

Bounded Discrete Walks

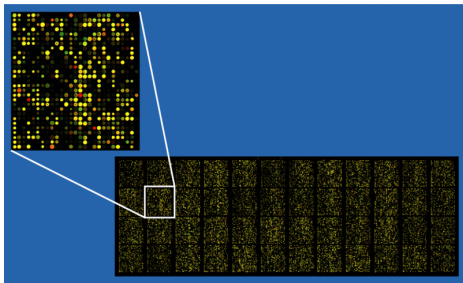
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CNRS - Team "CALIN", LIPN, University Paris 13

DNA micro-array and diagnostic in genetics?



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

- ▶ Γ := set of genes of a **background** population ($|\Gamma| = G$)
- ▶ γ := 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 $(B_i)_{0 \leq i \leq G+g}$ 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 $\left\{ \begin{array}{l} \circ \text{ genes of } \Gamma \\ \bullet \text{ genes of } \gamma \end{array} \right.$

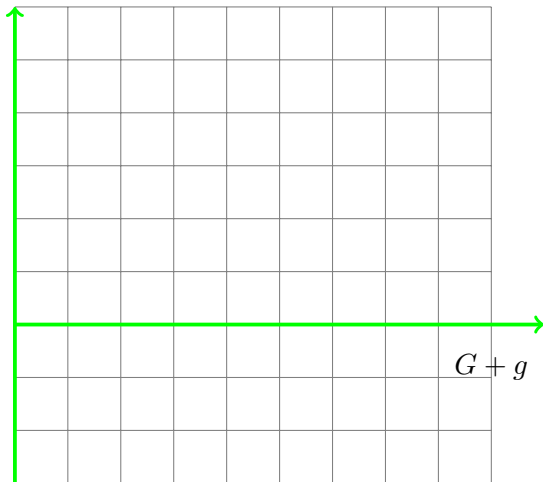
Pattern of level expression

High level	→	Low level
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$$\bullet \rightsquigarrow X_j = +2 \quad (+6/3)$$

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

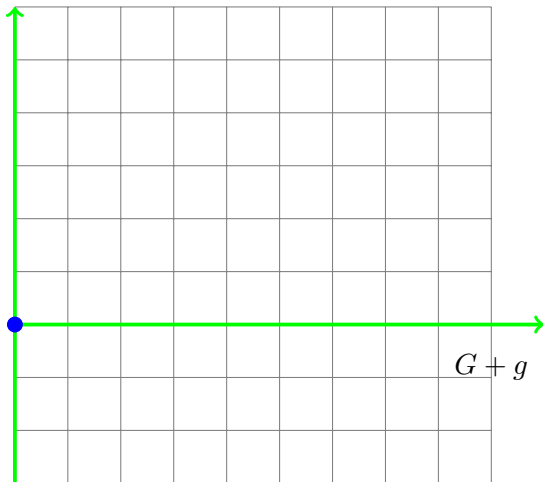


$$B_i = \sum_{1 \leq j \leq i} X_j$$

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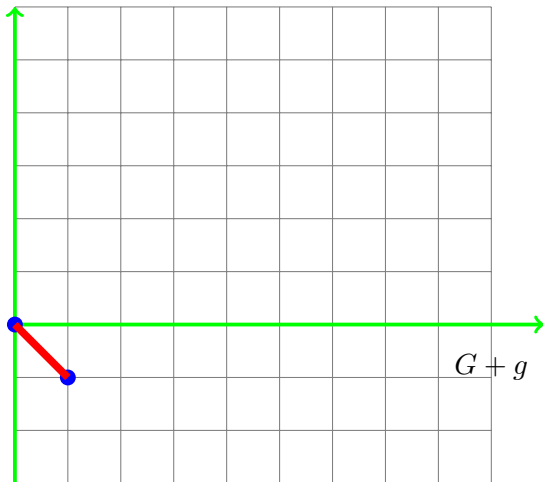


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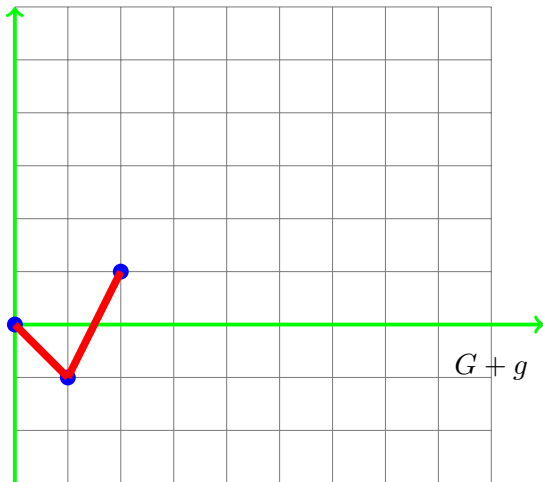


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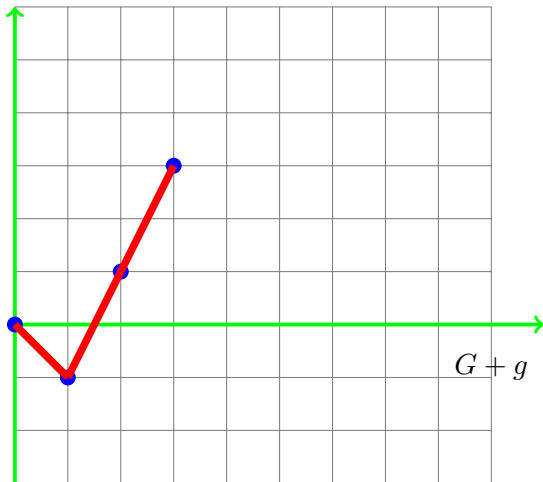


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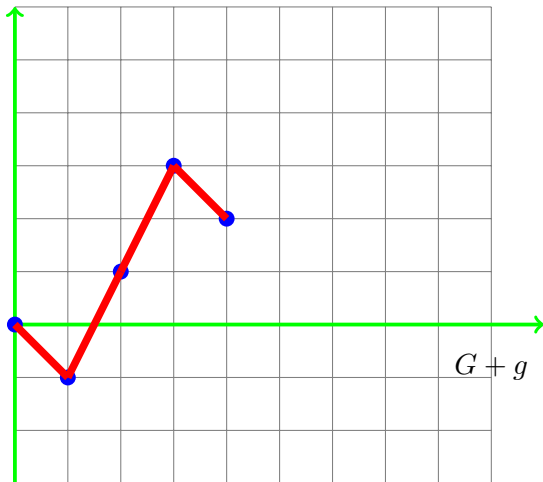


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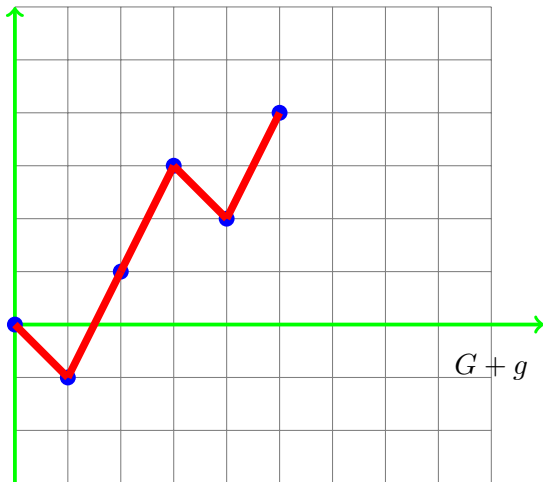


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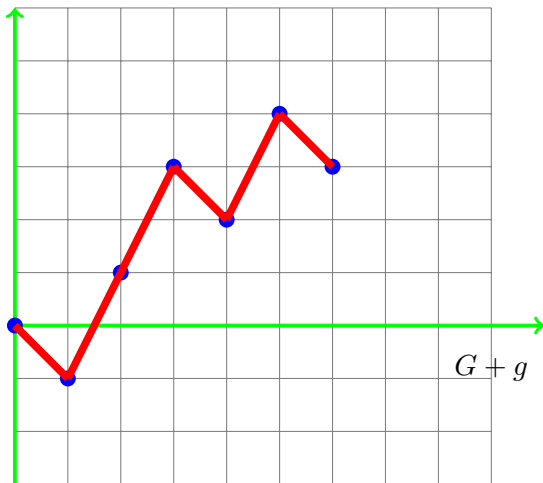


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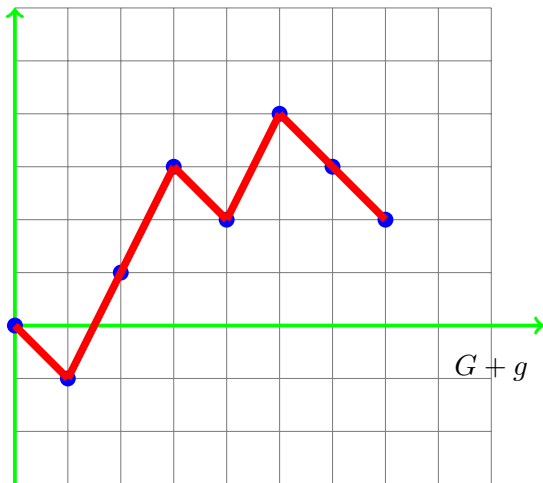


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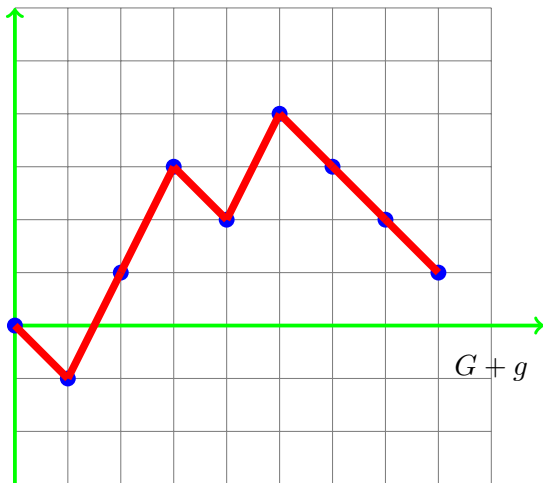


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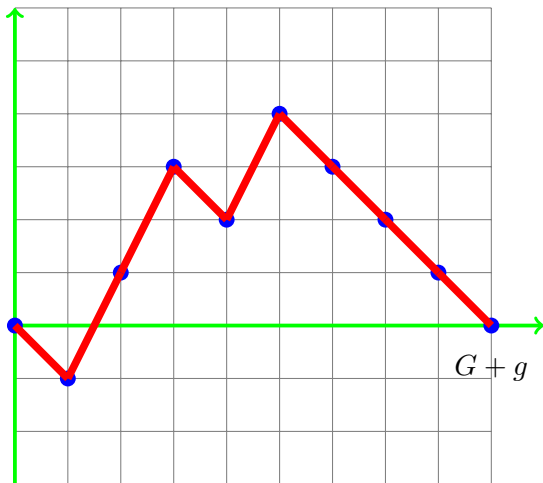


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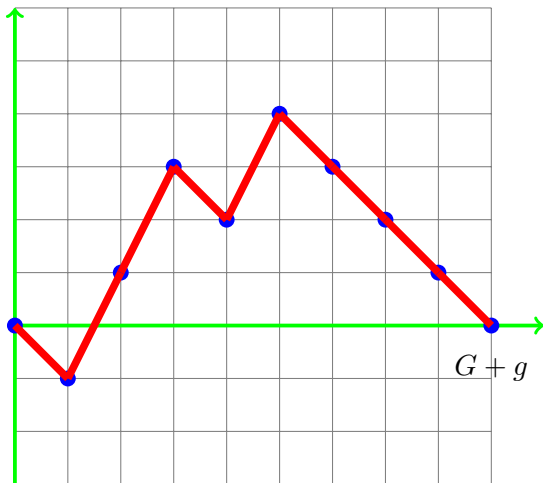


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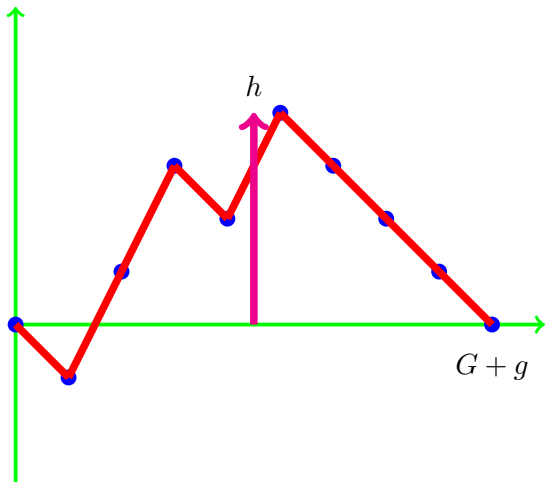


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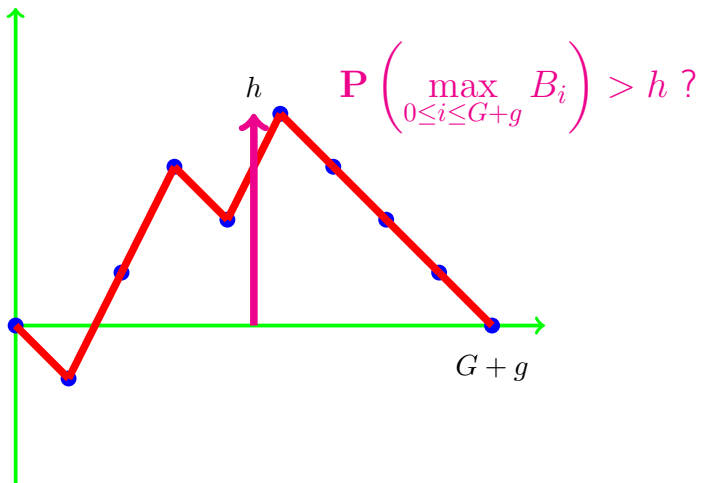


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Tail distribution for the height - Keller *et al.*

Keller, Backes and Lenhof (2007) compute

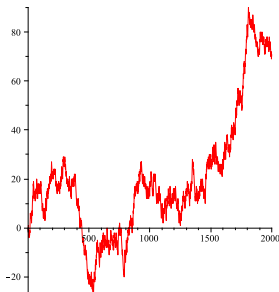
$$p\text{-value}(G, g, h) := \mathbf{P} \left(\max_{0 \leq i \leq G+g} B_i > h \right)$$

by a **dynamical programming** method in **complexity**

$$O(G \times g)$$

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

Brownian motion as limit of discrete walks



Strong approximations of discrete walks by Brownian motion

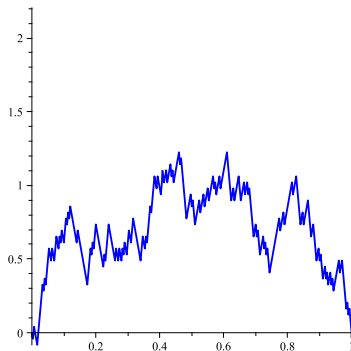
- Komlós, Major, Tusnády (1976), Chatterjee (2010)

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

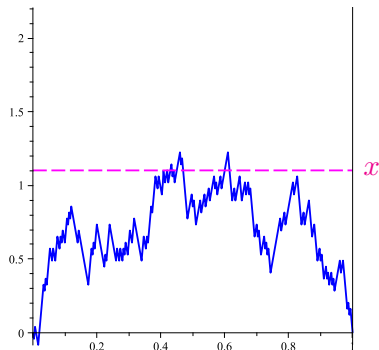
Approximations of bridges

- Kaigh (1976), Borisov (1978)

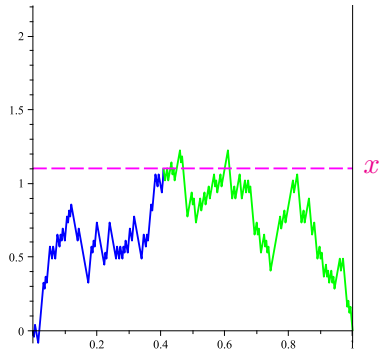
Désiré André reflexion principe



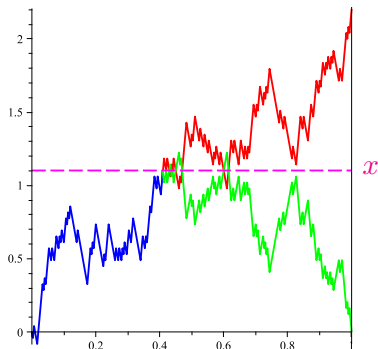
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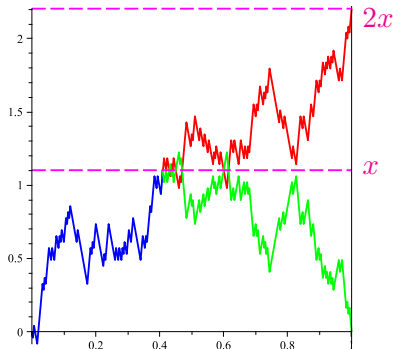


Désiré André reflexion principle



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).

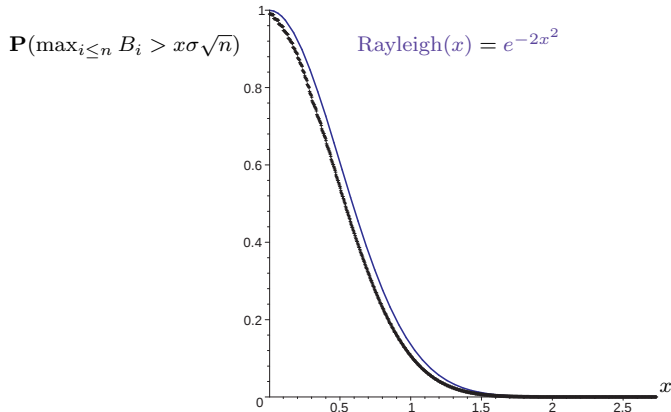
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$$\Phi(2x) = \mathbf{P}(W(1) = 2x) = \frac{1}{\sqrt{2\pi}} e^{-2x^2}$$

$$\mathbf{P}\left(\max_{t \in [0,1]} B_t \geq x\right) = \frac{\Phi(2x)}{\Phi(0)} = \text{Rayleigh}(x) = e^{-2x^2}$$

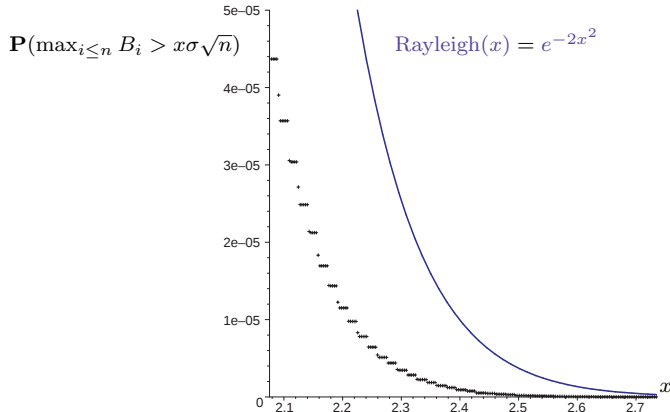
Brownian bridge versus simulations



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

10^8 simulations

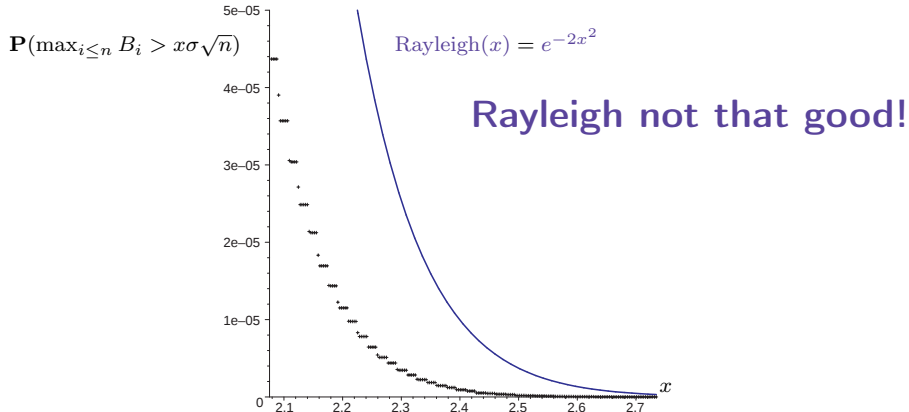
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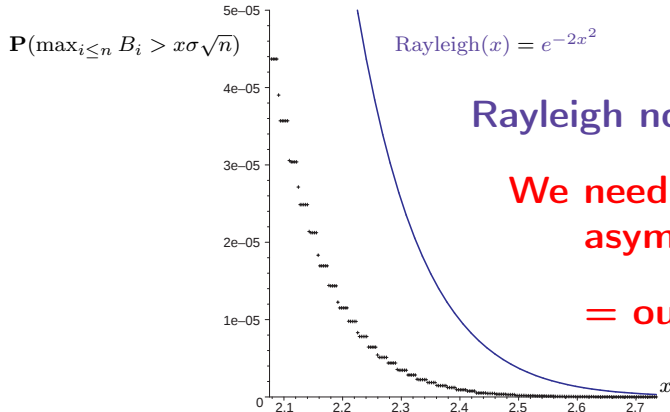
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Brownian bridge versus simulations



Rayleigh not that good!

We need more precise asymptotics!

= our work!

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

$\sigma = \sqrt{G \times g}$ 10^8 simulations

Summary of the talk

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

Directed discrete walks

Model = generalized Dyck walks

= discrete “bridges”

- ▶ Knuth (1973)
- ▶ Gessel (1980)
- ▶ Labelle & Yeah (1990), Merlini & al. (1996), Duchon (2000)
- ▶ Banderier and Flajolet (2002)
- ▶ Bousquet-Mélou (2009)
- ▶ Bousquet-Mélou and Ponty (2009)

Model

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

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Typical generating function

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

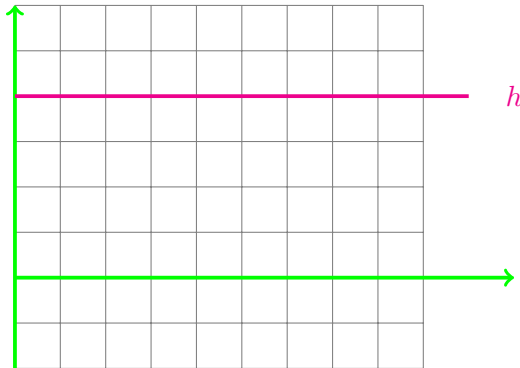
where

- ▶ $f_{n,k}$ is the probability that a walk remaining in an horizontal strip (by instance $] -\infty, +h[$) has **altitude** k at **time** n .

$[z^n][u^0]F(z, u)$ corresponds to **bridges** of **length** n

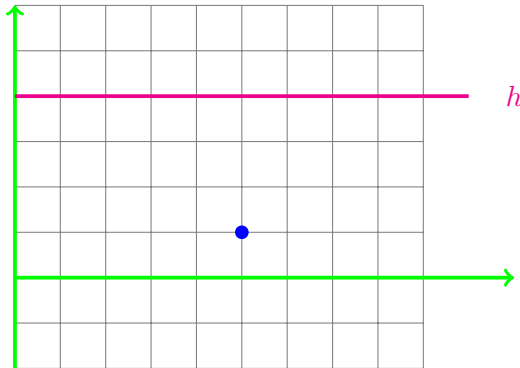
Getting the generating function

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



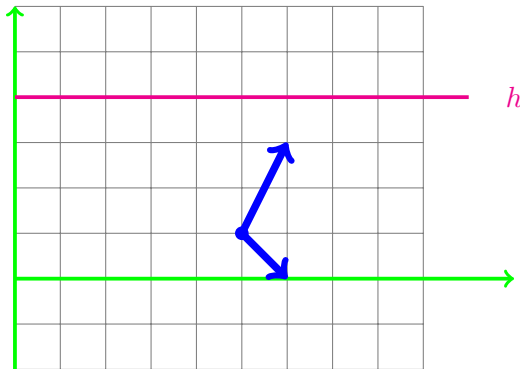
Getting the generating function

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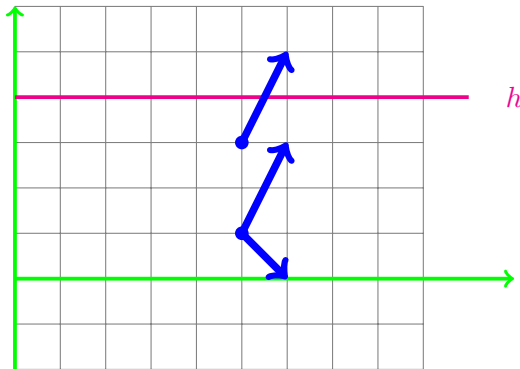
$$X_i \in \{-1, +2\} \quad P(u) = u^2 + \frac{1}{u}$$



$$f_{k+1}(u) = f_k(u) \times P(u)$$

Getting the generating function

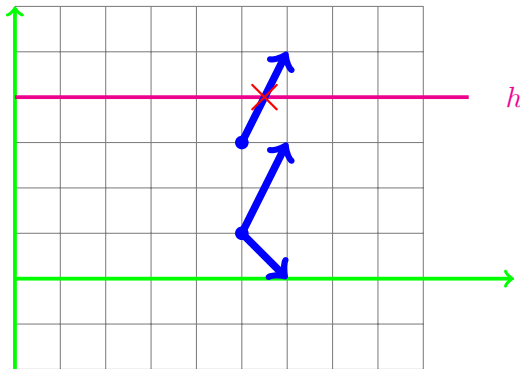
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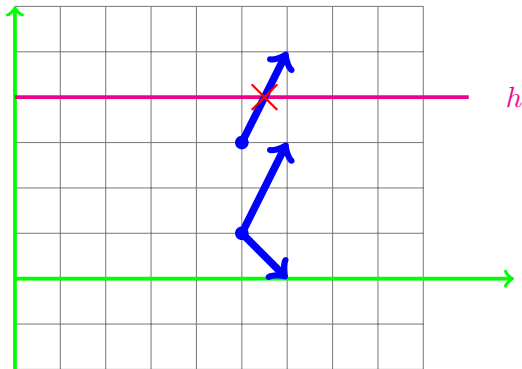
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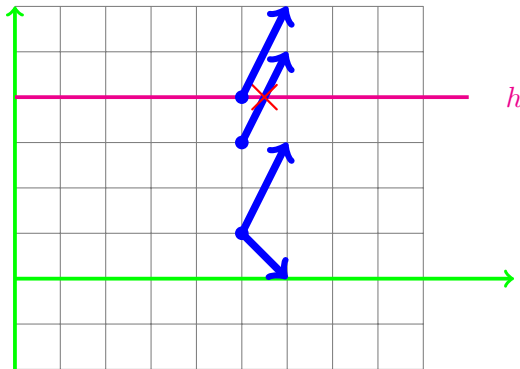


$$f_{k+1}(u) = f_k(u) \times P(u)$$

$$-u^{h+1}[u^{h+1}]f_k(u) \times P(u)$$

Getting the generating function

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

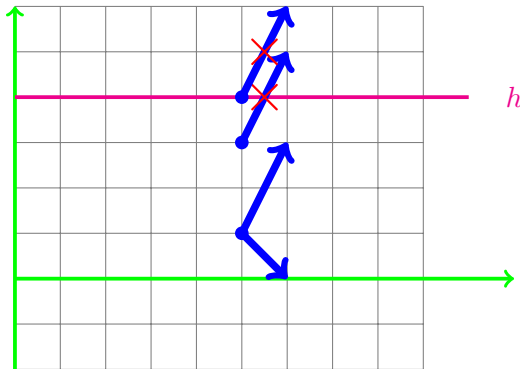


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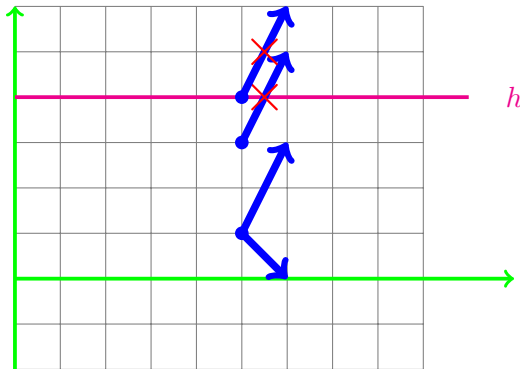


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Getting the generating function

$$X_i \in \{-1, +2\} \quad P(u) = u^2 + \frac{1}{u} \quad f_0(u) = 1$$

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

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

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

Kernel method

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

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

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

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

$$P(u) = p_{-c}u^{-c} + p_{-c+1}u^{-c+1} + \cdots + p_{d-1}u^{d-1} + p_d u^d$$

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

d unknown functions $F_{h+j}(z)$, but the equation $1 - zP(u) = 0$ has

$$\left\{ \begin{array}{ll} d \text{ large roots } v_i(z) & \text{such that } v_i(z) \sim \frac{1}{z}^{1/d} \quad \text{as } z \rightarrow 0 \\ c \text{ small roots } u_j(z) & \text{such that } u_j(z) \sim z^{1/c} \quad \text{as } z \rightarrow 0 \end{array} \right.$$

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$$\begin{cases} v_1(z)^{h+1}F_{h+1}(z) + \cdots + v_1(z)^{h+d}F_{h+d}(z) = 1/z, \\ \dots \\ v_d(z)^{h+1}F_{h+1}(z) + \cdots + v_d(z)^{h+d}F_{h+d}(z) = 1/z \end{cases}$$

General case - Any finite set of integer jumps

$$P(u) = p_{-c}u^{-c} + p_{-c+1}u^{-c+1} + \cdots + p_{d-1}u^{d-1} + p_d u^d$$

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

d unknown functions $F_{h+j}(z)$, but the equation $1 - zP(u) = 0$ has

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

$$\begin{cases} v_1(z)^{h+1}F_{h+1}(z) + \cdots + v_1(z)^{h+d}F_{h+d}(z) = 1/z, \\ \cdots \\ v_d(z)^{h+1}F_{h+1}(z) + \cdots + v_d(z)^{h+d}F_{h+d}(z) = 1/z \end{cases}$$

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

Nice expression for the generating function $F^{]-\infty, h]}$

$$\begin{cases} v_1(z)^{h+1}F_{h+1}(z) + \dots + v_1(z)^{h+d}F_{h+d}(z) = 1/z, \\ \dots \\ v_d(z)^{h+1}F_{h+1}(z) + \dots + v_d(z)^{h+d}F_{h+d}(z) = 1/z \end{cases}$$

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

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

Nice expression for the generating functions

$$F^{[-\infty, h]}(z, u) = \frac{1}{1 - zP(u)} - F^{[>h]}(z, u)$$

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

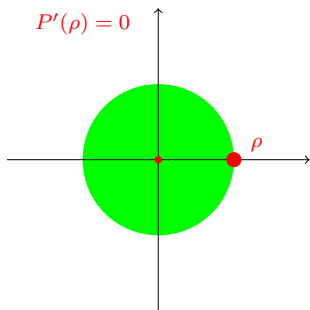
Theorem (Banderier-N. 2010)

Walks going **beyond** the barrier $+h$ verify

$$F^{[>h]}(z, u) = \frac{1}{1 - zP(u)} \sum_{j=1}^d \frac{u^{h+1}}{v_j(z)^{h+1}} \prod_{\substack{1 \leq i \leq d \\ i \neq j}} \frac{u - v_i(z)}{v_j(z) - v_i(z)}$$

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

Roots properties (Banderier-Flajolet)



for $\epsilon < |z| < \rho$

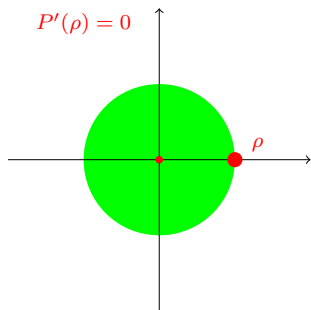
$$\max_{i \geq 2} |u_i(z)|$$

$$< |u_1(z)|$$

$$< |v_1(z)|$$

$$< \min_{j \geq 2} |v_j(z)|$$

Roots properties (Banderier-Flajolet)



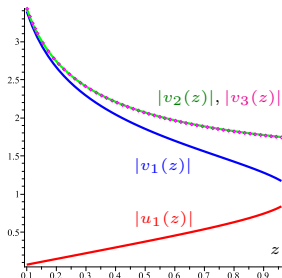
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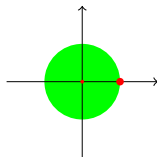


$$X_i \in \{+3, -1\} \quad \begin{cases} \mathbf{E}(X) = P'(1) = 0 \ (\rho = 1) \\ P(1) = 1 \end{cases}$$

$$z \sim 1^- \quad \begin{cases} u_1(z) = 1 - \sqrt{\frac{2}{P'''(1)}(1-z)} + O(1-z) \\ v_1(z) = 1 + \sqrt{\frac{2}{P'''(1)}(1-z)} + O(1-z) \end{cases}$$

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

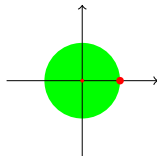
$$\frac{u^{h+1}}{v_j(z)^{h+1}} = \frac{u^{h+1}}{v_1(z)^{h+1}} \left(\frac{v_1(z)}{v_j(z)} \right)^{h+1} = O(A^h)$$



$$\left(j \geq 2, \quad A = \max_{j \geq 2} \sup_{|z| < \rho - \epsilon} \frac{|v_1(z)|}{|v_j(z)|} < 1 \right)$$

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$$\begin{aligned} \Rightarrow F^{[>h]}(z, u) &= \frac{1}{1 - zP(u)} \sum_{j=1}^d \frac{u^{h+1}}{v_j(z)^{h+1}} \prod_{\substack{1 \leq i \leq d \\ i \neq j}} \frac{u - v_i}{v_j - v_i} \\ &= \frac{1}{1 - zP(u)} \frac{u^{h+1}}{v_1(z)^{h+1}} \frac{Q(u)}{Q(v_1(z))} \left(1 + O(A^h) \right) \end{aligned}$$

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

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

Theorem. Banderier-Flajolet: walks terminating at altitude $-k$

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

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$$\begin{aligned} [u^0]F^{[>\mathbf{h}]}(z, u) &= [u^0] \frac{1}{1 - zP(u)} \frac{u^{\mathbf{h}+1}}{v_1(z)^{\mathbf{h}+1}} \frac{Q(u)}{Q(v_1(z))} (1 + O(A^h)) \\ &= \frac{1}{v_1(z)^{\mathbf{h}+1} Q(v_1(z))} \sum_{i=0}^{d-1} q_i(z) [u^0] \frac{u^{\mathbf{h}+\mathbf{i}+1}}{1 - zP(u)} (1 + O(A^h)) \end{aligned}$$

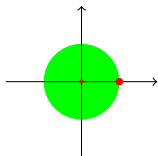
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$$= z \left(\frac{u_1(z)}{v_1(z)} \right)^{\mathbf{h}} \times \frac{u'_1(z) Q(u_1(z))}{v_1(z) Q(v_1(z))} \times (1 + O(C^h))$$

$$\sup_{\substack{\epsilon < |z| < \rho \\ j \geq 2}} \frac{|u_1(z)|}{|u_j(z)|} < B \quad C = \max(A, B)$$

Extracting asymptotically $[z^n][u^0]F^{[>x\sigma\sqrt{n}]}(z, u)$

$$P(1) = 1, \quad P'(1) = 0, \quad \rho = 1, \quad \sigma^2 = P''(1)$$

$$z \sim 1^- \left\{ \begin{array}{l} u_1(z) = 1 - \sqrt{\frac{2}{\sigma^2}(1-z)} + O(1-z) \\ v_1(z) = 1 + \sqrt{\frac{2}{\sigma^2}(1-z)} + O(1-z) \\ \frac{Q(u_1(z))}{Q(v_1(z))} = \frac{Q(1) + O(\sqrt{1-z})}{Q(1) + O(\sqrt{1-z})} = 1 + O(\sqrt{1-z}) \end{array} \right.$$

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

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

Asymptotics for upper bounded bridges

$$P(1) = 1, \quad P'(1) = 0, \quad \rho = 1, \quad \sigma^2 = P''(1)$$

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

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but for unconditioned 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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Moreover we get a **concentration** property around $\sigma\sqrt{n}$

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

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

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

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

Full asymptotics for Łukasiewicz bridges

Proposition (Banderier-N. 2010)

Łukasiewicz bridges verify asymptotically

$$[u^0]F^{[>h]}(z, u) = z \left(\frac{u_1(z)}{v_1(z)} \right)^h \times \frac{-v'_1(z)u_1(z)}{v_1(z)^2} \times (1 + O(C^h))$$

Full asymptotics for Łukasiewicz bridges

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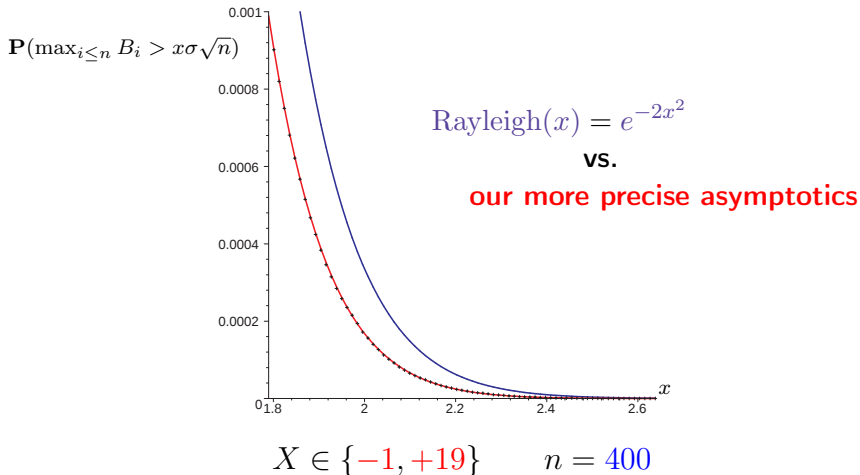
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use **gdev** of **inria-algolib** for expansions of $u_1(z)$ and $v_1(z)$

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

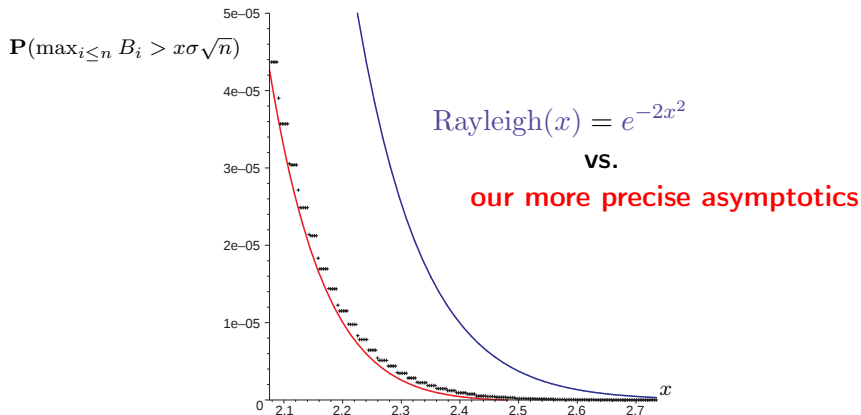
$$\beta_n^{>x\sigma\sqrt{n}} = \mathbf{P} \left(\max_{0 \leq i \leq n} B_i > x\sigma\sqrt{n} \right), \quad \begin{cases} \zeta = \sigma^2 = P''(1), \\ \xi = P'''(1), \quad \theta = P''''(1) \end{cases}$$

Back to simulations



if $X_i = \{-1, +d\}$, moments of $P(u)$ and p -values expressible as functions of d .

Heuristics for bioinformatics - rational jumps



$$X \in \{-11, +93\} \rightsquigarrow X' \in \left\{-1, +\frac{93}{11}\right\} \quad n = 104$$

Acknowledgements

