RESEARCH

Efficent Structure Searching with Inverted Indices

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Abstract

The rapid growth of chemical databases has put much burden on our ability to efficiently search and mine chemical structures. Even for modest sized chemical databases (e.g., $\approx 10^6$), supporting full structure searching efficiently remains a challenging task. Herein we describe an efficient indexing scheme—based on inverted indices—for chemical graphs that enables fast structure searching. We demonstrate the utility and effectiveness of our approach through a self-contained implementation available at https://spotlite.nih.gov/opensource/structure-indexer

Content

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Section title

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Sub-sub-sub heading for section Text for this sub-sub-sub-heading ... In this section we examine the growth rate of the mean of Z_0, Z_1 and Z_2. In addition, we examine a common modeling assumption and note the importance of considering the tails of the extinction time T_x in studies of escape dynamics. We will first consider the expected resistant population at vT_x for some $v > 0$, (and temporarily assume $\alpha = 0$)

$$E\big[Z_1(vT_x)\big] = E\left[\mu T_x \int_0^{v\wedge 1} Z_0(uT_x) \exp\big(\lambda_1 T_x(v-u)\big)\, du\right].$$

If we assume that sensitive cells follow a deterministic decay $Z_0(t) = xe^{\lambda_0 t}$ and approximate their extinction time as $T_x \approx -\frac{1}{\lambda_0}\log x$, then we can heuristically estimate the expected value as

$$E\big[Z_1(vT_x)\big] \quad = \quad \frac{\mu}{r}\log x \int_0^{v\wedge 1} x^{1-u} x^{(\lambda_1/r)(v-u)}\, du$$

$$= \frac{\mu}{r} x^{1-\lambda_1/\lambda_0 v} \log x \int_0^{v \wedge 1} x^{-u(1+\lambda_1/r)}\, du$$
$$= \frac{\mu}{\lambda_1 - \lambda_0} x^{1+\lambda_1/rv} \left(1 - \exp\left[-(v \wedge 1)\left(1 + \frac{\lambda_1}{r}\right) \log x\right]\right). \quad (1)$$

Thus we observe that this expected value is finite for all $v > 0$ (also see [?, ?, ?, ?, ?]).

Competing interests
The authors declare that they have no competing interests.

Author's contributions
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Figures

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Figure 2 Sample figure title. Figure legend text.

Tables

Table 1 Sample table title. This is where the description of the table should go.

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A1	0.1	0.2	0.3
A2	...	..	.
A3	..	.	.

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