Combinatorial Losses through Generalized Gradients of Integer Linear Programs

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Abstract

When samples have internal structure, we often see a mismatch between the objective optimized during training and the model's goal during inference. For example, in sequence-to-sequence modeling we are interested in high-quality translated sentences, but training typically uses maximum likelihood at the word level. Learning to recognize individual faces from group photos, each captioned with the correct but unordered list of people in it, is another example where a mismatch between training and inference objectives occurs. In both cases, the natural training-time loss would involve a combinatorial problem — dynamic programming-based global sequence alignment and weighted bipartite graph matching, respectively — but solutions to combinatorial problems are not differentiable with respect to their input parameters, so surrogate, differentiable losses are used instead. Here, we show how to perform gradient descent over combinatorial optimization algorithms that involve continuous parameters, for example edge weights, and can be efficiently expressed as integer, linear, or mixed-integer linear programs. We demonstrate usefulness of gradient descent over combinatorial optimization in sequence-to-sequence modeling using differentiable encoder-decoder architecture with softmax or Gumbel-softmax, and in weakly supervised learning involving a convolutional, residual feed-forward network for image classification.

1 Introduction

Combinatorial optimization problems [1][2], such as shortest path in a weighted directed graph, minimum spanning tree in a weighted undirected graph, or optimal assignment of tasks to workers, play a central role in many computer science applications. Yet, these fundamental problems, and the highly refined, efficient algorithms for solving them, have been largely absent in statistical learning involving deep predictive models. While we can use the Ford–Fulkerson algorithm to efficiently solve the shortest path problem, the total length of the shortest path as a function of the edge weights is not differentiable. This precludes using shortest distances as a criterion in training models that rely on differentiability of the objective function with respect to the model parameters.

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Deep predictive models learn to approximate a multivariate function or distribution based on training data. The model is composed of transformations that involve tunable parameters, which are most often fitted by optimizing a loss – a measure of approximation quality – using methods based on derivatives, such as variants of gradient descent. Efficient evaluation of gradients is thus a prerequisite for a transformation to be considered a useful building block in neural networks. Each transformation in the model should be differentiable with respect to its parameters. It should also be differentiable with respect to its input, to pass the gradient information to prior transformations.

While differentiability has been key in advancing from linear perceptron to non-linear, multi-layer neural networks \cite{3}, top-performing architectures go beyond classically-defined differentiability. For example, practical architectures use non-smooth elements such as max-pooling layer \cite{4} and ReLU activation function \cite{5}, even though these are not differentiable; a network involving them may not be locally convex and even subgradients may not be well-defined. Clearly, differentiability in the whole domain is a requirement that can be relaxed. This has been often achieved formally through the definition of subgradient \cite{6}, or a less well-known notion of Clarke subdifferential \cite{7}, a generalized gradient that eliminates the convexity assumption inherent in the definition of subgradient.

1.1 Our Contribution

Our main result shows that a broad class of combinatorial problems can be integrated into models trained using variants of gradient descent.

**Theorem. (Informal)** For an efficiently solvable combinatorial problem that can be efficiently expressed as a mixed-integer linear program, generalized gradients of the problem's objective value with respect to real-valued parameters defining the problem exist and can be efficiently computed.

Using the above result, we show how generalized gradients of combinatorial problems can provide sentence-level loss for text summarization using differentiable encoder-decoder models that involve softmax or Gumbel softmax \cite{8}, and an multi-element loss for training classification models when only weakly supervised, bagged training data is available.

2 Generalized Gradient Descent over Combinatorial Problems

2.1 Generalized Gradients

A function $f : \mathcal{X} \rightarrow \mathbb{R}$ defined over a convex, bounded open set $\mathcal{X} \subseteq \mathbb{R}^p$ is Lipschitz continuous on an open set $B \subseteq \mathcal{X}$ if there is a finite $K \in \mathbb{R}$ such that $\forall x, y \in B \; |f(x) - f(y)| \leq K||x - y||$. For a differentiable function, it suffices that its gradient is bounded on $B$ for the function to be Lipschitz continuous on $B$. A function is locally Lipschitz-continuous if for every point $x_0$ in its domain, there is a neighborhood $B_0$, an open ball centered at $x_0$, on which the function is Lipschitz-continuous. We then have the following definition of a generalized gradient.

**Definition 1.** \cite{7} Let $f : \mathcal{X} \rightarrow \mathbb{R}$ be Lipschitz-continuous in the neighborhood of $x \in \mathcal{X}$. Then, the Clarke subdifferential $\partial f(x)$ of $f$ at $x$ is defined as

$$
\partial f(x) = \text{conv} \left\{ \lim_{x_k \rightarrow x} \nabla f(x_k) \right\},
$$

2
where the limit is over all convergent sequences of \(x_k\) where gradient exists, and \(\text{conv}\) denotes convex hull, that is, the smallest polyhedron that contains all vectors from a given set. Each element of the set \(\partial f(x)\) is called a generalized gradient of \(f\) at \(x\).

The Rademacher theorem \([9]\) states that for any locally Lipschitz-continuous function the gradient exists almost everywhere; convergent sequences can be found.

The convex hull has one element if \(f\) has gradient at \(x\); then, all convergent sequences converge to \(\nabla f(x)\). If \(f\) is locally convex in the neighborhood of \(x\), then \(\partial f(x)\) is equal to the subdifferential of \(f\) at \(x\), the set of all subgradients, that is, vectors \(g \in \mathbb{R}^p\) such that for any \(y \in X\), \(f(y) - f(x) \geq \langle g, y - x \rangle\). In optimization algorithms, generalized gradients can be used in the same way as subgradients \([10]\), that is, nondifferentiability may affect convergence in certain cases.

### 2.2 Linear Programs and their Generalized Gradients

We will consider here feasible, bounded programs. For \(c \in \mathbb{R}^p\), \(b \in \mathbb{R}^m\), and for an \(m \times p\) matrix \(A = [a_{ij}]\), a primal and dual formulation of a linear program (LP) \([11]\)

\[
\begin{align*}
\min_u & \quad z = c^T u \\
\text{s.t.} & \quad Au = b \\
& \quad u \geq 0,
\end{align*}
\]

are solved by the same finite optimal objective value \(z^* = \text{LP}(c, A, b)\) and have the sets of optimal primal solutions \(U^* = \{u^*\} \subset \mathbb{R}^p\) and dual solutions \(V^* = \{v^*\} \subset \mathbb{R}^m\).

The objective value \(z^* = \text{LP}(c, A, b)\) of a linear program is not a differentiable function of the program’s parameters \(c, A, b\). However, generalized gradients can be defined.

**Proposition 2.** \([12]; [13]; [14]\) If \(z^* = \text{LP}(c, A, b)\) is finite at \((c, A, b)\) and in some neighborhood of \((c, A, b)\), then generalized gradients of \(z^*\) with respect to \(c, b,\) and \(A\) exist and are

\[
\begin{align*}
\partial z^*(c) &= U^*, \\
\partial z^*(b) &= V^*, \\
\partial z^*(A) &= \left\{ -vu^T : (u, v) \in V^* \times U^* \right\}.
\end{align*}
\]

Further, if the primal and dual solutions \(u^*\) and \(v^*\) are unique, \(z^* = \text{LP}(c, A, b)\) has gradients \(u^*, v^*,\) and \(-v^*u^T\) at \((c, A, b)\) with respect to \(c, b,\) and \(A\).

Consider the gradient of \(z^*\) with respect to \(c\). In the absence of any constraints, the gradient of \(c^T u\) with respect to \(c\) is simply \(u\). Once the constraints are introduced, the resulting LP for a single \((c, A, b)\) may have multiple primal or dual solution vectors corresponding to the same objective value. The feasible set is a multidimensional convex polyhedron, and the optimal solution set is either a single vertex of the polyhedron, or a whole face. Consider a set of parameters \((c, A, b)\) for which optimal primal and dual solutions are unique. Then, there is a neighborhood of \(c\) in which \(c + \varepsilon \Delta c\) has the same solution \(u\), and the objective value changes to \((c^T + \varepsilon \Delta c^T)u\) – the gradient is still \(u\). At some point, though, \(c\) changes so much that, while \(u\) is still an optimal solution, is not the only one: one of the feasible set polyhedron faces that contains \(u\) as a vertex becomes the solution set. For that \(c\), gradient does not exist, but the whole face of the polyhedron, including \(u\), defines the generalized gradient. Next, as
c changes further, the solution becomes unique again, it is a different vertex $u'$ of the same face of the polyhedron; gradient of $z^*$ with respect to $c$ exists again, it is $u'$. For a bounded, feasible LP, the set of gradients depends on the set of primal and dual solutions. The set of gradients is bounded, hence $z^*$ is Lipschitz-continuous in neighborhoods where it is finite, and generalized gradients exist.

2.3 Combinatorial Problems

Combinatorial problems such as shortest path or minimum spanning tree in a graph, unlike LPs, are defined over discrete domains – typically sets, represented by binary numbers or integers. Let $n$ be scalar or a vector describing the size of the combinatorial problem, for example the number of nodes and the number of edges in a graph. Given an algorithm for solving instances of the combinatorial problem of size $n$ in polynomial time poly($n$), we can construct a poly($n$)-sized Boolean circuit for the algorithm. For each poly($n$)-sized circuit, there is an LP with poly($n$) variables and constraints that gives the same solution (see [15], Chap. 7).

Reducing a combinatorial problem to an LP via a Boolean circuit is cumbersome, but typically a combinatorial problem can be phrased as a smaller, much more intuitive linear program if we add a constraint that the solution vector involves only integers – these are integer programs (IP), or mixed-integer linear programs (MILP) if only some variables are constrained to be integer. For example, graph problems such as shortest path, minimum spanning tree, and traveling salesman problem can all be specified as an integer program involving binary variables. The decision variant of IP is NP-complete, thus any decision problem in NP can be reduced to an integer program [15].

The following result shows that any integer program can be reduced to a linear program.

Proposition 3. [16] Consider an integer linear program

$$ \min_u \ z = c^T u \quad \text{s.t.} \quad Au = b, \quad u \geq 0, \quad u \in \mathbb{Z}^p, $$

Then, there exists a corresponding ideal formulation, a linear program

$$ \min_u \ z = c^T u \quad \text{s.t.} \quad A'u = b', \quad u \geq 0, $$

with the same solution $u$ and objective value $z^*$.

For a feasible, bounded $p$-dimensional integer program, we can view the pair $(A, b)$ as a convex polyhedron $\mathcal{A}$, the set of all feasible solutions. Then, the pair $(A', b')$ in the ideal formulation LP is defined as the set of constraints specifying the feasible set $\mathcal{A}' = \text{conv} \{A \cap \mathbb{Z}^p\}$. Convex hull of a subset of a convex set $\mathcal{A}$ is a subset of $\mathcal{A}$, thus, $\mathcal{A}'$ is convex, contains all integer solutions from $\mathcal{A}$, and no other integer solutions. The extension to MILPs is straightforward. Note that the number of linear constraints in the ideal formulation may be exponential in $p$, and/or in $m$, the number of the original constraints in $\mathcal{A}$; thus, the existence of the ideal formulation LP for a MILP may not have practical utility for solving it. However, special useful cases exist; for example, if matrix $A$ is totally unimodular [17] and $b \in \mathbb{Z}$, then $\mathcal{A}' = \mathcal{A}$ and $b' = b$; all vertices of the feasible set $\mathcal{A}$ are guaranteed to be integers.

2.4 Gradient Descent over Combinatorial Optimization

We are now prepared to introduce the result that shows how to perform efficient gradient-based optimization over solution to the combinatorial problems. We restrict our attention to
combinatorial problems that are defined, for a given problem size $n$ and given structure, by a vector of real-valued parameters $w \in W \subseteq \mathbb{R}^{\text{poly}(n)}$ – for example, by edge weights for a graph with a given topology – and that have a single, finite, real optimal objective value for every $w \in W$ – for example, a finite distance along the shortest path from source to target node. We further assume that the set $W$ of possible parameters $w$ is simply connected – that there are no holes consisting of forbidden parameters in it, although forbidden $w$ outside of $W$, such as weight vectors leading to a graph with negative-weight cycles reachable from the shortest path source, may exist. These assumptions are met for typical combinatorial optimization problems.

First, we introduce several notions of efficiency of transforming a combinatorial problem into a linear program that will be convenient in defining the generalized gradients of combinatorial problems.

**Definition 4.** Let $P(w)$ be a combinatorial problem that is parameterized by a continuous vector $w \in W \subseteq \mathbb{R}^{\text{poly}(n)}$, where $W$ is simply connected, and $n$ is a scalar or a vector describing the size of the problem $P$. Then, a combinatorial problem is

- **primal-dual $\partial$-efficient** if it can be phrased as a mixed integer linear program involving $p = \text{poly}(n)$ variables, with $m' = \text{poly}(n)$ constraints in the ideal formulation of the MILP, and the parameters of the ideal formulation depend on $w$ through (sub)differentiable functions, $c = c(w), A' = A'(w), b' = b'(w)$.

- **primal $\partial$-efficient** if it can be phrased as a mixed integer linear program involving $p = \text{poly}(n)$ variables, the parameters $w$ of the problem influence the cost vector $c$ through a (sub)differentiable function $c = c(w)$, and do not influence the constraints $A,b$.

- **dual $\partial$-efficient** if it can be phrased as a mixed integer linear program in which the number of constraints in the ideal formulation is $m' = \text{poly}(n)$, the parameters $w$ of the problem influence $b'$ through a (sub)differentiable function $b' = b'(w)$, and do no influence the constraint matrix $A$ nor the cost vector $c$.

For example, minimal spanning tree in an undirected graph is primal $\partial$-efficient, we have an IP with one binary variable per edge, and the weight of the edge only influences the cost vector $c$. It is not primal-dual $\partial$-efficient – we have to prohibit cycles in the solution, for example by a constraint for each cycle in the graph, thus the number of constraints is not poly($n$) for arbitrary graphs. However, these constraints are specified fully by the topology of the graph, not by the edge weights, so $w$ does not influence $A'$ nor $b'$. In typical cases, the functions $c = c(w), b' = b'(w)$ and $A' = A'(w)$ are identity or constant; for example, in the program for MST, the cost vector is composed directly of edge weights, and $A$ an $b$ are constant, do not depend on weights.

Our main result is the following theorem.

**Theorem 5.** Consider a combinatorial problem $P(w)$ of size $n$, a parameter vector $w$ from the interior of the parameter domain $W$, and an algorithm $\Pi(w)$ for solving it in time $\text{poly}(n)$. Let $z^*$ be the optimal objective value returned by $\Pi$. Then,

- if $P$ is primal $\partial$-efficient, then the generalized gradients $\partial z^*(w)$ exist, and can be efficiently computed from $U^*$, the set of primal solution of the integer program corresponding to $P$;
• if \( P \) is dual \( \partial \)-efficient, then the generalized gradients of \( \partial z^*(w) \) exist, and can be efficiently computed from \( V^* \), the set of all dual solution to the ideal formulation of the integer program corresponding to \( P \);

• if \( P \) is primal-dual \( \partial \)-efficient, then the generalized gradients of \( A \) over \( w \) exist, and can be efficiently computed from \( U^* \) and \( V^* \), as defined above.

Proof. For the first case, definition 4 states that in the mixed integer linear program corresponding to \( P \), only the cost vector \( c \) depends on \( w \), through a (sub)differentiable function \( c = c(w) \). Since \( w \) is in the interior of the parameter domain \( W \), the objective value is finite over some neighborhood of \( w \). Then,
\[
\partial z^*(w) = \partial z^*(c) \frac{\partial c}{\partial w} = \frac{\partial c}{\partial w} U^*,
\]
where by proposition 2 the generalized gradient \( z^*(c) \) exists and is equal to \( U^* \).

For the second case, from proposition 3 we have that the ideal formulation LP exists. Then, from definition 4 and proposition 2 we have that
\[
\partial z^*(w) = \partial z^*(b') \frac{\partial b'}{\partial w} = \frac{\partial b}{\partial w} V^*.
\]
The third case is a direct extension of the first two cases. \( \Box \)

2.5 Combinatorial Losses in Deep Learning

Combinatorial algorithms can be used to expand the range of transformations that can be efficiently utilized in neural networks. One immediate area of application is using them to specify a loss function. Consider a network \( F(x; \beta) \) parameterized by a vector of tunable parameters \( \beta \). The network transforms a batch of input samples \( x \) into a batch of outputs \( y \). Let us also consider a batch \( y' \) of some external information, such as target real images in generative networks. Then, in the broadest primal-dual \( \partial \)-efficient case, \( y \) is used, possibly with \( x \) or \( y' \), to formulate parameters \( (c, A, b) = g(x, y, y') \) of a linear program corresponding to the combinatorial problem, through some function \( g \). For brevity, we assume below that the combinatorial algorithm \( \Pi \) takes input directly in the form of \( (c, A, b) \); the general case where the algorithm takes \( w = g(x, y, y') \) and where we have \( c = c(w), b = b(w) \) and \( A = A(w) \) are easily derived through adding terms in the backward pass. For a given \( \beta \) and given batch \( (x, y, y') \), we can then define loss as a function of the optimal objective value of the linear program, \( L(x, y, y') = h(z^*(c, A, b)) \). This approach allows us to obtain the generalized gradient of the loss with respect to \( \beta \) as long as functions \( g \) and \( h \) are differentiable. For clarity, in Algorithm 1, we did not consider functions \( h \) depending not just on \( z \) but also on \( x, y, y' \), but the extension is straightforward.

3 Weighted Bipartite Graph Matching for Weakly-supervised Learning

To illustrate gradient descent over a combinatorial loss, we first focus on a simple image recognition problem. Consider a photo of a group of people with a caption listing each of the persons in the picture, but missing the "from left to right" part. Given a collection of such
Algorithm 1 Minimization of a combinatorial loss

**Input:** batch \( x \subseteq X, y \subseteq Y, y' \subseteq Y' \), network \( F(x; \beta) \), differentiable functions \( g, h \), combinatorial algorithm \( \Pi \)

**Output:** Loss and its generalized gradient, \( L(\beta), \partial L(\beta) \)

1: **procedure** COMBLOSSMIN(\( x, y, y', \beta, F, g, h, A \))
2:     forward pass \( y = F(x; \beta) \)
3:     forward pass \( (c, A, b) = g(x, y, y') \)
4:     use combinatorial algorithm to find optimal value \( z^* = \Pi(c, A, b) \), a primal solution \( u^* \), and a dual solution \( v^* \)
5:     forward pass \( L(\beta) = h(z^*) \)
6:     backward pass through \( h \): \( \partial L/\partial z \)
7:     backward pass through \( A \): \( \partial z^*(c) = u^*, \partial z^*(b) = v^*, \partial z^*(A) = -v^*u^* \)
8:     backward pass through \( g \) and \( F \)
9:     \( \partial L(\beta) = \frac{\partial L}{\partial \beta} \left( u^* \frac{\partial c}{\partial \beta} - v^* u^T \frac{\partial A}{\partial \beta} + v^* \frac{\partial c}{\partial \beta} \right) \)
10: **return** \( L(\beta), \partial L(\beta) \)
11: **end procedure**

labeled photos, can a model learn to recognize individual faces? Similarly, consider a shopping cart and a printout from the register. Given a collection of unordered shopping carts together with matching receipts, can a model learn to recognize individual shopping items? These are example of a weakly-supervised learning where the goal is to learn to classify previously unseen feature vectors, but a training sample is a bag of feature vectors accompanied by a bag of correct labels, instead of a feature-vector and a correct label. We are not told which class belongs to which sample, which prevents us from directly using the standard cross-entropy loss.

3.1 Generalized Gradient over the Hungarian Method

Consider a \( d \)-class classification problem, and a network \( F(x_i; \beta) \) that for sample \( x_i \) returns a \( d \)-dimensional vector of class probabilities, \( p_i \), with \( p_i \) denoting the predicted conditional probability of class \( j \) given feature vector \( x_i \). Let \( y_i \) denote a \( d \)-dimensional, one-hot representation of the true class label of sample \( x_i \).

In weakly supervised learning involving bags (see Fig. 1), a single element of the training set is an ordered tuple of \( X = (x_j)_{j=1}^d \) of \( d \) feature vectors, and a tuple of permuted labels \( Y = (y_{\sigma(i)})_{i=1}^d \) as one-hot-vectors, for some permutation \( \sigma \); we will refer to the \( j \)-th element of the tuple \( Y \) as \( Y_j \). The permutation \( \sigma \) is unknown, thus using a loss \( \ell(p_j, Y_j) = \ell(p_j, y_{\sigma(i)}) \) makes no sense, since most likely \( i \neq j \).

While the permutation is unknown, with repeated presentation of bags of samples and bags of corresponding labels, we do have some information connecting the feature vector to classes. Intuitively, we can try to match feature vectors in the bag to the class labels using the information in the model’s probability distribution, that is, find the permutation \( \hat{\sigma} \) optimal in the average loss sense

\[
\min_{\hat{\sigma}} \sum_{j=1}^d \ell(p_j, \hat{\sigma}(Y_j)).
\]
Figure 1: A single training sample – a bag of size four. Each edge has a corresponding weight $C_{jk} = \ell(p_j, Y_k)$, where $p_j$ is the vector of predicted class probabilities for $j$-th image in the bag, and $Y_k$ is the one-hot vector for $k$-th label in the bag. Maximum weighted bipartite matching is depicted in red, assuming the model makes correct predictions for each image in the bag.

Figure 2: Training and test error for CIFAR100 with reshuffling of the training set into bags after each epoch. Mean, and the 95% confidence interval of the mean, are shown.

If the class conditional probabilities $p_j$ resulting from the model perfectly match the one-hot vectors, the optimal $\hat{\sigma}$ will be the inverse of the permutation $\sigma$.

A $d$-element permutation can be represented by a $d \times d$ permutation matrix $M$. To find $M$, we define with a $d \times d$ matrix $C$ with $C_{jk} = \ell(p_j, Y_k)$ – the elements $C_{jk}$ correspond to edge weight in a bipartite graph with feature vectors on one side, and labels on the other side. Alternatively, $C$ specifies the cost matrix in the optimal assignment problem. We use a combinatorial solver, for example the Hungarian method with computational complexity $O(d^3)$, to find the optimal solution, that is, the permutation matrix $C^* = \arg \min_C \langle C, M \rangle_F$ that minimizes the Frobenius inner product of $C$ and $M$.

3.2 Experiments

In our tests, we use the standard CIFAR100 benchmark image dataset as the source of feature vectors and labels. We used the WideResNet architecture [18] involving residual, convolutional
blocks as the network $F$. We trained 5 independent supervised models, with cross-entropy loss $\ell(p, y) = -\langle \log p, y \rangle$, where the logarithm is applied element-wise. We also explored bag sizes of 2, 4, 8, 16, and 32, and trained 5 independent models for each bag size with the combinatorial loss based on weighted bipartite graph matching, with cross-entropy as the loss defining the edge weights $C_{jk}$. We used data augmentation involving flipping and cropping. Batch size was set to 128 elements divided into bags. We trained the networks for 150 epochs using Nesterov accelerated stochastic gradient descent with momentum, with the initial learning rate of 0.1, reduced by a multiplicative factor of 0.1 in epochs 60, 100, 120, and 140.

To see how well the combinatorial loss can match results from supervised learning with no bags, we used a shuffling approach in which contents of the training set are randomly assigned into bags after each epoch (CIFAR100-shuffle). To avoid situations where the combinatorial loss is aided by bags with mostly one class, we ignored any bag that has less than 75% of different classes, that is, for bag of size 8, we only consider bags that consist of at least 6 different classes. Training and test error for CIFAR100 with reshuffling of the training set into bags after each epoch (Fig. 3) shows that for bag sizes reaching up to eight elements, weak supervision through weighted bipartite graph matching is, in the long run, almost as effective as supervised learning, that is, bag of size one. Once the size of the bag increases past eight, models trained using weak supervision start exhibiting higher error; for bags of 32 elements, the model is no better than a random decision.

We also evaluated a more realistic approach in which the assignment of images to bags is done only once, prior to training, and stays fixed during training. In this scenario, we see immediate, moderate increase in both training and test set error (Fig. 2). In addition to CIFAR100, we also performed experiments with CIFAR10, which has only ten classes, to see how well the weakly-supervised learning works when the bag size is larger than the number of classes; we used fixed bags for CIFAR10. Since the number of classes is low compared to bag sizes, we relaxed the bag content criterion to 50%; a bag of size 10 has to contain at least 5 different classes. The results in Fig. 2 show that for the number of elements in the bag equal to the number of classes, the test set error is only slightly higher than in the supervised setting, with mean(std.dev.) of 9.25(0.48) vs 7.12(0.08). Even for bags of size 30, that is, three times the number of classes, the method performs better than random guessing.

Taken together, the results show that the generalized gradient over combinatorial opti-
mization is effective in providing training signal to train a large neural network.

4 Graph Shortest Path for Sentence-level Loss in Sequence-to-Sequence Models

For a more widely applicable scenario where a combinatorial loss is advantageous, we turn to sequence-to-sequence natural language models.

4.1 Generalized Gradients over Global Sequence Alignment

We used a standard encoder-decoder architecture for the model. The encoder takes the source sequence on input and prepares a context vector capturing the source sequence. The decoder is a recurrent network that outputs the predicted sequence one token at a time, based on the context vector and the output of the previous step. The output of the decoder at a step $t$ is a vector of probabilities $p_t$ over the set of all possible output tokens.

Existing encoder-decoder models use cross-entropy loss to compare predicted probabilities $p_t$ to the target word at position $t$, encoded as one-hot vector $y_t$. Instead of a sequence-level optimization, position-specific cross entropy loss results in an averaged token-level optimization. We hypothesize this has detrimental effect on the training process of differentiable sequence-to-sequence models that involve softmax or Gumbel-softmax [8] as the mechanism for feeding the output of the previous step of the decoder as input for the next step. For example, a recurrent model that learned to output almost all of the target sentence correctly but is still making the mistake of missing one word early in the sentence will have very high loss at all the words following the missing word – correcting the mistake should involve keeping most of the model and focusing on the missing word, but with position-specific loss, all

![Figure 4: A directed acyclic graph (DAG) corresponding to the global sequence alignment between the target sequence and the sequence predicted by the RNN model. Each node, except the end of sequence indicator $<>/>$, has out-degree of three: a diagonal edge corresponding to a match between the predicted and the target sequence, a horizontal edge corresponding to a gap in the predicted sequence, and a vertical edge corresponding to a gap in the target sequence. Optimal sequence alignment is depicted in red, with the weights – the alignment costs – of the selected edges in blue.](image)
Table 1: Results for the GIGAWORD text summarization task using ROUGE-1, ROUGE-2, and ROUGE-L metrics. Results are given as mean(std.dev.) over five independent runs.

| Loss Type                  | ROUGE-1   | ROUGE-2   | ROUGE-L   | Epoch   |
|----------------------------|-----------|-----------|-----------|---------|
|                            | Softmax   |           |           |         |
| Combinatorial (GSA)        | 33.87(0.38)| 11.59(0.18)| 29.49(0.30)| 10.80(1.30) |
| Maximum likelihood (MLE)   | 32.26(0.32)| 10.62(0.37)| 27.46(0.30)| 11.40(0.89)  |
|                            | Gumbel-softmax |   |           |         |
| Combinatorial (GSA)        | 33.22(0.41)| 10.56(0.25)| 28.66(0.36)| 12.20(3.77)  |
| Maximum likelihood (MLE)   | 31.36(0.20)| 9.74(0.11)| 26.38(0.15)| 15.40(3.91)  |

the outputs are considered wrong and in need of correction. Gaps or spurious words in the output sequence can be treated naturally if we consider global sequence alignment (GSA) as the loss. Global sequence alignment [19] is a combinatorial problem in which two sequences are aligned by choosing, at each position, to either match a token from one sequence to a token from the other, or to introduce a gap in one or the other sequence; each choice has a cost (see Fig. 4). In sequence-to-sequence modeling, the cost of matching the decoder’s output from position \( i \) to the target sequence token as position \( k \) will be given by \( -\log p_i, y_k \). The cost of a gap, that is, of a horizontal or a vertical move in Fig. 4 is specified in a way that promotes closing of the gap; we use the cost of diagonal move from that position as the cost of the gap, multiplied by a scalar \( \gamma > 1 \) to prioritize closing the gaps over improving the matchings. In our experiments, we used \( \gamma = 1.5 \).

The GSA problem can be reduced to a shortest path problem in a weighted directed acyclic graph, with the matching and gap costs corresponding to edge weights; it can be solved via dynamic programming in time \( O(l_ml_n) \), where \( l_m \) and \( l_n \) are the lengths of the two sequences. Single-source shortest path problem in a graph with \( p \) nodes and \( m \) edges is primal-dual \( \partial \)-efficient, it can be stated as a linear program with \( p \) variables and \( m + 1 \) constraints (see [1], Ch. 29.2), with the edge weights forming the right-hand side of the constraints. Thus, by Theorem 5, the generalized gradient of the minimum global sequence alignment with respect to matching and gap costs is efficiently available.

4.2 Experiments

In evaluating the combinatorial GSA loss, we used text summarization task involving the GIGAWORD dataset [20] as an example of a sequence-to-sequence problem. We used the same preprocessing as [21], that is, we used 200K examples in training. We used the validation set to select the best model epoch, and reported results on a separate test set. We used ROUGE 1, 2, and L scores [22] as the measure of quality of the summarizations produced by the network.

We used an encoder-decoder sequence-to-sequence architecture with bidirectional forward-backward RNN encoder and an attention-based RNN decoder [23], as implemented in PyTorch-Texar [24]. While this architecture is no longer the top performer in terms of ROUGE metric – currently, large pre-trained self-attention models such as BERT are the state-of-the-art [25] – it is much more efficient in training. In both the encoder and the de-
During training, to have a differentiable decoder, we use two alternative approaches. First, we feed the probabilities resulting from softmax layer applied to the outputs of the RNN directly. Second, inputs to the RNN are provided by the straight-through Gumbel-softmax distribution \[8\], which is an approximation of the categorical distribution from which one-hot, single-token outputs are sampled. In both softmax and Gumbel-softmax, we use annealing of the temperature parameter \(\tau\). As it has been used previously \[26\], we start with a high value of the temperature parameter \(\tau\) and reduced it as training progresses. Specifically, we started with \(\tau = 5\), and reduced it by 0.5 in each epoch until value of 1.0 is reached. Then, we kept reducing it by 0.1 until 0.1 is reached, and by 0.01 until 0.01 is reached.

The results of the tests, presented in Table \[1\], show that the combinatorial loss based on the global sequence alignment leads to improved text summarization results in all three ROUGE metrics compared to position-specific maximum likelihood training, both for the softmax and the Gumbel-softmax approach.

To analyze how common the situations in which the optimal alignment of the predicted and the target sequence involves gaps, in the model trained using MLE we also computed optimal alignment, without using it as source of gradients for optimization. The results (Fig. 5) show that while at the initial epochs both the position-specific MLE training and the GSA-based training lead to alignments with few gaps, as the model’s performance improves, the GSA model optimizes the sequences in fragments, with many more gaps than the position-specific MLE model. The results further show that the improved test set performance is achieved despite much higher MLE loss, indicating that position-specific loss is not best suited for training differentiable sequence-to-sequence models.

5 Related Work

Several authors used linear programs indirectly in their loss, by using a differentiable approximation. For example, WGAN-TS \[27\], a recently proposed improved method for training Wasserstein GANs \[28\] solves a dual LP to obtain the exact empirical Wasserstein distance. Then, to circumvent lack of differentiability of linear programs, WGAN-TS proceeds by training a neural network to approximate the LP solution in order to obtain gradients. Similarly, in seq2seq-OT \[21\], an approximation is used to model optimal transport between word embeddings serving as a regularizer in training sequence-to-sequence models.
Acknowledgments

T.A. is supported by NSF grant IIS-1453658.

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