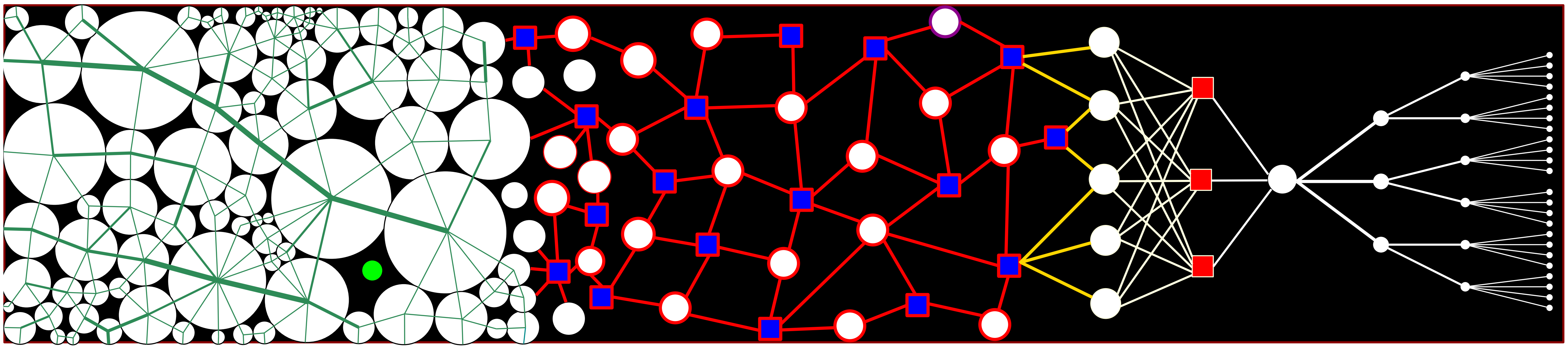


Jamming and Machine Learning

Pierfrancesco Urbani -IPhT, CNRS, CEA Saclay

Packing spheres

<u>The problem</u>: given a set of N spheres of a given diameter and a box of volume V, find an arrangement of the spheres in such a way that they do not overlap

$$\mathcal{V}_d(D)$$

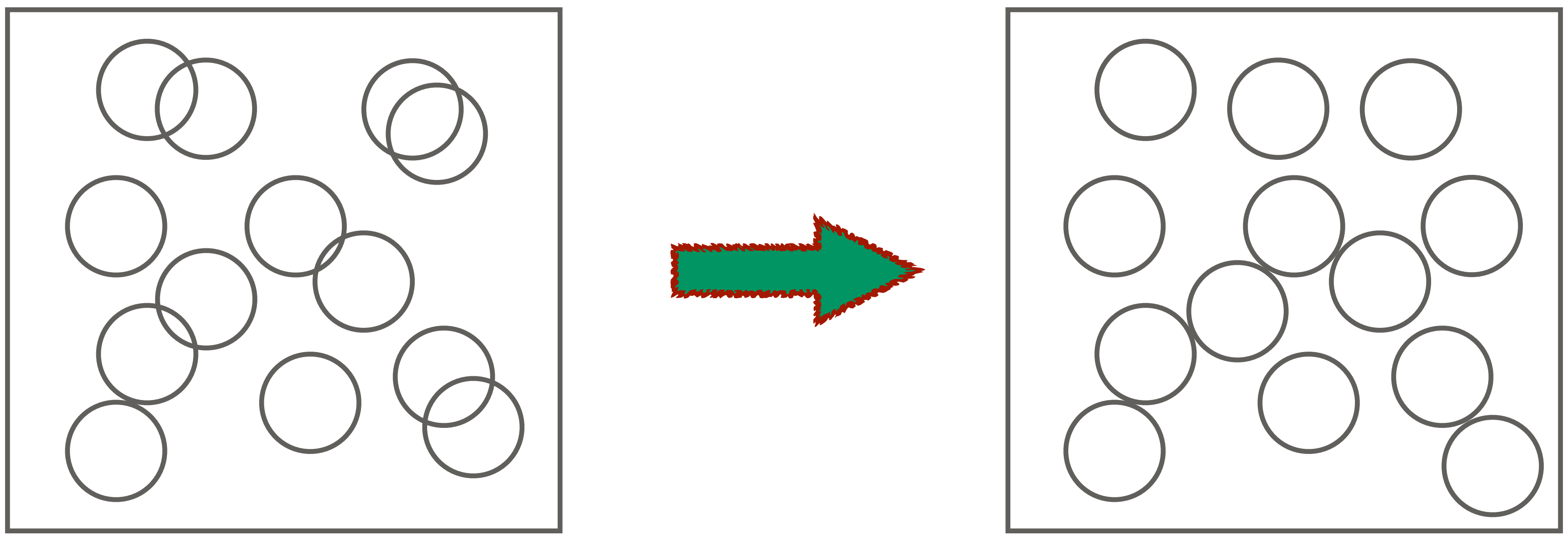
Volume of one sphere of diameter D in d dimensions

$$\varphi = \frac{N\mathcal{V}_d(D)}{V}$$

Packing fraction = fraction of the volume occupied by the spheres

This is a constraint satisfaction problem with <u>continuous</u> variables (CCSP)

The simplest algorithm

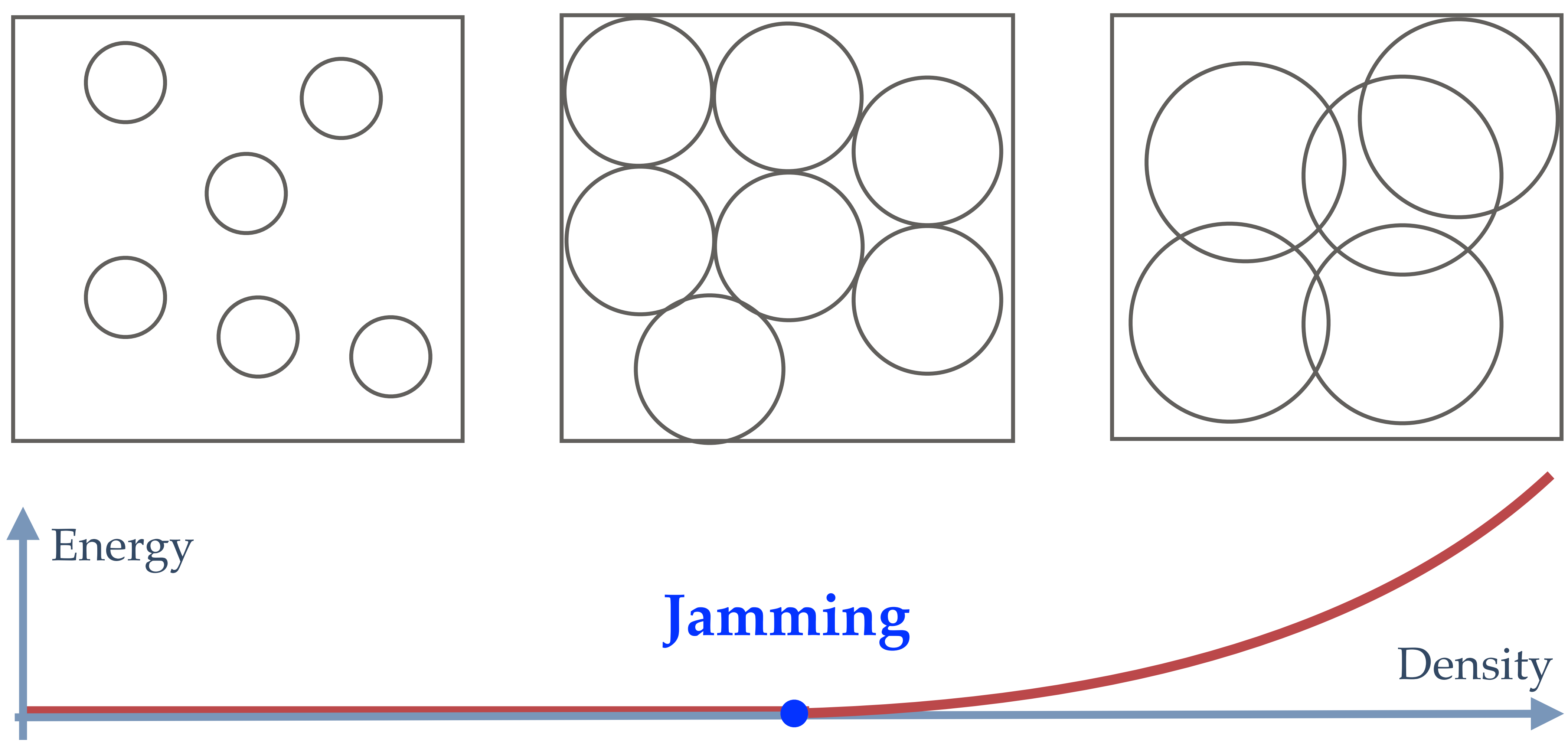


Minimize the energy through gradient descent

$$H[\underline{x}] = \frac{1}{2} \sum_{\langle i,j \rangle} h_{ij}^2 \theta(-h_{ij}) \qquad h_{ij} = |x_i - x_j| - D$$

Gap Variable

The jamming transition



Cost (loss) function: $H[\underline{x}_i] = \frac{1}{2} \sum_{\langle i,j \rangle} h_{ij}^2 \theta(-h_{ij}) \qquad h_{ij} = |x_i - x_j| - D$

A smarter algorithm

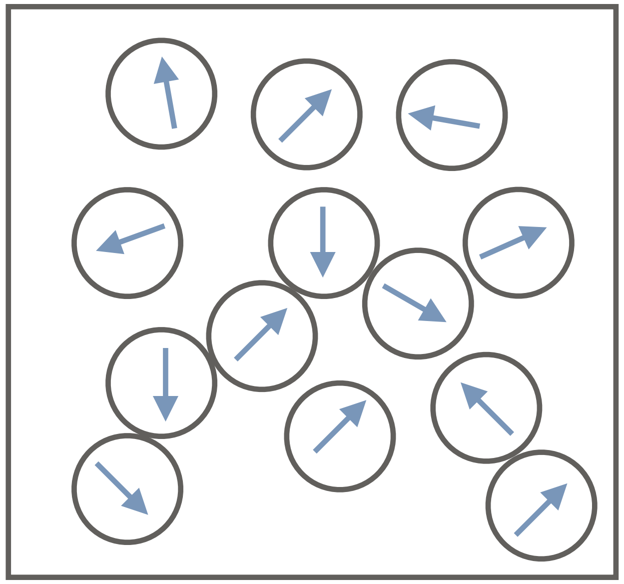
Kirkpatrick, Gelatt, Vecchi, Science 220.4598 (1983)

1. Start from a (very easy to find) low density configuration of *Hard Spheres*.

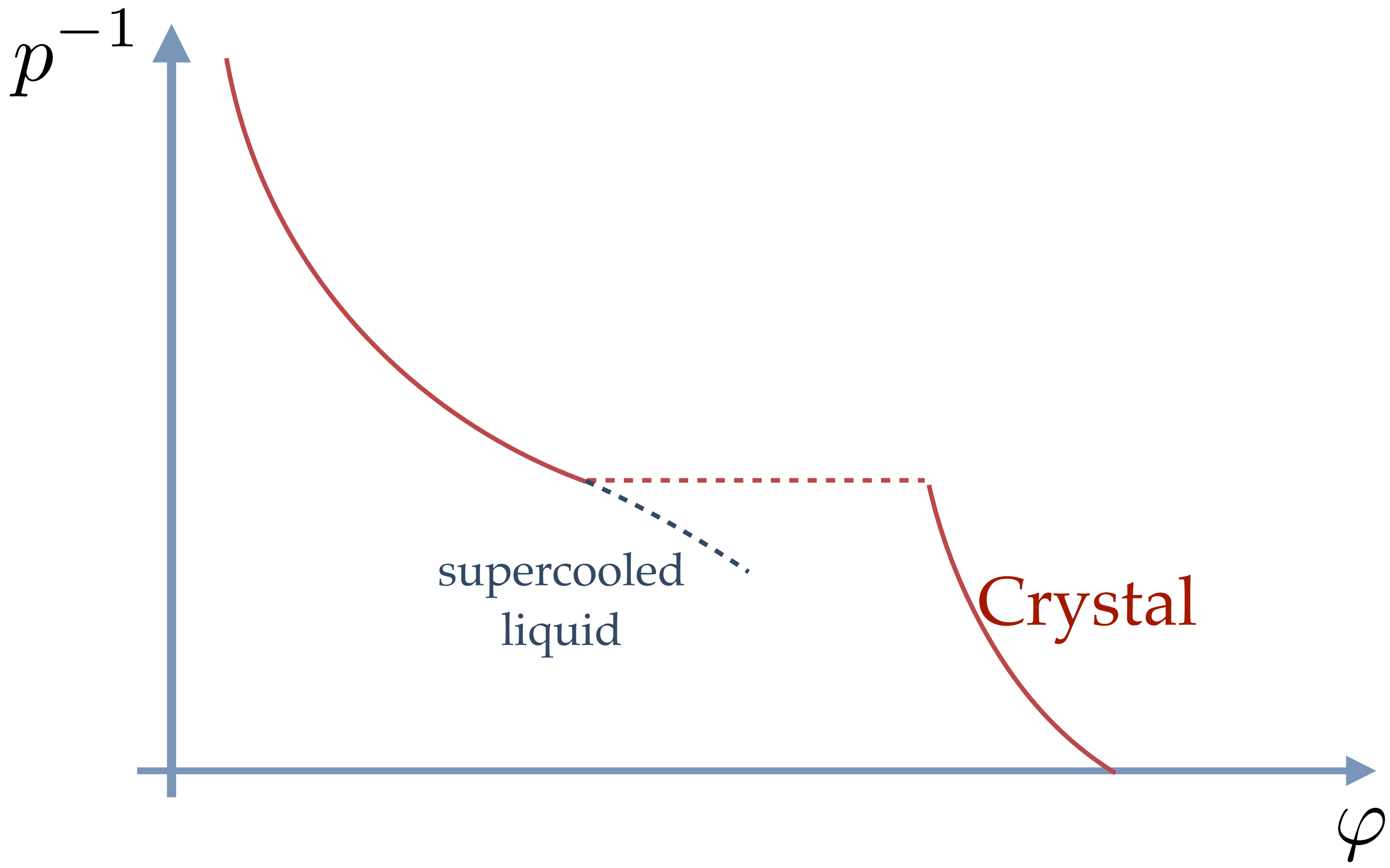
2. Initialize the spheres with random velocities

3. Inflate the spheres up to the target packing fraction

Lubachevsky, Stillinger, J. Stat. Phys., 1990

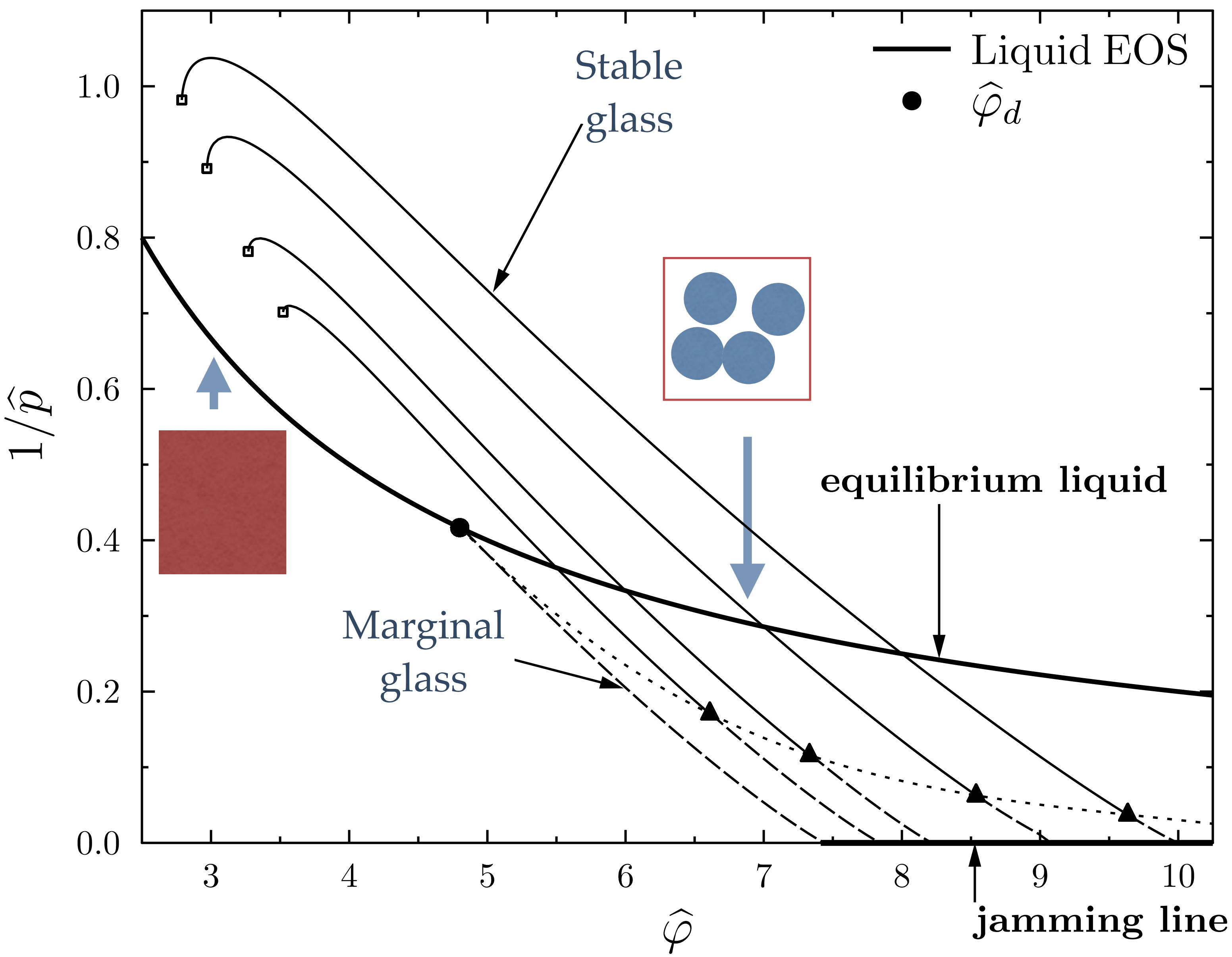


In three dimensions



Finding the crystal in higher dimension is harder.
Furthermore we do not even know who are the crystals (apart some very very special cases)

Infinite dimension



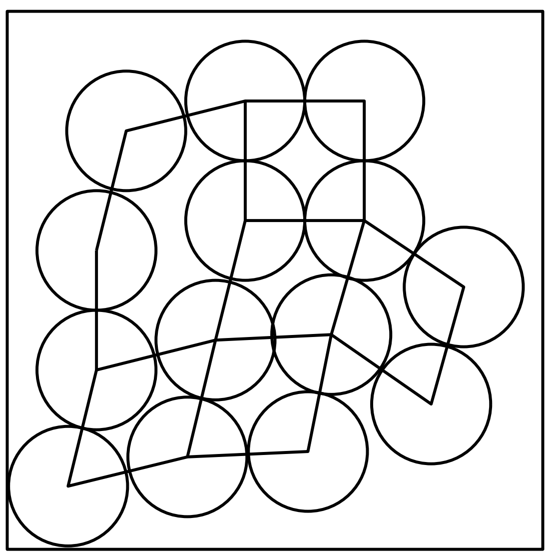
Charbonneau, Kurchan, Parisi, Urbani, Zamponi, Nature communications 5 (2014): 3725.

Rainone, Urbani, Yoshino, Zamponi PRL **114** (1) 015701 (2015)

Rainone, Urbani Journal of Statistical Mechanics: Theory and Experiment 2016.5 (2016): 053302

Microstructure of packings

Isostaticity



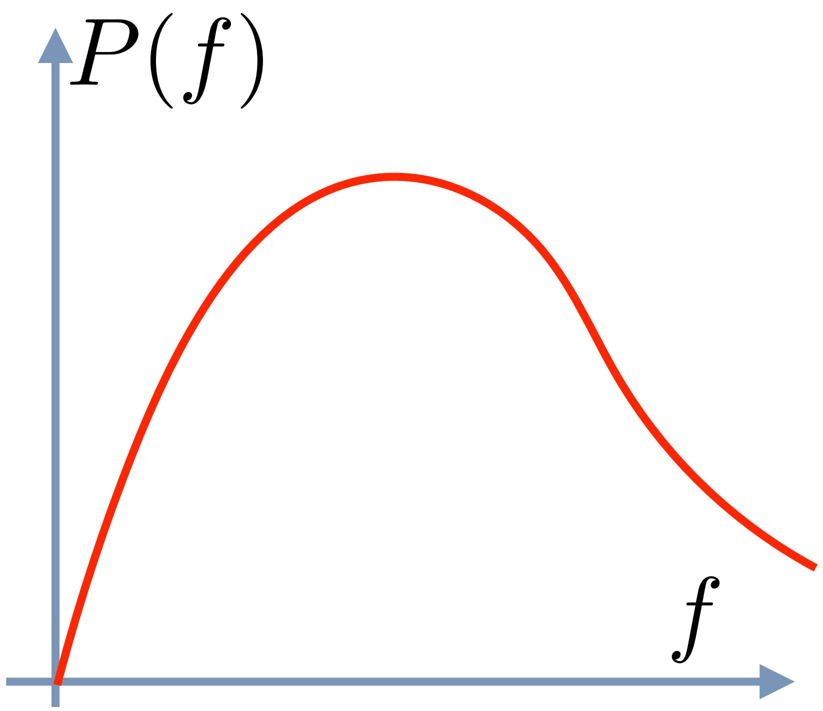
Given a packing one can look at the contact network. Define z as the average degree of the network.

Experimental observation: $z = 2d$

Tkachenko and Witten, Phys. Rev. E 60, 687 (1999)
O'hern, Silbert, Liu, Nagel, Physical Review E 68 (1), 011306
Wyart, Silbert, Nagel, Witten, Physical Review E 72, 051306 (2005).
AJ Liu, SR Nagel, Annu. Rev. Condens. Matter Phys. 1 (1), 347-369

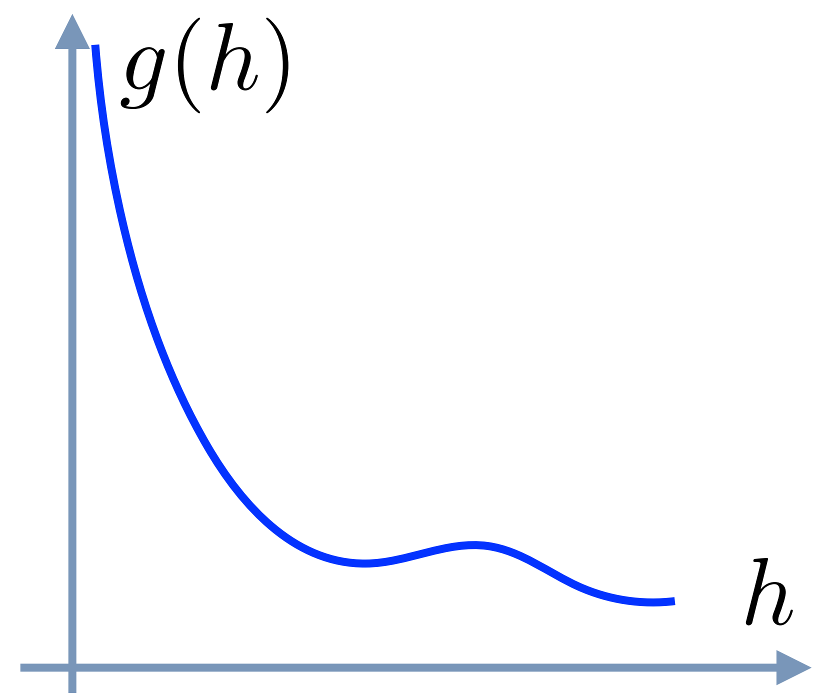
Microstructure of packings

Force distribution

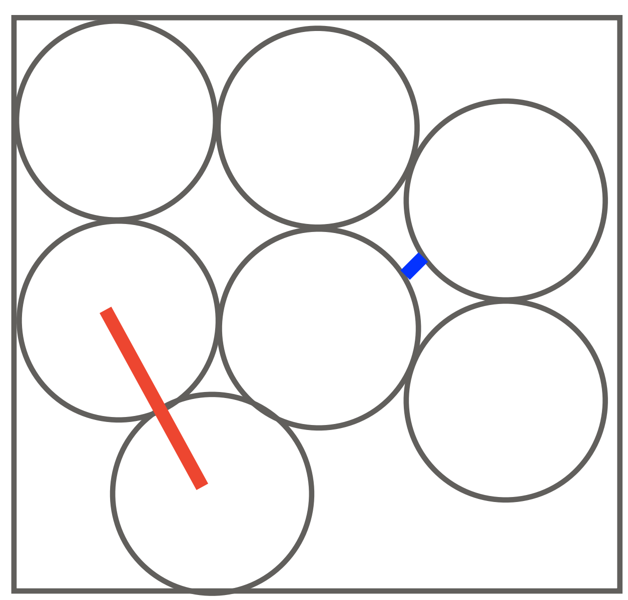


$$P(f) \sim f^{\theta}$$

Gap distribution

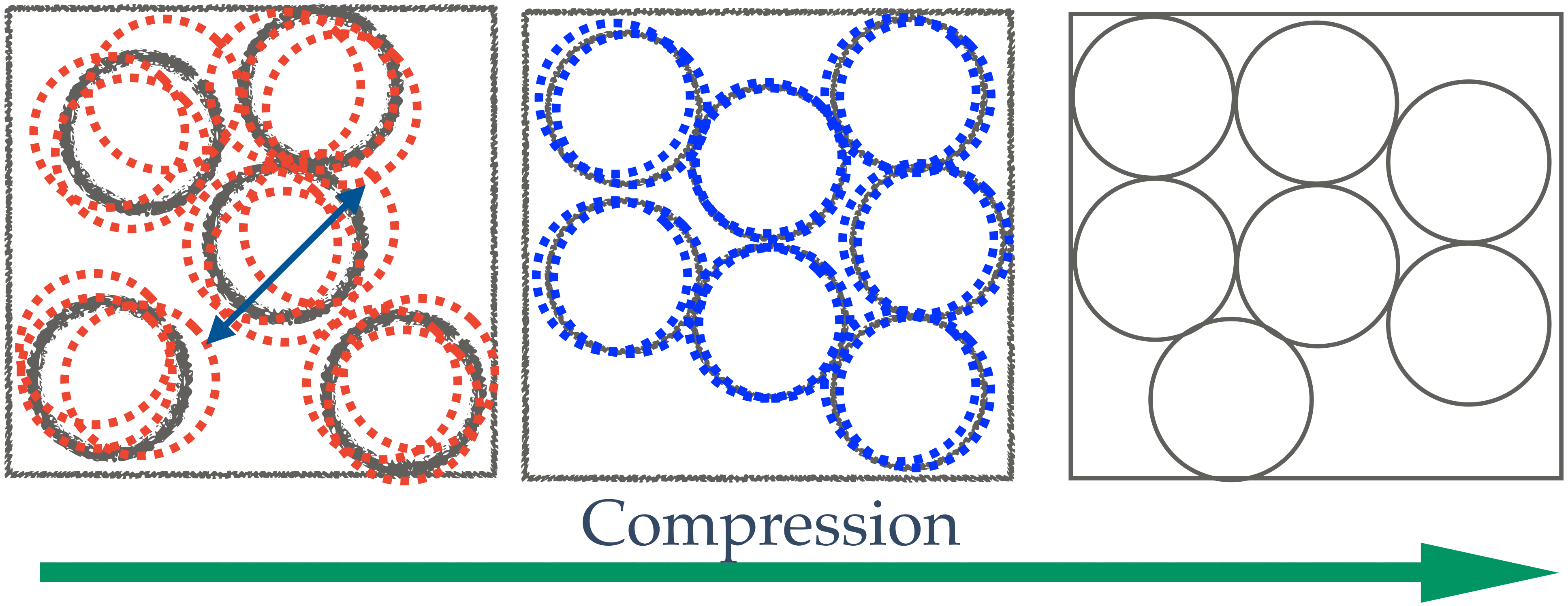


$$g(h) \sim h^{-\alpha}$$



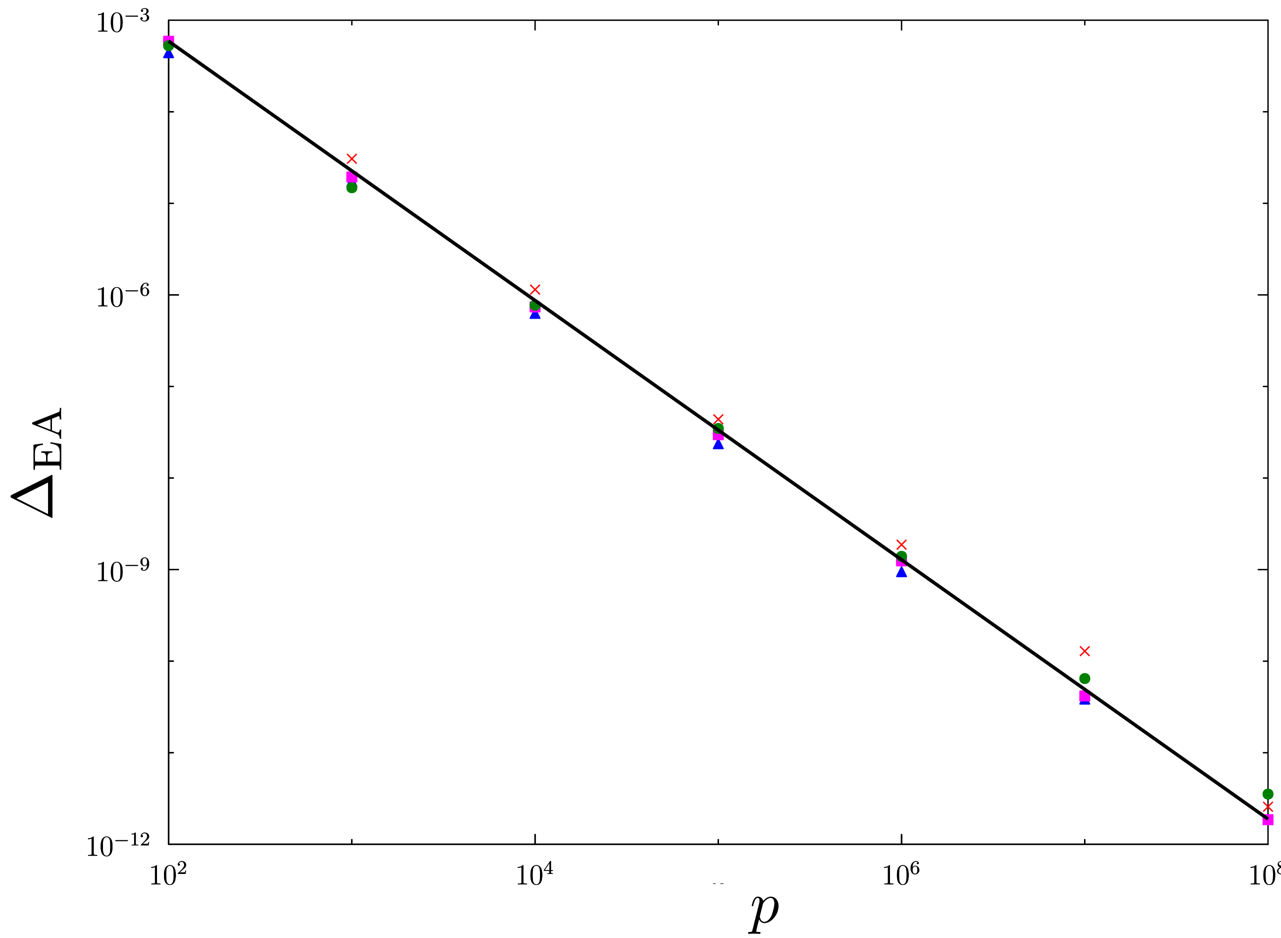
Lerner, Düring, Wyart,
Soft Matter 9 (34), 8252-8263

Cage size



$$\Delta_{\mathrm{EA}} \sim p^{-\kappa}$$

Critical properties of jamming



$$g(f) \sim f^{\theta}$$
$$\theta = 0.42311\ldots$$

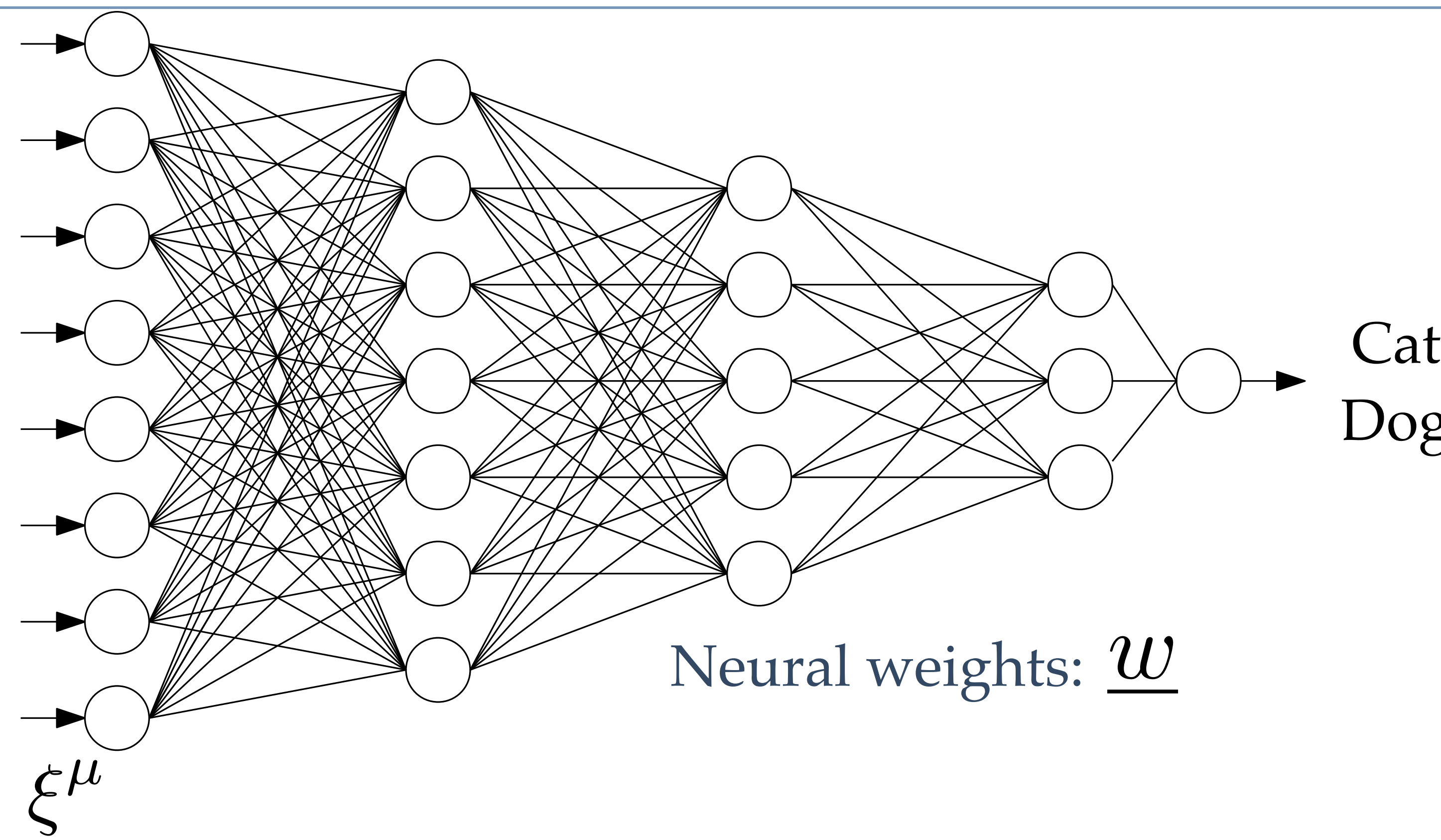
$$P(h) \sim h^{-\alpha}$$
$$\alpha = 0.41269\ldots$$

$$\Delta_{EA} \sim p^{-\kappa}$$
$$\kappa = 1.41574\ldots$$

& isostaticy

Charbonneau, Kurchan, Parisi, Urbani, Zamponi, Nature communications 5 (2014): 3725.
Charbonneau, Kurchan, Parisi, Urbani, Zamponi, Ann. Rev. Cond. Mat. 8, 265-288 (2017)

Supervised learning



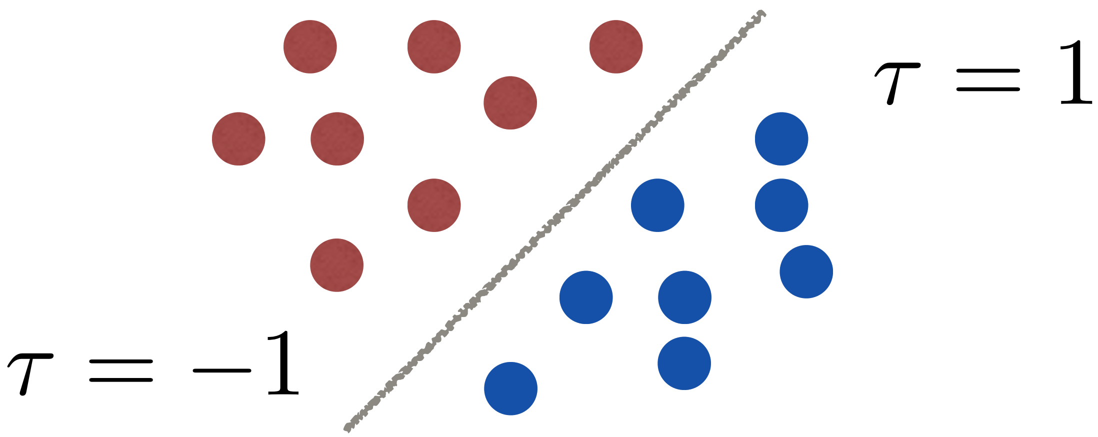
For each picture in the training set we want

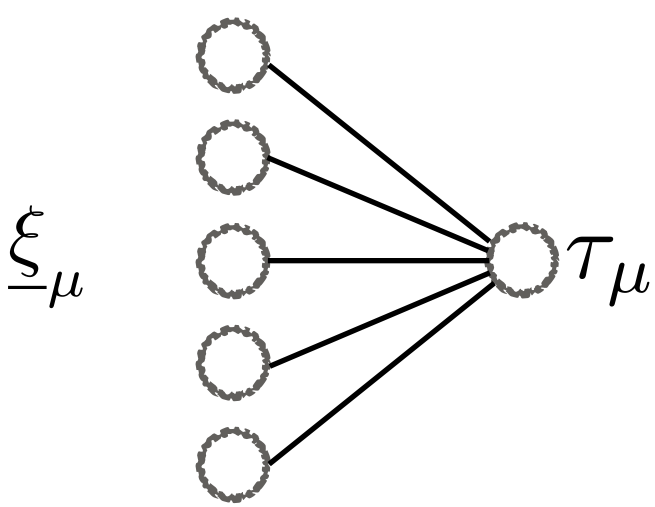
$$\theta\left[f(\underline{w}, \underline{\xi}^{\mu})\right] = 1 \quad \text{Dog}$$

$$\theta\left[f(\underline{w}, \underline{\xi}^{\mu})\right] = 0 \quad \text{Cat}$$

The supervised learning problem becomes a SAT problem for continuous variables, the weights $\underline{w}$.

The perceptron





$$\tau_\mu = \mathrm{sgn}\left(\frac{1}{\sqrt{N}}\underline{\xi}^\mu \cdot \underline{w}\right)$$

$$\tau_\mu \frac{1}{\sqrt{N}}\underline{\xi}^\mu \cdot \underline{w} > 0$$

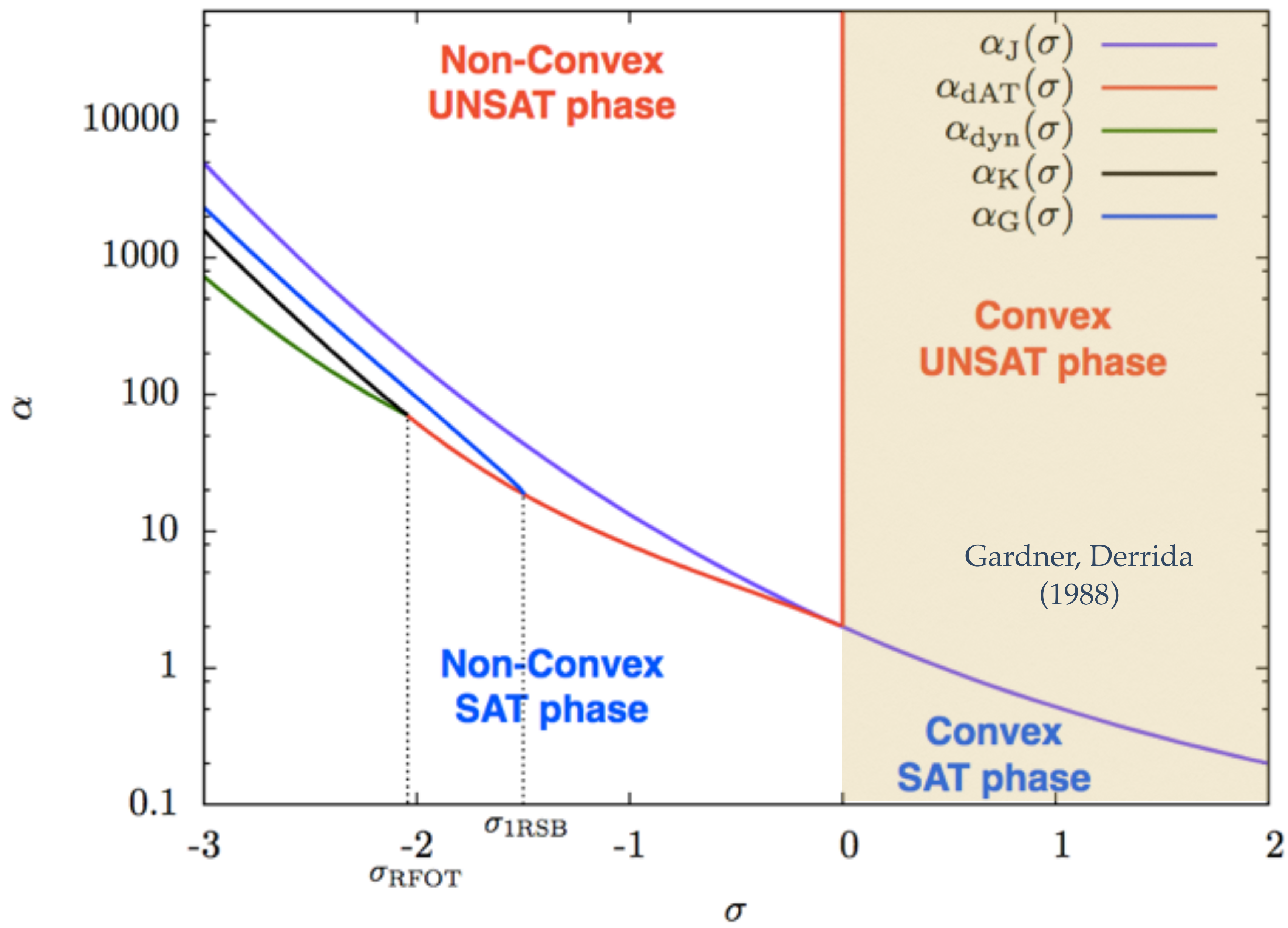
$$\tau_\mu \frac{1}{\sqrt{N}}\underline{\xi}^\mu \cdot \underline{w} > \sigma$$ add stability

Perceptron phase diagram

S Franz, G Parisi
J. Phys. A: Math. Th 49 (14), 145001

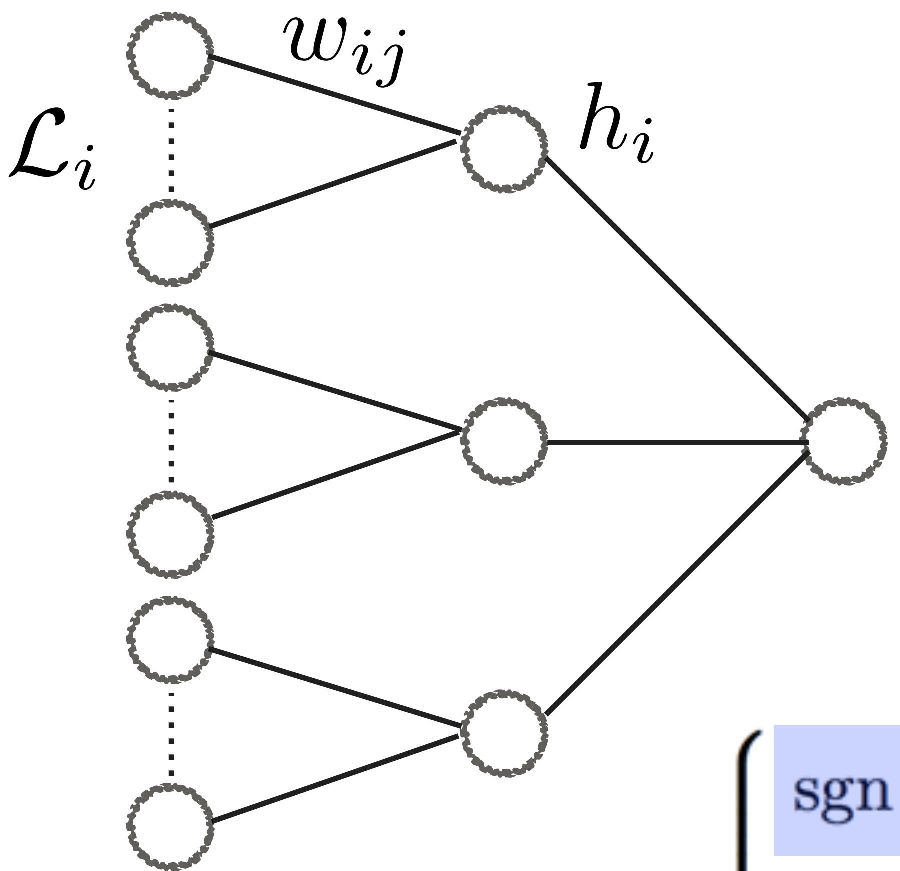
Franz, Parisi, Sevelev, Urbani, Zamponi
SciPost Phys. 2, 019 (2017)

IPhT Lectures 2017



Jamming in multilayer networks

Franz, Hwang, Urbani, arXiv:1809.09945



$$h_i\left[\underline{w},\underline{\xi}\right] = \sum_{j\in\mathcal{L}_i} w_{i,j}\xi_j$$

$$\mathcal{F}[\underline{h}]=\begin{cases} \mathrm{sgn}\left[\prod_{i=1}^{K} h_i\right] & \textbf{parity} \\ \mathrm{sgn}\left[\sum_{i=1}^{K} \mathrm{erf} h_i\right] & \textbf{soft committee} \\ \mathrm{sgn}\left[\frac{1}{K}\sum_{i=1}^{K} \rho_{\mathrm{ReLU}}(h_i,\sigma)-\sigma\right] & \textbf{ReLU 2-layer} \end{cases}$$

Monasson, Zecchina, Barkai, Hansel, Kanter, Sompolinsky, Saad, Solla…

Jamming in multilayer networks

Franz, Hwang, Urbani, arXiv:1809.09945

Gap variables or stabilities

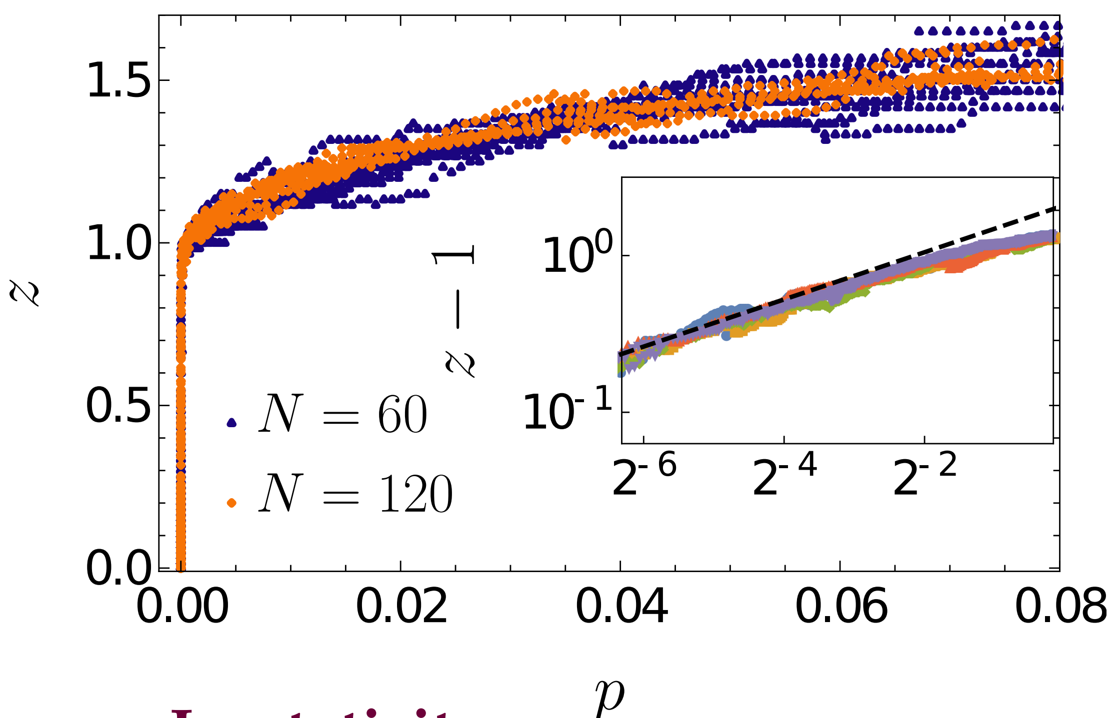
Given input-output associations

$$\{\xi^\mu, \tau_\mu\}$$

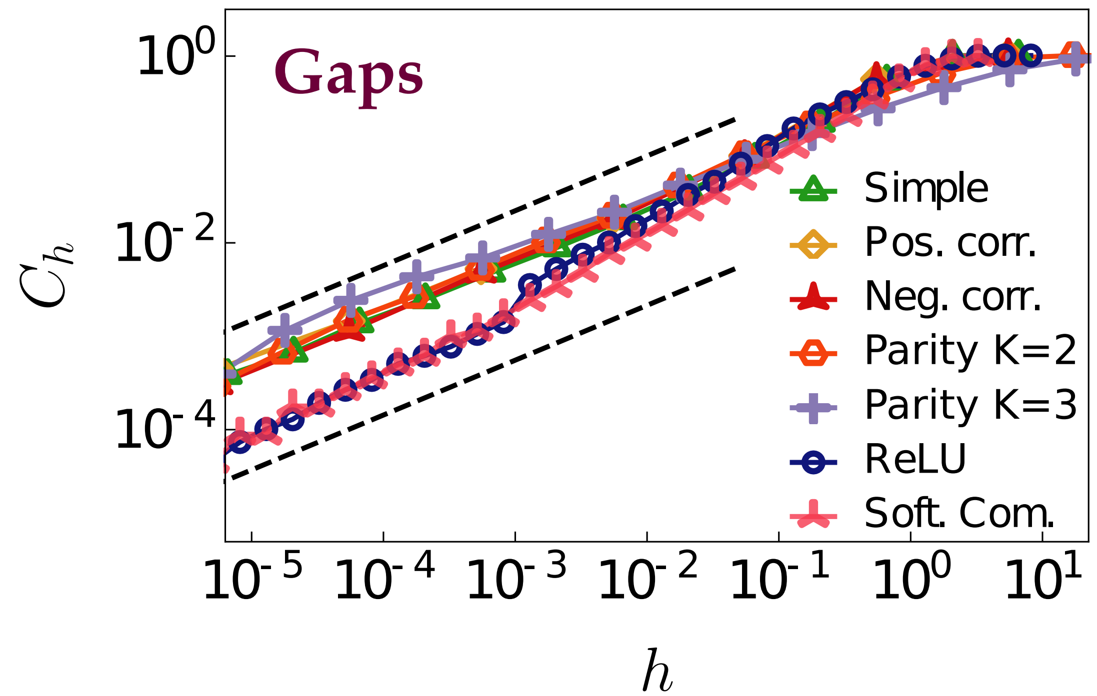
Parity $\Delta^\mu = \tau^\mu \prod_{i=1}^{K} h_i[\underline{\underline{w}}, \underline{\xi}^\mu] - \sigma$

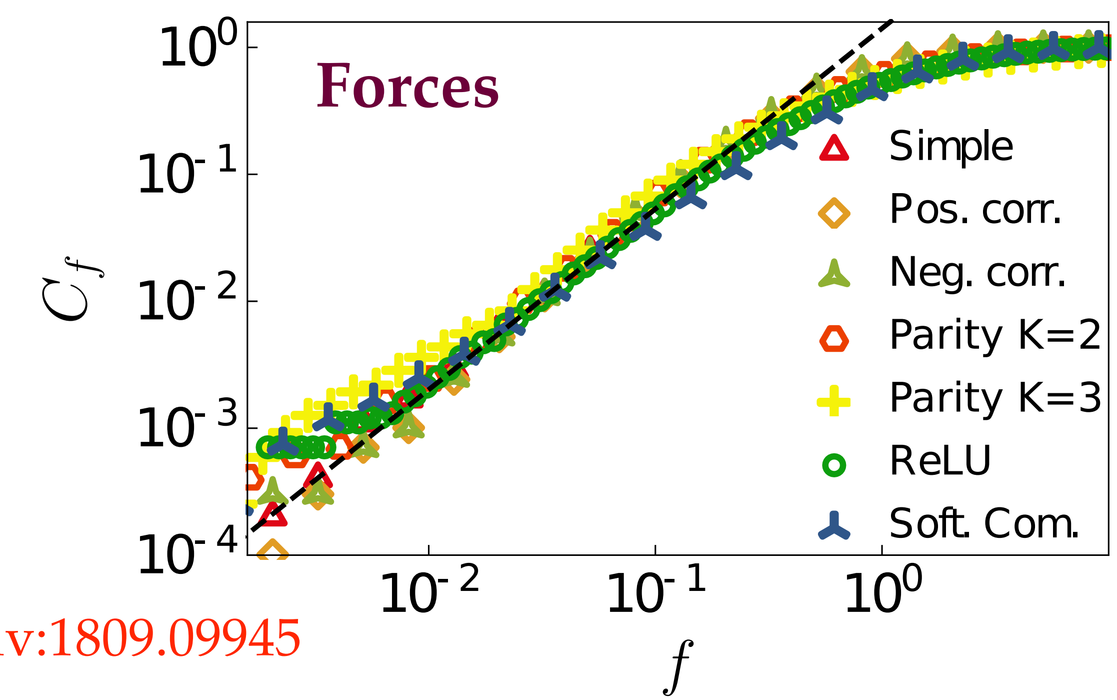
Find $\underline{w}$ such that $\Delta_\mu > 0 \quad \forall \mu$

Results at jamming



Isostaticity





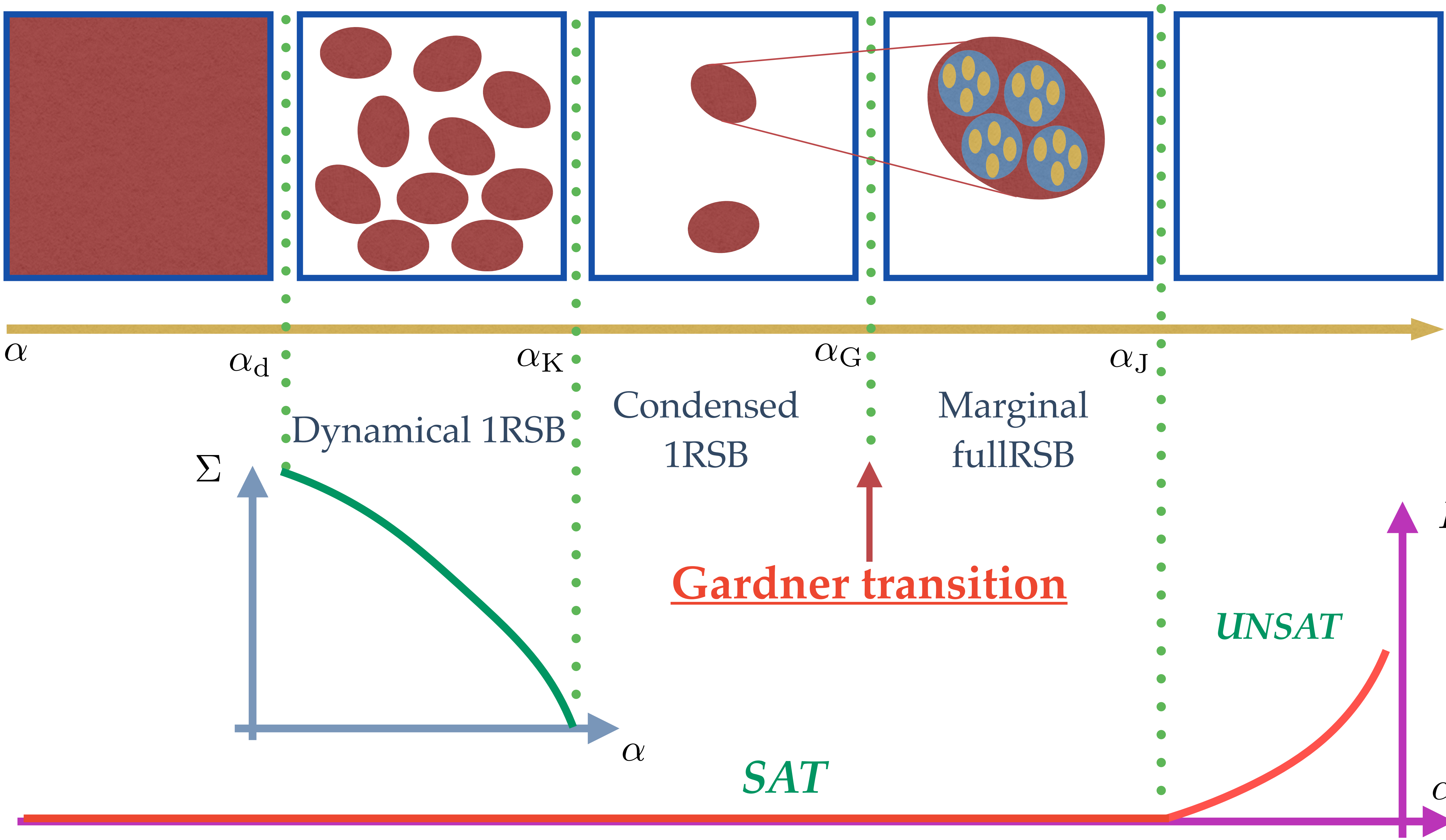
The hard spheres universality class is recovered

Franz, Hwang, Urbani, arXiv:1809.09945

The space of solutions

Franz, Parisi:
J. Phys. A:
Math. and Theo. 49 (14), 145001

Franz, Parisi, Sevelev,
Urbani, Zamponi
SciPost Phys. 2, 019 (2017)



Conclusions

1 - **Packing spheres and jamming**
observations, criticality
theory in infinite *d*

2 - **Continuous constraint satisfaction problems**
Space of solutions

3 - **Supervised learning**

4 - **Multilayer Supervised learning**

Perspectives

1. Develop new search algorithms based on the landscape

2. Universality at jamming. Why?

3. How the generalization properties depend on the landscape?