Lecture 6

Freedoms and Constraints
This is not a sphere.
Is this a sphere?
K-Sat problem

given the expression, is there some assignment of TRUE and FALSE values to the variables that will make the entire expression true?

Electronic Design Automation,
Formal verification,
Routing….

NP-complete problem… but with plenty of solutions discoverable with fast and efficient algorithms.
We want to maximize the number of accessible configurations but constraints reduce the portion of accessible phase space.
Biological cells

Lewis law

Constraints:

\[ \sum_{n} p_n = 1 \]
\[ \sum_{n} n \ p_n = 6 \]
\[ \sum_{n} A(n) \ p_n = \frac{A}{N} \]

Maximizing entropy by reducing constraints

\[ A(n) = a \ n + b \]

Euler relation: \( V - E + F = \chi \) with \( \chi = o(1) \)

\[ 3 \ V = 2 \ E \]
\[ <n>F = 2E \]
\[ <n> = 6 - 6 \ \chi/F \]

Froths (minimally connected cellular reticulates)

D. Weaire and N. Rivier, Soap, cells and statistics - random patterns in two dimensions, Contemporary Physics, 25, 1984, p.59 - 99
Maximize entropy whilst satisfying constraints

Lagrange Multipliers:

\[ p_n = \exp\left(\gamma - \lambda^\gamma f_n^\gamma\right) \]
If we call $f = \varepsilon$ and $\lambda = \beta$...

$$p(\varepsilon) = p_0 \exp(-\beta \varepsilon)$$

Boltzmann distribution $\beta^{-1} = K_B T$

Constraints are associated with average properties ($<E> = U$) which are fixed by the Lagrange multipliers ($\beta$). The Lagrange multipliers introduce boundaries, defining the portion of phase space one can explore (at a given “temperature”).
The Boltzmann-kind distribution is quite general because it is the consequence of a constraint maximization theory. Other distributions can emerge when different forms of entropy are considered.

\[ S = - \sum_{\varepsilon} p(\varepsilon) \ln \frac{p(\varepsilon)}{\Omega(\varepsilon)} \]  
Boltzamann - Gibbs entropy

\[ \sum_{\varepsilon} \varepsilon \ p(\varepsilon) = U \]

\[ p(\varepsilon) = \frac{\Omega(\varepsilon) \exp(-\beta \varepsilon)}{Z} \]

\[ S^* = - \sum_{\varepsilon} p(\varepsilon) \ln^* \left( \frac{p(\varepsilon)}{\Omega(\varepsilon)} \right) \]  
generalized entropy

\[ p(\varepsilon) = \frac{\Omega(\varepsilon) \exp^*(-\beta \varepsilon)}{Z} \]


Statistical Mechanics approach:
• Define an energy $E$ with $E = 0$ for the solution and $E>0$ otherwise.
• Study the partition function: sum over the configurations at finite temperature

$$Z = \sum_{\text{conf}} e^{-\beta E(\text{conf})}$$
• Search for solutions that minimize the free energy

$$A = U - TS = -k_B \ln Z.$$
OPTIMIZATION PROBLEMS

K-SAT problem:
\[
\left\{ x_1, x_2, \ldots, x_n \right\} \quad n \text{ variables} \quad 2^n \text{ states}
\]
\[
c_i = (x_{i_1} \lor \bar{x}_{i_2} \ldots \lor x_{i_k}) \quad \text{clause: excludes one combination over } 2^k \text{ possibilities}
\]

Constraint: this \( c_1 \land c_2 \land \ldots \land c_m \) must be satisfied (true)

Pseudo energy: \( E = -m = -\text{ # of clauses} \)

Optimization: minimize energy whilst satisfying the constraint

Up to a given \( m^* \) the problem is easily solvable, afterwards finding a solution becomes extremely rare.

\[
2^k \ln 2 - k \leq \frac{m^*}{n} \leq 2^k \ln 2
\]


Sphere packings:

Search for the densest packing.

No overlapping spheres.

Sphere Packing

constraint = no overlapping spheres
(pseudo)energy = # spheres in contact
optimization = max # of spheres in V
Graph Coloring

Coloring the vertices of a graph such that no two adjacent vertices share the same color (vertex coloring).

**constraint** = *no two connected vertices with the same color*

**optimization** = *min # of colors*

**(pseudo)energy** = *# of links*
Thomson Problem

What is the arrangement of $N$ electrical charges on a sphere, which minimizes the energy associated with their interactions?

$$V = \frac{e^2}{4\pi\varepsilon_0} \sum_{i \neq j} \frac{1}{r_i - r_j}$$
Tammes problem
Given a minimal distance between them, how many points can be put on the sphere?

Universal Optimal Configurations
Can we find packings that are optimal for entire classes of possible potentials?

For instance, in three dimensions there are only six possible configurations that are optimal for any kind of repulsive potential (generalized Thomson problem):

n = 1 a single point;

n = 2 two antipodal points;

n = 3 an equilateral triangle on the equator;

n = 4 a regular tetrahedron;

n = 6 a regular octahedron;

n = 12 a regular icosahedron.

Energy - Constraints

- solutions
- connected
- mostly connected
- dynamically isolated regions
- regions disappearing
- 1-state regions
- no solutions

Ergodicity breaking
Constraints define boundaries

Boundaries become very important in high dimensions

In a system with 1000 degrees of freedom 99.99% of the phase space is located within 1% from the boundary.

\[ \frac{V_b}{V} = 1 - \left( \frac{r - \delta}{r} \right)^f \]

The dynamics becomes slow because the system is trapped in the boundaries, and it spends all time visiting local minima.

The average number of neighboring minima increases exponentially with the number of degree of freedom:

\[ X_{f=1} = 2 \]
\[ X_{f=2} = 6 \]
\[ X_{f=3} \sim 10/16 \]

\[ X_f \sim 2^{f+1} \]

Complex dynamical features in a simple system: Froth.

\[ \langle n \rangle = 6 \]
\[ E = \mu_2 N = \sum_i (n_i - 6)^2 \]

Figure 4. Persistence function $C(t_w + \tau, t_w)$ for $t_w = (4^k)/N$ with $k = 1, \ldots, 5$. (a) At high temperatures ($\beta = 0.5$) the persistence function is independent of $t_w$ and decreases exponentially fast. (b) At low temperatures ($\beta = 10^8$) $C(t_w + \tau, t_w)$ depends on $t_w$ and shows a slow decay. The curves correspond to fits of the form $C(t_w + \tau, t_w) \sim C_0 (\tau/t_w)^{\alpha}$ with $\alpha = 2.5$, $t_w = 2N$ and $C_0 = N$. 

Figure 5. Schematic illustration of an energy landscape. The process of avalanches is described using a low-dimensional model. 

$T$ Aste and D Sherrington
Glass dynamics

Figure 2. (a) $\mu_2$ versus the number of attempted moves in units of $N$ at $\beta = 0.5$ with starting configurations (i) and (ii) (triangles down and up). (b) $\beta = 3$. The lines are the theoretical predictions for thermodynamical equilibrium.

Figure 3. (a) $\mu_2$ versus temperature ($T = \beta^{-1}$) with starting configurations (i) and (ii) (triangles down and up) dynamically equilibrated for 11000N moves. The full curve is the theoretical prediction at the thermodynamical equilibrium. (b) Side distributions ($p(n)$) at low temperatures in the ‘glass phase’ ($\beta = 3, 10, 100$). The curve is the equilibrium prediction for $\beta = 2.4$. (c) Side distributions at high temperatures in the ‘liquid phase’ ($\beta = 0, 0.5, 1$). The full curves are the theoretical equilibrium predictions.
Natural Disorder?

Most undifferentiated biological tissues are space-filling assemblies of cells where the side distribution is centered around $n = 6$ and the second moment $\mu_2$ takes values between 0.5 and 1.2; for instance, $\mu_2 = 0.53$ in the human epidermis, $0.6 \mu_2 \approx 1$ in vegetable leaves, $\mu_2 = 0.68$ in the cucumber epithelia and $\mu_2 = 1.00$ in the human amnion.
Additional material
Satisfying the K-SAT problem

Probability to get a \textit{false} answer from a k-clause

\[
\frac{1}{2^k}
\]

Probability to get a \textit{true} answer from a k-clause

\[
1 - \frac{1}{2^k}
\]

Probability to get \(m\) “\textit{true}” answers

\[
\left(1 - \frac{1}{2^k}\right)^m
\]

Expected number of \textit{true} answers

If we have \(n\) variables

\[
2^n \left(1 - \frac{1}{2^k}\right)^m
\]

Expected number of true answers \(\geq 1\) \(\iff\) \(m < n \ 2^k \ln 2\)