# 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)

## Lagrange Duality

## Convex Relaxations

$$
\begin{aligned}
& \begin{array}{ll}
\stackrel{\mathbf{c}}{\mathbf{C}} \underset{\mathbf{x}}{\operatorname{minimize}} & f_{0}(\mathbf{x}) \\
\text { subject to } & f_{i}(\mathbf{x}) \leq 0 \\
& h_{i}(\mathbf{x})=0 \\
\hline \mathbf{0} & 1 \leq i \leq m \\
L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu})=f_{0}(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} f_{i}(\mathbf{x})+\sum_{i=1}^{p} \nu_{i} h_{i}(\mathbf{x})
\end{array} \\
& \underset{\boldsymbol{\lambda}, \boldsymbol{\nu}}{\operatorname{maximize}} g(\boldsymbol{\lambda}, \boldsymbol{\nu})=\inf _{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \\
& \text { subject to } \lambda \geq 0
\end{aligned}
$$

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## Lagrange Duality

## Convex Relaxations

| $\underset{\mathbf{c}}{\mathbf{E}} \underset{\mathbf{x}}{\operatorname{minimize}}$ | $f_{0}(\mathbf{x})$ |
| :--- | :--- |
| subject to | $f_{i}(\mathbf{x}) \leq 0$ |
|  | $h_{i}(\mathbf{x})=0 \quad 1 \leq i \leq m$ |
|  |  |

$L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu})=f_{0}(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} f_{i}(\mathbf{x})+\sum_{i=1}^{p} \nu_{i} h_{i}(\mathbf{x})$
Dual

$$
\begin{array}{ll}
\underset{\boldsymbol{\lambda}, \boldsymbol{\nu}}{\operatorname{maximize}} & g(\boldsymbol{\lambda}, \boldsymbol{\nu})=\inf _{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \\
\text { subject to } & \boldsymbol{\lambda} \geq \mathbf{0}
\end{array}
$$



## Optimization Theory and Convexity

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## Lagrange Duality

## Convex Relaxations


$L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu})=f_{0}(\mathbf{x})+\sum_{i=1}^{m} \lambda_{i} f_{i}(\mathbf{x})+\sum_{i=1}^{p} \nu_{i} h_{i}(\mathbf{x})$

$$
\begin{array}{ll}
\underset{\boldsymbol{\lambda}, \boldsymbol{\nu}}{\operatorname{maximize}} & g(\boldsymbol{\lambda}, \boldsymbol{\nu})=\inf _{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \\
\text { subject to } & \boldsymbol{\lambda} \geq \mathbf{0}
\end{array}
$$



## Optimization Theory and Distributed Solutions

## Decomposition framework



$$
\begin{array}{ll}
\operatorname{minimize} & f_{1}\left(x_{1}\right)+f_{2}\left(x_{2}\right) \\
\text { subject to } & x_{1} \in \mathcal{C}_{1}, \quad x_{2} \in \mathcal{C}_{2} \\
& h_{1}\left(x_{1}\right)+h_{2}\left(x_{2}\right) \preceq 0
\end{array}
$$

Primal decomposition (resources)

```
minimize }\mp@subsup{f}{1}{}(\mp@subsup{x}{1}{}
subject to }\mp@subsup{x}{1}{}\in\mp@subsup{\mathcal{C}}{1}{},\quad\mp@subsup{h}{1}{}(\mp@subsup{x}{1}{})\preceqt
minimize }\mp@subsup{f}{2}{}(\mp@subsup{x}{2}{}
subject to }\mp@subsup{x}{2}{}\in\mp@subsup{\mathcal{C}}{2}{},\quad\mp@subsup{h}{2}{}(\mp@subsup{x}{2}{})\preceq-t
```

Dual decomposition (prices)

```
minimize }\mp@subsup{f}{1}{}(\mp@subsup{x}{1}{})+\mp@subsup{\lambda}{}{T}\mp@subsup{h}{1}{}(\mp@subsup{x}{1}{}
subject to }\mp@subsup{x}{1}{}\in\mp@subsup{\mathcal{C}}{1}{}\mathrm{ ,
minimize }\mp@subsup{f}{2}{}(\mp@subsup{x}{2}{})+\mp@subsup{\lambda}{}{T}\mp@subsup{h}{2}{}(\mp@subsup{x}{2}{}
subject to }\mp@subsup{x}{2}{}\in\mp@subsup{\mathcal{C}}{2}{}\mathrm{ .
```


## Sorting as a Mathematical Program

Given a list of numbers

$$
\left\{u_{1}, u_{2}, \ldots, u_{N}\right\}
$$

find a permutation such that

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

## Optimization problem

$$
\begin{aligned}
f_{\mathbf{u}}: \mathcal{S}_{N} & \rightarrow \mathbb{R} \\
\pi & \mapsto f_{\mathbf{u}}(\pi)
\end{aligned}
$$

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

Sorting as a Mathematical Program


Permutation matrices

$$
\begin{gathered}
\sum_{i=1}^{N} \mathrm{P}_{i j}=\sum_{j=1}^{N} \mathrm{P}_{i j}=1 \\
\mathrm{P}_{i j} \in\{0,1\}
\end{gathered}
$$

$\mathcal{S}_{3}$
-


## Sorting as a Mathematical Program



Permutation matrices

$$
\begin{gathered}
\sum_{i=1}^{N} \mathrm{P}_{i j}=\sum_{j=1}^{N} \mathrm{P}_{i j}=1 \\
\mathrm{P}_{i j} \geq 0
\end{gathered}
$$

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

## Sorting as a Mathematical Program

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

$$
\begin{array}{rc}
\text { maximize } & \sum_{i=1}^{N} i \sum_{j=1}^{N} \mathrm{P}_{i j} u_{j} \\
\text { subject to } & \sum_{j=1}^{N} \mathrm{P}_{i j}=1, i=1, \ldots, N, \\
& \sum_{i=1}^{N} \mathrm{P}_{i j}=1, j=1, \ldots, N, \\
& \mathrm{P}_{i j} \geq 0, i, j=1, \ldots, N .
\end{array}
$$

All the structure of the permutation is encoded on the constraints

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

## Sorting as a Mathematical Program

## Dual linear program

$$
\begin{array}{rc}
\text { minimize } & \sum_{i=1}^{N} r_{i}+\sum_{j=1}^{N} c_{j} \\
\text { subject to } & r_{i}+c_{j} \geq i u_{j} \quad i, j=1, \ldots, N .
\end{array}
$$

## Auction algorithm

Bidding phase:

$$
\begin{gathered}
\text { Best value } \rightarrow v_{i j^{*}}=\max _{j}\left(i u_{j}-c_{j}\right), \\
\text { Second best value } \rightarrow w_{i j^{*}}=\max _{j \neq j^{*}}\left(i u_{j}-c_{j}\right), \\
\text { Bid } \rightarrow b_{i}=p_{i}+v_{i j^{*}}-w_{i j^{*}}+\epsilon
\end{gathered}
$$

Assignment phase:

$$
c_{j}=\max _{i} b_{i j}
$$

$$
i_{j}=\arg \max _{i} b_{i j} \Rightarrow \mathrm{P}_{i j}:= \begin{cases}1, & \text { if } i=i_{j} \\ 0, & \text { otherwise }\end{cases}
$$



## Sorting as a Mathematical Program

## Another approach

(Permutation as a product of standard transpositions)
maximize

$$
f_{\mathbf{u}}(\pi)=[1,2, \ldots, N] \mathrm{E}_{N / 2} \mathrm{O}_{N / 2} \cdots \mathrm{E}_{1} \mathrm{O}_{1} \mathbf{u}
$$

subject to

$$
0 \leq c_{k l} \leq 1, k=1, \ldots, N / 2, l=1, \ldots, N .
$$

Convex Relaxation
Gauss-Seidel iteration

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

$\mathrm{E}_{k}^{(t+1)}=\arg \min _{\mathrm{E}}[1,2, \ldots, N] \underbrace{\mathrm{E}_{N / 2}^{(t)} \mathrm{O}_{N / 2}^{(t)} \cdots \mathrm{E}_{k+1}^{(t)} \mathrm{O}_{k+1}^{(t)}}_{(t)} \mathrm{E}_{\substack{(t+1) \\ \mathrm{E}_{k-1}^{(t+1)} \mathrm{O}_{k-1}^{(t+1)} \cdots \mathrm{E}_{1}^{(t+1)} \mathrm{O}_{1}^{(t+1)}}}^{u}$

## Sorting as a Mathematical Program

## Another approach

(Permutation as a product of standard transpositions)


Convex Relaxation


## Sudoku as a Linear Program

$x_{i j k}=\left\{\begin{array}{ll}1 & \text { if symbol in cell }(i, j) \text { is } s_{k}, \\ 0 & \text { otherwise. }\end{array} \quad\right.$ Blank Sudoku
cells: $\quad \sum_{k=1}^{n} x_{i j k}=1, \quad$ for all $i, j=1, \ldots, n$.

| 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 |

rows: $\quad \sum_{j=1}^{n} x_{i j k}=1, \quad$ for all $i, k=1, \ldots, n$.
cols: $\quad \sum_{i=1}^{n} x_{i j k}=1, \quad$ for all $j, k=1, \ldots, n$.
blocks: $\sum_{i=(I-1) m+1}^{I m} \sum_{j=(J-1) m+1}^{J m} x_{i j k}=1, \quad$ for all $I, J=1, \ldots, m$
$k=1, \ldots, n$.
$x_{11 k}=\delta_{2 k}, x_{14 k}=\delta_{4 k}, x_{16 k}=\delta_{9 k}, \ldots$

## Sudoku as a Linear Program

## Formulation I:

## Givens:

$$
\begin{aligned}
& x_{p q r}=0, \quad \text { if any of these } \begin{cases}p=i, q=j, r \neq k & \text { (cell), } \\
p \neq i, q=j, r=k \quad \text { (row), } \\
p=i, q \neq j, r=k \quad \text { (column), } \\
\lfloor p / m\rfloor=\lfloor i / m\rfloor,\lfloor q / m\rfloor=\lfloor j / m\rfloor, r=k \quad \text { (block), }\end{cases} \\
& x_{p q r}=1, \quad \text { if } p=i, q=j, r=k .
\end{aligned}
$$

| find | $\mathbf{x}$ |
| ---: | :---: |
| subject to | $\mathbf{x} \in \mathcal{B} \cap \mathcal{G}$, |
|  | $\mathbf{x} \in\{0,1\}^{n^{2}}$, |

## Sudoku as a Linear Program

## Formulation I:

## Givens:

$$
\begin{aligned}
& x_{p q r}=0, \quad \text { if any of these } \begin{cases}p=i, q=j, r \neq k & \text { (cell), } \\
p \neq i, q=j, r=k \quad \text { (row), } \\
p=i, q \neq j, r=k \quad \text { (column), } \\
\lfloor p / m\rfloor=\lfloor i / m\rfloor,\lfloor q / m\rfloor=\lfloor j / m\rfloor, r=k \quad \text { (block), }\end{cases} \\
& x_{p q r}=1, \quad \text { if } p=i, q=j, r=k .
\end{aligned}
$$

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

## Sudoku as a Linear Program

## Formulation I:

## Givens:

$$
\begin{aligned}
& x_{p q r}=0, \quad \text { if any of these }\left\{\begin{array}{l}
p=i, q=j, r \neq k \quad \text { (cell), } \\
p \neq i, q=j, r=k \quad \text { (row), } \\
p=i, q \neq j, r=k \quad \text { (column), } \\
\lfloor p / m\rfloor=\lfloor i / m\rfloor,\lfloor q / m\rfloor=\lfloor j / m\rfloor, r=k \quad \text { (block), }
\end{array}\right. \\
& x_{p q r}=1, \quad \text { if } p=i, q=j, r=k .
\end{aligned}
$$

$$
\begin{array}{cc}
\text { minimize } & f(\mathbf{x}) \equiv 0 \\
\text { subject to } & \mathbf{x} \in \mathcal{B} \cap \mathcal{G}, \\
& 0 \leq \mathbf{x},
\end{array}
$$

## Sudoku as a Linear Program

## Formulation 2:

$$
\begin{array}{cc}
\text { minimize } & f_{G}(\mathbf{x}) \\
\text { subject to } & \mathbf{x} \in \mathcal{B}, \\
& \mathbf{x} \in\{0,1\}^{n^{2}} .
\end{array}
$$

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

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

## Sudoku as a Linear Program

## Formulation 2:

$$
\begin{aligned}
& \text { minimize } \quad f_{G}(\mathbf{x}) \\
& \text { subject to } \quad \mathbf{x} \in \mathcal{B} \text {, } \\
& 0 \leq \mathbf{x} \text {, } \\
& f_{G}(\mathbf{x}) \equiv \sum_{i, j, k=1}^{n} c_{i j k} x_{i j k} \\
& c_{i j k}= \begin{cases}-1 & \text { if there is a given } k \text { in cell }(i, j), \\
1 & \text { if there is a given } \neq k \text { at }(i, j) \text { or }=k \text { at }(i, \neq j) \text { or at }(\neq i, j), \\
0 & \text { otherwise }\end{cases}
\end{aligned}
$$

## Sudoku as a Linear Program

## Algorithms:

## GLPK (GNU Linear Programming Kit)

## http://www.gnu.org/software/glpk/

I. Simplex (several flavours)
2. Interior point (primal-dual)

Transformations:

| minimize | $f(\mathrm{x})$ |
| ---: | :---: | :---: |
| subject to | $\mathrm{Ax}=\mathrm{b}$ |
|  | $\mathrm{x} \geq 0$ |$\quad \square$| minimize | $f(\mathrm{x})$ |
| ---: | :--- |
|  |  |
|  |  |
| subject to | $\mathrm{APx}=\mathrm{b}$ |
| $\mathrm{x} \geq \mathbf{0}$ |  |

## Sudoku as a Lattice Gas

## Multicomponent non-additive hard-core lattice gas

| 2 |  |  | 4 |  | 9 |  | 7 | 5 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  |  |  |  | 8 | 2 |  |
| 9 | 2 | 7 |  | 4 |  | 6 |  | 8 |
| 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

$$
\begin{gathered}
\mathcal{F}\left[\rho_{i j k}\right]=\sum\left\{\phi\left(\mathrm{ROW}_{i k}\right)+\phi\left(\mathrm{COL}_{j k}\right)+\phi\left(\mathrm{BLOCK}_{I J}\right)+\phi\left(\mathrm{POINT}_{i j}\right)\right. \\
\left.-\phi\left(\mathrm{row}_{i k: I J}\right)-\phi\left(\mathrm{col}_{j k: I J}\right)-\phi\left(\mathrm{point}_{i j k}\right)\right\} \\
\phi(\eta)=\eta \ln \eta+(1-\eta) \ln (1-\eta)
\end{gathered}
$$

## Euler-Lagrange Eqs.:

$$
\begin{array}{r}
\rho_{i j k}\left(1-\rho_{i j k}\right)\left(1-\sum_{l: B(i, j)} \rho_{i l k}\right)\left(1-\sum_{l: B(i, j)} \rho_{l j k}\right)=z_{i j k}\left(1-\sum_{l} \rho_{i j l}\right)\left(1-\sum_{l} \rho_{i l k}\right) \\
\times\left(1-\sum_{l} \rho_{l j k}\right)\left(1-\sum_{l, m: B(i, j)} \rho_{l m k}\right)
\end{array}
$$

## Sudoku as a Quadratic Program

$$
\begin{array}{cc}
\text { maximize } & \|\mathbf{x}\|_{2}^{2} \\
\text { subject to } & \mathbf{x} \in \mathcal{B} \cap \mathcal{G} \\
& \mathbf{x} \geq \mathbf{0}
\end{array}
$$

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

