

Supervised learning of GRFs1A. ML-estimator for Gibbs random fields

$S = \{s_i \in K \mid i \in V\}$ is a GRF w.r.t. the graph (V, E) and has p.d.

$$p_u(s) = \frac{1}{Z(u)} \exp \sum_{ij \in E} \psi_{ij}(s_i, s_j)$$

Its parameters are unknown. We are given an i.i.d. sample of training data $\mathcal{T}^m = \{s^j \in K^V \mid j=1, \dots, m\}$

MLE

$$u_* \in \operatorname{argmax}_{u \in \mathcal{U}} \frac{1}{m} \sum_{j=1}^m \log p_u(s^j) = \operatorname{argmax}_{u \in \mathcal{U}} L(u, \mathcal{T}^m)$$

Since the GRF is an exponential family, we can write

$$L(u, \mathcal{T}^m) = \frac{1}{m} \sum_{s \in \mathcal{T}^m} \langle \Phi(s), u \rangle - \log Z(u)$$

- $L(u, \mathcal{T}^m)$ is concave in u
- The model is identifiable up to re-parametrisations
i.e. $L(u) = \mathbb{E}_{\mathcal{T}^m \sim p_{u_0}} (\log p_u(\mathcal{T}^m))$ has maximum at u_0
up to re-parametrisations
- If \mathcal{U} is compact, then the MLE is consistent.

How to solve the task

$$L(u, \mathcal{T}^m) = \frac{1}{m} \sum_{s \in \mathcal{T}^m} \langle \Phi(s), u \rangle - \log Z(u) \rightarrow \max_{u \in \mathcal{U}}$$

Computing the gradient

$$\nabla L(u, \mathcal{T}^m) = \frac{1}{m} \sum_{s \in \mathcal{T}^m} \Phi(s) - \mathbb{E}_u[\Phi]$$

amounts to computing pairwise marginals for all edges of the graph!

B. Pseudo-likelihood estimator for GRFs

Can we do simpler? Besag, 1995 \Rightarrow Recall that a GRF on a graph (V, E) is defined by fixing the (consistent) family of conditional distributions

$$P_u(s_i | S_{N_i}) = \frac{1}{Z_i(u, S_{N_i})} \exp \sum_{j \in N_i} u_{ij}(s_i, s_j) \quad \forall i \in V$$

(see Gibbs sampler) Hence we may use the pseudo-likelihood

$$\tilde{L}(u, \mathcal{T}^m) = \frac{1}{m} \sum_{s \in \mathcal{T}^m} \sum_i \log p_u(s_i | S_{N_i}) \rightarrow \max_{u \in \mathcal{Q}} \tilde{L}(u, \mathcal{T}^m)$$

instead of MLE. We obtain

$$\begin{aligned} \tilde{L}(u, \mathcal{T}^m) &= \frac{1}{m} \sum_{s \in \mathcal{T}^m} \sum_{i \in V} \sum_{j \in N_i} u_{ij}(s_i, s_j) - \frac{1}{m} \sum_{s \in \mathcal{T}^m} \sum_{i \in V} \log Z_i(u, S_{N_i}) \\ &= 2 \sum_{ij \in E} \frac{1}{m} \sum_{s \in \mathcal{T}^m} u_{ij}(s_i, s_j) - \sum_{i \in V} \frac{1}{m} \sum_{s \in \mathcal{T}^m} \log Z_i(u, S_{N_i}) \end{aligned}$$

Computing $\tilde{L}(u, \mathcal{T}^m)$ and $\nabla \tilde{L}(u, \mathcal{T}^m)$ has complexity $\mathcal{O}(m|E||K|^2)$. Properties of pseudo-likelihood estimators:

- (1) $\tilde{L}(u, \mathcal{T}^m)$ is concave in u .
- (2) pseudo-likelihood estimators are consistent
- (3) their variance (in \mathcal{T}^m) is higher than the variance of MLE
- (4) PLE can not be used for unsupervised learning
(MLE + EM algorithm allows unsupervised learning)

Example 1 Conditional random fields for semantic segmentation

Combine a convolutional neural network with a CRF

Denote: $D \subset \mathbb{Z}^2$ - image domain

$x: D \rightarrow \mathbb{R}^3$ - image

$S: D \rightarrow K$ - segmentation

CNN network $a = f(x, w)$, $a \in \mathbb{R}^{D \times K}$ computes features for each pixel $i \in D$ and each segment label $k \in K$.

This could be e.g. a U-net

CRF model:

$$p_{\theta}(S|x) = \frac{1}{Z(x, \theta)} \exp \left[\sum_{i,j \in E} u_{ij}(s_i, s_j) + \sum_{i \in V} f_{s_i}(x, w) \right]$$

where $\theta = (u, w)$. Such models can be learned end-to-end by PLE. □