Machine Learning

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University of Illinois at Urbana-Champaign, 2018

L12: Structured Prediction (ILP, LP relaxation, message passing, graph cut)

Getting to know structured inference algorithms

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Reading material:

• Getting to know structured inference algorithms

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• D. Koller and N. Friedman; Probabilistic Graphical Models: Principles and Techniques;

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Algorithms:

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Algorithms:

- Exhaustive search
- Dynamic programming

$$\mathbf{y}^* = \arg\max_{\hat{\mathbf{y}}} \sum_r f_r(\hat{\mathbf{y}}_r)$$

Algorithms:

- Exhaustive search
- Dynamic programming
- Integer linear program
- Linear programming relaxation
- Message passing
- Graph-cut

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$$\max_{b_1,b_2,b_{12}} \begin{bmatrix} b_1(1) \\ b_1(2) \\ b_2(1) \\ b_2(2) \\ b_{12}(1,1) \\ b_{12}(2,1) \\ b_{12}(1,2) \\ b_{12}(2,2) \end{bmatrix}^{\top} \begin{bmatrix} f_1(1) \\ f_1(2) \\ f_2(1) \\ f_2(2) \\ f_{12}(1,1) \\ f_{12}(2,1) \\ f_{12}(2,2) \end{bmatrix}$$

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Integer Linear Program (LP) equivalence: variables $b_r(\mathbf{y}_r)$

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$$b_1$$

$$\begin{bmatrix}
b_1(1) \\
b_1(2) \\
b_2(1) \\
b_2(2) \\
b_{12}(1,1) \\
b_{12}(2,1) \\
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\begin{bmatrix}
f_1(1) \\
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s.t.

A. G. Schwing & M. Telgarsky (Uofl)
$$D_1(1) = \mathbf{y}_1 \\
\mathbf{y}_2 \\
\mathbf{y}_1 \\
\mathbf{y}_2 \\
\mathbf{y}_1 \\
\mathbf{y}_2 \\
\mathbf{y}_2 \\
\mathbf{y}_3 \\
\mathbf{y}_4 \\
\mathbf{y}_7 \\
\mathbf{y}_7$$

$$b_r(y_r) \in \{0, 1\}$$

 $\forall r, \mathbf{y}_r$

$$\mathbf{y}^* = \arg\max_{\hat{\mathbf{y}}} \sum_{r} f_r(\hat{\mathbf{y}}_r)$$







Integer Linear Program (LP) equivalence: variables $b_r(\mathbf{y}_r)$

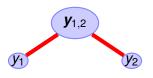
$$\max_{b_1,b_2,b_{12}} \begin{bmatrix} b_1(1) \\ b_1(2) \\ b_2(1) \\ b_2(2) \\ b_{12}(1,1) \\ b_{12}(2,1) \\ b_{12}(1,2) \\ b_{12}(2,2) \end{bmatrix}^{\!\!\top} \! \begin{bmatrix} f_1(1) \\ f_1(2) \\ f_2(1) \\ f_2(2) \\ f_{12}(1,1) \\ f_{12}(2,1) \\ f_{12}(1,2) \\ f_{12}(2,2) \end{bmatrix} \text{ s.t. } \begin{matrix} b_r(\boldsymbol{y}_r) \in \{0,1\} \\ \sum_{\boldsymbol{y}_r} b_r(\boldsymbol{y}_r) = 1 \\ \text{ s.t. } \end{matrix}$$

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 $\forall r, \mathbf{y}_r$

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$$oldsymbol{y}^* = rg \max_{\hat{oldsymbol{y}}} \sum_r f_r(\hat{oldsymbol{y}}_r)$$

Integer linear program:

$$\max_{b_1,b_2,b_{12}} \begin{bmatrix} b_1(1) \\ b_1(2) \\ b_2(1) \\ b_1(2(1,1) \\ b_1(2(2,1) \\ b_1(2(1,2) \\ b_1(2(2,2) \end{bmatrix}^\top \begin{bmatrix} f_1(1) \\ f_1(2) \\ f_2(1) \\ f_2(2) \\ f_{12}(1,1) \\ f_{12}(2,1) \\ f_{12}(1,2) \\ f_{12}(1,2) \\ f_{12}(2,2) \end{bmatrix} \quad \text{s.t.} \quad \sum_{\boldsymbol{y}_r} b_r(\boldsymbol{y}_r) = 1 \quad \forall r \\ \sum_{\boldsymbol{y}_r > \boldsymbol{y}_r > \boldsymbol{$$

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Integer linear program:

$$\begin{aligned} b_r(\boldsymbol{y}_r) &\in \{0,1\} & \forall r, \boldsymbol{y}_r \\ b_r(\boldsymbol{y}_r) &\geq 0 & \forall r, \boldsymbol{y}_r \end{aligned}$$

$$\max_{b_r} \sum_{r,\boldsymbol{y}_r} b_r(\boldsymbol{y}_r) f_r(\boldsymbol{y}_r) \qquad \text{s.t.} \quad \sum_{\boldsymbol{y}_r} b_r(\boldsymbol{y}_r) = 1 & \forall r \\ \sum_{\boldsymbol{y}_r} b_p(\boldsymbol{y}_p) &= b_r(\boldsymbol{y}_r) \end{aligned}$$

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$$b_r(\mathbf{y}_r) \ge 0 \qquad \forall r, \mathbf{y}_r$$

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Marginalization

$$m{y}^* = rg \max_{\hat{m{y}}} \sum_r f_r(\hat{m{y}}_r)$$

Integer linear program:

$$b_r(\mathbf{y}_r) \in \{0,1\} \quad \forall r, \mathbf{y}_r$$

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s.t. Local probability b_r

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$$\text{Marginalization}$$

- Advantage: global optimum, very good solvers available
- Disadvantage: very slow for larger problems

Linear Programming Relaxation

$$m{y}^* = rg \max_{\hat{m{y}}} \sum_r f_r(\hat{m{y}}_r)$$

LP relaxation:

$$b_r(\mathbf{y}_r) \in \{0,1\} \quad \forall r, \mathbf{y}_r$$

$$\max_{b_r} \sum_{r, \mathbf{y}_r} b_r(\mathbf{y}_r) f_r(\mathbf{y}_r)$$

s.t. Local probability b_r

Marginalization

s.t. $b \in C$

Linear Programming Relaxation

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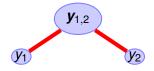
s.t. Local probability b_r

Marginalization

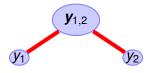
- Advantage: global optimum for LP, very good solvers available
- Disadvantage: no global optimum for ILP, slow for larger problems

Exploit: Graph structure defined via marginalization constraints

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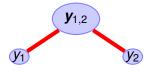


Exploit: Graph structure defined via marginalization constraints



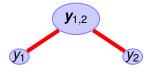
How:

Exploit: Graph structure defined via marginalization constraints



How: Compute the dual function

Exploit: Graph structure defined via marginalization constraints



How: Compute the dual function

Message passing solvers:

• Advantage: Efficient due to analytically computable sub-problems

• Disadvantage: Special care required to find LP relaxation optimum

$$\max_{b} \sum_{r, \mathbf{y}_r} b_r(\mathbf{y}_r) f_r(\mathbf{y}_r) \quad \text{s.t.} \quad \begin{cases} b_r(\mathbf{y}_r) \geq 0 & \forall r, \mathbf{y}_r \\ \sum_{\mathbf{y}_r} b_r(\mathbf{y}_r) = 1 & \forall r \\ \sum_{\mathbf{y}_p \setminus \mathbf{y}_r} b_p(\mathbf{y}_p) = b_r(\mathbf{y}_r) & \forall r, p \in P(r), \mathbf{y}_r \end{cases}$$

$$\max_{b} \sum_{r, \mathbf{y}_r} b_r(\mathbf{y}_r) f_r(\mathbf{y}_r) \quad \text{s.t.} \quad \left\{ \begin{array}{l} b_r(\mathbf{y}_r) \geq 0 & \forall r, \mathbf{y}_r \\ \sum_{\mathbf{y}_r} b_r(\mathbf{y}_r) = 1 & \forall r \\ \sum_{\mathbf{y}_p \setminus \mathbf{y}_r} b_p(\mathbf{y}_p) = b_r(\mathbf{y}_r) & \forall r, p \in P(r), \mathbf{y}_r \end{array} \right.$$

Lagrangian:

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Lagrangian:

$$L() = \sum_{r, \mathbf{y}_r} b_r(\mathbf{y}_r) f_r(\mathbf{y}_r) + \sum_{r, \rho \in P(r), \mathbf{y}_r} \lambda_{r \to \rho}(\mathbf{y}_r) \left(\sum_{\mathbf{y}_\rho \setminus \mathbf{y}_r} b_\rho(\mathbf{y}_\rho) - b_r(\mathbf{y}_r) \right)$$

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$$= \sum_{r,\mathbf{y}_r} b_r(\mathbf{y}_r) \left(f_r(\mathbf{y}_r) - \sum_{\rho \in P(r)} \lambda_{r \to \rho}(\mathbf{y}_r) + \sum_{c \in C(r)} \lambda_{c \to r}(\mathbf{y}_c) \right)$$

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Maximize Lagrangian w.r.t. primal variables subject to remaining constraints:

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Dual function:

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$$g(\lambda) = \sum_{r} \max_{\boldsymbol{y}_{r}} \left(f_{r}(\boldsymbol{y}_{r}) - \sum_{\rho \in P(r)} \lambda_{r \to \rho}(\boldsymbol{y}_{r}) + \sum_{c \in C(r)} \lambda_{c \to r}(\boldsymbol{y}_{c}) \right)$$

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Convex program

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- Lagrange multipliers are messages

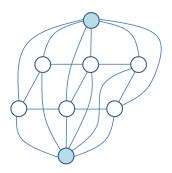
- Convex program
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- Lagrange multipliers are messages

Lagrange multipliers are messages defined on edges of the graph. They shift 'energy' such that local maximization (dual) is identical to global maximization (primal).

 Efficient algorithms to compute the minimum cost cut in a weighted graph

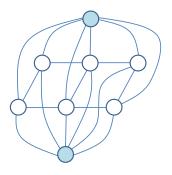
- Efficient algorithms to compute the minimum cost cut in a weighted graph
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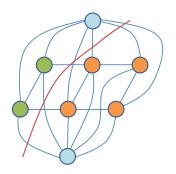
For binary problems $y_d \in \{1, 2\}$:

 Convert scoring function F into auxiliary graph (not the same graph as before!)



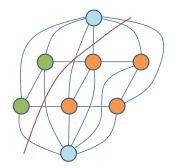
For binary problems $y_d \in \{1,2\}$:

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- Compute a weighted cut cost corresponding to the labeling score



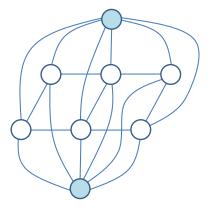
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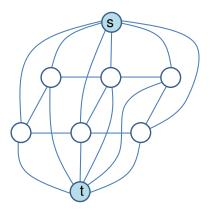


What are the nodes and what are the weights on the edges in this auxiliary graph?

What are the nodes in the auxiliary graph?

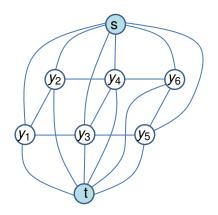


What are the nodes in the auxiliary graph?



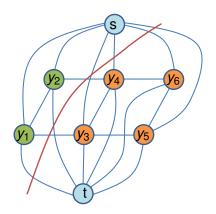
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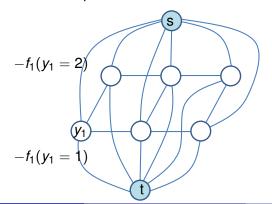
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Recall that local scoring functions are arrays:

$$\begin{bmatrix} f_{12}(1,1) & f_{12}(1,2) \\ f_{12}(2,1) & f_{12}(2,2) \end{bmatrix} = f(1,1) - f(2,1) + f(2,2)$$

$$+ \begin{bmatrix} 0 & 0 \\ f(2,1) - f(1,1) & f(2,1) - f(1,1) \end{bmatrix}$$

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What weights do we assign to edges?

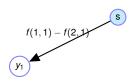
Recall that local scoring functions are arrays:

$$\begin{bmatrix} f_{12}(1,1) & f_{12}(1,2) \\ f_{12}(2,1) & f_{12}(2,2) \end{bmatrix} = f(1,1) - f(2,1) + f(2,2)$$

$$+ \begin{bmatrix} 0 & 0 \\ f(2,1) - f(1,1) & f(2,1) - f(1,1) \end{bmatrix}$$

$$+ \begin{bmatrix} f(2,1) - f(2,2) & 0 \\ f(2,1) - f(2,2) & 0 \end{bmatrix}$$

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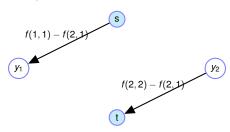
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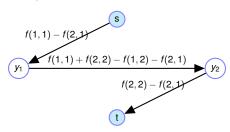
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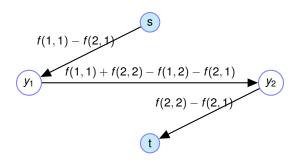
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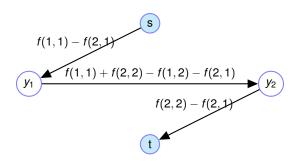
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Graph-cut solvers compute a min-cut:



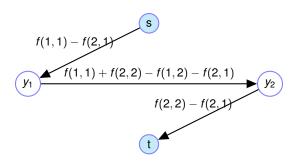


Requirement for optimality:



Requirement for optimality: Pairwise edge weights are positive

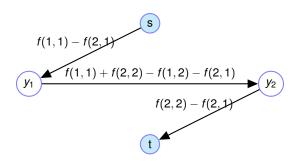
$$f(1,1) + f(2,2) - f(1,2) - f(2,1) \ge 0$$
 sub-modularity



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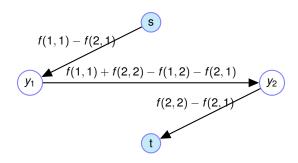
For higher order functions?



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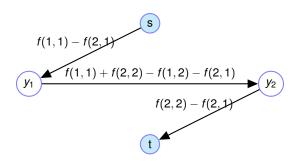
For higher order functions? More complicated graph constructions



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For higher order functions? More complicated graph constructions For more than two labels?



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For higher order functions? More complicated graph constructions For more than two labels? Move making algorithms

Inference:

$$\mathbf{y}^* = \arg\max_{\hat{\mathbf{y}}} \sum_r f_r(\mathbf{w}, x, \hat{\mathbf{y}}_r)$$

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Efficiency and accuracy of inference algorithms is problem dependent:

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- Graph-cut

Quiz:

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 What is the advantage of ILP and LP relaxation compared to dynamic programming and exhaustive search?

Quiz:

- What is the advantage of ILP and LP relaxation compared to dynamic programming and exhaustive search?
- When is a graph-cut algorithm optimal?

Important topics of this lecture

More inference algorithms for structured spaces

Up next:

Learning models for structured output spaces