Random copolymer adsorption

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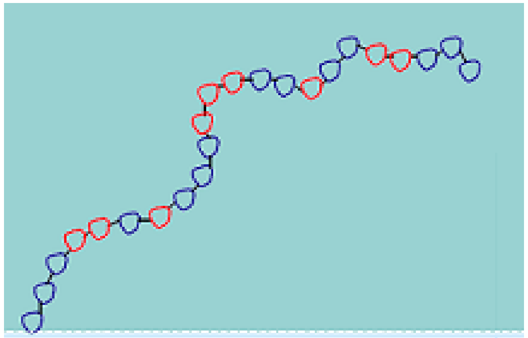
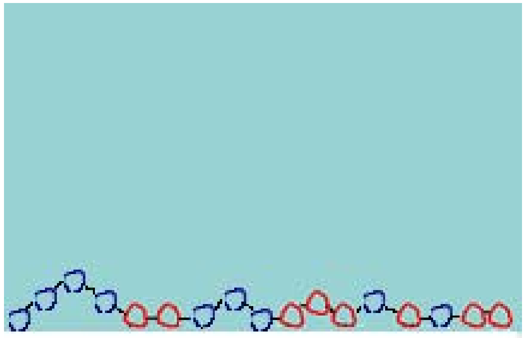
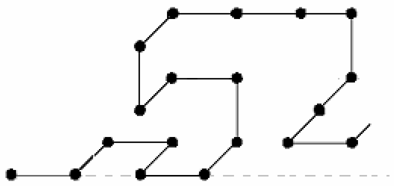


Desorbed

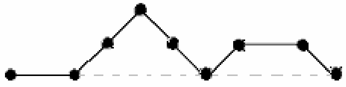


Adsorbed

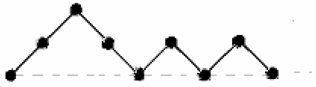
- Dilute solution (polymer-polymer interactions can be ignored).
- System in equilibrium.
- Polymer's conformations: self-avoiding walks, Motzkin paths, Dyck paths.



Self avoiding walk



Motzkin path



Dyck path

- Degree of polymerization: n

- Two types of monomers: A and B.
  - Monomer sequence (*colouring*) is random.
  - χ_i is *colour* of monomer *i* ($\chi_i = 1 \rightarrow$ A)
  - i.i.d. Bernoulli random variables, $P(\chi_i=1) = p$

- Energy of conformation ω for fixed colour χ :
  - $E(\omega|\chi) = -\alpha\, n_{A,S}$.
  - $\alpha = -1/kT$
  - $n_{A,S}$: number of A monomers at the surface.

- Conformations with same energy are equally likely, so

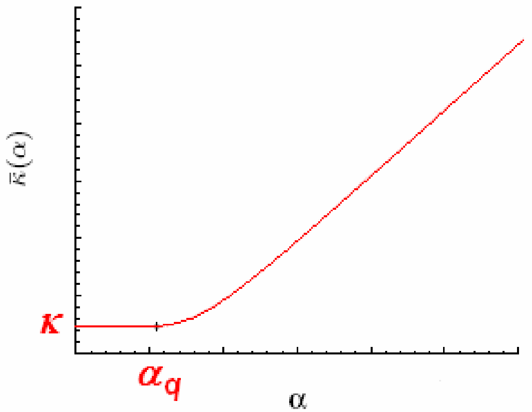
$$Z_n(\alpha|\chi) \;=\; \sum_{n_{A,S}=0}^{n} c_n(n_{A,S}|\chi)\; e^{\alpha n_{A,S}}$$

  - $c_n(n_{A,S}|\chi)$: number of walks with $n_{A,S}$ vertices coloured A at the surface.

- Intensive free energy at fixed χ : $\kappa_n(\alpha|\chi) = n^{-1}\log Z_n(\alpha|\chi)$
- Quenched average free energy : $\bar{\kappa}_n^q(\alpha) = \langle n^{-1}\log Z_n(\alpha|\chi)\rangle_\chi$
- Limiting quenched average free energy (exists):

$$\bar{\kappa}(\alpha) = \lim_{n\to\infty} \bar{\kappa}_n^q(\alpha)$$

  - Indicates if polymer prefers desorbed or adsorbed phase.



$$\kappa = \begin{cases} \log 2 & \textit{Dyck paths} \\ \log 3 & \textit{Motzkin paths} \end{cases}$$

  - As $\alpha \to \infty$, asymptotic to a line with slope $\begin{cases} p/2 & \textit{Dyck paths} \\ p & \textit{Motzkin paths} \end{cases}$
- Q: What is the value of α_q ?
- Q: What is $\bar{\kappa}(\alpha)$ for $\alpha > \alpha_q$?

- Annealed average free energy:

$$\bar{\kappa}_n^a(\alpha) = n^{-1} \log\langle Z_n(\alpha|\chi)\rangle_\chi \ \geq \ \bar{\kappa}_n^q(\alpha)$$

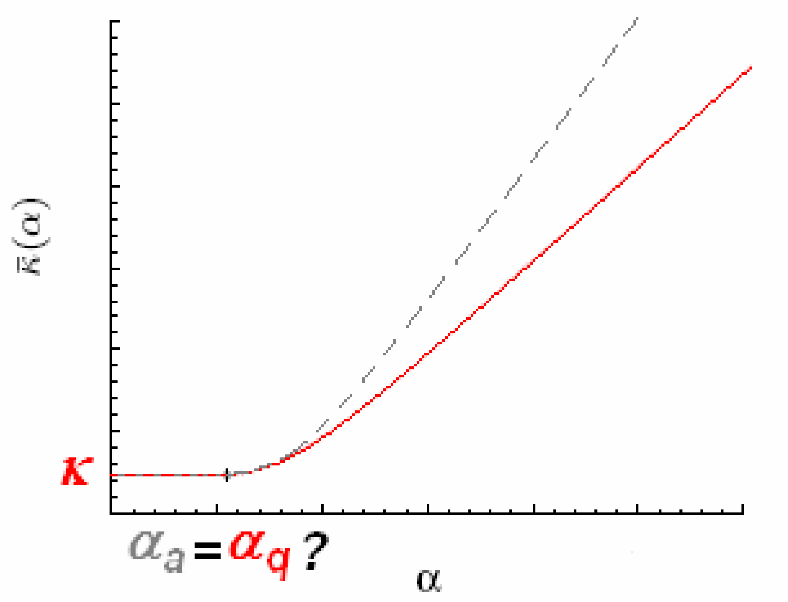
- Limiting annealed average free energy:

$$\bar{\kappa}^a(\alpha) = \lim_{n\to\infty} \bar{\kappa}_n^a(\alpha) \ \geq \ \bar{\kappa}^q(\alpha)$$

- So, $\alpha_a = \begin{cases} \log(1+1/p) & \textit{Dyck paths} \\ \log(1+1/2p) & \textit{Motzkin paths} \end{cases} \quad \leq \alpha_q$

- As $\alpha \to \infty$, $\bar{\kappa}^a(\alpha)$ is asymptotic to a line with slope

$$\begin{cases} 1/2 \neq p/2 & \textit{Dyck paths} \\ 1 \neq p & \textit{Motzkin paths} \end{cases}$$



The Morita Approximation (Constrained Annealing)

- Consider the constrained annealed average free energy

$$\bar{\kappa}_n^{c.a.}(\alpha,\lambda) = n^{-1}\log\left\langle Z_n(\alpha|\chi)\; e^{\Lambda(\lambda|\chi)}\right\rangle_\chi$$

with the Lagrangian

$$\Lambda(\lambda|\chi) = \sum_{C\subseteq[n]} \lambda_C \left[p^{|C|} - \prod_{i\in C}\chi_i\right]$$

- Minimization of $\bar{\kappa}_n^{c.a.}(\alpha,\lambda)$ with respect to λ_C constrains

$$Prob(\text{all the walk vertices in } \; C \; \text{ are coloured } \; A) = \langle\prod_{i\in C}\chi_i\rangle = p^{|C|}$$

- Mazo (1963), Morita (1964), and Kuhn (1996) showed that $\bar{\kappa}_n^q(\alpha)$ can be obtained as the solution to

$$\min_{\lambda} \bar{\kappa}_n^{c.a.}(\alpha,\lambda)$$

- Setting some λ's to zero and minimizing $\bar{\kappa}_n^{c.a.}\left(\alpha, \hat{\lambda}\right)$ to obtain $\bar{\kappa}_n^{u.b.}(\alpha)$ yields an upper bound on $\bar{\kappa}_n^{q}(\alpha)$
  - In particular, we obtain

$$\bar{\kappa}_n^{q}(\alpha) \;\le\; \bar{\kappa}_n^{u.b.}(\alpha) \le \; \bar{\kappa}_n^{a}(\alpha)$$

and so

$$\bar{\kappa}^{q}(\alpha) \;\le\; \bar{\kappa}^{u.b.}(\alpha) \le \; \bar{\kappa}^{a}(\alpha)$$

  - e.g.,
    - annealed

$$\Lambda(\lambda|\chi) = 0$$

$$\bar{\kappa}_n^{c.a.}(\alpha, \lambda) = n^{-1} \log \langle Z_n(\alpha|\chi)\rangle_\chi = \bar{\kappa}_n^{a}(\alpha)$$

    - 1st order Morita:

$$\Lambda(\lambda|\chi) = \lambda \sum_{i=1}^{n} (\chi_i - p)$$

$$\bar{\kappa}_n^{c.a.}(\alpha, \lambda) = n^{-1} \log \left\langle Z_n(\alpha|\chi)\; e^{\lambda \sum_{i=1}^{n} (\chi_i - p)} \right\rangle_\chi \le \bar{\kappa}_n^{a}(\alpha)$$

- Minimization to obtain $\bar{\kappa}_n^{u.b.}(\alpha)$ is quite complex.

$$\bar{\kappa}^{u.b.}(\alpha) \;=\; \lim_{k\to\infty} (k\sigma)^{-1} \min_{\lambda^{(\sigma)}} \log \left\langle Z_{k\sigma}(\alpha|\chi)\; e^{\Lambda\left(\lambda^{(\sigma)}|\chi\right)} \right\rangle_{\chi}$$

- Upper bound it by

$$\bar{\kappa}^{(\sigma)}(\alpha) \;=\; \min_{\lambda^{(\sigma)}} \lim_{k\to\infty} (k\sigma)^{-1} \log \left\langle Z_{k\sigma}(\alpha|\chi)\; e^{\Lambda\left(\lambda^{(\sigma)}|\chi\right)} \right\rangle_{\chi} \;\geq\; \bar{\kappa}^{u.b.}(\alpha)$$

  – Consider the grand canonical partition function

$$G^{(\sigma)}\left(z, \alpha, \lambda^{(\sigma)}\right) \;=\; \sum_{k=0}^{\infty} z^{k\sigma} Z_{k\sigma}\left(\alpha|\chi\right) e^{\Lambda\left(\lambda^{(\sigma)}|\chi\right)}$$

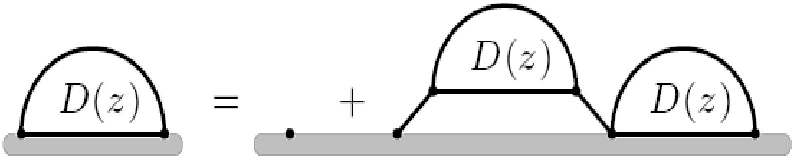
  – with radius of convergence $r_G\left(\alpha, \lambda^{(\sigma)}\right)$.

  – We obtain

$$\bar{\kappa}^{(\sigma)}(\alpha) \;=\; \min_{\lambda^{(\sigma)}} \left\{ -\log r_G\left(\alpha, \lambda^{(\sigma)}\right) \right\}$$

- G_σ in terms of a homopolymer generating function B_σ.
  - B_σ keeps track of the number of segments ω of the path that have the same sequence of surface touches.
  - Obtained via factorization,
    - e.g., d_n: number of n-step Dyck paths.

$$D(z) = \sum_{n\geq 0} d_{2n} z^{2n}$$



$$D(z) = 1 + z^2 D(z)^2 = \frac{1-\sqrt{1-4z^2}}{2z^2}$$

- G_σ in terms of a homopolymer generating function B_σ.
  - B_σ keeps track of the number of segments ω of the path that have the same sequence of surface touches.

- The radii of convergence are related by $r_G\left(\alpha, \lambda^{(\sigma)}\right) = r_B \cdot e^{q^{(\sigma)}\left(\lambda^{(\sigma)}\right)}$
- where
  - $r_B = \min\{|z_1|, |z_2|, \cdots, |z_{1+n_r}|\}$
  - z_1: branch cut from the desorbed phase (square root)
  - the other z_i's are the n_r poles from the adsorbed phase.
  - $\Lambda(\lambda|\chi) = \sum_{C\subseteq[n]} \lambda_C \left[p^{|C|} - \prod_{i\in C} \chi_i\right] = q^{(\sigma)}\left(\lambda^{(\sigma)}\right) - \sum_{C\subseteq[n]} \lambda_C \prod_{i\in C} \chi_i$

Direct Renewal approach

- Consider only colouring constraints on sequences of **non-overlapping** vertices.

$$\underbrace{\chi_1, \chi_2, \cdots, \chi_\sigma}_{1} \cdots \underbrace{\chi_{\sigma(i-1)+1}, \chi_{\sigma(i-1)+2}, \cdots, \chi_{\sigma i}}_{i} \cdots \underbrace{\chi_{\sigma(n-1)+1}, \chi_{\sigma(k-1)+2}, \cdots, \chi_{\sigma k}}_{k}$$

Direct Renewal approach

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$$\underbrace{\chi_1, \chi_2, ..., \chi_\sigma}_{1} \cdots \underbrace{\chi_{\sigma(i-1)+1}, \chi_{\sigma(i-1)+2}, ..., \chi_{\sigma i}}_{i} \cdots \underbrace{\chi_{\sigma(n-1)+1}, \chi_{\sigma(k-1)+2}, ..., \chi_{\sigma k}}_{k}$$

- As an example, consider the case $\sigma = 2$ for Motzkin paths. Then
  - $\lambda^{(2)} = (\lambda_0, ..., \lambda_3)$

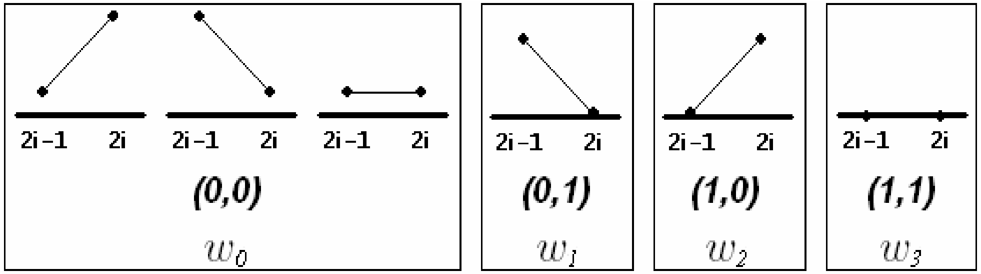
$$\left\langle Z_{2k}\left(\alpha|\chi\right) e^{\Lambda\left(\lambda^{(2)}|\chi\right)} \right\rangle = e^{-2kq^{(2)}(\lambda^{(2)})} \sum_{\omega\in\Omega_{2k}} \prod_{i=1}^{k} \left[p^2 e^{\alpha(\Delta_{2i-1}(\omega)+\Delta_{2i}(\omega))+\lambda_3}\right.$$

$$\left. +p(1-p)e^{\alpha(\Delta_{2i-1}(\omega))+\lambda_2} + (1-p)pe^{\alpha(\Delta_{2i}(\omega))+\lambda_1} + (1-p)^2 e^{\lambda_0}\right]$$

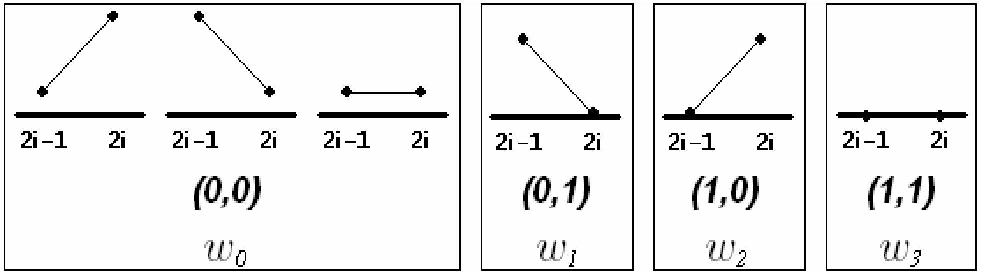
  - $\Delta_i = 1$ if vertex i is at surface.
  - Term in square brackets depends only on sequence

$$(\Delta_{2i-1}(\omega), \Delta_{2i}(\omega))$$

$$(\Delta_{2i-1}(\omega), \Delta_{2i}(\omega))$$



$$(\Delta_{2i-1}(\omega), \Delta_{2i}(\omega))$$



- Then

$$G^{(2)}\left(z, \alpha, \lambda^{(2)}\right) \;=\; B^{(2)}\left(ze^{-q^{(2)}(\lambda^{(2)})}, w_0, \ldots, w_3\right)$$

where

- $$B^{(2)}\left(z, w_0, \ldots, w_3\right) \;=\; \sum_{n\geq 0} z^n \sum_{n_0,\ldots,n_3} b_n(n_0, \ldots, n_3) \prod_{j=0}^{3} w_j^{n_j}$$
- $b_n(n_0, \ldots, n_3)$ is the number of Motzkin paths of length *n* with n_j s he sequence $(\Delta_{2i-1}(\omega), \Delta_{2i}(\omega))$ as the sequence of bits in *j* base *2* .
- $$w_i = p^2 e^{\alpha(s_1+s_0)+\lambda_3} + p(1-p)e^{\alpha s_1+\lambda_2} + (1-p)pe^{\alpha s_0+\lambda_1} + (1-p)^2 e^{\lambda_0}$$

Transfer Matrix approach

- Consider the following colouring constraints:

$$\underbrace{\chi_0, \underbrace{\chi_1, \cdots, \chi_{\sigma-1}}_{1}}, \underbrace{\chi_\sigma, \underbrace{\chi_{\sigma+1}, \cdots, \chi_{2\sigma-1}}_{2}}, \underbrace{\chi_{2\sigma}}, \ldots, \underbrace{\chi_{\sigma(k-1)}, \underbrace{\chi_{\sigma(k-1)+1}, \cdots, \chi_{\sigma k-1}}_{k}}, \chi_{\sigma k}.$$

$$\chi_0, \underbrace{\underbrace{\chi_1, \cdots, \chi_{\sigma-1}}_{1}, \chi_\sigma}, \underbrace{\underbrace{\chi_{\sigma+1}, \cdots, \chi_{2\sigma-1}}_{2}, \chi_{2\sigma}}, \ldots, \underbrace{\chi_{\sigma(k-1)}}, \underbrace{\underbrace{\chi_{\sigma(k-1)+1}, \cdots, \chi_{\sigma k-1}}_{k}, \chi_{\sigma k}}.$$

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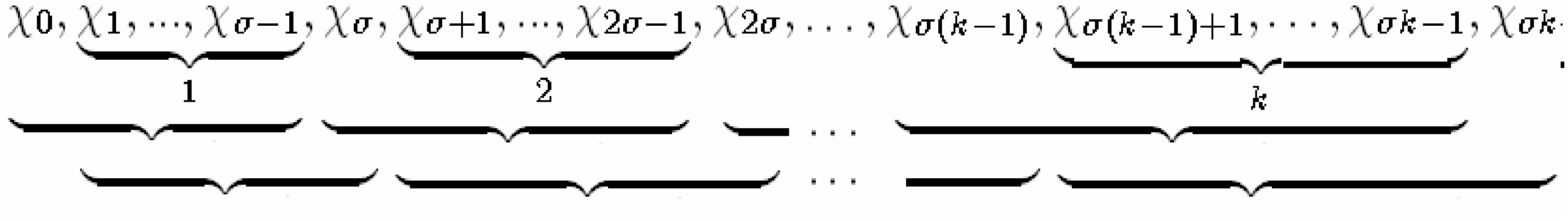


$$\chi_0, \underbrace{\chi_1, \dots, \chi_{\sigma-1}}_{1}, \chi_\sigma, \underbrace{\chi_{\sigma+1}, \dots, \chi_{2\sigma-1}}_{2}, \chi_{2\sigma}, \dots, \chi_{\sigma(k-1)}, \underbrace{\chi_{\sigma(k-1)+1}, \dots, \chi_{\sigma k-1}}_{k}, \chi_{\sigma k}.$$

- As an example, consider $\sigma = 2$ for Motzkin paths. Then
  - $\lambda^{(2)} = (\lambda_0, \dots, \lambda_4)$
  - $\left\langle Z_{2k}\,(\alpha|\chi)\, e^{\Lambda\left(\lambda^{(2)}|\chi\right)} \right\rangle = e^{-2kq^{(2)}(\lambda^{(2)})} \sum_{\omega \in \Omega_{2k}} Q^{(2)}\left(\alpha, \lambda^{(2)}|\omega\right)$

$$Q^{(2)}(\alpha, \lambda^{(2)}|\omega) = \int \left(\prod_{i=1}^{2k} d\chi_i\right) \prod_{i=1}^{k} \prod_{j=0}^{1} \sqrt{w_p(\chi_{2i-2+j})w_p(\chi_{2i-1+j})}$$

$$\times \exp\left[\lambda_{2+N(i,j)} + \frac{\lambda_{1-\chi_{2i-1}} + \chi_{2i-2+j}\Delta_{2i-2+j}(\omega) + \chi_{2i-1+j}\Delta_{2i-1+j}(\omega)}{2}\right]$$

- Need to find a sequence of *2×2* real matrices $T^{(i)}(\alpha, \lambda^{(2)}|\omega)$ such that

$$Q^{(2)}(\alpha, \lambda^{(2)}|\omega) = Tr\left(\prod_{i=1}^{k} T^{(i)}(\alpha, \lambda^{(2)}|\omega)\right)$$

- Using the properties of the trace of a real matrix

$$Q^{(2)}(\alpha, \lambda^{(2)}|\omega) \leq 2\prod_{i=1}^{k}\sqrt{\eta\left(T^{(i)}(\alpha, \lambda^{(2)}|\omega){T^{(i)}}^{t}(\alpha, \lambda^{(2)}|\omega)\right)}$$

where $\eta(\cdot)$ denotes the eigenvalue with largest modulus.

- $T^{(i)}$ only depends on ω through seq. $\Delta^{(i)} = (\Delta_{2i-2}(\omega), \Delta_{2i-1}(\omega), \Delta_{2i}(\omega))$
- Index the *8* possible matrices by the binary string $\Delta^{(i)}$ in base *10*.
- Then, $Q^{(2)}(\alpha, \lambda^{(2)}|\omega) \;\leq\; \prod_{j=0}^{7} \left(\eta(T_j T_j^t)\right)^{n_j(\omega)/2}$
- and $G^{(2)}\left(z, \alpha, \lambda^{(2)}\right) \;\leq\; \hat{B}^{(2)}\left(ze^{-q^{(2)}(\lambda^{(2)})}, w_0, \ldots, w_7\right)$
- with $w_j = \eta(T_j T_j^t)^{1/2}$
- The matrix $T^{(i)}$ is symmetric if $\Delta_{2i-2} = \Delta_{2i}$.

Lower bounds

- We can obtain a lower bound using the fact that

$$Z_{k\sigma}(\alpha|\chi) \geq (Z_\sigma(\alpha|\chi))^k$$

so that

$$\bar{\kappa}(\alpha) \;\geq\; \sigma^{-1} \left\langle \log Z_\sigma(\alpha|\chi) \right\rangle_\chi \;:=\; \bar{\kappa}^{(\sigma)}_{lb.ee}(\alpha)$$

- Another lower bound can be obtained from

$$Z_\sigma(\alpha|\chi) \;\geq\; c_{\sigma,E_{min}} e^{-E_{min}/kT} \;=\; c_\sigma(n_{A,S}|\chi) e^{\alpha n_{A,S}}$$

so that

$$\bar{\kappa}(\alpha) \;\geq\; \alpha\sigma^{-1} \left\langle n_{A,S} \right\rangle + \sigma^{-1} \left\langle \log c_\sigma(n_{A,S}|\chi) \right\rangle \;:=\; \bar{\kappa}^{(\sigma)}_{lb.me}(\alpha)$$

Monte Carlo

- Quenched average free energy:

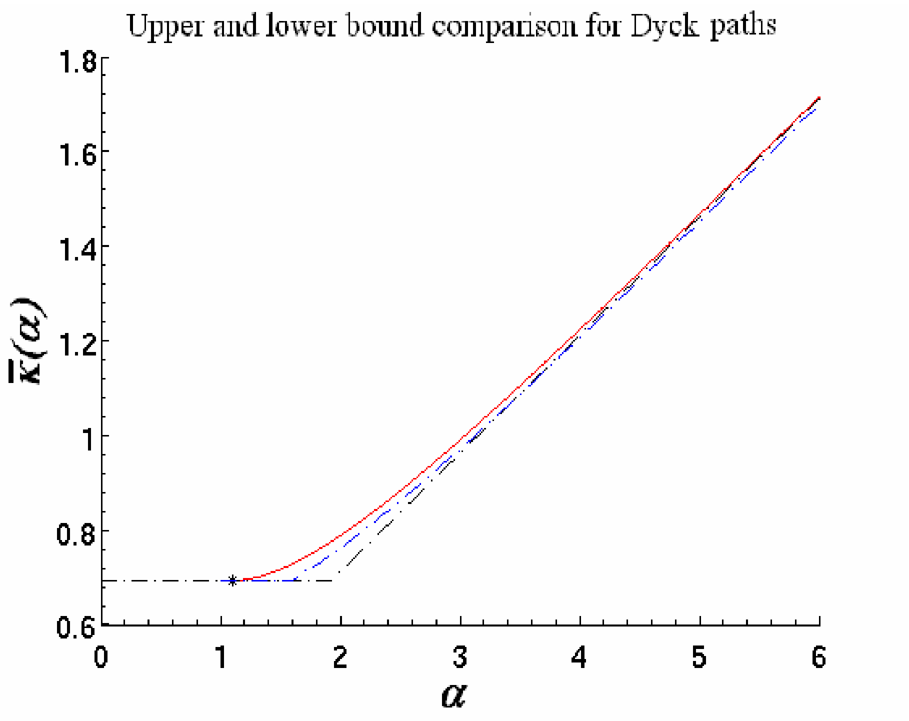
$$\bar{\kappa}_n^q(\alpha) = \langle n^{-1} \log Z_n(\alpha|\chi) \rangle_\chi$$

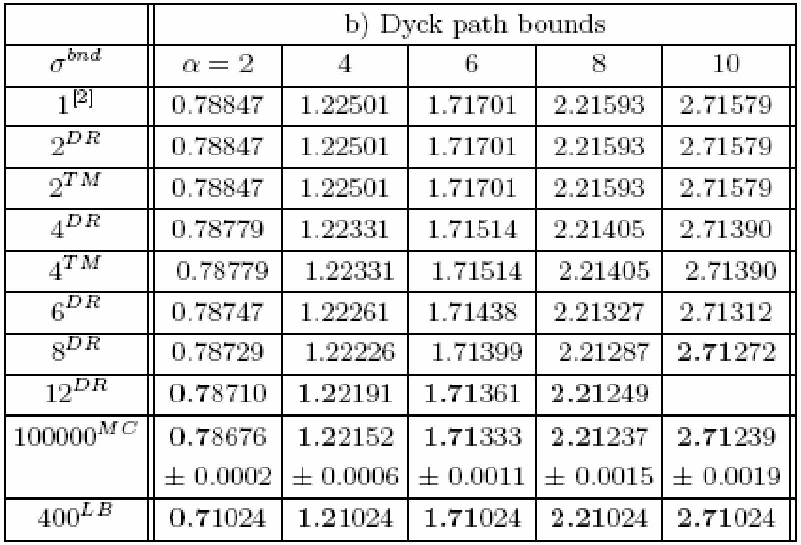
- Limiting quenched average free energy:

$$\bar{\kappa}(\alpha) = \lim_{n\to\infty} \bar{\kappa}_n^q(\alpha)$$

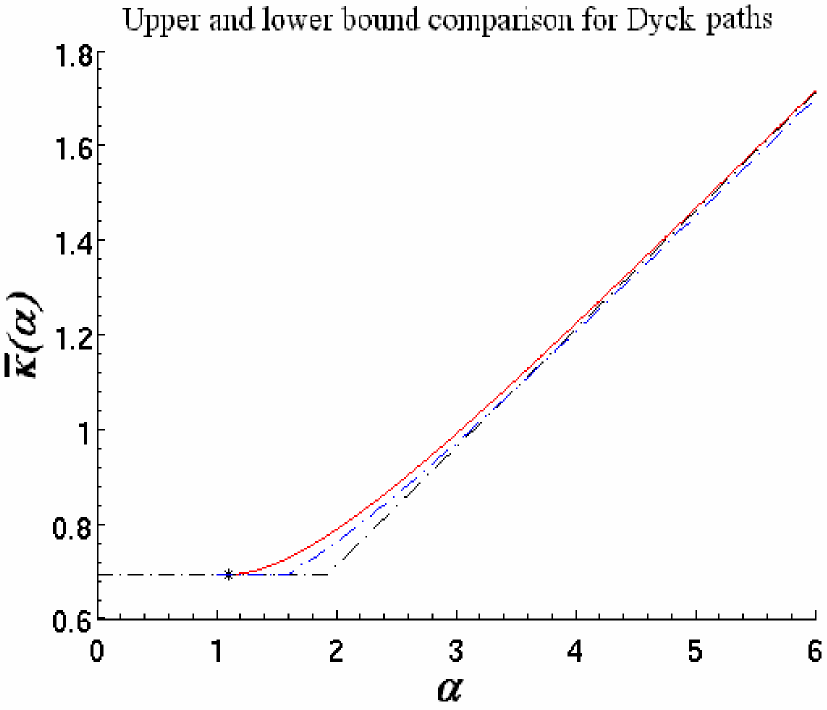
- Fir fixed n, average over a random set of colors

Q: What is $\bar{\kappa}(\alpha)$ for $\alpha > \alpha_q$?

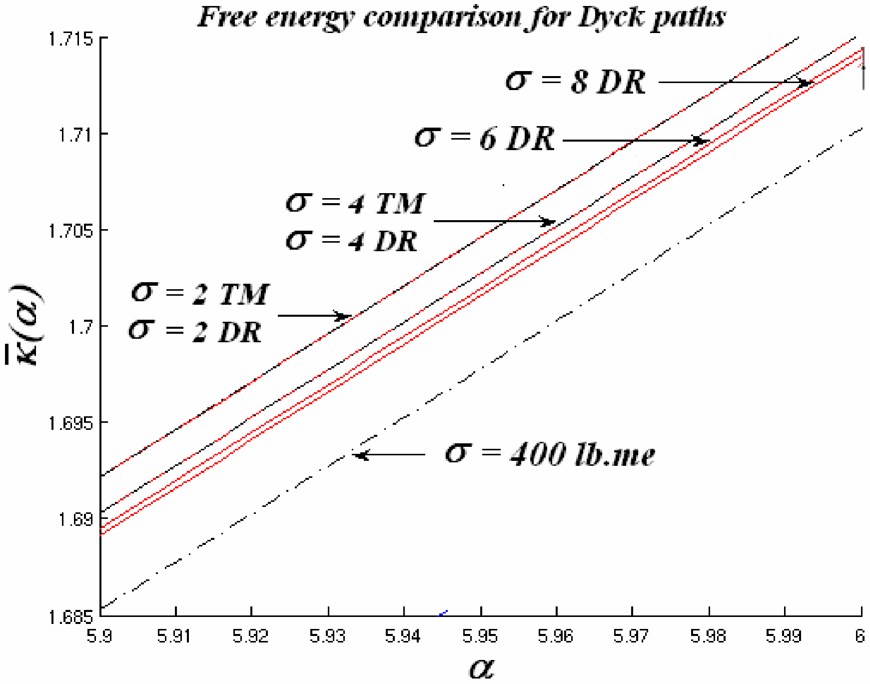

Upper and lower bound comparison for Dyck paths



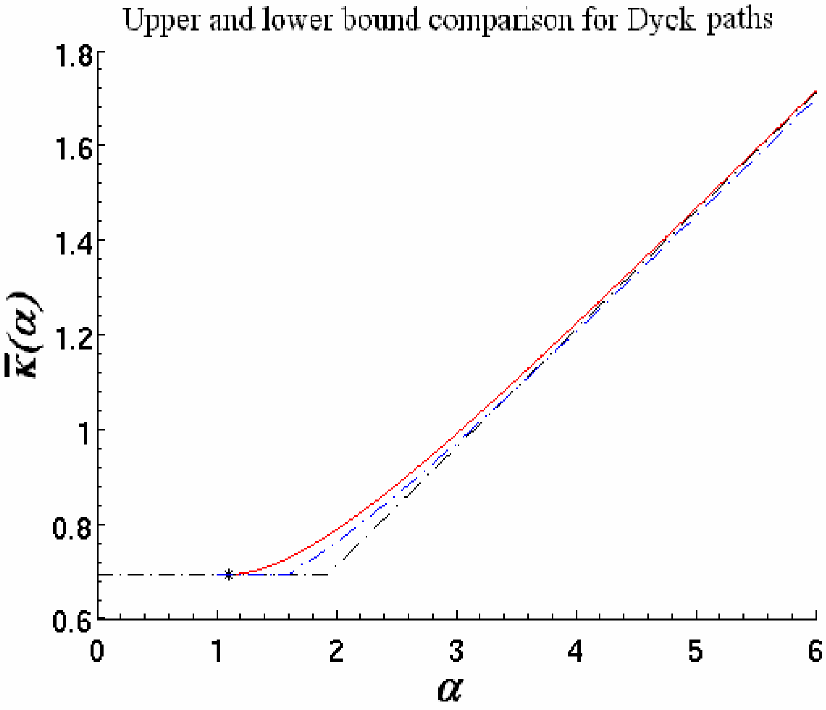
	b) Dyck path bounds				
σ^{bnd}	$\alpha = 2$	4	6	8	10
$1^{[2]}$	0.78847	1.22501	1.71701	2.21593	2.71579
2^{DR}	0.78847	1.22501	1.71701	2.21593	2.71579
2^{TM}	0.78847	1.22501	1.71701	2.21593	2.71579
4^{DR}	0.78779	1.22331	1.71514	2.21405	2.71390
4^{TM}	0.78779	1.22331	1.71514	2.21405	2.71390
6^{DR}	0.78747	1.22261	1.71438	2.21327	2.71312
8^{DR}	0.78729	1.22226	1.71399	2.21287	**2.71272**
12^{DR}	**0.78710**	**1.22191**	**1.71361**	**2.21249**	
100000^{MC}	**0.78676** ± 0.0002	**1.22152** ± 0.0006	**1.71333** ± 0.0011	**2.21237** ± 0.0015	**2.71239** ± 0.0019
400^{LB}	**0.71024**	**1.21024**	**1.71024**	**2.21024**	**2.71024**

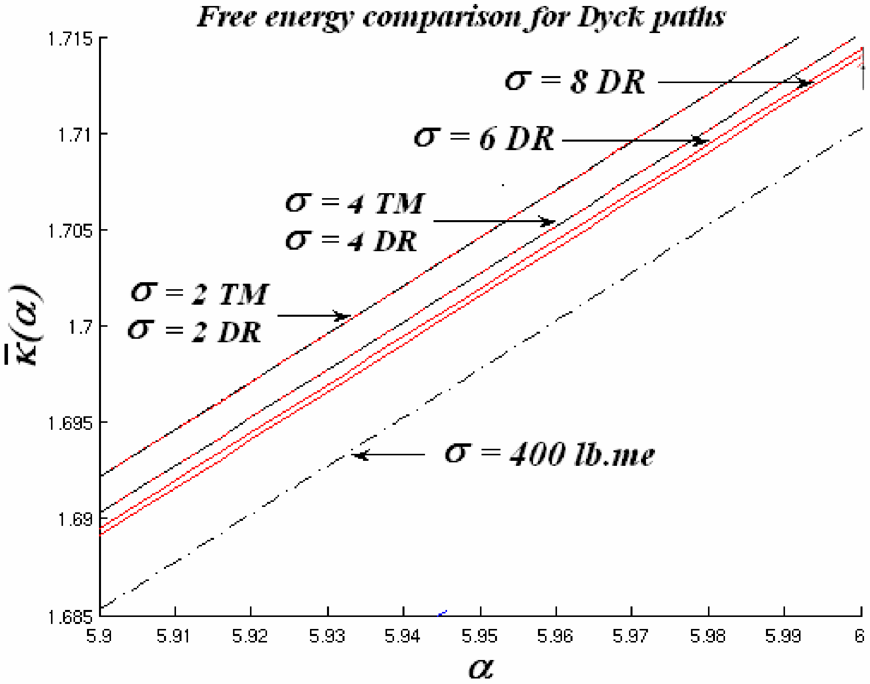


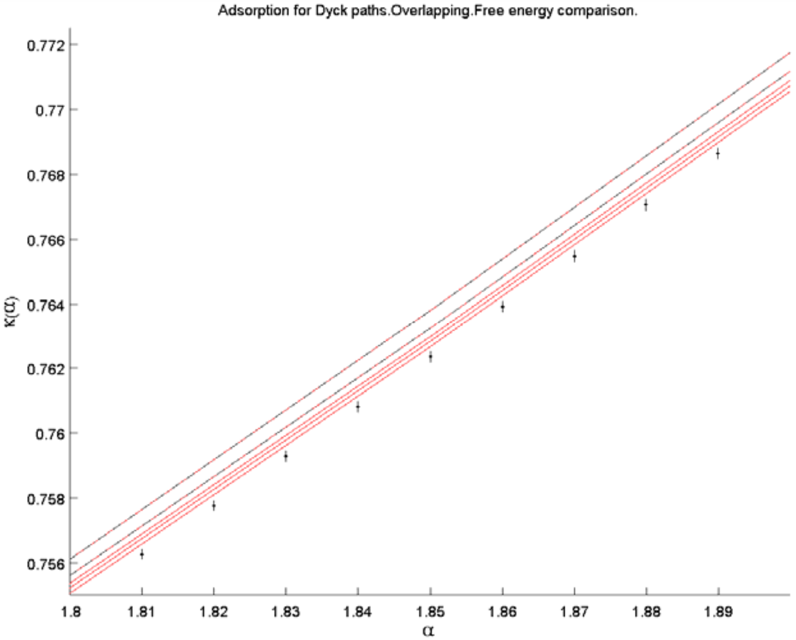
Upper and lower bound comparison for Dyck paths

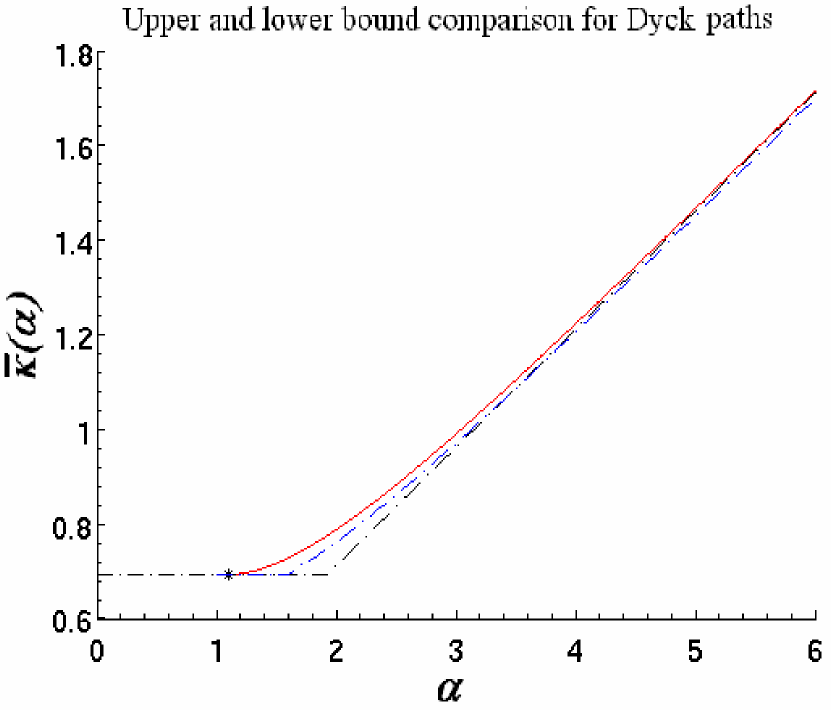


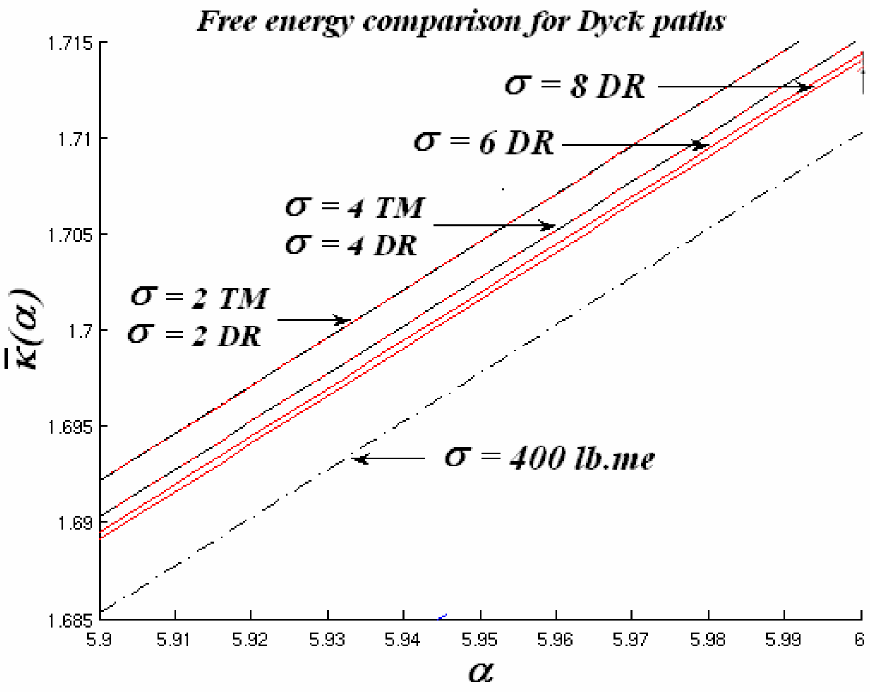
Free energy comparison for Dyck paths

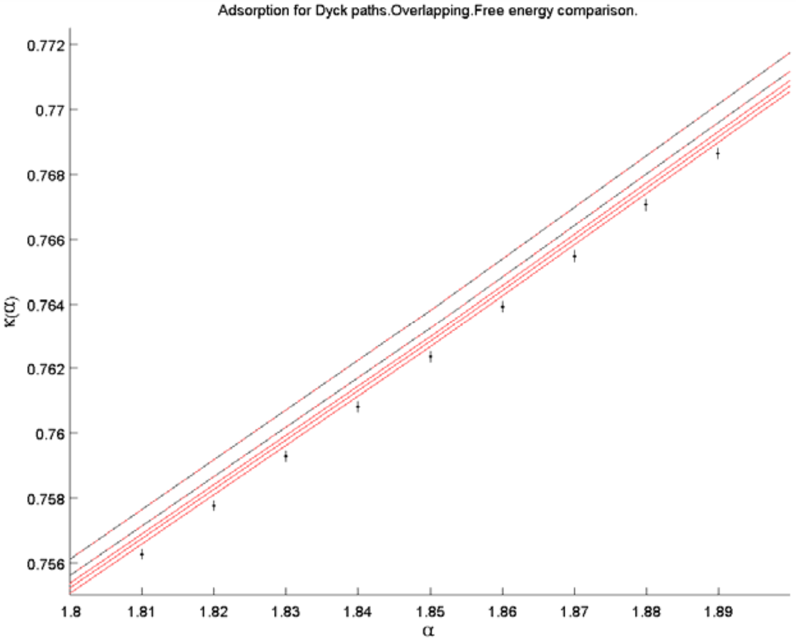

Upper and lower bound comparison for Dyck paths
$\overline{\kappa}(\alpha)$
1.8
1.6
1.4
1.2
1
0.8
0.6
0
1
2
3
4
5
6
α

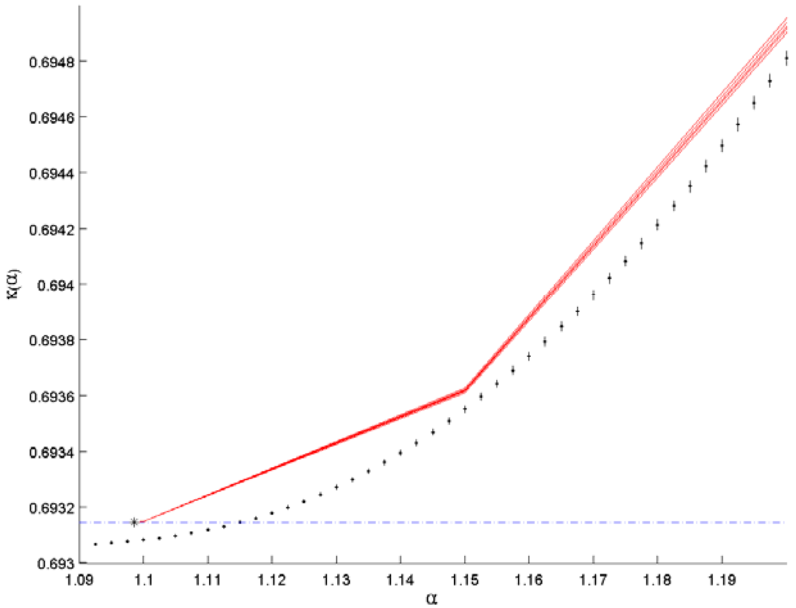

Free energy comparison for Dyck paths
$\overline{\kappa}(\alpha)$
1.715
1.71
1.705
1.7
1.695
1.69
1.685
5.9
5.91
5.92
5.93
5.94
5.95
5.96
5.97
5.98
5.99
6
α
σ = 8 DR
σ = 6 DR
σ = 4 TM
σ = 4 DR
σ = 2 TM
σ = 2 DR
σ = 400 lb.me

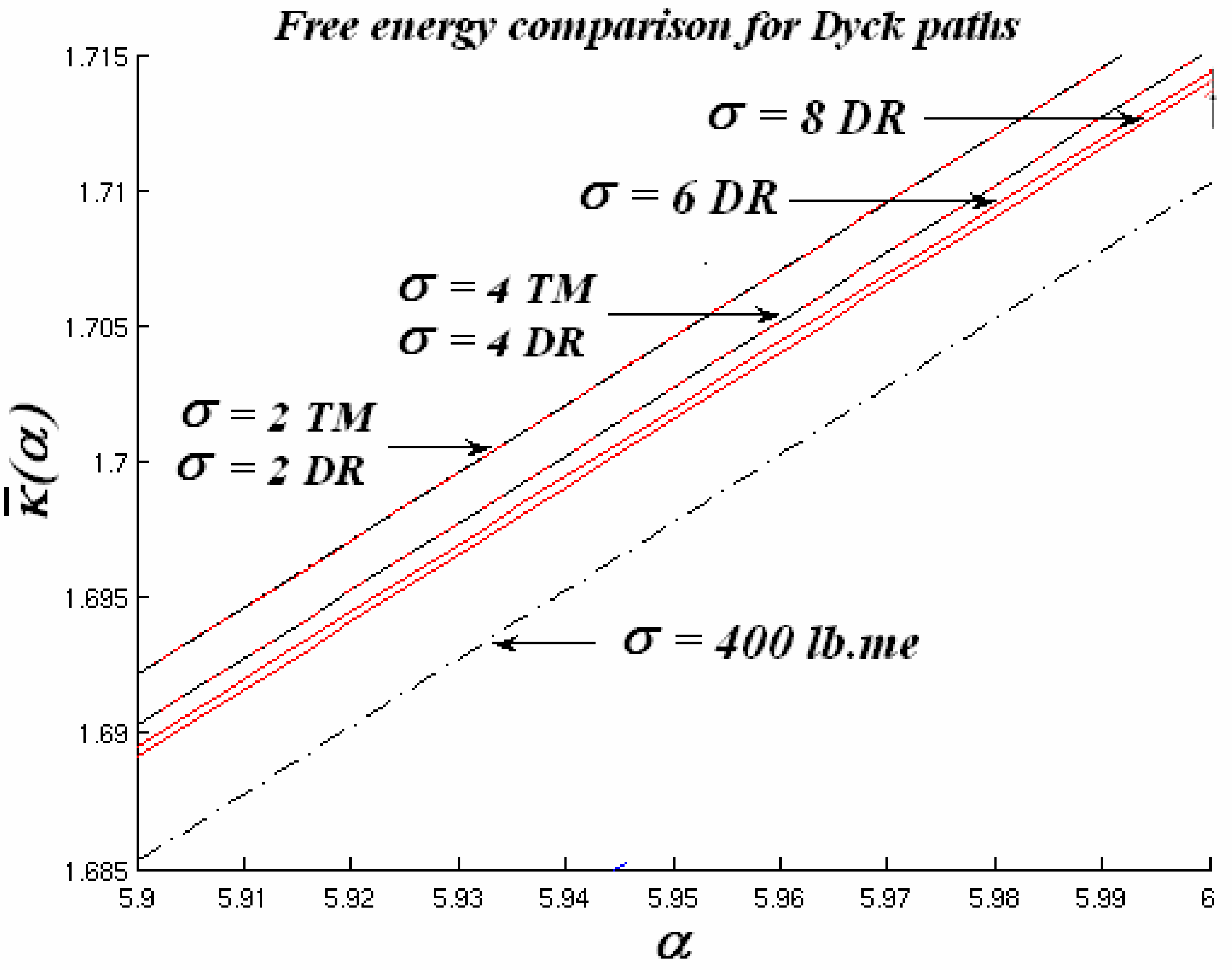

Adsorption for Dyck paths.Overlapping.Free energy comparison.
$\kappa(\alpha)$
0.772
0.77
0.768
0.766
0.764
0.762
0.76
0.758
0.756
1.8
1.81
1.82
1.83
1.84
1.85
1.86
1.87
1.88
1.89
α


Upper and lower bound comparison for Dyck paths


Free energy comparison for Dyck paths

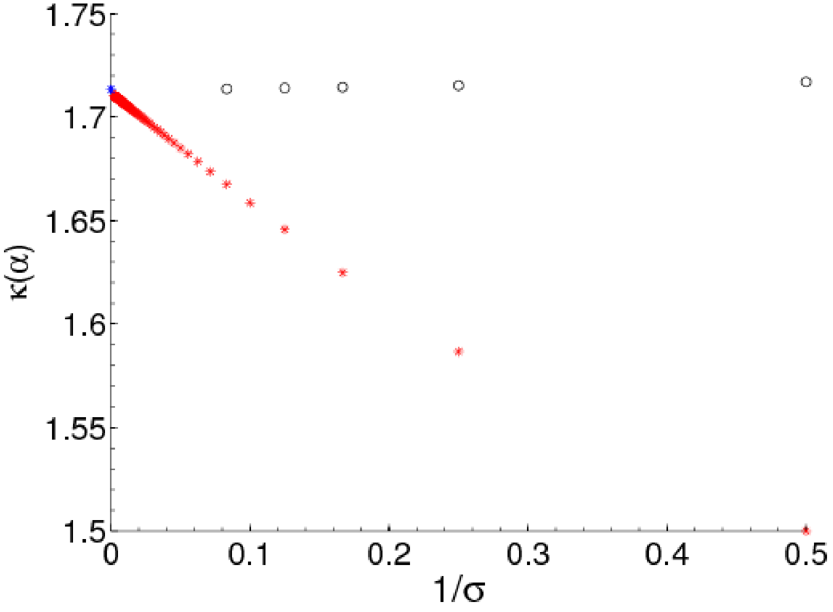

Adsorption for Dyck paths.Overlapping.Free energy comparison.



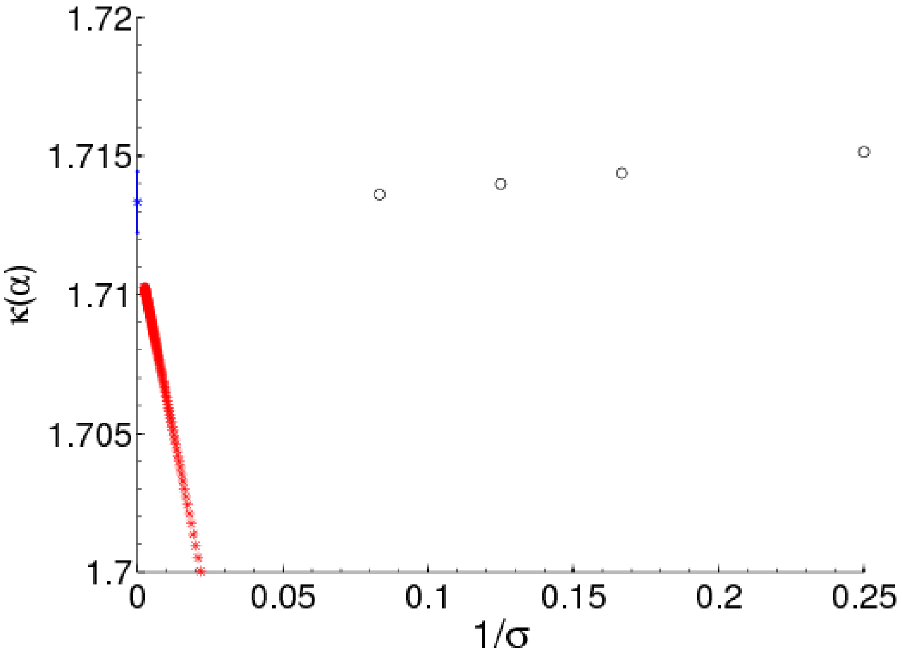


Free energy comparison for Dyck paths
$\bar{\kappa}(\alpha)$
α
1.715
1.71
1.705
1.7
1.695
1.69
1.685
5.9
5.91
5.92
5.93
5.94
5.95
5.96
5.97
5.98
5.99
6
σ = 8 DR
σ = 6 DR
σ = 4 TM
σ = 4 DR
σ = 2 TM
σ = 2 DR
σ = 400 lb.me

$\alpha = 6$

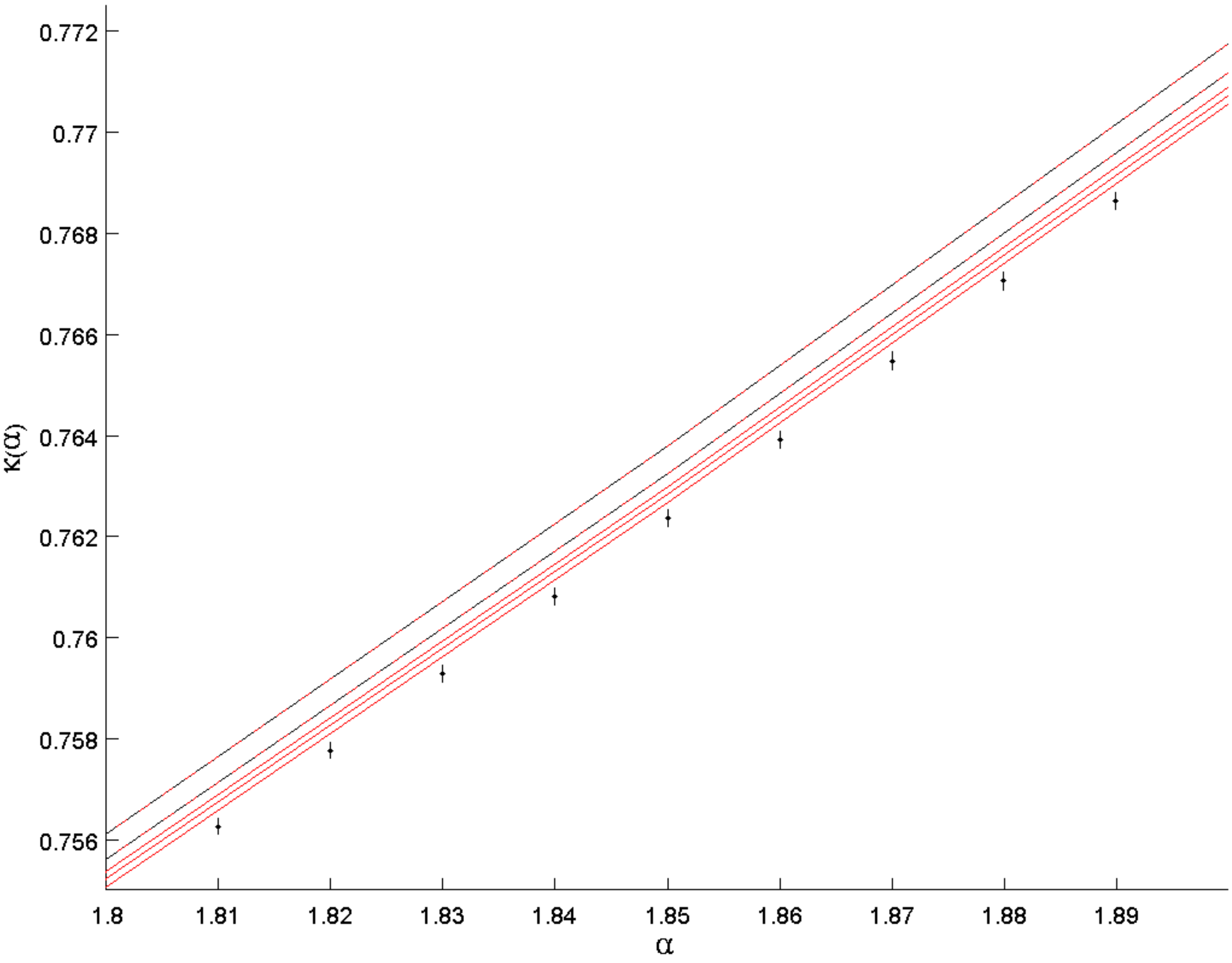


κ(α)
1.75
1.7
1.65
1.6
1.55
1.5
0
0.1
0.2
0.3
0.4
0.5
1/σ

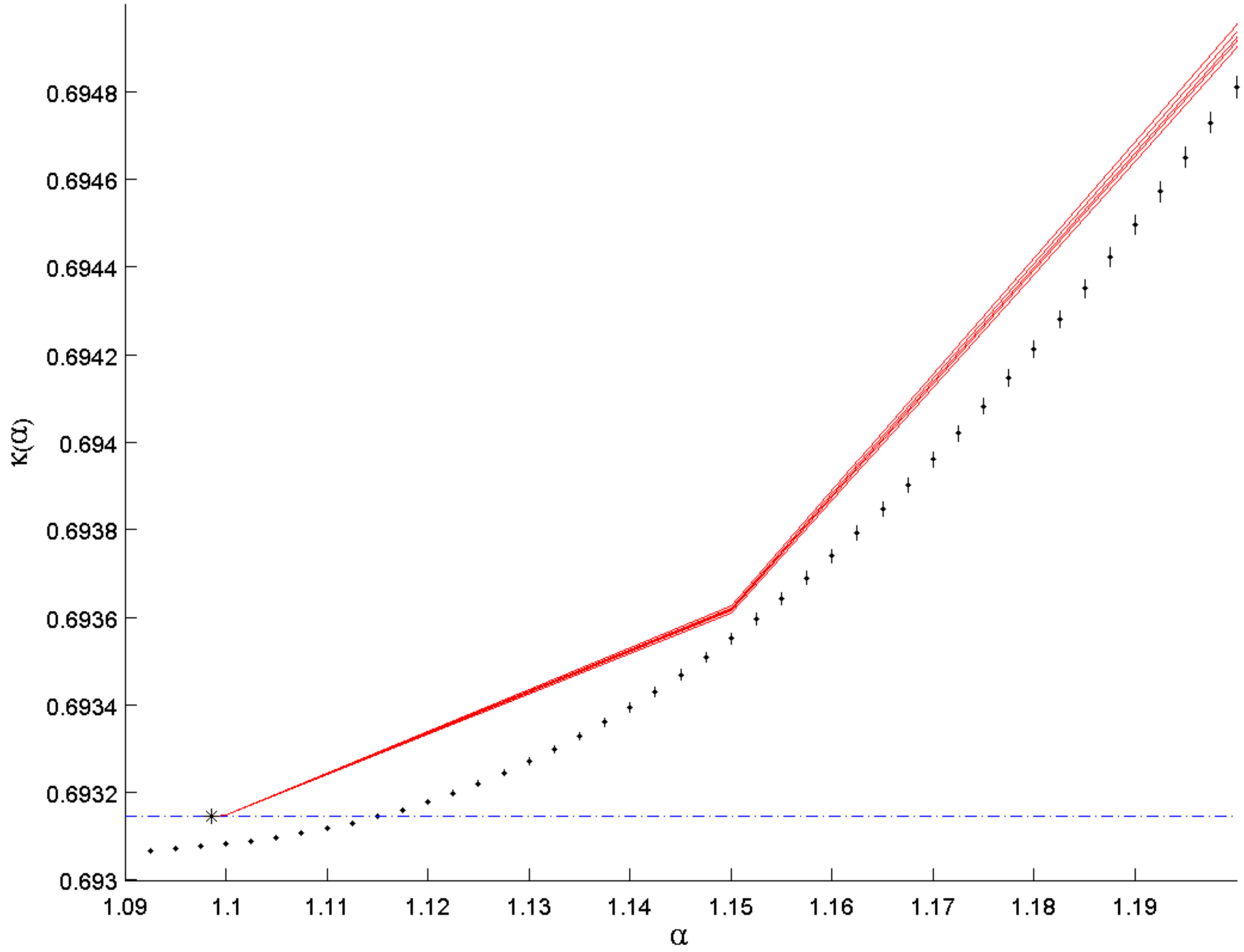


κ(α)
1.72
1.715
1.71
1.705
1.7
0
0.05
0.1
0.15
0.2
0.25
1/σ

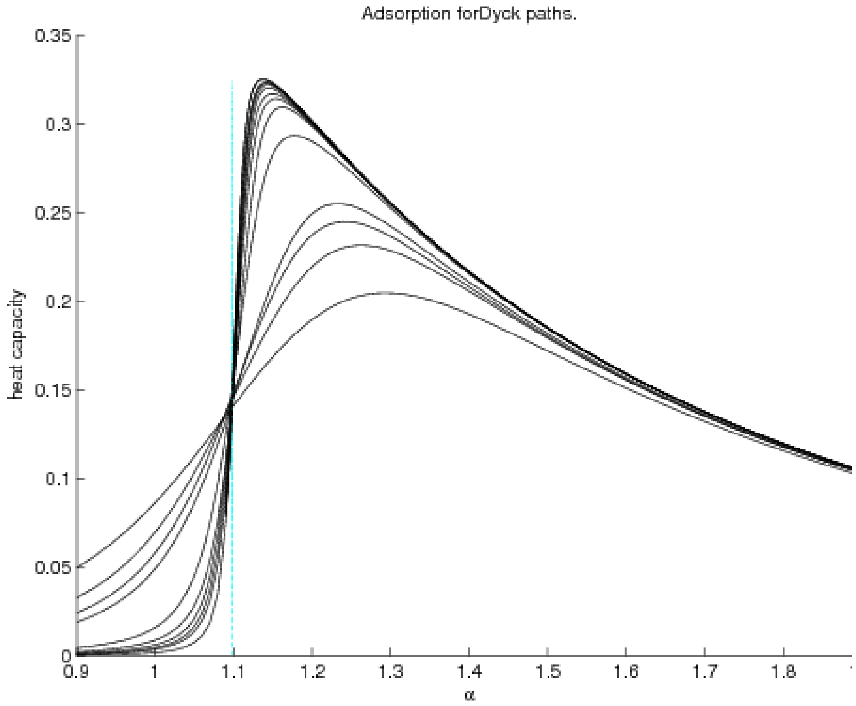
Adsorption for Dyck paths.Overlapping.Free energy comparison.

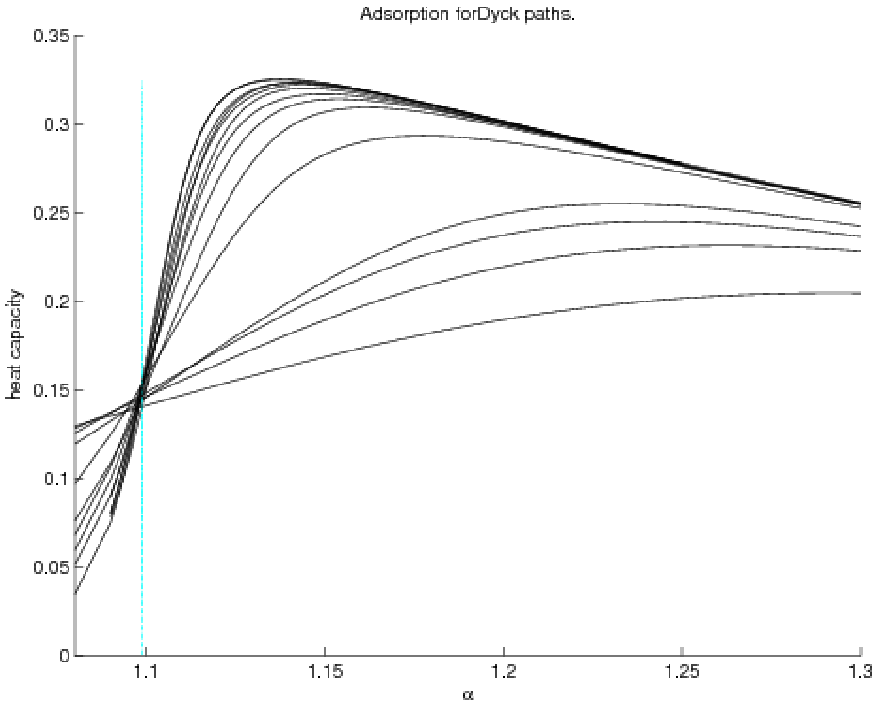


Adsorption for Dyck paths.Non-overlapping.Free energy comparison.



Heat capacity

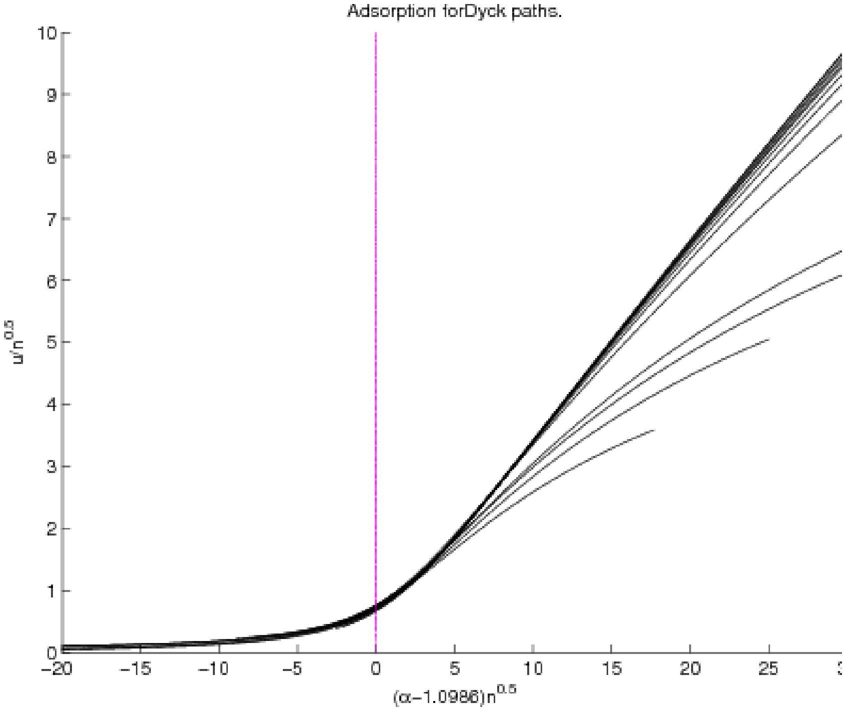


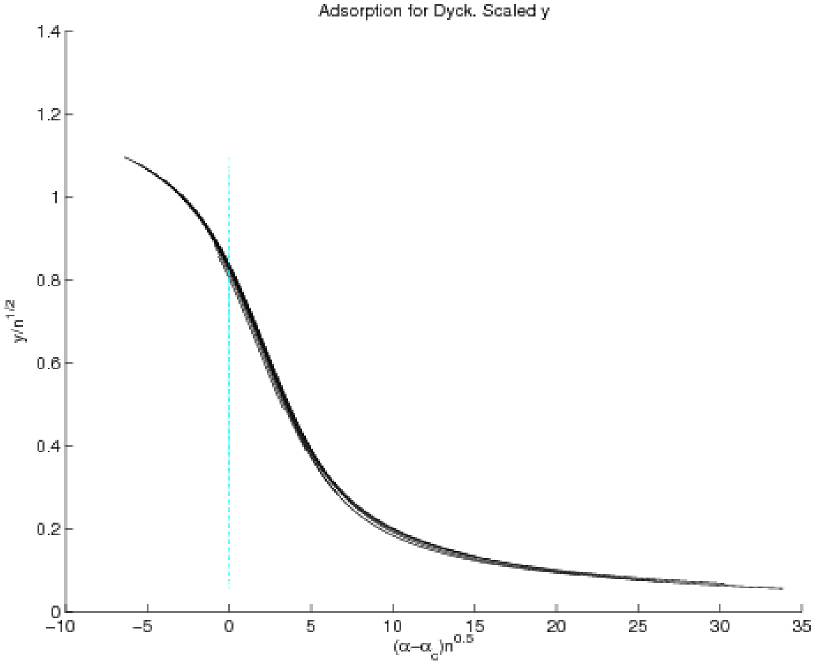


Scaling

$$\langle n_{A,S} \rangle \sim n^{\phi} f_1\left(\left(\alpha - \alpha_c\right) n^{\phi}\right)$$

$$y_{end} \sim n^{1/2} f_2\left(\left(\alpha - \alpha_c\right) n^{\phi}\right)$$





$$\phi = 0.5 \qquad \alpha_c = \log(3)$$

Thanks.

Direct Renewal approach

- Consider only colouring constraints on sequences of **non-overlapping** vertices.

$$\underbrace{\chi_1, \chi_2, ..., \chi_\sigma}_{1} \cdots \underbrace{\chi_{\sigma(i-1)+1}, \chi_{\sigma(i-1)+2}, ..., \chi_{\sigma i}}_{i} \cdots \underbrace{\chi_{\sigma(n-1)+1}, \chi_{\sigma(k-1)+2}, ..., \chi_{\sigma k}}_{k}$$

- As an example, consider the case $\sigma = 2$ for Motzkin paths. Then
  - $\lambda^{(2)} = (\lambda_0, ..., \lambda_3)$

$$\left\langle Z_{2k}\left(\alpha|\chi\right) e^{\Lambda\left(\lambda^{(2)}|\chi\right)}\right\rangle = e^{-2kq^{(2)}(\lambda^{(2)})} \sum_{\omega\in\Omega_{2k}} \prod_{i=1}^{k} \Big[p^2 e^{\alpha(\Delta_{2i-1}(\omega)+\Delta_{2i}(\omega))+\lambda_3}$$

$$+p(1-p)e^{\alpha(\Delta_{2i-1}(\omega))+\lambda_2} + (1-p)pe^{\alpha(\Delta_{2i}(\omega))+\lambda_1} + (1-p)^2 e^{\lambda_0}\Big]$$

  - $q^{(2)}\left(\lambda^{(2)}\right) = \frac{1}{2}\left(\lambda_3 p^2 + \lambda_2 p(1-p) + \lambda_1(1-p)p + \lambda_0(1-p)^2\right)$
  - $\Delta_i = 1$ if vertex i is at surface.
  - Term in square brackets depends only on sequence

$$(\Delta_{2i-1}(\omega), \Delta_{2i}(\omega))$$

Transfer Matrix approach

- Consider the following colouring constraints:

$$\underbrace{\chi_0, \underbrace{\chi_1, \dots, \chi_{\sigma-1}}_{1}}, \underbrace{\chi_\sigma, \underbrace{\chi_{\sigma+1}, \dots, \chi_{2\sigma-1}}_{2}}, \chi_{2\sigma}, \dots, \underbrace{\chi_{\sigma(k-1)}, \underbrace{\chi_{\sigma(k-1)+1}, \dots, \chi_{\sigma k-1}}_{k}}, \chi_{\sigma k}.$$

- As an example, consider $\sigma = 2$ for Motzkin paths. Then
  - $\lambda^{(2)} = (\lambda_0, ..., \lambda_4)$
  - $\left\langle Z_{2k}(\alpha|\chi)\, e^{\Lambda\left(\lambda^{(2)}|\chi\right)} \right\rangle = e^{-2kq^{(2)}(\lambda^{(2)})} \sum_{\omega \in \Omega_{2k}} Q^{(2)}\left(\alpha, \lambda^{(2)}|\omega\right)$
  - $q^{(2)}\left(\lambda^{(2)}\right) = \frac{\lambda_0}{2}p + \frac{\lambda_1}{2}(1-p) + \lambda_2 p^2 + 2\lambda_3 p(1-p) + \lambda_4(1-p)^2$

$$Q^{(2)}(\alpha, \lambda^{(2)}|\omega) = \int \left(\prod_{i=1}^{2k} d\chi_i\right) \prod_{i=1}^{k} \prod_{j=0}^{1} \sqrt{w_p(\chi_{2i-2+j})w_p(\chi_{2i-1+j})}$$

$$\times \exp\left[\lambda_{2+N(i,j)} + \frac{\lambda_{1-\chi_{2i-1}} + \chi_{2i-2+j}\Delta_{2i-2+j}(\omega) + \chi_{2i-1+j}\Delta_{2i-1+j}(\omega)}{2}\right]$$

- Need to find a sequence of *2×2* real matrices $T^{(i)}(\alpha, \lambda^{(2)}|\omega)$ such that

$$Q^{(2)}(\alpha, \lambda^{(2)}|\omega) = Tr\left(\prod_{i=1}^{k} T^{(i)}(\alpha, \lambda^{(2)}|\omega)\right)$$

- Using the properties of the trace of a real matrix

$$Q^{(2)}(\alpha, \lambda^{(2)}|\omega) \leq 2\prod_{i=1}^{k}\sqrt{\eta\left(T^{(i)}(\alpha, \lambda^{(2)}|\omega){T^{(i)}}^{t}(\alpha, \lambda^{(2)}|\omega)\right)}$$

  where $\eta(\cdot)$ denotes the eigenvalue with largest modulus.

- Let $T^{(i)}(\alpha, \lambda|\omega) = T^{(i,0)}(\alpha, \lambda^{(2)}|\omega)T^{(i,1)}(\alpha, \lambda^{(2)}|\omega)$ where

$$T^{(i,j)}(\alpha, \lambda^{(2)}|\omega) =$$

$$\begin{pmatrix} (1-p)e^{\lambda_2+\frac{\lambda_1}{2}} & \sqrt{(1-p)p}e^{\frac{\alpha\Delta_{2i-1+j}(\omega)}{2}+\lambda_3+\frac{\lambda_j}{2}} \\ \sqrt{(1-p)p}e^{\frac{\alpha\Delta_{2i-2+j}(\omega)}{2}+\lambda_3+\frac{\lambda_{1-j}}{2}} & pe^{\frac{\alpha\Delta_{2i-2+j}(\omega)}{2}+\frac{\alpha\Delta_{2i-1+j}(\omega)}{2}+\lambda_4+\frac{\lambda_0}{2}} \end{pmatrix}$$