Robust Conditional Probabilities

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Abstract: Conditional probabilities are a core concept in machine learning. For example, optimal prediction of a label $Y$ given an input $X$ corresponds to maximizing the conditional probability of $Y$ given $X$. A common approach to inference tasks is learning a model of conditional probabilities. However, these models are often based on strong assumptions (e.g., log-linear models), and hence their estimate of conditional probabilities is not robust and is highly dependent on the validity of their assumptions.

Here we propose a framework for reasoning about conditional probabilities without assuming anything about the underlying distributions, except knowledge of their second order marginals, which can be estimated from data. We show how this setting leads to guaranteed bounds on conditional probabilities, which can be calculated efficiently in a variety of settings, including structured-prediction. Finally, we apply them to semi-supervised deep learning, obtaining results competitive with variational autoencoders.

1 Introduction

In classification tasks the goal is to predict a label $Y$ for an object $X$. Assuming that the joint distribution of these two variables is $p^*(x, y)$ then optimal prediction\footnote{In the sense of minimizing prediction error.} corresponds to returning the label $y$ that maximizes the conditional probability $p^*(y|x)$. Thus, being able to reason about conditional probabilities is fundamental to machine learning and probabilistic inference.

In the fully supervised setting, one can sidestep the task of estimating conditional probabilities by directly learning a classifier in a discriminative fashion. However, in unsupervised or semi-supervised settings, a reliable estimate of the conditional distributions becomes important. For example, consider an unlabeled input $X$. If we had a reliable estimate of $p^*(y|x)$ we could decide whether to label the example or not, which could be used further within self-training\cite{20, 33} or active learning contexts. Furthermore, as we show in our empirical results, such conditional probability estimates can be used as a regularizer for semi-supervised learning.

There are of course many approaches to “modelling” conditional distributions, from logistic regression to conditional random fields. However, these do not come with any guarantees of approximations to the true underlying conditional distributions of $p^*$ and thus cannot be used to reliably reason about these. This is due to the fact that such models make assumptions about the conditionals (e.g., conditional independence or parametric), which are unlikely to be satisfied in practice.

As an illustrative example for our motivation and setup, consider a set of $n$ binary variables $X_1, ..., X_n$ whose distribution we are interested in. Suppose we have enough data to conclude that $P[X_1 = 1 | X_2 = 1] = 1$. This lets us reason about many other probabilities. For example, we know that $P[X_1 = 1 | X_2 = 1, ..., X_n = x_n] = 1$ for any setting of the $x_3, ..., x_n$ variables. This is a simple but powerful observation, as it translates knowledge about probabilities over small subsets to probability over large subsets. Now, what happens when $P[X_1 = 1 | X_2 = 1] = 0.99$? In other words, what can we say about $P[X_1 = 1 | X_2 = 1, ..., X_n = 0]$ given information about conditional probability $P[X_i = x_i | X_j = x_j]$. As we show here, it is still possible to reason about such conditional probabilities even under this partial knowledge.

Motivated by the above, we propose a novel model-free approach for reasoning about conditional probabilities. Specifically, we shall show how conditional probabilities can be lower bounded without making strong assumptions about the underlying distribution. The only assumption we make is...
that certain low-order marginals of the distribution are known. We then show how these can be used to infer lower bounds on conditional distributions that are guaranteed to hold. One of the surprising outcomes of our analysis is that these lower bounds can be calculated efficiently, and often have an elegant closed form. Finally, we show how these bounds can be used as a regularizer in a semi-supervised setting, obtaining results that are competitive with variational autoencoders \cite{14}.

## Problem Setup

We begin by defining notations to be used in what follows. Let $X$ denote features and $Y$ denote labels. Assume we have $n$ features, denoted by random variables $X_1, \ldots, X_n$. If we have a single label we will denote it by $Y$. Otherwise, a multivariate label will be denoted by $Y_1, \ldots, Y_r$. We assume all variables are discrete (i.e., can take on a finite set of values). Assume that $X, Y$ are generated by some unknown underlying distribution $p^*(X, Y)$. Here we will assume that although we do not know $p^*$ we have access to the expected value of some vector function $f : X, Y \rightarrow \mathbb{R}^d$ under $p^*$,\footnote{Abusing notation, we use $X$ to denote both the random variable and its range of values.} Namely we assume we are given a vector $a$ defined by $a = E_{p^*}[f(X, Y)]$. Since $a$ does not uniquely specify a distribution $p^*$, we will be interested in the set of all distributions where the expected value of $f(X, Y)$ is $a$. Denote this set by $\mathcal{P}(a)$, namely:

\begin{equation}
\mathcal{P}(a) = \{ q \in \Delta : E_q[f(X, Y)] = a \}
\end{equation}

where $\Delta$ is the probability simplex of the appropriate dimension.

We shall specifically be interested in the case where the expected values correspond to simple marginals of the distribution $p^*$, such as those of a single feature and a label:

$$
\mu_i(x_i, y) = \sum_{\bar{x}_1, \ldots, \bar{x}_n : \bar{x}_1 = x_i} p^*(\bar{x}_1, \ldots, \bar{x}_n, y).
$$

Similarly we may have access to the set of pairwise marginals $\mu_{ij}(x_i, x_j, y)$ for all $i, j \in E$, where the set $E$ corresponds to edges of a graph $G$ (see also \cite{7}). When the label is multivariate we may also incorporate marginals of the form $\mu_{lk}(y_l, y_k)$, then $(l, k) \in E$ and we treat labels as part of the graph.

We denote the set of all such marginals by $\mu$. And, as in Eq. (1) we define $\mathcal{P}(\mu)$ to be the set of distributions whose marginals are given by $\mu$. As we shall see later, the structure of the graph $G$ will have implications on the types of bounds we can derive. Specifically, if $G$ is tree shaped (i.e., has no cycles), tight bounds can be derived.

### 2.1 The Robust Conditionals Problem

Our approach is to reason about conditional distributions using only the fact that $p^* \in \mathcal{P}(\mu)$. Our key goal is to lower bound these conditionals, since this will allow us to conclude that certain labels are highly likely in cases where the lower bound is large. We shall also be interested in upper and lower bounding joint probabilities, since these will play a key role in bounding the conditionals.

Our goal is thus to solve the following optimization problems.

\begin{equation}
\min_{p \in \mathcal{P}(\mu)} p(x, y), \max_{p \in \mathcal{P}(\mu)} p(x, y), \min_{p \in \mathcal{P}(\mu)} p(y | x).
\end{equation}

In all three problems, the constraint set is linear in $p$. However, note that $p$ is specified by an exponential number of variables (one per assignment $x_1, \ldots, x_n$) and thus it is not feasible to plug these constraints into an LP solver. In terms of objective, the min and max problems are linear, and the conditional is fractional linear. In what follows we show how all three problems can be solved efficiently for tree shaped graphs.

\footnote{For simplicity we assume the expectation is exact. Generally it is of course only approximate, but concentration bounds can be used to quantify this accuracy as a function of data size. Furthermore, most of the methods described here can be extended to inexact marginals (e.g., see \cite{6} for an approach that can be applied here).}
3 Related Work

The problem of reasoning about a distribution based on its expected values has a long history, with many beautiful mathematical results. An early example is the classical Chebyshev inequality, which bounds the tail of a distribution given its first and second moments. This was significantly extended in the Chebyshev Markov Stieltjes inequality [2]. More recently, various generalized Chebyshev inequalities have been developed [3, 24, 29]. A typical statement of these is that several moments are given, and one seeks the minimum measure of some set $S$ under any distribution that agrees with the moments. As [3] notes, most of these problems are NP hard, with isolated cases of tractability. Such inequalities have been used to obtain minimax optimal linear classifiers in [17]. The moment problems we consider here are very different from those considered previously, in terms of the finite support we require, our focus on bounding probabilities and conditional probabilities of assignments.

The above approaches consider worst case bounds on probabilities of certain events for distributions in $P(a)$. A different approach is to pick a particular distribution in $P$ and use it as an approximation (or model) of $p^*$. The most common choice for such a distribution is the maximum entropy distribution in $P(a)$. Such log-linear models have found widespread use in statistics and machine learning. In particular, most graphical models can be viewed as maximum entropy distributions (e.g., see [15, 16]). However, the probabilities given by the maximum entropy model cannot be related to the true probabilities in any sense (e.g., upper or lower bound). This is where our approach markedly differs from entropy based assumptions. Another approach to reducing modeling assumptions is robust optimization, where data and certain model parameters are assumed not to be known precisely, and optimality is sought in a worst case adversarial setting. Such an approach has been applied to machine learning in various settings (e.g., see [34, 19]), establishing close links to regularization. None of these approaches considers bounding probabilities as is our focus here.

Finally, another elegant moment approach is that based on kernel mean embedding [25, 26]. In this approach, one maps a distribution into a set of expected values of a set of functions (possibly infinite). The key observation is that this mean embedding lies in an RKHS, and hence many operations, such as computing distribution similarity and covariances can be done implicitly. Most of the applications of this idea assume that the set of functions is rich enough to fully specify the distribution (i.e., characteristic kernels [27]). The focus is thus different from ours, where moments are not assumed to be fully informative, and the set $P(a)$ contains many possible distributions. It would however be interesting to study possible uses of RKHS in our setting.

4 Calculating Robust Conditional Probabilities

The optimization problems in Eq. (2) are linear programs (LP) and fractional LPs, where the number of variables scales exponentially with $n$. Yet, as we show in this section and Section 5, it turns out that in many non-trivial cases, they can be efficiently solved. Our focus below is on the case where the pairwise marginals correspond to a set $E$ that forms a tree structured graph. The tree structure assumption is common in literature on Graphical Models, only here we do not make an inductive assumption on the generating distribution (i.e., we make none of the conditional independence assumptions that are implied by tree-structured graphical models). In the following sections we study solutions of robust conditional probabilities under the tree assumption. We will also discuss some extensions to the cyclic case. Finally, note that although the derivations here are for pairwise marginals, these can be extended to the non-pairwise case by considering clique-trees [e.g., see 31]. Pairs are used here to allow a clearer presentation.

In what follows, we first show that the conditional lower bound has a simple structure as stated in Theorem 4.1. This result does not immediately suggest an efficient algorithm since its denominator includes an exponentially sized LP. Next, in Section 4.2 we show how this LP can be reduced to a polynomially sized one, resulting in an efficient algorithm for the lower bound. Finally, in Section 5 we show that in certain cases there is no need to use a general purpose LP solver and the problem can be solved either in closed form or via combinatorial algorithms. Detailed proofs are provided in the appendix.
4.1 From Conditional Probabilities To Maximum Probabilities with Exclusion

The main result of this section will reduce calculation of the robust conditional probability for \( p(y \mid x) \), to one of maximizing the probability of all labels other than \( y \). This reduction by itself will not allow for efficient calculation of the desired conditional probabilities, as the new problem is also a large LP that needs to be solved. Still the result will take us one step further towards a solution, as it reveals the probability mass a minimizing distribution \( p \) will assign to \( x, y \).

This part of the solution is related to a result from [10], where the authors derive the solution of \( \min_{p \in \mathcal{P}(\mu)} p(x, y) \). They prove that under the tree assumption this problem has a simple closed form solution, given by the functional \( I(x, y ; \mu) \):

\[
I(x, y ; \mu) = \left[ \sum_i (1 - d_i) \mu_i(x, y) + \sum_{ij \in E} \mu_{ij}(x, x_j, y) \right]^+ .
\] (3)

Here \([.]_+ \) denotes the ReLU function \([z]_+ = \max\{z, 0\}\) and \( d_i \) is the degree of node \( i \) in \( G \). The above expression is suitable in case of a single label, it extends naturally to the multivariate case when we consider labels as part of the graph.

It turns out that robust conditional probabilities will assign the event \( x, y \) its minimal possible probability as given in Eq. (3). Moreover, it will assign all other labels their maximum possible probability. This is indeed a behaviour that may be expected from a robust bound, we formalize it in the main result for this part:

**Theorem 4.1.** Let \( \mu \) be a vector of tree-structured pairwise marginals, then

\[
\min_{p \in \mathcal{P}(\mu)} p(y \mid x) = \frac{I(x, y ; \mu)}{I(x, y ; \mu) + \max_{\mu \in \mathcal{P}(\mu)} \sum_{y \neq y} p(x, y)} .
\] (4)

The proof of this theorem is rather technical and we leave it for the appendix.

We note that the above result also applies to the “structured-prediction” setting where \( y \) is multivariate and we also assume knowledge of marginals \( \mu(y_i, y_j) \). In this case, the expression for \( I(x, y ; \mu) \) will also include edges between \( y_i \) variables, and incorporate their degrees in the graph.

The important implication of Theorem 4.1 is that it reduces the minimum conditional problem to that of probability maximization with an assignment exclusion. Namely:

\[
\max_{p \in \mathcal{P}(\mu)} \sum_{y \neq y} p(x, y) .
\] (5)

Although this is still a problem with an exponential number of variables, we show in the next section that it can be solved efficiently.

4.2 Minimizing and Maximizing Probabilities

To provide an efficient solution for Eq. (5), we turn to a class of joint probability bounding problems. Assume we constrain each variable \( X_i \) and \( Y_j \) to a subset \( \bar{X}_i, \bar{Y}_j \) of its domain and would like to reason about the probability of this constrained set of joint assignments:

\[
U = \{ x, y \mid x_i \in \bar{X}_i, y_j \in \bar{Y}_j \ \forall i \in [n], j \in [r] \} .
\] (6)

Under this setting, an efficient algorithm for

\[
\max_{p \in \mathcal{P}(\mu)} \sum_{u \in U \setminus \{x, y\}} p(u),
\]

provides one to Eq. (5) and by the results of last section, also for robust conditional probabilities. To see this is indeed the case, assume we are given an assignment \( (x, y) \). Then setting \( \bar{X}_i = \{ x_i \} \) for all features and \( \bar{Y}_j = \{ 1, \ldots, |Y_j| \} \) for labels (i.e. \( U \) does not restrict labels), gives exactly Eq. (5).

To derive the algorithm, we will find a compact representation of the LP, with a polynomial number of variables and constraints. The result is obtained by using tools from the literature on Graphical Models.
It shows how to formulate probability maximization problems over $U$ as problems constrained by the local marginal polytope [31]. Its definition in our setting slightly deviates from its standard definition, as it does not require that probabilities sum up to 1:

**Definition 1.** The set of locally consistent pseudo marginals over $U$ is defined as:

$$\mathcal{M}_L(U) = \{ \tilde{\mu} | \sum_{x_i \in \bar{X}_i} \tilde{\mu}_{ij}(x_i, x_j) = \mu_{ij}(x_j) \quad \forall (i, j) \in E, x_j \in \bar{X}_j \}.$$ 

The partition function of $\tilde{\mu}$, $Z(\tilde{\mu})$, is given by $\sum_{x_i \in \bar{X}_i} \tilde{\mu}_i(x_i)$.

Our observation then is that Eq. (5) can be folded into a problem with polynomially many variables and constraints, by simply maximizing the partition function over $\mathcal{M}_L(U)$.

**Theorem 4.2.** Let $U$ be a universe of assignments as defined in Eq. (6), $x \in U$ and $\mu$ a vector of tree-structured pairwise marginals, then the values of the following problems:

$$\max_{\mu \in \mathcal{M}_L(U)} \sum_{u \in U} p(u), \quad \max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U \setminus \{x,y\}} p(u),$$

are equal (respectively to):

$$\max_{\tilde{\mu} \in \mathcal{M}_L(U)} Z(\tilde{\mu}), \quad \max_{\tilde{\mu} \in \mathcal{M}_L(U)} \sum_{l(x,y) \in \mathcal{P}(\mu)} Z(\tilde{\mu}).$$

The LPs in Eq. (7) involve a polynomial number of constraints and variables and can thus be solved efficiently.

Proofs of this result can be obtained either by exploiting strong duality of LPs and the max-reparameterization property of functions that decompose over trees [32, 5], or by using the junction-tree theorem [31]. In the appendix we provide a proof based on the latter.

To conclude this section, we restate the main result: the robust conditional probability problem Eq. (2) can be solved in polynomial time by combining Theorems 4.1 and 4.2. As a by-product of this derivation we also presented efficient tools for bounding answers on a large class of probabilistic queries. While this is not the focus of the current paper, these tools may be useful in probabilistic modelling, where we often combine estimates of low order marginals with assumptions on the data generating process. Bounds like the ones presented in this section give a quantitative estimate of the uncertainty that is induced by data and circumvented by our assumptions.

## 5 Closed Form Solutions and Combinatorial Algorithms

The results of the previous section imply that the minimum conditional can be found by solving a poly-sized LP. Although this results in polynomial runtime, it is interesting to improve as much as possible on the complexity of this calculation. One reason is that application of the bounds might require solving them repeatedly within some larger learning problem. For instance, in classification tasks it may be necessary to solve Eq. (4) for each sample in the dataset. An even more demanding procedure will come up in our experimental evaluation, where we learn features that result in high confidence under our bounds. There, we need to solve Eq. (4) over mini-batches of training data only to calculate a gradient at each training iteration. Since using an LP solver in these scenarios is impractical, we next derive more efficient solutions to some special cases of Eq. (4).

### 5.1 Closed Form for Multiclass Problems

The multiclass setting is a special case of Eq. (4) when $y$ is a single label variable (e.g., a digit label in mnist with values $y \in \{0, \ldots, 9\}$). In this case the problem in Eq. (2) is: $\min_{p \in \mathcal{P}(\mu)} p(y \mid x)$. The solution of course depends on the type of marginals provided in $\mathcal{P}(\mu)$. Here we will assume that we have access to joint marginals of the label $y$ and pairs of features $x_i, x_j$ corresponding to edges $ij \in E$ of a graph $G$. We note that we can obtain similar results for the cases where some additional “unlabeled” statistics $\bar{\mu}_{ij}(x_i, x_j)$ are known.

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4We omit the labels $Y_1, \ldots, Y_r$ from this definition for notational convenience. Formally, the consistency constraints are also enforced for edges with nodes that correspond to labels.
It turns out that in both cases Eq. (5) has a simple solution. Here we write it for the case without unlabeled statistics.

**Lemma 5.1.** Let $x \in \mathcal{X}$ and $\mu$ a vector of tree-structured pairwise marginals, then

$$\min_{p \in \mathcal{P}(\mu)} p(y \mid x) = \frac{I(x, y; \mu)}{I(x, y; \mu) + \sum_{y \neq y^*} \min_{ij} \mu_{ij}(x_i, x_j, y^*)}. \quad (8)$$

This lemma is based on a result that states $\max_{p \in \mathcal{P}(\mu)} p(x, y) = \min_{ij} \mu_{ij}(x_i, x_j, y^*)$, it can either be proved by analyzing results in Thm. 4.2, or with a duality based argument which is how we prove it in the appendix.

### 5.2 Combinatorial Algorithms and Connection to Maximum Flow Problems

In some cases, fast algorithms for the optimization problem in Eq. (5) can be derived by exploiting a tight connection of our problems to the Max-Flow problem. The problems are also closely related to the weighted Set Cover problem. To observe the connection to the latter, consider an instance of Set-Cover defined as follows. The universe is all assignments $x$. Sets are defined for each $i, j, x_i, x_j$ and are denoted by $S_{ij, x_i, x_j}$. The set $S_{ij, x_i, x_j}$ contains all assignments $\bar{x}$ whose values at $i, j$ are $x_i, x_j$. Moreover, the set $S_{ij, x_i, x_j}$ has weight $w(S_{ij, x_i, x_j}) = \mu_{ij}(x_i, x_j)$. Note that the number of items in sets is exponential, but there is a polynomial amount of sets. Now assume we would like to use these sets to cover some set of assignments $U$ with the minimum possible weight. It turns out that under the tree structure assumption, this problem is closely related to the problem of maximizing probabilities.

**Lemma 5.2.** Let $U$ be a set of assignments and $\mu$ a vector of tree-structured marginals. Then:

$$\max_{p \in \mathcal{P}(\mu)} \sum_{u \in U} p(u), \quad (9)$$

has the same value as the standard LP relaxation [30] of the Set-Cover problem above.

The connection to Set-Cover may not give a path to efficient algorithms, but it does illuminate some of the results presented earlier. It is simple to verify that $\min_{ij} \mu_{ij}(x_i, x_j, y)$ is a weight of a cover of $x, y$, while Eq. (3) equals one minus the weight of a set that covers all assignments but $x, y$. A connection that we may exploit to obtain more efficient algorithms is to Max-Flow. When the graph defined by $E$ is a chain, we show in the appendix that the value of Eq. (9) can be found by solving a flow problem on a simple network. We note that using the same construction, Eq. (5) turns out to be Max Flow under a budget constraint [1]. This may prove very beneficial for our goals, as it allows for efficient calculation of the robust conditionals we are interested in. Our conjecture is that this connection goes beyond chain graphs, but leave this for exploration in future work. The proofs for results in this section may also be found in the appendix.

### 6 Experiments

To evaluate the utility of our bounds, we consider their use in settings of semi-supervised deep learning and structured prediction. For the bounds to be useful, the marginal distributions need to be sufficiently informative. In some datasets, the raw features already provide such information, as we show in Section 6.3. In other cases, such as images, a single raw feature (i.e., a pixel) does not provide sufficient information about the label. These cases are addressed in Section 6.1 where we show how to learn new features which do result in meaningful bounds. Using deep networks to learn these features turns out to be an effective method for semi-supervised settings, reaching results close to those demonstrated by Variational Autoencoders [14]. It would be interesting to use such feature learning methods for structured prediction too; however this requires incorporation of the max-flow algorithm into the optimization loop, and we defer this to future work.

#### 6.1 Deep Semi-Supervised Learning

Here we describe how our bounds can be used for semi-supervised learning. We learn a neural network whose last layer serve as the features $\mathcal{Z}_i$. The marginals of these with the label $Y$ are used in
We trained the models described above on the MNIST dataset, using 100 labeled samples (see [14] for a similar setup). We set the two regularization parameters required for the entropy regularizer and the one required for our minimum probability regularizer with five fold cross validation. We used 10% of the training data as a validation set and compared error rates on the 10000 samples of the test set. Results are shown in Figure 1. They show that on the 1000 sample case we are slightly outperformed by VAE and for 100 samples we lose by 1%. Ladder networks outperform the other baselines.

We compare our results with those obtained by Variational Autoencoders and Ladder Networks. Although we do not expect to get the same high accuracies these methods obtain, getting comparable numbers with a simple regularizer (compared to the elaborate techniques used in these works) like the one we suggest, is an encouraging sign for the possibility of learning features that induce high confidence. We also compare to an architecture similar to ours, but that uses minimum entropy regularization [12] on a softmax layer connected to z (i.e., it does not use our bounds at all). In this case we also add \( \ell_2 \) regularization on the weights of the soft-max layer, since otherwise entropy can always be driven to zero in the separable case. Finally, we also experimented with adding a hinge loss as a regularizer (as in Transductive SVM [13]), but omit it from the comparison because it did not yield significant improvement over a purely supervised MLP and entropy regularization.

6.2 MNIST Dataset

We trained the models described above on the MNIST dataset, using 100 and 1000 labeled samples (see [14] for a similar setup). We set the two regularization parameters required for the entropy regularizer and the one required for our minimum probability regularizer with five fold cross validation. We used 10% of the training data as a validation set and compared error rates on the 10000 samples of the test set. Results are shown in Figure 1. They show that on the 1000 sample case we are slightly outperformed by VAE and for 100 samples we lose by 1%. Ladder networks outperform the other baselines.

| N   | Ladder [23] | VAE [14] | Robust Probs | Entropy | MLP+Noise |
|-----|-------------|----------|--------------|---------|-----------|
| 100 | 1.06(±0.37) | 3.33(±0.14) | 4.44(±0.22) | 18.93(±0.54) | 21.74(±1.77) |
| 1000| 0.84(±0.08) | 2.40(±0.02) | 2.48(±0.03) | 3.15(±0.03)  | 5.70(±0.20) |

Figure 1: Error rates of several semi-supervised learning methods on the MNIST dataset with few training samples.

Accuracy vs. Coverage Curves: In self-training and co-training methods, a classifier adds its most confident predictions to the training set and then repeats training. A crucial factor in the success
of such methods is the error in the predictions we add to the training pool. Classifiers that use confidence over unlabelled data as a regularizer are natural choices for base classifiers in such a setting. Therefore an interesting comparison to make is the accuracy we would get over the unlabelled data, had the classifier needed to choose its $k$ most confident predictions.

We plot this curve as a function of $k$ for the entropy regularizer and our min-probabilities regularizer. Samples in the unlabelled training data are sorted in descending order according to confidence. Confidence for a sample in entropy regularized MLP is calculated based on the value of the logit that the predicted label received in the output layer. For the robust probabilities classifier, the confidence of a sample is the minimum conditional probability the predicted label received. As can be observed in Figure 6.2, our classifier ranks its predictions better than the entropy based method. We attribute this to our classifier being trained to give robust bounds under minimal assumptions.

![Figure 2: Accuracy for $k$ most confident samples in unlabelled data. Blue curve shows results for the Robust Probabilities Classifier, green for the Entropy Regularizer. Confidence is measured by conditional probabilities and logits accordingly.](image)

### 6.3 Multilabel Structured Prediction

As mentioned earlier, in the structured prediction setting it is more difficult to learn features that yield high certainty. We therefore provide a demonstration of our method on a dataset where the raw features are relatively informative. The Genbase dataset taken from [28], is a protein classification multilabel dataset. It has 662 instances, divided into a training set of 463 samples and a test set of 199, each sample has 1185 binary features and 27 binary labels. We ran a structured-SVM algorithm, taken from [21] to obtain a classifier that outputs a labelling $\hat{y}$ for each $x$ in the dataset (the error of the resulting classifier was 2%). We then used our probabilistic bounds to rank the classifier’s predictions by their robust conditional probabilities. The bounds were calculated based on the set of marginals $\mu_{ij}(x_i, y_j)$, estimated from the data for each pair of a feature and a label $X_i, Y_j$. This set of marginals corresponds to a non-tree structure and we handled it as discussed in Section 7. Observing the values of our bounds, it turned out that 85% of these were above 0.99, indicating a high level of certainty that this is the correct label. Indeed only 0.59% of these 85% were actually errors. The remaining errors made by the classifier were assigned min conditional probability zero by our bounds, indicating low level of certainty.

### 7 Discussion

We presented a method for bounding conditional probabilities of a distribution based only on knowledge of its low order marginals. Our results can be viewed as a new type of moment problem, bounding a key component of machine learning systems, namely the conditional distribution. As we show, calculating these bounds raises many challenging optimization questions, which surprisingly result in closed form expressions in some cases.

While the results were limited to the tree structured case, some of the methods have natural extensions to the cyclic case that still result in robust estimations. For instance, the local marginal polytope in Eq. (7) can be taken over a cyclic structure and still give a lower bound on maximum probabilities. Also in the presence of the cycles, it possible to find the spanning tree that induces the best bound on
Eq. (3) using a maximum spanning tree algorithm. Plugging these solutions into Eq. (4) results in a tighter approximation which we used in our experiments.

Our method can be extended in many interesting directions. Here we addressed the case of discrete random variables, although we also showed in our experiments how these can be dealt with in the context of continuous features. It will be interesting to calculate bounds on conditional probabilities given expected values of continuous random variables. In this case, sums-of-squares characterizations play a key role [18, 22], and their extension to the conditional case is an exciting challenge. It will also be interesting to study how these bounds can be used in the context of unsupervised learning. One natural approach here would be to learn constraint functions such that the lower bound is maximized.

Finally, we plan to study the implications of our approach to diverse learning settings, from self-training to active learning and safe reinforcement learning.
References

[1] R. K. Ahuja and J. B. Orlin. A capacity scaling algorithm for the constrained maximum flow problem. *Networks*, 25(2):89–98, 1995.

[2] N. I. Akhiezer. *The classical moment problem: and some related questions in analysis*, volume 5. Oliver & Boyd, 1965.

[3] D. Bertsimas and I. Popescu. Optimal inequalities in probability theory: A convex optimization approach. *SIAM Journal on Optimization*, 15(3):780–804, 2005.

[4] A. Charnes and W. W. Cooper. Programming with linear fractional functionals. *Naval Research Logistics Quarterly*, 9(3-4):181–186, 1962.

[5] R. G. Cowell, P. Dawid, S. L. Lauritzen, and D. J. Spiegelhalter. *Probabilistic networks and expert systems: Exact computational methods for Bayesian networks*. Springer Science & Business Media, 2006.

[6] M. Dudík, S. J. Phillips, and R. E. Schapire. Maximum entropy density estimation with generalized regularization and an application to species distribution modeling. *Journal of Machine Learning Research*, 8(Jun):1217–1260, 2007.

[7] E. Eban, E. Mezuman, and A. Globerson. Discrete Chebyshev classifiers. In *Proceedings of the 31st International Conference on Machine Learning (ICML)*. JMLR Workshop and Conference Proceedings Volume 32, pages 1233–1241, 2014.

[8] E. Eban, E. Mezuman, and A. Globerson. Discrete chebyshev classifiers. In *Proceedings of the 31th International Conference on Machine Learning, ICML 2014, Beijing, China, 21-26 June 2014*, pages 1233–1241, 2014.

[9] L. R. Ford Jr and D. R. Fulkerson. *Flows in networks*. Princeton university press, 2015.

[10] M. Fromer and A. Globerson. An LP view of the M-best MAP problem. In *NIPS*, volume 22, pages 567–575, 2009.

[11] A. Globerson and T. S. Jaakkola. Fixing max-product: Convergent message passing algorithms for map lp-relaxations. In *Advances in neural information processing systems*, pages 553–560, 2008.

[12] Y. Grandvalet and Y. Bengio. Semi-supervised learning by entropy minimization. In *Advances in neural information processing systems*, pages 529–536, 2005.

[13] T. Joachims. Transductive inference for text classification using support vector machines. In *Proceedings of the Sixteenth International Conference on Machine Learning (ICML 1999), Bled, Slovenia, June 27 - 30, 1999*, pages 200–209, 1999.

[14] D. P. Kingma, S. Mohamed, D. J. Rezende, and M. Welling. Semi-supervised learning with deep generative models. In *Advances in Neural Information Processing Systems 27: Annual Conference on Neural Information Processing Systems 2014, December 8-13 2014, Montreal, Quebec, Canada*, pages 3581–3589, 2014.

[15] D. Koller and N. Friedman. *Probabilistic graphical models: principles and techniques*. MIT press, 2009.

[16] J. Lafferty, A. McCallum, and F. Pereira. Conditional random fields: Probabilistic models for segmenting and labeling sequence data. In *Proceedings of the 18th International Conference on Machine Learning*, pages 282–289. Morgan Kaufmann, San Francisco, CA, 2001.

[17] G. R. Lanckriet, L. E. Ghaoui, C. Bhattacharyya, and M. I. Jordan. A robust minimax approach to classification. *Journal of Machine Learning Research*, 3(Dec):555–582, 2002.

[18] J. B. Lasserre. Global optimization with polynomials and the problem of moments. *SIAM Journal on Optimization*, 11(3):796–817, 2001.
[19] R. Livni, K. Crammer, and A. Globerson. A simple geometric interpretation of SVM using stochastic adversaries. In Proceedings of the 15th International Conference on Artificial Intelligence and Statistics (AI-STATS), pages 722–730. JMLR: W&CP, 2012.

[20] D. McClosky, E. Charniak, and M. Johnson. Effective self-training for parsing. In Proceedings of the main conference on human language technology conference of the North American Chapter of the Association of Computational Linguistics, pages 152–159. Association for Computational Linguistics, 2006.

[21] A. C. Muller and S. Behnke. pystruct - learning structured prediction in python. Journal of Machine Learning Research, 15:2055–2060, 2014.

[22] P. A. Parrilo. Semidefinite programming relaxations for semialgebraic problems. Mathematical programming, 96(2):293–320, 2003.

[23] A. Rasmus, M. Berglund, M. Honkala, H. Valpola, and T. Raiko. Semi-supervised learning with ladder networks. In Advances in Neural Information Processing Systems 28: Annual Conference on Neural Information Processing Systems 2015, December 7-12, 2015, Montreal, Quebec, Canada, pages 3546–3554, 2015.

[24] J. E. Smith. Generalized chebychev inequalities: theory and applications in decision analysis. Operations Research, 43(5):807–825, 1995.

[25] A. Smola, A. Gretton, L. Song, and B. Schölkopf. A hilbert space embedding for distributions. In International Conference on Algorithmic Learning Theory, pages 13–31. Springer, 2007.

[26] L. Song, K. Fukumizu, and A. Gretton. Kernel embeddings of conditional distributions: A unified kernel framework for nonparametric inference in graphical models. IEEE Signal Processing Magazine, 30(4):98–111, 2013.

[27] B. K. Sriperumbudur, K. Fukumizu, and G. R. G. Lanckriet. Universality, characteristic kernels and rkhs embedding of measures. J. Mach. Learn. Res., 12:2389–2410, July 2011. ISSN 1532-4435.

[28] G. Tsoumakas, E. Spyromitros-Xioufis, J. Vilcek, and I. Vlahavas. Mulan: A java library for multi-label learning. Journal of Machine Learning Research, 12:2411–2414, 2011.

[29] L. Vandenberghe, S. Boyd, and K. Comanor. Generalized chebyshev bounds via semidefinite programming. SIAM review, 49(1):52–64, 2007.

[30] V. V. Vazirani. Approximation algorithms. Springer Science & Business Media, 2013.

[31] M. J. Wainwright and M. I. Jordan. Graphical models, exponential families, and variational inference. Foundations and Trends in Machine Learning, 1(1-2):1–305, 2008.

[32] M. J. Wainwright, T. S. Jaakkola, and A. S. Willsky. Tree consistency and bounds on the performance of the max-product algorithm and its generalizations. Statistics and Computing, 14(2):143–166, 2004.

[33] D. Weiss, C. Alberti, M. Collins, and S. Petrov. Structured training for neural network transition-based parsing. In Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), pages 323–333, Beijing, China, July 2015. Association for Computational Linguistics.

[34] H. Xu, C. Caramanis, and S. Mannor. Robustness and regularization of support vector machines. J. Mach. Learn. Res., 10:1485–1510, December 2009. ISSN 1532-4435.
Proofs

This appendix provides detailed proofs of theoretical results in the paper.

We first recall a property of functions that decompose over a tree structure. Assume we have a directed tree $G$ with $n$ nodes. Denote by $r$ its root, and by $pa(i)$ the parent of node $i$. Note that any undirected tree can be turned into a directed one by directing it away from an arbitrarily selected root.

Now consider a function $\lambda(x_1, \ldots, x_n)$ over $n$ discrete variables. We will abbreviate $x_1, \ldots, x_n$ by $x$ wherever clear from context. Assume that $\lambda(x)$ is defined as follows:

$$\lambda(x) = \lambda_r(x_r) + \sum_{i \neq r} \lambda_{i,pa(i)}(x_i, x_{pa(i)}) + \lambda_i(x_i).$$

where $\lambda_r, \lambda_i$ and $\lambda_{i,j}$ are given singleton and pairwise functions. Then $\lambda(x)$ can be reparameterised using min “marginals”, as defined below (See [5, 31] for proof of this result for max marginals and generalizations that include min operators):

$$\lambda(x) = \bar{\lambda}_r(x_r) + \sum_{i \neq r} \bar{\lambda}_{i,pa(i)}(x_i, x_{pa(i)}) - \bar{\lambda}_{pa(i)}(x_{pa(i)})$$

$$\bar{\lambda}_i(x_i) = \min_{z: z_i = x_i} \lambda(z), \quad \bar{\lambda}_{ij}(x_i, x_j) = \min_{z: z_i, z_j = x_i, x_j} \lambda(z)$$

Such $\lambda$ functions will arise, whenever we take the dual of a problem whose variables are a probability distribution constrained to satisfy some marginal distributions. Specifically, the multipliers $\bar{\lambda}_i(x_i), \bar{\lambda}_{ij}(x_i, x_j)$ will be those that correspond respectively to the primal constraints:

$$\sum_{z: z_i = x_i} p(z) = \mu_i(x_i), \quad \sum_{z: z_i, z_j = x_i, x_j} p(z) = \mu_{ij}(x_i, x_j).$$

A Proof of Lem. 5.1

Let us begin with the proof of Lem. 5.1, in which we derive the form of solutions used in our experiments.

Proof. We start by writing the problem down in the following manner:

$$\min_{p \in P(\mu)} \frac{p(x, y)}{p(x, y) + \sum_{\tilde{y} \neq y} p(x, \tilde{y})}.$$

It is obvious that in order to minimize the objective, the higher $p(x, \tilde{y})$ is for $\tilde{y} \neq y$ and the lower $p(x, y)$, the lower objective we get. We now notice that each of the assignments can be maximized or minimized independently, because they appear in totally distinct constraints in $P(\mu)$. This is true because all constraints in $P(\mu)$ are of the form:

$$\sum_{z: z_i = x_i, x_j} p(z, \tilde{y}) = \mu_{ij}(x_i, x_j, \tilde{y}).$$

Hence, for any pair $y_1 \neq y_2$, non of the variables in $\{p(x_1, y_1) \mid x_1 \in \mathcal{X}\}$ appear in the same constraint with a variable in $\{p(x_2, y_2) \mid x_2 \in \mathcal{X}\}$, so all variables $p(x, \tilde{y}), p(x, y)$ can be maximized or minimized separately. We already know from [10] that

$$\min_{p \in P(\mu)} p(x, y) = I(x, y; \mu).$$

It is left to show that

$$\max_{p \in P(\mu)} p(x, \tilde{y}) = \min_{ij} \mu_{ij}(x_i, x_j, \tilde{y}),$$

then the result of the lemma follows immediately. To prove the above equality we take the dual LP of the left hand side:

$$\min \lambda \cdot \mu$$

s.t. $\lambda(x, y) \geq 1$

$$\lambda(z, \tilde{y}) \geq 0 \quad \forall z \neq x \lor \tilde{y} \neq y.$$
Here $\lambda(\cdot)$ are the dual variables, which we can think of as a function that decomposes over a directed tree:

$$\lambda(x, y) = \lambda_r(x_r, y) + \sum_{i \notin r} \lambda_{i,pa(i)}(x_i, x_{pa(i)}, y) + \lambda_i(x_i, y).$$

The inner product $\lambda \cdot \mu$ is given by:

$$\sum_{i, \lambda_i} \lambda_i(z_i) \mu_i(z_i) + \sum_{ij \in E, \lambda_{ij}} \lambda_{ij}(z_i, z_j) \mu_{ij}(z_i, z_j). \quad (13)$$

Let us take the min-reparameterization of this function and then take its expectation over a distribution $p \in \mathcal{P}(\mu)$. The following inequality holds for any feasible $\lambda$:

$$\mathbb{E}_p [\lambda(x, y)] = \sum_{z_r} \mu_r(z_r) \tilde{\lambda}_r(z_r, y) + \sum_{i \notin r, \lambda_i} \mu_i,pa(i)(z_i, \bar{z}_{pa(i)}) (\tilde{\lambda}(z_i, \bar{z}_{pa(i)}, y) - \tilde{\lambda}_{pa(i)}(\bar{z}_{pa(i)}, y))$$

$$\geq \mu_r(x_r) \tilde{\lambda}_r(x_r, y) + \sum_{i \notin r} \mu_{i,pa(i)}(x_i, x_{pa(i)})(\tilde{\lambda}(x_i, x_{pa(i)}, y) - \tilde{\lambda}_{pa(i)}(x_{pa(i)}, y)).$$

The inequality is true because any feasible $\lambda$ is non-negative, hence $\tilde{\lambda}_r(z_r) \geq 0$ and because min-marginals over a pair of variables are always larger than those over one of them. We will conclude the proof by observing that:

- The right hand side of the inequality is a combination of the $\mu$s that are consistent with $x, y$ and the coefficients of this combination sum up to:

$$\tilde{\lambda}_r(x_r, y) + \sum_{i \notin r} \tilde{\lambda}(x_i, x_{pa(i)}, y) - \tilde{\lambda}_{pa(i)}(x_{pa(i)}, y) = \lambda(x, y) \geq 1.$$

The equality holds due to the reparameterization property in Eq. (11) and $\lambda$’s feasibility. Since the sum is higher than 1, the right hand side is also larger than any convex combination of the $\mu$s, which in turn is larger than the smallest element in the combination. We arrive at the conclusion that:

$$\mathbb{E}_p [\lambda(x, y)] \geq \min_{ij} \mu_{ij}(x_i, x_j, y).$$

- It also holds that $\lambda \cdot \mu = \mathbb{E}_p [\lambda(x)]$, hence the objective of any feasible solution is larger than $\min_{ij} \mu_{ij}(x_i, x_j, y)$. On the other hand, setting $\lambda_{ij}(x_i, x_j, y) = 1$ for a minimizing pair $i, j$ and all other variables to 0 results in a feasible solution with exactly this objective. It follows that this must be the optimal value of the problem.

\[ \square \]

**B Notations for Remainder of the Proofs**

To allow for a more convenient notation, from now on we treat labels as hidden variables. That is, instead of $n$ features and $r$ labels, we assume there are just $n$ variables $X_1, \ldots, X_n$. The first $m$ are hidden (these will play the role of a label) and the last $n - m$ are observed, where $m$ may be between 0 and $n - 1$. For an assignment $x$, we refer to the hidden part as $x_h$ and the observed as $x_o$. The split into hidden and observed variables will mainly serve us in the proof of Thm. 4.1, in other proofs it is just more convenient to not split expressions to $x, y$.

We also denote the subvector of $\mu$ over hidden variables and edges between them as $\mu_h$. That is, considering the items of $\mu$ are expressions $\mu_i(z_i), \mu_{ij}(z_i, z_j), \mu_h$. $\mu_h$ is the subvector containing items where $i \in h, i, j \in h$ respectively. Define a similar vector $\mu_\bar{h}$ for observed variables and edges between them. The vectors $I_r, I_h, I_o$ are defined to have the same indices as $\mu, \mu_h$ respectively, their value is 1 in indices consistent with $x$ (i.e. $z_i, z_j = x_i, x_j$ or $z_i = x_i$ for entries that contain $\mu_{ij}(z_i, z_j), \mu_i(z_i)$ respectively) and 0 otherwise. We will use the shorthand $I_x$ for the vector $I(x; \mu)I_x$.

Some notations related to graphical properties of hidden and observed nodes will be required. The number of connected components in the subgraph of hidden variables and edges between them is
We start by proving the connection to Set-Cover and then move on to Max-Flow. We will also use two variants on the local marginal polytope [31]:

$$\lambda$$

Let us write down the dual of Eq. (9):

$$\bar{\lambda}(x) = \lambda_r(x_r) + \sum_{i \not\in r} \lambda_{i,pa(i)}(x_i, x_{pa(i)}) - \lambda_{pa(i)}(x_{pa(i)}).$$

This is already very similar to the LP Relaxation of Set-Cover, but with the significant difference that variables \(\lambda\) are unrestricted, where in the Set-Cover LP they are non-negative. This is where the tree structure plays an important role. Consider the min-reparameterization of any feasible solution \(\lambda(x)\):

$$\delta(x) = \lambda_r(x_r) + \sum_{i \not\in r} \delta_{i,pa(i)}(x_i, x_{pa(i)}) - \delta_{pa(i)}(x_{pa(i)}).$$

Since \(\delta\) is feasible for Eq. (15), setting \(\lambda = \delta\) gives a feasible solution to Eq. (14) with the same objective as \(\delta\)'s in Eq. (15). That is, this problem is more constrained than Eq. (14). Yet given a
We conclude that while the set cover LP Relaxation is more constrained, all feasible solutions of Eq. (14) can be mapped to feasible solutions of this relaxation in a manner that preserves the objective. Hence the problems have the same value.

\( \lambda \cdot \mu = E_p[\lambda(x)] = E_p[\delta(x)] = \delta \cdot \mu. \)

We conclude that while the set cover LP Relaxation is more constrained, all feasible solutions of Eq. (14) can be mapped to feasible solutions of this relaxation in a manner that preserves the objective. Hence the problems have the same value.

Let us emphasize the following two points:

- This part of the lemma did not exploit the specific choice of \( U \) (being consisted of all assignments where variables take values in a certain set \( X_i \)). That is, it holds for any choice of \( U \), not only those of the form mentioned in Eq. (6).
- The constraints for \( x \notin U \) in Eq. (15) are redundant because \( \delta \geq 0 \). Removing these constraints and moving back from Eq. (15) to its dual, expressed with variables \( p \), we get another formulation of Eq. (9). We will use this in the next part of the proof and also later on, thus state it as a corollary.

**Corollary C.1.** Let \( U \) be a universe of assignments (not necessarily of the form in Eq. (6)) and \( \mu \) a tree-structured vector of marginals. The following LP has the same value as Eq. (9):

\[
\max_{p \geq 0} \sum_{u \in U} p(u) \tag{16}
\]

subject to:

\[
\sum_{u \in U: u_i = z_i} p(u) \leq \mu_i(z_i) \quad \forall i \in V, z_i
\]

\[
\sum_{u \in U: u_i = z_i} p(u) \leq \mu_i(z_i) \quad \forall i \in V, z_i
\]

**C.2 Equivalence to Max-Flow**

As stated in the Section 5.2, when the underlying graph is a chain, Eq. (9) is a Max-Flow problem. The equivalence to Max-Flow is apparent when thinking of every assignment \( x \in U \) as a path in a flow network. Assume our statistics \( \mu \) are \( \mu_{1,2}, \mu_{2,3}, \cdots, \mu_{n-1,n} \), then define a flow network with source and sink \( s, t \) and a node \((i, x_i)\) for each variable \( i \) and \( x_i \in X_i \) (i.e. one node for each variable-assignment pair). The edges of the network are \((i, x_i) \rightarrow (i+1, x_{i+1})\) for each \( 0 \leq i \leq n-1 \) and \( x_i, x_{i+1} \in X_i \times X_{i+1} \), they will have capacity \( \mu_{i,i+1}(x_i, x_{i+1}) \). Additionally we will have edges \( s \rightarrow (1, x_1), (n, x_n) \rightarrow t \) for each \( x_1 \) and \( x_n \) with unbounded capacity.

It is simple to see that there is a one-to-one correspondence between paths from \( s \) to \( t \) and assignments in \( U \). This is where \( U \)'s special structure, stated in Eq. (6) of the paper comes into play. Also, the paths that go through each edge \((i, x_i) \rightarrow (i+1, x_{i+1})\) are exactly those of assignments \( z \) where \( z_i, z_{i+1} = x_i, x_{i+1} \). According to flow decomposition [9], the LP in Eq. (16) solves the Max-Flow problem on this network (where the flow is expressed as the sum of flows in all \( s-t \) paths in the network), with a single exception that it does not contain the constraints:

\[
\sum_{u \in U: u_i = z_i} p(u) \leq \mu_i(z_i) \quad \forall i \in V, z_i.
\]

Thus to finish the proof we will get convinced that these added constraints are redundant. Consider a solution \( p \) that only satisfies the constraints of pairwise marginals in Eq. (16), we will show it also
satisfies the constraints above. Let $i \in [n]$ and $x_i \in \bar{X}_i$ and let $j$ be a neighbour of $i$ in the chain (the graph is connected, so there always is a neighbour), then:
\[
\sum_{u \in U} p(u) = \sum_{u_j \in X_j, \ u_i = x_i} \sum_{u \in U} p(u) \leq \sum_{u_j \in X_j} \mu_{ij}(x_i, u_j) \leq \mu_i(x_i).
\]
This shows the constraint is satisfied and concludes our proof.

The next proof, that of Thm. 4.2, is for results on maximizing probabilities. When the underlying graph is a chain, these results are similar to the equivalence to Max-Flow that we just proved. When the graph is not a chain, they will give an LP that does not directly correspond to a Max-Flow problem, but is still of polynomial size. That is, it can be solved efficiently with a standard LP solver, but not necessarily with a combinatorial algorithm. Our conjecture is that combinatorial algorithms can be derived for other cases, but we defer this to future work.

**D Proof of Thm. 4.2**

The theorem reformulates the following problems:
\[
\max_{\mu \in \mathcal{M}_L(U)} \max_{\mu \leq \mu} Z(\mu), \quad \max_{\mu \in \mathcal{M}_L(U)} \max_{\mu \leq \mu} Z(\mu).
\]

Our goal is to show that they have the same optimum as:
\[
\max_{I(\mu) \leq 0} Z(\mu).
\]

**Proof.** To show equality of the optimal values, let us offer a mapping between feasible solutions of the pairs of problems. From our previous results, both problems in Eq. (17) can be written in the form of Eq. (16) with $U$ and $U \setminus x$ respectively. We will start by mapping feasible solutions of these problems to feasible solutions of Eq. (18).

Choose an arbitrary root for the tree, $r \in V$, and turn the undirected tree to a directed one rooted in $r$. Consider a feasible solution $p$ to the reformulated problem in Eq. (16) and define:
\[
\tilde{\mu}_{i,pa(i)}(u_i, u_{pa(i)}) = \sum_{z \in U : z_i = u_i} p(z) \quad \forall (u_i, u_{pa(i)}) \in \bar{X}_i \times \bar{X}_{pa(i)}
\]
\[
\tilde{\mu}_i(u_i) = \sum_{z \in U : z_i = u_i} p(z) \quad \forall u_i \in \bar{X}_i
\]

It is simple to prove that $\tilde{\mu} \in \mathcal{M}_L(U)$, because for any pair $ij \in E$ it holds that:
\[
\sum_{u_j \in X_j} \tilde{\mu}_{ij}(u_i, u_j) = \sum_{u_j \in X_j} \sum_{z \in U : z_i = u_i, z_j = u_j} p(z) = \sum_{z \in U : z_i = u_i} p(z) = \tilde{\mu}_i(u_i).
\]

And from $p$’s feasibility we also get $\tilde{\mu} \leq \mu$. This can be seen from inequalities of the following type:
\[
\tilde{\mu}_{ij}(u_i, u_j) = \sum_{z \in U : z_i = u_i, z_j = u_j} p(z) \leq \mu_{ij}(u_i, u_j).
\]

We conclude that $\tilde{\mu}$ is a feasible solution to Eq. (18) with objective:
\[
Z(\tilde{\mu}) = \sum_{u_r \in X_r} \tilde{\mu}_r(z_r) = \sum_{u_r \in X_r} \sum_{z \in U : z_r = u_r} p(z) = p(U).
\]

This mapping only considered the first problem in Eq. (17). We can use the exact same construction when considering $U \setminus x$ as follows. Feasible solutions to Eq. (16) are functions $p : U \setminus x \to \mathbb{R}_+$, so extending $p$’s domain to $U$ by setting $p(x) = 0$, the above equations remain unaltered. It is left to show that the resulting $\tilde{\mu}$ satisfies $I(x; \mu) \leq 0$. If we examine the term $I(x; \mu)$, when $d_i$ is the degree of node $i$ in the graph, we get that:
\[
\sum_i (1 - d_i)\tilde{\mu}_i(x_i) + \sum_{ij} \tilde{\mu}_{ij}(x_i, x_j) = \sum_{u \in U} \alpha_u p(u),
\]
\[
\alpha_u \triangleq \sum_i I_{u_i = x_i} - \sum_{ij} I_{(u_i = x_i) \lor (u_j = x_j)}.
\]
Simple counting arguments show that $\alpha_x = 1$, while $\alpha_u \leq 0$ for all $u \neq x$. Since we set $p(x) = 0$, it follows that $\sum_{u \in U} \alpha_u p(u) \leq 0$ and also $I(x; \mu)$.

It is left to provide a mapping from solutions of Eq. (18) to solutions of Eq. (17). We will provide a proof for the case where

$$U = \{ u \mid u_i \subseteq X, \forall i \in [n] \}.$$ 

More specifically, we will construct a function $p : U \rightarrow \mathbb{R}_+$ whose marginals are $\tilde{\mu}$ and summing it over all of its domain gives $Z(\tilde{\mu})$. The construction is the same one used when proving that the local marginal polytope is equal to the marginal polytope for tree graphs [31]. To complete the proof, we will also need to show a construction when $p$’s domain is $U \setminus x$ (and $U$ defined the same as above). We refer the reader to [10] where this detailed construction can be found. There the sum of $p$ over its domain is 1, yet applying this construction to $\mu$ gives a function that sums up to $Z(\tilde{\mu})$.

The function $p$ we suggest for the problem over domain $U$ is:

$$p(u) = \tilde{\mu}_r(u_r) \prod_{i \neq r} \frac{\tilde{\mu}_{i,pa(i)}(u_i, u_{pa(i)})}{\tilde{\mu}_{pa(i)}(u_i)}.$$ 

Assume $r$ is set arbitrarily and $1, \ldots, n$ is a topological ordering of the nodes. Notice that any choice of $r$ and an ordering yields the same function $p$. It is simple to see that the function marginalizes to $\tilde{\mu}$ if we let $ij \in E$, set $i$ as the root and eliminate all variables other than $i, j$. To show that $p$’s sum over its domain $U$ is exactly the partition function, eliminate all the variables to get:

$$\sum_{x \in U} p(x) = \sum_{u_1 \in X_1} \tilde{\mu}_1(u_1) \left( \sum_{u_2 \in X_2} \frac{\tilde{\mu}_{2,pa(2)}(u_2, u_{pa(2)})}{\tilde{\mu}_{pa(2)}(u_2)} \right) \cdots \left( \sum_{u_n \in X_n} \frac{\tilde{\mu}_{n,pa(n)}(u_n, u_{pa(n)})}{\tilde{\mu}_{pa(n)}(u_n)} \right) = \sum_{u_1 \in X_1} \tilde{\mu}_1(u_1).$$ 

Here we implicitly numbered the root node as 1. To conclude, we showed a mapping from $\tilde{\mu}$ to a function $p$ that is feasible for Eq. (17), completing the proof.

For the case $U \setminus x$, as stated earlier, [10] offer a construction of a function that marginalizes to $\tilde{\mu}$ and achieves $p(x) = I(x; \mu)$. Thus enforcing $I(x; \mu) \leq 0$ ensures there is a mapping from $\tilde{\mu}$ to a function $p$ with the same objective.

Notice the equality in the above equation holds because of $U$’s special structure that includes all the assignments that take values in sets $X_i$. Different choices of $U$ do not necessarily yield this equation, thus the theorem does not hold for all choices of $U$.

### E Proof of Thm. 4.1

We recall the problem at hand of minimizing conditional probabilities:

$$\min_{p \in P(\mu)} p(x_h \mid x_o),$$ 

where we assume w.l.o.g that $x_h = x_1, \ldots, x_m$ are hidden variables, $x_o = x_{m+1}, \ldots, x_n$ are observed, and $x$ is the fixed assignment to both. Using the Charnes-Cooper variable transformation [4] between $p(z_h, z_o)$ and $\frac{p(z_h, z_o)}{p(x)}$ for all $z$, and taking the dual of the resulting LP, we arrive at the following problem:

$$\max \lambda_x$$

$$\text{s.t.} \lambda_r(z_r) + \sum_{i \neq r} \lambda_{i,pa(i)}(z_i, z_{pa(i)}) + \lambda_i(z_i) \leq 0 \quad \forall z : z_o \neq x_o$$

$$\lambda_r(z_r) + \sum_{i \neq r} \lambda_{i,pa(i)}(z_i, z_{pa(i)}) + \lambda_i(z_i) \leq -\lambda_x \quad \forall z : z_o = x_o, z_h \neq x_h,$$

$$\lambda_r(x_r) + \sum_{i \neq r} \lambda_{i,pa(i)}(x_i, x_{pa(i)}) + \lambda_i(x_i) \leq 1 - \lambda_x$$

$$\lambda \cdot \mu \geq 0.$$
The transformation is correct under the assumption that $p(x_o) > 0$, which is reasonable to assume when we observe $x_o$ and try to infer $x_h$.

The rest of the proof can now be decomposed into two main parts, one manipulates Eq. (19) and the other manipulates the second problem in Eq. (18):

**Lemma E.1.** Let $U$ be a set of the shape defined in Eq. (6) of the paper and $\mu$ a vector of tree shaped marginals. If

$$\max_{\mu \in \mathcal{M}_U} \sum_{u \in U} p(u) > \max_{\mu \in \mathcal{M}_U} \sum_{u \in U \setminus x} p(u),$$

then it holds that:

$$\max_{\mu \in \mathcal{M}_U, \mu \leq \mu} Z(\mu) = \max_{\mu \in \mathcal{M}_U, \mu - \mu_x = 0} Z(\mu).$$

**Lemma E.2.** Eq. (19) has the same optimal value as:

$$\min \mu_x$$

s.t. $\mu \in \mathcal{M}_U$, $0 \leq \mu \leq \tau \mu_h - \mu_x \bar{x}$

$$\mu \tau \mu \geq 1$$

$$\sum_{z_i} \mu_i(z_i) = \tilde{\tau} \quad \forall i \in h$$

$$\mu_x + \tilde{\tau} = 1$$

$$I(x_h; \mu) + (1 - |P_h|) \tilde{\tau} \leq 0$$

$$\tau \mu I(x; \mu) - \mu_x - I(x_h; \mu) + (|P_h| - 1) \tilde{\tau} \leq 0.$$

The decision variables in Eq. (21) are $\bar{x}$, $\tilde{\tau}$, $\tau \mu$, $\mu_x$, where $\bar{x}$ are pseudo-marginals on hidden variables and pairs of them that are connected by an edge. This form is very similar to that of problems in Eq. (18), and indeed their solutions are similar. Using Lem. E.1, we will show that a simple modification to the solution of the second problem in Eq. (18) leads to a solution of Eq. (21). This modification is shown in the following two lemmas, that also conclude the proof of Thm. 4.1. For now we assume the correctness of Lem. E.2 and Lem. E.1, their proofs are deferred to the end of this document.

To fit our problem into the formulation of Lem. E.1, define $U$ using $\bar{X}_i = \{x_i\}$ for all observed variables $i \in o$ and $\bar{X}_j$ unrestricted for all hidden variables $j \in h$. Under this definition we have:

$$\max_{\mu \in \mathcal{M}_U} \sum_{u \in U} p(u) = \max_{\mu \in \mathcal{M}_U} p(x_o),$$

$$\max_{\mu \in \mathcal{M}_U} \sum_{u \in U \setminus x} p(u) = \max_{\mu \in \mathcal{M}_U} \sum_{z_h \neq x_h} p(x_o, z_h).$$

We are now ready to use the above lemmas and conclude the proof.

**Lemma E.3.** If $I(x; \mu) \leq 0$ then

$$\min_{\mu \in \mathcal{M}_U} p(x_h \mid x_o) = 0,$$

unless $\max_{\mu \in \mathcal{M}_U} \sum_{z_h \neq x_h} p(z_h, x_o) = 0$ and then the value is 1.

**Proof.** We assume that $p(x_o)$ is constrained to be larger than 0, otherwise the robust conditional probability problem is ill-defined. So it is trivial that if

$$\max_{\mu \in \mathcal{M}_U} \sum_{z_h \neq x_h} p(x_o, z_h) = 0,$$

then $p(x) = p(x_o)$ and the conditional is 1.

Now assume towards contradiction that $\min_{\mu \in \mathcal{M}_U} p(x_h \mid x_o) > 0$, clearly we must have:

$$\max_{\mu \in \mathcal{M}_U} \sum_{u \in U} p(u) > \max_{\mu \in \mathcal{M}_U} \sum_{u \in U \setminus x} p(u),$$

which contradicts Lem. E.1.
because otherwise equality must hold, so a maximizing distribution of the right hand side will have to achieve a conditional probability of 0. Then the conditions of Lem. E.1 hold and we have:

$$\max_{p \in P(\mu)} \sum_{z_h, \neq x_h} p(x_o, z_h) = \max_{\tilde{\mu} \in \mathcal{M}_L(U), \mu \leq \tilde{\mu}} Z(\tilde{\mu}).$$

Denote the value of the above problems as $\tilde{\tau}_1$, so $\tilde{\tau}_1 > 0$, let $\tilde{\mu}_1$ be an optimal solution to the problem on the right hand side and $\tilde{\mu}_{1,h}$ its sub-vector that corresponds to hidden variables and edges between them. Consider taking $\tilde{\tau}_1 = 1, \mu_x = 0$, we will show there exists a value of $\tau_\mu$ such that $\tilde{\mu}, \bar{\tau}, \mu_x, \tau_\mu$ is a feasible solution to Eq. (21). The value of this solution is $\mu_x = 0$, which contradicts the assumption that the minimum is strictly positive and concludes the proof.

To see such a value of $\tau_\mu$ exists, note the following three points:

- $\tilde{\mu}_1 \in \mathcal{M}_L(U), \tilde{\mu}_1 \leq \mu$ and normalizes to $\tilde{\tau}_1$. So it also holds that $\tilde{\mu} \in \mathcal{M}_L, \tilde{\mu} \leq \tilde{\tau}_1^{-1} \mu_h$, hence the first constraint of Eq. (21) is satisfied for any $\tau_\mu \leq \tilde{\tau}_1^{-1}$. Also from these results it is straightforward to see that the third and fourth constraints are satisfied.

- Because we enforced $p(x_o) > 0$, it holds that $\mu_o > 0$. Thus the second constraint of Eq. (21) can also be satisfied if we take a large enough value for $\tau_\mu$ (i.e. larger than one over the minimal item in $\mu_o$).

- Finally, we will show that

$$I(x_h; \tilde{\mu}) + (1 - |P_h|)\tilde{\tau} = 0. \quad (22)$$

This means the fifth constraint is satisfied and more importantly, because $I(x; \mu) \leq 0$, the last constraint is satisfied for any positive value of $\tau_\mu$.

To show that Eq. (22) holds, notice that:

$$I(x; \tilde{\mu}) = \sum_{i} (1 - d_i)\tilde{\mu}_i(x_i) + \sum_{i,j \in E} \tilde{\mu}_{ij}(x_i, x_j)$$

$$= \sum_{i \in o} (1 - d_i)\tilde{\tau}_1 + \sum_{i \in h} (1 - d_i)\tilde{\mu}_{1,i}(x_i) + \sum_{i,j \in E_h} \tilde{\mu}_{1,ij}(x_i, x_j)$$

$$+ \sum_{i,j \in E_{oh}} \tilde{\mu}_{1,ij}(x_j) + \sum_{i \in o} \tilde{\tau}_1$$

$$= 0$$

Since the subgraph of observed nodes is a forest, it has $|E_o| = |o| - |P_o|$ edges. Furthermore, $\sum_{i \in o} d_i = |E_{oh}| + 2|E_o|$ so we can rewrite the above expression as:

$$I(x; \tilde{\mu}) = (|P_o| - |E_{oh}|)\tilde{\tau}_1 + \sum_{i \in h} (1 - d_i^h)\tilde{\mu}_{1,i}(x_i) + \sum_{i,j \in E_h} \tilde{\mu}_{1,ij}(x_i, x_j).$$

Notice we also combined the summation over $ij \in E_{oh}$ to that over $i \in h$, changing $d_i$ to $d_i^h$. The entire graph being a tree, it must also hold that $|E_{oh}| = |P_h| + |P_o| - 1$. Plugging this into our expression, we get:

$$I(x; \tilde{\mu}) = I(x_h; \tilde{\mu}_{1,h}) + (1 - |P_h|)\tilde{\tau} = 0.$$
Now because of the way we set $\tilde{\mu}$, we arrive at:

$$\frac{I(x; \tilde{\mu}_1)}{\tilde{\tau}_1} = I(x_h; \bar{\mu}) + (1 - |P_h|)\tilde{\tau} = 0,$$

which gives Eq. (22).

Combining the items above, we see that taking $\tau_{\mu}$ larger than $\tilde{\tau}_1^{-1}$ and all entries of $\mu_o^{-1}$, gives a feasible solution as required.

Lemma E.4. If $I(x; \mu) > 0$ then $\min_{\mu \in \mathcal{P}(\mu)} p(x_h | x_o) = \frac{I(x; \mu)}{I(x; \mu) + \max_{\mu \in \mathcal{P}(\mu)} \sum_{x_h \neq x_h} p(x_h, x_o)}$.

Proof. Obviously the right hand side is a lower bound on the minimum, we need to show there is a feasible solution that gives this bound. When $I(x; \mu) > 0$ it is easy to see that the conditions of Lem. E.1 hold. So defining $\mu_1, \tilde{\tau}_1$ as we did in the proof of Lem. E.3, we can assume $\mu_1 \leq \mu - 1_{x}, I(x_h; \mu_1) + (1 - |P_h|) = 0$. Now consider setting:

$$\tau_{\mu} = \frac{1}{I(x, \mu)} + \tilde{\tau}_1, \quad \tilde{\mu} = \mu_1 h, \tilde{\tau}_1, \quad \tilde{\tau} = \tilde{\tau}_1 \tau_{\mu}, \quad \mu_x = I(x; \mu) \tau_{\mu}.$$

Since $\tilde{\tau}_1$ is defined as the value of the maximization problem in the denominator of the bound stated in the lemma, it can be seen that the value of $\mu_x$ is equal to this bound. So if this solution is feasible for Eq. (21), $\mu_x$ is also an upper bound on the robust conditional probability and it must also be the optimal value. We will simply go through each constraint in Eq. (21) and show this solution satisfies it:

- $\tilde{\mu} \in \mathcal{M}^h \cup 0 \leq \tilde{\mu} \leq \tau_{\mu} \mu_h - \mu_x \ll_{x_h}$: since $\tilde{\mu}_1 \in \mathcal{M}(U)$ and linear constraints stay satisfied after multiplying all variables by a positive scalar, we have $\tilde{\mu} \in \mathcal{M}^h \cup 0$. Satisfaction of capacity constraints is also a direct consequence of $\tilde{\mu}_1$ satisfying capacity constraints:

$$\mu = \mu_1 h, \tilde{\tau}_1 \leq (\mu_h - 1_{x}) \tau_{\mu} = \tau_{\mu} \mu_h - \mu_x \ll_{x_h}.$$

- $\mu_i(x_i) \tau_{\mu} \geq 1 \quad \forall i \in o, \mu_{ij}(x_i, x_j) \tau_{\mu} \geq 1 \quad \forall i j \in E_o$: Notice that $\tilde{\mu}_1$ also has components for observed variables $i \in o$ that satisfy $\tilde{\tau}_1 = m_{ij}(x_i) \leq \mu_i(x_i) - I(x; \mu)$ and $\tilde{\tau}_1 = m_{ij}(x_i, x_j) \leq \mu_{ij}(x_i, x_j) - I(x; \mu)$ for $i j \in E_o$. This gives us the constraints easily:

$$\tilde{\tau}_1 + I(x; \mu) = \frac{1}{\tau_{\mu}} \leq \mu_i(x_i) \quad \forall i \in o,$$

and the same holds for every $i j \in E_o$.

- $\sum_{z_i} \tilde{\mu}_i(z_i) = \tilde{\tau}_1 \quad \forall i \in h, \mu_x + \tilde{\tau} = 1$: Easy to see from our setting of $\tilde{\mu}, \tilde{\tau}, \mu_x$, because $\mu_1$ normalizes to $\tilde{\tau}_1$.

- $I(x_h; \tilde{\mu}) + (1 - |P_h|)\tilde{\tau} \leq 0, \tau_{\mu} I(x; \mu) - \mu_x - I(x_h; \tilde{\mu}) + (|P_h| - 1)\tilde{\tau} \leq 0$: Using $I(x_h; \tilde{\mu}) + (1 - |P_h|)\tilde{\tau} = 0$ (this was proved in the proof of Lem. E.3) and because we set $\mu_x = I(x; \mu) \tau_{\mu}$, it is easy to confirm these two constraints are satisfied.

We are left with the task of proving Lem. E.2 and Lem. E.1, this is the topic of the next section.

E.1 Proofs of Lem. E.2 and Lem. E.1

The problem we are concerned with, Eq. (19), has an exponential number of constraints. We will see shortly that these constraints can be treated as constraints on the value of 2nd-best MAP problems [10], one over the tree shaped field $\lambda(z)$ and the other over the forest shaped $\lambda(z_h, x_o)$. To prove our results we will use a relaxation of these problems. Specifically, we will use the tightness of this relaxation in trees and forests to switch these constraints with a polynomially sized set, that is easier to handle analytically. Hence we turn to derive the set of linear constraints, this is done in a very similar manner to the derivation in [11].
E.1.1 Second Best MAP using Dual Decomposition

As proved by the authors in [10], the 2nd-best MAP problem over a field $\lambda(z)$, with excluded assignment $x$ can be written as follows:

$$\max_{\mu} \lambda \cdot \mu$$

s.t. $\mu \in \mathcal{M}_L, \bar{I}(x; \hat{\mu}) \leq |P| - 1,$

where $|P|$ is the number of connected components. This is in fact a relaxation of the 2nd-best MAP problem, but it is exact when the graph is a tree or a forest. The dual of this problem is:

$$\min_{\delta, \delta_x} \sum_i \delta_i + \sum_{ij} \delta_{ij} + (|P| - 1)\delta_x$$

s.t. $\lambda_i(z_i) + \sum_j \delta_{ij}(z_i) + (d_i - 1)\delta_x \mathbb{I}_{z_i = x_i} \leq \delta_i \quad \forall i, z_i$

$$\lambda_{ij}(z_i, z_j) - \delta_{ij}(z_i) - \delta_{ij}(z_j) - \delta_x \mathbb{I}_{z_i, z_j = x_i, x_j} \leq \delta_{ij} \quad \forall ij, (z_i, z_j)$$

$$\delta_x \geq 0$$

At the optimum, $\delta_i, \delta_{ij}$ will just be equal to the maximum of the left hand side over different values of $z_i, z_j$ (since the problem is a minimization problem), hence we can solve:

$$\min_{\delta, \delta_x \geq 0} \sum_i \max_{z_i} \left\{ \lambda_i(z_i) + \sum_j \delta_{ij}(z_i) + (d_i - 1)\delta_x \mathbb{I}_{z_i = x_i} \right\} +$$

$$\sum_{ij \in G} \max_{z_i, z_j} \left\{ \lambda_{ij}(z_i, z_j) - \delta_{ij}(z_i) - \delta_{ij}(z_j) - \delta_x \mathbb{I}_{z_i, z_j = x_i, x_j} \right\} + (|P| - 1)\delta_x$$

To formulate a set of linear constraints that are satisfied if and only if this MAP value is smaller than a constant $c$, we can use auxiliary variables and a polynomial number of constraints, as done in [8]:

$$\sum_i \alpha_i + \sum_{ij} \alpha_{ij} + (|P| - 1)\delta_x \leq c$$

$$\lambda_i(z_i) + \sum_j \delta_{ij}(z_i) + (d_i - 1)\delta_x \mathbb{I}_{z_i = x_i} \leq \alpha_i \quad \forall i, z_i$$

$$\lambda_{ij}(z_i, z_j) - \delta_{ij}(z_i) - \delta_{ij}(z_j) - \delta_x \mathbb{I}_{z_i, z_j = x_i, x_j} \leq \alpha_{ij} \quad \forall ij, (z_i, z_j)$$

$$\delta_x \geq 0.$$
We already showed in the proof of Lem. E.3 that the term \( \sum_{i \in o} (d_i - 1) - |E_o| \) is equal to \( |P_h| - 1 \), turning the above constraint to:

\[
\tau_{\mu} \tilde{I}(x; \mu) - \mu_x - \tilde{I}(x_h; \tilde{\mu}) + (|P_h| - 1) \tilde{\tau} \leq 0.
\]
So we end up with the following problem:

\[
\begin{align*}
\min & \quad \mu_x \\
\text{s.t.} & \quad \mu_x + \tilde{\tau} = 1 \\
& \quad \tilde{\mu}_i(z_i) - \mu_i(z_i) \tau_i + \mathbb{I}_{z_i = x_i, \mu_x} \leq 0 \quad \forall i \in h, z_i \\
& \quad \tilde{\mu}_{ij}(z_i, z_j) - \mu_{ij}(z_i, z_j) \tau_{ij} + \mathbb{I}_{z_i = x_i, z_j = x_j, \mu_x} \leq 0 \quad \forall ij \in E_h, (z_i, z_j) \\
& \quad \mu_i(x_i) \tau_i \geq 1 \quad \forall i \in o \\
& \quad \mu_{ij}(x_i, x_j) \tau_{ij} \geq 1 \quad \forall ij \in E_o \\
& \quad \tilde{\mu}_i(z_i) + \mathbb{I}_{z_i = x_i, \mu_x} - \mu_i(z_i) \tau_i \leq 0 \quad \forall ij \in E_{ho} \\
& \quad \mu_{ij}(z_i, z_j) = \tilde{\mu}_i(z_i) \quad \forall ij \in E_h, z_i \\
& \quad \sum_{z_j} \tilde{\mu}_{ij}(z_i, z_j) = \tilde{\tau} \quad \forall i \in h \\
& \quad \tau_i I(x; \mu) - \mu_x - I(x_h; \tilde{\mu}) + (|P_h| - 1)\tilde{\tau} \leq 0 \\
& \quad I(x_h; \tilde{\mu}) + (1 - |P_h|)\tilde{\tau} \leq 0
\end{align*}
\]

Simplifying notation using the vectors \( \mu_h, \mathbb{I}_x, \mu_o \) that we defined in Section B, the problem takes the shape of Eq. (21) \( \square \)

**Proof of Lem. E.2.** From Thm. 4.2 we know that:

\[
\max_{\tilde{\mu} \in M(U), \tilde{\mu} \leq \mu} Z(\tilde{\mu}) = \max_{p \in \mathcal{P}(\mu)} \sum_{u \in U} p(u),
\]

\[
\max_{\tilde{\mu} \in M(U), \tilde{\mu} \leq \mu} Z(\tilde{\mu}) = \max_{p \in \tilde{\mathcal{P}}(\mu)} \sum_{u \in U, x} p(u).
\]

Now for each \( i, (i, j) \in E \), consider replacing constraints in \( \mathcal{P}(\mu) \) as follows:

\[
\sum_{z: z_i, z_j = x_i, x_j} p(z) = \mu_{ij}(x_i, x_j) \rightarrow \sum_{z: z_i, z_j \neq x_i, x_j, z \neq x} p(z) \leq \mu_{ij}(x_i, x_j) - I(x, \mu),
\]

\[
\sum_{z: z_i = x_i} p(z) = \mu_i(x_i) \rightarrow \sum_{z: z_j = x_j, z \neq x} p(z) \leq \mu_i(x_i) - I(x, \mu).
\]

We will denote this set by \( \tilde{\mathcal{P}}(\mu) \). Since for any \( p \in \mathcal{P}(\mu) \) we know that \( p(x) \geq I(x, \mu) \), it holds that \( \mathcal{P}(\mu) \subseteq \tilde{\mathcal{P}}(\mu) \), which means the maximum of the new problem is higher than that of the original for both problems (on \( U \) and \( U \setminus x \)):

\[
\max_{p \in \mathcal{P}(\mu)} \sum_{u \in U} p(u) \leq \max_{p \in \tilde{\mathcal{P}}(\mu)} \sum_{u \in U} p(u)
\]

\[
\max_{p \in \mathcal{P}(\mu)} \sum_{u \in U, x} p(u) \leq \max_{p \in \tilde{\mathcal{P}}(\mu)} \sum_{u \in U, x} p(u)
\]

Taking the dual of this new problem on \( U \setminus x \) we obtain:

\[
\min_{\lambda} \lambda \cdot (\mu - \mathbb{I}_x) \\
\text{s.t.} \quad \lambda(z) \geq 1 \quad \forall z \in U \setminus x \\
\lambda(z) \geq 0 \quad \forall z \notin U \\
\lambda_{ij}(x_i, x_j) \geq 0, \lambda_i(x_i) \geq 0 \quad \forall i \in V, (i, j) \in E
\]

From the result in Cor. C.1, we can consider the variables to be non-negative (i.e. \( \lambda \geq 0 \)), the second constraint is redundant and can be removed. Furthermore, the first constraint is in fact a constraint on the value of the 2nd-best MAP problem on \( -\lambda(z) \) (i.e. minimization of \( \lambda(z) \) while excluding \( x \)).
Adapting the constraints in Eq. (23) to a minimization problem and switching into our problem we get:

\[
\min_{\lambda \geq 0, \alpha \geq 0, \delta} \lambda \cdot (\mu - I_x)
\]

subject to:
\[
\begin{align*}
\sum_i \alpha_i + \sum_{ij} \alpha_{ij} & \geq 1 \\
\lambda_i (z_i) + \sum_j \delta_{ij} (z_i) + (1 - d_i) \delta_x I_{z_i = x_i} & \geq \alpha_i \quad \forall i, z_i \in \bar{X}_i \\
\lambda_{ij} (z_i, z_j) - \delta_{ij} (z_i) - \delta_{ij} (z_j) + \delta_x I_{z_i = x_i, z_j} & \geq \alpha_{ij} \quad \forall ij, (z_i, z_j) \in \bar{X}_i \times \bar{X}_j.
\end{align*}
\]

Taking the dual of this problem, it is easy to see it equals to:

\[
\max_{\tilde{\mu} \in \mathcal{M}_I (U), \tilde{\mu} \leq \mu - I_x} Z(\tilde{\mu}).
\]

The constraints of this problem are more strict than the ones in the original, therefore its value is lower:

\[
\max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U' \setminus x} p(u) = \max_{I(x; \tilde{\mu}) \leq 0} Z(\tilde{\mu}) \geq \max_{I(x; \tilde{\mu}) \leq 0} Z(\tilde{\mu}) = \max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U' \setminus x} p(u).
\]

We gather that an equality must hold:

\[
\max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U' \setminus x} p(u) = \max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U' \setminus x} p(u) = \max_{I(x; \tilde{\mu}) \leq 0} Z(\tilde{\mu}).
\]

To complete the proof we need to show the existence a solution \( \tilde{\mu} \) that is optimal for the problem on the right hand side and satisfies \( I(x; \tilde{\mu}) = 0 \). Then assume towards contradiction that Eq. (20) holds and there is no optimal solution where \( I(x; \tilde{\mu}) = 0 \). Since the problem is feasible, some optimal solution \( \mu^* \) does exist and from complementary slackness, there is a corresponding solution \( \lambda^*, 0, \alpha^*, \delta^* \) to Eq. (25). Since the value of \( \delta_x = 0 \), then \( \lambda^*, \alpha^*, \delta^* \) is also a feasible solution to the dual of:

\[
\max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U} p(u),
\]

which means \( \lambda^* \cdot (\mu - I_x) \) is an upper bound on this problem. To conclude, we concatenate the inequalities we have so far:

\[
\max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U} p(u) \leq \max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U} p(u) \leq \lambda^* \cdot (\mu - I_x) = \max_{\mu \in \mathcal{P}(\mu)} \sum_{u \in U} p(u).
\]

This inequality contradicts the hard inequality we assumed at the statement of the lemma, therefore there exists an optimal solution where \( I(x; \tilde{\mu}) = 0 \) and we can incorporate this equality into the constraints without changing the value of the problem. \( \square \)