Bounded Discrete Walks

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Tortoiseshell cats - Chats Isabelle



The patchy colours of a tortoiseshell cat are the result of different levels of expression of pigmentation genes in different areas of the skin.

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DNA micro-array and diagnostic in genetics?



measuring fluorescence of a spot provides the level of expression of the corresponding gene.

• $\Gamma :=$ set of genes of a background population $(|\Gamma| = G)$

•
$$\gamma :=$$
 set of genes of a particular family $(|\gamma| = g)$

Question. Are the levels of expression of the genes of γ with respect to the level of expressions of the genes of Γ characteristic of an exceptional behaviour? (Disease, *etc*)

Random walks model

• Keller, Backes and Lenhof (2007) Order the genes by level of expression.

Build a walk $(B_i)_{0 \le i \le G+g}$ such that $B_0 = 0$ and

$$B_i = \begin{cases} +G & \text{if the gene at rank } i \text{ belongs to } \gamma, \\ -g & \text{if the gene at rank } i \text{ belongs to } \Gamma \end{cases}$$

These walks are therefore bridges as $B_{G+g} = Gg - gG = 0$.

exceptional overexpression of the genes of $\gamma \implies$ **exceptional height** of the bridge with respect to the height of a bridge chosen at random among the $\binom{G+g}{g}$ possible bridges.

Example

$$G = 6, \quad g = 3$$

represent by
$$\begin{cases} \circ & \text{genes of } \Gamma \\ \bullet & \text{genes of } \gamma \end{cases}$$



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$$\rightsquigarrow X_j = +2 \quad (+6/3)$$

• $\rightsquigarrow X_j = -1 \quad (-3/3)$



$$\underline{B_i} = \sum_{1 \le j \le i} X_j$$

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Tail distribution for the height - Keller et al.

Keller, Backes and Lenhof (2007) compute

$$p$$
-value $(G, g, h) := \mathbf{P}\left(\max_{0 \le i \le G+g} B_i > h\right)$

by a dynamical programming method in complexity

 $O(G \times g)$

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Our result: heuristics in **complexity** O(1)

Brownian motion as limit of discrete walks



Strong approximations of discrete walks by Brownian motion

Komlós, Major, Tusnády (1976), Chatterjee (2010)

$$\mathbf{P}\left\{\max_{1\leq k\leq n}|S_k - W(k)| > C\log n + x\right\} < Ke^{-\lambda x} \quad (W(k) \text{ Wiener process})$$

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Little done for approximations of bridges

Kaigh (1976)



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Caveat: This nice reflexion trick won't work in the discrete case if the walk has a drift or its jumps are other than +1, 0, -1. Another approach is needed then! (=our work).



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bridge length n = G + g = 104 G = +93 -g = -11

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 10^8 simulations



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 $\sigma = \sqrt{G \times g}$ 10⁸ simulations



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Summary of the talk

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- Model
- Generating functions for bounded walks
- Asymptotic limit law for bridges
- Łukasiewicz bridges
- Back to simulations

Directed discrete walks

Model = generalized Dyck walks

= discrete "excursions/bridges/meanders"

- Knuth (1973)
- Gessel (1980)
- Labelle & Yeah (1990), Merlini & al. (1996), Duchon (2000)

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- Banderier and Flajolet (2002)
- Bousquet-Mélou (2009)
- Bousquet-Mélou and Ponty (2009)

Model

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- ▶ i.i.d. integer jumps $X_i \in \{-c, \ldots, +d\}$
- characteristic polynomial $P(u) = p_{-c}u^{-c} + \dots + p_du^d$
- $\blacktriangleright \mathbf{E}(X_i) = P'(1) = 0$

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Typical generating function

$$F(z,u) = \sum_{n=0}^{\infty} f_n(u) z^n = \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} f_{n,k} u^k z^n$$

where

f_{n,k} is the probability that a walk remaining in an horizontal strip (by instance] −∞, +h]) has altitude *k* at time *n*.
 [*zⁿ*][*u*⁰]*F*(*z, u*) corresponds to bridges of length *n*

Getting the generating function $X_i \in \{-1, +2\}$ $P(u) = u^2 + \frac{1}{u}$ h

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Getting the generating function



Getting the generating function $X_i \in \{-1, +2\}$ $P(u) = u^2 + \frac{1}{u}$ $f_0(u) = 1$

$$f_{k+1}(u) = f_k(u) \times P(u) - \begin{cases} u^{h+1}[u^{h+1}]f_k(u) \times P(u) \\ + u^{h+2}[u^{h+2}]f_k(u) \times P(u) \end{cases}$$

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$$\sum_{k=0}^{\infty} f_{k+1}(u) z^{k+1} = F(z, u) - f_0(u)$$
$$= zP(u) \sum_{k=0}^{\infty} f_k(u) z^k - \begin{cases} z u^{h+1} F_{h+1}(z) \\ + z u^{h+2} F_{h+2}(z) \end{cases}$$

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 $F(z,u)(1-zP(u)) = 1 - zu^{h+1}F_{h+1}(z) - zu^{h+2}F_{h+2}(z)$

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Kernel method

Knuth, Tutte, Brown, Bousquet-Mélou, Petkovšek, etc.

$$X_i \in \{-1, +2\}$$
 $P(u) = \frac{1}{u} + u^2$

$$F(z,u)(1-zP(u)) = 1 - zu^{h+1}F_{h+1}(z) - zu^{h+2}F_{h+2}(z)$$

 $F(z, u), F_{h+1}(z), F_{h+2}(z)$ unknown functions

but the roots u(z) of 1 - zP(u) = 0 cancel the left member of the equation

two roots u(z) provide a linear system of two equations whose solutions are $F_{h+1}(z)$ and $F_{h+2}(z)$

General case - Any finite set of integer jumps

$$P(u) = p_{-c}u^{-c} + p_{-c+1}u^{-c+1} + \dots + p_{d-1}u^{d-1} + p_d u^d$$
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d unknown functions $F_{h+j}(z)$, but the equation 1 - zP(u) = 0 has

 $\begin{cases} d \text{ large roots } v_i(z) & \text{ such that } v_i(z) \sim \frac{1}{z}^{1/d} & \text{ as } z \to 0\\ c \text{ small roots } u_j(z) & \text{ such that } u_j(z) \sim z^{1/c} & \text{ as } z \to 0 \end{cases}$

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Vandermonde determinants $\mathbb{V}(...)$, Schur functions, occurring also when considering the area (Banderier-Gittenberger)

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$$F(z,u)(1-zP(u))$$

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$$= 1 - \sum_{j=1}^{d} \frac{\operatorname{Subs}(v_j = u, \mathbb{V}(v_1, \dots, v_d))}{v_1^h \dots v_d^h \mathbb{V}(v_1, \dots, v_d)}$$
$$= 1 - \sum_{j=1}^{d} \frac{\operatorname{Subs}\left(v_j = u, \begin{vmatrix} \dots & \dots & \dots & \dots & \dots \\ v_j^{h+d} & \dots & v_j^{h+j} & \dots & v_j^{h+1} \\ \dots & \dots & \dots & \dots & \dots \\ v_1^h \dots v_d^h \mathbb{V}(v_1, \dots, v_d) \end{vmatrix}\right)}{v_1^h \dots v_d^h \mathbb{V}(v_1, \dots, v_d)}$$

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$$=1-\sum_{j=1}^{u}\frac{u^{h+1}}{v_{j}^{h+1}}\prod_{\substack{1\leq i\leq d\\i\neq j}}\frac{u-v_{i}}{v_{j}-v_{i}}$$

Nice expression for the generating functions

$$F^{]-\infty,h]}(z,u) = \frac{1}{1-zP(u)} - \frac{1}{1-zP(u)} \sum_{j=1}^{d} \frac{u^{h+1}}{v_j^{h+1}} \prod_{\substack{1 \le i \le d \\ i \ne j}} \frac{u-v_i}{v_j-v_i}$$

N.B.:
$$\frac{1}{1-zP(u)}$$
 counts all the walks.

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Theorem (Banderier-N. 2010) Walks going beyond the barrier +h verify $F^{[>h]}(z,u) = \frac{1}{1-zP(u)} \sum_{j=1}^{d} \frac{u^{h+1}}{v_j(z)^{h+1}} \prod_{\substack{1 \le i \le d \\ i \ne j}} \frac{u-v_i}{v_j-v_i}$

Gives fast computation scheme for the n-th coefficients via holonomy theory.

Roots properties (Banderier-Flajolet)



Left: behaviour of the characteristic polynomial $P(u) = u^3 + \frac{1}{u}$. Right: domination property of the roots of $1 - zP(u) = 1 - z(u^3 + \frac{1}{u})$ in $]0, \rho]$, where τ is the unique positive solution of P'(z) = 0 and $\rho = 1/P(\tau)$. $P'(\tau) = 0 \implies u_1(\rho) = v_1(\rho)$. $u_1(z) < v_1(z) < |v_2(z)| = |v_3(z)|$ for $z \in]0, \rho[$.

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Roots properties (Banderier-Flajolet)

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Roots properties (Banderier-Flajolet)



Asymptotics simplifications for $F^{[>h]}$ as $h\longrightarrow\infty$

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$$\frac{u^{h+1}}{v_j(z)^{h+1}} = \frac{u^{h+1}}{v_1(z)^{h+1}} \left(\frac{v_1(z)}{v_j(z)}\right)^{h+1} = O(A^h) \quad \longrightarrow \quad \\ \left(j \ge 2, \quad A = \max_{j \ge 2} \sup_{|z| < \rho - \epsilon} \frac{|v_1(z)|}{|v_j(z)|} < 1\right)$$

Asymptotics simplifications for $F^{[>h]}$ as $h \longrightarrow \infty$

$$\implies F^{[>h]}(z,u) = \frac{1}{1-zP(u)} \sum_{j=1}^{d} \frac{u^{h+1}}{v_j(z)^{h+1}} \prod_{\substack{1 \le i \le d \\ i \ne j}} \frac{u-v_i}{v_j-v_i}$$
$$= \frac{1}{1-zP(u)} \frac{u^{h+1}}{v_1(z)^{h+1}} \frac{Q(u)}{Q(v_1(z))} \left(1+O(A^h)\right)$$

where
$$Q(x) = \prod_{2 \le i \le d} (x - v_i(z))$$

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Asymptotics simplifications for $[u^0]F^{[>h]}$ (bridges)

Thm. Banderier-Flajolet

$$(-k < -c)$$
 $[u^{-k}] \frac{1}{1 - zP(u)} = z \sum_{j=1}^{c} \frac{u'_j(z)}{u_j(z)^{-k+1}}$

Asymptotics simplifications for $[u^0]F^{[>h]}$ (bridges)

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Asymptotics simplifications for $[u^0]F^{[>h]}$ (bridges)

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$$(-k < -c) \qquad [u^{-k}] \frac{1}{1 - zP(u)} = z \sum_{j=1}^{c} \frac{u_j'(z)}{u_j(z)^{-k+1}} = [u^0] \frac{u^k}{1 - zP(u)}$$

$$Q(u) = \prod_{2 \le j \le d} (u - v_j(z)) = \sum_{i=0}^{d-1} q_i(z) u^i$$

$$[u^{0}]F^{[>h]}(z,u) = [u^{0}]\frac{1}{1-zP(u)}\frac{u^{h+1}}{v_{1}(z)^{h+1}}\frac{Q(u)}{Q(v_{1}(z))}\left(1+O(A^{h})\right)$$

$$= \frac{1}{v_{1}(z)^{h+1}Q(v_{1}(z))}\sum_{i=0}^{d-1}q_{i}(z)[u^{0}]\frac{u^{h+i+1}}{1-zP(u)}\left(1+O(A^{h})\right)$$

$$= z\left(\frac{u_{1}(z)}{v_{1}(z)}\right)^{h} \times \frac{u'_{1}(z)Q(u_{1}(z))}{v_{1}(z)Q(v_{1}(z))} \times \left(1+O(C^{h})\right)$$

$$\sup_{\substack{\epsilon < |z| < \rho \\ j \ge 2}}\frac{|u_{1}(z)|}{|u_{j}(z)|} < B \quad C = \max(A, B)$$

Extracting asymptotically $[z^n][u^0]F^{[>x\sigma\sqrt{n}]}(z,u)$ $P(1) = 1, P'(1) = 0, \rho = 1, \sigma^2 = P''(1)$ $z \sim 1^{-} \begin{cases} u_1(z) = 1 - \sqrt{\frac{2}{\sigma^2}(1-z)} + O(1-z) \\ v_1(z) = 1 + \sqrt{\frac{2}{\sigma^2}(1-z)} + O(1-z) \\ \frac{Q(u_1(z))}{Q(v_1(z))} = \frac{Q(1) + O(\sqrt{1-z})}{Q(1) + O(\sqrt{1-z})} = 1 + O(\sqrt{1-z}) \end{cases}$

$$[u^{0}]F^{[>x\sigma\sqrt{n}]}(z,u) = z\left(\frac{u_{1}(z)}{v_{1}(z)}\right)^{x\sigma\sqrt{n}} \times \frac{u_{1}'(z)Q(u_{1}(z))}{v_{1}(z)Q(v_{1}(z))} \times (1+O(C^{n}))$$

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Extracting asymptotically $[z^n][u^0]F^{[>x\sigma\sqrt{n}]}(z,u)$ $P(1) = 1, P'(1) = 0, \rho = 1, \sigma^2 = P''(1)$ $z \sim 1^{-} \begin{cases} u_1(z) = 1 - \sqrt{\frac{2}{\sigma^2}(1-z)} + O(1-z) \\ v_1(z) = 1 + \sqrt{\frac{2}{\sigma^2}(1-z)} + O(1-z) \\ \frac{Q(u_1(z))}{Q(v_1(z))} = \frac{Q(1) + O(\sqrt{1-z})}{Q(1) + O(\sqrt{1-z})} = 1 + O(\sqrt{1-z}) \end{cases}$

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$$=\frac{z}{\sigma\sqrt{2}}\frac{\left(1-2\sqrt{\frac{2}{\sigma^2}(1-z)}\right)^{x\sigma\sqrt{n}}}{\sqrt{1-z}}\times\left(1+O(\sqrt{1-z})\right)\times(1+O(C^n))$$

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$$[u^{0}]F^{[>x\sigma\sqrt{n}]}(z,u) = z\left(\frac{u_{1}(z)}{v_{1}(z)}\right)^{x\sigma\sqrt{n}} \times \frac{u_{1}'(z)Q(u_{1}(z))}{v_{1}(z)Q(v_{1}(z))} \times (1+O(C^{n}))$$

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Semi-large powers Banderier-Flajolet-Soria-Schaeffer (2001)

Asymptotics for upper bounded bridges $P(1) = 1, P'(1) = 0, \rho = 1, \sigma^2 = P''(1)$ $[z^n][u^0]F^{[>x\sigma\sqrt{n}]} = \frac{\sqrt{n}}{\sigma\sqrt{2}} \times e^{-2x^2} \times \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right)$

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Asymptotics for upper bounded bridges $P(1) = 1, P'(1) = 0, \rho = 1, \sigma^2 = P''(1)$ $[z^n][u^0]F^{[>x\sigma\sqrt{n}]} = \frac{\sqrt{n}}{\sigma\sqrt{2}} \times e^{-2x^2} \times \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right)$

but for unconditionned bridges (Banderier-Flajolet)

$$[z^n][u^0]F^{]-\infty,+\infty[} = \frac{\sqrt{n}}{\sigma\sqrt{2}} \times \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right)$$

Theorem (Banderier-N. 2010)

$$\mathbf{P}\left(\max_{0\leq i\leq n} B_i > x\sigma\sqrt{n}\right) = e^{-2x^2} \times \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right)$$

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Asymptotics for upper bounded bridges $P(1) = 1, P'(1) = 0, \rho = 1, \sigma^2 = P''(1)$ $[z^n][u^0]F^{[>x\sigma\sqrt{n}]} = \frac{\sqrt{n}}{\sigma\sqrt{2}} \times e^{-2x^2} \times \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right)$

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Moreover we get a concentration property around $\sigma \sqrt{n}$

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Full asymptotics for Łukasiewicz bridges $X_i \in \{-1, \dots, +d\}$ only one small root

 $Q(u_1(z))$ and $Q(v_1(z))$ expressible as functions of $u_1(z)$ and $v_1(z)$ only

$$Q(u) = \prod_{j=2}^{d} (u - v_j(z)) = \frac{u(1 - zP(u))}{p_d z(u - u_1(z))(u - v_1(z))}$$

 $P'(u(z)) = -1/ig(z^2 u'(z)ig)$ for any root u(z) of the kernel

$$Q(u_1(z)) = \left. \frac{1}{p_d z} \frac{\partial}{\partial u} \frac{u(1 - zP(u))}{u - v_1(z)} \right|_{u = u_1(z)} = \frac{1}{p_d z^2} \frac{u_1(z)}{u_1'(z)(u_1(z) - v_1(z))}$$

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Full asymptotics for Łukasiewicz bridges

Proposition (Banderier-N. 2010) Łukasiewicz bridges verify asymptotically

$$[u^0]F^{[>h]}(z,u) = z \left(\frac{u_1(z)}{v_1(z)}\right)^h \times \frac{-v_1'(z)u_1(z)}{v_1(z)^2} \times (1 + O(C^h))$$

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Full asymptotics for Łukasiewicz bridges

Proposition (Banderier-N. 2010) Łukasiewicz bridges verify asymptotically

$$[u^0]F^{[>h]}(z,u) = z \left(\frac{u_1(z)}{v_1(z)}\right)^h \times \frac{-v_1'(z)u_1(z)}{v_1(z)^2} \times (1+O(C^h))$$

use gdev for expansions of $u_1(z)$ and $v_1(z)$

$$\begin{split} \frac{\beta_n^{2x\sigma\sqrt{n}}}{\exp(-2x^2)} &= 1 + \frac{(-(2/3)x\xi/\zeta^{3/2} - 6x/\sqrt{\zeta})}{\sqrt{n}} + \frac{1}{n} \left((-2 - \frac{10}{9}\frac{\xi^2}{\zeta^3} + \frac{2}{3}\frac{\theta}{\zeta^2} - \frac{16}{3\zeta} - \frac{8}{3}\frac{\xi}{\zeta^2})x^4 \right. \\ &+ \left(\frac{24}{\zeta} + \frac{5}{3}\frac{\xi^2}{\zeta^3} + 3 - \frac{\theta}{\zeta^2} + \frac{20}{3}\frac{\xi}{\zeta^2}\right)x^2 - \frac{5}{\zeta} - \frac{3}{8} - \frac{7}{6}\frac{\xi}{\zeta^2} - \frac{5}{24}\frac{\xi^2}{\zeta^3} + \frac{1}{8}\frac{\theta}{\zeta^2} + \frac{5}{24}\frac{\xi^3}{\zeta^3} - \frac{1}{8}\frac{\theta^2 - 3\zeta^2}{\zeta^2} \right) \\ &+ O\left(\frac{1}{n^{3/2}}\right) \end{split}$$

$$\beta_n^{>x\sigma\sqrt{n}} = \mathbf{P}\left(\max_{0 \le i \le n} B_i\right) > x\sigma\sqrt{n}, \qquad \begin{cases} \zeta = \sigma^2 = P''(1), \\ \xi = P'''(1), \quad \theta = P''''(1) \end{cases}$$

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Heuristics for bioinformatics - rational jumps



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Upper and lower bounded Brownian bridges

$$\mathbf{P}\left(\max_{t\in[0,1]}|B_t| > x\right) = 2\sum_{k\ge 1} (-1)^{k+1} e^{-2k^2x^2}$$

Fourier theory:

$$G(x) = \sum_{k=-\infty}^{\infty} e^{-\pi k^2 x^2} \implies G(x) = \frac{1}{x} G\left(\frac{1}{x}\right)$$

$$\mathbf{P}\left(\max_{t\in[0,1]}|B_t| < x\right) = 2G\left(\frac{4x}{\sqrt{2\pi}}\right) - G\left(\frac{2x}{\sqrt{2\pi}}\right)$$

for small x, use the functional equation relating G(x) and G(1/x)

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