Evidential Uncertainty Quantification: A Variance-Based Perspective Supplementary Material

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A. Derivations

A.1. Problem Setup

In a C-class classification problem, it is assumed that the label vector $\boldsymbol{y} = [y_1, y_2, \dots, y_C]^\top$ is a one-hot random vector that follows a categorical distribution with parameters $\boldsymbol{\mu}$. The class probabilities $\boldsymbol{\mu}$ follow a Dirichlet distribution with concentration parameters $\boldsymbol{\alpha}$.

$$\boldsymbol{y} \sim \mathrm{Cat}(\boldsymbol{\mu}) \qquad \boldsymbol{\mu} \sim \mathrm{Dir}(\boldsymbol{\alpha}) \tag{1}$$

in which $\mathrm{Cat}(\cdot)$ and $\mathrm{Dir}(\cdot)$ denote categorical distribution and Dirichlet distribution respectively.

The class probability vector is $\boldsymbol{\mu} = [\mu_1, \mu_2, \dots, \mu_C]^\top$, in which $\mu_c \in [0, 1]$ and $\sum_{c=1}^{C} \mu_c = 1$. The Dirichlet parameters are specified by $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \dots, \alpha_C]^\top$ in which $\alpha_c > 0$ for $c \in \{1, 2, \dots, C\}$. The Dirichlet strength is denoted by $\alpha_0 = \sum_{c=1}^{C} \alpha_c$.

The expected class probabilities are $\bar{\boldsymbol{\mu}} = \mathbb{E}[\boldsymbol{\mu}] = \frac{\boldsymbol{\alpha}}{\alpha_0}$. For class c, the expected probabilty is $\bar{\mu}_c = \mathbb{E}[\mu_c] = \frac{\alpha_c}{\alpha_0}$.

A.2. Covariance Matrices

The covariance matrix of $\boldsymbol{y}$ is defined as

$$\mathrm{Cov}[\boldsymbol{y}] := \mathbb{E}[(\boldsymbol{y} - \mathbb{E}[\boldsymbol{y}])(\boldsymbol{y} - \mathbb{E}[\boldsymbol{y}])^\top] \tag{2}$$

which can be decomposed into aleatoric and epistemic components based on the law of total covariance.

$$\underbrace{\mathrm{Cov}[\boldsymbol{y}]}_{\text{total}} = \underbrace{\mathbb{E}[\mathrm{Cov}[\boldsymbol{y}|\boldsymbol{\mu}]]}_{\text{aleatoric}} + \underbrace{\mathrm{Cov}[\mathbb{E}[\boldsymbol{y}|\boldsymbol{\mu}]]}_{\text{epistemic}} \tag{3}$$

A.2.1 Aleatoric Covariance

The aleatoric covariance matrix can be calculated as

$$\mathrm{Cov}[\boldsymbol{y}]^{alea} = \mathbb{E}[\mathrm{Cov}[\boldsymbol{y}|\boldsymbol{\mu}]] = \mathbb{E}[\mathrm{Diag}(\boldsymbol{\mu}) - \boldsymbol{\mu}\boldsymbol{\mu}^\top] \tag{4}$$

in which $\mathrm{Diag}(\cdot)$ represents a diagonal matrix with the specified vector in its diagonal.

For $i \in \{1, 2, \dots, C\}$,

$$\begin{aligned}
\mathrm{Cov}[\boldsymbol{y}]^{alea}_{i,i} &= \mathbb{E}[\mu_i - \mu_i^2] && (5)\\
&= \mathbb{E}[\mu_i] - \mathbb{E}[\mu_i^2] && (6)\\
&= \mathbb{E}[\mu_i] - \mathbb{E}^2[\mu_i] - \mathrm{Var}[\mu_i] && (7)\\
&= \bar{\mu}_i - \bar{\mu}_i^2 - \frac{\bar{\mu}_i - \bar{\mu}_i^2}{\alpha_0 + 1} && (8)\\
&= \frac{\alpha_0}{\alpha_0 + 1}(\bar{\mu}_i - \bar{\mu}_i^2) && (9)
\end{aligned}$$

For $i, j \in \{1, 2, \dots, C\}$ such that $i \neq j$,

$$\begin{aligned}
\mathrm{Cov}[\boldsymbol{y}]^{alea}_{i,j} &= \mathbb{E}[-\mu_i\mu_j] && (10)\\
&= -\mathbb{E}[\mu_i\mu_j] && (11)\\
&= -\mathrm{Cov}[\mu_i, \mu_j] - \mathbb{E}[\mu_i]\mathbb{E}[\mu_j] && (12)\\
&= -\frac{-\bar{\mu}_i\bar{\mu}_j}{\alpha_0 + 1} - \bar{\mu}_i\bar{\mu}_j && (13)\\
&= -\frac{\alpha_0}{\alpha_0 + 1}\bar{\mu}_i\bar{\mu}_j && (14)
\end{aligned}$$

Therefore, the aleatoric covariance matrix can be expressed as

$$\mathrm{Cov}[\boldsymbol{y}]^{alea} = \frac{\alpha_0}{\alpha_0 + 1}(\mathrm{Diag}(\bar{\boldsymbol{\mu}}) - \bar{\boldsymbol{\mu}}\bar{\boldsymbol{\mu}}^\top) \tag{15}$$

A.2.2 Epistemic Covariance

The epistemic covariance matrix can be derived as

$$\mathrm{Cov}[\boldsymbol{y}]^{epis} = \mathrm{Cov}[\mathbb{E}[\boldsymbol{y}|\boldsymbol{\mu}]] = \mathrm{Cov}[\boldsymbol{\mu}] \tag{16}$$

For $i \in \{1, 2, \dots, C\}$,

$$\mathrm{Cov}[\boldsymbol{y}]^{epis}_{i,i} = \mathrm{Var}[\mu_i] = \frac{\bar{\mu}_i - \bar{\mu}_i^2}{\alpha_0 + 1} \tag{17}$$

For $i, j \in \{1, 2, \dots, C\}$ such that $i \neq j$,

$$\mathrm{Cov}[\boldsymbol{y}]^{epis}_{i,j} = \mathrm{Cov}[\mu_i, \mu_j] = \frac{-\bar{\mu}_i\bar{\mu}_j}{\alpha_0 + 1} \tag{18}$$

Therefore, the epistemic covariance matrix can be expressed as

$$\mathrm{Cov}[\boldsymbol{y}]^{epis} = \frac{1}{\alpha_0 + 1}(\mathrm{Diag}(\bar{\boldsymbol{\mu}}) - \bar{\boldsymbol{\mu}}\bar{\boldsymbol{\mu}}^\top) \tag{19}$$

A.2.3 Total Covariance

The total covariance matrix can be derived as the sum of aleatoric and epistemic components.

$$\begin{aligned} \mathrm{Cov}[\boldsymbol{y}] &= \mathrm{Cov}[\boldsymbol{y}]^{alea} + \mathrm{Cov}[\boldsymbol{y}]^{epis} && (20) \\ &= \mathrm{Diag}(\bar{\boldsymbol{\mu}}) - \bar{\boldsymbol{\mu}}\bar{\boldsymbol{\mu}}^\top && (21) \end{aligned}$$

A.3. Evidential Class Uncertainties

The evidential uncertainties of class $c \in \{1, 2, \ldots, C\}$ not only can be directly retrieved from the diagonal of the corresponding covariance matrix but also can be calculated by decomposing the variance of the class random variable y_c based on the law of total variance. The two approaches yield the same result.

$$\underbrace{\mathrm{Var}[y_c]}_{\text{total}} = \underbrace{\mathbb{E}[\mathrm{Var}[y_c|\boldsymbol{\mu}]]}_{\text{aleatoric}} + \underbrace{\mathrm{Var}[\mathbb{E}[y_c|\boldsymbol{\mu}]]}_{\text{epistemic}} \tag{22}$$

The aleatoric, epistemic, and total class uncertainties can respectively be quantified as follows

$$\begin{aligned} U_c^{alea} &= \mathbb{E}[\mathrm{Var}[y_c|\boldsymbol{\mu}]] && (23) \\ &= \mathbb{E}[\mu_c(1 - \mu_c)] && (24) \\ &= \mathbb{E}[\mu_c] - \mathbb{E}[\mu_c^2] && (25) \\ &= \mathbb{E}[\mu_c] - \mathbb{E}^2[\mu_c] - \mathrm{Var}[\mu_c] && (26) \\ &= \bar{\mu}_c - \bar{\mu}_c^2 - \frac{\bar{\mu}_c - \bar{\mu}_c^2}{\alpha_0 + 1} && (27) \\ &= \frac{\alpha_0}{\alpha_0 + 1}(\bar{\mu}_i - \bar{\mu}_c^2) && (28) \end{aligned}$$

$$\begin{aligned} U_c^{epis} &= \mathrm{Var}[\mathbb{E}[y_c|\boldsymbol{\mu}]] && (29) \\ &= \mathrm{Var}[\mu_c] && (30) \\ &= \frac{1}{\alpha_0 + 1}(\bar{\mu}_c - \bar{\mu}_c^2) && (31) \end{aligned}$$

$$\begin{aligned} U_c &= U_c^{alea} + U_c^{epis} && (32) \\ &= \bar{\mu}_i - \bar{\mu}_c^2 && (33) \end{aligned}$$

The derivation is the same as the covariance derivation on the diagonal entries.