18-1ec 2020
Analysis of Mass Speoha

- Proteomias
- Mertabolomics


Proteomich
classical protocol:

- separation: $2 D \mathrm{gel}$

- use mass-spectrometer chorge to measure mass of
indinidual "blobs".
I. glternative: Tandem mass spec
- digest all pooteins
- separate pepides
by HPLC $\rightarrow$ "blobs"
- ears "blob' ( $=1$ peptide) is mass - measured (cst Ms)
- let peptides fly thinorgh a
peptide collisionchamber $\rightarrow$ grable into

$$
\begin{aligned}
& \text { prefix }(b) \text { ions } \\
& \\
& \\
& \text { suffix }(y) \text { ions }
\end{aligned}
$$

Lion yon suffix (y )ions $\overline{\bar{b}} \bar{\equiv}$
and MS: measure moises of att these ions.
Problem: reconstruct protein (diffionto) or peptide (easter) sequence from sets of $b$-and $y$ ions.

give: parent mass $W$ ion mass with alphabet $\sum$ wits mass function $\mu: \Sigma \rightarrow \mathbb{N}$
wantids peptide sequence
approach: NC spectrum graph

for each lon with weight $w_{i}: N_{i}, C_{i}$ with coos dinates

$$
\begin{aligned}
& \operatorname{coovd}\left(N_{0}\right)=0 \\
& \operatorname{cosd}\left(C_{0}\right)=W-18 \\
& \operatorname{coosd}\left(N_{i}\right)=U_{i}-1 \quad \text { for } i=1.1 \\
& \operatorname{cososh}\left(C_{i}\right)=W-W_{i}+1
\end{aligned}
$$

edges $\quad x \rightarrow y=\left\{\begin{array}{l}(1) x, y \text { dump orighete fr } \\ \text { the same ion } I_{k}\end{array}\right.$
(2) $\operatorname{cond}(x)<\operatorname{cosed}(g)$
(3) $\operatorname{cosid}(y)-\operatorname{cosid}(x)$ equals the total mass of Some amino acid (s)
Task (inthe ideal case):
fund a pats from $N_{0}$ do Co through the NC spectrum graph suds that for each ion $I_{k}$, lither $N_{k}$ or $C_{k}$ is used, but nev bots.
Algaith u using DP:
depth - fist scares, with extra condition never to visit $N_{k}$ if $C_{r}$ has already been visited, and vice vasa.
Analysis: dds: $\theta(|E|)$ time extracted: O(IVI) time
overall ran tine: $\frac{\theta(|E| /|V|)}{(\text { fine })}$
bet: potential combinatorial explosion is the ourfont of sequences
III. Protein mass fin gerpricting

$Q Q^{n} a_{0}^{m 2}$ g glom $\mathrm{m}^{m-2}$ and mass $m$, find all $s^{\prime} \in D B$ that contain $m$ as a substring mass.

Q1B: GiveDB and spectrim

$$
Q=\left\{m_{1}, \ldots, m_{r}\right\},
$$

Aho-Comsich
Q2: GirenDB and $Q$ preprocess DB, suidithat questions la and 15 can be oustered faster.
$\rightarrow$ Yes (chech lifereture)
0.3: Given mass $m \in \mathbb{N}$, which strings have mass m?

"mones changing problem coins: 5t,2申, 10申, 20
(a) order matters a RERE
(b) arder des wit matter

Solution by example:

$$
\begin{aligned}
& \Sigma=\{A, B, C\} \\
& \mu(A)=4, \mu(B)=5, \mu(C)=7 \\
& W=13
\end{aligned}
$$

ideas tabulate the numbs of stings with a give mass from oo to $w$


$$
\left|\begin{array}{ll}
A & B \\
B & A \\
A & A
\end{array}\right|
$$

(a) sorbed

$$
A_{2} B_{1} C_{0}
$$

"imodurd (b)
"Componers
composition - mes

