# Reparameterization: a Universal Tool for Optimization and Counting

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10/05/2017

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# WCSP/MRF

- A set of discrete variables X, each with a domain D
- We define a joint function on all variables  $f: D^{\mathbf{X}} \to S$
- By decomposing the joint function to a set C of functions of small arity (*factors*)
- Concise way of describing complicated functions

#### Function Aggregation – WCSP

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$$S \equiv \mathbb{R}^+ \cup \{0,\infty\}$$

$$f(\mathbf{x}) = \sum_{c \in \mathcal{C}} c(\mathbf{x})$$

- f represents a cost or energy or potential
- Each c is a cost function

### Function Aggregation – MRF

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 $S \equiv \mathbb{R}^+ \cup \{0\}$ 

$$f(\mathbf{x}) = \prod_{c \in \mathcal{C}} c(\mathbf{x})$$

• Each c is a probability table

$$P(\mathbf{x}) = \frac{f(\mathbf{x})}{Z}$$
$$Z = \frac{1}{\sum_{\mathbf{x}'} \prod_{c \in \mathcal{C}} c(\mathbf{x}')}$$

### WCSP/MRF Equivalence

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• Given MRF P, a WCSP P' has

$$c'(\mathbf{x}) = -\log c(\mathbf{x})$$

Then

$$Z = \frac{exp(-f'(\mathbf{x})) \propto P(\mathbf{x})}{\sum_{\mathbf{x}'} \prod_{c \in \mathcal{C}} exp(-c(\mathbf{x}'))}$$

• So we deal with costs only

#### MAP

- Maximum a posteriori estimation
- Compute assignment with maximum probability in MRF
  - By equivalence to WCSP, same problem as cost minimization
- Optimization of an NP-hard set, hence FP<sup>NP</sup>
- Generalizes Boolean satisfiability, constraint satisfaction

#### Partition Function

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- Compute Z, the normalization constant (probability mass of the function)
- *P<sup>PP</sup>*-complete
- By Toda's theorem, this is Beyond PH

# Marginal MAP

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- Partition X into variable sets A, B
- Compute assignment  $\mathbf{x}_A$  that maximizes probability mass of  $f|_{\mathbf{x}_A}$
- $NP^{PP}$

## Aside: WCSP as COP

- WCSP combines crisp CSP with arbitrary polynomial objective
  - Clever dual bounds
- Small arity is not necessary
- Can use the machinery developed in CSP for more expressiveness
  - Higher level language
  - Propagators
    - Global Cost Functions an underexplored area
- New scenarios
  - MAP: What's the most likely to succeed schedule
  - Marginal MAP: What choices can I make that make schedules more likely to succeed

#### Reparameterization

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- Use a naive way to compute a bound
- Local transformation that leaves the problem unchanged
  - but improves naive bound
  - If we touch factors *S*, require

$$\forall \mathbf{x} \sum_{c \in S} c(\mathbf{x}) = \sum_{c \in S} c'(\mathbf{x})$$

Dates back to at least the Held-Karp lower bound for TSP

## WCSP reparameterization

#### $MOVE(c_1, c_2, \mathbf{x}, \alpha)$

- Shifts α units of cost between c<sub>1</sub> and c<sub>2</sub> on the common assignment x
- Shift direction: sign of  $\alpha$ .
- *α* constrained: no negative costs!
- Commonly restricted to scope(c<sub>1</sub>) ⊂ scope(c<sub>2</sub>) and in particular |scope(c<sub>1</sub>)| = 1:

PROJECT( $\{i\}, \{i, j\}, a, \alpha$ )





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 $PROJECT(\{1,2\},\{2\},a,-1)$ 

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 $PROJECT(\{1,2\},\{1\},b,-1)$ 



 $\Downarrow$  Project()({1},  $\emptyset$ , [], 1)

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 $\Downarrow \quad \text{Project}()(\{1\}, \emptyset, [], 1)$ 

 $c_{\varnothing} = 1$ 

#### Lower bounds for cost minimization

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• The sum of the lower bound of each function  $\min_{\mathbf{x}} \sum_{c} c(\mathbf{x}) \leq \sum_{c} \min_{\mathbf{x} \in c} c(\mathbf{x})$ 

## Min Sum Diffusion

- 1 Choose overlapping factors  $c_1, c_2$
- **2** For every **x** in the intersection, choose  $\alpha$  so that  $c_1(\mathbf{x}) = c_2(\mathbf{x})$
- 3 Repeat until convergence
  - Averages factors
  - Will converge as number of iterations goes to infinity, as long as each pair of factors is chosen infinitely often
  - Will converge to arc consistent state

### Block Coordinate Descent

- Min Sum Diffusion is a Block Coordinate Descent algorithm
- Differentiate on subproblem, order of updates
- At best will converge to optimum of linear relaxation
- Perform pruning

#### Branch-and-bound

- 1 Start with root node, corresponding to initial problem
- 2 Pick an open node
- 3 Compute dual bound
  - 1 If the primal bound is violated, *close* node; else
  - 2 Make a binary choice, replace by two new nodes
- Go to step 2

#### Upper bound for Partition Function

• Product of mass of all factors

$$Z = \sum_{\mathbf{x}} \prod_{c} exp(-c(\mathbf{x})) \leq \prod_{c} \sum_{\mathbf{x}} exp(-c(\mathbf{x}))$$

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• Proof: by distributing the product over the sum

# Approximate Z

- Branch and bound
- Ignore subtrees as long as the contribution is small enough
- 1 Start with root node, corresponding to initial problem, U = 0
- 2 Pick an open node
- 3 Compute Z upper bound u
  - **1** If  $u < \varepsilon U$ , *close* node; else
  - 2 If full assignment, add its weight to U; else
  - 3 Make a binary choice, replace by two new nodes
- 4 Go to step 2

# Marginal MAP

- Prune subtree as soon as upper bound for Z(f<sub>xA</sub>) is lower than incumbent
- 1 Start with root node, corresponding to initial problem
- 2 Pick an open node
- **3** Compute  $Z(f|_{\mathbf{x}_A})$  upper bound u
  - **1** If  $u < \varepsilon U$ , *close* node; else
  - If all A variables have been assigned, compute Z(f<sub>xA</sub>), replacing incumbent if needed; else
  - 3 Make a binary choice on variables in *A*, replace by two new nodes
- 4 Go to step 2

## Conclusions

- Reparameterization is a universal tool
  - Maintains cost/probability of all assignments, so always applicable
  - Non-trivial improvement of trivial bounds
- Precise connection to linear programming in cost minimization
- Hierarchies of strengthening reparameterizations which change network
- Linear programming cuts

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