\mathrm{H}''[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*]] + \mathrm{H}''[\omega^*])^{-1} + Id\right) \tag{134}$$

$$= \tfrac{1}{2}\log\det\left(\mathbb{E}_{\mathrm{p}(x^{\mathrm{eval}})}[\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]]\,(\mathrm{H}''[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1} + Id\right) \tag{135}$$

$$\leq \tfrac{1}{2}\mathrm{tr}\left(\mathbb{E}_{\mathrm{p}(x^{\mathrm{eval}})}[\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]]\,(\mathrm{H}''[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^*])^{-1}\right). \tag{136}$$

Note the $\leq \ldots \geq$, which invalidates the chain. Obviously, the errors could cancel out, but a principled statement seems hardly possible using this deduction.

### B.3 Approximate Predictive Information Gain

Similarly to Proposition 5.3, we can approximate the predictive information gain. We assume that we have access to an (empirical) distribution $\hat{\mathrm{p}}(x^{\mathrm{eval}}, y^{\mathrm{eval}})$:

**Proposition B.1.** *For a generalized linear model (or with the GGN approximation), when we take the expectation over* $\hat{\mathrm{p}}(x^{eval}, y^{eval})$*, we have:*

$$\arg\max_{x^{acq}} \mathrm{I}[Y^{eval}; y^{acq} \mid X^{eval}, x^{acq}, \mathcal{D}^{train}] = \arg\min_{x^{acq}} \mathrm{I}[\Omega; Y^{eval} \mid X^{eval}, y^{acq}, x^{acq}, \mathcal{D}^{train}] \tag{137}$$

*with*

$$\begin{aligned}
&\mathrm{I}[\Omega; Y^{eval} \mid X^{eval}, y^{acq}, x^{acq}, \mathcal{D}^{train}] && (138)\\
&\quad= \mathbb{E}_{\hat{\mathrm{p}}(x^{eval}, y^{eval})}\, \mathrm{I}[\Omega; y^{eval} \mid x^{eval}, y^{acq}, x^{acq}, \mathcal{D}^{train}]\\
&\quad\approx \mathbb{E}_{\hat{\mathrm{p}}(x^{eval}, y^{eval})}[\tfrac{1}{2}\log\det\left(\mathrm{H}''[y^{eval} \mid x^{eval}, \omega^*]\,(\mathrm{H}''[y^{acq} \mid x^{acq}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1} + Id\right)] && (139)\\
&\quad\leq \tfrac{1}{2}\log\det\left(\mathbb{E}_{\hat{\mathrm{p}}(x^{eval}, y^{eval})}[\mathrm{H}''[y^{eval} \mid x^{eval}, \omega^*]]\,(\mathrm{H}''[y^{acq} \mid x^{acq}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1} + Id\right) && (140)\\
&\quad\leq \tfrac{1}{2}\mathrm{tr}\left(\mathbb{E}_{\hat{\mathrm{p}}(x^{eval}, y^{eval})}[\mathrm{H}''[y^{eval} \mid x^{eval}, \omega^*]]\,(\mathrm{H}''[y^{acq} \mid x^{acq}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1}\right). && (141)
\end{aligned}$$

All of this follows immediately. Only for the second inequality, we need to use Jensen's inequality and that the log determinant is on the positive semidefinite symmetric cone (Cover and Thomas, 1988). Like for the information gain, there is no difference between having access to labels or not when we have a GLM or use the GGN approximation.

### B.4 Approximate Joint (Expected) Predictive Information Gain

A comparison of EPIG and JEPIG shows that JEPIG does not require an expectation over $\hat{\mathrm{p}}(x^{\mathrm{eval}})$ but uses a set of *evaluation samples* $\{x_i^{\mathrm{eval}}\}$. As such, we can easily adapt Proposition 5.4 to JEPIG and obtain:

**Proposition B.2** (JEPIG)**.** *For a generalized linear model (or with the GGN approximation), we have:*

$$\arg\max_{\{x_i^{acq}\}} \mathrm{I}[\{Y_i^{eval}\}; \{Y_i^{acq}\} \mid \{x_i^{eval}\}, \{x_i^{acq}\}, \mathcal{D}^{train}] = \arg\min_{\{x_i^{acq}\}} \mathrm{I}[\Omega; \{Y_i^{eval}\} \mid \{x_i^{eval}\}, \{Y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}] \tag{142}$$

*with*

$$\begin{aligned}
&\mathrm{I}[\Omega; \{Y_i^{eval}\} \mid \{x_i^{eval}\}, \{Y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}]\\
&\quad\approx \tfrac{1}{2}\log\det\left(\mathrm{H}''[\{Y_i^{eval}\} \mid \{x_i^{eval}\}, \omega^*]\,(\mathrm{H}''[\{Y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1} + Id\right) && (143)\\
&\quad\leq \tfrac{1}{2}\mathrm{tr}\left(\mathrm{H}''[\{Y_i^{eval}\} \mid \{x_i^{eval}\}, \omega^*]\,(\mathrm{H}''[\{Y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1}\right). && (144)
\end{aligned}$$

And similarly for JPIG, we obtain without relying on GGN approximations or GLMs:

**Proposition B.3** (JPIG)**.** *We have:*

$$\arg\max_{\{x_i^{acq}\}} \mathrm{I}[\{y_i^{eval}\}; \{y_i^{acq}\} \mid \{x_i^{eval}\}, \{x_i^{acq}\}, \mathcal{D}^{train}] = \arg\min_{\{x_i^{acq}\}} \mathrm{I}[\Omega; \{y_i^{eval}\} \mid \{x_i^{eval}\}, \{y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}] \tag{145}$$

*with*

$$\begin{aligned}
&\mathrm{I}[\Omega; \{y_i^{eval}\} \mid \{x_i^{eval}\}, \{Y_i^{acq}\}, \{x_i^{acq}\}, \mathcal{D}^{train}]\\
&\quad\approx \tfrac{1}{2}\log\det\left(\mathrm{H}''[\{y_i^{eval}\} \mid \{x_i^{eval}\}, \omega^*]\,(\mathrm{H}''[\{y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1} + Id\right) && (146)\\
&\quad\leq \tfrac{1}{2}\mathrm{tr}\left(\mathrm{H}''[\{y_i^{eval}\} \mid \{x_i^{eval}\}, \omega^*]\,(\mathrm{H}''[\{y_i^{acq}\} \mid \{x_i^{acq}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{train}])^{-1}\right). && (147)
\end{aligned}$$

**Comparison between (E)PIG and J(E)PIG approximations.** As observed information and Fisher information are additive, the difference between the approximations when we have an empirical, that is finite,

evaluation distribution $\hat{\mathrm{p}}(x^{\mathrm{eval}})$ with $M$ samples is a factor of $E$ inside the log determinant or trace:

$$\mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}},y^{\mathrm{eval}})}[\mathrm{H}''[y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]] = \frac{1}{E}\sum_i \mathrm{H}''[{y^{\mathrm{eval}}}_i \mid {x^{\mathrm{eval}}}_i, \omega^*] = \frac{1}{E}\,\mathrm{H}''[\{y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \omega^*]. \tag{148}$$

For the log determinant, $\log\det(A + Id) \neq \log\det(\frac{1}{E}A + Id)$ obviously, but for the trace approximation, we see that both approximations are equal up to a constant factor. For example:

$$\begin{aligned}
&\tfrac{1}{2}\mathrm{tr}(\mathbb{E}_{\hat{\mathrm{p}}(x^{\mathrm{eval}})}\left[\mathrm{H}''[Y^{\mathrm{eval}} \mid x^{\mathrm{eval}}, \omega^*]\right](\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}])^{-1}) && (149)\\
&= \tfrac{1}{2}\mathrm{tr}(\frac{1}{E}\mathrm{H}''[\{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \omega^*](\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}])^{-1}) && (150)\\
&= \tfrac{1}{2E}\mathrm{tr}(\mathrm{H}''[\{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \omega^*](\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}])^{-1}). && (151)
\end{aligned}$$

The same holds for the other upper-bounds that use the trace.

## C Similarity Matrices and One-Sample Approximations of the Fisher Information

**Proposition 6.1.** *Given $\mathcal{D}^{train}$, $\{x_i^{acq}\}$ and (sampled) $\{y_i^{acq}\}$, we have for the EIG:*

$$\begin{aligned}
\mathrm{I}[\Omega; \{Y_i^{acq}\} \mid \{x_i^{acq}\}, \mathcal{D}^{train}] &\overset{\approx}{\leq} \tfrac{1}{2}\log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]}[\mathcal{D}^{acq} \mid \omega^*] + Id\right) && (75)\\
&\leq \tfrac{1}{2}\mathrm{tr}\, S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{train}]}[\mathcal{D}^{acq} \mid \omega^*] && (76)
\end{aligned}$$

*Proof.*

$$\begin{aligned}
\mathrm{I}[\Omega; \{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \mathcal{D}^{\mathrm{train}}] &\overset{\approx}{\leq} \tfrac{1}{2}\log\det\left(\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*]\ \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]^{-1} + Id\right) && (152)\\
&= \tfrac{1}{2}\log\det\left((\mathrm{H}''[\{Y_i^{\mathrm{acq}}\} \mid \{x_i^{\mathrm{acq}}\}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}])\ \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]^{-1}\right) && (153)\\
&\approx \tfrac{1}{2}\log\det\left((\hat{\mathrm{H}}'[\mathcal{D}^{\mathrm{acq}} \mid \omega^*]^T\hat{\mathrm{H}}'[\mathcal{D}^{\mathrm{acq}} \mid \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}])\ \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]^{-1}\right) && (154)\\
&= \tfrac{1}{2}\log\det\left(\hat{\mathrm{H}}'[\mathcal{D}^{\mathrm{acq}} \mid \omega^*]\,\mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]^{-1}\hat{\mathrm{H}}'[\mathcal{D}^{\mathrm{acq}} \mid \omega^*]^T + Id\right) && (155)\\
&= \tfrac{1}{2}\log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]}[\mathcal{D}^{\mathrm{acq}} \mid \omega^*] + Id\right), && (156)
\end{aligned}$$

where we have used the matrix determinant lemma:

$$\det(AB + M) = \det(BM^{-1}A + Id)\,\det M. \tag{157}$$

□

**Connection to the Joint (Expected) Predictive Information Gain.** Following eq. (57), JEPIG can be decomposed as the difference between two EIG terms, which we can further divide into three terms that are only conditioned on $\mathcal{D}^{\mathrm{train}}$:

$$\begin{aligned}
&\mathrm{I}[\{Y_i^{\mathrm{eval}}\}; Y^{\mathrm{acq}} \mid \{x_i^{\mathrm{eval}}\}, x^{\mathrm{acq}}, \mathcal{D}^{\mathrm{train}}] && (158)\\
&\quad = \mathrm{I}[\Omega; \{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \mathcal{D}^{\mathrm{train}}] - \mathrm{I}[\Omega; \{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, Y^{\mathrm{acq}}, x^{\mathrm{acq}}, \mathcal{D}^{\mathrm{train}}]\\
&\quad = \mathrm{I}[\Omega; \{Y_i^{\mathrm{eval}}\} \mid \{x_i^{\mathrm{eval}}\}, \mathcal{D}^{\mathrm{train}}] - \mathrm{I}[\Omega; \{Y_i^{\mathrm{eval}}\}, Y^{\mathrm{acq}} \mid \{x_i^{\mathrm{eval}}\}, x^{\mathrm{acq}}, \mathcal{D}^{\mathrm{train}}] + \mathrm{I}[\Omega; Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \mathcal{D}^{\mathrm{train}}] && (159)
\end{aligned}$$

Using Proposition 6.1, we can approximate this as:

$$\begin{aligned}
&\mathrm{I}[\{Y_i^{\mathrm{eval}}\}; Y^{\mathrm{acq}} \mid \{x_i^{\mathrm{eval}}\}, x^{\mathrm{acq}}, \mathcal{D}^{\mathrm{train}}] && (160)\\
&\approx \tfrac{1}{2}\log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]}[\mathcal{D}^{\mathrm{eval}} \mid \omega^*] + Id\right) - \tfrac{1}{2}\log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]}[\mathcal{D}^{\mathrm{acq}}, \mathcal{D}^{\mathrm{eval}} \mid \omega^*] + Id\right) && (161)\\
&\quad + \tfrac{1}{2}\log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]}[\mathcal{D}^{\mathrm{acq}} \mid \omega^*] + Id\right) && (162)
\end{aligned}$$

Furthermore, we can apply the approximation in Proposition 6.2 and find that the $\log \lambda$ terms cancel because $|\mathcal{D}^{\text{acq}}| + |\mathcal{D}^{\text{train}}| = |\mathcal{D}^{\text{acq}} \cup \mathcal{D}^{\text{train}}|$. Taking the limit $\lambda \to 0$, we obtain:

$$\mathrm{I}[\{Y_i^{\text{eval}}\}; Y^{\text{acq}} \mid \{x_i^{\text{eval}}\}, x^{\text{acq}}, \mathcal{D}^{\text{train}}] \tag{163}$$

$$\approx \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{\text{eval}} \mid \omega^*] + \lambda Id\right) - \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{\text{acq}}, \mathcal{D}^{\text{eval}} \mid \omega^*] + \lambda Id\right) + \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{\text{acq}} \mid \omega^*] + \lambda Id\right) \tag{164}$$

$$\to \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{\text{eval}} \mid \omega^*]\right) - \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{\text{acq}}, \mathcal{D}^{\text{eval}} \mid \omega^*]\right) + \tfrac{1}{2} \log\det\left(S[\mathcal{D}^{\text{acq}} \mid \omega^*]\right). \tag{165}$$

Finally, the first term is independent of $\mathcal{D}^{\text{acq}}$, and if we are interested in approximately maximizing JEPIG, we can maximize as proxy objective:

$$\log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\text{train}}]}[\mathcal{D}^{\text{acq}} \mid \omega^*] + Id\right) - \log\det\left(S_{\mathrm{H}''[\omega^* \mid \mathcal{D}^{\text{train}}]}[\mathcal{D}^{\text{acq}}, \mathcal{D}^{\text{eval}} \mid \omega^*] + Id\right), \tag{166}$$

or

$$\log\det\left(S[\mathcal{D}^{\text{acq}} \mid \omega^*]\right) - \log\det\left(S[\mathcal{D}^{\text{acq}}, \mathcal{D}^{\text{eval}} \mid \omega^*]\right). \tag{167}$$

# D Connection to Other Acquisition Functions in the Literature

## D.1 SIMILAR (Kothawade et al., 2021) and PRISM (Kothawade et al., 2022)

**Connection to LogDetMI.** If we apply the Schur decomposition to $\log\det S[\mathcal{D}^{\text{acq}}, \mathcal{D}^{\text{eval}} \mid \omega^*]$ from eq. (167), we obtain the following:

$$\log\det S[\mathcal{D}^{\text{acq}} \mid \omega^*] - \log\det S[\mathcal{D}^{\text{acq}}, \mathcal{D}^{\text{eval}} \mid \omega^*] \tag{168}$$

$$= \log\det S[\mathcal{D}^{\text{acq}} \mid \omega^*] - \log\det S[\mathcal{D}^{\text{eval}} \mid \omega^*] \tag{169}$$

$$- \log\det(S[\mathcal{D}^{\text{acq}} \mid \omega^*] - S[\mathcal{D}^{\text{acq}}; \mathcal{D}^{\text{eval}} \mid \omega^*] S[\mathcal{D}^{\text{eval}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{eval}}; \mathcal{D}^{\text{acq}} \mid \omega^*]),$$

where $S[\mathcal{D}^{\text{acq}}; \mathcal{D}^{\text{eval}} \mid \omega^*]$ is the nonsymmetric similarity matrix between $\mathcal{D}^{\text{acq}}$ and $\mathcal{D}^{\text{eval}}$ etc.

Dropping $\log\det S[\mathcal{D}^{\text{eval}} \mid \omega^*]$ which is independent of $\mathcal{D}^{\text{acq}}$, we can instead maximize:

$$\log\det S[\mathcal{D}^{\text{acq}} \mid \omega^*] - \log\det(S[\mathcal{D}^{\text{acq}} \mid \omega^*] - S[\mathcal{D}^{\text{acq}}; \mathcal{D}^{\text{eval}} \mid \omega^*] S[\mathcal{D}^{\text{eval}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{eval}}; \mathcal{D}^{\text{acq}} \mid \omega^*], ) \tag{170}$$

which is exactly the LogDetMI objective of SIMILAR (Kothawade et al., 2021) and PRISM (Kothawade et al., 2022).

We can further rewrite this objective by extracting $S[\mathcal{D}^{\text{acq}} \mid \omega^*]$ from the second term, obtaining:

$$\log\det S[\mathcal{D}^{\text{acq}} \mid \omega^*] - \log\det(S[\mathcal{D}^{\text{acq}} \mid \omega^*] - S[\mathcal{D}^{\text{acq}}; \mathcal{D}^{\text{eval}} \mid \omega^*] S[\mathcal{D}^{\text{eval}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{eval}}; \mathcal{D}^{\text{acq}} \mid \omega^*]) \tag{171}$$

$$= -\log\det(Id - S[\mathcal{D}^{\text{acq}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{acq}}; \mathcal{D}^{\text{eval}} \mid \omega^*] S[\mathcal{D}^{\text{eval}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{eval}}; \mathcal{D}^{\text{acq}} \mid \omega^*]). \tag{172}$$

**Connection to LogDetCMI.** Using information-theoretic decompositions, it is easy to show that:

$$\mathrm{I}[\{Y_i^{\text{eval}}\}; Y^{\text{acq}} \mid \{x_i^{\text{eval}}\}, x^{\text{acq}}, \{Y_i\}, \{x_i\}, \mathcal{D}^{\text{train}}] \tag{173}$$

$$= \mathrm{I}[\{Y_i^{\text{eval}}\}; Y^{\text{acq}}, \{Y_i\} \mid \{x_i^{\text{eval}}\}, x^{\text{acq}}, \{x_i\}, \mathcal{D}^{\text{train}}] - \mathrm{I}[\{Y_i^{\text{eval}}\}; \{Y_i\} \mid \{x_i\}, \mathcal{D}^{\text{train}}]. \tag{174}$$

These are two JEPIG terms, and using above approximations, including (172), leads to the LogDetCMI objective:

$$\log \frac{\det(Id - S[\mathcal{D}^{\text{acq}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{acq}}; \mathcal{D}^{\text{eval}} \mid \omega^*] S[\mathcal{D}^{\text{eval}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{eval}}; \mathcal{D}^{\text{acq}} \mid \omega^*])}{\det(Id - S[\mathcal{D}^{\text{acq}}, \mathcal{D} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{acq}}, \mathcal{D}; \mathcal{D}^{\text{eval}} \mid \omega^*] S[\mathcal{D}^{\text{eval}} \mid \omega^*]^{-1} S[\mathcal{D}^{\text{eval}}; \mathcal{D}^{\text{acq}}, \mathcal{D} \mid \omega^*])}. \tag{175}$$

### D.2 Expected Gradient Length

**Proposition 7.3.** *The EIG for a candidate sample $x^{acq}$ approximately lower-bounds the EGL:*

$$2\,\mathrm{I}[\Omega; Y^{acq} \mid x^{acq}] \overset{\approx}{\leq} \mathbb{E}_{\mathrm{p}(y^{acq}|x^{acq},\omega^*)} \left\|\mathrm{H}'[y^{acq} \mid x^{acq}, \omega^*]\right\|^2 + \textit{const.} \tag{88}$$

*Proof.* The EIG is equal to the conditional entropy up to a constant term, via eq. (51) in Proposition 5.2:

$$\mathrm{I}[\Omega; Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}] \overset{\approx}{\leq} \tfrac{1}{2} \log\det\left(\mathrm{H}''[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{176}$$

We apply a diagonal approximation for the Fisher information and Hessian, noting that the determinant of the diagonal matrix upper-bounds the determinant of the full matrix:

$$\leq \tfrac{1}{2} \log\det\left(\mathrm{H}''_{diag}[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''_{diag}[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{177}$$

$$= \tfrac{1}{2} \sum_k \log\left(\mathrm{H}''_{diag,kk}[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''_{diag,kk}[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{178}$$

We use $\log x \leq x - 1$ and that $\mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]$ is constant:

$$\leq \tfrac{1}{2} \sum_k \left(\mathrm{H}''_{diag,kk}[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''_{diag,kk}[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{179}$$

$$\leq \tfrac{1}{2} \sum_k \mathrm{H}''_{diag,kk}[Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{const.} \tag{180}$$

From Proposition 4.3, we know that the Fisher information is equivalent to the outer product of the Jacobians: $\mathrm{H}''[Y^{\mathrm{acq}}|x^{\mathrm{acq}}, \omega^*] = \mathbb{E}_{\mathrm{p}(y^{\mathrm{acq}}|x^{\mathrm{acq}},\omega^*)}[\mathrm{H}'[y^{\mathrm{acq}}|x^{\mathrm{acq}}, \omega^*]\ \mathrm{H}'[y^{\mathrm{acq}}|x^{\mathrm{acq}}, \omega^*]^T]$, and we finally obtain for the diagonal elements:

$$= \tfrac{1}{2} \sum_k \mathbb{E}_{\mathrm{p}(y^{\mathrm{acq}}|x^{\mathrm{acq}},\omega^*)}\left[\mathrm{H}'_k[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*]^2\right] + \mathrm{const.} \tag{181}$$

$$= \tfrac{1}{2}\, \mathbb{E}_{\mathrm{p}(y^{\mathrm{acq}}|x^{\mathrm{acq}},\omega^*)}\left[\left\|\mathrm{H}'[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*]\right\|^2\right] + \mathrm{const.} \tag{182}$$

□

### D.3 Deep Learning on a Data Diet

**Proposition 7.4.** *The IG for a candidate sample $x^{acq}$ approximately lower-bounds the gradient norm score (GraNd) at $\omega^*$ up to a second-order term:*

$$2\,\mathrm{I}[\Omega; y^{acq} \mid x^{acq}] \overset{\approx}{\leq} \mathbb{E}_{\mathrm{q}(\omega)}[\left\|\mathrm{H}'[y^{acq} \mid x^{acq}, \omega]\right\|^2] - \mathbb{E}_{\mathrm{q}(\omega)}[\mathrm{tr}\left(\frac{\nabla^2_\omega\, \mathrm{p}(y \mid x, \omega)}{\mathrm{p}(y \mid x, \omega)}\right)] + \textit{const.} \tag{89}$$

*Proof.* For any fixed $\omega^*$, the IG is equal to the conditional entropy up to a constant term, via Proposition 5.3:

$$\mathrm{I}[\Omega; Y^{\mathrm{acq}} \mid x^{\mathrm{acq}}] \overset{\approx}{\leq} \tfrac{1}{2} \log\det\left(\mathrm{H}''[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{183}$$

As in the previous proof, we apply a diagonal approximation for the Hessian, noting that the determinant of the diagonal matrix upper-bounds the determinant of the full matrix:

$$\leq \tfrac{1}{2} \log\det\left(\mathrm{H}''_{diag}[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''_{diag}[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{184}$$

$$= \tfrac{1}{2} \sum_k \log\left(\mathrm{H}''_{diag,kk}[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''_{diag,kk}[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{185}$$

Again, we use $\log x \leq x - 1$ and that $\mathrm{H}''[\omega^* \mid \mathcal{D}^{\mathrm{train}}]$ is constant:

$$\leq \tfrac{1}{2} \sum_k \left(\mathrm{H}''_{diag,kk}[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{H}''_{diag,kk}[\omega^* \mid \mathcal{D}^{\mathrm{train}}]\right) + \mathrm{const.} \tag{186}$$

$$\leq \tfrac{1}{2} \sum_k \mathrm{H}''_{diag,kk}[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] + \mathrm{const.} \tag{187}$$

From Lemma A.1, we know that the Hessian is equivalent to the outer product of the Jacobians plus a second-order term: $\mathrm{H}''[y^{\mathrm{acq}} \,|\, x^{\mathrm{acq}}, \omega^*] = \mathrm{H}'[y^{\mathrm{acq}} \,|\, x^{\mathrm{acq}}, \omega^*]\ \mathrm{H}'[y^{\mathrm{acq}} \,|\, x^{\mathrm{acq}}, \omega^*]^T - \frac{\nabla^2_\omega \mathrm{p}(y^{\mathrm{acq}}|x^{\mathrm{acq}},\omega^*)}{\mathrm{p}(y^{\mathrm{acq}}|x^{\mathrm{acq}},\omega^*)}$, and we finally obtain for the diagonal elements:

$$= \tfrac{1}{2} \sum_k \mathrm{H}'_k[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*]^2 - \tfrac{1}{2} \operatorname{tr}\left( \frac{\nabla^2_\omega \mathrm{p}(y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*)}{\mathrm{p}(y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*)} \right) + \mathrm{const.} \tag{188}$$

$$= \tfrac{1}{2} \left\| \mathrm{H}'[y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*] \right\|^2 - \tfrac{1}{2} \operatorname{tr}\left( \frac{\nabla^2_\omega \mathrm{p}(y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*)}{\mathrm{p}(y^{\mathrm{acq}} \mid x^{\mathrm{acq}}, \omega^*)} \right) + \mathrm{const.} \tag{189}$$

Taking an expectation over $\omega^* \sim \mathrm{q}(\omega)$ yields the statement. □