
Label-Wise Uncertainty Decomposition for Multi-Label Classification by Maximizing Type II Likelihood

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Abstract

Currently, the way deep learning models recognize uncertainty remains inconsistent with human perception. In multi-label classification, quantifying uncertainty at the label level presents challenges, as each label may exhibit distinct model confidence levels. Understanding and decomposing label-specific uncertainty is essential for interpreting model behavior and ensuring reliable predictions. We build a hierarchical Bayesian methodology for multi-label classification that leverages a Type II likelihood and Empirical Bayes. Then we estimate and decompose label-wise uncertainties step by step. Our approaches offer four main contributions: (1) Type II likelihood maximization is data likelihood centric; (2) it can decompose label-wise uncertainty into the First-order Model Variance, Second-order Model Variance, Model Bias and Optimal Spread; (3) our label-wise uncertainty represented by Second-order Model Variance is intuitively interpretable when combined with observational data; and (4) when applied to out-of-distribution (OOD) detection task, it achieves a 6.88% lower FPR95 score on NUS-WIDE.

1 INTRODUCTION

The growing adoption of deterministic neural networks (NN) in safety-critical domains, such as medical diagnosis and autonomous driving, necessitates the development of reliable methods for uncertainty quantification. Model confidence is also essential for understanding the model’s behavior, enabling interpretable predictions and informed decision-making in complex domains. When considering multi-label classification tasks, this challenge becomes even more pronounced as the model must simultaneously predict multiple labels that may exhibit interdependencies, varying levels of

noise associated with different labels, and differing degrees of uncertainty across instances.

Unlike single-label multi-class classification, where each instance is assigned one label, multi-label classification allows multiple labels to exist simultaneously per instance. Consequently, individual labels can exhibit varying levels of uncertainty arising from input-dependent noise or intricate interdependencies. For example, in an image classification task, a stable foreground person may be assigned a label with low uncertainty due to clear visual features, while a moving car in the background, blurred by motion, may yield a label with high uncertainty due to ambiguity in its detection. Understanding label-wise uncertainty is crucial for interpreting the model’s reasoning, as it reveals how confidently the model assigns each label and highlights potential ambiguities in its predictions. However, merely making simple use of probability is often not enough.

Adapting uncertainty estimation techniques to multi-label classification remains challenging. Wang et al. [2021] proposed a label-wise uncertainty measurement based on an energy function, a method that leverages the overconfidence Nguyen et al. [2015] of neural networks targeting OOD detection. Sale et al. [2024] discussed how the mutual information or the total variance decomposition can be used to find the label-wise uncertainty in a multi-class classification problem. The Gibbs classifier is commonly adopted in EDL research Sensoy et al. [2018], Zhao et al. [2023], Charpentier et al. [2020]. And the Subjective Logic (SL) Jøssang et al. [2018], Jøssang [2016] from evidence theories also plays a crucial role in defining the epistemic uncertainty Hüllermeier and Waegeman [2021] of EDL research. As a sampling-based expected loss classifier, the Gibbs classifier does not fully optimize the likelihood of the observed data under the model; it also considers the variance factor in the hierarchical model, which is discussed in Section 2.4.

A key aspect of Bayesian inference involves assigning prior distributions to hierarchical models to quantify and estimate uncertainty Gelman [2006]. Sensoy et al. [2018] in-

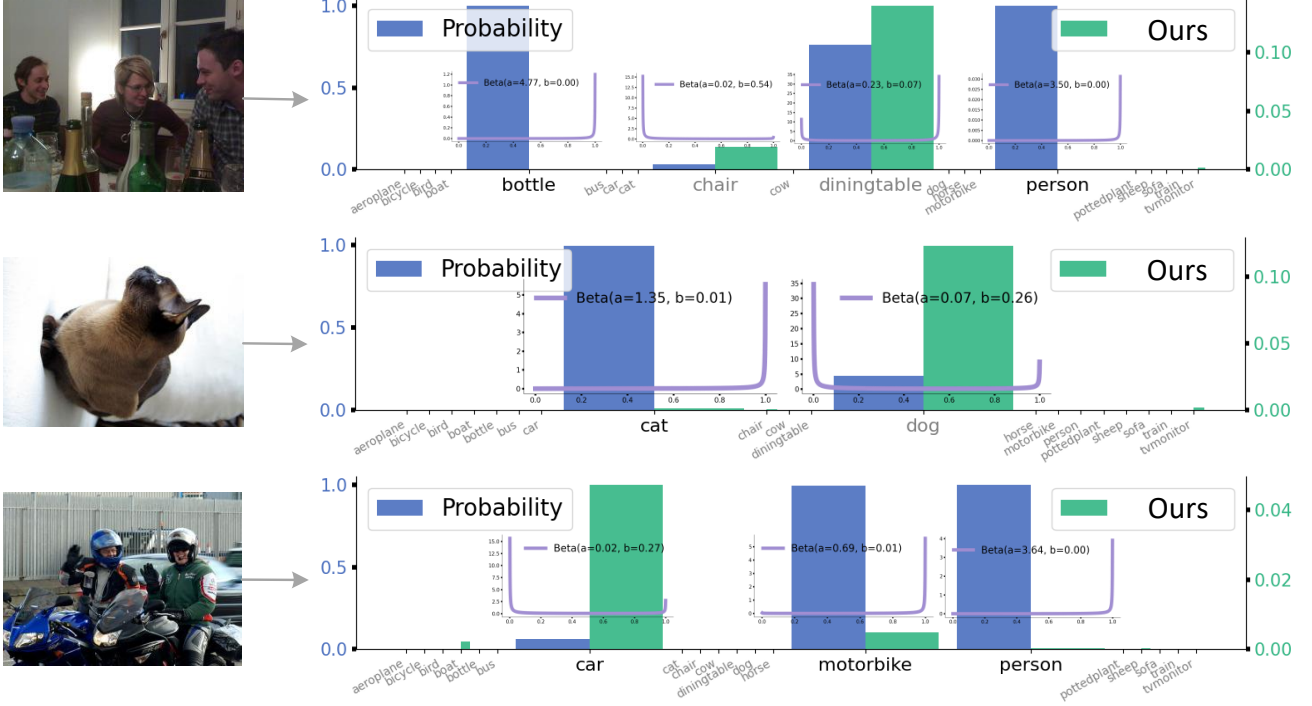


Figure 1: Given an input, the neural network is trained to predict the hyperparameters of a Type II likelihood instead of directly outputting the probability. The black labels represent the ground truth labels. The purple distribution represents the posterior Beta distribution for each label. The blue bar indicates predictive probability of the label, and the green bar represents the Second-Order Model Variance in (5). Across these three examples, our model demonstrates interpretable uncertainty regarding the labels: "dining table," visible but not ground truth; "dog," likely misidentified as a dog; and "car," exhibiting motion blur. This aligns well with human visual understanding of the corresponding scenes.

Introduces Evidential Deep Learning methods, a framework for modeling predictive uncertainty in multi-class classification problems by parameterizing a Dirichlet prior over first-order distribution. Malinin and Gales [2018] proposed a new framework for modeling predictive uncertainty called Prior Networks, which explicitly models distributional uncertainty. Gaussian distribution is commonly used to model and capture heteroscedastic uncertainty Lakshminarayanan et al. [2017]. The paper Nix and Weigend [1994] addressed regression problems by modeling the observed value as a sample from a heteroscedastic Gaussian distribution. Building on Gaussian, Amini et al. [2020] introduced a hierarchical evidential framework by incorporating an additional Gaussian and an inverse-gamma distribution to govern the original Gaussian's mean and variance. However, these approaches could not capture label-wise uncertainty, and some are still controversial. Bengs et al. [2022], Shen et al. [2024], Meinert et al. [2023] showed that evidential uncertainty methods do not incentivize the learner to represent epistemic uncertainty in a faithful way. Hence, further exploration of the remaining gaps in evidential learning is essential. In this paper, we systematically build a hierarchical model for multi-label classification by Bayesian inference and theoretically prove its correctness as both a learning criterion

and uncertainty measurement. To achieve this, we make the following key contributions.

1. We explore a maximizing Type II likelihood learning criterion for multi-label classification. We prove the criterion to be data likelihood-centric.
2. We propose a methodology for decomposing uncertainty at the label level, which is directly tied to the definition of the Type II likelihood.
3. Experiments show that the Second-Order Model Variance from the decomposition (5) is more intuitively interpretable. And its statistical effectiveness is proven by label-wise OOD detection tasks.

As illustrated in Figure 1, given an input, the neural network is trained to predict the parameters of a Type II likelihood or marginal likelihood. In the context of the first image depicting a party scene, the model shows uncertainty about the labels for the chair and dining table. Notably a portion of the dining table is visible in this image but not treated as ground truth.

2 METHODOLOGY

In multi-label classification, a sample can be associated with multiple labels simultaneously, requiring the prediction of a binary label vector $\mathbf{y} = (y_1, y_2, \dots, y_K)^\top \in \{0, 1\}^K$ from input feature $\mathbf{x} \in \mathbb{R}^d$. The objective is to learn a function f such that $f(\theta, \mathbf{x})$ helps approximate a probability vector $M = [\mu_1, \mu_2, \dots, \mu_K]$, where μ_k represents the probability of the k -th label of the input $\mathbf{x}$.

In this work, we focus on the Type II Maximum Likelihood (ML) methodology. While Type I ML is simpler and computationally efficient due to its deterministic nature, Type II ML provides a more comprehensive framework for capturing and exploiting uncertainty. Further introduction on both Type I and Type II ML approaches can be found in Appendix A.

2.1 TYPE I MAXIMUM LIKELIHOOD OF MULTI-LABEL CLASSIFICATION

The binary cross-entropy loss Rumelhart et al. [1986] function is used for multi-label classification tasks due to the independent nature of the problem. It is particularly effective as it treats each label as a separate binary classification, allowing the model to independently evaluate the presence or absence of each label. Let y_{ik} be the ground truth label for the i -th sample ($y_{ik} \in \{0, 1\}$) and k -th label. $\hat{y}_{ik}$ represents the raw logit output of the model f for the i -th input $\mathbf{x}_i$. $\sigma(\hat{y}_{ik}) = \frac{1}{1+e^{-\hat{y}_{ik}}}$ is the sigmoid function applied to the logits, converting them to probabilities μ . N denotes the total number of samples. The binary cross-entropy empirical risk using the sigmoid function can be defined as:

$$\hat{\mathcal{R}}_{\mathcal{D}}^{\text{BCE}}(f(\theta)) = -\frac{1}{NK} \sum_{i=1}^N \sum_{k=1}^K \left[y_{ik} \cdot \log(\sigma(\hat{y}_{ik})) + (1 - y_{ik}) \cdot \log(1 - \sigma(\hat{y}_{ik})) \right],$$

where is derived from the negative log-likelihood of a Bernoulli distribution, and the target is to maximize the Type I likelihood of the observed data. For a single label, the likelihood is given by:

$$p(y | \mu) = \mu^y (1 - \mu)^{1-y}, \quad (1)$$

where $\mu \in [0, 1]$ represents the predicted probability of the positive label $y = 1$.

In Type I ML, the hyperparameter μ is assumed as highly peaked, and uncertainty is often represented through the spread of the predicted probabilities, Entropy, etc. However, these methods only capture the uncertainty based on the probability values themselves. It cannot account for the uncertainty underneath the probability, such as cases where predictions with the same probability value may correspond

to fundamentally different confidence levels. So, label-wise uncertainty needs more sufficient model evidence to tell how the model's reasoning process.

2.2 DERIVE THE LABEL-WISE TYPE II LIKELIHOOD

In this section, we focus on deriving the Type II likelihood for individual labels. Type II ML Berger and Wolpert [1988] extends Type I by marginalizing over model parameters, effectively integrating out uncertainty in a Bayesian setting. In a fully Bayesian treatment, prior distributions are assigned for the Type I ML given by (1) over the hyperparameter μ and model parameters θ . This makes predictions by marginalizing with respect to the hyperparameter of Type I likelihood and as well as with respect to the parameters θ . In deep neural networks, incorporating hyperpriors for all model parameters Kendall and Gal [2017] remains challenging. Key difficulties include the intractability of directly inferring the posterior distribution of the weights given the data and the high computational cost associated with sampling during inference Amini et al. [2020]. Hence in our evidential approximation, we obtain the predictive distribution by introducing hyperpriors over hyperparameters of Type I likelihood. Since the likelihood for each binary label is a Bernoulli distribution, we assign its conjugate prior, a Beta distribution, over the latent probability μ . The Beta distribution is expressed as:

$$\mathcal{B}(\mu; a, b) = \frac{\mu^{a-1} (1 - \mu)^{b-1}}{\text{Beta}(a, b)},$$

where a and b are positive hyperparameters. $\text{Beta}(a, b)$ is the Beta function Kotz et al. [2019]. Then the predictive distribution is obtained by marginalizing over hyperparameters so that:

$$p(t | \mathbf{x}, \mathcal{D}) = \int \int p(t | \mu) p(\mu | a, b) p(a, b | \mathbf{x}, \mathcal{D}) d\mu da db, \quad (2)$$

where μ , a and b are treated as latent variables and μ is governed by the a and b . t represents the target label of a new given input $\mathbf{x}$. Here, $p(t | \mu)$ follows a Bernoulli distribution for a single label, while $p(\mu | a, b)$ represents the conjugate Beta prior over μ . The term $p(a, b | \mathbf{x}, \mathcal{D})$ denotes the posterior distribution of the hyperparameters a and b given the input $\mathbf{x}$ and the observed data $\mathcal{D}$, encapsulating the model's learned uncertainty about the underlying label probabilities.

Assumption 2.1 (Highly Peaked Hyperparameters). The posterior distribution $p(a, b | \mathcal{D})$ is sharply peaked around its mode (a^*, b^*) .

Since exploring the underlying distribution of a and b is much more complex, it assumes that the distribution places

most of its mass around a specific value. This allows us to approximate the posterior by a delta function centered at (a^*, b^*) , i.e., $p(a, b | \mathcal{D}) \approx \delta(a - a^*) \delta(b - b^*)$ enabling a simpler estimation of the predictive distribution. With Assumption 2.1, for frequent labels with many matching examples, the (Empirical Bayes) mode of μ will indeed sharpen, but for rare labels or small datasets, the mode of μ may sit atop a broad distribution. Now the predictive distribution is derived by integrating over μ , where a and b are set to their sharply peaked values a^* and b^* , leading to:

$$\begin{aligned} p(t | \mathbf{x}, \mathcal{D}) &\simeq p(t | \mathcal{D}, a^*, b^*) \\ &= \int p(t | \mu) p(\mu | \mathcal{D}, a^*, b^*) d\mu. \end{aligned}$$

To learn the a^* and b^* , from Bayes' theorem, the posterior distribution for a and b is expressed as:

$$p(a, b | \mathcal{D}) \propto p(\mathcal{D} | a, b) p(a, b).$$

Assumption 2.2 (Flat Prior $p(a, b)$). The prior distribution $p(a, b)$ is relatively flat (non-informative).

Assumption 2.2 means it does not favor any particular value of a and b a priori, but a relatively uninformative prior compared with the data, which anchors the Empirical Bayes interpretation. This allows the posterior $p(a, b | \mathcal{D})$ to be determined by $p(\mathcal{D} | a, b)$, simplifying the estimation of a^* and b^* by maximizing the Type II likelihood $p(\mathcal{D} | a, b)$, which is defined as a marginal distribution:

$$p(\mathcal{D} | a, b) = \prod_{i=1}^N \prod_{k=1}^K \int_0^1 p(y_{ik} | \mu_{ik}) p(\mu_{ik} | \mathbf{x}_i, a_{ik}, b_{ik}) d\mu_{ik}.$$

The Beta prior distribution, combined with the Bernoulli likelihood, enables the computation of a label-wise marginal likelihood. The Type II likelihood for one single label is expressed as:

$$p(y | a, b) = \int_0^1 \mu^y (1 - \mu)^{1-y} \frac{\mu^{a-1} (1 - \mu)^{b-1}}{\text{Beta}(a, b)} d\mu.$$

As the inference is shown in Appendix B, the above formula results in:

$$p(y | a, b) = \left(\frac{a}{a+b} \right)^y \left(\frac{b}{a+b} \right)^{1-y}. \quad (3)$$

We can also understand that each observed target label y is drawn independently but not identically from the distribution parameterized by a and b . These parameters encapsulate our belief about the distribution of labels and are subject to estimation. The graph model in Figure 2 shows the relationship between variables.

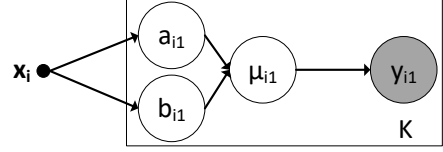


Figure 2: The graph model illustrates building a Beta prior to control the Bernoulli distribution, treating μ as a latent variable determined by a and b , enabling label-wise uncertainty estimation for the number of K labels.

2.3 MAXIMIZE THE TYPE II LIKELIHOOD BY NEURAL NETWORK

The Type II binary cross-entropy loss is derived from the Type II likelihood in (3) by taking a negative logarithm. We approximate second-order hyperparameters a and b by $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$. The loss function is defined as:

$$\begin{aligned} \mathcal{L}_{\text{Type II}}(f(\theta)) &= \log(a(\mathbf{x}, \theta) + b(\mathbf{x}, \theta)) \\ &\quad - y \log(a(\mathbf{x}, \theta)) - (1 - y) \log(b(\mathbf{x}, \theta)). \end{aligned} \quad (4)$$

The hyperparameters parameterize the Beta prior $\mathcal{B}(\mu; a, b)$ and are estimated via Empirical Bayes Robbins [1992] by maximizing the marginal likelihood $p(\mathcal{D} | a, b)$.¹ The loss function, defined in (4), penalizes the model based on its predictive confidence for the label y , with $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$ dynamically adjusting to balance the estimated probability and associated uncertainty.

In neural network, we use $\hat{a}_{ik}$ and $\hat{b}_{ik}$ represent the raw logit from the neural network $f(\mathbf{x}_i, \theta)$ of the input $\mathbf{x}_i$ and k -th label. We adopt the *softplus* function to ensure positivity and numerical stability during learning. The softplus function $s(x)$ is defined as: $s(x) = \ln(1 + e^x)$, where $s(x) > 0$ for all x . Then a_{ik} and b_{ik} can be represented by $s(\hat{a}_{ik})$ and $s(\hat{b}_{ik})$. To generalize this learning process across a dataset with N samples and K classes, we define the empirical risk as Type II binary cross-entropy loss denoted as $\hat{\mathcal{R}}_{\mathcal{D}}^{\text{Type II}}$:

$$\begin{aligned} \hat{\mathcal{R}}_{\mathcal{D}}^{\text{Type II}}(f(\theta)) &= \frac{1}{NK} \sum_{i=1}^N \sum_{k=1}^K \left[\log(s(\hat{a}_{ik}) + s(\hat{b}_{ik})) \right. \\ &\quad \left. - y_{ik} \log(s(\hat{a}_{ik})) - (1 - y_{ik}) \log(s(\hat{b}_{ik})) \right]. \end{aligned}$$

2.4 BAYESIAN CLASSIFIER OR GIBBS CLASSIFIER

In Section 2.2 and Section 2.3, we suggested a Bayesian classifier by the Type II likelihood. The loss function in (4) is actually a Bayesian classifier, which is given by:

$$\mathcal{L}_{\text{Type II}} = -\log \mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})} [\mu_{ik}],$$

¹The prior $\mathcal{B}(\mu; a, b)$ is an empirical prior, as its parameters a and b are learned by maximizing the marginal likelihood $p(\mathcal{D} | a, b)$.

where μ_{ik} represents the probability of the k -th class for the i -th sample, and $\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})$ is drawn from a Beta distribution parameterized by $a_{ik}(\mathbf{x}_i, \theta)$ and $b_{ik}(\mathbf{x}_i, \theta)$, which depend on input feature $\mathbf{x}_i$ and the model parameters.

In contrast, the Gibbs classifier adopts a different approach. It randomly samples μ_{ik} from the same Beta distribution, $\text{Beta}(a_{ik}, b_{ik})$, and computes the expected loss by averaging the negative log-probability over these samples. The loss function for the Gibbs classifier can be defined:

$$\mathcal{L}_{\text{Gibbs}} = \mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})} [-\log \mu_{ik}].$$

Unlike the Bayesian classifier, the Gibbs classifier does not directly minimize the expected likelihood but instead relies on optimizing the overall performance of the expected loss.

By Jensen’s inequality, for a convex function g , we have: $g(\mathbb{E}[X]) \leq \mathbb{E}[g(X)]$, which corresponds to $\mathcal{L}_{\text{Type II}} \leq \mathcal{L}_{\text{Gibbs}}$. Equality holds if and only if g is linear over the μ_{ik} or μ_{ik} is deterministic (i.e., the Beta distribution is degenerate, with all mass at a single point). Since the negative logarithm is convex, equality requires μ_{ik} to have zero variance, which occurs only in the degenerate case. Applying to $g(\mu_{ik}) = -\log \mu_{ik}$ and $X = \mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})$, we obtain:

$$\begin{aligned} & -\log \mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})} [\mu_{ik}] \\ & \leq \mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})} [-\log \mu_{ik}]. \end{aligned}$$

The inequality implies that, under the same distributional assumption $\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})$, the Bayesian classifier yields a lower or equal risk compared to the Gibbs classifier. The following proposition formalizes this result.

Proposition 2.3 (Bayesian Classifier is More likelihood-driven). *Let $\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})$ represent the class probability for the i -th sample and k -th class, parameterized by $a_{ik}(\mathbf{x}, \theta)$ and $b_{ik}(\mathbf{x}, \theta)$. Define the Bayesian classifier loss as $\mathcal{L}_{\text{Type II}} = -\log \mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})} [\mu_{ik}]$ and the Gibbs classifier loss as $\mathcal{L}_{\text{Gibbs}} = \mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})} [-\log \mu_{ik}]$. Then, by Jensen’s inequality, $\mathcal{L}_{\text{Type II}} \leq \mathcal{L}_{\text{Gibbs}}$, with equality if and only if μ_{ik} is deterministic. Thus, under the assumption that $\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})$, the Bayesian classifier is at least as effective as the Gibbs classifier as a learning criterion to maximize the data likelihood, and more effective when the Beta distribution has non-zero variance.*

Furthermore, a second-order Taylor expansion of the negative logarithm around the mean of the Beta distribution reveals that the Gibbs loss incorporates a penalty term proportional to the variance of μ_{ik} , effectively accounting for uncertainty in the class probabilities. According to Appendix C, we can read:

$$\mathcal{L}_{\text{Gibbs}} = \mathcal{L}_{\text{Type II}} + \frac{\text{Var}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})} [\mu_{ik}]}{2\mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})}^2 [\mu_{ik}]} + \mathbb{E}[R].$$

where R is the higher-order remainder. In contrast, the Type II loss does not include this second-order term, making it

Table 1: Average Precision scores with variability across seeds for different loss functions on ResNet architectures.

LOSS FUNCTION	RESNET-34	RESNET-50
$\mathcal{L}_{\text{BCE}}$	0.919 ± 0.001	0.926 ± 0.001
$\mathcal{L}_{\text{BCE}}(\text{SOFTMAX})$	0.918 ± 0.001	0.927 ± 0.001
$\mathcal{L}_{\text{Type II}}(a, b > 1)$	0.929 ± 0.001	0.940 ± 0.001
$\mathcal{L}_{\text{GIBBS}}$	0.789 ± 0.035	0.822 ± 0.057
$\mathcal{L}_{\text{Type II}}$	0.947 ± 0.001	0.958 ± 0.001

less sensitive to variance and thus potentially more robust in scenarios with concentrated posteriors, but less penalizing of high-uncertainty predictions. This suggests that the Gibbs classifier is more conservative, as it explicitly penalizes variance to encourage more certain predictions.

We compare the average precision score on the Pascal VOC 2012 real-world dataset for the Bayesian classifier $\mathcal{L}_{\text{Type II}}$, the Gibbs classifier $\mathcal{L}_{\text{Gibbs}}$, and other training criteria. The other criteria include binary cross entropy loss $\mathcal{L}_{\text{BCE}}$, softmax binary cross entropy loss $\mathcal{L}_{\text{BCE}}(\text{softmax})$, and $\mathcal{L}_{\text{Type II}}(a, b \geq 1)$. The latter represents the setting where hyperparameters a and b are constrained to be greater than or equal to 1, a common configuration in evidential deep learning. As shown in Table 1, the Type II learning criterion achieves superior performance on the dataset. We also discussed the effect of a non-informative prior weight, which is popularly used in EDL Sensoy et al. [2018], Charpentier et al. [2020], Zhao et al. [2023], Bengs et al. [2022] by Subjective Logic. It will make the Beta distribution a Bell shape when we set $a > 1$ and $b > 1$. This can also be found in Appendix D.

2.5 UNCERTAINTY ESTIMATION AND DECOMPOSITION

As Proposition 2.3 demonstrates, the learning criterion of $\mathcal{L}_{\text{Type II}}$ achieves a data likelihood that is greater than or equal to that of the Gibbs classifier. This superior data likelihood indicates that the Type II learning enables the model to develop a more compact connection with the underlying patterns present in the training data. Consequently, the Bayesian classifier’s enhanced understanding of training data is crucial for inferring human-interpretable uncertainty measurements. This framework also allows us to model label-wise heteroscedastic uncertainty, contrasting with homoscedastic uncertainty which assumes a uniform uncertainty level across all data instances.

Set the parameter μ^* is the theoretical true data-generating distribution $p(t \mid \mu^*)$. Both μ and μ^* are themselves uncertain: in a hierarchical Bayesian framework, μ is drawn from a second-order distribution $p(\mu \mid m)$ induced by $f(x)$, giving the Markov chain $m \rightarrow \mu \rightarrow t$, while μ^* is drawn

from $p(\mu^* | m^*)$, giving the parallel chain $m^* \rightarrow \mu^* \rightarrow t$. The main uncertainty decomposition in our framework is expressed through the pointwise risk $(\mu^* - t)^2$, which measures the squared deviation of the mean of the theoretical true data-generating distribution from the observed target. To decompose this risk into interpretable components from a model prediction perspective, we deconstruct it into:

$$\begin{aligned} E_{\mu^*} E_{\mu} E_{t|\mu} [(\mu^* - t)^2] &= \underbrace{E_{\mu} [\text{Var}_{t|\mu}(t)]}_{\text{First-order Model Variance}} \\ &+ \underbrace{\text{Var}_{\mu}(\mu)}_{\text{Second-order Model Variance}} + \underbrace{(\bar{\mu} - \mu^*)^2}_{\text{Model Bias}} + \underbrace{\text{Var}_{\mu^*}(\mu^*)}_{\text{Optimal Spread}}. \end{aligned} \quad (5)$$

The first-order model variance $E_{\mu} [\text{Var}_{t|\mu}(t)]$ captures the irreducible scatter of the observed target t around the model's predictive parameter μ , averaged over the model's own second-order distribution $p(\mu | a, b)$. The second-order model variance $\text{Var}_{\mu}(\mu)$ captures how much the model's predictive parameter μ itself fluctuates across the second-order distribution $p(\mu | a, b)$, reflecting the model's own parametric uncertainty. The model bias $(\bar{\mu} - \mu^*)^2$ measures the squared discrepancy between the mean of the model's predictive distribution and the mean of the true data-generating distribution, capturing the systematic misalignment between the model and the ground truth. The optimal spread $\text{Var}_{\mu^*}(\mu^*)$ captures the inherent variability of the true data-generating parameter μ^* across the optimal distribution $p(\mu^* | m^*)$, representing irreducible uncertainty that exists even under the theoretically perfect predictor.

The First-order Model Variance $E_{\mu} [\text{Var}_{t|\mu}(t)]$ can be derived by:

$$E_{\mu} [\text{Var}_{t|\mu}(t)] = \frac{ab}{(a+b)(a+b+1)}$$

And the Second-order Model variance is the Beta variance:

$$\text{Var}_{\mu}(\mu) = \frac{ab}{(a+b)^2(a+b+1)}$$

Due to the inaccessibility of μ^* , we will not approach Model Bias and Optimal Spread via the predictive hyperparameters. All uncertainties are heteroscedastic uncertainties across different labels for each input, derived in Appendix E.1. More introduction about the Second-order Model Variance we defined can be found in Appendix E.3. And according to the Appendix E.2, the total uncertainty of the model can be defined by:

$$\begin{aligned} \text{Var}_{p(t|a,b)}(t) &= \frac{ab}{(a+b)^2} = \underbrace{\frac{ab}{(a+b)(a+b+1)}}_{\text{First-order Model Variance}} \\ &+ \underbrace{\frac{ab}{(a+b)^2(a+b+1)}}_{\text{Second-order Model Variance}} \end{aligned}$$

The total uncertainty of the model approaches to the true underlying probability $\mu^* = \frac{a^*(\mathbf{x}, \mathcal{D})}{a^*(\mathbf{x}, \mathcal{D}) + b^*(\mathbf{x}, \mathcal{D})}$, estimated by $\frac{a(\mathbf{x}, \theta, \mathcal{D})}{a(\mathbf{x}, \theta, \mathcal{D}) + b(\mathbf{x}, \theta, \mathcal{D})}$. Under the Robbins–Monro conditions on step sizes, stochastic gradient descent converges to μ^* , which means the total uncertainty of the model $\text{Var}_{p(t|a,b)}(t)$ converges to a certainty level. The proof is deferred to Appendix F.1.

Proposition 2.4 (The Total Uncertainty of the Model Will Stabilize with More Data). *As the model learns more underlying patterns of data, the total uncertainty of the model will converge towards a level dictated by the inherent variability of the model parameters.*

In a standard Bayesian framework with a Beta(a, b) prior, observing a new data point y leads to a posterior distribution $p(\mu|y, a, b) \propto p(y|\mu)p(\mu|a, b)/p(y|a, b)$, which results in a Beta posterior with updated parameters: Beta($a+1, b$) if $y = 1$, and Beta($a, b+1$) if $y = 0$. This demonstrates that with each consistent observation, the parameters of the posterior increase, indicating a stronger and more concentrated belief about the underlying parameter μ .

While the neural network $f(\theta)$ does not perform a direct integer update on $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$, the principle of Bayesian updating still guides its learning. When a new data point $(\mathbf{x}, y)$ is observed consistent with the learned patterns, the neural network will adjust its weights θ to perform an analogous update to the prior for that input $\mathbf{x}$. This update can be conceptually represented as:

$$\begin{aligned} p(\mu|y, a(\mathbf{x}, \theta), b(\mathbf{x}, \theta)) &\propto \\ p(y|\mu)p(\mu|a(\mathbf{x}, \theta), b(\mathbf{x}, \theta)) &/p(y|a(\mathbf{x}, \theta), b(\mathbf{x}, \theta)) \end{aligned}$$

Leading to a posterior that resembles a Beta distribution with updated hyperparameters: Beta($a(\mathbf{x}, \theta) + \delta_a(\mathbf{x}, y), b(\mathbf{x}, \theta)$) if y reinforces the learned pattern, or Beta($a(\mathbf{x}, \theta), b(\mathbf{x}, \theta) + \delta_b(\mathbf{x}, y)$) if y contradicts it (though in the case of consistently patterned data, the reinforcement scenario will be dominant over time). Here, $\delta_a(\mathbf{x}, y) \geq 0$ and $\delta_b(\mathbf{x}, y) \geq 0$ represent the positive adjustments to the respective hyperparameters based on the consistency of the new data y with the learned pattern for input $\mathbf{x}$.

Assumption 2.5 (Positive Increasing Hyperparameters a and b). Assume a neural network learns to recognize consistent patterns in a dataset, mapping input features $\mathbf{x}$ to Beta prior hyperparameters $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$ by maximizing the marginal likelihood. As the network observes consistently patterned data points $(\mathbf{x}, y)$, it refines weights θ to produce positive adjustments $\delta_a(\mathbf{x}, y) \geq 0$ and $\delta_b(\mathbf{x}, y) \geq 0$, leading to increasing values of $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$. This reflects a strengthening belief in the predictive distribution's parameters, analogous to Bayesian posterior updates.

Assumption 2.5 is relatively heuristic, and Appendix F.2 has empirical proof talking about it. The neural network's

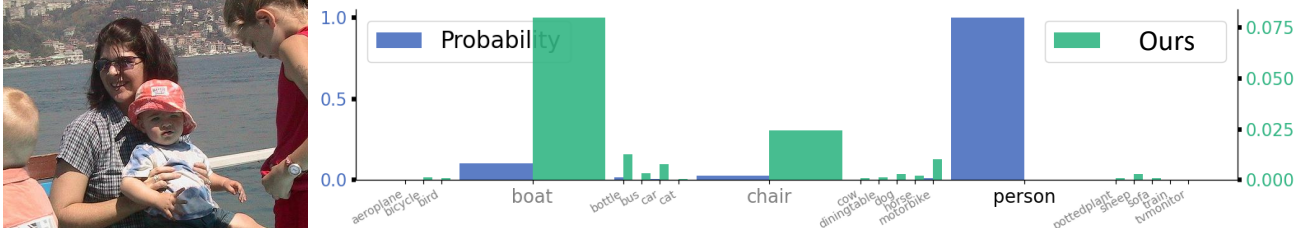


Figure 3: For the ground truth label "person," the Second-order Model Variance is low, indicating high certainty, consistent with the clear depiction of a woman sitting on a chair in an open area. In contrast, higher Second-order Model Variance is observed for the non-ground-truth labels "boat" and "chair," suggesting a lack of knowledge. This aligns with the scene, where multiple boats are visible across the river and a partial chair appears near the woman, potentially confusing the model.

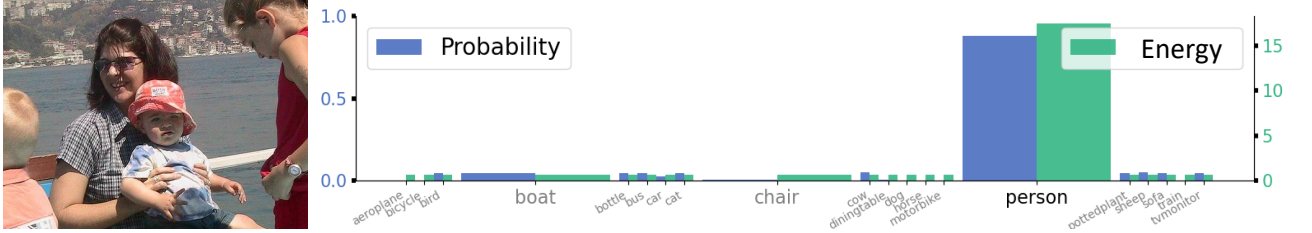


Figure 4: The energy-based method Wang et al. [2021] focuses on the high-probability "person" label, incorrectly indicating uncertainty despite its clear presence in the image.

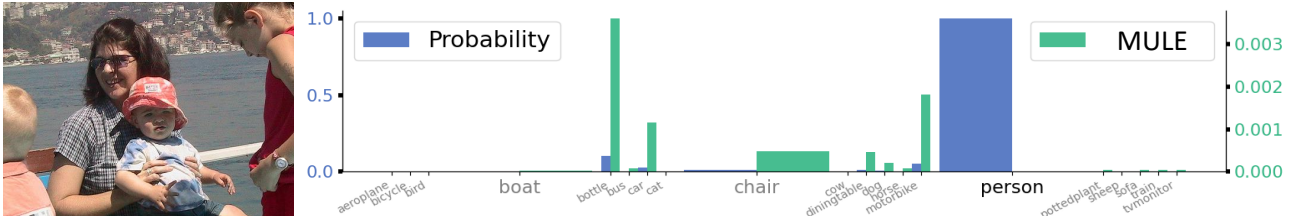


Figure 5: While MULE Zhao et al. [2023] demonstrates certainty for the existence of the ground truth "person" label, the nature of the captured uncertainty for other labels remains less interpretable.

objective is to maximize the marginal likelihood over the training data. For consistently patterned data, the marginal likelihood will be higher for prior hyperparameters $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$ that result in a concentrated prior accurately predicting the outcomes for specific input features. Over increasing amounts of consistent data, the neural network will continuously refine its weights θ to increase the values of $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$ for those inputs according to 2.5. This increase signifies a growing confidence in the learned prior and a reduction in the Second-Order Model Variance for those well-understood input patterns. Consider the proportion of the Second-Order Model Variance in the total uncertainty of the model:

$$\text{Var}_{p(t|a,b)}(t) = \underbrace{\frac{ab}{(a+b)(a+b+1)}}_{\text{First-order Model Variance}} \left(1 + \frac{1}{a+b}\right)$$

where, with the increase of $a+b$, the proportion of the Second-Order Model Variance in the total uncertainty is decreasing. It shows that the Second-Order Model Variance is the dominant term of the total uncertainty of the

model when $a+b < 1$, vice versa. Specifically, according to the validation experiments on the real-world dataset in Appendix F.2, the Second-order Model Variance will decrease, and $a+b$ will increase with more and more training data samples, reflecting reduced label uncertainty due to increased confidence. Formally, it is specified as follows:

Proposition 2.6 (The Second-order Model Variance Will Decrease with More Data). *Under the aforementioned Assumption 2.5, with an increase in consistently patterned data and for the sample size N , the Second-order Model Variance $\text{Var}_{\mu \sim p(\mu|a(\mathbf{x}, \theta, \mathcal{D}^{(N)}), b(\mathbf{x}, \theta, \mathcal{D}^{(N)}))}[\mu]$ has a higher proportion within the total uncertainty of the model compared to $\text{Var}_{\mu \sim p(\mu|a(\mathbf{x}, \theta, \mathcal{D}^{(N+1)}), b(\mathbf{x}, \theta, \mathcal{D}^{(N+1)}))}[\mu]$.*

Interestingly, when we discuss the Beta shape during learning in Section 2.4, we set $a, b > 1$ as a comparison method in table 1. It defaults to a relatively smaller proportion of Second-order Model Variance within the total uncertainty of the model, and it does not perform well during training, which implies keep the model thirsty (a high proportion of Second-order Model Variance) could help the learning.

Table 2: OOD detection performance comparison across different datasets ($\mathcal{D}_{in}$). The results are reported in terms of FPR95 ($\downarrow$), AUROC ($\uparrow$), and AUPR ($\uparrow$). Lower FPR95 and higher AUROC/AUPR indicate better performance. Our proposed methods, **Evidence₁** and **Evidence₂**, leverage well-calibrated evidential outputs, achieving superior OOD detection. Notably, incorporating Beta uncertainty in **Evidence₂** significantly reduces FPR95, demonstrating improved reliability.

$\mathcal{D}_{in}$ OOD SCORE	MS-COCO	PASCAL-VOC FPR95 $\downarrow$ /AUROC $\uparrow$ /AUPR $\uparrow$	NUS-WIDE
MAXLOGIT	43.53 / 89.11 / 93.74	45.06 / 89.22 / 83.14	56.46 / 83.58 / 94.32
MSP	79.90 / 73.70 / 85.37	74.05 / 79.32 / 72.54	88.50 / 60.81 / 87.00
ODIN	43.53 / 89.11 / 93.74	45.06 / 89.22 / 83.16	56.46 / 83.58 / 94.32
MAHALANOBIS	46.86 / 88.59 / 93.85	41.74 / 88.65 / 81.12	62.67 / 84.02 / 95.25
LOF	80.44 / 73.95 / 86.01	86.34 / 69.21 / 58.93	85.21 / 67.75 / 89.61
ISOLATION FOREST	94.39 / 49.04 / 66.87	93.22 / 50.67 / 35.78	95.69 / 53.12 / 83.32
JOINTENERGY	33.48 / 92.70 / 96.25	41.01 / 91.10 / 86.33	48.98 / 88.30 / 96.40
EVIDENCE₁	34.14 / 91.08 / 95.14	39.28 / 91.67 / 86.38	44.82 / 88.57 / 96.53
EVIDENCE₂	29.30 / 92.67 / 96.04	37.35 / 92.13 / 88.40	42.10 / 86.35 / 95.74

3 EXPERIMENTS

We present a series of experiments to illustrate the effectiveness of our methodology. The results demonstrate that the Second-order Model Variance by uncertainty decomposition offers deeper and more informative insights into the model’s reasoning process, enhancing the interpretability. Furthermore, we assess our method using OOD experiments, showcasing its capability to achieve a more reliable and well-calibrated OOD score. All the experiments are conducted on the NVIDIA RTX A4500.

3.1 ON THE REAL-WORLD DATASET

To provide an intuitive understanding of label-specific model reasoning on real-world data, we begin by showcasing a detailed result for a representative input. This example elucidates how the Second-order Model Variance offers insights into the potential ambiguities at the individual label level.

This experiment was conducted with a batch size of 16 and used Stochastic Gradient Descent (SGD) as the optimizer with a momentum of 0.9. The initial learning rates are set to 1.5×10^{-4} for the ResNet backbone and 5×10^{-2} for the fully connected layer. A Cosine Annealing learning rate scheduler with $T_{max} = 12$ is applied to adjust the learning rate smoothly over 30 training epochs. The experiment used the Pascal VOC 2012 dataset and was conducted by Resnet-34 He et al. [2016]. We compared our method with the energy-based method Wang et al. [2021] and Multi-label evidential learning (MULE) Zhao et al. [2023]. Figure 3, Figure 4 and Figure 5 show three different multi-label uncertainty measurements. Our label-wise Second-order Model Variance provides a human-interpretable reasoning process, revealing how the model weighs visual evidence and highlights ambiguities, thereby enhancing reliability in multi-

label classification tasks. More comparative examples are available in Appendix G.1. And we also shows more examples about how the distributional label-wise uncertainty explains the model’s thinking in Appendix G.2.

3.2 OOD EXPERIMENTS

To further show the statistical effectiveness of our method, we examine OOD experiments for multilabel classification. OOD detection for multi-label classification aims to identify whether an input belongs to the in-distribution $\mathcal{D}_{in}$ or the out-of-distribution $\mathcal{D}_{out}$. An input is considered an OOD if it does not contain any label in the in-distribution data. Inputs from $\mathcal{D}_{out}$ lack labels present in $\mathcal{D}_{in}$, often representing anomalies encountered during deployment. Consequently, classification models are unable to classify an object as none of the known categories. Instead, they tend to be overconfident in predictions, for example, assigning high probability to previously unseen objects Hendrycks et al. [2019]. We can interpret the Beta distribution hyperparameter a as the predicted belief mass. In an out-of-distribution (OOD) scenario, a high value of a may indicate an overconfident prediction, making it a useful signal for OOD detection. A straightforward approach is to compute the sum of the hyperparameter a across all labels as the OOD score, expressed as $\sum_{k=1}^K a_{ik}$. The OOD experiments result of this approach is presented as Evidence₁ in Table 2.

Besides, we propose another OOD score that focuses on identifying labels with both a high predicted belief mass and a high Second-order Model Variance. It means a high belief mass, but a lack of knowledge is more like an overconfidence label. To achieve this, we incorporate the confidence associated with each label, represented by the Second-order Model Variance from (5). Our objective is to detect labels with an overconfident predicted belief mass while accounting for their uncertainty. A higher score corresponds to a higher probability that the sample is OOD. It can be defined

as:

$$\text{Evidence}_2 = \sum_{k=1}^K a_{ik} \frac{\text{Var}_{\mu_{ik}}(\mu_{ik})}{\sum_{j=1}^K \text{Var}_{\mu_{ij}}(\mu_{ij})}.$$

Table 2 shows our OOD results by using evidence and the experiment setting follows the Wang et al. [2021]. The base-lines are Maxlogit Hendrycks et al. [2019], MSP Hendrycks and Gimpel [2016], ODIN Liang et al. [2017], Mahalanobis Lee et al. [2018], LOF Breunig et al. [2000], Isolation Forest Liu et al. [2008] and Joint Energy Wang et al. [2021]. The backbone used is DenseNet-121, pretrained on ImageNet-1K Deng et al. [2009]. For the in-distribution dataset $\mathcal{D}_{\text{in}}$, we use MS-COCO Lin et al. [2014], PASCAL-VOC Everingham et al. [2015], and NUS-WIDE Chua et al. [2009]. For the out-of-distribution dataset $\mathcal{D}_{\text{out}}$, we select the same set of 20 classes as in Hendrycks et al. [2019] chosen from ImageNet-22K. These classes are specifically selected to avoid overlap with ImageNet-1K, as the multi-label classifiers are pretrained on ImageNet-1K.

From Table 2, we can see that the Evidential training method shows a better OOD performance. When using the OOD score defined as Evidence₂, the results demonstrate a significant reduction in the false positive rate at 95% true positive rate (FPR95) compared to others. Our method using Evidence₂ achieves a 6.88% lower FPR95 score than the second-best Joint Energy on the NUS-WIDE dataset. Evidence₂ is specifically designed to identify overconfident predictions by jointly considering high belief mass and the Second-order Model Variance, which is particularly effective at suppressing false positives at high true positive rates (FPR95), but may not globally optimize the full ranking of OOD scores as captured by AUROC and AUPR.

4 CONCLUSION AND LIMITATION

Our work introduces a novel perspective for addressing label-wise uncertainty in multi-label classification tasks. We theoretically prove that, among currently popular second-order learners, the Type II likelihood maximization is data likelihood centric, while the Gibbs classifier will consider the variance factors. We decompose label-wise uncertainty into the First-order Model Variance, Second-order Model Variance, Model Bias, and Optimal Spread. In our OOD experiments, we leverage the Second-order Model Variance to demonstrate its efficacy, and the result shows a great improvement, specifically on the FPR95 metric. Our paper also has several limitations. The model variance and data noise remain underexplored. And in Section 2.5, we give a relatively heuristic Bayesian update rule explanation based on data consistency. More effort is needed to analyze the scalability of data consistency.

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Label-Wise Uncertainty Decomposition for Multi-Label Classification by Maximizing Type II Likelihood (Supplementary Material)

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A TYPE I & II MAXIMUM LIKELIHOOD

Type I ML directly optimizes the likelihood of the observed data with respect to the model parameters. The parameter values are determined directly by maximizing the likelihood $P(\mathcal{D}|\theta)$, where $\mathcal{D}$ is the observed data with ground truth and θ represents the parameters of model f .

Type II ML is an approximation framework, which is also called Evidence Approximation MacKay [1992], setting the hyperparameters m to specific values determined by maximizing the marginal likelihood function obtained by first integrating over the parameters θ . This gives rise to the marginal likelihood as shown:

$$p(\mathcal{D}|m) = \int p(\mathcal{D}|\theta)p(\theta|m) d\theta.$$

The marginal likelihood $p(\mathcal{D}|m)$ is a function that describes how likely the observed data $\mathcal{D}$ is, given the parameters m . It essentially answers the question: "How well do the parameters m explain the observed data $\mathcal{D}$?" It serves as the foundation for optimization, where the model adjusts m to maximize the agreement between predictions and observed data.

Once the marginal likelihood is derived, the next step involves estimating the hyperparameters m by maximizing the marginal likelihood expression with respect to m . This is often referred to as Type II Maximum Likelihood estimation, which seeks to identify the set of hyperparameters m that best explain the observed data under the given model. By maximizing this marginal likelihood, we effectively integrate out latent variables or nuisance parameters, allowing the model to focus solely on optimizing the hyperparameters to enhance its overall fit. The estimation will be:

$$\hat{m} = \arg \max_m p(\mathcal{D}|m).$$

B INFERENCE OF TYPE II LIKELIHOOD

The Beta prior distribution, combined with the Bernoulli likelihood, enables the computation of a label-wise marginal likelihood. The marginal likelihood for one single label is expressed as:

$$\begin{aligned} p(y | a, b) &= \int_0^1 \mu^y (1 - \mu)^{1-y} \frac{\mu^{a-1} (1 - \mu)^{b-1}}{\text{Beta}(a, b)} d\mu \\ &= \frac{1}{\text{Beta}(a, b)} \int_0^1 \mu^{y+a-1} (1 - \mu)^{1-y+b-1} d\mu \\ &= \frac{\text{Beta}(y + a, 1 - y + b)}{\text{Beta}(a, b)}. \end{aligned}$$

Here, the Beta function $\text{Beta}(a, b)$ serves as a normalization constant. Using the relationship between the Beta and Gamma

functions, where $\text{Beta}(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$, we rewrite the marginal likelihood as:

$$p(y|a, b) = \frac{\Gamma(y+a)\Gamma(1-y+b)}{\Gamma(1+a+b)} \cdot \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}.$$

To further illustrate this, consider the two possible cases for the binary ground truth y :

$$p(y|a, b) = \begin{cases} \frac{\Gamma(a)\Gamma(1+b)}{\Gamma(1+a+b)} \cdot \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}, & \text{if } y = 0, \\ \frac{\Gamma(1+a)\Gamma(b)}{\Gamma(1+a+b)} \cdot \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}, & \text{if } y = 1. \end{cases}$$

Finally, leveraging the property of the Gamma function, $\Gamma(x+1) = x\Gamma(x)$, we simplify the above expression into the Type II Maximum Likelihood (Type II ML) form. This results in the evidential likelihood:

$$p(y|a, b) = \left(\frac{a}{a+b}\right)^y \left(\frac{b}{a+b}\right)^{1-y}.$$

C DERIVATION OF THE RELATIONSHIP VIA TAYLOR EXPANSION

For simplicity, we denote $\mu = \mu_{ik} \sim \text{Beta}(a, b)$, with mean $\mu_0 = \mathbb{E}[\mu] = \frac{a}{a+b}$ and variance $\sigma^2 = \text{Var}(\mu) = \frac{ab}{(a+b)^2(a+b+1)}$. The difference between the losses is

$$\delta = \mathcal{L}_{\text{Gibbs}} - \mathcal{L}_{\text{Type II}} = -\mathbb{E}[\log \mu] + \log \mu_0.$$

Perform a second-order Taylor expansion of $g(\mu) = -\log \mu$ around μ_0 :

$$g(\mu) = g(\mu_0) + g'(\mu_0)(\mu - \mu_0) + \frac{1}{2}g''(\mu_0)(\mu - \mu_0)^2 + R,$$

where $g(\mu_0) = -\log \mu_0$, $g'(\mu_0) = -\frac{1}{\mu_0}$ and $g''(\mu_0) = \frac{1}{\mu_0^2}$, and R is the higher-order remainder. Taking the expectation,

$$\mathbb{E}[g(\mu)] = g(\mu_0) + \frac{1}{2\mu_0^2}\sigma^2 + \mathbb{E}[R].$$

Thus,

$$\mathcal{L}_{\text{Gibbs}} = \mathcal{L}_{\text{Type II}} + \frac{\sigma^2}{2\mu^2} + \mathbb{E}[R].$$

For small σ^2 , $\mathbb{E}[R]$ is negligible, yielding the approximation

$$\mathcal{L}_{\text{Gibbs}} \approx \mathcal{L}_{\text{Type II}} + \frac{\sigma^2}{2\mu^2}.$$

This approximation highlights that the Gibbs loss adds a term proportional to the variance, penalizing uncertainty, whereas the Type II loss does not.

D COMPARISON ON REAL-WORLD DATASET

As we can see from Figure 6, when both the hyperparameters a and b of a Beta distribution are less than 1, the distribution exhibits a U-shaped, meaning most of the probability density is concentrated near 0 and 1. Beta distribution in U-shape reflects that the true probability p is likely to be close to one of the extremes.

For $a, b > 1$, the Beta distribution is unimodal (bell shape), with the mode positioned between 0 and 1. The constraint $a, b > 1$ is commonly used for numerical stability and smoother predictions Sensoy et al. [2018], Bao et al. [2021], as it incorporates a non-informative prior greater than 1. However, relaxing this constraint of non-informative prior allows the distribution to take U-shaped or L-shaped forms, reflecting a strong preference for probabilities near 0 and 1. This

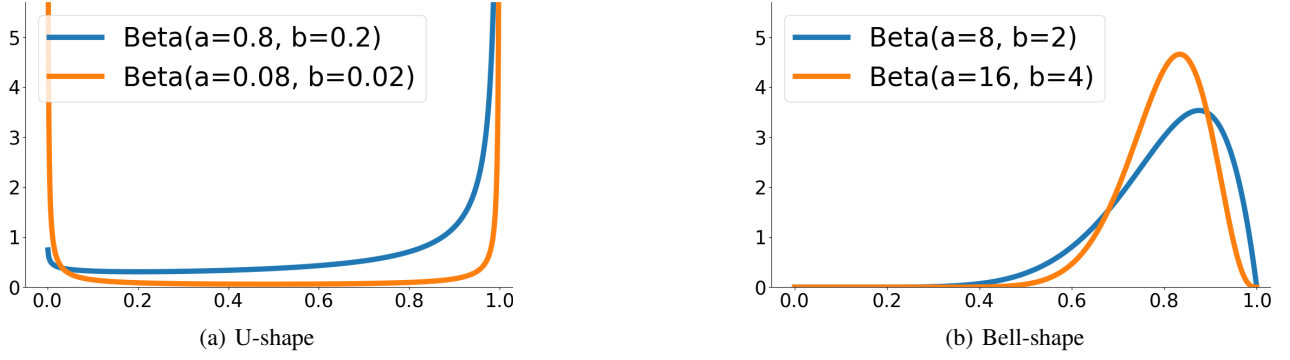


Figure 6: Given the predicted probability is 80%, different shapes of Beta distribution.

increased flexibility provides more expressive modeling for Type II ML estimation. The result in table 2 also shows that in the context of binary classification, without the restriction of $a, b > 1$, the Type II maximum likelihood actually can flexibly to adjust the hyperparameters to achieve the maximum and have better performance. Binary classification typically involves clear separations between two classes, making such extreme probabilities more plausible. The U-shaped and L-shaped Beta distributions align with the nature of the task and the available data. This belief suits scenarios where predictions are expected to lean strongly toward one of the two classes.

E TWO UNCERTAINTY METHODS

E.1 UNCERTAINTY DECOMPOSITION

Set the parameter μ^* is of the theoretical true data-generating distribution $p(t | \mu^*)$. Both μ and μ^* are themselves uncertain: in a hierarchical Bayesian framework, μ is drawn from a second-order distribution $p(\mu | m)$ induced by $f(x)$, giving the Markov chain $m \rightarrow \mu \rightarrow t$, while μ^* is drawn from $p(\mu^* | m^*)$, giving the parallel chain $m^* \rightarrow \mu^* \rightarrow t$. The main uncertainty decomposition in our framework is expressed through the pointwise risk $(\mu^* - t)^2$, which measures the squared deviation of the mean of theoretical true data-generating distribution from the observed target. The central question is how to decompose this risk into interpretable components from predictive model perspective by anchoring at the theoretical optimal μ^* .

We begin from the first-order predictive variance:

$$Var_{t|\mu}(t) = E_{t|\mu}[(\mu - t)^2].$$

Inserting $\mu^* \sim p(\mu^* | m^*)$ by adding and subtracting:

$$Var_{t|\mu}(t) = E_{t|\mu}[(\mu - \mu^* + \mu^* - t)^2].$$

Expanding and using $E_{t|\mu}[t] = \mu$, so that the cross-term gives $2(\mu - \mu^*)(\mu^* - \mu) = -2(\mu - \mu^*)^2$:

$$\begin{aligned} Var_{t|\mu}(t) &= (\mu - \mu^*)^2 + E_{t|\mu}[(\mu^* - t)^2] - 2(\mu - \mu^*)^2 \\ &= E_{t|\mu}[(\mu^* - t)^2] - (\mu - \mu^*)^2. \end{aligned}$$

Take $E_{\mu|m}$, Expanding $E_{\mu}[(\mu - \mu^*)^2]$ by adding and subtracting $\bar{\mu} = E_{\mu}[\mu]$:

$$E_{\mu}[(\mu - \mu^*)^2] = Var_{\mu}(\mu) + (\bar{\mu} - \mu^*)^2.$$

Hence:

$$E_{\mu}[Var_{t|\mu}(t)] = E_{\mu}E_{t|\mu}[(\mu^* - t)^2] - Var_{\mu}(\mu) - (\bar{\mu} - \mu^*)^2. \quad (6)$$

Take $E_{\mu^*|m^*}$. Since $Var_{t|\mu}(t)$ does not depend on μ^* by the Markov structure $m \rightarrow \mu \rightarrow t$, the left-hand side of (6) is unchanged by E_{μ^*} . Expanding $E_{\mu^*}[(\bar{\mu} - \mu^*)^2]$ by adding and subtracting $\bar{\mu}^* = E_{\mu^*}[\mu^*]$:

$$E_{\mu^*}[(\bar{\mu} - \mu^*)^2] = (\bar{\mu} - \bar{\mu}^*)^2 + Var_{\mu^*}(\mu^*).$$

Taking E_{μ^*} of (6) and rearranging gives the main result of this section:

$$E_{\mu^*} E_{\mu} E_{t|\mu} [(\mu^* - t)^2] = \underbrace{E_{\mu} [\text{Var}_{t|\mu}(t)]}_{\text{First-order Model Variance}} + \underbrace{\text{Var}_{\mu}(\mu)}_{\text{Second-order Model Variance}} + \underbrace{(\bar{\mu} - \bar{\mu}^*)^2}_{\text{Model Bias}} + \underbrace{\text{Var}_{\mu^*}(\mu^*)}_{\text{Optimal Spread}}.$$

where we replace the m to a, b and the First-order Model Variance $E_{\mu} [\text{Var}_{t|\mu}(t)]$ can be derived by:

$$\begin{aligned} E_{\mu} [\text{Var}_{t|\mu}(t)] &= E_{\mu \sim p(\mu|a,b)} [\mu(1 - \mu)] = E_{\mu \sim p(\mu|a,b)} [\mu] - E_{\mu \sim p(\mu|a,b)} [\mu^2] \\ &= E_{\mu \sim p(\mu|a,b)} [\mu] - [\text{Var}_{\mu \sim p(\mu|a,b)}(\mu) + (E_{\mu \sim p(\mu|a,b)}[\mu])^2] \\ &= \frac{a}{a+b} - \frac{ab}{(a+b)^2(a+b+1)} - \left(\frac{a}{a+b}\right)^2 \\ &= \frac{ab}{(a+b)(a+b+1)}. \end{aligned}$$

And the Second-order Model Variance is the Beta variance:

$$\text{Var}_{\mu}(\mu) = \text{Var}_{\mu \sim p(\mu|a,b)} [\mu] = \frac{ab}{(a+b)^2(a+b+1)}.$$

The four terms are interpreted as follows. The first-order model variance $E_{\mu} [\text{Var}_{t|\mu}(t)]$ captures the irreducible scatter of the observed target t around the model's predictive parameter μ , averaged over the model's own second-order distribution $p(\mu | a, b)$. The second-order model variance $\text{Var}_{\mu}(\mu)$ captures how much the model's predictive parameter μ itself fluctuates across the second-order distribution $p(\mu | a, b)$, reflecting the model's own parametric uncertainty. The model bias $(\bar{\mu} - \bar{\mu}^*)^2$ measures the squared discrepancy between the mean of the model's predictive distribution and the mean of the true data-generating distribution, capturing the systematic misalignment between the model and the ground truth. The optimal spread $\text{Var}_{\mu^*}(\mu^*)$ captures the inherent variability of the true data-generating parameter μ^* across the optimal distribution $p(\mu^* | m^*)$, representing irreducible uncertainty that exists even under the theoretically perfect predictor.

It is worth noting that the First-Order Model Variance can also be called Within-group Variance, and the Second-Order Model Variance can also be called Between-group variance. Another conventional names for them is aleatoric uncertainty and epistemic uncertainty. But we think aleatoric is more about the Optimal Spread instead of the Second-Order Model Variance. So we may not directly call it in this way.

E.2 THE TOTAL MODEL VARIANCE

As we mentioned before, for notational simplicity, we denote these data-driven hyperparameters $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$ as a and b . The predictive distribution is approximated by:

$$p(t | \mathbf{x}, \mathcal{D}) \approx p(t | a, b) = \int_0^1 p(t | \mu) \text{Beta}(\mu | a, b) d\mu.$$

The total variance of the real predictive distribution can be represented by:

$$\text{Var}_{p(t|\mathbf{x},\mathcal{D})}(t) = E_{p(t|\mathbf{x},\mathcal{D})}[t^2] - (E_{p(t|\mathbf{x},\mathcal{D})}[t])^2.$$

Since $t^2 = t$, $E_{p(t|\mathbf{x},\mathcal{D})}[t^2] = E_{p(t|\mathbf{x},\mathcal{D})}[t]$. The mean is:

$$E_{p(t|\mathbf{x},\mathcal{D})}[t] = p(t = 1 | \mathbf{x}, \mathcal{D}) \approx \int_0^1 \mu \text{Beta}(\mu | a, b) d\mu = \frac{a}{a+b}.$$

Thus, the total model variance conditioned on the $\mathbf{x}$ and $\mathcal{D}$ can be approximated by:

$$\begin{aligned} \text{Var}_{p(t|\mathbf{x},\mathcal{D})}(t) &\approx \text{Var}_{p(t|a,b)}(t) = \frac{a}{a+b} - \left(\frac{a}{a+b}\right)^2 = \frac{ab}{(a+b)^2} \\ &= \underbrace{\frac{ab}{(a+b)(a+b+1)}}_{\text{First-order Model Variance}} + \underbrace{\frac{ab}{(a+b)^2(a+b+1)}}_{\text{Second-order Model Variance}} \end{aligned}$$

where the approximated model variance is equal to the sum of the First-order Model Variance and Second-order Model Variance.

E.3 SECOND-ORDER MODEL VARIANCE

To visualize the behavior of the predictive distribution across different combinations of the Beta distribution hyperparameters a and b , we present heatmaps in Figure 7, which illustrate the mean and variance of the predictive distribution $p(\mu | \mathbf{x}, \mathcal{D}) \approx \text{Beta}(\mu | a, b)$. The left heatmap depicts the mean $\mathbb{E}_{p(\mu | \mathbf{x}, \mathcal{D})}[\mu] \approx \frac{a}{a+b}$, representing the predicted probability, while the right heatmap shows Second-order Model Variance $\text{Var}_{p(\mu | \mathbf{x}, \mathcal{D})}(\mu) \approx \frac{ab}{(a+b)^2(a+b+1)}$, a measure of fluctuation for First-order parameter μ . These visualizations reveal how the interplay of a and b generates a wide range of probability estimates and uncertainty levels, with variance peaking when a and b are small and balanced (indicating maximum uncertainty) and decreasing as either parameter dominates, reflecting a more confident prediction.

To further explore this distributional uncertainty of Second-order Model Variance, Figure 8 contrasts it with traditional entropy-based uncertainty in a 3D representation. The left subfigure (Figure 8(a)) plots entropy for a binary classification case, where uncertainty remains constant for a fixed probability $p = 0.5$ (maximum entropy), offering a static measure of ignorance. In contrast, the right subfigure (Figure 8(b)) depicts a 3D surface of Second-order Model Variance as a function of a and b , highlighting its dynamic nature. Unlike entropy, which provides a uniform uncertainty measure for a given p , the Beta distribution’s variance varies with a and b , enabling a richer representation of uncertainty that captures the model’s confidence in the predictive distribution. This variability is particularly valuable in multi-label classification, where label-wise uncertainty (e.g., for a stable person vs. a moving car) can differ significantly due to distinct $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$ inferred by the neural network.

The dependency of variance on a and b aligns with our Empirical Bayes framework, where these hyperparameters are learned by maximizing the Type II likelihood. As consistent data patterns reinforce the model (per Assumption 2.5), $a(\mathbf{x}, \theta)$ and $b(\mathbf{x}, \theta)$ increase, reducing variance and concentrating the posterior, as observed in the heatmaps. This adaptability offers deeper insights into model confidence, facilitating applications such as OOD detection, where precise uncertainty quantification enhances reliability. The 3D visualization underscores the potential for leveraging Second-order Model Variance in safety-critical domains, where understanding label-specific confidence is crucial for interpreting model behavior and ensuring robust predictions.

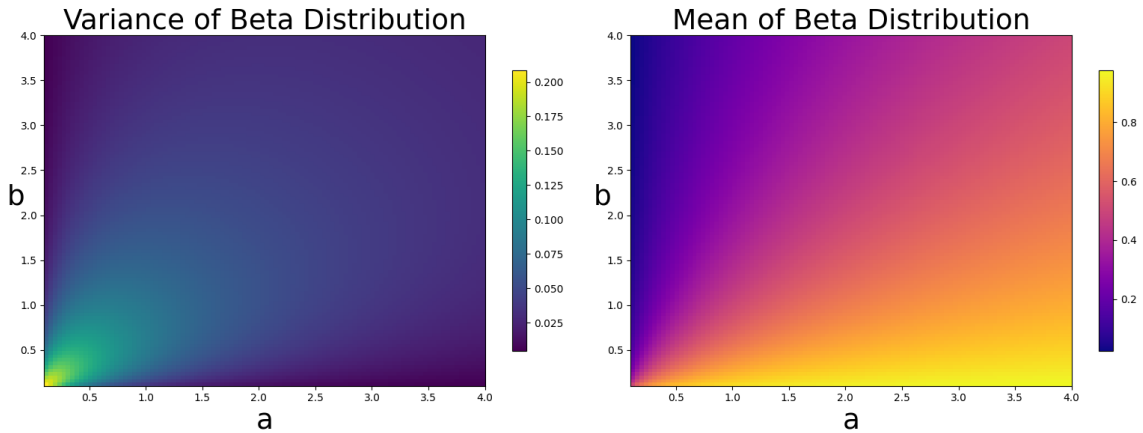


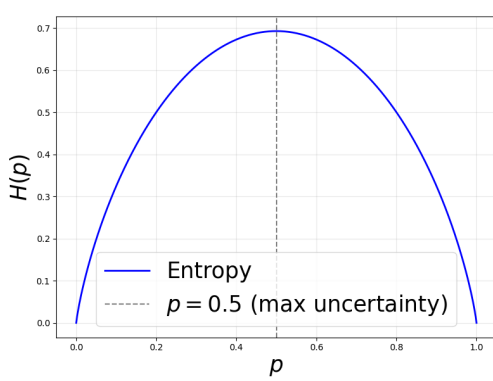
Figure 7: The combination of the parameters a and b in the Beta distribution results in a variety of probabilities and variances.

F BEHAVIOR OF TOTAL UNCERTAINTY AND SECOND-ORDER MODEL VARIANCE

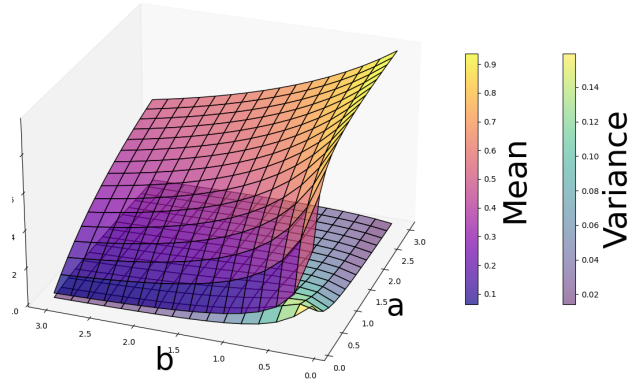
F.1 CONVERGENCE OF TOTAL UNCERTAINTY

Proof. The estimated total uncertainty of the model is given by:

$$\text{Var}_{p(t | a(\mathbf{x}, \theta, \mathcal{D}), b(\mathbf{x}, \theta, \mathcal{D}))}(t) = \frac{a(\mathbf{x}, \theta, \mathcal{D})b(\mathbf{x}, \theta, \mathcal{D})}{(a(\mathbf{x}, \theta, \mathcal{D}) + b(\mathbf{x}, \theta, \mathcal{D}))^2} = \hat{\mu}(1 - \hat{\mu}),$$



(a) Entropy uncertainty (binary case)



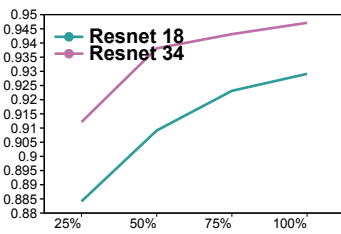
(b) Uncertainty using the variance of Beta distribution

Figure 8: For a given fixed probability, entropy provides a constant measure of uncertainty, whereas the Beta distribution allows for variable uncertainty depending on its hyperparameters, offering deeper insights into model confidence.

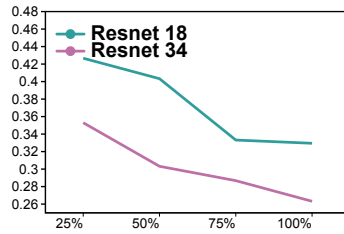
where $\hat{\mu}$ is the estimated mean of the predictive distribution of the label.

Maximizing the Type II likelihood $\mathbb{E}_{\mu_{ik} \sim \text{Beta}(a_{ik}, b_{ik})}[\mu_{ik}]$ does not directly maximize the Type I likelihood, because Type II integrates over all possible values of μ according to the prior. However, the outcome of maximizing Type II is a Beta distribution whose mean $\frac{a}{a+b}$ serves as a good point estimate for μ , and this point estimate is the value that would maximize the Type I likelihood for the observed data. The per-sample gradient of the Type-II loss is an unbiased estimate of the gradient of the binary cross-entropy risk. Under the Robbins–Monro conditions on step sizes, SGD then converges to the true parameter. So $\hat{\mu}$ will converge towards the true underlying probability μ^* of the label associated with the input $\mathbf{x}$. Therefore, the total uncertainty of the model will converge to: $\mu^*(1 - \mu^*)$, which represents the inherent Bernoulli variance associated with the consistent underlying pattern. It signifies that even with perfect learning of the pattern, there will still be irreducible randomness in the label according to the underlying likelihood. The total uncertainty of the model will not necessarily converge to zero unless the underlying pattern is deterministic ($\mu^* = 0$ or $\mu^* = 1$). Instead, it converges to a level dictated by the inherent stochasticity of the consistently patterned data. $\square$

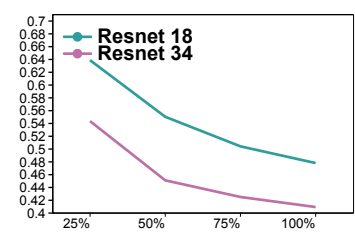
F.2 DECREASE OF SECOND-ORDER MODEL VARIANCE



(a) AP Score



(b) Second-Order Model Variance



(c) Type II Loss

Figure 9: Second-Order Model Variance Reduction with Increasing Data on Pascal VOC 2012

Figure 9 provides experimental validation for Proposition 2.6. As the training data incrementally increased from 25% to 100%, the average precision (shown in Figure 9(a)) progressively improved while the associated risk (depicted in Figure 9(c)) decreased. Concurrently, the Second-Order Model Variance, as quantified in (5), exhibited a corresponding reduction. The experimental setting is the same as in Section 3.

We report empirical evidence that directly supports the growth of $a + b$ with the addition of training data. As shown in Table 3, when increasing the training fraction from 75% to 100% on the Pascal VOC 2012 dataset, the median $a + b$

Table 3: Per-class $a + b$ values and test AP on Pascal VOC 2012 dataset at training fractions of 75% and 100%.

Train Frac	Test AP	Aero	Bike	Bird	Boat	Bottle	Bus	Car	Cat	Chair	Cow	Table	Dog	Horse	Moto	Person	Plant	Sheep	Sofa	Train	TV
0.75	0.9244	0.4553	0.4009	0.2727	0.3984	0.2953	0.5788	0.2282	0.2349	0.3350	0.5834	0.5363	0.2289	0.4694	0.3358	0.1871	0.2990	0.5149	0.4389	0.4470	0.4078
1.00	0.9285	0.5231	0.3807	0.3475	0.4163	0.2888	0.5180	0.2098	0.2483	0.3656	0.6323	0.5061	0.2004	0.4771	0.3669	0.2322	0.3148	0.5300	0.5392	0.5152	0.4304

increases from 0.3824 to 0.4021 on the test set. Furthermore, out of 20 object classes, 14 show a clear increase in their per-label $a + b$ values, while only 6 decrease, which is consistent with the theoretical findings in Proposition 2.6. The overall test Average Precision (AP) also improves from 0.9244 to 0.9285. It suggests that more training data leads to a more concentrated posterior $p(\mu \mid a, b)$, which is reflected empirically by the growth of $a + b$.

G INTUITIVE EXPERIMENTS

G.1 ADDITIONAL COMPARATIVE EXAMPLES

We present further comparative experiments, where blue bars represent the model’s predictive probability for each label, and green bars illustrate the corresponding uncertainty as quantified by different methods across figures. The black labels are the ground truth.

The first comparative example, shown in Figure 10, examines a scene containing a dog and chairs, with a very likely dining table. Our method’s distributional uncertainty indicates high certainty regarding the obvious presence of the dog. And it reflects the model’s bias for the low predictive probability of the dining table. The method also captures a moderate uncertainty for the chairs, which appears reasonable given the potentially ambiguous viewing angle of these objects. In contrast, both the Energy-based method Wang et al. [2021] and Multi-label Evidential Learning (MULE) Zhao et al. [2023] suggest uncertainty for the dog label, a result that lacks clear interpretability based on the visual evidence. In another instance

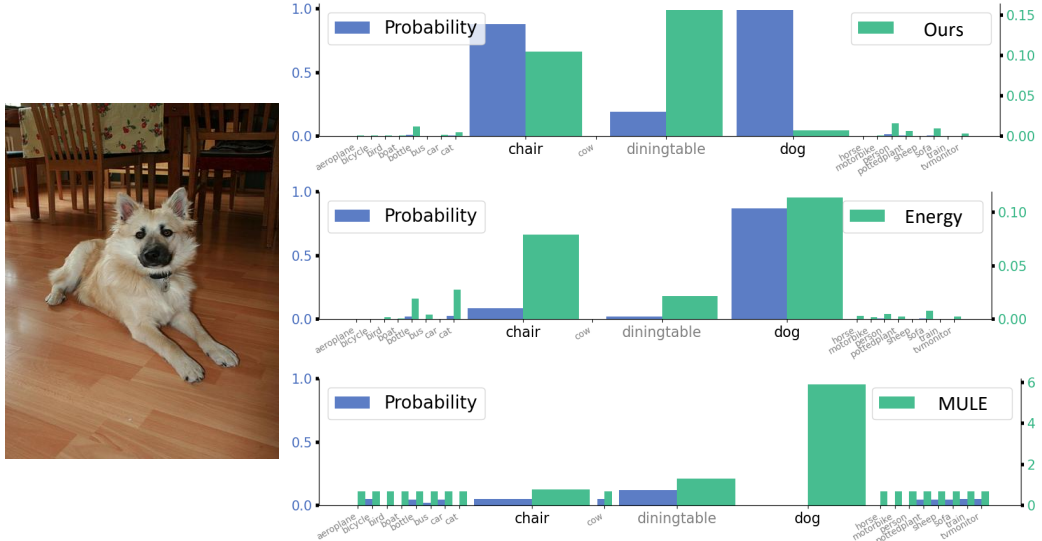


Figure 10: High Second-order Model Variance for the low predictive probability of the dining table.

shown in Figure 11, where "cat" and "tvmonitor" are the ground truth labels, the predictive probabilities of all three models exhibit similar trends: low for "tvmonitor" and high for "cat." However, our method uniquely provides an interpretable uncertainty assessment, indicating certainty for the high probability assigned to "cat" and uncertainty for the low probability associated with "tvmonitor." This aligns with a human understanding of the scene.

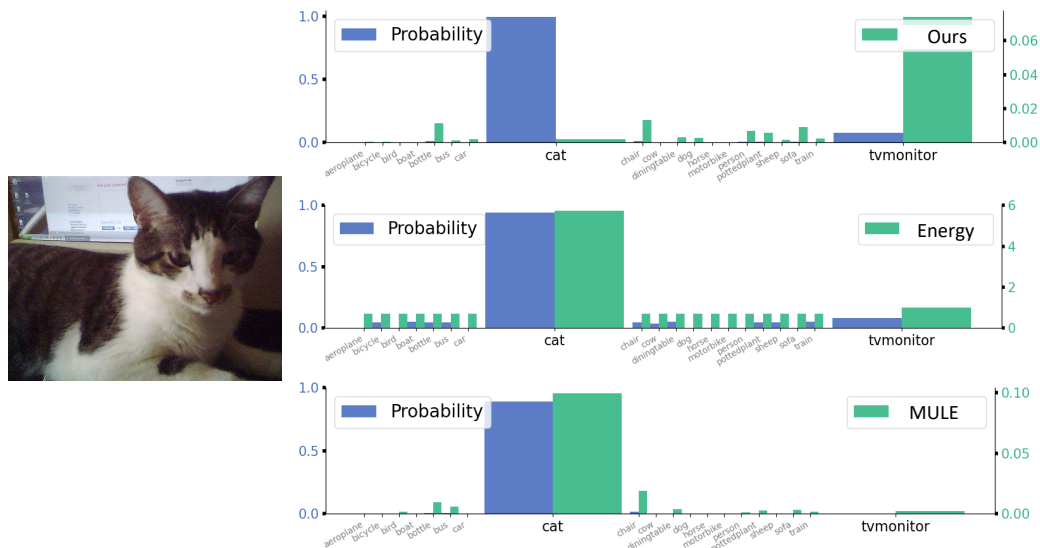


Figure 11: High Second-order Model Variance for the low predictive probability of the TV monitor.

G.2 MORE ANALYSIS ON REAL WORLD DATA

We can examine more results in Figure 12 from the Pascal VOC 2012 dataset conducted by Resnet-34 He et al. [2016]. The blue bar represents predictive probability. Meanwhile, the green bar represents the model distributional uncertainty. The black label indicates the ground truth, while the gray labels represent non-ground truth labels. Starting with data ambiguity, several examples demonstrate the challenges within the dataset. In the first image on the left, a potted plant is visible but excluded from the ground truth, resulting in high variance in the model’s predictive probability. Similarly, the second image contains a figure resembling the KFC logo or the people on the ground, yet lacks a "person" ground truth label. The third image depicts a piece of furniture that could be classified as either a chair or a sofa, adding inherent ambiguity. The fifth image on the left shows a blurry car in the background, further confusing the model. On the right side, the first image highlights a person behind a cute dog, yet the label "person" is missing from the ground truth, contributing to uncertainty. Turning to the model’s limited knowledge, several cases reveal perplexity. For instance, the fourth image on the left features a crashed motorcycle with high label nervousness due to limited prior knowledge. Similarly, the fifth image on the right depicts a sheep being sheared. It is interesting to discuss the explainable variance levels illustrated in Figure 12, which reflect human-interpretable label-wise uncertainties. The model’s "feeling" can range from confident to confused. These results provide insights into the model’s internal reasoning and offer an intuitive answer to the question: "Does the model exhibit 'nervousness' in each label-wise prediction?"

The result shows that our approach enables a deeper and label-wise understanding of the model’s predictive probability. Whether grappling with ambiguous ground truths, such as blurry objects or misclassified categories, or facing scenarios outside its learned knowledge, like unusual contexts or rare events, the method highlights areas of uncertainty that impact decision-making. This ability to expose and explain uncertainty provides valuable insights for improving model robustness and interpretability, helping to align predictions with reasoning in real-world applications.

And the code will be released at <https://github.com/Minghao87/Label-Wise-Uncertainty-Decomposition>.

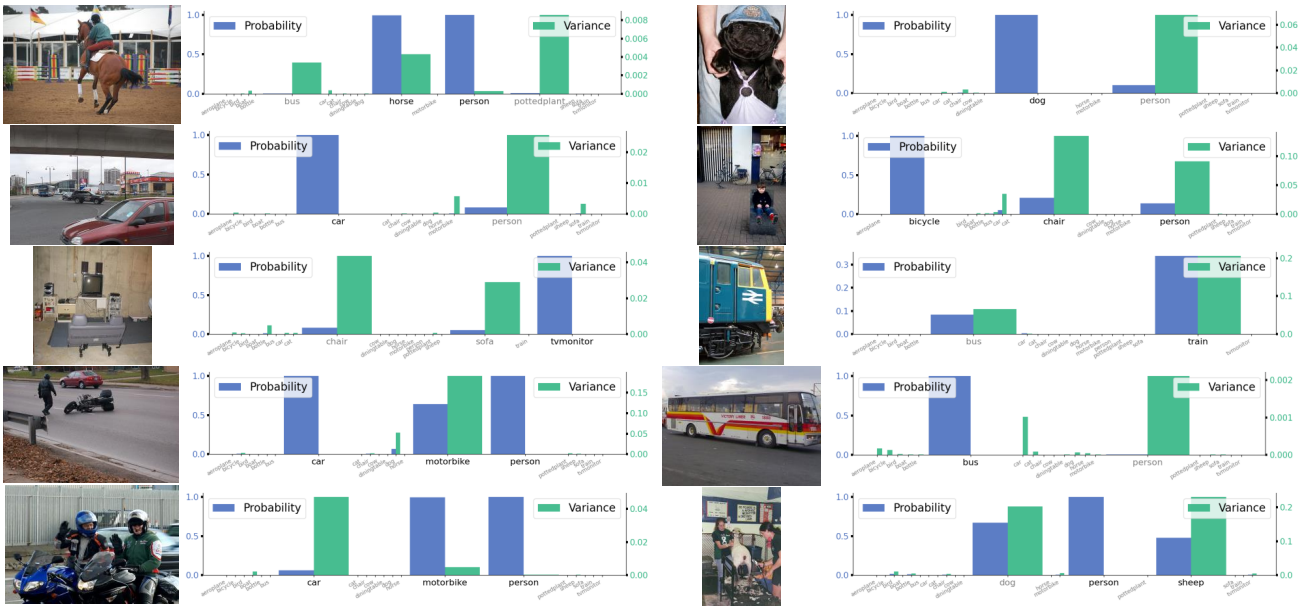


Figure 12: This figure presents real-world data experiment results, showcasing the model's fine-grained label-wise Second-Order Model Variance.