
Learning with Differentiable Perturbed Optimizers

Quentin Berthet¹ Mathieu Blondel¹ Olivier Teboul¹ Marco Cuturi¹ Jean-Philippe Vert¹ Francis Bach²

Abstract

Machine learning pipelines often rely on optimization procedures to make discrete decisions (e.g. sorting, picking closest neighbors, finding shortest paths or optimal matchings). Although these discrete decisions are easily computed in a forward manner, they cannot be used to modify model parameters using first-order optimization techniques because they break the back-propagation of computational graphs. In order to expand the scope of learning problems that can be solved in an end-to-end fashion, we propose a systematic method to transform a block that outputs an optimal discrete decision into a differentiable operation. Our approach relies on stochastic perturbations of these parameters, and can be used readily within existing solvers without the need for ad hoc regularization or smoothing. These perturbed optimizers yield solutions that are differentiable and never locally constant. The amount of smoothness can be tuned via the chosen noise amplitude, whose impact we analyze. The derivatives of these perturbed solvers can be evaluated efficiently. We also show how this framework can be connected to a family of losses developed in structured prediction, and describe how these can be used in unsupervised and supervised learning, with theoretical guarantees. We demonstrate the performance of our approach on several machine learning tasks in experiments on synthetic and real data.

1. Introduction

Many applications of machine learning benefit from the possibility to train by gradient descent compositional models using end-to-end differentiability. Yet, there remain many fields in which discrete decisions are required at intermediate steps of a data processing pipeline, notably those involving sequences of decisions and/or discrete objects (e.g., in

robotics, graphics or biology). This is the result of many factors: discrete decisions provide a much sought-for interpretability of what a black-box is actually doing and discrete solvers are built upon decades of advances in combinatorial algorithms (Schrijver, 2003) to make quick decisions (e.g., sorting, picking closest neighbors, exploring options with beam-search, and more generally with knapsack, routing and shortest paths problems). Even though these discrete decisions can be easily computed, in what would be called a forward pass in a deep learning context, the derivatives of these decisions with respect to inputs are degenerate (small changes in the inputs either yield no change or discontinuous changes in the outputs). As a consequence, discrete solvers break the back-propagation of computational graphs, and cannot be incorporated in end-to-end learning.

In order to expand the set of operations that can be incorporated in differentiable models, we propose and investigate a systematic method to transform blocks with discrete optimizers as outputs into differentiable operations. Our approach relies on the method of stochastic perturbations, the theory of which was developed and applied to several tasks of machine learning recently (see, e.g. Hazan et al., 2016, for a survey). In a nutshell, we perturb the inputs of a discrete solver with random noise, and consider the perturbed optimal solutions of the problem. The method is both easy to analyze theoretically and trivial to implement. Using the formal expectation of these perturbed solutions, we show that they are never locally constant and everywhere differentiable, with successive derivatives being expectations of simple expressions.

Related work. Our work is part of growing efforts to modify operations in order to make them differentiable, that we now review.

Differentiating through an argmax. Several works have studied the introduction of regularization in the optimization problem in order to make the argmax differentiable. However these works are usually problem-specific, since a new optimization problem needs to be solved. Examples include assignments (Adams & Zemel, 2011) and more generally optimal transport (Bonneel et al., 2016; Cuturi, 2013), differentiable dynamic programming (Mensch & Blondel, 2018), differentiable submodular optimization (Djolonga & Krause, 2017). An exception is the so-called

¹Google Research, Brain team, Paris, France ²Inria, ENS, PSL Research University, Paris, France. Correspondence to: Q. Berthet <qberthet@google.com>, M. Blondel <mblondel@google.com>.

SparseMAP algorithm (Niculae et al., 2018), which is based on Frank-Wolfe or active-set algorithms for solving the L_2 -regularized-problem, and on implicit differentiation for computing a Jacobian. Like our proposal, SparseMAP only requires access to a linear maximization oracle. However, it is sequential in nature, while our approach is trivial to parallelize. More recently Agrawal et al. (2019) analyze implicit differentiation on solutions of convex optimization. They express the derivatives of the argmax exactly, leading to zero Jacobian almost everywhere for optimization over polytopes. Vlastelica et al. (2019) propose a new scheme to interpolate in a piecewise-linear manner between locally constant regions. Their aim is to keep the same value for the Jacobian of the argmax for a large region of inputs, allowing for zero Jacobians as well.

Perturbation methods. The idea of using the expectation of a perturbed max and argmax, commonly known as the ‘‘Gumbel trick’’, dates back to Gumbel (1954), and the notion of random choice models (Luce, 1959; McFadden et al., 1973; Guadagni & Little, 1983). They are exploited in online learning and bandit problems in order to promote exploration, and induce robustness to adversarial data (see, e.g., Abernethy et al., 2016, for a survey). In relation with our work, they are used for action spaces that are combinatorial in nature (Neu & Bartók, 2016). The Gumbel trick has also been used together with a softmax to obtain differentiable sampling (Jang et al., 2016; Maddison et al., 2016).

The use of perturbation techniques as an alternative to MCMC techniques for sampling was pioneered by Papan-dreou & Yuille (2011). They are used to compute the expected statistics arising in the gradient of conditional random fields. They show the exactness for the fully perturbed (but intractable case) and propose ‘‘low-rank’’ perturbations as an approximation. These results are extended by Hazan & Jaakkola (2012), who proved that the maximum with low-rank perturbations, in expectation, provides an upper-bound on the log partition and proposed to replace the log partition in conditional random fields loss by that expectation. Their results, however, are limited to discrete product spaces. Shortly after, Hazan et al. (2013) derived new lower bounds on the partition function and proposed a new unbiased sequential sampler for the Gibbs distribution based on low-rank perturbations. These results were further refined by Gane et al. (2014) and Orabona et al. (2014). Shpakova & Bach (2016) further studied these bounds and proposed a doubly stochastic scheme. Balog et al. (2017) explored other distributions from extreme value theory, including the Fréchet and Weibull distributions. Apart from Lorberbom et al. (2019), who use a finite difference method, we are not aware of any prior work using perturbation techniques to differentiate through an **argmax**. As reviewed above, all papers focus on (approximately) sampling from the Gibbs distribution, upper-bounding the log partition function, or

differentiating through the **max**.

Our contributions.

- We propose a new general method to transform discrete optimizer outputs, inspired by the stochastic perturbation literature. This versatile method is easy to apply to any blackbox solvers without ad-hoc modifications.
- Our stochastic smoothing allows **argmax** differentiation, through the formal perturbed maximizer. We show that its Jacobian is well-defined and non-zero everywhere, thereby avoiding vanishing gradients.
- The successive derivatives of the perturbed maximum and argmax are expressed as simple expectations, which are easy to approximate with Monte-Carlo methods.
- This particular approach to operator smoothing yields natural connections to the recently-proposed Fenchel-Young losses by Blondel et al. (2019). We show that the equivalence via duality with regularized optimization makes Fenchel-Young losses particularly natural. We propose a doubly stochastic scheme for minimization of these losses, for unsupervised and supervised learning.
- We demonstrate the performance of our approach on several machine learning tasks in experiments on synthetic and real data.

2. Perturbed maximizers

Given a finite set of distinct points $\mathcal{Y} \subset \mathbb{R}^d$ and \mathcal{C} its convex hull, we consider a general discrete optimization problem parameterized by an input $\theta \in \mathbb{R}^d$ as follows:

$$F(\theta) = \max_{y \in \mathcal{C}} \langle y, \theta \rangle, \quad y^*(\theta) = \arg \max_{y \in \mathcal{C}} \langle y, \theta \rangle. \quad (1)$$

As detailed in Section 2.2 below, this formulation encompasses a variety of discrete operations such as picking the maximum value or the top k largest values of a vector; ranking the entries of a vector; or computing the shortest path over a weighted graph, to name just a few. In all cases, \mathcal{C} is a polytope and these problems are linear programs (LP). For almost every θ , the argmax is unique, and $y^*(\theta) = \nabla_{\theta} F(\theta)$. While widespread, these functions do not have the convenient properties of blocks in end-to-end learning methods, such as smoothness or differentiability. In particular, $\theta \mapsto y^*(\theta)$ is piecewise constant: its gradient is zero almost everywhere, and undefined otherwise.

To address these issues, we simply add to θ a random noise vector εZ , where $\varepsilon > 0$ is a temperature parameter and Z has a positive and differentiable density $d\mu(z) \propto \exp(-\nu(z))dz$ on \mathbb{R}^d , ensuring that $y^*(\theta + \varepsilon Z)$ is almost surely (a.s.) uniquely defined. This induces a prob-

ability distribution p_θ on \mathcal{Y} given by $p_\theta(y) = P(y^*(\theta + \varepsilon Z) = y)$.

Taking expectations w.r.t. the random perturbation leads to smoothed versions of F and y^* (see Figure 1):

Definition 2.1. For all $\theta \in \mathbb{R}^d$, and $\varepsilon > 0$, we define the **perturbed maximum** as

$$F_\varepsilon(\theta) = \mathbf{E}[F(\theta + \varepsilon Z)] = \mathbf{E}[\max_{y \in \mathcal{C}} \langle y, \theta + \varepsilon Z \rangle] \text{ and}$$

the **perturbed maximizer** as

$$\begin{aligned} y_\varepsilon^*(\theta) &:= \mathbf{E}_{p_\theta(y)}[Y] = \mathbf{E}[\arg \max_{y \in \mathcal{C}} \langle y, \theta + \varepsilon Z \rangle] \\ &= \mathbf{E}[\nabla_\theta \max_{y \in \mathcal{C}} \langle y, \theta + \varepsilon Z \rangle] = \nabla_\theta F_\varepsilon(\theta). \end{aligned}$$

This creates a general and natural model on the variable Y , when observations are solutions of optimization problems, with uncertain costs. It enables the modeling of phenomena where agents chose an optimal $y \in \mathcal{C}$ based on uncertain knowledge of θ , or varying circumstances. We view this as a generalization, or alternative to the Gibbs distribution, rather than an approximation thereof.

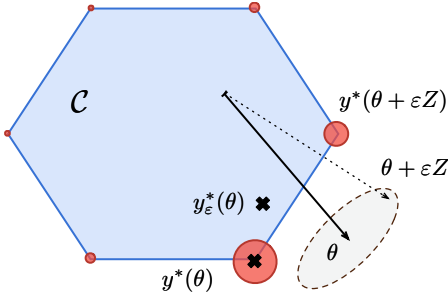


Figure 1. Over a polytope \mathcal{C} , stochastic perturbations on θ induce a probability over \mathcal{Y} (in red) on $Y = y^*(\theta + \varepsilon Z)$. The perturbed maximizer y_ε^* is the expectation of Y under p_θ .

Models of random optimizers for linear problems with perturbed inputs are the subject of a wide literature in machine learning, under the name of Perturb-and-MAP (Papandreou & Yuille, 2011; Hazan & Jaakkola, 2012), and perturbed leader method in online learning (Hannan, 1957; Kalai & Vempala, 2003; Abernethy et al., 2014). We refer to it here as the *perturbed model*. A notorious example is when \mathcal{Y} is the set of one-hot-encoding of d classes, \mathcal{C} is the unit simplex, and Z has the Gumbel distribution (Gumbel, 1954). In that case it is well-known that p_θ is the Gibbs distribution, proportional to $\exp(\langle y, \theta \rangle / \varepsilon)$, $F_\varepsilon(\theta)$ is the log-sum-exp function of θ , and $y_\varepsilon^*(\theta)$ is the vector of softmax (or exponential weights) of the components of θ . The following result shows that the perturbed maximizer can also be defined as the solution of a convex problem, by Fenchel-Rockafellar duality.

Proposition 2.1. Let Ω be the Fenchel dual of F_1 , with domain \mathcal{C} . We have that

$$y_\varepsilon^*(\theta) = \arg \max_{y \in \mathcal{C}} \{ \langle y, \theta \rangle - \varepsilon \Omega(y) \}. \quad (2)$$

As F_ε generalizes the log-sum-exp function for Gumbel noise on the simplex, its dual Ω is a generalization of the negative entropy (which is the Fenchel dual of log-sum-exp). These connections have been studied in many parts of statistical and machine learning (Wainwright et al., 2008). In the literature on bandit problems and online learning, these links between regularization and perturbation for linear optimization problems are well-studied, and applied to gradient-based algorithms (Abernethy et al., 2014; 2016).

This model, and the perturbed functions of Definition 2.1 inherit several important properties from this formulation. First, it allows to take derivatives with respect to the input θ of F_ε and of y_ε^* (Proposition 2.2). These derivatives are also easily expressed as expectations involving F and y^* with noisy inputs, as discussed in Section 3. In turn, this yields fast computational methods for these functions and their derivatives, described in Section 3.1. Further, by the duality point of view describing y_ε^* as a regularized maximizer, there exists a natural convex loss for this model that can be efficiently optimized in θ , for data $y_i \in \mathcal{Y}$. We describe this formalism in Section 4. All proofs are in the appendix.

2.1. Properties of the model

This model modifies the maximum and maximizer by perturbation. Because of the simple action of the stochastic noise, we can analyze their properties precisely.

Proposition 2.2. Assume \mathcal{C} is a convex polytope with non-empty interior, and μ has positive differentiable density. The perturbed model p_θ and the associated functions F_ε , Ω , and y_ε^* have the following properties, for $R_C = \max_{y \in \mathcal{C}} \|y\|$ and $M_\mu = \mathbf{E}[\|\nabla_z \nu(Z)\|^2]^{1/2}$:

- F_ε is strictly convex, twice differentiable, R_C -Lipschitz-continuous and its gradient is $R_C M_\mu / \varepsilon$ -Lipschitz-continuous.
- Ω is $1/(R_C M_\mu)$ -strongly convex, differentiable, and Legendre-type.
- $y_\varepsilon^*(\theta)$ is in the interior of \mathcal{C} and is differentiable in θ .
- Impact of the temperature $\varepsilon > 0$: we have that

$$F_\varepsilon(\theta) = \varepsilon F_1\left(\frac{\theta}{\varepsilon}\right), F_\varepsilon^*(y) = \varepsilon \Omega(y), y_\varepsilon^*(\theta) = y_1^*\left(\frac{\theta}{\varepsilon}\right).$$

We develop in further details the simple expressions for derivatives of F_ε and y_ε^* in Section 3. By this proposition, since F_ε is strictly convex, it is nowhere locally linear, so

y_ε^* is nowhere locally constant. Formally, $y_\varepsilon^* = \nabla_\theta F_\varepsilon$ is a *mirror map*, a one-to-one mapping from \mathbb{R}^d unto the interior of \mathcal{C} . The gradient of $\varepsilon\Omega$ is its functional inverse, by convex duality between these functions (see, e.g. surveys Wainwright et al., 2008; Bubeck et al., 2015, and references therein).

Remark 1. For these properties to hold, it is crucial that \mathcal{C} has non-empty interior, i.e., that \mathcal{Y} does not lie in an affine subspace of lower dimension. To adapt to cases where \mathcal{C} lies in a subspace, we consider the set of inputs θ up to vectors orthogonal to \mathcal{C} , or represent \mathcal{Y} in a lower-dimensional subspace. As an example, over the unit simplex and Gumbel noise, the log-sum-exp is not strictly convex, and in fact linear along the all-ones vector $\mathbf{1}$. In such cases, the model is only well-specified in θ up to the space orthogonal to \mathcal{C} , which does not affect prediction tasks.

For any positive temperature, these properties imply that there is an informative, well-defined and nonzero gradient in θ . The limiting behavior at extreme temperatures can also be explicitly derived from these properties.

Proposition 2.3. *With the conditions of Proposition 2.2, for θ such that $y^*(\theta)$ is a unique maximum:*

- When $\varepsilon \rightarrow 0$, $F_\varepsilon(\theta) \rightarrow F(\theta)$ and $y_\varepsilon^*(\theta) \rightarrow y^*(\theta)$.
- When $\varepsilon \rightarrow \infty$, $y_\varepsilon^*(\theta) \rightarrow y_1^*(0) = \arg \min_{y \in \mathcal{C}} \Omega(y)$.

For every $\varepsilon > 0$, we have $F(\theta) - F_\varepsilon(\theta) \leq C\varepsilon$,

$$\langle y^*(\theta), \theta \rangle - \langle y_\varepsilon^*(\theta), \theta \rangle \leq C'\varepsilon,$$

for constants C and C' .

The properties of the distributions p_θ in this model are well studied in the perturbations literature (see, e.g. Hazan et al., 2016, for a survey). They notably do not have a simple closed-form expression, but can be very easy to sample from. By the argmax definition, simulating $Y \sim p_\theta$, only requires to sample μ (e.g., Gaussian, or vector of i.i.d. Gumbel), and to solve the original optimization problem. It is the case in the applications we consider (e.g., max, ranking, shortest paths). This is in stark contrast to the Gibbs distribution, which has the opposite properties.

2.2. Examples

Many operations frequently used in machine learning can be written as optimal decisions over a discrete set and can be written as the problem in Equation (1). They correspond to a linear program (typically with integral solutions), but we emphasize again that this structure need not be known or exploited to use the perturbed maximizers in practice.

Maximum. The max function from \mathbb{R}^d to \mathbb{R} , that returns the largest of d entries of a vector θ is ubiquitous in machine

learning, the hallmark of any classification task. It is equal to an LP over the unit simplex \mathcal{C} , $F(\theta) = \max_{i \in [d]} \theta_i$ with $\mathcal{C} = \{y \in \mathbb{R}^d : y \geq 0, \mathbf{1}^\top y = 1\}$.

Top k . The function from \mathbb{R}^d to \mathbb{R} that returns the sum of the k largest entries of a vector θ is also commonly used. Akin to the maximum, it is the value of an LP (cf. Appendix for more details).

Ranking. The function returning the ranks (in descending order) of a vector $\theta \in \mathbb{R}^d$ can be written as the argmax of a linear program over the *permutahedron*, the convex hull of permutations of any vector v with distinct entries. Using different reference vectors v yield different perturbed operations, and $v = (1, 2, \dots, d)$ is commonly used.

Shortest paths. For a graph $G = (V, E)$ and positive costs over edges $c \in \mathbb{R}^E$, the problem of finding a shortest path (i.e. with minimal total cost) from vertices s to t can be written in our setting with $\theta = -c$ as an LP (see Appendix).

Other discrete problems. Finding linear assignments, minimum spanning trees, maximum flows and even applying logical operators can be written in this form. The strength of our method is that it adapts to any setting where the scores to be maximized correspond to a linear function $\langle y, \theta \rangle$, for some embedding of the possible outputs in \mathbb{R}^d .

3. Differentiation of soft maximizers

As noted above, for the right noise distributions, the perturbed maximizer y_ε^* is differentiable in its inputs, with non-zero Jacobian. Further, the derivatives associated to this model can be expressed as simple expectations.

Proposition 3.1. (Abernethy et al., 2016, Lemma 1.5) *For noise Z with distribution $d\mu(z) \propto \exp(-\nu(z))dz$ and twice differentiable ν , the following hold:*

$$\begin{aligned} F_\varepsilon(\theta) &= \mathbf{E}[F(\theta + \varepsilon Z)], \\ y_\varepsilon^*(\theta) &= \nabla_\theta F_\varepsilon(\theta) = \mathbf{E}[y^*(\theta + \varepsilon Z)] \\ &= \mathbf{E}[F(\theta + \varepsilon Z) \nabla_z \nu(Z) / \varepsilon], \\ J_\theta y_\varepsilon^*(\theta) &= \nabla_\theta^2 F_\varepsilon(\theta) = \mathbf{E}[y^*(\theta + \varepsilon Z) \nabla_z \nu(Z)^\top / \varepsilon] \\ &= \mathbf{E}[F(\theta + \varepsilon Z) (\nabla_z \nu(Z) \nabla_z \nu(Z)^\top - \nabla_z^2 \nu(Z)) / \varepsilon^2]. \end{aligned}$$

We discuss in the following subsection efficient techniques to evaluate in practice $y_\varepsilon^*(\theta)$ and its Jacobian, or to generate stochastic gradients, based on these expressions.

Remark 2. Being able to compute the perturbed maximizer and its Jacobian allows to optimize functions that depend on θ through $y_\varepsilon^*(\theta)$. This can be used to alter the costs to promote solutions with certain desired properties. Moreover, in a supervised learning setting, this allows to train models containing blocks with inputs $\theta = g_w(X)$ (for some features

X_i) and outputs $y_{\text{pred}} = y_\varepsilon^*(g_w(X_i))$, for response y_i

$$F(w) = L(\theta = g_w(X_i)) = \ell(y_{\text{pred}} = y_\varepsilon^*(\theta); y_i).$$

For first-order methods, back-propagating $\nabla_w F(w)$ requires not only the usual architecture-dependent $J_w g_w(X_i)$, but also a gradient in θ of the loss $L(\theta)$. If this block is a strict discrete maximizer y^* , as noted above, the computational graph is broken. However, with our proposed modification, we have that

$$\nabla_\theta L(\theta, y_i) = J_\theta y_\varepsilon^*(g_w(X_i)) \nabla_{y_{\text{pred}}} \ell(y_\varepsilon^*(g_w(X_i)); y_i), \quad (3)$$

and the gradient can be fully backpropagated. Perturbed maximizers can therefore be used in end-to-end prediction models, for any loss ℓ on the predicted maximizer. Furthermore, we describe in Section 4 a loss that can be directly optimized in θ by first-order methods. It comes with a strong algorithmic advantage, as it requires only to compute the perturbed maximizer and not its Jacobian.

3.1. Practical implementation

For any θ , the perturbed maximizer $y_\varepsilon^*(\theta)$ is a solution of a convex optimization problem (Eq. 2). If Ω has a simple form, $y_\varepsilon^*(\theta)$ can be computed either explicitly or through convex optimization (e.g. exponential weights for the entropy on the simplex).

More generally, by their expressions as expectations, the perturbed maximizer and its Jacobian in the input θ can be stochastically approximated with Monte-Carlo methods. This only requires to efficiently sample from μ , and to solve the maximization problem over \mathcal{C} , which is a much weaker requirement (see, e.g., examples in Section 2.2).

Definition 3.1. Given $\theta \in \mathbb{R}^d$, let $(Z^{(1)}, \dots, Z^{(M)})$ be M i.i.d. copies of Z and, for $\ell = 1, \dots, M$,

$$y^{(\ell)} = y^*(\theta + \varepsilon Z^{(\ell)}) = \arg \max_{y \in \mathcal{C}} \langle y, \theta + \varepsilon Z^{(\ell)} \rangle.$$

A Monte-Carlo estimate $\bar{y}_{\varepsilon, M}(\theta)$ of $y_\varepsilon^*(\theta)$ is:

$$\bar{y}_{\varepsilon, M}(\theta) = \frac{1}{M} \sum_{\ell=1}^M y^{(\ell)}.$$

Since $\mathbf{E}[y^{(\ell)}] = y_\varepsilon^*(\theta)$ for every $\ell \in [M]$, by definition of p_θ , this yields an unbiased estimate of $y_\varepsilon^*(\theta)$.

Note that the formulae in Proposition 3.1 give several manners to stochastically approximate F_ε , y_ε^* , and their derivatives by using $F(\theta + \varepsilon Z^{(\ell)})$, $y^*(\theta + \varepsilon Z^{(\ell)})$ and $\nabla_z \nu(Z^{(\ell)})$ and averages. This yields unbiased estimates for F_ε , y_ε^* , and its Jacobian. The plurality of these formulae gives the user several options for practical implementation, depending on

how convenient it is to compute the maximum or the maximizer, how numerically stable they are, or what the impact of the $1/\varepsilon$ factors are.

If y_ε^* or its derivatives are used in stochastic gradient descent for training in supervised learning, a full approximation of the gradients is not always necessary. Indeed, taking only $M = 1$ (or a small number) of observations is acceptable here, as the gradients are stochastic in the first place. We call this scheme doubly stochastic, as it is stochastic with respect to both training samples and noise.

A great strength of this method is the absence of conceptual overhead, or of supplementary computations. Only sampling from the chosen noise distribution and solutions of the problem are required. Further, even though our analysis relies on the specific structure of the problem as an LP, these algorithms do not. The Monte-Carlo estimates can be obtained by using a function y^* as a blackbox, without requiring knowledge of the problem or of the algorithm that solves it.

Implementation details. Two methods in which this implementation can be optimized are parallelization and warm starts. Indeed, to alleviate the dependency in M of the running time, we can independently sample the $Z^{(\ell)}$ and compute the $y^{(\ell)} = y^*(\theta + \varepsilon Z^{(\ell)})$ in parallel. On the other hand, on certain algorithms, starting from a solution or near-solution can lead to significant speed-ups. Using $y^*(\theta)$ as initialization can improve running times dramatically, especially at lower temperatures.

4. Perturbed model learning with Fenchel-Young losses

There is a large literature on learning parameters of a Gibbs distribution based on data $(Y_i)_{i=1, \dots, n}$, through maximization of the likelihood:

$$\bar{\ell}_n(\theta) = \frac{1}{n} \sum_{i=1}^n \log p_{\text{Gibbs}, \theta}(Y_i) = \frac{1}{n} \sum_{i=1}^n \langle Y_i, \theta \rangle - \log Z(\theta). \quad (4)$$

They can be optimized by taking gradients of the empirical log-likelihood, of the form

$$\nabla_\theta \bar{\ell}_n(\theta) = \bar{Y}_n - \mathbf{E}_{\text{Gibbs}, \theta}[Y],$$

thus earning the name of moment-matching procedures. The expectation of the Gibbs distribution is however hard to evaluate in some cases. This motivates its replacement by p_θ (perturb-and-MAP in this literature), and to use this method to learn the parameters in this model (Papandreou & Yuille, 2011), as a proxy for log-likelihood.

This minimization is equivalent to maximizing a term akin to Equation (4), substituting the log-partition $Z(\theta)$ with $F_\varepsilon(\theta)$.

We show here that this approach can be formally analyzed by the use of Fenchel-Young losses (Blondel, 2019) in this context. The use of these losses also drastically improves the algorithmic aspects of the learning tasks, because of the specific expression of the gradients in θ of the loss.

Definition 1. In the perturbed model, the *Fenchel-Young* loss $L_\varepsilon(\cdot; y)$ is defined for $\theta \in \mathbb{R}^d$ by

$$L_\varepsilon(\theta; y) = F_\varepsilon(\theta) + \varepsilon \Omega(y) - \langle \theta, y \rangle.$$

It is—among other things—nonnegative, convex in θ , and minimized with value 0 if and only if θ is such that $y_\varepsilon^*(\theta) = y$. It is equal to the Bregman divergence associated to $\varepsilon \Omega$

$$L_\varepsilon(\theta; y) = D_{\varepsilon \Omega}(y, \hat{y}_\varepsilon^*(\theta)).$$

As θ and y interact in this loss only through a scalar product, for random Y we have

$$\mathbf{E}[L_\varepsilon(\theta; Y)] = L_\varepsilon(\theta; \mathbf{E}[Y]) + C,$$

where C does not depend on θ . This is particularly convenient in analyzing the performance of Fenchel-Young losses in generative models. The gradient of the loss is

$$\nabla_\theta L_\varepsilon(\theta; y) = \nabla_\theta F_\varepsilon(\theta) - y = y_\varepsilon^*(\theta) - y.$$

The Fenchel-Young loss can therefore be interpreted as a loss in θ that is a function of $y_\varepsilon^*(\theta)$. Moreover, it can be optimized in θ with first-order methods simply by computing the soft maximizer, without having to compute its Jacobian. It is therefore a particular case of the situation described in Eq. (3), allowing to even bypass virtually the perturbed maximizer block in the output, and to directly optimize a loss between observations y_i and model outputs $\theta = g_w(X_i)$.

These ideas are developed in the following two subsections, in the cases of unsupervised and supervised learning.

4.1. Unsupervised learning - parameter estimation

For a given sequence of observations $(Y_i)_{1 \leq i \leq n} \in \mathcal{Y}^n$, a natural problem is to find the parameter θ that best fits these observations with the Fenchel-Young loss. We show here that this approach is particularly appropriate if the Y_i 's are generated by the perturbed model

$$Y_i = \arg \max_{y \in \mathcal{C}} \langle \theta_0 + \varepsilon Z_i, y \rangle,$$

that is, $Y_i \sim p_{\theta_0}(y)$, for some unknown θ_0 . In this unsupervised model, we therefore have a natural *empirical* \bar{L}_n and *population* loss L_{θ_0} , given a sample of size n

$$\bar{L}_{\varepsilon, n}(\theta) = \frac{1}{n} \sum_{i=1}^n L_\varepsilon(\theta; Y_i) = L_\varepsilon(\theta; \bar{Y}_n) + C(Y),$$

$$\begin{aligned} L_{\varepsilon, \theta_0}(\theta) &= \mathbf{E}[\bar{L}_{\varepsilon, n}(\theta)] = \mathbf{E}_{\theta_0}[L_\varepsilon(\theta; Y)] \\ &= L_\varepsilon(\theta; y_\varepsilon^*(\theta_0)) + C(\theta_0). \end{aligned}$$

Their gradients are given by

$$\begin{aligned} \nabla_\theta \bar{L}_{\varepsilon, n}(\theta) &= \nabla_\theta F_\varepsilon(\theta) - \bar{Y}_n = y_\varepsilon^*(\theta) - \bar{Y}_n, \\ \nabla_\theta L_{\varepsilon, \theta_0}(\theta) &= y_\varepsilon^*(\theta) - y_\varepsilon^*(\theta_0). \end{aligned}$$

The empirical loss is minimized for $\hat{\theta}_n$ such that $y_\varepsilon^*(\hat{\theta}_n) = \bar{Y}_n$ and the population loss when $y_\varepsilon^*(\theta) = y_\varepsilon^*(\theta_0)$. As a consequence, the whole battery of statistical results, from asymptotic to non-asymptotic, can be leveraged, and we present the simplest one (asymptotic normality).

Proposition 4.1. When n goes to ∞ , with the assumptions of Proposition 2.2 on the model, we have

$$\begin{aligned} \sqrt{n}(\hat{\theta}_n - \theta_0) &\rightarrow \mathcal{N}(0, (\nabla_\theta^2 F_\varepsilon(\theta_0))^{-1} \Sigma_Y (F_\varepsilon(\theta_0))^{-1}), \\ &\text{in distribution, where } \Sigma_Y \text{ is the covariance of } Y \sim p_{\theta_0}. \end{aligned}$$

In practice, θ can be fitted by stochastic optimization. Taking the loss only on observation i yields

$$\nabla_\theta L_\varepsilon(\theta; Y_i) = y_\varepsilon^*(\theta) - Y_i.$$

As a consequence, as usually in stochastic optimization, $\nabla_\theta L_\varepsilon(\theta; Y_i)$ is a stochastic gradient either for $\bar{L}_{\varepsilon, n}$ (w.r.t. a random i uniform from $[n]$) or for $L_{\varepsilon, \theta_0}$ (w.r.t. Y_i drawn from $p_{\theta_0}(y)$).

The methods described in Section 3.1 to stochastically approximate the gradient are particularly adapted here. Indeed, following Shpakova & Bach (2016), given an observation Y_i and a current value θ , a *doubly stochastic* version of the gradient is obtained by

$$\bar{\gamma}_{i, M}(\theta) = \frac{1}{M} \sum_{\ell=1}^M y^*(\theta + \varepsilon Z^{(\ell)}) - Y_i. \quad (5)$$

This can also be incorporated with a procedure where batches of data points are used to compute an approximate gradients, where the number of artificial samples M and the batch size can be chosen separately.

4.2. Supervised learning

This loss can also be applied to a supervised learning task with observations (X_i, y_i) , in a model class of parametrized functions g_w , for $w \in \mathbb{R}^d$. The Fenchel-Young loss between y_i and $\theta = g_w(X_i)$ is, in this case as well, a natural and convenient loss to minimize. We consider

$$L_{\varepsilon, \text{emp}}(w) = \frac{1}{n} \sum_{i=1}^n L_\varepsilon(g_w(X_i); y_i)$$

As in the unsupervised setting, this loss can be motivated by a generative model for some parameter w_0 such that

$$Y_i = \arg \max_{y \in \mathcal{C}} \langle g_{w_0}(X_i) + \varepsilon Z^{(i)}, y \rangle. \quad (6)$$

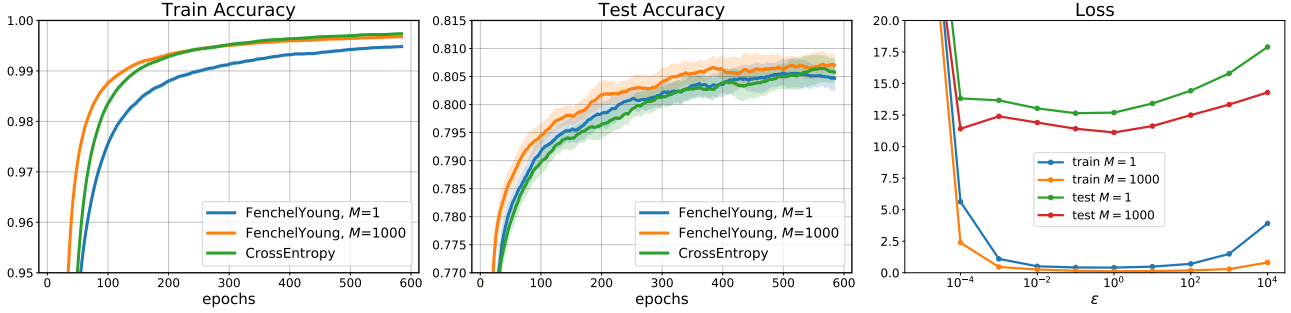


Figure 2. Results for image classification with perturbed argmax. **Left.** Accuracy in training, using the cross-entropy and the FY loss for two sample sizes. **Center.** Test accuracy for these three methods. **Right.** Impact of the parameter ϵ on the test and train ℓ_2^2 loss.

This gives a natural distribution for discrete outputs that are optimizers, where the *population loss* $\mathbf{E}[L_{\epsilon, \text{emp}}(w)]$ is

$$L_{\epsilon, \text{pop}}(w) := \frac{1}{n} \sum_{i=1}^n L_{\epsilon}(g_w(X_i); y_{\epsilon}^*(g_{w_0}(X_i))) + C(w_0)$$

The population loss is therefore minimized at w_0 . The gradient of the empirical loss is given by

$$\nabla_w L_{\epsilon, \text{emp}}(w) = \frac{1}{n} \sum_{i=1}^n J_w g_w(X_i) \cdot (y_{\epsilon}^*(g_w(X_i)) - y_i).$$

Each term in the sum, gradient of the loss for a single observation, is therefore a stochastic gradient for $L_{\epsilon, \text{emp}}$ (w.r.t. i uniform in $[n]$) or for $L_{\epsilon, \text{pop}}$ (w.r.t. to a random Y_i from $p_{g_{w_0}(X_i)}$). As in unsupervised learning, a doubly stochastic gradient is obtained by averaging M perturbed argmax.

5. Experiments

We demonstrate how perturbed maximizers can be used in a supervised learning setting, as described in Section 4. We do so in several tasks with features X_i and responses y_i in a discrete set of optimizers \mathcal{Y} . In this section, since we focus on the prediction task, the issues raised in Remark 1 do not apply. We can write these maxima over polytopes \mathcal{C} that might have empty interior, for ease of notation.

When learning with the Fenchel-Young losses, we simulate doubly stochastic gradients $\nabla_w L_{\epsilon}(g_w(X_i); Y_i)$ of the empirical loss with M artificial perturbations (see Equation 5)

$$\tilde{\gamma}_{i,M} = J_w g_w(X_i) \cdot (\bar{y}_{M,\epsilon}(g_w(X_i)) - y_i)$$

We give here a proof of concept of the adaptivity of this method to several tasks, and exhibit its performance for simple models (small neural networks, linear models).

We will open-source a package allowing to make any black-box solver differentiable in just a few lines of code.

5.1. Perturbed max

We use the perturbed argmax with Gaussian noise in an image classification task. We train a vanilla-CNN made of 4 convolutional and 2 fully connected layers on the CIFAR-10 dataset for 600 epochs with minibatches of size 32. The 10 network outputs are the entries of θ and we minimize the Fenchel-Young loss between $\theta = g_w(X_i)$ and y_i , with different temperatures ϵ and number of perturbations M .

We analyze the impact of these two algorithmic parameters on the optimization and generalization abilities. We exhibit the final loss and accuracy for different number of perturbations in the doubly stochastic gradient ($M = 1, 1000$), and observe competitive performance compared to using the standard cross-entropy loss (Figure 2, left and center).

We also highlight the importance of the temperature parameter ϵ on the algorithm (see Figure 2, right). Very low temperatures do not smooth the maximizers enough and no fitting occurs, even on training data. At very high temperatures, the perturbed maximizer carries less information about θ , and gradient estimates are closer to pure noise, which degrades the ability to fit to training and to generalize to the testing data.

5.2. Perturbed ranking

We create a ranking task by, at each instance i , projecting n vectors $V_{i,(j)}$ of dimension d along an unknown direction w_0 . The label $y_i \in \mathbb{R}^n$ is then given by the vector of ranks of $w_0^\top V_{i,(j)}$, for $j \in [n]$. This provides a simple experiment with permuted vectors as labels, for which the Fenchel-Young loss is convex in w : we fit $\theta = g_w(X_i) = w^\top X_i$ to the response y_i . Since θ is linear in w , the loss is also convex in w and we explore here the performance of our framework in a simple setting. On our experiments, we use instances of $n = 100$ vectors in dimension $d = 9$ - with 3840 instances in the training set and 960 on the test set.

To explore the complexity of this task, we create a range of datasets, where the projections are perturbed with Gaus-

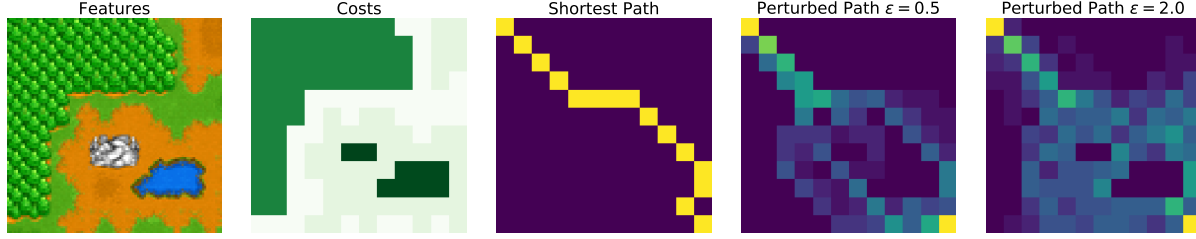


Figure 3. In the shortest paths experiment, training features are images. Shortest paths are computed based on terrain costs, hidden to the network. Training responses are shortest paths based on this cost. We illustrate the impact of the temperature ε on perturbed shortest paths.

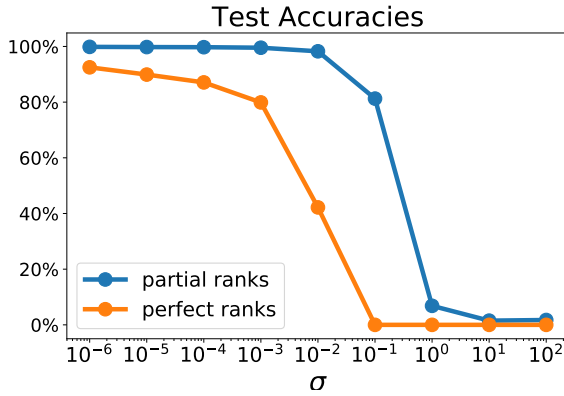


Figure 4. The accuracy, measured in percentage of perfect ranks (complete recovery) and partial ranks (mean of correct positions), under different noise variances on the labels.

sian noise of variance σ before being ranked. They follow precisely the distribution of the generative model described in Equation 6, and the population loss is indeed minimized at w_0 . For correct labels ($\sigma = 0$), our doubly stochastic scheme allows us to accurately generalize after 10 epochs to the test data (see Figure 4). Even under small variances, we are able to accurately predict a high proportion of the correct ranks, and predictably fail for larger variances.

5.3. Perturbed shortest path

We replicate the experiment of Vlastelica et al. (2019), aiming to learn the travel costs in graphs based on features, given examples of shortest path solutions (see Figure 3). On a dataset of 10,000 RGB images of size 96×96 illustrating Warcraft terrains in the form of 12×12 2D grid networks. The responses are a shortest path between the top-left and bottom-right corners, for costs hidden to the network corresponding, to the terrain type. These responses y_i are represented as 12×12 boolean matrices indicating the vertices along the shortest path. We train a purely convolutional neural network made of 3 layers with a Fenchel-Young loss

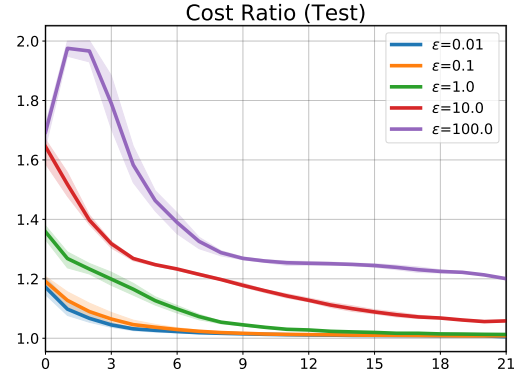


Figure 5. Accuracy of the predicted path, measured by the ratio of costs between the predicted path and the actual shortest path, for several values of the temperature parameter ε .

between the predicted costs $\theta = g_w(X_i)$ and the shortest path y_i . We optimize over 21 epochs with batches of size 64, temperature parameter and $M = 1$, a single perturbation. We are able, only after a few epochs, to generalize very well for $\varepsilon = 0.01$, and to accurately predict the shortest path on the test data (see Figure 5). We show here the impact of the temperature parameter on a finer metric based on the ratio between the optimal and the predicted cost.

6. Conclusion

Despite a large body of work on perturbations techniques for machine learning, most existing works focused on approximating sampling, log-partitions and expectations under the Gibbs distribution. Together with novel theoretical insights, we proposed a framework for differentiating through, not only a max, but also an argmax, without ad-hoc modification of the underlying solver. In addition, by defining an equivalent regularizer Ω , we showed how to construct Fenchel-Young losses and proposed a doubly stochastic scheme, enabling both unsupervised and supervised learning. Experiments validated the ease of application of our framework to various tasks.

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A. Proofs of technical results

Proof of Proposition 2.1. The function $\varepsilon\Omega$ is the Fenchel dual of F_ε (see Proposition 2.2, impact of the temperature), and is defined on \mathcal{C} . As such, as in (Abernethy et al., 2014), we have that

$$F_\varepsilon(\theta) = \sup_{y \in \mathcal{C}} \{ \langle \theta, y \rangle - \varepsilon\Omega(y) \}.$$

It is maximized at $\nabla_\theta F_\varepsilon(\theta) = y_\varepsilon^*(\theta)$, by Fenchel-Rockafellar duality (see, e.g. Wainwright et al., 2008, Appendix A). \square

Proof of Proposition 2.2. The proof of these properties makes use of the notion of the *normal fan* of \mathcal{C} . It is the set of all *normal cones* to all faces of the polytope \mathcal{C} (Rockafellar & Wets, 2009). For each face, such a cone is the set of vectors in \mathbb{R}^d such that the linear program on \mathcal{C} with this vector as cost is maximized on this face. They form a partition of \mathbb{R}^d , and these cones are full dimensional if and only if they are associated to a vertex of \mathcal{C} . These vertices are a subset \mathcal{E} of \mathcal{Y} , corresponding to extreme points of \mathcal{C} .

As a consequence of this normal cone structure, since μ has a positive density, it assigns positive mass to sets if and only if they have non-empty interior, so for any $\theta \in \mathbb{R}^d$, and any $\varepsilon > 0$, $p_\theta(y) > 0$ if and only if $y \in \mathcal{E}$. In most applications, $\mathcal{E} = \mathcal{Y}$ to begin with (all y are potential maximizer for some vector of costs, otherwise they are not included in the set), and all points in \mathcal{Y} have positive mass.

Properties of F_ε

- F_ε is strictly convex

The function F is convex, as a maximum of convex (linear) functions. By definition of F_ε , for every $\lambda \in [0, 1]$ and $\theta, \theta' \in \mathbb{R}^d$, for $\theta_\lambda = \lambda\theta + (1 - \lambda)\theta'$ we have

$$\lambda F_\varepsilon(\theta) + (1 - \lambda)F_\varepsilon(\theta') = \mathbf{E}[\lambda F(\theta + \varepsilon Z) + (1 - \lambda)F(\theta' + \varepsilon Z)] \leq \mathbf{E}[F(\lambda\theta + (1 - \lambda)\theta' + \varepsilon Z)] = F_\varepsilon(\theta_\lambda).$$

The inequality holds with equality if and only if it holds within the expectation for almost all z since the distribution of Z is positive on \mathbb{R}^d . If the function F_ε is not strictly convex, there exists therefore θ and θ' such that

$$\lambda F(\theta + \varepsilon z) + (1 - \lambda)F(\theta' + \varepsilon z) = F(\lambda\theta + (1 - \lambda)\theta' + \varepsilon z)$$

for all $\lambda \in [0, 1]$, for almost all $z \in \mathbb{R}^d$. In this case, F is linear on the segment $[\theta + \varepsilon z, \theta' + \varepsilon z]$ for almost all $z \in \mathbb{R}^d$.

If $\theta - \theta'$ is contained in the boundary between the normal cones to y_1 and y_2 , for all distinct $y_1, y_2 \in \mathcal{E}$, we have $\langle y_1 - y_2, \theta - \theta' \rangle = 0$ for all such pairs of y , so θ is orthogonal to the span of all the pairwise differences of y . However, since \mathcal{C} has no empty interior, it is not contained in a strict affine subspace of \mathbb{R}^d so $\theta - \theta' = 0$. As a consequence, for distinct θ and θ' , there exists $z \in \mathbb{R}^d$ such that $\theta + \varepsilon z$ and $\theta' + \varepsilon z$ are in the interior of two normal cones to different $y \in \mathcal{E}$. As a consequence, the same holds under perturbations of z in a small enough ball of \mathbb{R}^d , so F cannot be linear on almost all segments $[\theta + \varepsilon z, \theta' + \varepsilon z]$, and F_ε is strictly convex.

- F_ε is twice differentiable, as a direct consequence of Proposition 3.1.

- F_ε is R_C -Lipschitz

F is the maximum of finitely many functions that are R_C -Lipschitz. It therefore also satisfies this property. F_ε is an expectation of such functions, therefore it satisfies the same property.

- F_ε is $R_C M_\mu / \varepsilon$ -gradient Lipschitz.

We have, by Proposition 3.1, for θ and θ' in \mathbb{R}^d

$$\nabla_\theta F_\varepsilon(\theta) - \nabla_\theta F_\varepsilon(\theta') = \mathbf{E}[(F(\theta + \varepsilon Z) - F(\theta' + \varepsilon Z)) \nabla_z \nu(Z) / \varepsilon].$$

As a consequence, by the Cauchy-Schwarz inequality, and Lipschitz property of F , it holds that

$$\begin{aligned} \|\nabla_\theta F_\varepsilon(\theta) - \nabla_\theta F_\varepsilon(\theta')\| &\leq \mathbf{E}[\|F(\theta + \varepsilon Z) - F(\theta' + \varepsilon Z)\|^2]^{1/2} \mathbf{E}[\|\nabla_z \nu(Z)\|^2 / \varepsilon^2]^{1/2} \\ &\leq R_C \|\theta - \theta'\| \mathbf{E}[\|\nabla_z \nu(Z)\|^2]^{1/2} / \varepsilon = (R_C M_\mu / \varepsilon) \|\theta - \theta'\|. \end{aligned}$$

Properties of Ω

The function $\varepsilon\Omega$ is the Fenchel dual of F_ε , which is strictly convex and $R_C M_\mu/\varepsilon$ smooth. As a consequence, Ω is differentiable on the image of y_ε^* – the interior of \mathcal{C} – and it is $1/R_C M_\mu$ -strongly convex.

- Legendre type property

The regularization function Ω is differentiable on the interior. If there is a point y of its boundary such that $\nabla_y \Omega$ does not diverge when approaching y , then taking θ such that $\theta - \varepsilon \nabla_y \Omega(y) \in \mathcal{N}_C(y)$ (where $\mathcal{N}_C(y)$ is the normal cone to \mathcal{C} at y), then $y_\varepsilon^*(\theta) = y$. However, y_ε^* takes image in the interior of \mathcal{C} (see immediately below), leading to a contradiction.

Properties of y_ε^*

- The perturbed maximizer is in the interior of \mathcal{C}

Since the distribution of Z has positive density, the probability that $\theta + \varepsilon Z \in \mathcal{N}_C(y)$ (i.e. $p_\theta(y)$) is positive for all $y \in \mathcal{E}$. As a consequence, since

$$y_\varepsilon^*(\theta) = \sum_{y \in \mathcal{E}} y p_\theta(y),$$

with all positive weights $p_\theta(y)$, y_ε^* is in the interior of the convex hull \mathcal{C} of \mathcal{E} .

- The function y_ε^* is differentiable, by twice differentiability of F_ε , by Proposition 3.1.

Influence of temperature parameter $\varepsilon > 0$

We have for all θ

$$F_\varepsilon(\theta) = \mathbf{E}[\max_{y \in \mathcal{C}} \langle y, \theta + \varepsilon Z \rangle] = \varepsilon \mathbf{E}[\max_{y \in \mathcal{C}} \langle y/\varepsilon, \theta + Z \rangle] = \varepsilon F_1(\theta/\varepsilon).$$

As a consequence

$$(F_\varepsilon)^*(y) = \max_{z \in \mathbb{R}^d} \{\langle y, z \rangle - F_\varepsilon(z)\} = \varepsilon \max_{z \in \mathbb{R}^d} \{\langle y, z/\varepsilon \rangle - \varepsilon F_1(z/\varepsilon)\} = \varepsilon (F_1)^*(y) = \varepsilon \Omega(y).$$

Since $y_\varepsilon^*(\theta) = \nabla_\theta F_\varepsilon(\theta)$, and since $F_\varepsilon(\theta) = \varepsilon F_1(\theta/\varepsilon)$, we have $y_\varepsilon^*(\theta) = y_1^*(\theta/\varepsilon)$. \square

Proof of Proposition 2.3. We recall that we assume that θ yields a unique maximum to the linear program on \mathcal{C} . This is true almost everywhere, and assumed here for simplicity of the results. We discuss briefly at the end of this proof how this can be painlessly extended to the more general case.

Limit at low temperatures ($\varepsilon \rightarrow 0$)

Since F is convex (see proof of Proposition 2.2), so by Jensen's inequality

$$\begin{aligned} F(\mathbf{E}[\theta + \varepsilon Z]) &\leq \mathbf{E}[F(\theta + \varepsilon Z)] \\ F(\theta) &\leq F_\varepsilon(\theta). \end{aligned}$$

Further, we have for all $Z \in \mathbb{R}^d$

$$\max_{y \in \mathcal{C}} \langle \theta + \varepsilon Z, y \rangle \leq \max_{y \in \mathcal{C}} \langle \theta, y \rangle + \varepsilon \max_{y' \in \mathcal{C}} \langle Z, y' \rangle$$

Taking expectations on both sides yields that

$$F_\varepsilon(\theta) \leq F(\theta) + \varepsilon F_1(\theta).$$

As a consequence, when $\varepsilon \rightarrow 0$, combining these two inequalities yields that $F_\varepsilon(\theta) \rightarrow F(\theta)$.

Regarding the behavior of the perturbed maximizer $y_\varepsilon^*(\theta)$, we follow the arguments of (Peyré & Cuturi, 2019, Proposition 4.1). By Proposition 2.1 and the definition of $y^*(\theta)$, we have

$$0 \leq \langle y^*(\theta), \theta \rangle - \langle y_\varepsilon^*(\theta), \theta \rangle \leq \varepsilon [\Omega(y^*(\theta)) - \Omega(y_\varepsilon^*(\theta))]$$

Since Ω is continuous, it is bounded on \mathcal{C} , and the right hand term above is bounded by $C\varepsilon$, for some $\varepsilon > 0$. As a consequence, when $\varepsilon \rightarrow 0$, $\langle y_\varepsilon^*(\theta), \theta \rangle \rightarrow \langle y^*(\theta), \theta \rangle$. For any sequence $\varepsilon_n \rightarrow 0$, the sequence $y_n = y_{\varepsilon_n}^*(\theta)$ is in a compact

\mathcal{C} . Therefore, it has a subsequence $y_{\varphi(n)}$ that converges to some limit $y_\infty \in \mathcal{C}$. However, since $\langle y_{\varphi(n)}^*, \theta \rangle \rightarrow \langle y^*(\theta), \theta \rangle$, we have $\langle y_\infty, \theta \rangle = \langle y^*(\theta), \theta \rangle$, by continuity. Since $y^*(\theta)$ is a unique maximizer, $y_\infty = y^*(\theta)$. As a consequence, all convergent subsequences of y_n converge to the same limit $y^*(\theta)$: it is the unique accumulation point of this sequence. It follows directly that y_n converges to $y^*(\theta)$, as it lives in a compact set, which yields the desired result.

Limit at high temperatures By Proposition 2.2, $y_\varepsilon^*(\theta) = y_1(\theta/\varepsilon)$, so the desired result follows by continuity of the perturbed maximizer.

Nonasymptotic inequalities. These inequalities follow directly from those proved to establish limits at low temperatures.

If θ is such that the maximizer is not unique (which occurs only on a set of measure 0), the only result affected is the convergence of $y_\varepsilon^*(\theta)$ when $\theta \rightarrow 0$. Following the same proof of (Peyré & Cuturi, 2019, Proposition 4.1), it can be shown to converge to the minimizer of Ω over the set of maximizer. This point is always unique, as the minimizer of a strongly convex function over a convex set. \square

Proof of Proposition 4.1. We follow the classical proofs in M-estimation (see, e.g. van der Vaart, 2000, Section 5.3). First, the estimator is consistent as a virtue of the continuous mirror map between \mathbb{R}^d and $\text{int}(\mathcal{C})$. For n large enough $\bar{Y}_n \in \text{int}(\mathcal{C})$, since the probability of each extreme point of \mathcal{C} is positive. By definition of the estimator and stationarity condition for $\hat{\theta}_n$, we have in these conditions

$$\nabla_\theta F_\varepsilon(\hat{\theta}_n) = \bar{Y}_n, \quad \nabla_\theta F_\varepsilon(\theta_0) = y_\varepsilon^*(\theta_0).$$

By the law of large numbers, \bar{Y}_n converges to its expectation $y_\varepsilon^*(\theta_0)$ a.s. Since $\varepsilon \nabla_y \Omega$, the inverse of $\nabla_\theta F_\varepsilon$, is also continuous (by the fact that Ω is convex smooth), so we have that $\hat{\theta}_n$ converges to θ_0 a.s.

We write the first order conditions for $\bar{L}_{\varepsilon,n}$ at $\hat{\theta}_n$ and the Taylor expansion with Lagrange remainder for all coordinates, one by one

$$0 = \nabla_\theta \bar{L}_{\varepsilon,n}(\hat{\theta}_n) = \nabla_\theta \bar{L}_{\varepsilon,n}(\theta_0) + A_n(\hat{\theta}_n - \theta_0), \quad (7)$$

where A is such that, for all coordinates $i \in [d]$

$$A_i = (\nabla_{\bar{\theta}}^2 \bar{L}_{\varepsilon,n}(\bar{\theta}^{(i)}))_i$$

for some $\bar{\theta}^{(i)} \in [\hat{\theta}_n, \theta_0]$. We note here that since the estimator is not necessarily in dimension 1, A_n cannot be written directly as $\nabla_{\bar{\theta}}^2 \bar{L}_{\varepsilon,n}(\bar{\theta})$ for some $\bar{\theta} \in [\hat{\theta}_n, \theta_0]$, since the Taylor expansion with Lagrange remainder is not true in its multivariate form. However, doing it coordinate-by-coordinate as here allows to circumvent this issue.

We have that $\nabla^2 \bar{L}_{\varepsilon,n} = \nabla^2 F_\varepsilon$. Since $\hat{\theta}_n \rightarrow \theta_0$ a.s. we have that $\bar{\theta}^{(i)} \rightarrow \theta_0$ for all $i \in [d]$, so $A_n \rightarrow \nabla^2 F_\varepsilon(\theta_0)$ a.s. Rearranging terms in Eq. (7), we have

$$\begin{aligned} \sqrt{n}(\hat{\theta}_n - \theta_0) &= -A_n^{-1} \cdot \sqrt{n} \nabla_\theta \bar{L}_{\varepsilon,n}(\theta_0) \\ &= -A_n^{-1} \cdot \sqrt{n}(\bar{Y}_n - y_\varepsilon^*(\theta_0)) \end{aligned}$$

By the central limit theorem, $\sqrt{n}(\bar{Y}_n - y_\varepsilon^*(\theta_0)) \rightarrow \mathcal{N}(0, \Sigma_Y)$ in distribution. As a consequence, by convergence of A_n and Slutsky's lemma, we have the convergence in distribution

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \rightarrow \mathcal{N}(0, (\nabla_{\bar{\theta}}^2 F_\varepsilon(\theta_0))^{-1} \Sigma_Y (F_\varepsilon(\theta_0))^{-1}).$$

\square

B. Examples of discrete decision problems as linear programs

Our method applies seamlessly to all decision problems over discrete sets. Indeed, any problem of the form $\max_{y \in \mathcal{Y}} s(y)$, for some score function $s : \mathcal{Y} \rightarrow \mathbb{R}$, can at least be written in the form

$$\max_{x \in \Delta^{|\mathcal{Y}|}} \langle x, s \rangle,$$

by representing \mathcal{Y} as the vertices of the unit simplex in $\mathbb{R}^{|\mathcal{Y}|}$. However, for most interesting decision problem that can actually be solved in practice, the score function takes a simpler form $s(y) = \langle y, \theta \rangle$, for some representation of $y \in \mathbb{R}^d$ and some θ . We give here a non-exhaustive list of examples of interesting problems of this type.

Maximum. The max function from \mathbb{R}^d to \mathbb{R} , that returns the largest among the d entries of a vector θ is ubiquitous in machine learning, the hallmark of any classification task. It is equal to $F(\theta)$ over the standard unit simplex.

$$F(\theta) = \max_{i \in [d]} \theta_i, \quad \mathcal{C} = \{y \in \mathbb{R}^d : y \geq 0, \mathbf{1}^\top y = 1\}.$$

On this set, using Gumbel noise yields the log-sum-exp for F_ε , the Gibbs distribution for p_θ , and the softmax for y_ε^* . Using other noise distributions for Z will change the model.

Top k . The function from \mathbb{R}^d to \mathbb{R} that returns the sum of the k largest entries of a vector θ is also commonly used. It fits our framework over the set

$$\mathcal{C} = \{y \in \mathbb{R}^d : 0 \leq y \leq 1, \mathbf{1}^\top y = k\}.$$

Ranking. The function returning the ranks (in descending order) of a vector $\theta \in \mathbb{R}^d$ can be written as the argmax of a linear program over the *permutahedron*, the convex hull of permutations of any vector v with distinct entries

$$\mathcal{C} = \mathcal{P}_v = \text{cvx}\{P_\sigma v : \sigma \in \Sigma_d\}.$$

Using different reference vectors v yield different perturbed operations, and $v = (1, 2, \dots, d)$ is commonly used.

Shortest paths. For a graph $G = (V, E)$ and positive costs over edges $c \in \mathbb{R}^E$, the problem of finding a shortest path (i.e. with minimal total cost) from vertices s to t can be written in our setting with $\theta = -c$ and

$$\mathcal{C} = \{y \in \mathbb{R}^E : y \geq 0, (\mathbf{1}_{\rightarrow i} - \mathbf{1}_{i \rightarrow})^\top y = \delta_{i=s} - \delta_{i=t}\}.$$

Assignment. The linear assignment problem, and more generally the optimal transport problem, can also be written as a linear program. In the case of the assignment problem, it is the *Birkhoff polytope* of doubly-stochastic matrices, whose extreme points are the permutation matrices

$$\mathcal{C} = \{Y \in \mathbb{R}^{d' \times d'} : Y_{ij} \geq 0, \mathbf{1}^\top Y = \mathbf{1}^\top, Y\mathbf{1} = \mathbf{1}\}.$$

There is a large literature on regularization of this problem, with entropic penalty (Cuturi, 2013). This is one of the rare cases where the regularized version of the problem is actually computationally lighter, in stark contrast with the general case in our setting.

Combinatorial problems. Many other problems, such in combinatorial optimization can be formulated exactly (e.g. minimum spanning tree, maximum flow), or approximately via convex relaxations (e.g. traveling salesman problem, knapsack), via relaxations in linear programs. Differentiable versions of these exact or approximate solutions can therefore be obtained via perturbation methods.

Relaxations with atomic norms A wide variety of high-dimensional statistical learning problems can be tackled by regularization via atomic, or otherwise sparsity-inducing norms (Chandrasekaran et al., 2012; Bach et al., 2012). Our framework also allows us to consider versions of these estimators that are differentiable in their inputs.