17/07/2017 FRANCESCO ZAMPONI TUTORIAL LECTURE at the other end of copybook.

OUTLINE I PERCEPTRON 1 Definitions 2 Replica method 3 SAT UNSAT transition 4 Summary SCIPOST PHYS 2, 019 (2017)

THE PERCEPTRON

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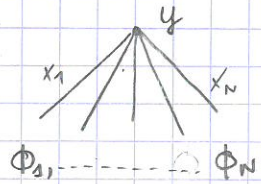
1 Definitions

1a Perceptron:



output function of linear combination of inputs:

$$y = \mathrm{sgn}(\vec{X}\cdot\vec{\Phi}) \quad \text{(Rosenblatt 1957)}.$$

teacher-student scenario: teacher chooses $\vec{x}^*$, produces (output, input) pairs: $\vec{\Phi}^1$ y^1, $\vec{\Phi}^2$ y^2, $\vdots$

Can the student infer a good $\hat{\vec{x}}$?

1b. Constraint satisfaction.

Conversely: suppose being given $\vec{\Phi}^1, y_1 \dots \vec{\Phi}^n y^n$ not generated from a $\vec{x}^*$.

Question: Can I find $\vec{x}$ s.t. $\forall \mu = 1 \dots M$ $y^\mu = \mathrm{sgn}(\vec{x}\cdot\vec{\Phi}^\mu)$? constrained satisfaction pb.

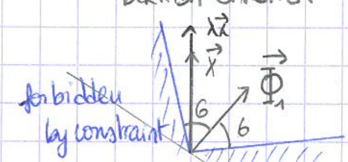
↳ Further simplification, random iid data: $\begin{cases} \Phi_i^\mu \sim \mathcal{N}(0, \frac{1}{N}) \\ y^\mu \sim \pm 1 \quad p = 1/2 \end{cases}$ random CSP

no classification generalisation here.

↳ then y^μ do not really matter.

We can assume/restrict ourselves to $\underbrace{\cancel{y^\mu}\,\vec{x}\cdot\vec{\Phi}^\mu \geq 0}_{\text{constraint}}$ + threshold $\boxed{\vec{X}\cdot\vec{\Phi}^\mu \geq \sigma > 0}$

DERRIDA-GARDNER

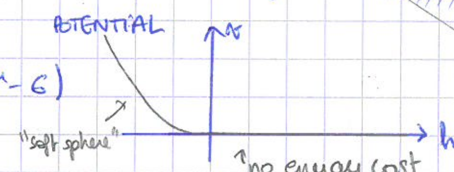


↳ if $\vec{x}$ is solution $\lambda\vec{x}$ is as well $\Rightarrow$ impose normalization

final problem: $\begin{cases} \Phi^\mu \text{ iid } \mathcal{N}(0, 1/N) \\ \text{Find } \vec{x} \text{ s.t. } \begin{cases} \vec{x}\cdot\vec{x} = N \leftarrow \text{"spherical"} \\ \forall \mu = 1 \dots M \;\; R_\mu(\vec{x}) = \vec{x}\cdot\vec{\Phi}^\mu \geq \sigma \end{cases} \end{cases}$

1c - Stat mech formulation

Hamiltonian $H(\vec{x}) = \sum_{\mu=1}^{M} v(R_\mu(\vec{x})) = \sum_{\mu=1}^{M} v(\vec{x}\cdot\vec{\Phi}^\mu - \sigma)$



$\begin{cases} H(\vec{x}) = 0 \iff \vec{x} \text{ solution} \\ H(\vec{x}) > 0 \iff \vec{x} \text{ not solution} \end{cases}$

↳ to a zero number of solutions: $Z = \int \mathcal{D}\vec{x}\, e^{-\beta H(\vec{x})}$

↳ $\int dx_1 \dots dx_N\, \delta(\sum_i x_i^2 - N)$.

Partition function $Z = \int \mathcal{D}\vec{x} \prod_{i=1}^{M} \int dr_\mu\, e^{-\beta v(r^\mu - \sigma)}\, \delta(r^\mu - R^\mu(\vec{x}))$

$$\propto \int \mathcal{D}\vec{x} \prod_{\mu=1}^{M} \int dr_\mu\, dk_\mu\, e^{-\beta v(r^\mu - \sigma) + i k^\mu (r^\mu - \vec{x}\cdot\vec{\Phi}^\mu)} \qquad \to F = -T\log Z.$$

2 Replica method

2a - In general

$$F = -T\,\overline{\log Z}^{\,\Phi} = \lim_{n\to 0} -T\,\partial_n \overline{Z^n} = -T \lim_{n\to 0} \partial_n \log \overline{Z^n}$$

(average over disorder)

$$\overline{Z^n} = \prod_{a=1}^{n} \int \mathcal{D}\vec{x}_a \prod_\mu dr_a^\mu\, dk_a^\mu\, e^{-\beta v(r_a^\mu - \sigma) + i k_a^\mu r_a^\mu}\, \overline{e^{-i k_a^\mu \vec{x}_a\cdot\vec{\Phi}^\mu}}$$

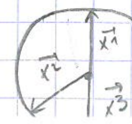
average over Φ gaussian integral

second order term of taylor e: $\overline{e^{-i k_a^\mu \vec{x}_a\cdot\vec{\Phi}^\mu}} = e^{-\frac{1}{2}\sum_{a,b,\mu} k_a^\mu k_b^\mu Q_{ab}}$ with $Q_{ab} = \frac{1}{N}\vec{x}_a\cdot\vec{x}_b$ $n \times n$ matrix

$$\Rightarrow \overline{Z^n} = \int \mathcal{D}\vec{x}_a \left(\prod_\mu dr_a^\mu\, dk_a^\mu\right) e^{-\beta\sum_{a\mu} v(r_a^\mu - \sigma) + i\sum_{a\mu} k_a^\mu r_a^\mu - \frac{1}{2}\sum_{ab\mu} k_a^\mu k_b^\mu Q_{ab}}$$

$$= \int \mathcal{D}\vec{x}_a \Bigg(\underbrace{\int dr_a\, dk_a\, e^{-\beta\sum_a v(r_a - \sigma) + i\sum_a k_a r_a - \frac{1}{2}\sum_{ab} k_a k_b Q_{ab}}}_{I(Q)}\Bigg)^M$$

↳ rotationally invariant for all the replicas



(we can integrate over the k's, gaussian)

$$\overline{Z^n} \propto \int d\hat{q}\; e^{\frac{N}{2}\log\det\hat{q}} \prod_a \delta(q_{aa}-1)\; I(\hat{q})^M$$

$d\hat{q} \to \prod_{a\leq b} dq_{a,b}$

spherical constraint

$$I(\hat{q}) = \int d\lambda_a\; e^{-\frac{1}{2}\sum_{ab} q_{ab}^{-1}\lambda_a\lambda_b}\; e^{\sum_a \nu(\lambda_a - \sigma)} \Big/ \sqrt{(2\pi)^n \det\hat{q}}\,.$$

+ should have some constraint to which q we are integrating over, but the logdet takes care of that by penalizing the invalid.

Action

$$\boxed{\overline{Z^n} = \int \prod_{a<b} dq\; e^{NA(\hat{q})}} \qquad \boxed{A(\hat{q}) = \underbrace{\frac{1}{2}\log\det\hat{q}}_{\text{entropic term for rotations}} + \underbrace{\alpha\log I(\hat{q})}_{\text{constraint term}}} \qquad \alpha = M/N.$$

$\begin{cases} \text{no more int on } a=b,\ q_{aa}=1 \\ q_{ab} = q_{ba} \text{ SYMMETRIC} \end{cases}$

$\to$ thermodynamic limit $N\to\infty$, $M\to\infty$, $\alpha = M/N$

$$\frac{1}{N}\log\overline{Z^n} = \max_{\hat{q}} A(\hat{q})$$

$\hat{q}$: $\begin{cases} \text{diagonal}=1 \\ \text{symmetric} \end{cases}$

To finish the computation ①: fix n $\to$ $\max A(\hat{q})$ ②: continue $n\in\mathbb{R}^+$ ③ ∂_n + $\lim_{n\to 0}$ -

COMMENTS "If everything goes well, you can reconstruct the log from all the integer moments".

"Replicas interfer because they have the same disorder Φ"

2b Replica symmetric

The first think we can do to be able to perform the analytical continuous is to that all the replicas are equivalent, $\det\hat{q}$, $I(\hat{q})$ are all symmetric in the replicas.

Assuming that the replica symmetry is not spontaneously broken:

$\hat{q}^*$ is RS $\to$ $\hat{q} = \begin{pmatrix} 1 & q & q & q \\ q & \ddots & & \\ q & & \ddots & \\ q & & & 1 \end{pmatrix} = (1-q)\hat{\mathbb{1}} + q\hat{J}$, $\hat{J} \to \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \ddots & & \\ 1 & & & \\ 1 & & & \end{bmatrix}$ closed algebra, stable under ⊕ and ⊗

With this great simplification:

$$\det(\hat{q}) = (1-q)^{n-1}(1+(n-1)q)$$

$\downarrow$ action under RS ansatz: $a_{RS}(q) = \frac{1}{2}(n-1)\log(1-q) + \frac{1}{2}\log(1+(n-1)q) + \alpha\log I(q)$

(it works, can check $\lim_{n\to 0} q(n) = q^*$ consistent)

$\downarrow$ hopping for maximization/deviation to commute...

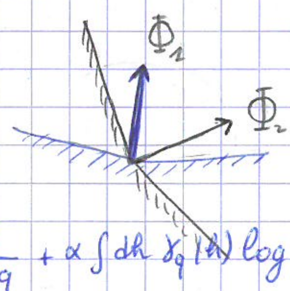
$$\lim_{n\to 0}\partial_n a_{RS}(q) = \frac{1}{2}\log(1-q) + \frac{1}{2}\frac{q}{1-q} + \alpha\int dh\,\frac{e^{-h^2/2q}}{\sqrt{2\pi q}}\log\int dz\,\frac{e^{-z^2/1-q}}{\sqrt{2\pi(1-q)}}\,e^{-\beta z(h-\sigma)}$$

a bit of work... convolutions of potential + gaussians

$\downarrow$ find minimum q^*: $f = \frac{F}{N} = -Ta_{RS}(q^*)$.

3 SAT/UNSAT transition

3a the satisfiable phase



When $T\to 0$ $q\to q^{(0)}$

$e^{-\beta v(h)} \xrightarrow{T\to 0} \Theta(h)$

there are solutions, not null space allowed by the constraints $\to$ replicas will fluctuate in this volume $\to$ $q^{(0)} < 1$.

$$\downarrow a_{RS}(q) = \frac{1}{2}\log(1-q) + \frac{1}{2}\frac{q}{1-q} + \alpha\int dh\,\gamma_q(h)\log\left(\Theta\left(\frac{h-\sigma}{\sqrt{2(1-q)}}\right)\right)$$

result of the convolution

$\Theta(x) = \frac{1}{2}(1+\mathrm{erf}(x))$

when approaching SAT/UNSAT, less and less solutions: $q\to 1$ for $\alpha\to\alpha_{SAT}^-$.

Moreover, from the SAT phase: $\begin{cases} e=0 \text{ (no broken constraint)} \\ s \text{ finite} \end{cases}$ $\to$ $S = \min_q a_{RS}(q) \to f = -Ta(q^*)$.

$\hookrightarrow$ equation for q: $0 = \frac{\partial a}{\partial q}$ $\quad \frac{1}{2}\frac{q}{(1-q)^2} + \alpha\frac{d}{dq}\int dh\,\underbrace{\gamma_q(h)}_{W(0,q)}\,\log\Theta\left(\frac{h-\sigma}{\sqrt{2(1-q)}}\right) = 0$

$q\to 1$: $\begin{cases} \to 0 & h>\sigma \\ \to -\frac{(h-\sigma)^2}{2(1-q)} & h<\sigma \end{cases}$

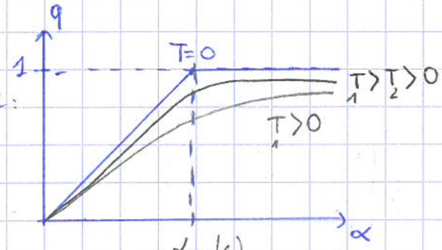
$\hookrightarrow$ Approaching SAT/UNSAT transition:

with $\begin{cases} q\to 1 \\ \frac{\partial a}{\partial q} = 0 \end{cases}$ $\Rightarrow$ $\boxed{\alpha = \frac{1}{\int^{\sigma} dh\,\gamma_1(h)(h-\sigma)^2} = \alpha_{SAT}(\sigma)}$ $\quad \alpha_{SAT}(\sigma=0) = 2$!

$\alpha\uparrow$

3b Unsatisfiable phase – assuming $v(h) = \frac{h^2}{2}\Theta(-h)$

let's fix σ and vary α from SAT to UNSAT phase:



Hence in the unsat phase $q \to 1$ when $T \to 0$

↳ Ansatz assuming harmonic: $q = 1 - \chi T$

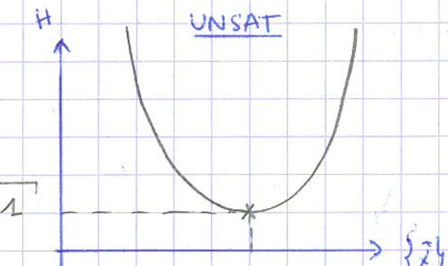
plugging into free energy: $f = -T a(q) \xrightarrow[q=1-\chi T]{T\to 0} -\frac{1}{2\chi} + \frac{\alpha}{2}\int_{-\infty}^{\sigma} dh\, \gamma(h)\frac{(h-a)^2}{1+\chi} = -\frac{1}{2\chi} + \frac{\alpha}{2\alpha_s(\sigma)}\frac{1}{1+\chi}$

$f \xrightarrow{T\to 0} e - \underbrace{TS}_{\to T\log T \to 0} \to 0 \Rightarrow \boxed{\frac{1}{\chi} = \sqrt{\frac{\alpha}{\alpha_s(\sigma)}} - 1}$ $\qquad e = \frac{1}{2}\left(\sqrt{\frac{\alpha}{\alpha(\sigma)}} - 1\right)^2$

Approching SAT/UNSAT from unsat phase at $T=0$: $\chi \to +\infty$

$e \propto (\alpha - \alpha_s(\sigma))^2 \to$ depends on potential

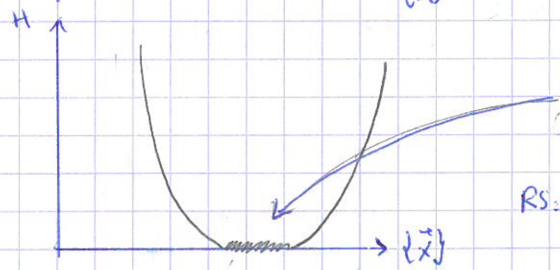
3c landscape



RS: only one minimum

can be checked numerically by doing gradient descent on sphere: $\dot{x} = -\frac{\partial H}{\partial x}$

↳ harmonic + value of $e(\alpha)$.



$\begin{cases} e = 0 \\ s = \text{finite} \end{cases}$

RS: connected unique space of solutions!

3d Isostaticity

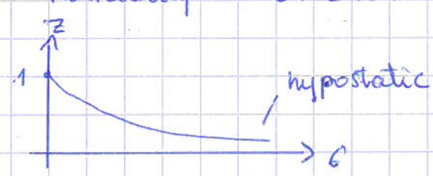
Property of jamming: number of particles touching = number of degrees of freedom (dof).

In the context of the perceptron, we wish to compute how many constraints saturate when approaching the transition:

$h_\mu = R_\mu(\vec{x}) - \sigma \geq 0 \to h_\mu = 0$?

↳ Denote by zM the number of saturated constraints $\Rightarrow$ isostaticity $\Leftrightarrow zM = N$.

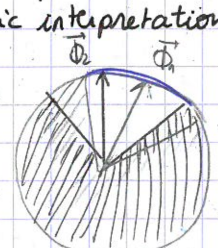
We can compute $z = \int_{-\infty}^{0} \frac{dh}{\sqrt{2\pi}} e^{-\frac{(h+\sigma)^2}{2}} = H\left(\frac{\sigma}{\sqrt{2}}\right)$



4 Non convex perceptron $\sigma < 0$

4a Geometric interpretation

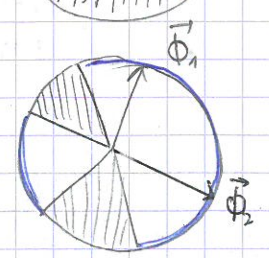
$\sigma > 0$



space of solution = intersection of convex domains, portion of surface of sphere

↳ always convexe!

$\sigma < 0$



already with two constraints → two disconnected part to the set of solutions!

Castellani-Cavagna spin glass theory for pedestrians

4b Phase diagram and Replica Symmetry Breaking

RS: $q_{ab} = \begin{pmatrix} 1 & & q_0 \\ & \ddots & \\ q_0 & & 1 \end{pmatrix}$

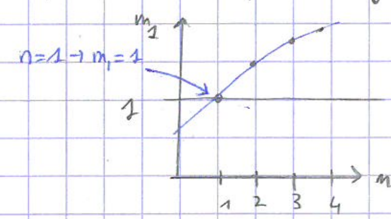
→ replicas at distance q_0.

→ guess structure of q_{ab} easy to continue analytically!

1RSB: $\hat{q} = \begin{pmatrix} \begin{matrix} 1 & q_1 \\ q_1 & 1 \end{matrix} & & q_0 \\ & \begin{matrix} 1 & q_1 \\ q_1 & 1 \end{matrix} & \\ q_0 & & \begin{matrix} 1 & q_1 \\ q_1 & 1 \end{matrix} \end{pmatrix}$ (blocks of size m_1, total size n)

Why?
→ closed at
→ well seems more and more good idea.

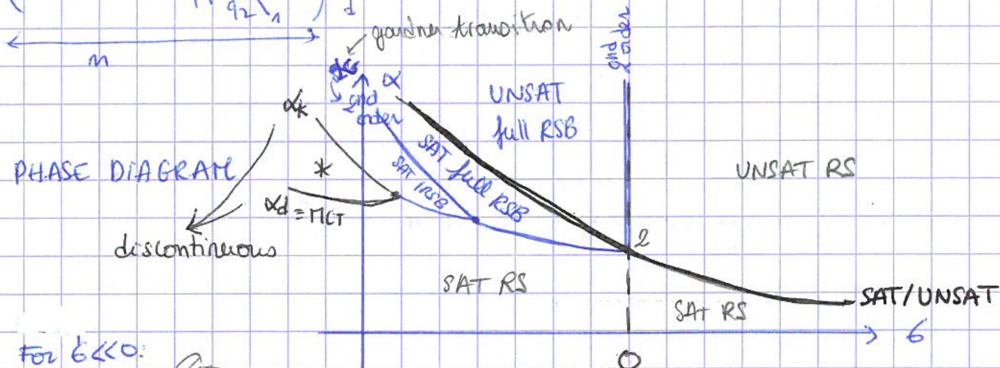
↳ replicas are either at distance q_0 or distance q_1
⇒ in resolution minimize over m_1, q_1, q_0!
↳ $n \to 0$ $0 < m_1 < 1$
+ m_1 = probability at distance q_1.



→ you can keep going:
2RSB → either distance q_2, q_1, q_0.

$\begin{pmatrix} \begin{matrix} \begin{matrix} 1 & q_2 \\ q_2 & 1 \end{matrix} & q_1 \\ q_1 & \begin{matrix} 1 & q_2 \\ q_2 & 1 \end{matrix} \end{matrix} & q_0 \\ q_0 & \begin{matrix} \begin{matrix} 1 & q_2 \\ q_2 & 1 \end{matrix} & q_1 \\ q_1 & \begin{matrix} 1 & q_2 \\ q_2 & 1 \end{matrix} \end{matrix} \end{pmatrix}$ (inner blocks of size m_2, blocks of size m_1, total size n)

PHASE DIAGRAM



For $\sigma \ll 0$:

SAT RS: q_0!

(*): exponential number of clusters q_0, q_1

after α_K: dominate by few cluster (still q_0, q_1)

SAT full RSB: infinite clusters of clusters

↳ the SAT/UNSAT falling to full RSB SAT has all the same properties of jamming.

II SPHERES

II 1 Sphere packing as a CSP

1a General formulation

in d dimension → positions of the particles: $\underline{X} = \{\vec{x}_1, \vec{x}_2 \cdots \vec{x}_N\}$ either $x_i \in V \subset \mathbb{R}^d$ (on a sphere) $x_i \in \mathbb{R}^{d+1} / x_i^2 + \ldots = R^2$
↳ periodic boundary condition
, locally flat for $d \to \infty$
, invariant under any rot.

Constraints: $\mu = \langle ij \rangle = 1 \ldots \frac{N(N-1)}{2}$ $h_\mu(\vec{x}) = |\vec{x}_i - \vec{x}_j| - \sigma$

Hamiltonian: $H = \sum_{ij} v(h_\mu(\vec{x})) = \sum_{ij} v(|x_i - x_j| - \sigma)$

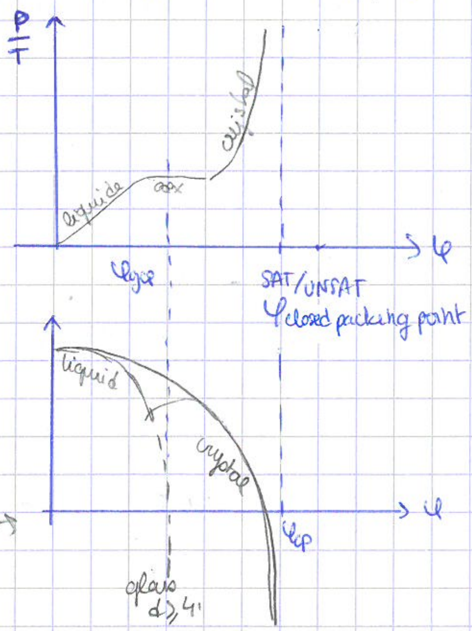
at least σ apart

Partition function $Z = \int d\underline{X}\, e^{-\beta H}$

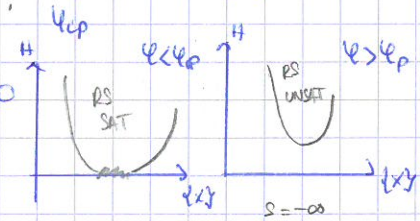
2 spheres in $d\to\infty$ 3 Criticality of jamming.

1b Problems: crystal, disorder.

Two important differences with perceptron → no quenched disorder
→ optimal will have packing fraction of the crystal.



→ CRYSTAL LIKE PERCEPTRO



How to study instead disordered phase?

① Introduce back some disorder in the system: → polydispersity $h_\mu(\vec{x}) = |x_i - x_j| - \sigma_{ij}$
→ disorder in the constraints $h_\mu(\vec{x}) = |\vec{x}_i - \vec{x}_j + A_{ij}| - \sigma$ (MKK) Flo Jorge

② Increase dimension $d \geq 4$ → very hard to crystallize, will never nucleate.

20/07/2017 entropy of quantum systems > 0
entropy classically 1 harmonic oscillator → $-\infty$, volume = 1.

entropy crisis = Kauzmann → configurational entropy → 0.

1c Franz Parisi potential "replica without disorder".

Take equilibrium configuration R:

$$V(Q) = -T\int d\vec{R}\ \frac{e^{-\beta H(\vec{R})}}{Z} \log \int dx\, e^{-\beta H(x)}\, \delta(Q - Q(X,R))$$

→ can be defined without any disorder
→ need replicas for ⟨log⟩!

⇒ we do a replica computation, R playing the role of the quenched disorder - which we average over finally.

II 2 Hard spheres (SAT phase) in dimension $d\to\infty$.

[Frisch, Rivier, Klein, Wyler '80s
Frisch, ... '99 PRE]

2a

Virial expansions (low density expansions)

$$-\beta F(\rho(x)) = \underbrace{\int dx\ \rho(x)\left[\log \rho(x) - 1\right]}_{\text{ideal gas}} + \int dx dy\ \rho(x)\rho(y)\, \underbrace{f(x-y)}_{\text{mayer function } e^{-\beta v(x-y)} - 1} + \ldots$$

↳ plugging a uniform density in space $\rho(x) = \rho$, impose translational invariance → liquid ≠ crystal.