VIBI: Explaining a Black-Box using Deep Variational Information Bottleneck Approach

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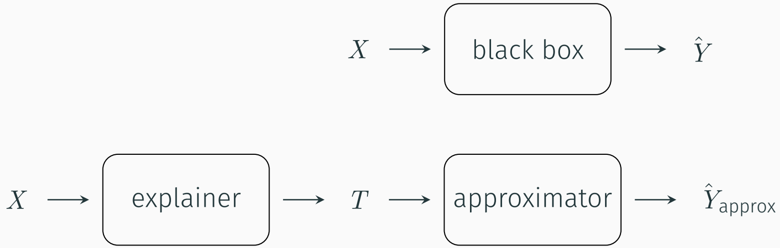
Overview

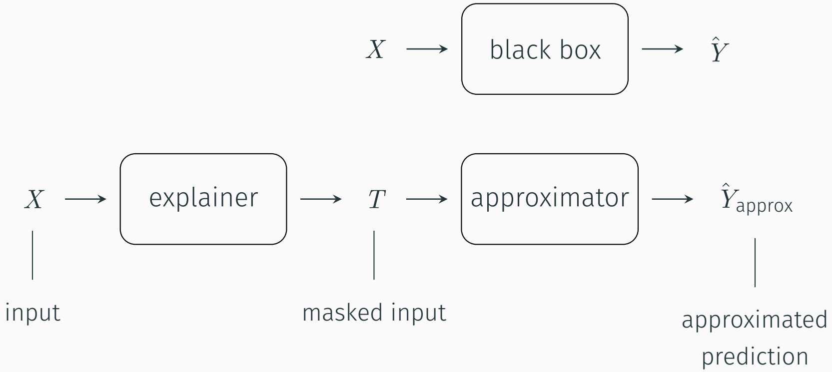
1. Introduction to VIBI
2. Information Bottleneck & Variational Bound
3. Gumbel Softmax
4. Results

Introduction to VIBI

VIBI


X
black box
$\hat{Y}$
X
explainer
T
approximator
$\hat{Y}_{\text{approx}}$

VIBI



X
black box
$\hat{Y}$
X
explainer
T
approximator
$\hat{Y}_{\text{approx}}$
input
masked input
approximated prediction

Notation and Conventions

s : scalar

$\mathbf{x}$: vector

X : random variable

$$p(\mathbf{x}) = p_X(X = \mathbf{x})$$

$$p(\mathbf{x}, \mathbf{y}) = p_{X,Y}(X = \mathbf{x},\, Y = \mathbf{y})$$

$$p(\mathbf{x} \,|\, \mathbf{y}) = p_{X|\,Y}(X = \mathbf{x} \,|\, Y = \mathbf{y}) = \frac{p_{X,Y}(X = \mathbf{x},\, Y = \mathbf{y})}{p_Y(Y = \mathbf{y})}$$

Markov-Chain Assumption

Markov-chain assumption:

$$Y \longleftrightarrow X \longleftrightarrow T$$

- Y is the *discrete* RV over the **class labels**, $\mathbf{y} \in \mathcal{Y} = \{1, \ldots, 10\}$.

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- X is the *continuous* RV over the **image space**, $\mathbf{x} \in \mathcal{X} = [0, 1]^d$

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- T is the RV over $\mathcal{T} = \mathcal{X}$

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- Y is the *discrete* RV over the **class labels**, $\mathbf{y} \in \mathcal{Y} = \{1, \ldots, 10\}$.
- X is the *continuous* RV over the **image space**, $\mathbf{x} \in \mathcal{X} = [0, 1]^d$
- T is the RV over $\mathcal{T} = \mathcal{X}$

d is the image dimension ($28 \times 28 = 784$ in the case of the MNIST dataset).

Markov-Chain Assumption

Markov-chain assumption:

$$Y \longleftrightarrow X \longleftrightarrow T$$

The Markov-chain assumption leads to the joint-distribution

$$p(\mathbf{x}, \mathbf{y}, \mathbf{t}) = p(\mathbf{y} \mid \mathbf{t}, \mathbf{x}) p(\mathbf{t}, \mathbf{x})$$

Markov-Chain Assumption

Markov-chain assumption:

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The Markov-chain assumption leads to the joint-distribution

$$\begin{aligned} p(\mathbf{x}, \mathbf{y}, \mathbf{t}) &= p(\mathbf{y} \mid \mathbf{t}, \mathbf{x}) p(\mathbf{t}, \mathbf{x}) \\ &= p(\mathbf{y} \mid \mathbf{t}, \mathbf{x}) p(\mathbf{t} \mid \mathbf{x}) p(\mathbf{x}) \end{aligned}$$

Markov-Chain Assumption

Markov-chain assumption:

$$Y \longleftrightarrow X \longleftrightarrow T$$

The Markov-chain assumption leads to the joint-distribution

$$\begin{aligned} p(\mathbf{x}, \mathbf{y}, \mathbf{t}) &= p(\mathbf{y} \mid \mathbf{t}, \mathbf{x}) p(\mathbf{t}, \mathbf{x}) \\ &= p(\mathbf{y} \mid \mathbf{t}, \mathbf{x}) p(\mathbf{t} \mid \mathbf{x}) p(\mathbf{x}) \\ &= p(\mathbf{y} \mid \mathbf{t}) p(\mathbf{t} \mid \mathbf{x}) p(\mathbf{x}) \end{aligned}$$

Markov-Chain Assumption

The explainer network models a probability distribution $p(\mathbf{z} \,|\, \mathbf{x})$ over cognitive chunks. Z is drawn as a k-hot vector from $p(\mathbf{z} \,|\, \mathbf{x})$. The resulting explanation is given by $\mathbf{t} = \mathbf{x} \odot \mathbf{z}$

Full markov-chain:

$$Y \longleftrightarrow X \longleftrightarrow (X, Z) \longleftrightarrow T$$

Information Bottleneck & Variational Bound

Information Bottleneck

The Information Bottleneck (IB) objective as stated by Tishby, Pereira, and Bialek, 2000:

$$\max_{p_{T|X},\, p_{Y|T},\, p_T} I(T;Y) - \beta I(X;T)$$

Variational Bound - $I(X;T)$ Upper Bound

Markov-chain:

$$Y \longleftrightarrow X \longleftrightarrow (X, Z) \longleftrightarrow T$$

$$I(X;T) \leq I(X;X,Z)$$

Variational Bound - $I(X;T)$ Upper Bound

Markov-chain:

$$Y \longleftrightarrow X \longleftrightarrow (X, Z) \longleftrightarrow T$$

$$\begin{aligned} I(X;T) &\leq I(X;X,Z) \\ &= I(X;Z) + I(X;X \,|\, Z) \end{aligned}$$

Variational Bound - $I(X;T)$ Upper Bound

Markov-chain:

$$Y \longleftrightarrow X \longleftrightarrow (X, Z) \longleftrightarrow T$$

$$\begin{aligned} I(X;T) &\leq I(X;X,Z) \\ &= I(X;Z) + I(X;X \mid Z) \\ &= I(X;Z) + H(X \mid Z) + H(X \mid Z) - H(X,X \mid Z) \end{aligned}$$

Variational Bound - $I(X;T)$ Upper Bound

Markov-chain:

$$Y \longleftrightarrow X \longleftrightarrow (X, Z) \longleftrightarrow T$$

$$\begin{aligned}
I(X;T) &\leq I(X;X,Z) \\
&= I(X;Z) + I(X;X \mid Z) \\
&= I(X;Z) + H(X \mid Z) + H(X \mid Z) - H(X, X \mid Z) \\
&= I(X;Z) + H(X \mid Z)
\end{aligned}$$

Variational Bound - $I(X;T)$ Upper Bound

Markov-chain:

$$Y \longleftrightarrow X \longleftrightarrow (X,Z) \longleftrightarrow T$$

$$\begin{aligned}
I(X;T) &\leq I(X;X,Z) \\
&= I(X;Z) + I(X;X \mid Z) \\
&= I(X;Z) + H(X \mid Z) + H(X \mid Z) - H(X,X \mid Z) \\
&= I(X;Z) + H(X \mid Z) \\
&\leq I(X;Z) + H(X)
\end{aligned}$$

Variational Bound - $I(X; Z)$ Upper Bound

$$I(X; Z) = \int p(\mathbf{x}, \mathbf{z}) \log \left(\frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{x}) p(\mathbf{z})} \right) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z}$$

Variational Bound - $I(X;Z)$ Upper Bound

$$
\begin{aligned}
I(X;Z) &= \int p(\mathbf{x},\mathbf{z}) \log\left(\frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{x})p(\mathbf{z})}\right) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}\mid\mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z}
\end{aligned}
$$

Variational Bound - $I(X;Z)$ Upper Bound

$$
\begin{aligned}
I(X;Z) &= \int p(\mathbf{x},\mathbf{z}) \log \left(\frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{x})p(\mathbf{z})} \right) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z} \mid \mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z} \mid \mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{z}) \log p(\mathbf{z}) \, \mathrm{d}\mathbf{z}
\end{aligned}
$$

Variational Bound - $I(X;Z)$ Upper Bound

$$
\begin{aligned}
I(X;Z) &= \int p(\mathbf{x},\mathbf{z}) \log \left(\frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{x})p(\mathbf{z})} \right) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z} \mid \mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z} \mid \mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \underbrace{\int p(\mathbf{z}) \log p(\mathbf{z}) \, \mathrm{d}\mathbf{z}}_{D_{\mathsf{KL}}(p||r) + H(p,r)}
\end{aligned}
$$

Variational Bound - $I(X;Z)$ Upper Bound

$$
\begin{aligned}
I(X;Z) &= \int p(\mathbf{x},\mathbf{z}) \log\left(\frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{x})p(\mathbf{z})}\right) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}\,|\,\mathbf{x})\, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z})\, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}\,|\,\mathbf{x})\, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \underbrace{\int p(\mathbf{z}) \log p(\mathbf{z})\, \mathrm{d}\mathbf{z}}_{D_{\mathsf{KL}}(p||r)+H(p,r)} \\
&\leq \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}\,|\,\mathbf{x})\, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{z}) \log r(\mathbf{z})\, \mathrm{d}\mathbf{z}
\end{aligned}
$$

Variational Bound - $I(X;Z)$ Upper Bound

$$
\begin{aligned}
I(X;Z) &= \int p(\mathbf{x},\mathbf{z}) \log \left(\frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{x})p(\mathbf{z})} \right) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z} \mid \mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z} \mid \mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \underbrace{\int p(\mathbf{z}) \log p(\mathbf{z}) \, \mathrm{d}\mathbf{z}}_{D_{\mathsf{KL}}(p||r) + H(p,r)} \\
&\leq \int p(\mathbf{x},\mathbf{z}) \log p(\mathbf{z} \mid \mathbf{x}) \, \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z} - \int p(\mathbf{z}) \log r(\mathbf{z}) \, \mathrm{d}\mathbf{z} \\
&= \int p(\mathbf{x},\mathbf{z}) \log \left(\frac{p(\mathbf{z} \mid \mathbf{x})}{r(\mathbf{z})} \right) \mathrm{d}\mathbf{z}
\end{aligned}
$$

Variational Bound - $I(X;T)$ Upper Bound

$$I(X;T) \leq \int p(\mathbf{x},\mathbf{z}) \log \left(\frac{p(\mathbf{z} \mid \mathbf{x})}{r(\mathbf{z})} \right) \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{x} + C$$

Variational Bound - $I(X;T)$ Upper Bound

$$
\begin{aligned}
I(X;T) &\leq \int p(\mathbf{x},\mathbf{z}) \log\left(\frac{p(\mathbf{z}\,|\,\mathbf{x})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{x} + C \\
&= \int p(\mathbf{x}) p(\mathbf{z}\,|\,\mathbf{x}) \log\left(\frac{p(\mathbf{z}\,|\,\mathbf{x})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{x} + C
\end{aligned}
$$

Variational Bound - $I(X;T)$ Upper Bound

$$
\begin{aligned}
I(X;T) &\leq \int p(\mathbf{x},\mathbf{z}) \log\left(\frac{p(\mathbf{z}\mid\mathbf{x})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{x} + C \\
&= \int p(\mathbf{x}) p(\mathbf{z}\mid\mathbf{x}) \log\left(\frac{p(\mathbf{z}\mid\mathbf{x})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{x} + C \\
&\approx \frac{1}{N}\sum_{n=1}^{N} \int p(\mathbf{z}\mid\mathbf{x}^{(n)}) \log\left(\frac{p(\mathbf{z}\mid\mathbf{x}^{(n)})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z} + C
\end{aligned}
$$

Variational Bound - $I(X;T)$ Upper Bound

$$
\begin{aligned}
I(X;T) &\leq \int p(\mathbf{x},\mathbf{z}) \log\left(\frac{p(\mathbf{z}\mid\mathbf{x})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{x} + C \\
&= \int p(\mathbf{x}) p(\mathbf{z}\mid\mathbf{x}) \log\left(\frac{p(\mathbf{z}\mid\mathbf{x})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{x} + C \\
&\approx \frac{1}{N}\sum_{n=1}^{N} \int p(\mathbf{z}\mid\mathbf{x}^{(n)}) \log\left(\frac{p(\mathbf{z}\mid\mathbf{x}^{(n)})}{r(\mathbf{z})}\right) \mathrm{d}\mathbf{z} + C \\
&= \frac{1}{N}\sum_{n=1}^{N} D_{\mathsf{KL}}\left(f_{\mathsf{xpl}}(\mathbf{x}^{(n)}) \,||\, r\right) + C
\end{aligned}
$$

Variational Bound - $I(X;T)$ Upper Bound

$$
\begin{aligned}
I(X;T) &\leq \int p(\mathbf{x}, \mathbf{z}) \log \left(\frac{p(\mathbf{z} \mid \mathbf{x})}{r(\mathbf{z})} \right) \mathrm{d}\mathbf{z} \mathrm{d}\mathbf{x} + C \\
&= \int p(\mathbf{x}) p(\mathbf{z} \mid \mathbf{x}) \log \left(\frac{p(\mathbf{z} \mid \mathbf{x})}{r(\mathbf{z})} \right) \mathrm{d}\mathbf{z} \mathrm{d}\mathbf{x} + C \\
&\approx \frac{1}{N} \sum_{n=1}^{N} \int p(\mathbf{z} \mid \mathbf{x}^{(n)}) \log \left(\frac{p(\mathbf{z} \mid \mathbf{x}^{(n)})}{r(\mathbf{z})} \right) \mathrm{d}\mathbf{z} + C \\
&= \frac{1}{N} \sum_{n=1}^{N} D_{\mathsf{KL}} \left(f_{\mathsf{xpl}}(\mathbf{x}^{(n)}) \,||\, r \right) + C \quad =: U_{X,T}
\end{aligned}
$$

Variational Bound - $I(T;Y)$ Lower Bound

$$I(T;Y) = \int p(\mathbf{t},\mathbf{y}) \log \left(\frac{p(\mathbf{t},\mathbf{y})}{p(\mathbf{t})p(\mathbf{y})} \right) \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}$$

Variational Bound - $I(T;Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &= \int p(\mathbf{t},\mathbf{y}) \log \left(\frac{p(\mathbf{t},\mathbf{y})}{p(\mathbf{t})p(\mathbf{y})} \right) \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y} \mid \mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} - \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}
\end{aligned}
$$

$$
\begin{aligned}
I(T;Y) &= \int p(\mathbf{t},\mathbf{y}) \log\left(\frac{p(\mathbf{t},\mathbf{y})}{p(\mathbf{t})p(\mathbf{y})}\right) \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y} \mid \mathbf{t})\, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} - \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y})\, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{y}) \int p(\mathbf{y} \mid \mathbf{t}) \log p(\mathbf{y} \mid \mathbf{t})\, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} - \int p(\mathbf{y}) \log p(\mathbf{y})\, \mathrm{d}\mathbf{y}
\end{aligned}
$$

Variational Bound - $I(T;Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &= \int p(\mathbf{t},\mathbf{y}) \log\left(\frac{p(\mathbf{t},\mathbf{y})}{p(\mathbf{t})p(\mathbf{y})}\right) \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} - \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{y}) \int p(\mathbf{y}\,|\,\mathbf{t}) \log p(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} - \int p(\mathbf{y}) \log p(\mathbf{y})\,\mathrm{d}\mathbf{y} \\
&\overset{\text{(var. approx)}}{\geq} \int p(\mathbf{y}) \int p(\mathbf{y}\,|\,\mathbf{t}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} + H(Y)
\end{aligned}
$$

Variational Bound - $I(T;Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &= \int p(\mathbf{t},\mathbf{y}) \log\left(\frac{p(\mathbf{t},\mathbf{y})}{p(\mathbf{t})p(\mathbf{y})}\right) \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y}\,|\,\mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} - \int p(\mathbf{t},\mathbf{y}) \log p(\mathbf{y}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{y}) \int p(\mathbf{y}\,|\,\mathbf{t}) \log p(\mathbf{y}\,|\,\mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} - \int p(\mathbf{y}) \log p(\mathbf{y}) \, \mathrm{d}\mathbf{y} \\
&\overset{\text{(var. approx)}}{\geq} \int p(\mathbf{y}) \int p(\mathbf{y}\,|\,\mathbf{t}) \log q(\mathbf{y}\,|\,\mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} + H(Y) \\
&\geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y}\,|\,\mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}
\end{aligned}
$$

Variational Bound - $I(T;Y)$ Lower Bound

$$I(T;Y) \geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y} \mid \mathbf{t}) \,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}$$

Variational Bound - $I(T;Y)$ Lower Bound

$$\begin{aligned} I(T;Y) &\geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y} \mid \mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\ &= \int p(\mathbf{t},\mathbf{y},\mathbf{x}) \log q(\mathbf{y} \mid \mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \end{aligned}$$

Variational Bound - $I(T;Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &\geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y} \mid \mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y},\mathbf{x}) \log q(\mathbf{y} \mid \mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&= \int p(\mathbf{x}) p(\mathbf{t} \mid \mathbf{x}) p(\mathbf{y} \mid \mathbf{x}) \log q(\mathbf{y} \mid \mathbf{t}) \, \mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x}
\end{aligned}
$$

Variational Bound - $I(T; Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &\geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y} \,|\, \mathbf{t}) \,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y},\mathbf{x}) \log q(\mathbf{y} \,|\, \mathbf{t}) \,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&= \int p(\mathbf{x}) p(\mathbf{t} \,|\, \mathbf{x}) p(\mathbf{y} \,|\, \mathbf{x}) \log q(\mathbf{y} \,|\, \mathbf{t}) \,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&\approx \frac{1}{N} \sum_{n=1}^{N} \int p(\mathbf{t} \,|\, \mathbf{x}^{(n)}) \int p(\mathbf{y} \,|\, \mathbf{x}^{(n)}) \log q(\mathbf{y} \,|\, \mathbf{t}) \,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{t}
\end{aligned}
$$

Variational Bound - $I(T;Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &\geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y},\mathbf{x}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&= \int p(\mathbf{x})p(\mathbf{t}\,|\,\mathbf{x})p(\mathbf{y}\,|\,\mathbf{x}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&\approx \frac{1}{N}\sum_{n=1}^{N} \int p(\mathbf{t}\,|\,\mathbf{x}^{(n)}) \int p(\mathbf{y}\,|\,\mathbf{x}^{(n)}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{t} \\
&\approx \frac{1}{NM} \sum_{\substack{n=1\ldots N \\ m=1\ldots M}} \int p(\mathbf{y}\,|\,\mathbf{x}^{(n)}) \log q(\mathbf{y}\,|\,\mathbf{t}^{(m;n)})\,\mathrm{d}\mathbf{y}
\end{aligned}
$$

Variational Bound - $I(T;Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &\geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y} \mid \mathbf{t}) \,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y},\mathbf{x}) \log q(\mathbf{y} \mid \mathbf{t}) \,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&= \int p(\mathbf{x}) p(\mathbf{t} \mid \mathbf{x}) p(\mathbf{y} \mid \mathbf{x}) \log q(\mathbf{y} \mid \mathbf{t}) \,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&\approx \frac{1}{N} \sum_{n=1}^{N} \int p(\mathbf{t} \mid \mathbf{x}^{(n)}) \int p(\mathbf{y} \mid \mathbf{x}^{(n)}) \log q(\mathbf{y} \mid \mathbf{t}) \,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{t} \\
&\approx \frac{1}{NM} \sum_{\substack{n=1\ldots N \\ m=1\ldots M}} \int p(\mathbf{y} \mid \mathbf{x}^{(n)}) \log q(\mathbf{y} \mid \mathbf{t}^{(m;n)}) \,\mathrm{d}\mathbf{y} \\
&\approx -\frac{1}{NM} \sum_{\substack{n=1\ldots N \\ m=1\ldots M}} H\left(b(\mathbf{x}^{(n)}), f_{\mathsf{apx}}(\mathbf{t}^{(m;n)})\right)
\end{aligned}
$$

Variational Bound - $I(T;Y)$ Lower Bound

$$
\begin{aligned}
I(T;Y) &\geq \int p(\mathbf{t},\mathbf{y}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y} \\
&= \int p(\mathbf{t},\mathbf{y},\mathbf{x}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&= \int p(\mathbf{x})p(\mathbf{t}\,|\,\mathbf{x})p(\mathbf{y}\,|\,\mathbf{x}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{t}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&\approx \frac{1}{N}\sum_{n=1}^{N} \int p(\mathbf{t}\,|\,\mathbf{x}^{(n)}) \int p(\mathbf{y}\,|\,\mathbf{x}^{(n)}) \log q(\mathbf{y}\,|\,\mathbf{t})\,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{t} \\
&\approx \frac{1}{NM} \sum_{\substack{n=1\ldots N\\ m=1\ldots M}} \int p(\mathbf{y}\,|\,\mathbf{x}^{(n)}) \log q(\mathbf{y}\,|\,\mathbf{t}^{(m;n)})\,\mathrm{d}\mathbf{y} \\
&\approx -\frac{1}{NM} \sum_{\substack{n=1\ldots N\\ m=1\ldots M}} H\left(b(\mathbf{x}^{(n)}), f_{\mathsf{apx}}(\mathbf{t}^{(m;n)})\right) \qquad =: L_{T,Y}
\end{aligned}
$$

Variational Bound - Combined

$$I(T;Y) - \beta I(X;T) \gtrapprox L_{T,Y} - \beta U_{X,T}$$

$$\max_{\boldsymbol{\theta}} \quad L_{T,Y} - \beta U_{X,T}$$

Variational Bound - Combined

$$I(T;Y) - \beta I(X;T) \gtrapprox L_{T,Y} - \beta U_{X,T}$$

$$\begin{aligned} & \max_{\boldsymbol{\theta}} \quad L_{T,Y} - \beta U_{X,T} \\ \iff & \min_{\boldsymbol{\theta}} -L_{T,Y} + \beta U_{X,T} \end{aligned}$$

Variational Bound - Combined

$$I(T;Y) - \beta I(X;T) \gtrapprox L_{T,Y} - \beta U_{X,T}$$

$$\begin{aligned} & \max_{\boldsymbol{\theta}} \quad L_{T,Y} - \beta U_{X,T} \\ \iff & \min_{\boldsymbol{\theta}} -L_{T,Y} + \beta U_{X,T} \quad =: J_{\text{IB}} \end{aligned}$$

Variational Bound - Combined

$$I(T;Y) - \beta I(X;T) \gtrapprox L_{T,Y} - \beta U_{X,T}$$

$$\begin{aligned}
& \max_{\boldsymbol{\theta}} \quad L_{T,Y} - \beta U_{X,T} \\
\iff & \min_{\boldsymbol{\theta}} -L_{T,Y} + \beta U_{X,T} \qquad =: J_{\mathsf{IB}} \\
\iff & \min_{\boldsymbol{\theta}} \frac{1}{NM} \sum_{\substack{n=1\ldots N \\ m=1\ldots M}} H\Big(b(\mathbf{x}^{(n)}), f_{\mathsf{apx}}(\mathbf{t}^{(m;n)})\Big) \\
& \qquad + \beta \frac{1}{N} \sum_{n=1\ldots N} D_{\mathsf{KL}}\Big(f_{\mathsf{xpl}}(\mathbf{x}^{(n)}) \,||\, r\Big)
\end{aligned}$$

Variational Bound - Combined

$$I(T;Y) - \beta I(X;T) \gtrapprox L_{T,Y} - \beta U_{X,T}$$

$$\begin{aligned}
&\max_{\boldsymbol{\theta}} \quad L_{T,Y} - \beta U_{X,T} \\
\iff &\min_{\boldsymbol{\theta}} -L_{T,Y} + \beta U_{X,T} \quad =: J_{\mathsf{IB}} \\
\iff &\min_{\boldsymbol{\theta}} \frac{1}{NM} \sum_{\substack{n=1\ldots N \\ m=1\ldots M}} H\Big(\underbrace{b(\mathbf{x}^{(n)})}_{p(\mathbf{y}\,|\,\mathbf{x})}, \underbrace{f_{\mathsf{apx}}(\mathbf{t}^{(m;n)})}_{q(\mathbf{y}\,|\,\mathbf{t})} \Big) \\
&\qquad + \beta \frac{1}{N} \sum_{n=1\ldots N} D_{\mathsf{KL}}\Big(\underbrace{f_{\mathsf{xpl}}(\mathbf{x}^{(n)})}_{p(\mathbf{z}\,|\,\mathbf{x})} \;||\; r \Big)
\end{aligned}$$

Gumbel Softmax

Sampling T

$$\mathbf{t} = \mathbf{x} \odot \mathbf{z}$$

$$p(\mathbf{t} \mid \mathbf{x}) = p(\mathbf{z} \mid \mathbf{x}) \stackrel{?}{=} f_{\mathsf{xpl}}(\mathbf{x})$$

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outputs of f_{xpl} network are unnormalized logits...

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$$p(\mathbf{t} \mid \mathbf{x}) = p(\mathbf{z} \mid \mathbf{x}) \stackrel{?}{=} f_{\text{xpl}}(\mathbf{x})$$

$$p(\mathbf{z}^* \mid \mathbf{x}) = \text{relaxed\_k\_hot}_\tau(f_{\text{xpl}}(\mathbf{x}))$$

outputs of f_{xpl} network are unnormalized logits...

Gumbel Softmax

$$\mathbf{g} = -\log(-\log(\boldsymbol{\varepsilon}))\,,\ \boldsymbol{\varepsilon} \sim \mathcal{U}[0,1]$$
$$\mathbf{c} = \mathsf{softmax}\left(\frac{\log(\mathbf{p}) + \mathbf{g}}{\tau}\right)$$

Gumbel Softmax

$$\mathbf{g} = -\log(-\log(\varepsilon)) \,, \; \varepsilon \sim \mathcal{U}[0,1]$$
$$\mathbf{c} = \text{softmax}\left(\frac{\log(\mathbf{p}) + \mathbf{g}}{\tau}\right)$$

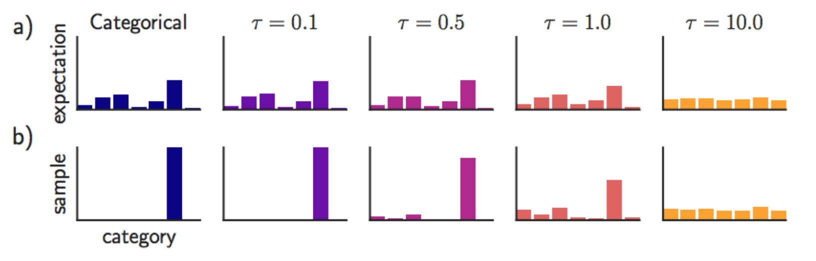

Figure 1: Relaxed categorical gumbel softmax distribution with varying temperature τ (Jang, Gu, and Poole, 2017).

Gumbel Softmax

$$\mathbf{g} = -\log(-\log(\boldsymbol{\varepsilon}))\,,\ \boldsymbol{\varepsilon} \sim \mathcal{U}[0,1]$$
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Gumbel Softmax

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$$\mathbf{c} = \text{softmax}\left(\frac{\log(\mathbf{p}) + \mathbf{g}}{\tau}\right)$$

Sample k relaxed one-hot vectors $\{\mathbf{c}^{(n)}\}_{n=1}^{k}$.

$$\mathbf{z}_i^* = \max_n \mathbf{c}_i^{(n)}$$

Resulting vector z^* will be at most k-hot.

Results

Authors' - Results

Figure 2: Interpretable results from MNIST black box classifier (Bang et al., 2019).

Authors' - Results

	chunk size	k	L2X	VIBI (Ours)					
			0	0.001	0.01	0.1	1	10	100
Accuracy	1×1	64	0.694	0.690	0.726	0.689	0.742	0.729	**0.766**
	1×1	96	0.814	0.831	0.780	0.806	**0.859**	0.765	0.826
	1×1	160	0.903	0.907	0.905	0.917	0.917	**0.928**	0.902
	2×2	16	0.735	**0.795**	0.750	0.771	0.732	0.753	0.769
	2×2	24	0.776	0.855	0.834	0.856	**0.868**	0.854	0.847
	2×2	40	0.811	0.914	0.914	0.915	0.903	0.918	**0.935**
	2×2	80	0.905	0.949	0.940	0.939	**0.962**	0.941	0.923
	4×4	4	0.650	0.655	0.650	**0.775**	0.717	0.682	0.681
	4×4	6	0.511	**0.858**	0.706	0.701	0.708	0.690	0.730
	4×4	10	0.835	0.835	0.824	**0.933**	0.875	0.854	0.782
	4×4	20	0.954	**0.962**	0.815	0.934	0.929	0.946	0.943

Figure 3: Ablations for β parameter on MNIST (Bang et al., 2019).

Authors' - Results

	chunk size	k	Approximator Fidelity					Rationale Fidelity	
			Saliency	LIME	SHAP	L2X	VIBI (Ours)	L2X	VIBI (Ours)
IMDB	sentence	1	38.7 ± 0.9	72.7 ± 0.8	49.5 ± 1.0	87.6 ± 0.6	**87.7 ± 0.6**	72.7 ± 0.8	**73.1 ± 0.8**
	word	5	41.9 ± 0.9	**75.6 ± 0.8**	50.1 ± 1.0	73.8 ± 0.8	74.4 ± 0.8	63.8 ± 0.8	**65.7 ± 0.8**
	5 words	1	42.4 ± 0.9	29.0 ± 0.8	49.7 ± 1.0	75.9 ± 0.7	**76.4 ± 0.7**	60.1 ± 0.9	**63.2 ± 0.8**
	5 words	3	41.4 ± 0.9	67.9 ± 0.8	49.1 ± 1.0	83.3 ± 0.7	**83.5 ± 0.7**	**69.4 ± 0.8**	66.0 ± 0.8
MNIST	2×2	16	91.2 ± 0.6	77.0 ± 0.8	94.2 ± 0.5	93.4 ± 0.5	**94.8 ± 0.4**	73.5 ± 0.9	**77.1 ± 0.8**
	2×2	24	93.8 ± 0.5	80.7 ± 0.8	95.4 ± 0.4	95.1 ± 0.4	**95.3 ± 0.4**	77.6 ± 0.8	**85.6 ± 0.7**
	2×2	40	95.7 ± 0.4	85.9 ± 0.7	95.4 ± 0.4	**96.7 ± 0.4**	96.2 ± 0.4	81.1 ± 0.8	**91.5 ± 0.5**
	4×4	4	86.3 ± 0.7	60.9 ± 1.0	94.8 ± 0.4	**95.3 ± 0.4**	94.8 ± 0.4	65.0 ± 0.9	**77.5 ± 0.8**
	4×4	6	90.6 ± 0.6	63.7 ± 0.9	93.6 ± 0.5	**95.7 ± 0.4**	95.6 ± 0.4	51.1 ± 1.0	**70.1 ± 0.9**
	4×4	10	94.9 ± 0.4	70.5 ± 0.9	95.1 ± 0.4	96.5 ± 0.4	**96.7 ± 0.4**	83.5 ± 0.7	**93.3 ± 0.5**

Figure 4: Comparison with other interpretability frameworks (Bang et al., 2019).

CIFAR10 Results

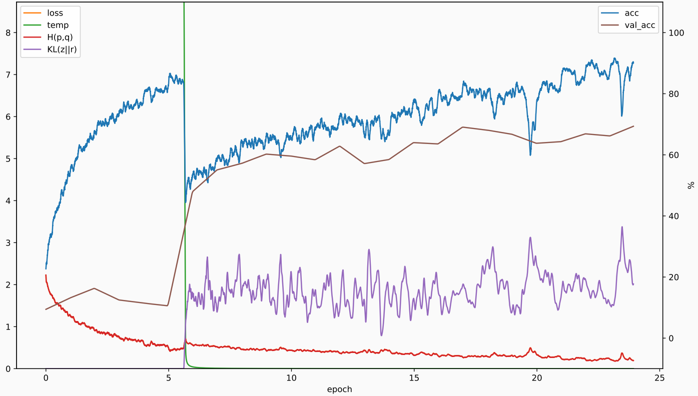
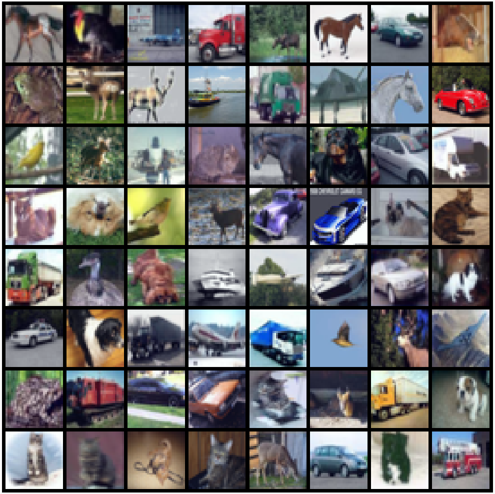


Figure 5: CIFAR10 VIBI training metrics. Explainer is a *Unet*, $k = 64$, β = 0.001

CIFAR10 Results

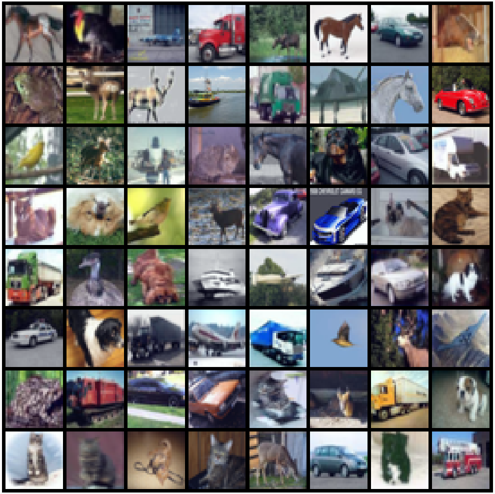


CIFAR10 test set batch.

CIFAR10 Results

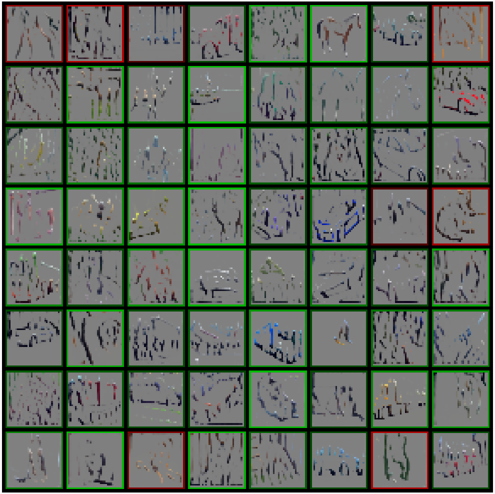
CIFAR10 VIBI **distribution** over explanation. Explainer is a *Unet*, $k = 64$, β = 0.001

CIFAR10 Results



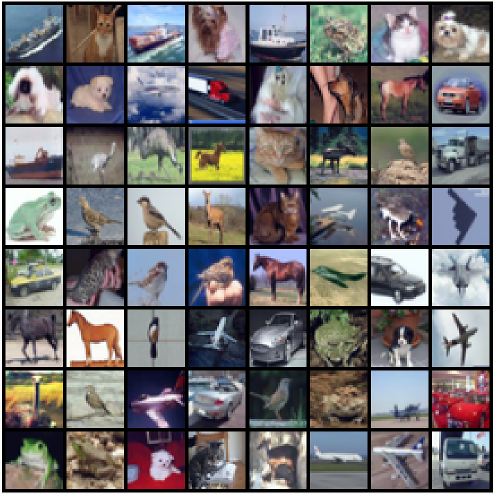
CIFAR10 test set batch.

CIFAR10 Results



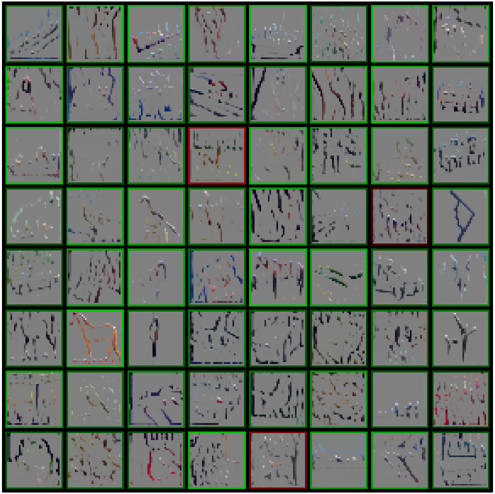
CIFAR10 VIBI explanations with black box prediction context. Explainer is a *Unet*, $k = 64$, β = 0.001

CIFAR10 More Results



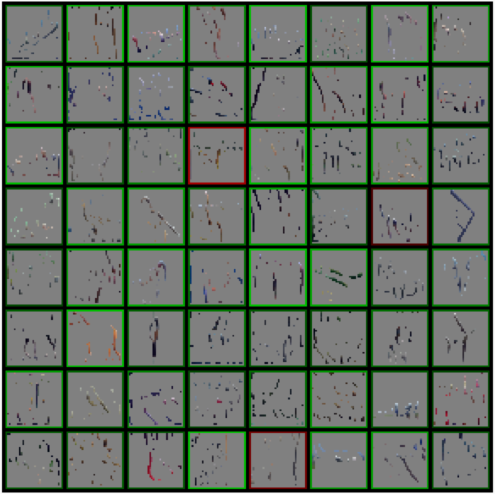
CIFAR10 test set batch.

CIFAR10 More Results



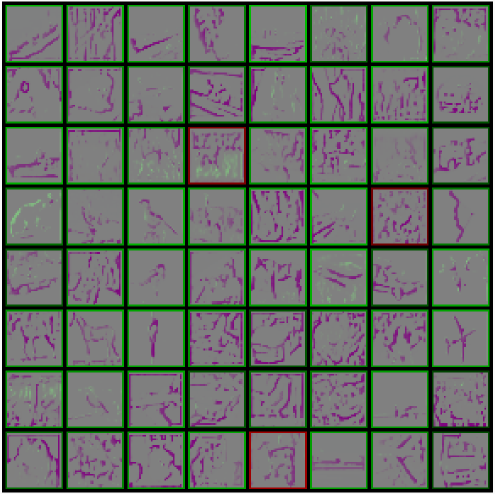
CIFAR10 VIBI **distribution** over explanation with black box prediction context.
Explainer is a *Unet*, $k = 64$, $\beta = 0.001$

CIFAR10 More Results



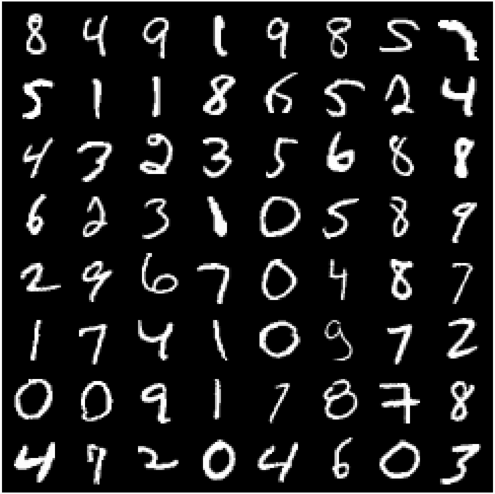
CIFAR10 VIBI **top-k** explanations with black box prediction context. Explainer is a ***Unet***, $k = 64$, $\beta = 0.001$

CIFAR10 More Results



CIFAR10 VIBI top-k explanations with black box prediction context. Explainer is a ***Unet***, $k = 64$, $\beta = 0.001$, ***out_channels*** $= 3$

MNIST Results

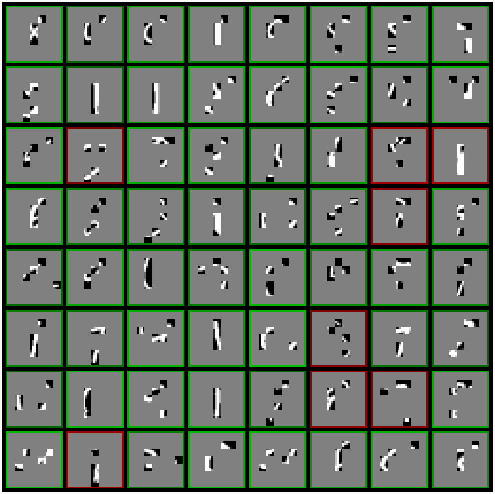


MNIST test set batch.

MNIST Results

MNIST VIBI **distribution** over explanations with black box prediction context.
Explainer is a ***ResNet***, $k = 4$, $\beta = 0.01$, ***chunk_size=4x4***

MNIST Results



MNIST VIBI **top-k** explanations with black box prediction context. Explainer is a *ResNet*, $k = 4$, $\beta = 0.01$, *chunk_size=4x4*

References

- Seojin Bang et al. *Explaining a black-box using Deep Variational Information Bottleneck Approach*. 2019. arXiv: *1902.06918 [cs.LG]*.
- Eric Jang, Shixiang Gu, and Ben Poole. *Categorical Reparameterization with Gumbel-Softmax*. 2017. arXiv: *1611.01144 [stat.ML]*.
- Naftali Tishby, Fernando C Pereira, and William Bialek. "The information bottleneck method". In: *arXiv preprint physics/0004057* (2000).

Code available at github.com/willisk/VIBI