CRF, CTC, Word2Vec

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Structured Prediction
Consider generating a sequence of \( y_1, \ldots, y_N \in Y^N \) given input \( x_1, \ldots, x_N \).

Predicting each sequence element independently models the distribution \( P(y_i | X) \).

\[
\begin{array}{cccc}
  x_1 & x_2 & x_3 & \cdots & x_N \\
  y_1 & y_2 & y_3 & \cdots & y_N \\
\end{array}
\]

However, there may be dependencies among the \( y_i \) themselves, which is difficult to capture by independent element classification.
Maximum Entropy Markov Models

We might model the dependencies by assuming that the output sequence is a Markov chain, and model it as

$$P(y_i | X, y_{i-1}).$$

Each label would be predicted by a softmax from the hidden state and the previous label.

The decoding can be then performed by a dynamic programming algorithm.
However, MEMMs suffer from a so-called *label bias* problem. Because the probability is factorized, each $P(y_i | X, y_{i-1})$ is a distribution and **must sum to one**.

Imagine there was a label error during prediction. In the next step, the model might “realize” that the previous label has very low probability of being followed by any label – however, it cannot express this by setting the probability of all following labels low, it has to “conserve the mass”.


Conditional Random Fields

Let $G = (V, E)$ be a graph such that $\mathbf{y}$ is indexed by vertices of $G$. Then $(\mathbf{X}, \mathbf{y})$ is a **conditional random field**, if the random variables $\mathbf{y}$ conditioned on $\mathbf{X}$ obey the Markov property with respect to the graph, i.e.,

$$P(y_i | \mathbf{X}, y_j, i \neq j) = P(y_i | \mathbf{X}, y_{j \forall} : (i, j) \in E).$$

By a **fundamental theorem of random fields**, the density of a conditional random field can be factorized over the cliques of the graph $G$:

$$P(\mathbf{y} | \mathbf{X}) = \prod_{\text{clique } C \text{ of } G} P(\mathbf{y}_C | \mathbf{X}).$$
Linear-Chain Conditional Random Fields (CRF)

Usually often assume that dependencies of $y$, conditioned on $X$, form a chain.

$$\begin{align*}
&x_1 \quad x_2 \quad x_3 \quad \cdots \quad x_N \\
&\downarrow \quad \downarrow \quad \downarrow \quad \cdots \quad \downarrow \\
&y_1 \quad y_2 \quad y_3 \quad \cdots \quad y_N
\end{align*}$$

Then, the cliques are *nodes* and *edges*, and we usually factorize the probability as:

$$P(y|X) \propto \exp \left( \sum_{i=1}^{N} \log P(y_i|x_i) + \sum_{i=2}^{N} \log P(y_i, y_{i-1}) \right).$$
Linear-Chain Conditional Random Fields (CRF)

Linear-chain Conditional Random Field, usually abbreviated only to CRF, acts as an output layer. It can be considered an extension of softmax – instead of a sequence of independent softmaxes, it is a sentence-level softmax, with additional weights for neighboring sequence elements.

We start by defining a score of a label sequence $y$ as

$$s(X,y;\theta,A) = \sum_{i=1}^{N} (A_{y_{i-1},y_{i}} + f_{\theta}(y_{i}|X))$$

and define the probability of a label sequence $y$ using softmax:

$$p(y|X) = \text{softmax}_{z \in Y^{N}} (s(X,z))_{y}.$$  

For cross-entropy (and also to avoid underflow), we need a logarithm of the probability:

$$\log p(y|X) = s(X,y) - \text{logsumexp}_{z \in Y^{N}} (s(X,z)), \text{ where}$$

$$\text{logsumexp}_{x} (f(x)) = \log(\sum_{x} e^{f(x)}).$$
Linear-Chain Conditional Random Fields (CRF)

Computation

We can compute $p(y|X)$ efficiently using dynamic programming. We denote $\alpha_t(k)$ the logarithmic probability of all $t$-element sequences with the last label $y$ being $k$.

The core idea is the following:

$$\alpha_t(k) = f_\theta(y_t = k|X) + \text{logsumexp}_{j \in Y}(\alpha_{t-1}(j) + A_{j,k}).$$

For efficient implementation, we use the fact that

$$\ln(a + b) = \ln a + \ln(1 + e^{\ln b - \ln a}), \text{ so}$$

$$\text{logsumexp}_x(f(x)) = \max_x(f(x)) + \log(\sum_x e^{f(x)} - \max_x(f(x))).$$
Conditional Random Fields (CRF)

**Inputs:** Network computing $f_\theta(y_t = k | X)$, an unnormalized probability of output sequence element probability being $k$ at time $t$.

**Inputs:** Transition matrix $A \in \mathbb{R}^{Y \times Y}$.

**Inputs:** Input sequence $X$ of length $N$, gold labeling $g \in Y^N$.

**Outputs:** Value of $\log p(g | X)$.

**Time Complexity:** $\mathcal{O}(N \cdot Y^2)$.

- For $t = 1, \ldots, N$:
  - For $k = 1, \ldots, Y$:
    - $\alpha_t(k) \leftarrow f_\theta(y_t = k | X)$
    - If $t > 1$:
      - $\alpha_t(k) \leftarrow \alpha_t(k) + \text{logsumexp} \left( \alpha_{t-1}(j) + A_{j,k} \mid j = 1, \ldots, Y \right)$
  - Return $\sum_{t=1}^{N} f_\theta(y_t = g_t | X) + \sum_{t=2}^{N} A_{g_{t-1},g_t} - \text{logsumexp}_{k=1}^{Y} (\alpha_N(k))$
Conditional Random Fields (CRF)

Decoding
We can perform decoding optimally, by using the same algorithm, only replacing \( \log \text{sumexp} \) with \( \max \) and tracking where the maximum was attained.

Applications
The CRF output layer is useful for span labeling tasks, like

- named entity recognition,
- dialog slot filling.

It can be also useful for image segmentation.

Figure 1 of paper “Multi-Task Cross-Lingual Sequence Tagging from Scratch”, https://arxiv.org/abs/1603.06270.
Let us again consider generating a sequence of $y_1, \ldots, y_M$ given input $x_1, \ldots, x_N$, but this time $M \leq N$ and there is no explicit alignment of $x$ and $y$ in the gold data.

Figure 7.1 of the dissertation "Supervised Sequence Labelling with Recurrent Neural Networks" by Alex Graves.
Connectionist Temporal Classification

We enlarge the set of output labels by a \((\text{blank})\) and perform a classification for every input element to produce an \emph{extended labeling}. We then post-process it by the following rules (denoted as \(B\)):

1. We collapse multiple neighboring occurrences of the same symbol into one.
2. We remove the blank \(-\).

Because the explicit alignment of inputs and labels is not known, we consider \emph{all possible} alignments.

Denoting the probability of label \(l\) at time \(t\) as \(p_i^t\), we define

\[
\alpha^t(s) \overset{\text{def}}{=} \sum_{\text{extended labelings } \pi: \mathcal{B}(\pi_{1:t}) = y_{1:s}} \prod_{t' = 1}^{t} p_{\pi_{t'}}^t.
\]
In CRF, we normalize the whole sentences, therefore we need to compute unnormalized probabilities for all the (exponentially many) sentences. Decoding can be performed optimally. In CTC, we normalize per each label. However, because we do not have explicit alignment, we compute probability of a labeling by summing probabilities of (generally exponentially many) extended labelings.
Computation

When aligning an extended labeling to a regular one, we need to consider whether the extended labeling ends by a \textit{blank} or not. We therefore define

\[
\alpha^t_-(s) \overset{\text{def}}{=} \sum_{\text{extended labelings } \pi:} \prod_{t'=1}^{t} p_{\pi_t'}^t
\]

\[
\alpha^t_+(s) \overset{\text{def}}{=} \sum_{\text{extended labelings } \pi:} \prod_{t'=1}^{t} p_{\pi_t'}^t
\]

and compute \( \alpha^t(s) \) as \( \alpha^t_-(s) + \alpha^t_+(s) \).
Computation – Initialization

We initialize \( \alpha_s \) as follows:

- \( \alpha^1_-(0) \leftarrow p^1_- \)
- \( \alpha^1_*(1) \leftarrow p^1_y \)

Computation – Induction Step

We then proceed recurrently according to:

- \( \alpha^t_-(s) \leftarrow p^t_-(\alpha^t-1_*(s) + \alpha^t-1_-(s)) \)
- \( \alpha^t_*(s) \leftarrow \begin{cases} p^t_{y_s} (\alpha^t-1_*(s) + \alpha^t-1_-(s - 1) + \alpha^t-1_*(s - 1)), & \text{if } y_s \neq y_{s-1} \\ p^t_{y_s} (\alpha^t-1_*(s) + \alpha^t-1_-(s - 1)), & \text{if } y_s = y_{s-1} \end{cases} \)
CTC Decoding

Unlike CRF, we cannot perform the decoding optimally.

The key observation is that while an optimal extended labeling can be extended into an optimal labeling of a larger length, the same does not apply to regular (non-extended) labeling. The problem is that regular labeling corresponds to many extended labelings, which are modified each in a different way during an extension of the regular labeling.

\[
p(\text{blank}) = p(-) \\
= 0.7 \times 0.6 \\
= 0.42
\]

\[
p(\text{A}) = p(\text{AA}) + p(\text{A}) + p(-\text{A}) \\
= 0.3 \times 0.4 + 0.3 \times 0.6 + 0.7 \times 0.4 \\
= 0.58
\]

*Figure 7.5 of the dissertation "Supervised Sequence Labelling with Recurrent Neural Networks" by Alex Graves.*
Beam Search

To perform beam search, we keep \( k \) best regular (non-extended) labelings. Specifically, for each regular labeling \( y \) we keep both \( \alpha_\cdot^t(y) \) and \( \alpha_*^t(y) \), which are probabilities of all (modulo beam search) extended labelings of length \( t \) which produce the regular labeling \( y \); we therefore keep \( k \) regular labelings with highest \( \alpha_\cdot^t(y) + \alpha_*^t(y) \).

To compute the best regular labelings for longer prefix of extended labelings, for each regular labeling in the beam we consider the following cases:

- adding a blank symbol, i.e., contributing to \( \alpha_{\cdot}^{t+1}(y) \) both from \( \alpha_\cdot^t(y) \) and \( \alpha_*^t(y) \);
- adding a non-blank symbol, i.e., contributing to \( \alpha_*^{t+1}(\cdot) \) from \( \alpha_\cdot^t(y) \) and to possibly different \( \alpha_*^{t+1}(\cdot) \) from \( \alpha_*^t(y) \).

Finally, we merge the resulting candidates according to their regular labeling and keep only the \( k \) best.
Unsupervised Word Embeddings

The embeddings can be trained for each task separately.

However, a method of precomputing word embeddings have been proposed, based on *distributional hypothesis*:

**Words that are used in the same contexts tend to have similar meanings.**

The distributional hypothesis is usually attributed to Firth (1957):

*You shall know a word by a company it keeps.*
Mikolov et al. (2013) proposed two very simple architectures for precomputing word embeddings, together with a C multi-threaded implementation *word2vec*.
### Table 8: Examples of the word pair relationships, using the best word vectors from Table 4 (Skip-gram model trained on 783M words with 300 dimensionality).

<table>
<thead>
<tr>
<th>Relationship</th>
<th>Example 1</th>
<th>Example 2</th>
<th>Example 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>France - Paris</td>
<td>Italy: Rome</td>
<td>Japan: Tokyo</td>
<td>Florida: Tallahassee</td>
</tr>
<tr>
<td>big - bigger</td>
<td>small: larger</td>
<td>cold: colder</td>
<td>quick: quicker</td>
</tr>
<tr>
<td>Miami - Florida</td>
<td>Baltimore: Maryland</td>
<td>Dallas: Texas</td>
<td>Kona: Hawai\i</td>
</tr>
<tr>
<td>Einstein - scientist</td>
<td>Messi: midfielder</td>
<td>Mozart: violinist</td>
<td>Picasso: painter</td>
</tr>
<tr>
<td>Sarkozy - France</td>
<td>Berlusconi: Italy</td>
<td>Merkel: Germany</td>
<td>Koizumi: Japan</td>
</tr>
<tr>
<td>copper - Cu</td>
<td>zinc: Zn</td>
<td>gold: Au</td>
<td>uranium: plutonium</td>
</tr>
<tr>
<td>Berlusconi - Silvio</td>
<td>Sarkozy: Nicolas</td>
<td>Putin: Medvedev</td>
<td>Obama: Barack</td>
</tr>
<tr>
<td>Microsoft - Windows</td>
<td>Google: Android</td>
<td>IBM: Linux</td>
<td>Apple: iPhone</td>
</tr>
<tr>
<td>Microsoft - Ballmer</td>
<td>Google: Yahoo</td>
<td>IBM: McNealy</td>
<td>Apple: Jobs</td>
</tr>
<tr>
<td>Japan - sushi</td>
<td>Germany: bratwurst</td>
<td>France: tapas</td>
<td>USA: pizza</td>
</tr>
</tbody>
</table>

Considering input word $w_i$ and output $w_o$, the Skip-gram model defines

$$p(w_o|w_i) \overset{\text{def}}{=} \frac{e^{W_{w_o}^\top V_{w_i}}}{\sum_w e^{W_w^\top V_{w_i}}}.$$
Instead of a large softmax, we construct a binary tree over the words, with a sigmoid classifier for each node.

If word \( w \) corresponds to a path \( n_1, n_2, \ldots, n_L \), we define

\[
p_{HS}(w | w_i) \overset{\text{def}}{=} \prod_{j=1}^{L-1} \sigma([+1 \text{ if } n_{j+1} \text{ is right child else } -1] \cdot W_{n_j}^{\top} V_{w_i}).
\]
Instead of a large softmax, we could train individual sigmoids for all words.

We could also only sample several negative examples. This gives rise to the following negative sampling objective (instead of just summing all the sigmoidal losses):

$$l_{NEG}(w_o, w_i) \stackrel{\text{def}}{=} \log \sigma(W^\top_{w_o} V_{w_i}) + \sum_{j=1}^{k} \mathbb{E}_{w_j \sim P(w)} \log \left(1 - \sigma(W^\top_{w_j} V_{w_i})\right).$$

The usual value of negative samples $k$ is 5, but it can be even 2 for extremely large corpora.

Each expectation in the loss is estimated using a single sample.

For $P(w)$, both uniform and unigram distribution $U(w)$ work, but $U(w)^{3/4}$ outperforms them significantly (this fact has been reported in several papers by different authors).
### Recurrent Character-level WEs

<table>
<thead>
<tr>
<th>increased</th>
<th>John</th>
<th>Noahshire</th>
<th>phding</th>
</tr>
</thead>
<tbody>
<tr>
<td>reduced</td>
<td>Richard</td>
<td>Nottinghamshire</td>
<td>mixing</td>
</tr>
<tr>
<td>improved</td>
<td>George</td>
<td>Bucharest</td>
<td>modelling</td>
</tr>
<tr>
<td>expected</td>
<td>James</td>
<td>Saxony</td>
<td>styling</td>
</tr>
<tr>
<td>decreased</td>
<td>Robert</td>
<td>Johannesburg</td>
<td>blaming</td>
</tr>
<tr>
<td>targeted</td>
<td>Edward</td>
<td>Gloucestershire</td>
<td>christening</td>
</tr>
</tbody>
</table>

Table 2: Most-similar in-vocabulary words under the C2W model; the two query words on the left are in the training vocabulary, those on the right are nonce (invented) words.
### Table 6: Nearest neighbor words (based on cosine similarity) of word representations from the large word-level and character-level (before and after highway layers) models trained on the PTB. Last three words are OOV words, and therefore they do not have representations in the word-level model.

<table>
<thead>
<tr>
<th>In Vocabulary</th>
<th>Out-of-Vocabulary</th>
</tr>
</thead>
<tbody>
<tr>
<td>while</td>
<td>computer-aided</td>
</tr>
<tr>
<td>although</td>
<td>misled</td>
</tr>
<tr>
<td>letting</td>
<td></td>
</tr>
<tr>
<td>though</td>
<td></td>
</tr>
<tr>
<td>minute</td>
<td></td>
</tr>
<tr>
<td>chile</td>
<td>computer-guided</td>
</tr>
<tr>
<td>whole</td>
<td></td>
</tr>
<tr>
<td>meanwhile</td>
<td></td>
</tr>
<tr>
<td>white</td>
<td></td>
</tr>
<tr>
<td>meanwhile</td>
<td>computer-guided</td>
</tr>
<tr>
<td>whole</td>
<td></td>
</tr>
<tr>
<td>though</td>
<td></td>
</tr>
<tr>
<td>nevertheless</td>
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<td></td>
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<td>although</td>
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<td>letting</td>
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<tr>
<td>nevertheless</td>
<td></td>
</tr>
</tbody>
</table>

Another simple idea appeared simultaneously in three nearly simultaneous publications as *Charagram*, *Subword Information* or *SubGram*.

A word embedding is a sum of the word embedding plus embeddings of its character $n$-grams. Such embedding can be pretrained using same algorithms as *word2vec*.

The implementation can be

- dictionary based: only some number of frequent character $n$-grams is kept;
- hash-based: character $n$-grams are hashed into $K$ buckets (usually $K \sim 10^6$ is used).
Table 7: Nearest neighbors of rare words using our representations and skipgram. These hand picked examples are for illustration.

Figure 2: Illustration of the similarity between character n-grams in out-of-vocabulary words. For each pair, only one word is OOV, and is shown on the x-axis. Red indicates positive cosine, while blue negative.

*Figure 2 of paper "Enriching Word Vectors with Subword Information", https://arxiv.org/abs/1607.04606.*
The word2vec enriched with subword embeddings is implemented in publicly available fastText library [https://fasttext.cc/](https://fasttext.cc/).

Pre-trained embeddings for 157 languages (including Czech) trained on Wikipedia and CommonCrawl are also available.