Large Deviations in Renewal Models of Statistical Mechanics

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Outline

Basics

$\{(S_i, R_i)\}_{i\geq 1}$ sequence of i.i.d. random vectors on $(\Omega, \mathcal{F}, \mathbb{P})$ so that

- $S_i \in \{1, 2, \ldots\} \cup \{\infty\}$ is a "waiting time";
- $T_i := S_1 + \ldots + S_i$ is a "renewal time" and $T_0 := 0$;
- $R_i \in \mathbb{R}^d$ is a "reward" associated with S_i.

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For each integer time $t \geq 0$

- $X_t := \mathbb{1}(t \notin \{T_i\}_{i\geq 0})$ is the (non-)renewal indicator;
- $N_t := \sup\{i \geq 0 : T_i \leq t\}$ is the number of renewals by t;
- $W_t := \sum_{i=1}^{N_t} R_i$ is the total reward by t and $W_t := 0$ if $N_t = 0$.

Constrained Renewal Model (1)

Renewal equation:

$$\mathbb{P}[X_t = 0] = \begin{cases} 1 & \text{if } t = 0; \\ \sum_{s=1}^{t} p(s)\, \mathbb{P}[X_{t-s} = 0] & \text{if } t > 0, \end{cases}$$

where $p(s) := \mathbb{P}[S_1 = s]$ is the “waiting time distribution”.

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$\mathbb{P}[X_t = 0] > 0$ *for all t sufficiently large if* $\gcd\{s \geq 1 : p(s) > 0\} = 1$.

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If $\gcd\{s \geq 1 : p(s) > 0\} = 1$, then conditioning on $\{X_t = 0\}$

- is well-defined for all t sufficiently large;
- yields the new model $(\Omega, \mathcal{F}, \mathbb{P}_t)$ with $\dfrac{d\mathbb{P}_t}{d\mathbb{P}} := \dfrac{1 - X_t}{\mathbb{P}[X_t = 0]}$.

Constrained Renewal Model (2)

Distribution of waiting times:

$$\mathbb{P}_t\left[S_1 = s_1, \ldots, S_n = s_n, N_t = n\right] = \frac{\mathbb{1}\left(\sum_{k=1}^{n} s_k = t\right)}{\mathbb{P}[X_t = 0]} \prod_{k=1}^{n} p(s_k).$$

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Distribution of renewal indicators:

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with $\#_{s|t}(x_0, \ldots, x_t) := \sum_{i=1}^{t-s+1} (1 - x_{i-1}) \left(\prod_{k=i}^{i+s-2} x_k \right) (1 - x_{i+s-1})$.

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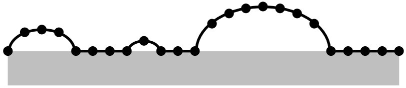
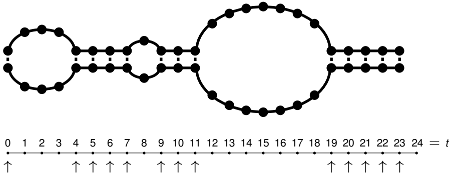
...and they look like finite-volume Gibbs states!

Polymer Localization and DNA Denaturation

Pinned polymer (Fisher):



DNA molecule (Poland-Scheraga):



t monomers (per strand)

- in n stretches of lengths s_k with $s_1 + \cdots + s_n = t$ and only the first monomer bound;
- with binding energy ϵ;
- with loop entropy σ_s so that $\sigma_s \leq b\,s$.

Statistical weight:

$$\prod_{k=1}^{n} \exp(\sigma_{s_k} - \epsilon + \eta s_k).$$

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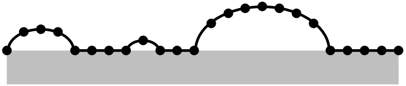

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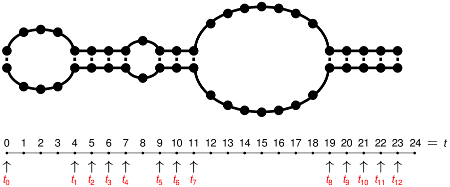

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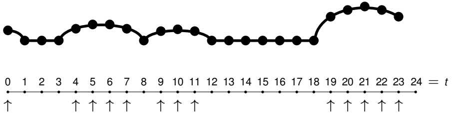
Take η so that $p(s) := \exp(\sigma_s - \epsilon + \eta s)$ satisfies $\sum_{s=1}^{\infty} p(s) \leq 1$!

Protein Folding

Protein (Wako-Saitô-Muñoz-Eaton):



t peptide bonds

- $x_i = 1$ native, $x_i = 0$ non-native;
- interact only if belong to the same native stretch;
- with contact energy ϵ_{j-i+1} so that $u_s := \sum_{k=1}^{s}(s-k)\epsilon_k \geq b\,s$;
- order with entropic loss σ.

Statistical weight:

$$\exp\left[-\sum_{i=0}^{t-1}\sum_{j=i}^{t-1}\epsilon_{j-i+1}\prod_{k=i}^{j}x_k+\sigma\sum_{i=0}^{t-1}(1-x_i)+\eta t\right]$$

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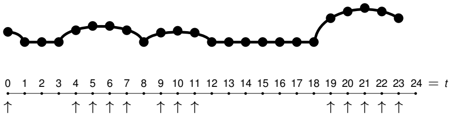

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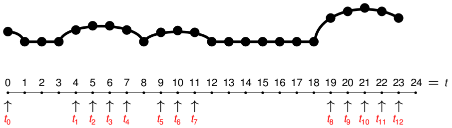

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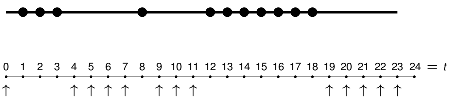
Strained Epitaxy

Crystal film (Tokar-Dreyssé):



t lattice sites

- $x_i = 1$ occupied, $x_i = 0$ empty;
- particles interact only if belong to the same cluster;
- with energetic gain u_s so that $u_s \geq b\, s$;
- with chemical potential μ.

Statistical weight:

$$\exp\left[-\sum_{s=1}^{t} u_s \,\#_{s|t}(x_0, \ldots, x_{t-1}, 0) + \mu \sum_{i=0}^{t-1} x_i + (\eta - \mu) t\right]$$

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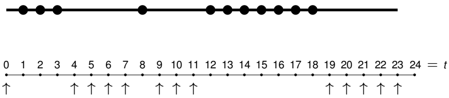

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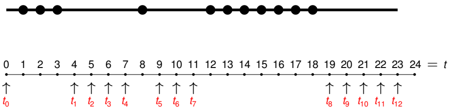

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Total Reward $W_t := \sum_{i=1}^{N_t} R_i$ in Statistical Mechanics

In pinned-polymer model and Poland-Scheraga model

- $R_i := 1 \implies W_t$ counts bound monomers;
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In all cases

- $R_i := \big(\mathbb{1}(S_i = 1), \ldots, \mathbb{1}(S_i = d)\big) \implies W_t$ counts waiting times;
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Quantifying Rare Events

Problem: study $\mathbb{P}_t\left[\frac{W_t}{t} \in A\right]$ for large t and some $A \subseteq \mathbb{R}^d$ measurable.

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Weak large deviations principle if (b) valid only for F compact.

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Main Results

Let $\zeta(k)$ be the extended real number defined for each $k \in \mathbb{R}^d$ by

$$\zeta(k) := \inf\left\{ z \in \mathbb{R} : \mathbb{E}\Big[\exp\left(k \cdot R_1 - z\,S_1\right)\mathbb{1}(S_1 < \infty)\Big] \leq 1 \right\} > -\infty.$$

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Theorem

$$\lim_{t\uparrow\infty} \frac{1}{t} \ln \mathbb{E}_t\left[\exp(k \cdot W_t)\right] =: c(k) \textit{ exists and } c(k) = \zeta(k) - \zeta(0).$$

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Theorem

(a) *W_t satisfies a weak LDP with rate function I.*

(b) *If $0 \in \text{int}\{k \in \mathbb{R}^d : c(k) < \infty\}$, then W_t satisfies an LDP with I.*

Remark

c non-differentiable on $\text{int}\{k \in \mathbb{R}^d : c(k) < \infty\}$ in general

$\Downarrow$

Gärtner-Ellis Theorem does not apply

(based on a change of measure)

$\Downarrow$

an original proof is needed!

(based on subadditivity arguments like for Cramér's Theorem)

Final Remarks

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On the physical side

- rate function I with singularities.