# Searching for Scalable Solutions to really Large Problems: Theory

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# Optimization theory as a modeling tool

- Decoding over noisy channels
- Optimal routing
- Scheduling
- Resource allocation
- Solving Linear Systems
- MAP inference

Can be formulated as a (combinatorial) optimization problem

# **Optimization Theory and Convexity**

"...the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity." R.Tyrrell Rockafellar (SIAM Review, 2003)



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# **Optimization Theory and Distributed Solutions**

# Decomposition framework



 $\begin{array}{ll} \text{minimize} & f_1(x_1) + f_2(x_2) \\ \text{subject to} & x_1 \in \mathcal{C}_1, \quad x_2 \in \mathcal{C}_2 \\ & h_1(x_1) + h_2(x_2) \preceq 0 \end{array}$ 

#### Primal decomposition (resources)

$$\begin{array}{ll} \text{minimize} & f_1(x_1) \\ \text{subject to} & x_1 \in \mathcal{C}_1, \quad h_1(x_1) \preceq t, \\ \\ \text{minimize} & f_2(x_2) \\ \\ \text{subject to} & x_2 \in \mathcal{C}_2, \quad h_2(x_2) \preceq -t. \end{array}$$

#### Dual decomposition (prices)

Given a list of numbers

$$\{u_1, u_2, \ldots, u_N\}$$

find a permutation such that

$$u_{\pi(1)} \le u_{\pi(2)} \le \ldots \le u_{\pi(N)}$$

#### **Optimization problem**

$$f_{\mathbf{u}} \colon \mathcal{S}_N \to \mathbb{R}$$
  
 $\pi \mapsto f_{\mathbf{u}}(\pi)$ 

 $f_{\mathbf{u}}$  reaches the maximum when the permutation sorts the list



Permutation matrices





**Birkhoff-von Neumann Theorem**: The convex hull of the set of permutation matrices is the set of doubly stochastic matrices

Linear program  $f_{\mathbf{u}}(\pi) = 1u_{\pi(1)} + 2u_{\pi(2)} + \dots + Nu_{\pi(N)}$ 

 $\begin{array}{ll} \mbox{maximize} & \sum_{i=1}^{N} i \sum_{j=1}^{N} \mathsf{P}_{ij} u_j \\ \mbox{subject to} & \sum_{j=1}^{N} \mathsf{P}_{ij} = 1, \, i = 1, \dots, N, \\ & \sum_{i=1}^{N} \mathsf{P}_{ij} = 1, \, j = 1, \dots, N, \\ & \mathsf{P}_{ij} \geq 0, \, i, j = 1, \dots, N. \end{array}$ 

All the structure of the permutation is encoded on the constraints

**DUALITY:** Relax the original problem by transfering the constraints to the objective function

#### Dual linear program

$$\begin{array}{ll} \mbox{minimize} & \sum_{i=1}^N r_i + \sum_{j=1}^N c_j \\ \mbox{subject to} & r_i + c_j \geq i u_j \quad i, j = 1, \dots, N. \end{array}$$

#### Auction algorithm

Bidding phase:

Best value 
$$\rightarrow v_{ij^*} = \max_j (iu_j - c_j),$$
  
Second best value  $\rightarrow w_{ij^*} = \max_{j \neq j^*} (iu_j - c_j)$   
Bid  $\rightarrow b_i = p_i + v_{ij^*} - w_{ij^*} + \epsilon$ 

Assignment phase:

$$c_{j} = \max_{i} b_{ij},$$
  
$$i_{j} = \arg\max_{i} b_{ij} \Rightarrow \mathsf{P}_{ij} := \begin{cases} 1, & \text{if } i = i_{j}, \\ 0, & \text{otherwise.} \end{cases}$$



#### Another approach (Permutation as a product of standard transpositions)

maximize  $f_{\mathbf{u}}(\pi) = [1, 2, ..., N] \mathsf{E}_{N/2} \mathsf{O}_{N/2} \cdots \mathsf{E}_1 \mathsf{O}_1 \mathbf{u}$ subject to  $0 \le c_{kl} \le 1, \ k = 1, ..., N/2, \ l = 1, ..., N.$ Convex Relaxation

Gauss-Seidel iteration

$$O_{k}^{(t+1)} = \arg\min_{O}[1, 2, \dots, N] \underbrace{\mathsf{E}_{N/2}^{(t)} \mathsf{O}_{N/2}^{(t)} \cdots \mathsf{E}_{k+1}^{(t)} \mathsf{O}_{k+1}^{(t)} \mathsf{E}_{k}^{(t)}}_{(t)} O \underbrace{\mathsf{E}_{k-1}^{(t+1)} \mathsf{O}_{k-1}^{(t+1)} \cdots \mathsf{E}_{1}^{(t+1)} \mathsf{O}_{1}^{(t+1)}}_{(t+1)} \mathbf{u}}_{(t+1)}$$

$$\mathsf{E}_{k}^{(t+1)} = \arg\min_{\mathsf{E}}[1, 2, \dots, N] \underbrace{\mathsf{E}_{N/2}^{(t)} \mathsf{O}_{N/2}^{(t)} \cdots \mathsf{E}_{k+1}^{(t)} \mathsf{O}_{k+1}^{(t)}}_{(t)} \mathsf{E} \underbrace{\mathsf{O}_{k}^{(t+1)} \mathsf{E}_{k-1}^{(t+1)} \mathsf{O}_{k-1}^{(t+1)} \cdots \mathsf{E}_{1}^{(t+1)} \mathsf{O}_{1}^{(t+1)}}_{(t+1)} \mathbf{u}}_{(t+1)}$$

Another approach (Permutation as a product of standard transpositions)

maximize subject to

$$f_{\mathbf{u}}(\pi) = [1, 2, \dots, N] \mathsf{E}_{N/2} \mathsf{O}_{N/2} \cdots \mathsf{E}_1 \mathsf{O}_1 \mathbf{u}$$
$$0 \le c_{kl} \le 1, \ k = 1, \dots, N/2, \ l = 1, \dots, N.$$
Convex Relaxation



$$c_{ijk} = \begin{cases} 1 & \text{if symbol in cell } (i,j) \text{ is } s_k, \\ 0 & \text{otherwise.} \end{cases}$$
Blank Sudoku

2			4		9		7	5
						8	2	
	8		1		5	9		3
9	2	7		4		6		8
8		3		9		5	4	1
5		2	3		6		8	
	9	8						
6	4		9		8			2

$$\begin{array}{ll} \text{cells:} & \sum_{k=1}^{n} x_{ijk} = 1, & \text{for all } i, j = 1, \dots, n. \\ \text{rows:} & \sum_{j=1}^{n} x_{ijk} = 1, & \text{for all } i, k = 1, \dots, n. \\ \text{cols:} & \sum_{i=1}^{n} x_{ijk} = 1, & \text{for all } j, k = 1, \dots, n. \\ \text{blocks:} & \sum_{i=(I-1)m+1}^{Im} \sum_{j=(J-1)m+1}^{Jm} x_{ijk} = 1, & \text{for all } I, J = 1, \dots, m \\ & k = 1, \dots, n. \end{array}$$

$$x_{11k} = \delta_{2k}, \ x_{14k} = \delta_{4k}, \ x_{16k} = \delta_{9k}, \dots$$

# Formulation I:

#### Givens:

$$\begin{aligned} x_{pqr} &= 0, \quad \text{if any of these} \begin{cases} p = i, q = j, r \neq k \quad (\text{cell}), \\ p \neq i, q = j, r = k \quad (\text{row}), \\ p = i, q \neq j, r = k \quad (\text{column}), \\ \lfloor p/m \rfloor &= \lfloor i/m \rfloor, \lfloor q/m \rfloor = \lfloor j/m \rfloor, r = k \quad (\text{block}), \end{cases} \end{aligned}$$

$$x_{pqr} = 1$$
, if  $p = i, q = j, r = k$ .



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 $\begin{array}{ll} \mbox{minimize} & f(\mathbf{x}) \equiv 0 \\ \mbox{subject to} & \mathbf{x} \in \mathcal{B} \cap \mathcal{G}, \\ & \mathbf{x} \in \{0,1\}^{n^2}. \end{array}$ 

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$$x_{pqr} = 1$$
, if  $p = i, q = j, r = k$ 



# Formulation 2:



$$f_G(\mathbf{x}) \equiv \sum_{i,j,k=1}^n c_{ijk} x_{ijk}$$

 $c_{ijk} = \begin{cases} -1 & \text{if there is a given } k \text{ in cell } (i,j), \\ 1 & \text{if there is a given } \neq k \text{ at } (i,j) \text{ or } = k \text{ at } (i,\neq j) \text{ or at } (\neq i,j), \\ 0 & \text{otherwise} \end{cases}$ 

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# Algorithms:

# GLPK (GNU Linear Programming Kit) http://www.gnu.org/software/glpk/

I. Simplex (several flavours)

2. Interior point (primal-dual)

#### Transformations:



#### Sudoku as a Lattice Gas

# Multicomponent non-additive hard-core lattice gas

2			4		9		7	5
						8	2	
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8		3		9		5	4	1
5		2	3		6		8	
	9	8						
6	4		9		8			2

#### Sudoku as a Lattice Gas

#### Free-energy density Functional Theory

 $\mathcal{F}[\rho_{ijk}] = \sum \left\{ \phi(\text{ROW}_{ik}) + \phi(\text{COL}_{jk}) + \phi(\text{BLOCK}_{IJ}) + \phi(\text{POINT}_{ij}) - \phi(\text{row}_{ik:IJ}) - \phi(\text{col}_{jk:IJ}) - \phi(\text{point}_{ijk}) \right\}$ 

$$\phi(\eta) = \eta \ln \eta + (1 - \eta) \ln(1 - \eta)$$

#### Euler-Lagrange Eqs.:

$$\rho_{ijk}(1-\rho_{ijk})\left(1-\sum_{l:B(i,j)}\rho_{ilk}\right)\left(1-\sum_{l:B(i,j)}\rho_{ljk}\right) = z_{ijk}\left(1-\sum_{l}\rho_{ijl}\right)\left(1-\sum_{l}\rho_{ilk}\right) \times \left(1-\sum_{l}\rho_{ljk}\right)\left(1-\sum_{l,m:B(i,j)}\rho_{lmk}\right)$$

#### Sudoku as a Quadratic Program

# maximize $\|\mathbf{x}\|_2^2$ subject to $\mathbf{x} \in \mathcal{B} \cap \mathcal{G}$ $\mathbf{x} \geq \mathbf{0}$

Non-convex problem! NP-hard if the quadratic term matrix is definite negative

# Some Final Comments

- LP vs. Semidefinite Relaxations.
- Distributed Solvers.

- Optimization methods as a tool to derive local Message Passing algortihms.
- Connections with BP-like algorithms