



Optically solving

the Distance Geometry Problem*

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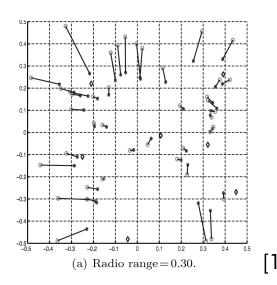
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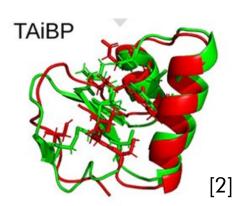
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Motivation

Sensor network localization



Molecular conformation



Distance Geometry Problem



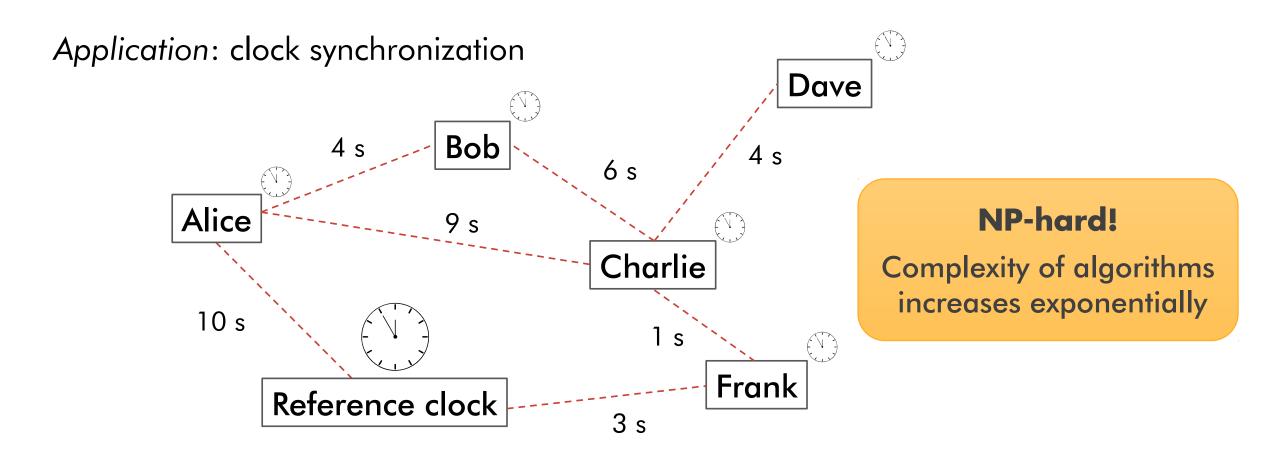
- [1] Biswas et al., ACM Trans. Sens. Netw. 2 (2006)
- [2] Malliavin et al., J. Chem. Inf. Model. 59 (2019)

New computing platforms



Which problem?

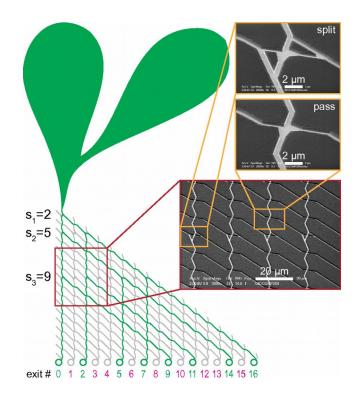
<u>Distance Geometry Problem in dimension 1</u>



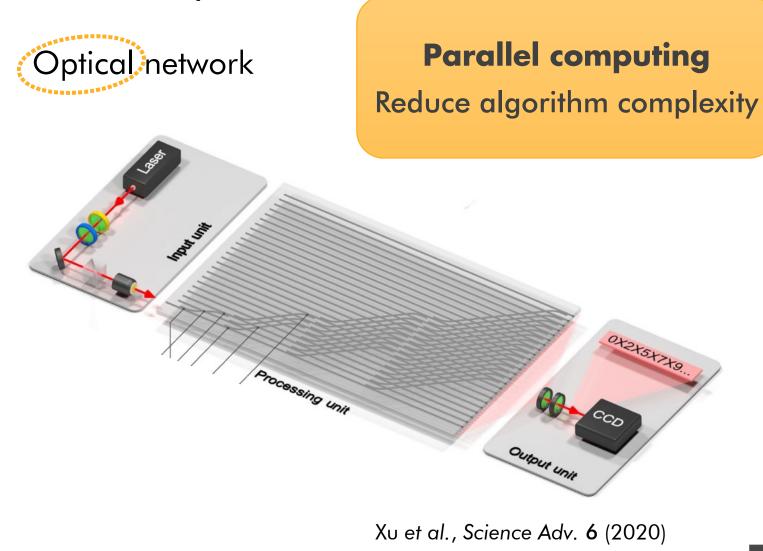
Which platform?

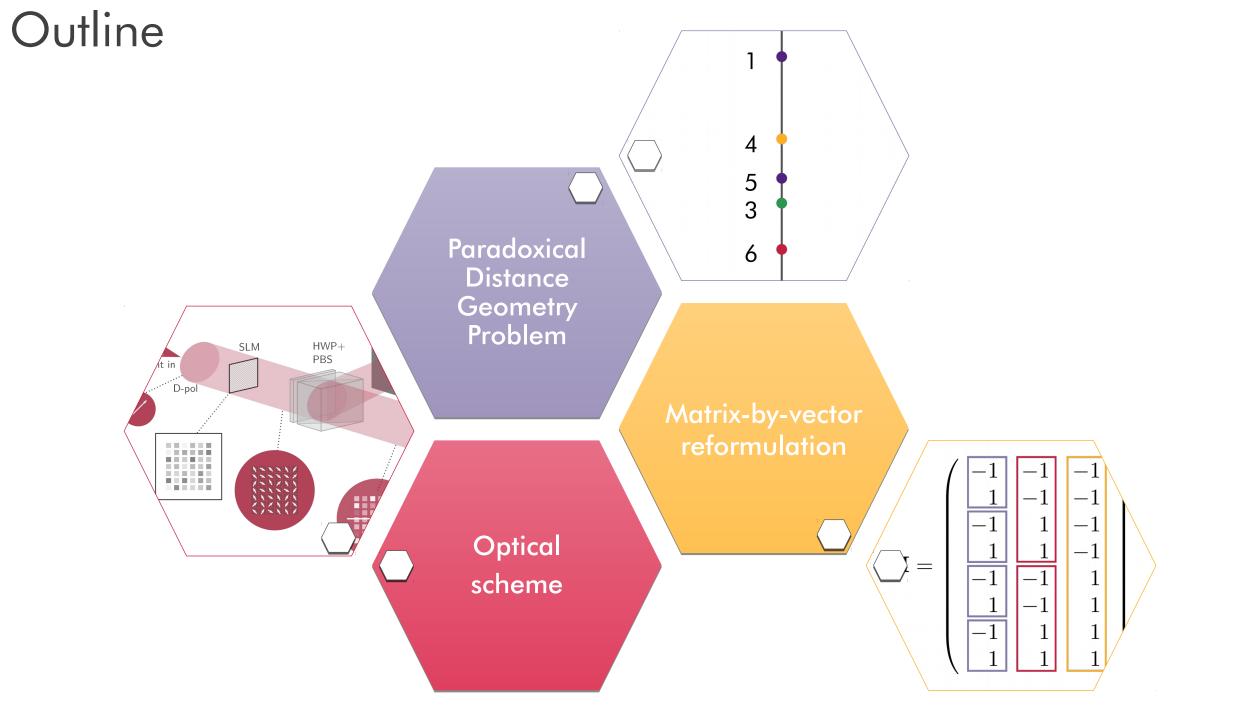
Solving Subset-Sum Problem in different platforms

Molecular network



Nicolau Jr. et al., PNAS 113 (2016)





Paradoxical DGP

Distance Geometry Problem

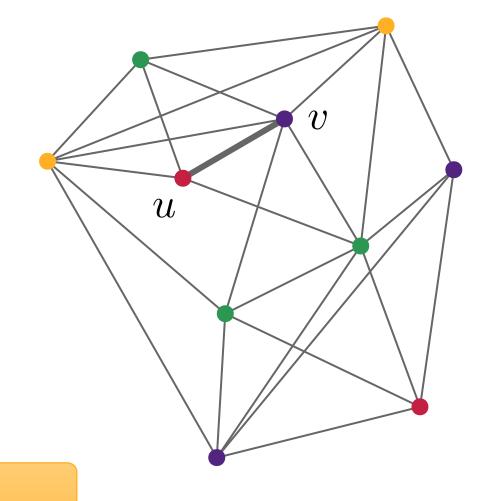
Graph
$$G = (V, E, d)$$

Vertices V

Edges E

Distances d *

* Weight $d(u,v) \in \mathbb{R}_+$ when $\{u,v\} \in E$



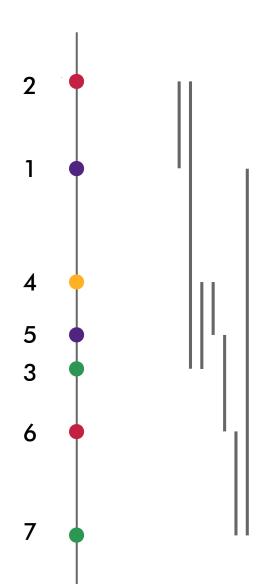
NP-hard!

Paradoxical DGP,

DGP₁: distance geometry problem in dimension 1

Definition of paradoxical DGP₁

- i. Vertex order exists: for every vertex (different from the first), the edge k $\{k-1,k\}$ belongs to E;
- ii. No other edge is in E except $\{1, n\}$ (distance from first to last vertex in the order, n = |V|).



Paradoxical DGP₁

DGP₁: distance geometry problem in dimension 1

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- → Presence of d(1, n) → only two solutions are possible;
- → d(1, n) involves the very first and the very last vertex → information can be exploited **only** in the last moment.

BuildUp algorithms

Construct possible DGP solutions:

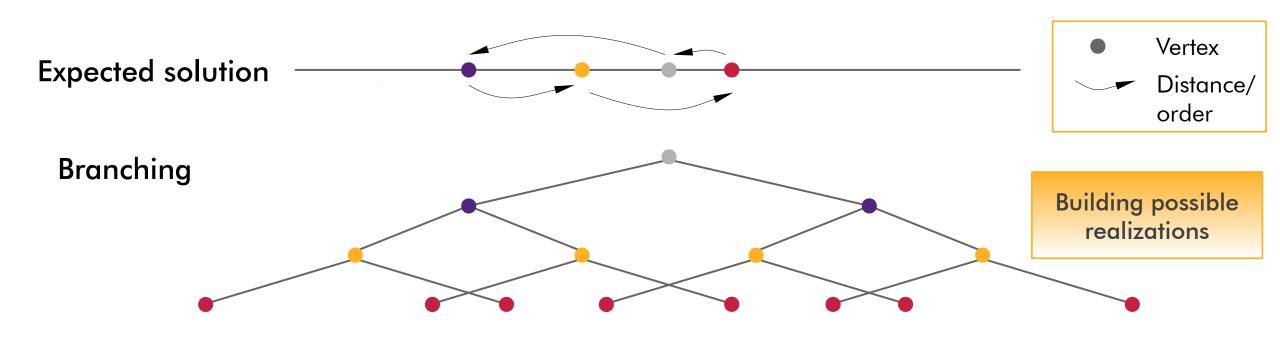
- i. One vertex position at a time;
- ii. Predefined vertex order.

→ can be used to generate a search tree (multiple realizations)

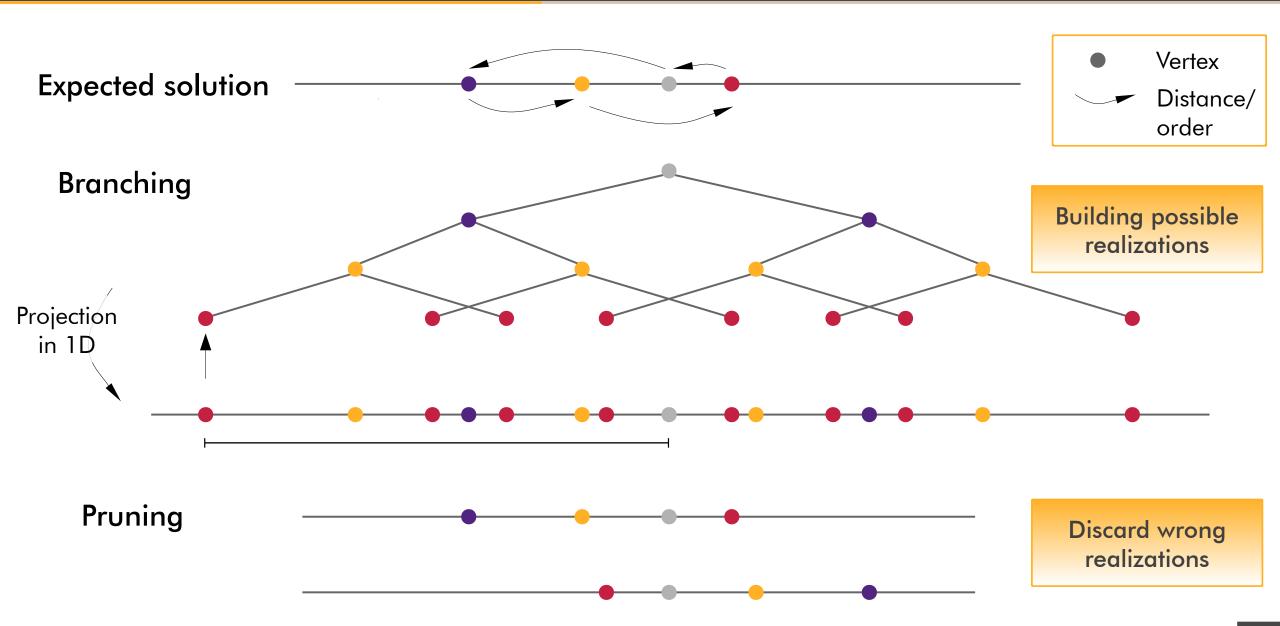
For paradoxical DGP₁

- *# of potential realizations keeps exponentially growing until reaching the last vertex;
- → at most two realizations are feasible (correspond to all distances)

Branch-and-Prune I



Branch-and-Prune I



Branch-and-Prune II

For a paradoxical DGP, instance:

- i. Initialize position of vertex 1: $x_1 = 0$
- ii. Possible positions for all subsequent vertices:

$$x_k = x_{k-1} + s_k d_{k-1,k}, \quad \forall k = 2, \dots, n,$$

 $d_{k-1,k} = d(k-1,d); \quad s_k = -1 \text{ or } s_k = +1$

- iii. Branching: computing 2p positions for the vertex k (p is the number of available positions for the preceding vertex).
- iv. Pruning: at the last layer n, $d_{1,n}$ is used to select only two solutions of the tree.

HERE: uniformize branching/pruning by including a "virtual" vertex n+1, for which $d_{n,n+1}=d_{1,n}$

 \rightarrow feasibility of a solution: $x_1 = x_{n+1}$

Matrix-by-vector reformulation

Basic idea

$$x_k = x_{k-1} + s_k d_{k-1,k}, \quad \forall k = 2, \dots, n,$$

 $s_k = -1 \text{ or } s_k = +1, \text{ and } x_1 = 0$

- \rightarrow A solution is represented by a boolean n-vector (s_k) : $(-1,+1,+1,\ldots,-1,-1)$
- ullet ... when multiplied by a vector containing the distances: $\mathbf{y}=(d_{12},d_{23},\ldots,d_{n-1,n},d_{1n})^T$
 - \rightarrow position of vertex n+1 (check feasibility)

$$x_{k+1} = (-1, +1, \dots, -1, -1) \begin{bmatrix} d_{12} \\ d_{23} \\ \vdots \\ d_{n-1,n} \\ d_{1n} \end{bmatrix} = -d_{12} + d_{23} + \dots - d_{n-1,n} - d_{1n}$$

Binary matrix

- \rightarrow Take all possible realizations at once \rightarrow binary matrix \mathbf{M} :
 - 2^n rows potential realizations with fictive vertex

 $x_1 = 0$

- *n* columns *n* vertices
- ightharpoonup Only one vertex in G: $\mathbf{M} = \begin{pmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \end{pmatrix}$, $\mathbf{y} = (d_{11}) \Rightarrow \mathbf{r} = \begin{pmatrix} -d_{11} \\ d_{11} \end{pmatrix}$.

Two vertices in
$$G$$
: $\mathbf{M} = \begin{pmatrix} \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix} \end{pmatrix}$, $\mathbf{y} = \begin{pmatrix} d_{12} \\ d_{12} \end{pmatrix}$ $\Rightarrow \mathbf{r} = \begin{pmatrix} -d_{12} - d_{12} \\ d_{12} - d_{12} \\ -d_{12} + d_{12} \\ +d_{12} + d_{12} \end{pmatrix}$.

Pattern length: 2^j

Binary matrix

- \rightarrow Take all possible realizations at once \rightarrow binary matrix M:
 - 2^n rows potential realizations with fictive vertex
 - *n* columns *n* vertices

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 Only one vertex in G : $\mathbf{M} = \begin{pmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \end{pmatrix}$, $\mathbf{y} = (d_{11}) \Rightarrow \mathbf{r} = \begin{pmatrix} -d_{11} \\ d_{11} \end{pmatrix}$.

$$\mathbf{M} = \begin{bmatrix} -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

Pattern length: 2^{j}

Matrix-by-vector multiplication reformulation

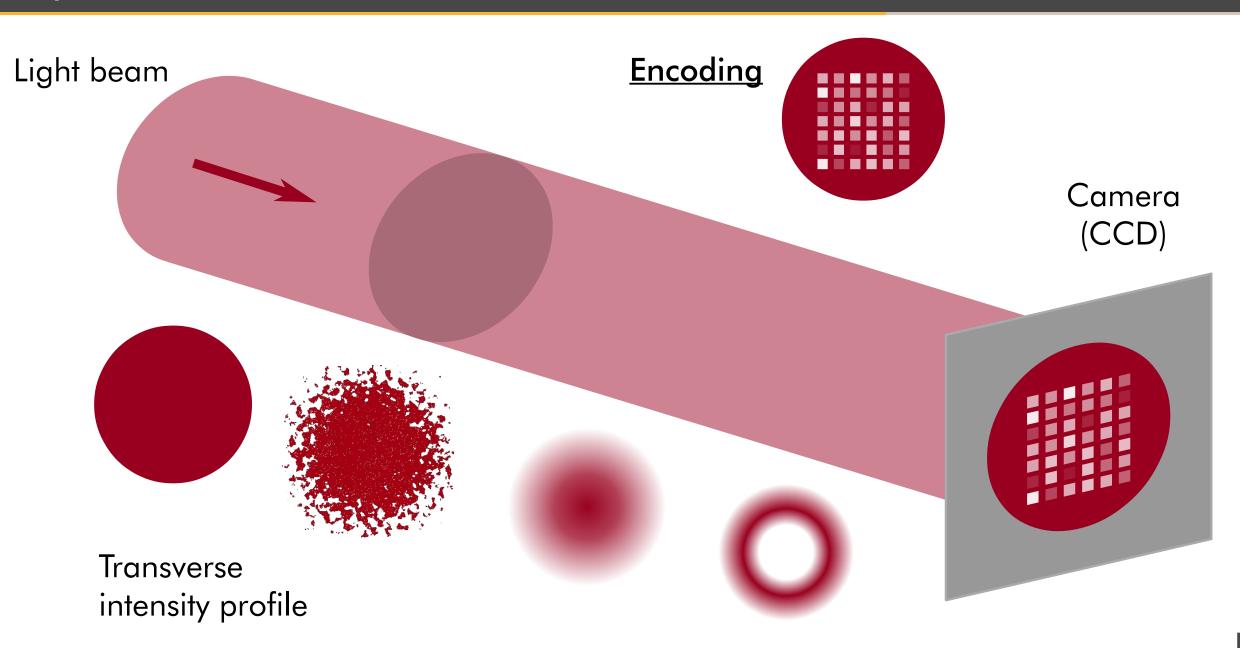
$$oldsymbol{ iny}$$
 Realizations vector: $\mathbf{r} = \mathbf{M} imes \mathbf{y}$

$$ightharpoonup$$
 Binary matrix: $\mathbf{M}_{ij} = \left\{ egin{array}{ll} -1 & ext{if } (i-1)2^{1-j} \mod 2 = 0, \\ 1 & ext{otherwise.} \end{array} \right.$

Feasible solutions: null components of r

Optical scheme

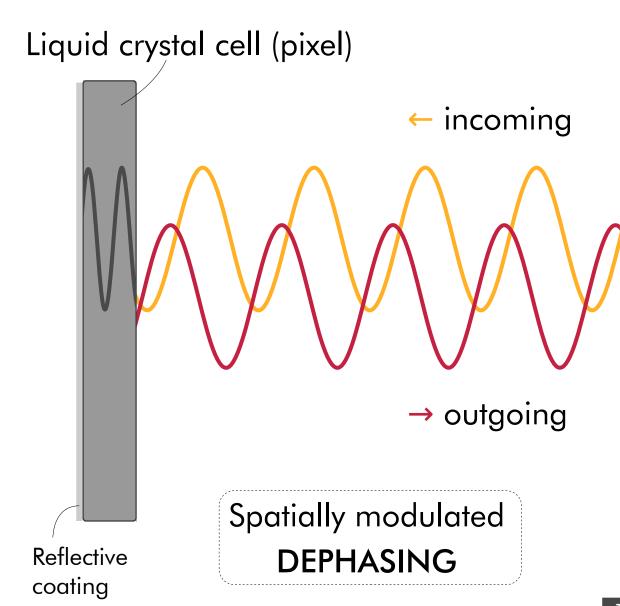
Optical matrices?



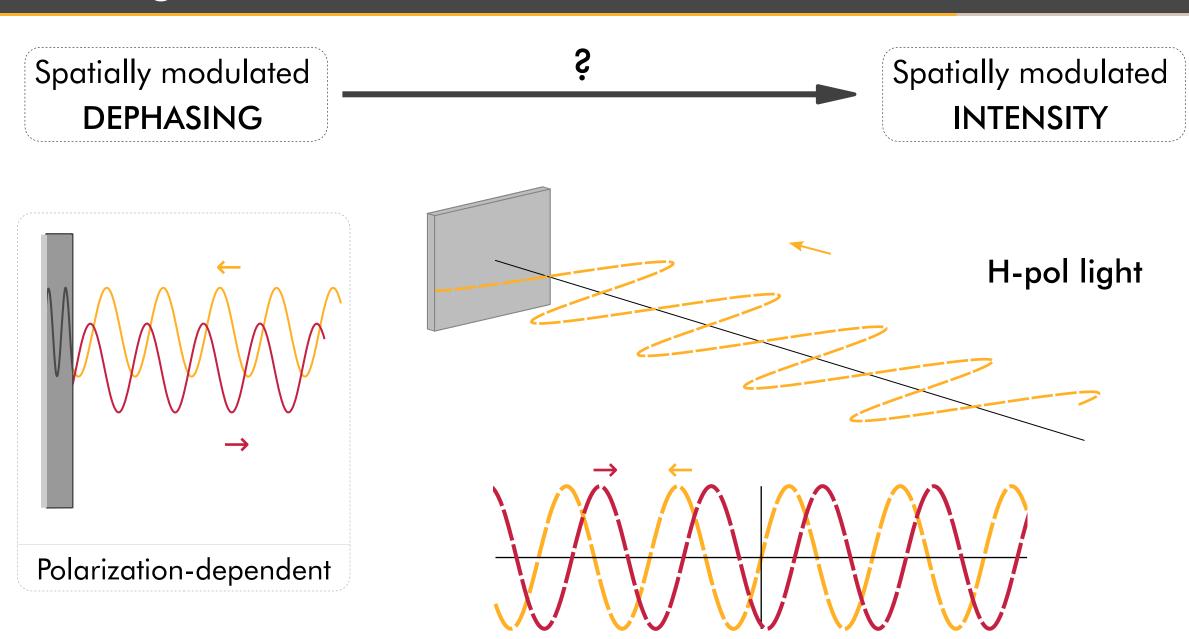
Encoding scheme I

SLM = spatial light modulator

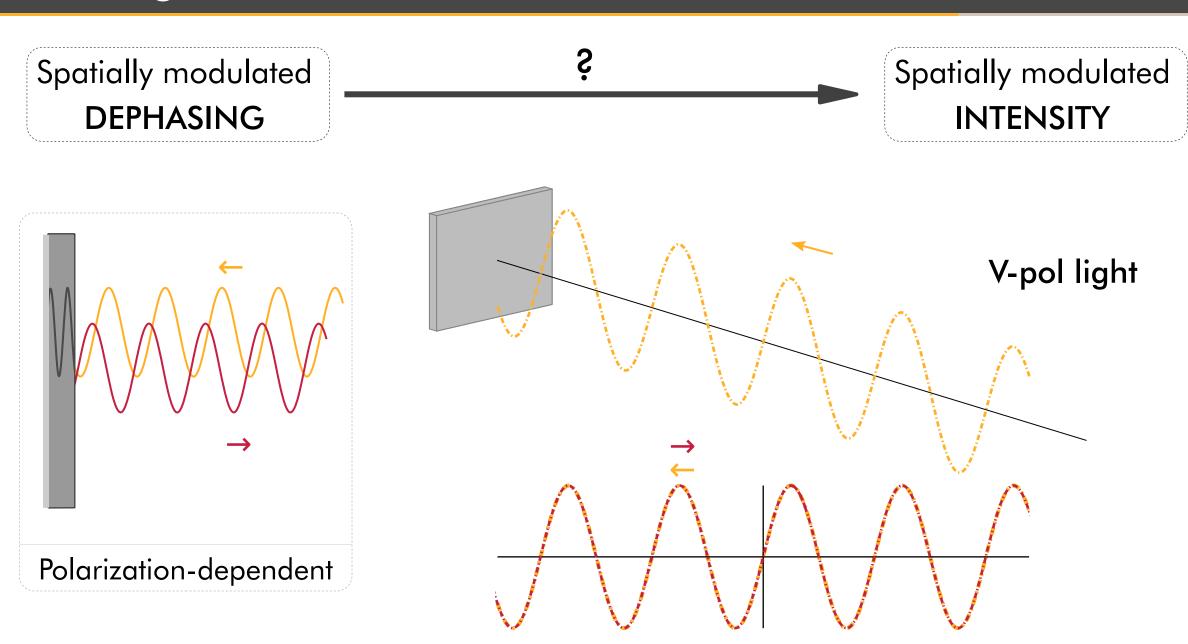




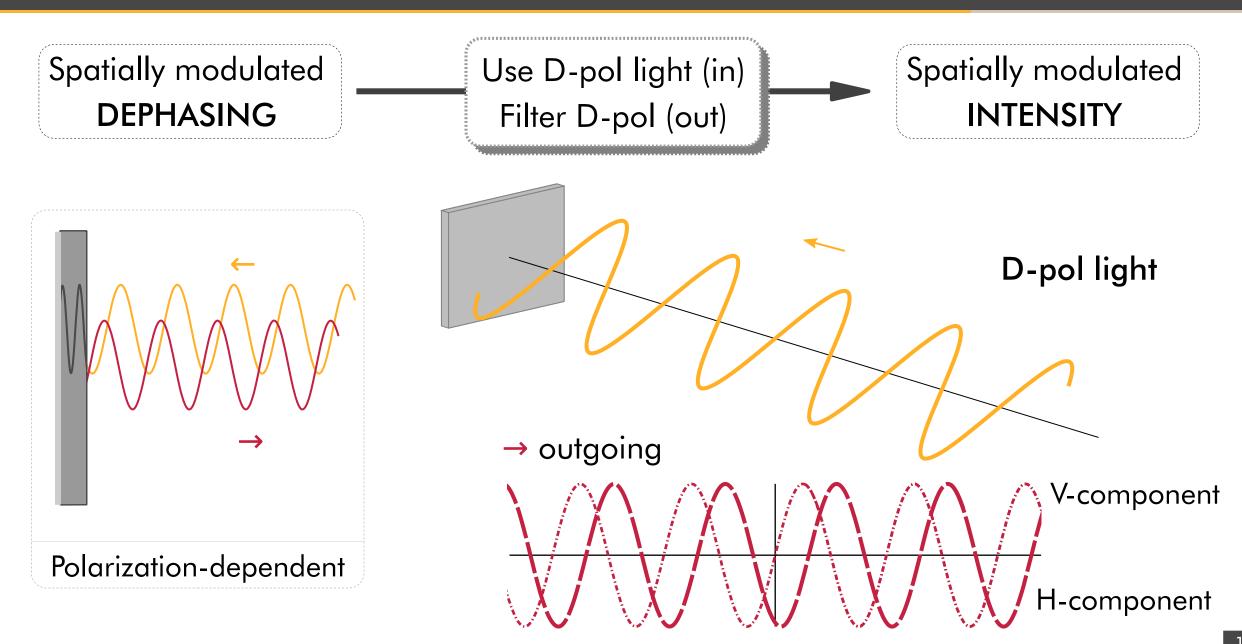
Encoding scheme II



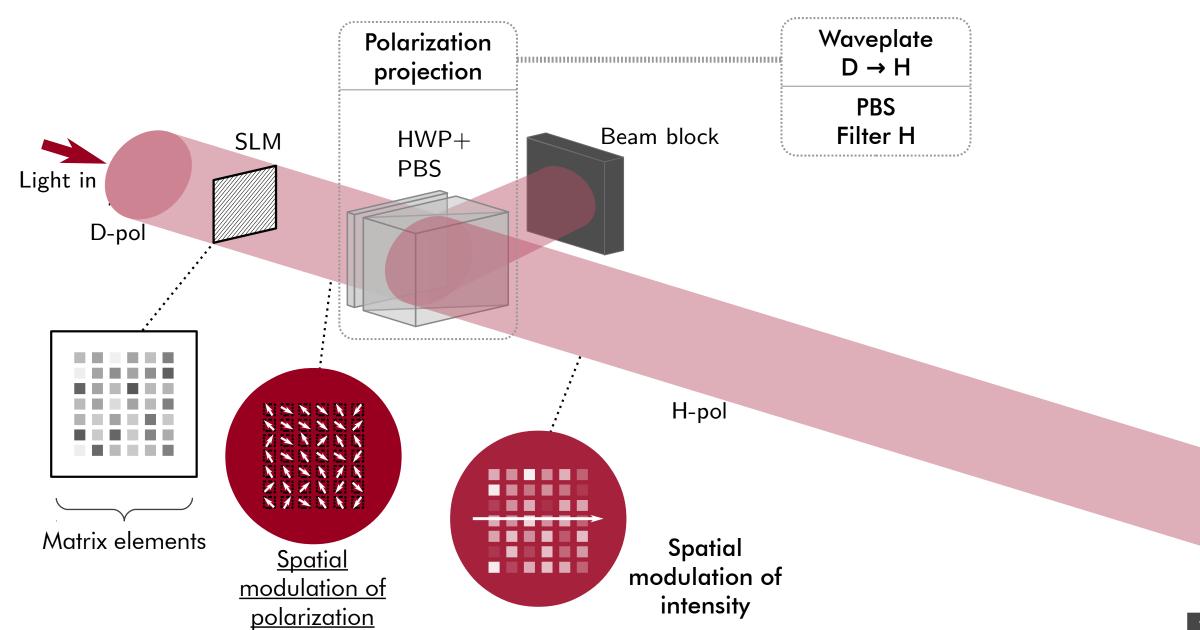
Encoding scheme II



Encoding scheme II

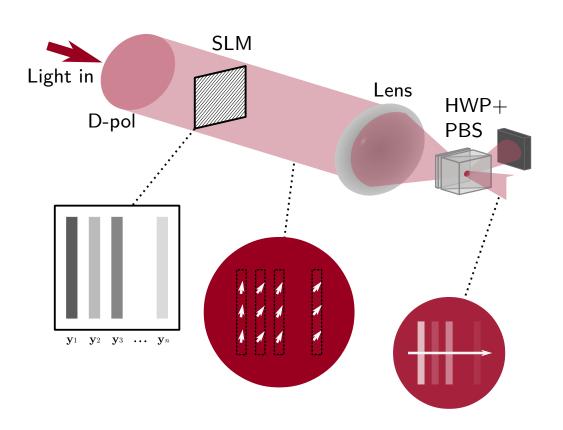


Preparing vectors and matrices



Processing

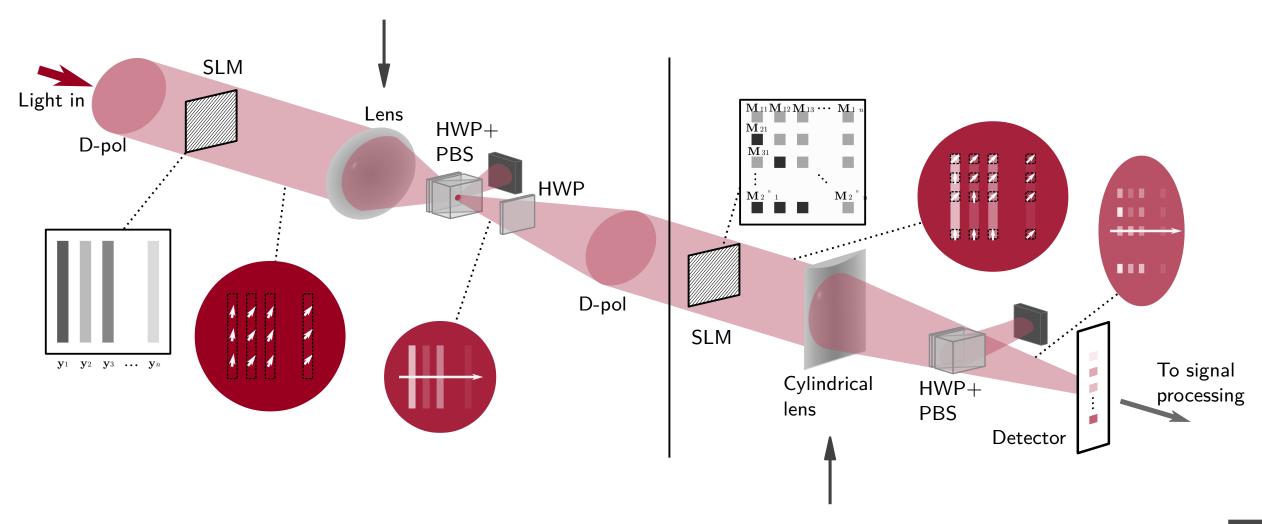
Input vector preparation



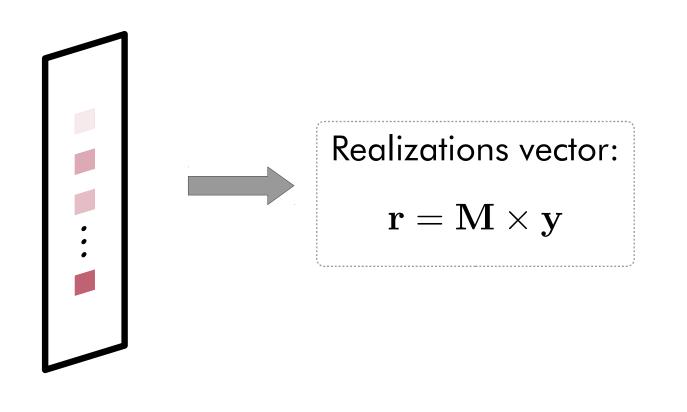
Processing

Input vector preparation

Matrix-by-vector multiplication



Output signal



Feasible solutions

- → presence of pixel with a reference intensity value
- corresponding to $x_1 = 0$

Detected signal

Discussion and Outlook

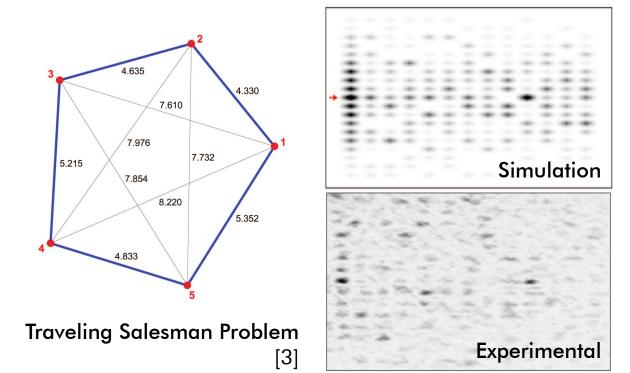
<u>Performance</u>

- A figure of merit MAC-operations/s
 - **Here**: 0.1 TOPS
 - Photonic chip: 2 TOPS [1]
 - CPU: 2.6 TOPS [2]
- Possible limitations
 - Noise level
 - Refreshing rate of SLM
 - SLM resolution

NP-hard!

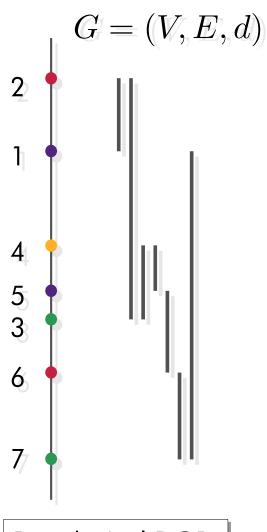
- Speeding up
 - Larger / faster SLM
 - Many SLMs in parallel
 - Alternative modulation scheme

Other optical schemes

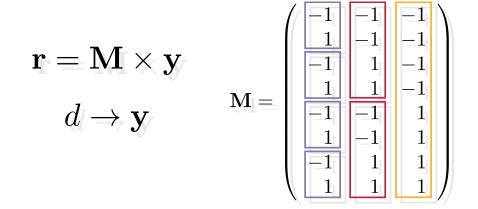


- [1] Feldmann et al., Nature **589** (2021)
- [2] Jouppi et al., Proc. ISCA '17 (2017)
- [3] Shaked et al., Appl. Optics 46 (2007)

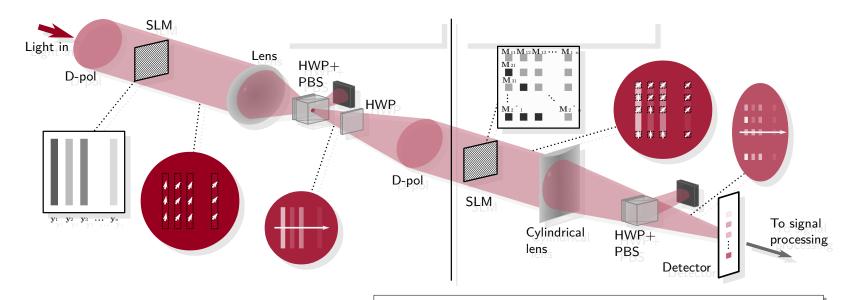
Summary







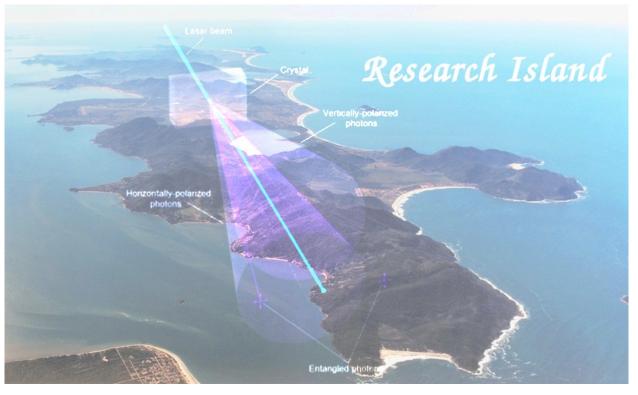
Matrix-by-vector reformulation allows for...



...Optical computing of matrix-byvector multiplication

Acknowledgements





Thank you for your attention!







Pesquisa e Inovação do



