MIDTERMS.
1 MIRIAM
2 CINDY
3 ADAM
4 VAN

INDEX CARD: FEEDBACK

Last time : Stat Mech

- Monte Carlo: USE RANDOM SAMPLES VS. FULL ENSEMBLE OF μstates

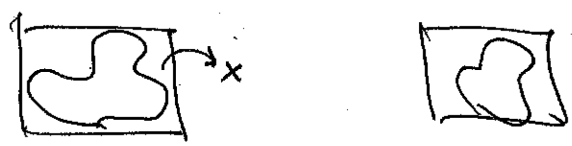
  AVG of a smaller # of microstates = AVG of full ensemble

  these have a probability dist.

  ... if SAMPLE is faithful to

- Markov Chain : generate sample sequentially
  - many "small" steps
    ↳ ERGODIC proper: these can access all allowed μ states

    eg: can't use marble game for disconnected fields



no way to sample the disconnected island

  - 2 kinds of prob:

want to sample → P_i (BOLTZMANN) PROB of i^{th} μ-STATE
↳ $= e^{-\beta E_i}/Z$

we make UP! → $p(i \to j)$ TRANSITION PROBABILITY to go from μstate i to μstate j.

2 RULES : ① conservation of transition prob.

$$\boxed{\sum_j P(i \to j) = 1}$$

② conservation of state prob.

$$P_j = \sum_i P_i \, p(i \to j)$$

prob of being somewhere = prob of going there from somewhere else × being in that "somewhere else"

from this: $\boxed{\text{ANSATZ}}$ ($\cong$ solution)

Detailed Balance :

$$\boxed{P_i \, p(i \to j) = P_j \, p(j \to i)}$$

notation: TRANSITION MATRIX : $T_{ij} = p(i \to j)$

"propagator" ... you see these ideas over & over & over again in physics.

ACTS ON VECTOR OF PROBABILITIES

$$\vec{P} = \begin{pmatrix} P_1 \\ \vdots \\ P_N \end{pmatrix}$$

$$\boxed{P_i T_{ij} = P_j T_{ji}}$$ (no sum implied!!)

$$P_j = \frac{e^{-\beta E_j}}{Z}$$

CAN CALCULATE IN A GIVEN SYSTEM

intractable, important

detailed balance $\Rightarrow \dfrac{T_{ij}}{T_{ji}} = \dfrac{P_j}{P_i} = \underbrace{e^{-\beta(E_j - E_i)}}_{\text{can calculate}}$

if we know the ratios of transition probabilities, we can determine our rules for MCMC!

$\boxed{\text{HOPE}}$ ← to best of my knowledge, no rigorous proof.

① if we have a sample that is BOLTZMANN DISTRIBUTED, IT STAYS BOLTZMANN

② if we have a sample that is not BOLTZMANN, it <u>BECOMES</u> BOLTZMANN.

PROB of being in i @ time t

ie $\boxed{\dfrac{\#\text{ states in } i}{\#\text{ states gen in } t \text{ steps}}}$

①: given $P_i(t)$,

$$
\begin{aligned}
P_j(t+\Delta t) &= \sum_i \underbrace{P_i(t)\, T_{ij}} \\
&= \sum_i P_j(t)\, T_{ji} \\
&= P_j(t) \boxed{\sum_i T_{ji}} = 1 \\
&= P_j(t)
\end{aligned}
$$

← SO PROB DIST. DOESN'T CHANGE.

can drop this t for large enough t.

THAT'S THE POINT OF DETAILED BALANCE

... but is P_i boltzmann?

② DOES MCMC <u>converge</u> to Boltzmann dist?

$\hookrightarrow$ $\boxed{\text{ERGODIC HOPE}}$

APP D of NEWMAN IS A NICE "PHYSICIST'S" PF.

<u>Sketch</u> : $\vec{P}(t) = T^t \vec{P}(0)$

DISCRETE # of STEPS

transition matrix

RANDOM initial state (set of probabilities)

suppose T has eigenvectors $\vec{V}_k$

$$\vec{P}(t) = T^t \sum_k c_k \vec{V}_k = \sum_k c_k \lambda_k \vec{V}_k$$

$\vec{P}(0)$ PROJECTION ONTO EIGENBASIS

eigenvals

$$= \lambda_1^t \sum_k c_k \left(\frac{\lambda_k}{\lambda_1}\right)^t \vec{V}_k$$

LARGEST EIGENVAL

$$(<1)^{t \gg 1} \longrightarrow 0$$

UNLESS $k = 1$

$$\frac{\vec{P}(t)}{\lambda_1^t} = c_1 \vec{V}_1$$

EIGENVEC of PROBABILITIES

- DETAILED BALANCE: $\sum_j T_{ji} P_j = P_i \sum_j T_{ji} = P_i$

$\boxed{\text{EIGEN VEC w/ } \lambda = 1}$

sketch of rest of pf

$\sum_j T_{ij} = 1 \longrightarrow \vec{\mathbb{1}} = (1, \cdots, 1)$ is a left eigenvector.

L & R are kind of weird... maybe I should have defined

$S_{ij} = T_{ji} = P(j \to i)$

if BOLTZMANN EIG VEC. only one w/ $\lambda = 1$, THEN ALL OTHERS ARE ORTHOG

must have neg entries (unmathematical)

if not: then $\exists$ SEPARATE SUBSPACE OF STATES

$$\mu\text{states} = (\mu\text{state})_1 \oplus (\mu\text{state})_2$$

T keeps you in here T keeps you in here

* this violates ergodicity!

hope ergodicity is true.

finally: T is non-neg. $\vec{p}(0)$ is non neg.

$\vec{p}(\infty)$ must also be non-neg.

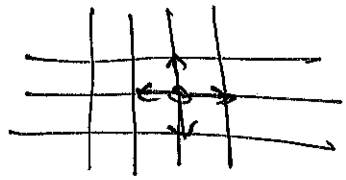
must be Boltzmann.

PRACTICAL: ② $T_{ij} = p(i \to j)$

standard choice of algorithm: METROPOLIS

EACH MOVE

1. IDENTIFY ALLOWED MOVES (move set)

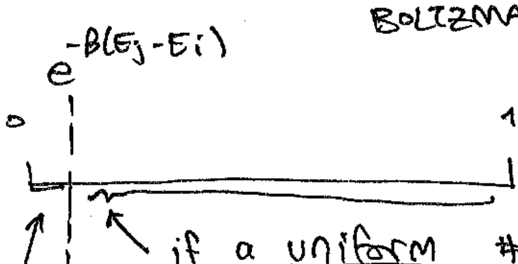


(also: ↺ "stay")

2. Pick one @ random w/ uniform distribution
3. if the configuration is lower energy, make the move.

otherwise: flip a WEIGHTED coin

↑ BOLTZMANN FACTOR: $e^{-\beta(E_j - E_i)}$ ← POSITIVE



if a uniform # from (0,1) lands here, then REJECT move

if uniform # from (0,1) lands here, then ACCEPT move to higher E state.

---

why it works:

$$T_{ij} = \begin{cases} 1 & \text{if } E_j < E_i \\ e^{-\beta(E_j - E_i)} & \text{if } E_i < E_j \end{cases}$$

DETAILED BALANCE!

$$\frac{T_{ij}}{T_{ji}} = \begin{cases} e^{-\beta(E_j - E_i)} & E_j < E_i \\ e^{-\beta(E_j - E_i)} & E_j > E_i \end{cases} \quad \boxed{= \frac{P_i}{P_j}}$$