

An optical processor for matrix-by-vector multiplication: an application to the distance geometry problem in 1D

NARA RUBIANO
DA SILVA



CENTRO SOCIAL DA CERVEZA, FLORIANOPOLIS

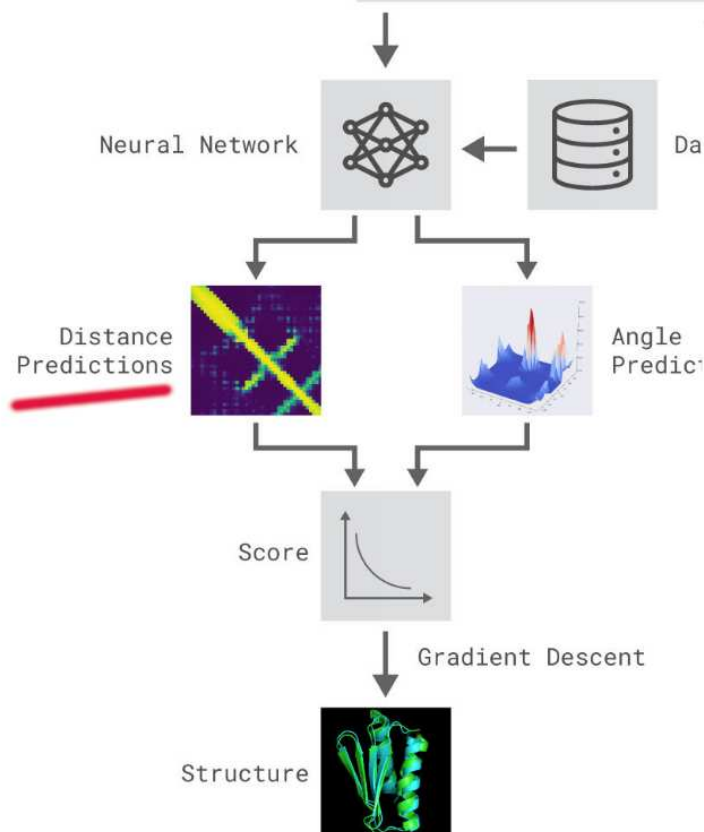


DOUGLAS GONÇALVES

PAULO H.S. RIBEIRO



DOUGLAS ANTONIO RAPHAEL PAULO & WIFE MARIA & BOYFRIEND



Accelerated Article Preview

Highly accurate protein structure prediction with AlphaFold

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John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A. A. Kohl, Andrew J. Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishub Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zielinski, Martin Steinegger, Michalina Pacholska, Tamas Berghammer, Sebastian Bodenstern, David Silver, Oriol Vinyals, Andrew W. Senior, Koray Kavukcuoglu, Pushmeet Kohli & Demis Hassabis

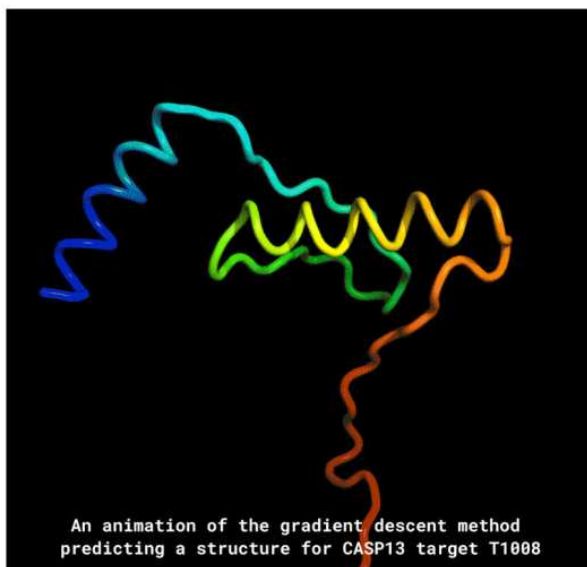
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RESEARCH ARTICLE

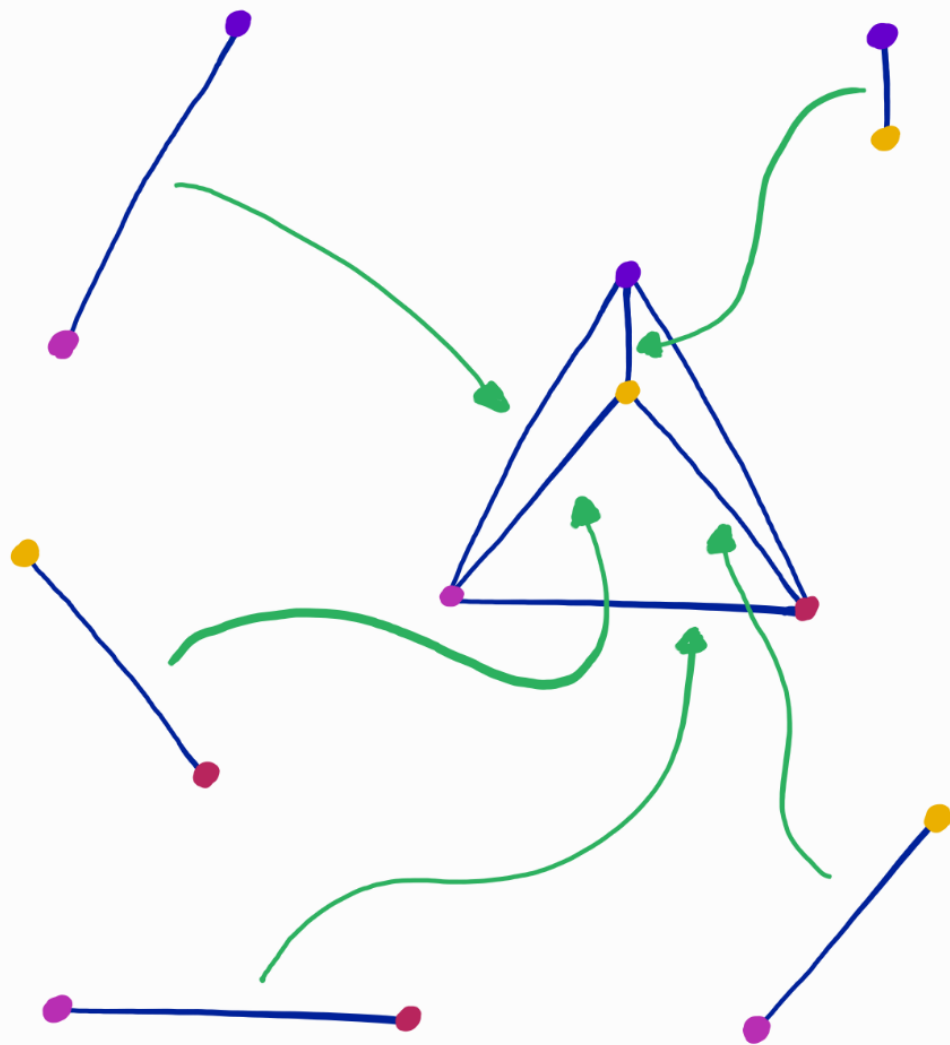
PROTEIN FOLDING

Accurate prediction of protein structures and interactions using a three-track neural network

Minkyung Baek^{1,2}, Frank DiMaio^{1,2}, Ivan Anishchenko^{1,2}, Justas Dauparas^{1,2}, Sergey Ovchinnikov^{3,4}, Gyu Rie Lee^{1,2}, Jue Wang^{1,2}, Qian Cong^{5,6}, Lisa N. Kinch⁷, R. Dustin Schaeffer⁶, Claudia Millán⁸, Hahnbeom Park^{1,2}, Carson Adams^{1,2}, Caleb R. Glassman^{9,10,11}, Andy DeGiovanni¹², Jose H. Pereira¹², Andria V. Rodrigues¹², Alberdina A. van Dijk¹³, Ana C. Ebrecht¹³, Diederik J. Opperman¹⁴, Theo Sagmeister¹⁵, Christoph Buhllheller^{15,16}, Tea Pavkov-Keller^{15,17}, Manoj K. Rathinaswamy¹⁸, Udit Dalwadi¹⁹, Calvin K. Yip¹⁹, John E. Burke¹⁸, K. Christopher Garcia^{9,10,11,20}, Nick V. Grishin^{6,7,21}



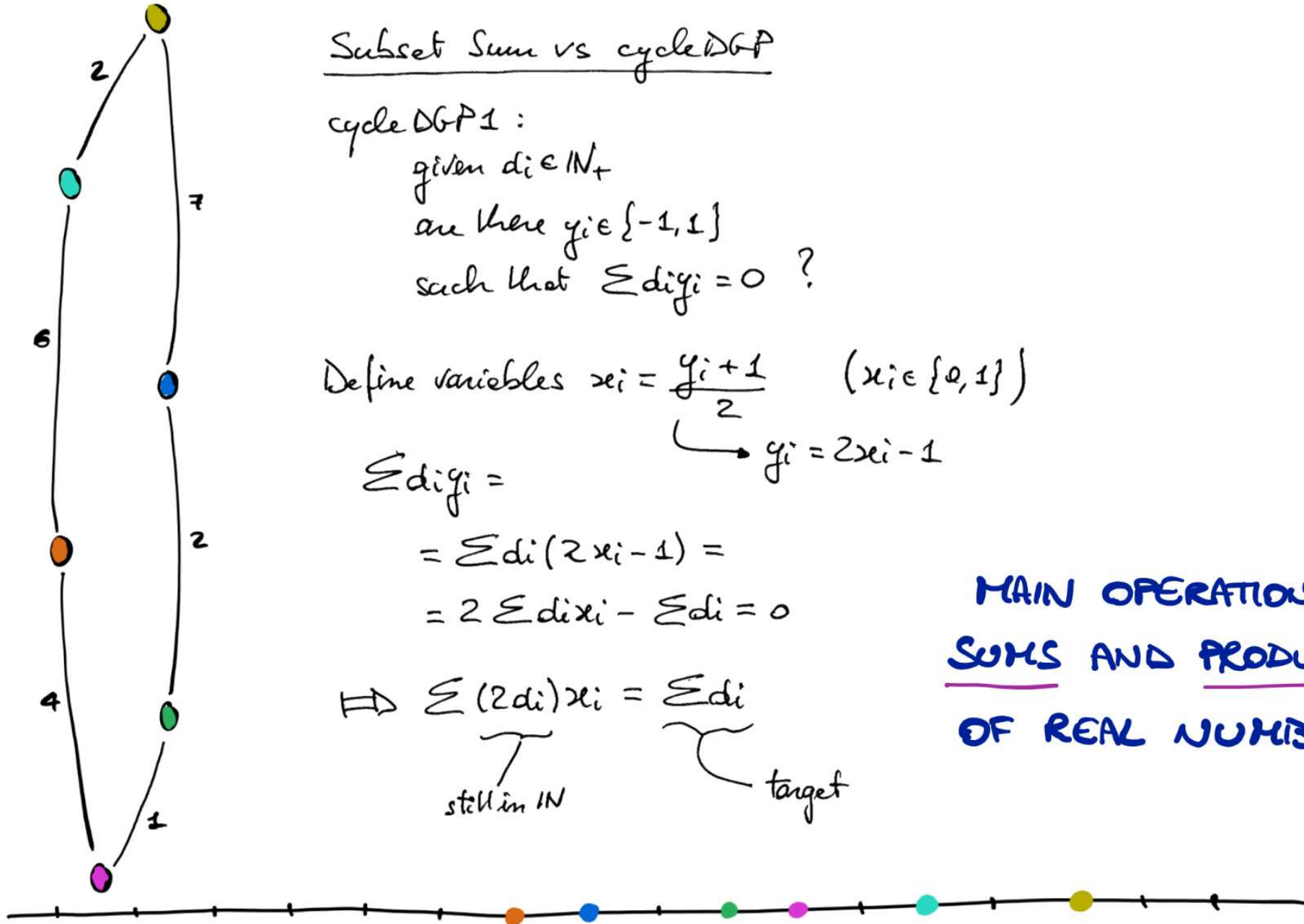
DISTANCE GEOMETRY



GIVEN A CERTAIN NUMBER OF STICKS WITH LABELED VERTICES, CONSTRUCT A GEOMETRICAL FIGURE WHERE EVERY VERTEX IS PLACED IN A UNIQUE POSITION.

THIS PROBLEM IS NP-HARD

A SPECIAL CLASS OF INSTANCES IN 1D



Subset Sum vs cycle DP

cycle DP 1:

given $d_i \in \mathbb{N}_+$

are there $y_i \in \{-1, 1\}$

such that $\sum d_i y_i = 0$?

Define variables $x_i = \frac{y_i + 1}{2}$ ($x_i \in \{0, 1\}$)

$$\hookrightarrow y_i = 2x_i - 1$$

$$\sum d_i y_i =$$

$$= \sum d_i (2x_i - 1) =$$

$$= 2 \sum d_i x_i - \sum d_i = 0$$

$$\Rightarrow \sum (2d_i) x_i = \sum d_i$$

$\underbrace{\hspace{1cm}}$
still in \mathbb{N}

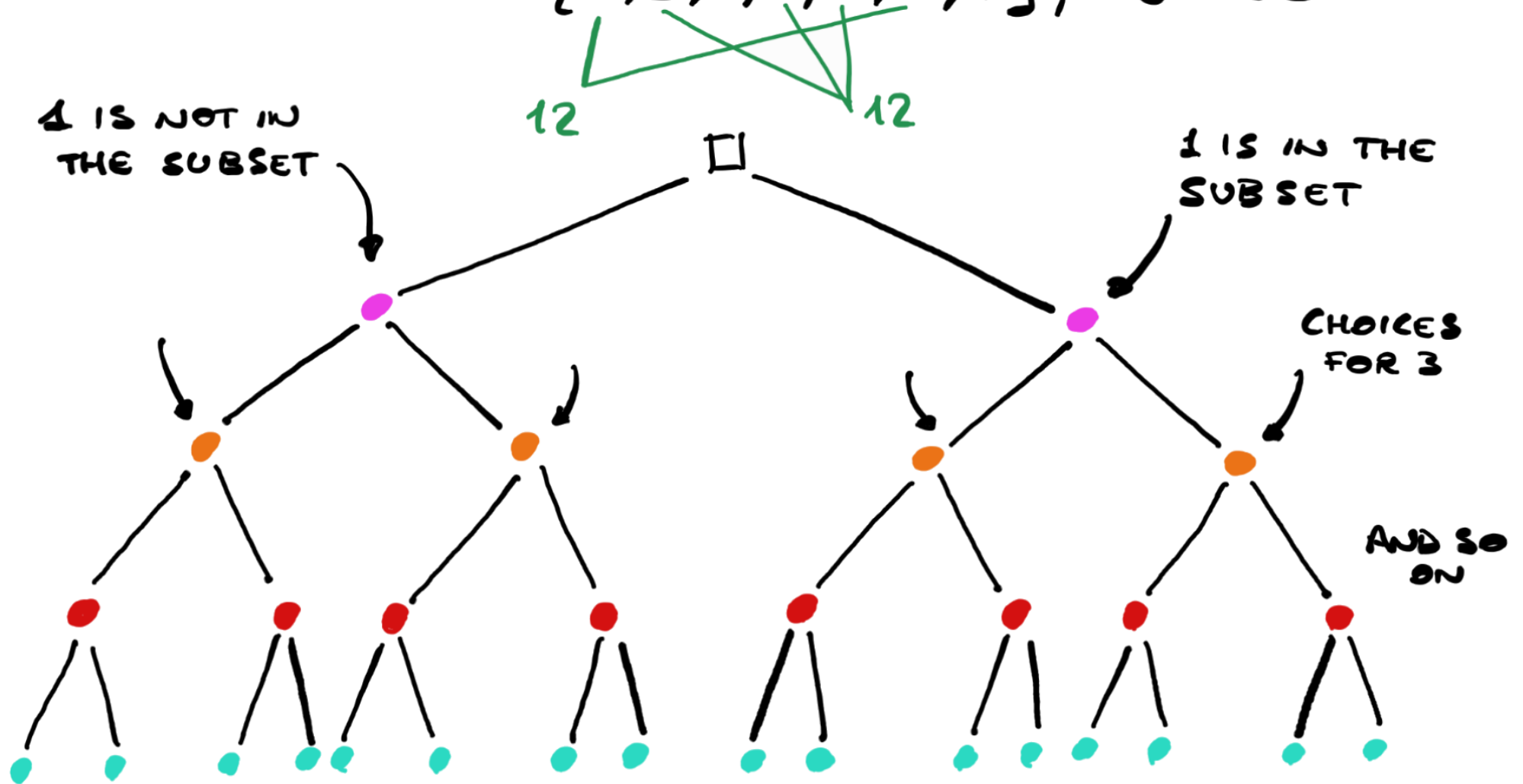
$\underbrace{\hspace{1cm}}$
target

MAIN OPERATIONS:
SUMS AND PRODUCTS
OF REAL NUMBERS

SUBSET SUM

IS THERE ANY SUBSET OF S WHOSE ELEMENTS SUM UP TO t ?

$$S = \{1, 3, 5, 7, 2, 11, 4\}; \quad t = 12$$



SUBSET SUM

EVEN IF IT HAS EXPONENTIAL WORST-CASE COMPLEXITY,
IT IS POSSIBLE TO DESIGN AD-HOC EFFICIENT IMPLEMENTATIONS

Optimization Strategy 1 – Reduce Memory Access

```
void SSP_simplebp_rec(  
    int i,  
    long partial,  
    long total,  
    uint64_t selected,  
    const SSP* ssp,  
    SSP_Solutions* result  
)
```

int i	edi
long partial	rsi
long total	rdx
uint64_t selected	rcx
const SSP* ssp	r8
SSP_Solutions* result	r9



SUBSET SUM

EVEN IF IT HAS EXPONENTIAL WORST-CASE COMPLEXITY,
IT IS POSSIBLE TO DESIGN AD-HOC EFFICIENT IMPLEMENTATIONS

SimpleBP in Assembly

Introduction Code Analysis **Optimization** Conclusion

Optimization Strategy 1 – Reduce Memory Access

```
void SSP_simplebp_rec(
    int i,
    long partial,
    long total,
    uint64_t selected,
    const SSP* ssp,
    SSP_Solutions* result
)
```

SimpleBP in Assembly

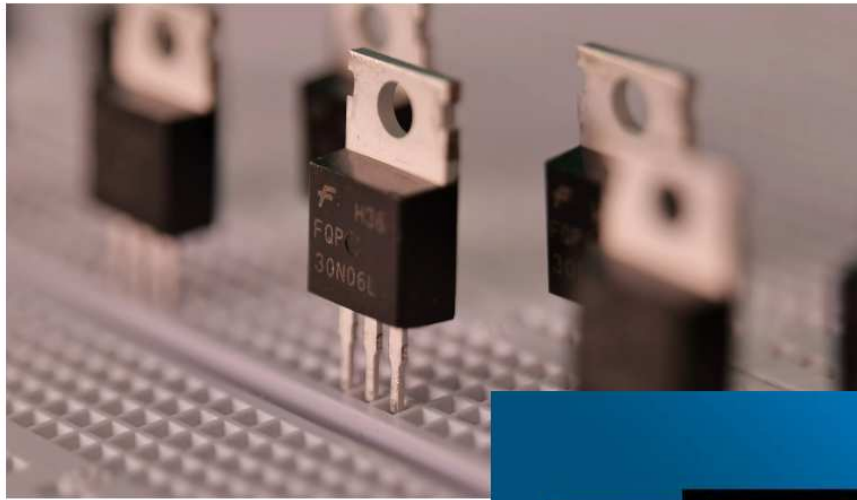
Introduction Code Analysis **Optimization** Conclusion

Optimization Strategy 1 – Reduce Memory Access

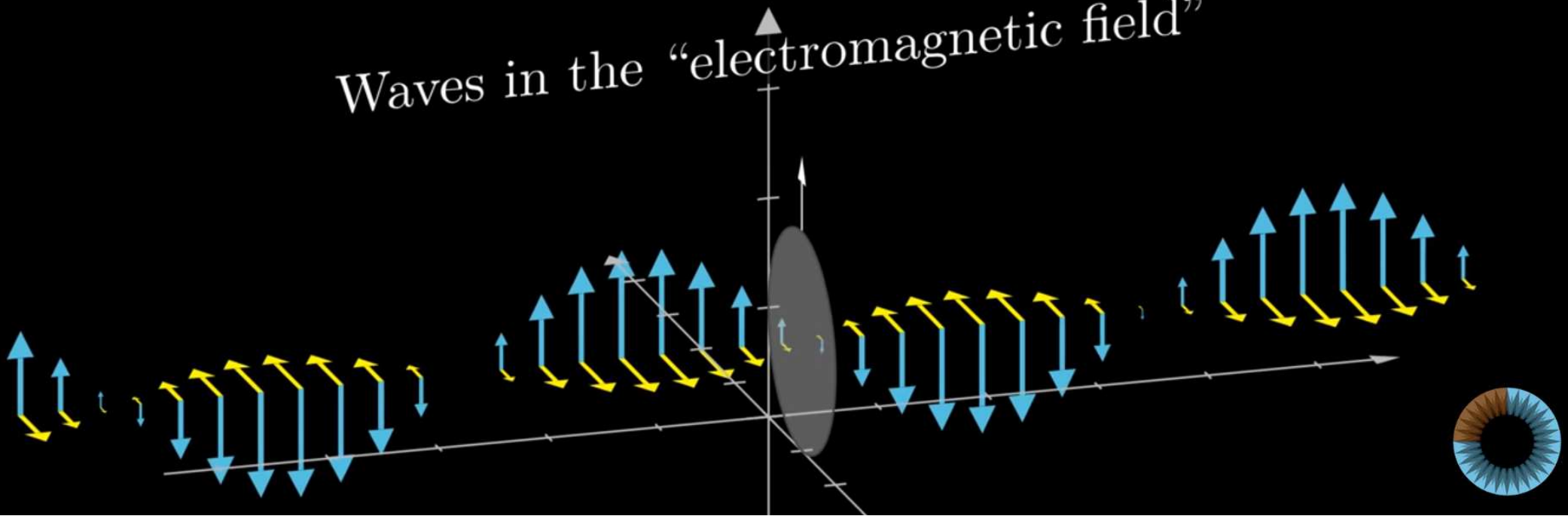
```
// did we find a new solution already?
if (partial == ssp->target)
{
    result->solutions[result->count] = selected;
    result->count++;
    return;
}
```

movq -32(%rbp), %rdx	# Load selected	movq (%r9), %rax	# Load result pointer
movq -48(%rbp), %rax	# Load result pointer	movl 8(%r9), %ecx	# Load count
movq (%rax), %rax	# Load solutions array	movq %r15, (%rax,%rcx,8)	# Store solution
movq -48(%rbp), %rcx	# Load result pointer	incl %ecx	# Increment count
movslq 8(%rcx), %rcx	# Load count	movl %ecx, 8(%r9)	# Store new count
movq %rdx, (%rax,%rcx,8)	# Store solution	jmp .LBB1_8	# Jump to return
movq -48(%rbp), %rax	# Load result pointer		
movl 8(%rax), %ecx	# Load count		
addl \$1, %ecx	# Increment count		
movl %ecx, 8(%rax)	# Store new count		
jmp .LBB1_8	# Jump to return		





Waves in the "electromagnetic field"



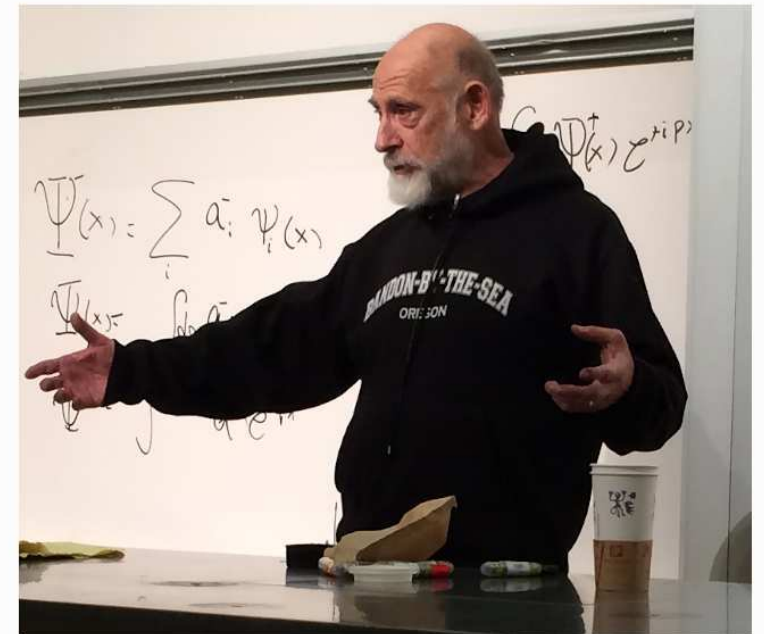
POLARIZATION FOR PHOTONS AND QBITS

LIGHT POLARIZATION IS ONE OF THE POSSIBLE WAYS TO IMPLEMENT QBITS WITH PHOTONS:

$$\alpha|H\rangle + \beta|V\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \alpha, \beta \in \mathbb{C}$$

BECAUSE OF THE NORMALIZATION CONSTRAINT ($\alpha^2 + \beta^2 = 1$) AND THE FACT THAT THE GLOBAL PHASE PLAYS NO ROLE ($e^{i\omega}$) ONE QBIT ONLY ADMITS TWO DEGREES OF FREEDOM.

JONES MATRICES ARE OPERATORS CAPABLE TO EMULATE THE EFFECT OF OPTIC DEVICES ON PHOTONS.



LEONARD SUSSKIND STANFORD UNIVERSITY

JONES MATRICES FOR POLARIZERS

FOCUS ON LINEAR POLARIZERS

HORIZONTAL

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$|H\rangle$

VERTICAL

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$|V\rangle$

DIAG. $+45^\circ$

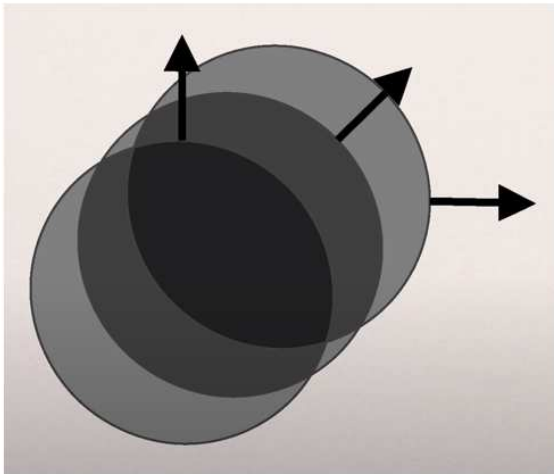
$$\frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$|D\rangle$

DIAG -45°

$$\frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$|A\rangle$

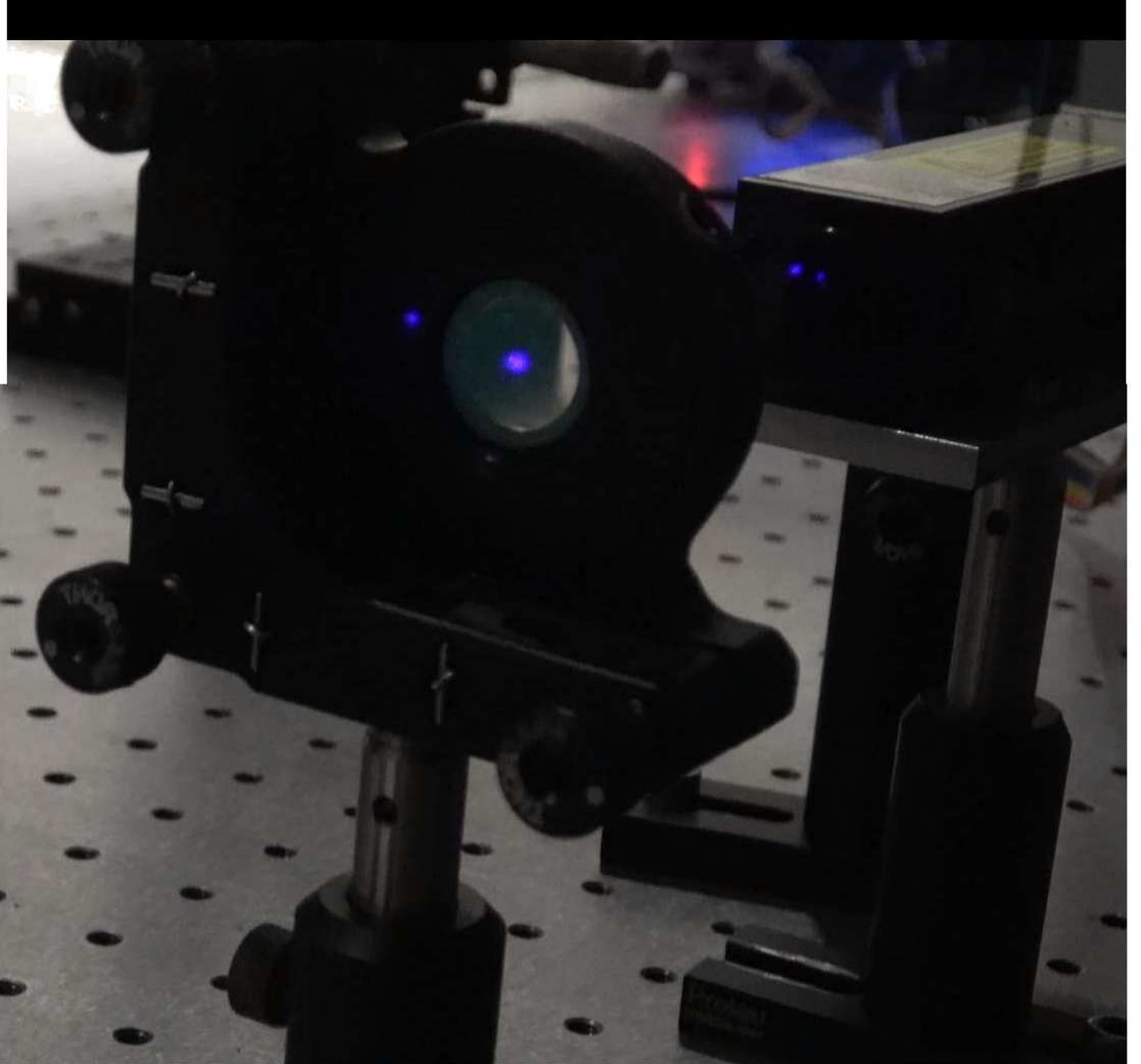


DEPENDING ON THE CURRENT STATE $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$,
PART OF THE LIGHT PASSES THROUGH,
ANOTHER PART IS INSTEAD ABSORBED.

THE HALF WAVE PLATE

IT ALLOWS US TO "TILT" THE POLARIZATION:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ -\beta \end{pmatrix}$$



DIFFERENTLY FROM POLARIZERS, NO LIGHT IS ABSORBED (IN IDEAL CONDITIONS)

ENCODING DATA WITH SPATIAL LIGHT MODULATORS



- IT IMPRINTS A GIVEN PHASE TO THE LIGHT BEAM REACHING EVERY PIXEL
- 2^m DIFFERENT DATA VALUES δ CAN BE ASSOCIATED TO THE PHASE (eg. $m = 8 \Rightarrow 256$ values)
- BUT HOW TO READ/EXPLOIT THESE DATA ONCE ENCODED?



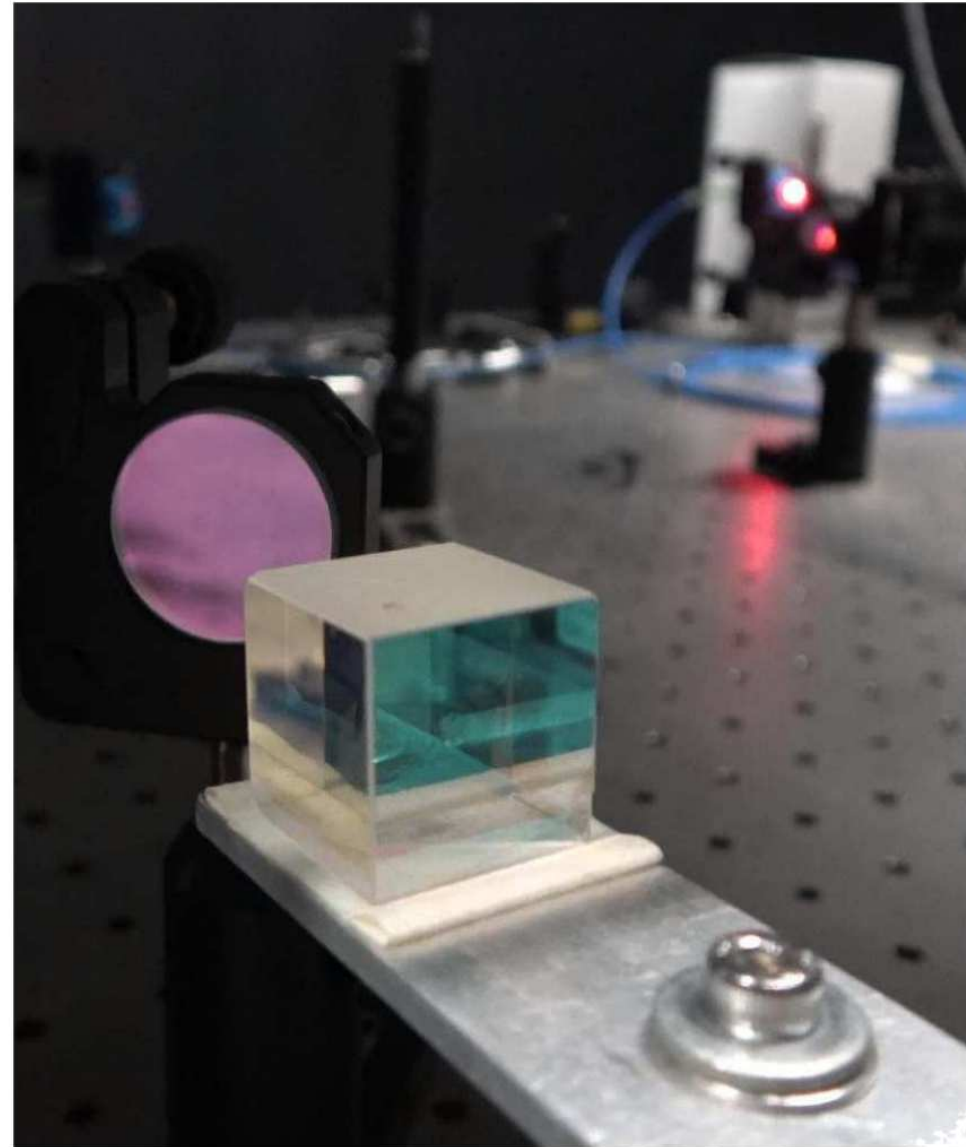
USE THE FACT THAT SLMs ALTER THE PHASE ONLY ALONG ONE OF THE 2 POLARIZATION COMPONENTS (eg. Horizontal)

$$\begin{pmatrix} e^{i\delta} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha e^{i\delta} & 0 \\ 0 & \beta \end{pmatrix}$$

FROM POLARIZATION MODULATION TO INTENSITY PROFILE

- USE A HALF-WAVE PLATE
($\theta = -45^\circ$, (D,A) \rightarrow (H,V))

- USE A POLARIZATION BEAM SPLITTER
(WE SELECT THE H COMPONENT ONLY)



THIS IS EQUIVALENT TO PERFORMING
A POLARIZATION PROJECTION ON H

MULTIPLYING TWO REAL NUMBERS ($a = 1 - \cos \delta_a, b = 1 - \cos \delta_b$)

MONOCHROMATIC
D-POLARIZED LIGHT
FROM LASER

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \xrightarrow{\text{SCH}} \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\delta_a} & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\delta_a} \\ 1 \end{pmatrix}$$

HWP flip
D \rightarrow H, A \rightarrow V

$$\frac{1}{2} \begin{pmatrix} e^{i\delta_a} - 1 \\ -e^{i\delta_a} - 1 \end{pmatrix} \leftarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} e^{i\delta_a} \\ 1 \end{pmatrix}$$

$$\frac{1}{2} \begin{pmatrix} e^{i\delta_a} - 1 \\ 0 \end{pmatrix} \xrightarrow{\text{SOME MATH}} (1 - \cos \delta_a) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

WE WRITE $e^{i\delta_a} - 1$ IN THE FORM $\alpha e^{i\beta}$
WE CAN THEN NEGLECT THE GLOBAL PHASE

MULTIPLYING TWO REAL NUMBERS ($a = 1 - \cos \delta_a, b = 1 - \cos \delta_b$)

MONOCHROMATIC
D-POLARIZED LIGHT
FROM LASER

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \xrightarrow{\text{STEP 1}} (1 - \cos \delta_a) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \xrightarrow{\text{D-pol.}} \frac{1}{2} (1 - \cos \delta_a) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

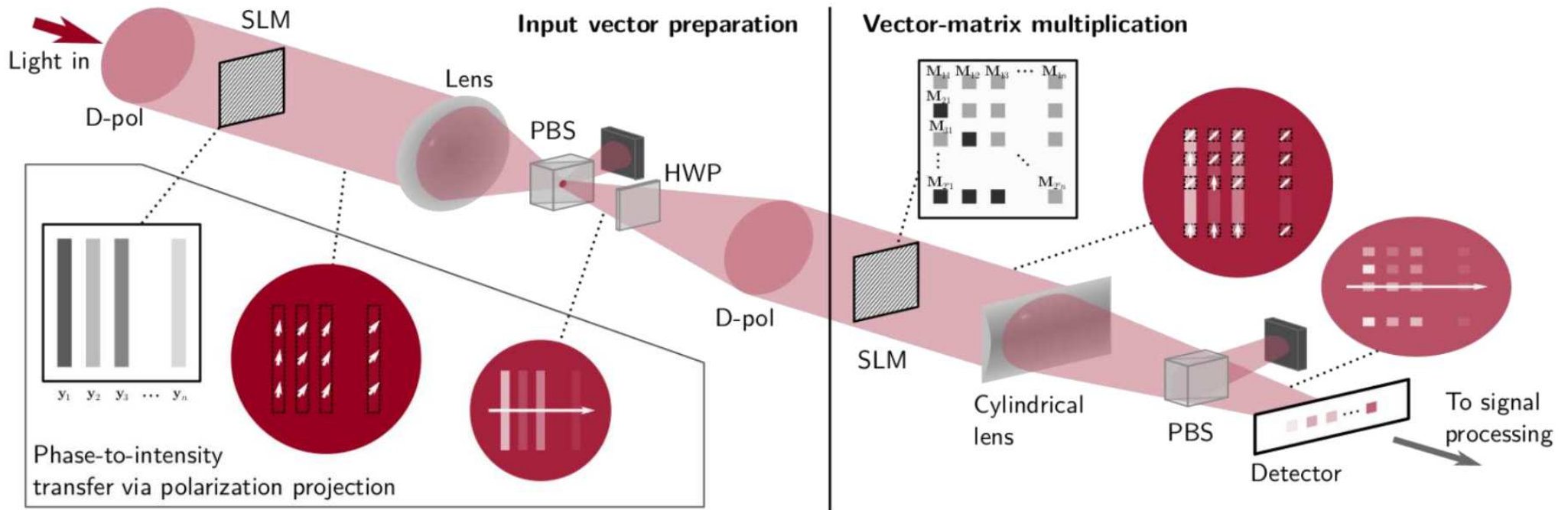
$$e \begin{pmatrix} 1 \\ 0 \end{pmatrix} \xleftarrow{\text{STEP 2}} \frac{(1 - \cos \delta_a)(1 - \cos \delta_b)}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \xleftarrow{\frac{1}{2} \begin{pmatrix} 1 - \cos \delta_a \\ 1 - \cos \delta_a \end{pmatrix}}$$

OUR INTENSITY
MEASURE

$$ab = \sqrt{2} c$$

IDENTICAL BUT WITH
DIFFERENT INPUT (δ_b)

OUR FULL-OPTICAL PROCESSOR



ONGOING RESEARCH:

- THEORY: OTHER DEGREES OF FREEDOM?
- PRACTISE: HARDWARE IMPLEMENTATION



Antonio Mucherino

Associate Professor

IRISA, University of Rennes

antonio.mucherino@irisa.fr

Hey guys, I've just tried this new **Google's NotebookLM** functionality, where you provide a bunch of sources and it generates for you an audio summary of its content in the form a podcast.

This is what it was produced from one of our papers: [a podcast about our optical processor](#)! Just amazing.

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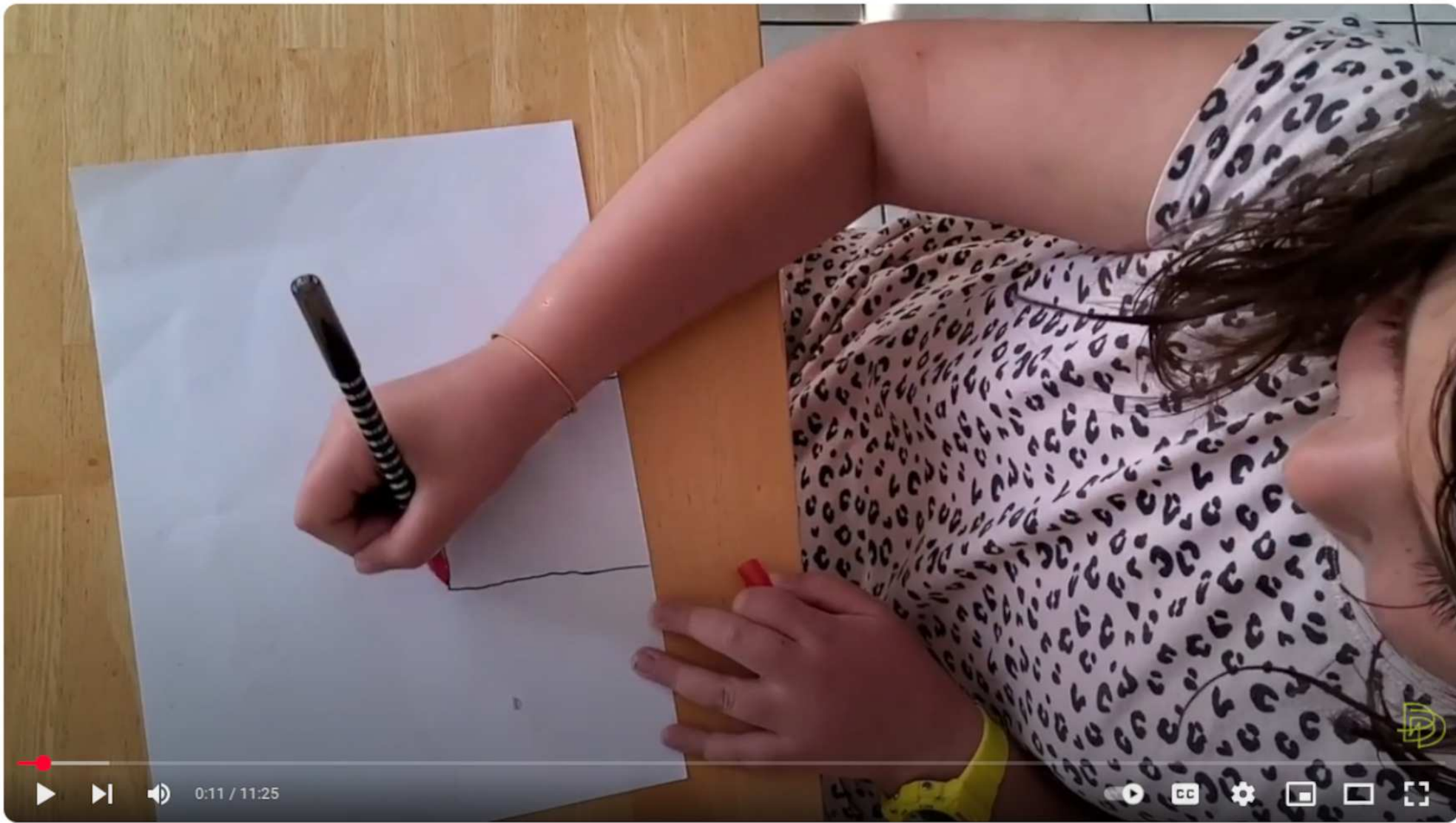
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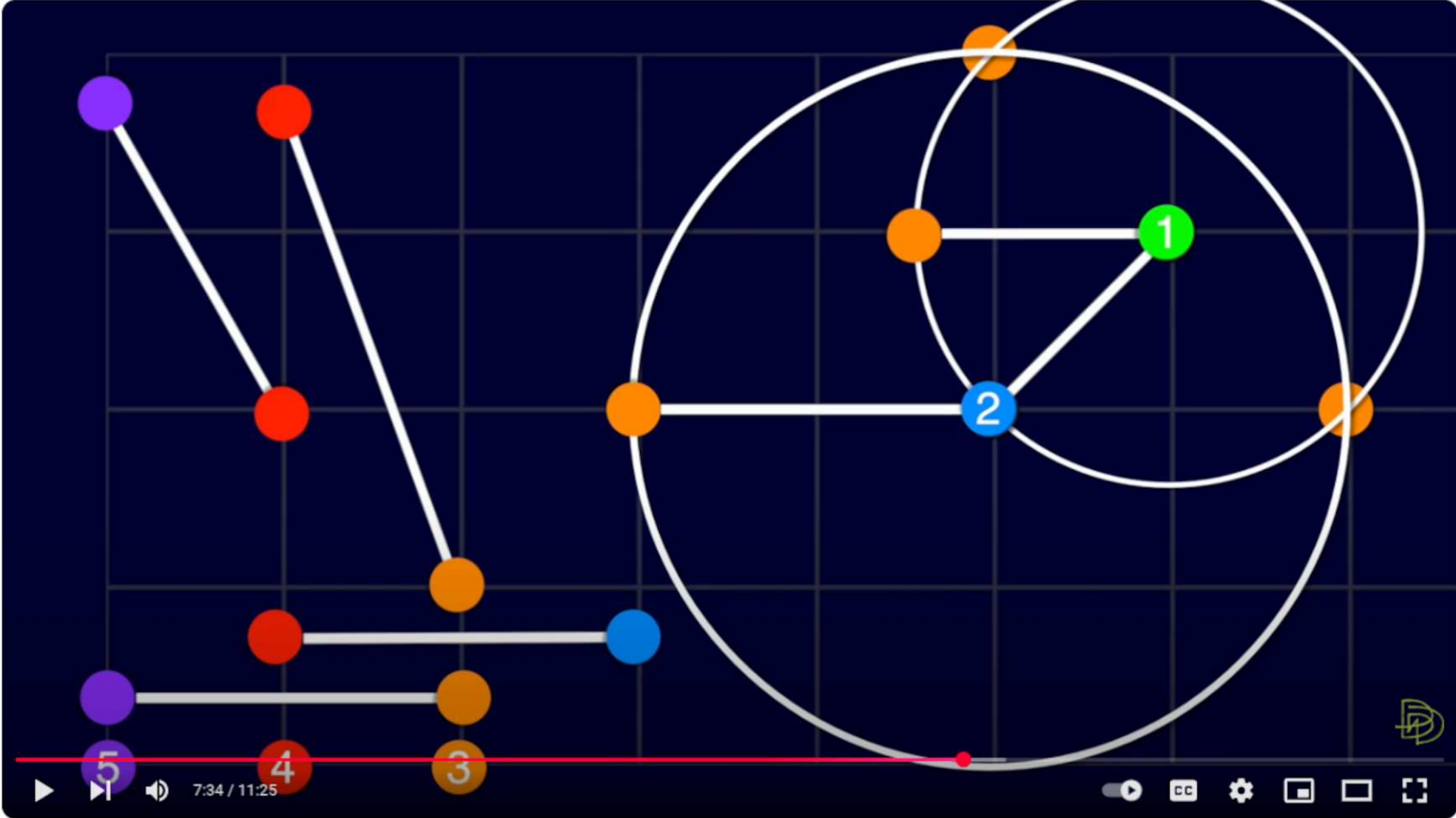
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Thanks!

EMAIL: ANTONIO.MUCHERINO@IRISA.FR

GITHUB: MUCHERINO

YOUTUBE: @DISTANCEGEOMETRY