Phase transitions in combinatorial optimization problems
Course at Helsinki Technical University, Finland, autumn 2007
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Lecture 5, 2. October 2007

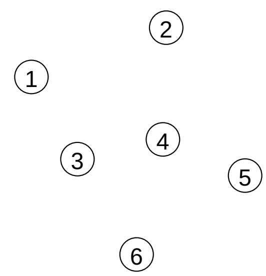
Announcements:

- Workshop 12. October in lecture room, 10:00-18:30
- 30-40 min per talk, 5 minutes discussion (at least ONE meaningful question per talk, before proceeding to next talk!!!!)
- Dinner afterwards (place to be announced, bill paid by lecturer)
- Submit summaries (about 5 pages printed) by 12. October →
  Another appointment per person 15/16. October, to discuss changes to summaries
- Summaries and pdfs of talk will be put on course web page

3.5.2 Markov chains

Given system with

- finite number of configurations $\{\underline{y}\}$
- probabilities $P(\underline{y})$



Here: $\underline{y}$ =states of N vertices → # Configurations $\mathcal{O}(2^{cN})$
→ enumeration not feasible
Usually $P(\underline{y}) \in \mathcal{O}(1)$ only for few configurations,
and exponentially small for most (*).

Aim: measurements of averages of $A(\underline{y})$:

$$\langle A \rangle := \sum_{\underline{y}} A(\underline{y}) P(\underline{y})\,, \tag{1}$$

(e.g. density of hard core gas)

Simplest approach: generate randomly L configurations $\{\underline{y}^i\}$ (all same probability) →

$$\langle A \rangle \approx \overline{A}^{(a)} \equiv \sum_{\underline{y}^i} A(\underline{y}^i) P(\underline{y}^i) / \sum_{\underline{y}^i} P(\underline{y}^i)\,.$$

(*) → result very inaccurate.

Better: generate configurations, those with large probability occur more often (<u>importance sampling</u>).

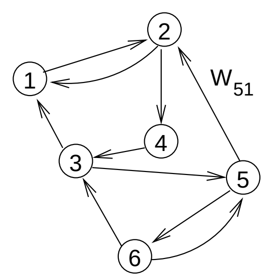
Ideal case: distributed according $P(\underline{y}^i) \rightarrow$

$$\langle A \rangle \approx \overline{A}^{(b)} \equiv \sum_{\underline{y}^i} A(\underline{y}^i)/L\,. \tag{2}$$

Direct generation according $P(\underline{y}^i)$ (like for Gaussian random numbers): does <u>not</u> work in almost all cases.

$\rightarrow$ <u>probabilistic dynamics</u> generating $\underline{y}(t)$ ($t = 0, 1, 2, \ldots$): $\underline{y}(1) \rightarrow \underline{y}(2) \rightarrow \ldots$.
Assumption: $\underline{y}(t+1) = f\big[\text{(pseudo) random number}, \underline{y}(t)\big]$ (<u>Markov chain</u>) (MC)

Description: transitions $\underline{y}(t) \rightarrow \underline{y}(t+1)$ by
<u>transition probabilities</u> $W_{\underline{y}\underline{z}} = W(\underline{y} \rightarrow \underline{z}) = W(\underline{y}|\underline{z})$
Assumpion: $W_{\underline{y}\underline{z}}$ independend of time t
Properties:

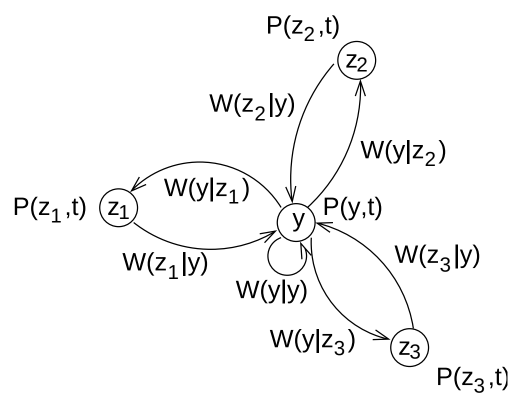


$$\begin{aligned} W_{\underline{y}\underline{z}} &\geq 0 \quad \forall \underline{y}, \underline{z} \quad (\textit{positivity}) \\ \sum_{\underline{z}} W_{\underline{y}\underline{z}} &= 1 \quad \forall y \quad (\textit{conservation})\,. \end{aligned} \tag{3}$$

<u>Markov process</u> (MP) = configurations + transition probabilities

$P(\underline{y}, t) :=$ probability that MC is at time t in $\underline{y}(t) = \underline{y}$
Aim: change of probability for t to $t+1$:

- transitions out of configuration $\underline{y}$: decreasing contribution to $P(\underline{y}, t+1)$
- transitions into $\underline{y}$: increasing contribution to $P(\underline{y}, t+1)$



<u>Master equation</u>

$$\Delta P(\underline{y}, t) := P(\underline{y}, t+1) - P(\underline{y}, t) = \sum_{\underline{z}} W_{\underline{z}\underline{y}} P(\underline{z}, t) - \sum_{\underline{z}} W_{\underline{y}\underline{z}} P(\underline{y}, t) \quad \forall \underline{y}. \tag{4}$$

Certain conditions (e. g., if there is only one eigenvalue $\lambda = 1$ for the matrix $(W_{\underline{y}\underline{z}})$), distributions $P(\underline{y}, t)$ converges towards the <u>stationary</u> (time-independent) distribution

$$P_{ST}(\underline{y}) \equiv \lim_{t \rightarrow \infty} P(\underline{y}, t)\,. \quad (\triangle)$$

(independently of $\underline{y}(0)$) $\rightarrow$ MP is called ergodic
meaning: one can reach each configuration from all other configurations.

$$\boxed{\text{Target: Choose } W_{\underline{y}\underline{z}} \text{ such that } P_{ST} = P}$$

$P(.)$ is time-independent: from Eq. (4) $\rightarrow$

$$0 = \Delta P(\underline{y}) = \sum_{z} W_{\underline{z}\underline{y}} P(\underline{z}) - \sum_{\underline{z}} W_{\underline{y}\underline{z}} P(\underline{y}) \quad \forall \underline{y}\,.$$

i.e. third condition: the "flows" of probability in and out of the configurations balance out.
One way to do it: balance holds for all pairs of configurations (detailed balance):

$$W_{\underline{z}\underline{y}} P(\underline{z}) - W_{\underline{y}\underline{z}} P(\underline{y}) = 0 \quad \forall \underline{y}, \underline{z}\,. \tag{5}$$

Formally: limit after $t \rightarrow \infty$ (in ($\triangle$))
In practice: First equilibration: wait till t_{eq}. Then measuring during MC simulation
Note: $\underline{y}(t)$, $\underline{y}(t+1)$ usually strongly correlated
$\rightarrow$ measure "distant" configurations $\underline{y}(t), \underline{y}(t+\Delta t), \underline{y}(t+2\Delta t), \ldots$
(Δt, t_{eq}, determined within simulation, via measuring quantities and their correlations)

3.5.3 Monte Carlo for hard-core gases

Configuration = vector $\underline{\nu} = \{\nu_i\}$ ($i \in V$

$$\nu_i = \begin{cases} 1 & \text{for } i \text{ is occupied by a particle} \\ 0 & \text{else }. \end{cases} \tag{6}$$

Hard-core constraint $\rightarrow$ indicator function

$$\chi(\underline{\nu}) = \prod_{\{i,j\} \in E} (1 - \nu_i \nu_j)\,. \tag{7}$$

$\chi = 1$ if configuration allowed.
Grand-canonical distribution (system coupled to "particle reservoir")

$$P(\underline{\nu}) = \frac{1}{\Xi} \chi(\underline{\nu}) e^{\mu \sum_i \nu_i} \tag{8}$$

- Ξ = grand-canonical partition function (normalization constant)
- μ = chemical potential
- $n = \sum_i \nu_i$ = # of particles.

For $\mu > 0$, the higher n the higher the statistical weight.
$\rightarrow$ for $\mu \rightarrow \infty$, only configurations with the highest density $\rho = \frac{1}{N}\sum_i \nu_i$ are obtained.
$\rightarrow$ # unoccupied vertices is minimized $\rightarrow$ minimum VC (used also in analytical calculations)

Not all $W_{\underline{zy}} \neq 0$: special types of transitions.
Here: two types: "move" (M) and "exchange" (E). For each MC step, chosen with probability 1/2 each.
For both: vertex i selected randomly (prob. $1/|V|$ each)

M If i unoccupied and exactly one neighbor j occupied
$\rightarrow$ particle at j is moved to vertex i
else: nothing happens.

E If vertex i unoccupied and all neighbors unoccupied
$\rightarrow$ particle inserted at i.
If some neighbors are occupied: nothing happens.

If i occ., particle removed w. prob. $\exp(-\mu)$.