

Energy Minimization and MAP inference

For a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$,

$$\min_{\mathbf{x}} \sum_{i \in \mathcal{V}} \theta_i(x_i) + \sum_{(i,j) \in \mathcal{E}} \theta_{ij}(x_i, x_j) \quad x_i \in \{1, \dots, K\}$$

is the discrete pairwise energy minimization problem

This problem:

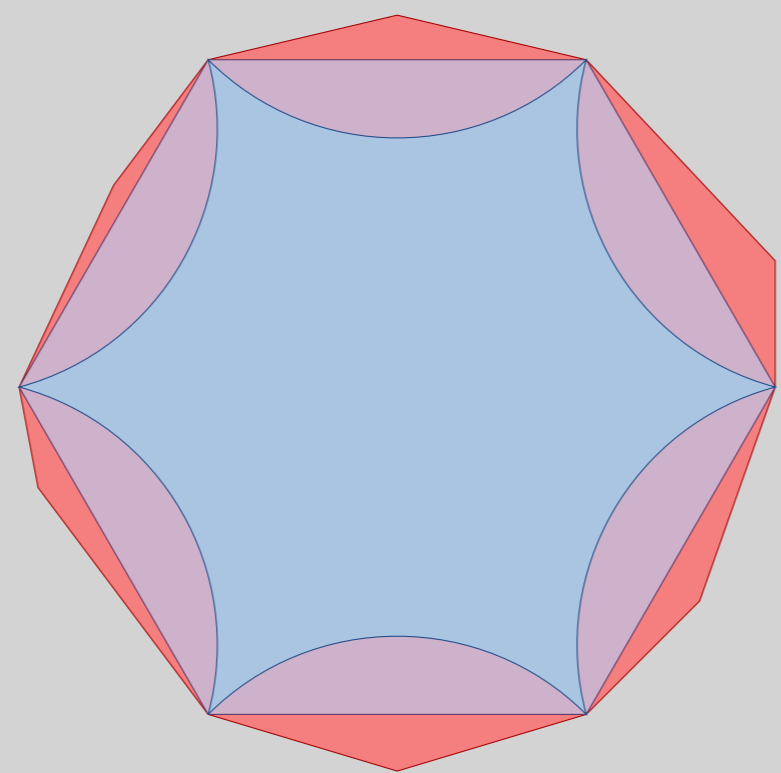
- In general graphs and energies is NP-hard
- Arises in the context of finding the MAP prediction in MRF

The potentials $\theta_i(x_i)$ and $\theta_{ij}(x_i, x_j)$ encode unary and pairwise dependencies

Relaxation Approaches

MAP as an integer quadratic program:

$$\begin{aligned} \min_{\boldsymbol{\mu}} \quad & \sum_{i \in \mathcal{V}} \boldsymbol{\theta}_i^T \boldsymbol{\mu}_i + \sum_{(i,j) \in \mathcal{E}} \boldsymbol{\mu}_i^T \boldsymbol{\Theta}_{ij} \boldsymbol{\mu}_j \\ \text{s.t.} \quad & \mu_{i;k} \in \{0, 1\} \quad \forall i, k \quad \text{and} \quad \sum_k \mu_{i;k} = 1 \quad \forall i. \end{aligned}$$



$\boldsymbol{\Theta}_{ij}$ represent the pairwise potentials in a matrix form.

Linear program (LP) relaxation:

Quadratic program (QP) relaxation:

$$\begin{aligned} \min_{\boldsymbol{\mu} \in \mathcal{L}_G} \quad & \sum_{i \in \mathcal{V}} \boldsymbol{\theta}_i^T \boldsymbol{\mu}_i + \sum_{(i,j) \in \mathcal{E}} \boldsymbol{\theta}_{ij}^T \boldsymbol{\mu}_{ij}, \\ \mathcal{L}_G = \left\{ \boldsymbol{\mu} \mid \right. & \left. \begin{aligned} & \sum_k \mu_{i;k} = 1 \\ & \sum_l \mu_{ij;kl} = \mu_{i;k} \\ & \mu_{i;k} \geq 0, \mu_{ij;kl} \geq 0 \end{aligned} \right\} \end{aligned}$$

$$\min_{\boldsymbol{\mu} \in \Delta_K^{|\mathcal{V}|}} \sum_{i \in \mathcal{V}} \boldsymbol{\theta}_i^T \boldsymbol{\mu}_i + \sum_{(i,j) \in \mathcal{E}} \boldsymbol{\mu}_i^T \boldsymbol{\Theta}_{ij} \boldsymbol{\mu}_j.$$

$\Delta_K^{|\mathcal{V}|}$ is a product space of $|\mathcal{V}|$ simplexes over K variables

Combined LP and QP Relaxation

$$\min_{\boldsymbol{\mu} \in \mathcal{L}_G} \underbrace{\sum_{i \in \mathcal{V}} \boldsymbol{\theta}_i^T \boldsymbol{\mu}_i + \sum_{(i,j) \in \mathcal{E}} \boldsymbol{\theta}_{ij}^T \boldsymbol{\mu}_{ij}}_{\text{standard LP objective}} + \beta \underbrace{\sum_{(i,j) \in \mathcal{E}} D_{KL}(\boldsymbol{\mu}_{ij}, \text{vec}(\boldsymbol{\mu}_i \boldsymbol{\mu}_j^T))}_{\text{penalty term for inconsistencies}}$$

$$D_{KL}(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sum_k \mu_k \log \left(\frac{\mu_k}{\nu_k} \right) \text{ is the Kullback-Leibler divergence}$$

- While $\beta = 0$ amounts to the LP relaxation, $\beta \rightarrow \infty$ recovers the QP
- Option: successively increase β to moderate the constraint enforcement

Convex-Concave Procedure (CCCP)

1. Decompose non-convex objective into convex u , v :

$$\min_{\boldsymbol{\mu} \in \mathcal{L}_G} u_{\beta}(\boldsymbol{\mu}) - v_{\beta}(\boldsymbol{\mu})$$

2. Iteratively solve problem where v is linearized:

$$\boldsymbol{\mu}^{t+1} = \operatorname{argmin}_{\boldsymbol{\mu} \in \mathcal{L}_G} u_{\beta}(\boldsymbol{\mu}) - \boldsymbol{\mu}^T \nabla v_{\beta}(\boldsymbol{\mu}^t)$$

CCCP for the Combined LP-QP Relaxation

$$u_{\beta}(\boldsymbol{\mu}) = \sum_{i \in \mathcal{V}} \boldsymbol{\theta}_i^T \boldsymbol{\mu}_i + \sum_{(i,j) \in \mathcal{E}} \boldsymbol{\theta}_{ij}^T \boldsymbol{\mu}_{ij} - \beta \sum_{(i,j) \in \mathcal{E}} H(\boldsymbol{\mu}_{ij})$$

d_i : degree of node i

$$v_{\beta}(\boldsymbol{\mu}) = -\beta \sum_{i \in \mathcal{V}} d_i H(\boldsymbol{\mu}_i)$$

$H(\boldsymbol{\mu})$: entropy of $\boldsymbol{\mu}$

The gradient of $v_{\beta}(\boldsymbol{\mu})$:

$$\frac{\partial v_{\beta}(\boldsymbol{\mu})}{\partial \mu_{i;k}} = \beta d_i (1 + \log(\mu_{i;k})) \quad \text{and} \quad \frac{\partial v_{\beta}(\boldsymbol{\mu})}{\partial \mu_{ij;kl}} = 0$$

LPQP Algorithm

Require: $\mathcal{G} = (\mathcal{V}, \mathcal{E}), \boldsymbol{\theta}$.

- 1: initialize $\boldsymbol{\mu} \in \mathcal{L}_G$ uniform, $\beta = \beta_0$.
- 2: **repeat**
- 3: $t = 0, \boldsymbol{\mu}^0 = \boldsymbol{\mu}$.
- 4: **repeat**
- 5: $\boldsymbol{\mu}^{t+1} = \operatorname{argmin}_{\boldsymbol{\tau} \in \mathcal{L}_G} u_{\beta}(\boldsymbol{\tau}) - \boldsymbol{\tau}^T \nabla v_{\beta}(\boldsymbol{\mu}^t)$.
- 6: $t = t + 1$.
- 7: **until** $\|\boldsymbol{\mu}^t - \boldsymbol{\mu}^{t-1}\|_2 \leq \epsilon_{dc}$.
- 8: $\boldsymbol{\mu} = \boldsymbol{\mu}^t$.
- 9: increase β .
- 10: **until** $\|\boldsymbol{\mu} - \boldsymbol{\mu}^0\|_2 \leq \epsilon_{\beta}$.
- 11: **return** $\boldsymbol{\mu}$.

Inner Optimization Problem – Message Passing

For a fixed β and $\tilde{\boldsymbol{\theta}}_i = \boldsymbol{\theta}_i - \beta d_i \log(\boldsymbol{\mu}_i^t)$ we solve,

$$\boldsymbol{\mu}^{t+1} = \operatorname{argmin}_{\boldsymbol{\mu} \in \mathcal{L}_G} \sum_{i \in \mathcal{V}} \tilde{\boldsymbol{\theta}}_i^T \boldsymbol{\mu}_i + \sum_{(i,j) \in \mathcal{E}} \boldsymbol{\theta}_{ij}^T \boldsymbol{\mu}_{ij} - \beta \sum_{(i,j) \in \mathcal{E}} H(\boldsymbol{\mu}_{ij})$$

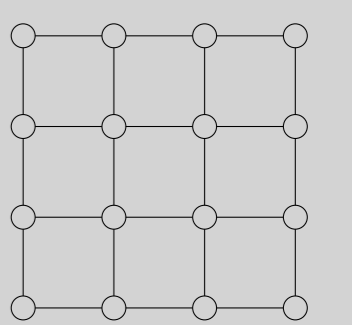
Using a variant of the norm-product belief propagation algorithm

$$\begin{aligned} m_{j \rightarrow i}(x_i) & \propto \left(\sum_{x_j} \theta_{ij}^{1/\beta}(x_i, x_j) \frac{\theta_j^{1/(d_j \beta)}(x_j) \prod_{k \in \mathcal{N}(j)} m_{k \rightarrow j}^{1/(d_j \beta)}(x_j)}{m_{i \rightarrow j}^{1/\beta}(x_j)} \right)^{\beta} \\ \mu_i(x_i) & \propto \left(-\theta_i(x_i) \prod_{j \in \mathcal{N}(i)} m_{j \rightarrow i}(x_i) \right)^{1/(d_i \beta)} \end{aligned}$$

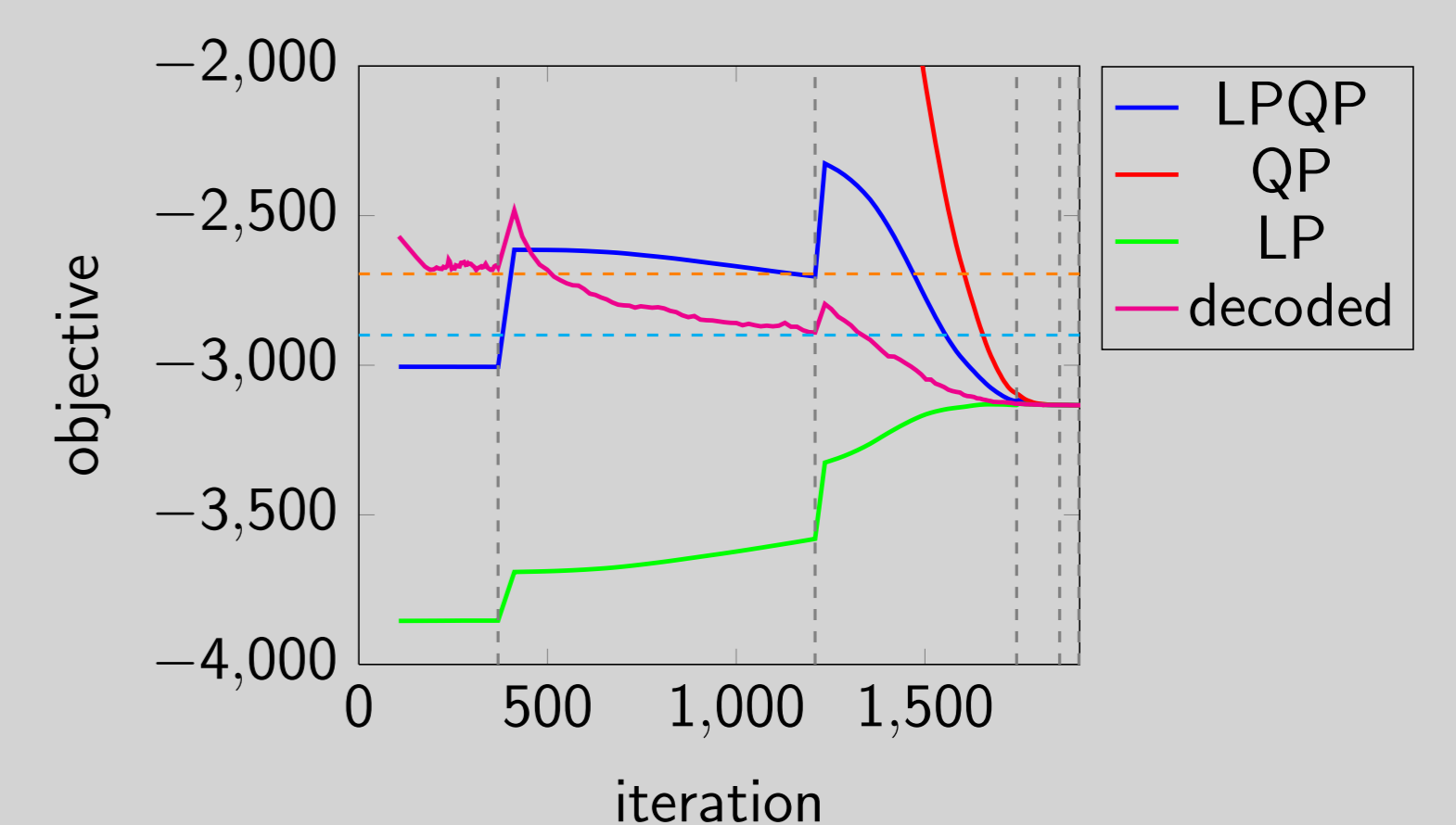
Synthetic Lattice Experiment

- Potts model for a lattice graph.
- Mixed attractive and repulsive potentials.
- For smaller σ : Unaries have less influence.

$$\begin{aligned} \theta_{i;k}(x_i) & \sim \text{Uniform}(-\sigma, \sigma) \\ \alpha_{ij} & \sim \text{Uniform}(-1, 1) \\ \theta_{ij}(x_i, x_j) & = \begin{cases} 0 & \text{if } x_i \neq x_j \\ \alpha_{ij} & \text{otherwise.} \end{cases} \end{aligned}$$

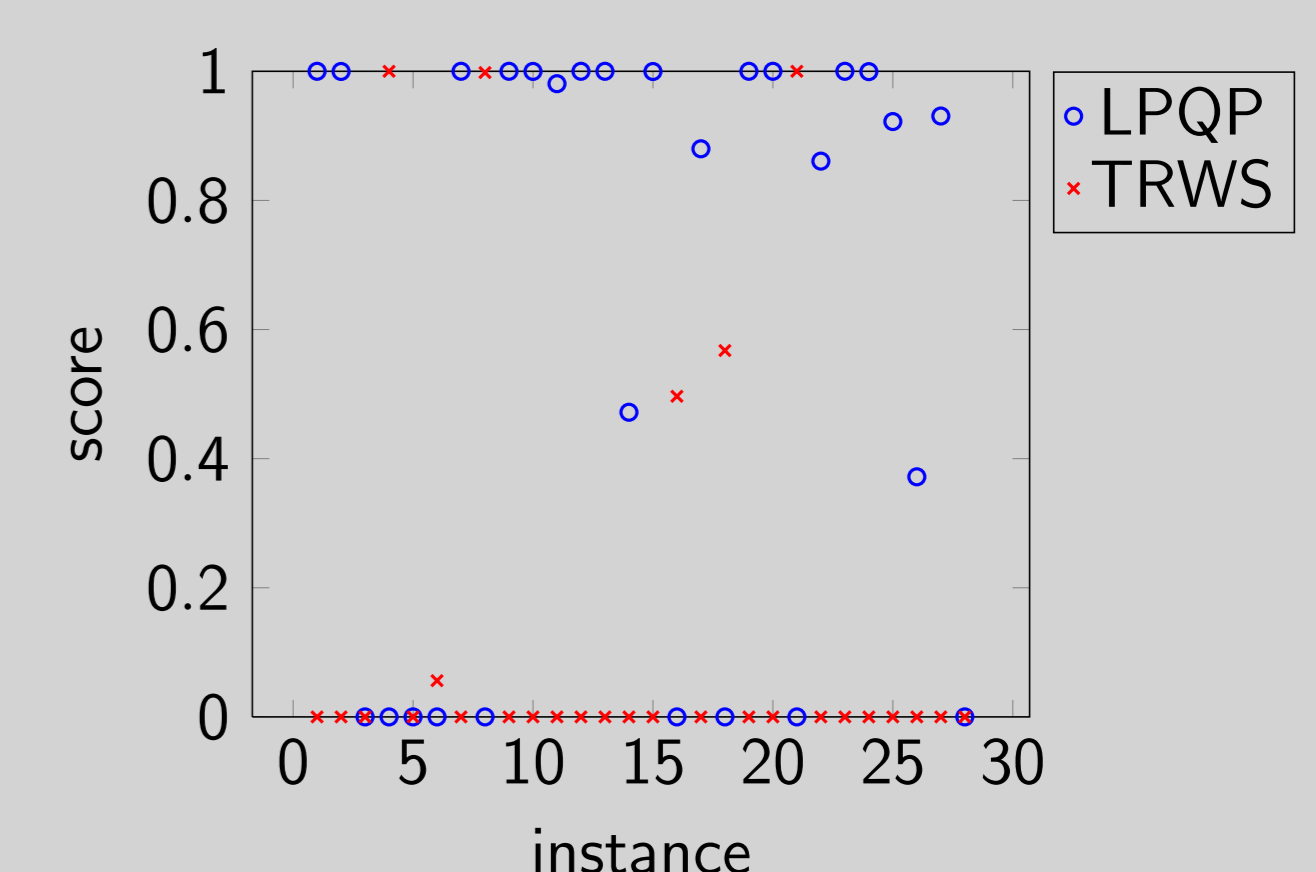


M (size)	60		90		120	
K (# states)	2	5	2	5	2	5
	$\sigma = 0.05$					
MPLP	0.73	0.99	0.53	0.97	0	0.95
LPQP	1	0.99	1	1	1	1
TRWS	0	0	0	0	0.40	0
	$\sigma = 0.5$					
MPLP	1	1	1	1	1	1
LPQP	0.99	0.94	0.99	0.93	1	0.96
TRWS	0	0	0	0	0	0



Protein Side-Chain Prediction Experiment

- 28 instances where LP not tight.
- True MAP state known through integer programming.
- LPQP only on six instances worse than TRWS.
- LPQP finds global minimum for 12 instances.



Conclusions

- Joint formulation of LP and QP relaxation.
- CCCP algorithm in its core uses norm-product belief-propagation for modified unary potentials.
- Competitive results in terms of MAP state found.

References

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