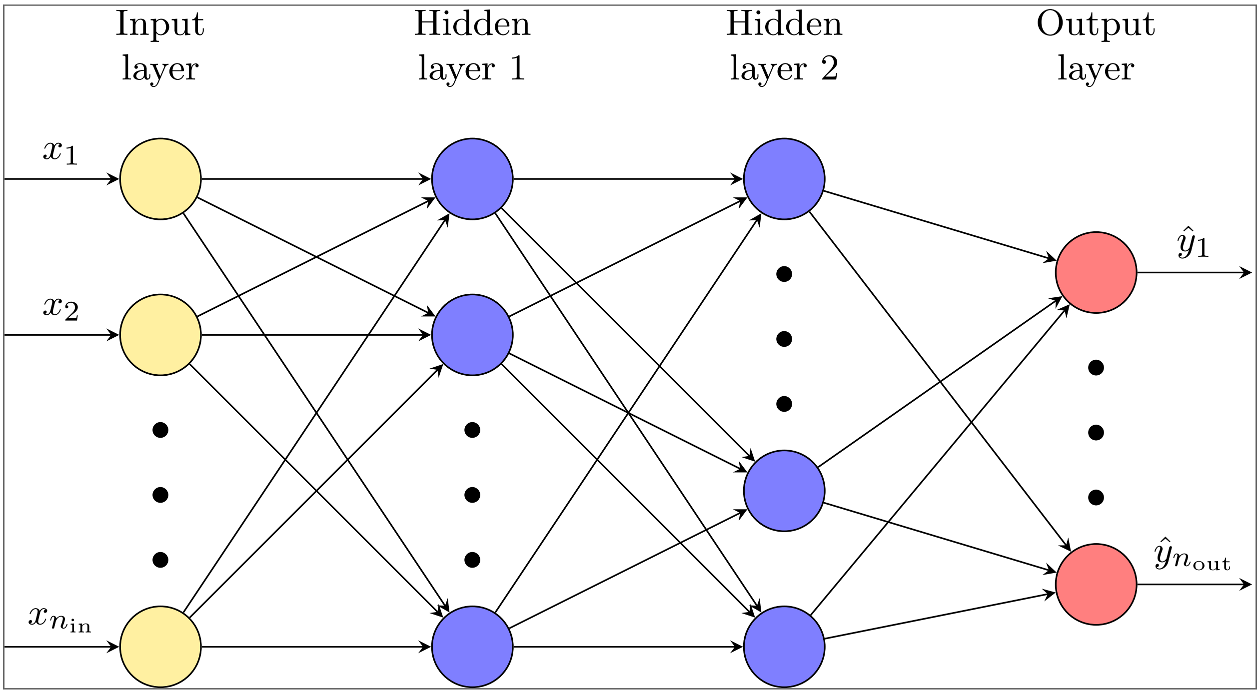
SchNet

and

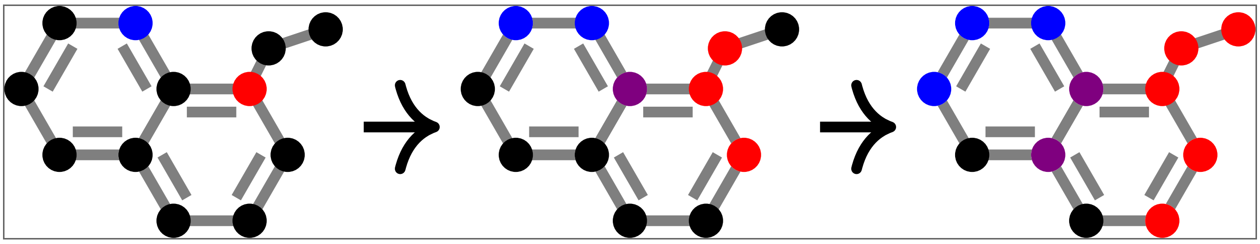
PaiNN

GNNs

and Message Passing

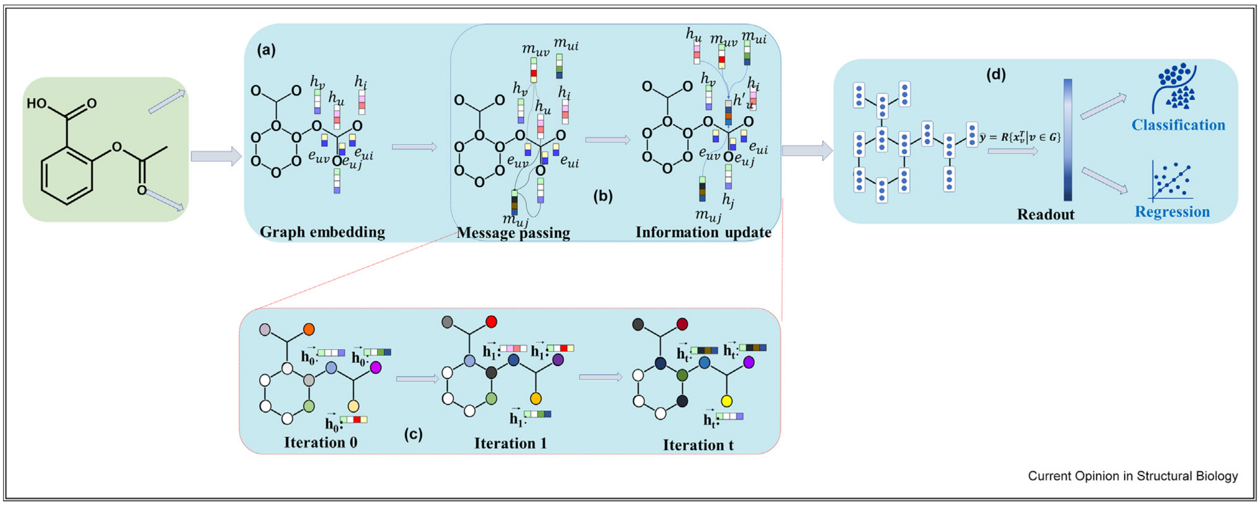

Input layer
Hidden layer 1
Hidden layer 2
Output layer
x_1
x_2
$x_{n_{\text{in}}}$
$\hat{y}_1$
$\hat{y}_{n_{\text{out}}}$

$$
\begin{bmatrix}
0 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
*
\begin{bmatrix}
1 & 0 & 1 \\
0 & 1 & 0 \\
1 & 0 & 1
\end{bmatrix}
=
\begin{bmatrix}
1 & 4 & 3 & 4 & 1 \\
1 & 2 & 4 & 3 & 3 \\
1 & 2 & 3 & 4 & 1 \\
1 & 3 & 3 & 1 & 1 \\
3 & 3 & 1 & 1 & 0
\end{bmatrix}
$$



$$\mathbf{m}_i^{t+1} = \sum_{j \in \mathcal{N}(i)} \mathbf{M}_t(\mathbf{s}_i^t, \mathbf{s}_j^t, \vec{r}_{ij})$$

$$\mathbf{s}_i^{t+1} = \mathbf{U}_t(\mathbf{s}_i^t, \mathbf{m}_i^{t+1})$$


(a)
Graph embedding
Message passing
(b)
Information update
(c)
Iteration 0
Iteration 1
Iteration t
(d)
Readout
Classification
Regression
Current Opinion in Structural Biology

Invariance

and

Equivariance

$$f : \mathbb{V} \to \mathbb{W} \qquad G : \begin{cases} \mathbb{V} \to \mathbb{V} \\ \mathbb{W} \to \mathbb{W} \end{cases}$$

---

f invariant *wrt* G:

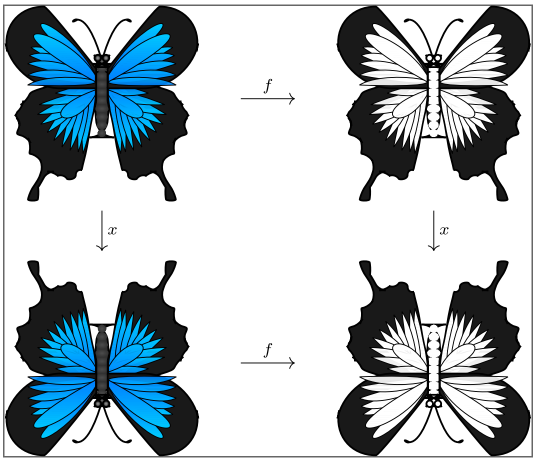
$$f(x \cdot v) = f(v) \quad \forall v \in \mathbb{V}, x \in G$$

f equivariant *wrt* G:

$$f(x \cdot v) = x \cdot f(v) \quad \forall v \in \mathbb{V}, x \in G$$

$$G = \{e, \sigma\}$$

$$f(r, g, b) = \begin{cases} (0, 0, 0) & \text{if } r = g = b = 0 \\ (255, 255, 255) & \text{otherwise} \end{cases}$$



$$f(x \cdot v) = x \cdot f(v)$$

$$R \cdot \vec{\mathrm{f}}(\vec{\mathrm{x}}) = \vec{\mathrm{f}}(R \cdot \vec{\mathrm{x}})$$

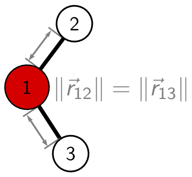
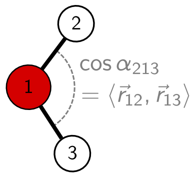
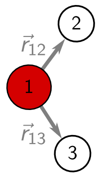
$$\mathbf{s}' = \mathbf{f}(\mathbf{s}) \qquad \vec{\mathbf{v}}' = \mathbf{s} \circ \vec{\mathbf{v}}$$

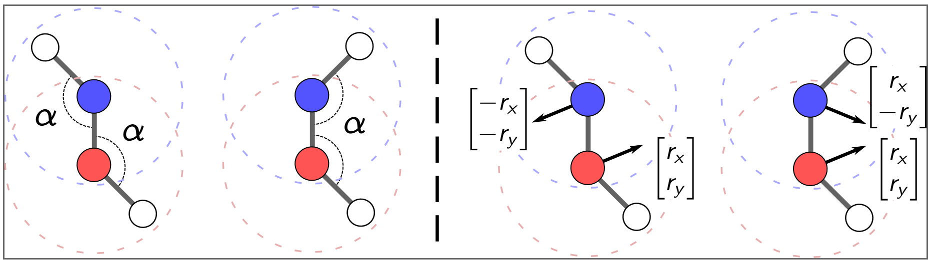
$$\mathbf{s}' = \|\mathbf{s}\|^2 \qquad \vec{\mathbf{v}}' = \mathbf{W}\vec{\mathbf{v}}$$

$$\mathbf{s}' = \langle \vec{\mathbf{v}}_1, \vec{\mathbf{v}}_2 \rangle \qquad \vec{\mathbf{v}}' = \vec{\mathbf{v}}_1 \times \vec{\mathbf{v}}_2$$

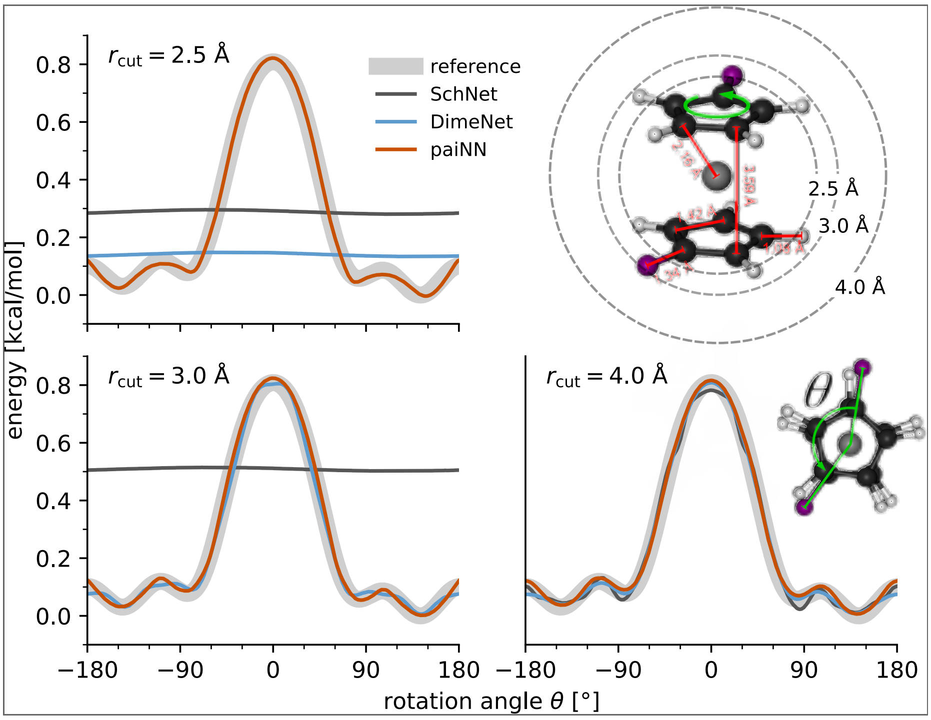
Equivariance

Rationale

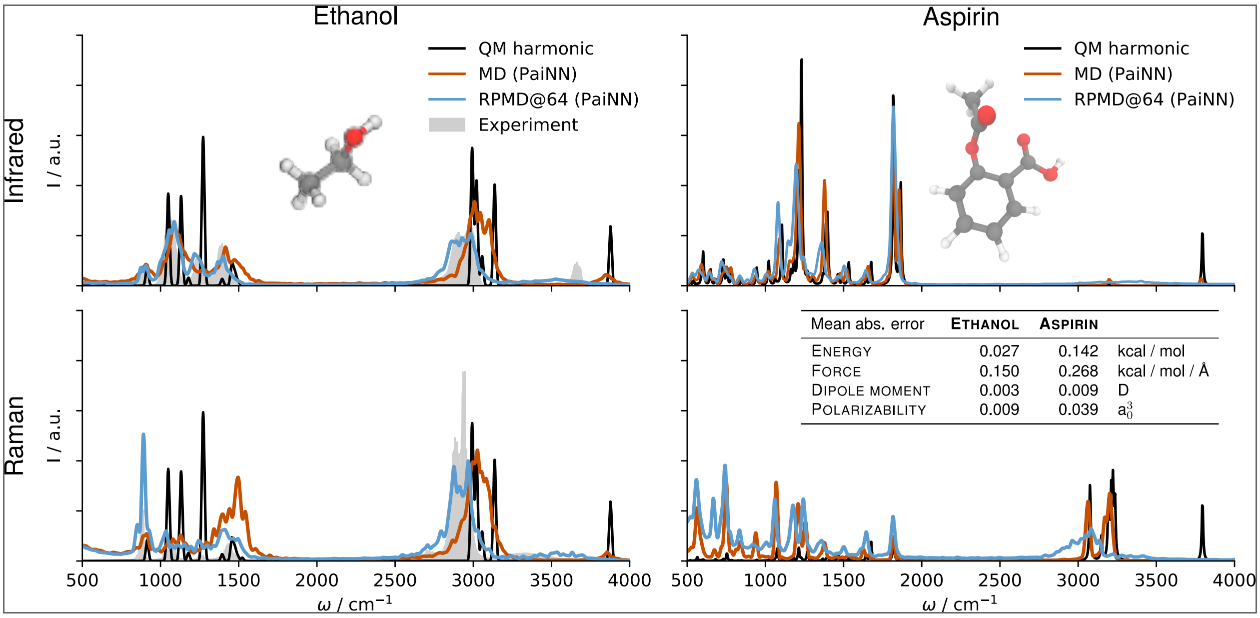
Features	**Distances**	**Angles**	**Directions**
H_2O			
Message M ***at atom*** i	$\sum_{j\in\mathcal{N}_i} \lVert\vec{r}_{ij}\rVert$	$\sum_{j\in\mathcal{N}_i}\sum_{k\in\mathcal{N}_i} \alpha_{jik}$	$\sum_{j\in\mathcal{N}_i} \frac{\vec{r}_{ij}}{\lVert\vec{r}_{ij}\rVert}$
Scaling with neighbors	$\mathcal{O}(\lvert\mathcal{N}\rvert)$	$\mathcal{O}(\lvert\mathcal{N}\rvert^2)$	$\mathcal{O}(\lvert\mathcal{N}\rvert)$
Resolve change of $\lVert\vec{r}_{1j}\rVert$	yes	no	no
Resolve change of α_{213}	no	yes	yes



$$\left\| \sum_{j=1}^{N} \frac{\vec{r}_{ij}}{\|\vec{r}_{ij}\|} \right\|^2 = \sum_{j,k} \left\langle \frac{\vec{r}_{ij}}{\|\vec{r}_{ij}\|}, \frac{\vec{r}_{ik}}{\|\vec{r}_{ik}\|} \right\rangle = \sum_{j=1}^{N} \sum_{k=1}^{N} \cos \alpha_{jik}$$



$r_{cut} = 2.5$ Å
reference
SchNet
DimeNet
paiNN
2.5 Å
3.0 Å
4.0 Å
$r_{cut} = 3.0$ Å
$r_{cut} = 4.0$ Å
θ
energy [kcal/mol]
rotation angle θ [°]



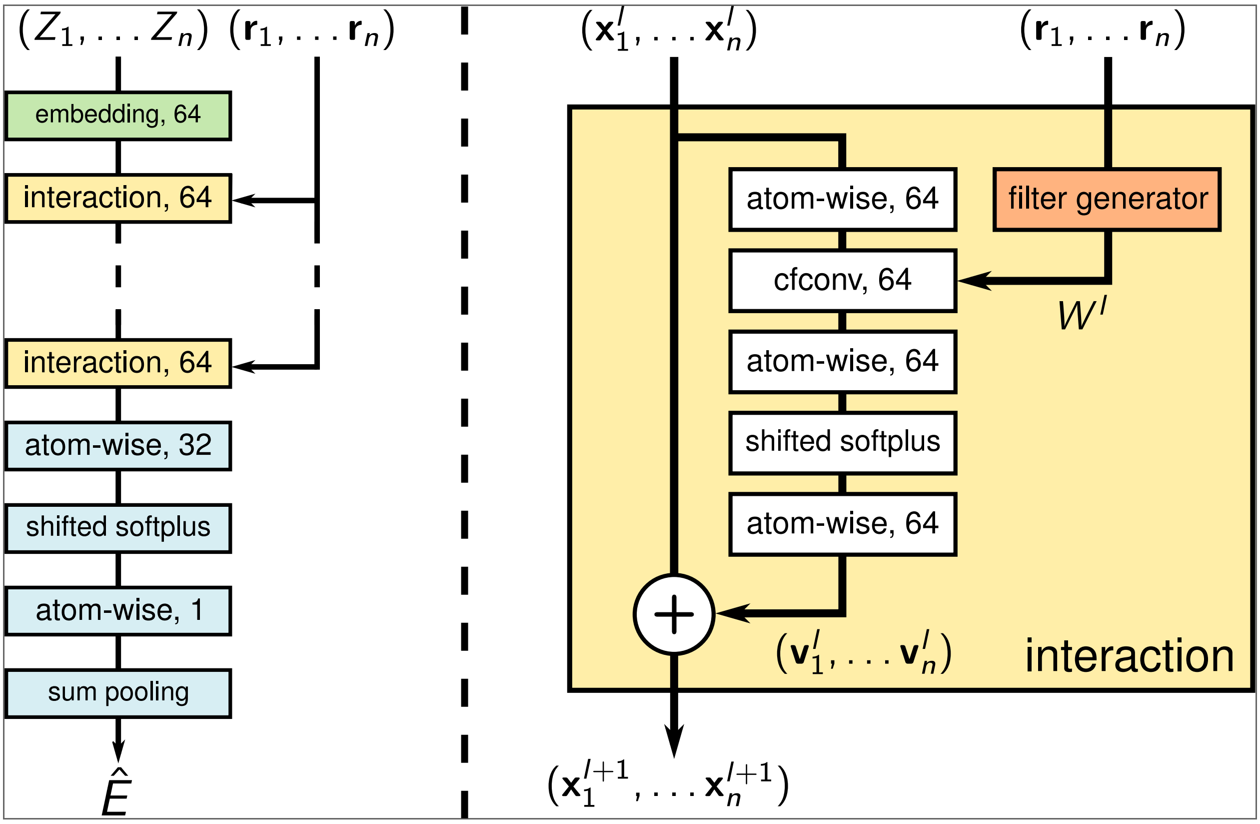
Mean abs. error	ETHANOL	ASPIRIN	
ENERGY	0.027	0.142	kcal / mol
FORCE	0.150	0.268	kcal / mol / Å
DIPOLE MOMENT	0.003	0.009	D
POLARIZABILITY	0.009	0.039	a_0^3

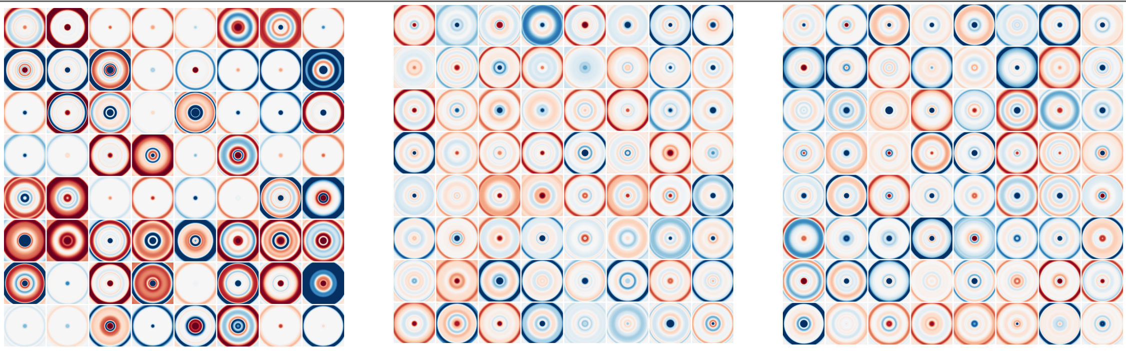
$$\vec{\mu} = \sum_{i=1}^{N} \vec{\mu}_{\text{atom}}(\vec{\mathbf{v}}_i) + q_{\text{atom}}(\mathbf{s}_i)\vec{r}_i$$

SchNet

workings

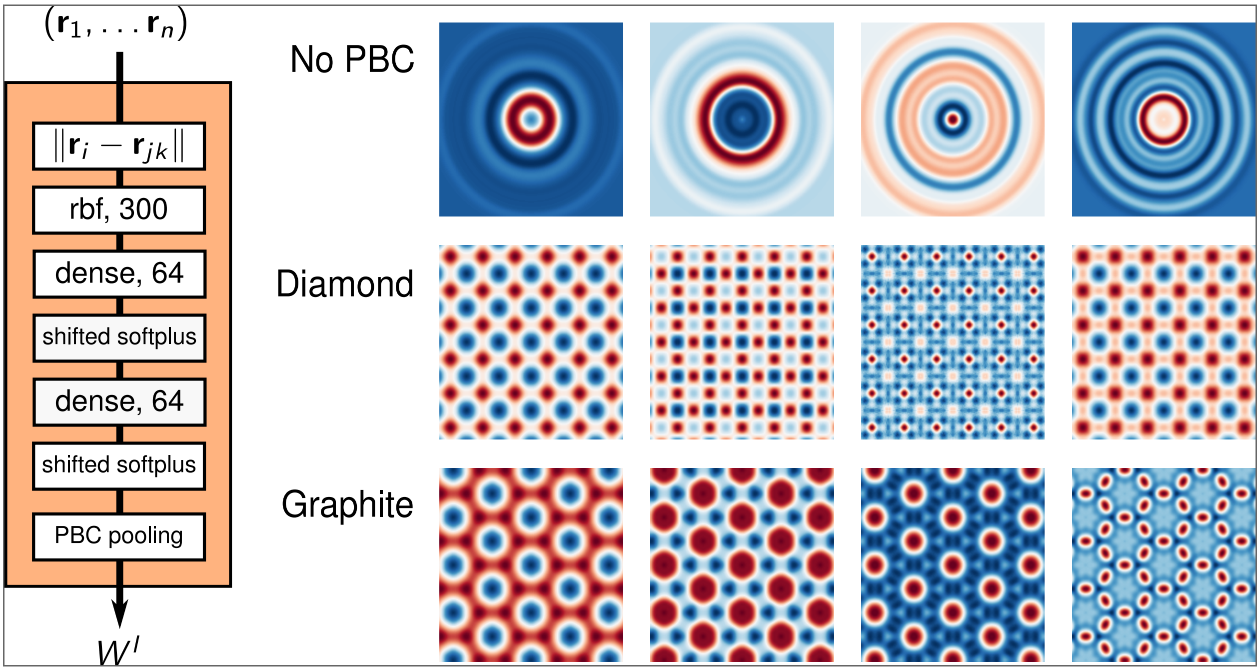
$$\mathrm{ssp}(x) = \ln(0.5e^{0.5} + 0.5)$$


$(Z_1, \dots Z_n)$
$(\mathbf{r}_1, \dots \mathbf{r}_n)$
embedding, 64
interaction, 64
interaction, 64
atom-wise, 32
shifted softplus
atom-wise, 1
sum pooling
$\hat{E}$
$(\mathbf{x}_1^l, \dots \mathbf{x}_n^l)$
$(\mathbf{r}_1, \dots \mathbf{r}_n)$
atom-wise, 64
filter generator
cfconv, 64
W^l
atom-wise, 64
shifted softplus
atom-wise, 64
$(\mathbf{v}_1^l, \dots \mathbf{v}_n^l)$
interaction
$(\mathbf{x}_1^{l+1}, \dots \mathbf{x}_n^{l+1})$



(a) 1st interaction block (b) 2nd interaction block (c) 3rd interaction block

Figure 3: 10x10 Å cuts through all 64 radial, three-dimensional filters in each interaction block of SchNet trained on molecular dynamics of ethanol. Negative values are blue, positive values are red.



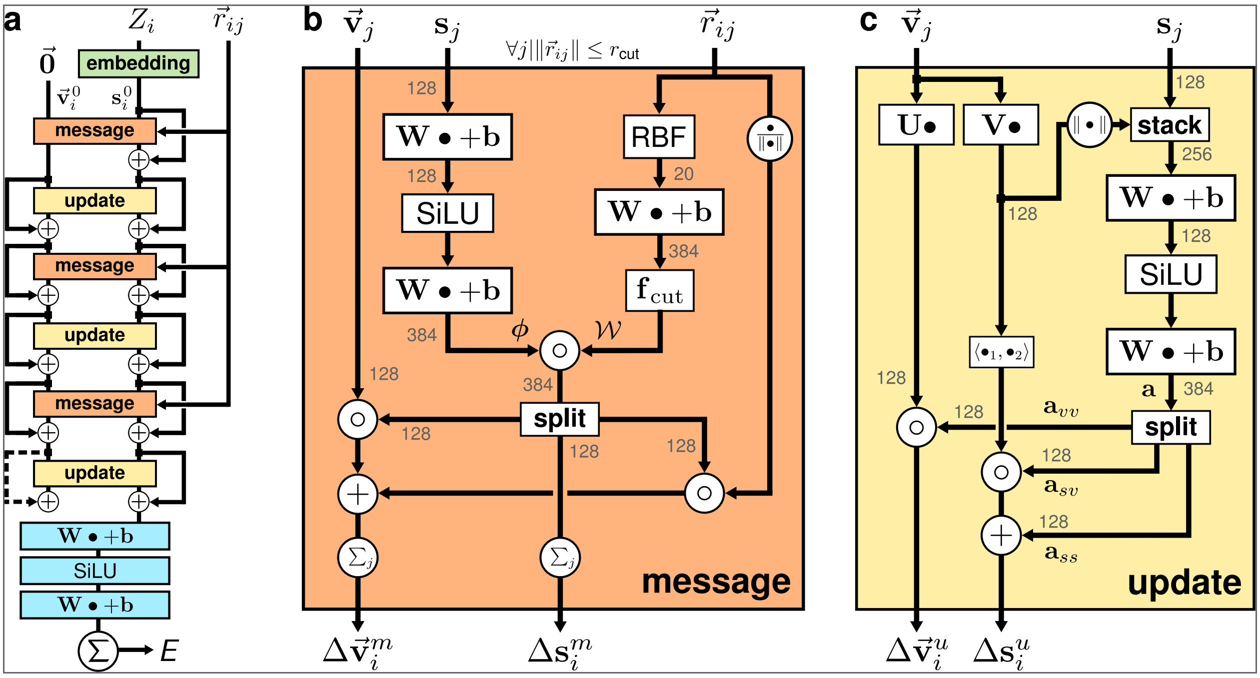
$$e_k(r_{ij}) = \exp(-\gamma \|r_{ij} - \mu_k\|^2)$$

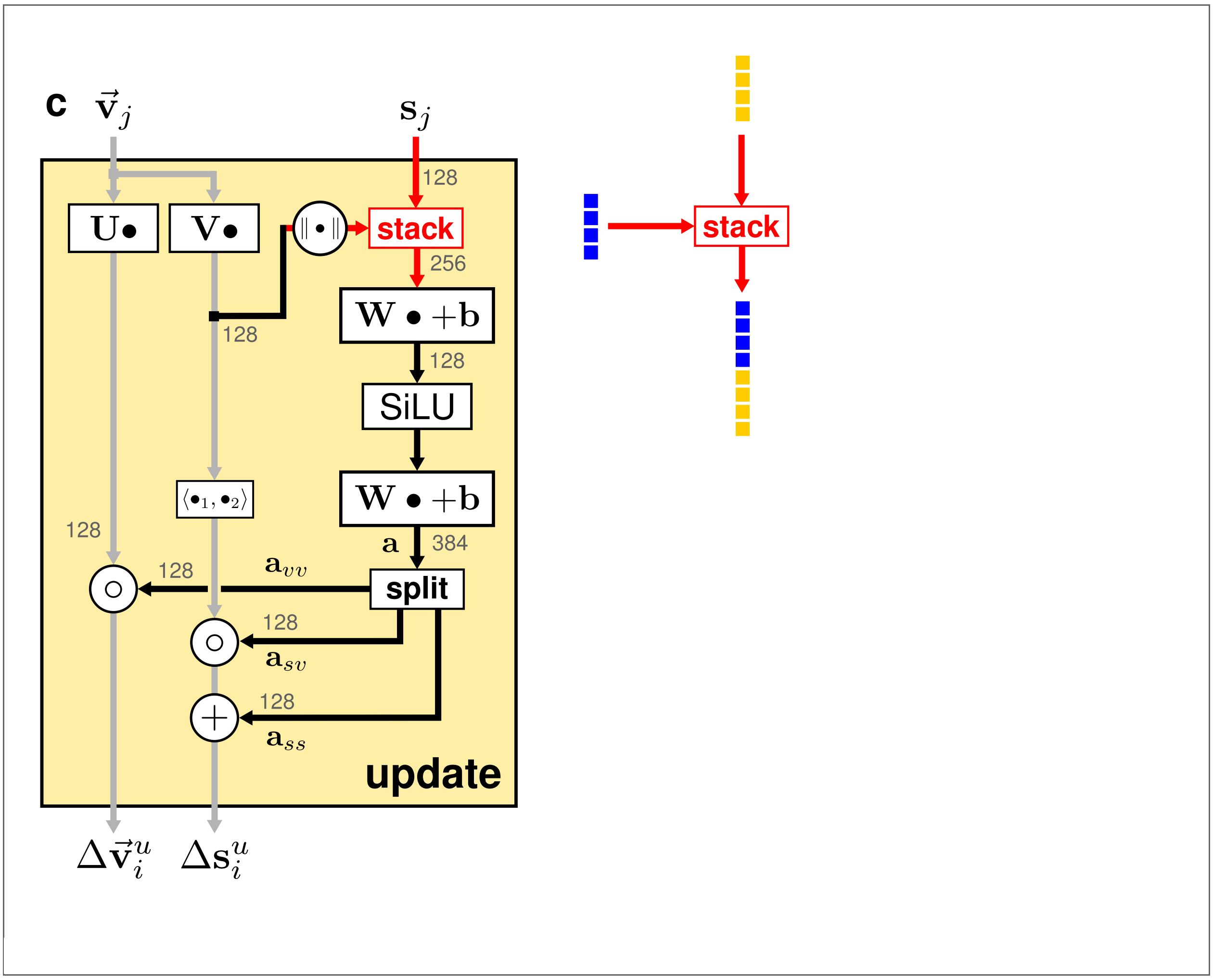
PaiNN

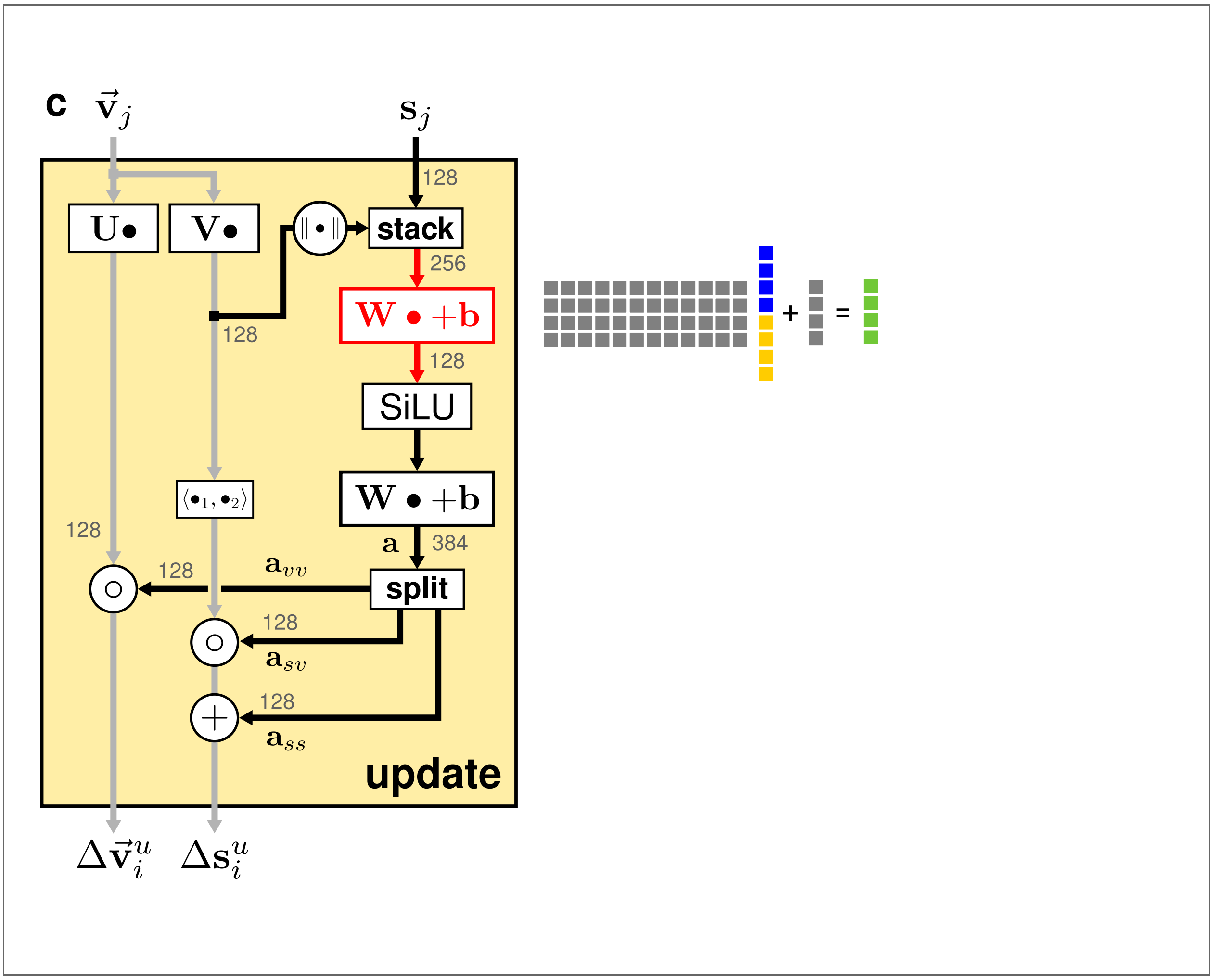
workings

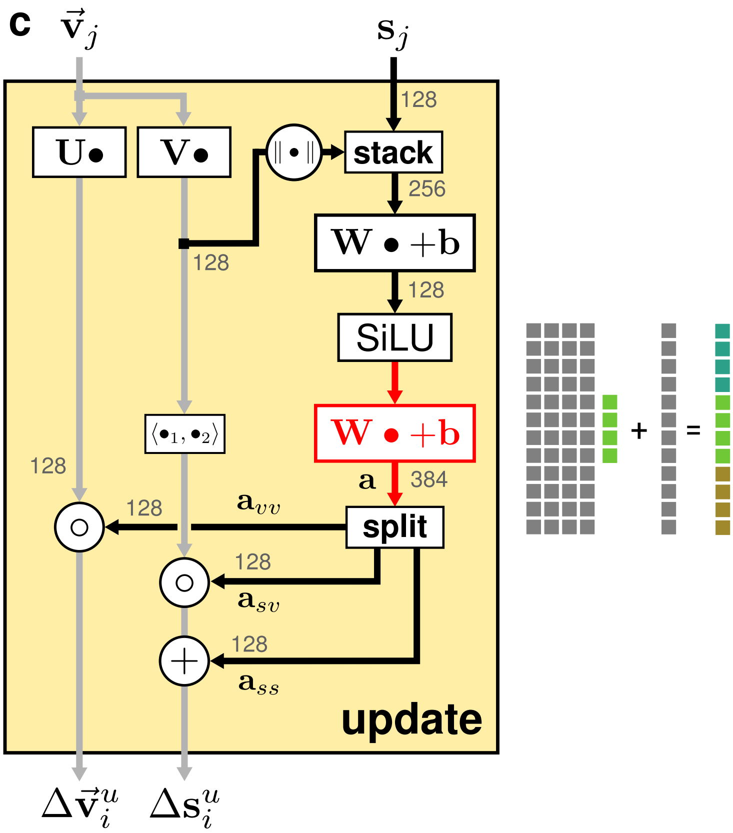
$$\mathrm{SiLU}(x) = \frac{x}{1 + e^{-k(x-x_0)}}$$

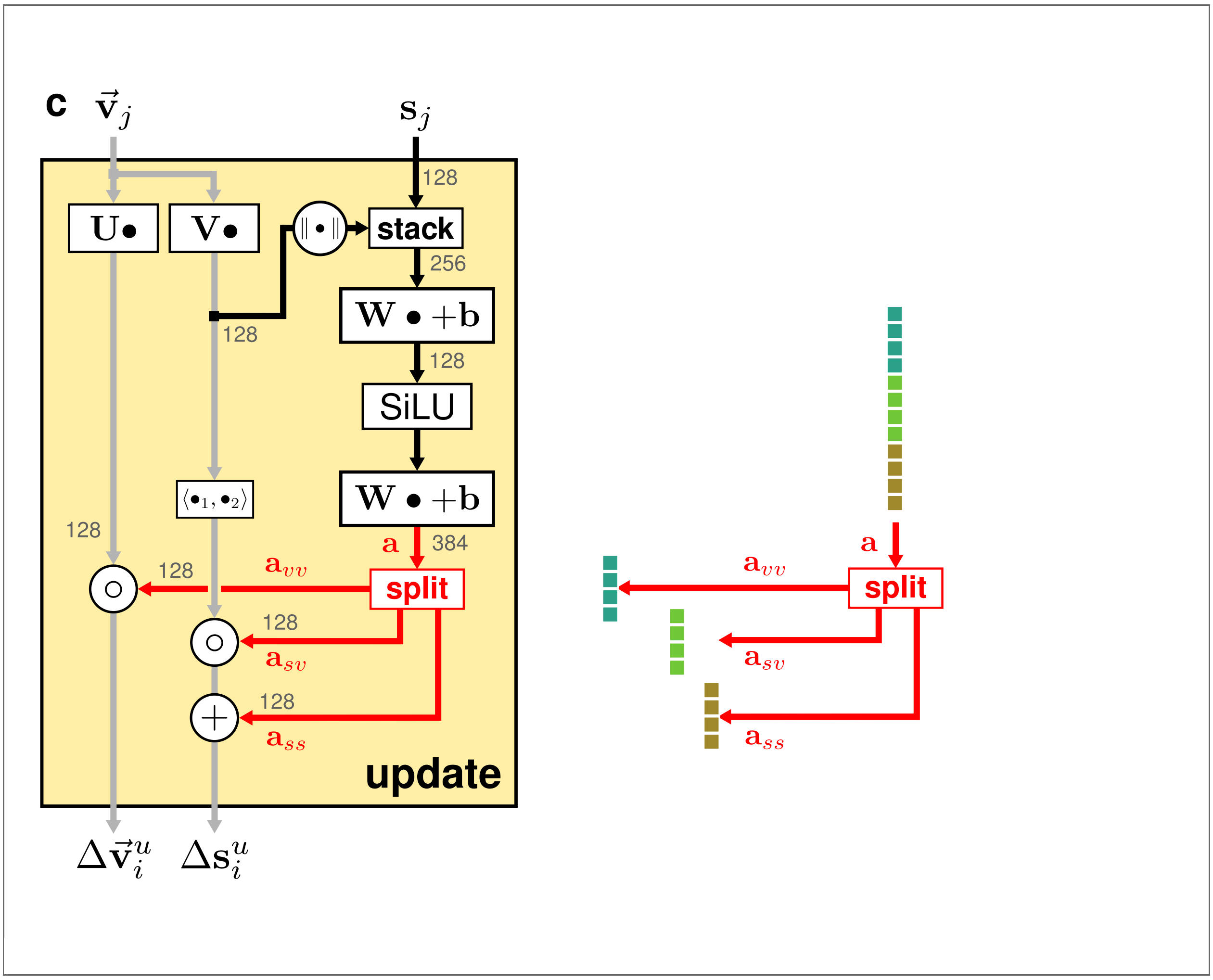
$$RBF(\vec{r}_{i,j}, n) = \frac{\sin\left(n\pi\frac{\|\vec{r}_{i,j}\|}{r_{\text{cut}}}\right)}{\|\vec{r}_{i,j}\|}$$

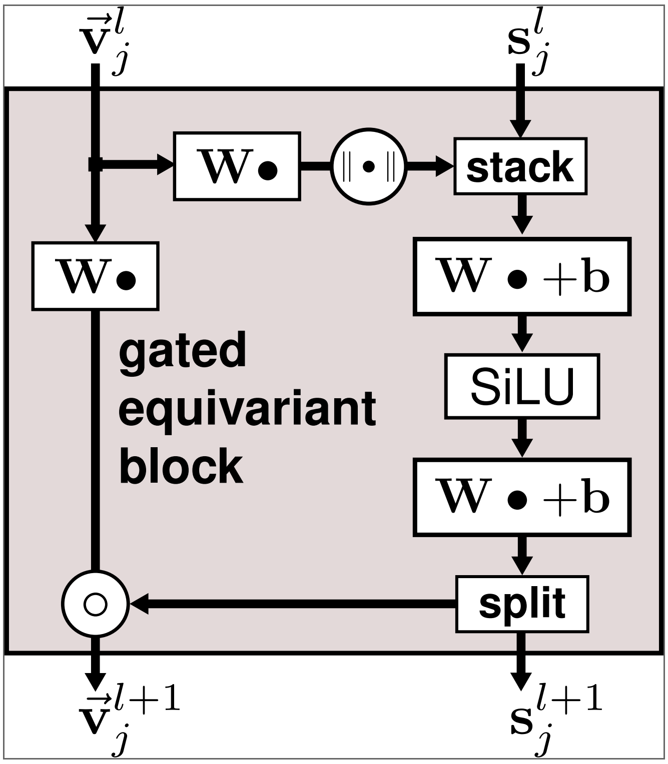

a
Z_i
$\vec{r}_{ij}$
$\vec{0}$
embedding
$\vec{\mathbf{v}}_i^0$
$\mathbf{s}_i^0$
message
update
message
update
message
update
$\mathbf{W}\bullet+\mathbf{b}$
SiLU
$\mathbf{W}\bullet+\mathbf{b}$
E
b
$\vec{\mathbf{v}}_j$
$\mathbf{s}_j$
$\vec{r}_{ij}$
$\forall j \| \vec{r}_{ij} \| \leq r_{\text{cut}}$
128
$\mathbf{W}\bullet+\mathbf{b}$
RBF
128
20
SiLU
$\mathbf{W}\bullet+\mathbf{b}$
384
$\mathbf{W}\bullet+\mathbf{b}$
$\mathbf{f}_{\text{cut}}$
384
ϕ
$\mathcal{W}$
128
384
split
128
128
128
message
$\Delta\vec{\mathbf{v}}_i^m$
$\Delta\mathbf{s}_i^m$
c
$\vec{\mathbf{v}}_j$
$\mathbf{s}_j$
128
$\mathbf{U}\bullet$
$\mathbf{V}\bullet$
stack
256
$\mathbf{W}\bullet+\mathbf{b}$
128
128
SiLU
$\langle\bullet_1,\bullet_2\rangle$
$\mathbf{W}\bullet+\mathbf{b}$
128
$\mathbf{a}$
384
128
$\mathbf{a}_{vv}$
split
128
$\mathbf{a}_{sv}$
128
$\mathbf{a}_{ss}$
update
$\Delta\vec{\mathbf{v}}_i^u$
$\Delta\mathbf{s}_i^u$


c
$\vec{\mathbf{v}}_j$
$\mathbf{s}_j$
128
U•
V•
‖•‖
stack
256
W • +b
128
128
SiLU
W • +b
⟨•1, •2⟩
128
a
384
128
$\mathbf{a}_{vv}$
split
128
$\mathbf{a}_{sv}$
128
$\mathbf{a}_{ss}$
update
$\Delta\vec{\mathbf{v}}_i^u$
$\Delta\mathbf{s}_i^u$
stack


c
$\vec{\mathbf{v}}_j$
$\mathbf{s}_j$
128
U•
V•
‖•‖
stack
256
W • +b
128
128
SiLU
W • +b
⟨•1, •2⟩
128
a
384
128
$\mathbf{a}_{vv}$
split
128
$\mathbf{a}_{sv}$
128
$\mathbf{a}_{ss}$
update
$\Delta\vec{\mathbf{v}}_i^u$
$\Delta\mathbf{s}_i^u$
+
=


c
$\vec{\mathbf{v}}_j$
$\mathbf{s}_j$
128
U•
V•
‖•‖
stack
256
W • +b
128
128
SiLU
⟨•1, •2⟩
W • +b
a
384
128
128
$\mathbf{a}_{vv}$
split
128
$\mathbf{a}_{sv}$
128
$\mathbf{a}_{ss}$
update
$\Delta\vec{\mathbf{v}}_i^u$
$\Delta\mathbf{s}_i^u$
+
=


c
$\vec{\mathbf{v}}_j$
$\mathbf{s}_j$
128
$\mathbf{U}\bullet$
$\mathbf{V}\bullet$
$\|\bullet\|$
stack
256
$\mathbf{W}\bullet+\mathbf{b}$
128
128
SiLU
$\langle\bullet_1,\bullet_2\rangle$
$\mathbf{W}\bullet+\mathbf{b}$
$\mathbf{a}$
384
128
128
$\mathbf{a}_{vv}$
split
128
$\mathbf{a}_{sv}$
128
$\mathbf{a}_{ss}$
update
$\Delta\vec{\mathbf{v}}_i^u$
$\Delta\mathbf{s}_i^u$
$\mathbf{a}$
$\mathbf{a}_{vv}$
split
$\mathbf{a}_{sv}$
$\mathbf{a}_{ss}$


$\vec{\mathbf{v}}_j^l$
$\mathbf{s}_j^l$
$\mathbf{W}\bullet$
$\|\bullet\|$
stack
$\mathbf{W}\bullet$
$\mathbf{W}\bullet+\mathbf{b}$
gated
equivariant
block
SiLU
$\mathbf{W}\bullet+\mathbf{b}$
$\circ$
split
$\vec{\mathbf{v}}_j^{l+1}$
$\mathbf{s}_j^{l+1}$

How does the prediction
of energies and forces
differ between SchNet and PaiNN?

$$\vec{F}_i = -\frac{\partial E}{\partial \vec{r}_i}$$

Speaker notes