Abstract

Structured prediction tasks in machine learning involve the simultaneous prediction of multiple labels. This is typically done by maximizing a score function on the space of labels, which decomposes as a sum of pairwise elements, each depending on two specific labels. Intuitively, the more pairwise terms are used, the better the expected accuracy. However, there is currently no theoretical account of this intuition. This paper takes a significant step in this direction.

We formulate the problem as classifying the vertices of a known graph $G = (V, E)$, where the vertices and edges of the graph are labelled and correlate semi-randomly with the ground truth. We show that the prospects for achieving low expected Hamming error depend on the structure of the graph $G$ in interesting ways. For example, if $G$ is a very poor expander, like a path, then large expected Hamming error is inevitable. Our main positive result shows that, for a wide class of graphs including 2D grid graphs common in machine vision applications, there is a polynomial-time algorithm with small and information-theoretically near-optimal expected error. Our results provide a first step toward a theoretical justification for the empirical success of the efficient approximate inference algorithms that are used for structured prediction in models where exact inference is intractable.
1 Introduction

An increasing number of problems in machine learning are being solved using structured prediction \cite{13,30,37}. Examples of structured prediction include dependency parsing for natural language processing, part-of-speech tagging named entity recognition, and protein folding. In this setting, the input $X$ is some observation (e.g., an image, a sentence) and the output is a set of labels (e.g., whether each pixel in the image is foreground or background, or the parse tree for the sentence). The advantage of performing structured prediction is that one can specify features that encourage sets of labels to take some value (e.g., a feature that encourages two neighboring pixels to take different foreground/background states whenever there is a big difference in their colors). The feature vector can then be used within an exponential family distribution over the space of labels, conditioned on the input. The parameters are learned using maximum likelihood estimation (as with conditional random fields \cite{30}) or using structured SVMs \cite{2,37}.

In the applications above, performance is typically quantified as the discrepancy between the correct “ground truth” labels $Y$ and the predicted labels $\hat{Y}$. The most common performance measure, which we study in this paper, is Hamming error, the number of disagreements between $Y$ and $\hat{Y}$. The optimal decision strategy for minimizing Hamming error is to use marginal inference, namely $\hat{Y}_i \leftarrow \text{arg max}_Y p(Y | X)$ for each $i$, where $p$ is the true generating distribution. However, in practice MAP inference is more often used. Namely, the assignment maximizing $p(Y | X)$ is returned. One advantage of using MAP inference is computational, as the partition function (normalization constant) no longer needs to be estimated during training or at test time. However, in the worst case, even MAP inference can be NP-hard, such as for binary pairwise Markov random fields with arbitrary potential functions.

It is now widely understood from a practical perspective that better performance (measured in terms of Hamming error) can be obtained by using a more complex model incorporating a strong set of features than a simple model for which exact inference can be performed. Despite the worst-case intractability of inference in these models, heuristic MAP inference algorithms often work well in practice, including those based on linear programming relaxations and dual decomposition \cite{29,35}, policy-based search \cite{16}, graph cuts \cite{28}, and branch-and-bound \cite{36}. By “work well in practice”, we mean that they obtain high accuracy predicting the true labels on test data, measured in terms of the actual loss function of interest such as Hamming error.

However, the theoretical understanding of the setup is fairly limited. For example, for many applications even the state-of-the-art structured prediction models are unable to achieve zero labeling error, and there is no characterization of the choice of feature sets and the generative settings for which high prediction accuracy can be expected, even ignoring computational limitations. Moreover, the good performance of these heuristic algorithms indicates that real-world instances are far from the theoretical worst case, and it is a major open problem to better characterize the complexity of inference problems to distinguish those that are in fact easy to solve from those that are computationally intractable. Finally, it is not well understood why MAP inference can provide such good results for these structured prediction problems and how much accuracy is lost relative to marginal inference.

The goal of this paper is to initiate the theoretical study of structured prediction for obtaining small Hamming error. Such an analysis must define a generative process for the $X, Y$ pairs, in order to properly define expected Hamming error. Our model assumes that the observed $X$ is a noisy version of $Y$ in the following sense: $X_i$ is a noisy version of the true $Y_i$ and $X_{i,j}$ is a noisy version of the variable $I(Y_i = Y_j)$. The resulting posterior for $Y$ given $X$ is then very similar to the data and
smoothness terms used for structured prediction in machine vision. Motivated by machine vision applications we also focus on the case where \( i, j \) pairs correspond to a two dimensional grid graph [35]. We also provide results for classes of non-grid and non-planar graphs.

As noted earlier, prediction is often performed by taking marginals of the posterior or its maximum. Both of these turn out to be computationally intractable in our setting. We are thus also interested in analyzing algorithms that are polynomial time and have guarantees on the expected Hamming error. Our main result is that there exists a polynomial-time algorithm that achieves the information-theoretic lower bound on the expected Hamming error, and is thus optimal (up to multiplicative constants). The algorithm is a two-step procedure which ignores the node evidence in the first step, solving a MaxCut problem on a grid (which can be done in polynomial time), and in the second step uses node observations to break symmetry. We use combinatorial arguments to provide a worst-case upper bound on the error of this algorithm. Our analysis is validated via experimental results on 2D grid graphs.

2 Related Work

Our goal is to recover a set of unobserved variables \( Y \) from a set of noisy observations \( X \). As such it is related to various statistical recovery settings, but distinct from those in several important aspects. Below we review some of the related problems.

**Channel Coding:** This is a classic recovery problem (e.g., see [4]) where the goal is to exactly recover \( Y \) (i.e., with zero error). Here \( Y \) is augmented with a set of “error-correcting” bits, deterministic functions of \( Y \), and the complete set of bits is sent through a noisy channel. In our model, \( X_{i,j} \) is a noisy version of the parity of \( Y_i \) and \( Y_j \). Thus our setting may be viewed as communication with an error correcting code where each error-correcting bit involves two bits of the original message \( Y \), and each \( Y_i \) appears in \( d_i \) check bits, where \( d_i \) is the number of edge observations involving \( Y_i \). Such codes cannot be used for errorless transmission (e.g., see our lower bound in Section 4). As a result, the techniques and results from channel coding do not appear to apply to our setting.

**Correlation Clustering (CC):** There are numerous variants of this problem, but in the typical setting \( Y \) is a partition of \( N \) variables into an unknown number of clusters and \( X_{u,v} \) specifies whether \( Y_u \) and \( Y_v \) are in the same cluster (with some probability of error as in [25] or adversarially as in [32]). The goal is to find \( Y \) from \( X \). Most CC works assume an unrestricted number of clusters [7, 25], although a few consider a fixed number of clusters (e.g. see [21]). Our results apply to the case of two clusters. The most significant difference is that most of the CC works study the objective of minimizing the number of edge disagreements. It is not obvious how to translate the guarantees provided in these works to a non-trivial bound on Hamming error (i.e., number of node disagreements) for our analysis framework.

**Approximately Stable Clusterings:** Work on approximation stability, initiated by Balcan et al. [5] and Bilu and Linial [9], also seek polynomial-time algorithms with low Hamming error with respect to a ground truth clustering. Instead of assuming that the input is derived from the ground truth by a random process, these papers make an incomparable assumption that all near-optimal solutions w.r.t. some objective function have low error w.r.t. the ground truth clustering. Approximation stable instances of correlation clustering problems were studied by Balcan and Braverman [6], who gave positive results when \( G \) is the complete graph and stated the problem of understanding general graphs as an open question.
**Recovery Algorithms in Other Settings:** The high-level goal of recovering ground truth from a noisy input has been studied in numerous other application domains. In the overwhelming majority of these settings, the focus is on maximizing the probability of exactly recovering the ground truth, a manifestly impossible goal in our setting. This is the case with, for example, planted cliques and graph partitions (e.g. [14, 19, 33]), detecting hidden communities [3], and phylogenetic tree reconstruction [15]. A notable exception is work by Braverman and Mossel [10] on sorting from noisy information, who give polynomial-time algorithms for the approximate recovery of a ground truth total ordering given noisy pairwise comparisons. Their approach, similar to the present work, is to compute the maximum likelihood ordering given the data, and prove that the expected distance between this ordering and the ground truth ordering is small.

**Recovery on Random Graphs:** Two very recent works [1, 11] have addressed the case where noisy pairwise observations of $Y$ are obtained for edges in a graph. In both of these, the focus is mainly on guarantees for random graphs (e.g., Erdős-Renyi graphs). Furthermore, the analysis is of perfect recovery (in the limit as $n \to \infty$) and its relation to the graph ensemble. The goal of our analysis is considerably more challenging, as we are interested in the Hamming error for finite $N$. Abbe et al. [1] explicitly state partial (as opposed to exact) recovery for sparse graphs with constant degrees as an open problem, which we solve in this paper.

**Percolation:** Some of the technical ideas in our study of grid graphs (Section 4) are inspired by arguments in percolation, the study of connected clusters in random (often infinite) graphs. For example, our use of “filled-in regions” in Section 4 is reminiscent of arguments in percolation theory (e.g., see p. 286 in [22]). In addition, we can directly adapt results from statistical physics that bound the connectivity constant of square lattices [12, 31] and the number of self-avoiding polygons of a particular length and area [24], to give precise constants for our theoretical results.

### 3 Preliminaries

We consider the setting of prediction on a graph $G = (V, E)$ where $V$ denotes the set of labels that we want to predict, and $E$ the observed pairwise relationships. Let $Y \in \{-1, +1\}^N$ denote the ground truth labels, where $N = |V|$. The setting is depicted in Figure 1.

**The Generative Model and Hamming Error:** A random process generates observations for the edges and nodes of $G$ as a function of the ground truth. It has two parameters, an edge noise $p \in [0, .5]$ and a node noise $q \in [0, .5]$. The generative model is as follows. For each edge $(u, v) \in E$, the edge observation $X_{uv}$ is independently sampled to be $Y_u Y_v$ with probability $1 - p$ (called a *good* edge), and $-Y_u Y_v$ with probability $p$ (called a *bad* edge). Observe that adjacent vertices are likely to have the same (or different) labels if the observation on the edge connecting them is $+1$ (or $-1$). Similarly, for each node $v \in V$, the node observation $X_v$ is independently sampled to be $Y_v$ with
probability $1 - q$ (good nodes), and $-Y_i$ with probability $q$ (bad nodes).

A labeling algorithm is a function $A : \{-1, +1\}^E \times \{-1, +1\}^V \rightarrow \{-1, +1\}^V$ from graphs with labeled edges and nodes (i.e., the noisy observations described above) to a labeling of the nodes $V$. We measure the performance of $A$ by the expectation of the Hamming error (i.e., the number of mispredicted labels) over the observation distribution induced by $A$. The overall error is then:

$$e_y(A) = \mathbb{E}_{X|Y=y}[\frac{1}{2} \| A(X) - y \| ] .$$

The overall error is then:

$$e(A) = \max_y e_y(A).$$

**MAP and Marginal Estimators:** The maximum likelihood (ML) estimator of the ground truth is given by $\hat{Y} ← \arg \max_X p(X | Y)$, where

$$p(X | Y) = \prod_{uv \in E} (1 - p)^{\frac{1}{2}(1 + X_{uv}Y_uY_v)} p^{\frac{1}{2}(1 - X_{uv}Y_uY_v)} \cdot \prod_{v \in V} (1 - q)^{\frac{1}{2}(1 + X_vY_v)} q^{\frac{1}{2}(1 - X_vY_v)}. \tag{3}$$

Taking the logarithm and ignoring constants, we see that maximizing $p(X | Y)$ is equivalent to

$$\max_Y \frac{1}{2} \sum_{uv \in E} X_{uv}Y_uY_v \log \frac{1 - p}{p} + \sum_{v \in V} X_vY_v \log \frac{1 - q}{q} , \tag{4}$$

or simply

$$\max_Y \sum_{uv \in E} X_{uv}Y_uY_v + \gamma \sum_{v \in V} X_vY_v ,$$

where $\gamma = \log \frac{1 - q}{q} / \log \frac{1 - p}{p}$.

Assuming a uniform prior over ground truths $Y$, MAP inference reduces to maximum likelihood inference, and marginal inference can be performed using $p(Y | X) \propto p(X | Y)$. Standard arguments prove that the algorithm that performs marginal inference using a uniform distribution over $Y$ achieves the smallest possible error according to Eq. [2] for completeness, we include a proof in Appendix [A]. In other words, marginal inference using a uniform prior minimizes the worst case expected error (i.e., it is minimax optimal).

**Approximate Recovery:** The interesting regime for structured prediction is when the node noise $q$ is large. In this regime there is no correlation decay, and correctly predicting a label requires a more global consideration of the node and edge observations. The intriguing question — and the question that reveals the importance of the structure of the graph $G$ — is whether or not there are algorithms with small error when the edge noise $p$ is a small constant. Precisely, we make the following definition.

**Definition 3.1 (Approximate Recovery)** For a family of graphs $\mathcal{G}$, we say that approximate recovery is possible if there is a function $f : [0, 1] \rightarrow [0, 1]$ with $\lim_{p \to 0} f(p) = 0$ such that, for every sufficiently small $p$ and all $N$ at least a sufficiently large constant $N_0(p)$, the minimum-possible error of an algorithm on a graph $G \in \mathcal{G}$ with $N$ vertices is at most $f(p) \cdot N$.

**A Non-Example:** Some graph families admit approximate recovery whereas others do not. To illustrate this and impart some intuition about our model, consider the family of path graphs. Assume that the node noise $q$ is extremely close to .5, so that node labels provide no information about the ground truth, while the edge noise $p$ is an arbitrarily small positive constant. If $G$ is a path graph on $N$ nodes with $N$ sufficiently large then, with high probability, for most pairs of
nodes, the unique path between them contains a bad edge. This implies that approximate recovery
is not possible.

A bit more formally, imagine that an adversary generates the ground truth \( Y \) by picking \( i \)
uniformly at random from \( \{1, 2, \ldots, N\} \), giving the first \( i \) nodes the label -1 and the last \( N - i \)
nodes the label +1. With high probability a constant fraction of the input’s edges are “-1” edges — one good edge consistent with the ground truth and the rest bad edges inconsistent with the ground truth. Intuitively, no algorithm can guess which is which, which means that every algorithm has expected error \( \Omega(N) \) with respect to the distribution over \( Y \), and hence error \( \Omega(N) \) with respect to a worst case choice of \( Y \). Thus, path graphs do not allow approximate recovery\(^1\).

4 Optimal Recovery in Grid Graphs

This section studies grid graphs. We devote a lengthy treatment to them for several reasons. First, grid graphs are central in applications such as machine vision. Second, the grid is a relatively poor expander and for this reason poses a number of interesting technical challenges. Third, our algorithm for the grid and other planar graphs is computationally efficient. Our grid analysis yields matching upper and lower bounds of \( \Theta(p^2N) \) on the information-theoretically optimal error.

4.1 The Algorithm

We study the algorithm \( \bar{A} \), which has two stages. The first stage ignores the node observations and computes a labeling \( \hat{Y} \) that maximizes the agreement with respect to edge observations only, i.e.

\[
\hat{Y} \leftarrow \arg \max \sum_{uv \in E} X_{uv} Y_u Y_v. \tag{5}
\]

Note that \( \hat{Y} \) and \( -\hat{Y} \) agree with precisely the same set of edge observations, and thus both maximize Eq. 5. The second stage of algorithm \( \bar{A} \) outputs \( \hat{Y} \) or \( -\hat{Y} \), according to a “majority vote” by the node observations. Precisely, it outputs \( -\hat{Y} \) if \( \sum_{v \in V} X_v Y_v < 0 \), and \( \hat{Y} \) otherwise.

| Algorithm 1 \( \bar{A}(X) \) |
|-------------------------------|
| **Require:** | Edge and node observations \( X \) |
| **Ensure:** | Node predictions \( \hat{Y} \) |
| \( \hat{Y} \leftarrow \arg \max \sum_{uv \in E} X_{uv} Y_u Y_v \) |
| if \( \sum_{v \in V} X_v Y_v < 0 \) then |
| \( \hat{Y} \leftarrow -\hat{Y} \) |
| end if |
| return \( \hat{Y} \) |

When the graph \( G \) is a 2D grid, or more generally a planar graph, this algorithm can be implemented in polynomial time by a reduction to the maximum-weight matching problem (see [20, 8]). By contrast, it is \( NP \)-hard to maximize the full expression in (4) [8].

\(^1\)It is not difficult to make this argument rigorous. See Section 4.3 for a rigorous, and more interesting, version of this lower bound argument.
### 4.2 An Upper Bound on the Error

Our goal is to prove the following theorem, which shows that approximate recovery on grids is possible.

**Theorem 4.1** If \( p < \frac{1}{39} \), then the algorithm \( \bar{A} \) achieves error \( e(\bar{A}) = O(p^2N) \).

**Analysis of First Stage:** We analyze the two stages of algorithm \( \bar{A} \) in order. We first show that after the first stage, the expected error of the better of \( \hat{Y} \), \(-\hat{Y}\) is \( O(p^2N) \). We then extend this error bound to the output of the second stage of the algorithm.

We begin by highlighting a simple but key lemma that characterizes a structural property of the maximizing assignment in Eq. 5. We use \( \delta(S) \) to denote the boundary of \( S \subset V \), i.e. the set of edges with exactly one endpoint in \( S \).

**Lemma 4.2 (Flipping Lemma)** Let \( S \) denote a maximal connected subgraph of \( G \) with every node of \( S \) incorrectly labelled by \( \hat{Y} \) or \(-\hat{Y}\). Then at least half the edges of \( \delta(S) \) are bad.

**Proof:** The computed labeling \( \hat{Y} \) (or \(-\hat{Y}\)) agrees with the edge observations on at least half the edges of \( \delta(S) \) — otherwise, flipping the labels of all nodes in \( S \) would yield a new labeling with agreement strictly higher than \( \hat{Y} \) (or \(-\hat{Y}\)). On the other hand, since \( S \) is maximal, for every edge \( e \in \delta(S) \), exactly one endpoint of \( e \) is correctly labeled. Thus every edge of \( \delta(S) \) is inconsistent with the ground truth. These two statements are compatible only if at least half the edges of \( \delta(S) \) are bad. □

Call a set \( S \) bad if at least half its boundary \( \delta(S) \) is bad. The Flipping Lemma motivates bounding the probability that a given set is bad, and then enumerating over sets \( S \). This approach can be made to work only if the collection of sets \( S \) is chosen carefully — otherwise, there are far too many sets and this approach fails to yield a non-trivial error bound.

To begin the analysis, let \( H \) denote the error of our algorithm on a random input. \( H \) seems difficult to analyze directly, so we introduce a simpler-to-analyze upper bound. This requires some definitions. Let \( C \) denote the subsets \( S \) of \( V \) such that the induced subgraph \( G[S] \) is connected. We classify subsets \( S \) of \( C \) into 6 categories (see Figure 2):

1. \( S \) contains no vertices on the perimeter of \( G \);
2. \( S \) contains vertices from exactly one side of the perimeter of \( G \);
3. \( S \) contains vertices from exactly two sides of the perimeter of \( G \), and these two sides are adjacent;
4. \( S \) contains vertices from exactly two sides of the perimeter of \( G \), and these two sides are opposite;
5. \( S \) contains vertices from exactly three sides of the perimeter of \( G \);
6. \( S \) contains vertices from all four sides of the perimeter of \( G \).

Let \( C_{\leq 6} \) denote the set of all \( S \subset V \) from one of the first 5 categories. For a set \( S \in C_{\leq 6} \), we define a corresponding filled in set \( F(S) \). Consider the connected components \( C_1, \ldots, C_k \) of \( G[V \setminus S] \) for such a subset \( S \). Call such a connected component 3-sided if it includes vertices from at least three
sides of the grid $G$. For every $S \in C_{<6}$ there is at least one 3-sided component; it is unique if $S$ has type 1, 2, 3, or 5. We define $F(S)$ as the union of $S$ with all the connected components of $G[V \setminus S]$ except for a single 3-sided one. Appendix B illustrates the filling-in procedure. $F(S)$ is not defined for type-6 components $S$. Observe that $F(S) \supseteq S$. Let $F = \{F(S) : S \in C_{<6}\}$ denote the set of all such filled-in components.

**Lemma 4.3** If $S_1, S_2$ are disjoint and not type 6, then $F(S_1), F(S_2)$ are distinct and not type 6.

*Proof:* If a set $S$ is not type 6, then every 3-sided component of $G[V \setminus S]$ contains one entire side of the grid perimeter. Since $F(S)$ excludes a 3-sided component, it cannot be type 6.

Also, for a set $S$ that is not type 6, the boundary of $F(S)$ is a non-empty subset of that of $S$. Thus, the non-empty set of endpoints of $\delta(F(S))$ that lie in $F(S)$ also lie in $S$. This implies that if $F(S_1) = F(S_2)$, then $S_1 \cap S_2 \neq \emptyset$. ■

The following error upper bound applies to whichever of $\hat{Y}, -\hat{Y}$ does not incorrectly classify a type-6 set (there is at most one type-6 set, so at least one of them has this property). Let $B$ denote the mislabeled vertices of such a labeling and let $B_1, \ldots, B_k$ denote the connected components (of types 1–5) of $G[B]$. The next lemma extends the Flipping Lemma.

**Lemma 4.4** For every set $B_i$, the filled-in set $F(B_i)$ is bad.

*Proof:* We first claim that $\hat{Y}$ agrees with the data on at least half the edges of $\delta(F(B_i))$; the same is true of $-\hat{Y}$. The reason is that flipping the label of every vertex of $F(B_i)$ increases the agreement with the data by the number of disagreeing edges of $\delta(F(B_i))$ minus the number of agreeing edges of $\delta(F(B_i))$, and this difference is non-positive by the optimality of $\hat{Y}$.

On the other hand, since $B_i$ is maximal, every neighbor of $B_i$ is correctly labeled in $\hat{Y}$. Since the neighborhood of $F(B_i)$ is a subset of $B_i$, this also holds for $F(B_i)$. Thus, $\hat{Y}$ disagrees with $Y$ on every edge of $\delta(F(B_i))$. ■

A crucial point is that Lemmas 4.3 and 4.4 imply that the random variable

\[ T = \sum_{F \in F} |F| \cdot 1_{F \text{ is bad}} \]  \hspace{1cm} (6)

is an upper bound on the error $H$ with probability 1. We now upper bound the easier-to-analyze quantity $T$. The first lemma provides an upper bound on the probability that a set $S$ is bad, as a function of its boundary size $|\delta(S)|$.

**Lemma 4.5** For every set $S$ with $|\delta(S)| = i$, $\Pr[S \text{ is bad}] \leq (3\sqrt{p})^i$. 

\[ \text{Figure 2: Examples of type 1, 2, 3, and 6 regions, left-to-right.} \]
Lemma 4.7

Let \( a \) be a positive integer. We do this by counting simple cycles in the dual graph.

For the next \( i \) choices for a starting point. There are at most 4 choices for the first edge, at most 3 choices for the next \((i - 2)\) edges, and at most one choice at the final step to return to the starting point.

\[
\Pr\left[ \sum_j Z_j \geq \frac{i}{2} \right] < \left( \frac{i}{2} \right) p^i \leq (2e)^2 p^i \leq (3\sqrt{p})^i
\]  

(7)

where \( Z_j \) is the indicator event of the \( i \)-th edge being bad. ■

The probability bound in Lemma 4.5 is naturally parameterized by the number of boundary edges. Because of this, we face two tasks in upper bounding \( T \). First, \( T \) counts the number of nodes of bad filled-in sets \( F \in F \), not boundary sizes. The next lemma states that the number of nodes of such a set cannot be more than the square of its boundary size.

Lemma 4.6

For \( F \in F \): (1) \(|F| \leq |\delta(F)|^2\); (2) if \( F \) is a type-1 region, then \(|F| \leq \frac{1}{10} |\delta(F)|^2\).

Proof: If \( F \) is a type 4 or 5 set, then \(|\delta(F)| \geq \sqrt{N} \) and the bound is trivial. If \( F \) is a type 1 set, let \( U \) be the smallest rectangle in the dual graph that contains \( F \). Let \( k, m \) denote the side lengths of \( U \). Then: \(|F| \leq km \leq \frac{1}{10} (2k + 2m)^2 \leq \frac{1}{10} |\delta(F)|^2\). Similarly for type 2 sets we have \(|F| \leq km \leq \min\{(2k + m)^2, (k + 2m)^2\} \leq |\delta(F)|^2\). Finally, for type 3 sets have \(|F| \leq km \leq (k + m)^2 \leq |\delta(F)|^2\).

The second task in upper bounding \( T \) is to count the number of filled-in sets \( F \in F \) that have a given boundary size. We do this by counting simple cycles in the dual graph.

Lemma 4.7

Let \( i \) be a positive integer.

(a) If \( i \) is odd or 2, then there are no type-1 sets \( F \in F \) with \(|\delta(F)| = i\);

(b) If \( i \) is even and at least 4, then there are at most \( \frac{N \cdot 2^{3i-2}}{2i} = N \cdot 2^{3i-2} \) type 1 sets \( F \in F \) with \(|\delta(F)| = i\);

(c) If \( i \) is at least 2, then there are at most \( 2\sqrt{N} \cdot 3^{i-2} \) type 2-5 sets \( F \in F \) with \(|\delta(F)| = i\).

Proof: Recall that, by construction, a filled-in set \( F \in F \) is such that both \( G[F] \) and \( G[V \setminus F] \) are connected. This is equivalent to the property that \( \delta(F) \) is a minimal cut of \( G \) — there is no subset \( S \) such that \( \delta(S) \) is a strict subset of \( \delta(F) \). In a planar graph such as \( G \), this is equivalent to the property that the dual of \( \delta(F) \) is a simple cycle in the dual graph \( G^d \) of \( G \) (e.g., see Section 4.6 of [17]).

Note that the dual graph \( G^d \) is just an \((n - 1) \times (n - 1)\) grid graph — with one vertex per “grid cell” of \( G \) — plus an extra vertex \( z \) of degree \( 4(\sqrt{N} - 1) \) that corresponds to the outer face of \( G \). The type-1 sets of \( F \) are in dual correspondence with the simple cycles of \( G^d \) that do not include \( z \), the other sets of \( F \) are in dual correspondence with the simple cycles of \( G^d \) that do include \( z \).

The cardinality of the boundary \(|\delta(F)|\) equals the length of the corresponding dual cycle.

Part (a) follows from the fact that \( G^d \setminus \{z\} \) is a bipartite graph, with only even cycles, and with no 2-cycles.

For part (b), we count simple cycles of \( G^d \) of length \( i \) that do not include \( z \). There are at most \( N \) choices for a starting point. There are at most 4 choices for the first edge, at most 3 choices for the next \((i - 2)\) edges, and at most one choice at the final step to return to the starting point.
Each simple cycle of $G^d \setminus \{z\}$ is counted $2i$ times in this way, once for each choice of the starting point and the orientation.

For part (c), we count simple cycles of $G^d$ of length $i$ that include $z$. We start the cycle at $z$, and there are at most $4\sqrt{N}$ choices for the first node. There are at most 3 choices for the next $i-2$ edges, and at most one choice for the final edge. This counts each cycle twice, once in each orientation.

Let $F_1 \subseteq F$ denote the type-1 sets of $F$. The computation below shows that

$$E[T] \leq c p^2 N + O(p\sqrt{N})$$

for a constant $c > 0$ that is independent of $p$ and $N$, which completes the analysis of the first stage of the algorithm $\bar{A}$. The intuition for why this computation works out is that Lemma 4.7 implies that there is only an exponential number of relevant regions to sum over; Lemma 4.6 implies that the Hamming error is quadratically related to the (bad) boundary size; and Lemma 4.5 implies that the probability of a bad boundary is decreasing exponentially in $i$ (with base $3\sqrt{p}$). Provided $p$ is at most a sufficiently small constant (independent of $N$), the probability term dominates and so the expected error is small.

Formally, we have

$$E[T] = \sum_{F \in F} |F| \cdot \Pr[F \text{ is bad}]$$

\[= \sum_{i=2}^{\infty} \sum_{F \in F_1 : |\delta(F)|=2i} |F| \cdot \Pr[F \text{ is bad}] + \sum_{j=2}^{\infty} \sum_{F \in F \setminus F_1 : |\delta(F)|=j} |F| \cdot \Pr[F \text{ is bad}]\]

\[\leq \sum_{i=2}^{\infty} N \cdot \frac{1}{i} \cdot \frac{3^{2i-2} 2^i}{i^2} \cdot (3\sqrt{p})^{2i} + \sum_{j=2}^{\infty} 2\sqrt{N} \cdot 3^{j-2} \cdot j^2 \cdot (3\sqrt{p})^j\]

\[\leq N \sum_{i=2}^{\infty} \frac{i}{16} (81p)^i + \sqrt{N} \sum_{j=2}^{\infty} \frac{2j^2}{9} (9\sqrt{p})^j\]

\[= N (cp^2) + O(p\sqrt{N}),\]

for a constant $c > 0$ that is independent of $p$ and $N$. In the derivation, (9) follows from the definition of $T$ and linearity of expectation, (10) follows from Lemmas 4.5 and 4.6, and (11) follows from Lemma 4.7. In the final line, we are assuming that $p < 1/81$.

**Remark 4.8** There are several ways to optimization the computation above. The requirement that $p < 1/81$ was needed for the infinite series to converge. To improve this, we can use the tighter upper bound of $(2ep)^{i/2}$ for the probability that a region of boundary size $i$ is bad (see Lemma 4.5). We can then replace the upper bound on the number of regions of each type in Lemma 4.7 with tighter results from statistical physics. In particular, the number of type-1 sets with boundary size $i$ can be upper bounded by $N\mu^i$ (Eq. 3.2.5 of [31]), where $\mu$ is the so-called connective constant of square lattices and is upper bounded by 2.65 [12]. The number of type 2–5 sets with boundary
length \( i \) can similarly be upper bounded by \( 4\sqrt{N}\mu^i e^{\kappa\sqrt{i}} \) for the same value of \( \mu \) and for some fixed constant \( \kappa > 0 \) [23]. Putting these together, we obtain that the infinite series for all region types is at most a constant when \( p < 1/39 \).

To compute an upper bound on the constant \( c \) in the term in [12] that is linear in \( N \), recall that this term can be attributed to the type-1 regions. We expand the sum in [9] over type-1 regions into two terms: one term that explicitly enumerates over type-1 regions whose corresponding simple cycle in \( G^d \) is of length \( i = 2 \) to 100, and a remainder term. The sum in the first term can be computed exactly as follows. For each value of \( i \), the probability that the region is bad is simply \( \sum_{k=i/2}^{i} (\frac{i}{k}) p^k (1-p)^{i-k} \). We can then use the bound \( \sum_{F \in F_1 : |\delta(F)| = i} |F| \leq N \sum_{a=1}^{i^2/16} a c_{a,i} \), where \( c_{a,i} \) is the number of distinct cycles in an infinite grid of length \( i \) and area \( a \) (up to translation). These cycles also go by the name of self-avoiding polygons in statistical physics, and the numbers \( c_{a,i} \) have been exhaustively computed up to \( i = 100 \) [24]. Finally, the infinite sum in the remainder can be shown to be upper bounded by \( 51 b^{51}/(1-b)^3 \) for \( b = 2ep(2.65)^2 \). The resulting function can then be shown to be upper bounded by \( 8Np^2 \) for \( p \leq 0.017 \).

**Analyzing the Second Stage:** Our analysis so far shows that the better of \( \hat{Y}, -\hat{Y} \) has small error with respect to the ground truth \( Y \). In the second phase, we use the node labels to choose between them via a “majority vote.” We next show that, provided \( q \) is slightly below \( \frac{1}{2} \), the better of \( \hat{Y}, -\hat{Y} \) is chosen in the second stage with high probability. This completes the proof of Theorem 4.1.

Our starting point for the second-stage analysis is the inequality \( \mathbb{E}[H_0] \leq N \cdot cp^2 \), where \( H_0 \) is the Hamming error of the better of \( \hat{Y}, -\hat{Y} \). Markov’s inequality implies that \( \Pr[H_0 \geq \frac{1}{kp} N cp^2] \leq kp^2 \), where \( k \) is a free parameter.

For the second stage, let \( B' \) be the set of wrong node observations. Chernoff bounds imply that, for every constant \( \delta > 0 \) and sufficiently large \( N \), \( \Pr[|B'| \geq (1+\delta)Nq] \leq \frac{1}{N^2} \). Observe that if the sum of the number of bad node observations and the number of misclassified nodes for the better of \( \hat{Y}, -\hat{Y} \) is less than \( N/2 \), then the two-stage algorithm \( \mathcal{A} \) would choose the better of \( \hat{Y}, -\hat{Y} \). Hence, with probability \( 1 - kp^2 - \frac{1}{N^2} \), the algorithm would choose the better of \( \hat{Y}, -\hat{Y} \) provided \( \frac{1}{kp^2} N cp^2 + (1+\delta)Nq < \frac{N}{2} \), or equivalently,

\[
\frac{c}{k} + (1+\delta)q < \frac{1}{2}.
\]

This inequality is satisfied for small \( \delta \) provided \( k > \frac{c}{1/2 - (1+\delta)q} \). Thus,

\[
\mathbb{E}[H] \leq 1 \cdot N cp^2 + (kp^2 + \frac{1}{N^2}) \cdot N \leq N \cdot ((c + 1)p^2 + kp^2) \leq N \cdot C p^2
\]

for \( N > N_0(p, q) \), where \( H \) is the error of the 2-step algorithm. (In second inequality we use that \( N > \frac{1}{p} \))

### 4.3 Lower Bound

In this section, we prove that every algorithm suffers worst-case (over the ground truth) expected error \( \Omega(p^2 N) \) on 2D grid graphs, matching the upper bound for the 2-step algorithm \( \mathcal{A} \) that we proved in Theorem 4.1. We use the fact that marginal inference is minimax optimal for Eq. 2 (see Appendix A). The expected error of marginal inference is independent of the ground truth (by
symmetry), so we can lower bound its expected error for the all-0 ground truth. Also, its error only decreases if it is given part of the ground truth.

Let \( G = (V,E) \) denote an \( n \times n \) grid with \( N = n^2 \) vertices. Let \( Y : V \to \{-1,+1\} \) denote the ground truth. We consider the case where \( Y \) is chosen at random from the following distribution. Color the nodes of \( G \) with black and white like a chess board. White nodes are assigned binary values uniformly and independently. Black nodes are assigned the label +1. Given \( Y \), input is generated using the random process described in Section 3.

Consider an arbitrary function from inputs to labellings of \( V \). We claim that the expected error of the output of this function, where the expectation is over the choice of ground truth \( Y \) and the subsequent random input, is \( \Omega(p^2N) \). This implies that, for every function, there exists a choice of ground truth \( Y \) such that the expected error of the function (over the random input) is \( \Omega(p^2N) \).

Given \( Y \), call a white node ambiguous if exactly two of the edges incident to it are labeled “+1” in the input. A white node is ambiguous with probability \( 6p^2(1-p)^2 \geq 5.1p^2 \) for \( p \leq 0.078 \). Since there are \( N/2 \) white nodes, and the events corresponding to ambiguous white nodes are independent, Chernoff bounds imply that there are at least \( \frac{5p^2}{2}N \) ambiguous white nodes with very high probability.

Let \( L \) denote the error contributed by ambiguous white nodes. Since the true labels of different white nodes are conditionally independent (given that all black nodes are known to have value +1), the function that minimizes \( \mathbb{E}[L] \) just predicts each white node separately. The algorithm that minimizes the expected value of \( L \) simply predicts that each ambiguous white node has true label equal to its input label. This prediction is wrong with constant probability, so \( \mathbb{E}[L] = \Omega(p^2N) \) for every algorithm. Since \( L \) is a lower bound on the Hamming error, the result follows.

5 Extensions

The section sketches several extensions of our model and results, to planar graphs beyond grids (Section 5.1), to expander graphs (Section 5.2), to graphs with a large minimum cut (Section 5.3), and to semi-random models (Section 5.4).

5.1 Approximate Recovery in Other Planar Graphs

Section 4 gives a polynomial-time algorithm for essentially information-theoretically optimal approximate recovery in grid graphs. While the analysis does use properties of grids beyond planarity, it is robust in that it applies to all planar graphs that share two key features with grids.

The path graph (see Section 3) shows that approximate recovery is not possible for all planar graphs; additional conditions are needed. The first property, which fails in “thin” planar graphs like a path but holds in many planar graphs of interest, is the following weak expansion property:

\((P1)\) (Weak expansion.) For some constants \( c_1,c_2 > 0 \), every filled-in set \( F \in \mathcal{F} \) satisfies \( |F| \leq c_1|\delta(F)|^{c_2} \).

(Filled-in sets can be defined analogously to the grid case.)

The second key property is that the number of filled-in sets with a given boundary size \( i \) should be at most exponential in \( i \). As in Lemma 4.7, a sufficient (but not necessary) condition for this property is that the dual graph has bounded degree (except possibly for the vertex corresponding to the outer face, which can have arbitrary degree).
(P2) \textit{(Bounded Dual Degree.)} Every face of \(G\), except possibly for the outer face, contains at most a constant \(c_3\) number of edges.

Our proof of computationally efficient approximate recovery (Theorem \(4.1\)) extends to show that approximate recovery is possible in every planar graph that satisfies properties (P1) and (P2); the precise bound on the function \(f(p)\) depends on the constants \(c_1, c_2, c_3\).

### 5.2 Approximate Recovery in Expander Graphs

Structured prediction on expander graphs is often applied to relational classification (e.g., predicting protein-protein interactions or web-page classification). This section proves that every family \(G\) of \(d\)-regular expanders admits approximate recovery. Recall the definition of such a family: for some constant \(c > 0\), for every \(G \in \mathcal{G}\) with \(N\) vertices and every set \(S \subseteq V\) with \(|S| \leq N/2\), \(|\delta(S)| \geq c \cdot d \cdot |S|\), where the boundary \(\delta(S)\) is the set of edges with exactly one endpoint in \(S\). We claim that \(G\) allows approximate recovery with \(f(p) = 3p/c\), and proceed to the proof.

The algorithm is the same as in Section 4; it is not computationally efficient for expanders. As in Section 4, analyzing the two-stage algorithm reduces to analyzing the better of the two solutions produced by the first stage. We therefore assume that the output \(\hat{Y}\) of the first stage has error \(H\) at most \(N/2\).

Fix a noise parameter \(p \in (0, \frac{1}{2})\), a graph \(G \in \mathcal{G}\) with \(N\) sufficiently large, and a ground truth. Let \(B\) denote the set of bad edges. Chernoff bounds imply that for all sufficiently large \(N\), the probability that \(|B| \geq 2p|E| = pdN\) is at most \(1/N^2\). When \(|B| > pdN\), we can trivially bound the error \(H\) by \(N/2\). When \(|B| \leq pdN\), we bound \(H\) from above as follows.

Let \(S\) denote the nodes of \(V\) correctly classified by the first stage \(\hat{Y}\) and \(C_1, \ldots, C_k\) the connected components of the (misclassified) nodes of the induced subgraph \(G[V \setminus S]\). Since \(H/2, |C_i| \leq N/2\) for every \(i\). We have

\[
H = \sum_{i=1}^{k} |C_i| \leq \frac{1}{cd} \cdot \sum_{i=1}^{k} |\delta(C_i)| \leq \frac{2}{cd} \cdot \sum_{i=1}^{k} |\delta(C_i) \cap B| \leq \frac{2}{cd} \cdot |B|,
\]

where the first inequality follows from the expansion condition, the second from the Flipping Lemma (Lemma 4.2), and the third from the fact that the \(\delta(C_i)\)'s are disjoint (since the \(C_i\)'s are maximal). Thus, when \(|B| \leq pdN\), \(H \leq \frac{2p}{c}N\). Overall, we have

\[
\mathbb{E}[H] \leq 1 \cdot \frac{2p}{c}N + \frac{1}{N^2} \cdot \frac{N}{2} \leq \frac{3p}{c}N
\]

for \(N\) sufficiently large, as claimed.

### 5.3 Graphs with a Large Min Cut

Approximate recovery is also possible in every graph family \(\mathcal{G}\) for which the global minimum cut \(c^*\) is bounded below by \(c \log N\) for a sufficiently large constant \(c\). This class of graphs is incomparable to the expanders considered in Section 5.2.

To see why a large minimum cut is sufficient, we modify the first-stage analysis in the proof of Theorem 4.1 as follows. Define \(C\) as the subsets \(S\) of \(V\) such that \(|S| \leq N/2\) and \(G[S]\) is connected, and \(C_i\) the subset of \(C\) corresponding to sets \(S\) with \(|\delta(S)| = i\). Recall that, for every \(\alpha \geq 1\), the number of \(\alpha\)-approximate minimum cuts of an undirected graph is at most \(N^{2\alpha}\) (e.g.,
see [27]). Thus, \( |C_i| \leq N^{2i/c^*} \), which is at most \( 2^{2i/c^*} \) when \( c^* \geq c \log_2 N \). That is, there can only be an exponential number of connected subgraphs with a given boundary size (cf., property (P1) in Section 5.1). A calculation along the lines of the proof of Theorem 4.1 then implies that approximate recovery is possible, provided the constant \( c \) is sufficiently large.

5.4 Semi-Random Models

All of our positive results make minimal use of the properties of the random process that generates inputs given the ground truth. Our proofs only need the fact that the probability that a boundary \( \delta(S) \) consists of at least half bad edges decays exponentially in the boundary size \( |\delta(S)| \) (Lemma 4.5). As such, our positive results are robust to many variations in the random model.

For example, the fact that every edge has the same noise parameter \( p \) is not important — our algorithms continue to have the exact same guarantees, with the same proofs, with the function \( f(p) \) replaced by \( f(p_{\text{max}}) \), where \( p_{\text{max}} \) is the maximum noise parameter of any edge. If bad edges are negatively correlated instead of independent, then the relevant Chernoff bounds (and hence Lemma 4.5) continue to hold (see e.g. [18]), and our results remain unchanged.

Most interestingly, our positive results can accommodate the following semi-random adversary (cf., [19]). Given a graph \( G \) and ground truth, as before nature independently designates each edge as good or bad with probability \( 1 - p \) and \( p \), and similarly for nodes (with probability \( 1 - q \) and \( q \)). Good nodes and edges are labelled according to the ground truth. An adversary, who knows what algorithm will be used on the input, selects arbitrary labels for the bad nodes and edges. Our basic models corresponds to the special case in which the adversary labels every bad node and edge to be inconsistent with the input. Such semi-random adversaries can often foil algorithms that work well in a purely random model, especially algorithms that are overly reliant on the details of the input distribution or that are “local” in nature.

In all of our proofs of our positive results, we effectively assume that every relevant set \( S \) that has a boundary \( \delta(S) \) with at least half bad edges contributes \( |S| \) to our algorithm’s error. Thus, an adversary maximizes our error upper bound by maximizing the number of bad nodes and edges. In other words, from the standpoint of our error bounds, a semi-random adversary is no worse than a random one.

6 Empirical Study

Our theoretical analysis suggests that statistical recovery on 2D grid graphs can attain an error that scales with \( p^2 \). Furthermore, we show that this error is achieved using the two-step algorithm in Section 4. Here we describe a synthetic experiment that compares the two-step algorithm to other recovery procedures. We consider a \( 20 \times 20 \) grid, with high node noise of 0.4 and variable edge noise levels. In addition to the two-step algorithm we consider the following:

- Marginal inference - predicting according to \( p(Y_i|X) \). As mentioned in Section 3 this is the optimal recovery procedure. Although it is generally hard to calculate, for the graph size we use it can be done in 20 minutes per model.

- Local LP relaxation - Instead of calculating \( p(Y_i|X) \) one can resort to approximation. One possibility is to calculate the mode of \( p(Y|X) \) (also known as the MAP problem). However, since we also experimented with a greedy hill climbing procedure, but results were poor and are not shown.

\[ \text{14} \]
this is also hard, we consider LP relaxations of the MAP problem. The simplest such relaxation assumes locally consistent pseudo-marginals.

- Cycle LP relaxation - A tighter version of the LPs above uses cycle constraints instead of pairwise. In fact, for planar graphs with no external field (as in the first step of our two step algorithm) this relaxation is tight. It is thus of interest to study it in our context. For both the cycle and local relaxations we use the code for [34].

Fig. 6 shows the expected error for the different algorithms, as a function of edge noise. It can be seen that the two step procedure almost matches the accuracy of the optimal marginal algorithm for low noise levels. As the noise increases the gap grows. Another interesting observation is that the local relaxation performs significantly worse than the other baselines, but that the cycle relaxation is close to optimal. The latter observation is likely to be due to the fact that with high node noise and low edge noise, the MAP problem is “close” to the no node-noise case, where the cycle relaxation is exact. However, an analysis of the Hamming error in this case remains an open problem.

![Figure 3: Average Hamming error for different recovery algorithms. Data is generated from a 20 × 20 grid with node noise \( q = 0.4 \) and variable edge noise \( p \). The true \( Y \) is the all zeros word. Results are averaged over 100 repetitions.](image)

7 Discussion

Structured prediction underlies many empirically successful systems in machine vision and NLP. In most of these (e.g., [29, 26]) the inference problems are intractable and approximate inference is used instead. However, there is little theoretical understanding of when structured prediction is expected to perform well, how its performance is related to the structure of the score function, which approximation algorithms are expected to work in which setting, etc.

In this work we present a first step in this direction, by analyzing the error of structured prediction for 2D grid models. One key finding is that a two-step algorithm attains the information theoretically optimal error in a certain regime of parameters. What makes this setting particularly interesting from a theoretical perspective is that exact inference (marginals and MAP) is intractable due to the intractability of planar models with external fields. Thus, it is rather surprising that a tractable algorithm achieves optimal performance.
Our work opens the door to a number of new directions, with both theoretical and practical implications. In the context of grid models, we have not studied the effect of the node noise $q$ but rather assumed it may arbitrary (less than 0.5). Our two step procedure uses both node and edge evidence, but it is clear that for small $q$, improved procedures are available. In particular, the experiments in Section 6 show that decoding with cycle LP relaxations results in empirical performance that is close to optimal. More generally, we would like to understand the statistical and computational properties of structured prediction for complex tasks such as dependency parsing \cite{parsing} and non-binary variables (as in semantic segmentation). In these cases, it would be interesting to understand how the structure of the score function affects both the optimal expected accuracy and the algorithms that achieve it.

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A Marginal Inference is the Minimax Optimal Algorithm

In this section, we prove marginal inference using the uniform prior, which we denote by $A_1$, is the minimax optimal algorithm (i.e., minimizes $e(A) = \max_y e_y(A)$). The marginal inference algorithm predicts each node separately by $\hat{Y}_i \leftarrow \arg \max_{Y_i} p(Y_i | X)$ using the uniform prior over $X$.

Assume for contradiction that there is an algorithm $A_0$ that yields strictly smaller error than marginal inference. Hence, by definition the of a minimax optimal algorithm, there exists ground truth assignments $y_0$ and $y_1$ such that $\max_y e_y(A_0) = e_{y_0}(A_0) < e_{y_1}(A_1)$. By symmetry, the marginal inference algorithm has equal error for every ground truth. Hence, $e_y(A_0) < e_y(A_1)$ for every ground truth assignments $y$.

On the other hand, marginal inference minimizes the expected Hamming error when the prior distribution over ground truth assignments is uniform. To see why, let $\hat{Y}_i(X)$ be an estimator of the $i$-th node. The expected Hamming error of $\hat{Y}_i$ assuming uniform prior on $Y_i$ is

$$\Pr[\hat{Y}_i(X) \neq Y_i] = \sum_X 1_{\hat{Y}_i(X) = +1} \cdot \frac{1}{2} \Pr[\mu^+_i(X)] + \sum_X 1_{\hat{Y}_i(X) = -1} \cdot \frac{1}{2} \Pr[\mu^-_i(X)]$$

where $\mu^+_i$ and $\mu^-_i$ are the distributions of $X$ conditioned on $Y_i = +1$ and $Y_i = -1$, respectively. Since $E_y[e_y(A)]$ is the sum of the expected error at individual nodes, marginal inference using the
uniform prior minimizes it. The optimality of marginal inference for the uniform prior contradicts the fact that $A_0$ performs better than marginal inference on all ground truth assignments.

Notice that this proof also works for the subset of ground truths considered in the proof of lower bound for the grids (Section 4.3).

B Illustration of Filled In Sets

Recall that for every subset $S$ we defined a corresponding filled in set $F(S)$. Figures B1–B3 illustrate the transformation from a subset $S$ to the corresponding filled-in set $F(S)$.

Figure 4: An example of a type 1 set (left) and a type 2 set (right) and the corresponding filled-in sets.

Figure 5: An example of a type 3 set (left) and a type 4 set (right) and the corresponding filled-in sets.

Figure 6: An example of a type 5 set and the corresponding filled-in set (left) and an example of type 6 set.