Statistical physics and statistical inference

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What is inference?

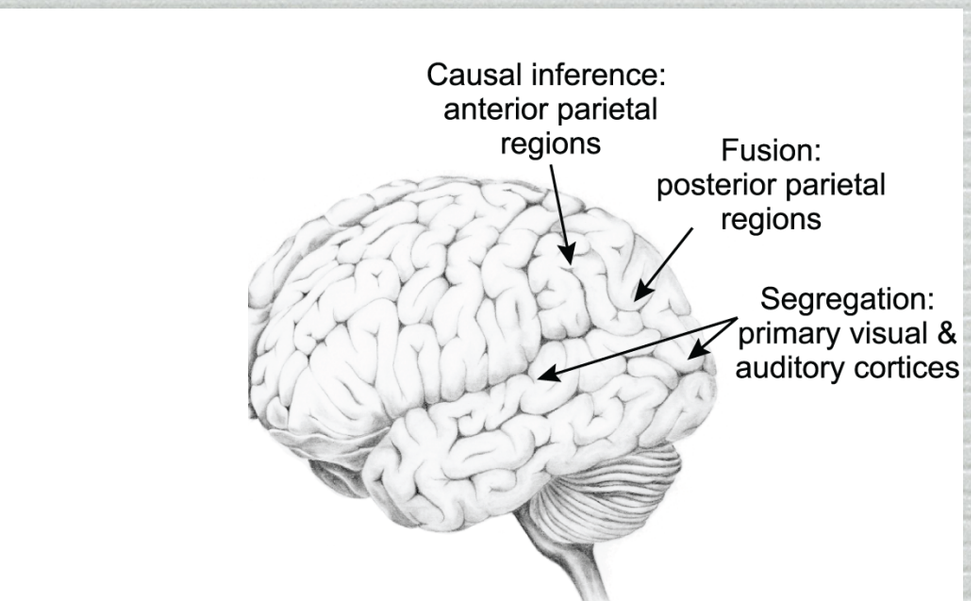
Brain, deduction, reasoning, learning…

Psychology : inference = production of new internal representations on the basis of previously held representations

eg : - perceptions → expectations → action

- conceptual thinking

Not necessarily conscious (while reasoning is)



see eg Mercier Sperber 2011

What is inference?

Statistics

Infer a hidden rule, or hidden variables, from data.

Restricted sense : find parameters of a probability distribution

Urn with 10.000 balls. Draw 100, find 70 white balls and 30 black

Best guess for the composition of the urn? How reliable? Probability that it has 6000 white- 4000 black?

If only black and white balls , with fraction x of white, probability to pick-up 70 white balls is $\binom{100}{70} x^{70}(1-x)^{30}$

Log likelihood of x : $L(x) = 70 \log x + 30 \log(1-x)$

Maximum at $x^* = .7$ Probability of .6 : $e^{L(.6)-L(.7)}$

Bayesian inference

Unknown parameters	x	|	Prior	$P(x)$
Measurements	y	|	Likelihood	$P(y\|x)$

Posterior $$P(x|y) = \frac{P(y|x)P(x)}{P(y)}$$

Bayesian inference

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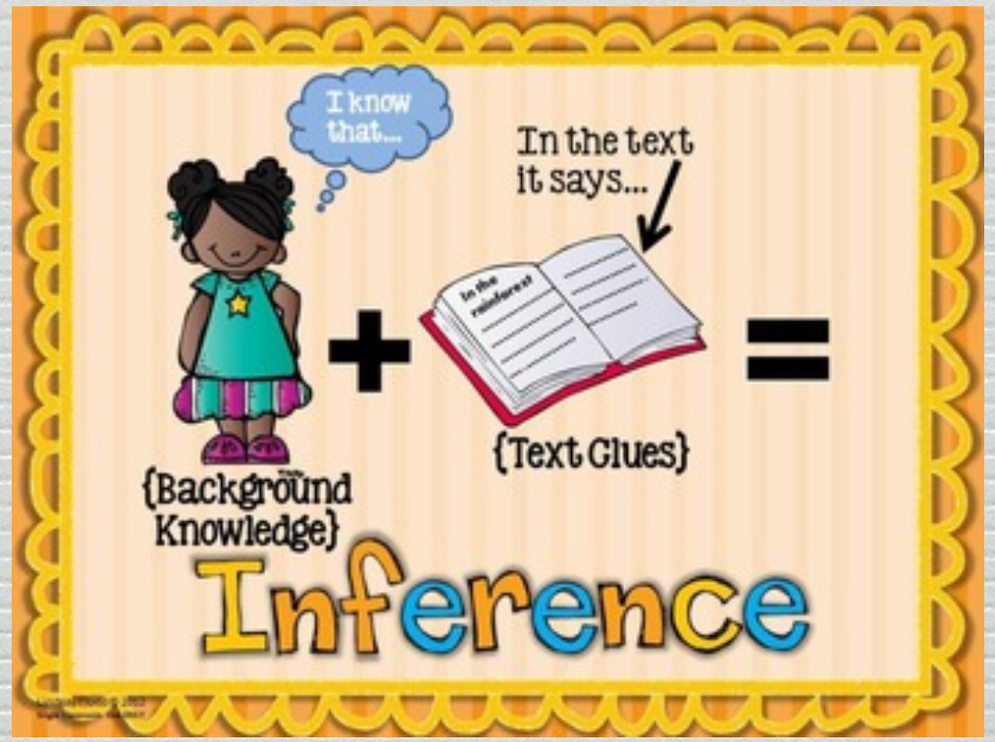
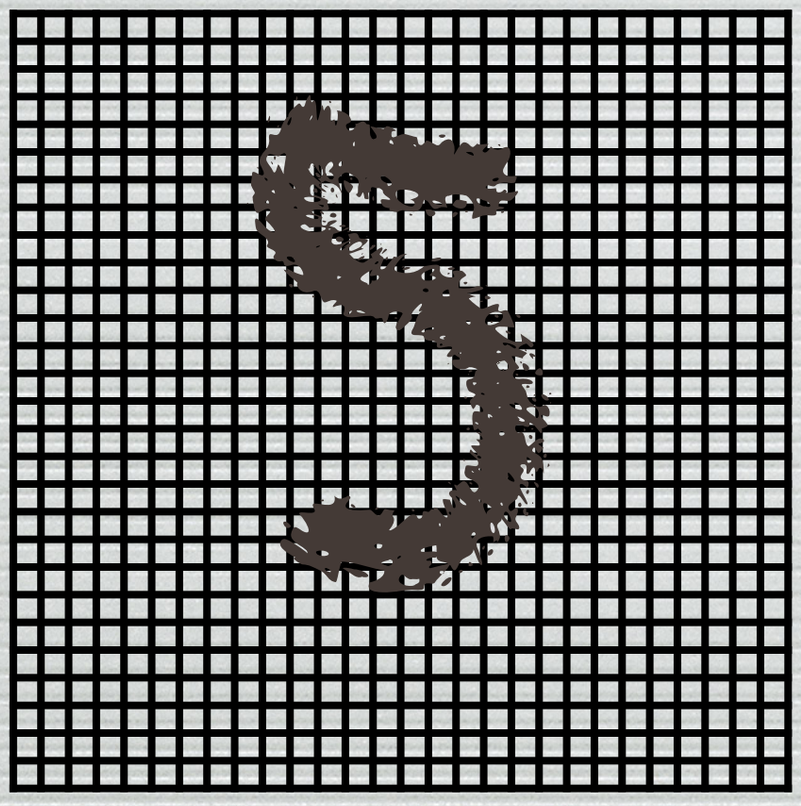
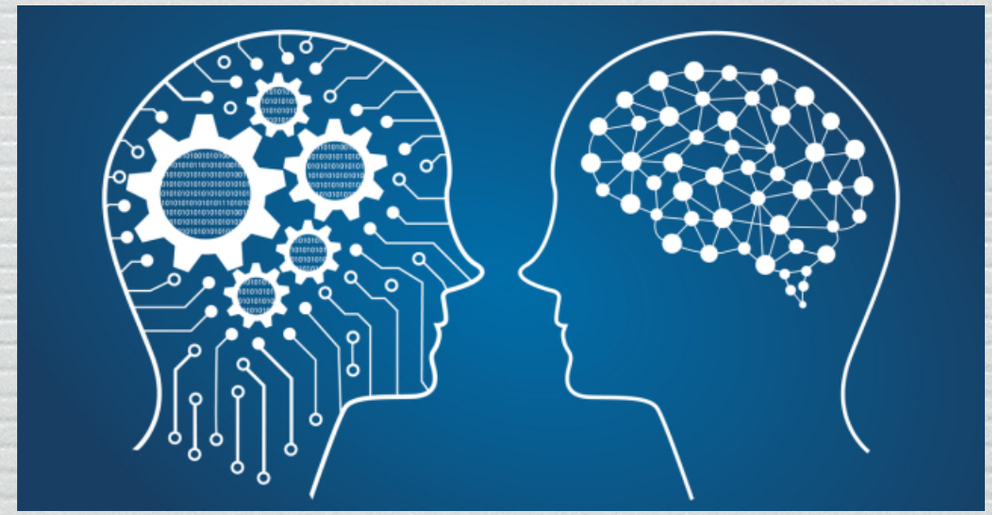


What is inference?

Artificial intelligence,
machine learning





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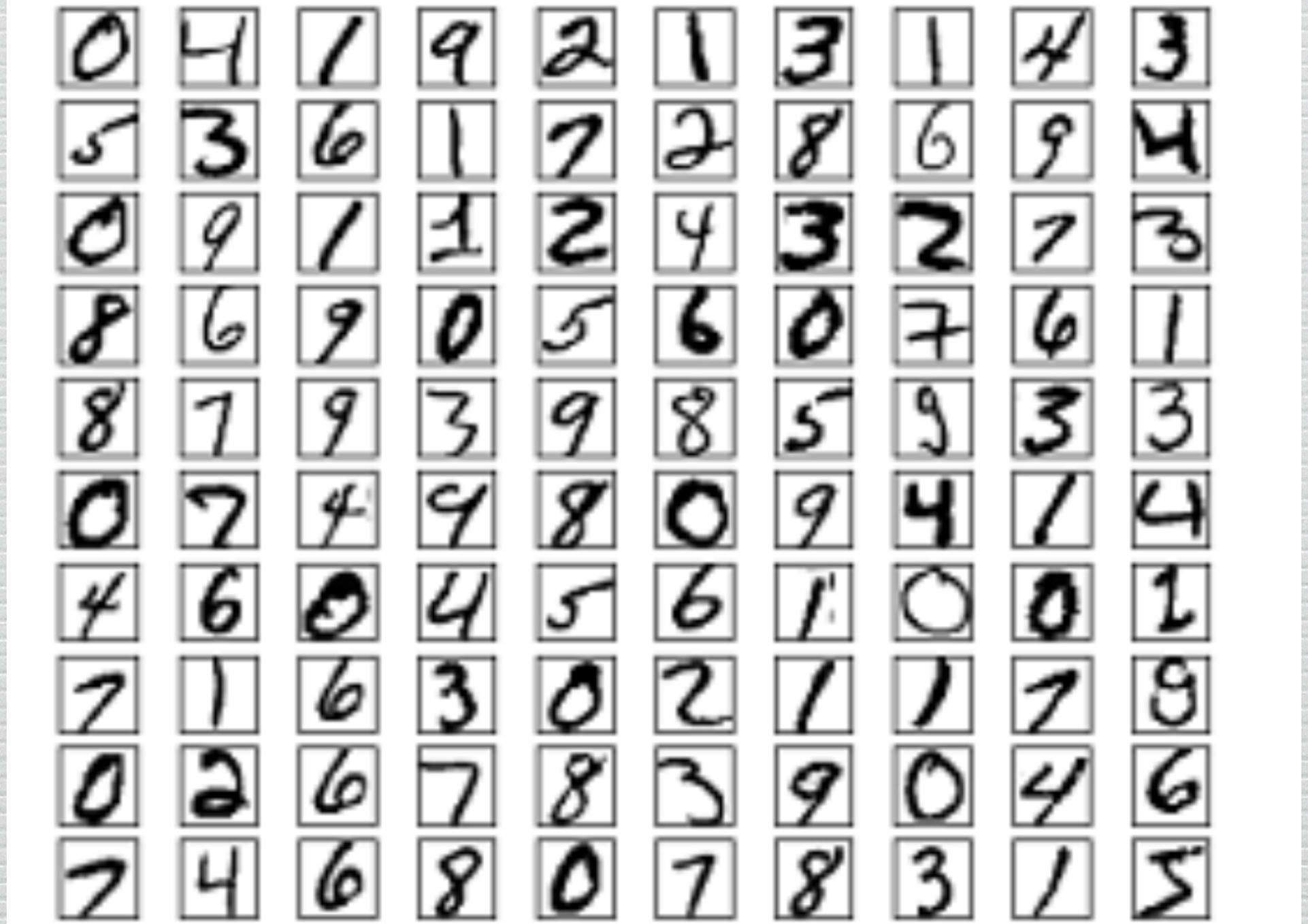
Find a machine that reads handwritten digits…

…inferring its parameters from examples



MNIST database : 70,000 images of digits, segmented, 28×28 pixels each, greyscale. Known output (supervised learning)

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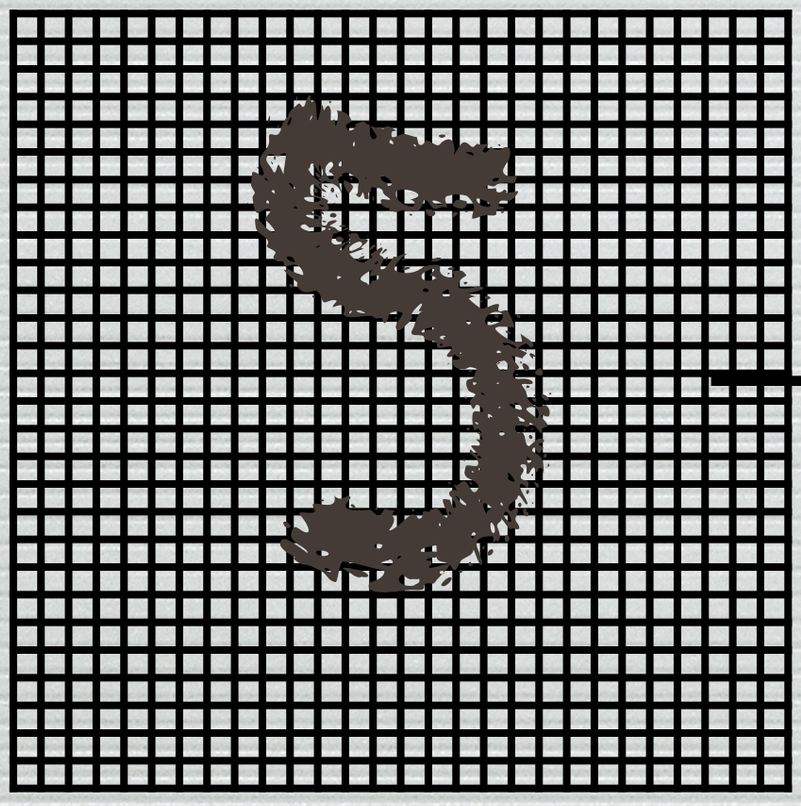
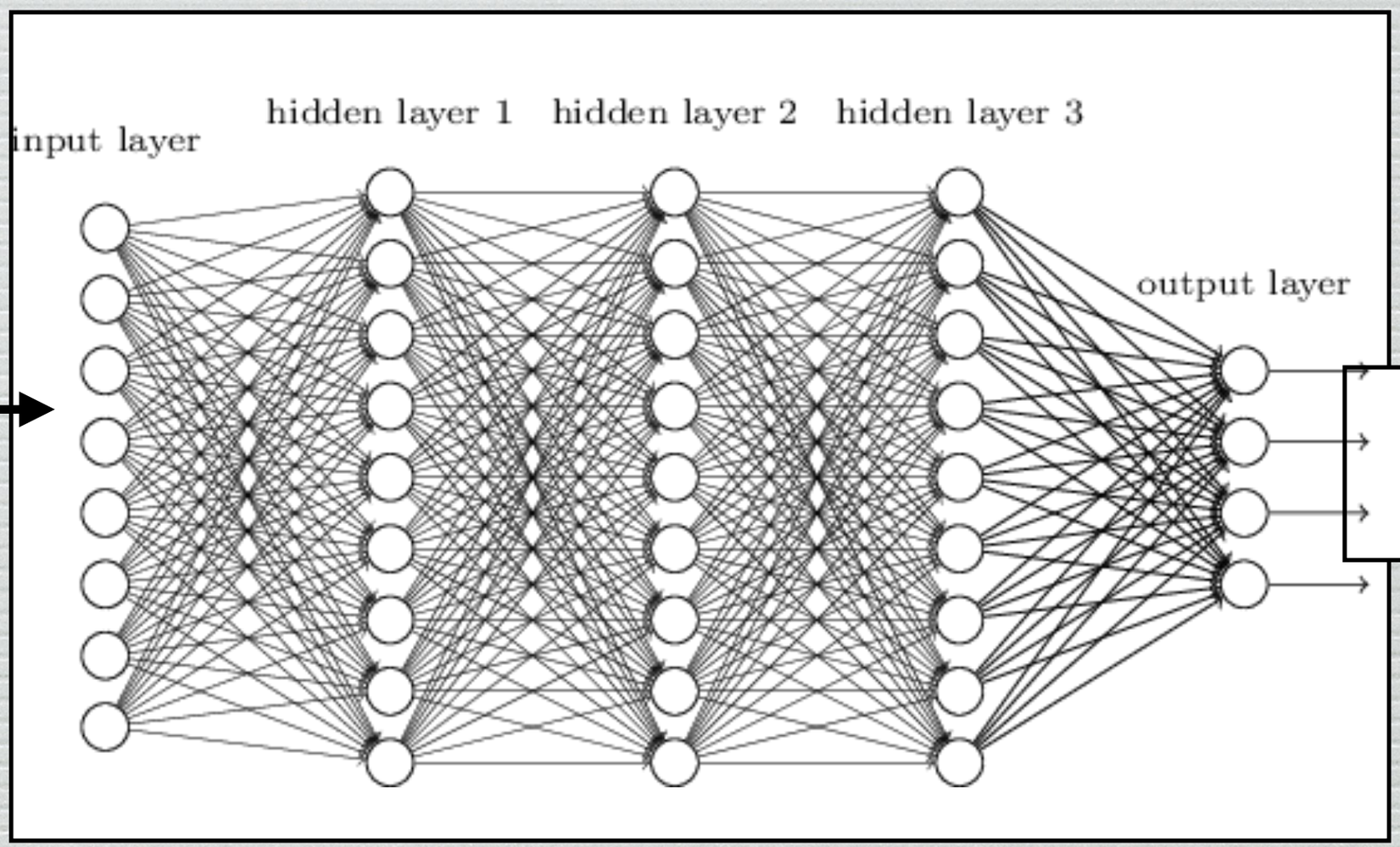
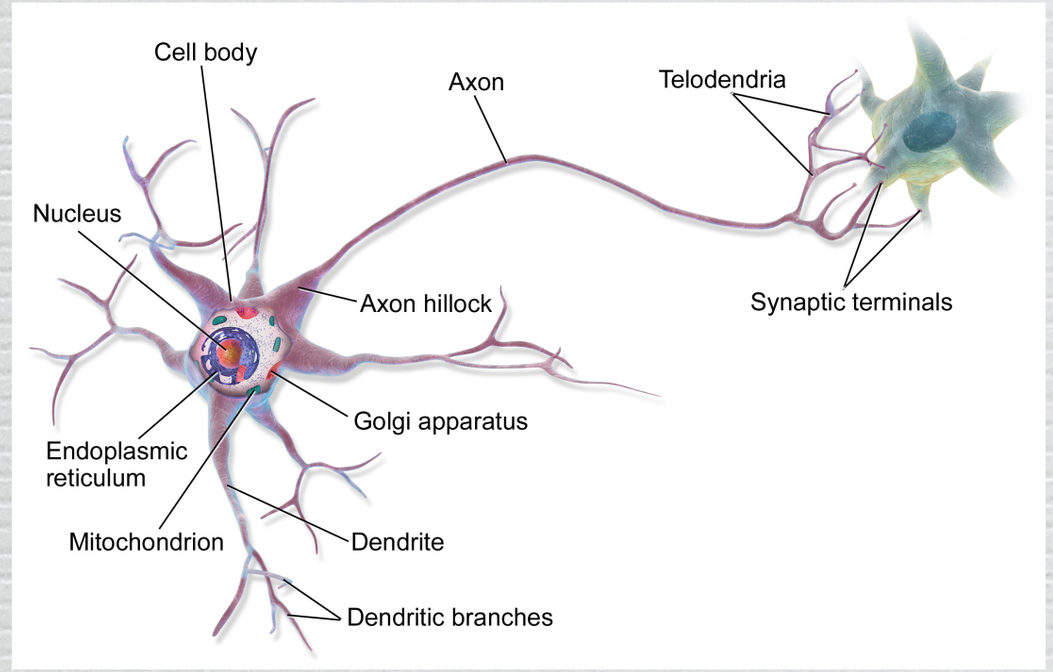
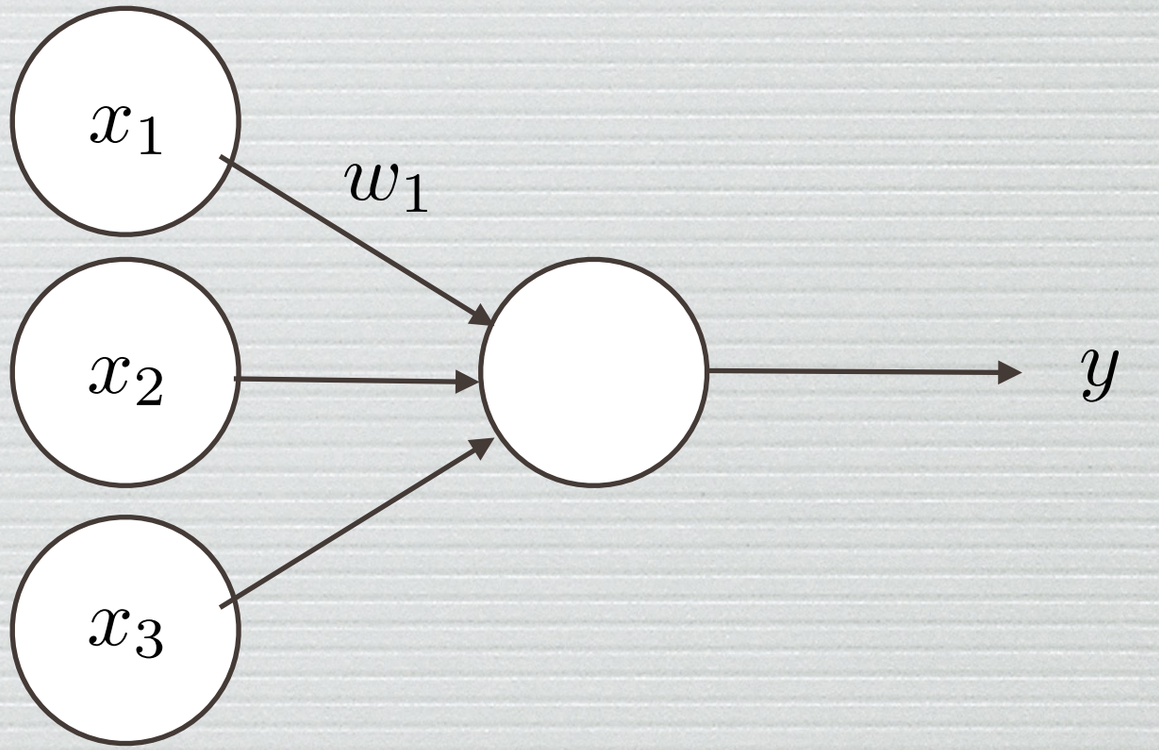




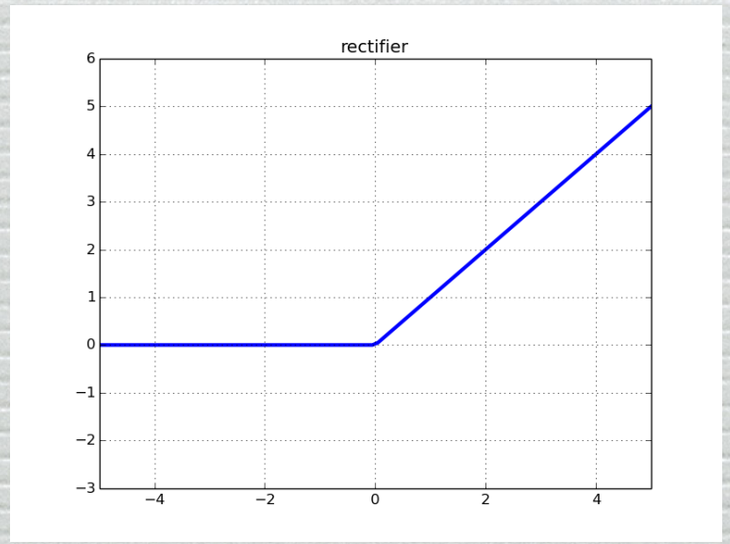
« Neural network » : artificial neurons

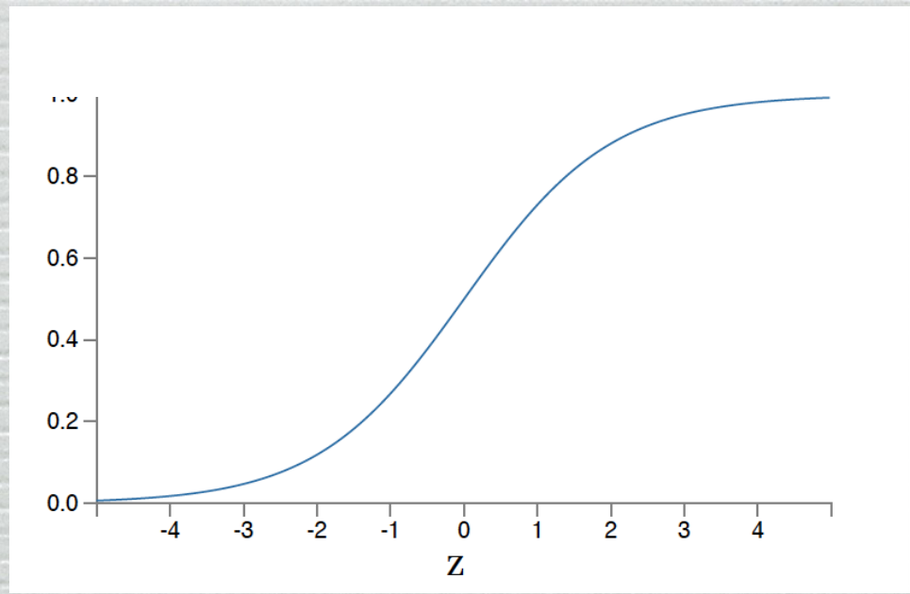




$$y = f(w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3)$$

Formal neural network





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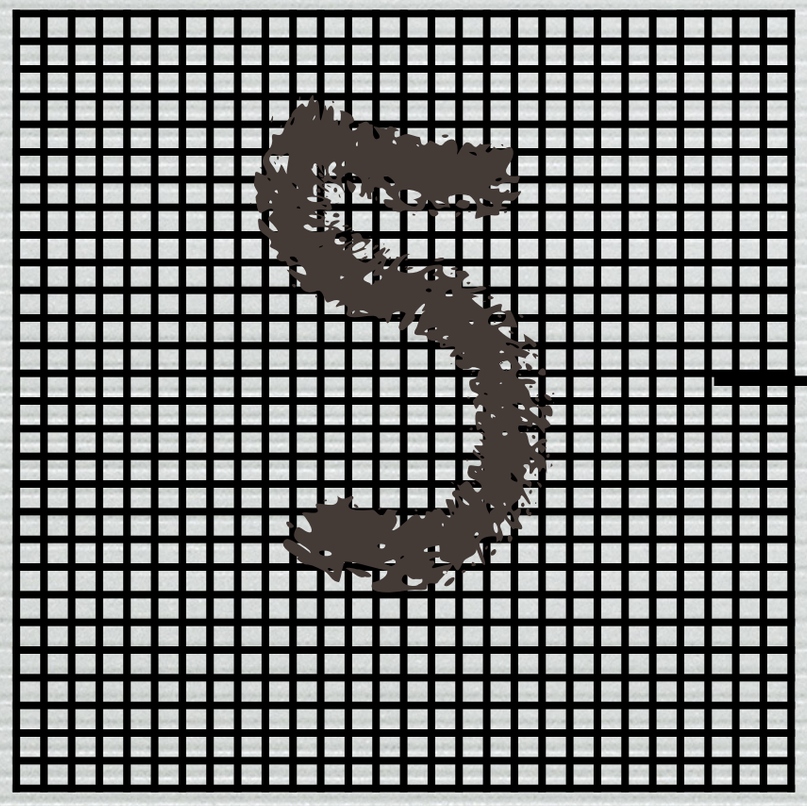
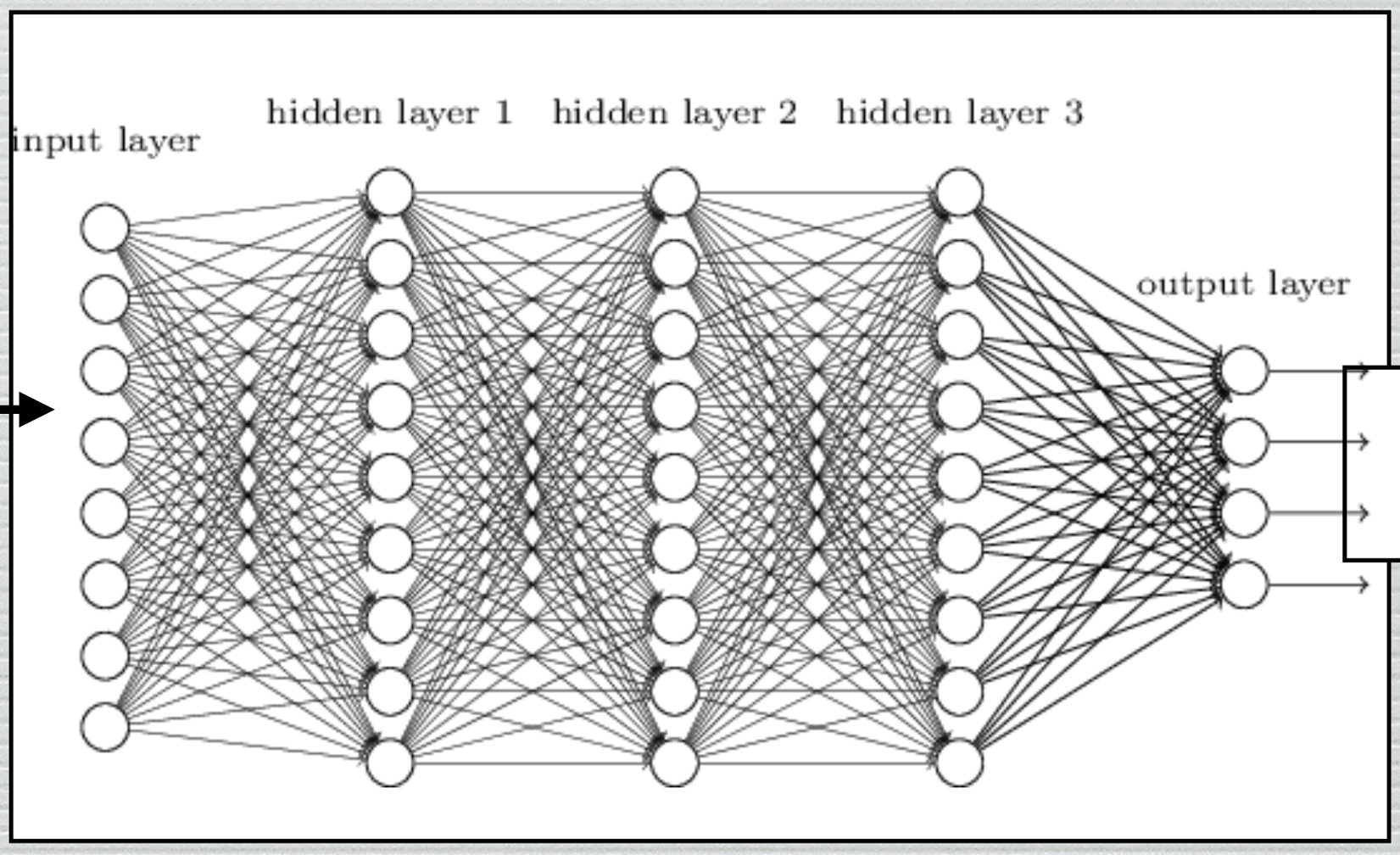


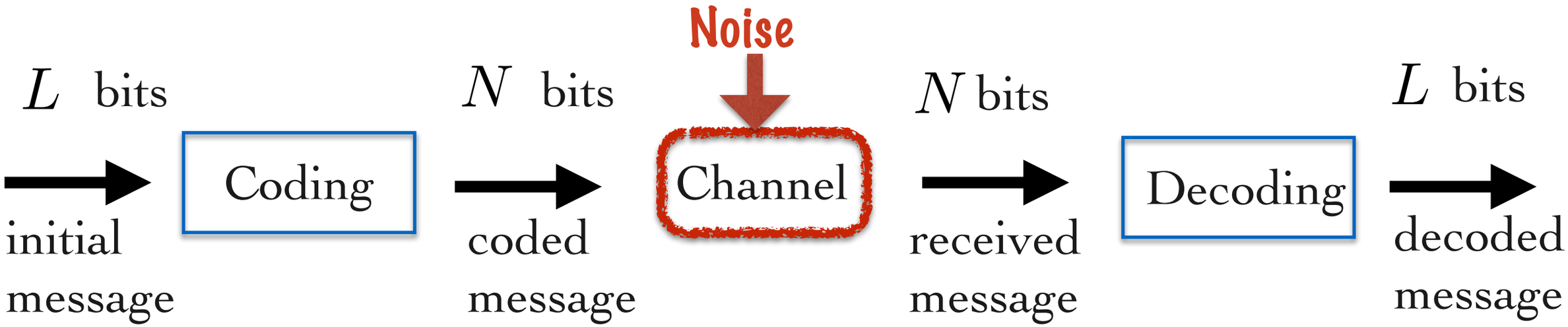


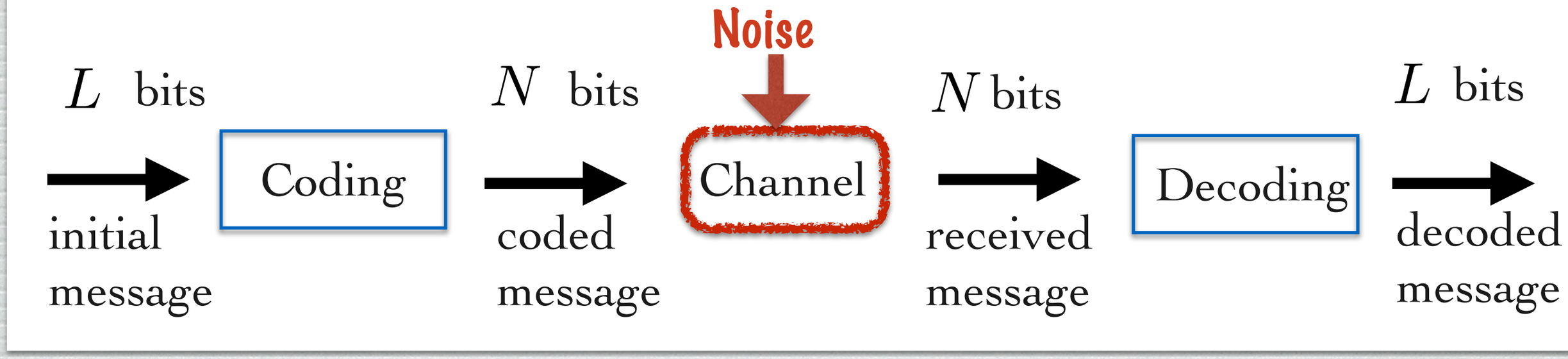
Machine with hundreds of thousands of parameters, trained on very large data base: infer the parameters from data (supervised learning)

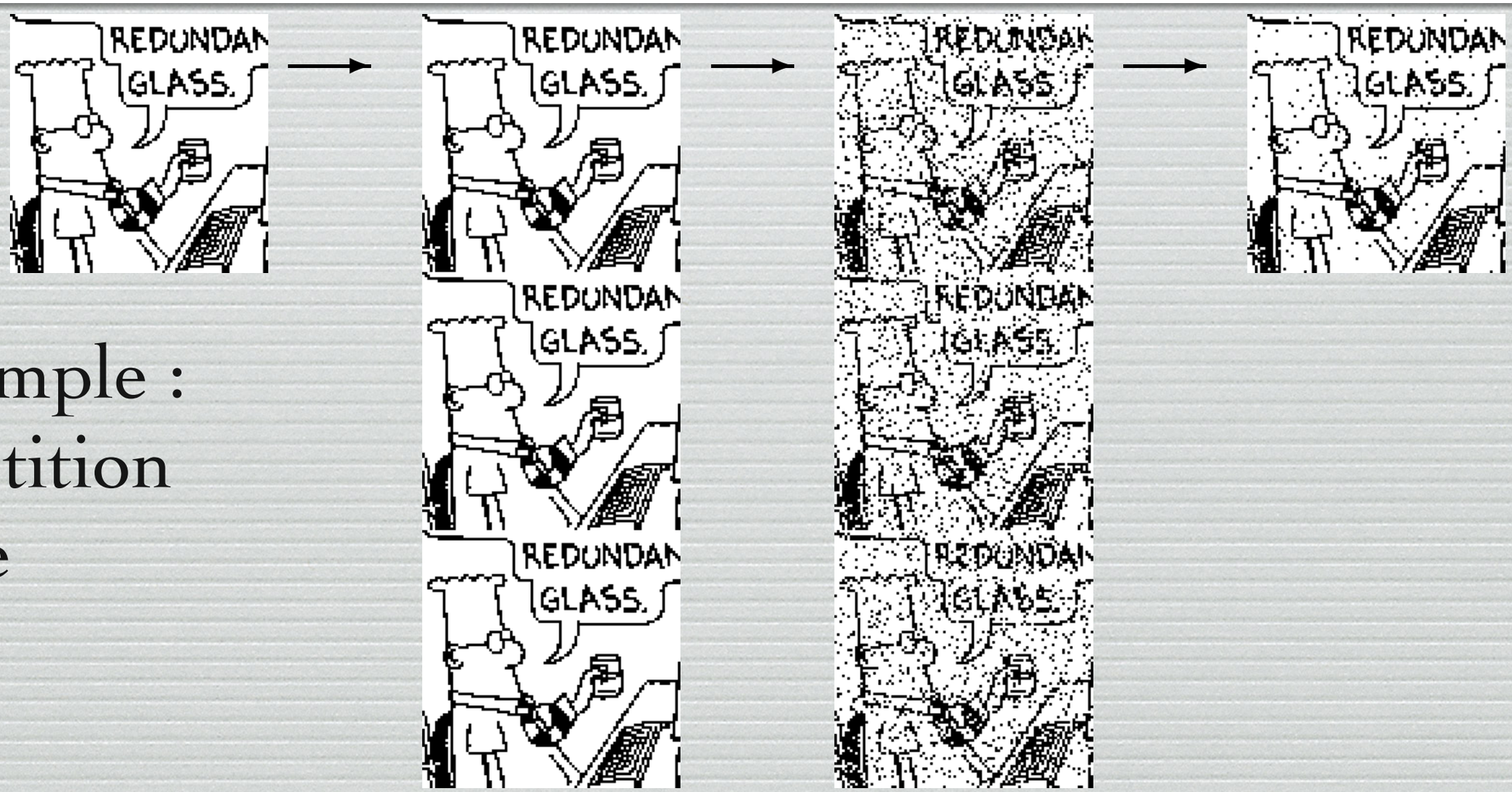
What is inference?

Information theory, communication, signal processing

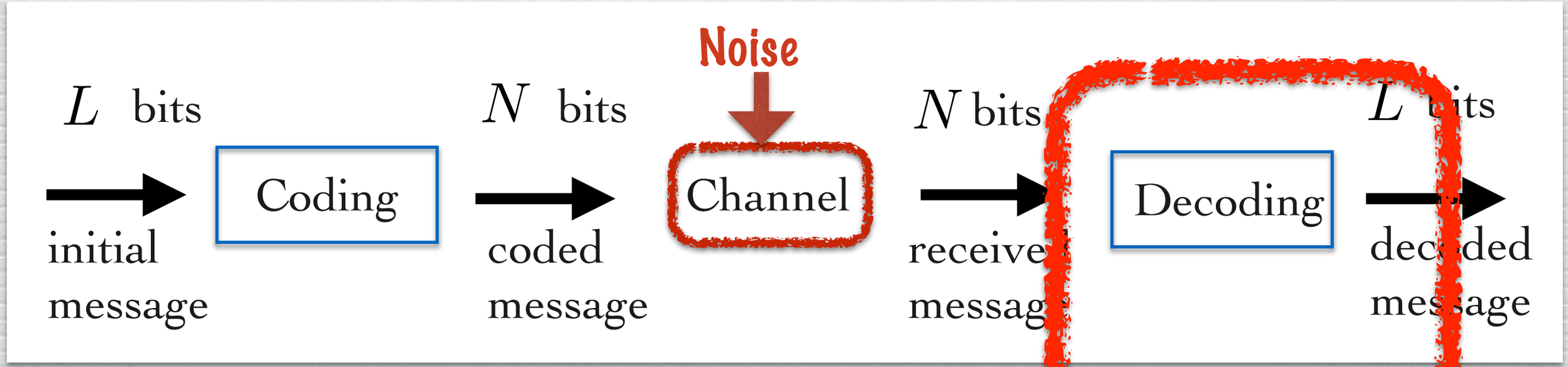
Information transfer : error correction by the use of redundancy

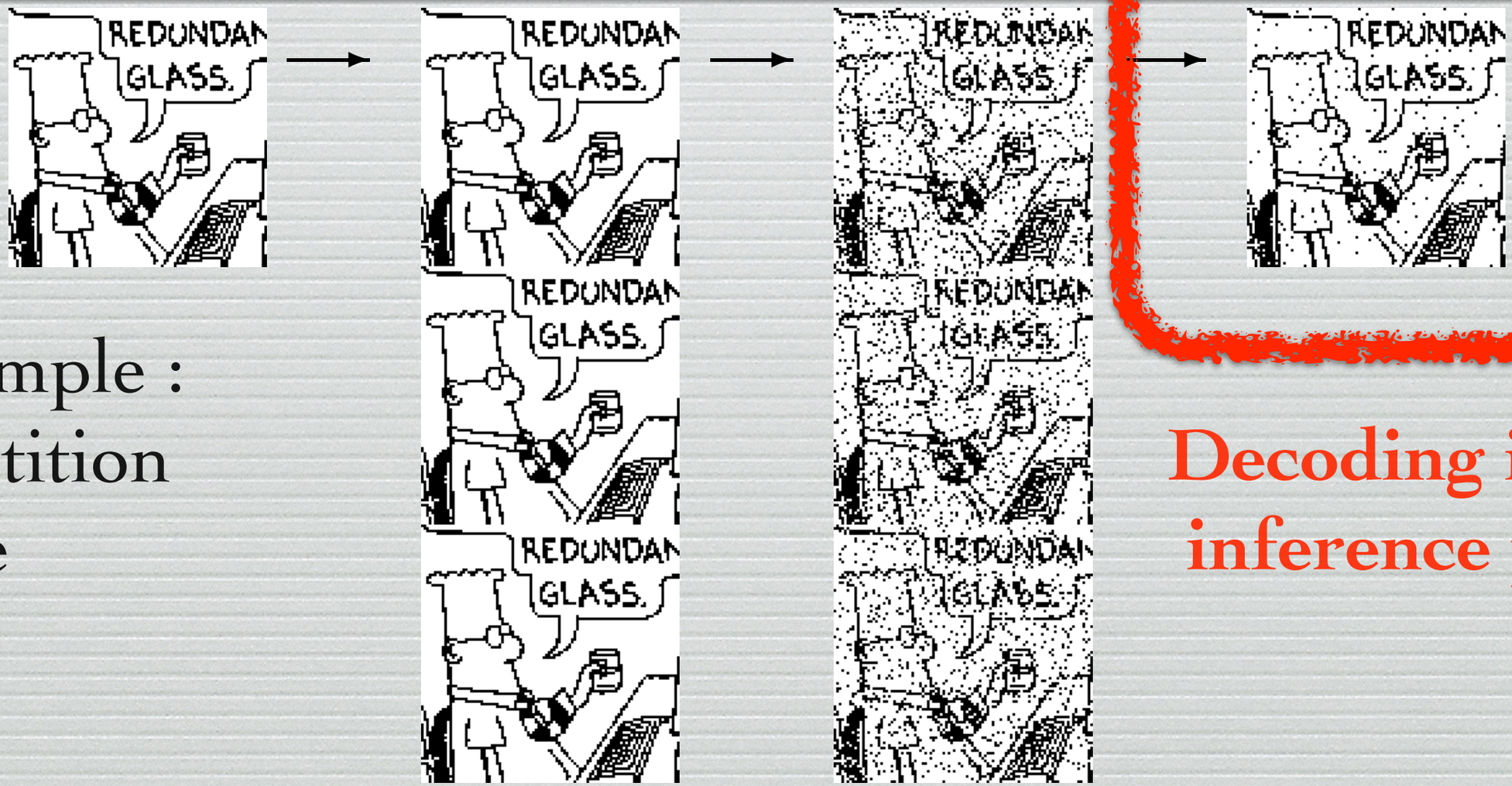

Noise
L bits
initial message
Coding
N bits
coded message
Channel
N bits
received message
Decoding
L bits
decoded message





Example : repetition code





Example : repetition code

Decoding is an inference process

Statistical inference

Challenge = rules with **many hidden parameters**. eg : machine learning with large machine and big data, decoding in commonication,…

$x = (x_1, \ldots, x_N) \quad N \gg 1$

Many measurements $y = (y_1, \ldots, y_M) \quad M \gg 1$

Measure of the amount of data $\alpha = M/N$

- **Algorithms**
- **Prediction on the quality of inference**, on the performance of the algorithms, on the type of situations where they can be applied

Bayesian inference with many unknown and many measurements

Unknown parameters $x = (x_1, \ldots, x_N)$ Prior $P^0(x)$

Measurements $y = (y_1, \ldots, y_M)$ $P(y|x)$

Bayesian inference $P(x|y) \propto P(y|x)P^0(x)$

Often (but not necessarily):

Independent measurements $P(y|x) = \prod_\mu P_\mu(y_\mu|x)$

Factorized prior $P^0(x) = \prod_i P_i^0(x_i)$

Posterior $P(x) = \frac{1}{Z(y)} \left(\prod_i P_i^0(x_i) \right) \exp\left[-\sum_\mu E_\mu(x, y_\mu) \right]$

$E_\mu(x, y_\mu) = -\log P_\mu(y_\mu|x)$

Bayesian inference with many unknown and many measurements

$$P(x) = \frac{1}{Z(y)} \left(\prod_i P_i^0(x_i) \right) \exp \left[- \sum_\mu E_\mu(x, y_\mu) \right]$$

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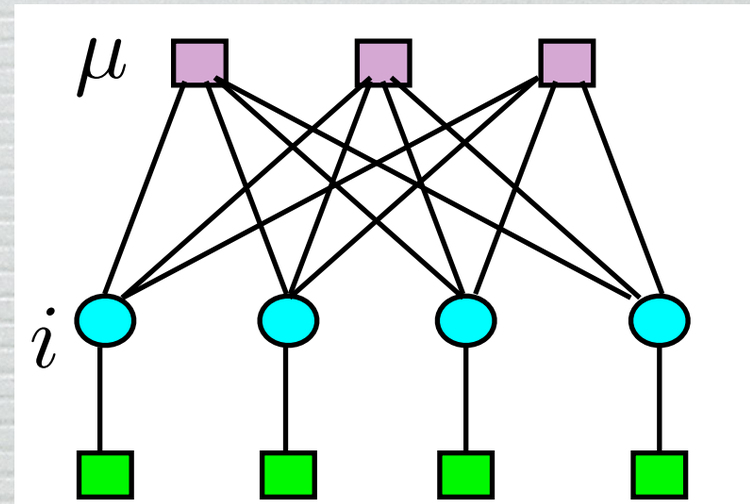


Statistical mechanics.

✦Discrete or continuous variables x_i

✦Interactions through $e^{-E_\mu(x,y_\mu)}$ can be

- pairwise : $E_\mu = J_\mu x_i(\mu) x_j(\mu)$
- multibody

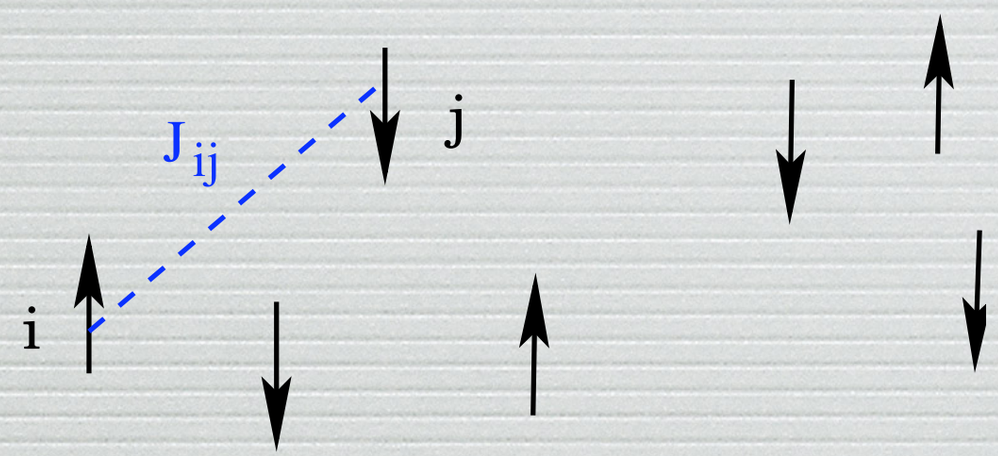
✦Disordered system, ensemble

✦Thermodynamic limit, phase transitions

« Spin glass »

Spin glasses

- Disordered magnetic systems e.g.: CuMn



$$s_i = \pm 1$$

$$E = -\sum_{i,j} J_{ij} s_i s_j$$

$$P(s_1, \ldots, s_N) = \frac{1}{Z} e^{-E/T}$$

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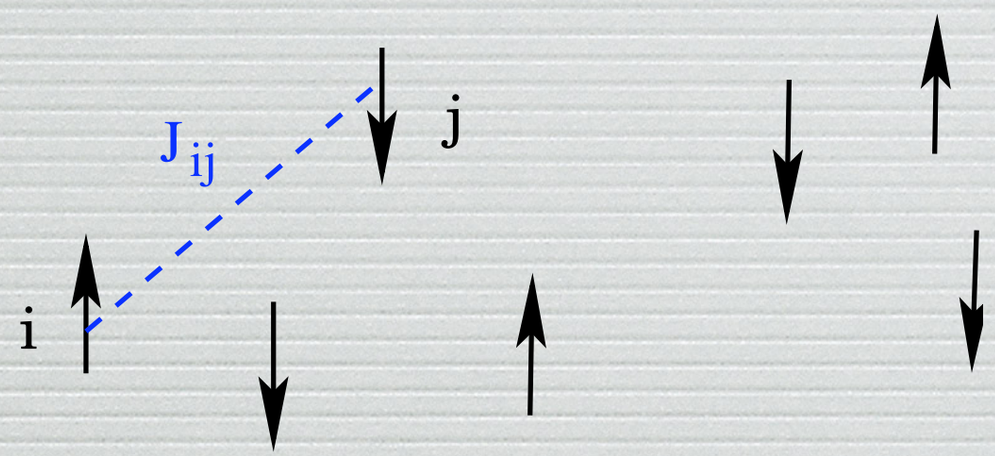

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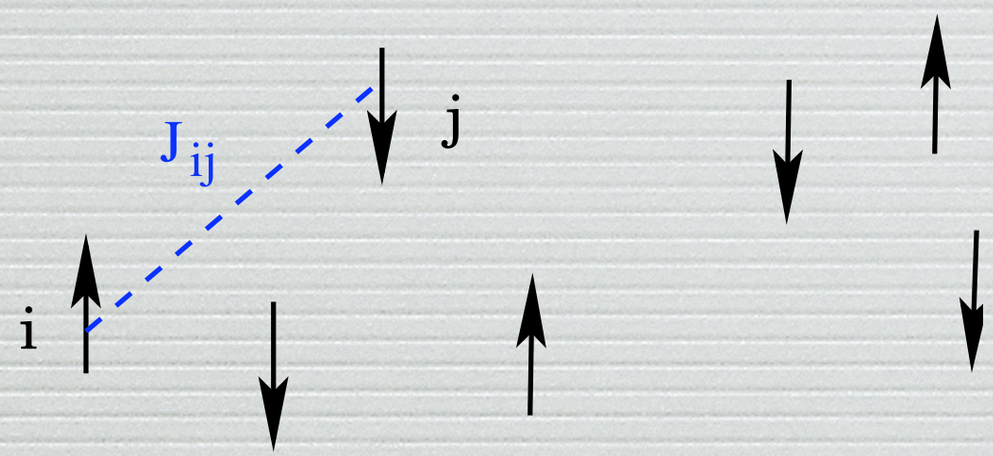
➡ Each spin ‘sees’ a different local field

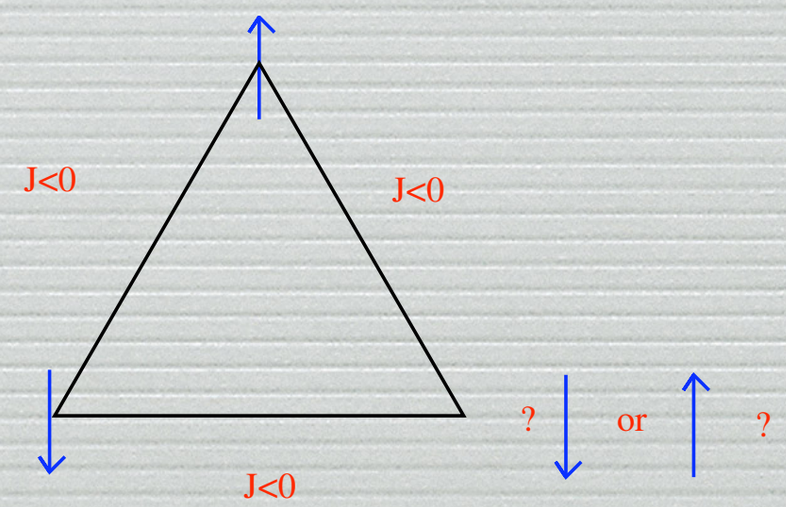
Phase transition with many states: spin glasses

- Many atoms, microscopic interactions are known, "disordered systems" e.g.: CuMn



➡ Each spin 'sees' a different local field

➡ Low temperature: frustration



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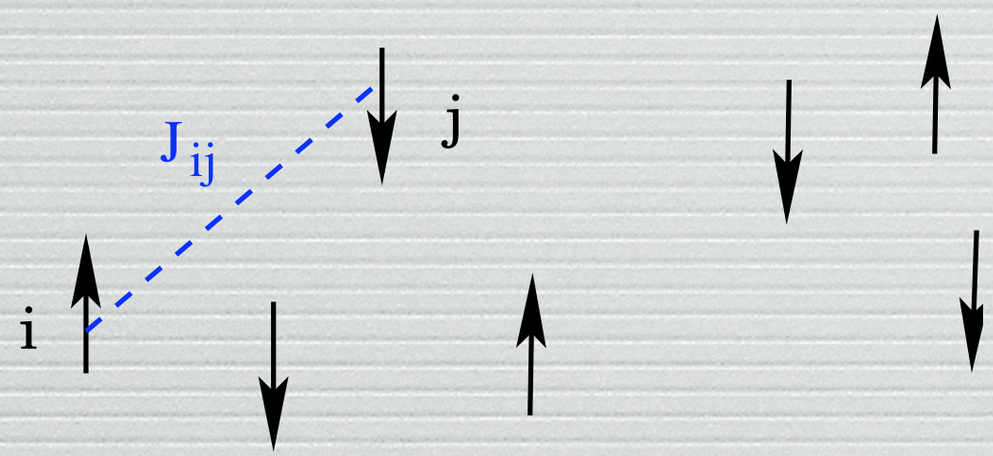
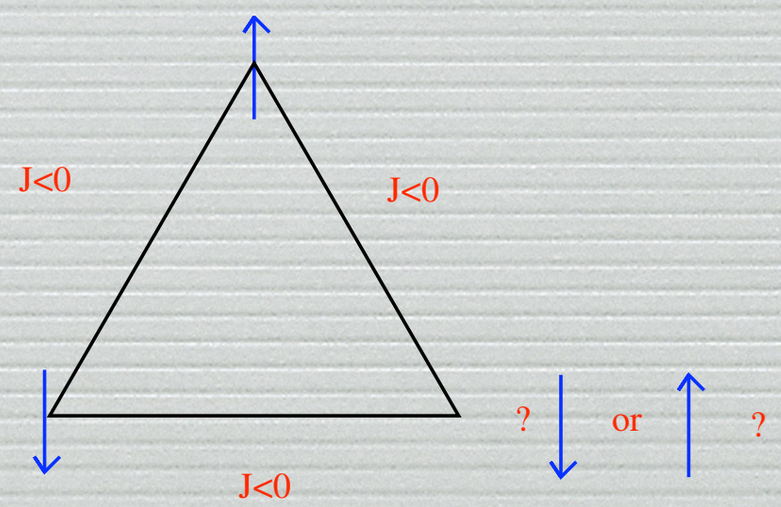


- Each spin 'sees' a different local field
- Low temperature: frustration
- Spins freeze in random directions
- Difficult to find min. of E



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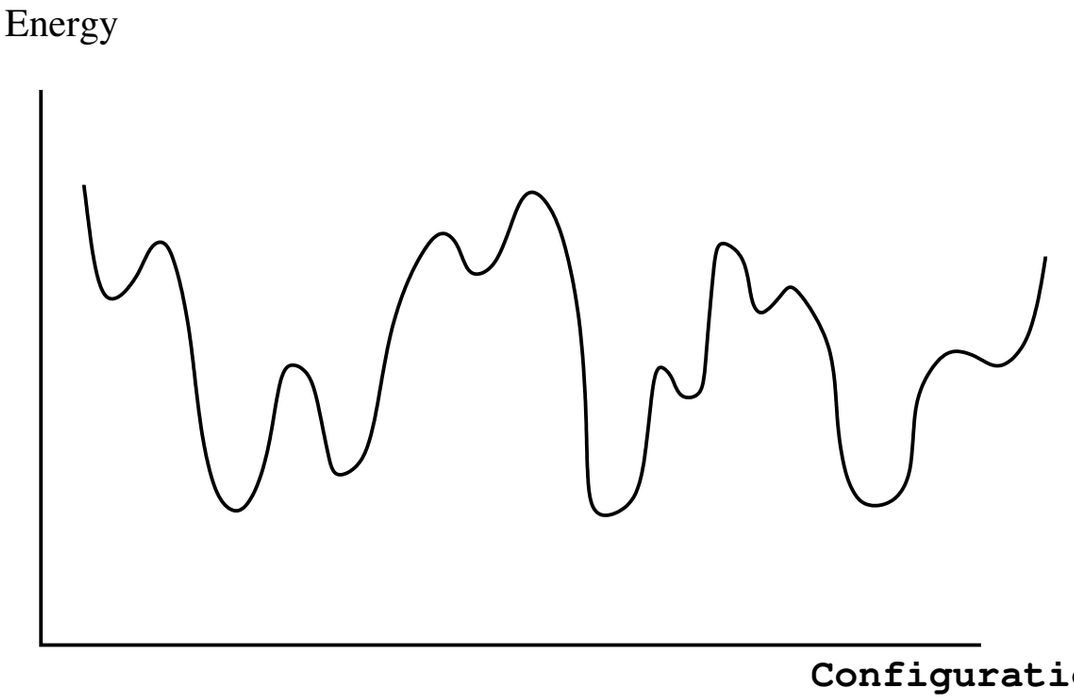

Many quasi-ground states unrelated by symmetries, many metastable states

Slow dynamics, aging

Spin glass

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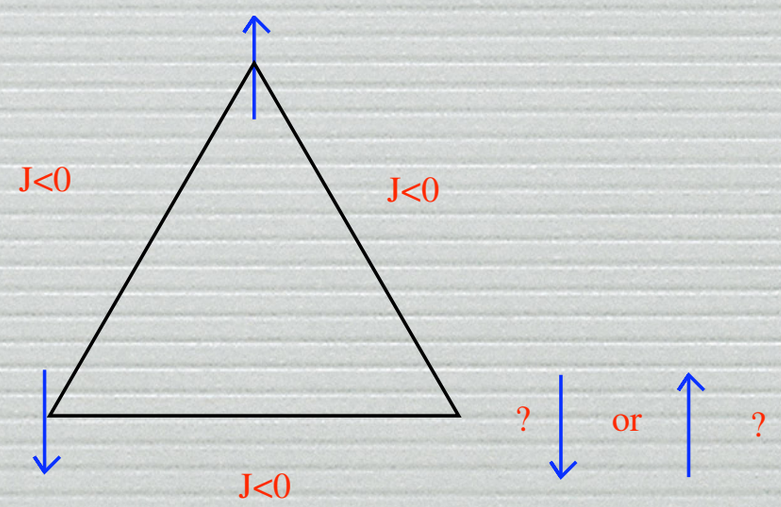

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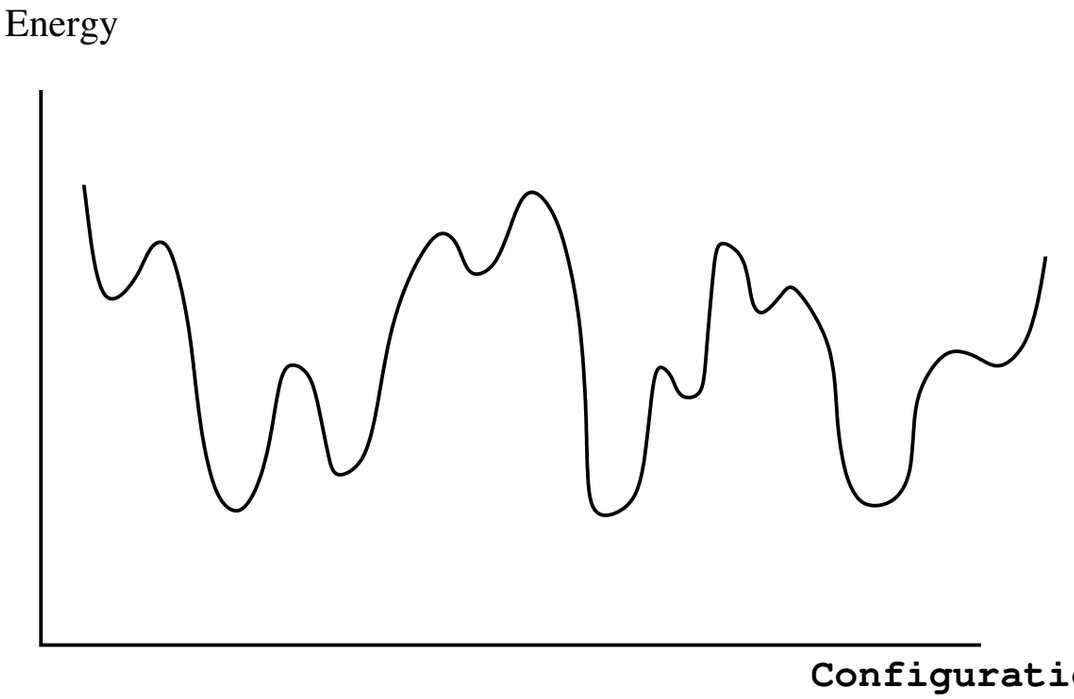

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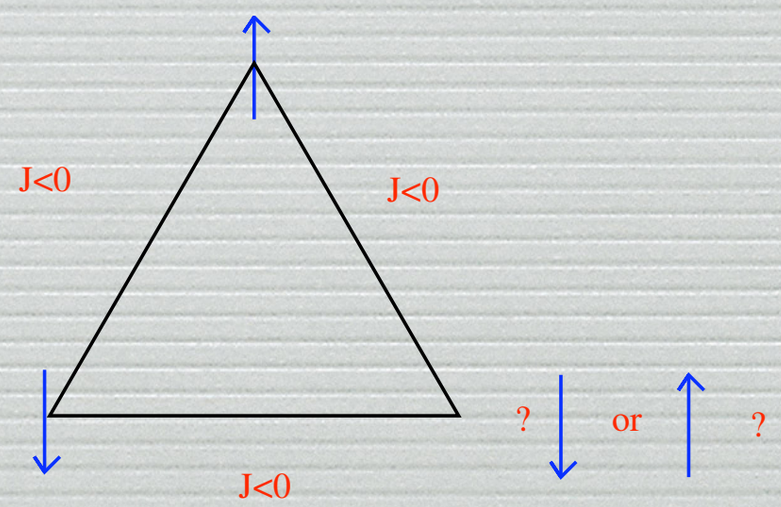

Useless, but thousands of papers...

Inference, spin-glass and crystal: tomography of binary mixtures

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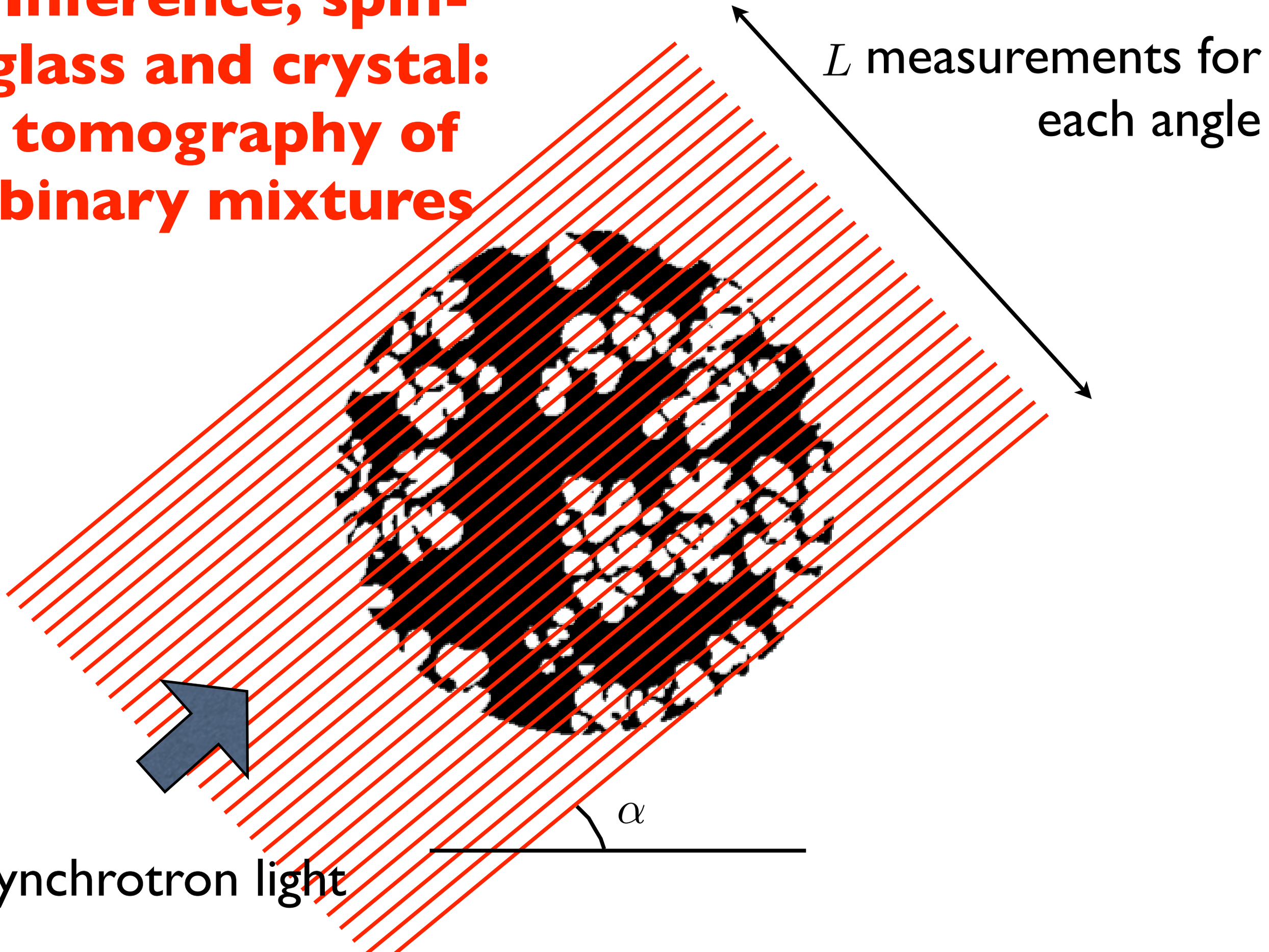
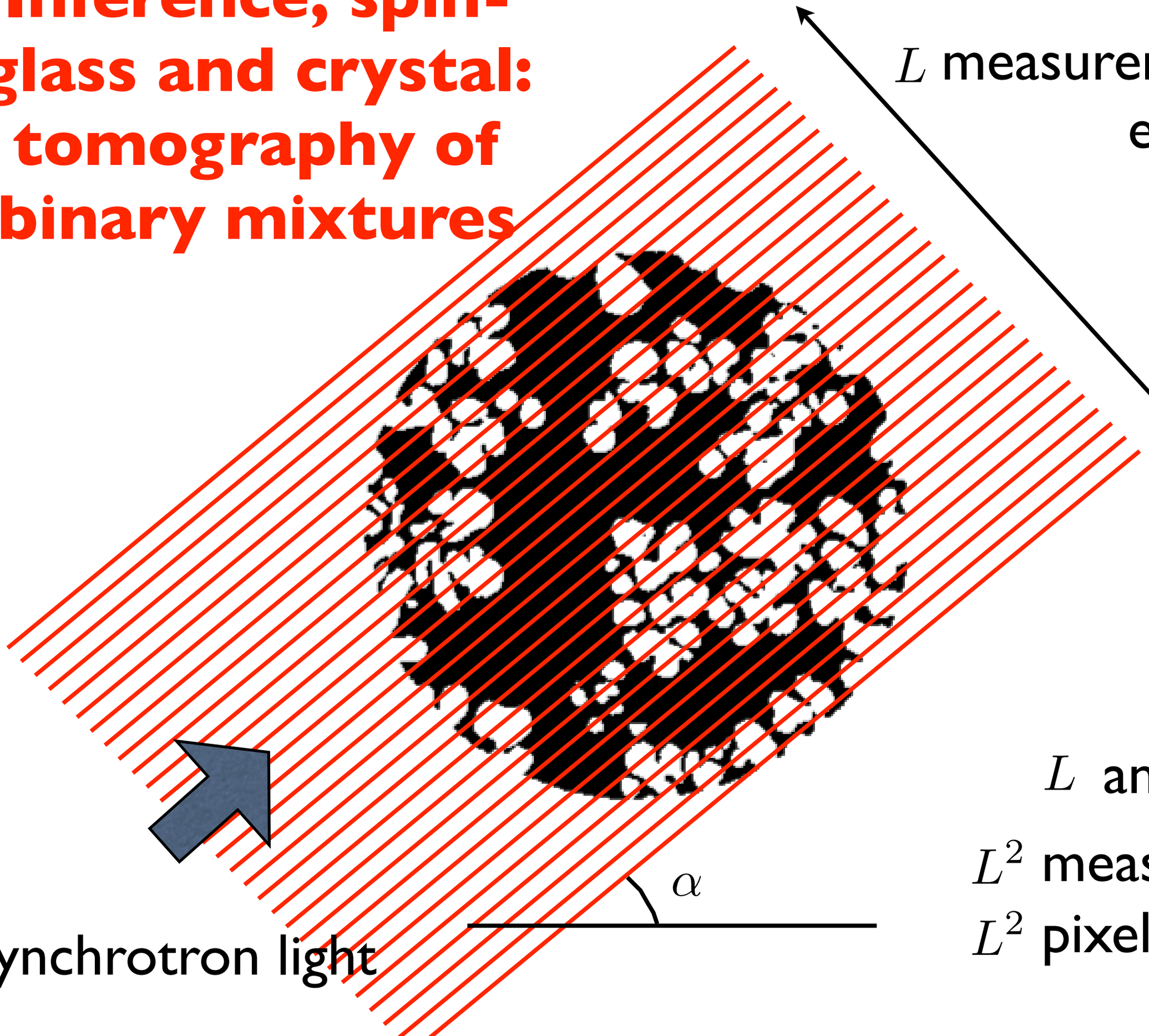


Inference, spin-glass and crystal: tomography of binary mixtures



L angles:

L^2 measurements

L^2 pixels

Tomography of binary mixtures

L angles:

L^2 measurements

L^2 pixels

sample size L

pixel size 1

$\updownarrow$ domain size ξ

If the size of domains is $\gg$ pixel: possible to reconstruct with $\ll L^2$ measurements

$\xi \gg 1$

Tomography of binary mixtures

sample size L

pixel size 1

$\updownarrow$ domain size ξ

If the size of domains is $\gg$ pixel: possible to reconstruct with $\ll L^2$ measurements

$\xi \gg 1$

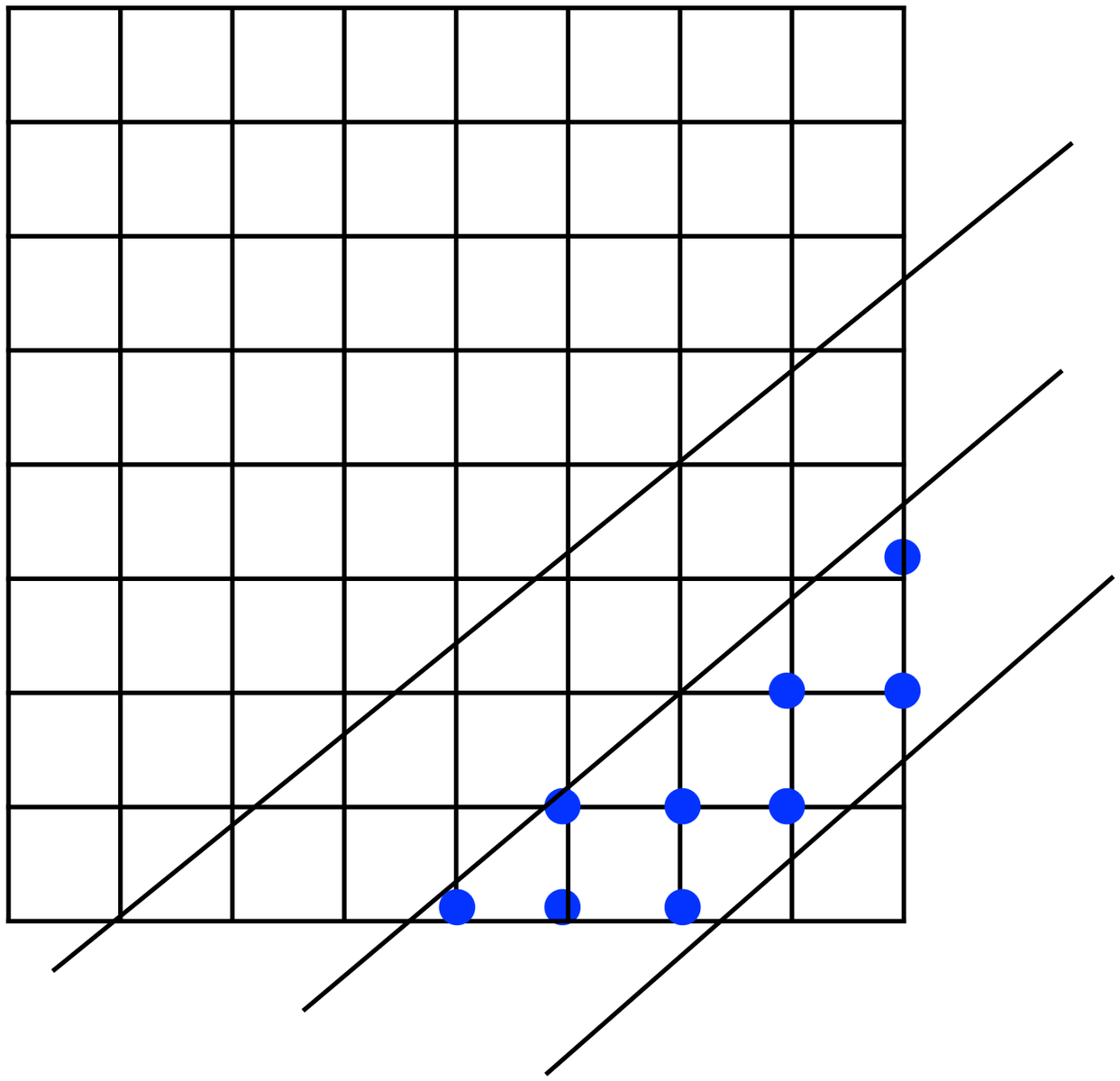
Tomography of binary mixtures

This picture, digitalized on 1000×1000 grid, can be reconstructed fom measurements with 16 angles

Gouillart et al.,
Inverse problems 2013

Compressed sensing

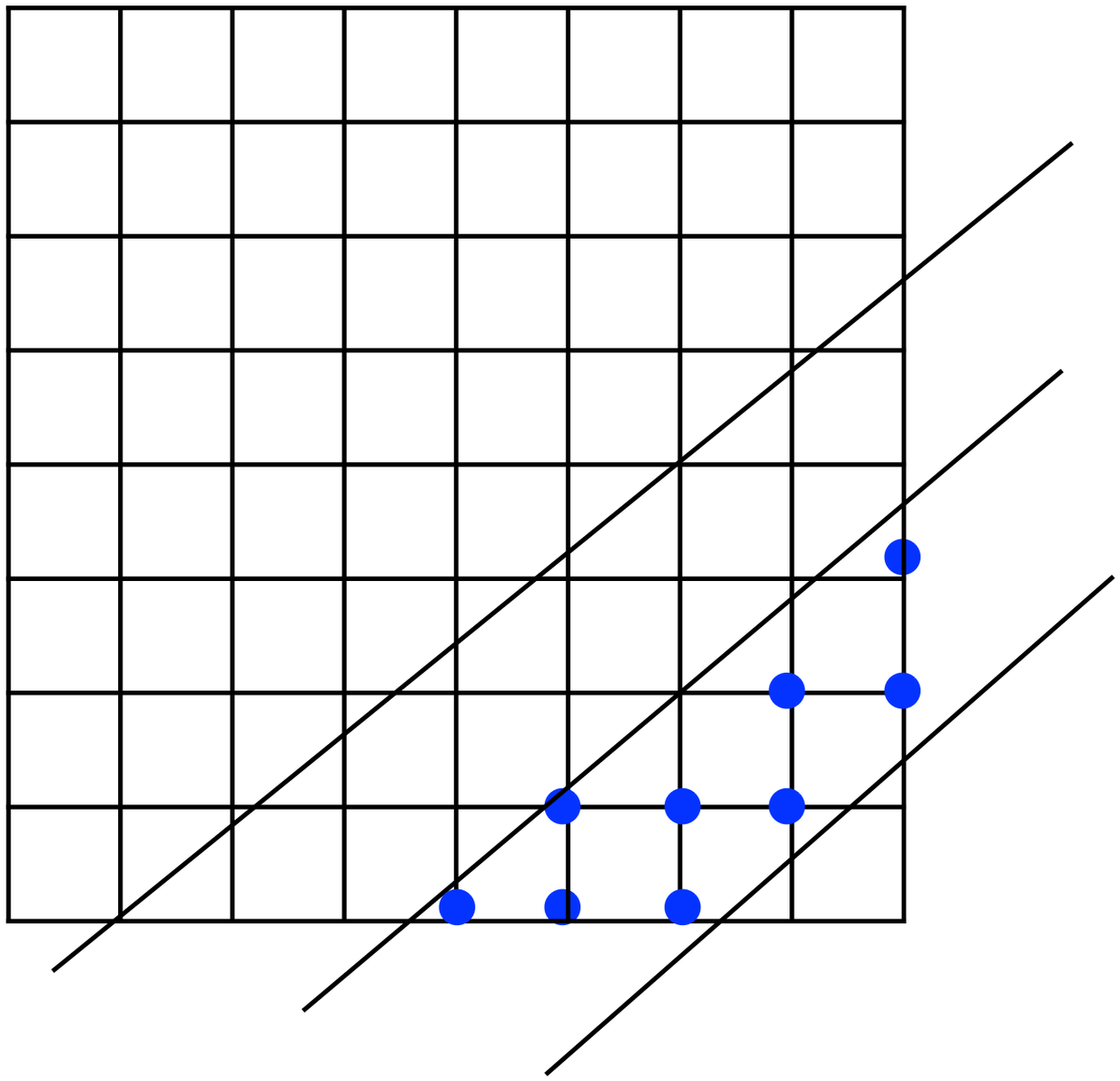
If the size of domains is $\gg$ pixel: possible to reconstruct with $\ll L^2$ measurements



μ $\quad y_\mu = \sum_{i \in \partial\mu} s_i$

Prior knowledge on $\{s_i\}$: neighboring pixels more likely to be equal

Studied with mean-field



μ $\quad$ $y_\mu = \sum_{i \in \partial\mu} s_i$

Prior knowledge on $\{s_i\}$: neighboring pixels more likely to be equal

$$P(S) = \prod_{ij \in \text{grid}} e^{J s_i s_j} \prod_\mu \delta\left(y_\mu, \sum_{i \in \partial\mu} s_i\right)$$

prior $\quad$ measurement

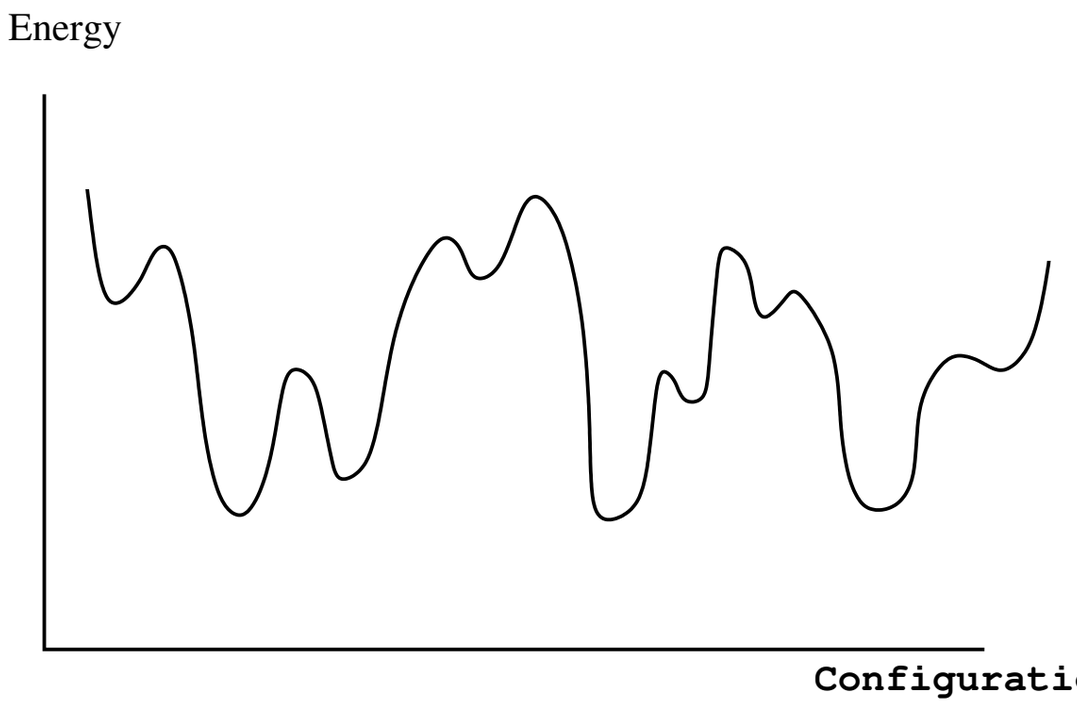
Studied with mean-field

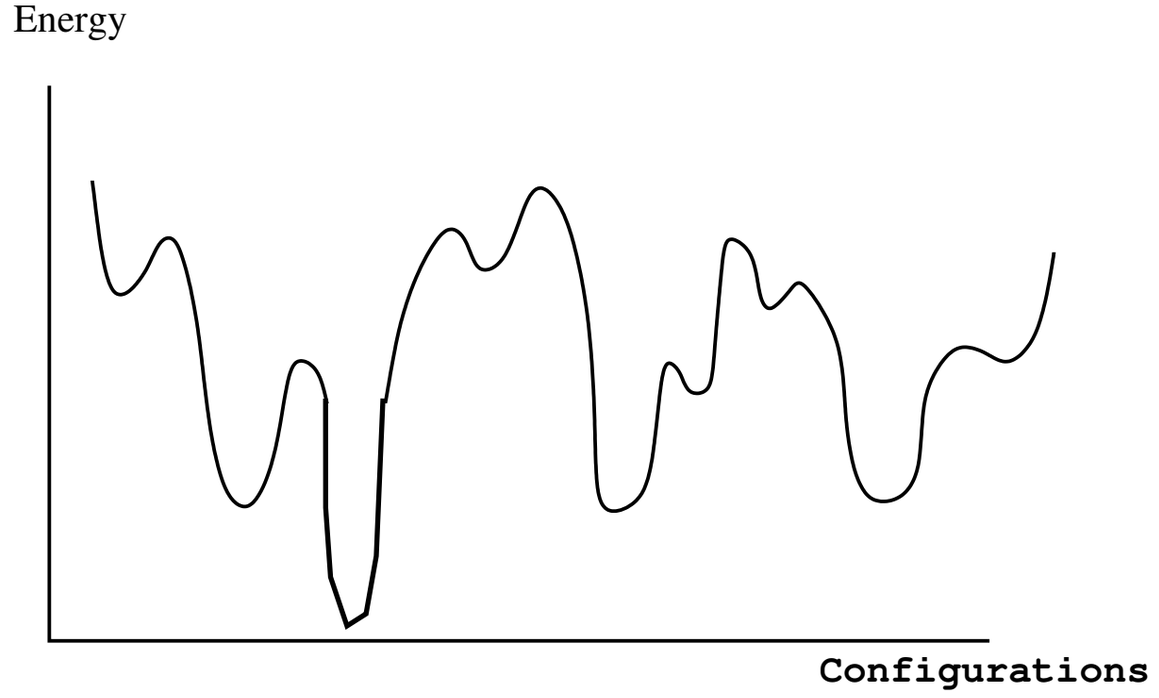
$$P(S) = \prod_{ij \in \text{grid}} e^{J s_i s_j} \prod_{\mu} \delta \left(y_\mu, \sum_{i \in \partial \mu} s_i \right)$$

If enough measurements: The most probable S (the ground state) gives the perfect composition of the sample.

« Crystal » : much more probable

But in some cases « crystal hunting » may be computationally very hard !





Spin glass with crystal

« Crystal » : much more probable

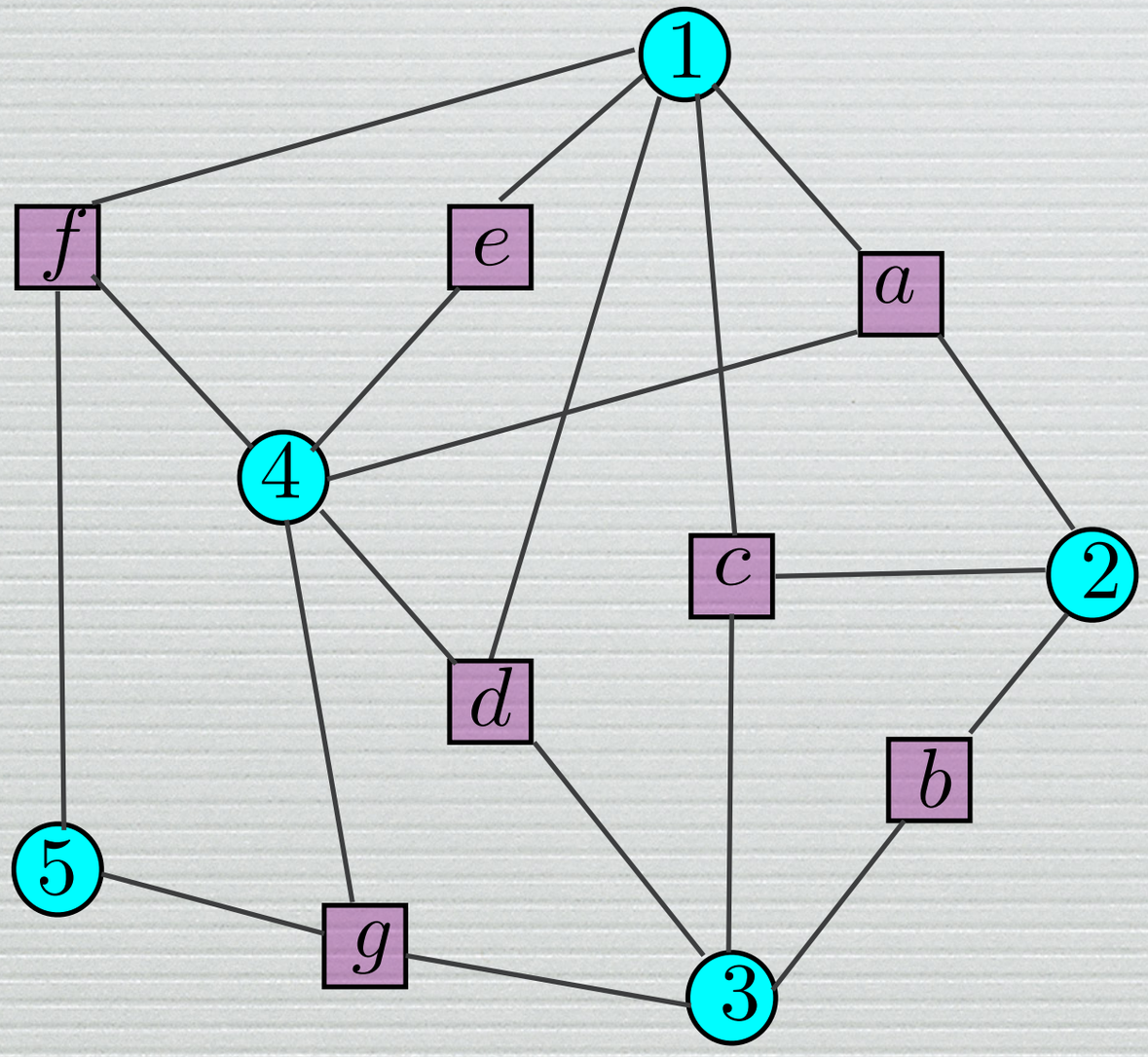
But in some cases « crystal hunting »
may be computationally very hard !

Inference with many unknowns : « crystal hunting » with mean-field based algorithms

Historical development of mean field equations :

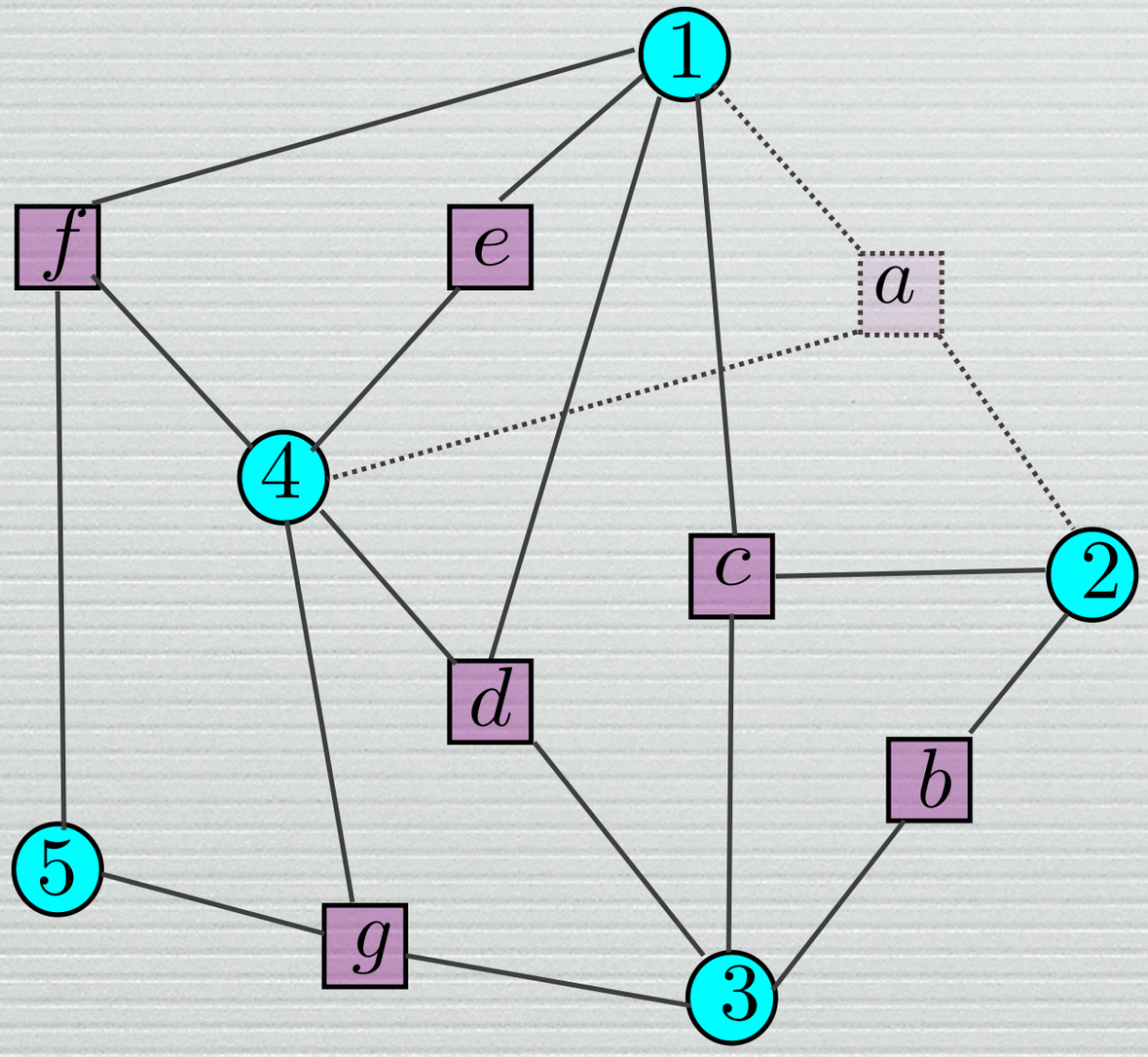
- In homogeneous ferromagnets:
  - Weiss (infinite range, 1907)
  - Bethe Peierls (finite connectivity, 1935)
- In glassy systems:
  - Thouless Anderson Palmer 1977,
  - M. Parisi Virasoro 1986 (infinite range)
  - M. Parisi 2001 (finite connectivity)
- As an algorithm:
  - Gallager 1963
  - Pearl 1986
  - M. Parisi Zecchina 2002
  - Kabashima 2003, 2008
  - Donoho Bayati Montanari 2009
  - Rangan 2010
  - Krzakala M. Zdeborova 2012 ...

BP = Bethe-Peierls = Belief Propagation



$$P(x_1, \cdots, x_5) = \psi_a(x_1, x_2, x_4)\psi_b(x_2, x_3) \cdots$$

BP equations

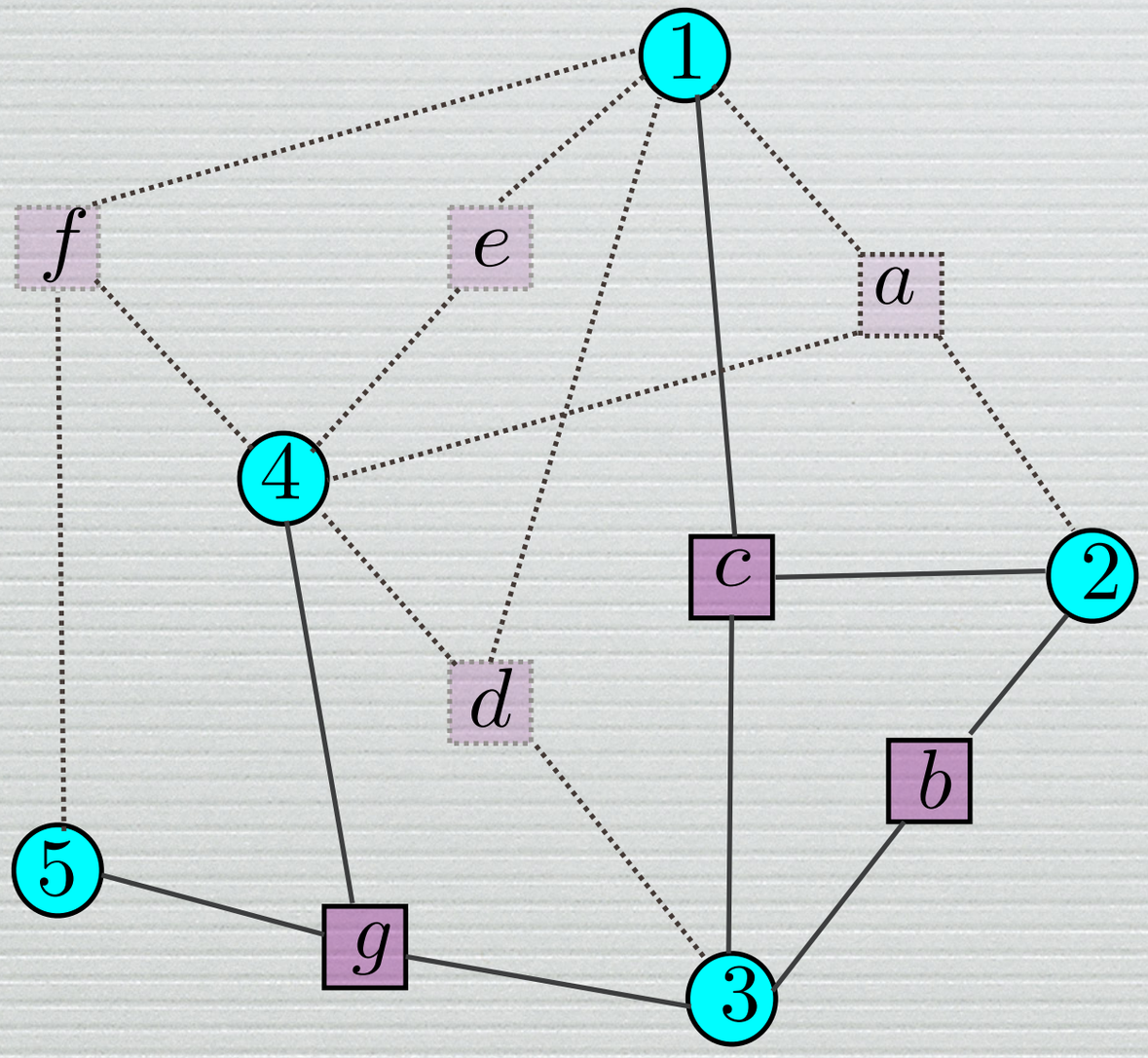


First type of messages:

Probability of x_1 in the absence of a:

$$m_{1\to a}(x_1)$$

BP equations

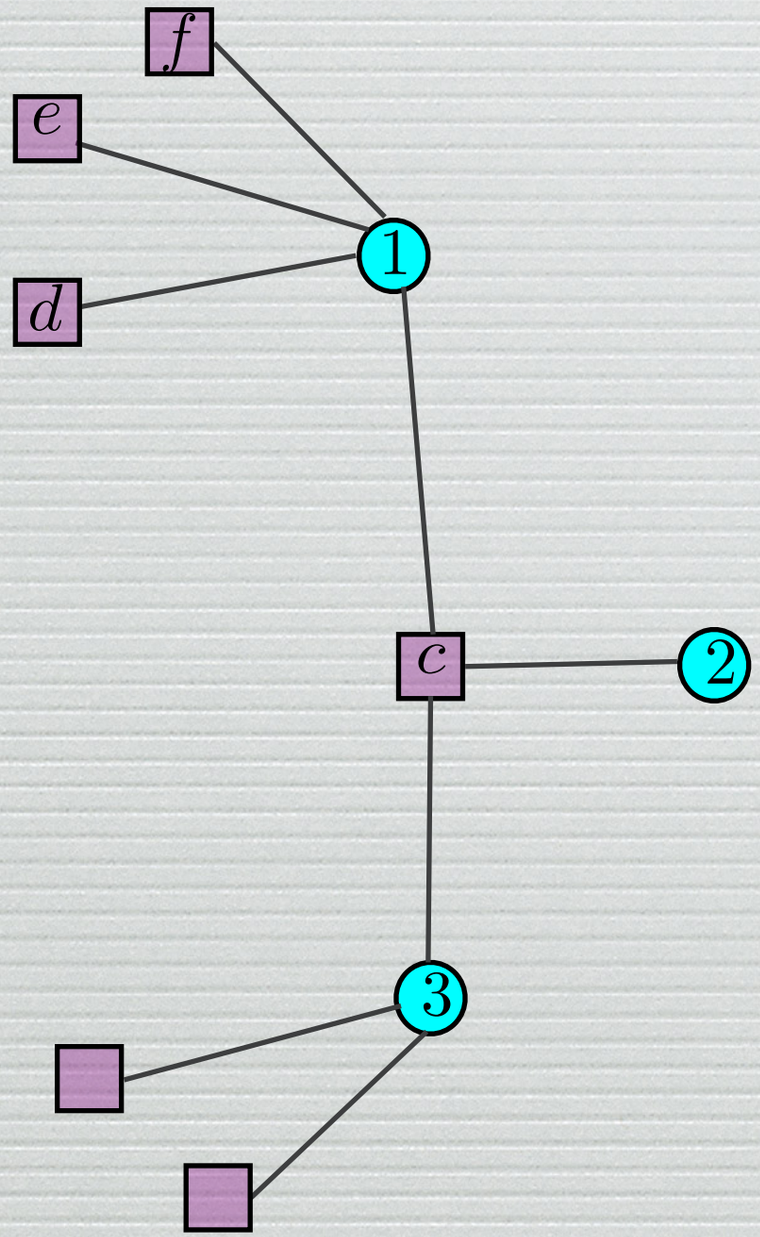


Second type of messages:

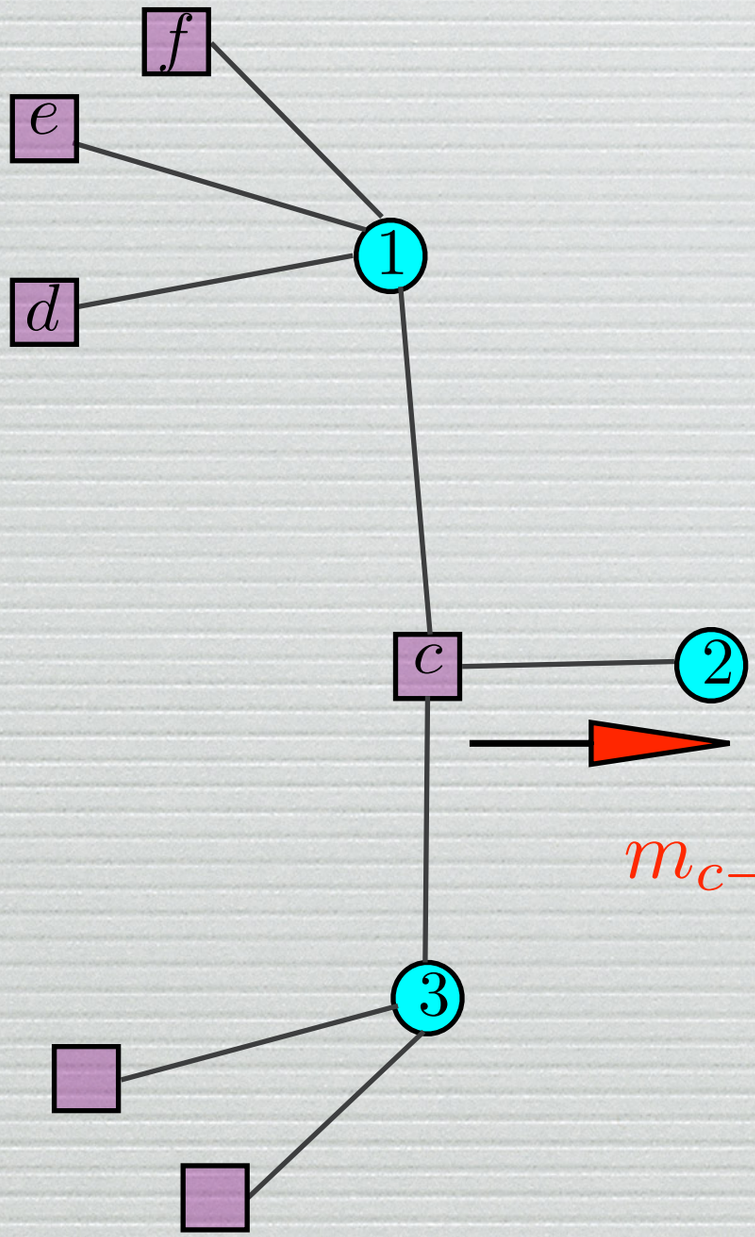
Probability of x_1 when it is connected only to c :

$$m_{c\to 1}(x_1)$$

BP equations

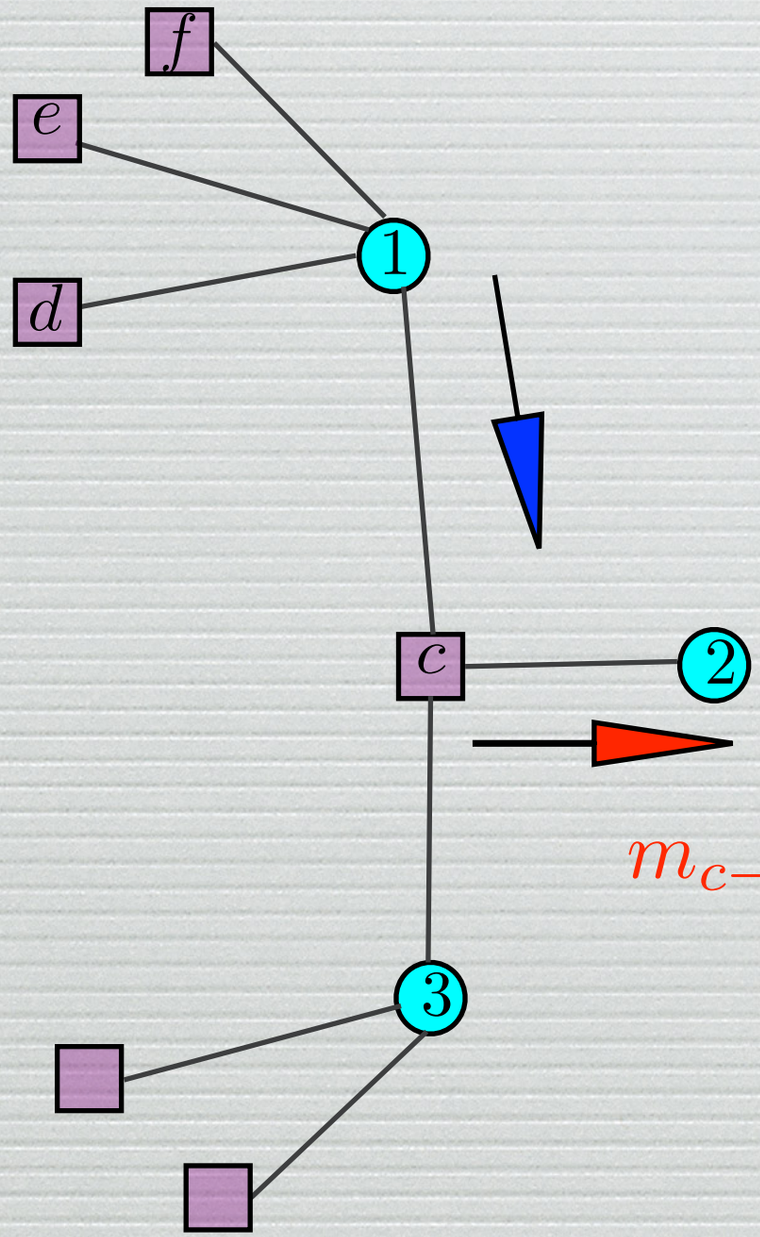


BP equations



$$m_{c\to 2}(x_2) = \sum_{x_1,x_3} \psi_c(x_1,x_2,x_3) m_{1\to c}(x_1) m_{3\to c}(x_3)$$

BP equations



$$m_{1\to c}(x_1) = C m_{d\to 1}(x_1) m_{e\to 1}(x_1) m_{f\to 1}(x_1)$$

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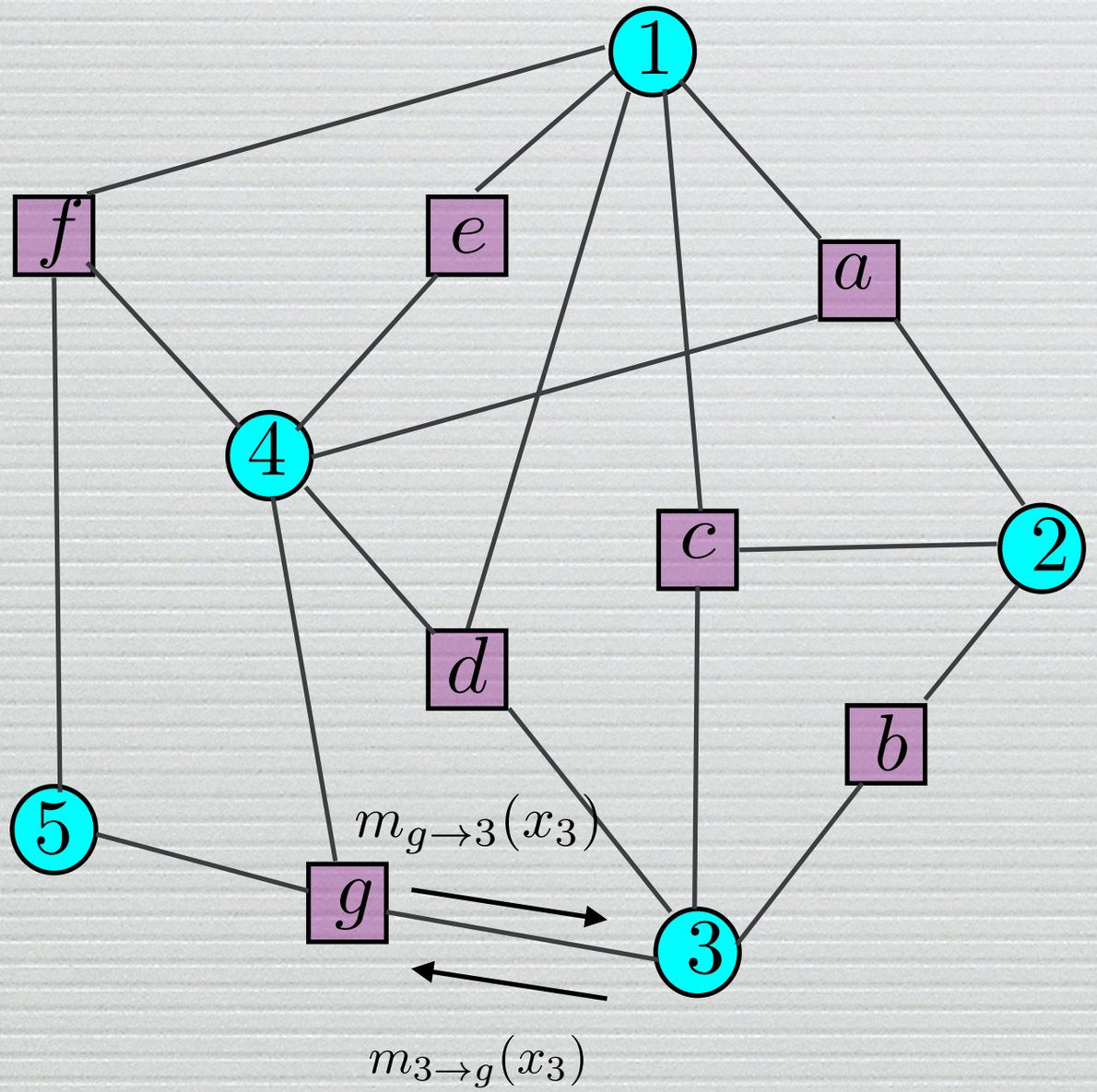
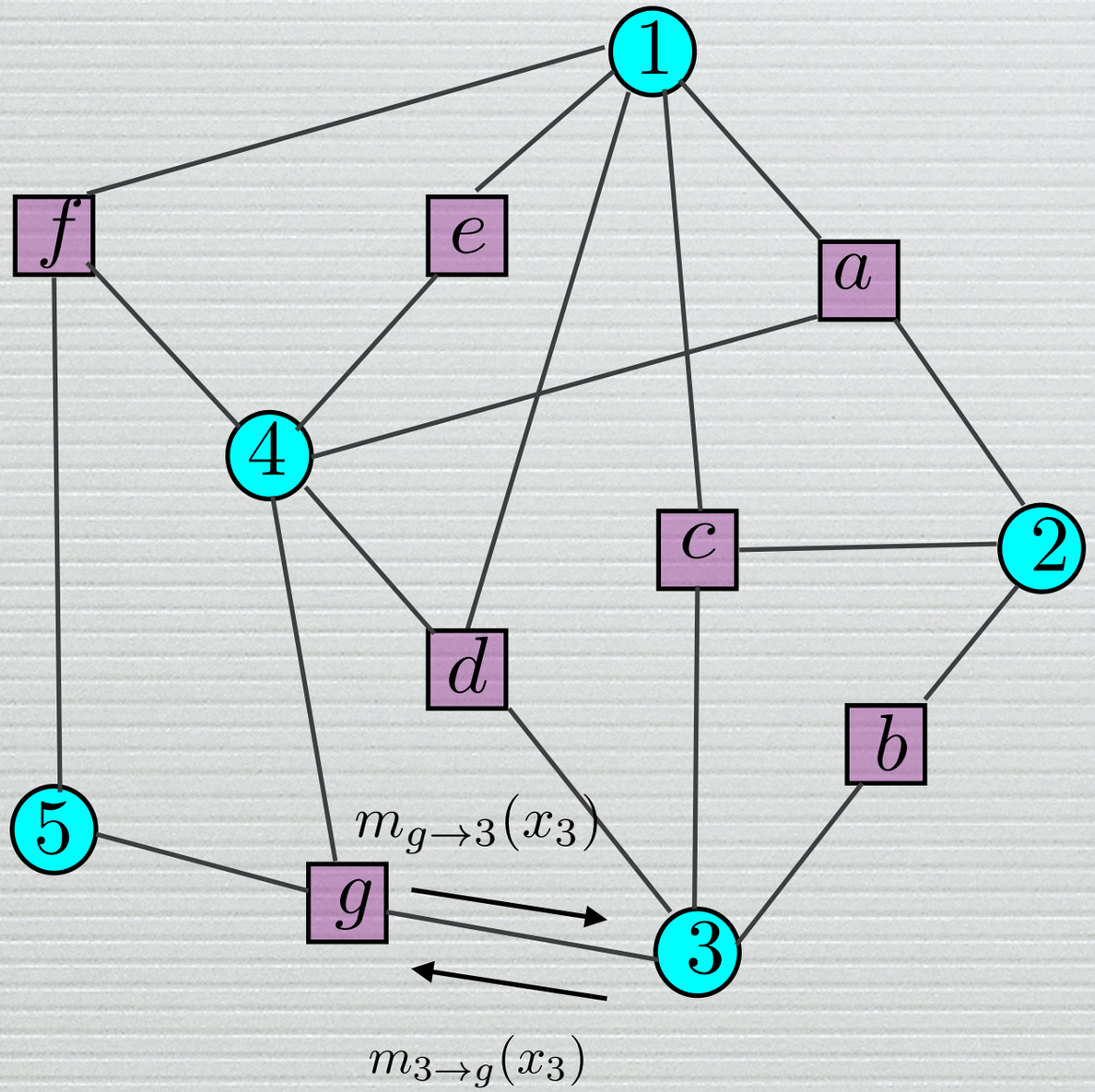


Propagate messages along the edges, update messages at vertices, using elementary local probabilistic rules

BP equations



Propagate messages along the edges, update messages at vertices, using elementary local probabilistic rules

Closed set of equations: two messages "propagate" on each edge of the factor graph.

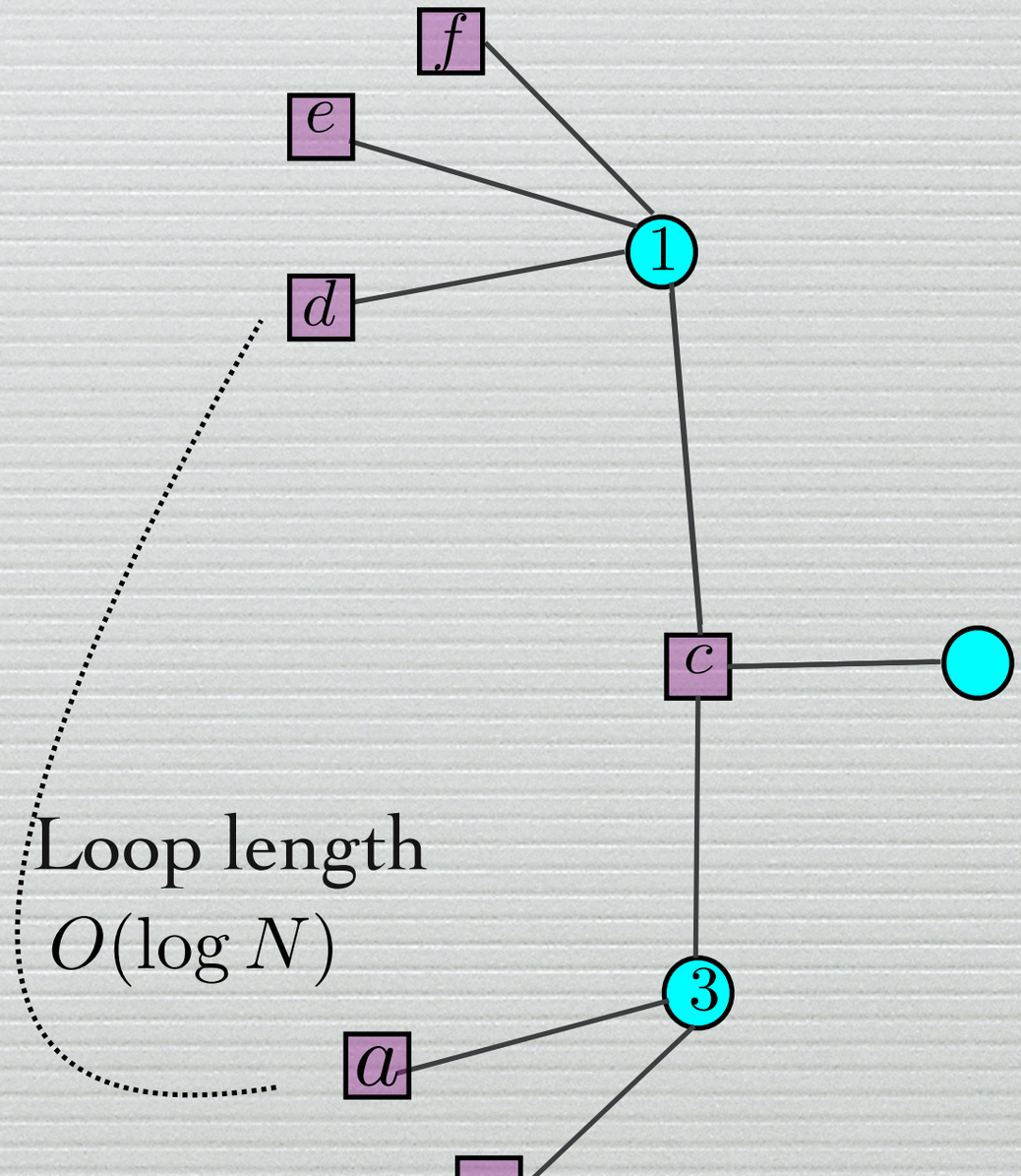
When is BP exact?

$$m_{1\to c}(x_1) = C m_{d\to 1}(x_1) m_{e\to 1}(x_1) m_{f\to 1}(x_1)$$

$$m_{c\to 2}(x_2) = \sum_{x_1,x_3} \psi_c(x_1,x_2,x_3) m_{1\to c}(x_1) m_{3\to c}(x_3)$$

Fluctuations are handled correctly, but beware of correlations

- Exact in one dimension (transfer matrix = dynamic programming)
- Exact on a tree (uncorrelated b.c)
- Exact on locally tree-like graphs (Erdös Renyi etc.) if correlations decay fast enough (single pure state) and uncorrelated disorder
- Exact in infinite range problems if correlations decay fast enough (single pure state) and uncorrelated disorder

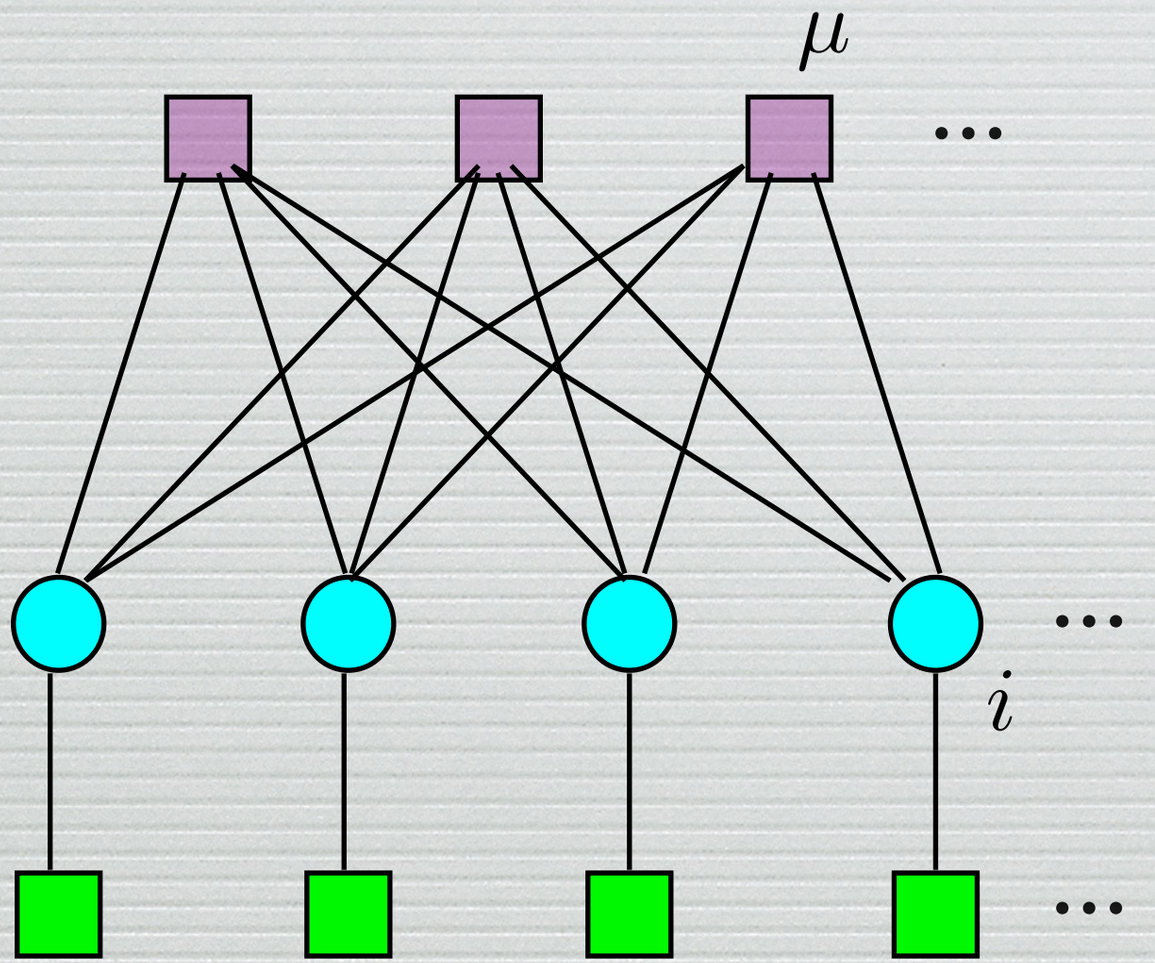


Two important developments

1) The special case of infinite-range models

2) What happens in a glass phase, when there are many pure states, and therefore many solutions ?

Infinite range models



$$m_{i\to\mu}(x_i) = \prod_{\nu(\neq\mu)} m_{\nu\to i}(x_i)$$

$$M_i(x_i) = \prod_{\nu} m_{\nu\to i}(x_i)$$

Small difference, treated perturbatively

Mean-field equations can be written only in terms of site pdfs: $M_i(x_i)$. TAP, AMP...

eg TAP equations for spin glasses:

$$H_i^{t+1} = \sum_k J_{ki} \tanh(\beta H_k^{t}) - \beta \tanh(\beta H_i^{t-1}) \sum_k J_{ki}^2 [1 - \tanh^2(\beta H_k^{t-1})]$$

Two important developments

1) The special case of infinite-range models

2) What happens in a glass phase, when there are many pure states, and therefore many solutions ?

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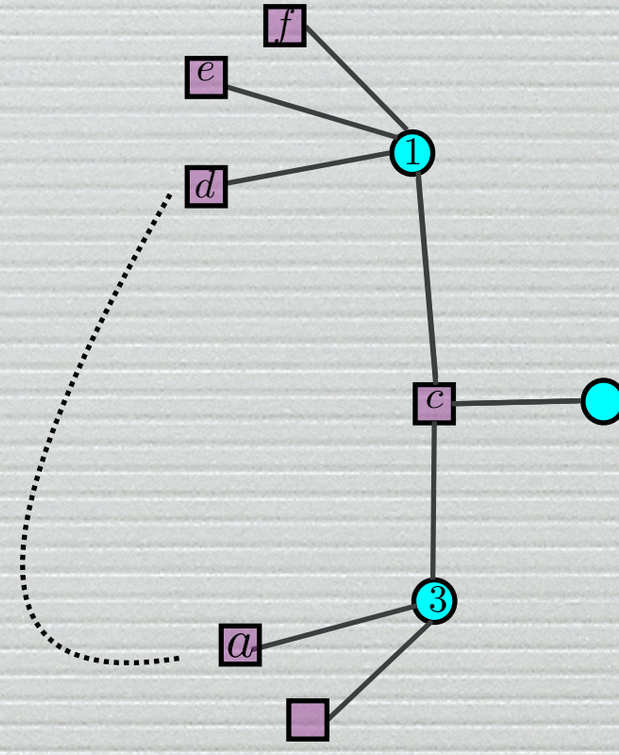
$$m_{i\to\mu}(x_i) = \prod_{\nu(\neq\mu)} m_{\nu\to i}(x_i)$$

Correct if, in absence of the i-j interaction, the correlations between k and ℓ can be neglected.



Loop length $O(\log N)$

2) What happens in a glass phase, when there are many pure states, and therefore many solutions ?

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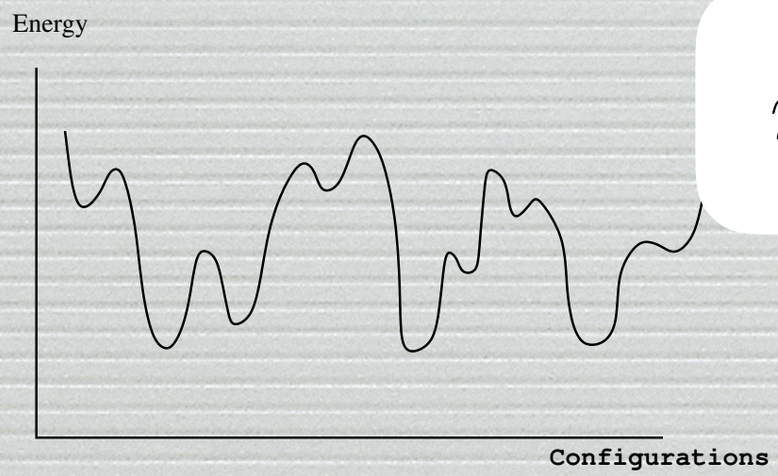
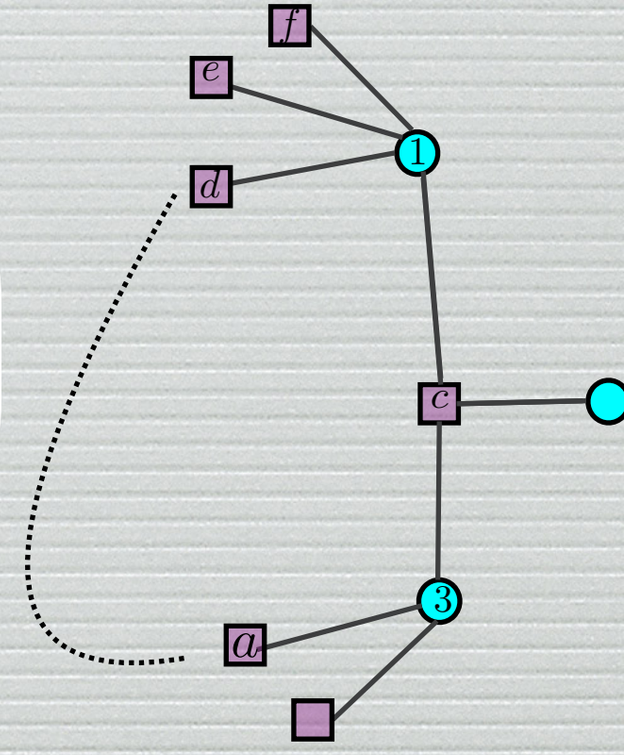


$$m^{\alpha}_{i\to\mu}(x_i) = \prod_{\nu(\neq\mu)} m^{\alpha}_{\nu\to i}(x_i)$$



Glassy phase: many states, many solutions of BP

Loop length $O(\log N)$

2) What happens in a glass phase, when there are many pure states, and therefore many solutions ?

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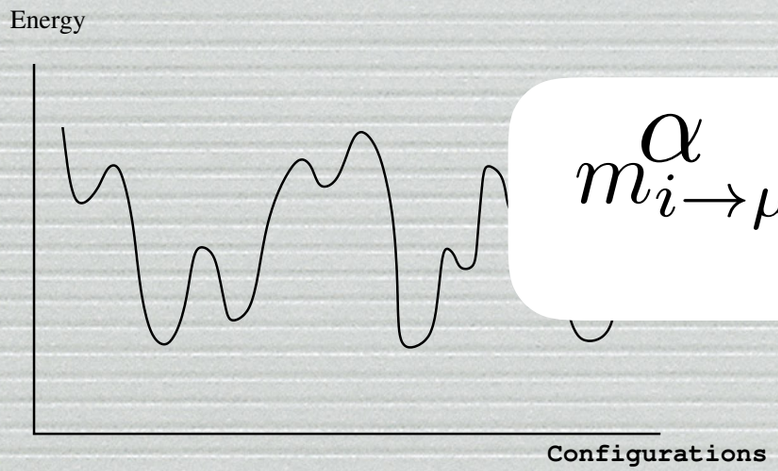

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Glassy phase: many states, many solutions of BP

Statistics of $m^{\alpha}_{i\to\mu}(x_i)$ over the many states α

$$P_{i\to\mu}(m)$$

related to

$$P_{\nu\to i}(m)$$

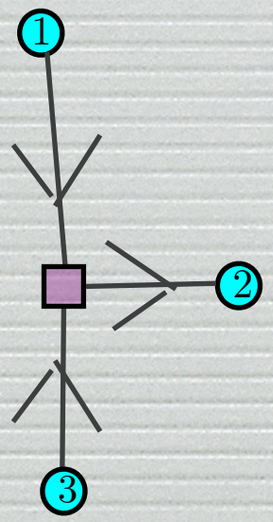
Survey propagation

M Parisi Zecchina 2002

Power of message passing algorithms

Approximate solution of very hard, and very large constraint satisfaction problems, ...FAST! (typically linear time)

- BP: Best decoders for LDPC error correcting codes
- SP: Best solver of random satisfiability problems
- BP: Best algorithm for learning patterns in neural networks (e.g. binary perceptron)
- Data clustering, graph coloring, Steiner trees, etc…
- Fully connected networks : TAP (=AMP). Compressed sensing, linear estimation, etc.



Local, simple update equations:
Each message is updated using information from incoming messages on the same node.
Distributed, solves hard global pb

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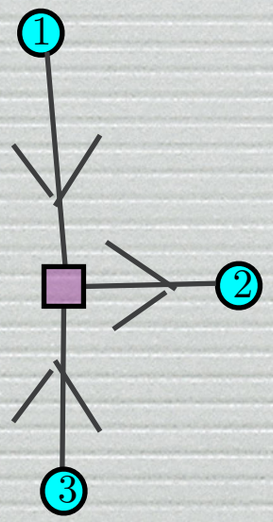

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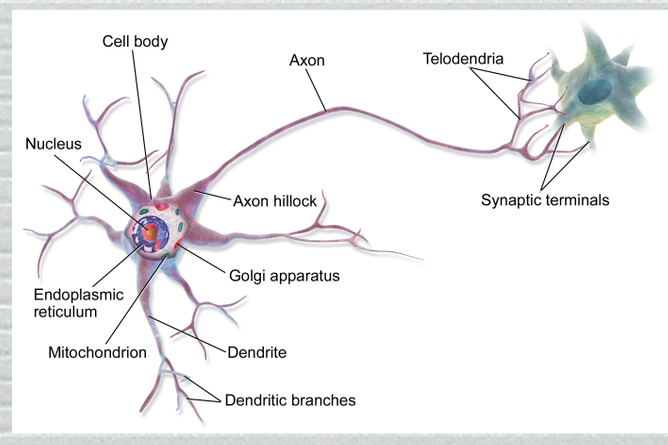


An example of fully connected model: Generalized Linear Regression

Unknowns: $x_i \quad i = 1, \ldots, N$

Linear combinations: $z_\mu = \sum_i F_{\mu i} x_i \qquad \mu = 1, \ldots, M$

Outputs y_μ generated from $P_{\rm out}(y_\mu | z_\mu)$

Prior factorized $\prod_i P(x_i)$

Bayes

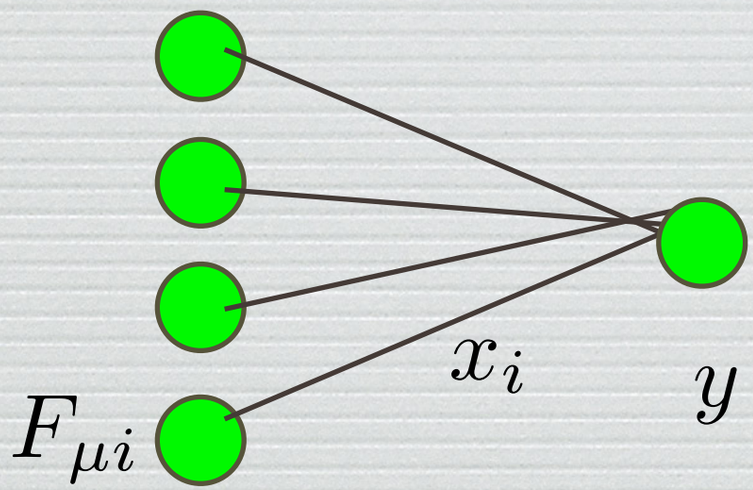
$$P(x|y) = \frac{1}{Z(y)} \prod_i P(x_i) \prod_\mu P_{\rm out}(y_\mu | \sum_i F_{\mu i} x_i)$$

Examples: tomography, linear regression, perceptron learning, compressed sensing…

$$P(x|y) = \frac{1}{Z(y)} \prod_i P(x_i) \prod_\mu P_{\text{out}}(y_\mu | \sum_i F_{\mu i} x_i)$$

Perceptron learning

Pattern μ



$$P_{out} = \delta(y_\mu, Sign(z_\mu))$$

Linear regression:

Individual μ : expression of disease y_μ

Value of factor i for individual μ : $F_{\mu i}$

Find the best weights of factors x_i

Minimize mean square error with regularization

$$\frac{1}{2} \sum_\mu (y_\mu - \sum_i F_{\mu i} x_i)^2 + \sum_i ||x_i||$$

$$P_{out} = e^{-(y_\mu - z_\mu)^2/(2\Delta)}$$

$$P(x_i) = e^{-||x_i||/\Delta}$$

$$P(x|y) = \frac{1}{Z(y)} \prod_i P(x_i) \prod_\mu P_{\rm out}(y_\mu | \sum_i F_{\mu i} x_i)$$

Compressed sensing

Unknown variables x_i

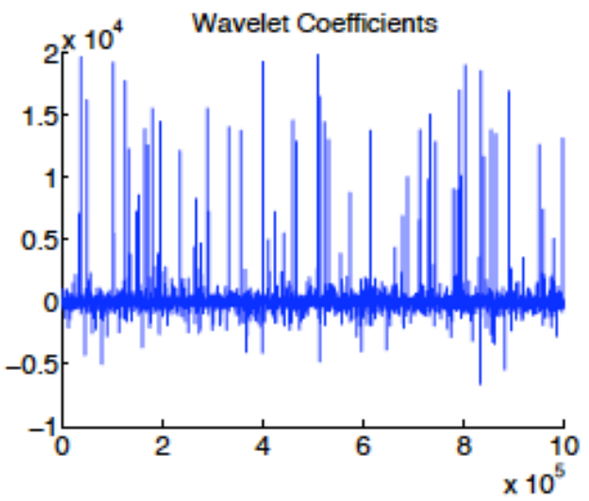
Linear measurements $y_\mu = \sum_i F_{\mu i} x_i + \eta_\mu$

$$P_{out} = e^{-(y_\mu - z_\mu)^2/(2\Delta)}$$

Compressed sensing regime : $M < N$

sparse prior (in appropriate basis)

$$P(x_i) = (1-\rho)\delta(x_i) + \rho\phi(x_i)$$



$$P(x|y) = \frac{1}{Z(y)} \prod_i P(x_i) \prod_\mu P_{\rm out}(y_\mu | \sum_i F_{\mu i} x_i)$$

$F_{\mu i}$: iid, known

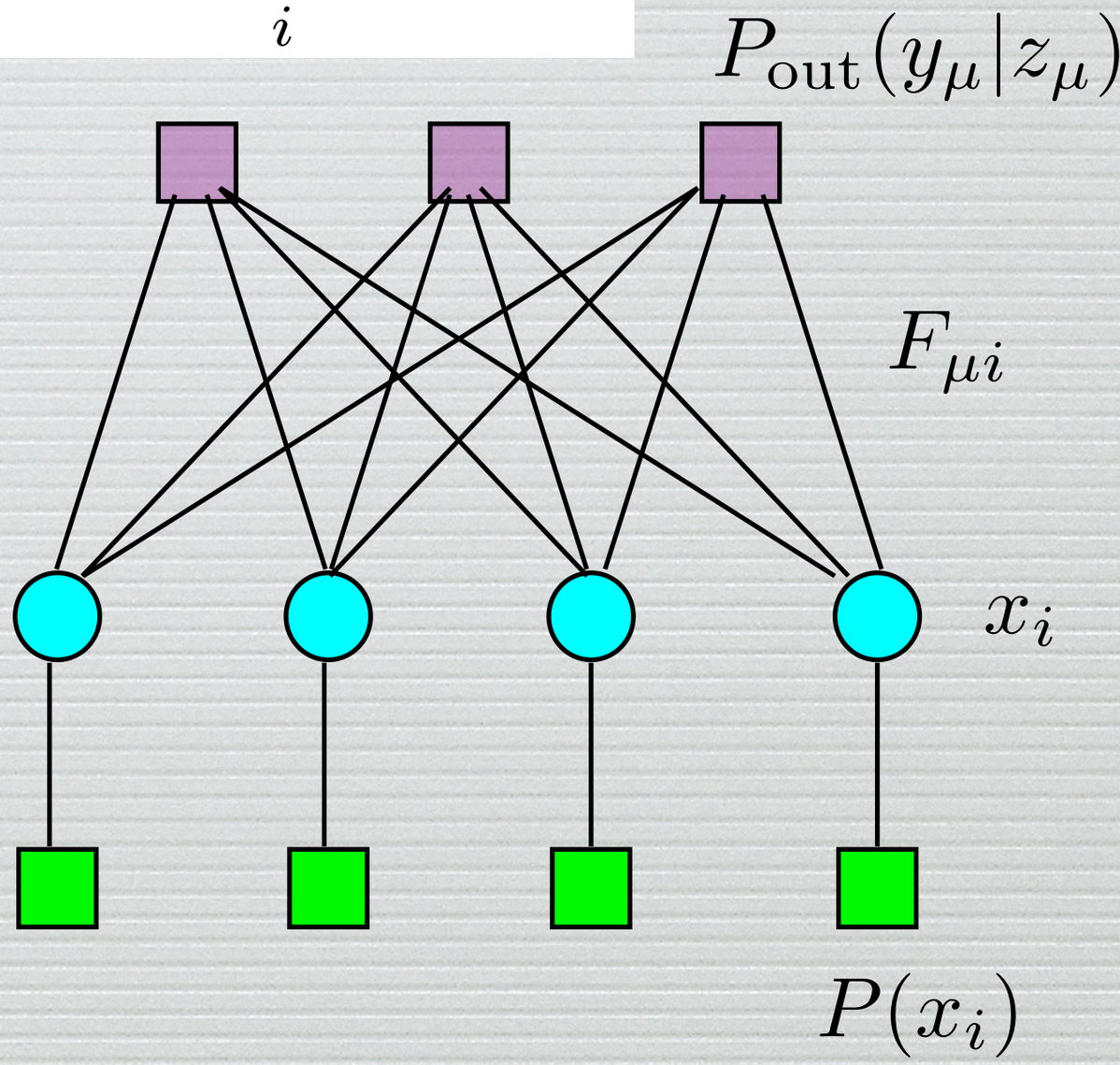
Spin glass with multispin interactions, infinite range: write mean field equations.

TAP equations written in terms of $a_i = \langle x_i \rangle$

$$c_i = \langle x_i^2 \rangle - \langle x_i \rangle^2$$

Iteration ⟶ algorithm : AMP

Statistical study ⟶ phase diagram



M 1989, OW 96, K 2003, K 2008 , DMM 2009, R2011, KMSSZ 2012

Benchmark: noiseless limit of compressed sensing with iid measurements

System of linear measurements

$$y = Fx$$

Measurements $y = \begin{pmatrix} y^1 \\ . \\ . \\ y^M \end{pmatrix}$

Signal $x = \begin{pmatrix} x_1 \\ . \\ . \\ x_N \end{pmatrix}$

$F = M \times N$ matrix

Random F : «random projections» (incoherent with signal)

Pb: Find x when $M < N$ and x is sparse

Phase diagram

«Thermodynamic limit»

$N \gg 1$ variables

$R = \rho N$ non-zero variables

$M = \alpha N$ equations

- Solvable by enumeration when $\alpha > \rho$ but $O(e^N)$

- ℓ_1 norm approach

Find a N - component vector x such that the M equations $y = Fx$ are satisfied and $||x||_1$ is minimal

- AMP = Bayesian approach

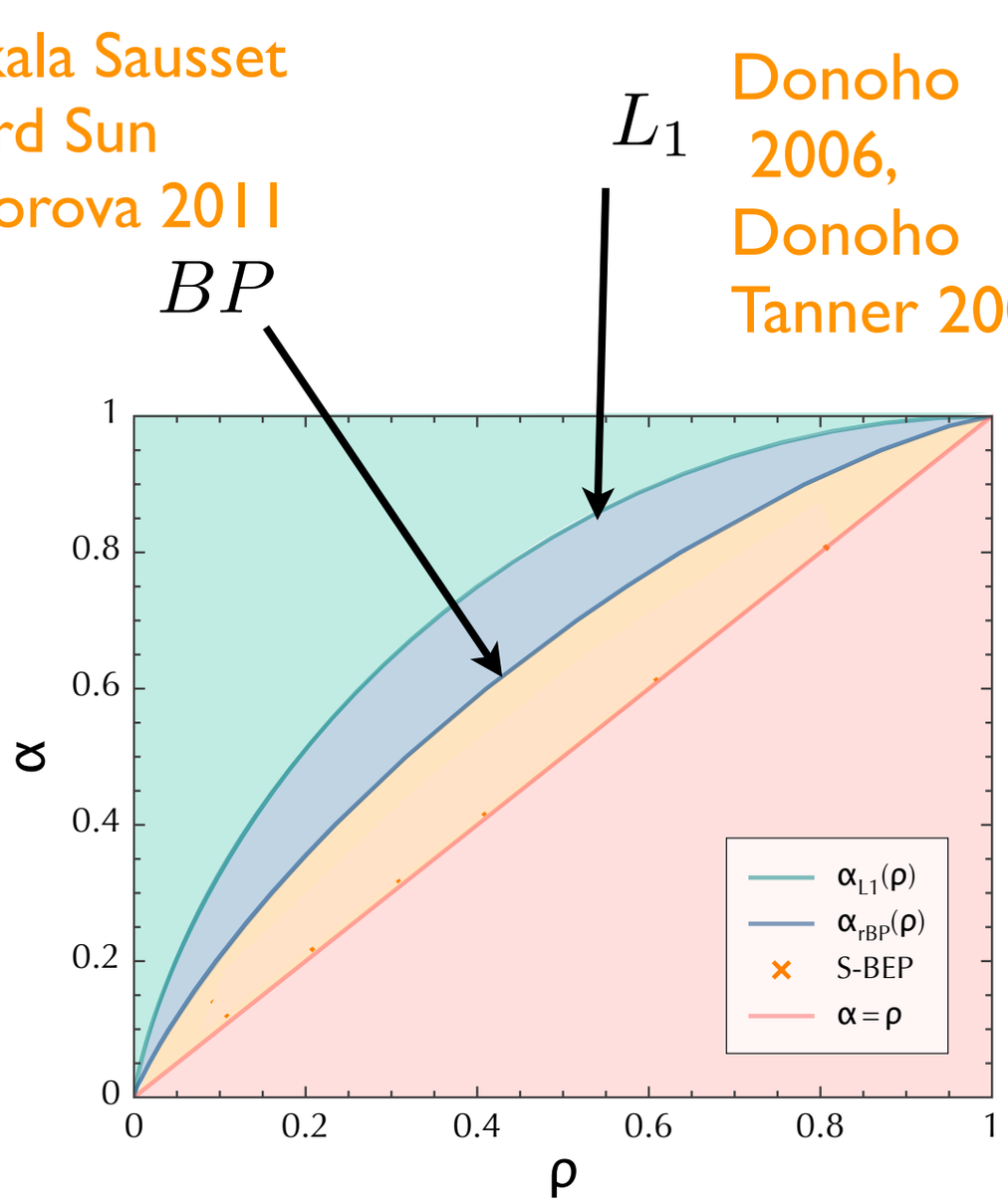
Planted: $\phi_T(x)$

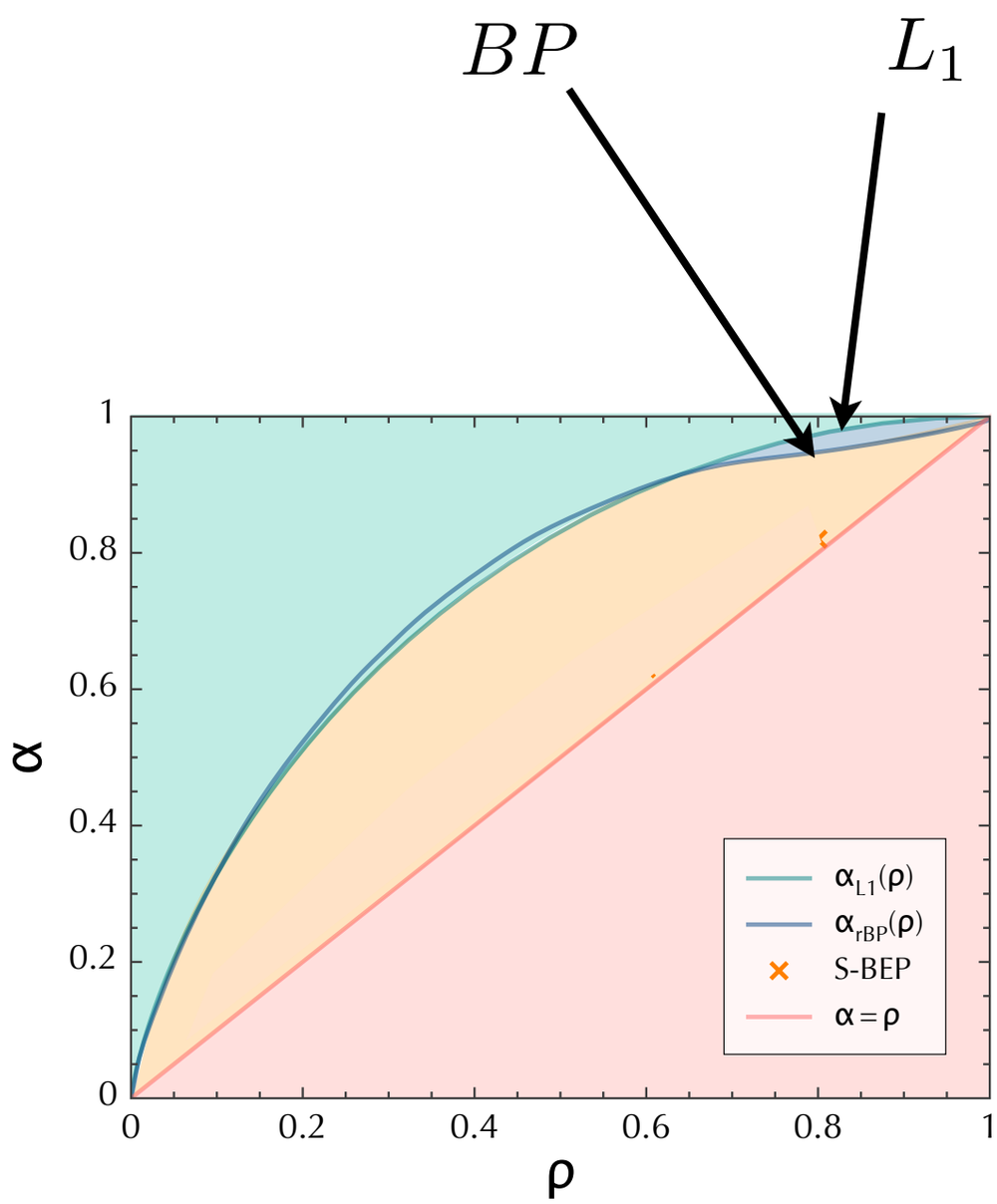
$$P(\mathbf{x}) = \prod_{i=1}^{N}[(1-\rho)\delta(x_i) + \rho\phi(x_i)] \prod_{\mu=1}^{P}\delta\left(y_\mu - \sum_i F_{\mu i}x_i\right)$$

Performance of AMP with Gauss-Bernoulli prior: phase diagram

Krzakala Sausset
Mézard Sun
Zdeborova 2011

Donoho
2006,
Donoho
Tanner 2005





Gaussian signal

$$\phi_T(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

Binary signal

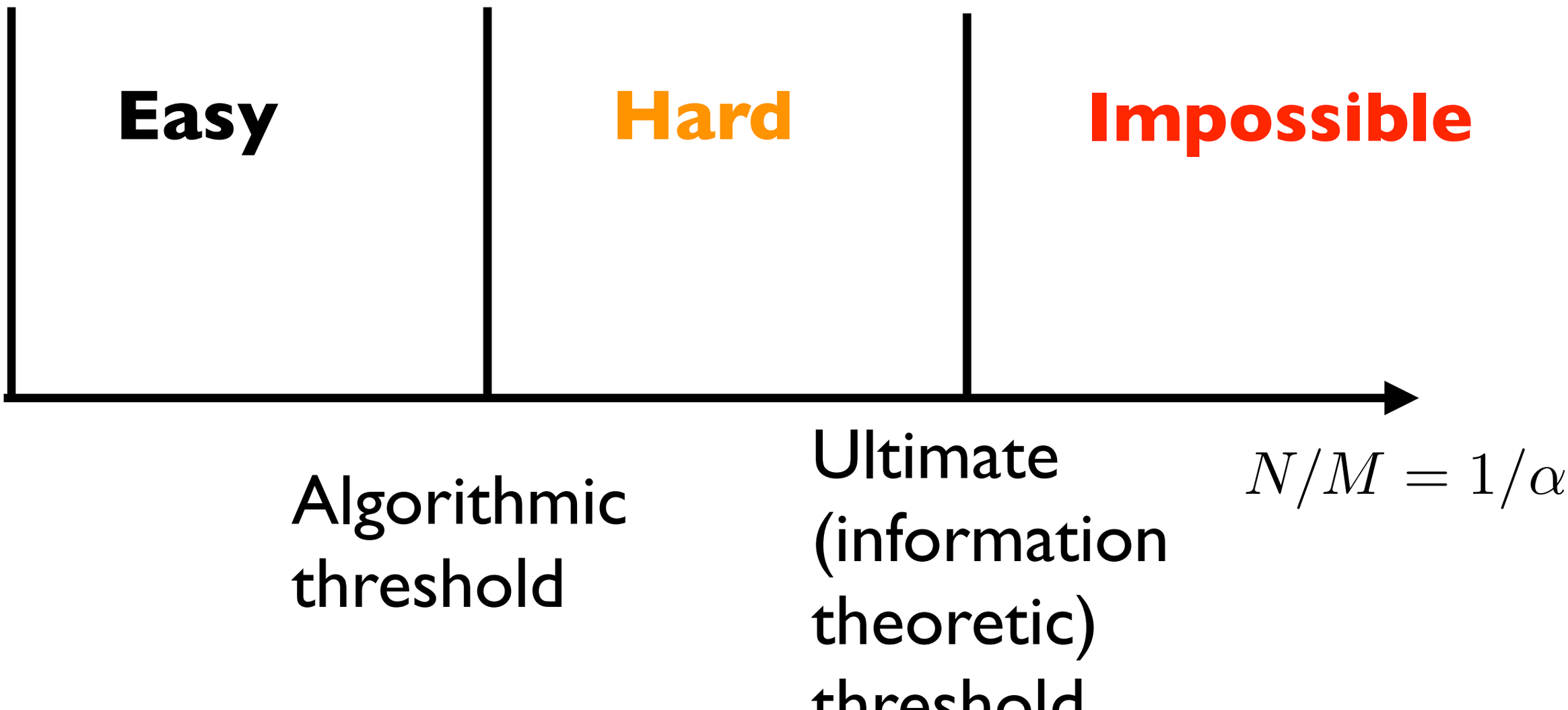
$$\phi_T(x) = \frac{1}{2}\left(\delta_{x,1} + \delta_{x,-1}\right)$$

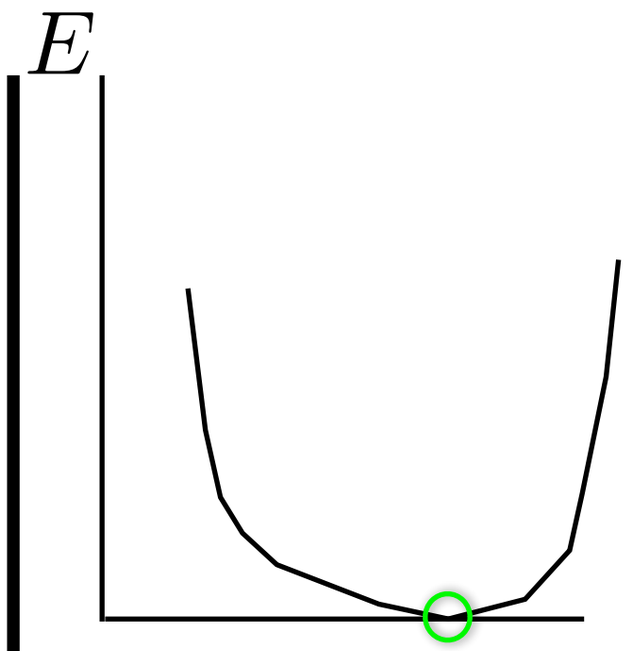
Analysis of random instances : phase transitions

N (real) variables, M measurements (linear functions)

Analysis of random instances : phase transitions

Reconstruction of signal using BP. Fixed ρ , decrease α





Crystal

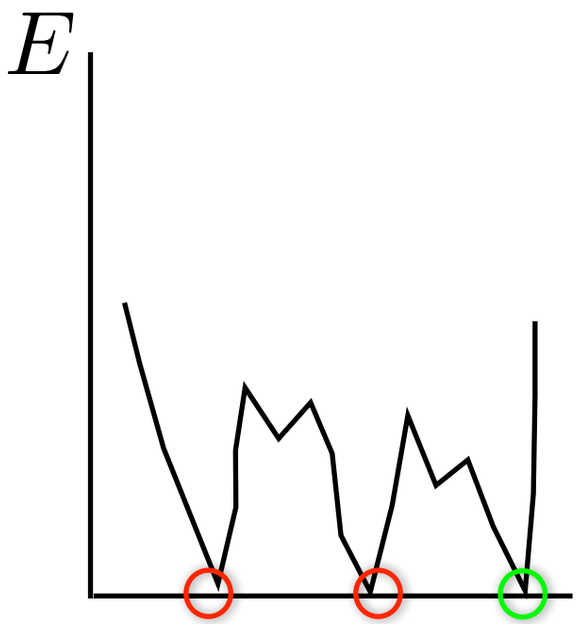
Easy

Belief Propagation

Crystal

Hard

«Seeded » BP



Many « crystals »

Impossible

Not enough measurements

N/M

Dynamical phase transition. Ubiquitous in statistical inference. Conjecture « All local algorithms freeze »… How universal?

Step 3: design the measurement matrix in order to get around the glass transition

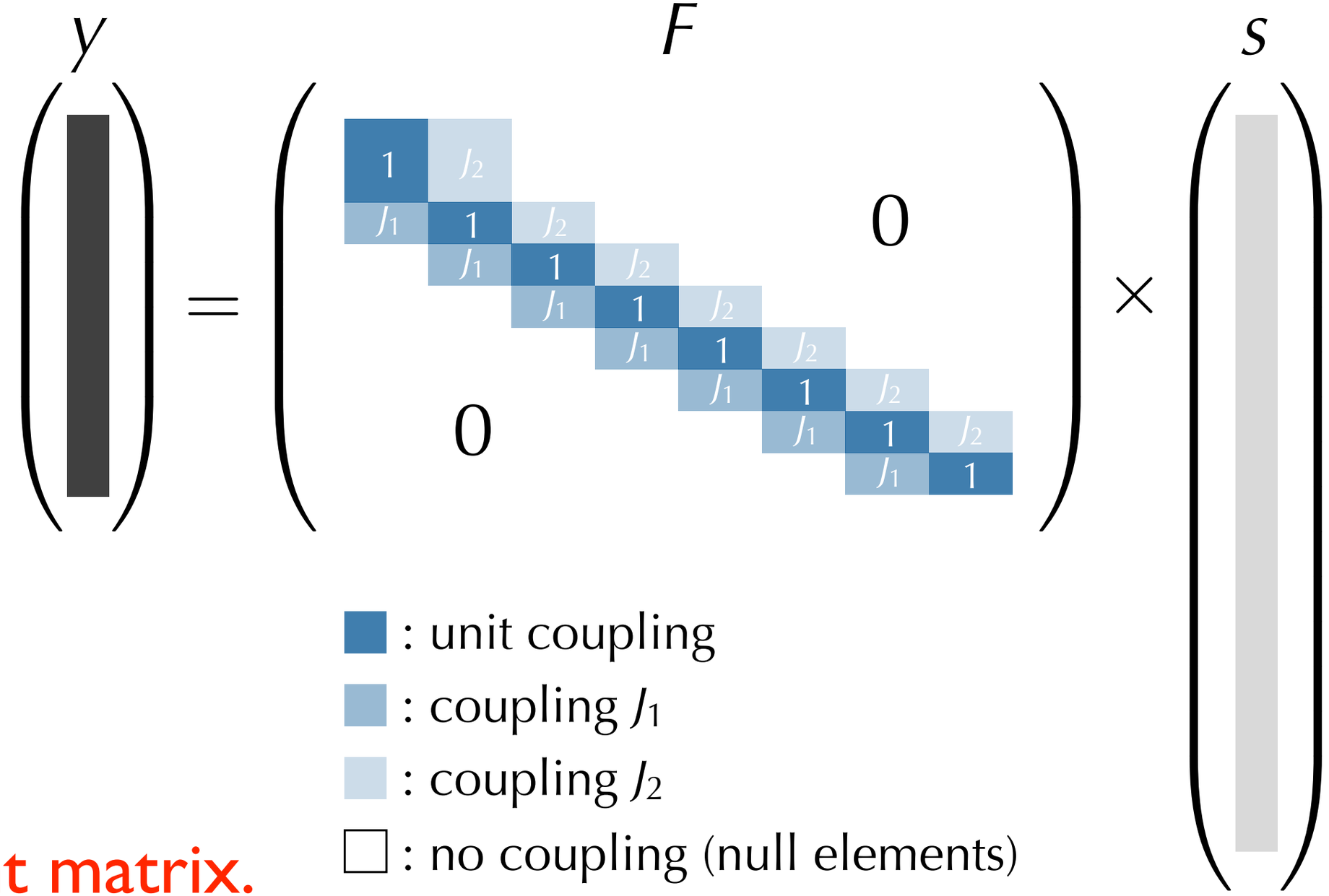
Getting around the glass trap: design the matrix F so that one nucleates the naive state (crystal nucleation idea,
...borrowed from error correcting codes : « spatial coupling »)

Felström-Zigangirov,
Kudekar Richardson Urbanke,
Hassani Macris Urbanke,
...

«Seeded BP»

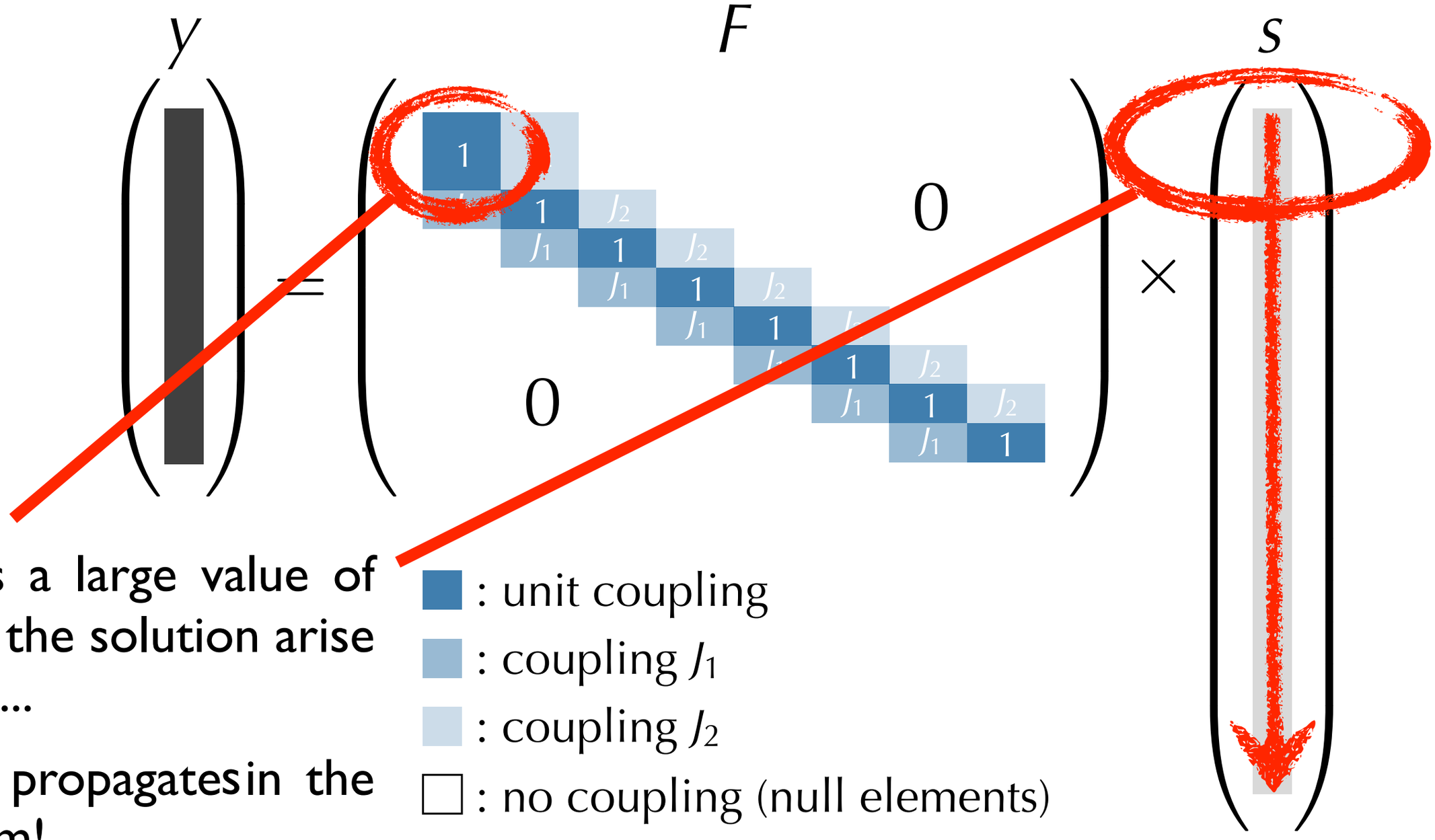
Nucleation and seeding

Nucleation and seeding



Structured measurement matrix. Variances of the matrix elements

$F_{\mu i} =$ independent random Gaussian variables, zero mean and variance $J_{b(\mu)b(i)}/N$



Block 1 has a large value of M such that the solution arise in this block...

... and then propagatesin the whole system!

■ : unit coupling

■ : coupling J_1

■ : coupling J_2

□ : no coupling (null elements)

$$L = 8$$

$$N_i = N/L$$

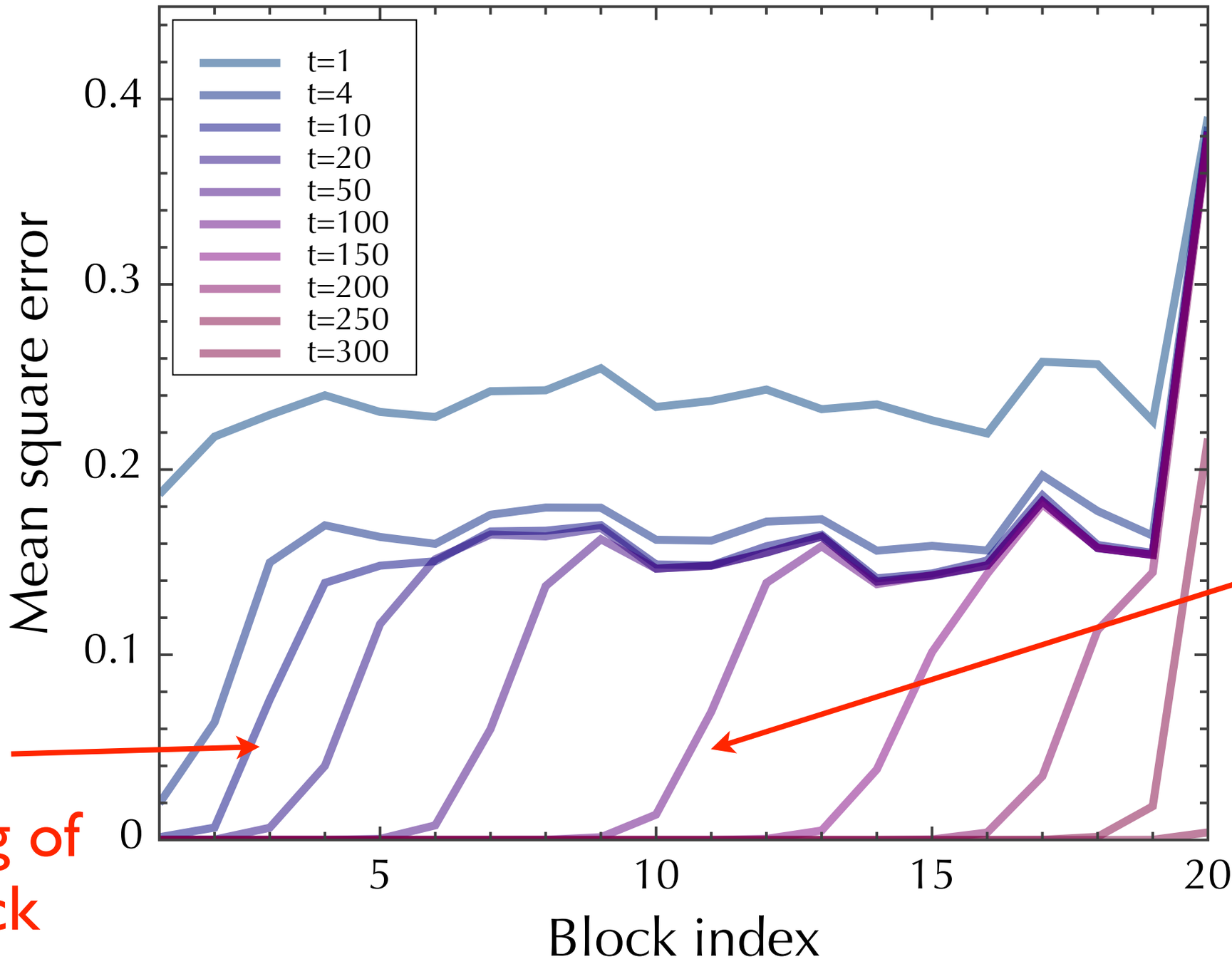
$$M_i = \alpha_i N/L$$

$$\alpha_1 > \alpha_{BP}$$

$$\alpha_j = \alpha' < \alpha_{BP} \qquad j \geq 2$$

$$\alpha = \frac{1}{L}\left(\alpha_1 + (L-1)\alpha'\right)$$

Numerical study



$t = 100$ decoding of blocks 1 to 9

$t = 10$ decoding of first block

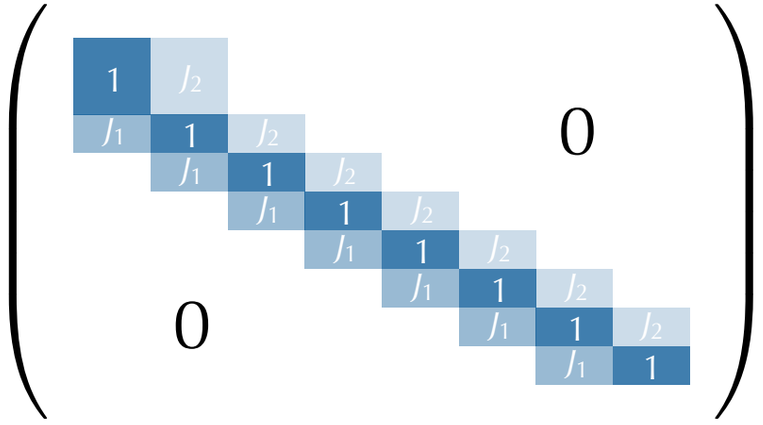
$L = 20$ $N = 50000$ $\rho = .4$ $J_1 = 20$ $\alpha_1 = 1$

$J_2 = .2$ $\alpha = .5$

Performance of the probabilistic approach + message passing + parameter learning+ seeding matrix

$$Z = \int \prod_{j=1}^{N} \mathrm{d}x_j \prod_{i=1}^{N} \left[(1-\rho)\delta(x_i) + \rho\phi(x_i)\right] \prod_{\mu=1}^{M} \delta\left(y_\mu - \sum_{i=1}^{N} F_{\mu i} x_i\right)$$

F



- Simulations
- Analytic approaches (replicas and cavity)

$$\rightarrow \alpha_c = \rho_0$$

Reaches the ultimate information-theoretic threshold

Proof: Donoho Javanmard Montanari

Performance of AMP with Gauss-Bernoulli prior: phase diagram

Krzakala Sausset
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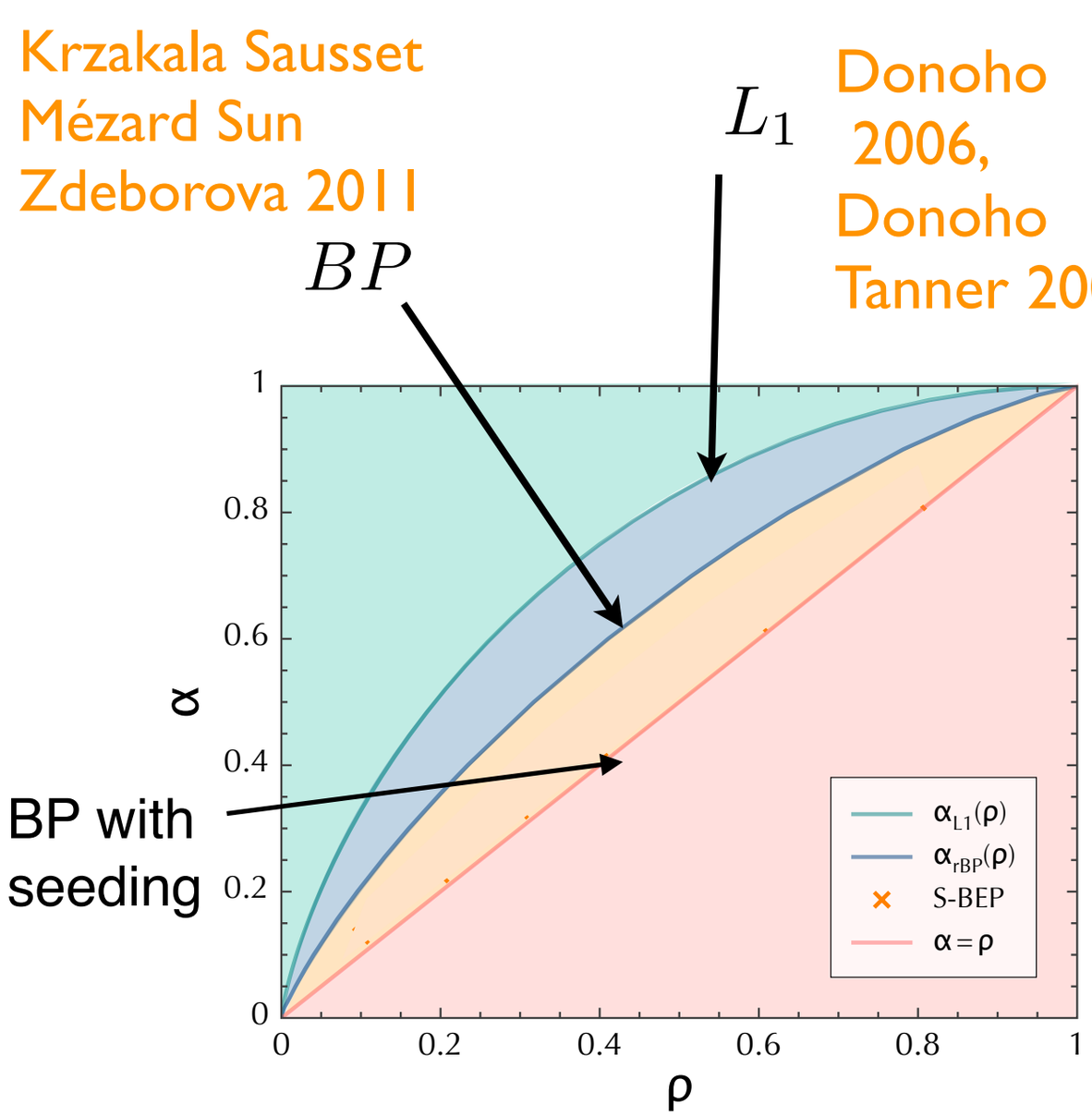
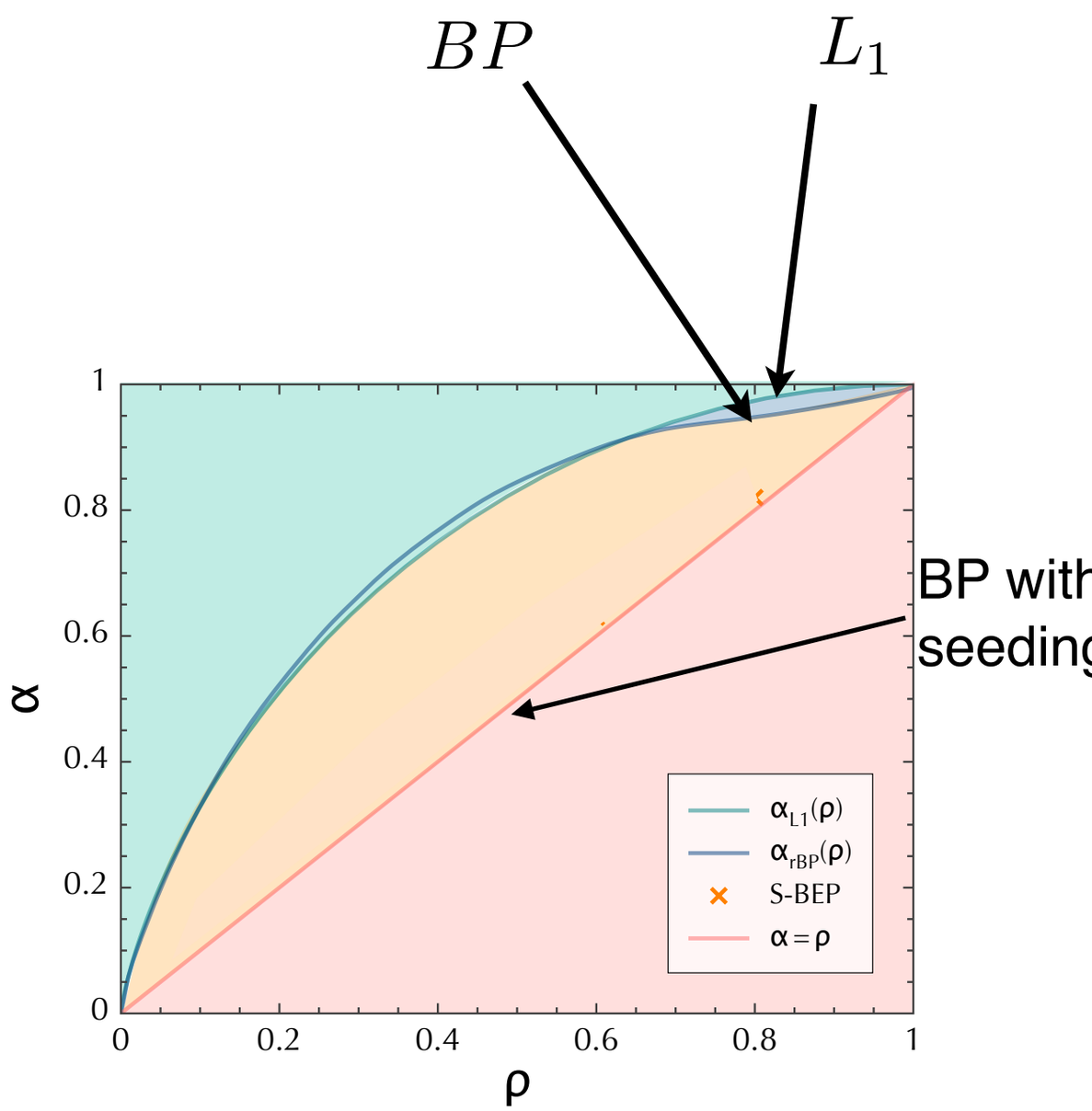
Tanner 2005





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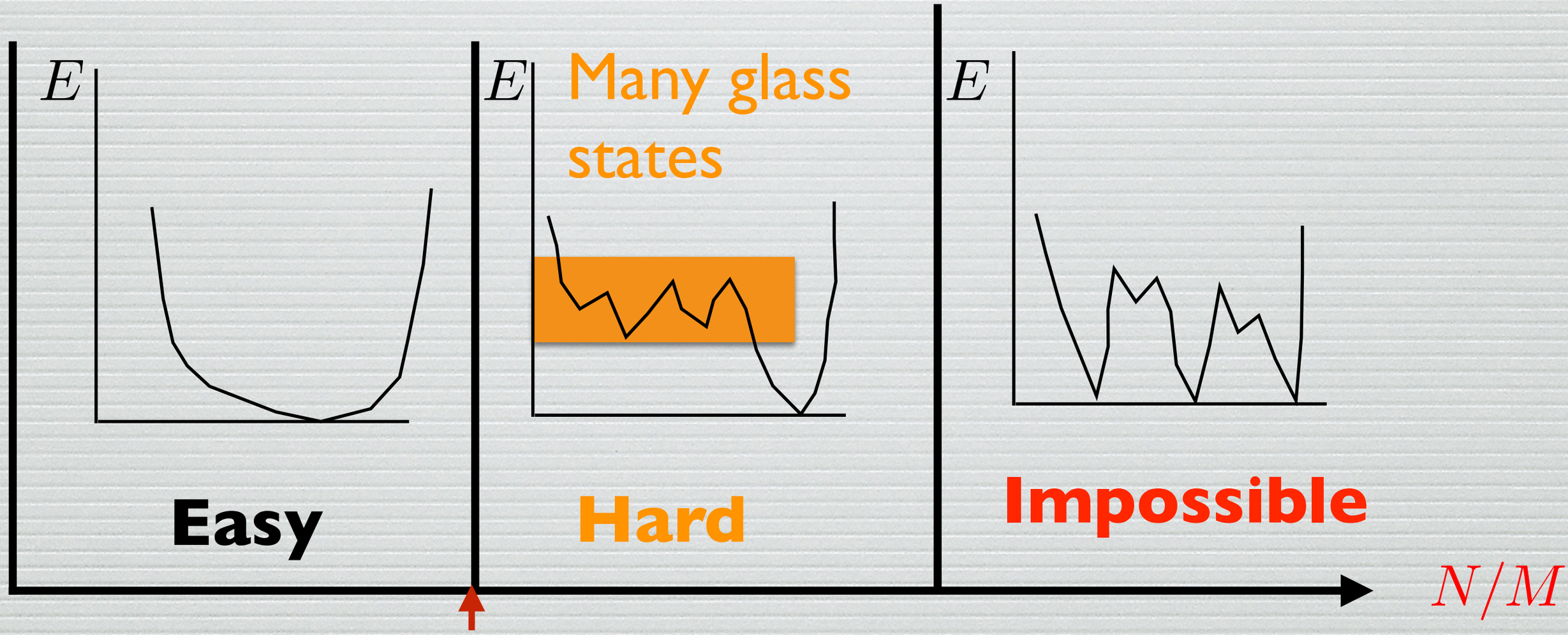


Phase transitions are crucial in large inference problems

Hard-Impossible = absolute limit (Shannon-like)

Easy- Hard = limit for large class of algorithms (local)

The spin glass cornucopia

A very sophisticated and powerful corpus of conceptual and methodological approaches has been developed (replicas, cavity, TAP,…) mostly in the years 1975-2000, and has found applications in many different fields of information theory and computer science

Portrait of Ottavio Strada,

Tintoretto, Venice 1567

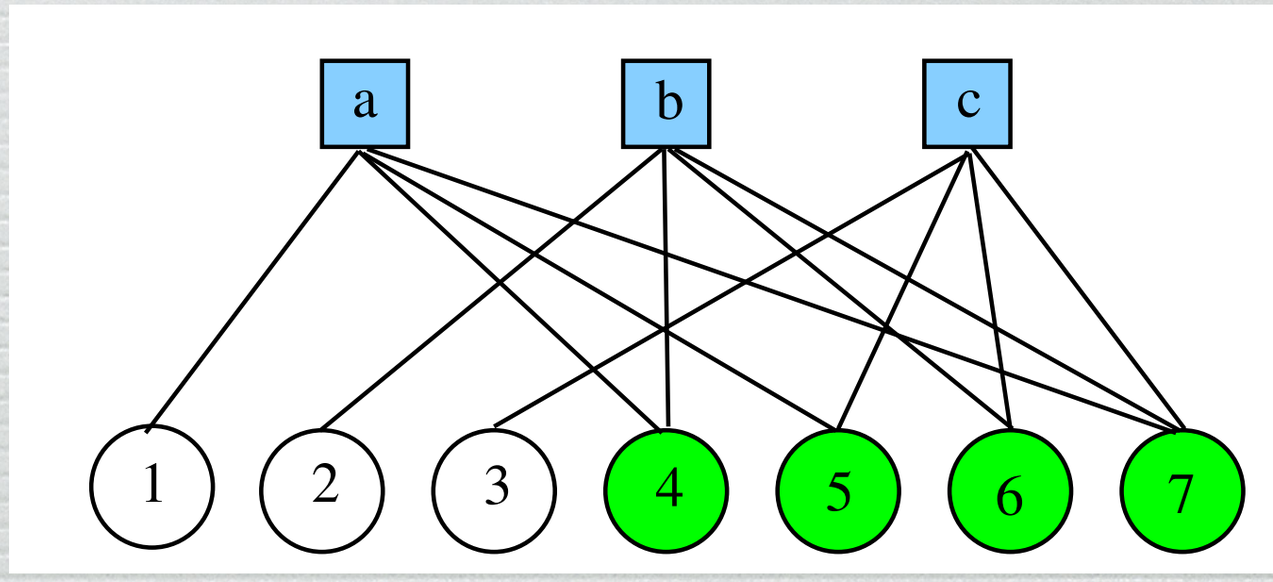
Rijk's Museum Amsterdam

Back to error correction

Efficient codes : parity checks (LDPC codes)

Add redundancy, with structure allowing to decode

$x_i \in \{0, 1\}$

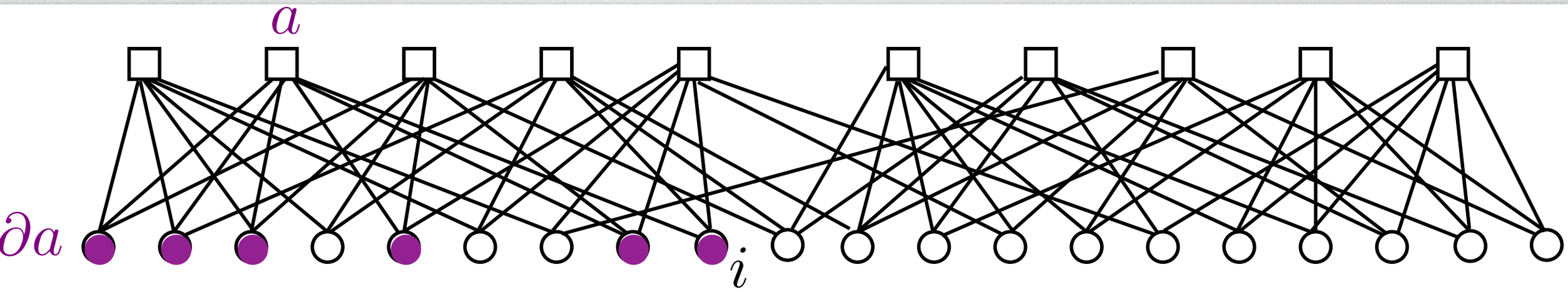


$$a: \quad x_1 + x_4 + x_5 + x_7 = 0 \pmod 2$$
$$b: \quad x_2 + x_4 + x_6 + x_7 = 0 \pmod 2$$
$$c: \quad x_3 + x_5 + x_6 + x_7 = 0 \pmod 2$$

2^4 codewords

among 2^7 words

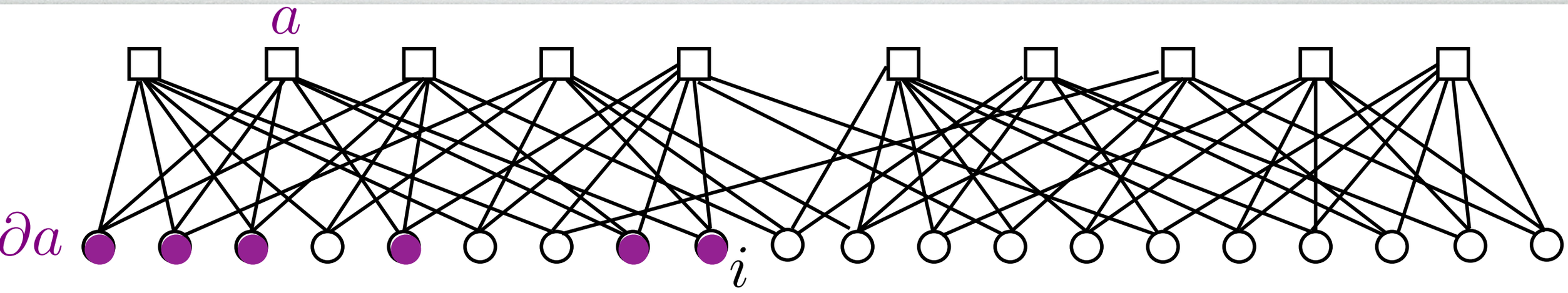
Error decoding: « crystal hunting » inference problem



$$P(x_1,\ldots,x_N|y_1,\ldots,y_N) = \frac{1}{Z}\prod_i \psi_i(x_i|y_i) \prod_a \mathbb{I}\left(\sum_{i\in\partial a} x_i = 0 \ (mod\ 2)\right)$$

Spin glass problem with multispin interactions, discontinuous glass transition (1 step RSB)

Error decoding: « crystal hunting » inference problem



$$P(x_1,\ldots,x_N|\underbrace{y_1,\ldots,y_N}_{\text{received}}) = \frac{1}{Z}\prod_i \psi_i(x_i|y_i)\ \prod_a \mathbb{I}\left(\sum_{i\in\partial a} x_i = 0\ (mod\ 2)\right)$$

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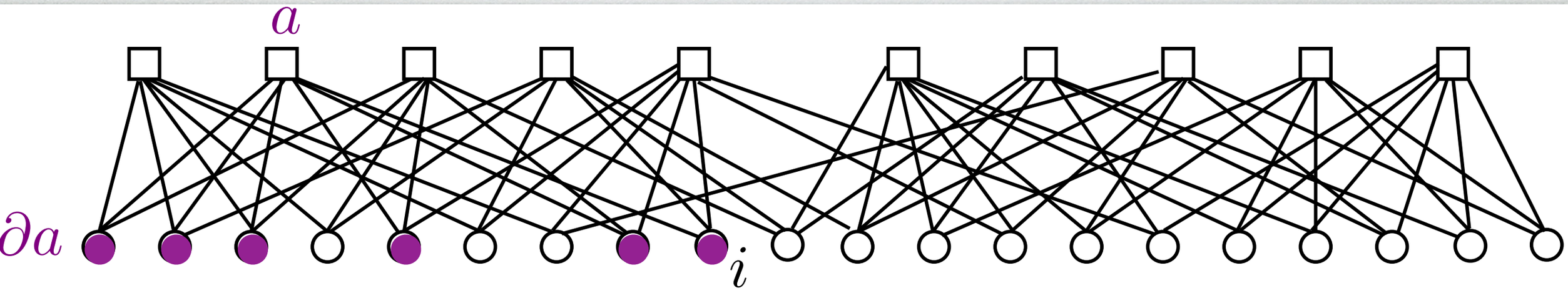
Error decoding: « crystal hunting » inference problem



$$P(x_1,\ldots,x_N|\underbrace{y_1,\ldots,y_N}_{\text{received}}) = \frac{1}{Z}\prod_i \psi_i(x_i|y_i) \prod_a \mathbb{I}\left(\sum_{i\in\partial a} x_i = 0 \ (mod\ 2)\right)$$

A priori knowledge of the channel

Spin glass problem with multispin interactions, discontinuous glass transition (1 step RSB)

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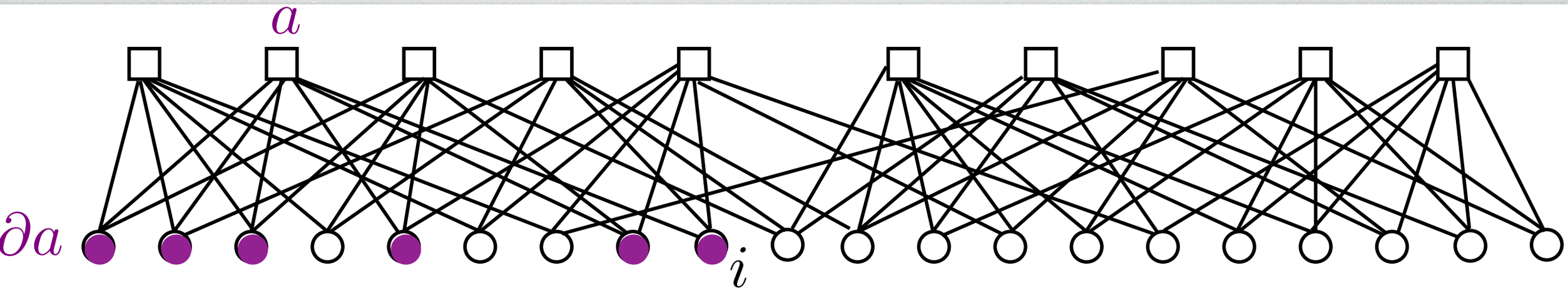

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A priori knowledge of the channel

Parity check constraints

Spin glass problem with multispin interactions, discontinuous glass transition (1 step RSB)

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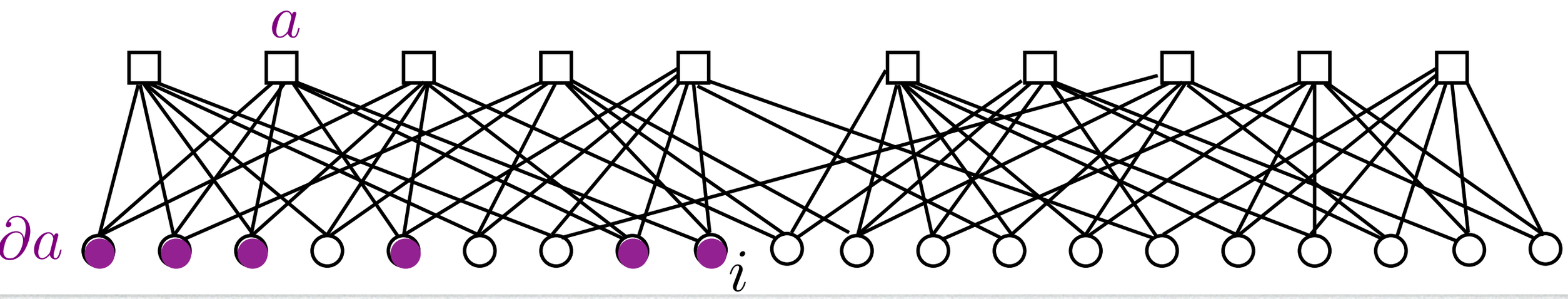

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One possible decoding algorithm: use belief-propagation mean-field equations relating the local fields

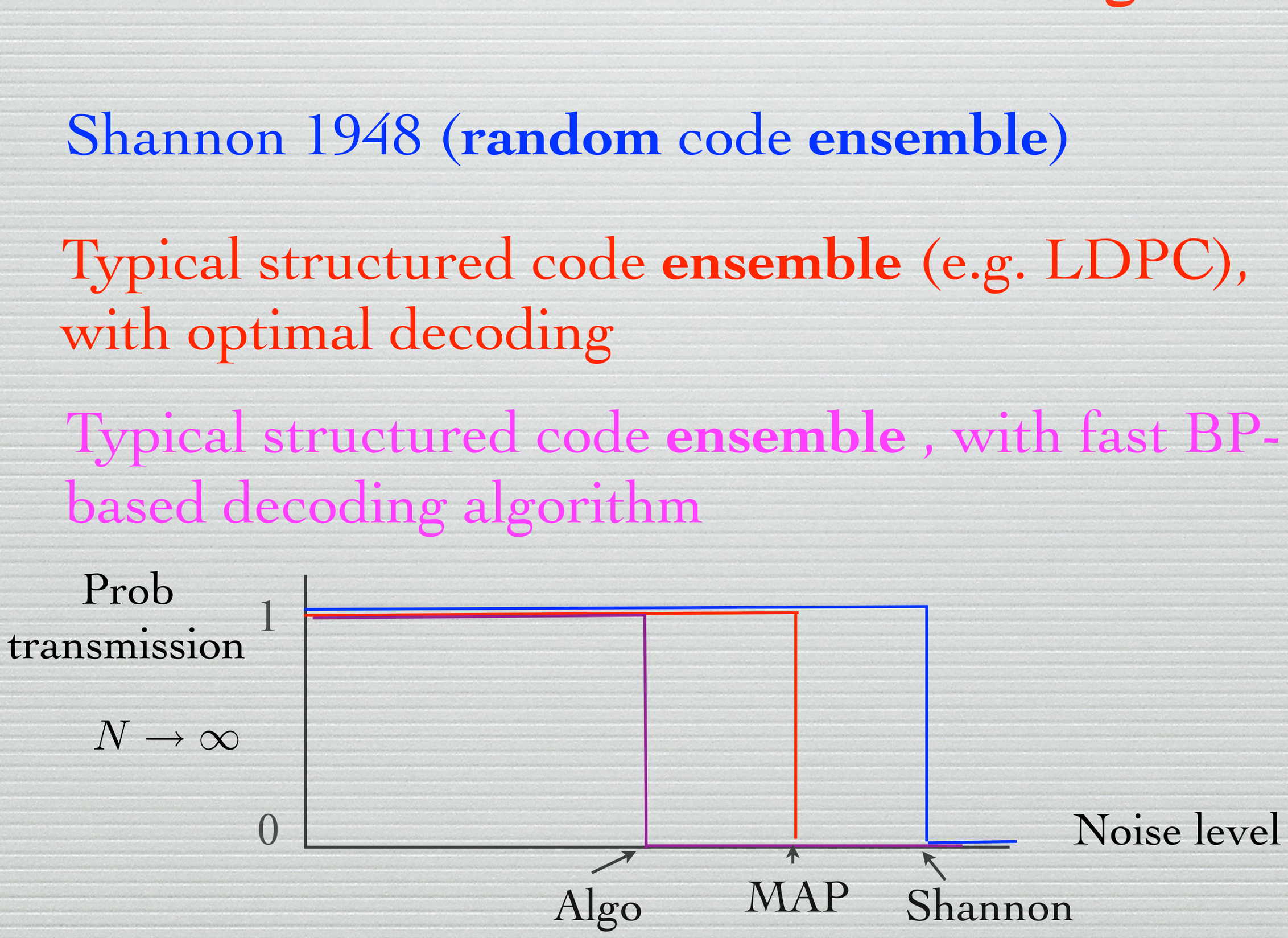
Solve them iteratively (Gallager)

Phase Transitions in Error correcting codes

Shannon 1948 (**random** code **ensemble**)

Typical structured code **ensemble** (e.g. LDPC), with optimal decoding

Typical structured code **ensemble** , with fast BP-based decoding algorithm



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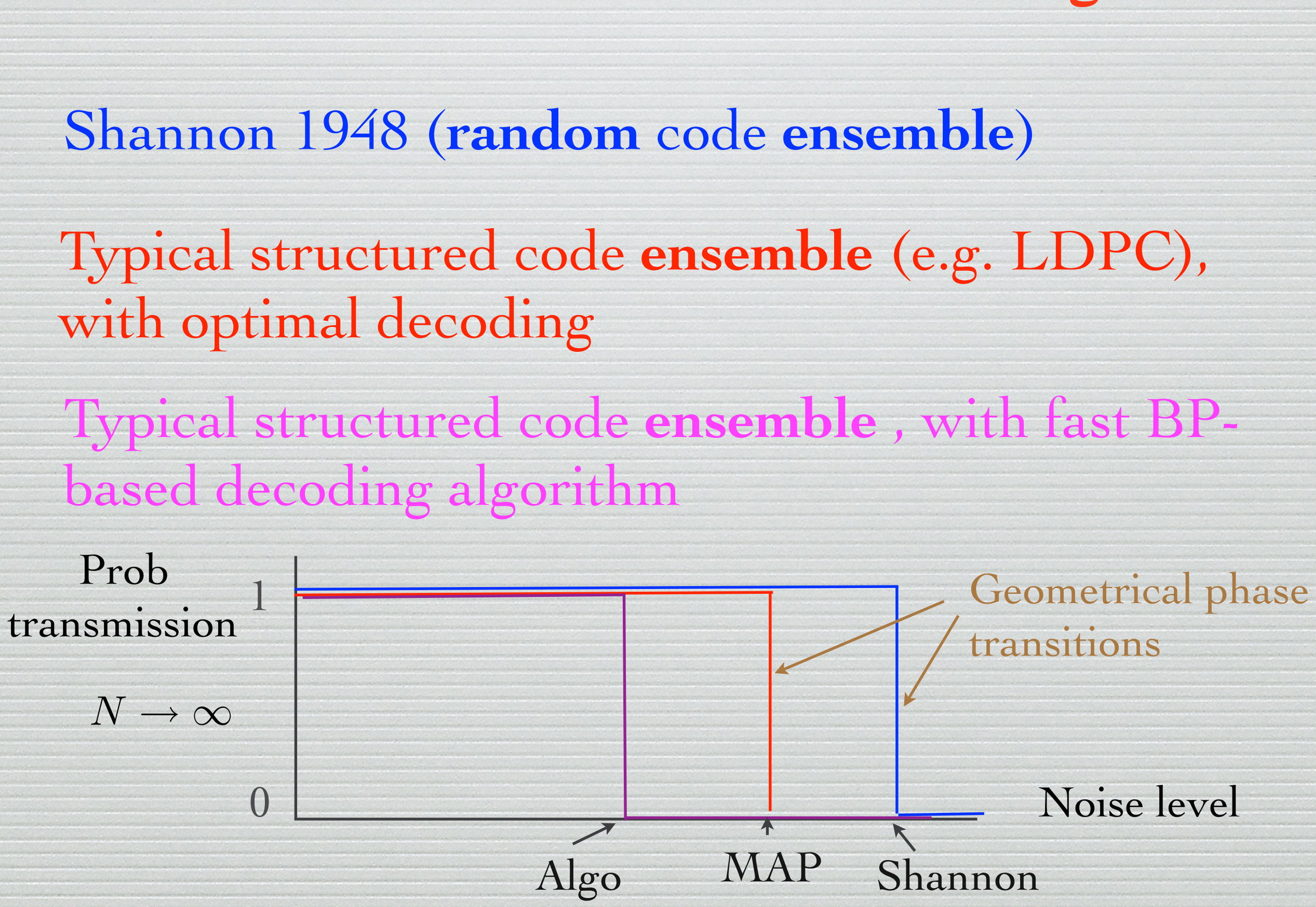

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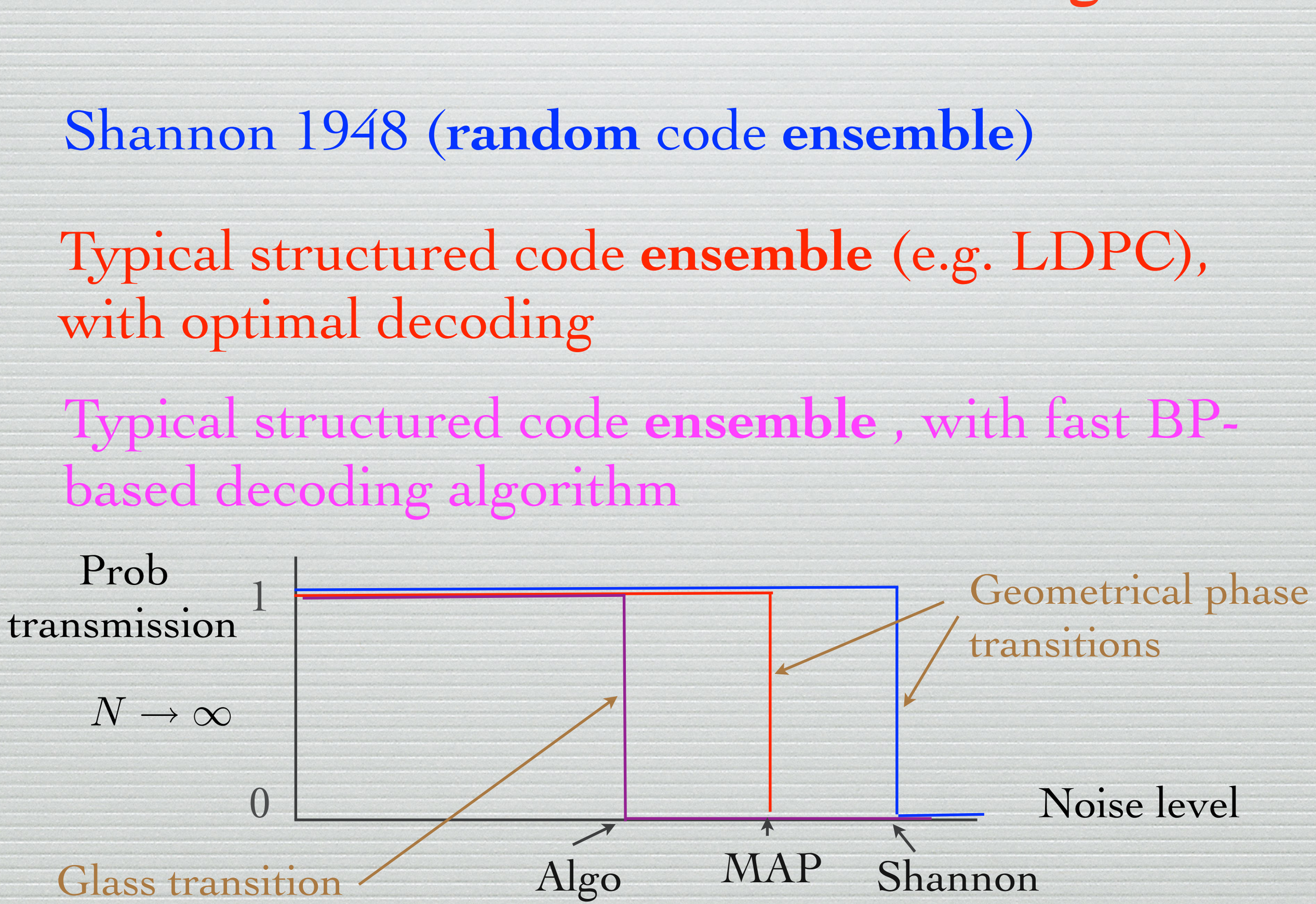
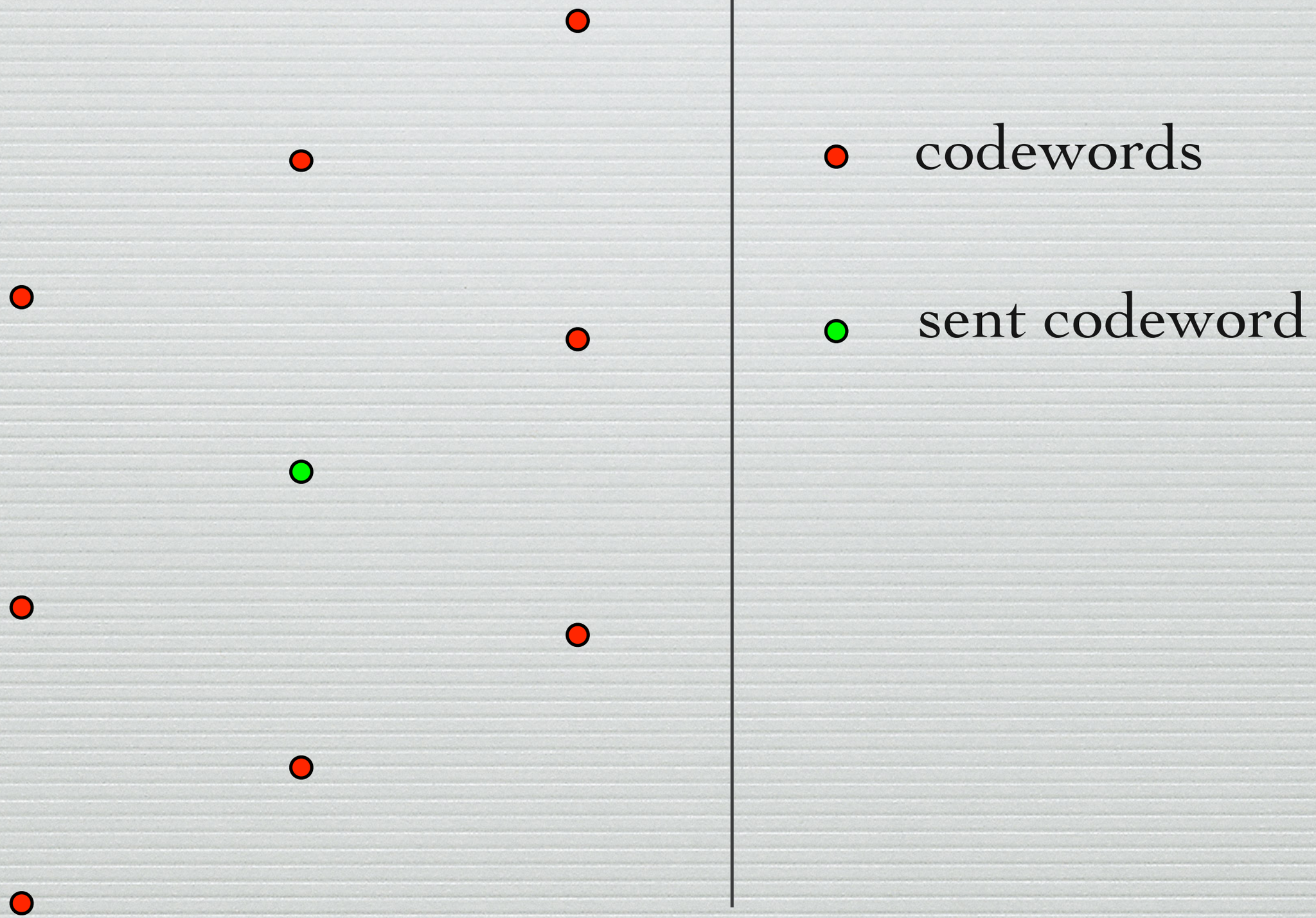


Error correction: decoding



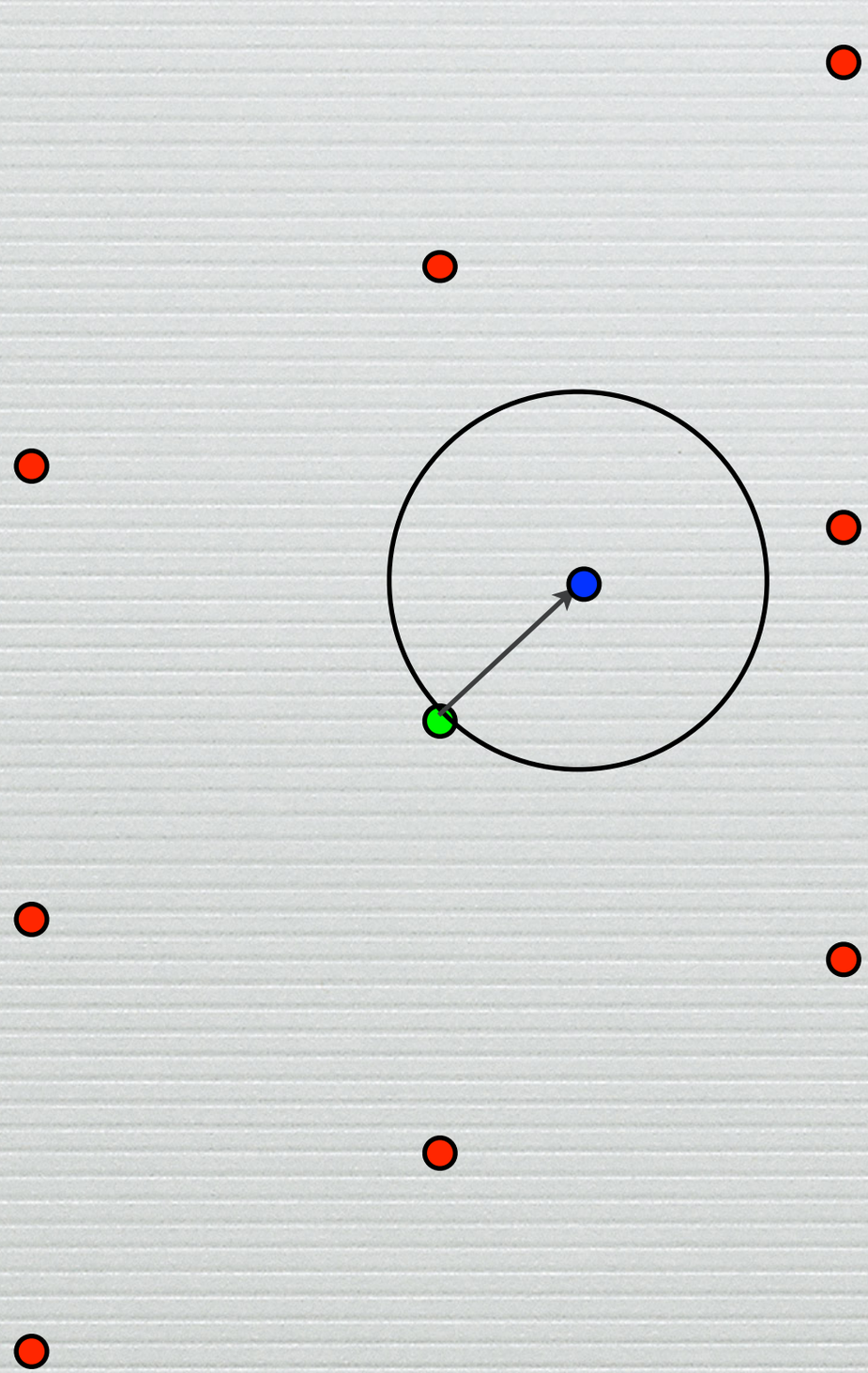
Error correction: decoding

codewords

sent codeword

received word

Error correction: decoding



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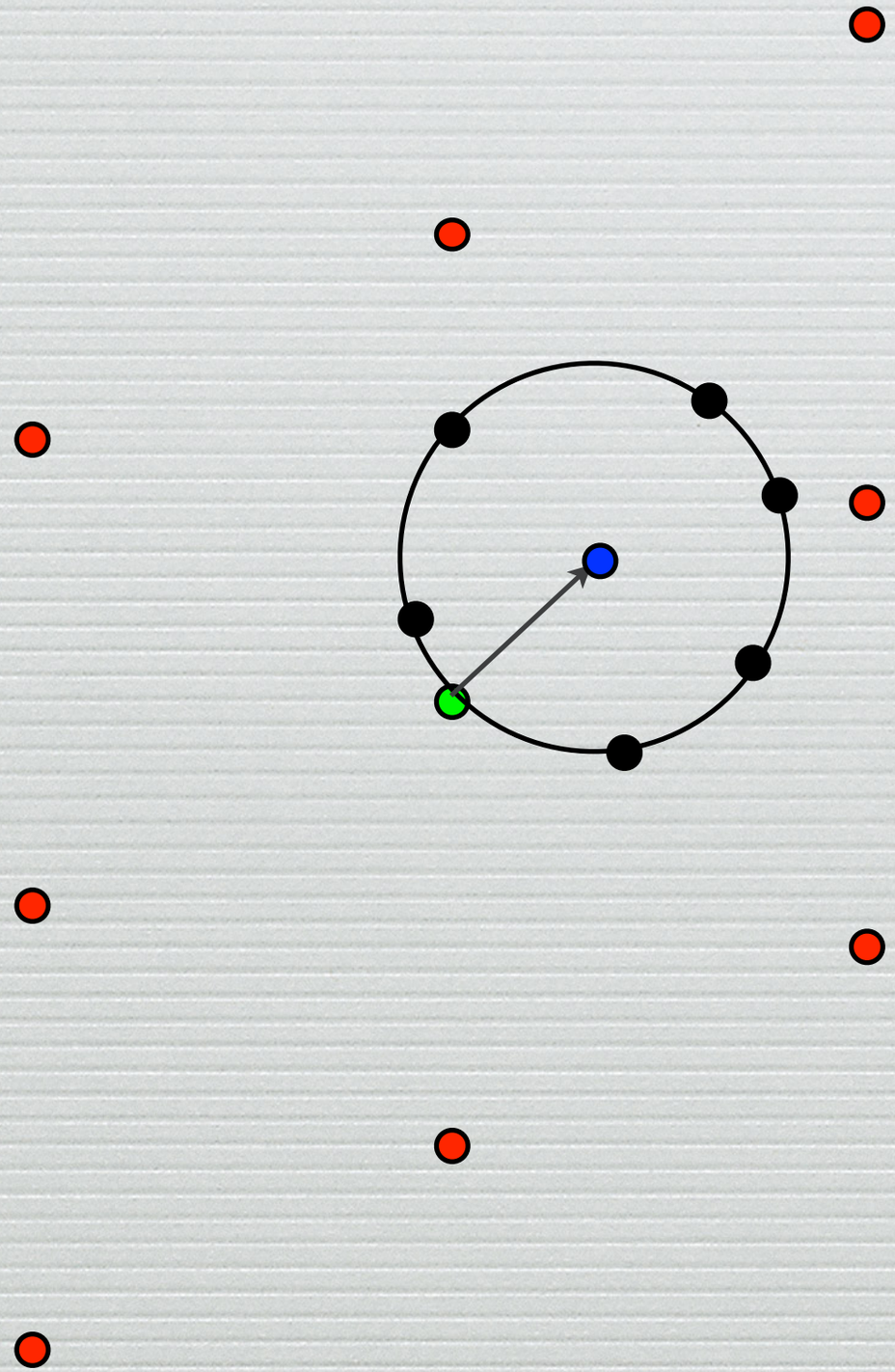
Error correction: decoding



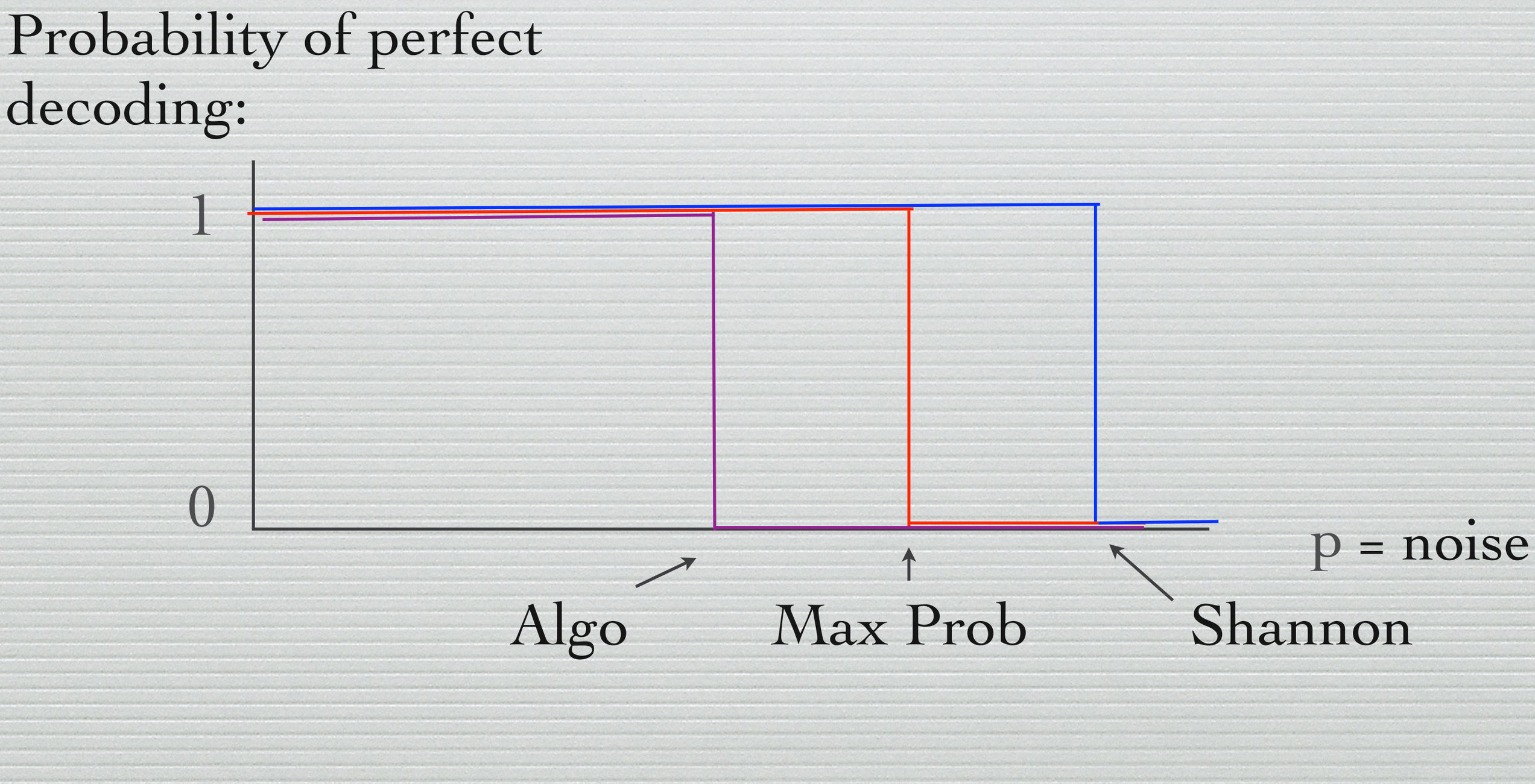
codewords

sent codeword

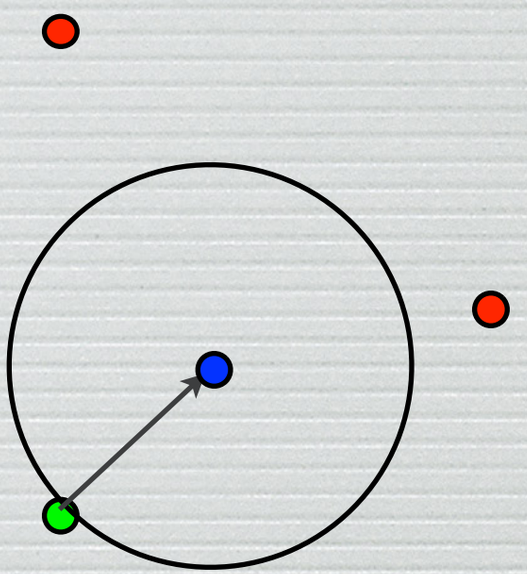
received word

metastable states

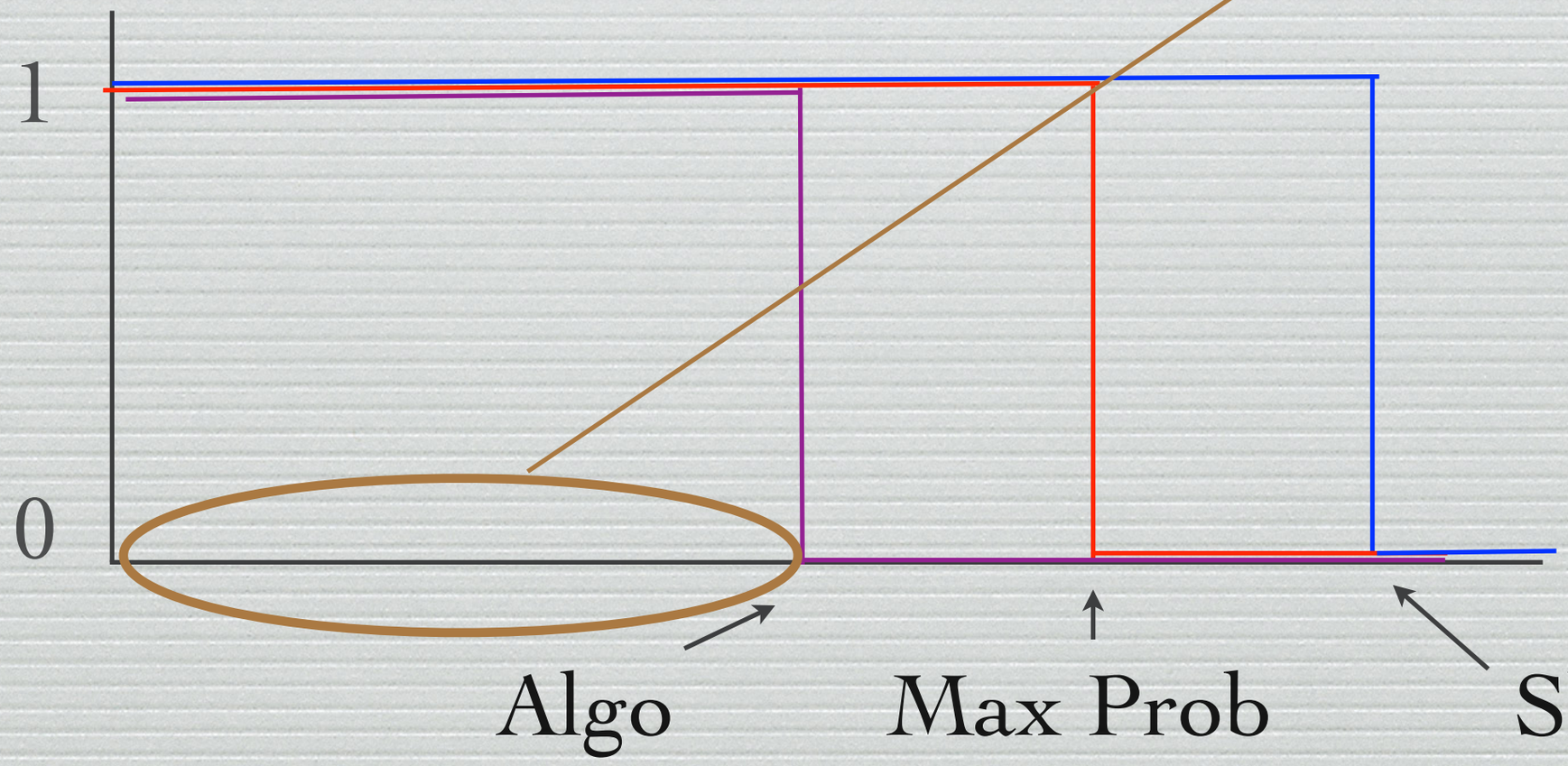
Phase transitions in decoding



Phase transitions in decoding

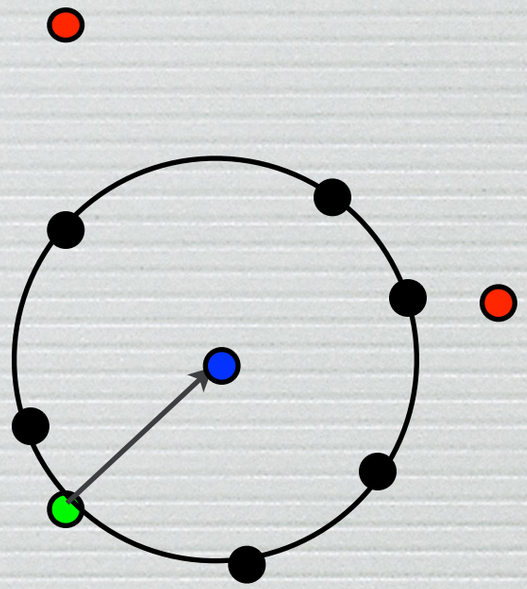


Probability of perfect decoding:

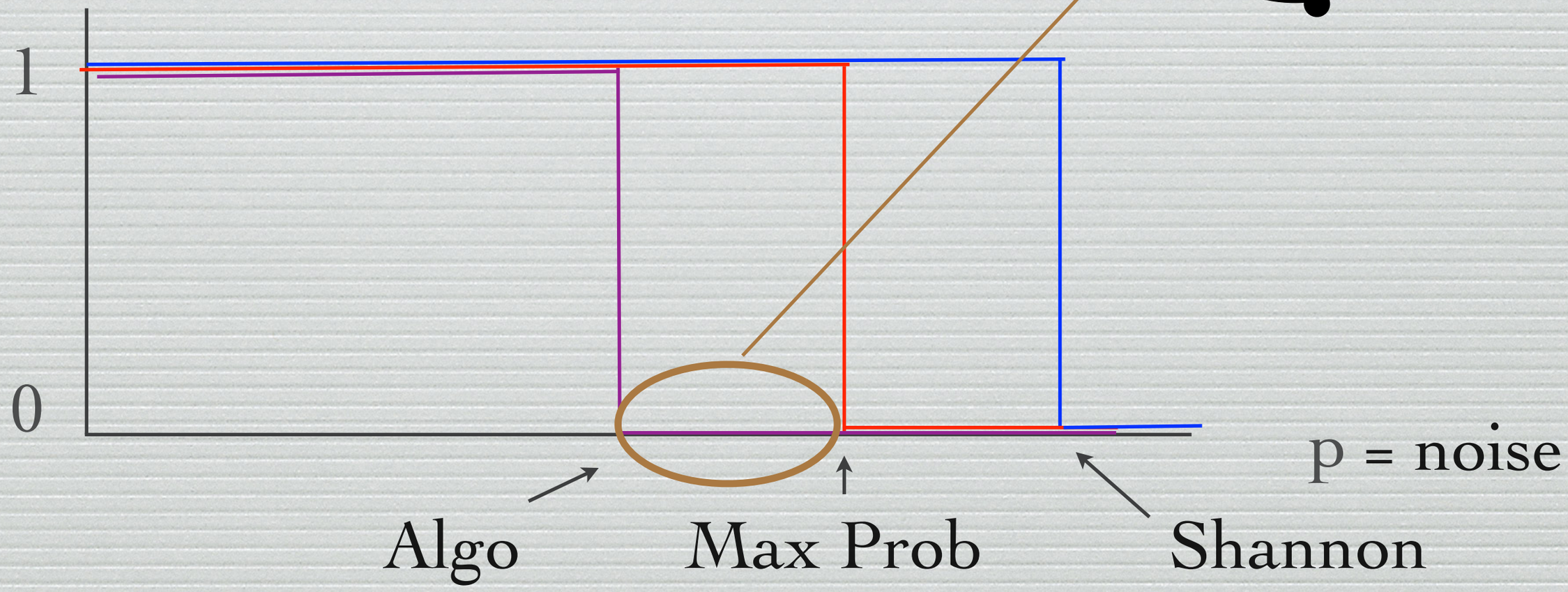


Phase transitions in decoding

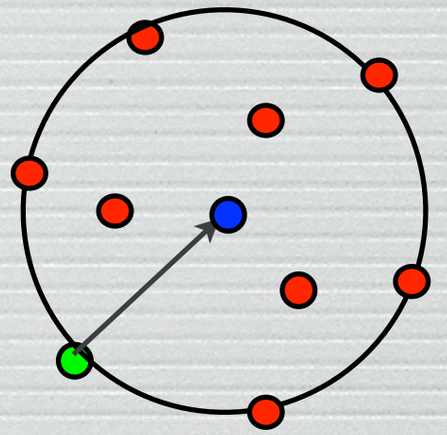
Metastables states=traps



Probability of perfect decoding:



Phase transitions in decoding



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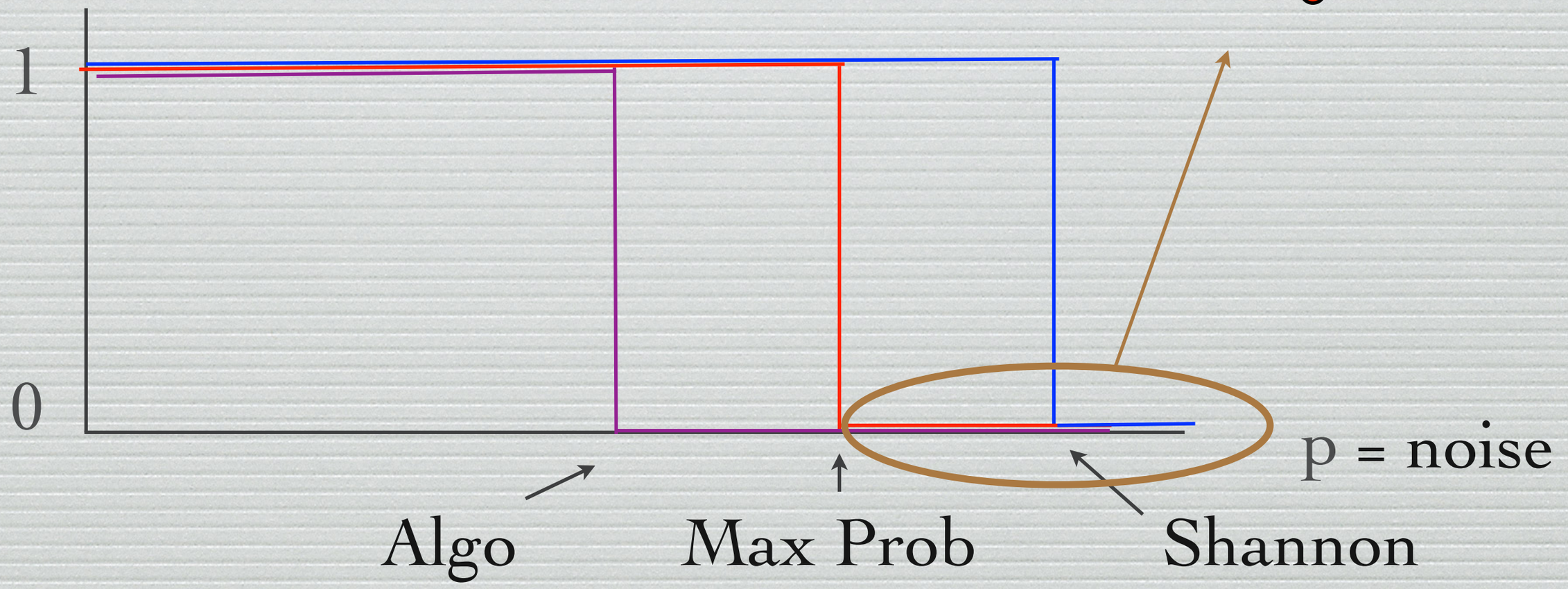

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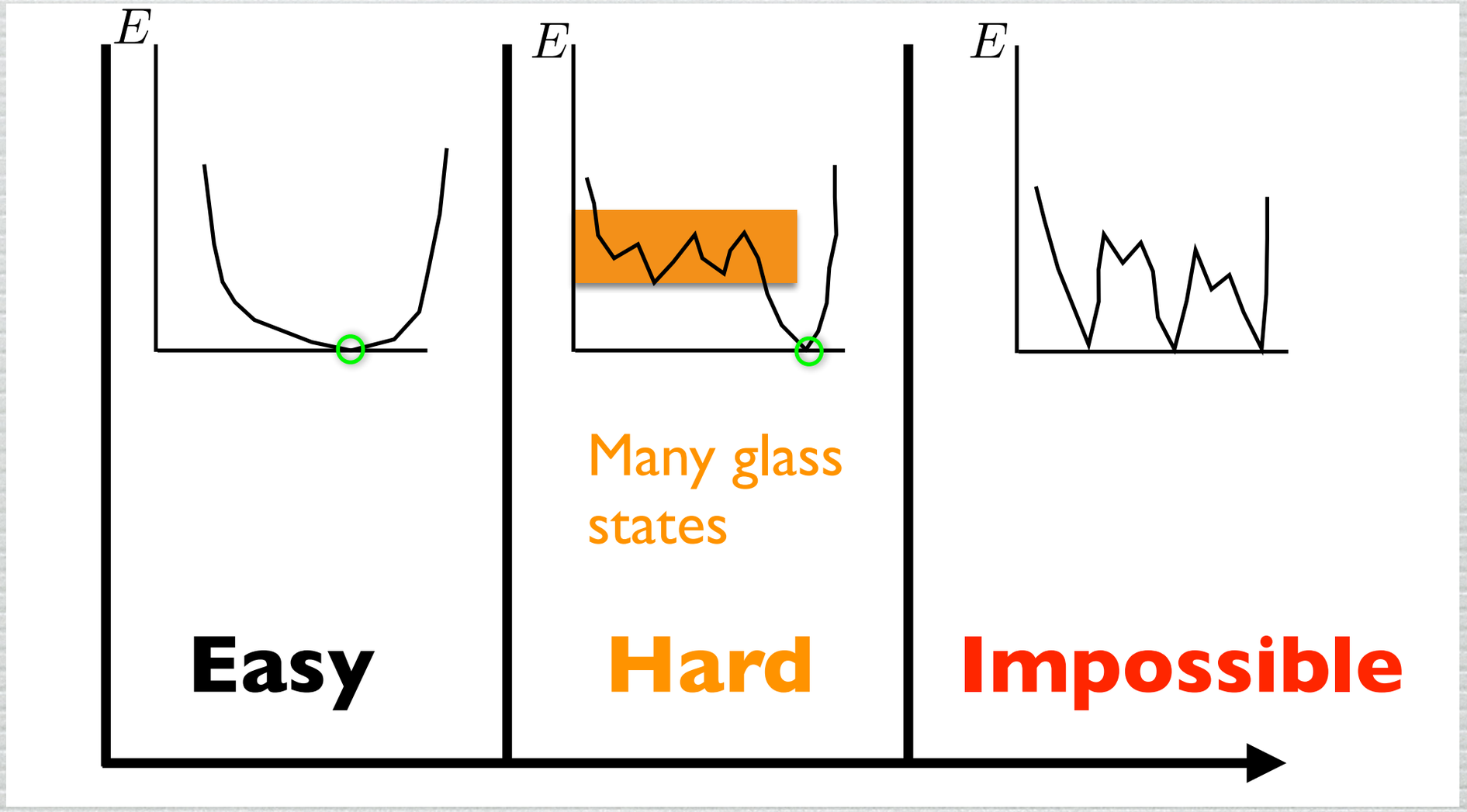

The spin glass cornucopia

A very sophisticated and powerful corpus of conceptual and methodological approaches has been developed (replicas, cavity, TAP,…) mostly in the years 1975-2000, and has found applications in many different fields of information theory and computer science

Portrait of Ottavio Strada,

Tintoretto, Venice 1567

Rijk's Museum Amsterdam