Inversion of Band-Limited Fourier Transforms of Binary Vectors and Matrices

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Motivation: Resolution limit and search for super-resolution

Scattering amplitude in the first Born approximation

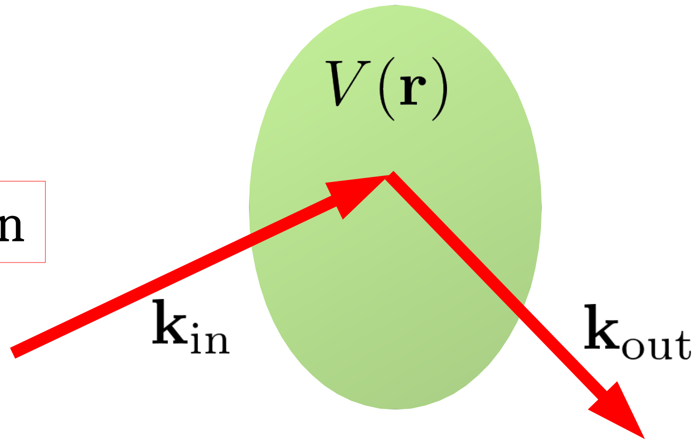
$$f(\mathbf{k}_{\rm in}, \mathbf{k}_{\rm out}) \propto \tilde{V}(\mathbf{k}_{\rm in} - \mathbf{k}_{\rm out})$$

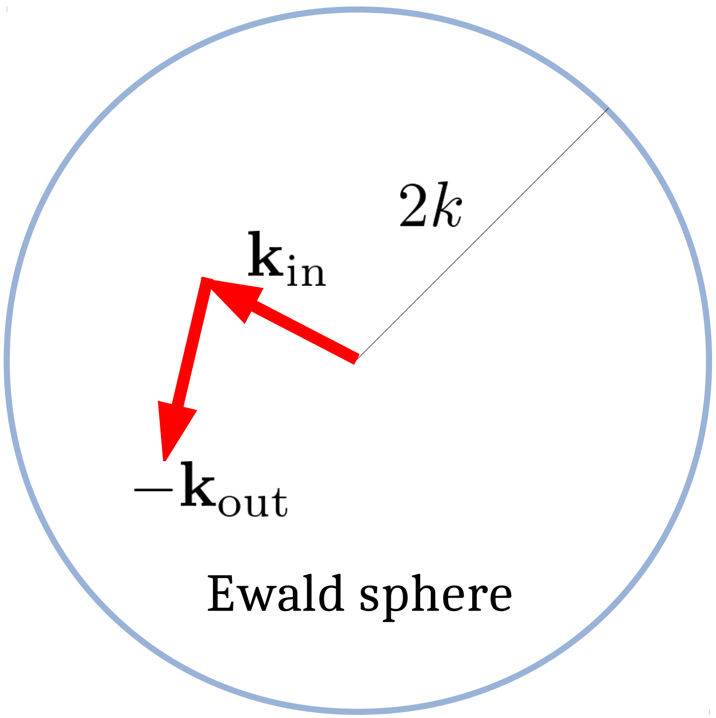
where

$$\tilde{V}(\mathbf{q}) = \int V(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3r$$

Scattering potential (can be complex)

$$|\mathbf{k}_{\rm in}| = |\mathbf{k}_{\rm out}| = k = \frac{\omega}{c}$$

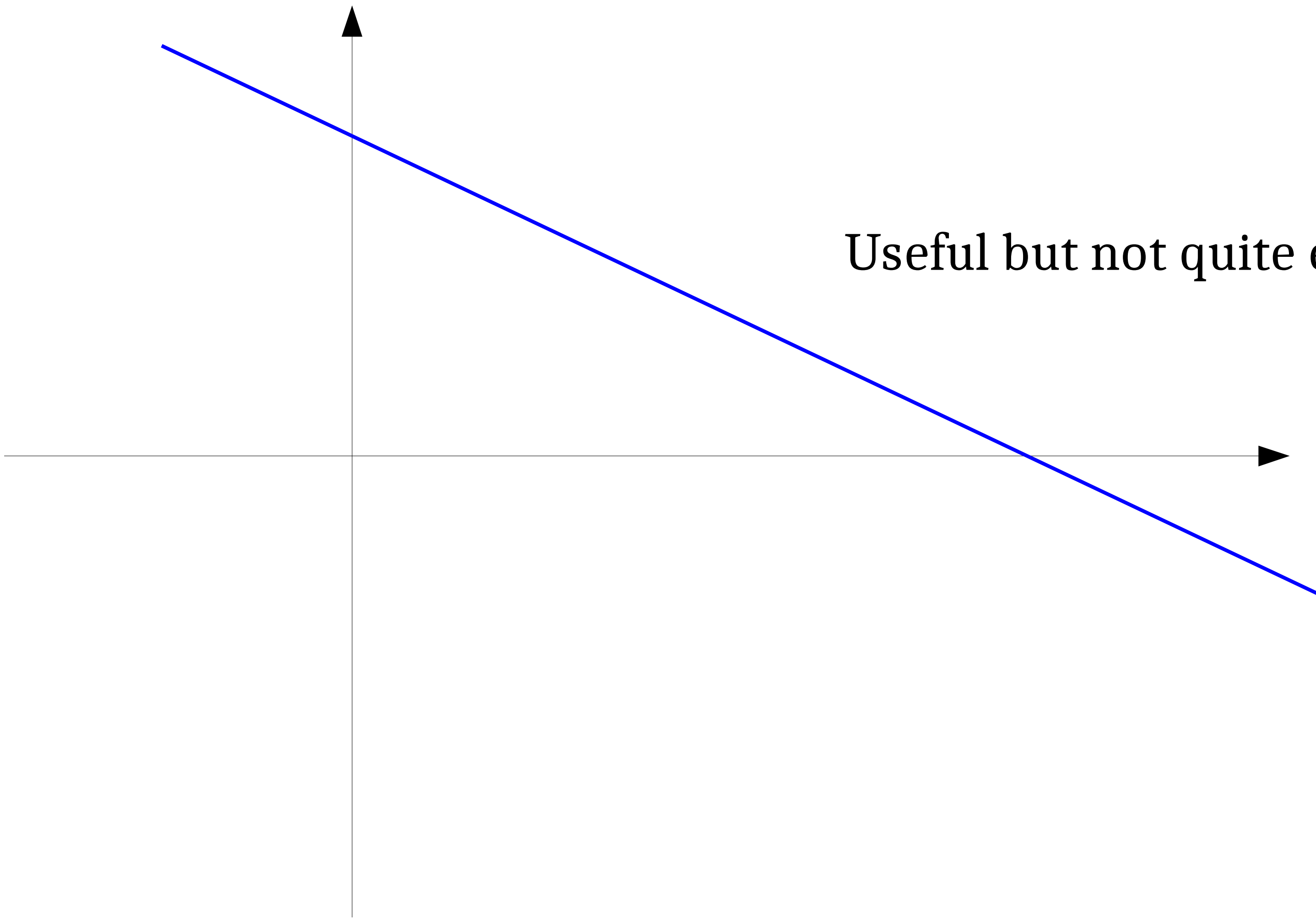




Methods to obtain super-resolution

- Use analytic continuation of Fourier data beyond the Ewald sphere
  - all measurements are discrete
  - it is not possible to analytically continue a discrete data set, at least, not without making assumptions about the unavailable frequencies (defeats the purpose)
- Near-field optics
  - ill-posed IP due to exponential decay of evanescent waves
  - requires a model for tip-object interaction
  - slow
- STORM (stochastic optical reconstruction microscopy), PALM (photo-activation localization mocroscopy)
  - not really tomographic imaging methods; rather, map-builders
  - sparsity is required + some additional assumptions
- Solve nonlinear ISP
  - V.A.Markel, Investigation of the effect of super-resolution in nonlinear inverse scattering, Phys.Rev. E 102, 053313, 2020
  - Conclusions are not optimistic
- Use physical constraints on the potential
  - subject of this talk

Physical constraints: Positivity (or more general bounds)



Useful but not quite enough

Simplest case of a compositional prior

$$\tilde{y}_m = \sum_{n=1}^{N} y_n e^{\mathrm{i}\,\xi nm}$$

$$y_n = \frac{1}{N} \sum_{m=-M}^{M} \tilde{y}_m e^{-\mathrm{i}\,\xi mn}$$

$$\xi = \frac{2\pi}{N}\,, \quad M = \frac{N-1}{2}$$

Here we assume for simplicity that N is odd

If we know all DFT coefficients $\tilde{y}_m$ with indexes in the range $-M \leq m \leq M$, we can reconstruct all y_m.

What if we know the DFT coefficients within the "band" $-L \leq m \leq L$ where $L < M$ and, in addition, that y_m can take only two values, say, a and b?

QUESTIONS:

Under which conditions can we reconstruct the original vector uniquely?

Is there a stable and sufficiently fast way to find the solution?

Reduction to binary vectors

$$y_n = a + (b-a)x_n \ , \quad x_n \in \{0,1\}$$

$$\Downarrow$$

$$\tilde{y}_m = aN\delta_{m0} + (b-a)\tilde{x}_m$$

$$\Downarrow$$

$$\tilde{x}_m = \frac{\tilde{y}_m - aN\delta_{m0}}{b-a}$$ $\Rightarrow$ It is sufficient to consider inversion of binary vectors

Problem:

Given a set of complex numbers ϕ_m with indexes in the range $-L \leq m \leq L$ where $L < M = \frac{N-1}{2}$, find a binary vector $\mathbf{x} = (x_1, x_2, \ldots, x_N)$ of length N, which satisfies

$$\sum_{n=1}^{N} e^{\mathrm{i}\,\xi mn} x_m = \phi_m \ , \quad \text{for } -L \leq m \leq L$$

Further details

1. $r \equiv \phi_0$ is the number of 1s in the vector $\mathtt{x}$ (the popcount). We assume that r is always known.

2. The set of all vectors $\mathtt{x}$ with given N and r is $\Omega(N, r)$ of the size $S[\Omega(N, r)] = \frac{N!}{r!(N-r)!}$

3. It is enough to consider $1 \leq r \leq (N-1)/2$ (symmetry). The cases $r = 1$ and $r = 2$ are exactly solvable. The case $r \sim N/2$ is the most difficult.

4. Distances:

$$\chi(\mathrm{x}, \mathrm{y}; L) = \left[\frac{1}{L} \sum_{m=-L}^{L} |\tilde{x}_m - \tilde{y}_m|^2 \right]^{\frac{1}{2}}$$

$$d(\mathrm{x}, \mathrm{y}) = \frac{1}{2} \sum_{n=1}^{N} |x_n - y_n|$$

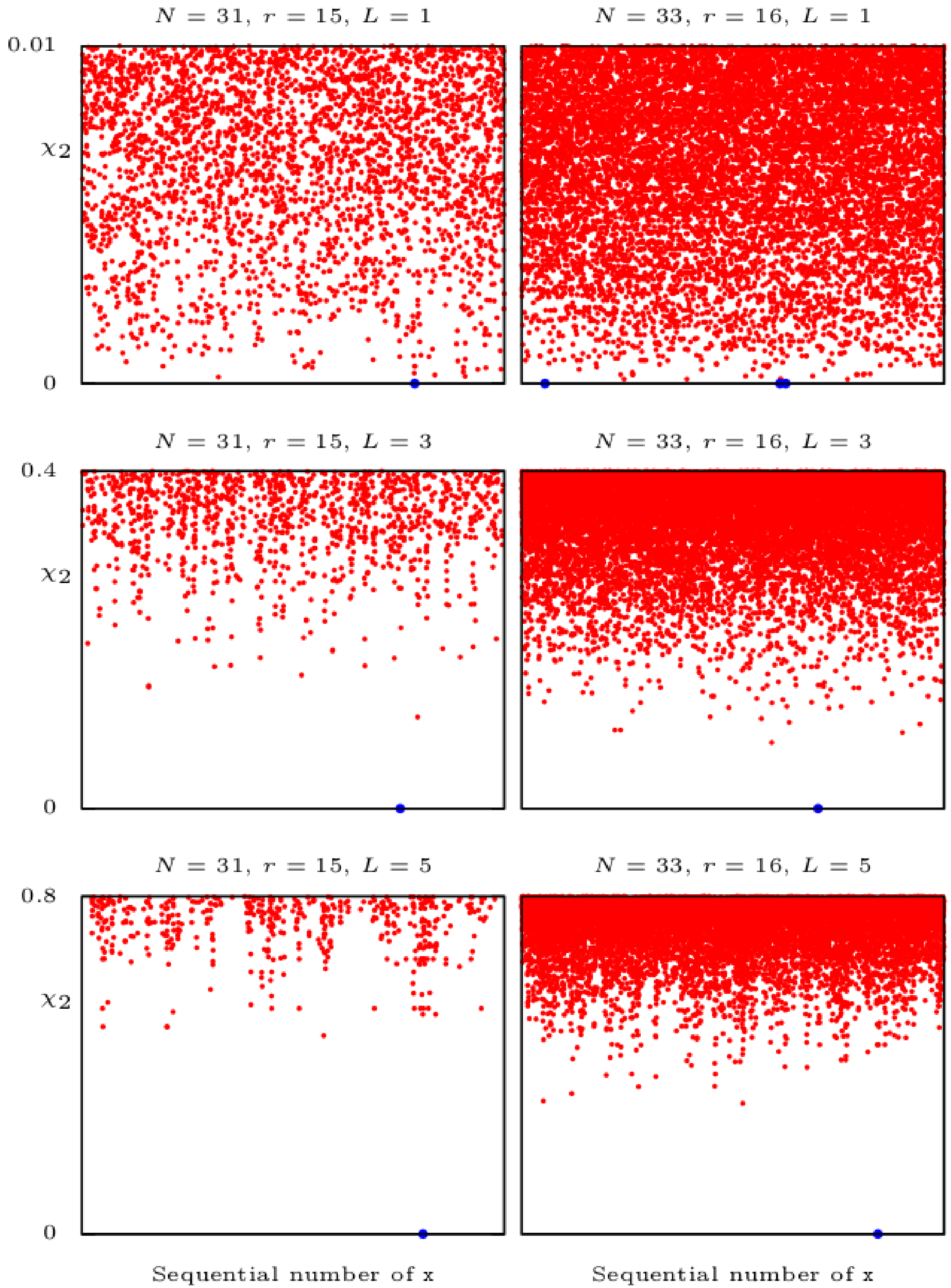
$$\chi(\mathrm{x}, \mathrm{y}; L) = 0$$

$$\Uparrow$$

$$d(\mathrm{x}, \mathrm{y}) = 0$$

$$\Updownarrow$$

$$\mathrm{x} = \mathrm{y}$$



Model (a) Model (b)

A numerical example:

Fourier space distances of all vectors with given N and r to a model

Model (a)

$$N = 31, \; r = 15, \; S[\Omega(N, r)] = 300,540,195$$

$$(1001011000011101101100011010100)$$

Model (b)

$$N = 33, \; r = 16, \; S[\Omega(N, r)] = 1,166,803,110$$

$$(100100110001100111001010100110110)$$

(a) N=31 is prime, and there is no false solutions in this example, even with L=1

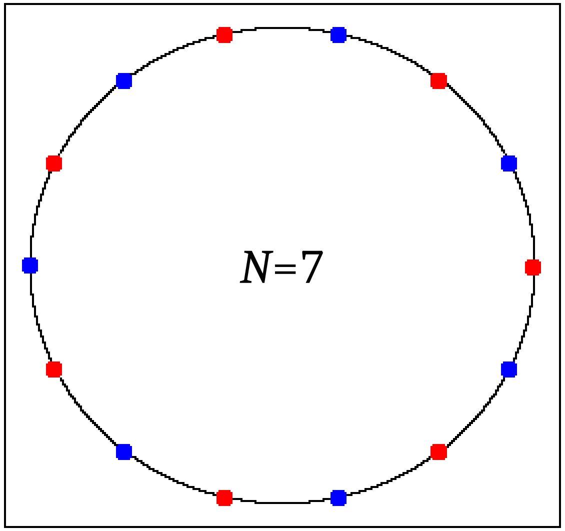
(b) N=33 is not prime, and there are 2 false solutions in this example with L=1 (and L=2); no false solutions with L=3

Uniqueness of inversion with *L*=1 for prime *N*

Let $\mathtt{x}, \mathtt{y} \in \Omega(N, r)$, $\mathtt{x} \neq \mathtt{y}$, and $\mathtt{z} = \mathtt{x} - \mathtt{y} \neq \mathtt{0}$.
Consider the first DFT coefficient of $\mathtt{z}$:

$$\tilde{z}_1 = \sum_{n=1}^{N} z_n e^{\mathrm{i}\,\xi n}\ , \qquad \xi = \frac{2\pi}{N}$$

$$\mathrm{z}_n = x_n - y_n \in \{0, +1, -1\}$$



For odd *N*:

Red dots: *N*-th order roots of unity

Blue dots: their opposites

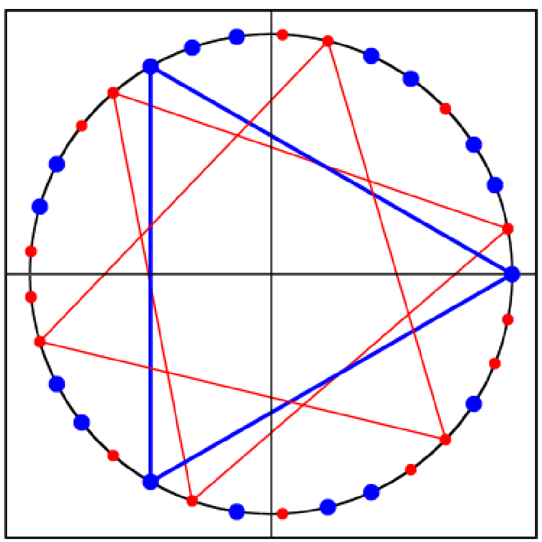
All dots: 2*N*-th order roots of unity

If *N* is prime, the non-zero terms in the sum cannot form a regular polygon. However, roots of unity sum to zero only if they can be partitioned into regular polygons (with possible cancellations of opposing roots – so-called asymmetric sums).

For prime N, all vectors in $\Omega(N,r)$ are $(L=1)$-distinguishable

If N is not prime, some of vectors in $\Omega(N,r)$ have $(L=1)$-indistinguishable pairs but others are still uniquely recoverable with $L=1$

If $N = pq$ where $1 < p \leq q$ are primes, then $\mathbf{x}$ is $(L = 1)$-indistinguishable from some other vector(s) in $\Omega(N, r)$ if and only if $\mathbf{x}$ contains at least one pair of either p- or q-gons in 0s and 1s (p-gon is a regular polygon with p vertices). Equivalently, $\mathbf{x}$ is $(L = 1)$-distinguishable from all other vectors in $\Omega(N, r)$ if and only if it does not contain any pairs of p- or q-gons.



Model (b) with N=33

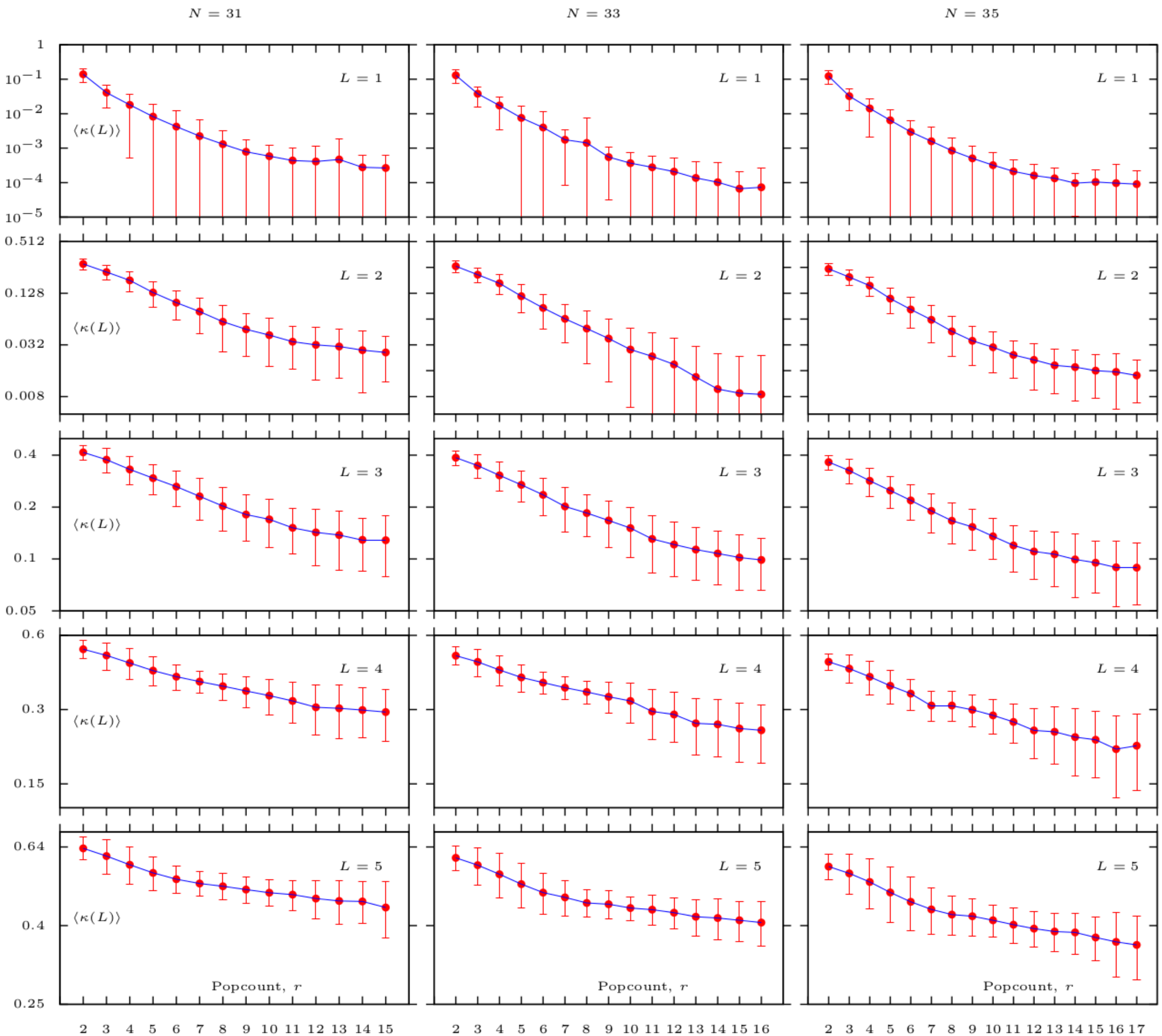
All roots of unity $e^{\mathrm{i}\frac{2\pi}{N}n}$ for $N = 33$

Large blue dot if $\mathbf{x}$ has 1 in n-th position

Small blue dot if $\mathbf{x}$ has 0 in n-th position

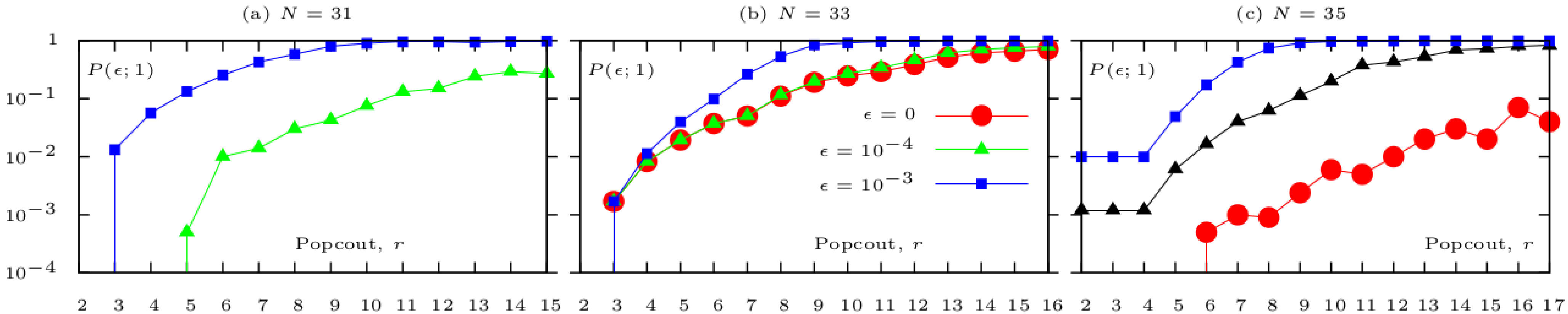
Two pairs of 3-gons

Difficult to compute the number of uniquely-recoverable vectors in $\Omega(N,r)$, but here is some statistical analysis



$$\kappa(\mathrm{x}; L) = \min_{\mathrm{y} \neq \mathrm{x}} \chi(\mathrm{x}, \mathrm{y}; L)$$

More statistical analysis...



$P(\epsilon; L)$ is the fraction of vectors in $\Omega(N, r)$ with at least one distinct neighbor that is at least as close in Fourier space as ϵ.

Data are shown for $L = 1$, however, we can describe the results for larger L a follows:

(a) $N = 31$: all displayed fractions are zero if $L > 1$.

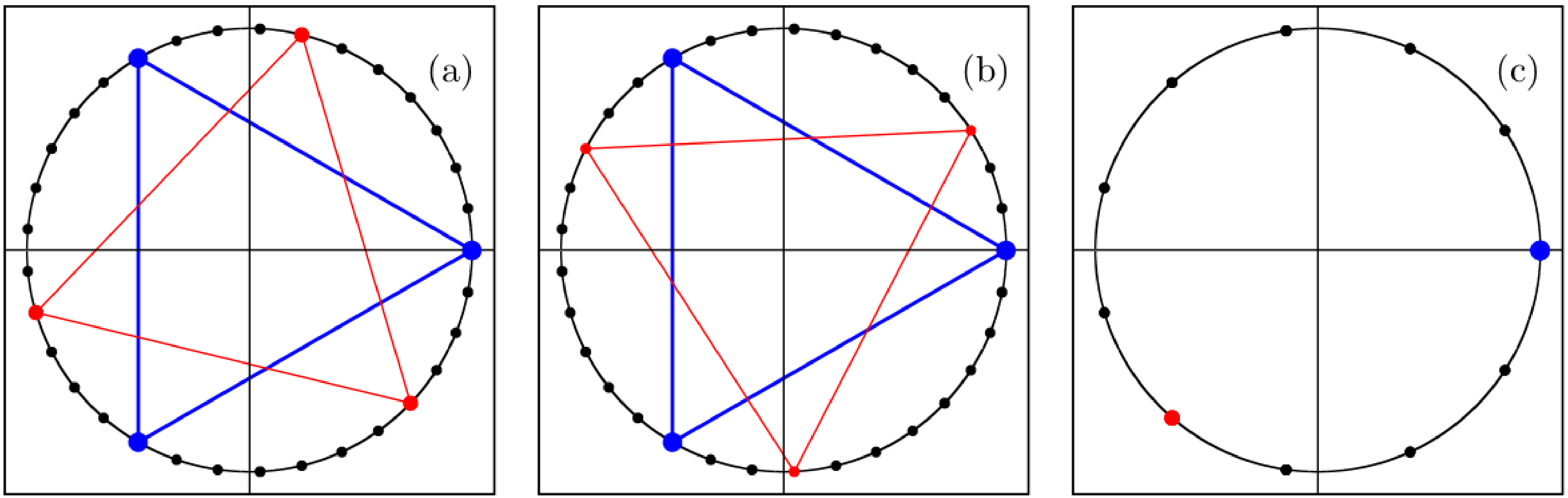
(b) $N = 33$: all fractions are either zero or too small to be shown if $L > 2$. $L = 2$ case is not significantly different from $L = 1$.

(c) $N = 35$: all fractions are zero or small for:

(i) $r < 5$ and $L \geq 1$
(ii) $5 \leq r < 7$ and $L \geq 5$
(iii) $7 \leq r \leq 17$ and $L \geq 7$

Uniqueness of inversion for non-prime N

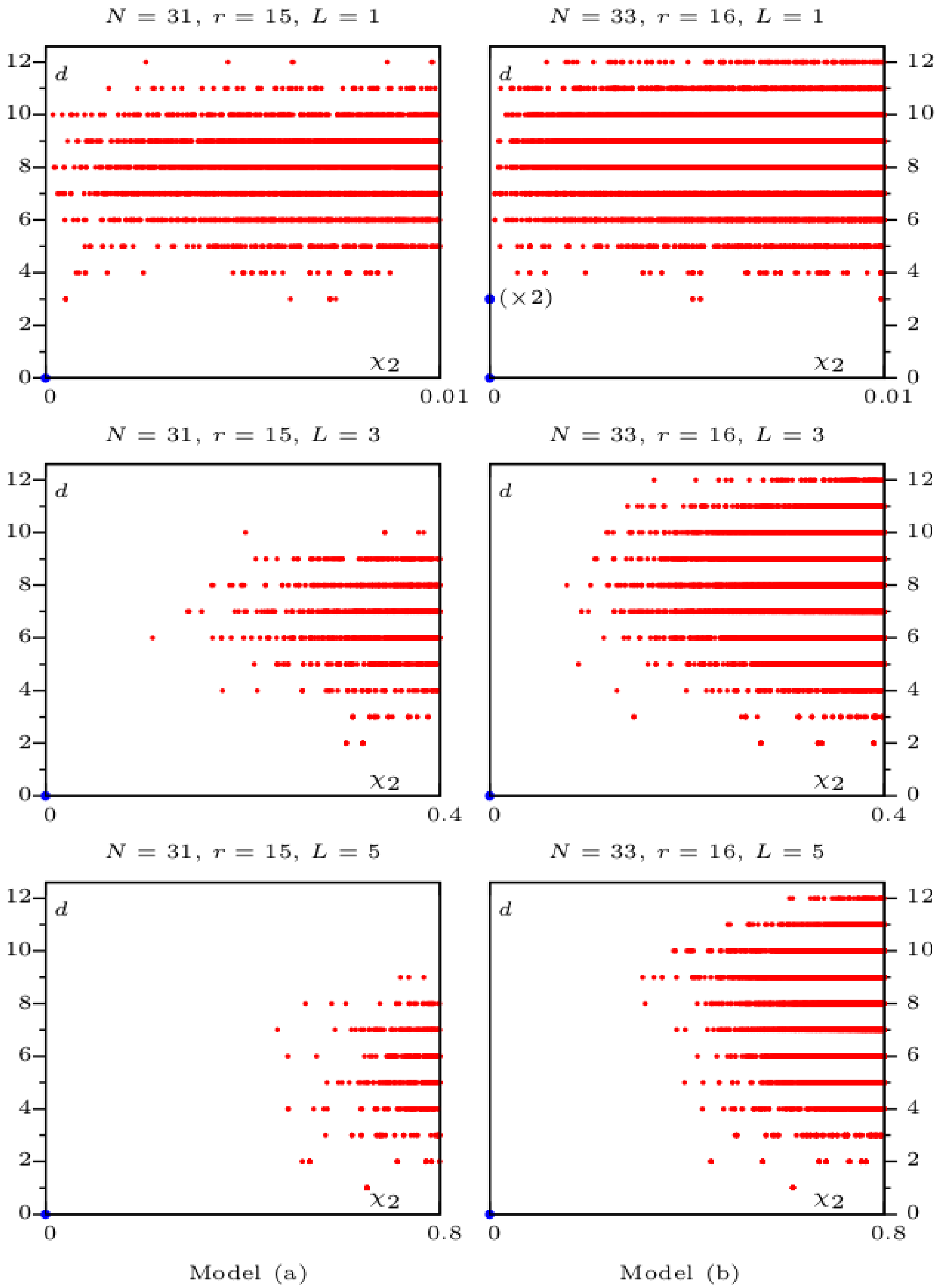
Let $N = pq$ with $1 < p \leq q$ primes and $1 < r \leq M = \frac{N-1}{2}$. Then the inverse problem of recovering *any* $\mathtt{x} \in \Omega(N, r)$ is uniquely solvable for $L \geq \min\left(\max(p, q), r\right)$.



m=1 m=2 m=3

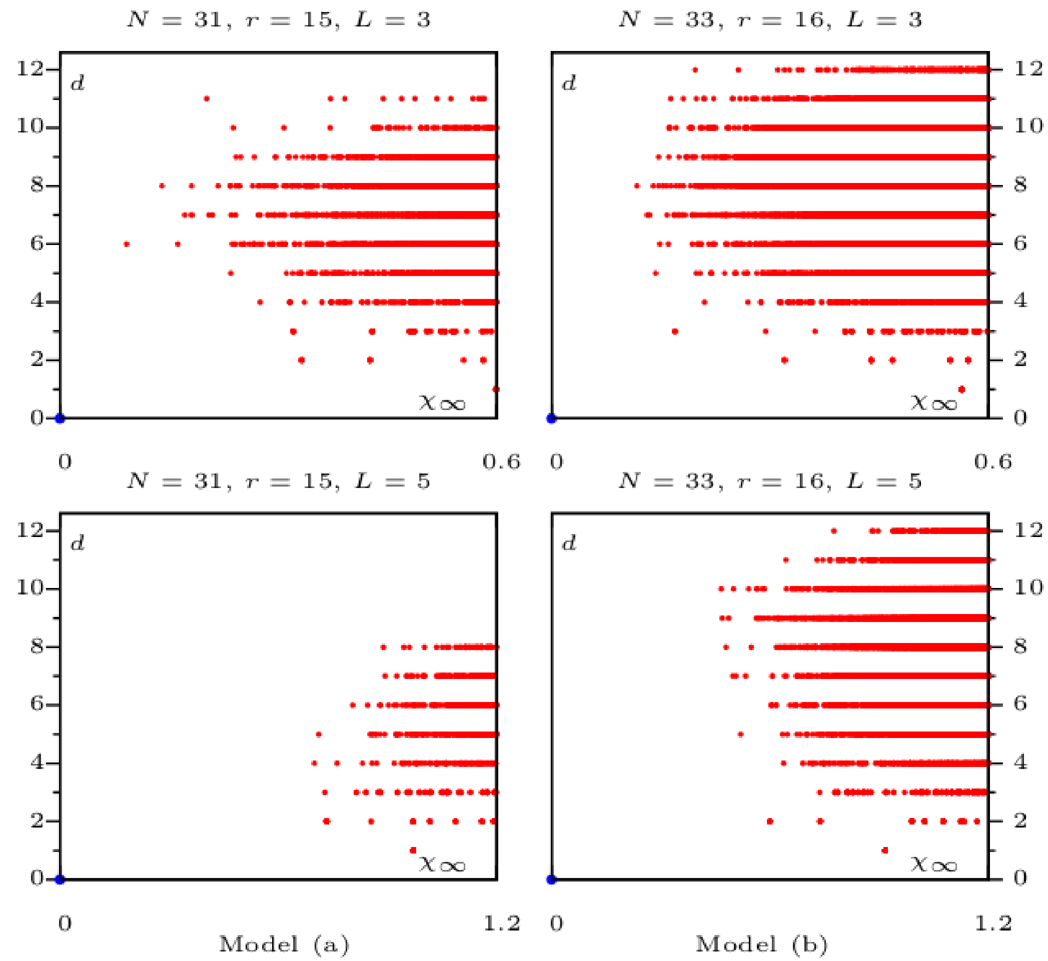
Non-zero terms in the sum $\tilde{z}_m = \sum_{n=1}^{N} e^{\mathrm{i}\,\xi m n} z_n$ for Model (b) with $N = 33$.

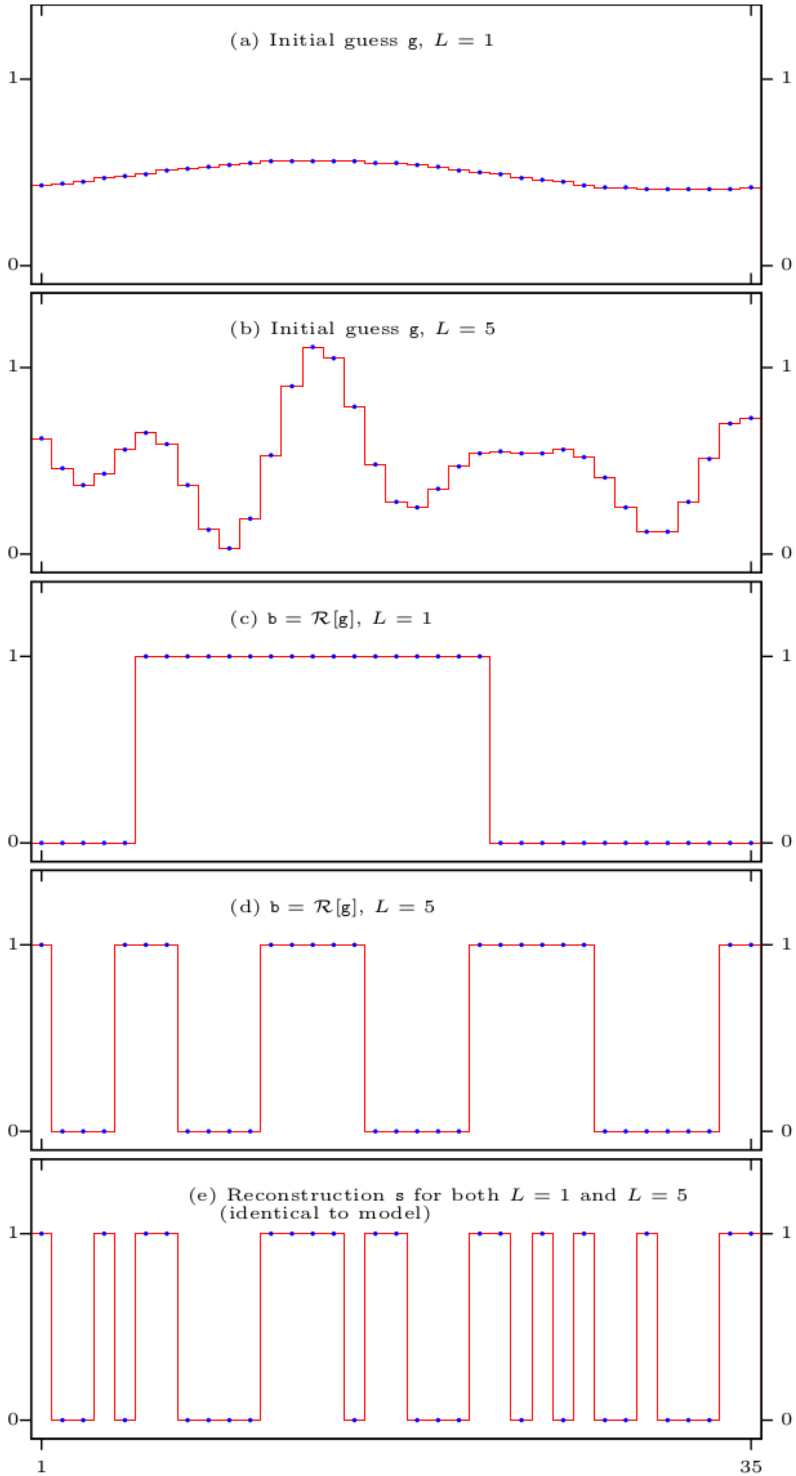
Here $\mathtt{z} = \mathtt{x} - \mathtt{y}$ where $\mathtt{x}$ and $\mathtt{y}$ is a pair of $(L = 1)$-indistinguishable vectors. Red dots correspond to $x_n - y_n = 1$, blue dots to $x_n - y_n = -1$.



How to reconstruct?

Optimization in Fourier space will not work





Combinatorial method: works for relatively small N

1. Start with band-limited inverse DFT (not binary)

2. Use thesholding to obtain a binary approximation (initial guess for the combinatorial search)

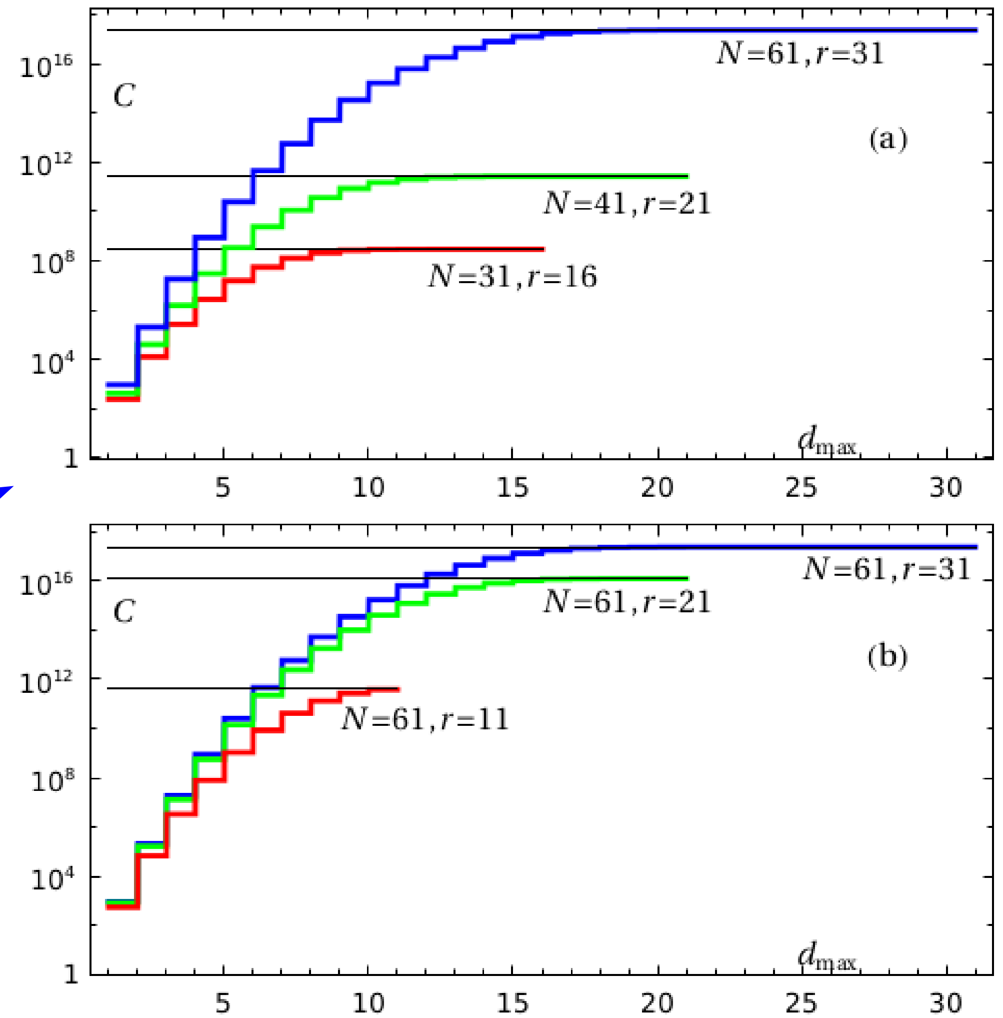
3. Use recursive pairwise switches to search for solution

a) Not the same as exhaustive search (faster)
b) Still NP-hard
c) Critically depends on initial guess
d) Useful to run a cycle over recursion depth

Reconstruction shown is for N=35, r=17

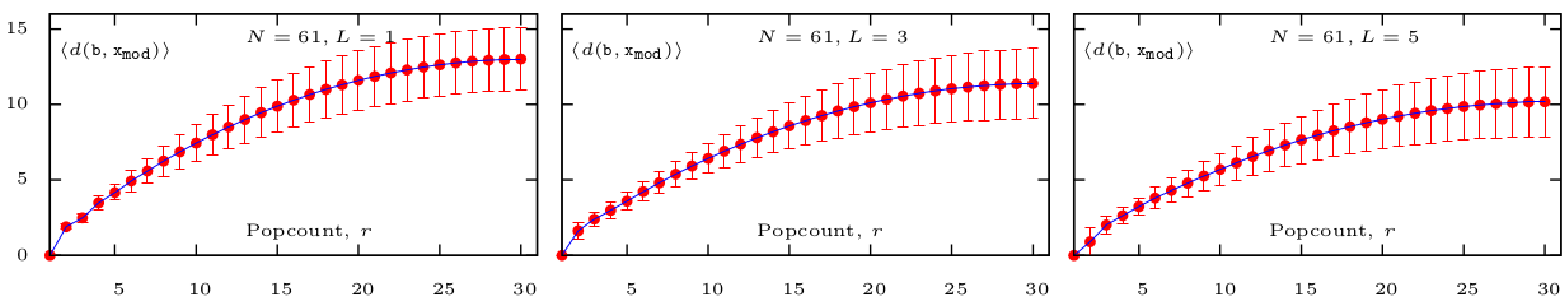
Exact solution found with L=1 and L=5 (faster with L=5)

Complexity of combinatorial inversion



Complexity for some N and r as a function of depth of recursion. Depth must be at least equal to the distance between initial guess and solution.

Average distance between initial guess and solution as a function of popcount for N=61, various L



Non-convex optimization (can work for larger *N*)

We start from the band-limited reconstruction but do not use thresholding at this stage. Instead, we work with non-binary vectors and optimize the functional

$$F[\mathbf{x}] = \sum_{n=1}^{N} x_n^2 (x_n - 1)^2$$

Updated vector stays consistent with the data

General update step: $\mathbf{x} \longleftarrow \mathbf{x} + \beta \mathbf{d}$

$$d_n = \sum_{m=L+1}^{M} \left[c_m \cos(\xi m n) + s_m \sin(\xi m n) \right]$$

Steepest descent direction:

$$c_m = 2 \sum_{n=1}^{N} u_n \cos(\xi m n) \ , \quad s_m = 2 \sum_{n=1}^{N} u_n \sin(\xi m n) \ ,$$

where

$$u_n = x_n (x_n - 1)(2 x_n - 1)$$

Non-convex optimization (cont.)

Finally, the length of the step β is determined from the cubic equation

$$a_0 + a_1\beta + a_2\beta^2 + a_3\beta^3 = 0$$

$$a_0 = \sum_{n=1}^{N} x_n(x_n - 1)(2x_n - 1)d_n$$

$$a_1 = \sum_{n=1}^{N} [2x_n(x_n - 1) + (2x_n - 1)^2]d_n^2$$

$$a_2 = 3\sum_{n=1}^{N} (2x_n - 1)d_n^3$$

$$a_3 = 2\sum_{n=1}^{N} d_n^4$$

The functional $F[\mathtt{x} + \beta\mathtt{d}]$ is a 4-th order polynomial with a positive senior coefficient. It either has one minimum or two minima and one maximum in between. If the above cubic has 3 real roots, the latter scenario is realized (but this is very rare). In any case, we select the nearest minimum.

Non-convex optimization (cont.)

Problem: there are many local minima

However, we can tell that a minimum is not the global minimum by looking at its depth

If we end up in a local minimum, make a random jump and search for a minimum again

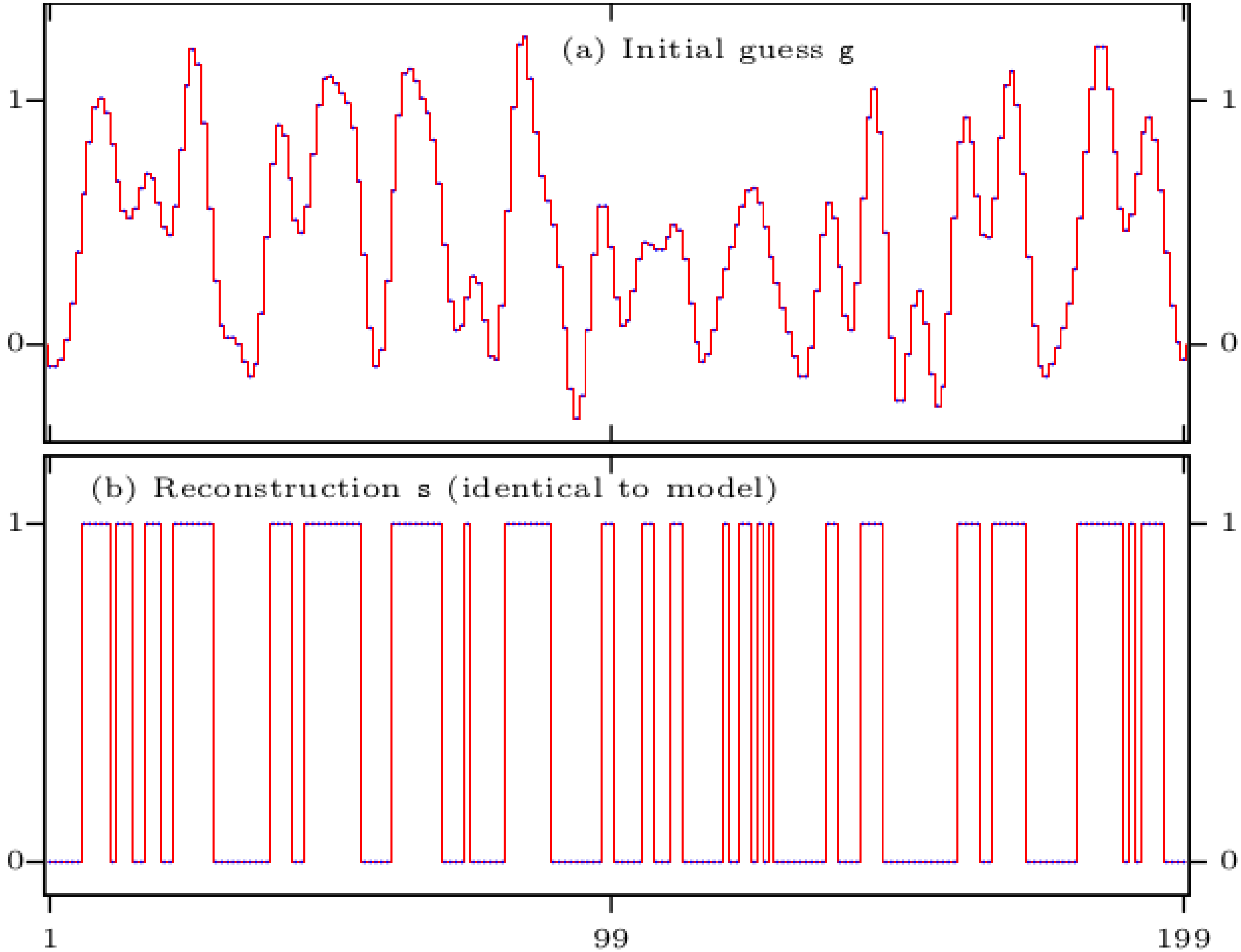
- can jump in random directions from the original initial guess
- can jump from the most recent minimum (random walk over local minima)

Random jumps work if the initial guess is not too far from the solution.

This requires that the number of known DFT coefficients is not too small.

The problem is hardest for random models and much simpler for models with structure (i.e., one or two pulses)

Non-convex optimization: Example with N=199, L=29



Blurred initial guess

If approximated by a binary vector, 16 bits are wrong

Reconstruction by non-convex optimization (about 50sec on my laptop)

Reconstruction is exact

Generalization to 2D

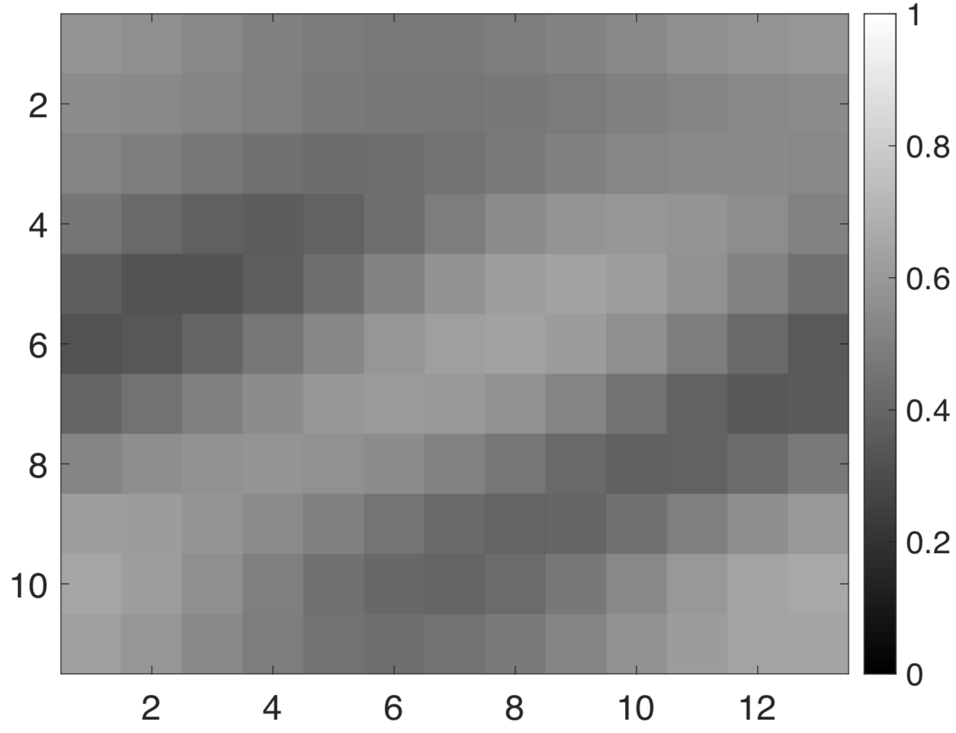
Rectangular images x_{nm} with prime dimensions $N_1 \neq N_2$ are uniquely determined by only four DFT coefficients including the popcount: $r = \tilde{x}_{00}$, $\tilde{x}_{01}$, $\tilde{x}_{10}$ and $\tilde{x}_{11}$. (But this is hardly enough for stability, at least for non-sparse images.)

(This is proved by mapping the DFT of a matrix onto that of a vector)

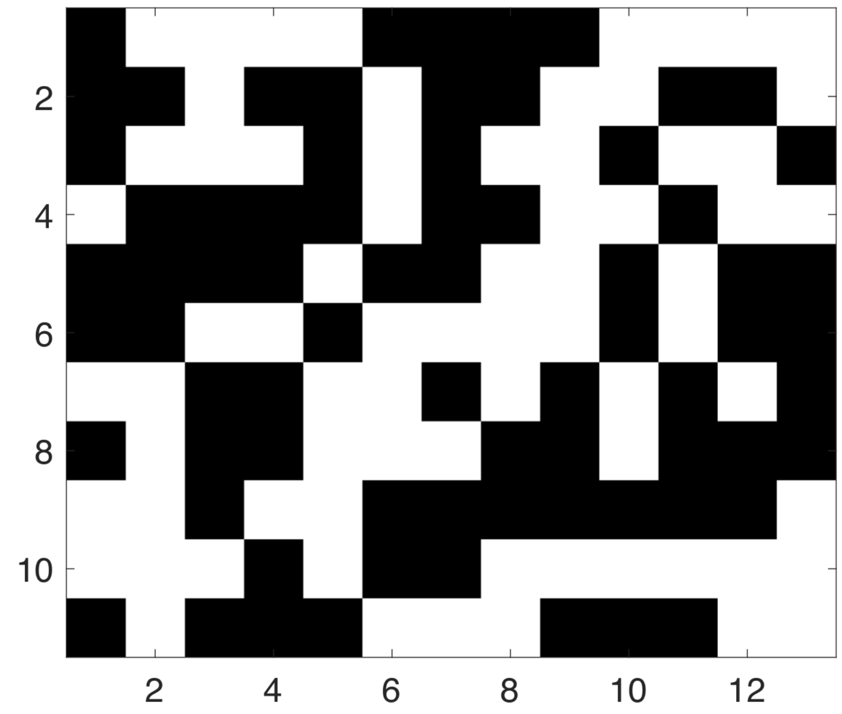
For square images x_{nm} with prime dimension $N = N_1 = N_2$ the mapping to a 1D vector does not quite work because of cancellations and in the expression $(N_1 n + N_2 m)/N_1 N_2$. The difference $\mathtt{z} = \mathtt{x} - \mathtt{y}$ does not sample all roots of unity of the order $N_1 N_2$.

In the case of square matrices or prime size, we need all DFT coefficients in the central square of dimension $L = \mathrm{floor}(\sqrt{N})$.

Example: Reconstruction of a rectangular 13x11 image from only four DFT coefficients (minimum required for uniqueness).

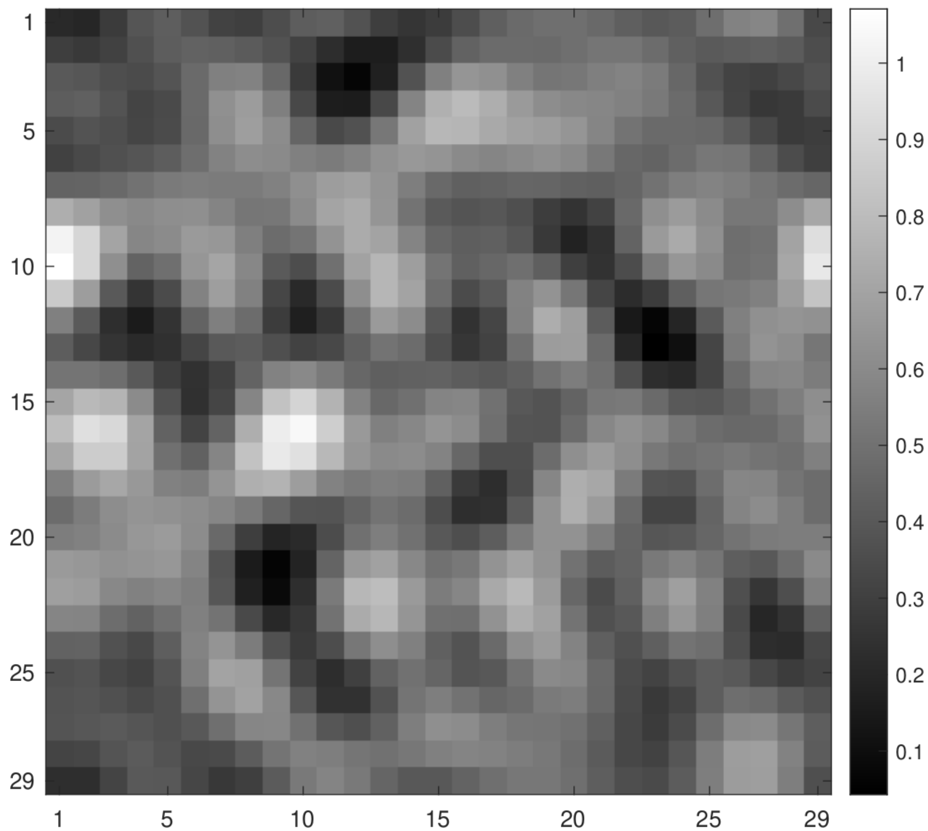


Severely low-pass filtered at L=1 (blurred) image



Reconstruction (exact)

Example: Reconstruction of a square 29x29 image with *L*=5 (band limit *M*=(29-1)/2=14)



Blurred image (band limit is approximately 1/3 of complete)

Reconstruction (exact)

No *a priori* knowledge (i.e., corners) was used

Concluding Remarks

- We can hope to reconstruct not very large images from severely blurred versions using the binarity constraint
- The reconstruction of QR code shown is reproduible (was tested on ~100 random images with consistent success).
- Random images are much harder to reconstruct than images with structure and connectivity. So, in many applications, the methods will be more powerful than in our simulations, which consider the most difficult case
- We are looking for exact reconstructions, not approximations
- The method can tolerate some noise in the data. The larger L, the better noise tolerance
- Connection to medical imaging – discrete tomography