How Hard is Inference for Structured Prediction?

David Sontag

Joint work with Amir Globerson, Tim Roughgarden, and Cafer Yildirim



Computer vision Image segmentation

input: image



output: segmentation





• Input: $x \in \mathcal{X}$ Output: labeling $y \in \mathcal{Y}$



• Given an input x, the "goodness" of a prediction y is characterized by a score function s(x,y) such that

s(x,y) = High if y is a good labeling for x Low if y is a bad labeling for x

• Pairwise models have a score that decomposes over edges of a graph, e.g.

$$s(x,y) = \sum_{ij \in E} s_{ij}(x,y_i,y_j) + \sum_{i \in V} s_i(x,y_i)$$

• Input: $x \in \mathcal{X}$ Output: labeling $y \in \mathcal{Y}$



• Given an input x, the "goodness" of a prediction y is characterized by a score function s(x,y) such that

• Consider the following distribution over labelings:

$$\Pr(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \exp\left\{\sum_{ij\in E} s_{ij}(x, y_i, y_j) + \sum_{i\in V} s_i(x, y_i)\right\}$$

• Conditional random fields (Lafferty et al. '01) use maximum likelihood learning, and predict using marginal inference $\arg \max_{y_i} \Pr(y_i \mid \mathbf{x})$ for all *i*

• Input: $x \in \mathcal{X}$ Output: labeling $y \in \mathcal{Y}$



• Given an input x, the "goodness" of a prediction y is characterized by a score function s(x,y) such that

• Consider the following distribution over labelings:

$$\Pr(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \exp\left\{\sum_{ij\in E} s_{ij}(x, y_i, y_j) + \sum_{i\in V} s_i(x, y_i)\right\}$$

• Max-margin learning (Collins '02, Taskar et al. '03, Tsochantaridis et al. '05) seeks large margin, and predicts using MAP inference $\arg \max_{\mathbf{y}} \Pr(\mathbf{y} \mid \mathbf{x})$

Inference is NP-hard. So why does approximate inference work so well?

- Both marginal and MAP inference are in general NP-hard
- Nonetheless, heuristic inference algorithms can get state-ofthe-art results for structured prediction



Input images

Stereo vision



Ground truth depth



Prediction (approximate MAP inference with graph cuts)

(Pal et al., "On Learning Conditional Random Fields for Stereo", IJCV 2010)

Inference is NP-hard. So why does approximate inference work so well?

- Both marginal and MAP inference are in general NP-hard
- Nonetheless, heuristic inference algorithms can get state-ofthe-art results for structured prediction Why?

Foreground-background segmentation



Input images



Ground truth



Prediction (approximate MAP inference with dual decomposition)

(Borenstein & Ullman '02, Domke '13)

Inference is NP-hard. So why does approximate inference work so well?

- Both marginal and MAP inference are in general NP-hard
- Nonetheless, heuristic inference algorithms can get state-ofthe-art results for structured prediction Why?
- These instances do not correspond to any known tractable family (they are not tree-structured, submodular, ...)
- Intuitively, however, they are *close* to something tractable
- This paper: We demonstrate a setting in which approximate inference algorithms provably obtain small Hamming error,

$$H(Y, \hat{Y}) = \sum_{i=1}^{N} \mathbb{1}[\hat{Y}_i \neq Y_i]$$

Y: Ground truth \hat{Y} : Prediction by approx inf

Key questions for theoretical analysis

- What are the information theoretic limits?
- What are the computational & statistical trade-offs?
 - How much worse is MAP inference compared to marginal inference?
 - What is the best prediction accuracy attainable in polynomial time?
 - Provable guarantees for linear programming relaxations?

q = node noise Generative process p = edge noise

- Goal is to predict a set of labels Y_1 , ..., Y_N , $Y_i \in \{-1, 1\}$, from observations X
- Our analysis assumes observations X generated from Y by the following process on graph G=(V,E):

 \circ X_i = -Y_i with probability **q**, and X_i = Y_i otherwise

○ For $ij \in E$, $X_{ij} = -Y_iY_j$ with probability p, and $X_{ij} = Y_iY_j$ otherwise



q = node noise Generative process p = edge noise

- Goal is to predict a set of labels Y_1 , ..., Y_N , $Y_i \in \{-1, 1\}$, from observations X
- Our analysis assumes observations X generated from Y by the following process on graph G=(V,E):

 \circ X_i = -Y_i with probability **q**, and X_i = Y_i otherwise

• For $ij \in E$, $X_{ij} = -Y_iY_j$ with probability p, and $X_{ij} = Y_iY_j$ otherwise



q = node noise Generative process p = edge noise

- Goal is to predict a set of labels Y_1 , ..., Y_N , $Y_i \in \{-1, 1\}$, from observations X
- Our analysis assumes observations X generated from Y by the following process on graph G=(V,E):

 \circ X_i = -Y_i with probability **q**, and X_i = Y_i otherwise

• For $ij \in E$, $X_{ij} = -Y_iY_j$ with probability p, and $X_{ij} = Y_iY_j$ otherwise

• The maximum likelihood (ML) estimator is:

$$\max_{Y} \quad \sum_{uv \in E} \frac{1}{2} X_{uv} Y_{u} Y_{v} \log \frac{1-p}{p} + \sum_{v \in V} \frac{1}{2} X_{u} Y_{u} \log \frac{1-q}{q}$$

• Even when G is a planar graph, this maximization problem is NPhard (reduction from max-cut) q = node noiseGenerative processp = edge noise

- Goal is to predict a set of labels Y_1 , ..., Y_N , $Y_i \in \{-1, 1\}$, from observations X
- Our analysis assumes observations X generated from Y by the following process on graph G=(V,E):

• $X_i = -Y_i$ with probability **q**, and $X_i = Y_i$ otherwise

○ For $ij \in E$, $X_{ij} = -Y_iY_j$ with probability p, and $X_{ij} = Y_iY_j$ otherwise

• The maximum likelihood (ML) estimator is:

2D grid tractable without a field $\begin{array}{ll} & \underset{Y}{\max} & \underset{uv \in E}{\sum} \ \frac{1}{2} X_{uv} Y_u Y_v \log \frac{1-p}{p} + \underset{v \in V}{\sum} \ \frac{1}{2} X_u Y_u \log \frac{1-q}{q} \end{array}$

• Even when G is a planar graph, this maximization problem is NPhard (reduction from max-cut)

Relating the generative process to CRFs



Empirical study of inference



Empirical study of inference



- Ground truth = all -1's
- Node noise q=0.4
- Results averaged over 100 trials

What are the information theoretic limits?

- <u>Theorem (lower bound)</u>: Every algorithm must have error $\Omega(p^2N)$, where N is the number of nodes
- Proof sketch:



Shaded nodes fixed to -1.

White nodes sampled uniformly, +1 with prob. $\frac{1}{2}$ -1, otherwise.

(b) Call a node *ambiguous* if exactly two of its edge observations are ≠ (i.e., -1) and two are = (i.e. +1)

How many? $\frac{N}{2} {4 \choose 2} p^2 (1-p)^2 \approx \frac{5N}{2} p^2$

(c) Best is to predict according to node observation. Will be wrong with probability q

(d) $E[H] \ge \frac{5N}{2}p^2q$, i.e. $\Omega(p^2N)$ q = node noise p = edge noise

Two-stage approximate inference

• We analyze the following approximate inference algorithm:

Require: Edge and node observations XStage 1 (uses only edge1: $\hat{Y} \leftarrow \arg \max_Y \sum_{uv \in E} X_{uv} Y_u Y_v$ Stage 1 (uses only edge2: if $\sum_{v \in V} X_v \hat{Y}_v < 0$ thenobservations)3: $\hat{Y} \leftarrow -\hat{Y}$ Stage 24: end ifoutput \hat{Y}

- MAP inference for Stage 1 is polynomial time using matching (Fisher '66) or solving cycle LP (Barahona '82)
- Intuition: after stage 1, either Ŷ or its flip –Ŷ is *close* in Hamming distance to the ground truth:



We choose one of these by looking at the node observations (stage 2)



Two-stage algorithm is optimal for grids

<u>Theorem (upper bound)</u>: The two-stage algorithm obtains error O(p²N) when p < 0.017

Key structural lemma

- Let $\delta(S)$ denote the outer boundary of a set of vertices S
- <u>An edge is bad</u> if $X_{uv} = -Y_u Y_v$
- Lemma 1 (Flipping Lemma): Let S denote a maximal connected subgraph of G with every node of S mispredicted by Ŷ. Then, at least half the edges of δ(S) are <u>bad</u>

Example:

 $\,\circ\,$ Suppose ground truth Y is all -1, and we mispredicted the middle node $\hat{Y}^{}_1$

 \circ Suppose for contradiction that all four edges of $\delta(S)$ are "=" (i.e., not bad)

 $\circ~$ Flipping \hat{Y}_1 to -1 strictly improves the objective, contradicting optimality of \hat{Y}

$$\hat{Y} \leftarrow \arg\max_{Y} \sum_{uv \in E} X_{uv} Y_u Y_v$$



"=" denotes X_{IIV}=1

Bounding number and size of maximally connected mispredicted sets

• Let $\delta(S)$ denote the outer boundary of a set of vertices S



- <u>A set S is bad</u> if at least half its outer boundary $\delta(S)$ is bad
- Lemma 2: For every set S with $|\delta(S)| = k$, $\Pr[S \text{ is bad}] \le (9p)^{k/2}$
- Lemma 3: For every set S, $|S| \le c |\delta(S)|^2$
- Lemma 4: There are at most 4N3^{k-2}/(2k) sets with |δ(S)| = k for even length k (and zero for odd k)
- Many large sets (Lemma 3+4), but unlikely to be bad (Lemma 2) Result is then shown using a Union Bound.

Discussion & Conclusions

- Results extend to other generative processes, planar graphs and d-regular expander graphs
- **Take away 1:** Think about approximate inference for structured prediction in terms of *recovering ground truth*
- **Take away 2**: When using dual decomposition or LP relaxations, look for tractable *and accurate* components
- Many open problems
 - Non-binary models (e.g., for stereo vision), and other prediction tasks such as dependency parsing
 - Analysis of cycle LP relaxation: might need new proof techniques

Extra slides

Error of an algorithm

• The *error* of an algorithm *A* is defined to be the *worst-case* (over *Y*) expected Hamming error:

$$err(\mathcal{A}) = \max_{y} \mathbb{E}_{X|Y=y} \left[H(y, \mathcal{A}(X)) \right]$$

- Marginal inference using a uniform prior for Y can be shown to be minimax optimal
 - *Statistically efficient,* but not *computationally efficient*

<u>Theorem (upper bound)</u>: The two-stage algorithm obtains error O(p²N)

$$\begin{split} H &= \sum_{\text{cycles } C} \sum_{S:\delta(S)=C} |S| \mathbb{1} \Big[S \text{ is maximally connected mispredicted set} \Big] \\ &\leq \sum_{k=4,6,8,\dots} \left(\max_{S:|\delta(S)|=k} |S| \right) \sum_{\text{cycles } C:|C|=k} \mathbb{1} \Big[\text{at least half of edges in } C \text{ are bad} \Big] \\ &\leq \sum_{k=4,6,8,\dots} k^2 \sum_{\text{cycles } C:|C|=k} \mathbb{1} \Big[\text{at least half of edges in } C \text{ are bad} \Big] \end{split}$$

$$E[H] \leq \sum_{k=4,6,8,...} k^2 \cdot (9p)^{k/2} \cdot 4N3^{k-2}/(2k)$$
 (Using results from percolation, can substantially improve constants)

$$\approx N \sum_{k=4,6,8,\dots}^{\infty} k \cdot (9p)^{k/2} 3^k = N \sum_{l=2}^{\infty} 2l \cdot (9p)^l 9^l \approx N \sum_{l=2}^{\infty} l(81p)^l = O(p^2 N)$$

Generalizations

- Planar graphs
 - Use two-step algorithm: still polynomial time
 - Need two properties
 - Weak expansion: $|F| \le c_1 |\delta(F)|^{c_2}$, for every set *F*
 - *Bounded dual degree* (used in bounding the number of sets)
- d-regular expander graphs
 - Use two-step algorithm: *not* computationally efficient
 - Expected Hamming error O(Np): different analysis



