

Supplementary material

A Proofs

A.1 Proof of Proposition 1

Recall that

$$\Pi_{\Omega}(\mathbf{x}) = \arg \min_{\mathbf{y} \in \Delta^d} f(\mathbf{y}), \quad \text{where} \quad f(\mathbf{y}) := \gamma \Omega(\mathbf{y}) - \mathbf{y}^T \mathbf{x}.$$

At an optimal solution, we have the fixed point iteration [36, §4.2]

$$\mathbf{y}^* = P_{\Delta^d}(\mathbf{y}^* - \nabla f(\mathbf{y}^*)). \quad (2)$$

Seeing \mathbf{y}^* as a function of \mathbf{x} , and P_{Δ^d} and ∇f as functions of their inputs, we can apply the chain rule to (2) to obtain

$$J_{\Pi_{\Omega}}(\mathbf{x}) = J_{P_{\Delta^d}}(\mathbf{y}^* - \nabla f(\mathbf{y}^*)) (J_{\Pi_{\Omega}}(\mathbf{x}) - J_{\nabla f \circ \mathbf{y}^*}(\mathbf{x})). \quad (3)$$

Applying the chain rule once again to $\nabla f(\mathbf{y}^*) = \gamma \nabla \Omega(\mathbf{y}^*) - \mathbf{x}$, we obtain

$$\begin{aligned} J_{\nabla f \circ \mathbf{y}^*}(\mathbf{x}) &= \gamma J_{\nabla \Omega}(\mathbf{y}^*) J_{\Pi_{\Omega}}(\mathbf{x}) - I \\ &= \gamma H_{\Omega}(\mathbf{y}^*) J_{\Pi_{\Omega}}(\mathbf{x}) - I. \end{aligned}$$

Plugging this into (3) and re-arranging, we obtain

$$(I + A(B - I)) J_{\Pi_{\Omega}} = A,$$

where we defined the shorthands

$$J_{\Pi_{\Omega}} := J_{\Pi_{\Omega}}(\mathbf{x}), \quad A := J_{P_{\Delta^d}}(\mathbf{y}^* - \gamma \nabla \Omega(\mathbf{y}^*) + \mathbf{x}) \quad \text{and} \quad B := \gamma H_{\Omega}(\mathbf{y}^*).$$

A.2 Proof of Proposition 3

Proof outline. Let $\mathbf{z}^* = P_{\text{TV}}(\mathbf{x})$ or $P_{\text{OSC}}(\mathbf{x})$. We use the optimality conditions of P_{TV} , respectively P_{OSC} in order to express \mathbf{z}^* as an explicit function of \mathbf{x} . Then, obtaining the Jacobians of $P_{\text{TV}}(\mathbf{x})$ and $P_{\text{OSC}}(\mathbf{x})$ follows by application of the chain rule to the two expressions. We discuss the proof for points where P_{TV} and P_{OSC} are differentiable; on the (zero-measure) set of nondifferentiable points (i.e. where the group structure changes) we may take one of Clarke's generalized gradients [11].

Jacobian of P_{TV} .

Lemma 1 *Let $\mathbf{z}^* = P_{\text{TV}}(\mathbf{x}) \in \mathbb{R}^d$ and G_i^* be the set of indices around i with the same value at the optimum, as defined in §3.2. Then, we have*

$$z_i^* = \frac{\sum_{j \in G_i^*} x_j + \lambda(s_{a_i} - s_{b_i})}{|G_i^*|}, \quad (4)$$

where $a_i = \min G_i^*, b_i = \max G_i^*$ are the boundaries of segment G_i^* , and

$$s_{a_i} = \begin{cases} 0 & \text{if } a = 1, \\ \text{sign}(z_{a_i-1}^* - z_i^*) & \text{if } a > 1 \end{cases} \quad \text{and} \quad s_{b_i} = \begin{cases} 0 & \text{if } b = d, \\ \text{sign}(z_i^* - z_{b_i+1}^*) & \text{if } b < d \end{cases}.$$

To prove Lemma 1, we make use of the optimality conditions of the fused lasso proximity operator [17, Equation 27], which state that \mathbf{z}^* satisfies

$$z_j^* - x_j + \lambda(t_j - t_{j+1}) = 0, \quad \text{where} \quad t_j \in \begin{cases} \{0\} & \text{if } i \in \{1, d\}, \\ \{\text{sign}(z_j^* - z_{j-1}^*)\} & \text{if } z_j^* \neq z_{j-1}^*, \\ [-1, 1] & \text{o.w.} \end{cases} \quad \forall j \in [d]. \quad (5)$$

The optimality conditions (5) form a system with unknowns z_j^*, t_j for $j \in [d]$. To express \mathbf{z}^* as a function of \mathbf{x} , we shall now proceed to eliminate the unknowns t_j .

Let us focus on a particular segment G_i^* . For readability, we drop the segment index i and use the shorthands $z := z_i^*$, $a := a_i$, and $b := b_i$. By definition, a and b satisfy

$$z_j^* = z \quad \forall a \leq j \leq b, \quad z_{a-1}^* \neq z \text{ if } a > 1, \quad z_{b+1}^* \neq z \text{ if } b < d.$$

It immediately follows from the definition of t_j in (5) that

$$t_a = \begin{cases} 0 & \text{if } a = 1, \\ \text{sign}(z - z_{a-1}^*) & \text{if } a > 1 \end{cases} \quad \text{and} \quad t_{b+1} = \begin{cases} 0 & \text{if } b = d, \\ \text{sign}(z_{b+1}^* - z) & \text{if } b < d \end{cases}.$$

In other words, the unknowns t_a and t_b are already uniquely determined. To emphasize that they are known, we introduce $s_a := t_a$ and $s_b := t_{b+1}$, leaving t_j only unknown for $a < j \leq b$.

By rearranging the optimality conditions (5) we obtain the recursion

$$\lambda t_j = x_j - z + \lambda t_{j+1} \quad \forall a \leq j \leq b.$$

We start with the first equation in the segment (at $j = a$), and unroll the recursion until reaching the stopping condition $j = b$.

$$\begin{aligned} \lambda s_a &= x_a - z + \lambda t_{a+1} \\ &= x_a - z + x_{a+1} - z + \cdots + x_b - z + \lambda s_b \\ &= \sum_{k=a}^b x_k - (b - a + 1)z + \lambda s_b \end{aligned}$$

Rearranging the terms, we obtain the expression

$$z = \frac{\sum_{k=a}^b x_k + \lambda(s_b - s_a)}{b - a + 1}.$$

Applying this calculation to each segment in \mathbf{z}^* yields the desired result. \square

The proof of Proposition 3 follows by applying the chain rule to (4), noting that the groups G_i^* are constant within a neighborhood of \mathbf{x} (observation also used for OSCAR in [7]). Therefore, for P_{TV} ,

$$\frac{\partial z_i^*}{\partial x_j} = \frac{1}{|G_i^*|} \left(\sum_{k \in G_i^*} \frac{\partial x_k}{\partial x_j} + \lambda \left(\frac{\partial s_b}{\partial x_j} - \frac{\partial s_a}{\partial x_j} \right) \right).$$

Since s_b and s_a are either constant or sign functions w.r.t. \mathbf{x} , their partial derivatives are 0, and thus

$$\frac{\partial z_i^*}{\partial x_j} = \begin{cases} \frac{1}{|G_i^*|} & \text{if } j \in G_i^*, \\ 0 & \text{o.w.} \end{cases}.$$

Jacobian of P_{OSC} .

Lemma 2 ([47, Theorem 1], [49, Proposition 3]) *Let $\mathbf{z}^* = P_{\text{OSC}}(\mathbf{x}) \in \mathbb{R}^d$ and G_i^* be the set of indices around i with the same value at the optimum: $G_i^* = \{j \in [d] : |z_i^*| = |z_j^*|\}$. Then, we have*

$$z_i^* = \text{sign}(x_i) \max \left(\frac{\sum_{j \in G_i^*} |x_j|}{|G_i^*|} - w_i, 0 \right), \quad (6)$$

$$\text{where } w_i = \lambda \left(d - \frac{u_i + v_i}{2} \right), \quad u_i = |\{j \in [d] : |z_j^*| < |z_i^*|\}|, \quad v_i = u_i + |G_i^*|.$$

Lemma 2 is a simple reformulation of Theorem 1, part *ii* from [47]. With the same observation that the induced groups do not change within a neighborhood of \mathbf{x} , we may differentiate (6) to obtain

$$\frac{\partial z_i^*}{\partial x_j} = \begin{cases} 0 & \text{if } z_i^* = 0, \\ \frac{\text{sign}(x_i)}{|G_i^*|} \sum_{k \in G_i^*} \frac{\partial |x_k|}{\partial x_k} \frac{\partial x_k}{\partial x_j} - \frac{\partial w_i}{\partial x_j} & \text{o.w.} \end{cases}.$$

Noting that $\frac{\partial w_i}{\partial x_j} = 0$, as w_i is derived only from group indices and the term $\frac{\partial |x_k|}{\partial x_k} \frac{\partial x_k}{\partial x_j}$ either vanishes (when $k \neq j$) or else equals $\text{sign}(x_j)$ with $x_j \neq 0$, we substitute $\text{sign}(z_j^*)$ for $\text{sign}(x_j)$ [47] to get

$$\frac{\partial z_i^*}{\partial x_j} = \begin{cases} \frac{\text{sign}(z_i^* z_j^*)}{|G_i^*|} & \text{if } j \in G_i^* \text{ and } z_i^* \neq 0, \\ 0 & \text{o.w.} \end{cases}.$$

B Computational complexity and implementation details

B.1 Sparsemax

Computing the forward and backward pass of sparsemax is a compositional building block in fusedmax, oscarmax, as well as in the general case; for this reason, we discuss it before the others.

Forward pass. The problem is exactly the Euclidean projection on the simplex, which can be computed exactly in worst-case $\mathcal{O}(d \log d)$ due to the required sort [31, 34, 15], or in expected $\mathcal{O}(d)$ time using a pivot algorithm similar to median finding [15]. Our implementation is based on sorting.

Backward pass. From [31] we have that the result of a Jacobian-vector product $J_{\Pi_\Omega} v$ has the same sparsity pattern as \mathbf{y}^* . If we denote the number of nonzero elements of \mathbf{x} by $\text{nnz}(\mathbf{x})$, we can see that \hat{v} in [31, eq. 14], and thus the Jacobian-vector product itself, can be computed in $\mathcal{O}(\text{nnz}(\mathbf{y}^*))$.

B.2 Fusedmax

We implement fusedmax as the composition of the fused lasso proximal operator with sparsemax.

Forward pass. We need to solve the proximal operator of fused lasso. The algorithm we use is $\mathcal{O}(d^2)$ in the worst case, but has strong performance on realistic benchmarks, close to $\mathcal{O}(d)$ [13].

Backward pass. Due to the structure of the Jacobian and the locality of fused groups, Jacobian-vector products $J_{\Pi_\Omega} v$ can be computed in $\mathcal{O}(d)$ using a simple algorithm that iterates over the output \mathbf{y}^* and the vector \mathbf{v} simultaneously, averaging the elements of \mathbf{v} whose indices map to fused elements of \mathbf{y}^* . Since only consecutive elements can be fused, this amounts to resetting to a new group as soon as we encounter an index i such that $y_i^* \neq y_{i-1}^*$.

B.3 Oscarmax

We implement oscarmax as the composition of the OSCAR proximal operator with sparsemax.

Forward pass. The proximal operator of the OSCAR penalty can be computed in $\mathcal{O}(d \log d)$ as a particular case of the ordered weighted ℓ_1 (OWL) proximal operator, using an algorithm involving a sort followed by isotonic regression [48].

Backward pass. The algorithm is similar in spirit to fusedmax, but because groups can reach across non-adjacent indices, a single pass is not sufficient. With no other information other than \mathbf{y}^* , the backward pass can be computed in $\mathcal{O}(d \log d)$ using a stable sort followed by a linear-time pass for finding groups. Further optimization is possible if group indices may be saved from the forward pass.

B.4 General case and sq-pnorm-max

Forward pass. For general Π_Ω we may use any projected gradient solver; we choose FISTA [4]. Each iteration requires a projection onto the simplex; in the case of sq-pnorm-max, this dominates every iteration, leading to a complexity of $\mathcal{O}(td \log d)$ where t is the number of iterations performed.

Backward pass. To compute Jacobian-vector products we solve the linear system from Proposition 1: $(I + A(B - I))(J_{\Pi_\Omega} v) = Av$. This is a $d \times d$ system, which at first sight suggests a complexity of $\mathcal{O}(d^3)$. However, we can use the structure of A to solve it more efficiently.

The matrix A is defined as $A := J_{P_{\Delta^d}}(\mathbf{y}^* - \nabla f(\mathbf{y}^*))$. As a sparsemax Jacobian, A is row- and column-sparse, and uniquely defined by its sparsity pattern. By splitting the system into equations corresponding to zero and nonzero rows of A , we obtain that the solution $J_{\Pi_\Omega} v$ must have the same sparsity pattern as the row-sparsity of A , therefore we only need to solve a subset of the system. From the fixed-point iteration $\mathbf{y}^* = P_{\Delta^d}(\mathbf{y}^* - \nabla f(\mathbf{y}^*))$, we have that the row-sparsity of A is the same as the sparsity of the forward pass solution \mathbf{y}^* . The backward pass complexity is thus $\mathcal{O}(\text{nnz}(\mathbf{y}^*)^3)$.

C Additional experimental results

C.1 Visualizing attention mappings in 3-d

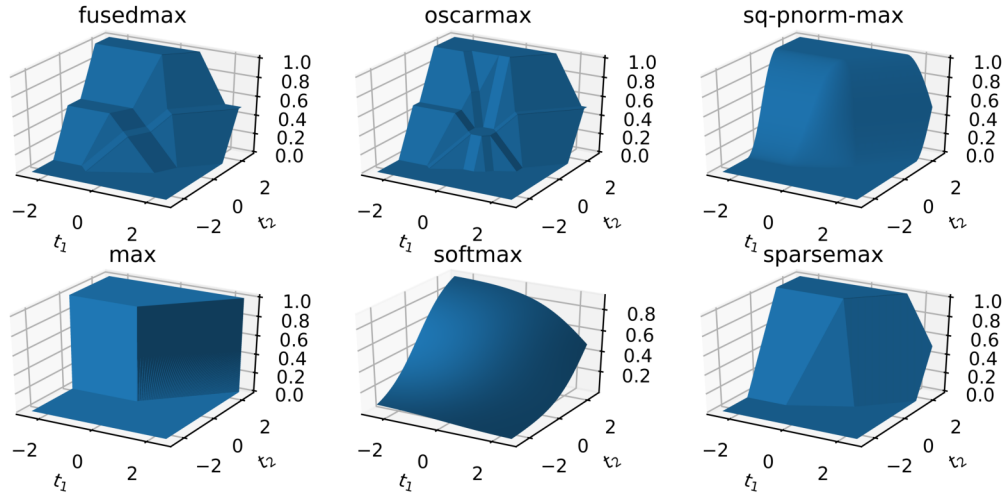


Figure 5: 3-d visualization of $\Pi_\Omega([t_1, t_2, 0])_2$ for several proposed and existing mappings Π_Ω . sq-pnorm-max with $p = 1.5$ resembles sparsemax but with smoother transitions. The proposed structured attention mechanisms, fusedmax and oscarmax, exhibit plateaus and ridges in areas where weights become fused together. We set $\gamma = 1$ and $\lambda = 0.2$.

C.2 Textual entailment results

Experimental setup. We build upon the implementation from [31], which is a slight variation of the attention model from [38], using GRUs instead of LSTMs. The GRUs encoding the premise and hypothesis have separate parameters, but the hypothesis GRU is initialized with the last state of the premise GRU. We use the same settings and methodology as [31]: we use fixed 300-dimensional GloVe vectors, we train for 200 epochs using ADAM with learning rate $3 \cdot 10^{-4}$, we use a drop-out probability of 0.1, and we choose an l_2 regularization coefficient from $\{0, 10^{-4}, 3 \cdot 10^{-4}, 10^{-3}\}$. Experiments are performed on machines with 2×Xeon X5675 3.06GHz CPUs and 96GB RAM.

Dataset and preprocessing. We use the SNLI v1 dataset [8]. We apply the minimal preprocessing from [31], skipping sentence pairs with missing labels and using the provided tokenization. This results in a training set of 549,367 sentence pairs, a development set of 9,842 sentence pairs and a test set of 9,824 sentence pairs. We report timing measurements in Table 3 and visualizations of the produced attention weights in Figure 6.

C.3 Machine translation results

Experimental setup. Because our goal is to demonstrate that our attention mechanisms can be drop-in replacements for existing ones, we focus on OpenNMT-py with default settings for all of our

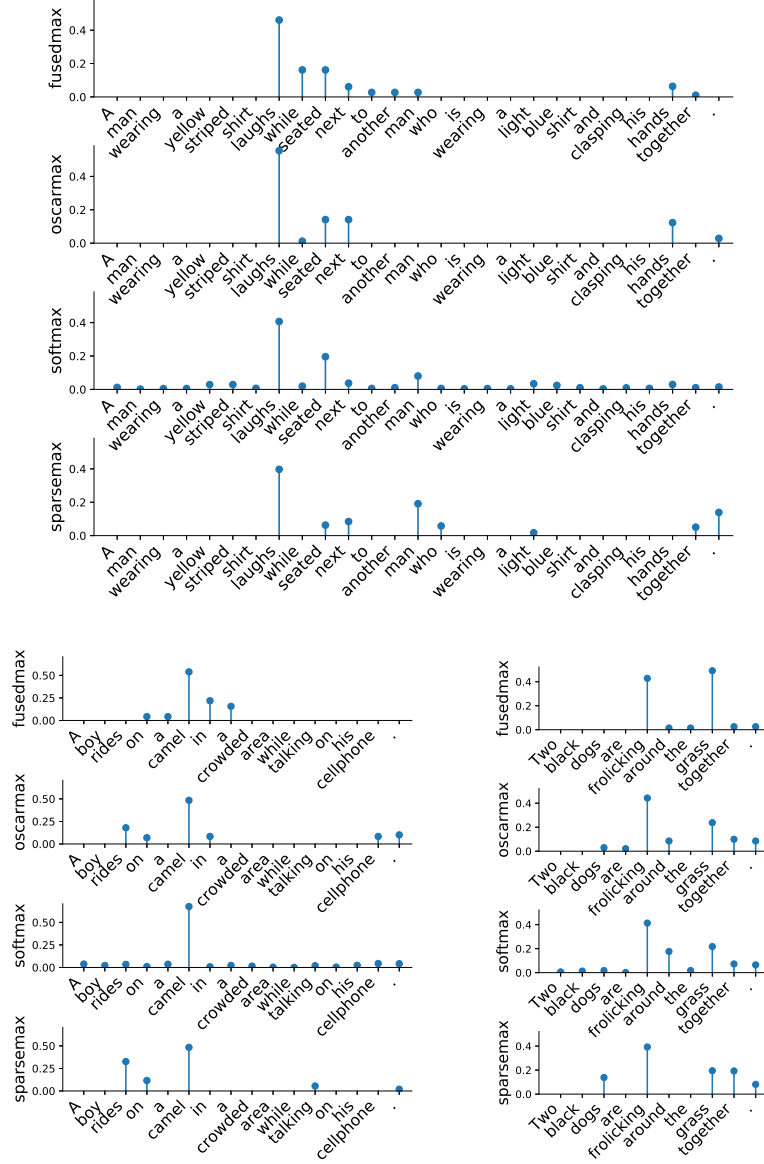


Figure 6: Attention weights on several examples also used in [38, 31]. The hypotheses considered are “Two mimes sit in complete silence.” (top), “A boy is riding an animal.” (left), and “Two dogs swim in the lake.” (right). All attention mechanisms result in correct classifications (top: contradiction; left: entailment; right: contradiction). As can be seen, fusedmax prefers contiguous support segments even when not all weights are tied.

sequence-to-sequence experiments. These defaults are: an unidirectional LSTM, 500 dimensions for the word vectors and for the LSTM hidden representations, drop-out probability of 0.3, global attention, and input-feeding [29]. Following the default, we train our models for 13 epochs with stochastic gradient updates (batches of size 64 and initial learning rate of 1, halved every epoch after the 8th). Weights (including word embeddings) are initialized uniformly over $[-0.1, 0.1]$, and gradients are normalized to have norm 5 if their norm exceeds this value. For test scores and visualizations, we use the model snapshot at the epoch with the highest validation set accuracy. All of the experiments in this section are performed on machines equipped with Xeon E5 CPUs and Nvidia Tesla K80 GPUs.

Datasets. We employ training and test datasets from multiple sources.

attention	time per epoch
softmax	1h 26m 40s \pm 51s
sparsemax	1h 24m 21s \pm 54s
fusedmax	1h 23m 58s \pm 50s
oscarmax	1h 23m 19s \pm 50s

Table 3: Timing results for training textual entailment on SNLI, using the implementation and experimental setup from [31]. With this C++ CPU implementation, fusedmax and oscarmax are as fast as sparsemax, and all three sparse attention mechanisms are slightly faster than softmax.

- BENCHMARK: Training, validation, and test data from the NMT-Benchmark project (<http://scorer.nmt-benchmark.net/>). All languages have \sim 1M training sentence pairs, and equal validation and test sets of size 1K (French) and 2K (Italian, Dutch and Swedish).
- BENCHMARK⁺: Training and validation data as above, but testing on all available *newstest* data. For Italian we use the 2009 data (\sim 2.5K sentence pairs), and for French we concatenate 2009–2014 (\sim 11K sentence pairs).
- WMT16, WMT17: Translation tasks at the first and second ACL Conferences for Machine Translation, available at <http://www.statmt.org/wmt16/translation-task.html> and <http://www.statmt.org/wmt17/translation-task.html>. Training, validation, and test sizes are, approximately, for Romanian 400K/2K/2K, for German 5.8M/6K/3K, for Finnish 2.6M/2K/2K, for Latvian 4.5M/2K/2K, and for Turkish 207K/1K/3K.

We use the preprocessing scripts from Moses [25] for tokenization, and, where needed, SGML parsing. We limit source and target vocabulary sizes to 50K lower-cased tokens and prune sentences longer than 50 tokens at training time and 100 tokens at test time. We do not perform recasing.

We report BLEU scores in Table 4 and showcase the enhanced interpretability induced by our proposed attention mechanisms in Figure 7. Timing measurements can be found in Table 5.

Table 4: Neural machine translation results: tokenized BLEU scores on test data.

	BENCHMARK				BENCHMARK ⁺		WMT16	WMT17			
	fr	it	nl	sv	fr	it	ro	de	fi	lv	tr
from English											
softmax	36.94	37.20	36.12	34.97	27.13	24.86	17.71	22.32	14.54	11.02	11.95
sparsemax	37.03	37.21	36.12	35.09	26.99	24.49	17.61	22.43	14.85	11.07	11.66
fusedmax	37.08	36.73	36.04	34.30	26.89	24.47	17.19	22.25	14.28	11.27	11.32
oscarmax	36.66	36.89	35.96	34.86	27.02	24.76	17.26	22.42	14.02	11.19	11.63
sq-pnorm-max	37.16	37.39	36.21	34.63	27.25	24.56	17.80	—	14.45	—	11.58
to English											
softmax	36.79	39.95	40.06	37.96	25.72	25.37	17.86	25.82	15.11	13.60	11.78
sparsemax	36.91	40.13	40.25	38.09	25.97	25.62	17.46	25.76	14.95	13.59	12.04
fusedmax	36.64	39.64	39.87	37.83	25.72	25.41	18.29	25.58	15.08	13.53	11.91
oscarmax	36.90	40.05	40.17	38.12	26.13	25.65	17.89	25.69	14.94	13.71	11.70
sq-pnorm-max	36.84	40.23	40.48	38.12	25.72	25.70	17.44	—	15.20	—	11.93

attention	time per epoch
softmax	2h
sparsemax	2h 18m
fusedmax	3h 5m
oscarmax	3h 25m
sq-pnorm-max	7h 5m

Table 5: Timing results for French-to-English translation using OpenNMT-py (all standard errors are under 2 minutes). For simplicity, all attention mechanisms, except softmax, are implemented on the CPU, thus incurring memory copies in both directions. (The rest of the pipeline runs on the GPU.) Even without special optimization, sparsemax, fusedmax, and oscarmax are practical, taking within 1.75x the training time of a softmax model on the GPU.

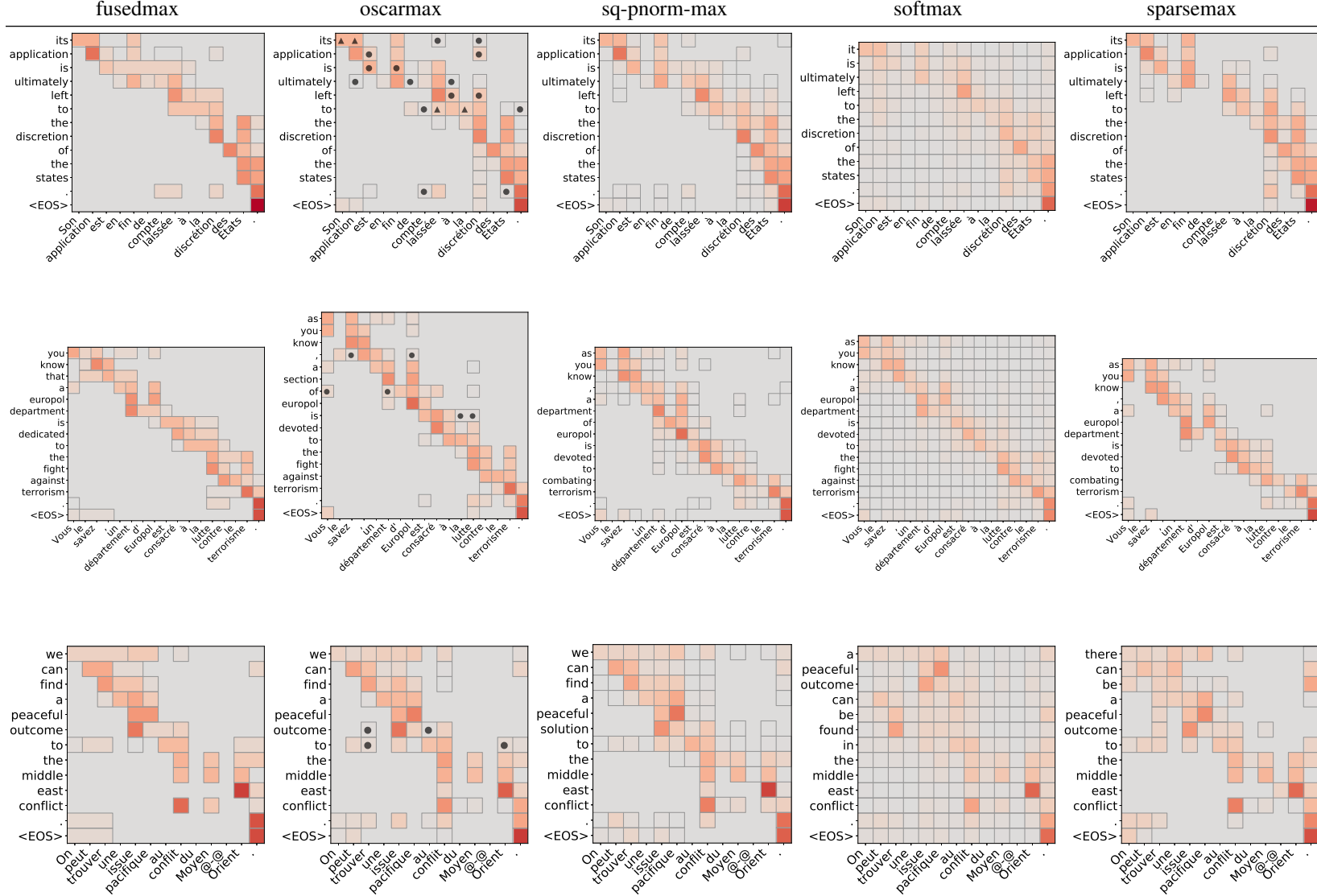


Figure 7: Attention alignment examples for French-to-English translation, following the conventions of Figure 1. “@-@” denotes a hyphen not separated by spaces. When oscarmax induces multiple clusters, we denote them using different bullets (e.g., ●, ▲, ■). Fusedmax often selects meaningful grammatical segments, such as “est consacré,” as well as determiner-noun constructions.

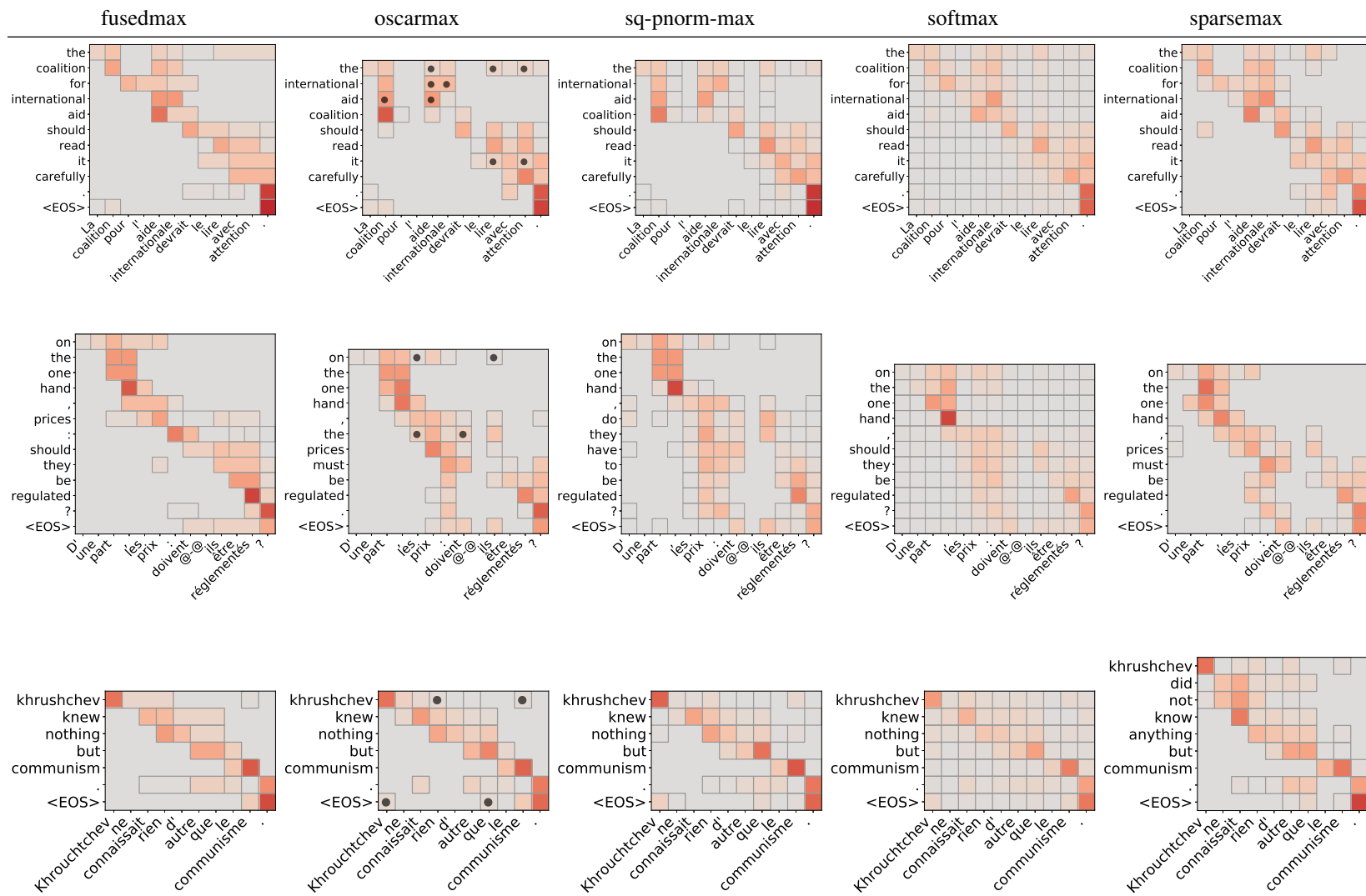


Figure 7 (continued): Further translation examples from French to English.

C.4 Sentence summarization results

Experimental setup and data. We use the exact same experimental setup and preprocessing as for machine translation, described in Appendix C.3. We use the preprocessed Gigaword sentence summarization dataset, made available by the authors of [39] at <https://github.com/harvardnlp/sent-summary>. Since, unlike [39], we do not perform any tuning on DUC-2003, we can report results on this dataset, as well. We observe that the simple sequence-to-sequence model is able to keep summaries short without any explicit constraints, informed only through training data statistics; therefore, in this section, we also report results without output truncation at 75 bytes (Table 6). We also provide precision and recall scores for ROUGE-L in Table 7. Finally, we provide attention weights plots for all studied attention mechanisms and a number of validation set examples in Figure 8.

Table 6: Sentence summarization F_1 scores for several ROUGE variations.

attention	Truncated				Not truncated			
	ROUGE-1	ROUGE-2	ROUGE-L	ROUGE-W _{1.2}	ROUGE-1	ROUGE-2	ROUGE-L	ROUGE-W _{1.2}
DUC 2003								
softmax	26.63	8.72	23.87	16.95	27.06	8.86	24.23	17.02
sparsemax	26.54	8.78	23.89	16.93	26.95	8.94	24.21	16.99
fusedmax	27.12	8.93	24.39	17.28	27.48	9.04	24.66	17.30
oscarmax	26.72	9.08	24.02	17.06	27.11	9.23	24.32	17.10
sq-pnorm-max	26.55	8.77	23.78	16.87	26.92	8.89	24.07	16.92
DUC 2004								
softmax	27.16	9.48	24.47	17.14	27.25	9.52	24.55	17.20
sparsemax	27.69	9.55	24.96	17.44	27.77	9.61	25.02	17.48
fusedmax	28.42	9.96	25.55	17.78	28.43	9.96	25.55	17.79
oscarmax	27.84	9.46	25.14	17.55	27.88	9.47	25.17	17.57
sq-pnorm-max	27.94	9.28	25.08	17.49	28.01	9.30	25.13	17.52
Gigaword								
softmax	35.13	17.15	32.92	24.17	35.01	17.10	32.77	24.00
sparsemax	36.04	17.78	33.64	24.69	35.97	17.75	33.54	24.55
fusedmax	36.09	17.62	33.69	24.69	35.98	17.60	33.59	24.54
oscarmax	35.36	17.23	33.03	24.25	35.26	17.20	32.92	24.10
sq-pnorm-max	35.94	17.75	33.66	24.71	35.86	17.73	33.54	24.55

Table 7: Sentence summarization: ROUGE-L precision, recall and F-scores.

attention	Truncated			Not truncated		
	P	R	F_1	P	R	F_1
DUC 2003						
softmax	29.57	20.67	23.87	30.40	20.80	24.23
sparsemax	29.59	20.58	23.89	30.37	20.68	24.21
fusedmax	30.02	21.11	24.39	30.75	21.15	24.66
oscarmax	29.64	20.78	24.02	30.40	20.87	24.32
sq-pnorm-max	29.45	20.50	23.78	30.23	20.56	24.07
DUC 2004						
softmax	30.54	21.00	24.47	30.59	21.13	24.55
sparsemax	30.99	21.57	24.96	31.03	21.64	25.02
fusedmax	32.19	21.80	25.55	32.19	21.81	25.55
oscarmax	31.89	21.46	25.14	31.91	21.51	25.17
sq-pnorm-max	31.42	21.55	25.08	31.46	21.63	25.13
Gigaword						
softmax	36.43	31.67	32.92	36.61	31.54	32.77
sparsemax	37.32	32.18	33.64	37.54	32.07	33.54
fusedmax	37.44	32.15	33.69	37.68	32.01	33.59
oscarmax	36.40	31.78	33.03	36.61	31.67	32.92
sq-pnorm-max	37.12	32.37	33.66	37.31	32.26	33.54

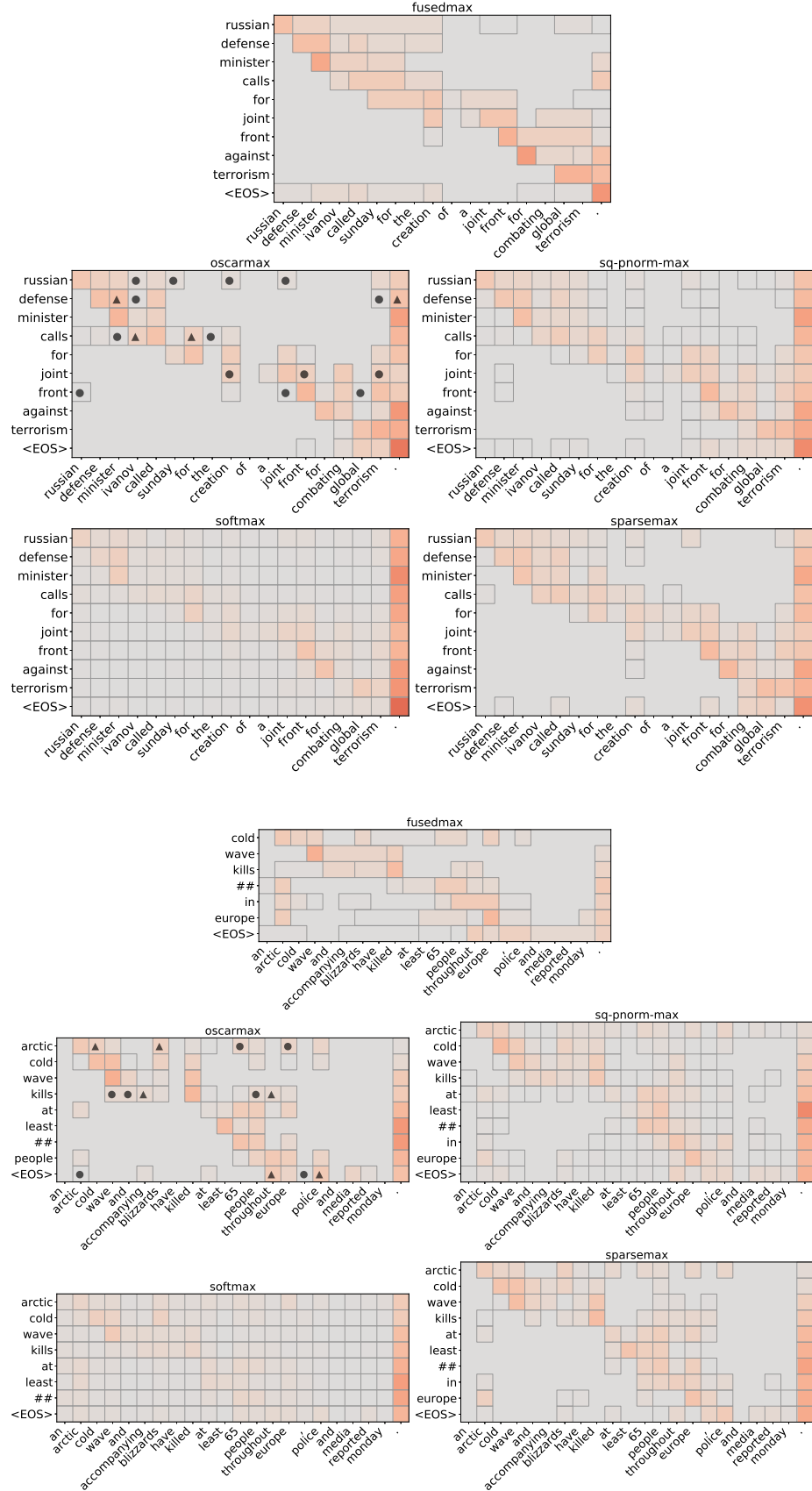


Figure 8: Summarization attention examples. The 1-d TV prior of fusedmax captures well the intuition of aligning long input spans with single expressive words, as supported by ROUGE scores.

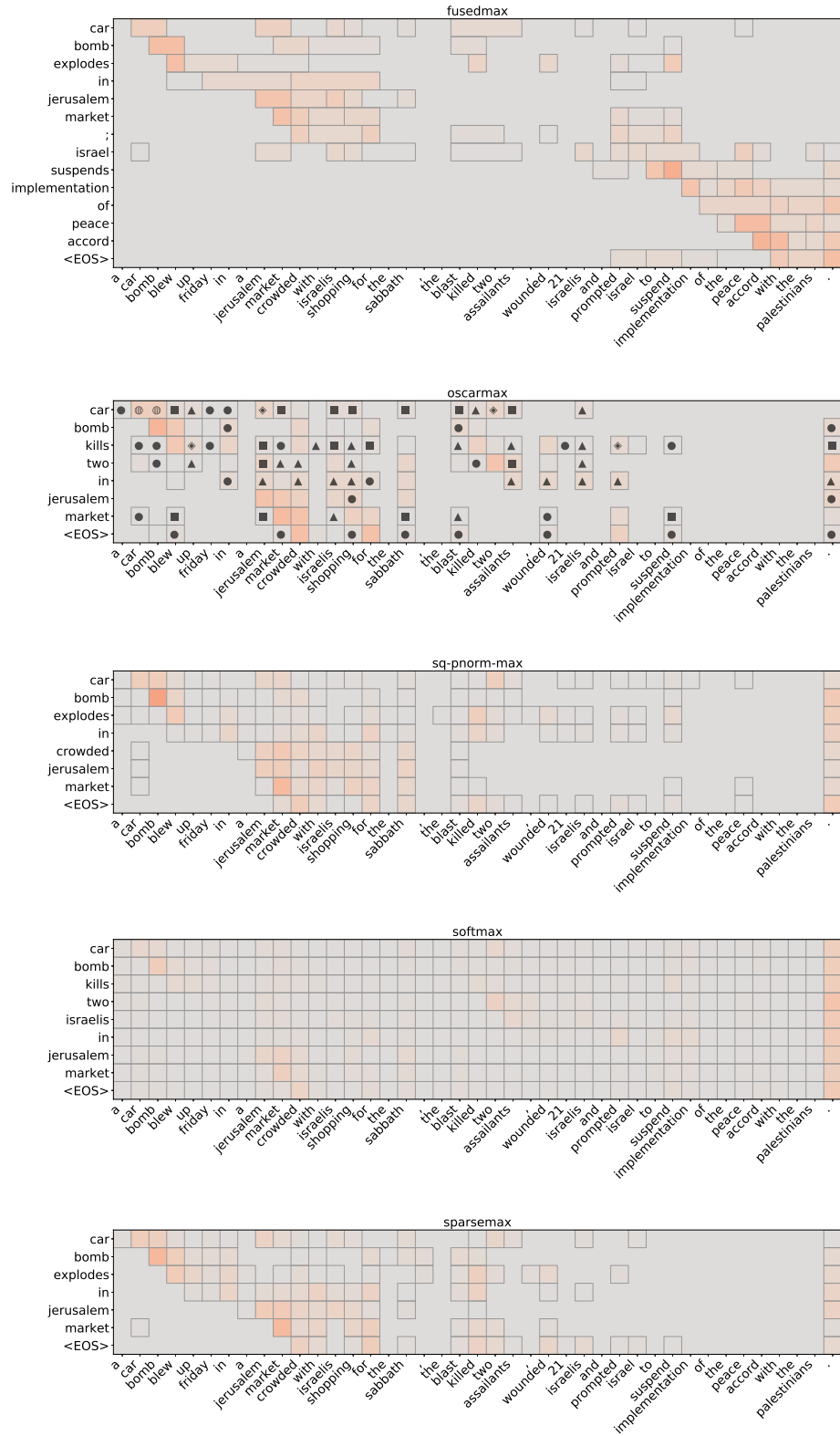


Figure 8 (continued): Summarization attention examples. Here, fusedmax recovers a longer but arguably better summary, identifying a separate but important part of the input sentence.

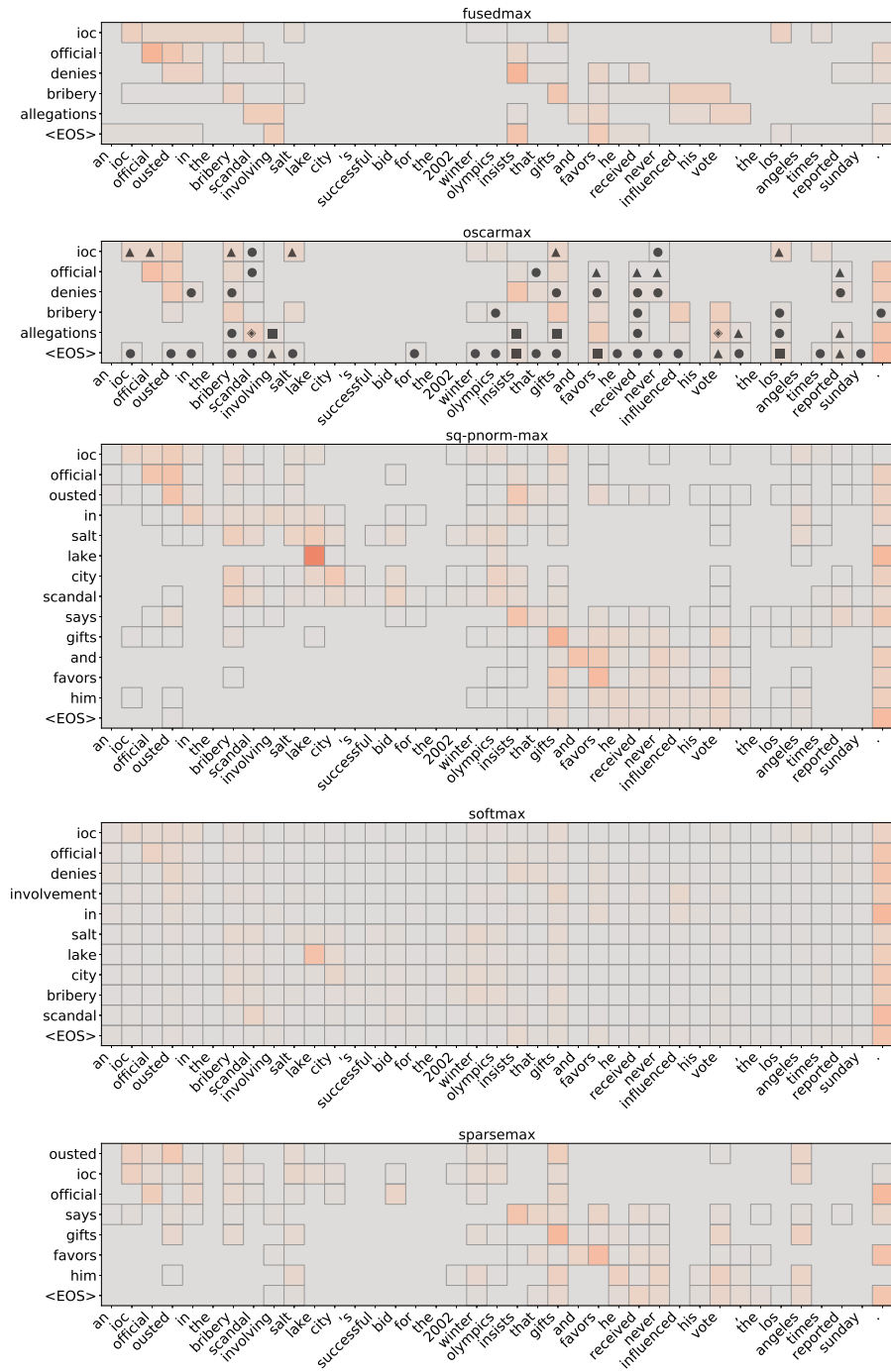


Figure 8 (continued): Summarization attention examples. Here, fusedmax and oscarmax produce a considerably shorter summary.