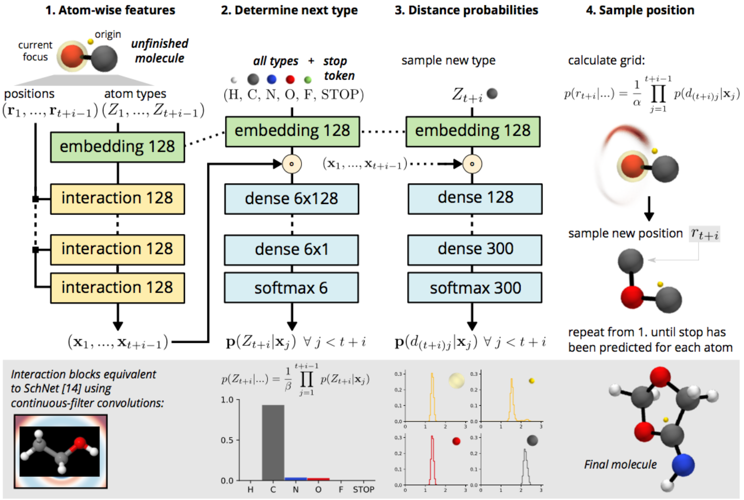
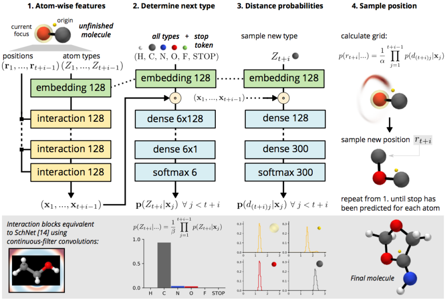
G-SchNet

October 29, 2020


1. Atom-wise features
2. Determine next type
3. Distance probabilities
4. Sample position
current focus
origin
unfinished molecule
positions
atom types
$(\mathbf{r}_1, \ldots, \mathbf{r}_{t+i-1})\ (Z_1, \ldots, Z_{t+i-1})$
embedding 128
interaction 128
interaction 128
interaction 128
$(\mathbf{x}_1, \ldots, \mathbf{x}_{t+i-1})$
all types + stop token
(H, C, N, O, F, STOP)
embedding 128
dense 6x128
dense 6x1
softmax 6
$\mathbf{p}(Z_{t+i}|\mathbf{x}_j)\ \forall\, j < t+i$
sample new type
Z_{t+i}
embedding 128
$(\mathbf{x}_1, \ldots, \mathbf{x}_{t+i-1})$
dense 128
dense 300
softmax 300
$\mathbf{p}(d_{(t+i)j}|\mathbf{x}_j)\ \forall\, j < t+i$
calculate grid:
$p(r_{t+i}|\ldots) = \frac{1}{\alpha} \prod_{j=1}^{t+i-1} p(d_{(t+i)j}|\mathbf{x}_j)$
sample new position r_{t+i}
repeat from 1. until stop has been predicted for each atom
Interaction blocks equivalent to SchNet [14] using continuous-filter convolutions:
$p(Z_{t+i}|\ldots) = \frac{1}{\beta} \prod_{j=1}^{t+i-1} p(Z_{t+i}|\mathbf{x}_j)$
1.0
0.5
0.0
H C N O F STOP
Final molecule

$$\mathbf{R}^{t}_{\leq i} = (\mathbf{r}_1, \ldots, \mathbf{r}_t, \mathbf{r}_{t+1}, \ldots, \mathbf{r}_{t+i})$$

$$\mathbf{R}^t_{\leq i} = (\mathbf{r}_1, ..., \mathbf{r}_t, \mathbf{r}_{t+1}, ..., \mathbf{r}_{t+i})$$
$$\mathbf{Z}^t_{<i} = (Z_1, ..., Z_t, Z_{t+1}, ..., Z_{t+i})$$



1. Atom-wise features
2. Determine next type
3. Distance probabilities
4. Sample position
current focus
origin
unfinished molecule
positions
atom types
$(\mathbf{r}_1, ..., \mathbf{r}_{t+i-1})$ $(Z_1, ..., Z_{t+i-1})$
embedding 128
interaction 128
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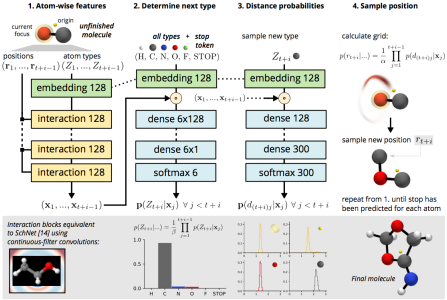
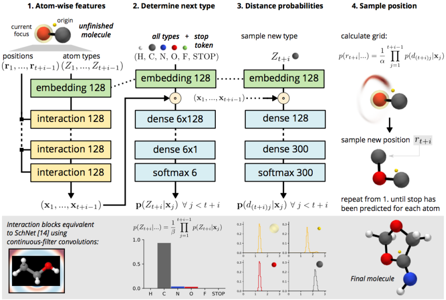
$(\mathbf{x}_1, ..., \mathbf{x}_{t+i-1})$
all types + stop token
(H, C, N, O, F, STOP)
embedding 128
dense 6x128
dense 6x1
softmax 6
$\mathbf{p}(Z_{t+i}|\mathbf{x}_j)\ \forall j < t+i$
sample new type
Z_{t+i}
embedding 128
$(\mathbf{x}_1, ..., \mathbf{x}_{t+i-1})$
dense 128
dense 300
softmax 300
$\mathbf{p}(d_{(t+i)j}|\mathbf{x}_j)\ \forall j < t+i$
calculate grid:
$p(r_{t+i}|...) = \frac{1}{\alpha}\prod_{j=1}^{t+i-1} p(d_{(t+i)j}|\mathbf{x}_j)$
sample new position r_{t+i}
repeat from 1. until stop has been predicted for each atom
Interaction blocks equivalent to SchNet [14] using continuous-filter convolutions:
$p(Z_{t+i}|...) = \frac{1}{\beta}\prod_{j=1}^{t+i-1} p(Z_{t+i}|\mathbf{x}_j)$
1.0
0.5
0.0
H
C
N
O
F
STOP
Final molecule



$$p(\mathbf{R}_{\leq n}, \mathbf{Z}_{\leq n}) = \prod_{i=1}^{n} \left[p\left(\mathbf{r}_{t+i}, Z_{t+i} | \mathbf{R}^t_{\leq i-1}, \mathbf{Z}^t_{\leq i-1}\right)\right] \cdot p(stop|\mathbf{R}^t_{\leq n}, \mathbf{Z}^t_{\leq n}) \tag{1}$$



$$p(\mathbf{R}_{\leq n}, \mathbf{Z}_{\leq n}) = \prod_{i=1}^{n} \left[p\left(\mathbf{r}_{t+i}, Z_{t+i} | \mathbf{R}^t_{\leq i-1}, \mathbf{Z}^t_{\leq i-1}\right) \right] \cdot p(stop | \mathbf{R}^t_{\leq n}, \mathbf{Z}^t_{\leq n}) \quad (1)$$

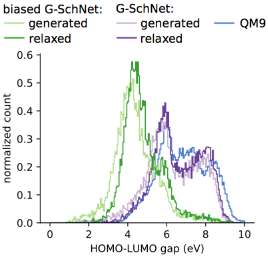
$$p\left(\mathbf{r}_{t+i}, Z_{t+i} | \mathbf{R}^t_{\leq i-1}, \mathbf{Z}^t_{\leq i-1}\right) = p(\mathbf{r}_{t+i} | Z_{t+i}, \mathbf{R}^t_{\leq i-1}, \mathbf{Z}^t_{\leq i-1})\, p(Z_{t+i} | \mathbf{R}^t_{\leq i-1}, \mathbf{Z}^t_{\leq i-1}) \quad (2)$$

$$\mathbf{p}_i^{\text{type}} = \frac{1}{\beta} \prod_{j=1}^{t+i-1} \mathbf{p}(Z_{t+i} | \mathbf{x}_j)$$

$$p(\mathbf{r}_{t+i}|\mathbf{R}^t_{\leq i-1}, \mathbf{Z}^t_{\leq i}) = \frac{1}{\alpha} \prod_{j=1}^{t+i-1} p(d_{(t+i)j}|\mathbf{R}^t_{\leq i-1}, \mathbf{Z}^t_{\leq i}). \tag{3}$$

$$\mathbf{p}_{ij}^{\text{dist}} = \mathbf{p}(d_{(t+i)j} | \mathbf{x}_j)$$

$$H\left(\mathbf{Q}_i, \mathbf{P}_i\right) = \underbrace{-\sum_{k=1}^{n_{\text{types}}} \left[\mathbf{q}_i^{\text{type}}\right]_k \cdot \log\left[\mathbf{p}_i^{\text{type}}\right]_k}_{\textit{cross-entropy of types}} \underbrace{-\frac{1}{t+i-1} \sum_{j=1}^{t+i-1} \sum_{l=1}^{n_{\text{bins}}} \left[\mathbf{q}_{ij}^{\text{dist}}\right]_l \cdot \log\left[\mathbf{p}_{ij}^{\text{dist}}\right]_l}_{\textit{average cross-entropy of distances}}$$


biased G-SchNet:
generated
relaxed
G-SchNet:
generated
relaxed
QM9
normalized count
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0
2
4
6
8
10
HOMO-LUMO gap (eV)