DISCRETE TOMOGRAPHY - A SURVEY

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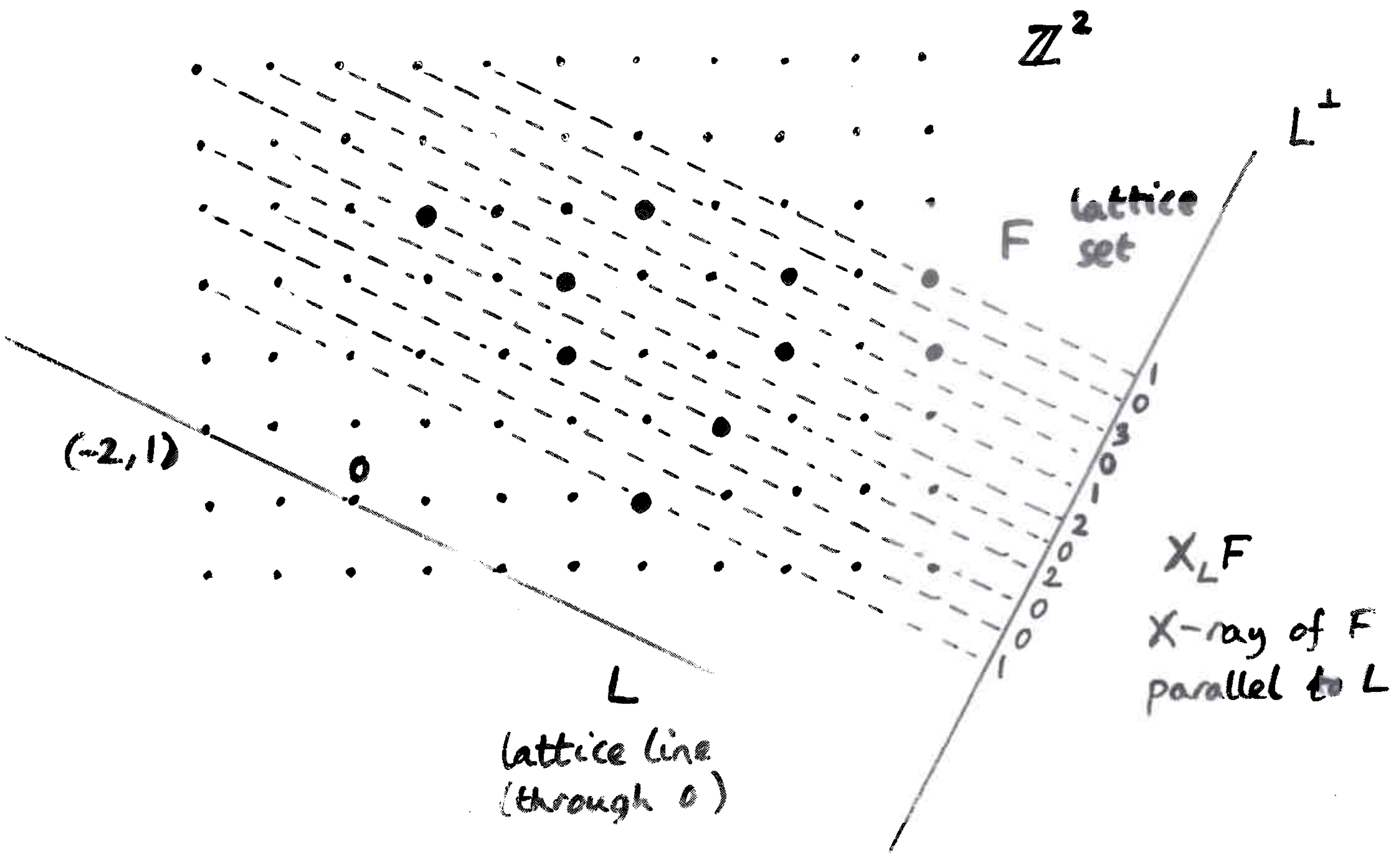
High Resolution Transmission Electron Microscopy

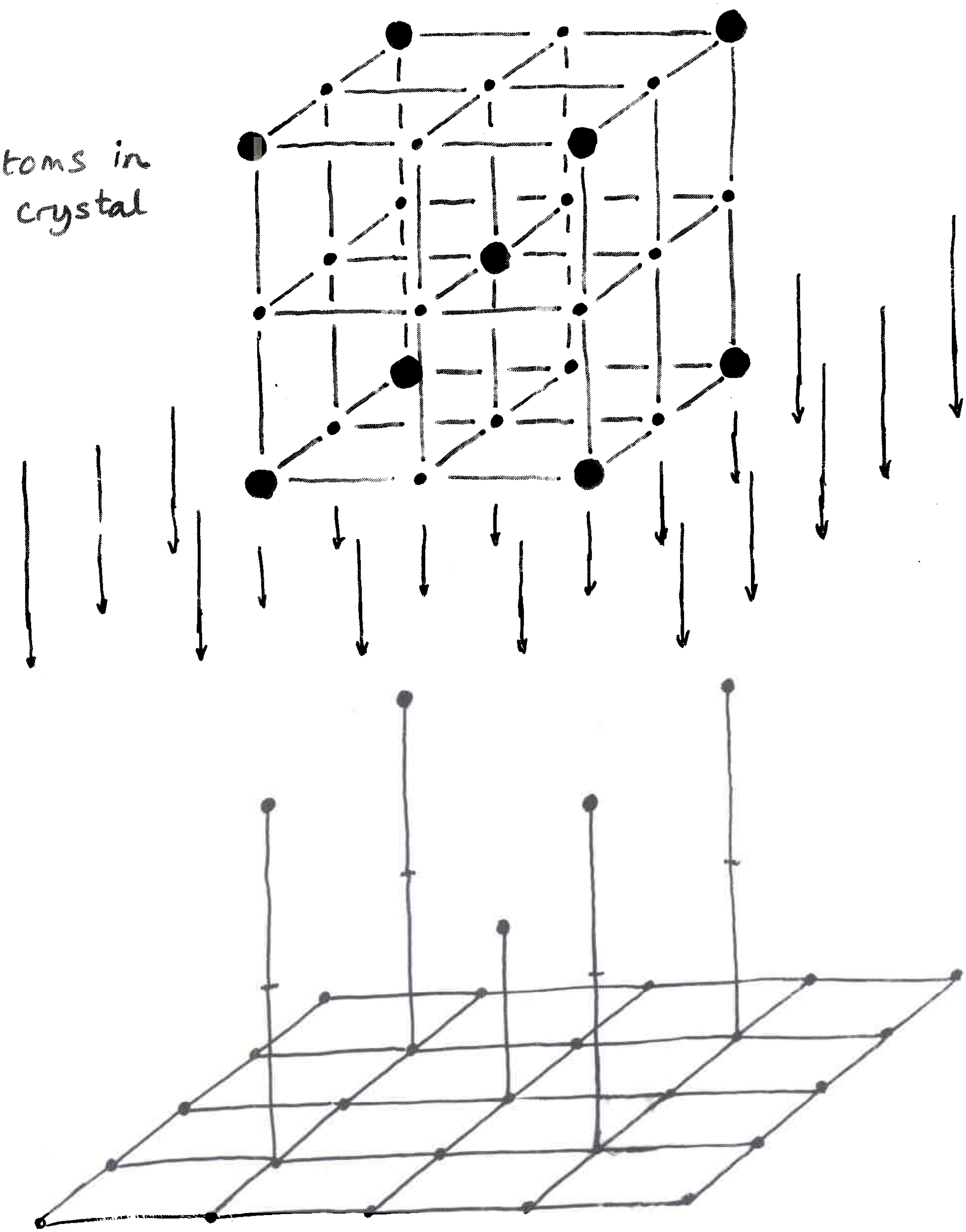
X-ray of a crystalline structure
↓
number of atoms on each of a family of parallel lines



DISCRETE TOMOGRAPHY

P. Schwander
L. A. Shepp 1994

Atoms in a crystal



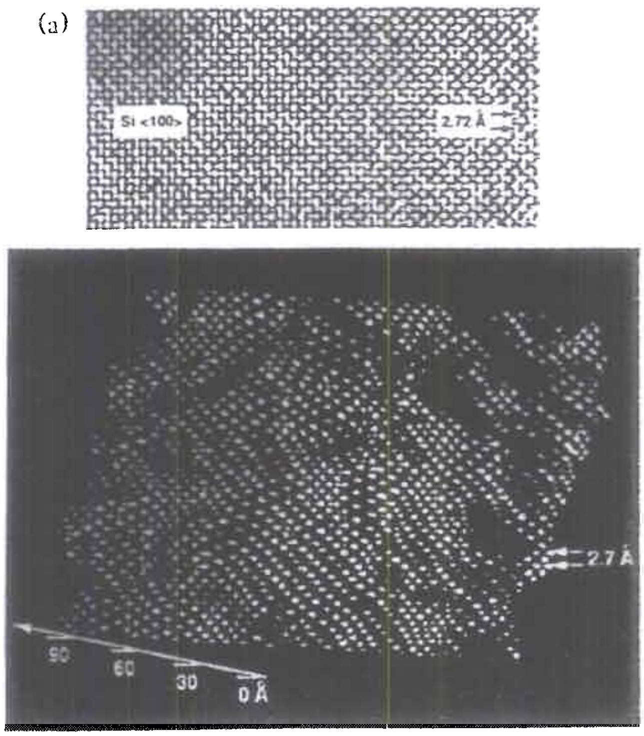


FIG. 3. (a) Lattice image of $SiO_2/Si/SiO_2$ sample, viewed in ⟨100⟩ plan view. The sample was formed by anisotropic etching of Si in KOH, followed by formation of a native oxide. Two Si/SiO_2 interfaces are seen superimposed. (b) QUANTITEM map of the thickness of crystalline Si sandwiched between the two SiO_2 layers. Height represents sample thickness. This topographic map, deduced from (a) above, directly reveals the superimposed roughness of the two Si/SiO_2 interfaces. Note the pyramidal hillocks produced by the anisotropic etch.

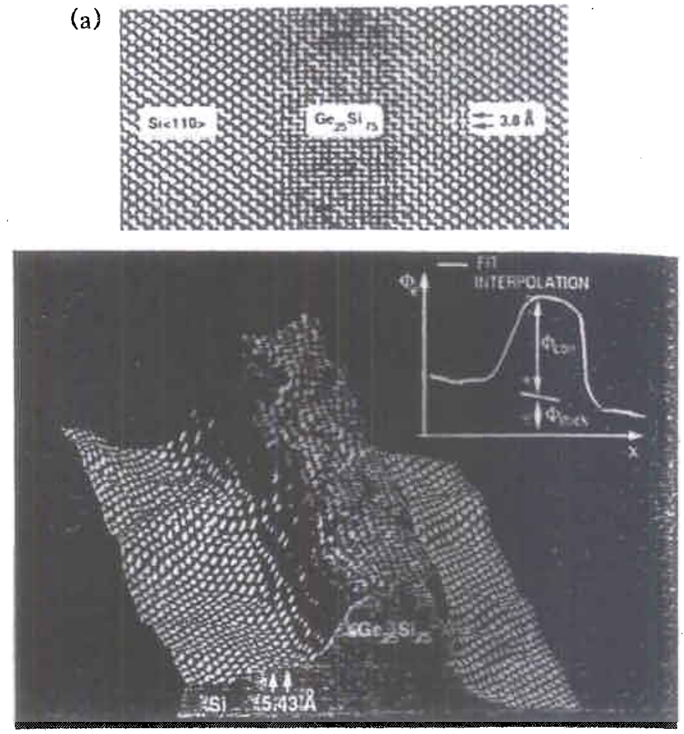


FIG. 4. (a) Lattice image of $Si/Ge_{0.25}Si_{0.75}/Si$ quantum well structure, viewed in ⟨110⟩ cross section. (b) Map of ellipse phase angle ϕ_e across the image shown in (a) above. Note the variations in the Si region, indicating significant thickness changes. Inset: schematic representation of the effect of composition on ϕ_e. The heavier GeSi causes ϕ_e to advance more rapidly. The variation of thickness across the field of view means that part of the change in ϕ_e is due to composition, part due to thickness change.

$\mathcal{F}^n$ = class of finite subsets of $\mathbb{Z}^n$ (lattice sets)

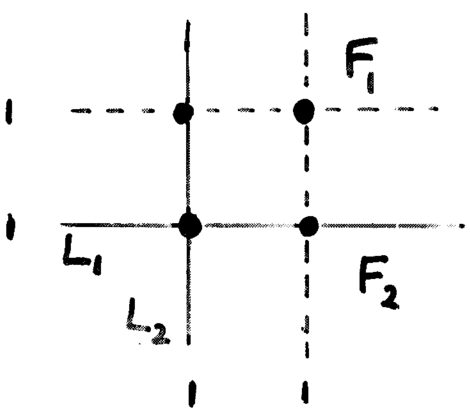
$\mathcal{L}^n$ = class of lattice lines through o in $\mathbb{E}^n$

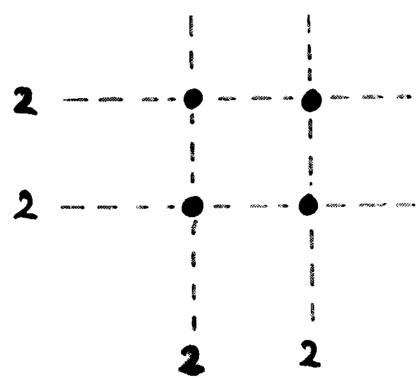
$\mathcal{E} \subset \mathcal{F}^n \qquad \mathcal{L} \subset \mathcal{L}^n$ (finite)

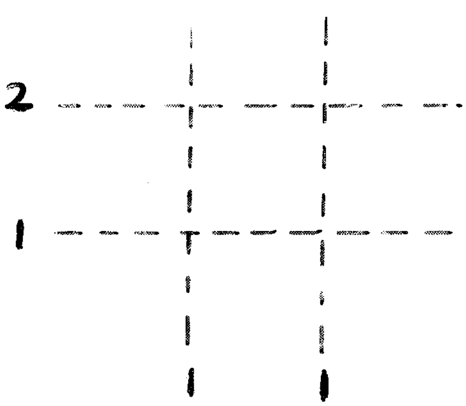
$E \in \mathcal{E}$ is **determined** by X-rays parallel to lines in $\mathcal{L}$ if $E' \in \mathcal{E}$ and $X_L E' = X_L E \;\; \forall L \in \mathcal{L} \Rightarrow E' = E$.

UNIQUENESS$(\mathcal{E},\mathcal{L})$	RECONSTRUCTION$(\mathcal{E},\mathcal{L})$
CONSISTENCY$(\mathcal{E},\mathcal{L})$	

$\mathcal{E} = \mathcal{F}^2, \quad |\mathcal{L}| = 2.$







??

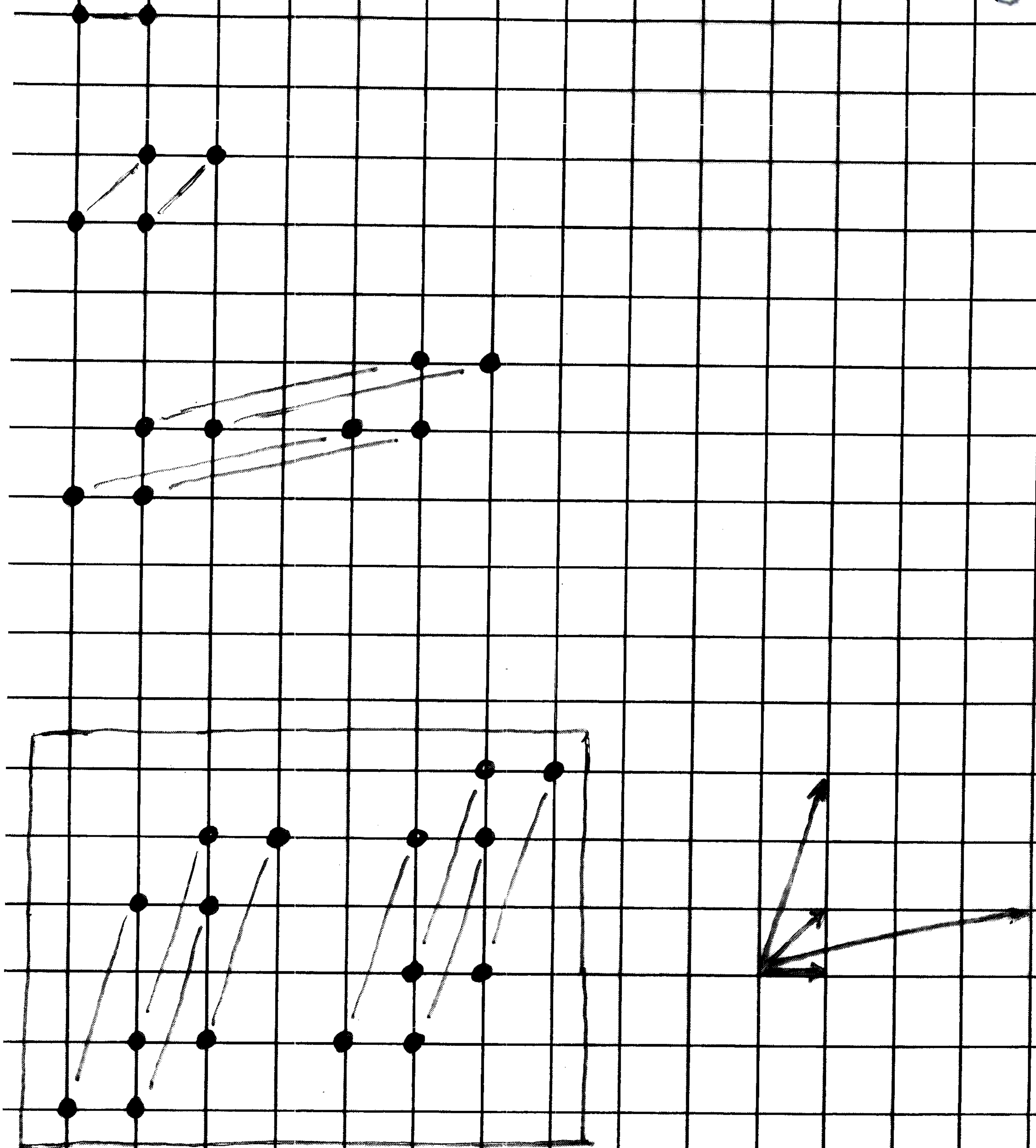
{0,1}-matrices

H. J. Ryser

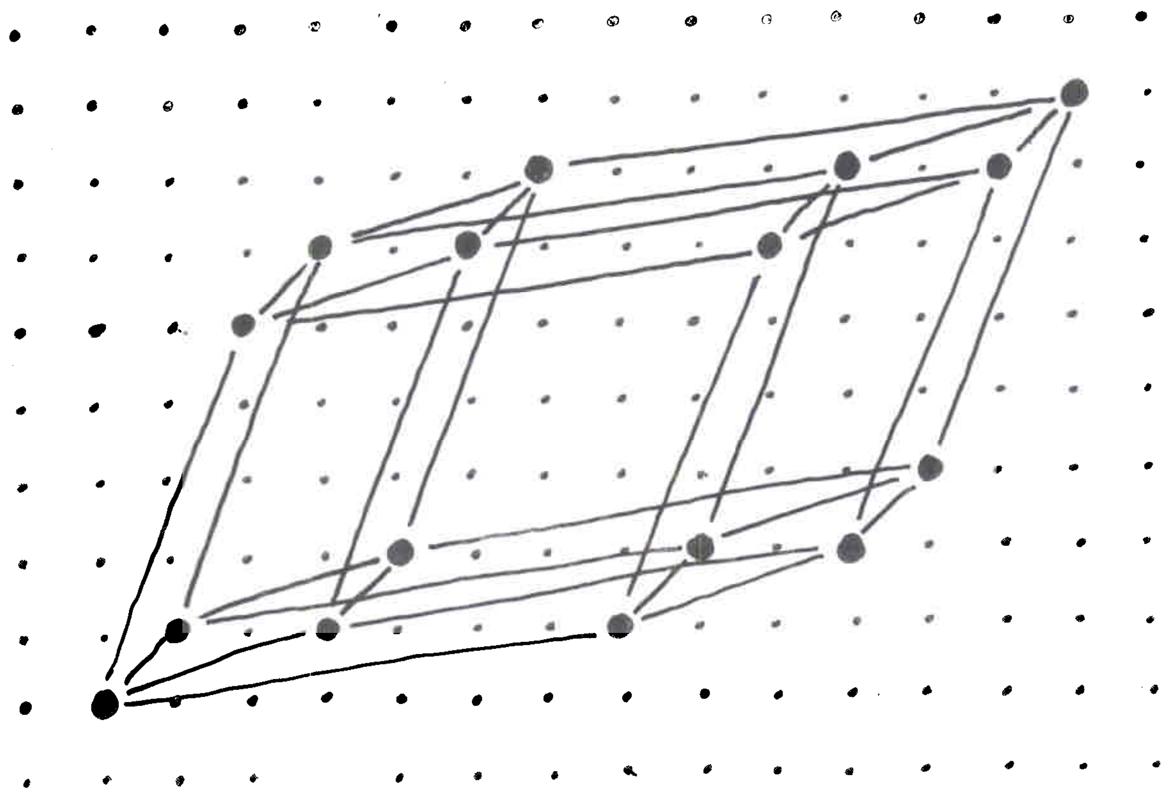
1956/7

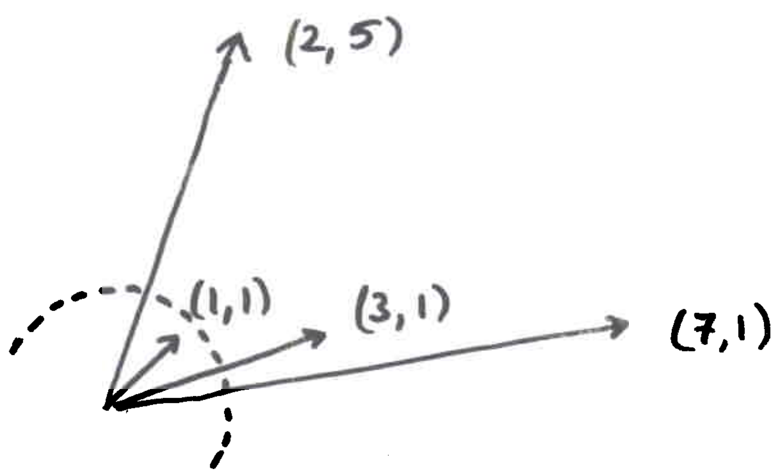
POLYNOMIAL TIME

(data security)



F_1 F_2





Note "complementary" examples – crystals with impurities.

Options

- restrict $\mathcal{F}^n$
- settle for less
  - check uniqueness algorithmically
  - determine a "typical" solution
  - determine the "core" of all solutions

Algorithmic preliminaries : **Precise data**

$S_1, \ldots, S_m \in \mathcal{S}^n$ ← different! $\mathcal{G} \subset \mathcal{F}^n$

CONSISTENCY$_{\mathcal{G}}(S_1, \ldots, S_m)$

Instance : $X_i : S_i^{\perp} \to \mathbb{N} \cup \{0\} \quad (i = 1, \ldots, m)$

Question : Does there exist $F \in \mathcal{G}$ such that $X_{S_i} F = X_i$ for $i = 1, \ldots, m$?

UNIQUENESS$_{\mathcal{G}}(S_1, \ldots, S_m)$

RECONSTRUCTION$_{\mathcal{G}}(S_1, \ldots, S_m)$

Results*:

1. CONSISTENCY$_{\mathcal{F}^n}(S_1, S_2)$ and UNIQUENESS$_{\mathcal{F}^n}(S_1, S_2)$ can be solved in polynomial time.

2. For $m \geq 3$, CONSISTENCY$_{\mathcal{F}^n}(S_1, \dots, S_m)$ and UNIQUENESS$_{\mathcal{F}^n}(S_1, \dots, S_m)$ are NP-complete.

there is a polynomial-time transformation from any other problem in NP.

↑ increasing complexity

problems that can be solved with a polynomial-time algorithm

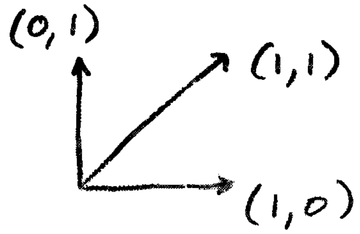
NP - "yes" instances can be checked in polynomial time

* R.J.G., P. Gritzmann, and D. Prangenberg, Discrete Math. 202 (1999), 45–71.

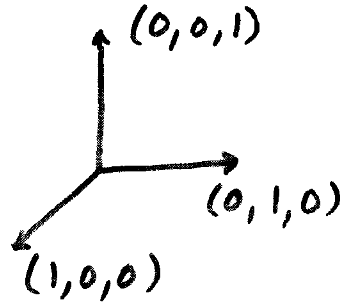
The plan:

1. Find a polynomial-time transformation from $\text{CONSISTENCY}_{\mathcal{J}^n}(S_1, \dots, S_m)$ to $\text{CONSISTENCY}_{\mathcal{J}^n}(S_1, \dots, S_{m+1})$.
2. Show $\text{CONSISTENCY}_{\mathcal{J}^n}(S_1^*, S_2^*, S_3^*)$ is NP-complete

$n = 2$



$n \geq 3$



1-IN-3-SAT

Instance: $r, s \in \mathbb{N}$, $V = \underbrace{\{x_1, \dots, x_r\}}^{\text{variables}}$,

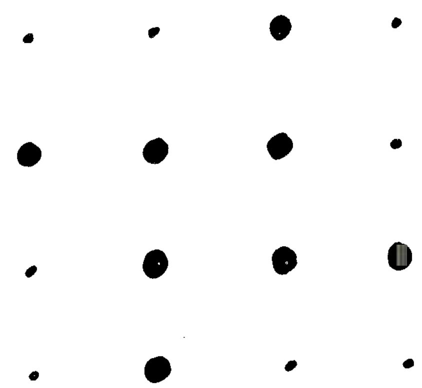
$\overbrace{\mathcal{C}}^{\text{clauses}} = \{C_1, \dots, C_s\}$, each C_i contains 3 literals.

Question: Is there a truth assignment for $\mathcal{C}$ that sets exactly one literal true in each clause?

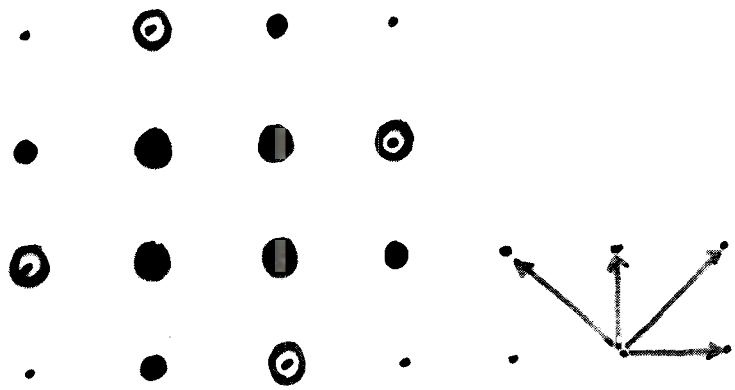
Example:

$$\underbrace{(x_1 \vee \neg x_2 \vee x_4)}^{C_1} \wedge \underbrace{(x_2 \vee x_3 \vee x_4)}^{C_2} \wedge \underbrace{(\neg x_1 \vee x_3 \vee x_5)}^{C_3}$$

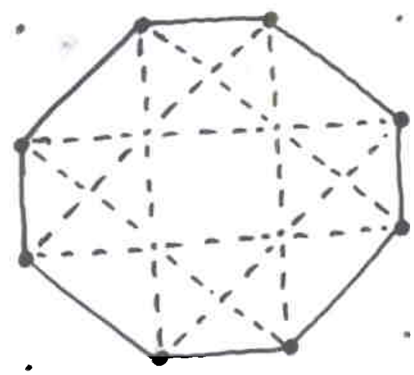
x_1	T
x_2	T
x_3	F
x_4	F
x_5	T



$\mathcal{G}^n$ = class of convex lattice sets in $\mathbb{Z}^n$.



$\mathcal{C}^n$ = class of convex lattice sets in $\mathbb{Z}^n$.



A lattice $\mathcal{L}$-polygon with $|\mathcal{L}| = 4$.

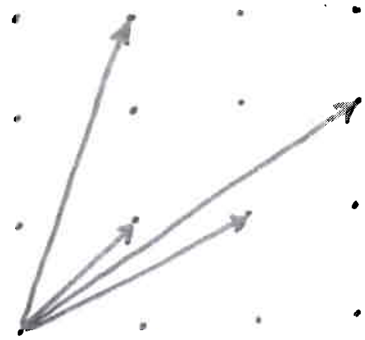
G. & P. GRITZMANN, Trans. A.M.S. 349 (1997), 2271-95.

Suppose $\mathcal{L} \subset \mathcal{L}^2$. Sets in $\mathcal{C}^2$ are determined by X-rays parallel to lines in $\mathcal{L}$ $\Leftrightarrow$ there does not exist a lattice $\mathcal{L}$-polygon.

1. If $|\mathcal{L}| \le 3$, there is a lattice $\mathcal{L}$-polygon (affinely regular hexagon).

2. If $|\mathcal{L}| \geq 4$ and $\exists$ a lattice $\mathcal{L}$-polygon, then cross-ratio of any 4 lines in $\mathcal{L}$ is $\frac{4}{3}$, $\frac{3}{2}$, 2, 3, or 4.

cross-ratio $= 5/4$

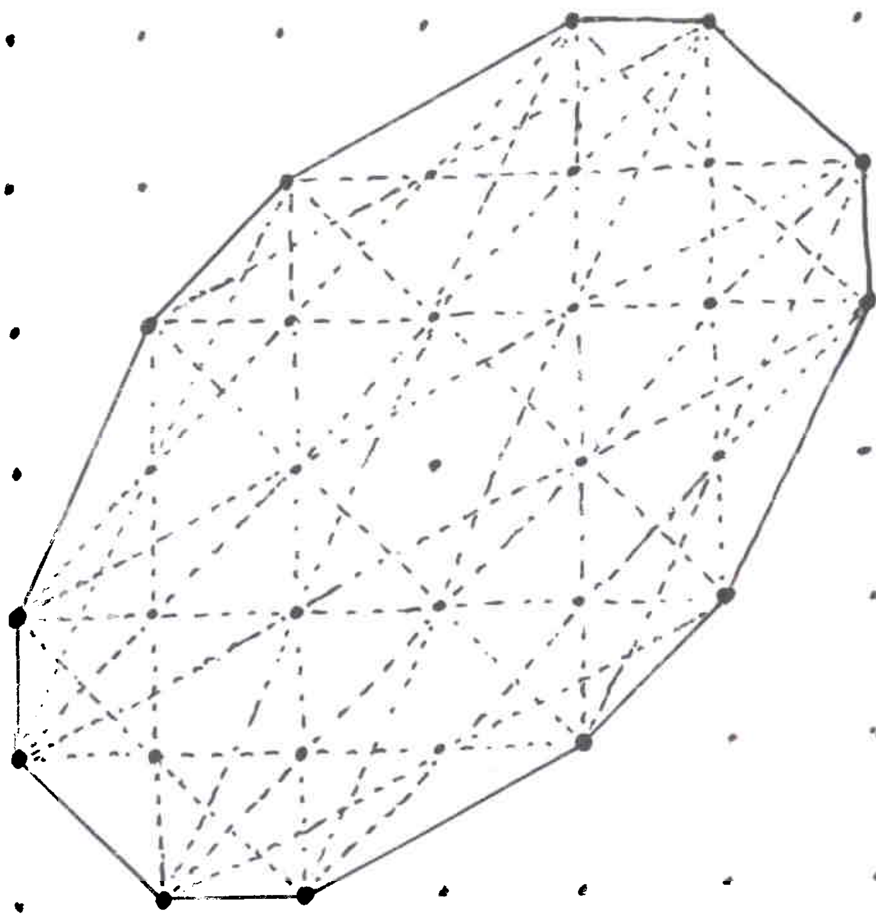


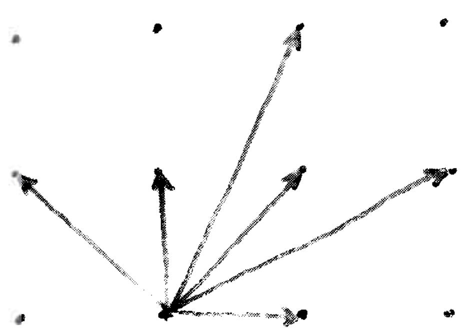
GOOD for X-rays

BAD for lattice $\mathcal{L}$-polygons!

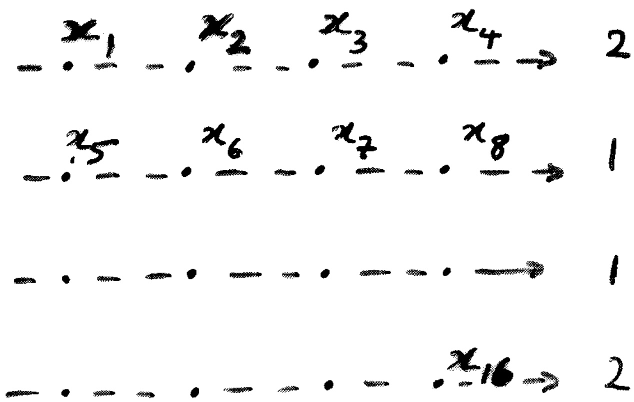
(p-adic valuations)

3. If $|\mathcal{L}| \geq 7$, there are no lattice $\mathcal{L}$-polygons.





LP-relaxation methods.



$x_1 + x_2 + x_3 + x_4 = 2$

$x_5 + x_6 + x_7 + x_8 = 1$

etc.

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & \cdots & 0 \\ & & & & & \cdots & & & & & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{16} \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ \vdots \end{bmatrix}$$

$$A \quad x \quad = \quad b$$

LP: "feasibility problem":

minimize 0
subject to $Ax = b$
$x_i = 0$ or 1

or:

maximize $x_1 + \cdots + x_N$
subject to $Ax \overset{=}{\leq} b$
$x_i = 0$ or 1

Relaxation: Replace $x_i \in \{0,1\}$ by $0 \leq x_i \leq 1$.

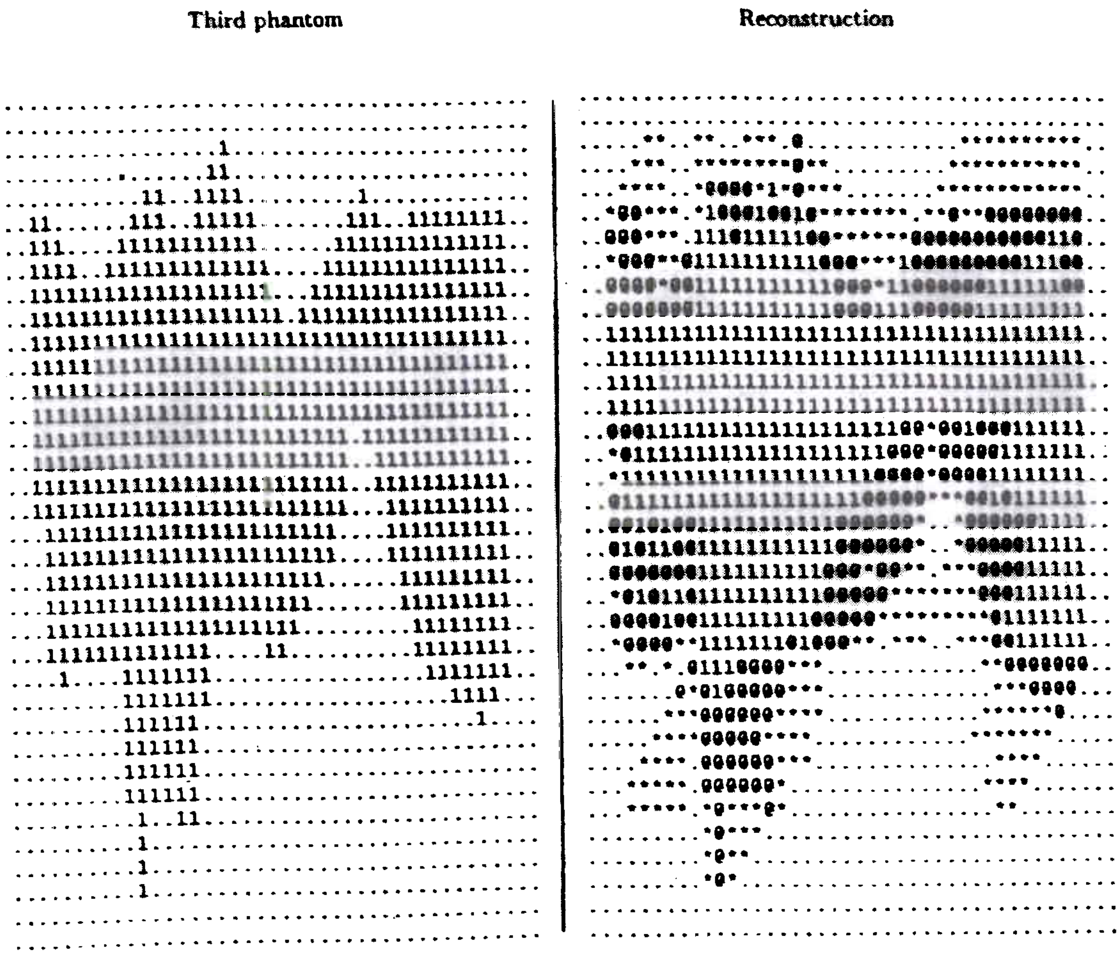


Fig. 9. Third phantom and reconstruction.

following linear program:

$$\begin{aligned} &\text{minimize} \quad 0 \\ &\text{subject to} \quad \sum_{z \in L} f(z) = v_S(L), \quad L \in \mathcal{L}, \\ &\qquad\qquad 0 \leqslant f(z) \leqslant 1, \quad z \in I, \end{aligned} \tag{7.1}$$

where I denotes a subset of $\mathbb{Z}^2$ which is assumed known to contain the phantom (we used $I = \{-30, -29, \ldots, 29, 30\}^2$).

To solve the linear program, we used an interior point solver called LOQO: see [12]. The reconstructions are shown on the right-hand sides in Fig. 7–9. In the reconstructions, each "dot" represents a lattice point having value 0, a "one" represents a lattice point having value 1, and each "asterisk" represents a lattice point having a value strictly between 0 and 1.

It is well known that interior point methods produce solutions that lie in the center of the face of optimality [1]. This means that any variable which can be away from

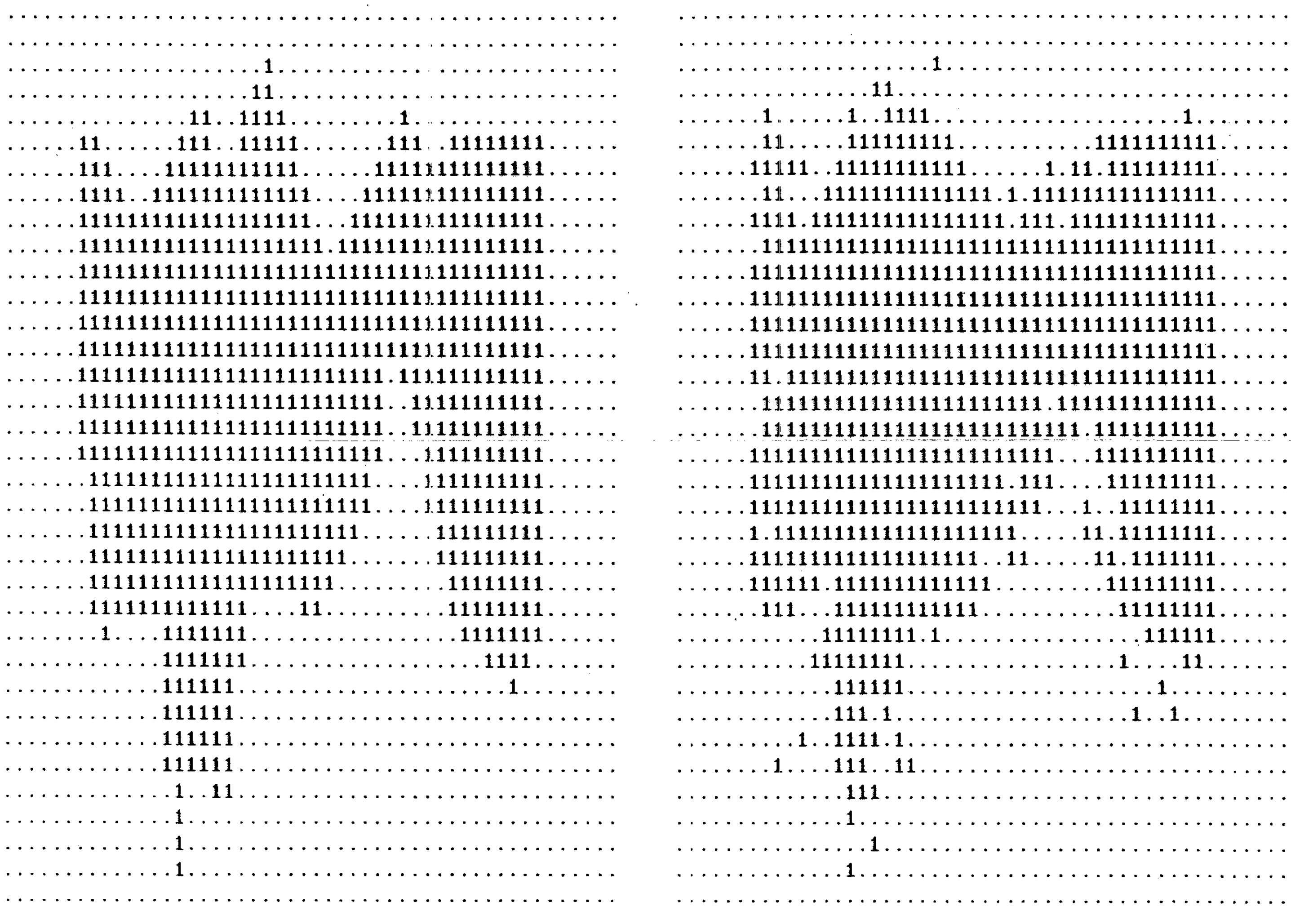


FIGURE 6. Phantom 3 of [14], and another set with the same X-rays in the directions $(1,0), (0,1), (1,1)$

$\leq x \leq u$, where A' and b' are normalizations of A and b, and u is a corresponding upı vector. This approach is particularly intriguing in the presence of noise. Then it l a specific regularization whose solutions have an interpretation as best-approximatic sense of maximum likelihood.

ill be interesting to see on the basis of real-world data 'how much' of the fractioı nents of any LP-based method mirrors non-uniqueness (and might hence be interpret proportion of those solutions that contain the corresponding point) and what is rea ifact introduced by the underlying relaxation. That there is at least a certain sı ce follows from the facts that there are instances of (1) which have a unique soluti

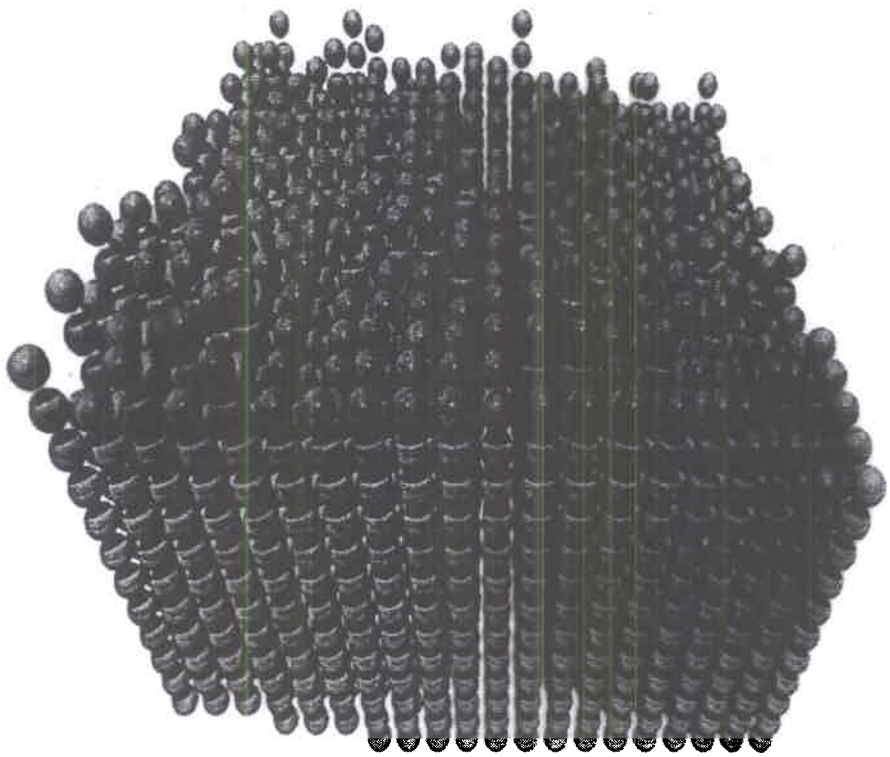


FIGURE 1. Reconstruction of a 3D-phantom by a branch-and-bound algorithm

Intern. J. Imaging Systems Technology 9(1998), 101-9.

Greedy algorithms

Best Inner Fit: Given data $X_1, \dots, X_m$, find $F \subset$ grid G of maximum cardinality such that $X_{S_i} F(T) \le X_i(T)$ for all lines T parallel to S_i and $i = 1, \dots, m$.

1. Initialize: $F = E = \phi$ and choose a direction, say S_1.
2. for each T parallel to S_1, do:

   2.1 For all $g \in G \cap T$, find

   $$w_g = \prod_{i=2}^{m} \frac{X_i(g+S_i) - |(g+S_i) \cap F|}{|(G \setminus (F \cup E)) \cap (g+S_i)|}$$

   2.2 Sort $G \cap T$ according to decreasing weights w_g, $g \in G \cap T$, and add the

   $$\min\{X_1(g+S_1), |\{g \in G \cap T : w_g > 0\}|\}$$

   first elements of $G \cap T$ to F and the remaining ones to E.

Theory: F will contain at least $1/m$ of the points in an optimal solution.

Practise: A proportion of $> .9$ is typical.

Good experimental results for 500×500 grid – 250,000 positions and examples with 125,000 atoms.

SIAM J. Optim. 11 (2000), 522-546.

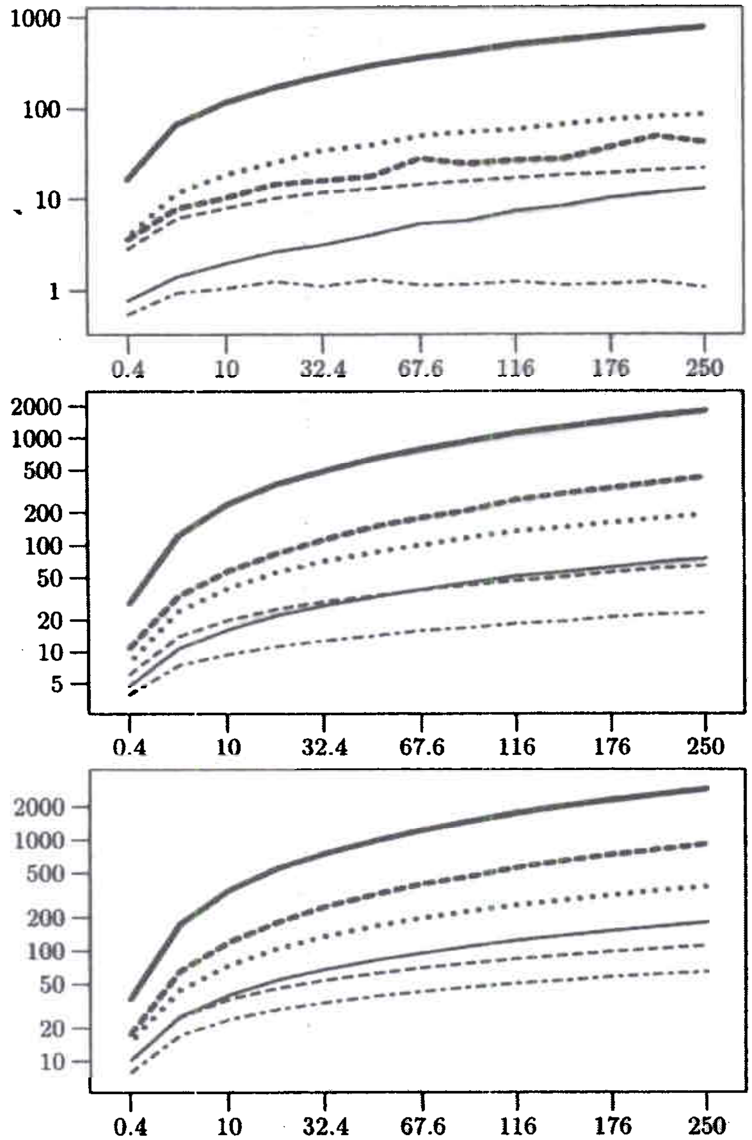
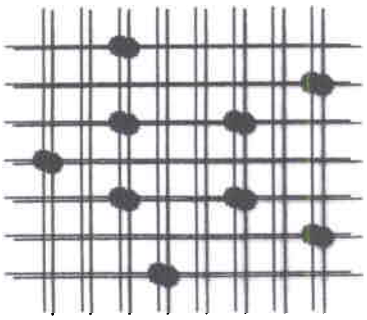
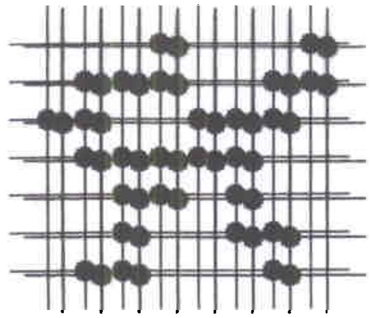


FIG. 10. *Absolute error for 3 (top), 4 (middle), and 5 (bottom) directions on instances of 50% density for GreedyA (/), ImprovementA (/), GreedyB (·˙), ImprovementB (/), GreedyC (/), and ImprovementC (/). The abscissa depicts the number of variables in thousands at a quadratic scale and the ordinate depicts the absolute error at a logarithmic scale.*

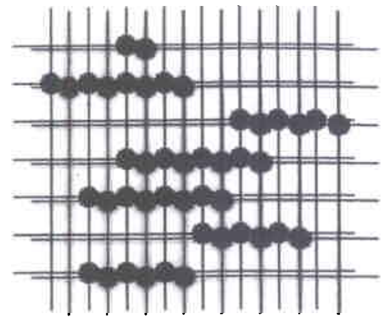
For GreedyC only lines with error at most 2 occur, while for ImprovementC a single instance with a line of error 5 came up. In contrast, GreedyA, GreedyB, ImprovementA, and ImprovementB always have a couple of lines with a huge error (see Figure 11). For instance, for GreedyA, ImprovementA, GreedyB, and ImprovementB instances occurred with lines of error 67, 130, 109, and 66. These huge errors do seem inappropriate in the physical application since it is more likely that many lines occur with small error rather than with very large error.



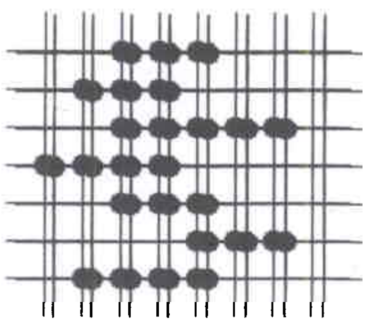
arbitrary



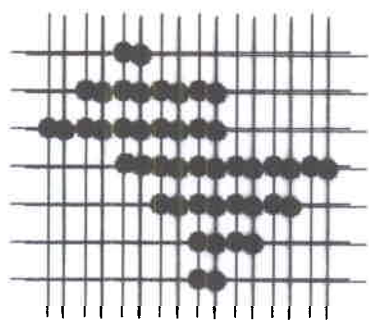
arbitrary polyomino



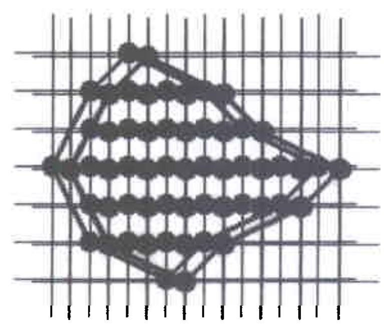
h-convex



h-convex polyomino



hv-convex polyomino

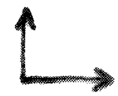


convex polyomino

Some classes of finite lattice sets.

Complexity results.

X-rays



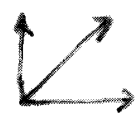
	arbitrary	polyomino
arbitrary	$\mathbb{P}$ Ryser '57	$\mathbb{NP}$ Woeginger '96
h-convex	$\mathbb{NP}$ BDNP '96	$\mathbb{NP}$ BDNP '96
hv-convex	$\mathbb{NP}$ Woeginger '96	$\mathbb{P}$ BDNP '96† Chrobak & Dürr '99†
convex	open	open

Chrobak & Dürr: Inf. Proc. Lett. 69 (1999), 283–289

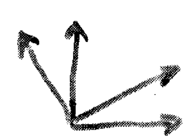
BDNP = Barcucci, Del Lungo, Nivat, Pinzani, Theor. Comp. Sci. 155 (1996), 321–347

	arbitrary	polyomino
arbitrary	$\mathbb{NP}$ GGP '99	$\mathbb{NP}$ BDVG '99
h-convex	$\mathbb{NP}$ BDVG '99	$\mathbb{NP}$ BDVG '99
hv-convex	$\mathbb{NP}$ BDVG '99	open
hvd-convex	$\mathbb{NP}$ BDVG '99	$\mathbb{P}$ BBDN '99
convex	open	open

de Vries
Gritzmann



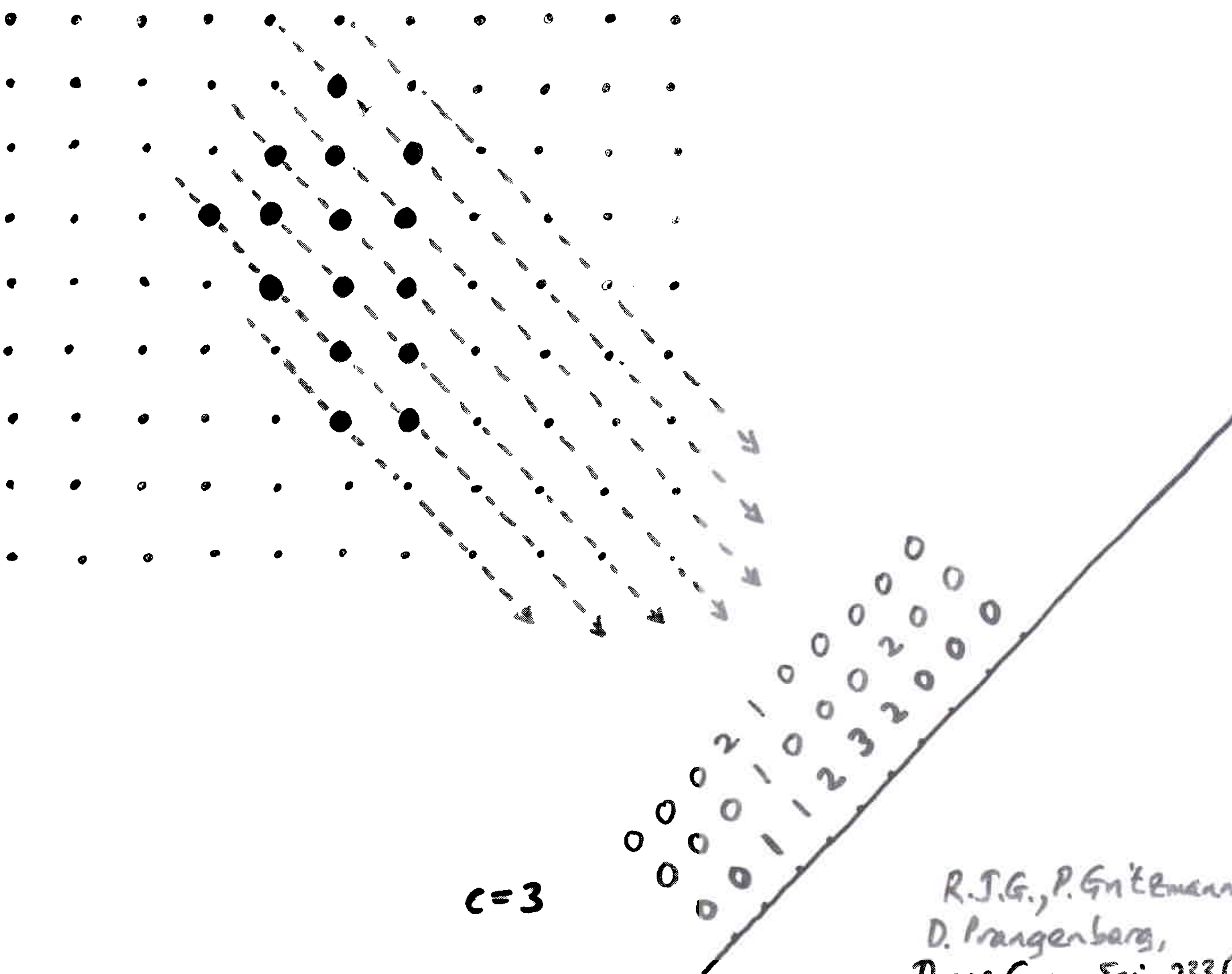
4 special directions



* Convex polyominoes (lattice sets) can be reconstructed in polynomial time (Brunetti & Daurat, Theor. Comp. Sci., to appear.)

† Algorithms compared by Balogh, Kuba, Dévényi, and Del Lungo, Linear Alg. Appl. 339 (2001), 23–35.

"Polyatomic" case:



R.J.G., P. Gritzmann & D. Prangenberg, Theor. Comp. Sci. 233 (2000), 91-106

If $c \geq 6$, POLY$_c$-CONSISTENCY$_{\mathcal{F}^n}(S_1, S_2)$ is NP-complete

- UNIQUENESS

Still open!

QUESTIONS: 1. What about $c = 2, \underbrace{3, 4, 5}$?

M. Chrobak & C. Dürr, Inf. Proc. Lett. 69 (1999), 283-289

2. Higher-dimensional X-rays?