Wiener Index and Dependencies in Random Digital Trees

(joint with Hsien-Kuei Hwang and Chung-Kuei Lee)

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June 21st, 2016

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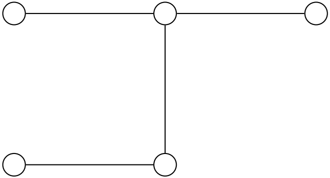

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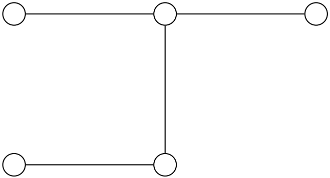

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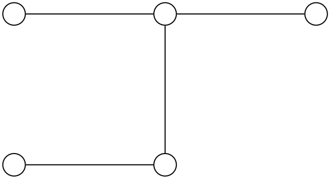

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In this talk, we will consider the Wiener index of rooted trees (trees arise as molecular graphs of acyclic organic molecules).

Families of Random Trees

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- Random plane trees;
- Random non-plane trees;
- Random binary trees;
- Random binary search trees;
- Random median-of-$(2k+1)$ search trees;
- Random quadtrees;
- Random digital search trees;
- Etc.

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Question: How does the Wiener index behave for such random trees?

Binary Search Trees

Example: Input: $4, 7, 6, 1, 8, 5, 3, 2$

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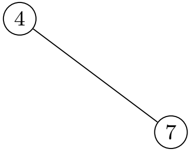

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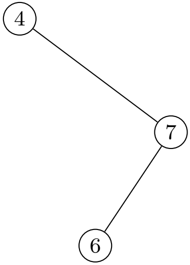

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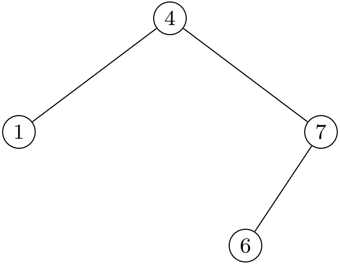

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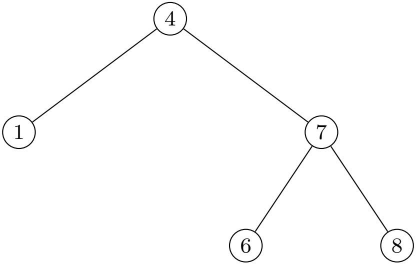

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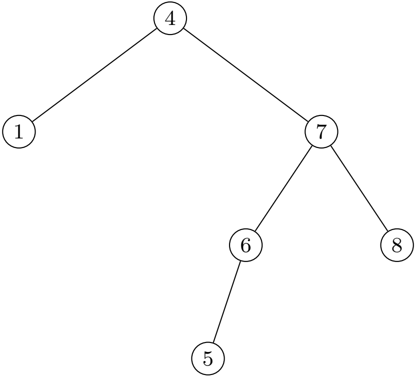

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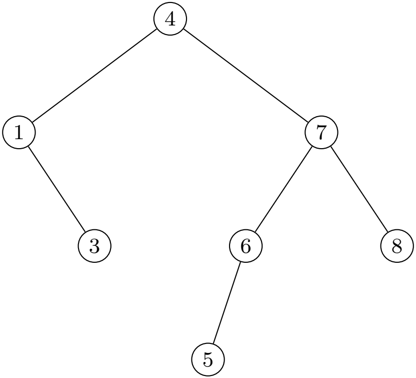

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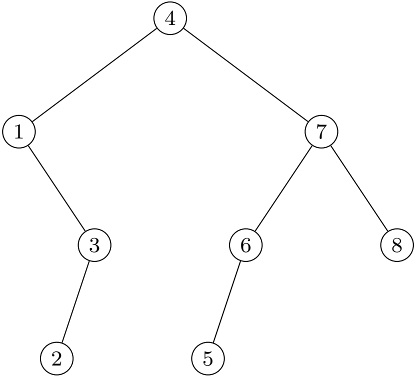

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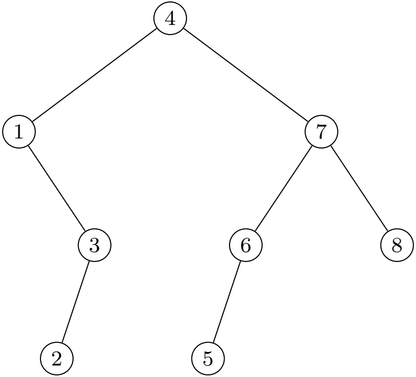

Random model: Input is a random permutation of size n.

Moments of Wiener Index

T_n ... total path length.

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Theorem (Neininger 2002)

We have,

$$\mathbb{E}(W_n) \sim 2n^2 \log n$$

and

$$\mathrm{Var}(T_n) \sim \frac{21 - 2\pi^2}{3} n^2,$$
$$\mathrm{Cov}(T_n, W_n) \sim \frac{20 - 2\pi^2}{3} n^3,$$
$$\mathrm{Var}(W_n) \sim \frac{20 - 2\pi^2}{3} n^4.$$

Limit Law of Wiener Index

Theorem (Neininger 2002)

We have,

$$\left(\frac{T_n - \mathbb{E}(T_n)}{n}, \frac{W_n - \mathbb{E}(W_n)}{n^2}\right) \xrightarrow{d} (T, W),$$

where (T, W) *is a solution of*

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \stackrel{d}{=} A \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} + B \begin{pmatrix} X_1^* \\ X_2^* \end{pmatrix} + \begin{pmatrix} b_1^* \\ b_2^* \end{pmatrix}$$

with

$$A = \begin{pmatrix} 0 & U \\ U^2 & U(1-U) \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1-U \\ (1-U)^2 & U(1-U) \end{pmatrix}$$

and b_1^*, b_2^* *are functions of* U.

Random Split Trees (i)

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Assume that

$$V_i \stackrel{d}{=} V_1 := V \qquad 2 \leq i \leq b.$$

V is called *splitter*.

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The resulting tree is called *random split tree of size* n.

Examples of Random Split Trees

Example 1: Binary search trees: $b = 2, s = s_0 = 1, s_1 = 0$ and V uniformly distributed on $[0, 1]$.

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Satisfied by Example 1 but NOT Example 2.

Moments of Wiener Index

Theorem (Munsonius 2012)

Under the assumption,

$$\mathbb{E}(W_n) \sim \frac{1}{\mu} n^2 \log n$$

with $\mu = -b\mathbb{E}(V \log V)$ *and*

$$\begin{aligned} \mathrm{Var}(T_n) &\sim \sigma_T^2 n^2, \\ \mathrm{Cov}(T_n, W_n) &\sim \sigma_C^2 n^3, \\ \mathrm{Var}(W_n) &\sim \sigma_W^2 n^4, \end{aligned}$$

where $\sigma_T^2, \sigma_C^2, \sigma_W^2 > 0$.

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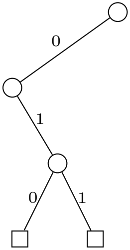

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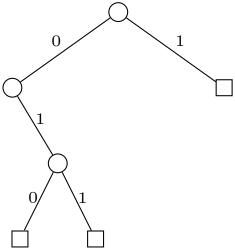

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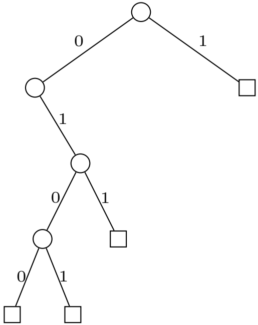

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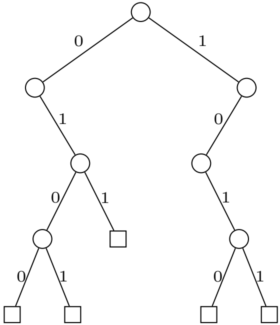

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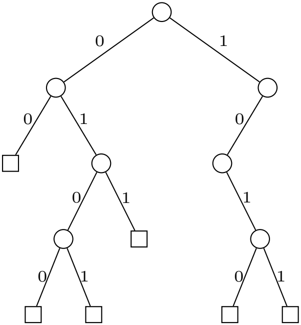

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- Analysis of tries is interesting and challenging.

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Question: How does a random trie look like?

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Computed recursively as follows: compute it for the two subtrees and add them up + add a toll.

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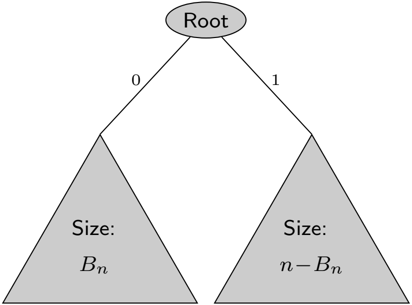
$$X_n \stackrel{d}{=} X_{B_n} + X^*_{n-B_n} + T_n$$

- $B_n \stackrel{d}{=} \text{Binomial}(n,p)$;
- $X_n \stackrel{d}{=} X^*_n$;
- X_n, X^*_n, B_n independent.
- T_n toll-function.



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Wiener Indices:

$$KW_n \stackrel{d}{=} KW_{B_n} + KW^*_{n-B_n} + B_n(K^*_{n-B_n} + n - B_n) + (n - B_n)(K_{B_n} + B_n);$$

$$NW_n \stackrel{d}{=} NW_{B_n} + NW^*_{n-B_n} + (S_{B_n} + 1)(N^*_{n-B_n} + S^*_{n-B_n}) + (S_{n-B_n} + 1)(N_{B_n} + S_{B_n}).$$

Mean and Variance - An Overview

Shape parameter	Mean	Variance
Size S_n	n	n
EPL K_n	$n\log n$	$\begin{cases} p\neq q: & n\log n \\ p=q: & n \end{cases}$
IPL N_n	$n\log n$	$n\log^2 n$
External Wiener Index KW_n	$n^2\log n$	$\begin{cases} p\neq q: & n^3\log n \\ p=q: & n^3 \end{cases}$
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$$\chi_k = \frac{2rk\pi i}{\log p}, \qquad (k \in \mathbb{Z}).$$

- For a function G:

$$\mathcal{F}[G](x) = \begin{cases} h^{-1}\sum_{k\in\mathbb{Z}} G(-1+\chi_k)e^{2k\pi i x}, & \text{if } \log p/\log q \in \mathbb{Q}; \\ h^{-1}G(-1), & \text{if } \log p/\log q \notin \mathbb{Q}. \end{cases}$$

Variance of Size S_n

Theorem (Régnier & Jacquet 1989; Kirschenhofer & Prodinger 1991; F., Hwang, Zacharovas 2014)

We have,

$$\mathrm{Var}(S_n) \sim \mathcal{F}[G_S](r \log_{1/p} n)n,$$

where

$$\begin{aligned} G_S(-1+\chi_k) =& \chi_k \Gamma(-1+\chi_k)\left(1 - \frac{\chi_k + 3}{2^{1+\chi_k}}\right) \\ & - \frac{1}{h}\sum_{j\in\mathbb{Z}} \Gamma(\chi_j + 1)\Gamma(\chi_{k-j}+1) \\ & - 2\sum_{j\geq 1} \frac{(-1)^j (j+1+\chi_k)\Gamma(j+\chi_k)\left(p^{j+1}+q^{j+1}\right)}{(j-1)!(j+1)(1-p^{j+1}-q^{j+1})}. \end{aligned}$$

Variance of EPL K_n

Theorem (Jacquet & Régnier 1986; Kirschenhofer, Prodinger, Szpankowski 1989; F., Hwang, Zacharovas 2014)

- $p \neq q$:

$$\mathrm{Var}(K_n) \sim h^{-3} pq \log^2(p/q) n \log n;$$

- $p = q$:

$$\mathrm{Var}(K_n) \sim \mathcal{F}[G_K](r \log_{1/p} n) n$$

Variance of EPL K_n

Theorem (Jacquet & Régnier 1986; Kirschenhofer, Prodinger, Szpankowski 1989; F., Hwang, Zacharovas 2014)

- $p \neq q$:

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where

$$G_K(-1+\chi_k) = \Gamma(\chi_k)\left(1 - \frac{\chi_k^2 - \chi_k + 4}{2^{\chi_k+2}}\right) + 2\sum_{\ell \geq 1} \frac{(-1)^\ell \Gamma(\chi_k+\ell)(\ell(\chi_k+\ell-1)-1)}{\ell!(2^\ell - 1)}.$$

Variance and Limit Law of IPL N_n

Theorem (F., Hwang, Zacharovas 2014)

We have,

$$\mathrm{Cov}(S_n, N_n) \sim h^{-1}\mathcal{F}[G_S](r\log_{1/p} n)n\log n$$

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$$\left(\frac{S_n - \mathbb{E}(S_n)}{\sqrt{\mathrm{Var}(S_n)}}, \frac{N_n - \mathbb{E}(N_n)}{\sqrt{\mathrm{Var}(N_n)}}\right)^{\mathsf{T}} \xrightarrow{d} \mathcal{N}(0, E_2),$$

where E_2 is the 2×2 unit matrix.

External Wiener Index KW_n

Theorem (F. & Lee 2015)

- $p \neq q$:

$$\mathrm{Cov}(K_n, KW_n) \sim h^{-3} pq \log^2(p/q) n^2 \log n;$$
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Internal Wiener Index NW_n

Theorem (F. & Lee 2015)

We have,

$$\mathrm{Cov}(S_n, NW_n) \sim 2h^{-1}\mathcal{F}[G_{\hat{S}}](r\log_{1/p} n)\mathcal{F}[G_S](r\log_{1/p} n)n^2\log n;$$

$$\mathrm{Cov}(N_n, NW_n) \sim 2h^{-2}\mathcal{F}[G_{\hat{S}}](r\log_{1/p} n)\mathcal{F}[G_S](r\log_{1/p} n)n^2\log^2 n;$$

$$\mathrm{Var}(NW_n) \sim 4h^{-2}(\mathcal{F}[G_{\hat{S}}](r\log_{1/p} n))^2\mathcal{F}[G_S](r\log_{1/p} n)n^3\log^2 n.$$

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Moreover,

$$\left(\frac{S_n - \mathbb{E}(S_n)}{\sqrt{\mathrm{Var}(S_n)}}, \frac{N_n - \mathbb{E}(N_n)}{\sqrt{\mathrm{Var}(N_n)}}, \frac{NW_n - \mathbb{E}(NW_n)}{\sqrt{\mathrm{Var}(NW_n)}}\right)^{\mathsf{T}} \xrightarrow{d} \mathcal{N}(0, E_3),$$

where E_3 is the 3×3 unit matrix.

Size S_n and EPL K_n

Remark

We have,

$$\rho(K_n, KW_n) \sim 1$$

and

$$\begin{aligned} \rho(S_n, N_n) &\sim 1, \\ \rho(S_n, NW_n) &\sim 1, \\ \rho(N_n, NW_n) &\sim 1, \end{aligned}$$

where $\rho(\cdot,\cdot)$ denotes the correlation coefficient.

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Question: how about the correlation between S_n and K_n?

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$\longrightarrow$ one expects strong positive correlation!

Covariance between S_n and K_n

Theorem (F. & Hwang 201?)

We have,

$$\mathrm{Cov}(S_n, K_n) \sim \mathcal{F}[G_{SK}](r \log_{1/p} n) n,$$

where

$$\begin{aligned} G_{SK}(-1+\chi_k) &= \Gamma(\chi_k)\left(1 - \frac{\chi_k + 2}{2^{\chi_k+1}}\right) \\ &\quad - \frac{1}{h} \sum_{j \in \mathbb{Z}\setminus\{0\}} \Gamma(\chi_{k-j}+1)(\chi_j - 1)\Gamma(\chi_j) \\ &\quad - \frac{\Gamma(\chi_k+1)}{h}\left(\gamma + 1 + \psi(\chi_k+1) - \frac{p\log^2 p + q \log^2 q}{2h}\right) \\ &\quad + \sum_{j \geq 2} \frac{(-1)^j (2j^2 - 2j + 1 + (2j-1)\chi_k)\Gamma(j-1\chi_k)(p^j + q^j)}{j!(1-p^j-q^j)}. \end{aligned}$$

Correlation Coefficient $\rho(S_n, K_n)$

Theorem (F. & Hwang 201?)

We have,

$$\rho(S_n, K_n) \sim \begin{cases} 0, & \text{if } p \neq q; \\ F(n), & \text{if } p = q, \end{cases}$$

where

$$F(n) = \frac{\mathcal{F}[G_{SK}](r \log_{1/p} n)}{\sqrt{\mathcal{F}[G_S](r \log_{1/p} n)\mathcal{F}[G_K](r \log_{1/p} n)}}$$

is a periodic function with

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Question: can this behavior be ascribed to the weakness of Pearson's correlation coefficient?

Limit Laws

Theorem (F. & Hwang 201?)

- $p \neq q$:

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where I_2 is the 2×2 identity matrix.

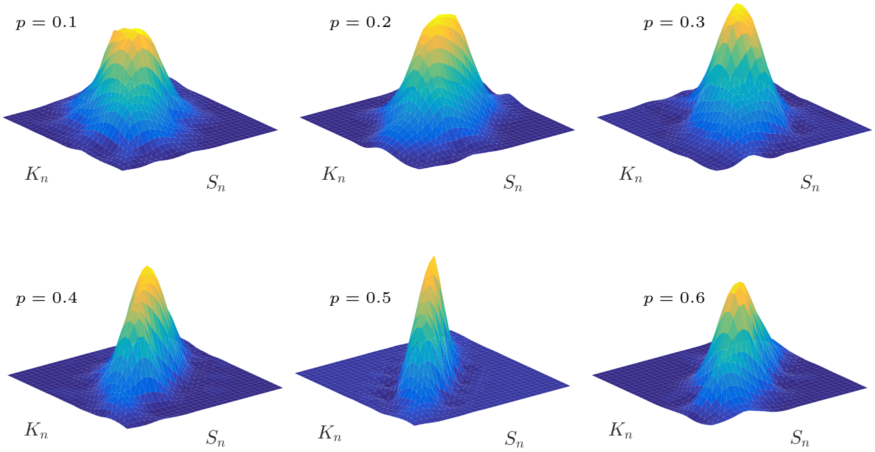
- $p = q$:

$$\Sigma_n^{-1/2} \begin{pmatrix} S_n - \mathbb{E}(S_n) \\ K_n - \mathbb{E}(K_n) \end{pmatrix} \xrightarrow{d} \mathcal{N}_2(0, I_2),$$

where Σ_n is the (asymptotic) covariance matrix:

$$\Sigma_n := n \begin{pmatrix} \mathscr{F}[G_S](r \log_{1/p} n) & \mathscr{F}[G_{SK}](r \log_{1/p} n) \\ \mathscr{F}[G_{SK}](r \log_{1/p} n) & \mathscr{F}[G_K](r \log_{1/p} n) \end{pmatrix}.$$

Joint Distribution of S_n and K_n



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- Similar surprising results for other shape parameters and other digital trees:

  M. Fuchs and H.-K. Hwang. Dependence between path length and size in random digital trees, preprint.