

## Energy Minimization and MAP Inference

For a graph  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  the pairwise MAP problem is:

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

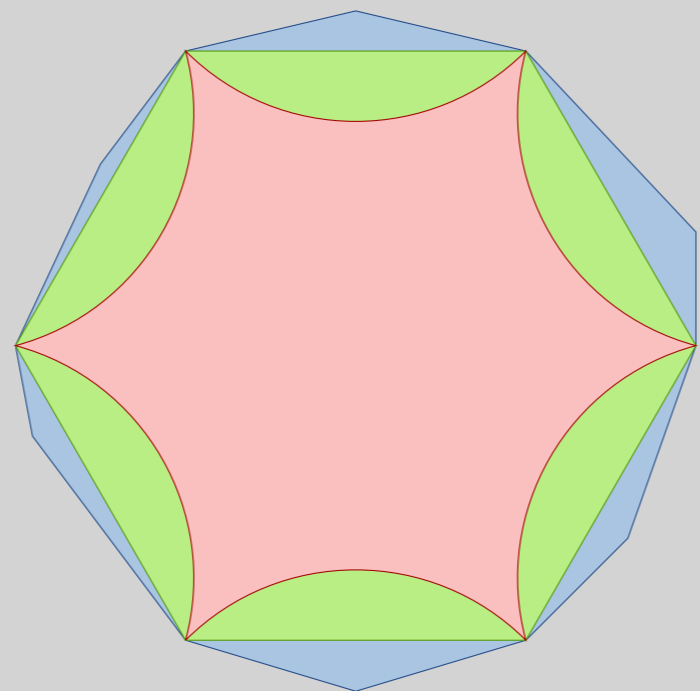
- MAP for general graphs and energies is NP-hard.
- The potentials  $\theta_i(x_i)$  and  $\theta_{ij}(x_i, x_j)$  encode costs of an assignment.

## Relaxation Approaches

MAP as an integer quadratic program:

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

$$\text{s.t. } \mu_{i,k} \in \{0, 1\} \quad \forall i, k \quad \text{and} \quad \sum_k \mu_{i,k} = 1 \quad \forall i.$$



Linear program (LP) relaxation:

$$\min_{\boldsymbol{\mu} \in \mathcal{L}_{\mathcal{G}}} \sum_{i \in \mathcal{V}} \boldsymbol{\theta}_i^T \boldsymbol{\mu}_i + \sum_{(i,j) \in \mathcal{E}} \boldsymbol{\theta}_{ij}^T \boldsymbol{\mu}_{ij},$$

$$\mathcal{L}_{\mathcal{G}} = \left\{ \boldsymbol{\mu} \mid \begin{array}{l} \sum_k \mu_{i,k} = 1 \\ \sum_l \mu_{ij,kl} = \mu_{i,k} \\ \mu_{i,k} \geq 0, \mu_{ij,kl} \geq 0 \end{array} \right\}$$

Quadratic program (QP) relaxation:

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

$$\text{s.t. } \boldsymbol{\mu}_{ij} = \text{vec}(\boldsymbol{\mu}_i \boldsymbol{\mu}_j^T)$$

## Combined LP and QP Relaxation

$$\min_{\boldsymbol{\mu} \in \mathcal{L}_{\mathcal{G}}} \boldsymbol{\theta}^T \boldsymbol{\mu} + \rho g(\boldsymbol{\mu})$$

- $g(\boldsymbol{\mu})$ : penalizes inconsistencies between  $\boldsymbol{\mu}_{ij}$  and  $\boldsymbol{\mu}_i \boldsymbol{\mu}_j^T$ .
- $\rho = 0$  amounts to the LP relaxation,  $\rho \rightarrow \infty$  recovers the QP.
- Non-convex objective (for  $\rho > 0$ ).
- Successively increase  $\rho$  to moderate the constraint enforcement.

## Kullback-Leibler Divergence Penalty Terms – Two Variants

Uniform

$$\sum_{(i,j) \in \mathcal{E}} D_{KL}(\boldsymbol{\mu}_{ij}, \boldsymbol{\mu}_i \boldsymbol{\mu}_j^T)$$

Tree-based for trees  $\mathcal{G}_a = (\mathcal{V}_a, \mathcal{E}_a)$

$$\sum_{a \in \mathcal{A}} \eta_a \left( \sum_{(i,j) \in \mathcal{E}_a} D_{KL}(\boldsymbol{\mu}_{ij}, \boldsymbol{\mu}_i \boldsymbol{\mu}_j^T) \right)$$

With  $D_{KL}(\cdot)$  the Kullback-Leibler divergence or mutual information

$$D_{KL}(\boldsymbol{\mu}_{ij}, \boldsymbol{\mu}_i \boldsymbol{\mu}_j^T) = \sum_{k,l} \mu_{ij,kl} \log \left( \frac{\mu_{ij,kl}}{\mu_{i,k} \mu_{j,l}} \right) = H(\boldsymbol{\mu}_i) + H(\boldsymbol{\mu}_j) - H(\boldsymbol{\mu}_{ij}).$$

With  $H(\mathbf{p}) = -\sum_k p_k \log(p_k)$  the entropy of  $\mathbf{p}$ .

## Concave-Convex Procedure (CCCP)

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

$$\min_{\boldsymbol{\mu} \in \mathcal{L}_{\mathcal{G}}} u_{\rho}(\boldsymbol{\mu}) - v_{\rho}(\boldsymbol{\mu})$$

2. Iteratively solve problem where  $v$  is linearized:

$$\boldsymbol{\mu}^{t+1} = \underset{\boldsymbol{\mu} \in \mathcal{L}_{\mathcal{G}}}{\text{argmin}} u_{\rho}(\boldsymbol{\mu}) - \boldsymbol{\mu}^T \nabla v_{\rho}(\boldsymbol{\mu}^t)$$

## Difference of Convex Functions for Combined Relaxation

- Several solvers for LP relaxations add entropy terms to objective.  $\rightarrow$  better convergence properties.
- LPQP has an entropy augmentation built-in!
- Linearized CCCP term simply modifies the unary potentials.

Uniform weighting

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

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

$$\frac{\partial v_{\rho}(\boldsymbol{\mu})}{\partial \mu_{i,k}} = \rho d_i (1 + \log \mu_{i,k})$$

Tree-based weighting

$$u_{\rho}(\boldsymbol{\mu}) = \boldsymbol{\theta}^T \boldsymbol{\mu} - \rho \sum_{a \in \mathcal{A}} \eta_a \left( \sum_{(i,j) \in \mathcal{E}_a} H(\boldsymbol{\mu}_{ij}) - \sum_{i \in \mathcal{V}_a} (d_i^a - 1) H(\boldsymbol{\mu}_i) \right)$$

$$v_{\rho}(\boldsymbol{\mu}) = -\rho \sum_{a \in \mathcal{A}} \eta_a \sum_{i \in \mathcal{V}_a} H(\boldsymbol{\mu}_i)$$

$$\frac{\partial v_{\rho}(\boldsymbol{\mu})}{\partial \mu_{i,k}} = \rho \sum_{a \in \mathcal{A}(i)} \eta_a (1 + \log \mu_{i,k})$$

$d_i$ : degree of node  $i$  in  $\mathcal{G}$ ,  $d_i^a$ : degree of node  $i$  in graph  $\mathcal{G}_a$ ,  $\eta_a$ : weight of graph  $\mathcal{G}_a$ .

## LPQP Algorithm

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

- 1: initialize  $\boldsymbol{\mu} \in \mathcal{L}_{\mathcal{G}}$  uniform,  $\rho = \rho_0$ .
- 2: **repeat**
- 3:  $t = 0, \boldsymbol{\mu}^0 = \boldsymbol{\mu}$ .
- 4: **repeat**
- 5:  $\boldsymbol{\mu}^{t+1} = \underset{\boldsymbol{\tau} \in \mathcal{L}_{\mathcal{G}}}{\text{argmin}} u_{\rho}(\boldsymbol{\tau}) - \boldsymbol{\tau}^T \nabla v_{\rho}(\boldsymbol{\mu}^t)$ .
- 6:  $t = t + 1$ .
- 7: **until**  $\|\boldsymbol{\mu}^t - \boldsymbol{\mu}^{t-1}\|_2 \leq \epsilon_{\text{dc}}$ .
- 8:  $\boldsymbol{\mu} = \boldsymbol{\mu}^t$ .
- 9: increase  $\rho$ .
- 10: **until**  $\|\boldsymbol{\mu} - \boldsymbol{\mu}^0\|_2 \leq \epsilon_{\rho}$ .
- 11: **return**  $\boldsymbol{\mu}$ .

## Inner Optimization Problem – Message Passing

For a fixed  $\rho$  and modified unary potentials  $\tilde{\boldsymbol{\theta}}_i(\boldsymbol{\mu}_i^t)$  need to solve a convex optimization problem.

- Uniform weighting (LPQP-U):

$$\boldsymbol{\mu}^{t+1} = \underset{\boldsymbol{\mu} \in \mathcal{L}_{\mathcal{G}}}{\text{argmin}} \tilde{\boldsymbol{\theta}}^T \boldsymbol{\mu} - \rho \sum_{(i,j) \in \mathcal{E}} H(\boldsymbol{\mu}_{ij}).$$

$\rightarrow$  Solved by norm-product belief-propagation.

- Tree-based weighting (LPQP-T):

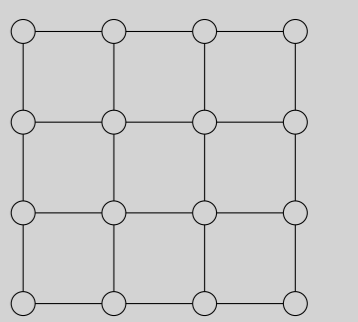
$$\boldsymbol{\mu}^{t+1} = \underset{\boldsymbol{\mu} \in \mathcal{L}_{\mathcal{G}}}{\text{argmin}} \tilde{\boldsymbol{\theta}}^T \boldsymbol{\mu} - \rho \sum_{a \in \mathcal{A}} \eta_a \left( \sum_{(i,j) \in \mathcal{E}_a} H(\boldsymbol{\mu}_{ij}) - \sum_{i \in \mathcal{V}_a} (d_i^a - 1) H(\boldsymbol{\mu}_i) \right).$$

$\rightarrow$  Solved by dual decomposition & the sum-product algorithm.

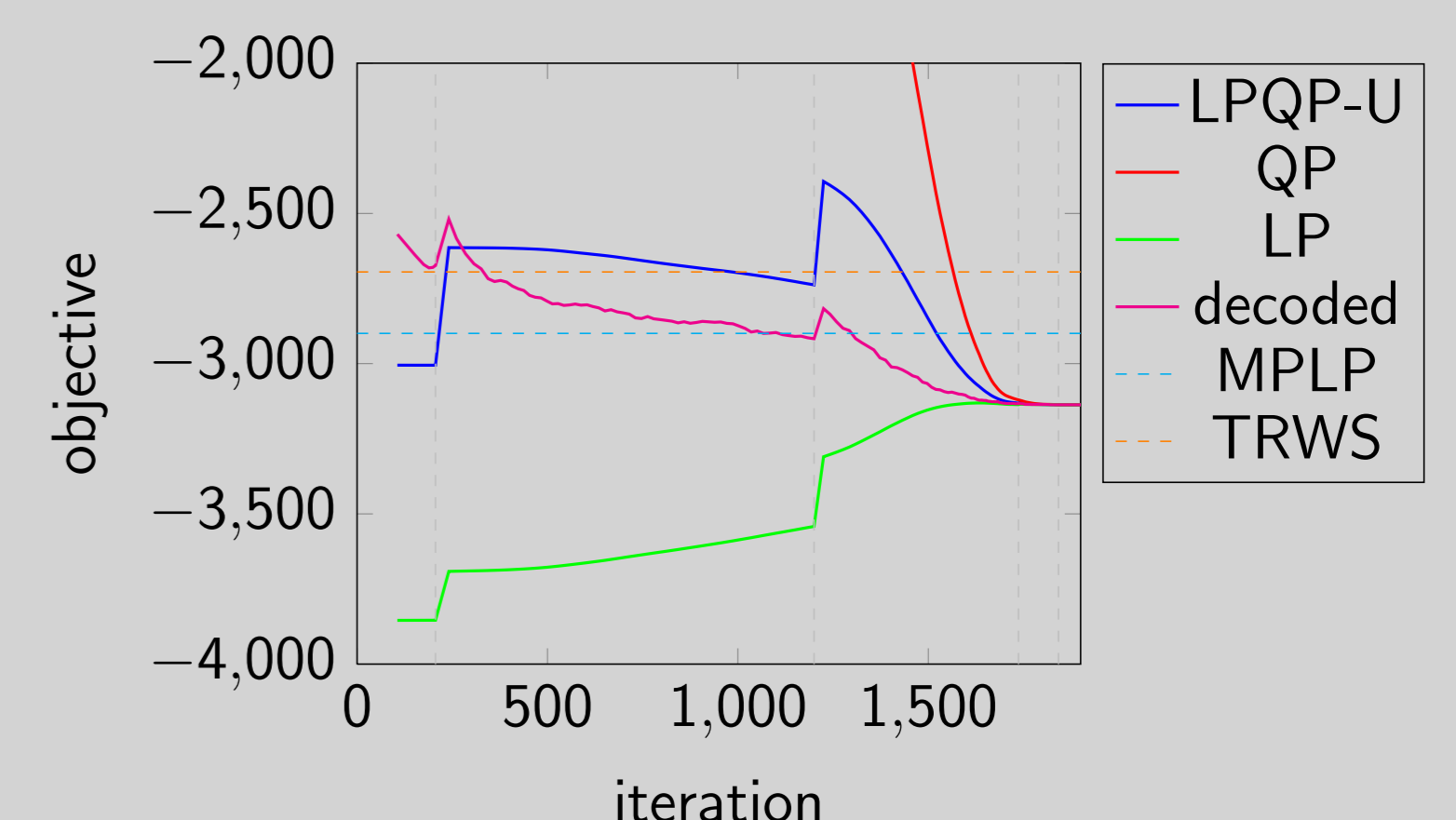
## Synthetic Potts Model Experiment

- Potts model for a lattice graph.
- Mixed attractive and repulsive potentials.
- Lower signal-to-noise ratio for smaller  $\sigma$ .

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



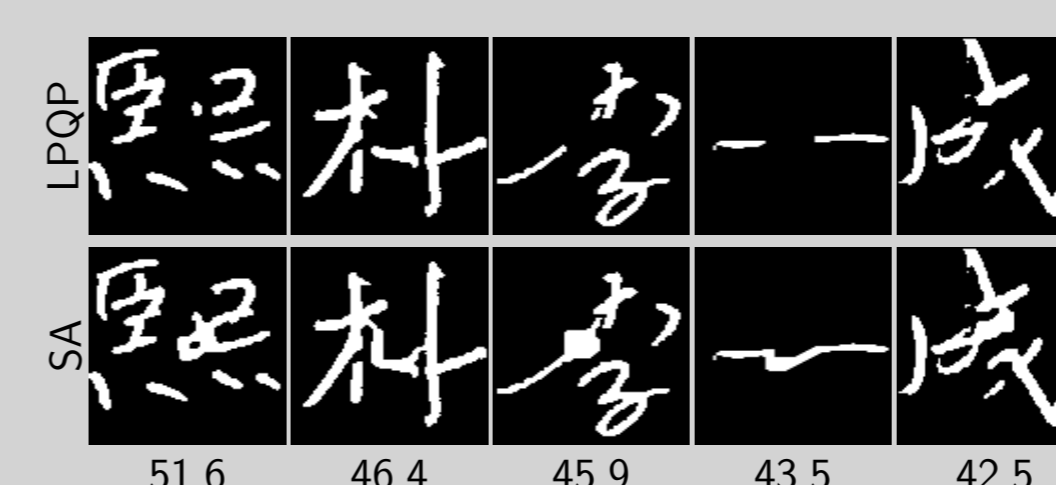
| M (size)     | 60              | 90   | 120  |      |      |
|--------------|-----------------|------|------|------|------|
| K (# states) | 2               | 5    | 2    | 5    | 2    |
|              | $\sigma = 0.05$ |      |      |      |      |
| MPLP         | 0.71            | 0.99 | 0.51 | 0.96 | 0.95 |
| LPQP-U       | 0.97            | 0.99 | 0.97 | 1    | 0.98 |
| LPQP-T       | 1               | 0.97 | 1    | 0.98 | 1    |
| TRWS         | 0               | 0    | 0    | 0    | 0.39 |
|              | $\sigma = 0.5$  |      |      |      |      |
| MPLP         | 1               | 1    | 1    | 1    | 0.99 |
| LPQP-U       | 0.99            | 0.92 | 0.99 | 0.91 | 1    |
| LPQP-T       | 0.99            | 0.95 | 0.99 | 0.94 | 0.96 |
| TRWS         | 0               | 0    | 0    | 0    | 0    |



$$\text{score for the evaluation: } s_i = \frac{\max_{1 \leq j \leq J} (e_j) - e_i}{\max_{1 \leq j \leq J} (e_j) - \min_{1 \leq j \leq J} (e_j)}$$

## Real-world Experiments (Proteins and Inpainting)

DTF Problem Dataset



Protein Prediction & Design

- Prediction. 28 instances where LP not tight. Recover true MAP for 2/3.
- Design. Average scores: LPQP-U: 0.93, MPLP: 1 and TRWS: 0.03.

Better solution for 43/100 instances

## Conclusions

- Joint formulation of LP and QP relaxation  $\rightarrow$  LPQP.
- LPQP solved by a message-passing algorithm for modified unary potentials.
- Get a smooth objective for free. Key to fast convergence.
- Competitive results in terms of MAP state found.

## References

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