

1 Efficient Inference of fully connected CRF

1.1 Definition of Conditional Random Fields

A conditional random field (\mathbf{I}, \mathbf{X}) is characterized by a Gibbs distribution

$$P(\mathbf{X}|\mathbf{I}) = \frac{1}{Z(\mathbf{I})} \exp \left(- \sum_{c \in C_{\mathcal{G}}} \phi_c(\mathbf{X}_c|\mathbf{I}) \right),$$

where $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a graph on \mathbf{X} and each clique c in a set of cliques $C_{\mathcal{G}}$ in \mathcal{G} induces a potential ϕ_c . The Gibbs energy of a labeling $\mathbf{x} \in \mathcal{L}^N$ is

$$E(\mathbf{x}|\mathbf{I}) = \sum_{c \in C_{\mathcal{G}}} \phi_c(\mathbf{x}_c|\mathbf{I}).$$

In the fully connected pairwise CRF model, \mathcal{G} is the complete graph on \mathbf{X} and $C_{\mathcal{G}}$ is the set of all unary and pairwise cliques. The corresponding Gibbs energy is :

$$E(\mathbf{x}) = \sum_i \psi_u(x_i) + \sum_{i < j} \psi_p(x_i, x_j),$$

1.2 Mean Field Approximation of Inference of CRF

Instead of computing the exact distribution $P(\mathbf{X})$, the mean field approximation would transfer the computations of CRF into a distribution $Q(\mathbf{X})$ with simpler structure. The ideal choice of the approximation measure should satisfy

- Q can be expressed product of independent marginals, $Q(\mathbf{X}) = \prod_i Q_i(X_i)$.
- Q will minimize the KL-divergence $\mathcal{D}(Q\|P)$.

By applying Lagrange multiplier method, we could obtain the necessary condition of the optimal measure is a system of nonlinear equations:

$$Q_i(x_i = l) = \frac{1}{Z_i} \exp \left\{ -\psi_u(x_i) - \sum_{l' \in \mathcal{L}} \mu(l, l') \sum_{m=1}^K w^{(m)} \sum_{j \neq i} k^{(m)}(f_i, f_j) Q_j(l') \right\}.$$

Recall that we have N different data samples and for each sample we have $L - 1$ parameters to be determined, *i.e.* $\{Q_i(x_i = l)\}_{l=1}^{L-1}$. Thus analytically solving this system of equations may still be hard. Practically, a fixed point iteration approximation could be an efficient way to obtain the numerical solution. The fixed-point iteration is given by the following procedure.

- Initialize Q by

$$Q_i(x_i) \leftarrow \frac{1}{Z_i} \exp \{-\phi_u(x_i)\}.$$

- $\hat{Q}_i^{(m)}(l) \leftarrow \sum_{j \neq i} k^{(m)}(f_i, f_j) Q_j(l)$
- $\hat{Q}_i(x_i) \leftarrow \sum_{l' \in \mathcal{L}} \mu^{(m)}(x_i, l') \sum_m w^{(m)} \hat{Q}_i^{(m)}(l')$
- $Q_i(x_i) \leftarrow \exp \left\{ -\psi_u(x_i) - \hat{Q}_i(x_i) \right\}$
- normalize $Q_i(x_i)$
- repeat until convergence.

2 End-to-end Learning and Inference of CRF

For the mean field approximation inference of a CRF, we can embed all the calculation into a CNN layer, and the iteration can be regarded as another RNN structure. Thus the inference step can be solely based on Neural Networks structure. For the training of this RNN-CRF layer, we use maximal log-likelihood strategy for the parameter updating. However, in this case the loss function of the Neural Networks will admit an intractable gradient.

$$\mathcal{L}(\theta) = \sum_{n=1}^N \log P(\mathbf{x}^{(n)} | \mathbf{I}^{(n)}; \theta) = - \sum_{n=1}^N [E(\mathbf{x} | \mathbf{I}^{(n)}; \theta) + \log Z(\mathbf{I}^{(n)}; \theta)] \quad (2.1)$$

$$\Rightarrow \nabla_{\theta} \mathcal{L}(\theta) = - \sum_{n=1}^N \nabla_{\theta} [E(\mathbf{x} | \mathbf{I}^{(n)}; \theta) + \log Z(\mathbf{I}^{(n)}; \theta)]. \quad (2.2)$$

and a straightforward calculation leads to

$$\nabla_{\theta} \mathcal{L}(\theta) \log Z(\mathbf{I}^{(n)}; \theta) = - \mathbb{E}_{\mathbf{x}^{(n)} \sim P(\mathbf{x}^{(n)} | \mathbf{I}^{(n)}; \theta)} \nabla_{\theta} E(\mathbf{x} | \mathbf{I}^{(n)}; \theta).$$

In order to address this issue, we use mean field approximation again for the calculation of the marginal expectation term in the gradient. Thus, we build an end-to-end CRF model.