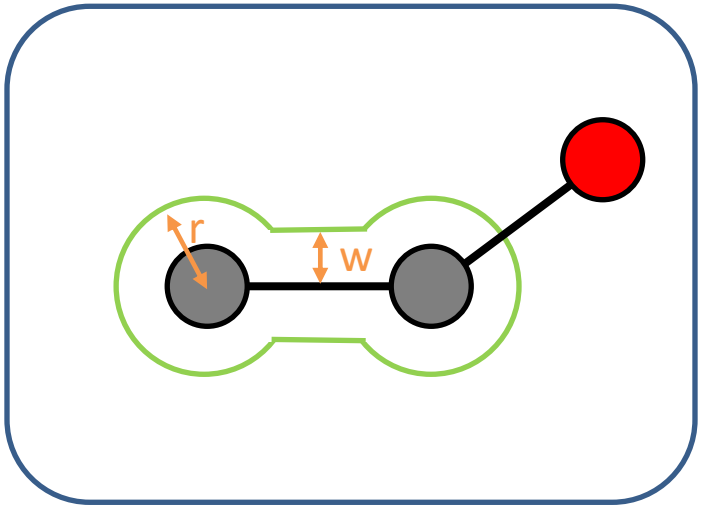
Lasso Substructure Highlighting

Parameter Definition

- *avg_len*: Average bond length
- *r*: circle radius
- *w*: width of bond

- *rel_radius*: radius relative to *avg_len*
  - $r = rel\_radius \cdot avg\_len$
  - $0 < r\_rel$

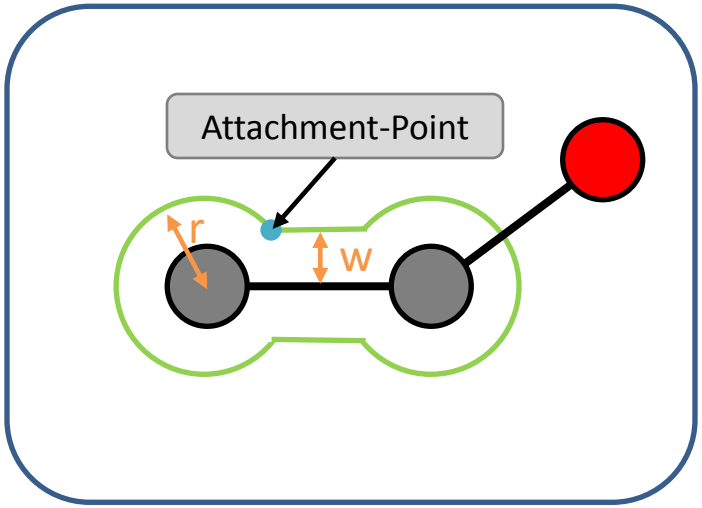
- *rel_width*: width relative to *r*
  - $w = rel\_width \cdot r$
  - $0 < rel\_width \leq 1$



Exemplary highlighting of carbons in ethanol

Attachment-Points

- Highlighting consists of:
  - circles around atoms
  - bond-edging
- Attachment-Points:
  - connection between circles and edging
  - saved as polar-coordinates
    - atom-position is origin
- Polar Coordinates:
  - distance to atom: *d*
  - angle in radiant: *alpha*
    - 0 corresponds to north

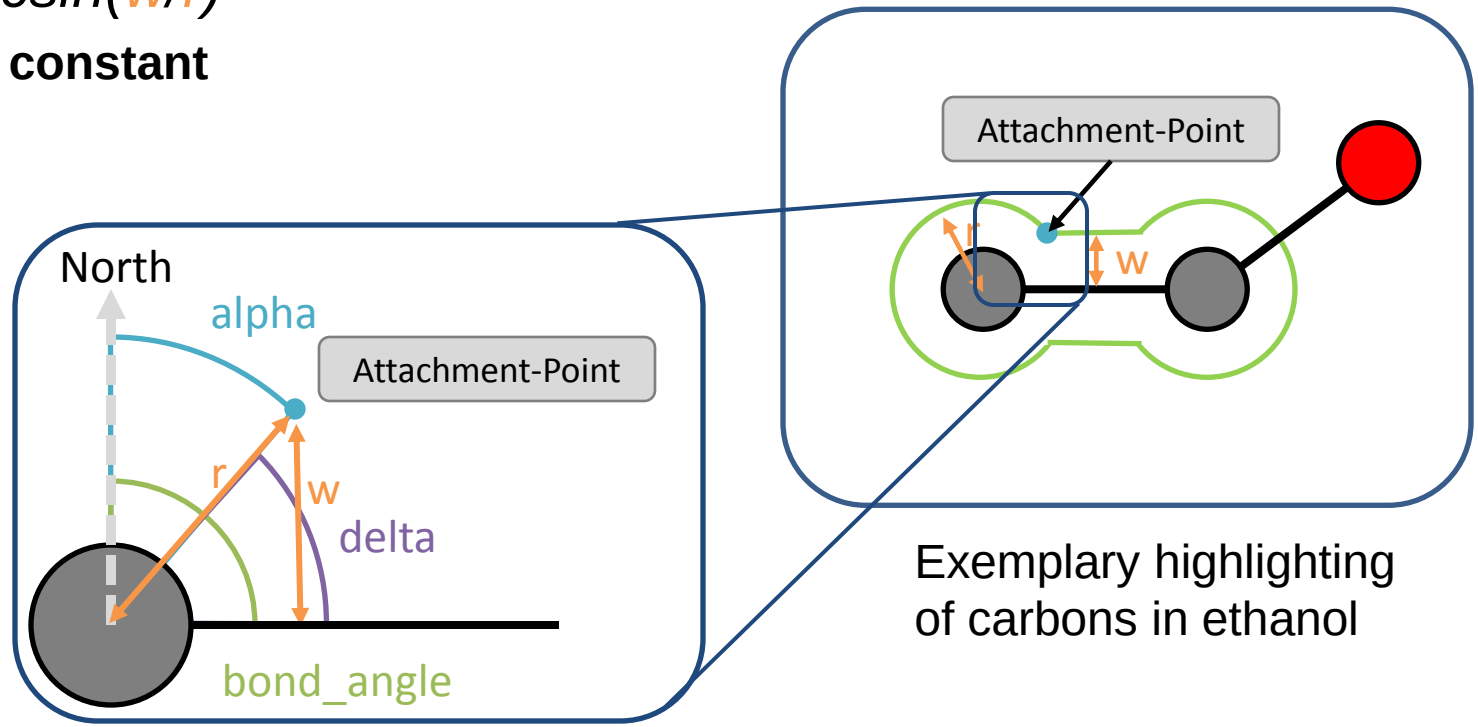


Exemplary highlighting of carbons in ethanol

Left Attachment-Point

- Calculations:
  - distance to atom: *d* = *r*
  - angle in radiant: *alpha* = bond_angle - delta

- *delta* = *arcsin(w/r)*
  - *delta* **is constant**

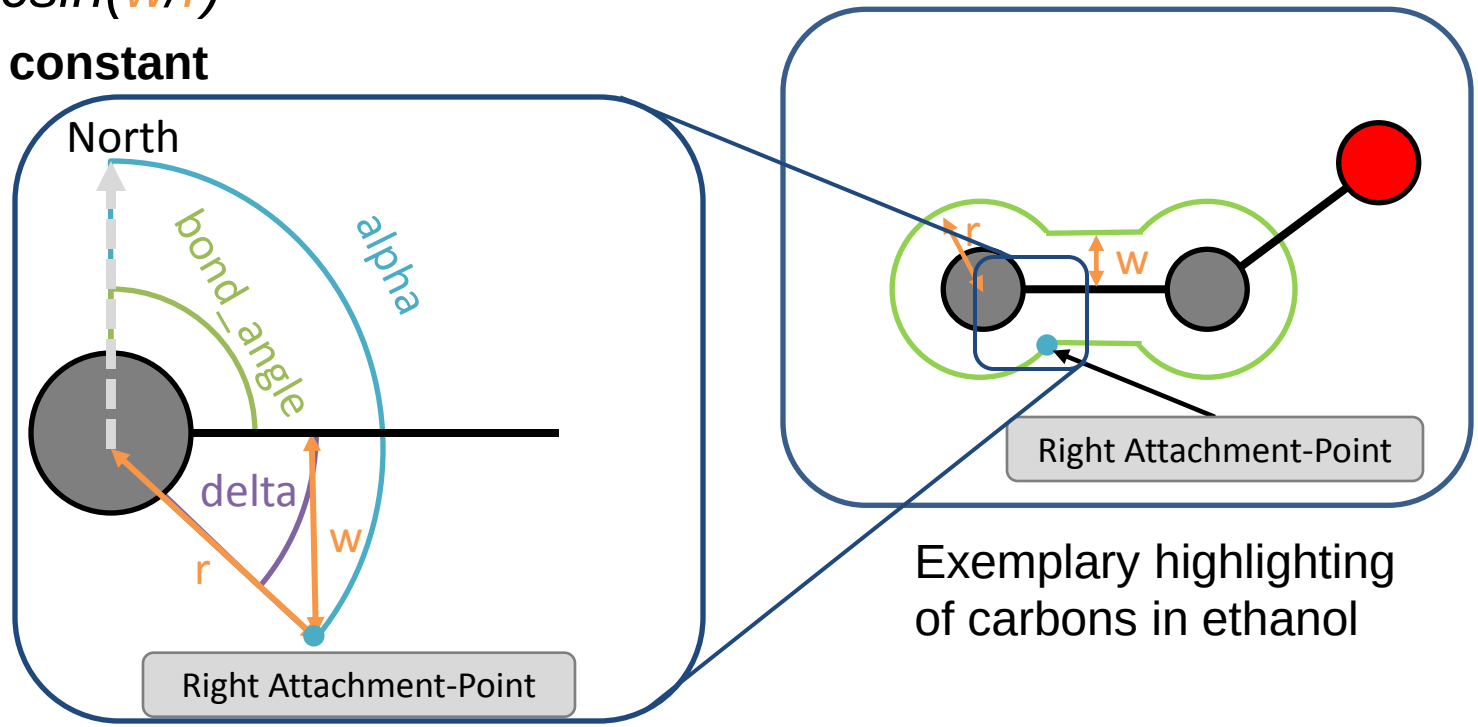


Exemplary highlighting of carbons in ethanol

Right Attachment-Point

- Calculations:
  - distance to atom: *d* = *r*
  - angle in radiant: *alpha* = bond_angle **+** delta

- *delta* = *arcsin(w/r)*
  - *delta* **is constant**

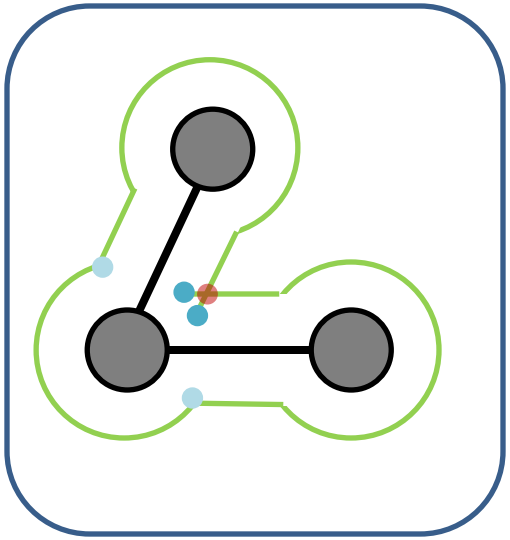


Exemplary highlighting of carbons in ethanol

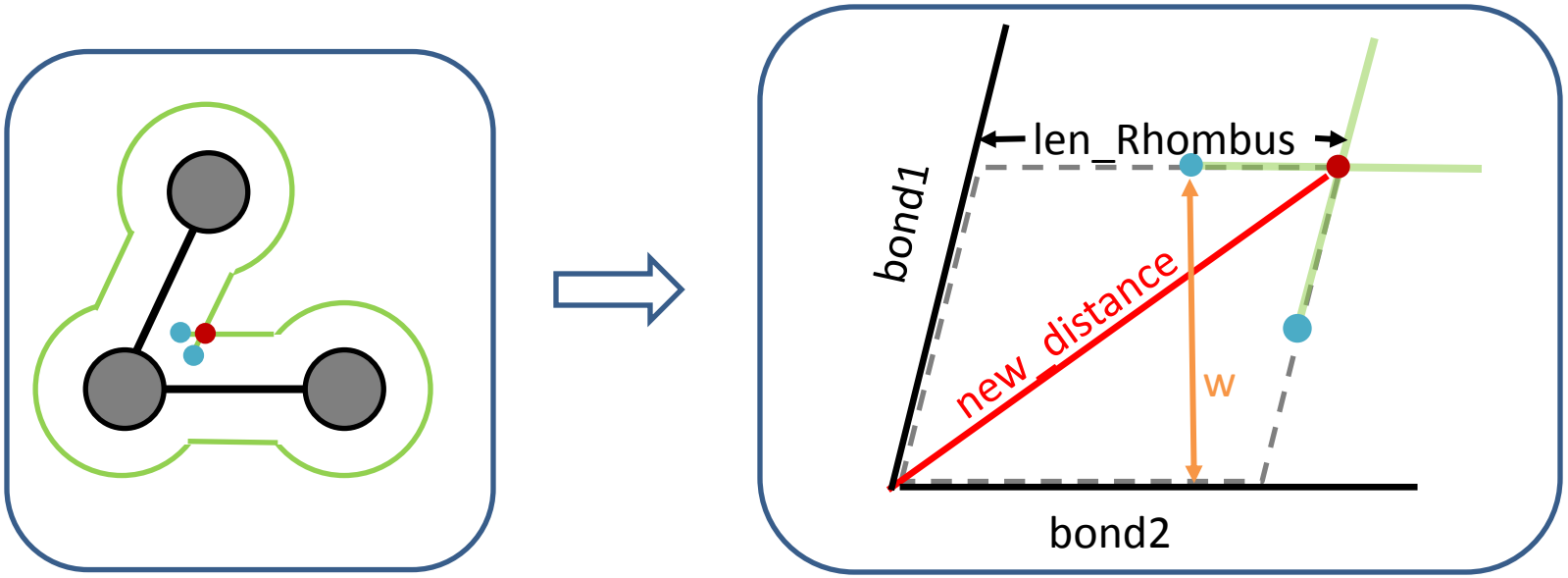
Intersecting Attachment-Points

- For atoms with small angles between bonds
  - right Attachment-Point (bond1_rAT) may have greater alpha than left Attachment-Point of following bond (bond2_lAT)

- New Attachment-Point needed
  - angle: mean of angles:
    - bond1_rAT & bond2_lAT
  - distance: next slide



Intersecting Attachment-Points



- Distance for new Attachment-Point:
  - Angle of rhombus:
    a_rhombus = *bond2.*angle - *bond1.*angle
  - Height of rhombus:
    h_rhombus = w
  - Side length:
    len_rhombus = *h_rhombus* / sin(*a_rhombus*)
  - new_distance = 2 *len_rhombus* · *cos(a_rhombus* / 2)

Workflow

1) Calculation of average bond length (*avg_len*)
2) Calculation of *w*, *r* and *delta* from *avg_len* (Slide 2 & 4)
3) Determining atoms and bonds between selected atoms
4) Calculation of Attachment-Points (AT)
    1) calculation of bond angles
    2) calculation of left and right ATt (Slide 4 & 5)
        - left AT: distance = r, angle = bond-angle – delta
        - right AT: distance = r, angle = bond-angle + delta
    3) checking for intersecting AT (Slide 6)
        - when $bond_i$ and $bond_{i+1}$ intersect:
          right AT of $bond_i$ & left AT of $bond_{i+1}$ are adapted (Slide 6 & 7)

Workflow

5) Drawing arches between:
   - right AT
   - and left AT of following bond
6) Drawing lines between:
   - left AT from atom i
   - and right AT from atom j
   - if ATs are for same bond
7) Drawing lines between:
   - right AT from atom i
   - and left AT from atom j
   - if ATs are for same bond