Weighted words collector

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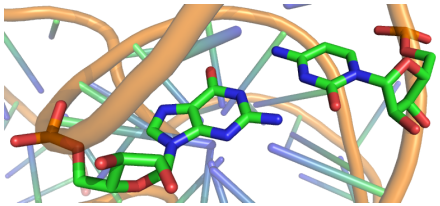
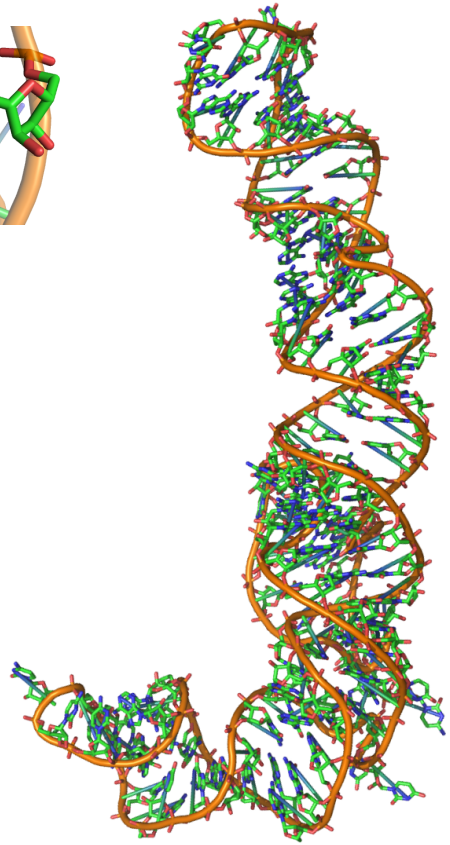
Motivation: RNA folding prediction through statistical sampling

- RNA Structure

  RNA = Sequence over $\{A, C, G, U\}$.
  RNA folds, creating hydrogen bonds.
  Such base-pairs stabilize structure.
  Free-energy E_S assigned to each structure S.





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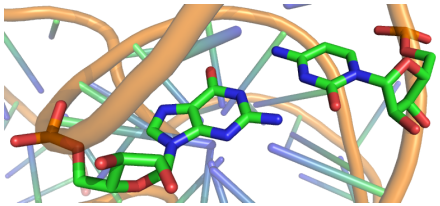

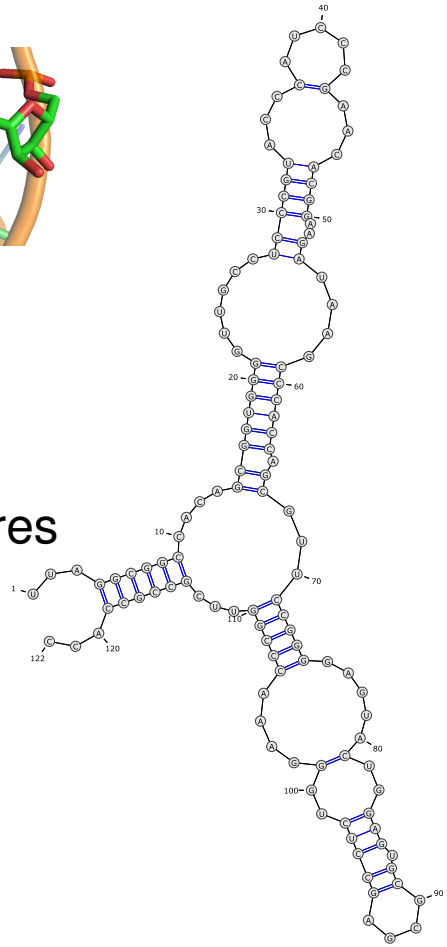

- Simplified energy model [Nussinov-Jacobson 78]

  Only non-crossing base-pairs allowed $\rightarrow$ Secondary Structures
  Free-Energy = $-$# Base-pairs

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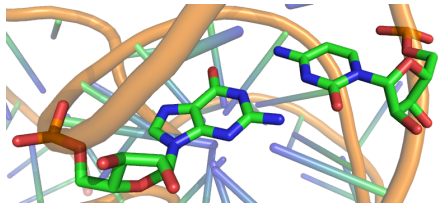

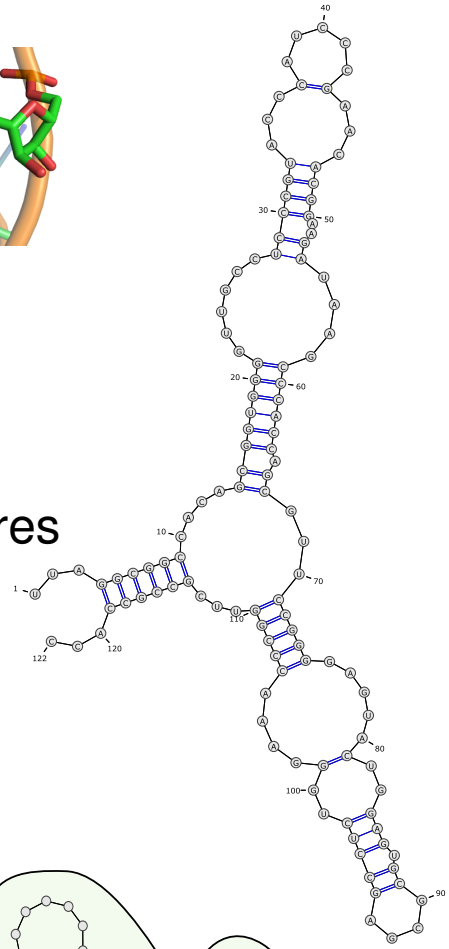

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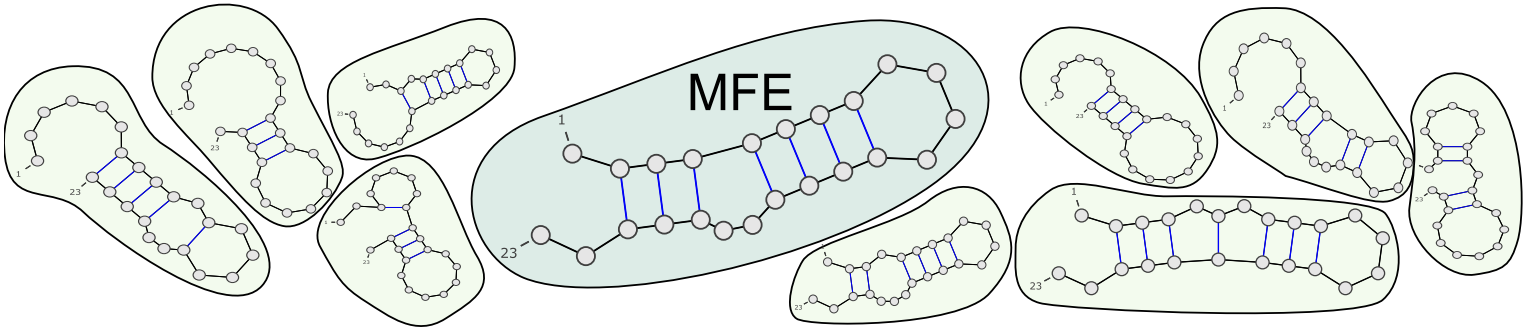
- Boltzmann equilibrium [McCaskill 90]

  Any structure S exists w.p. $p_S \propto e^{-\#E_S/RT}$.



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RNA *in silico* search: from sequence to functional secondary structure

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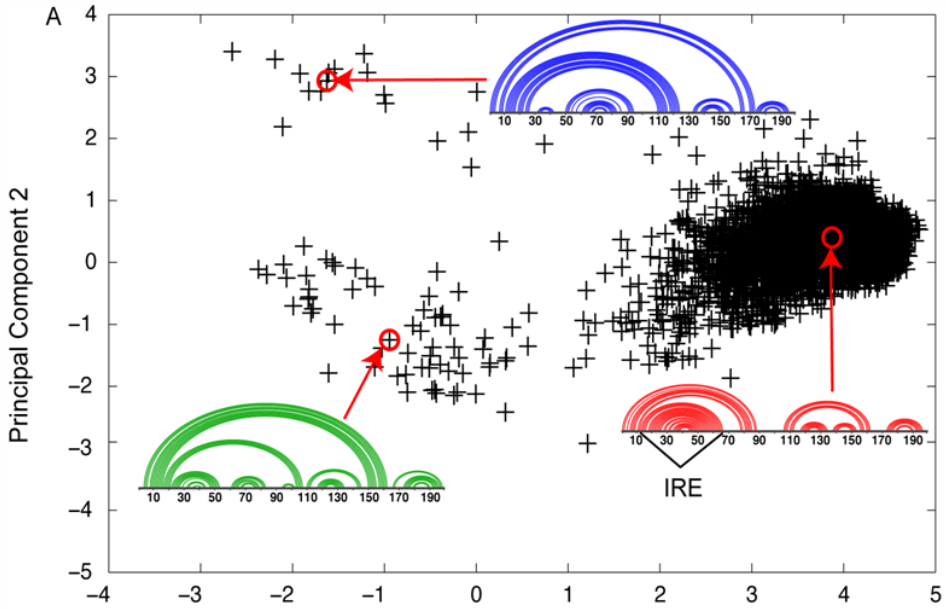

[Halvorsen *et al* 2010]

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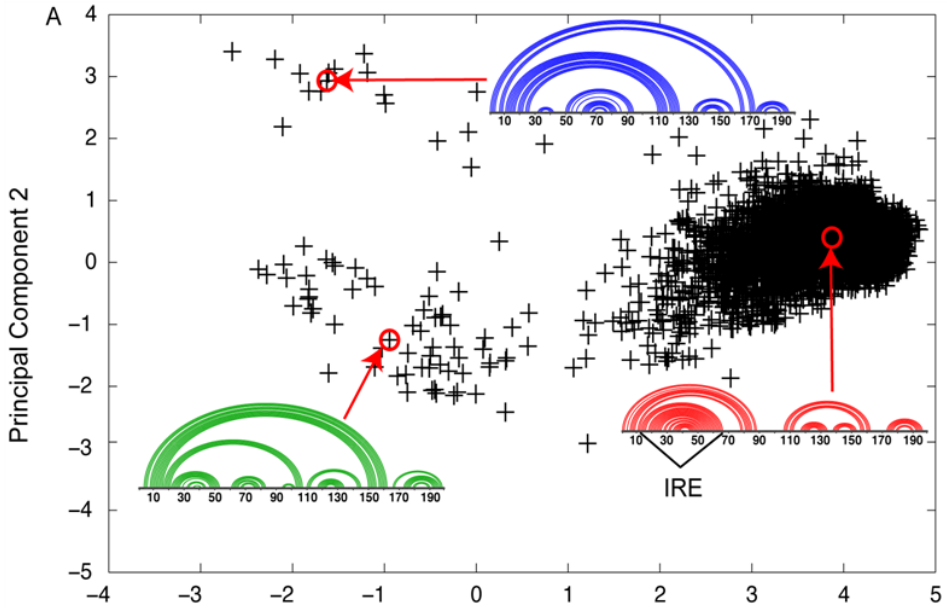

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2. Cluster them using some machine learning technique
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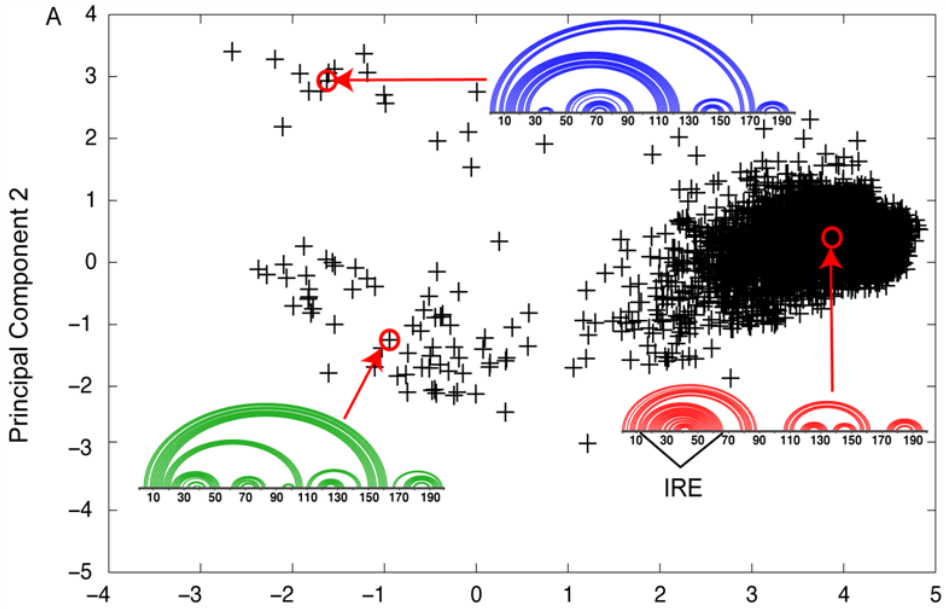

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2. Cluster them using some machine learning technique
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$\Rightarrow$ This simple idea greatly improved specificity of predictions.

Motivation: RNA folding prediction through statistical sampling

A closer look at the (meta)-algorithm:

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Redundancy is uninformative, one should aim for k distinct secondary structures.

Which additional cost is induced by the redundant generation?

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Coupon collector problem!

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The Coupon Collector problem (uniform)

10¢ per sticker
$m = 539$ stickers

$\Rightarrow$ 339 €!!!

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Average cost: - It takes a first coupon to get hooked!
- One must then buy, on the average, $\frac{m}{m-k}$ coupons to get the $k+1$-th coupon...

$$E[C_m] = 1 + \frac{m}{m-1} + \frac{m}{m-2} + \ldots + \frac{m}{m-k} + \ldots = m \cdot \mathcal{H}_m \underset{m\to\infty}{\sim} m \ln m.$$

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Theorem (Flajolet-Gardy-Thimonier,92)

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(i) [David-Barton,62] $p_i = \dfrac{2i}{m(m+1)} \quad \Rightarrow \quad E[C_m] \underset{m\to\infty}{\sim} \left(\frac{2\pi}{\sqrt{3}} - 3\right) \cdot m \cdot (m+1).$

(ii) [Hildebrand,93] $p_i = \dfrac{1}{iH_m} \quad \Rightarrow \quad E[C_m] \underset{m\to\infty}{\sim} m \cdot H_m \cdot \log m.$

A more general result

- Distribution defined by a sequence of positive numbers $\{a_1, ..., a_m\}$:

$$p_i = \frac{a_i}{\mu_m}, \qquad \text{with} \qquad \mu_m = \sum_{i=1}^{m} a_i.$$

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Theorem (Boneh-Papanicolaou,94)

If f satisfies:

$$(i)\ f(x) \nearrow \infty, \qquad (ii)\ \frac{f'(x)}{f(x)} \searrow, \qquad \text{and} \qquad (iii)\ \frac{f''(x)/f'(x)}{(f'(x)/f(x))\log(f'(x)/f)(x)} \to 0,$$

$$\text{Then} \qquad E[C_m] \underset{m\to\infty}{\sim} \mu_m \cdot f(m) \cdot \log \frac{f(m)}{f'(m)}$$

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What about sequences whose weights appear with multiplicities?
(e.g. unbounded #occurrences of some a_i as $m \to \infty$)

Word collector?

Random generation of words

Word collector?

Random generation of words

+

Coupon Collector

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=

Words collector

Which probability distribution on words?

Definition

i $\mathcal{L}$ *is a language over* $\Sigma = (a_1, ..., a_k)$, *and* $\mathcal{L}_n$ *its restriction to words of length n.*

ii *Weight of a letter* $a_i \to \pi_{a_i} \in \mathbb{R}^+$.

iii *Weight of a word* $\omega \in \mathcal{L}_n \to \pi(\omega) = \prod_{a \in \omega} \pi_a$

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Remark: Words having equal composition have equal probability:

$$\mathbb{P}[ababbabaaa] = \mathbb{P}[aababbbaaa] = \mathbb{P}[aaaaaabbbb] = \frac{\pi_a^6 \pi_b^4}{\mu_{10}}.$$

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Many coupons have equal weight, i.e. equal probabilities! $\Rightarrow$ Large multiplicities
$\Rightarrow$ None of the general theorems applies...

Asymptotics

Reminder:

$$E[C_m] = \int_0^\infty \Phi(t)dt \qquad \textit{with} \qquad \Phi(t) = 1 - \prod_{i=1}^{m} \left(1 - e^{-p_i t}\right).$$

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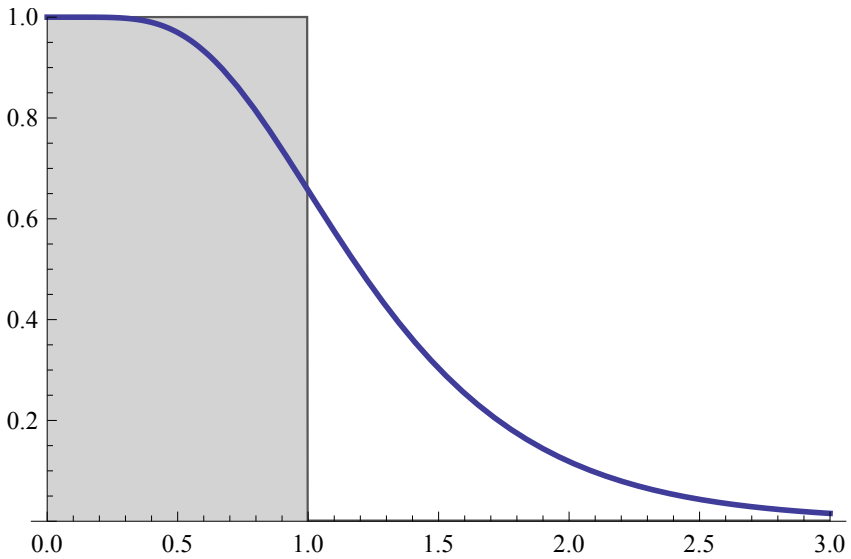

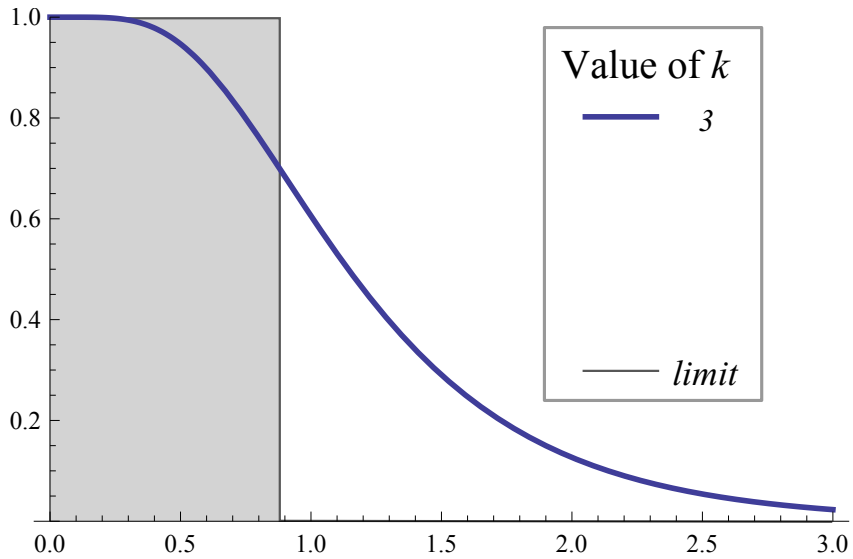

$\Psi(t)$ on $\{a, b\}^k$ ($m = 2^k$) upon well-chosen change of variable.
Left: Uniform distribution. Right: Weighted distribution, $\pi_a/\pi_b = 2/3$.

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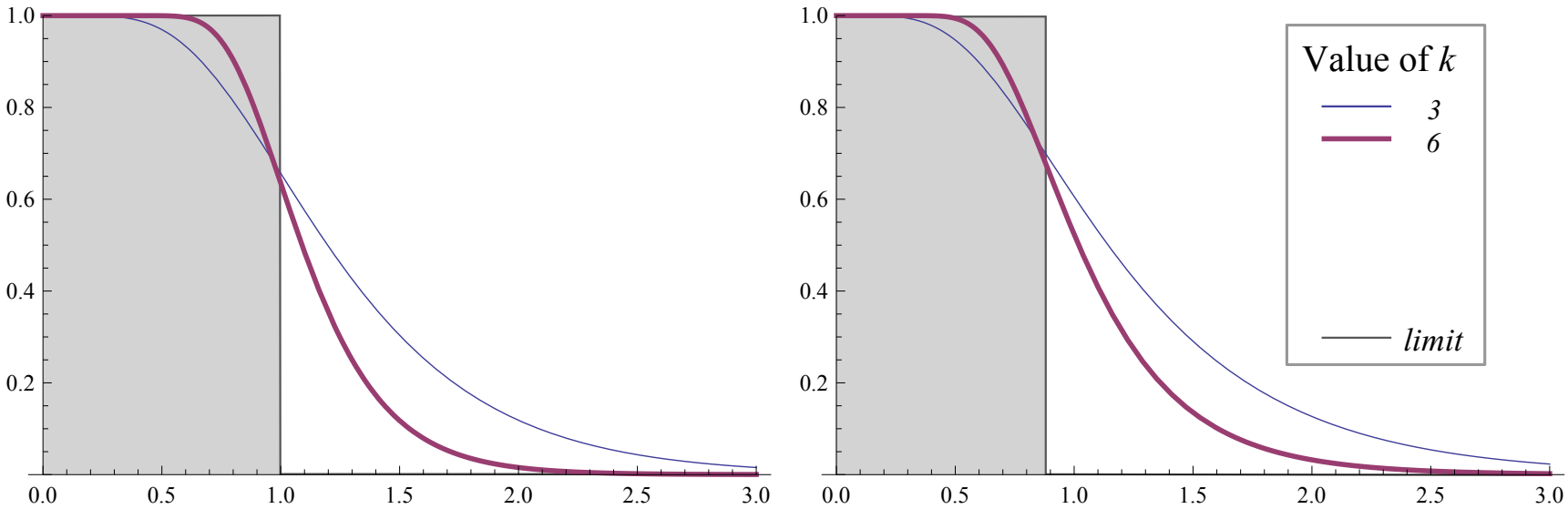

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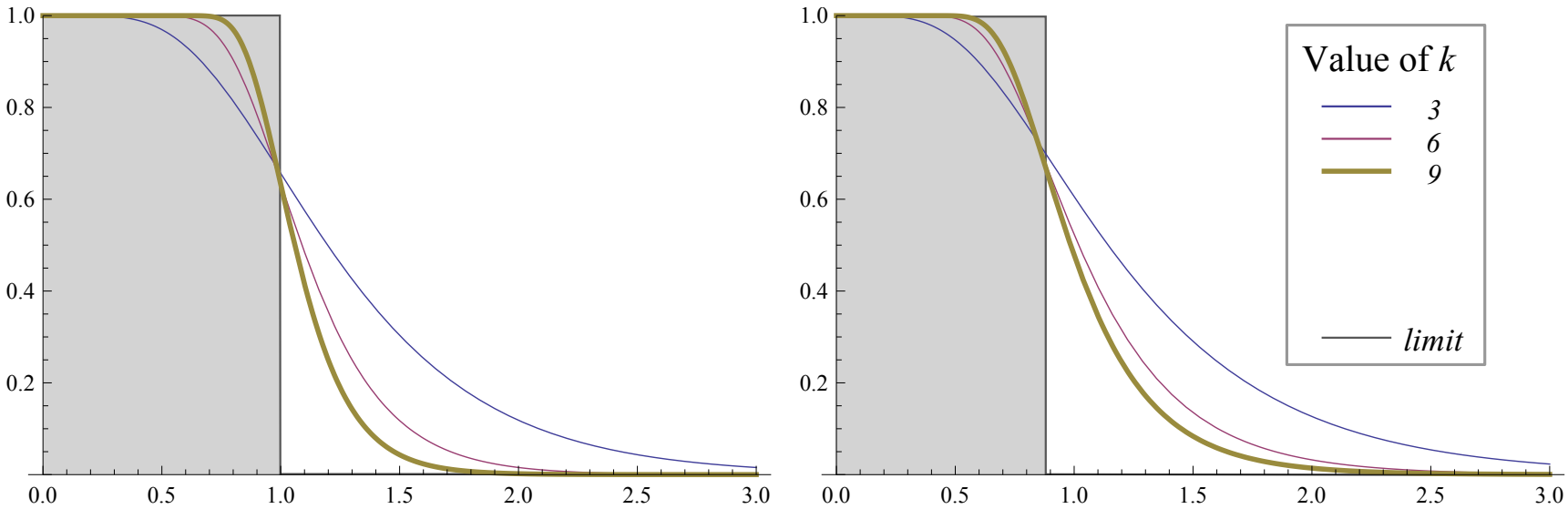

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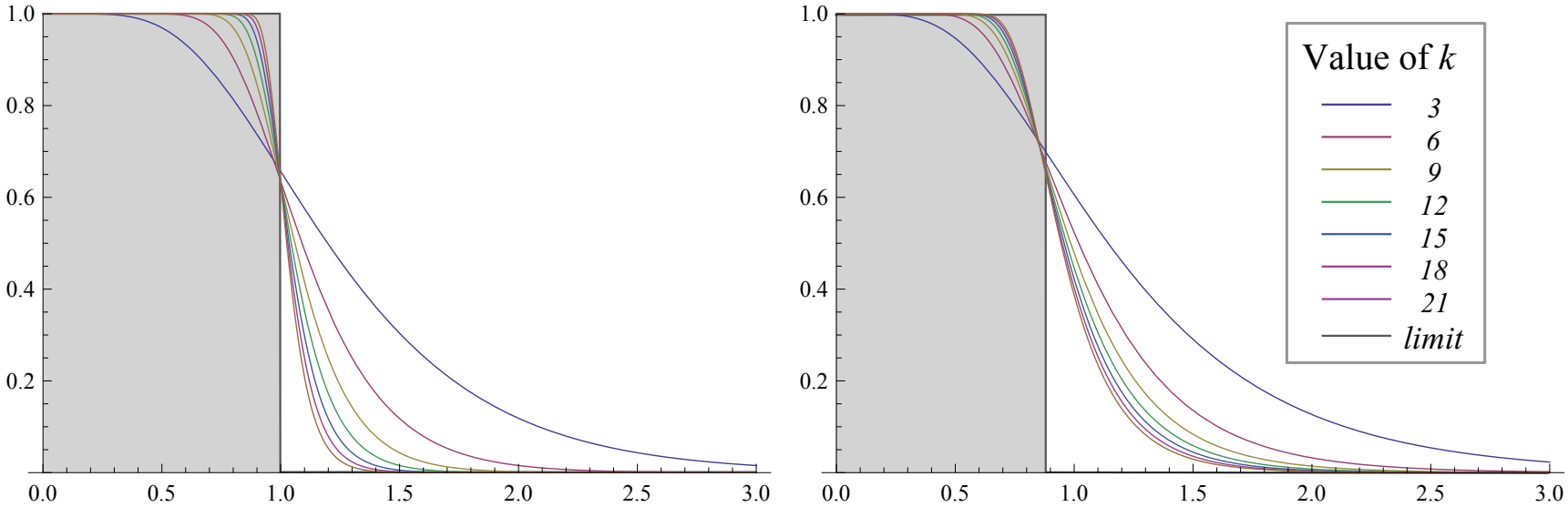

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If weight distribution satisfies hypotheses ***H1***, ***H2*** *et* ***H3***, *then*

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Asymptotics (continued)

Evaluating the integral? $\rightarrow$ **for distributions featuring large multiplicities**.

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Application: Σ^*

Description: Language $(a_1, ..., a_k)^*$ with $1 = \pi_{a_1} = ... = \pi_{a_j} < \pi_{a_{j+1}} \leq ... \leq \pi_{a_k}$.

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Proposition

$$E[C_m] \sim \begin{cases} \kappa_1 \cdot m^p \cdot \log\log m & \text{if } j = 1, \\ \kappa_2 \cdot m^p \cdot \log m & \text{otherwise.} \end{cases}$$

where $p = \log_k(\pi_{a_1} + \cdots + \pi_{a_k})$.

Asymptotic waiting time differs from the uniform case.

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Description: RNA sec. str. unambiguously generated by context-free grammar

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where θ: minimal distance between matching parentheses ($\theta = 1$ or 3).
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i Gen. fun. + Singularity analysis $\Rightarrow \mu_m \sim \kappa \cdot m \cdot (\log m)^{-3/2}$
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Proposition

$$E[C_m] \sim \kappa \cdot m^p \cdot (\log m)^{3p/2} \cdot \log\log m$$

where $p = \frac{\log \rho_\theta}{\log \eta_\theta} > 1$ *and* η_θ *(resp.* ρ_θ*) is the dom. sing. for the number (resp. cumulated weight) of RNA sec. str.*

Again, asymptotic waiting time differs from the uniform case.
Corollary: On average, a secondary structure is generated $\Theta((\eta_\theta/\rho_\theta)^n \cdot \log(n))$ times.

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Thanks for listening
Questions?