A jump-start into machine-learning

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TCP

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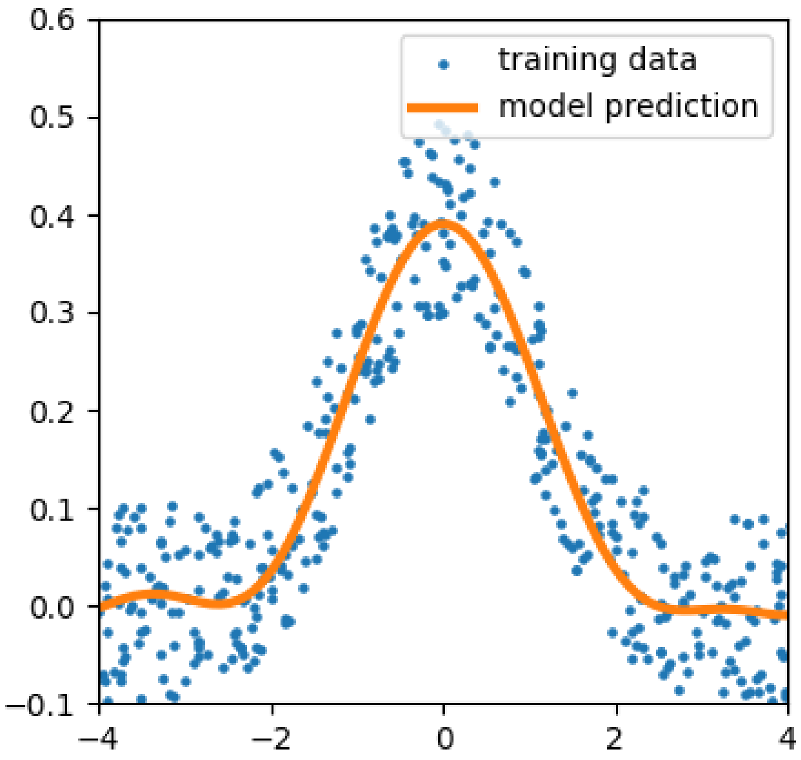
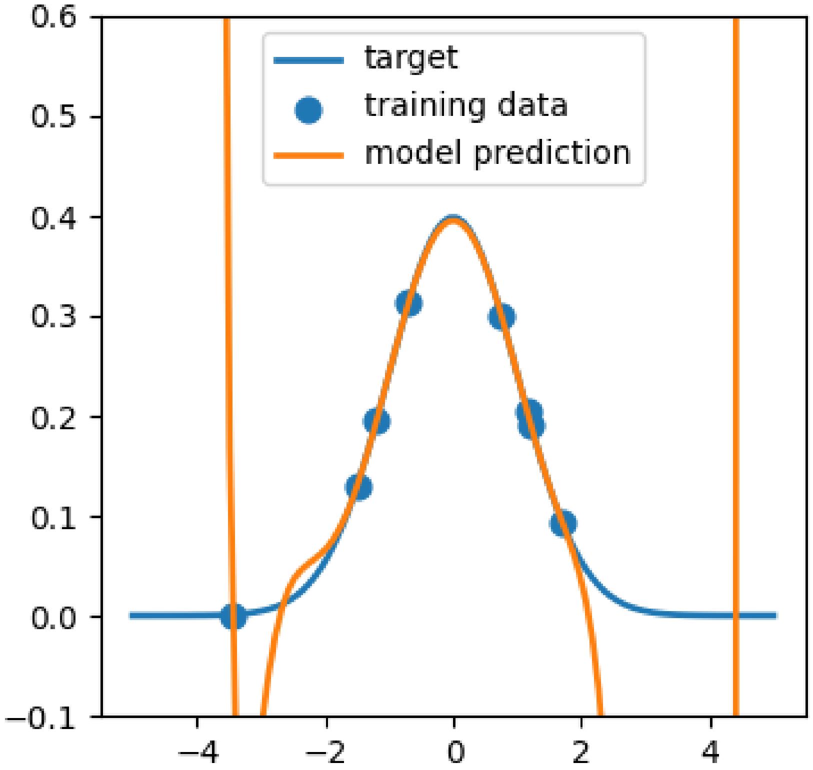
Regression for computational chemistry

Most applications: lots of noisy data



Our case: few data points with almost no noise



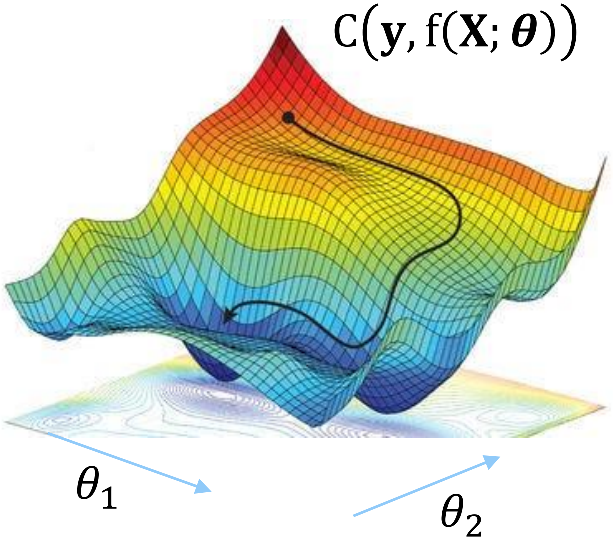
Anatomy of regression

1. Data: $(\boldsymbol{X}, \boldsymbol{y})$

2. Model: $f(\boldsymbol{x}; \boldsymbol{\theta})$
   $f: \boldsymbol{x} \rightarrow y$
   $\boldsymbol{\theta}$ are trainable parameters

3. Cost function: $\mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$
   mean squared error (MSE) $= \frac{1}{N}\sum_i\big(\boldsymbol{y}_i - f(\boldsymbol{x}_i, \boldsymbol{\theta})\big)^2$

4. Find $\min_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$ using gradient descent



Hutson, Science 2018

Pytorch example lj_1_overfit.py

1. Open anaconda prompt
2. conda activate ml_tutorial
3. Go to ml_tutorial folder
4. spyder &
5. In spyder open
   lj_1_overfit.py

Anatomy of regression

1. Data: $(\boldsymbol{X}, \boldsymbol{y})$
   - Instance/object of a customized dataset class
   - Implement 3 functions: __init__, __len__, and __get_item__
   - dataloader pulls random batches of data from the dataset

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x_1} \\ \boldsymbol{x_2} \\ \boldsymbol{x_3} \\ \vdots \end{pmatrix} \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{pmatrix}$$

Anatomy of regression

1. Data: $(\boldsymbol{X}, \boldsymbol{y})$

2. Model: $f(\boldsymbol{x}; \boldsymbol{\theta})$
   - Instance/object of a customized nn.module class
   - Implement 2 functions: __init__ and __forward__

Anatomy of regression

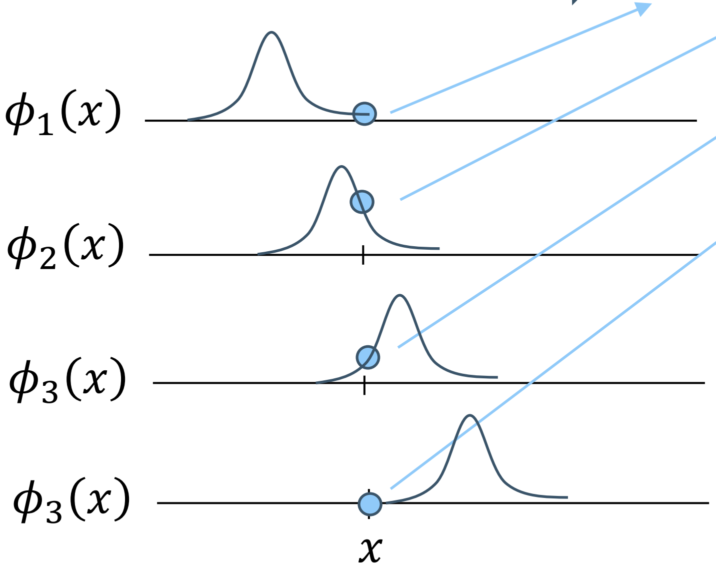
1. Data: $(\boldsymbol{X}, \boldsymbol{y})$

2. Model: $f(\boldsymbol{x}; \boldsymbol{\theta})$
   - Instance/object of a customized nn.module class
   - Implement 2 functions: __init__ and __forward__
   - Descriptor:

One hot encoding:

$$H = (1 \quad 0 \quad 0)$$
$$C = (0 \quad 1 \quad 0)$$
$$O = (0 \quad 0 \quad 1)$$

Continuous data: $x = 3.1$ ⇨ $(0.1 \quad 0.5 \quad 0.3 \quad 0.01 \quad 0 \quad 0)$



Anatomy of regression

1. Data: $(\boldsymbol{X}, \boldsymbol{y})$

2. Model: $f(\boldsymbol{x}; \boldsymbol{\theta})$
   - Instance/object of a customized nn.module class
   - Implement 2 functions: __init__ and __forward__
   - Descriptor
   - Neural network:

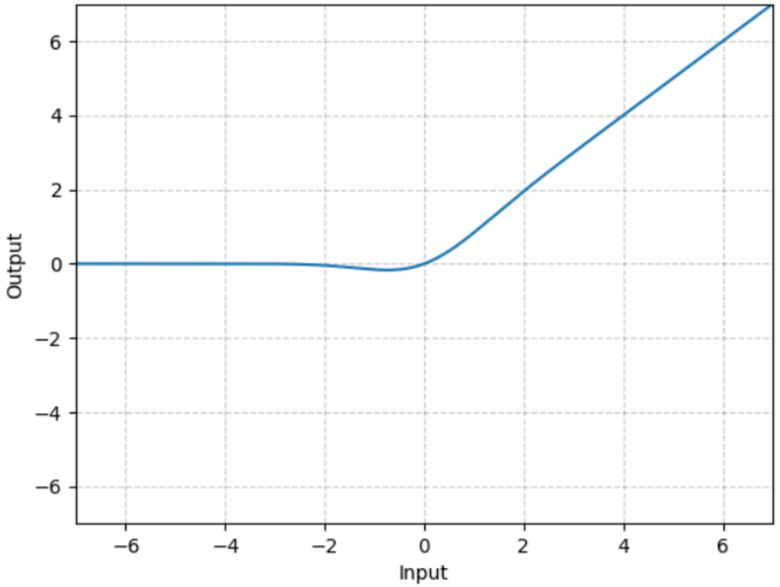
$$\boldsymbol{y_1} = \sigma(\boldsymbol{W_0 x} + \boldsymbol{b_0})$$

$$\boldsymbol{y_2} = \sigma(\boldsymbol{W_1 y_1} + \boldsymbol{b_1})$$

$$\boldsymbol{y_3} = \sigma(\boldsymbol{W_2 y_2} + \boldsymbol{b_2})$$

$$\mathrm{y}_{\mathrm{pred}} = \boldsymbol{w_3} \cdot \boldsymbol{y_3} + b_3$$

$\sigma(x)$ is the nonlinear activation function: GELU



Use a continuously differentiable activation function

Anatomy of regression

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2. Model: $f(\boldsymbol{x}; \boldsymbol{\theta})$

3. Cost function: $\mathrm{C}\left(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\right)$
   - Mean squared error

Anatomy of regression

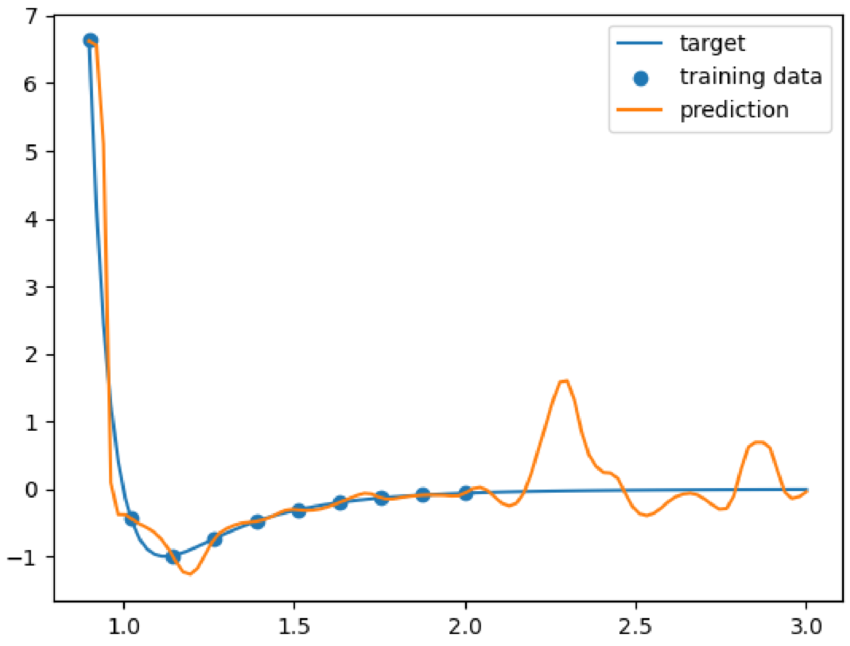
1. Data: $(\boldsymbol{X}, \boldsymbol{y})$
2. Model: $f(\boldsymbol{x}; \boldsymbol{\theta})$
3. Cost function: $\mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$
4. Find $\min_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$

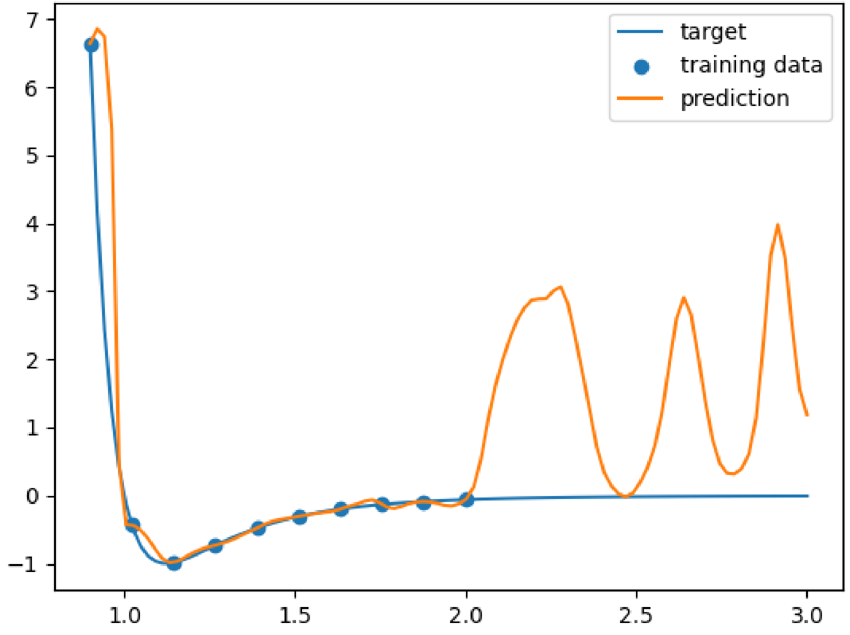
Batch 1	Batch 2	Batch 3	
(x_1, y_1), (x_3, y_3), (x_8, y_8)	(x_2, y_2), (x_5, y_5), (x_6, y_6)	(x_4, y_4), (x_7, y_7), (x_9, y_9)	$\cdots$
$\boldsymbol{\theta}' = \boldsymbol{\theta} - \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$	$\boldsymbol{\theta}' = \boldsymbol{\theta} - \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$	$\boldsymbol{\theta}' = \boldsymbol{\theta} - \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$	

1 Epoch

Overfitting

- NNs often have many more parameters than samples in the training data
- Run lj_1_overfit.py several times
  - 311 trainable parameters, 10 data points



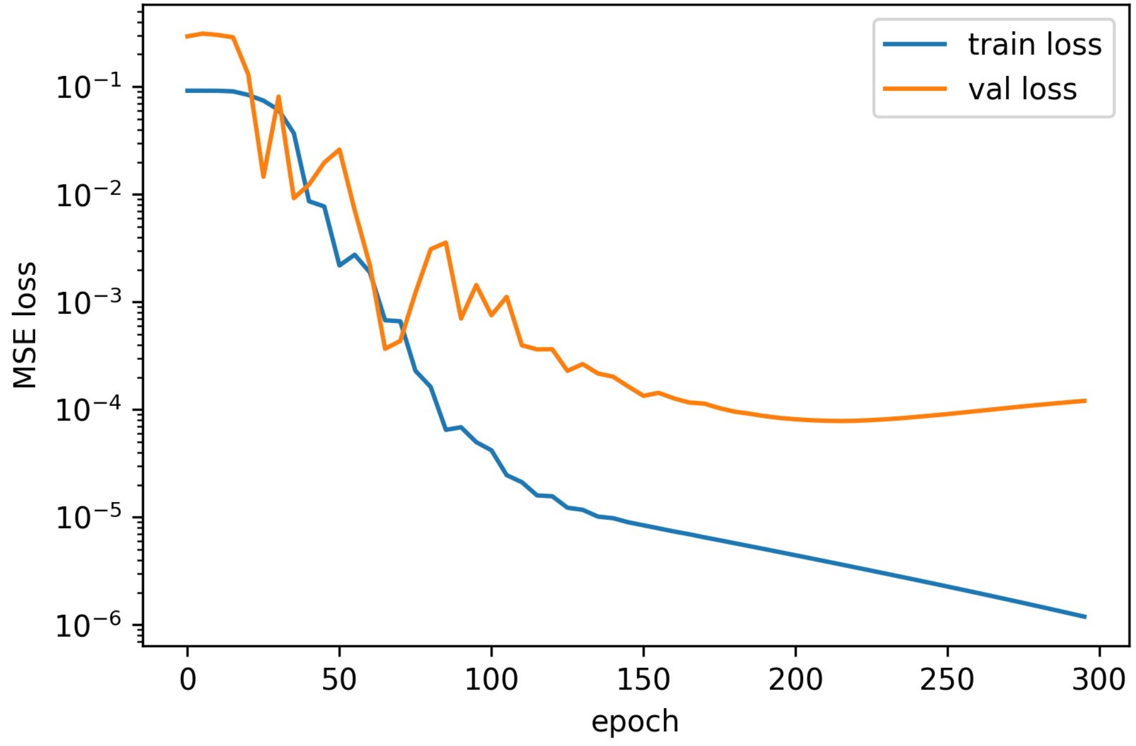


- Each model perfectly fits the training points, but doesn't do a great job in the interpolation region
- **You measure a model by testing on data it has never seen**
- The models do terrible in the extrapolation regime

Validation and test sets

- Separate your data into a training set, a validation set, and a test set
- Validation set used to measure overfitting and tune hyperparameters
- Test set is only used for the final model to get a final estimate of how accurate the model really is

- Run lj_2_overfit_with_validation.py
  - The main change in the code is lines 56-58



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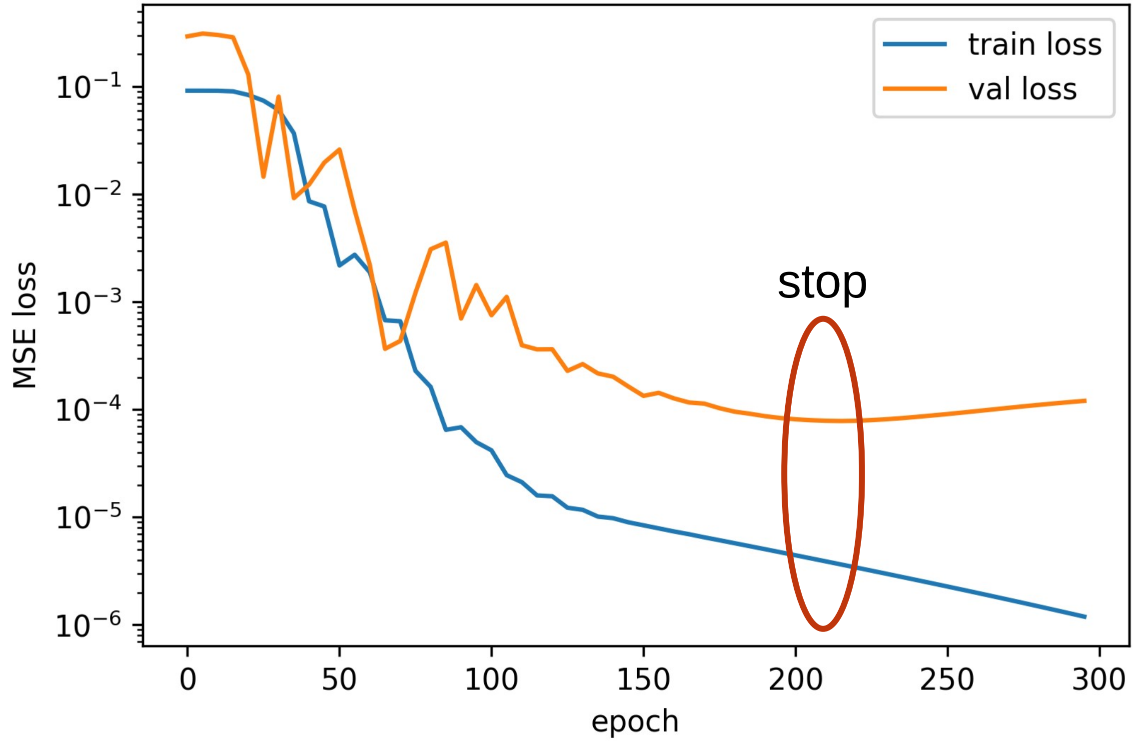
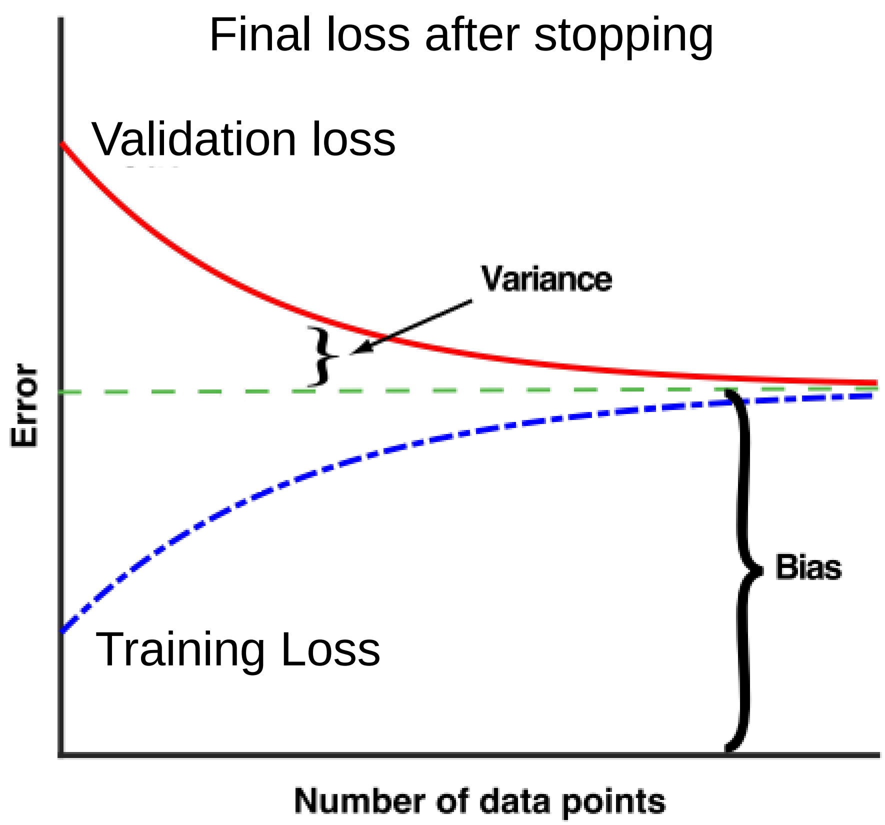
- To get the best performance model stop when there is a steady increase in validation loss and decrease in training loss (early stopping)



Learning curve

- With enough data the validation loss and training loss should converge



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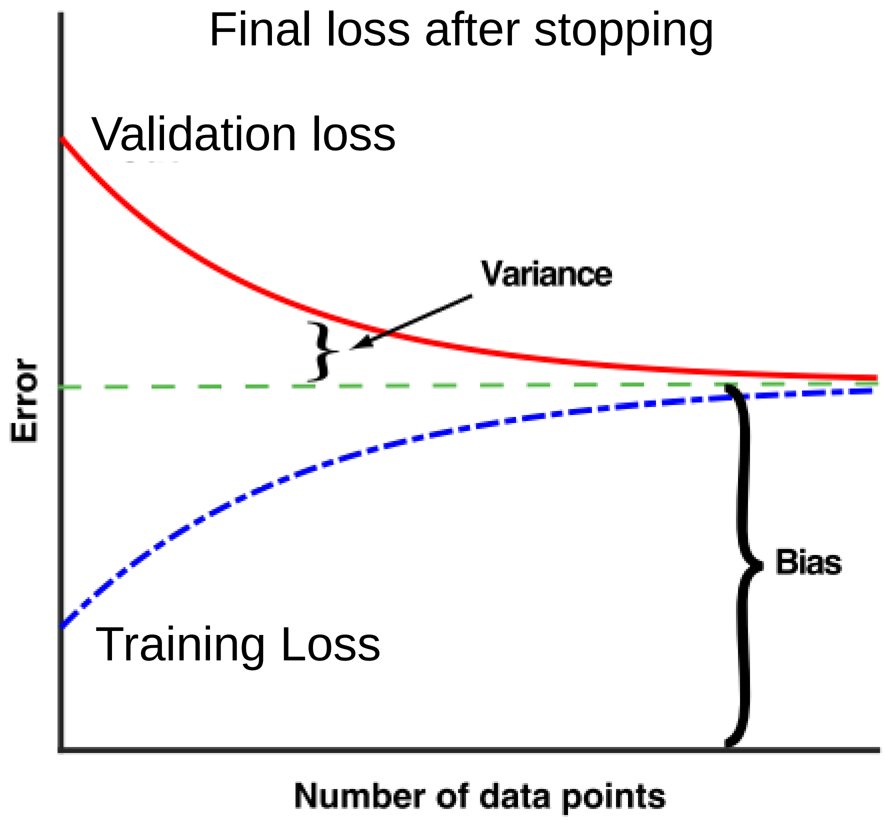
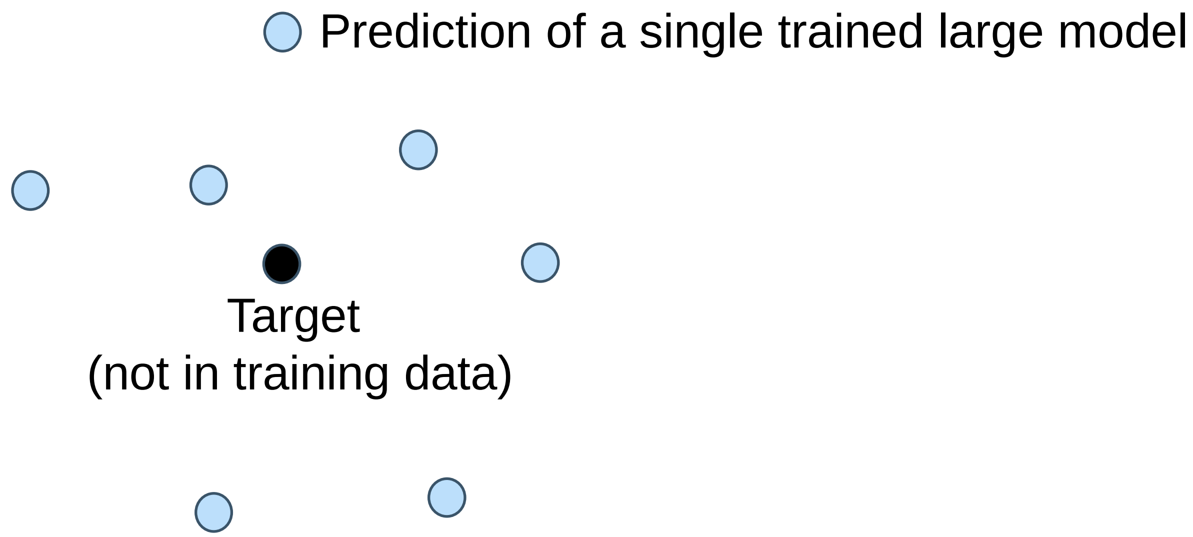
Learning curve

- With enough data the validation loss and training loss should converge
- Variance: a models trained with different, but equal number of points yield different results
  - The more parameters, the more variance in the model





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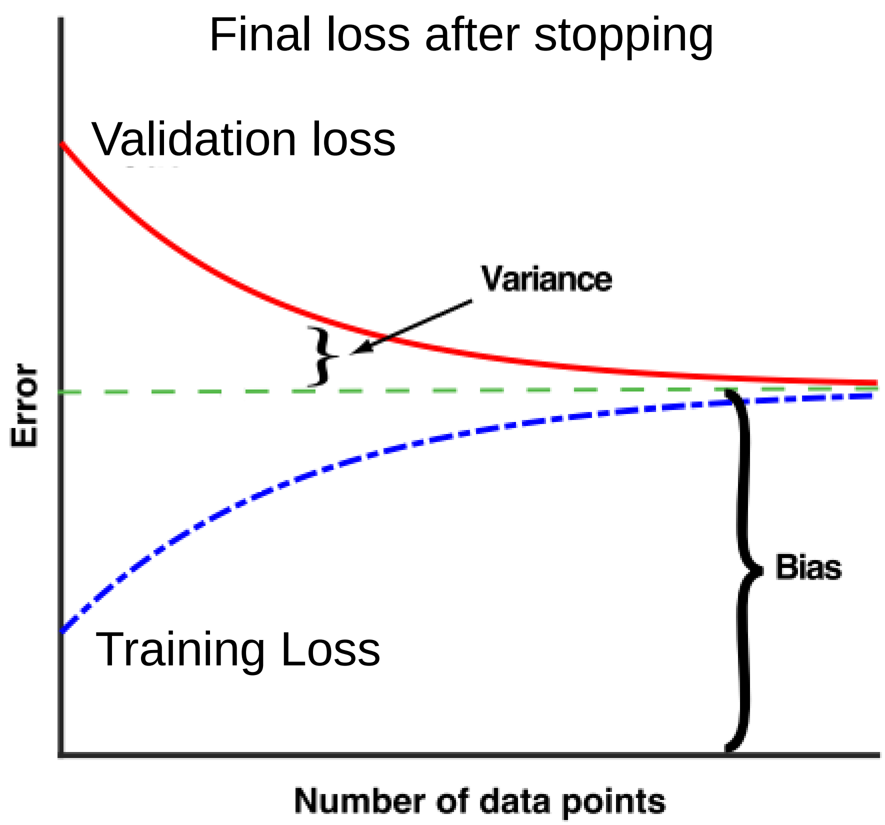

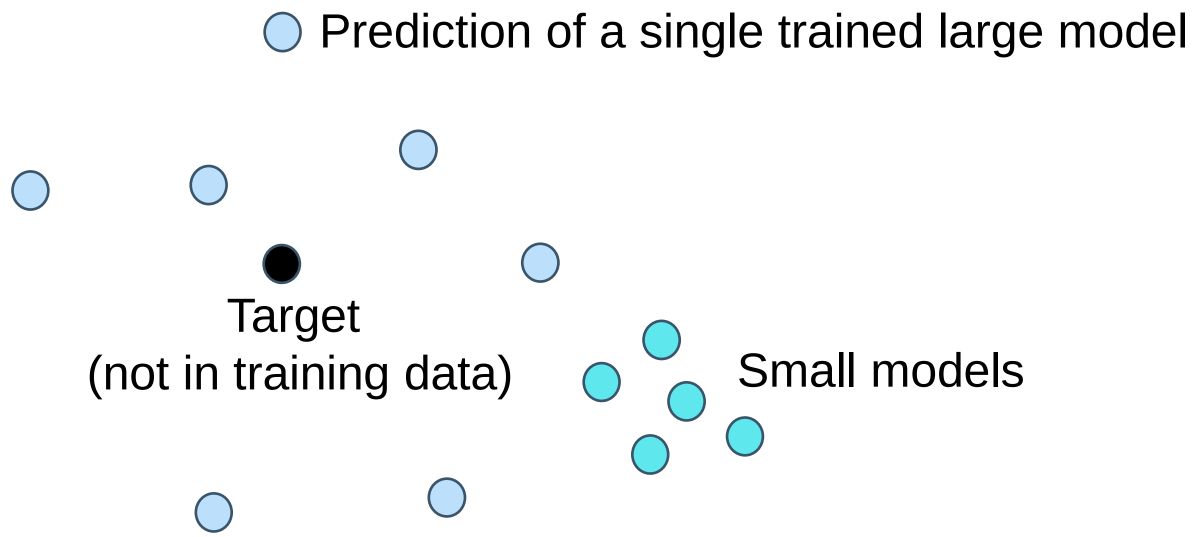

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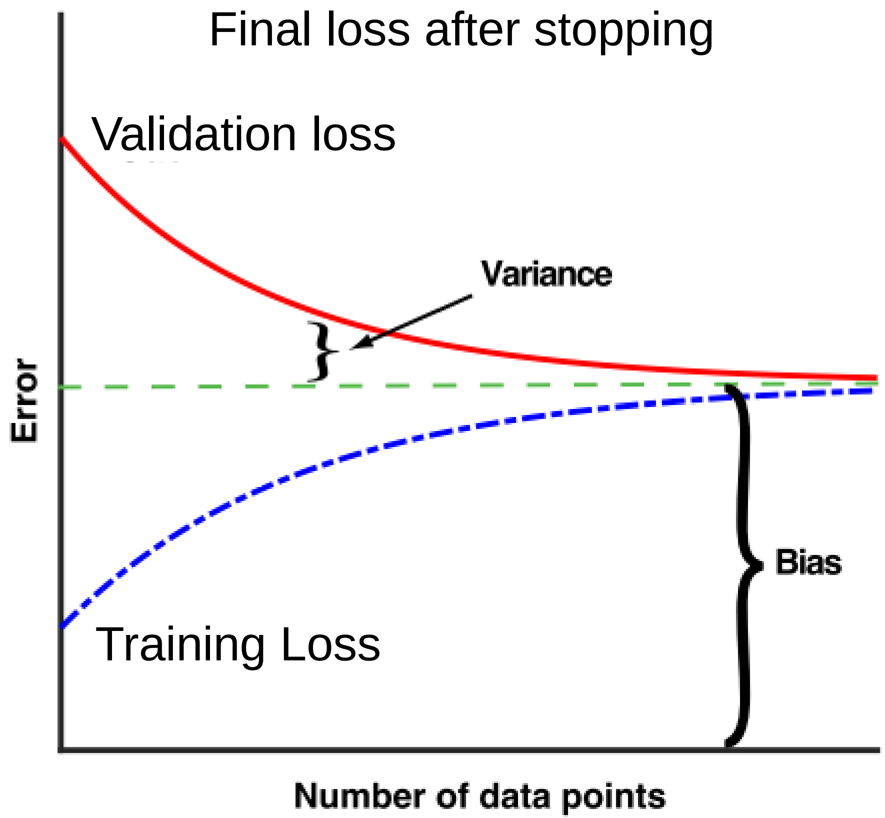
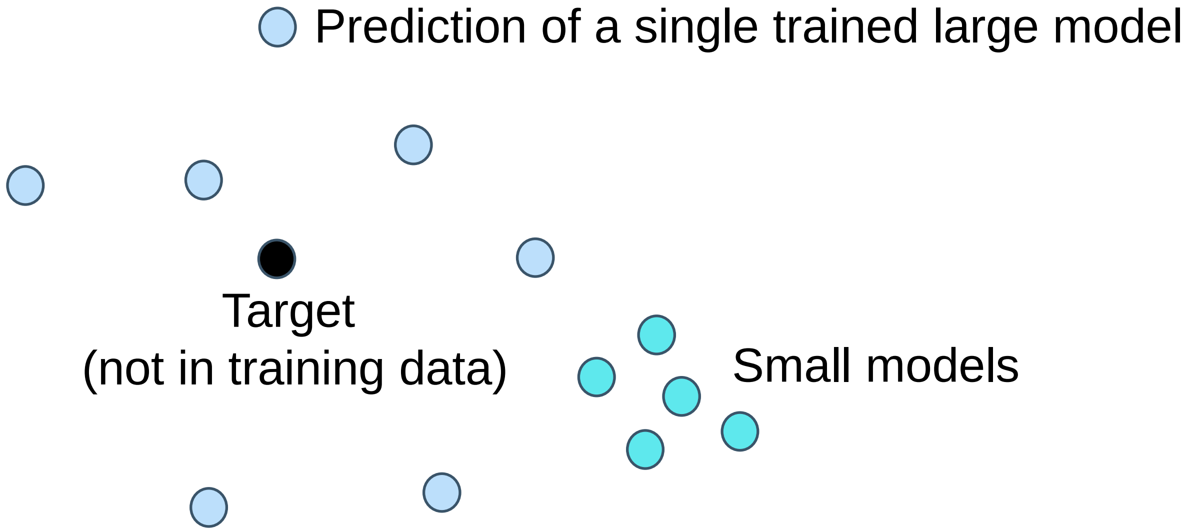
- Large high variance models overfit





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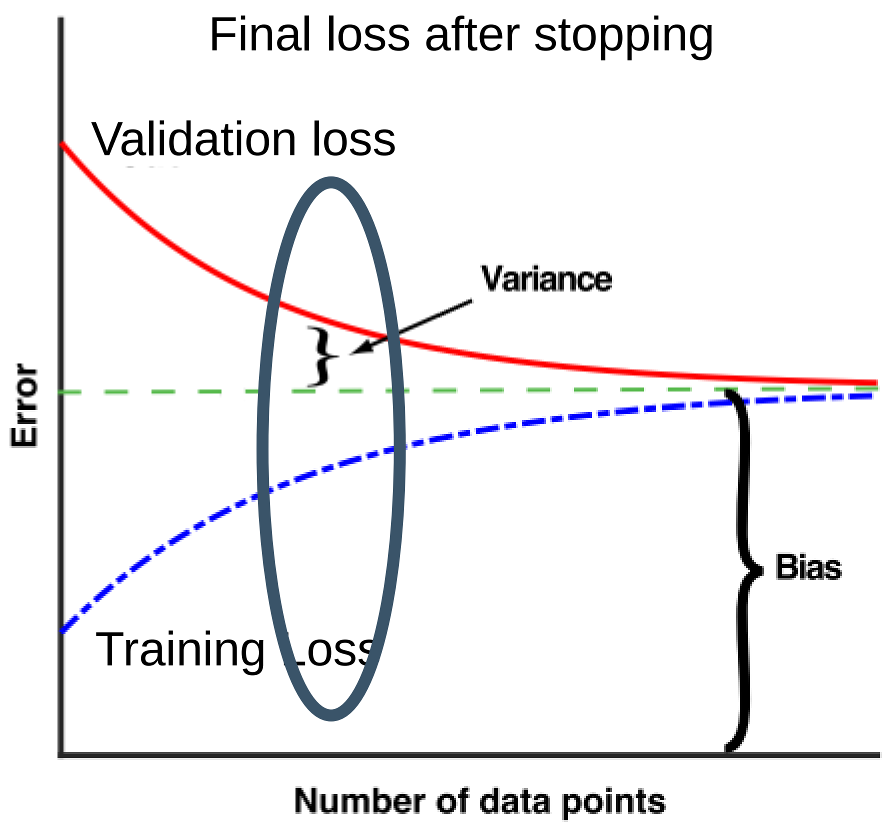

- Enough data lowers variance
- However, we are always working in the low data regime

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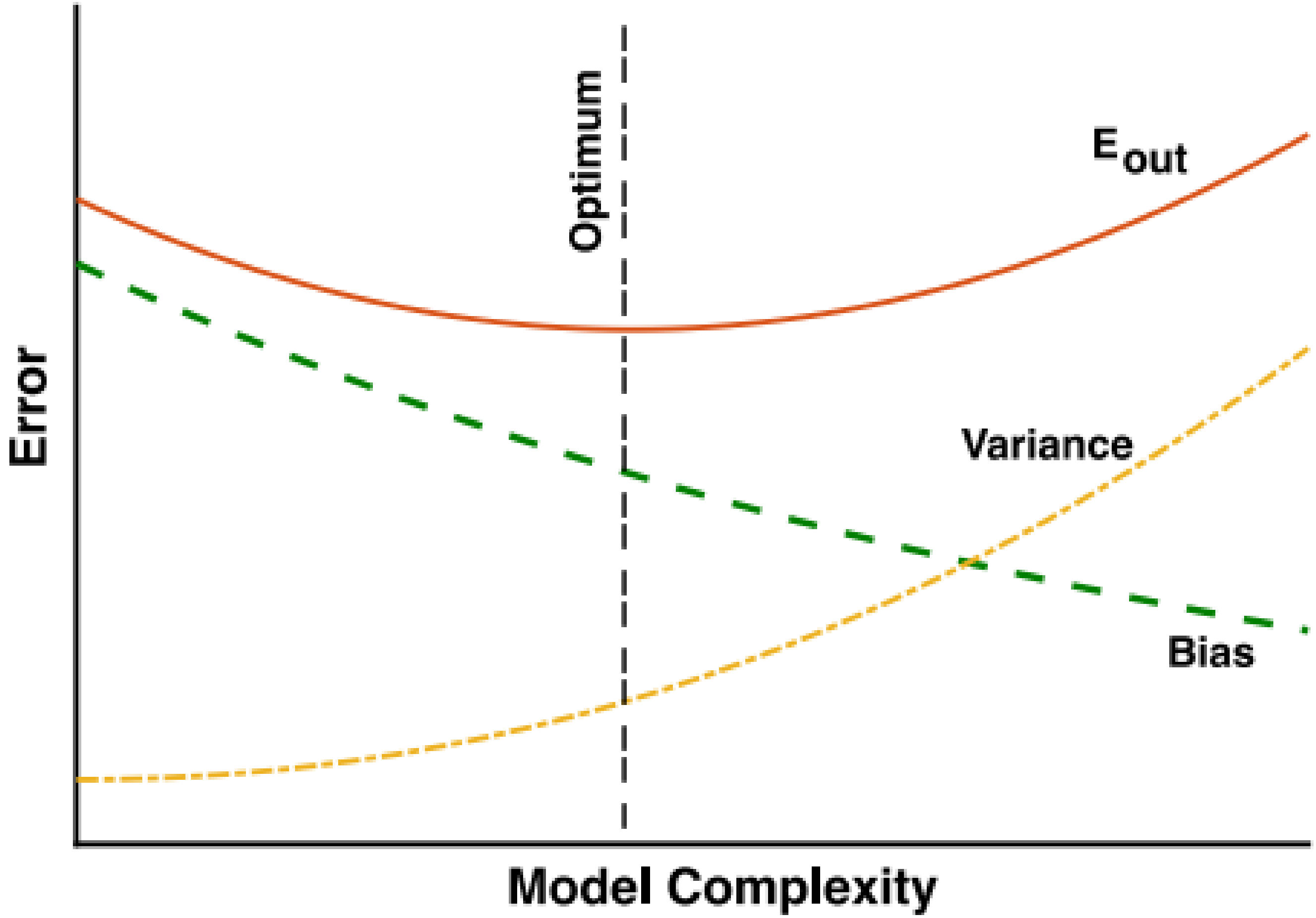
Bias variance tradeoff

- There is an optimum size of your model for a given amount of data.



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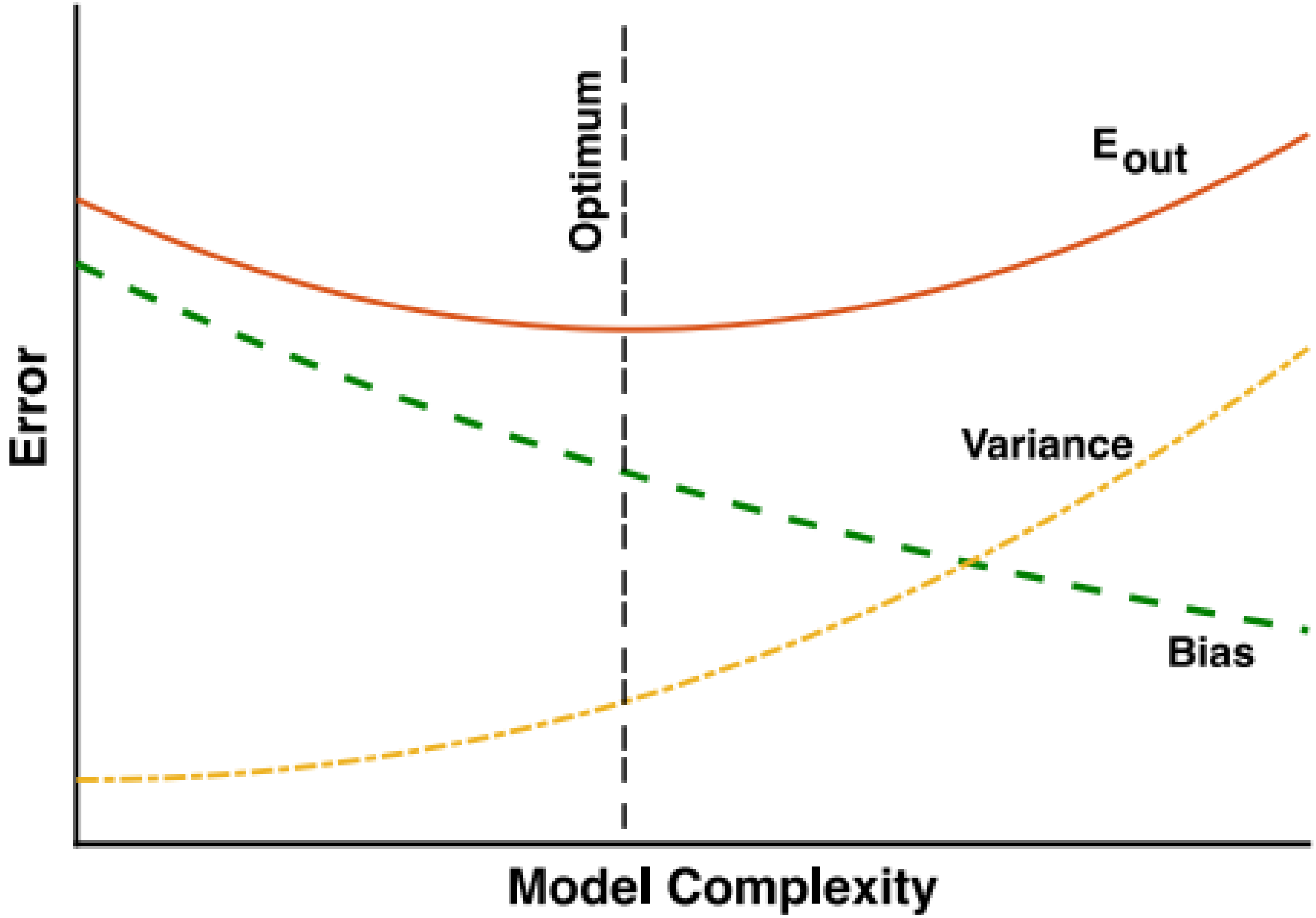

- L2 regularization (also known as weight decay):
  - lowers variance/prevents overfitting
  - Allows you to use larger models while getting lower errors

Use the right amount of regularization

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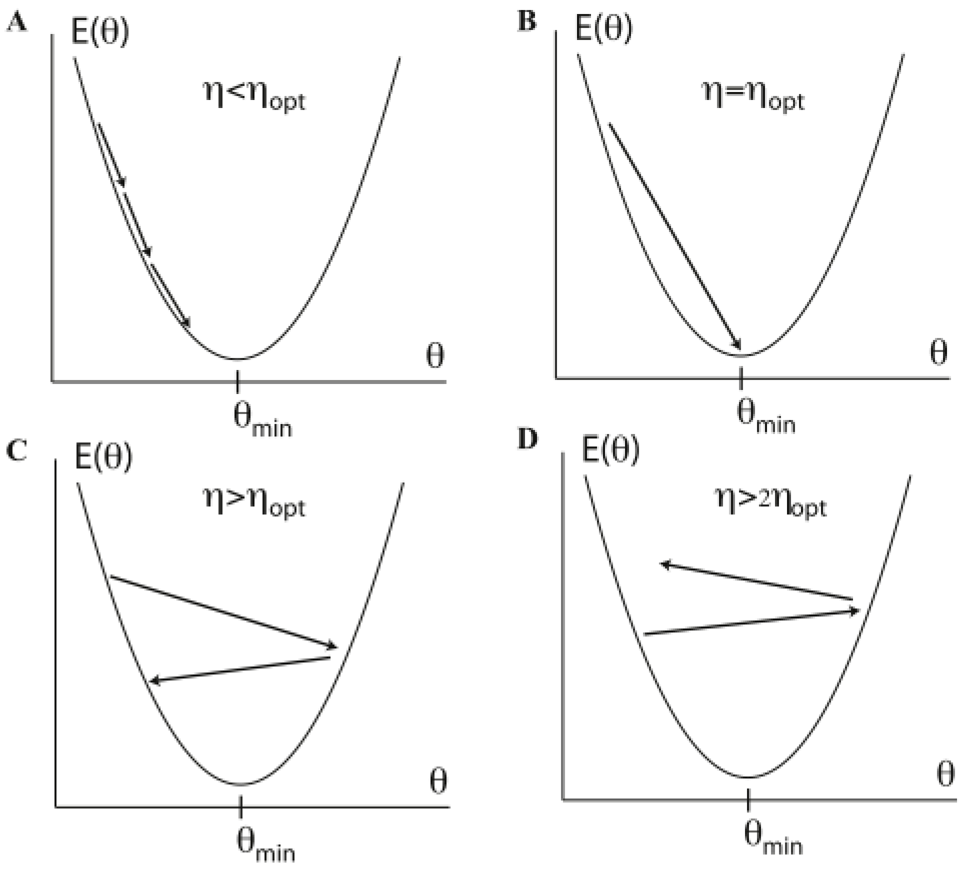
Find $\min_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$: Gradient descent

$$\boldsymbol{v}_t = -\eta \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

η step size
v_t update to weights



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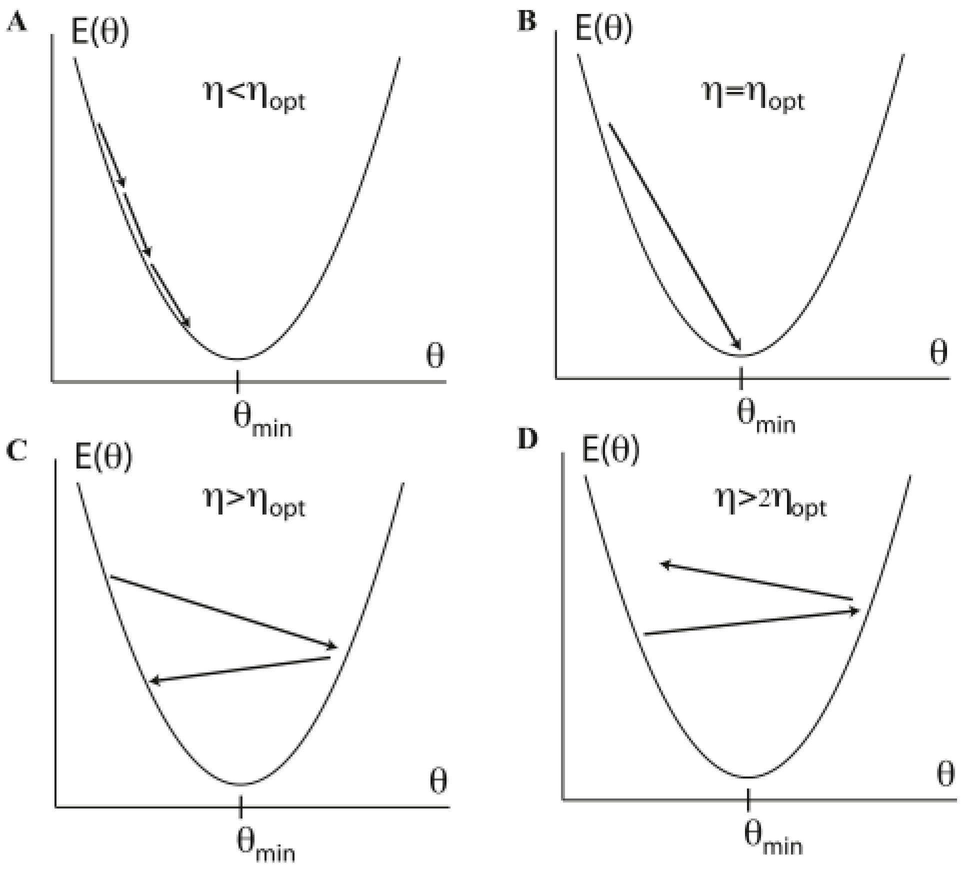

- Momentum algorithms
  - Build up speed in shallow directions

$$\boldsymbol{v}_t = \gamma \boldsymbol{v}_{t-1} - \eta \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

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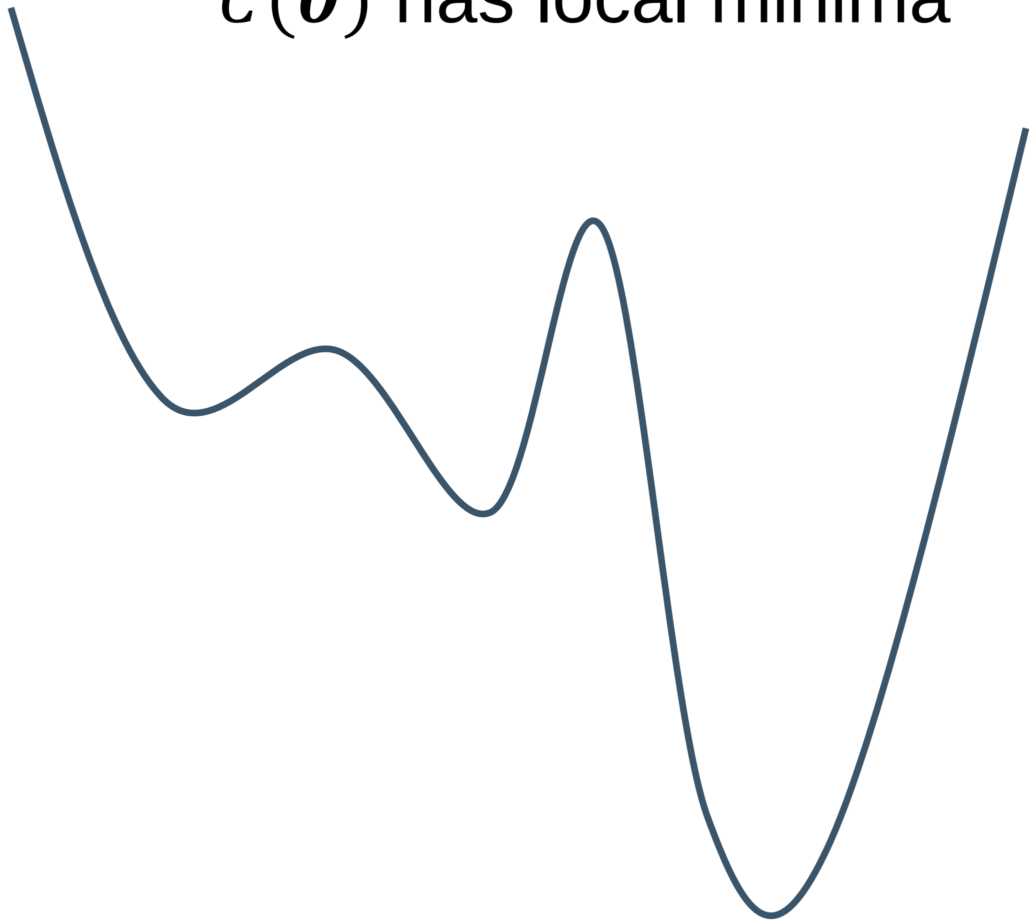
Momentum

$$\boldsymbol{v}_t = -\eta \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

$C(\boldsymbol{\theta})$ has local minima



- Momentum algorithms
  - Build up speed in shallow directions
  - Can get out of local minima

$$\boldsymbol{v}_t = \gamma \boldsymbol{v}_{t-1} - \eta \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

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Use stochasticity to get out of local minima

$$\boldsymbol{v}_t = -\eta \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}, \mathrm{f}(\mathbf{X}; \boldsymbol{\theta})\big)$$

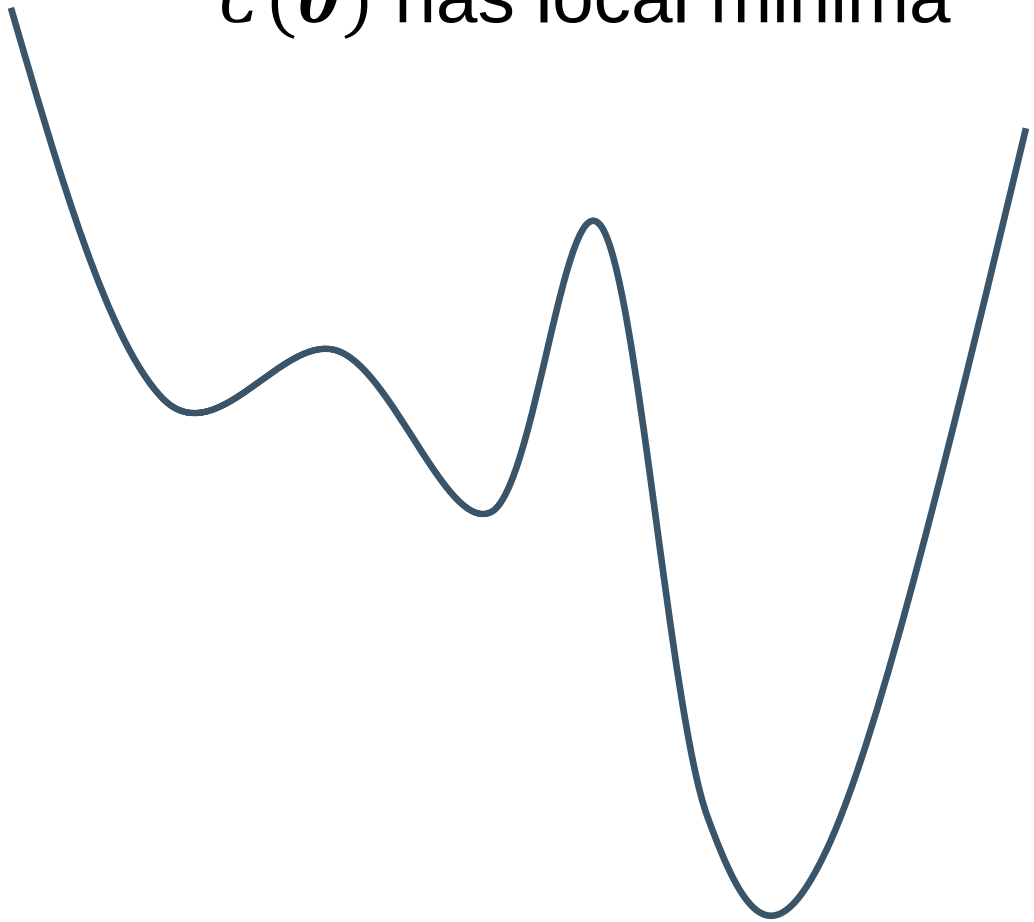
$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

Only compute v_t on a subset of X and y

$$\boldsymbol{v}_t = -\eta \nabla_{\boldsymbol{\theta}} \mathrm{C}\big(\mathbf{y}_{\mathrm{batch}}, \mathrm{f}(\mathbf{X}_{\mathrm{batch}}; \boldsymbol{\theta})\big)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

$C(\boldsymbol{\theta})$ has local minima



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A model to play with

- Run lj_3_hyperparameters.py

- Change hyperparameters at the top of the script and see how the training progression changes

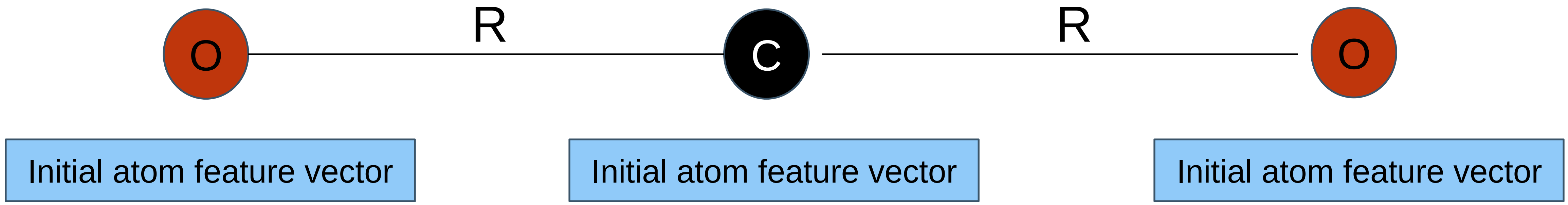
- Tensorboard to plot training progression
  - Using the anaconda prompt, in the ml_tutorial folder run:

  tensorboard --logdir=runs --reload_multifile True
  - Go to http://localhost:6006/ in your browser

Best practices when developing an NN

- Try to memorize a few data points first
- Try also using fake simple data
- Check your descriptors and targets to make sure you are feeding the NN what you think you are
- Hyperparameter tuning on even just a few epochs to screen out unpromising parameter values
- Use grid search/random search of hyperparameters

Architecture of message passing neural networks



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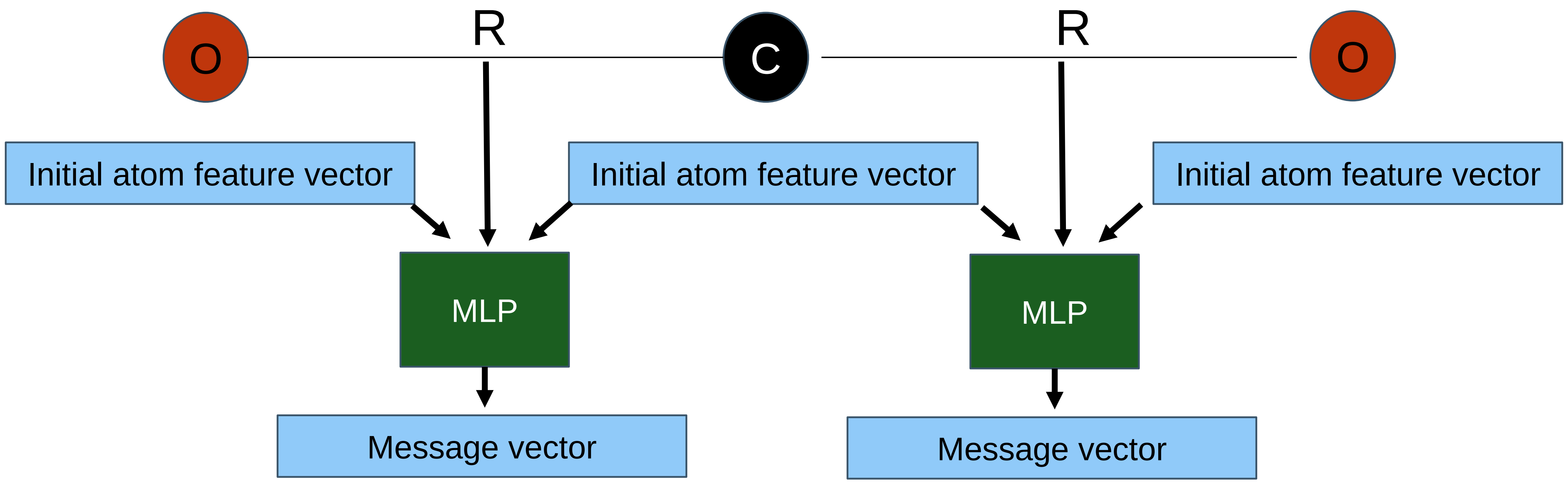

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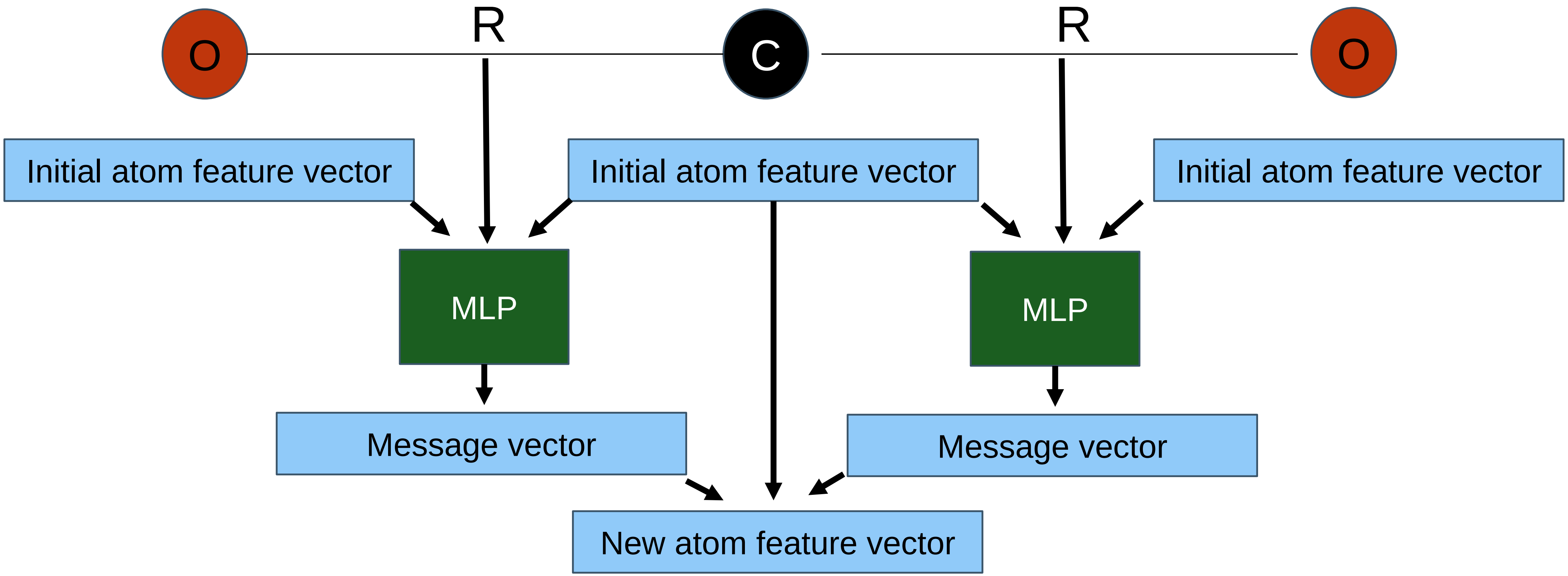

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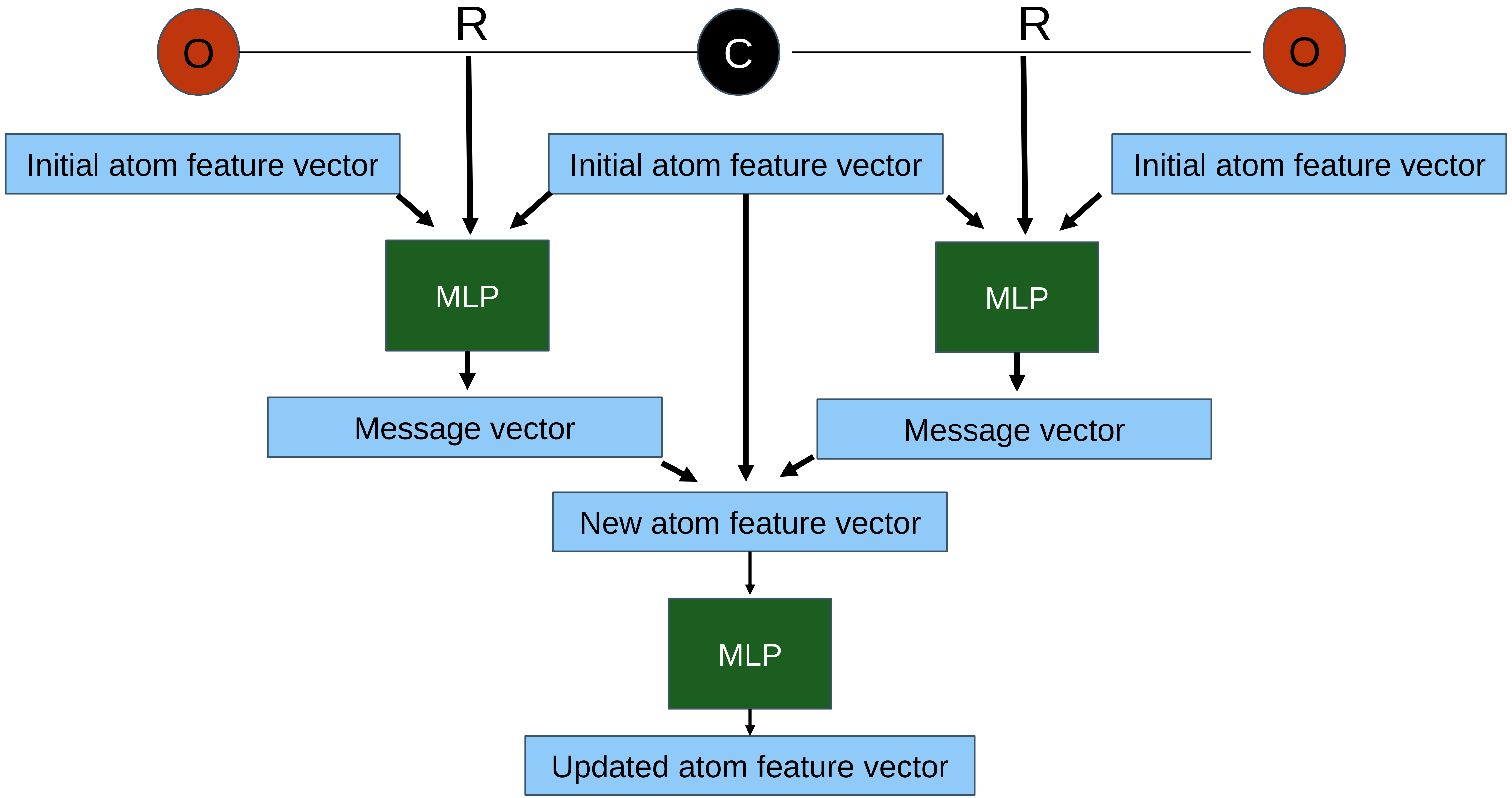

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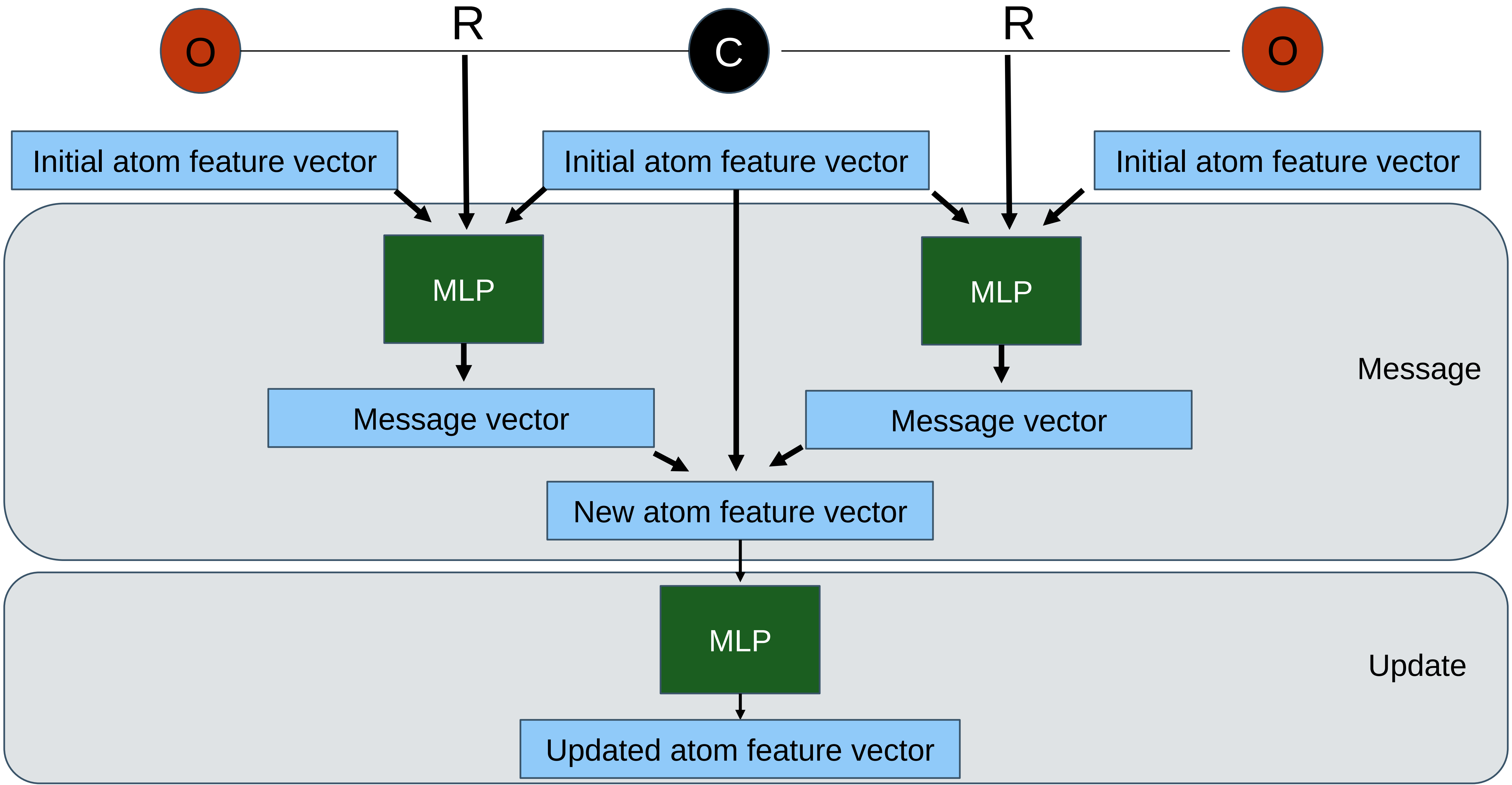

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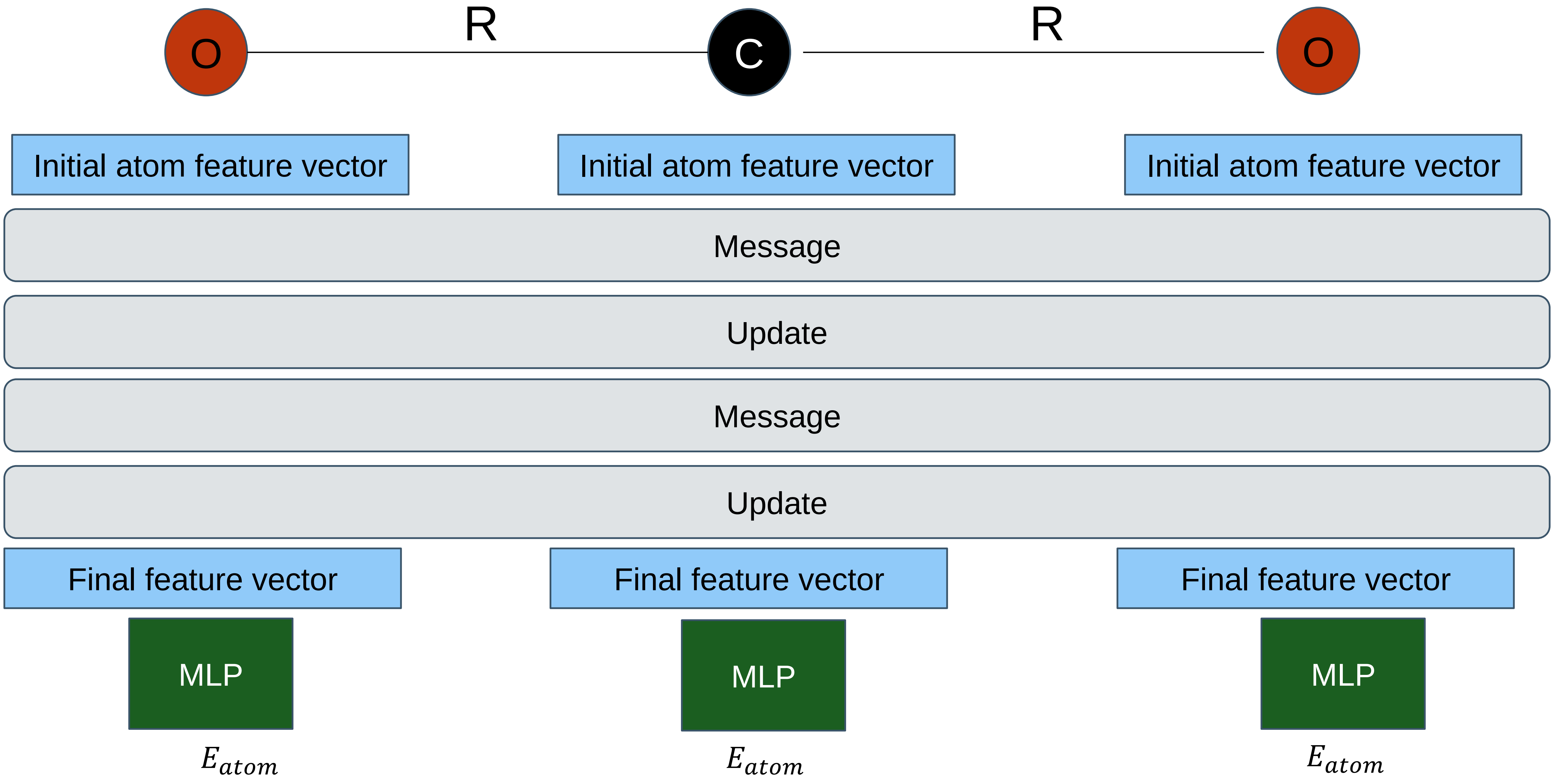

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