2.1.2 `pairs`: calculate base-pairing observables

Command: `pairs [-T `<u>`temperature`</u>`] [-multi] [-pseudo] [-material `<u>`parameters`</u>`]`
`[-dangles `<u>`treatment`</u>`] [-cutoff `<u>`cutoffvalue`</u>`] `<u>`prefix`</u>

Description: Computes *pair probabilities* $p(i_n \cdot j_m)$ for the complex corresponding to the specified strand ordering π. When `-multi` is selected, also computes the *expected number of base pairs* $E(i_{\{A\}} \cdot j_{\{B\}})$.

Additional option:

> `-cutoff `<u>`cutoffvalue`</u>
> Only probabilities and expected values at or above <u>`cutoffvalue`</u> (default: 0.001) are saved in the output file(s).

Input: Same format as for the executable `pfunc`.

Output: The output is written to the files:

- <u>`prefix`</u>`.ppairs`
  Contains the probability of each type of base pair in the complex. The relevant quantities are $p(i_n \cdot j_m)$, the probability that base i of strand n is paired to base j of strand m in the complex corresponding to strand ordering π. All strands in the complex are considered to be distinct. For example, the two strands labeled 2 in Example 2 are considered distinct. One might think of them as strand $2a$ and $2b$, and a given base of strand $2a$ may have different pair probabilities than the corresponding one in strand $2b$. The total number of bases in the complex is $N = \sum_{l=1}^{L} N_l$, so indexing bases from 1 to N, the pair probabilities can be stored in a symmetric $N \times N$ matrix. Augmentation by an $N + 1$st column containing the probability that each base is unpaired causes the rows to sum to unity.

  By default, the file is formatted as follows. Following header comments, the first entry is the integer N. The remaining entries come in triplets of the form $[i\ \ j\ \ p]$, where $1 \le i \le N$ and $1 \le j \le N+1$ are base numbers and p is the probability of the corresponding pair. Values corresponding to $j = N+1$ represent the probability that base i is unpaired. If `-pseudo` is selected, each row is augmented by two additional columns. The first is the probability that bases i and j form a nested pair and the second is the probability that bases i and j form a non-nested pair. In the case of $j = N + 1$, these additional columns store the probability that bases i and j do not form a nested pair and the probability that they do not form a non-nested pair, respectively.