

Learning Efficient Random Maximum A-Posteriori Predictors with Non-Decomposable Loss Functions

Authored by:

Tommi Jaakkola
Joseph Keshet
Tamir Hazan
Subhransu Maji

Abstract

In this work we develop efficient methods for learning random MAP predictors for structured label problems. In particular, we construct posterior distributions over perturbations that can be adjusted via stochastic gradient methods. We show that every smooth posterior distribution would suffice to define a smooth PAC-Bayesian risk bound suitable for gradient methods. In addition, we relate the posterior distributions to computational properties of the MAP predictors. We suggest multiplicative posteriors to learn super-modular potential functions that accompany specialized MAP predictors such as graph-cuts. We also describe label-augmented posterior models that can use efficient MAP approximations, such as those arising from linear program relaxations.

1 Paper Body

Learning and inference in complex models drives much of the research in machine learning applications ranging from computer vision, natural language processing, to computational biology [1, 18, 21]. The inference problem in such cases involves assessing the likelihood of possible structured-labels, whether they be objects, parsers, or molecular structures. Given a training dataset of instances and labels, the learning problem amounts to estimation of the parameters of the inference engine, so as to best describe the labels of observed instances. The goodness of fit is usually measured by a loss function. The structures of labels are specified by assignments of random variables, and the likelihood of the assignments are described by a potential function. Usually, it is feasible to only find the most likely or maximum a-posteriori (MAP) assignment, rather than sampling according to their likelihood. Indeed, substantial effort has gone into

developing algorithms for recovering MAP assignments, either based on specific parametrized restrictions such as super-modularity [2] or by devising approximate methods based on linear programming relaxations [21]. Learning MAP predictors is usually done by structured-SVMs that compare a ?loss adjusted? MAP prediction to its training label [25]. In practice, most loss functions used decompose in the same way as the potential function, so as to not increase the complexity of the MAP prediction task. Nevertheless, non-decomposable loss functions capture the structures in the data that we would like to learn. Bayesian approaches for expected loss minimization, or risk, effortlessly deal with nondecomposable loss functions. The inference procedure samples a structure according to its likelihood, and computes its loss given a training label. Recently [17, 23] constructed probability models through MAP predictions. These ?perturb-max? models describe the robustness of the MAP prediction to random changes of its parameters. Therefore, one can draw unbiased samples from these distributions using MAP predictions. Interestingly, when incorporating perturbmax models to Bayesian loss minimization one would ultimately like to use the PAC-Bayesian risk [11, 19, 3, 20, 5, 10]. Our work explores the Bayesian aspects that emerge from PAC-Bayesian risk minimization. We focus on computational aspects when constructing posterior distributions, so that they could be used 1

to minimize the risk bound efficiently. We show that any smooth posterior distribution would suffice to define a smooth risk bound which can be minimized through gradient decent. In addition, we relate the posterior distributions to the computational properties of MAP predictors. We suggest multiplicative posterior models to learn super-modular potential functions, that come with specialized MAP predictors such as graph-cuts [2]. We also describe label-augmented posterior models that can use MAP approximations, such as those arising from linear program relaxations [21].

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Background

Learning complex models typically involves reasoning about the states of discrete variables whose labels (assignments of values) specify the discrete structures of interest. The learning task which we consider in this work is to fit parameters w that produce to most accurate prediction $y \in Y$ to a given object x . Structures of labels are conveniently described by a discrete product space $Y = Y_1 \times \dots \times Y_n$. We describe the potential of relating a label y to an object x with respect to the parameters w by real valued functions $\phi(y; x, w)$. Our goal is to learn the parameters w that best describe the training data $(x, y) \in S$. Within Bayesian perspectives, the distribution that one learns given the training data is composed from a distribution over the parameter space $q(w)$ and over the labels space $P[y|w, x] \propto \exp \phi(y; x, w)$. Using the Bayes rule we derive the predictive distribution over the structures Z $P[y|x] = \int P[y|w, x] q(w) d w$ (1) Unfortunately, sampling algorithms over complex models are provably hard in theory and tend to be slow in many cases of practical interest [7]. This is in contrast to the maximum a-posteriori (MAP) prediction, which can be computed efficiently for many practical cases, even when sampling is

provably hard. (MAP predictor)

$$y_w(x) = \arg \max_{y_1, \dots, y_n} \phi(y; x, w) \quad (2)$$

Recently, [17, 23] suggested to change of the Bayesian posterior probability models to utilize the MAP prediction in a deterministic manner. These perturb-max models allow to sample from the predictive distribution with a single MAP prediction:

def (Perturb-max models) $P[y=x] = P_{\phi}(y=x) \quad (3)$ A is decomposed along a graphical model if it has the form $\phi(y; x, w) = \sum_i V_i(y_i; x, w) + \sum_{i,j \in E} \phi_{i,j}(y_i, y_j; x, w)$. If the graph has no cycles, MAP prediction can be computed efficiently using the belief propagation algorithm. Nevertheless, there are cases where MAP prediction can be computed efficiently for graph with cycles. A potential function is called supermodular if it is defined over $Y = \{1, 1\}^n$ and its pairwise interactions favor adjacent states to have the same label, i.e., $\phi_{i,j}(1, 1; x, w) + \phi_{i,j}(1, 1; x, w) \geq \phi_{i,j}(1, 1; x, w) + \phi_{i,j}(1, 1; x, w)$. In such cases MAP prediction reduces to computing the min-cut (graph-cuts) algorithm. Recently, a sequence of works attempt to solve the MAP prediction task for non-supermodular potential function as well as general regions. These cases usually involve potentials function that are described by a family R of subsets of variables $r \subseteq \{1, \dots, n\}$, called regions. We denote by y_r the set of labels that correspond to the region r , namely $(y_i)_{i \in r}$ and consider the following potential P functions $\phi(y; x, w) = \sum_{r \in R} \phi_r(y_r; x, w)$. Thus, MAP prediction can be formulated as an integer linear program:
$$\max_{y_r} \sum_{r \in R} \phi_r(y_r; x, w) \quad (4)$$

s.t.

y_r

$y_r \in \{0, 1\}$,

X

$y_r = 1$,

y_r

X

$y_s = y_r \quad \forall r \in R$

y_s

The correspondence between MAP prediction and integer linear program solutions is $y_w(x) = \arg \max_{y_i} \phi(y_i)$. Although integer linear program solvers provide an alternative to MAP prediction, they may be restricted to problems of small size. This restriction can be relaxed when one replaces the integral constraints $y_r \in \{0, 1\}$ with nonnegative constraints $y_r \geq 0$. These 2

linear program relaxations can be solved efficiently using different convex max-product solvers, and whenever these solvers produce an integral solution it is guaranteed to be the MAP prediction [21]. Given training data of object-label pairs, the learning objective is to estimate a predictive distribution over the structured-labels. The goodness of fit is measured by a loss function $L(y, y)$. As we focus on randomized MAP predictors our goal is to learn the parameters

w that minimize the expected perturb-max prediction loss, or randomized risk. We define the randomized risk at a single instance-label pair as X

$$R(w, x, y) = \mathbb{P}_{y \sim q_w} [L(y, x, y)]$$

Alternatively, the randomized risk takes the form $R(w, x, y) = \mathbb{E}_{y \sim q_w} [L(y, x, y)]$. The randomized risk originates within the PAC-Bayesian generalization bounds. Intuitively, if the training set is an independent sample, one would expect that best predictor on the training set to perform well on unlabeled objects at test time.

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Minimizing PAC-Bayesian generalization bounds

Our approach is based on the PAC-Bayesian risk analysis of random MAP predictors. In the following we state the PAC-Bayesian generalization bound for structured predictors and describe the gradients of these bounds for any smooth posterior distribution. The PAC-Bayesian generalization bound describes the expected loss, or randomized risk, when considering the true distributions over object-labels in the world $R(w) = \mathbb{E}_{(x,y)} [R(w, x, y)]$. It upper bounds the randomized risk by the empirical randomized risk $RS(w) = \frac{1}{n} \sum_{(x,y) \in S} R(w, x, y)$ and a penalty term which decreases proportionally to the training set size. Here we state the PAC-Bayesian theorem, that holds uniformly for all posterior distributions over the predictions. Theorem 1. (Catoni [3], see also [5]). Let $L(y, x, y) \in [0, 1]$ be a bounded loss function. Let $p(\cdot)$ be any probability density function and let $q_w(\cdot)$ be a family of probability density functions parameterized by w . Let $KL(q_w \parallel p) = \int q_w(\cdot) \log(q_w(\cdot)/p(\cdot))$. Then, for any $\eta \in (0, 1]$ and for any real number $\epsilon \geq 0$, with probability at least $1 - \epsilon$ over the draw of the training set the following holds simultaneously for all w

$KL(q_w \parallel p) + \log(1/\epsilon) \leq RS(w) + R(w) + \frac{1}{n} \exp(-\eta n) \sum_{(x,y) \in S} [\log q_w(\cdot)] L(y, x, y) - \sum_{(x,y) \in S} R(w, x, y)$ For completeness we present a proof sketch for the theorem in the appendix. This proof follows Seeger's PAC-Bayesian approach [19], and extended to the structured label case [13]. The proof technique replaces prior randomized risk, with the posterior randomized risk that holds uniformly for every w , while penalizing this change by their KL-divergence. This change-of-measure step is close in spirit to the one that is performed in importance sampling. The proof is then concluded by simple convex bound on the moment generating function of the empirical risk. To find the best posterior distribution that minimizes the randomized risk, one can minimize its empirical upper bound. We show that whenever the posterior distributions have smooth probability density functions $q_w(\cdot)$, the perturb-max probability model is smooth as a function of w . Thus the randomized risk bound can be minimized with gradient methods. Theorem 2. Assume $q_w(\cdot)$ is smooth as a function of its parameters, then the PAC-Bayesian bound is smooth as a function of w : $\frac{d}{dw} RS(w) = \mathbb{E}_{(x,y) \sim q_w} [\log q_w(\cdot)] L(y, x, y) - \sum_{(x,y) \in S} R(w, x, y)$

Moreover, the KL-divergence is a smooth function of w and its gradient takes the form: $\frac{d}{dw} KL(q_w \parallel p) = \mathbb{E}_{(x,y) \sim q_w} [\log q_w(\cdot)] \log(q_w(\cdot)/p(\cdot)) + 1$ R Proof: First we note that $R(w, x, y) = \int q_w(\cdot) L(y, x, y) d\cdot$. Since $q_w(\cdot)$ is a probability density function and $L(y, x, y) \in [0, 1]$ we can differentiate under

the integral (cf. [4] Theorem 2.27). $Z^{-1} \int \mathbb{R}(w, x, y) = \int q(w) L(y|x, w) d\mu(w)$

Using the identity $\int q(w) \log(q(w)) = -\int q(w) \log(q(w))$ the first part of the proof follows. The second part of the proof follows in the same manner, while noting that $\int q(w) \log(q(w)) = (\int q(w) \log(q(w)) + 1)$. The gradient of the randomized empirical risk is governed by the gradient of the log-probability density function of its corresponding posterior model. For example, Gaussian model with mean w and identity covariance matrix has the probability density function $q(w) = \exp(-k^2 w^2 / 2)$, thus the gradient of its log-density is the linear moment w , i.e., $\int w \log(q(w)) = -w$. Taking any smooth distribution $q(w)$, we can find the parameters w by descending along the stochastic gradient of the PAC-Bayesian generalization bound. The gradient of the randomized empirical risk is formed by two expectations, over the sample points and over the posterior distribution. Computing these expectations is time consuming, thus we use a single sample $y \sim q(w)$ $L(y|x, w)$ as an unbiased estimator for the gradient. Similarly we estimate the gradient of the KL-divergence with an unbiased estimator which requires a single sample of $\int w \log(q(w))(\log(q(w)/p(w)) + 1)$. This approach, called stochastic approximation or online gradient descent, amounts to use the stochastic gradient update rule

$w \leftarrow w - \eta \int w \log(q(w)) L(y|x, w) + \log(q(w)/p(w)) + 1$ where η is the learning rate. Next, we explore different posterior distributions from computational perspectives. Specifically, we show how to learn the posterior model so to ensure the computational efficiency of its MAP predictor.

4

Learning posterior distributions efficiently

The ability to efficiently apply MAP predictors is key to the success of the learning process. Although MAP predictions are NP-hard in general, there are posterior models for which they can be computed efficiently. For example, whenever the potential function corresponds to a graphical model with no cycles, MAP prediction can be efficiently computed for any learned parameters w . Learning unconstrained parameters with random MAP predictors provides some freedom in choosing the posterior distribution. In fact, Theorem 2 suggests that one can learn any posterior distribution by performing gradient descent on its risk bound, as long as its probability density function is smooth. We show that for unconstrained parameters, additive posterior distributions simplify the learning problem, and the complexity of the bound (i.e., its KL-divergence) mostly depends on its prior distribution. Corollary 1. Let $q_0(w)$ be a smooth probability density function with zero mean and set the posterior distribution using additive shifts $q(w) = q_0(w + w)$. Let $H(q) = \int q(w) \log(q(w))$ be the entropy function. Then $KL(q - p) = H(q_0) - \int q_0(w) \log(p(w + w))$. In particular, if $p(w) = \exp(-k^2 w^2)$ is Gaussian then $\int w KL(q - p) = w$. Proof: $KL(q - p) = H(q) - \int q(w) \log(p(w))$. By a linear change of variable, $w = w + w$ it follows that $H(q) = H(q_0)$ thus $\int w H(q) = 0$. Similarly $\int q(w) \log(p(w)) = \int q_0(w) \log(p(w + w))$. Finally, if $p(w)$ is Gaussian then $\int q_0(w) \log(p(w + w)) = -w^2 - \int q_0(w) [w^2]$. This result implies that every additively-

enforces the constraints of its parameters. This property suggests that using multiplicative rules are computationally favorable. Interestingly, using a prior model with Gamma distribution adds to the barrier function a linear regularization term kwk_1 that encourages sparsity. On the other hand, a prior model with a truncated Gaussian adds a square regularization term which drifts the nonnegative parameters away from zero. A computational disadvantage of the Gaussian prior is that its barrier function cannot be controlled by a parameter γ .

4.2 Learning posterior models with approximate MAP predictions

MAP prediction can be phrased as an integer linear program, stated in Equation (4). The computational burden of integer linear programs can be relaxed when one replaces the integral constraints with nonnegative constraints. This approach produces approximate MAP predictions. An important learning challenge is to extend the predictive distribution of perturb-max models to incorporate approximate MAP solutions. Approximate MAP predictions are described by the feasible set of their linear program relaxations, that is usually called the local polytope: $\mathcal{N} \times \mathcal{X} \times \mathcal{L}(\mathbf{R}) = \{(\mathbf{y}, \mathbf{r}) : \mathbf{b}(\mathbf{y}, \mathbf{r}) \geq 0, \mathbf{b}(\mathbf{y}, \mathbf{r}) = 1, \mathbf{r} \geq \mathbf{s}(\mathbf{y})\}$

where

Linear programs solutions are usually the extreme points of their feasible polytope. The local polytope is defined by a finite set of equalities and inequalities, thus it has a finite number of extreme points. The perturb-max model that is defined in Equation (3) can be effortlessly extended to the finite set of the local polytope extreme points [15]. This approach has two flaws. First, linear program solutions might not be extreme points, and decoding such a point usually requires additional

computational effort. Second, without describing the linear program solutions one cannot incorporate loss functions that take the structural properties of approximate MAP predictions into account when computing the randomized risk. Theorem 3. Consider approximate MAP predictions that arise from relaxation of the MAP prediction problem in Equation (4). $\mathbf{x}^* = \arg \max_{\mathbf{x}} \mathbf{b}(\mathbf{y}^*, \mathbf{r}^*)$ s.t. $\mathbf{b} \in \mathcal{L}(\mathbf{R})$

where

Then any optimal solution \mathbf{b}^* is described by a vector $\mathbf{y}^*, \mathbf{r}^*(\mathbf{x})$ in the finite power sets over the regions, $\mathcal{Y} \times \mathcal{R} : \mathbf{y}^*, \mathbf{r}^*(\mathbf{x}) = (\mathbf{y}^*, \mathbf{r}^*(\mathbf{x})) \in \mathcal{R}$

where

$$\mathbf{y}^*, \mathbf{r}^*(\mathbf{x}) = \{(\mathbf{y}, \mathbf{r}) : \mathbf{b}(\mathbf{y}, \mathbf{r}) \geq 0\}$$

Moreover, if there is a unique optimal solution \mathbf{b}^* then it corresponds to an extreme point in the local polytope. Proof: The program is convex over a compact set, thus strong duality holds. Fixing the Lagrange \mathbf{P} multipliers $\mathbf{r}^*(\mathbf{y})$ that correspond to the marginal constraints $\mathbf{y}^*, \mathbf{r}^*(\mathbf{y}) = \mathbf{b}(\mathbf{y}, \mathbf{r}^*(\mathbf{y}))$, and considering the probability constraints as the domain of the primal program, we derive the dual program $\mathcal{N} \times \mathcal{X} \times \mathcal{X} \times \mathcal{X} \max_{\mathbf{r}} \mathbf{r}^*(\mathbf{y}^*; \mathbf{x}, \mathbf{w}) + \sum_{\mathbf{c}} \mathbf{r}^*(\mathbf{y}^*) \cdot \mathbf{r}^*(\mathbf{p}(\mathbf{y}^*))$

where

tions. Our learned parameters outperform structured SVM approaches and Perturb-and-MAP moment matching

Figure 1: Two examples of image (left), input trimap (middle) and the final segmentation (right) produced using our learned parameters.

We use two different loss functions for training/testing for our approach to illustrate the flexibility of our approach for learning using various task specific loss functions. The GrabCut loss measures the fraction of incorrect pixels labels in the region specified as the boundary in the trimap. The PASCAL loss, which is commonly used in several image segmentation benchmarks, measures the ratio of the intersection and union of the foregrounds of ground truth segmentation and the solution. As a comparison we also trained parameters using moment matching of MAP perturbations [17] and structured SVM. We use a stochastic gradient approach with a decaying step size for 1000 iterations. Using structured SVM, solving loss-augmented inference $\max_y \{L(y, y^*) + \lambda(y; x, w)\}$ with the hamming loss can be efficiently done using graph-cuts. We also consider learning parameters with all-zero loss function, i.e., $L(y, y^*) = 0$. To ensure that the weights remain non-negative we project the weights into the non-negative side after each iteration. Table 1 shows the results of learning using various methods. For the GrabCut loss, our method obtains comparable results to the GMMRF framework of [1], which used hand-tuned parameters. Our results are significantly better when PASCAL loss is used. Our method also outperforms the parameters learned using structured SVM and Perturb-and-MAP approaches. In our experiments the structured SVM with the hamming loss did not perform well – the loss augmented inference tended to focus on maximum violations instead of good solutions which causes the parameters to change even though the MAP solution has a low loss (a similar phenomenon was observed in [22]). Using the all-zero loss tends to produce better results in practice as seen in Table 1. Figure 1 shows some examples images, the input trimap, and the segmentations obtained using our approach.

6

Related work

Recent years have introduced many optimization techniques that lend efficient MAP predictors for complex models. These MAP predictors can be integrated to learn complex models using structuredSVM [25]. Structured-SVM has a drawback, as its MAP prediction is adjusted by the loss function, therefore it has an augmented complexity. Recently, there has been an effort to efficiently integrate non-decomposable loss function into structured-SVMs [24]. However this approach does not hold for any loss function. Bayesian approaches to loss minimization treat separately the prediction process and the loss incurred, [12]. However, the Bayesian approach depends on the efficiency of its sampling procedure, but unfortunately, sampling in complex models is harder than the MAP prediction task [7]. The recent works [17, 23, 8, 9, 16] integrate efficient MAP predictors into Bayesian modeling. [23] describes the Bayesian perspectives, while [17, 8] describe their relations to the Gibbs distribution and moment matching. [9] provide unbiased samples from the Gibbs distribution using MAP predictors and [16] present their measure concentration properties.

Other strategies for producing \hat{f}

(pseudo) samples efficiently include Herding [26]. However, these approaches do not consider risk minimization. The perturb-max models in Equation (3) play a key role in PAC-Bayesian theory [14, 11, 19, 3, 20, 5, 10]. The PAC-Bayesian approaches focus on generalization bounds to the object-label distribution. However, the posterior models in the PAC-Bayesian approaches were not extensively studied in the past. In most cases the posterior model remained undefined. [10] investigate linear predictors with Gaussian posterior models to have a structured-SVM like bound. This bound holds uniformly for every γ and its derivation is quite involved. In contrast we use Catoni's PAC-Bayesian bound that is not uniform over γ but does not require the $\log \frac{1}{\gamma}$ term [3, 5]. The simplicity of Catoni's bound (see Appendix) makes it amenable to different extensions. In our work, we extend these results to smooth posterior distributions, while maintaining the quadratic regularization form. We also describe posterior distributions for non-linear models. In different perspective, [3, 5] describe the optimal posterior, but unfortunately there is no efficient sampling procedure for this posterior model. In contrast, our work explores posterior models which allow efficient sampling. We investigate two posterior models: the multiplicative models, for constrained MAP solvers such as graph-cuts, and posterior models for approximate MAP solutions.

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Discussion

Learning complex models requires one to consider non-decomposable loss functions that take into account the desirable structures. We suggest to use the Bayesian perspectives to efficiently sample and learn such models using random MAP predictions. We show that any smooth posterior distribution would suffice to define a smooth PAC-Bayesian risk bound which can be minimized using gradient decent. In addition, we relate the posterior distributions to the computational properties of the MAP predictors. We suggest multiplicative posterior models to learn supermodular potential functions that come with specialized MAP predictors such as graph-cuts algorithm. We also describe label-augmented posterior models that can use efficient MAP approximations, such as those arising from linear program relaxations. We did not evaluate the performance of these posterior models and further explorations of such models is required. The results here focus on posterior models that would allow for efficient sampling using MAP predictions. There are other cases for which specific posterior distributions might be handy, e.g., learning posterior distributions of Gaussian mixture models. In these cases, the parameters include the covariance matrix, thus would require to sample over the family of positive definite matrices.

A

Proof sketch for Theorem 1

Theorem 2.1 in [5]: For any distribution D over object-labels pairs, for any w -parametrized distribution q_w , for any prior distribution p , for any $\gamma \in (0, 1]$, and for any convex function $D : [0, 1] \times [0, 1] \rightarrow \mathbb{R}$, with probability at least $1 - \gamma$ over the draw of the training set the divergence $D(E_{q_w}(\cdot), E_p(\cdot))$

$R(\cdot)$ is upper bounded simultaneously for all w by $1 + \frac{1}{\epsilon} \log \frac{1}{\epsilon} \text{KL}(q_w - p) + \log E_{p \sim \mathcal{D}} \exp mD(RS(\cdot), R(\cdot)) - S$. For $D(RS(\cdot), R(\cdot)) = F(R(\cdot))$, the bound reduces to a simple convex bound on the moment generating function of the empirical risk: $E_{p \sim \mathcal{D}} \exp mD(RS(\cdot, x, y), R(\cdot, x, y)) = \exp(mF(R(\cdot)))$. Since the exponent function is a convex function of $RS(\cdot) = RS(\cdot) \cdot 1 + (1 - RS(\cdot)) \cdot 0$, the moment generating function bound is $\exp(\epsilon RS(\cdot)) \cdot RS(\cdot) \exp(\epsilon) + (1 - RS(\cdot))$. Since $E_{p \sim \mathcal{D}} RS(\cdot) = R(\cdot)$, the right term in the risk bound can be made 1 when choosing $F(R(\cdot))$ to be the inverse of the moment generating function bound. This is Catoni's bound [3, 5] for the structured labels case. To derive Theorem 1 we apply $\exp(\epsilon x) \geq 1 + \epsilon x$ to derive the lower bound $(1 - \exp(\epsilon)) E_{p \sim \mathcal{D}} RS(\cdot) \geq E_{p \sim \mathcal{D}} RS(\cdot) - \exp(\epsilon) R(\cdot)$. 8

2 References

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