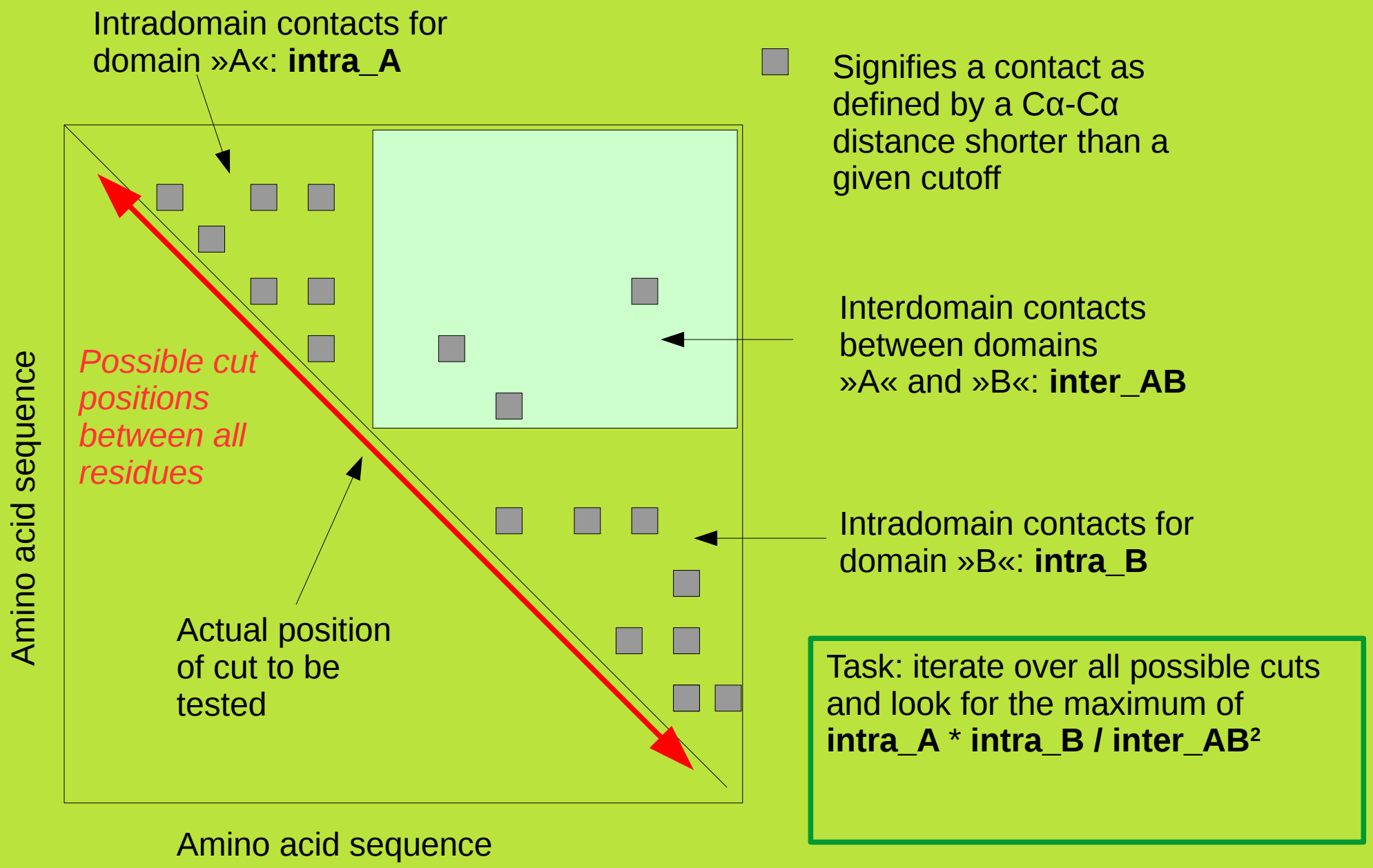
PRACTICAL TASK INFO
concept to be applied



Task: iterate over all possible cuts and look for the maximum of **intra_A * intra_B / inter_AB²**

PRACTICAL TASK INFO
pseudocode for the concept to be applied

```
# initialization
Read PDB, store coordinates of CA atoms
# build CA-CA proximity matrix
for x=2 to chainlength
  for y=1 to x
    if (distance(CA[x],CA[y]) <= cutoff) MATRIX[x][y]=1
# iterate over possible chain cuts
for x=2 to chainlength-1
  intA=intra(1,x)
  intB=intra(x+1,chainlength)
  extAB=inter(1,x,x+1,chainlength)
  print x, (intA*intB)/(extAB^2)
# subroutines
function intra(a,b)
  for x=a to b
    for y=a+1 to b
      intradomain+=MATRIX[x][y]
  return intradomain
function inter(a,b,c,d)
  for x=a to b
    for y=c to d
      interdomain+=MATRIX[x][y]
  Return interdomain
```

You can use any programming language you want. The instructor will provide some hints on how to start the implementation in Python (a Jupyter notebook).

Note that this is a pseudocode and contains the main steps only (e.g. variable initialization is omitted completely).

Application of the code to the structure 1GPZ