SOFTMAX IS NOT AN ARTIFICIAL TRICK:
AN INFORMATION-THEORETIC VIEW OF SOFTMAX IN NEURAL NETWORKS

A PREPRINT

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October 8, 2019

ABSTRACT

Despite great popularity of applying softmax to map the non-normalised outputs of a neural network to a probability distribution over predicting classes, this normalised exponential transformation still seems to be artificial. A theoretic framework that incorporates softmax as an intrinsic component is still lacking. In this paper, we view neural networks embedding softmax from an information-theoretic perspective. Under this view, we can naturally and mathematically derive log-softmax as an inherent component in a neural network for evaluating the conditional mutual information between network output vectors and labels given an input datum. We show that training deterministic neural networks through maximising log-softmax is equivalent to enlarging the conditional mutual information, i.e., feeding label information into network outputs. We also generalise our informative-theoretic perspective to neural networks with stochasticity and derive information upper and lower bounds of log-softmax. In theory, such an information-theoretic view offers rationality support for embedding softmax in neural networks; in practice, we eventually demonstrate a computer vision application example of how to employ our information-theoretic view to filter out targeted objects on images.

Keywords Softmax · Mutual Information · Neural Network

1 Introduction

Thanks to AlexNet [1], neural networks have attracted attention back in computer vision and machine learning communities and demonstrate spectacular performances in a wide range of applications [2]. A large number of neural networks, particularly in the classification tasks, applied softmax to map the non-normalised network outputs to a categorical probability distribution over classes [3], followed by taking a negative log-softmax as the cross-entropy between this estimated and true class distributions for minimisation [4].

Despite the tremendous popularity of employing softmax and its extraordinary performance in modelling categorical probability distributions [5], such a transformation of converting neural network outputs to probability distributions with softmax seem to be artificial. We desire to build up a theoretic framework that can naturally and mathematically derive log-softmax as an inherent ingredient in a neural network, instead of rigidly gluing the theories of neural networks and probabilities. In this paper, we present such an end-to-end theoretic view such that log-softmax is a smooth derivation for evaluating the conditional mutual information between network output vectors and labels given an input datum.

To the best of authors’ knowledge, we are the first to build a coherent information-theoretic view that incorporates log-softmax as its intrinsic building block. We summarise our contributions as the following:
1. We show that training deterministic neural networks through maximising log-sofmax is equivalent to enlarging the conditional mutual information, i.e., feeding label information into network outputs.

2. We generalise our informative-theoretic perspective to neural networks with stochasticity and derive information upper and lower bounds of log-softmax.

3. We demonstrate a computer vision application example of how to employ our information-theoretic view to filter out targeted objects on images.

In sum, our information-theoretic view can offer rationality support for embedding softmax in neural networks in theory, and can apply to solve concrete tasks and demonstrate impressive performance.

2 Preliminaries

2.1 Softmax

2.1.1 Definition

Neural networks embed the softmax function, abbreviated as softmax in this paper, to learn multi-class categorical distributions, particularly within the classification tasks. We first formally define softmax $f_s(\cdot)$. Let the training data consist of $M$ classes and $N$ labelled instances $\{(x_1, y_1), \ldots, (x_N, y_N)\}$, where $y_n \in \{1, \ldots, y, \ldots, M\}$, of each datum $(x_n, y_n)$, is an integer class label of the input datum $x_n \in \mathbb{R}^D$. We train a neural network $f_s(x_n) : \mathbb{R}^D \rightarrow \mathbb{R}^M$ to output the likelihood $z_m = \{z_1, \ldots, z_y, \ldots, z_M\} \in \mathbb{R}^M$, where the greater each $z_y$ is, the more likely this input datum $x$ belongs to the class $y$. Nonetheless, such $z_y$ is not a probability since it can be negative as well as greater than 1, violating probability axioms. Therefore, we employ softmax $f_s(\cdot)$, which is a normalised exponential function, to map each $z_y$ to be in the range of $(0, 1)$. Formally,

$$\text{softmax}(z, y) = f_s(z, y) = \frac{\exp \{z_y\}}{\sum_{m=1}^{M} \exp \{z_m\}}$$  \hspace{1cm} (1)

where $z_y$ denotes the $y$-th element of $z \in \mathbb{R}^M$. As a consequence, we can treat the joint outcomes of softmax $\{f_s(z, 1), \ldots, f_s(z, M)\}$ as a categorical probability distribution over the $M$ classes, since each element within $\{f_s(z, i)\}_{i=1}^{M}$ is bounded between 0 and 1, and all the elements within $\{f_s(z, i)\}_{i=1}^{M}$ sum up to 1.

2.1.2 Training

It is common to train neural networks embedding softmax to minimise the cross-entropy loss $L(f_\omega, x, y)$, which has the form

$$\min_\omega L(f_\omega, x, y) = -\log f_s(f_\omega(x), y) = -\log f_s(z, y) = -\log \frac{\exp \{z_y\}}{\sum_{m=1}^{M} \exp \{z_m\}}$$  \hspace{1cm} (2)

i.e., by adding negativity and log in front of softmax.

Equivalently and in this paper, we convert Eq.2 to an objective function $\text{obj}(f_\omega, x, y)$. As a result, instead of minimising Eq.2 with respect to the parameter $\omega$, we maximise the objective $\text{obj}(f_\omega, x, y)$ with respect to the same parameter, which has the form

$$\max_\omega \text{obj}(f_\omega, x, y) = \log f_s(f_\omega(x), y) = \log f_s(z, y) = \log \frac{\exp \{z_y\}}{\sum_{m=1}^{M} \exp \{z_m\}}$$  \hspace{1cm} (3)

through which we have turned the problem of learning a categorical distribution to an optimisation problem. Specifically, via maximising $\text{obj}$ in Eq.3 or minimising $L$ in Eq.2 with respect to parameter $\omega$, we can refine the learned conditional categorical distribution $\{f_\omega(x), i\}_{i=1}^{M}$ given input datum $x$.

2.2 The Donsker-Varadhan Lower Bound of Mutual Information

2.2.1 Mutual Information

In information theory, mutual information is a fundamental quantity for evaluating the relationship between two random variables, which is a key problem in science and engineering [6]. Without loss of generality, we denote the two random variables as $Z$ and $Y$, where $Z$ is a continuous and $Y$ is a discrete variable. Furthermore, their joint probability distribution is defined as $P_{Z \sim Z,Y \sim Y}(z, y)$, and their marginal probability distributions as $P_{Z \sim Z}(z)$ and
We generalise this neural network $P_{y \sim Y}(y)$ respectively. We abbreviate these three distributions as $P_{Z,Y}(z, y)$, $P_Z(z)$ and $P_Y(y)$. Then the mutual information of $Z$ and $Y$ can be expressed in the form as

$$\mathbb{I}(Z, Y) = \int_{z \in Z} \left( \sum_{y \in Y} P_{Z,Y}(z, y) \log \left( \frac{P_{Z,Y}(z, y)}{P_Z(z)P_Y(y)} \right) dz \right)$$  \hspace{1cm} (4)

We can express the mutual information in Eq. (4) as a KL divergence [8]. Formally,

$$\mathbb{I}(Z, Y) = D_{KL}(P_{Z,Y}(z, y) || P_Z(z)P_Y(y))$$  \hspace{1cm} (5)

Intuitively, the larger the divergence between the joint and marginal probabilities of the random variables $X$ and $Y$, the more dependence existing between $X$ and $Y$. In contrast, if $X$ and $Y$ are fully independent, then the mutual information between them vanishes [9].

Similarly, we have the definition of the conditional mutual information $\mathbb{I}(Z, Y|X)$ and its KL-divergence form, where $X$ is the conditional variable, formally as

$$\mathbb{I}(Z, Y|X) = \sum_{x \in X} \left( \int_{z \in Z} \left( \sum_{y \in Y} P_{Z,Y|X}(z, y|x) \log \left( \frac{P_{Z,Y|X}(z, y|x)}{P_{Z|X}(z|x)P_{Y|X}(y|x)} \right) dz \right) dx \right)$$  \hspace{1cm} (6)

$$= \sum_{x \in X} \left( D_{KL}(P_{Z,Y|X}(z, y|x)||P_{Z|X}(z|x)P_{Y|X}(y|x)) \right)$$

$$= \mathbb{E}_x \left[ D_{KL}(P_{Z,Y|X}(z, y|x)||P_{Z|X}(z|x)P_{Y|X}(y|x)) \right]$$  \hspace{1cm} (7)

where $\mathbb{E}_x$ is the abbreviation of expectation $\mathbb{E}_{z \sim X}$, and $P_{Z,Y|X}(z, y|x)$, $P_{Z|X}(z|x)$ as well as $P_{Y|X}(y|x)$ are the abbreviations of $P_{z \sim Z, y \sim Y|x \sim X}(z, y|x)$, $P_{z \sim Z|x \sim X}(z|x)$ as well as $P_{y \sim Y|x \sim X}(y|x)$.

2.2.2 The Donsker-Varadhan Representation

The KL form of mutual information in Eq. (7) is intractable due to the integration. We utilise a lower bound to the mutual information based on Donsker-Varadhan (DV) representation [10] to make mutual information computable. Formally,

$$\mathbb{I}(Z, Y|X) = \mathbb{E}_x \left[ D_{KL}(P_{Z,Y|X}(z, y|x)||P_{Z|X}(z|x)P_{Y|X}(y|x)) \right]$$

$$\geq \tilde{\mathbb{I}}^D_{\omega}(Z, Y|X)$$

$$:= \mathbb{E}_{z, y} \left[ T_{\omega}(z, y, x) \right] - \log \mathbb{E}_z \mathbb{E}_y \left[ \exp \{ T_{\omega}(z, y, x) \} \right]$$  \hspace{1cm} (8)

where $\omega$ is the parameter of the function $T_{\omega} : Z \times Y \times X \to \mathbb{R}$. In theory, given an optimal neural network to simulate $T_{\omega}$, Eq. (8) can be infinitesimally close to mutual information $\mathbb{I}(Z, Y|X)$.

3 Information Theoretic View

We now provide a coherent information-theoretic view, connecting log-softmax with conditional mutual information of neural network output vectors and labels, conditioned on an input datum.

We first provide notations. As previously have defined in Section 2.1.1 log-softmax corresponding to the input datum $x$ and label $y$ is as

$$\log f_{\omega}(z, y) \mid z = f_{\omega}(x)$$  \hspace{1cm} (9)

where $f_{\omega}(\cdot)$ is a neural network with parameter $\omega$.

We generalise this neural network $f_{\omega}(\cdot)$ from outputting a single result $z$ to producing a conditional Dirac delta distribution $\delta_{\omega}(Z|X = x)$ whose probability density function (PDF) is defined as

$$\delta_{\omega}(z|x) = \begin{cases} +\infty & z = f_{\omega}(x) \\ 0 & z \neq f_{\omega}(x) \end{cases}$$  \hspace{1cm} (10)

That is, instead of regarding $z$ as a direct output of the neural network $f_{\omega}(x)$ input with $x$, we consider it as a sampled result from a conditional distribution, formally written as $z \sim \delta_{\omega}(Z|X = x)$. That is, the output of the neural network $f_{\omega}(x)$ given $x$ becomes a conditional distribution. This more generalised definition does not impose any assumptions.
We now derive the relationship between expectation log-softmax, i.e., Eq. 16, and the DV representation of conditional
expectation.

We are interested in the expectation of log-softmax, i.e., Eq. 11:

\[ E_{z \sim f_x(x)} \log f_{s}(z, y) = \log f_{s}(f_{\omega}(x), y) \]  

(11)

where \( y \) is the label corresponding to the input datum \( x \).

We denote the conditional mutual information between the neural network output \( z \in Z \) and the class labels \( y \in Y \) conditioned on \( x \in X \) as \( \log Z, Y \mid X \), and we define a function \( T_{\omega}() \) such that

\[ T_{\omega}(z, y, x) = z_y \mid z \sim f_{\omega}(x) \]  

(12)

which depicts relationships among the neural network \( f_{\omega}() \), the input datum \( x \), and the label \( y \).

Furthermore, we denote the distribution of \( x \) as \( P(X) \), and the conditional categorical distribution of \( y \) given the input datum \( x \) as \( P(Y \mid X = x) \). Then, based on Eq. (12) we can denote the conditional mutual information between the neural network output \( z \in Z \) and the class labels \( y \in Y \) conditioned on \( x \in X \) as

\[ \tilde{T}_{\omega}^{DV}(Z, Y \mid X) = \]  

(13)

We are interested in the expectation of log-softmax, i.e., Eq. (11) under the distribution of \( x \), which can be written formally as

\[ E_{x \sim P(X)} \left[ E_{z \sim f_x(x), y \sim P(Y \mid X = x)} \left[ T_{\omega}(z, y, x) \right] - \log E_{z \sim f_x(x)} E_{y \sim P(y \mid x = x)} \left[ \exp \{ T_{\omega}(z, y, x) \} \right] \right] \]  

(14)

where both \( z \) and \( y \) correspond to the input datum \( x \) in Eq. (13). That is, they form positive sampling pairs.

For simplicity, we abbreviate Eq. (13) as

\[ E_{x} \left[ E_{z,y} \left[ T_{\omega}(z, y, x) \right] - \log E_{z} E_{y} \left[ \exp \{ T_{\omega}(z, y, x) \} \right] \right] \]  

(15)

and abbreviate Eq. (14) as

\[ E_{x} \left[ E_{z,y} \left[ \log f_{s}(z, y) \right] \right] \]  

(16)

### 3.1 Relationships Between Log-Softmax and Conditional Mutual Information

#### 3.1.1 Derivation

We now derive the relationship between expectation log-softmax, i.e., Eq. (16) and the DV representation of conditional lower bound of mutual information, i.e., Eq. (15). We show that excepting a constant \( \log M \), where \( M \) is the class number, they are of equivalence.

\[ E_{x} \left[ E_{z,y} \left[ \log f_{s}(z, y) \right] \right] = E_{x} E_{z,y} \left[ \log \frac{\exp \{ z_y \}}{\sum_{m=1}^{M} \exp \{ z_m \}} \right] \]

\[ = E_{x} E_{z,y} \left[ \log \frac{1}{M} \sum_{m=1}^{M} \exp \{ z_m \} \right] \]

\[ = E_{x} E_{z,y} \left[ \log \frac{1}{M} \exp \{ z_y \} - \log \frac{1}{M} \sum_{m=1}^{M} \exp \{ z_m \} \right] \]

\[ = E_{x} E_{z,y} \left[ z_y - \log \frac{1}{M} \sum_{m=1}^{M} \exp \{ z_m \} - \log M \right] \]  

(17)

The constant \( M \) is the class number, we further have

\[ E_{x} \left[ E_{z,y} \left[ \log f_{s}(z, y) \right] \right] = E_{x} E_{z,y} \left[ z_y - \log \frac{1}{M} \sum_{m=1}^{M} \exp \{ z_m \} - \log M \right] \]

\[ = E_{x} \left[ E_{z,y} \left[ z_y \right] - E_{z} \left[ \log \frac{1}{M} \sum_{m=1}^{M} \exp \{ z_m \} \right] \right] - \log M \]  

(18)
We employ probabilistic graphical models to help explaining the information flow during training with log-softmax. We abbreviate \( E \) and \( T \) as \( \hat{E} \) and \( \hat{T} \) given. Therefore, the conditional orthogonality between the network output vector \( z \) and the label \( y \) is broken. As a consequence, information can be passed from label \( y \) to network output vector \( z \).

### 3.1.2 Informative Flow of Training with Log-Softmax

In Section 3.1.1, we derive the theoretic relationship between the log-softmax and the DV conditional mutual information lower bound by assuming the distribution \( \delta_x(\mathbf{Z}|\mathbf{X}=x) \) to be a Dirac delta distribution. We in this section relax this assumption to derive a more general relationship between log-softmax and conditional mutual information of stochastic neural networks, i.e., the ones whose outputs can be stochastic.

#### 3.2 Generalisation to Neural Networks with Stochastic Outputs

We employ probabilistic graphical models to help explaining the information flow during training with log-softmax. We consider feed-forward and back-propagation separately. In the feed-forward stage as Figure 1a, the neural network output vector \( z \in \mathbf{Z} \) and the label \( y \in \mathbf{Y} \) are conditionally independent given the input datum \( x \in \mathbf{X} \). We feed information about \( y \in \mathbf{Y} \) to \( z \in \mathbf{Z} \) through back-propagation. During back-propagation as Figure 1b, the objective is given. Therefore, the conditional orthogonality between the network output vector \( z \in \mathbf{Z} \) and the label \( y \in \mathbf{Y} \) is broken. That is, \( z \not\perp y \). As a consequence, information can be passed from label \( y \) to network output vector \( z \).

#### 3.2.1 Lower Bound of Log-Softmax in Stochastic Neural Networks

Unlike in Eq. 22 where we can switch expectation of logarithm \( z \) to be logarithm of expectation \( z \) without losing equality, here we need to apply Jensen’s inequality and derive an inequality. Formally,

\[
\mathbb{E}_z \left[ \log \mathbb{E}_y[\exp\{T_\omega(z, y, x)\}] \right] \geq \log \mathbb{E}_z \left[ \mathbb{E}_y[\exp\{T_\omega(z, y, x)\}] \right] \tag{24}
\]
As a consequence, Eq. 23 now becomes
\[
\mathbb{E}_z \left[ \log \mathbb{E}_y \{ \exp \{ T_\omega (z, y, x) \} \} \right] \geq \mathbb{E}_x \left[ \mathbb{E}_{z,y}(x) \{ T_\omega (z, y, x) \} \right] - \log \mathbb{E}_z \mathbb{E}_y \left[ \exp \{ T_\omega (z, y, x) \} \right] - \log M \\
= \tilde{I}_{DV}^\omega (Z, Y|X) - \log M
\]
(25)

That is, the DV representation subtracting \( \log M \)
\[
\tilde{I}_{DV}^\omega (Z, Y|X) - \log M
\]
acts as a lower bound of logarithm softmax
\[
\mathbb{E}_x \left[ \mathbb{E}_{z,y}[\log f_s(z, y)] \right]
\]

### 3.2.2 Upper Bound of Log-Softmax in Stochastic Neural Networks

In Section 2.1.1, we have showed that softmax \( f_s(z, y) \) will return a value that is in the range of \((0, 1)\). Therefore, its logarithm \( \log f_s(z, y) \) will result in a negative number, so that \( \mathbb{E}_x \mathbb{E}_{z,y}[\log f_s(z, y)] \) will also be of negativity. In contrast, by definition, mutual information \( I(Z, Y|X) \) is non-negative due to its equivalence with KL-divergence. Thus, we have
\[
I(Z, Y|X) \geq \mathbb{E}_x \left[ \mathbb{E}_{z,y}[\log f_s(z, y)] \right]
\]
(26)

That is, conditional mutual information
\[
I(Z, Y|X)
\]
acts as an upper bound of the softmax expectation
\[
\mathbb{E}_x \left[ \mathbb{E}_{z,y}[\log f_s(z, y)] \right]
\]

### 3.2.3 A Sandwich Form of Log-Softmax in Stochastic Neural Networks

Combining Eq. 25 and 26 we have the sandwich form of the log-softmax expectation in stochastic neural networks
\[
I(Z, Y|X) \geq \mathbb{E}_x \left[ \mathbb{E}_{z,y}[\log f_s(z, y)] \right] \geq \tilde{I}_{DV}^\omega (Z, Y|X) - \log M
\]
(27)
When $\hat{I}^{DV}_\omega(Z, Y|X)$ obtains its optimality $\hat{I}^{DV}_\omega(Z, Y|X) = I(Z, Y|X)$, the sandwich form of Eq. 27 becomes
\[
\begin{align*}
I(Z, Y|X) & \geq \\
& \geq E_x E_{z, y} \log \text{softmax}(z, y) = E_x \left[ E_{z, y} [\log f_s(z, y)] \right] \\
& \geq I(Z, Y|X) - \log M
\end{align*}
\]

### 3.2.4 Interpretation of Information-Theoretic View of Log-Softmax in Stochastic Neural Networks

Optimising stochastic neural networks with log-softmax as the objective can diverge from maximising the conditional mutual information between neural network outputs and labels given the input datum. This is because, as the inequality in Eq. 25 indicates, maximising the expectation of log-softmax cannot ensure the enlargement of its lower bound, which is the conditional mutual information, despite they both share the same parameter $\omega$. Thus, training with log-softmax can cause stochastic neural networks to converge at a non-optimum from the informative perspective that the neural network output vector $z \in Z$ obtaining the most information about the label $y \in Y$.

### 4 Application Example: Information Masking (Info-Masking)

Our information-theoretic view of neural networks can be exploited for visualising and understanding convolutional neural networks. Here we present an example of how to employ it to conduct object masking. That is, to only keep objects relating to a particular class and disguise all the other irrelevant objects. Since we leverage our information-theoretic view, we name the approach as information masking (info-masking).

Specifically, our dataset consists of images, each is comprised of one or two MNIST digits [11], appearing either left or right. Our classification network aims to predict whether an image $x \in X$ containing a digit whose label is $y = t \in Y$. We assume we have trained a neural network $f_\omega$ embedding log-softmax that can accurately predict whether an image $x$ contains the target digit ($y = t$) or not ($y \neq t$).

We exploit the following proposition proposed in [12] and [13].

**Proposition 1** The optimal function $T^*_\omega$ in DV representation evaluates the point-wise conditional mutual information and an additional constant.

Due to Proposition 1, we can consider $T_\omega(z, y = t, x)$, i.e., $z_t$, as an approximation of the point-wise conditional mutual information between network output vector $z$ and class $y = t$, i.e., the network output vector containing the target digit.

We then explain the approach of Information-Masking (Info-Masking). Given an input image $x$, we split this image $x$ into small patches, and fetch the approximate point-wise mutual information between the learned feature $z$ and the class $y = t$, i.e., $z_i$ or $[f_\omega(x_i)]_i$, where $x_i$ is the $i$-th small patch of the image $x$. Afterwards, for each small patch $i$, we use a simple thresholding technique to filter out the patches whose mutual information is above 20% of the max value of the conditional mutual information, following [14]. That is, we mask the regions of image $x$ that contain too little information about the target, which also serves the reason for naming this approach as information masking (info-masking).

Figure 2 demonstrates the performance of our info-masking approach, where Figure 2a is the original image and Figure 2b is the processed outcome.

### 5 Related Work

The outputs of a multi-output classification network normally do not satisfy the axioms of probabilities, i.e., probabilities should maintain positivity and sum up to one [15].

### 5.1 Probability Transformation

The softmax non-linearity was originally proposed to bridge stochastic model paradigms and feed-forward non-linear “neural” networks, which also referred softmax non-linearity as normalised exponential [3]. As to stochastic models,
method maximises the class conditional probabilities based on Bayes’ theorem. Formally,
\[
\max P(\text{Class}|\text{Data}) = P(\text{Data}|\text{Class})P(\text{Class})/P(\text{Data})
\] (29)
In contrast to the stochastic model method, a standard “multi-layer perceptron” (MLP) neural network is trained to minimise the squared error minimisation between the predicted and true targets, by updating its weights through back-propagation [16]. Formally,
\[
\min_\theta J[(Y - F(x, \theta))^2]
\] (30)
where \(E\) represents “error”, \(F\) is a network and \(\theta\) is its parameters, \(Y\) stands for the true targets. However, the training method in Eq. 30 is intrinsically with over overfitting. As a consequence, softmax non-linearity was introduced to map neural network outputs \(F(x, \theta)\) to follow the axioms of probabilities. Then, the logarithm of softmax can be further considered as the cross-entropy between a “true” distribution and an estimated distribution.

5.2 Winner-Take-All Mapping
Softmax generalises maximum picking [17]. It stands for a smooth version of the winner-take-all activation, in the sense that outputs change smoothly, and the same inputs will produce equal outputs [3]. Moreover, the exponential can enhance the dominance of the largest value so that after transformation the largest value turns to be +1 while all the other transformed values become zero [18]. Work in [19] also shows an equivalence between the “Winner-Take-All” network and softmax.

6 Anomalies with Differential Entropy
The authors are aware that the conditional mutual information \(I(Z, Y|X)\) is zero when the distribution \(P(Z)\) is a Dirac delta distribution. Therefore, the DV representation acts as a lower bound of a conditional mutual information whose value is 0. This seems to be problematic since even under the optimal DV representation, i.e., the lower bound becomes the highest, \(Z\) seemingly still has no information about \(Y\), and most time this DV representation is negative. Nonetheless, our information-theoretic view is built upon differential entropy, which loses fundamental associations with the discrete entropy. We cannot interpret its values with the interpretations of discrete entropy. Therefore, we do not concern about the negativity of the DV representation and the zero information problem since the concerns mentioning above are based on the intuitions from the discrete information theory.

7 Acknowledgements
This is a preprint work. The authors welcome and thank any criticism and suggestion. Please feel free to contact the authors if you have any concerns.
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