分子のグラフ表現と機械学習

2020年10月20日(火)：日本化学会 第10回CSJ化学フェスタ2020
データサイエンスの世界をのぞいてみませんか？

たきがわ　いちがく
瀧川 一学

https://itakigawa.github.io/

北海道大学 化学反応創成研究拠点 (WPI-ICReDD)

本日の内容

GNN(Graph Neural Networks)で**グラフ表現**された分子を入力にして機械学習するやり方を**のぞいてみませんか**？

- 機械学習とは？
- 分子のグラフ表現
- 準備：深層学習のココロ (forwardとbackward)
- Graph Neural Networksとは？
- 自分でやってみるための情報
- おまけ：
  最近の話 (計算限界、分子生成、事前学習、...)

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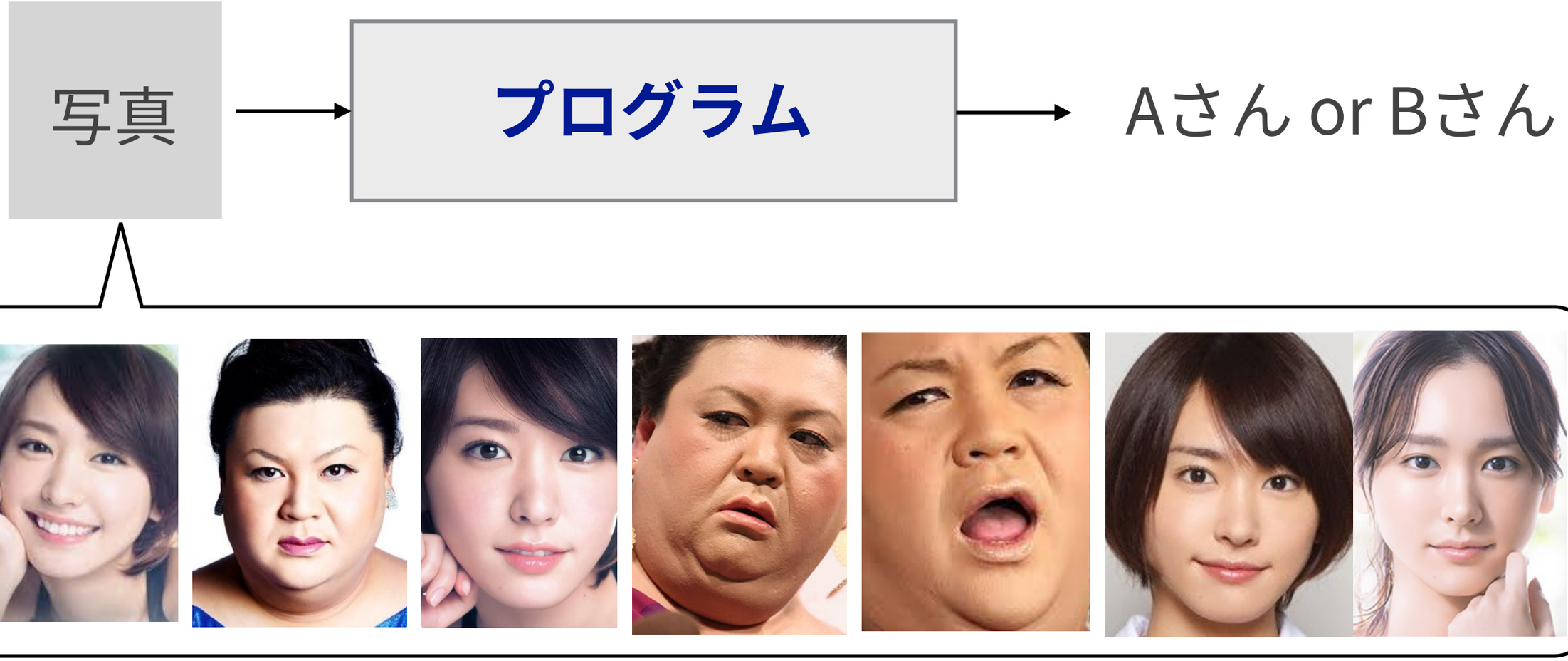
機械学習の出番

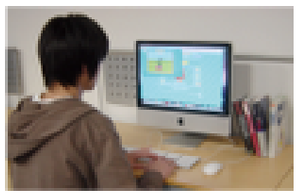
AさんとBさんの写真を分けるプログラムを作りたい



人間なら簡単に解けるけど手順は自分でも説明できない...

機械学習：新しいプログラミングのパラダイム

機械学習 = 多量の入出力の見本例からプログラムを
自動的に作成する(いいかげんな)技術



一般物体認識

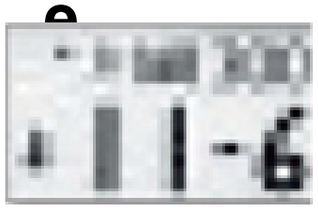
J’aime
la
musiqu
e

音声認識

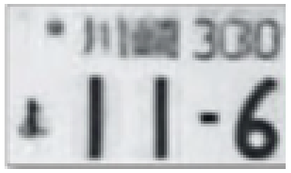
“ありがとう”

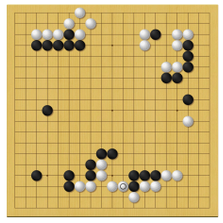
機械翻訳

I love music

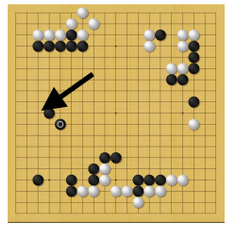


超解像

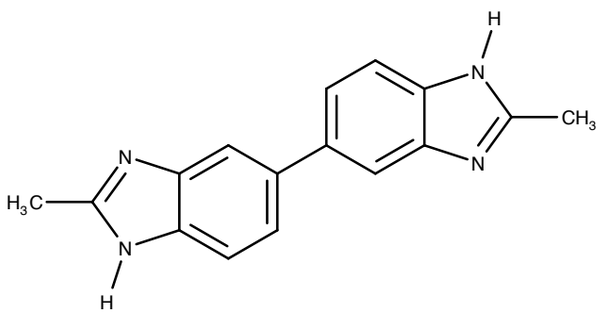




ゲームAI



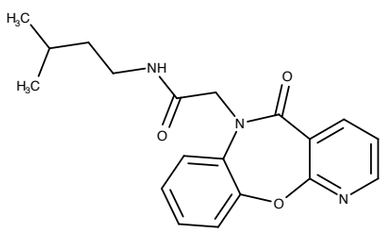
今日の例：分子の活性や物性の予測 (QSAR/QSPR)



分子の活性・物性の予測

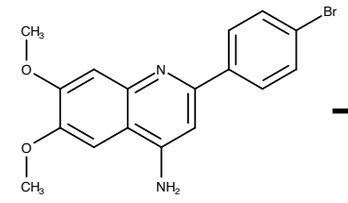
50%阻害濃度

0.739

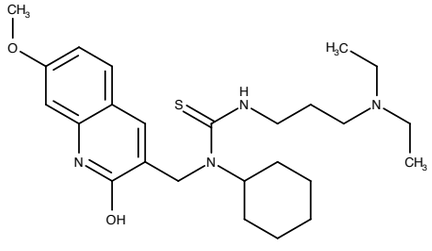


1.399

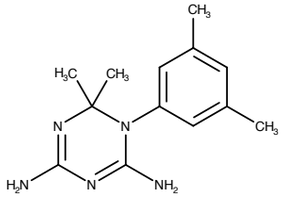
入出力の
見本例



-1.753

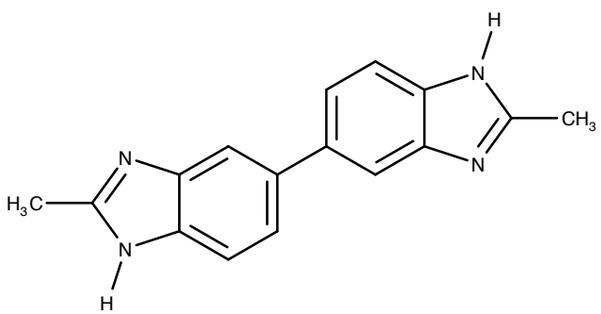


1.394



-3.171

分子のグラフ表現とGraph Neural Networks (GNNs)



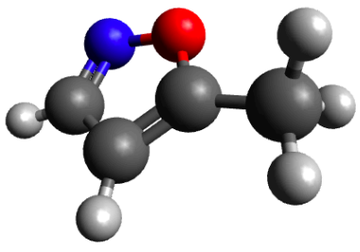
分子の活性・物性の予測

50%阻害濃度

0.739

色々やり方あるけれど今日はGNNをのぞいてみませんか？

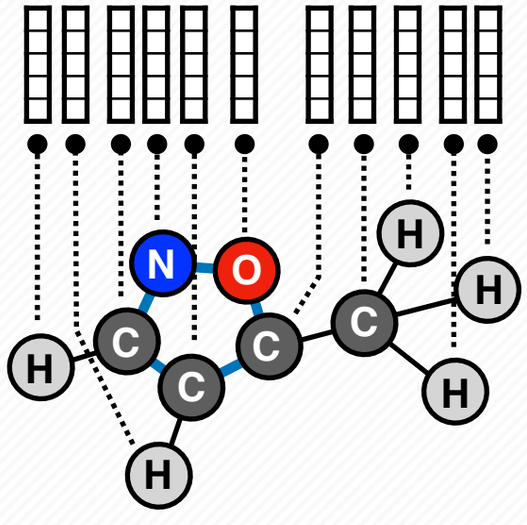
分子構造



分子記述子 (Hansch-藤田法など)

汎用機械学習

分子のグラフ表現



特徴ベクトル

分子フィンガープリント
(ECFP法など)

Graph
Neural
Networks

動機：GNNは広いモダリティを統一的に扱うことができる

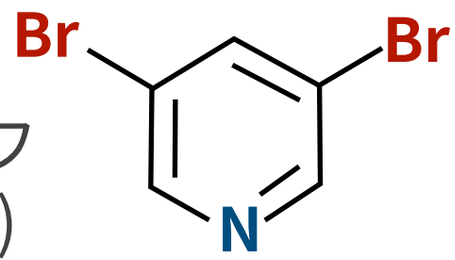
GNNで扱えるモダリティは
狭義の「グラフ」より広い

SMILES

文字列　Brc1cncc(Br)c1

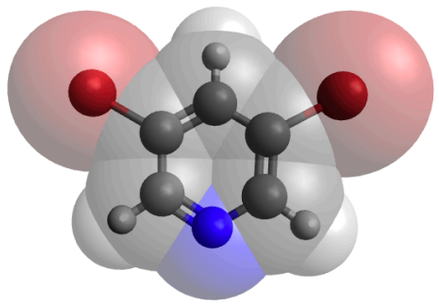
化学構造式

グラフ
(狭義)



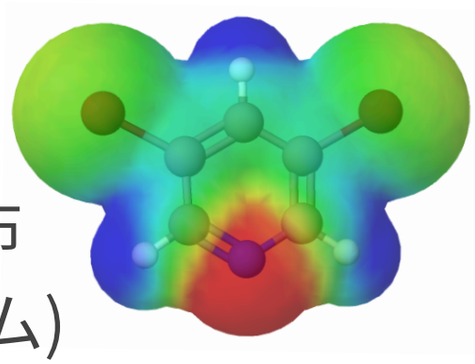
立体構造

幾何的
点集合

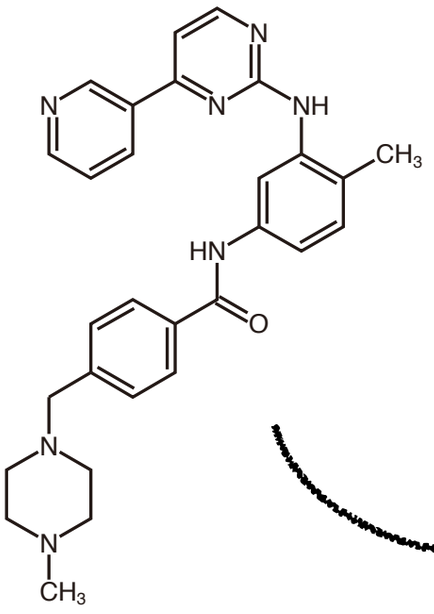


電子状態

空間的分布
(ボリューム)



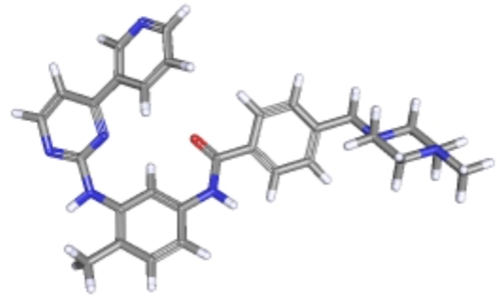
抗悪性腫瘍剤
(CID 5291)



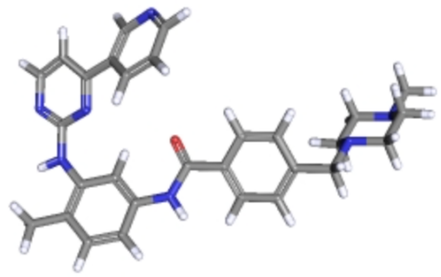
単結合の
回転の自由度

立体配座 (PubChem3D)

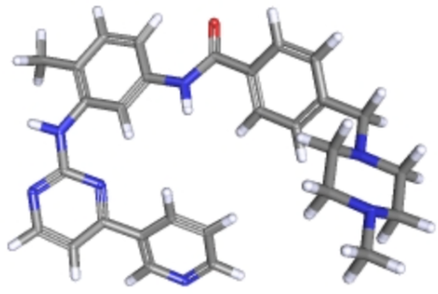
1



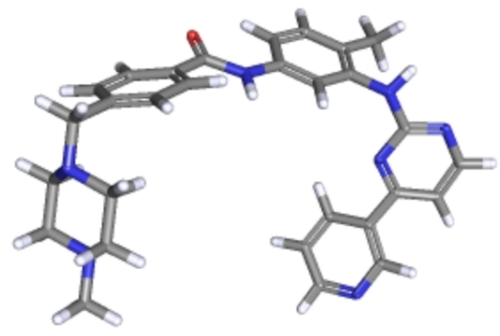
2



3



284



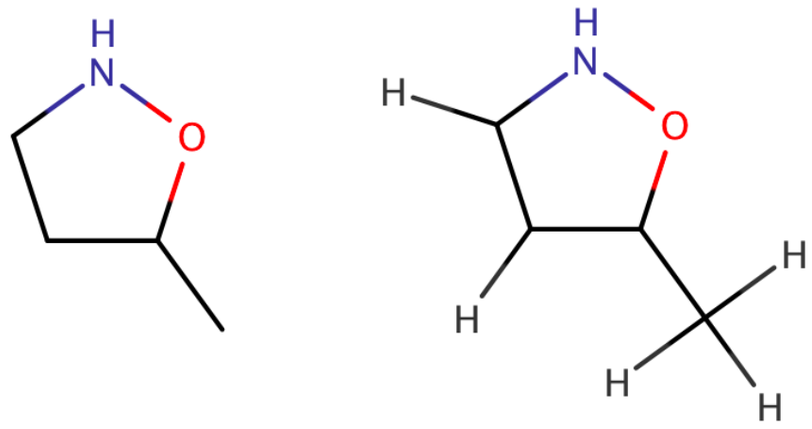
分子表現

1次元

CC1CCNO1

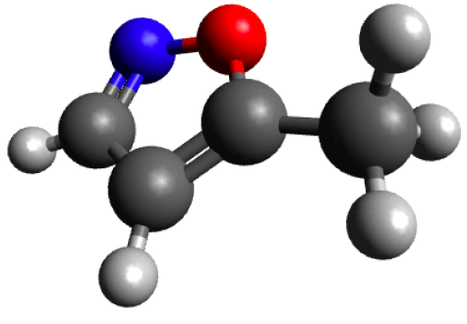
Canonical SMILES

2次元



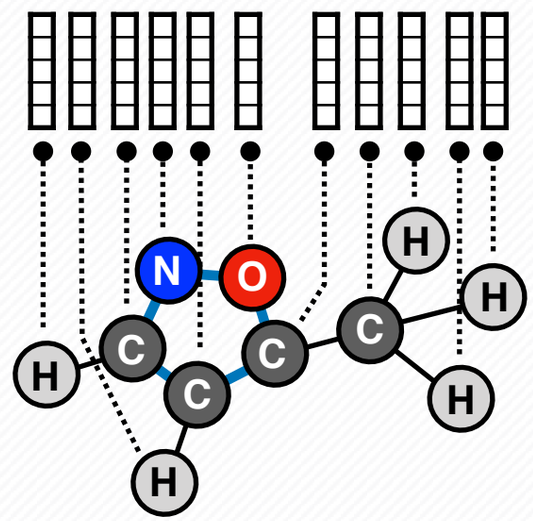
水素(Implicit)　　**水素(Explicit)**

3次元



MOL形式

分子のグラフ表現



特徴ベクトル

```
11 11  0  0  0  0            999
    0.0264    1.4944    0.0287 C
   -0.0850    0.0111    0.0449 C
   -1.0957   -0.8588   -0.2308 C
   -0.5082   -2.1326   -0.0113 C
    0.7433   -2.0451    0.3632 N
    1.0156   -0.6777    0.3997 O
    0.8032    1.8213   -0.6702 H
   -0.9230    1.9401   -0.2734 H
    0.2923    1.8782    1.0190 H
   -2.1005   -0.6271   -0.5415 H
   -0.9559   -3.1113   -0.1136 H
 1  2  1  0  0  0  0
 1  9  1  0  0  0  0
 2  6  1  0  0  0  0
 3  4  1  0  0  0  0
 3  2  2  0  0  0  0
 4  5  2  0  0  0  0
 5  6  1  0  0  0  0
 7  1  1  0  0  0  0
 8  1  1  0  0  0  0
10  3  1  0  0  0  0
11  4  1  0  0  0  0
```

原子核のxyz

化学結合

実際の分子グラフデータを見てみよう

QM9 Dataset (Ramakrishnan+ 2014)

133,885 分子： C, N, O, Fの組合せから成る**9原子**(H以外)までの分子の**安定3D構造**と**15種の物性値**を計算 (B3LYP/6-31G(2df,p) level)

OPEN

SUBJECT CATEGORIES

» Quantum chemistry

» Density functional theory

Quantum chemistry structures and properties of 134 kilo molecules

Raghunathan Ramakrishnan[1], Pavlo O. Dral[2,3], Matthias Rupp[1] & O. Anatole von Lilienfeld[1,4]

Sci Data **1,** 140022 (2014). https://doi.org/10.1038/sdata.2014.22

実際の分子グラフデータを見てみよう

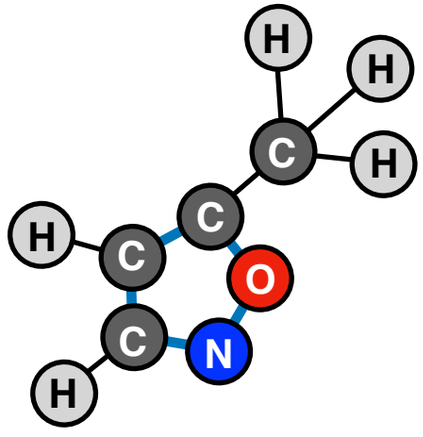
```
import matplotlib.pyplot as plt
import networkx as nx
import torch_geometric as pyg
```

```
data = pyg.datasets.qm9.QM9(root='/tmp/QM9')
print('分子グラフの数:', len(data))
```

```
分子グラフの数: 130831
```

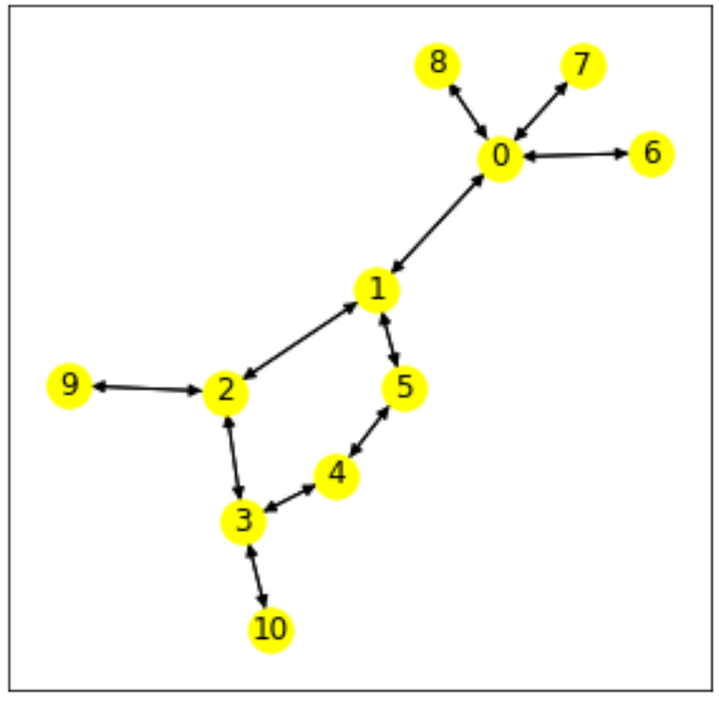
```
mol = data[717]
mol.name
```

718番目の
この分子の
molを観察




```
'gdb_727'
```

```
g = pyg.utils.convert.to_networkx(mol)
fig, ax = plt.subplots(figsize=(5, 5))
nx.draw_networkx(g, node_color="yellow")
fig.show()
```



実際の分子グラフデータを見てみよう

```
mol.y
```

```
tensor([[ 3.1194e+00,  4.8060e+01, -6.8763e+00, -1.9320e-01,  6.6831e+00,
          4.8378e+02,  2.3288e+00, -7.7632e+03, -7.7631e+03, -7.7631e+03,
         -7.7640e+03,  1.8293e+01, -4.7811e+01, -4.8092e+01, -4.8349e+01,
         -4.4744e+01,  9.2803e+00,  3.5644e+00,  2.6172e+00]])
```

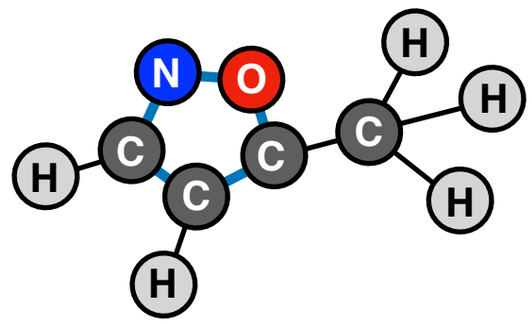
```
import pandas as pd
pd.Series(mol.y.numpy()[0])
```

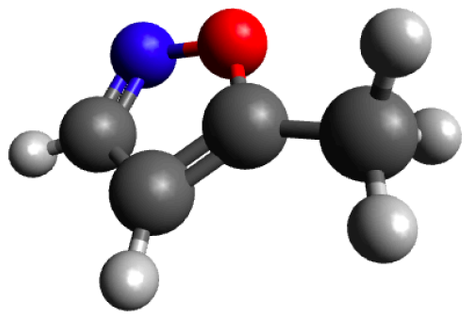
タテに表示

0	3.119400	Dipole moment
1	48.060001	Isotropic polarizability
2	-6.876316	Highest occupied molecular orbital (HOMO) energy
3	-0.193201	Lowest unoccupied molecular orbital (LUMO) energy
4	6.683115	Gap between HOMO and LUMO
5	483.779388	Electronic spatial extent
6	2.328750	Zero point vibrational energy
7	-7763.241699	Internal energy at 0K
8	-7763.098633	Internal energy at 298.15K
9	-7763.073242	Enthalpy at 298.15K
10	-7764.022949	Free energy at 298.15K
11	18.292999	Heat capavity at 298.15K
12	-47.811089	Atomization energy at 0K
13	-48.092346	Atomization energy at 298.15K
14	-48.349361	Atomization enthalpy at 298.15K
15	-44.743744	Atomization free energy at 298.15K
16	9.280260	Rotational constant A
17	3.564360	Rotational constant B
18	2.617160	Rotational constant C

```
dtype: float32
```

これらのDFT計算値を
(DFTしないで)予測するタスク





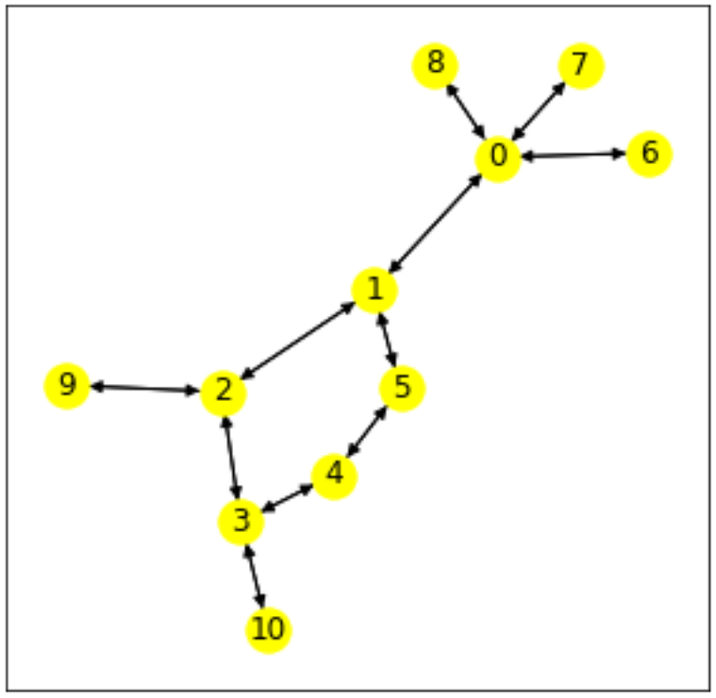
実際の分子グラフデータを見てみよう

```
mol.edge_index
```

```
tensor([[ 0,  0,  0,  0,  1,  1,  1,  2,  2,  2,  3,  3,  3,  4,  4,  5,  5,  6,
          7,  8,  9, 10],
        [ 1,  6,  7,  8,  0,  2,  5,  1,  3,  9,  2,  4, 10,  3,  5,  1,  4,  0,
          0,  0,  2,  3]])
```

```
for id, (s, t) in enumerate(zip(*mol.edge_index)):
  print(f'Edge: {id}, node[{s}] -> node[{t}]')
```

```
Edge: 0, node[0] -> node[1]
Edge: 1, node[0] -> node[6]
Edge: 2, node[0] -> node[7]
Edge: 3, node[0] -> node[8]
Edge: 4, node[1] -> node[0]
Edge: 5, node[1] -> node[2]
   ⋮
Edge: 20, node[9] -> node[2]
Edge: 21, node[10] -> node[3]
```



辺の向きも
考慮できる

Edge 0

node[0] 0 1 node[1]

Edge 4

実際の分子グラフデータを見てみよう

mol.z　頂点の原子番号

```
tensor([6, 6, 6, 6, 7, 8, 1, 1, 1, 1, 1])
```

mol.x　頂点の特徴ベクトル (11次元)

```
tensor([[0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 3.],
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 0.],
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 1.],
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 1.],
        [0., 0., 1., 0., 0., 7., 0., 0., 0., 0., 0.],
        [0., 0., 0., 1., 0., 8., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.]])
```

mol.pos　頂点の位置ベクトル (3次元)

```
tensor([[ 0.0264,  1.4944,  0.0287],
        [-0.0850,  0.0111,  0.0449],
        [-1.0957, -0.8588, -0.2308],
        [-0.5082, -2.1326, -0.0113],
        [ 0.7433, -2.0451,  0.3632],
        [ 1.0156, -0.6777,  0.3997],
        [ 0.8032,  1.8213, -0.6702],
        [-0.9230,  1.9401, -0.2734],
        [ 0.2923,  1.8782,  1.0190],
        [-2.1005, -0.6271, -0.5415],
        [-0.9559, -3.1113, -0.1136]])
```

辺の特徴ベクトル (4次元)

mol.edge_attr

```
tensor([[1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.]])
```

Single
Double
Triple
Aromatic

(one-hot encoding)

実際の分子グラフデータを見てみよう

mol.z　頂点の原子番号

```
tensor([6, 6, 6, 6, 7, 8, 1, 1, 1, 1, 1])
```

mol.x　頂点の特徴ベクトル (11次元)

```
tensor([[0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 3.],
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 0.],
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 1.],
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 1.],
        [0., 0., 1., 0., 0., 7., 0., 0., 0., 0., 0.],
        [0., 0., 0., 1., 0., 8., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.]])
```

mol.pos　頂点の位置ベクトル (3次元)

```
tensor([[ 0.0264,  1.4944,  0.0287],
        [-0.0850,  0.0111,  0.0449],
        [-1.0957, -0.8588, -0.2308],
        [-0.5082, -2.1326, -0.0113],
        [ 0.7433, -2.0451,  0.3632],
        [ 1.0156, -0.6777,  0.3997],
        [ 0.8032,  1.8213, -0.6702],
        [-0.9230,  1.9401, -0.2734],
        [ 0.2923,  1.8782,  1.0190],
        [-2.1005, -0.6271, -0.5415],
        [-0.9559, -3.1113, -0.1136]])
```

辺の特徴ベクトル (4次元)

mol.edge_attr

```
tensor([[1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.],
        [1., 0., 0., 0.]])
```

Single
Double
Triple
Aromatic

(one-hot encoding)

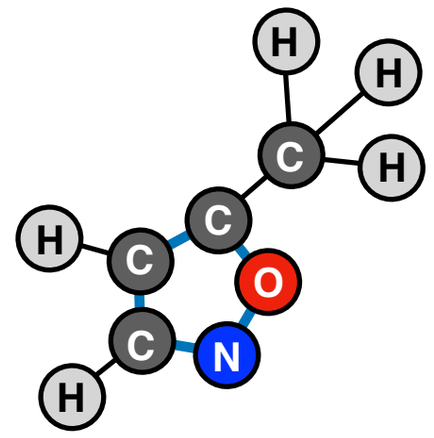
実際の分子グラフデータを見てみよう

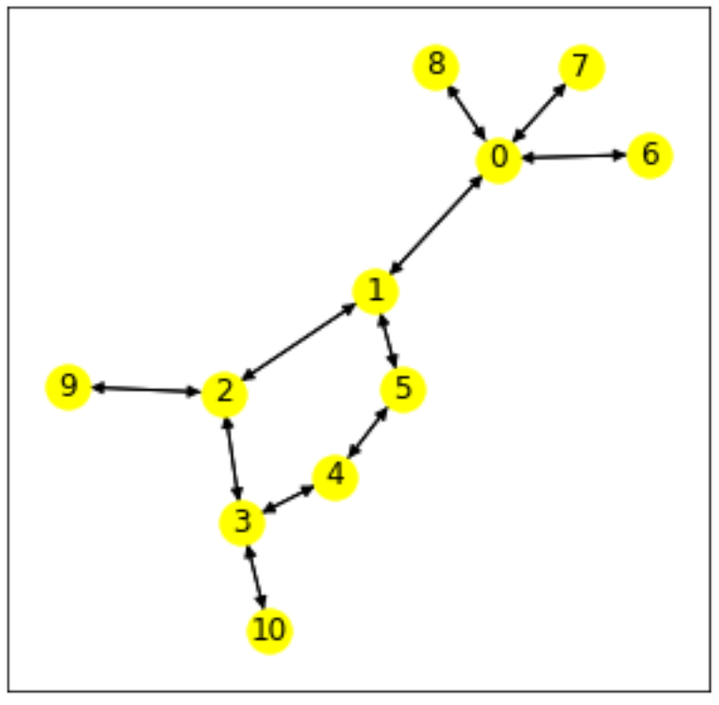
mol.x　　**頂点の特徴ベクトル (11次元)**

```
tensor([[0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 3.],   0
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 0.],   1
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 1.],   2
        [0., 1., 0., 0., 0., 6., 0., 0., 0., 0., 1.],   3
        [0., 0., 1., 0., 0., 7., 0., 0., 0., 0., 0.],   4
        [0., 0., 0., 1., 0., 8., 0., 0., 0., 0., 0.],   5
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],   6
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],   7
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],   8
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],   9
        [1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0.]])  10
```

H C N O F (one-hot encoding)

- 原子番号
- aromatic? (0/1)
- sp? (0/1)
- sp^2? (0/1)
- sp^3? (0/1)
- 結合するHの数



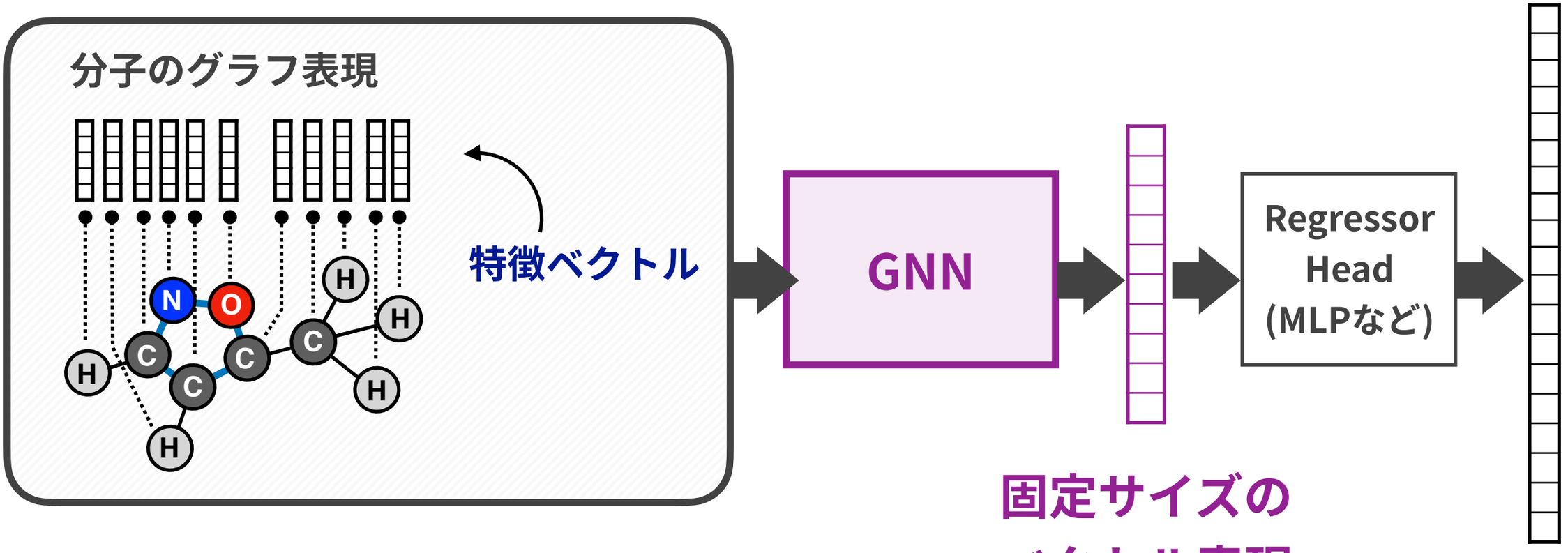


→ **これ以外にもいろいろ有りえることに注意**

https://pytorch-geometric.readthedocs.io/en/latest/_modules/torch_geometric/datasets/qm9.html

GNNがやること

可変サイズの分子グラフから「固定サイズのベクトル表現」への変換を学習



mol.x 頂点の特徴ベクトル (11次元)

mol.pos 頂点の位置ベクトル (3次元)

mol.edge_attr 辺の特徴ベクトル (4次元)

mol.edge_index 辺と結合原子ペアの対応

本日の内容

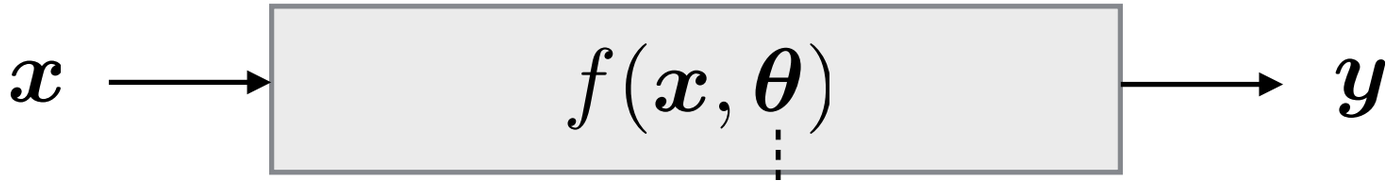
GNN(Graph Neural Networks)で**グラフ表現**された分子を入力にして機械学習するやり方を**のぞいてみませんか**？

- 機械学習とは？
- 分子のグラフ表現
- 準備：深層学習のココロ (forwardとbackward)
- Graph Neural Networksとは？
- 自分でやってみるための情報
- おまけ：
  最近の話 (計算限界、分子生成、事前学習、...)

機械学習のモデル

機械学習 = **多量の入出力の見本例**から**プログラム**を
自動的に作成する(いいかげんな)技術

機械学習モデル



$$\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)$$

多数のパラメタの値を動かして
出力が望む値になるようにする

モデルの学習 = パラメタの値を最適にする

予測値　教師の値

見本例を予測

$\boldsymbol{x}_1 \longrightarrow f(\boldsymbol{x}, \boldsymbol{\theta}) \longrightarrow \hat{y}_1 \quad y_1$

$\boldsymbol{x}_2 \longrightarrow f(\boldsymbol{x}, \boldsymbol{\theta}) \longrightarrow \hat{y}_2 \quad y_2$

$\boldsymbol{x}_n \longrightarrow f(\boldsymbol{x}, \boldsymbol{\theta}) \longrightarrow \hat{y}_n \quad y_n$

$\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)$

予測値と教師の値が近づくように
パラメタ $\boldsymbol{\theta}$ を調整

モデルの学習 = パラメタの値を最適にする

予測値と教師の値が近づくように
パラメタ θ を調整

関数 $\mathrm{loss}(\theta)$ の値が小さくなる
ようにパラメタ θ を調整

$$\mathrm{loss}(\theta) = \sum_{i=1}^{n} (\hat{y}_i - y_i)^2$$

パラメタ調整のやりかた：

- θ をランダム値で初期化
- $\mathrm{loss}(\theta)$ の値が小さくなるように θ をちょっとだけ変える

$$\begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix} \leftarrow \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix} + 0.01 \times \begin{bmatrix} \Delta\theta_1 \\ \Delta\theta_2 \\ \vdots \\ \Delta\theta_p \end{bmatrix}$$

学習率
(step size)

くりかえし

勾配降下法 (Gradient Descent)

- $\mathrm{loss}(\boldsymbol{\theta})$ の値が小さくなるように $\boldsymbol{\theta}$ を**ちょっとだけ**変える

$$\begin{bmatrix}\theta_1\\ \theta_2\end{bmatrix} \leftarrow \begin{bmatrix}\theta_1\\ \theta_2\end{bmatrix} + 0.01 \times \begin{bmatrix}f_1'(\theta_1,\theta_2)\\ f_2'(\theta_1,\theta_2)\end{bmatrix}$$

勾配ベクトル

$$f_1'(\theta_1,\theta_2) = \frac{\partial \mathrm{loss}(\theta_1,\theta_2)}{\partial \theta_1}$$

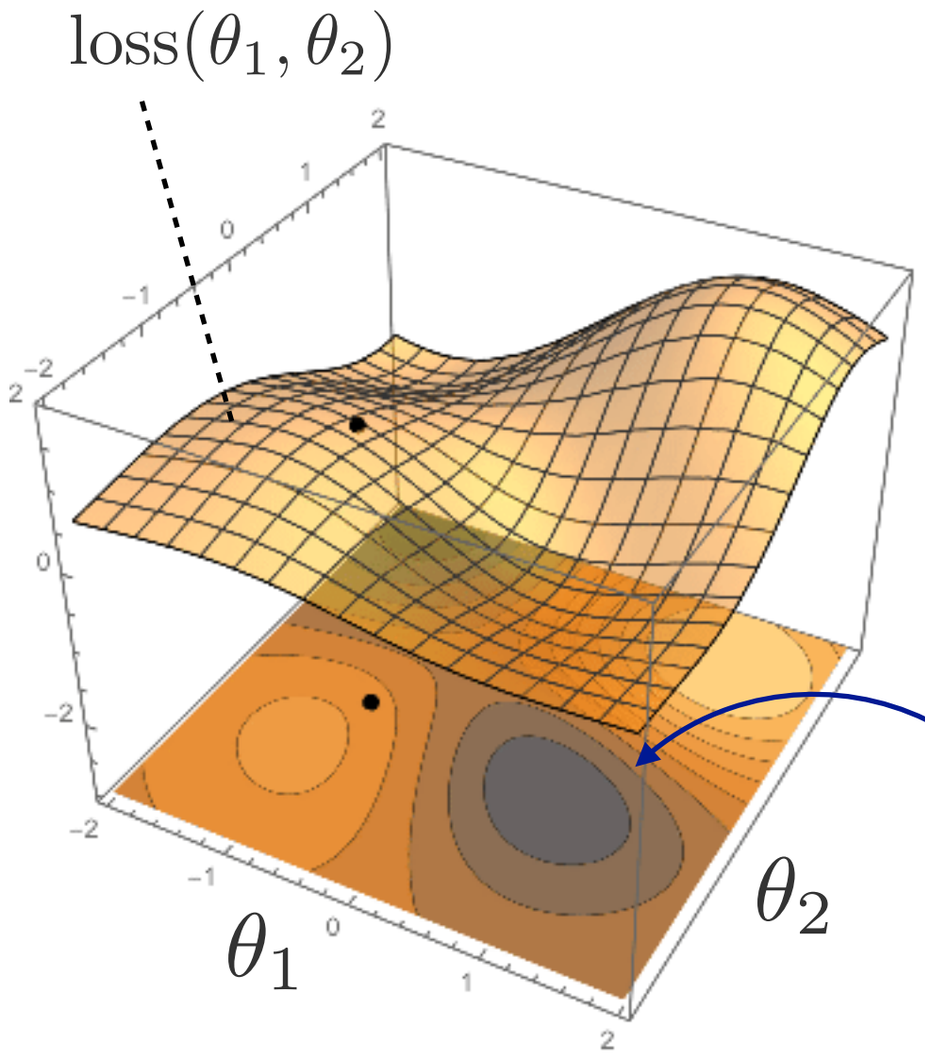
$$f_2'(\theta_1,\theta_2) = \frac{\partial \mathrm{loss}(\theta_1,\theta_2)}{\partial \theta_2}$$

偏微分

θ_1 や θ_2 を

少し動かしたときの

$\mathrm{loss}(\theta_1,\theta_2)$ の変化量



勾配ベクトルに比例する量を**ちょっと引く**と
最寄りの極小値に向かうことがわかっている

勾配降下法 (Gradient Descent)

- $\mathrm{loss}(\boldsymbol{\theta})$ の値が小さくなるように $\boldsymbol{\theta}$ を**ちょっとだけ**変える

$$\begin{bmatrix}\theta_1\\ \theta_2\end{bmatrix} \leftarrow \begin{bmatrix}\theta_1\\ \theta_2\end{bmatrix} + 0.01 \times \begin{bmatrix}f_1'(\theta_1,\theta_2)\\ f_2'(\theta_1,\theta_2)\end{bmatrix}$$

勾配ベクトル

$$f_1'(\theta_1,\theta_2) = \frac{\partial \mathrm{loss}(\theta_1,\theta_2)}{\partial \theta_1}$$

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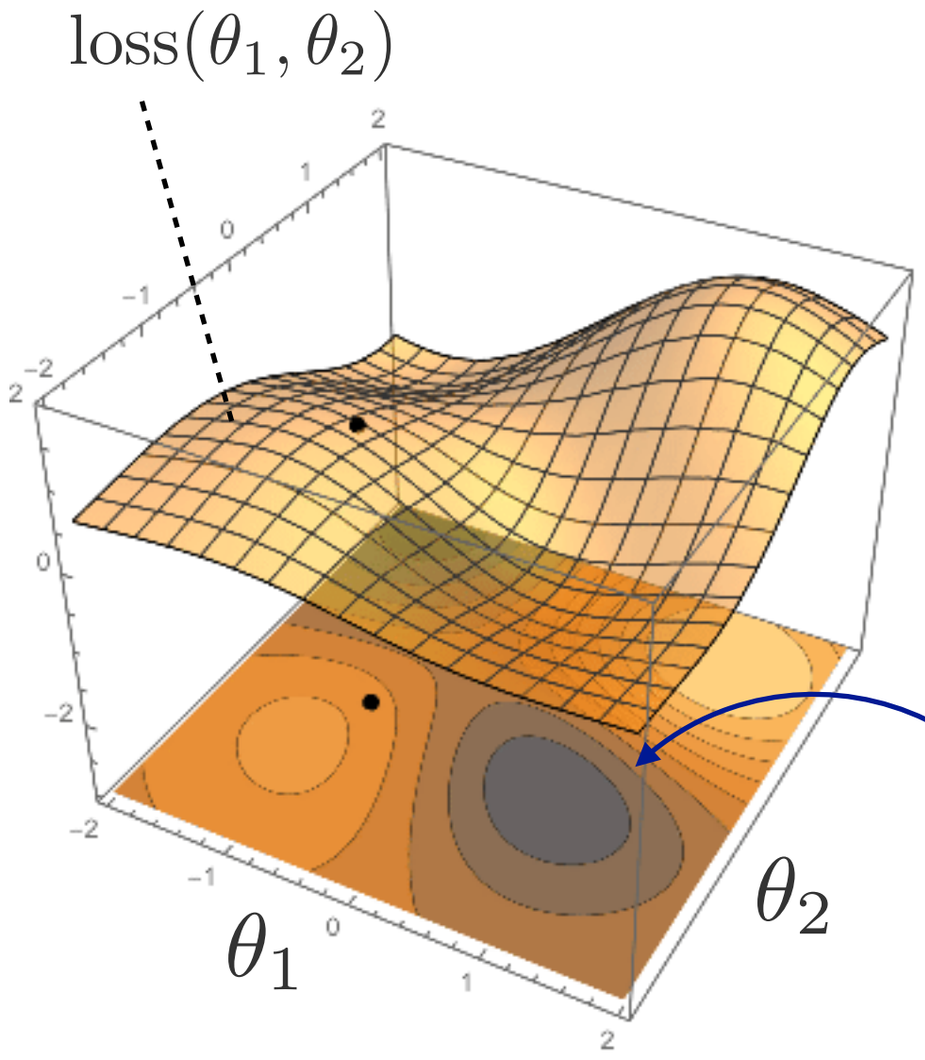
偏微分

θ_1 や θ_2 を

少し動かしたときの

$\mathrm{loss}(\theta_1,\theta_2)$ の変化量



勾配ベクトルに比例する量を**ちょっと引く**と
最寄りの極小値に向かうことがわかっている

計算グラフと自動微分：複雑なモデルの勾配の計算

機械学習モデル

$$\boldsymbol{x}_i \longrightarrow \boxed{f(\boldsymbol{x}, \boldsymbol{\theta})} \longrightarrow \hat{y}_i$$

小さくしたい尺度

$$\begin{aligned}\mathrm{loss}(\boldsymbol{\theta}) &= \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 \\ &= \sum_{i=1}^{n} (f(\boldsymbol{x}_i, \boldsymbol{\theta}) - y_i)^2\end{aligned}$$

勾配ベクトル

$$\begin{bmatrix} \partial \mathrm{loss}(\boldsymbol{\theta})/\partial\theta_1 \\ \partial \mathrm{loss}(\boldsymbol{\theta})/\partial\theta_2 \\ \vdots \\ \partial \mathrm{loss}(\boldsymbol{\theta})/\partial\theta_p \end{bmatrix}$$

計算グラフと自動微分：複雑なモデルの勾配の計算

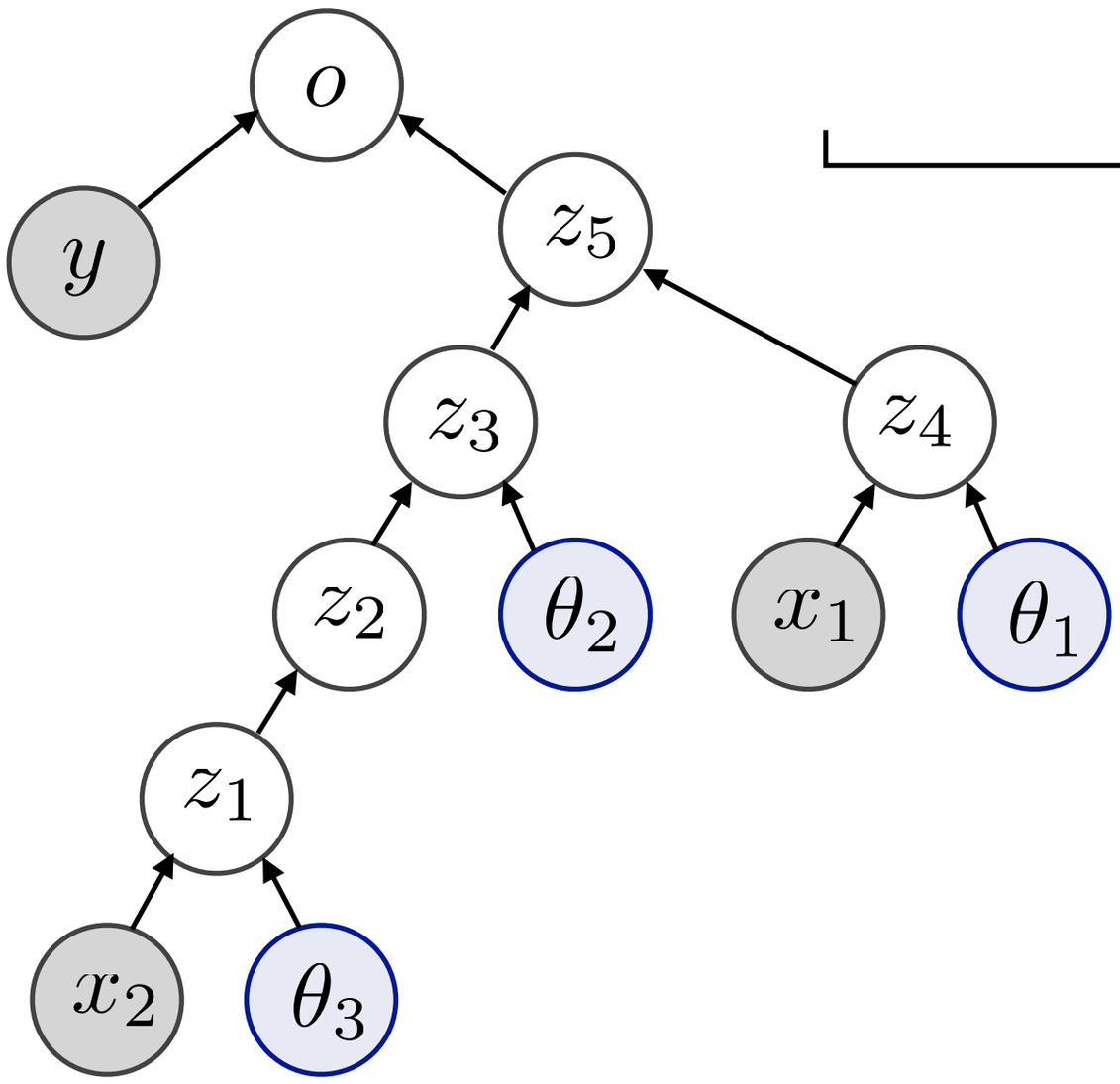
例 $g(\theta_1, \theta_2) = \big(\underline{f(x_1, x_2, \theta_1, \theta_2, \theta_3)} - y\big)^2$

$$= \underbrace{\theta_1 x_1}_{z_4} - \theta_2 \cos(\underbrace{\theta_3 + x_2}_{z_1})$$

z_2

z_3

z_5

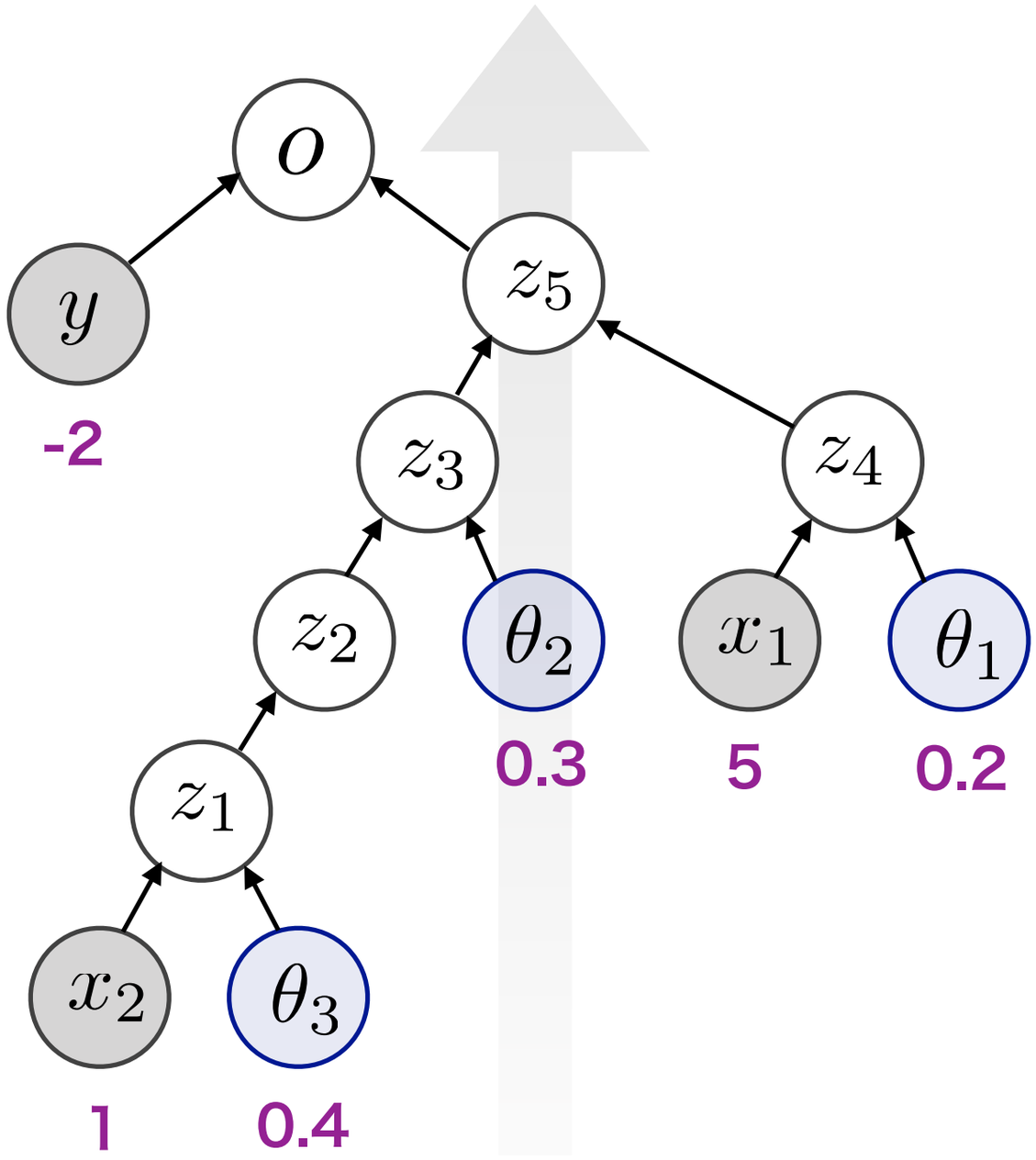


合成関数

$$z_1 = \theta_3 + x_2$$
$$z_2 = \cos(z_1)$$
$$z_3 = \theta_2 z_2$$
$$z_4 = \theta_1 x_1$$
$$z_5 = z_4 - z_3$$
$$o = (z_5 - y)^2$$

forward

このとき o は？



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1$$

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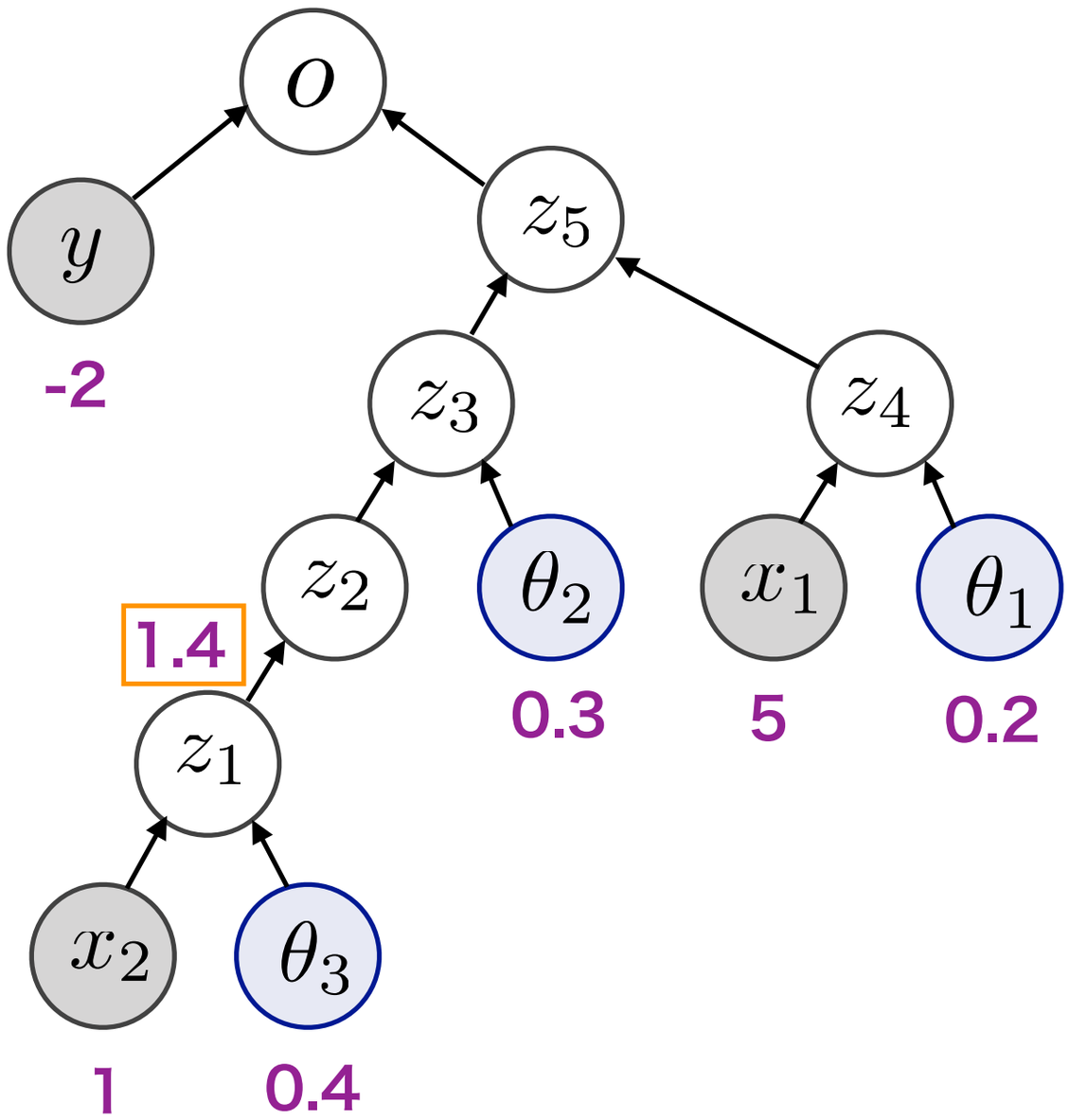
forward

このとき o は？



$$o = (z_5 - y)^2$$

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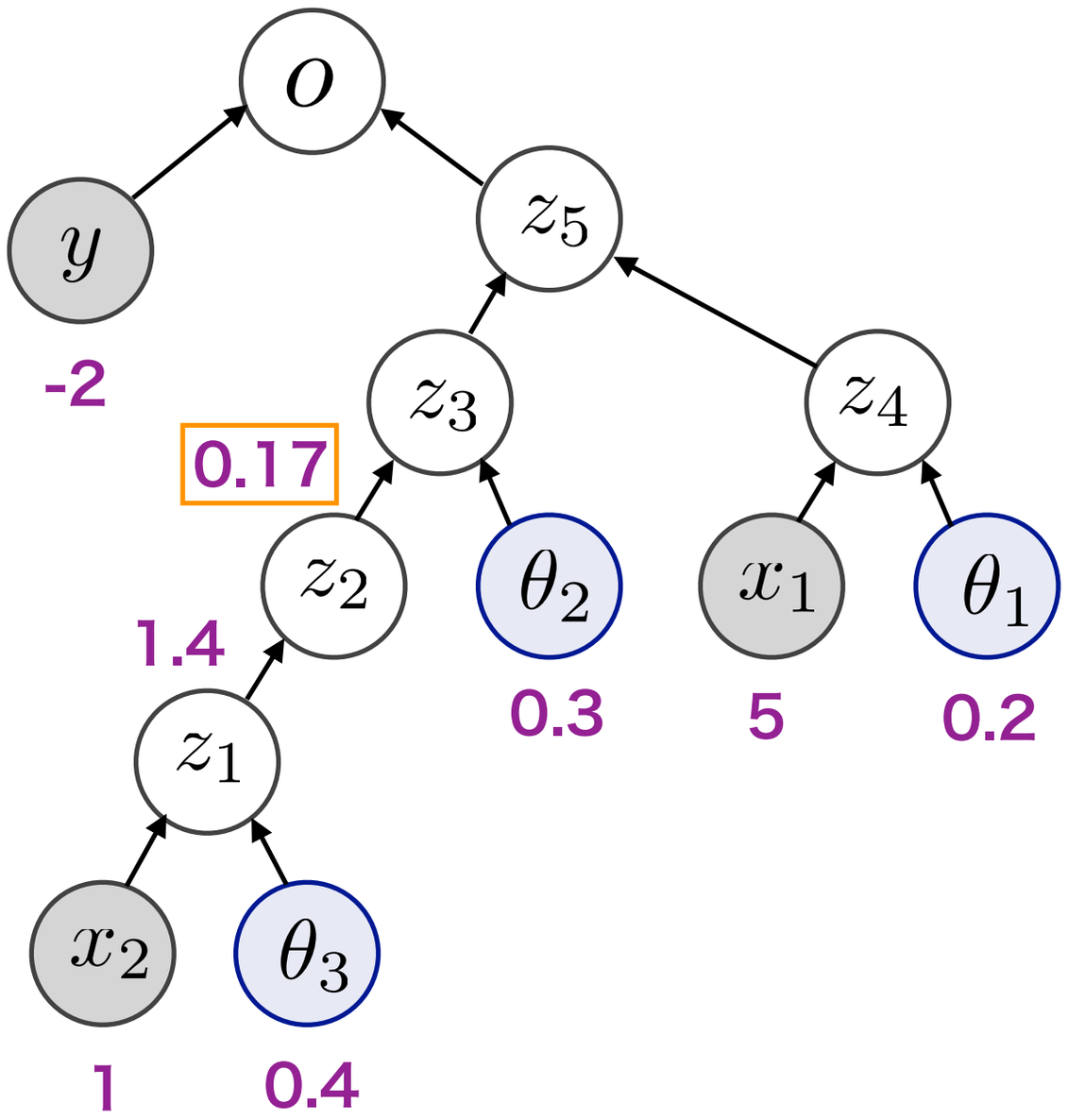
forward

このとき o は？



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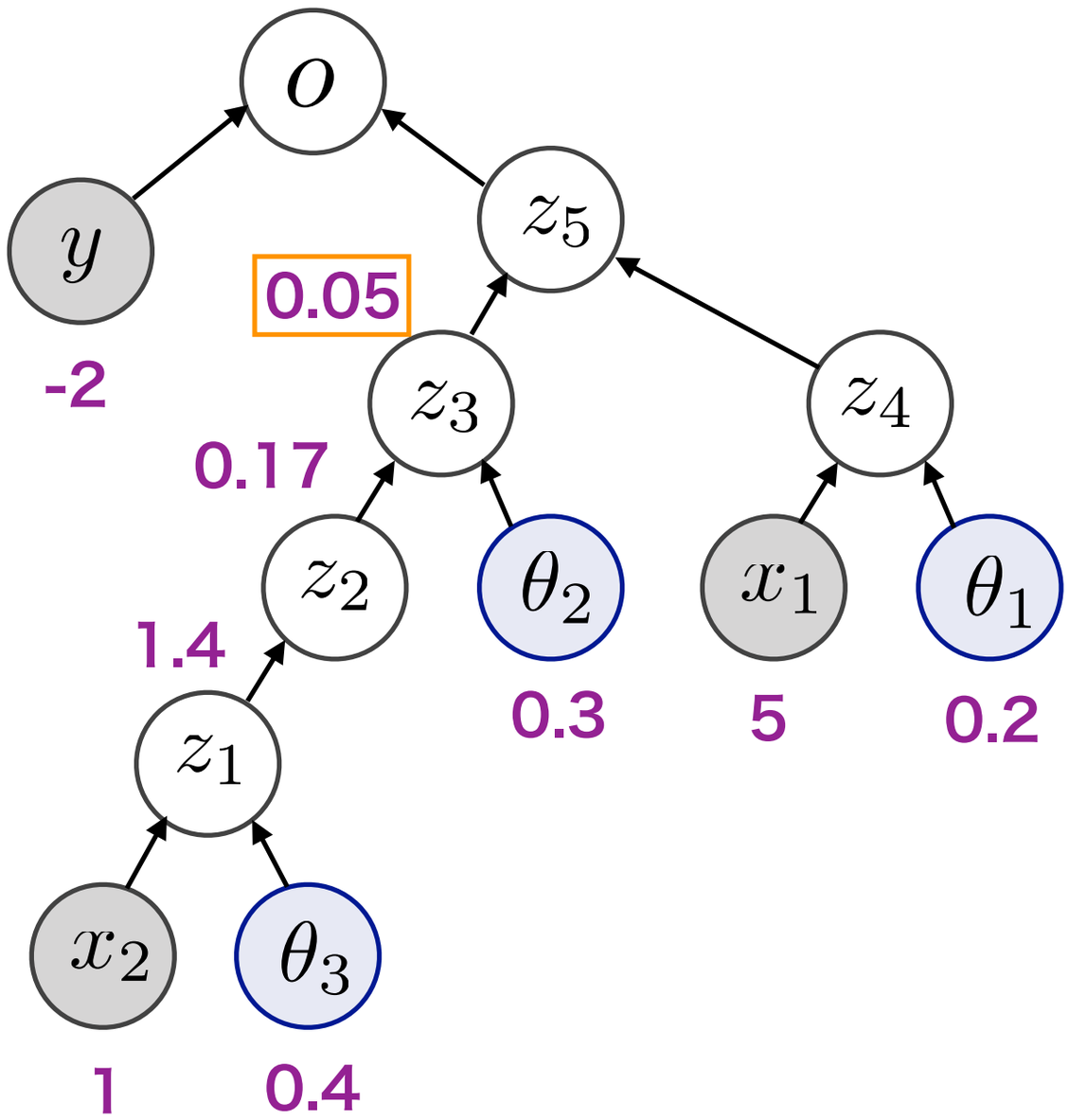
forward

このとき o は？



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$$z_4 = \theta_1 x_1$$

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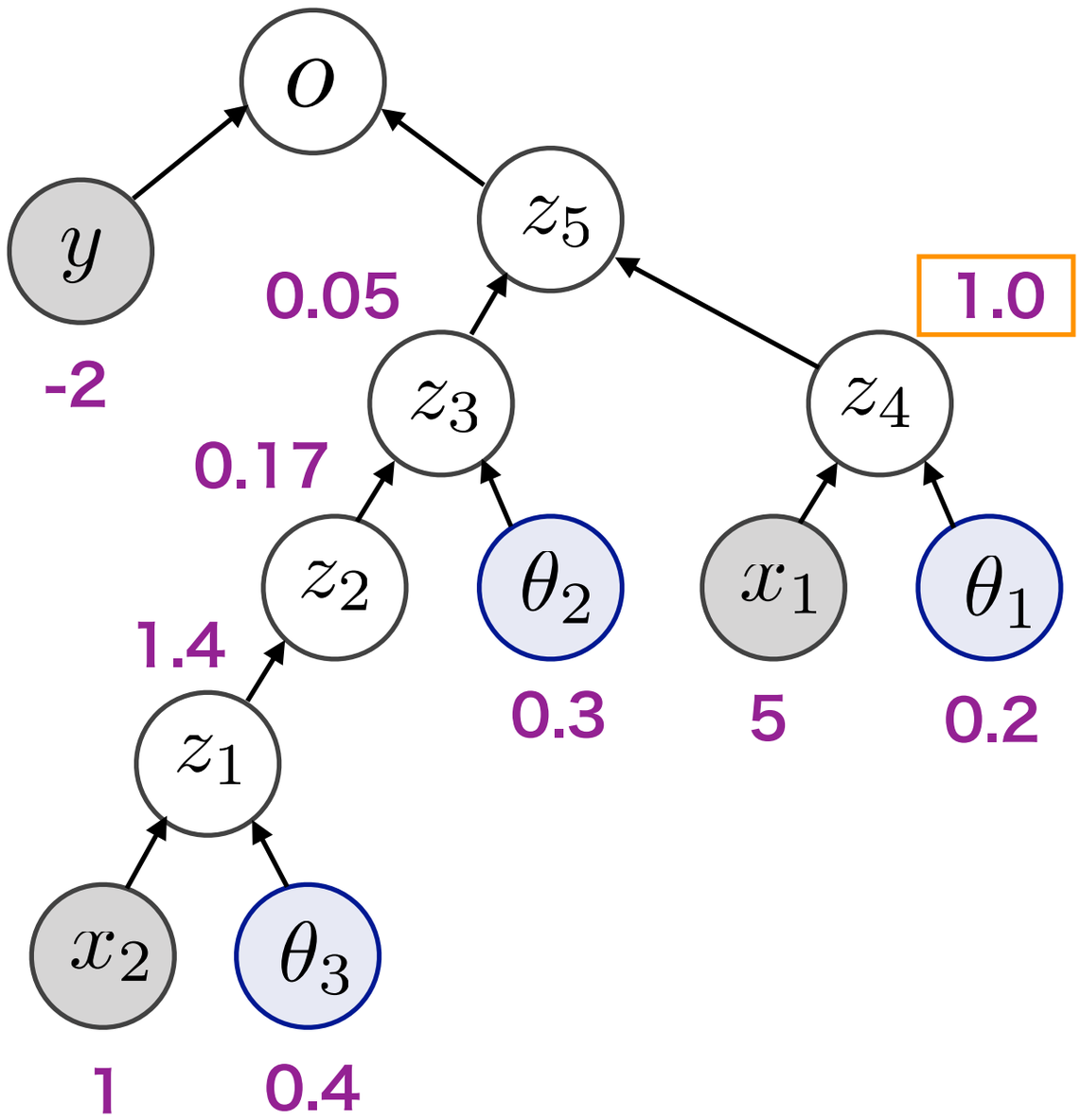
forward

このとき o は？



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1$$

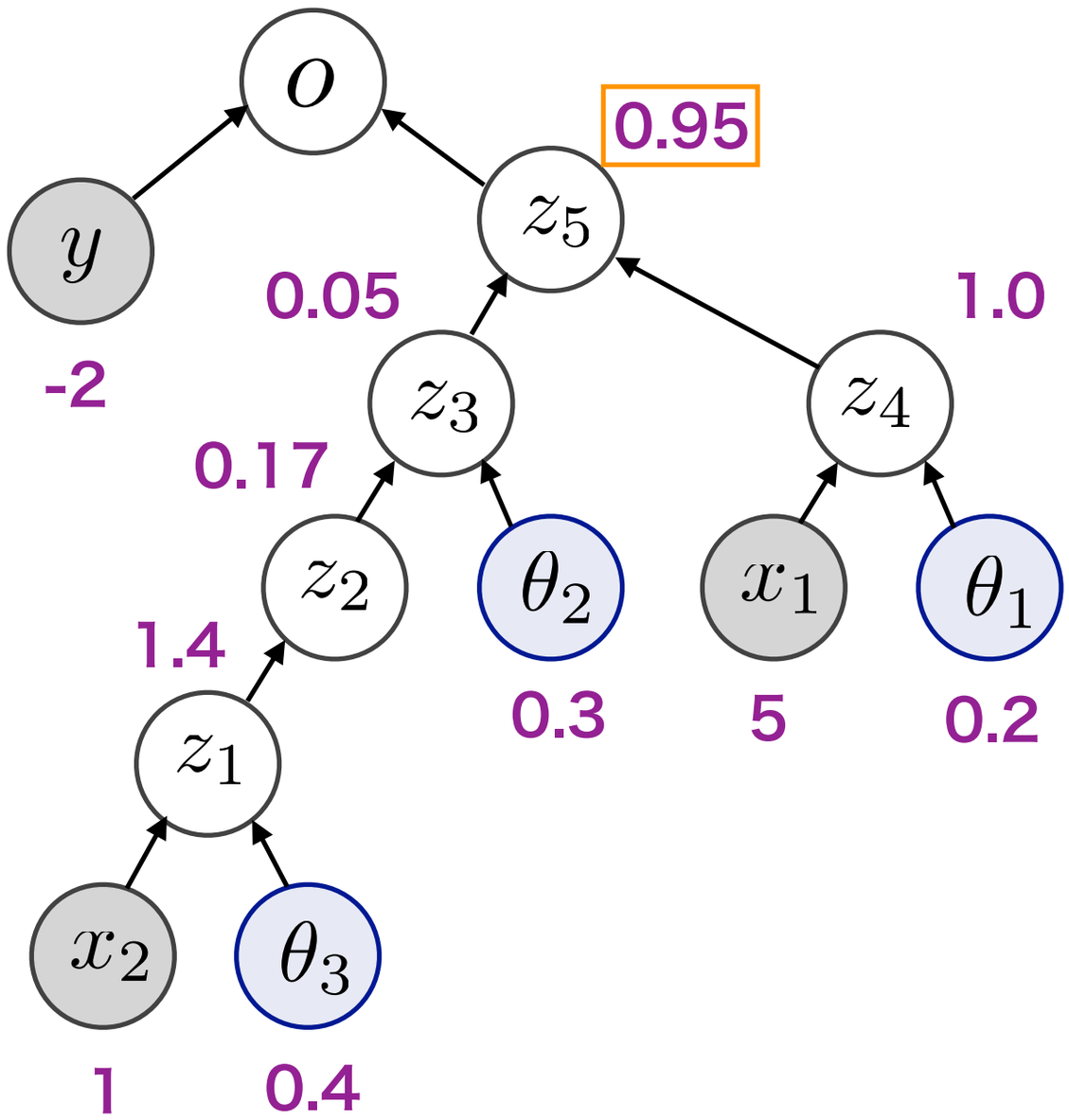
$$z_3 = \theta_2 z_2$$

$$z_2 = \cos(z_1)$$

$$z_1 = \theta_3 + x_2$$

forward

このとき o は？



$$o = (z_5 - y)^2$$

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$$z_4 = \theta_1 x_1$$

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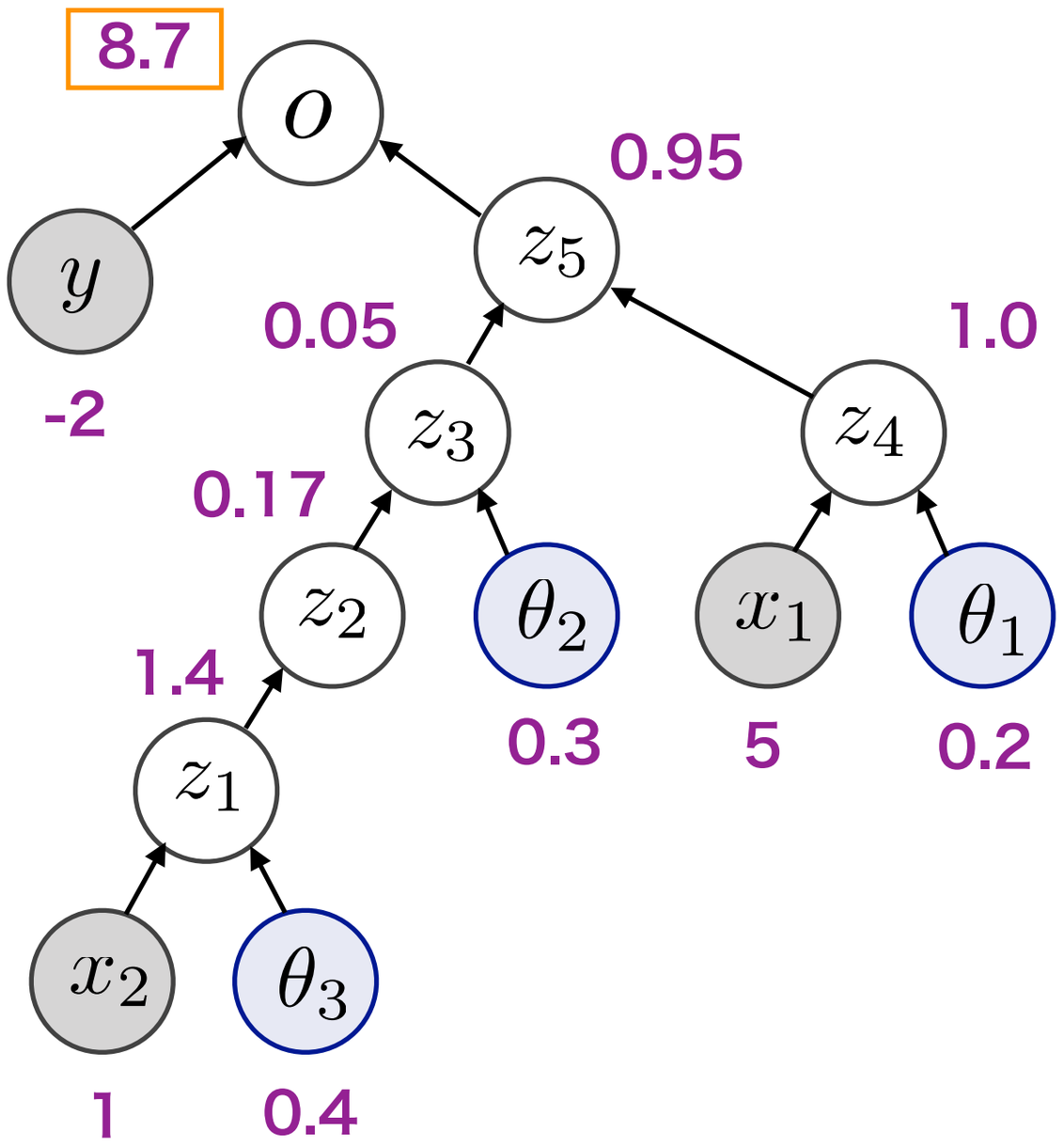
forward

このとき o は？



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1$$

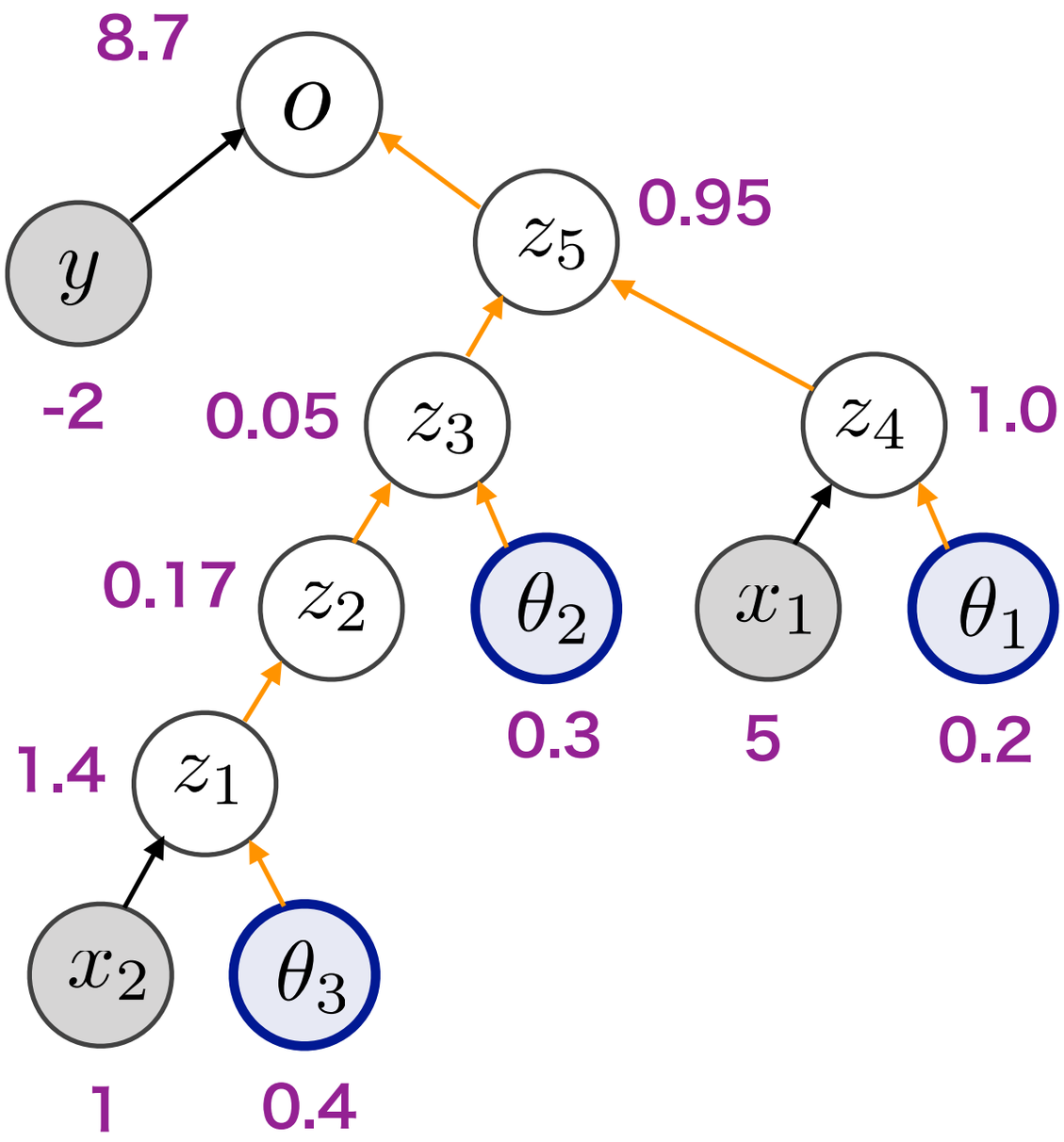
$$z_3 = \theta_2 z_2$$

$$z_2 = \cos(z_1)$$

$$z_1 = \theta_3 + x_2$$

forward

勾配を計算する変数は**ついでに各ステップの偏微分値**も計算しておく



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1$$

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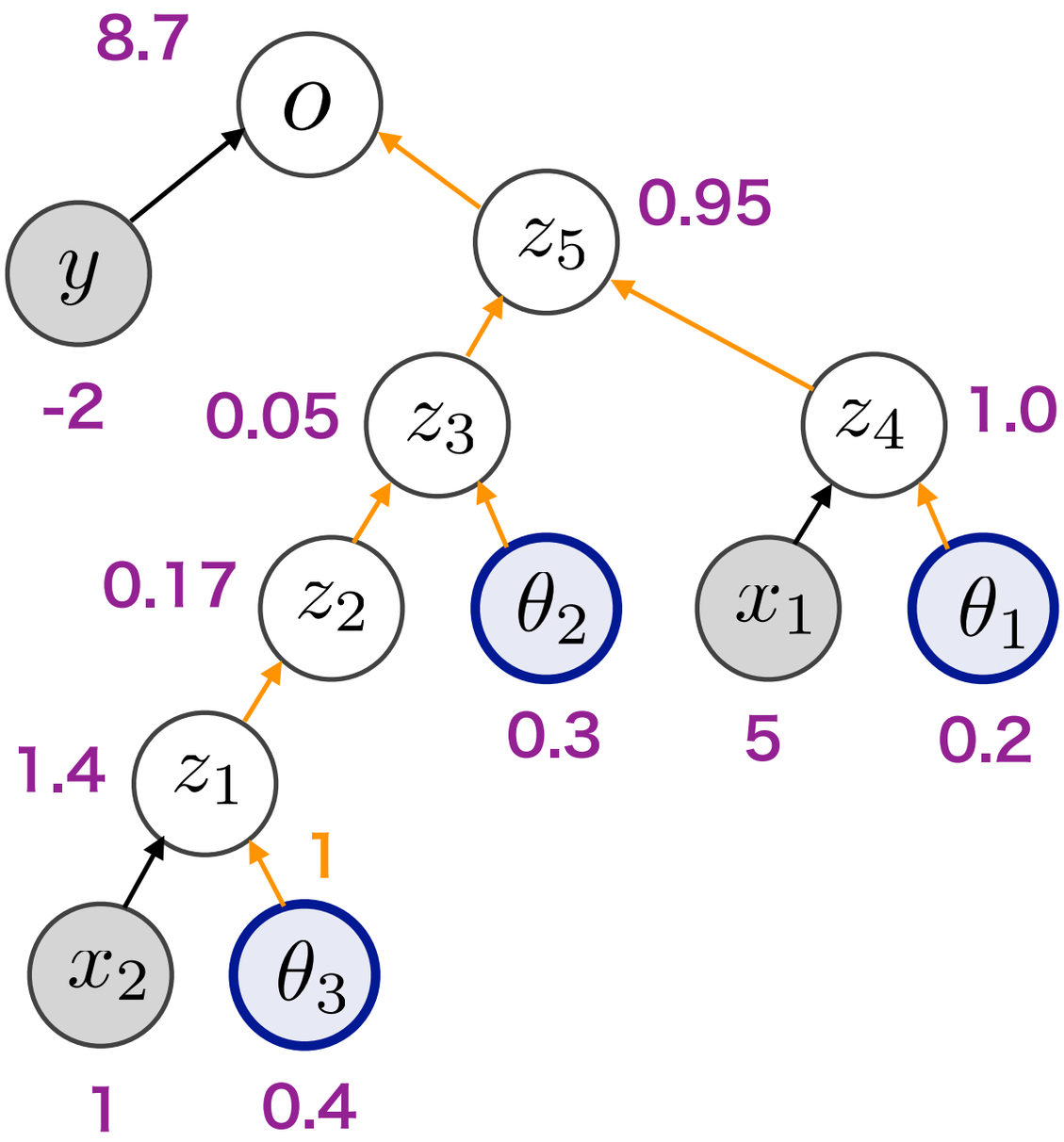
forward

勾配を計算する変数は**ついでに各ステップの偏微分値**も計算しておく



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1$$

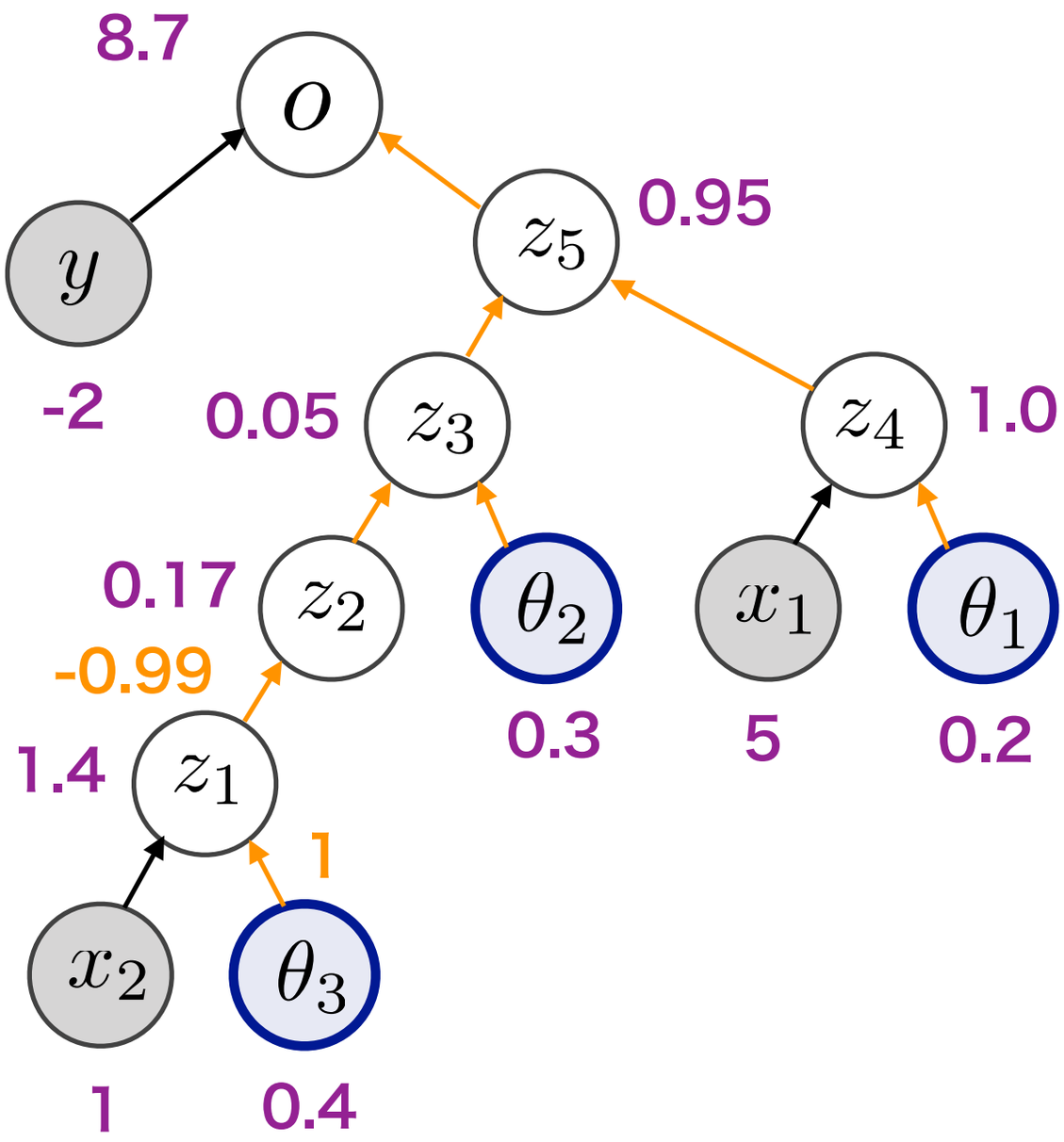
$$z_3 = \theta_2 z_2$$

$$z_2 = \cos(z_1)$$

$$z_1 = \theta_3 + x_2 \quad \partial z_1 / \partial \theta_3 = 1$$

forward

勾配を計算する変数は**ついでに各ステップの偏微分値**も計算しておく



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1$$

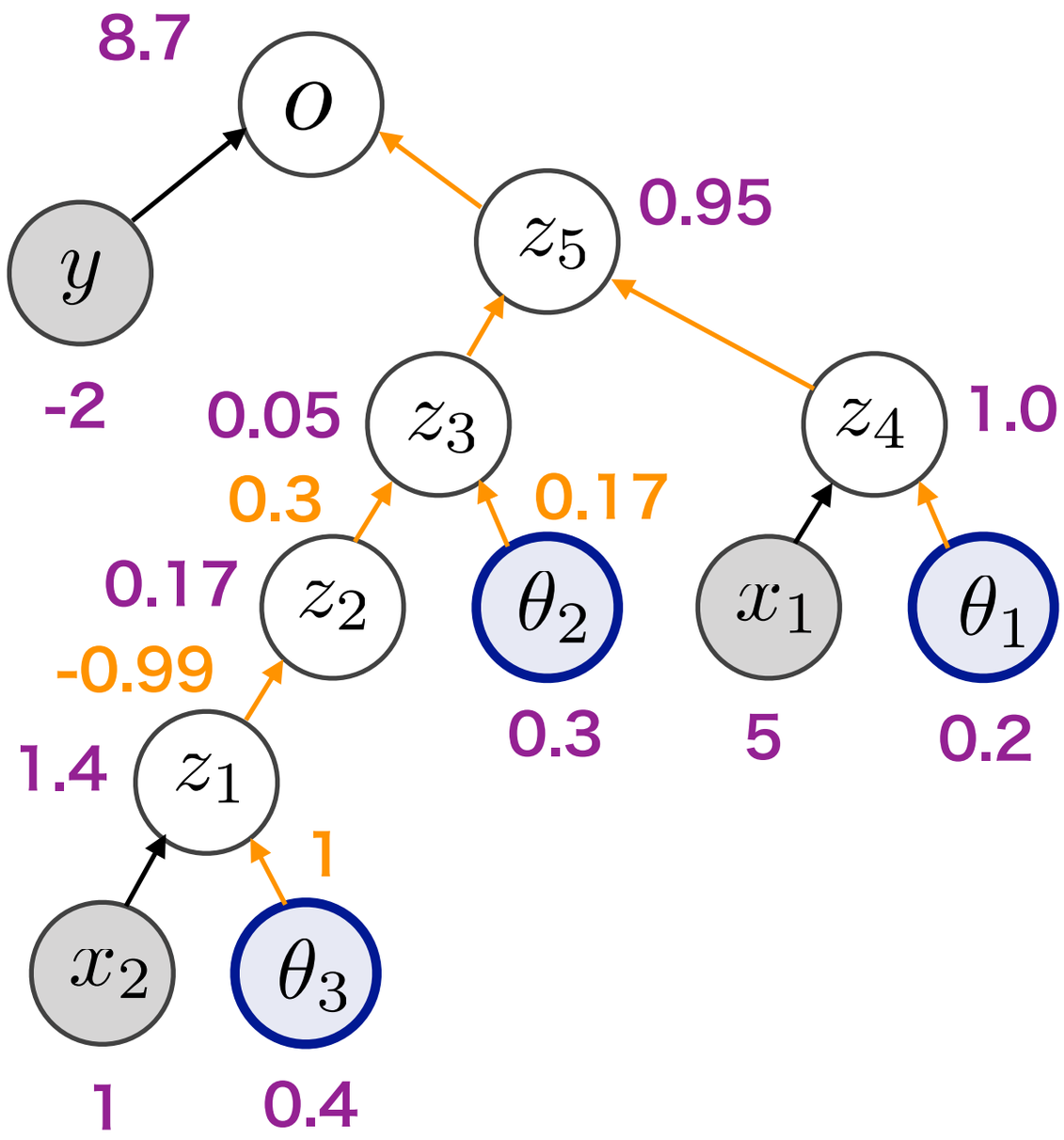
$$z_3 = \theta_2 z_2$$

$$z_2 = \cos(z_1) \qquad \partial z_2 / \partial z_1 = -\sin(z_1)$$

$$z_1 = \theta_3 + x_2 \qquad \partial z_1 / \partial \theta_3 = 1$$

forward

勾配を計算する変数は**ついでに各ステップの偏微分値**も計算しておく



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1$$

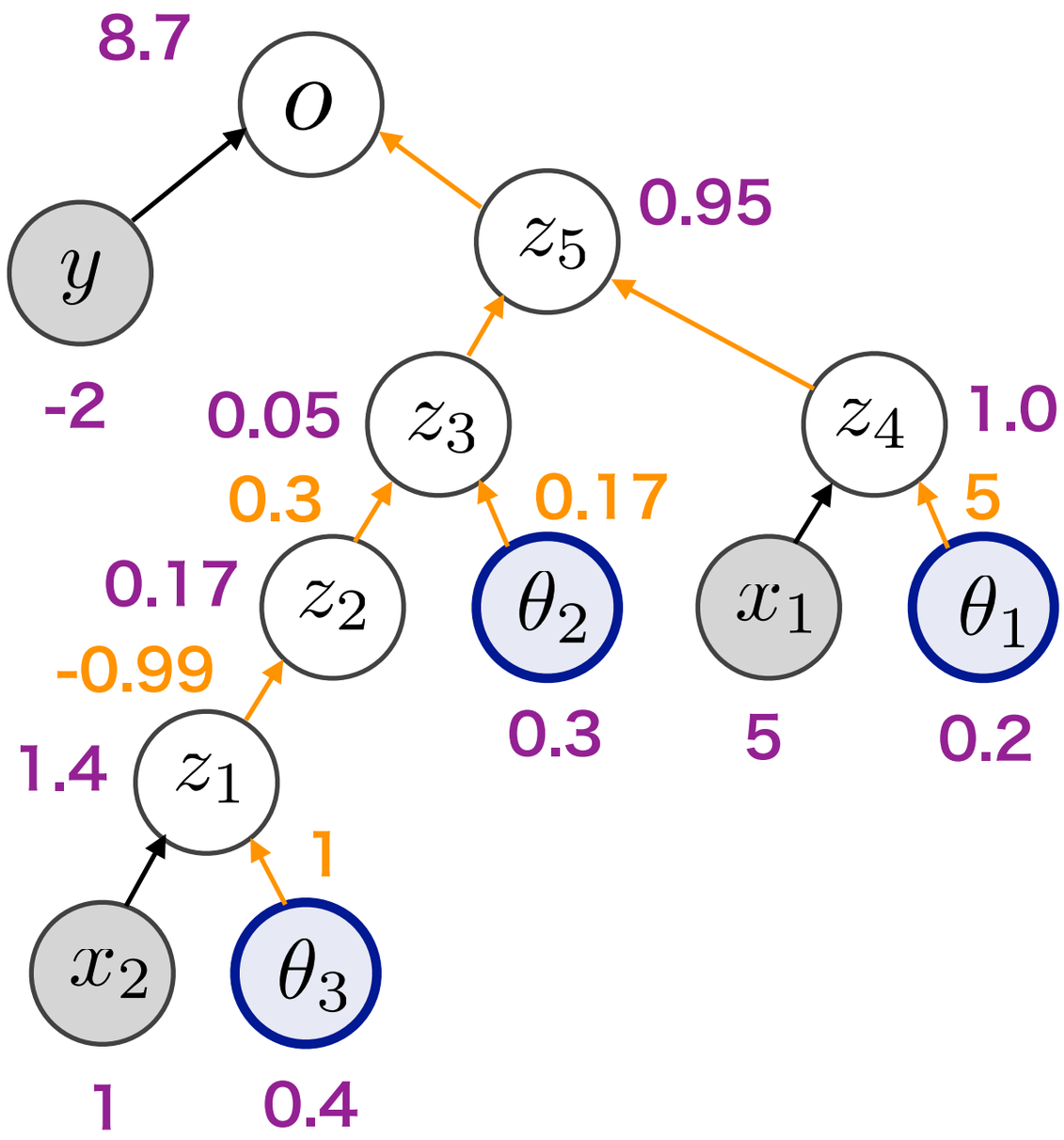
$$z_3 = \theta_2 z_2 \qquad \partial z_3/\partial z_2 = \theta_2 \quad \partial z_3/\partial \theta_2 = z_2$$

$$z_2 = \cos(z_1) \qquad \partial z_2/\partial z_1 = -\sin(z_1)$$

$$z_1 = \theta_3 + x_2 \qquad \partial z_1/\partial \theta_3 = 1$$

forward

勾配を計算する変数は**ついでに各ステップの偏微分値**も計算しておく



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3$$

$$z_4 = \theta_1 x_1 \qquad \partial z_4/\partial \theta_1 = x_1$$

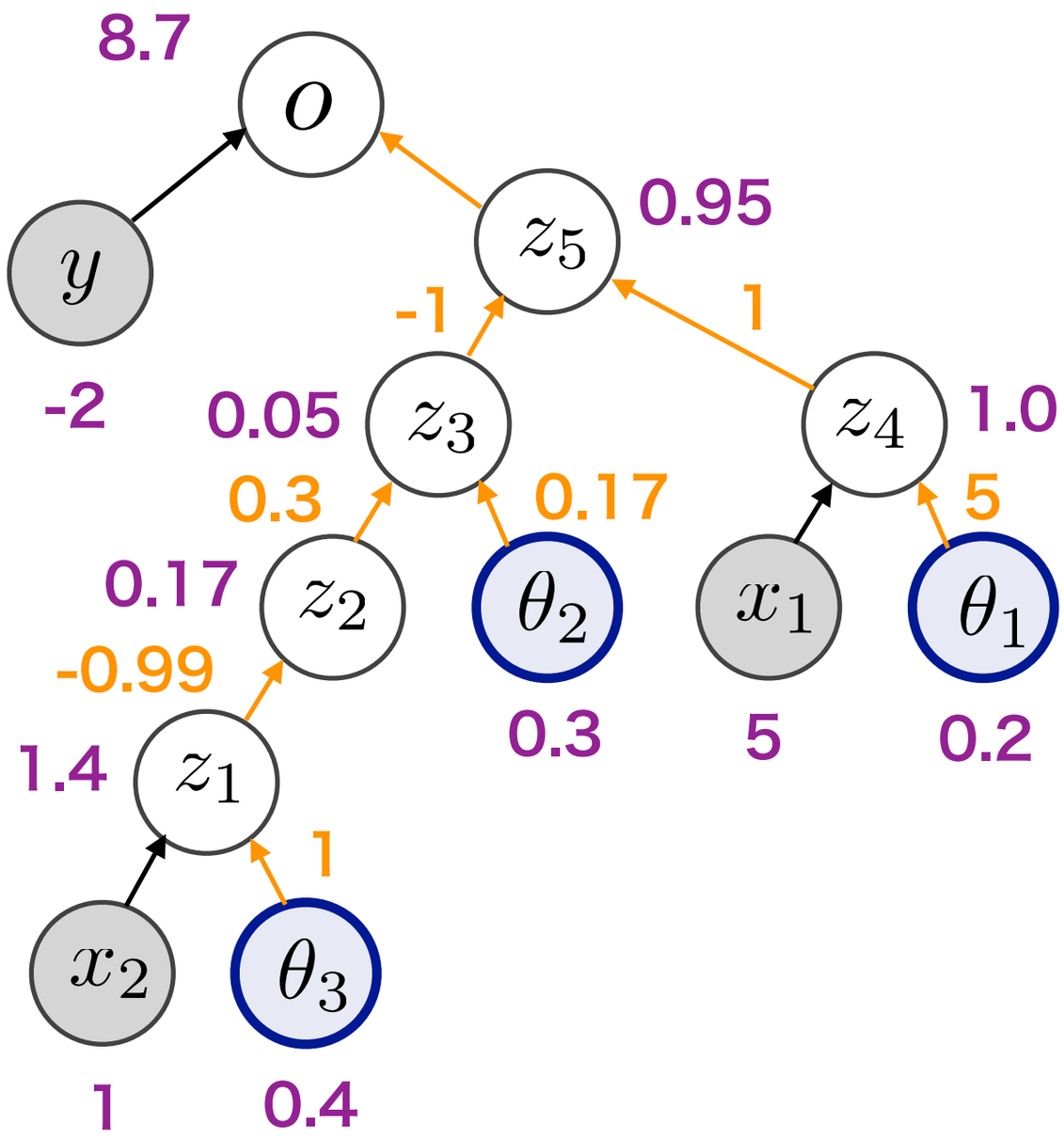
$$z_3 = \theta_2 z_2 \qquad \partial z_3/\partial z_2 = \theta_2 \quad \partial z_3/\partial \theta_2 = z_2$$

$$z_2 = \cos(z_1) \qquad \partial z_2/\partial z_1 = -\sin(z_1)$$

$$z_1 = \theta_3 + x_2 \qquad \partial z_1/\partial \theta_3 = 1$$

forward

勾配を計算する変数は**ついでに各ステップの偏微分値**も計算しておく



$$o = (z_5 - y)^2$$

$$z_5 = z_4 - z_3 \qquad \partial z_5/\partial z_4 = 1 \quad \partial z_5/\partial z_3 = -1$$

$$z_4 = \theta_1 x_1 \qquad \partial z_4/\partial \theta_1 = x_1$$

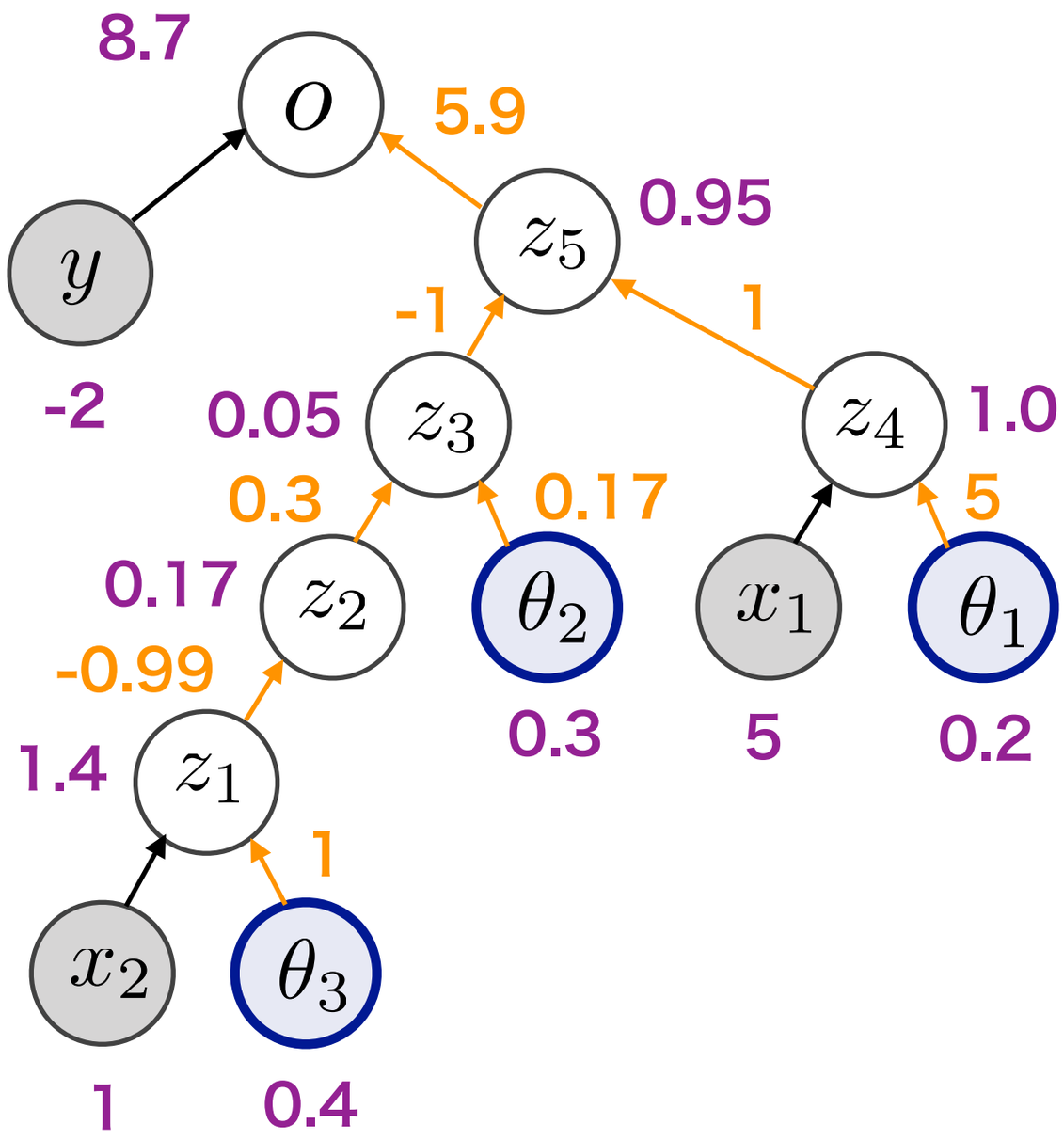
$$z_3 = \theta_2 z_2 \qquad \partial z_3/\partial z_2 = \theta_2 \quad \partial z_3/\partial \theta_2 = z_2$$

$$z_2 = \cos(z_1) \qquad \partial z_2/\partial z_1 = -\sin(z_1)$$

$$z_1 = \theta_3 + x_2 \qquad \partial z_1/\partial \theta_3 = 1$$

forward

勾配を計算する変数は**ついでに各ステップの偏微分値**も計算しておく



$$o = (z_5 - y)^2 \qquad \partial o/\partial z_5 = 2(z_5 - y)$$

$$z_5 = z_4 - z_3 \qquad \partial z_5/\partial z_4 = 1,\ \partial z_5/\partial z_3 = -1$$

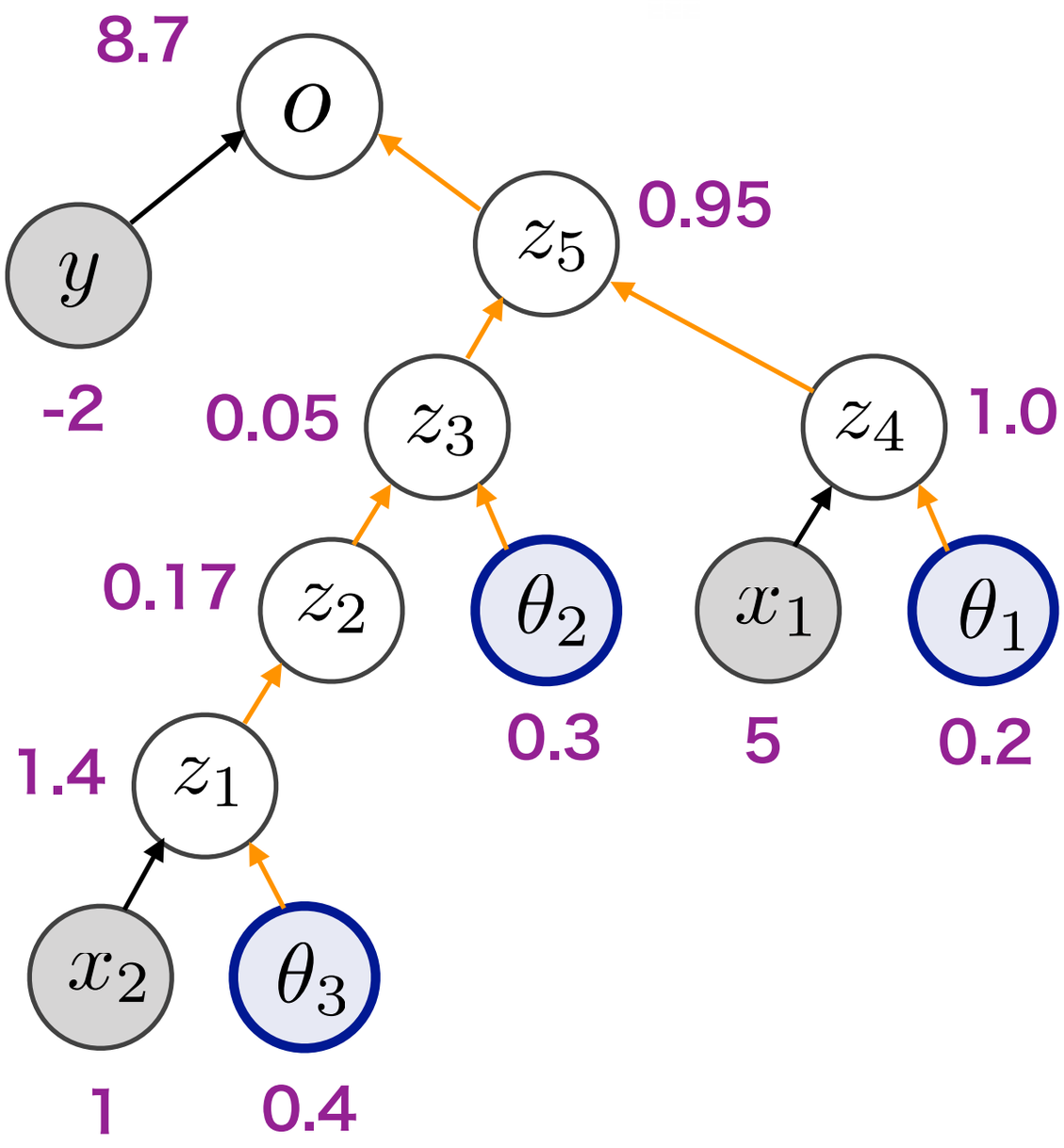
$$z_4 = \theta_1 x_1 \qquad \partial z_4/\partial \theta_1 = x_1$$

$$z_3 = \theta_2 z_2 \qquad \partial z_3/\partial z_2 = \theta_2,\ \partial z_3/\partial \theta_2 = z_2$$

$$z_2 = \cos(z_1) \qquad \partial z_2/\partial z_1 = -\sin(z_1)$$

$$z_1 = \theta_3 + x_2 \qquad \partial z_1/\partial \theta_3 = 1$$

forward



PyTorch

```
import torch
```

```
y = torch.tensor([-2])
x1 = torch.tensor([5])
x2 = torch.tensor([1])
theta1 = torch.tensor([0.2], requires_grad=True)
theta2 = torch.tensor([0.3], requires_grad=True)
theta3 = torch.tensor([0.4], requires_grad=True)
```

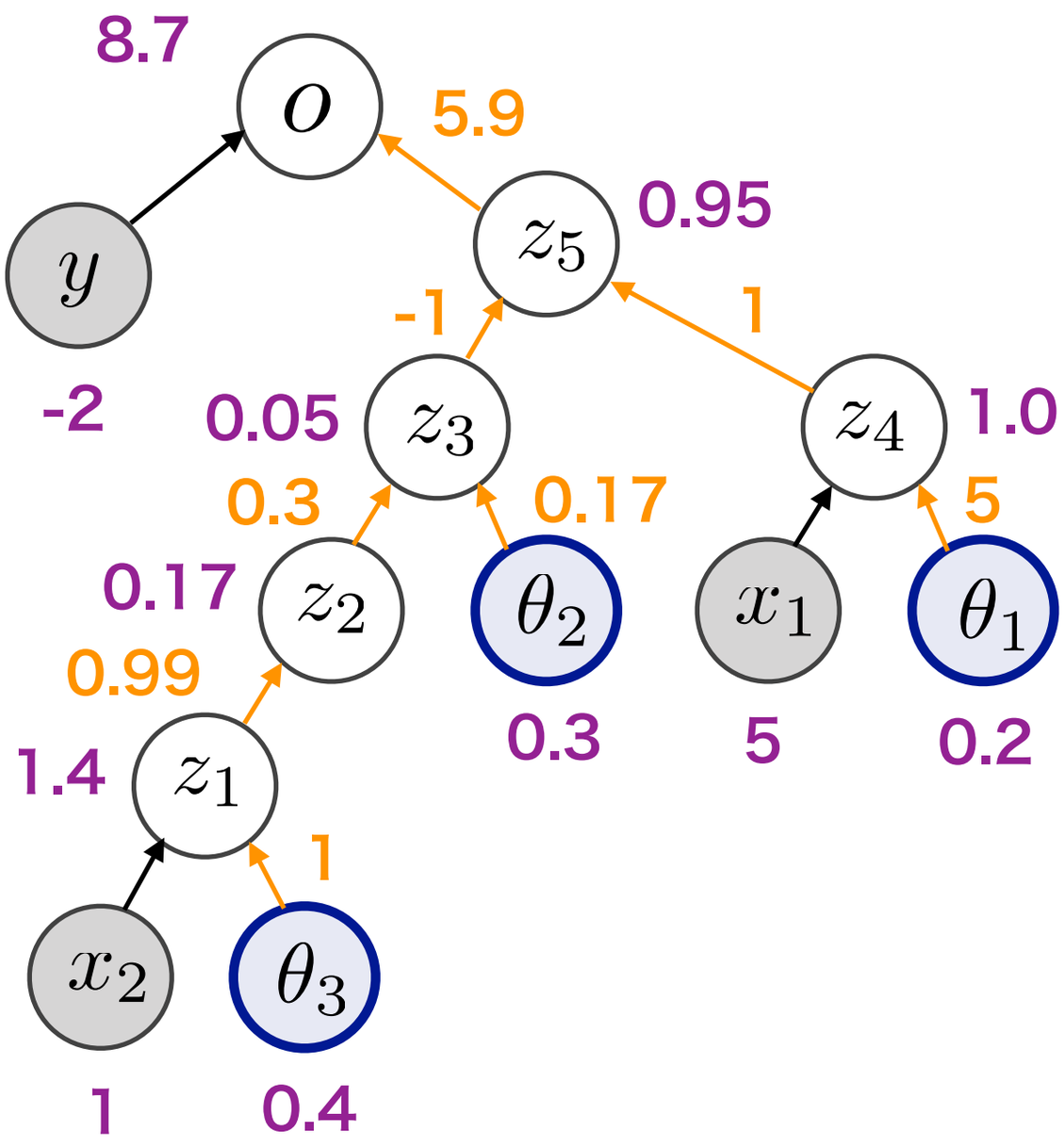
```
z1 = theta3 + x2
z2 = torch.cos(z1)
z3 = theta2 * z2
z4 = theta1 * x1
z5 = z4 - z3
o = (z5-y)**2
```

```
z1, z2, z3, z4, z5, o
```

```
(tensor([1.4000], grad_fn=<AddBackward0>),
 tensor([0.1700], grad_fn=<CosBackward>),
 tensor([0.0510], grad_fn=<MulBackward0>),
 tensor([1.], grad_fn=<MulBackward0>),
 tensor([0.9490], grad_fn=<SubBackward0>),
 tensor([8.6967], grad_fn=<PowBackward0>))
```

自動微分(リバースモード) "Back Propagation"

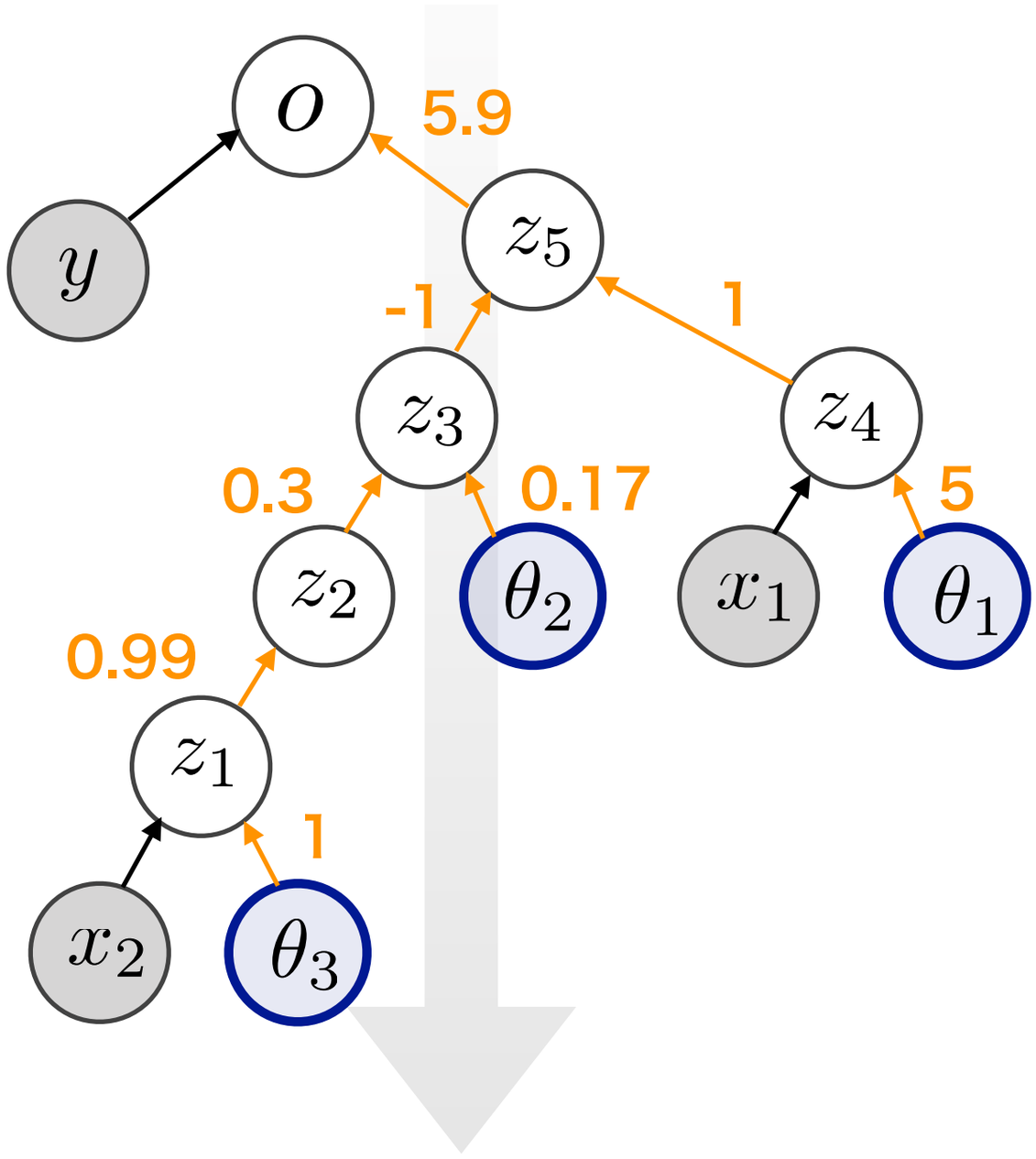
本当に計算したいのは**勾配を計算する変数**に関する**偏微分**



勾配ベクトル $= \begin{bmatrix} \frac{\partial o}{\partial \theta_1} \\ \frac{\partial o}{\partial \theta_2} \\ \frac{\partial o}{\partial \theta_3} \end{bmatrix}$

backward

本当に計算したいのは勾配を計算する変数に関する偏微分



左図を使って簡単に計算できる！

```
o.backward()
```

```
theta1.grad, theta2.grad, theta3.grad
```

```
(tensor([29.4901]), tensor([-1.0025]), tensor([1.7437]))
```

$$\frac{\partial o}{\partial \theta_1} = \frac{\partial o}{\partial z_5} \times \frac{\partial z_5}{\partial z_4} \times \frac{\partial z_4}{\partial \theta_1}$$

5.9　1　5　= 29.5

$$\frac{\partial o}{\partial \theta_2} = \frac{\partial o}{\partial z_5} \times \frac{\partial z_5}{\partial z_3} \times \frac{\partial z_3}{\partial \theta_2}$$

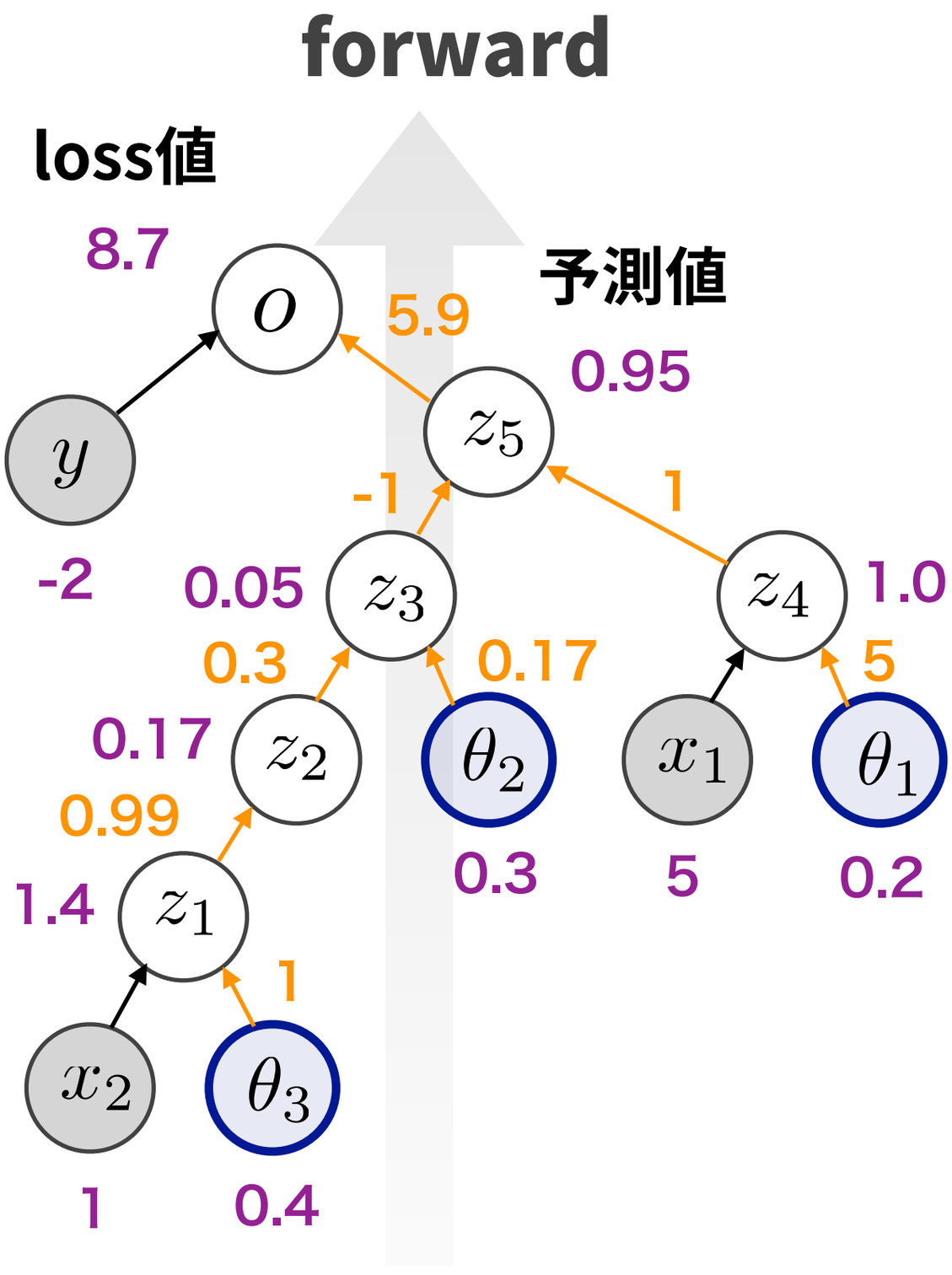
5.9　-1　0.17　= -1.00

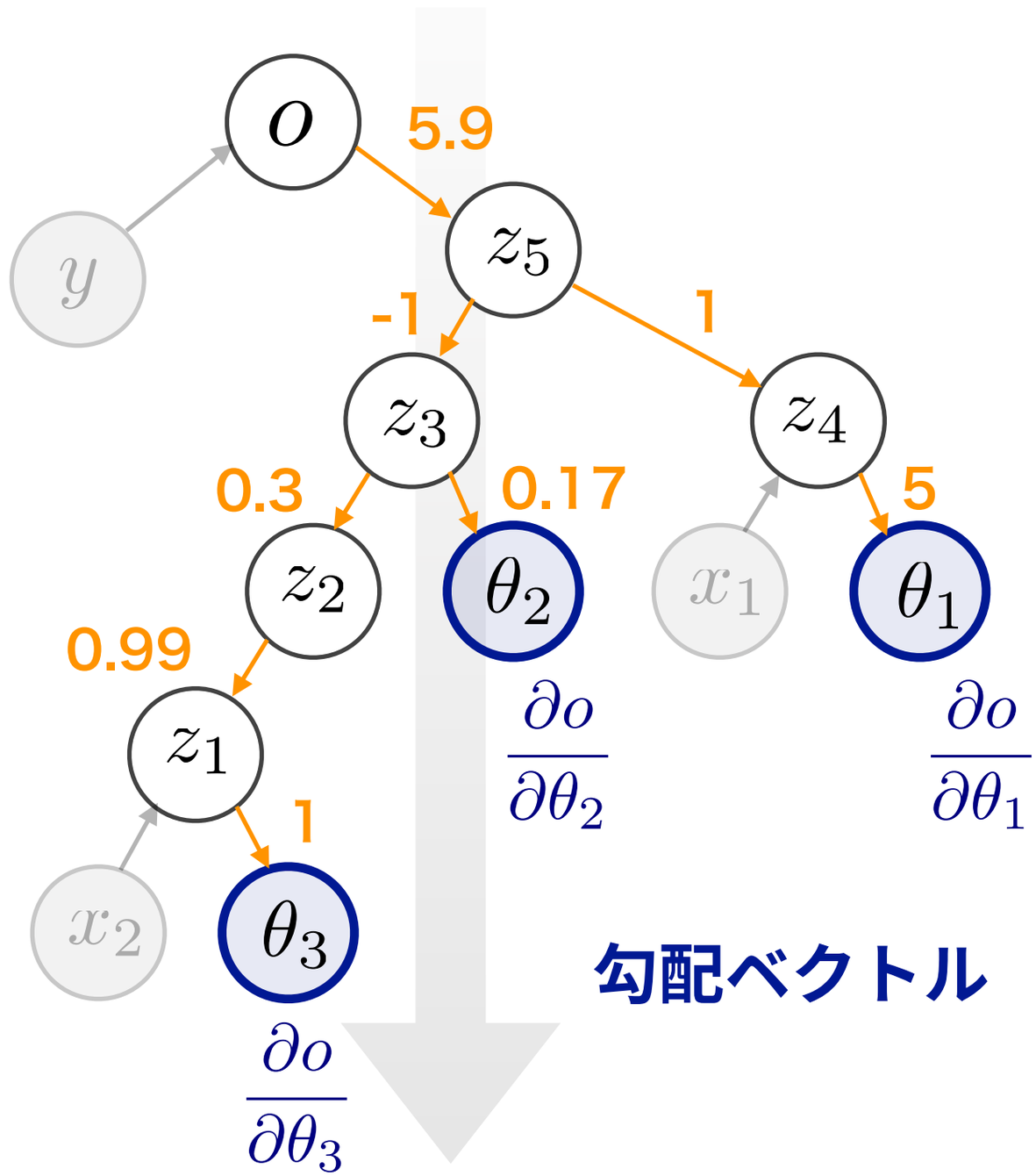
$$\frac{\partial o}{\partial \theta_3} = \frac{\partial o}{\partial z_5} \times \frac{\partial z_5}{\partial z_3} \times \frac{\partial z_3}{\partial z_2} \times \frac{\partial z_2}{\partial z_1} \times \frac{\partial z_1}{\partial \theta_3}$$

5.9　-1　0.3　-0.99　1

= 1.75

合成関数の自動微分 (forward & backward)





深層学習のココロ

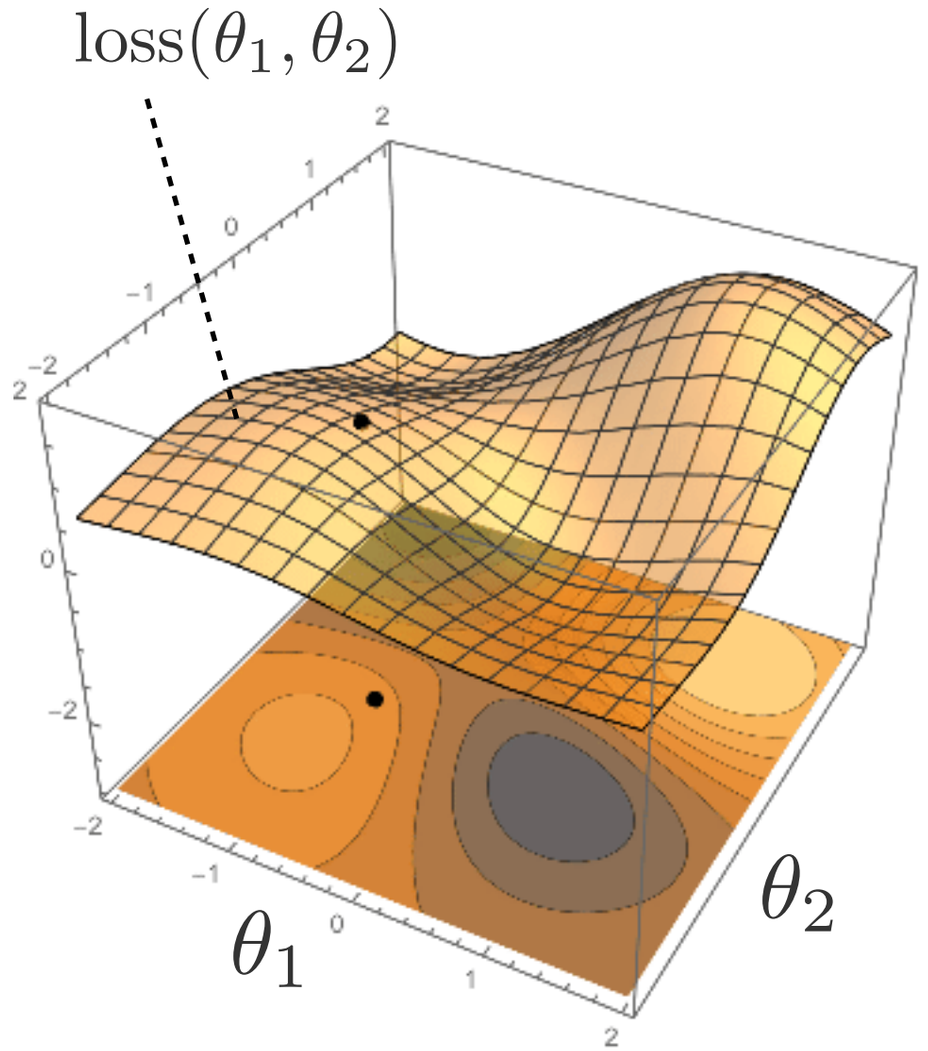
機械学習モデルが合成関数(計算グラフ)になってさえいれば
自動微分＋勾配降下法でパラメタを最適にできる！

$$\begin{bmatrix}\theta_1\\ \theta_2\\ \vdots\\ \theta_p\end{bmatrix} \leftarrow \begin{bmatrix}\theta_1\\ \theta_2\\ \vdots\\ \theta_p\end{bmatrix} + \eta \times \begin{bmatrix}\partial \mathrm{loss}(\boldsymbol{\theta})/\partial\theta_1\\ \partial \mathrm{loss}(\boldsymbol{\theta})/\partial\theta_2\\ \vdots\\ \partial \mathrm{loss}(\boldsymbol{\theta})/\partial\theta_p\end{bmatrix}$$

学習率
(step size)

勾配ベクトル

自動微分で計算



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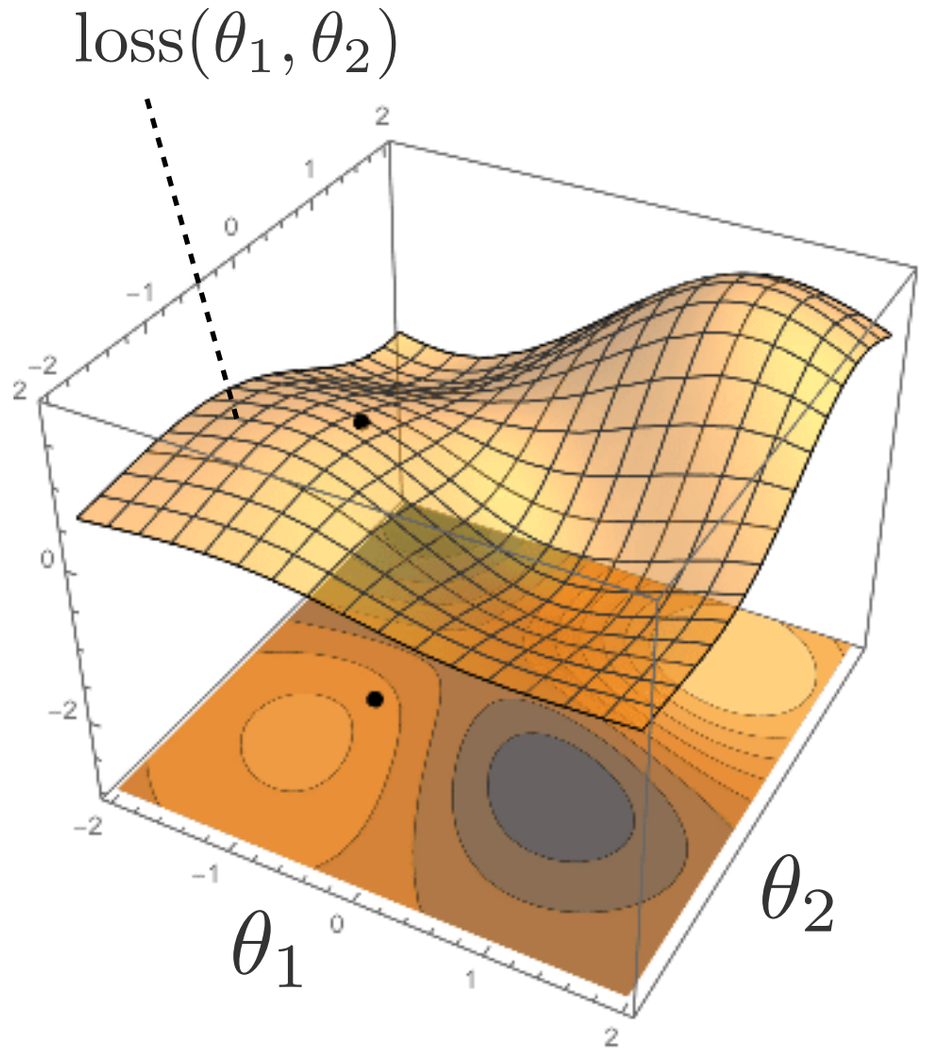
学習率
(step size)

勾配ベクトル

自動微分で計算



本日の内容

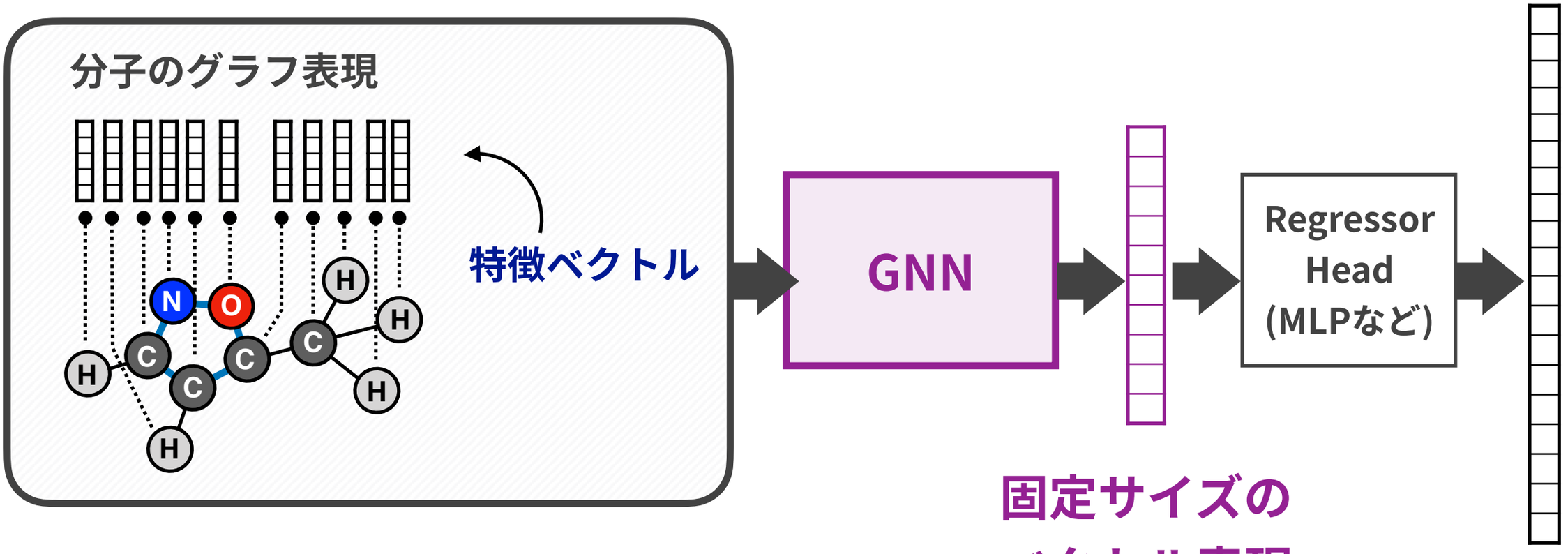
GNN(Graph Neural Networks)で**グラフ表現**された分子を入力にして機械学習するやり方を**のぞいてみませんか**？

- 機械学習とは？
- 分子のグラフ表現
- 準備：深層学習のココロ (forwardとbackward)
- Graph Neural Networksとは？
- 自分でやってみるための情報
- おまけ：

  最近の話 (計算限界、分子生成、事前学習、...)

GNN = 下記の変換を何らかの合成関数でデザインしたもの

可変サイズの分子グラフから「固定サイズのベクトル表現」への変換を学習



mol.x 頂点の特徴ベクトル (11次元)

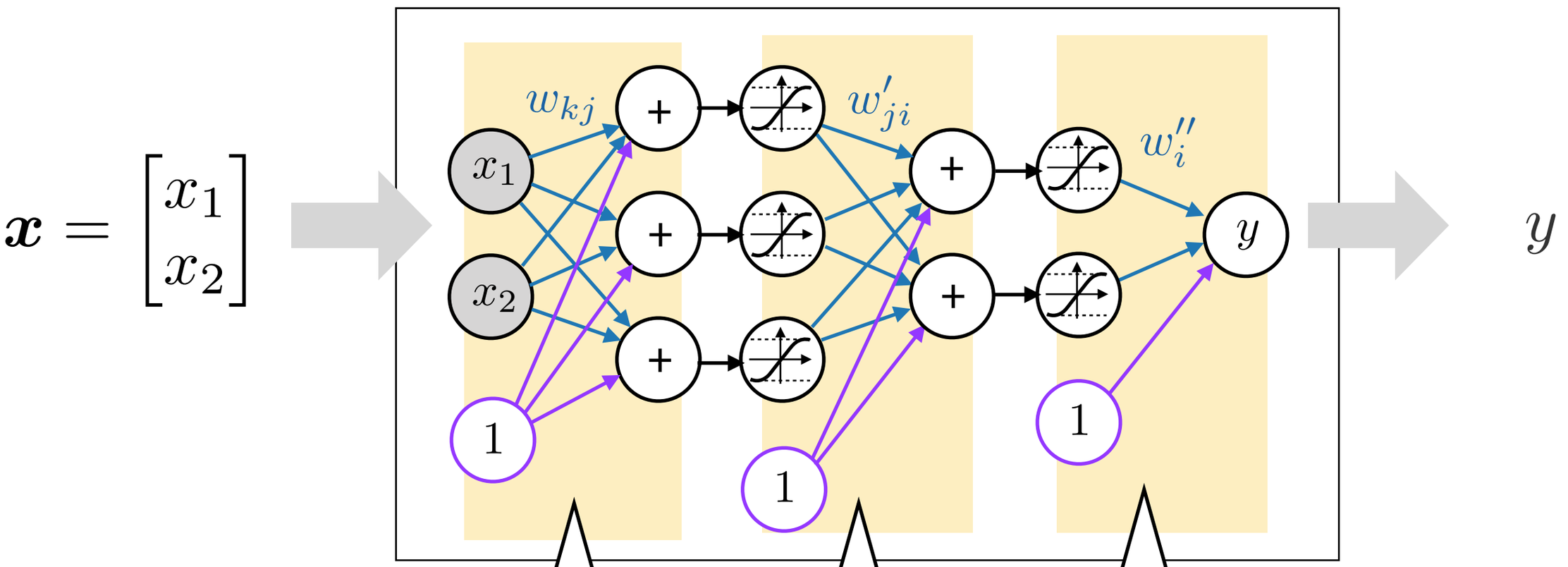
mol.pos 頂点の位置ベクトル (3次元)

mol.edge_attr 辺の特徴ベクトル (4次元)

mol.edge_index 辺と結合原子ペアの対応

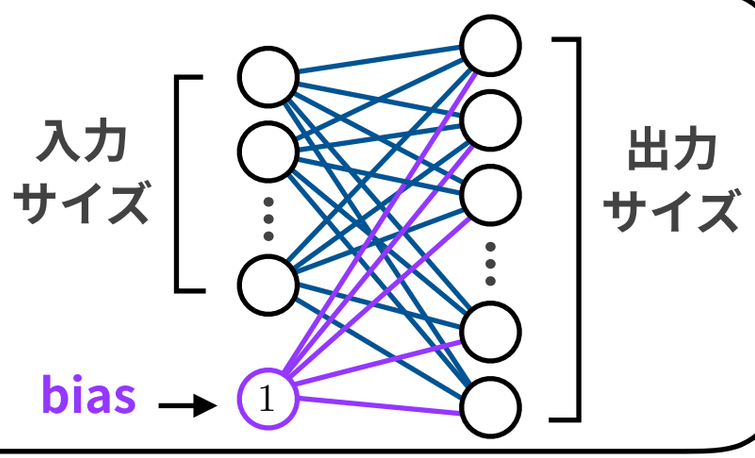
基本道具：MLP (多層パーセプトロン)

```
import torch.nn as nn
nn.Sequential(nn.Linear(2, 3), nn.ReLU(), nn.Linear(3, 2), nn.ReLu(), nn.Linear(2, 1))
```



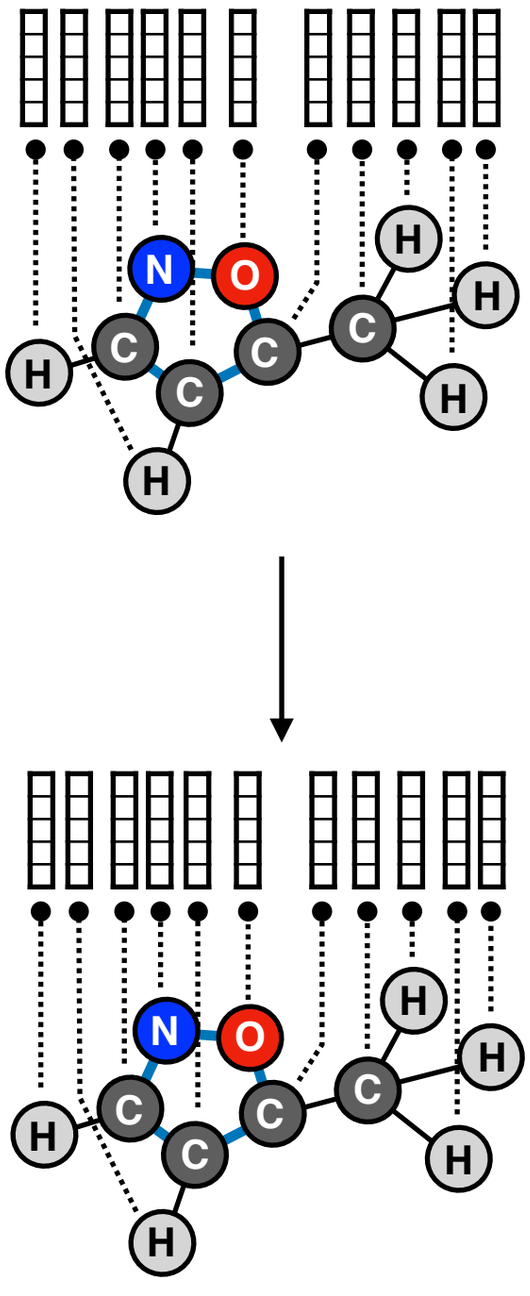
torch.nn.Linear

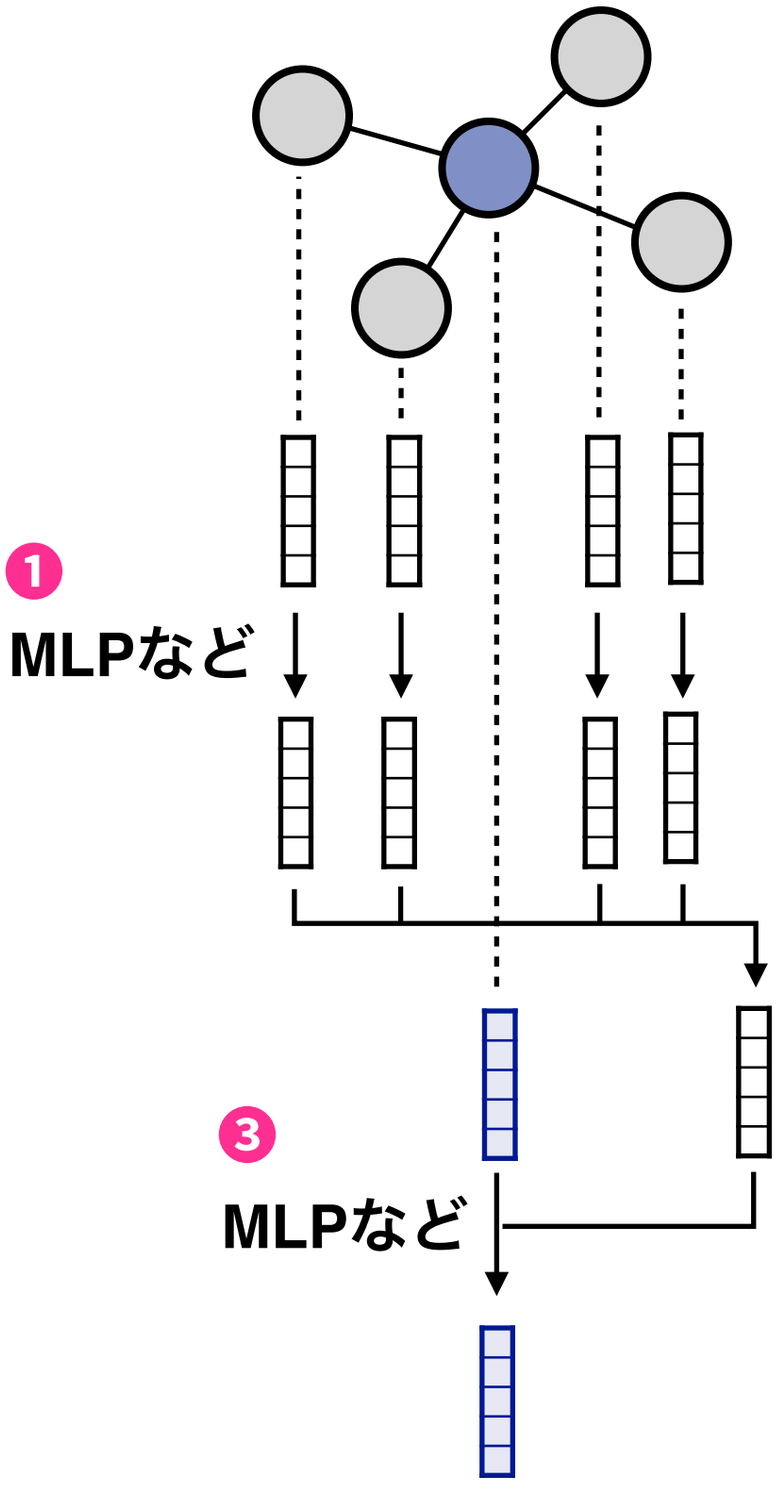
- **in_features** 入力サイズ
- **out_features** 出力サイズ
- **bias (True/False)** biasの有無



Message Passing (or Neighborhood Aggregation)

各特徴ベクトルの更新



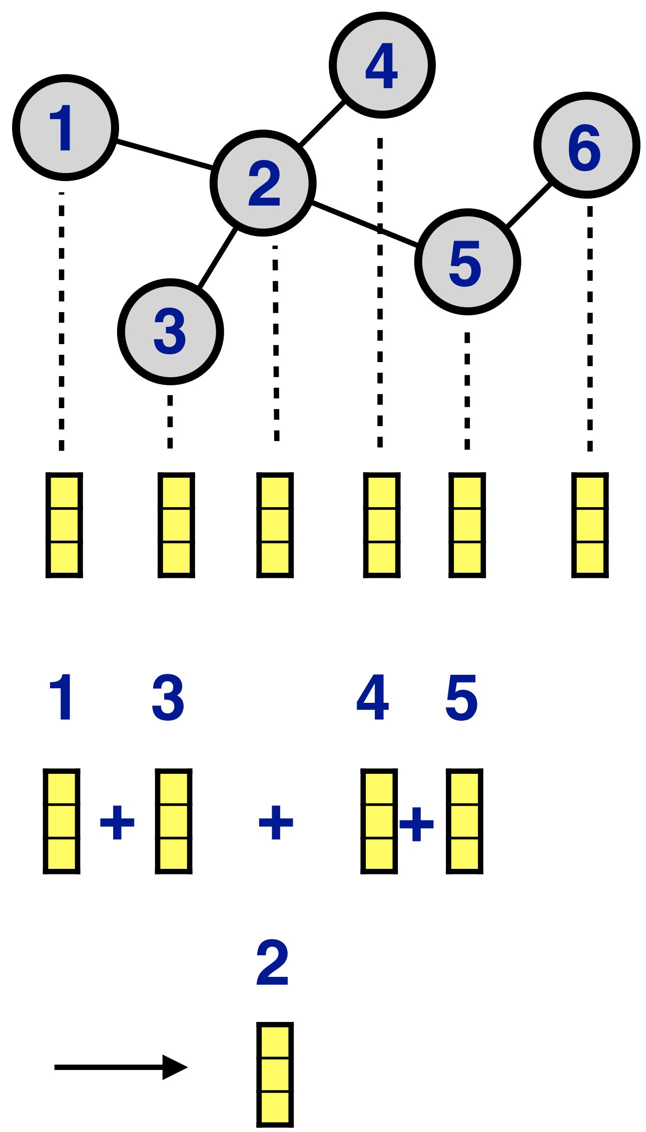


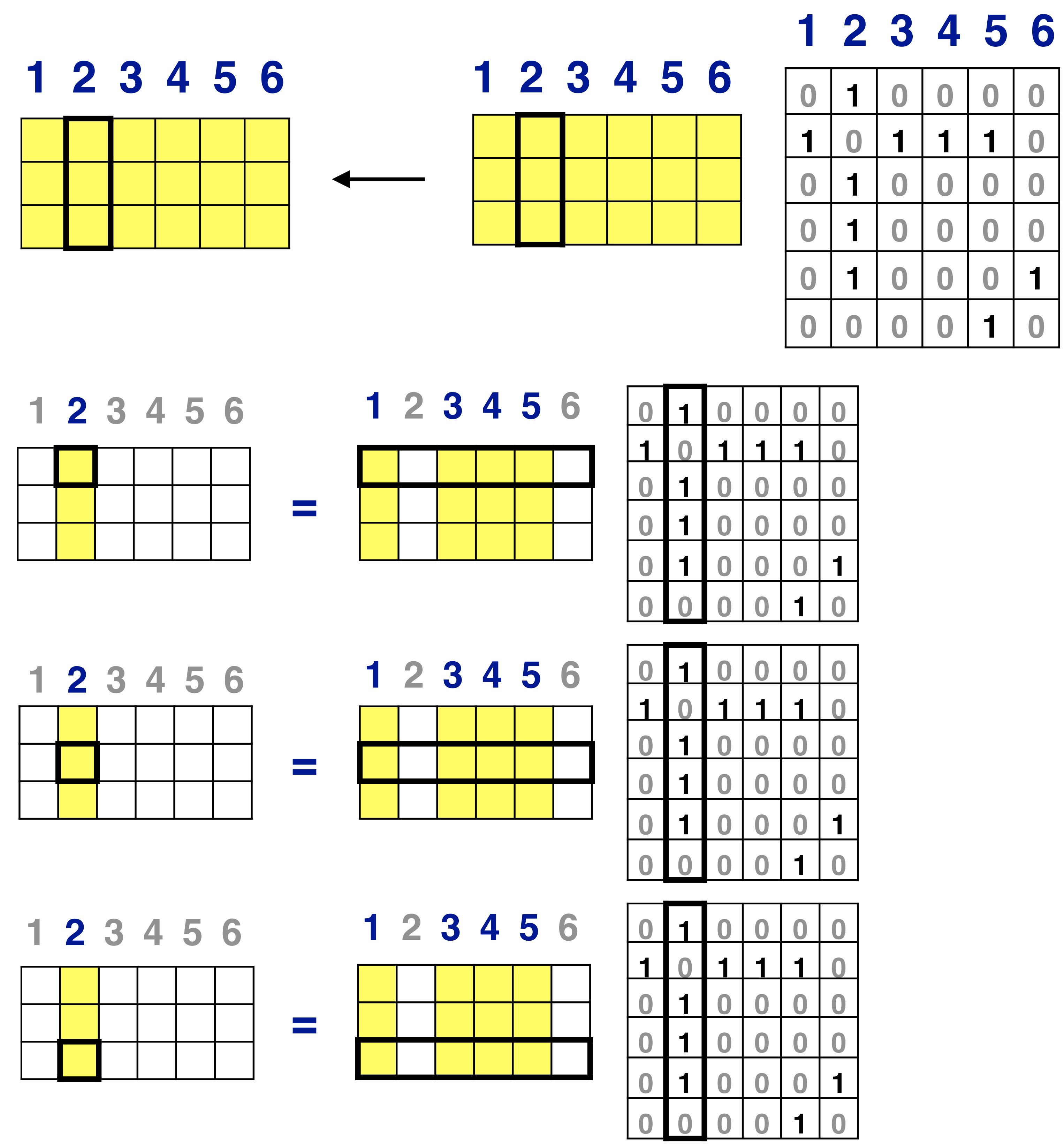
torch_geometric.nn.
MessagePassing

$$\mathbf{x}_i' = \gamma_{\Theta}\left(\mathbf{x}_i, \square_{j \in \mathcal{N}(i)}\, \phi_{\Theta}\left(\mathbf{x}_i, \mathbf{x}_j, \mathbf{e}_{j,i}\right)\right)$$

❸ ❷ ❶

Message Passing (or Neighborhood Aggregation)





隣接行列などを使っても
集約する操作は書ける

Message Passing (or Neighborhood Aggregation)

- **torch_geometric.nn.GCNConv** (Kipf and Welling, ICML2017)

$$\mathbf{X}' = \hat{\mathbf{D}}^{-1/2}\hat{\mathbf{A}}\hat{\mathbf{D}}^{-1/2}\mathbf{X}\mathbf{\Theta}$$

- **torch_geometric.nn.SAGEConv** (Hamilton et al, NIPS2017)

$$\mathbf{x}'_i = \mathbf{W}_1\mathbf{x}_i + \mathbf{W}_2 \cdot \text{mean}_{j \in \mathcal{N}(i)}\mathbf{x}_j$$

- **torch_geometric.nn.GraphConv** (Morris et al, AAAI2019)

$$\mathbf{x}'_i = \mathbf{\Theta}_1\mathbf{x}_i + \sum_{j \in \mathcal{N}(i)} \mathbf{\Theta}_2\mathbf{x}_j$$

- **torch_geometric.nn.GINConv** (Xu et al, ICLR2019)

$$\mathbf{x}'_i = h_{\mathbf{\Theta}}\left((1+\epsilon)\cdot\mathbf{x}_i + \sum_{j \in \mathcal{N}(i)}\mathbf{x}_j\right) \quad \textbf{or} \quad \mathbf{X}' = h_{\mathbf{\Theta}}\left((\mathbf{A} + (1+\epsilon)\cdot\mathbf{I})\cdot\mathbf{X}\right)$$

https://pytorch-geometric.readthedocs.io/en/latest/modules/nn.html

Message Passing (or Neighborhood Aggregation)

- **torch_geometric.nn.SchNet** (Schütt et al, NIPS2017)

$$\mathbf{x}_i' = \sum_{j \in \mathcal{N}(i)} \mathbf{x}_j \odot h_{\mathbf{\Theta}}(\exp(-\gamma(\mathbf{e}_{j,i} - \mu)))$$

⊙ 要素積

→ **xyzでの距離を辺重みにして集約時に活用する**

- **torch_geometric.nn.GATConv** (Veličković et al., ICLR2018)

$$\mathbf{x}_i' = \alpha_{i,i}\mathbf{\Theta}\mathbf{x}_i + \sum_{j \in \mathcal{N}(i)} \alpha_{i,j}\mathbf{\Theta}\mathbf{x}_j$$

$$\alpha_{i,j} = \frac{\exp\left(\text{LeakyReLU}\left(\mathbf{a}^\top [\mathbf{\Theta}\mathbf{x}_i \,\|\, \mathbf{\Theta}\mathbf{x}_j]\right)\right)}{\sum_{k \in \mathcal{N}(i) \cup \{i\}} \exp\left(\text{LeakyReLU}\left(\mathbf{a}^\top [\mathbf{\Theta}\mathbf{x}_i \,\|\, \mathbf{\Theta}\mathbf{x}_k]\right)\right)}$$

|| concat

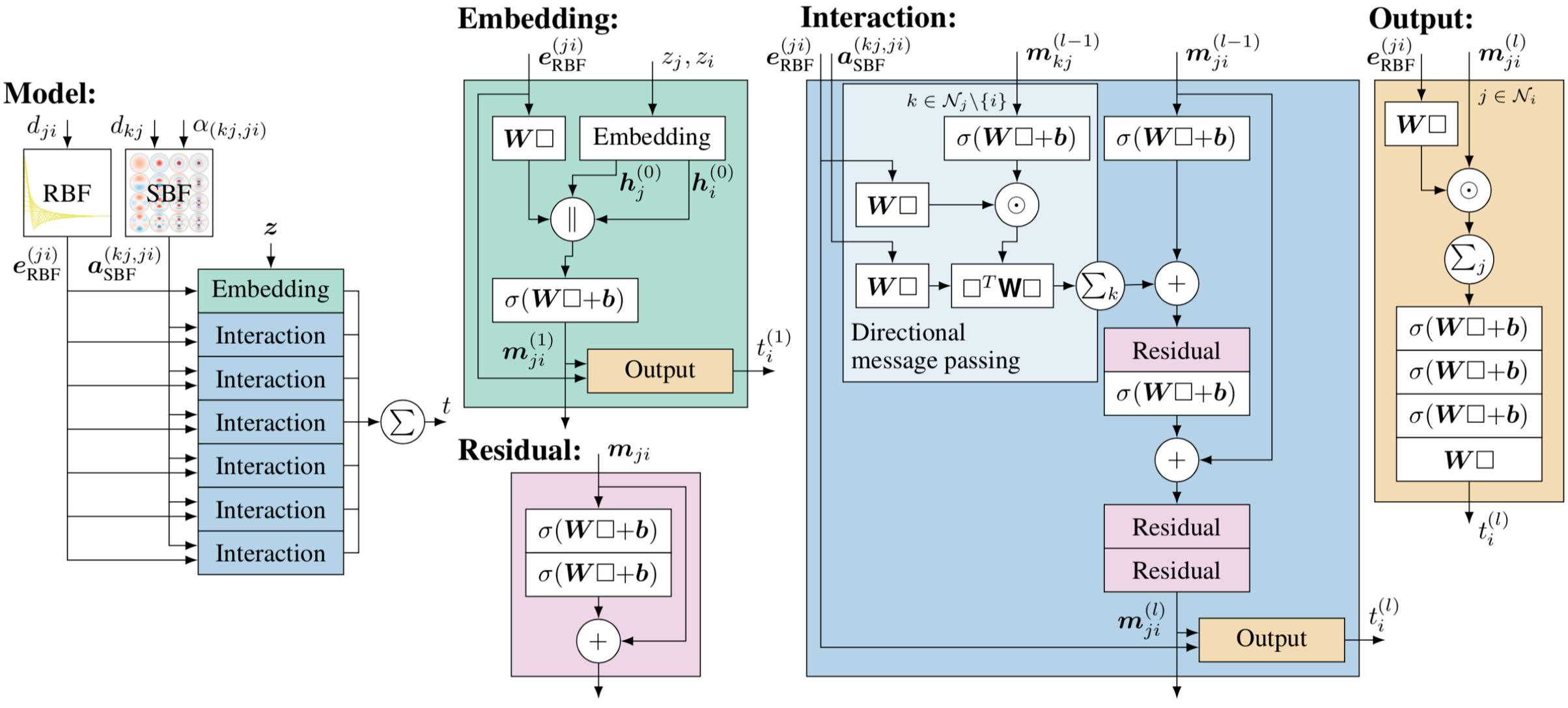
→ **集約操作はシンプルだがアテンション機構で重みを適応的に**

https://pytorch-geometric.readthedocs.io/en/latest/modules/nn.html

Message Passing (or Neighborhood Aggregation)

- **torch_geometric.nn.DimeNet** (Klicpera et al, ICLR2020)

  xyzに対して化学的なドメイン知識を活用して操作を作り込みまくった例



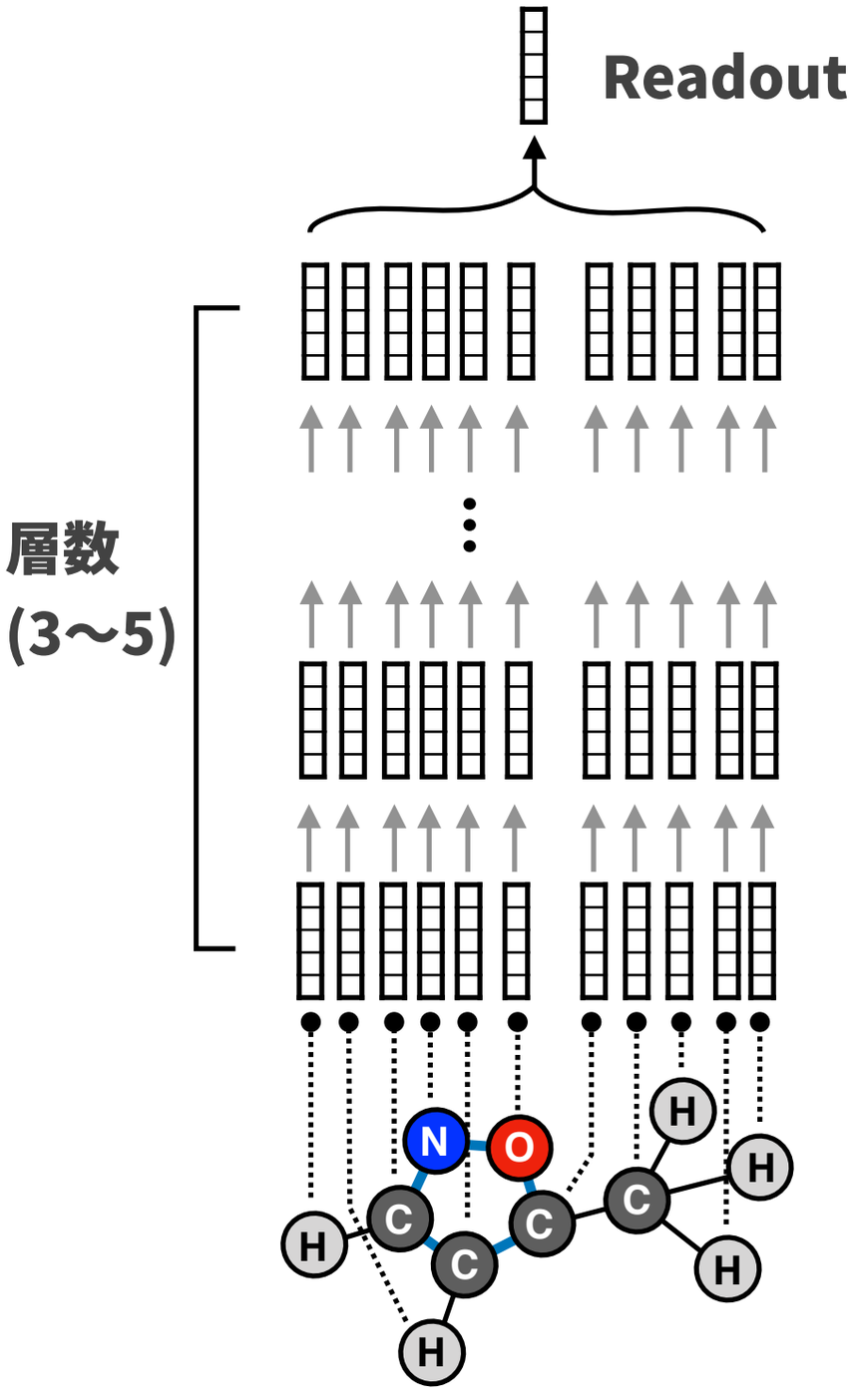
Message Passing (or Neighborhood Aggregation)

最初に例に出したQM9データでは従来手法を優越する予測精度

Table 1: MAE on QM9. DimeNet sets the state of the art on 11 targets, outperforming the second-best model on average by 31 % (mean std. MAE).

Target	Unit	PPGN	SchNet	PhysNet	MEGNet-s	Cormorant	**DimeNet**
μ	D	0.047	0.033	0.0529	0.05	0.13	**0.0286**
α	${a_0}^3$	0.131	0.235	0.0615	0.081	0.092	**0.0469**
ϵ_{HOMO}	meV	40.3	41	32.9	43	36	**27.8**
ϵ_{LUMO}	meV	32.7	34	24.7	44	36	**19.7**
$\Delta\epsilon$	meV	60.0	63	42.5	66	60	**34.8**
$\langle R^2 \rangle$	${a_0}^2$	0.592	**0.073**	0.765	0.302	0.673	0.331
ZPVE	meV	3.12	1.7	1.39	1.43	1.98	**1.29**
U_0	meV	36.8	14	8.15	12	28	**8.02**
U	meV	36.8	19	8.34	13	-	**7.89**
H	meV	36.3	14	8.42	12	-	**8.11**
G	meV	36.4	14	9.40	12	-	**8.98**
c_{v}	$\frac{\text{cal}}{\text{mol K}}$	0.055	0.033	0.0280	0.029	0.031	**0.0249**
std. MAE	%	1.84	1.76	1.37	1.80	2.14	**1.05**
logMAE	-	−4.64	−5.17	−5.35	−5.17	−4.75	**−5.57**

Readout: グラフに対する固定サイズ表現を得る



- torch_geometric.nn.**global_add_pool**
  torch_geometric.nn.**global_max_pool**
  torch_geometric.nn.**global_mean_pool**

  順番に依存しない集約操作　(sum, mean or max)

- torch_geometric.nn.**global_sort_pool**

  最後の要素でsortしてトップkをconcat

- torch_geometric.nn.**GlobalAttention**

$$\mathbf{r}_i = \sum_{n=1}^{N_i} \mathrm{softmax}\left(h_{\mathrm{gate}}(\mathbf{x}_n)\right) \odot h_{\mathbf{\Theta}}(\mathbf{x}_n),$$

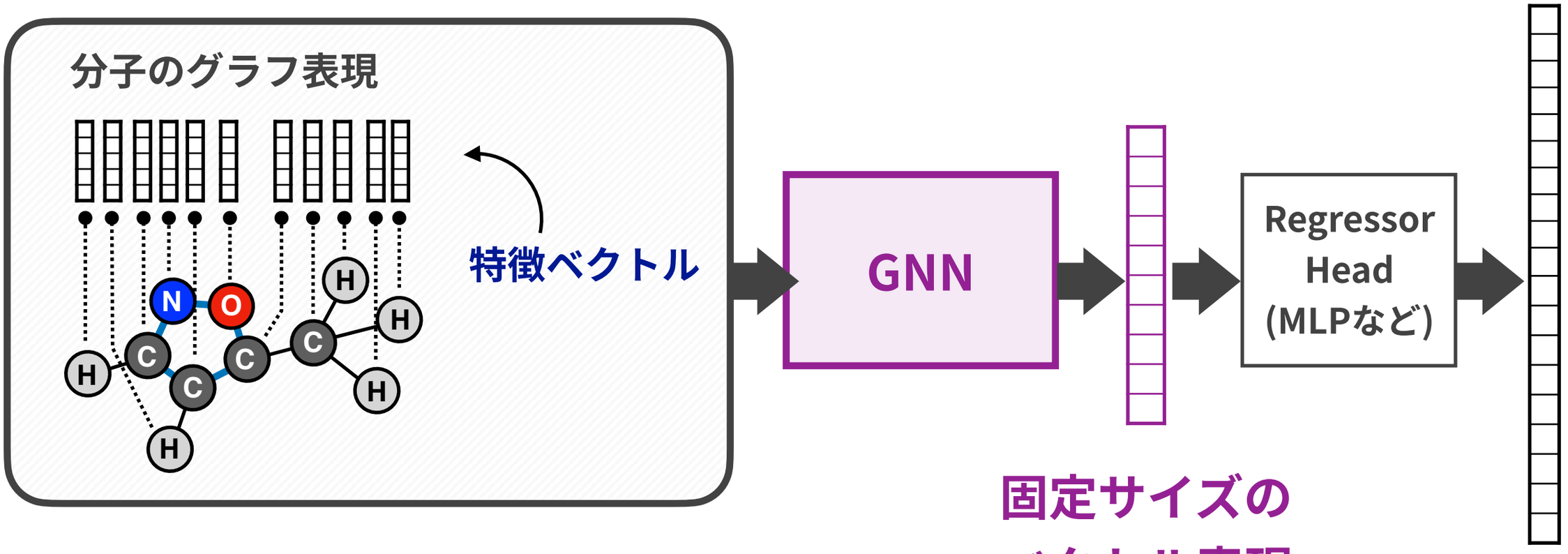
- torch_geometric.nn.**Set2Set**

$$\mathbf{q}_t = \mathrm{LSTM}(\mathbf{q}^*_{t-1})$$
$$\alpha_{i,t} = \mathrm{softmax}(\mathbf{x}_i \cdot \mathbf{q}_t)$$

$$\mathbf{r}_t = \sum_{i=1}^{N} \alpha_{i,t}\mathbf{x}_i$$
$$\mathbf{q}^*_t = \mathbf{q}_t \,\|\, \mathbf{r}_t,$$

GNN = 下記の変換を何らかの合成関数でデザインしたもの

可変サイズの分子グラフから「固定サイズのベクトル表現」への変換を学習



mol.x 頂点の特徴ベクトル (11次元)

mol.pos 頂点の位置ベクトル (3次元)

mol.edge_attr 辺の特徴ベクトル (4次元)

mol.edge_index 辺と結合原子ペアの対応

PyTorch Geometricの例 (Google Colab)

```
!pip install torch-scatter==latest+cu101 torch-sparse==latest+cu101 \
      torch-cluster==latest+cu101 -f https://pytorch-geometric.com/whl/torch-1.6.0.html
!pip install torch-geometric
```

```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch_geometric as pyg

from tqdm import tqdm

dataset = pyg.datasets.qm9.QM9(root='/tmp/QM9')
data_size = len(dataset)
loader = pyg.data.DataLoader(dataset[:int(data_size * 0.8)], batch_size=64, shuffle=True)
test_loader = pyg.data.DataLoader(dataset[int(data_size * 0.8):], batch_size=64, shuffle=True)
```

```
def mlp(input_dim, hidden_dim):
    return nn.Sequential(
        nn.Linear(input_dim, hidden_dim),
        nn.ReLU(),
        nn.Linear(hidden_dim, hidden_dim))
```

モデルとforward定義

```
class MyGNN(nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim):
        super(MyGNN, self).__init__()
        self.convs = nn.ModuleList()
        self.convs.append(pyg.nn.GINConv(mlp(input_dim, hidden_dim)))
        for l in range(2):
          self.convs.append(pyg.nn.GINConv(mlp(hidden_dim, hidden_dim)))
        self.head = nn.Sequential(
            nn.Linear(hidden_dim, hidden_dim), nn.Dropout(0.25),
            nn.Linear(hidden_dim, output_dim))

    def forward(self, data):
        x, edge_index, batch = data.x, data.edge_index, data.batch
        for conv in self.convs:
            x = conv(x, edge_index)
            x = F.relu(x)
            x = F.dropout(x, p=0.25, training=self.training)
        x = pyg.nn.global_mean_pool(x, batch)
        x = self.head(x)
        return x
```

Regressor Head (MLP)

← 出力を計算するforward

Message Passing (x 3層)

← Readout

学習：モデルのパラメタを最適にする

```
model = MyGNN(dataset.num_node_features, 32, dataset.num_classes)
```

```
opt = torch.optim.Adam(model.parameters(), lr=0.01)
error = torch.nn.MSELoss(reduction='sum')

for epoch in range(10):                          ←―― とりあえず10 epoch (数百必要)
    total_loss = 0
    model.train()
    for batch in tqdm(loader):                   ←―― グラフをbatch_size(64こ)づつfeed
        opt.zero_grad()
        pred = model(batch)                      ←―― モデルに入れて予測を得る
        loss = error(pred, batch.y)              ←―― lossを計算しbackward
        loss.backward()
        opt.step()                               ←―― 勾配降下(パラメタ更新)
        total_loss += loss.item() * batch.num_graphs
    total_loss /= len(loader.dataset)
    print("loss", total_loss, epoch)
```

注意

- QM9のタスクの場合はほぼxyz(x.pos)の情報が必要だが、単純なGNNはx.edge_attrも使わないので適宜改変が必要
- 例えばx.edge_attrに原子間距離を加えてConvで活用?

```
QM9_dist = []
for g in dataset:
    edge_attr = torch.empty(g.num_edges, g.num_edge_features + 1)
    for id, (s, t) in enumerate(zip(*g.edge_index)):
        d = torch.norm(g.pos[s]-g.pos[t])
        edge_attr[id] = torch.cat([g.edge_attr[id], d.reshape(1)])
    data = pyg.data.Data(x=g.x, z=g.z, pos=g.pos, edge_index=g.edge_index,
                         edge_attr=edge_attr, y=g.y, name=g.name, idx=id)
    QM9_dist.append(data)
```

- そのまま使う場合はSchNetやDimeNetが向いている
- 公式コードサンプルもチェック

  https://github.com/rusty1s/pytorch_geometric/tree/master/examples

Open Graph Benchmark https://ogb.stanford.edu

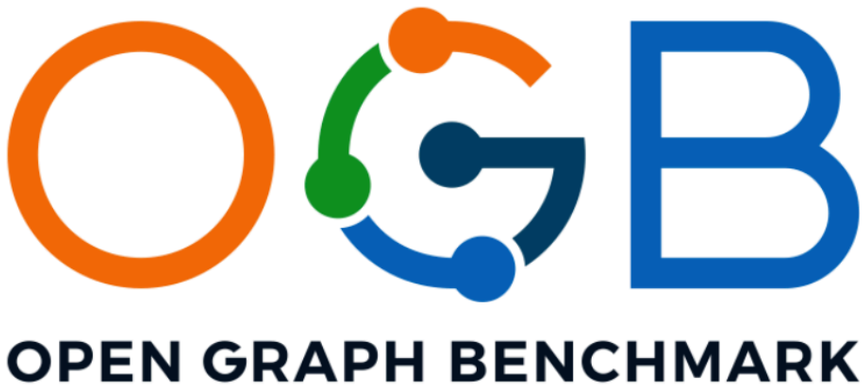
Get Started Updates Datasets Leaderboards Paper Team Github

Open Graph Benchmark

Benchmark datasets, data loaders and evaluators for graph machine learning

GET STARTED VIEW UPDATES

The Open Graph Benchmark (OGB) is a collection of realistic, large-scale, and diverse benchmark datasets for machine learning on graphs. OGB datasets are automatically downloaded, processed, and split using the OGB Data Loader. The model performance can be evaluated using the OGB Evaluator in a unified



本日の内容

GNN(Graph Neural Networks)で**グラフ表現**された分子を入力にして機械学習するやり方を**のぞいてみませんか**？

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- 分子のグラフ表現
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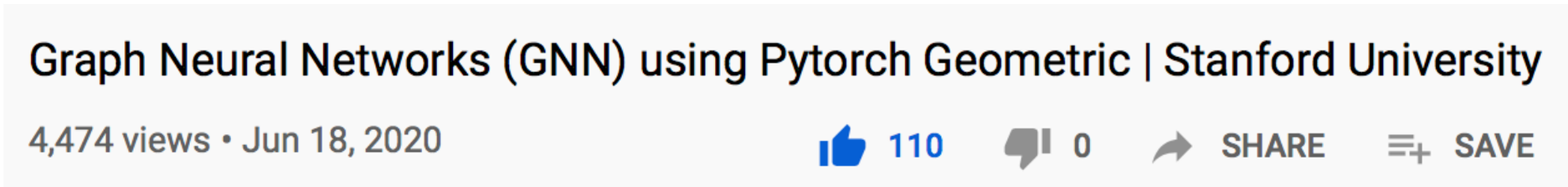
Graph Neural Networksを知るための３つのソース

- **CS224W: Machine Learning with Graphs (Stanford)**

  http://web.stanford.edu/class/cs224w/



YouTube **https://youtu.be/-UjytpbqX4A**

- **KDD2020 Tutorial**
  Deep Graph Learning: Foundations, Advances and Applications

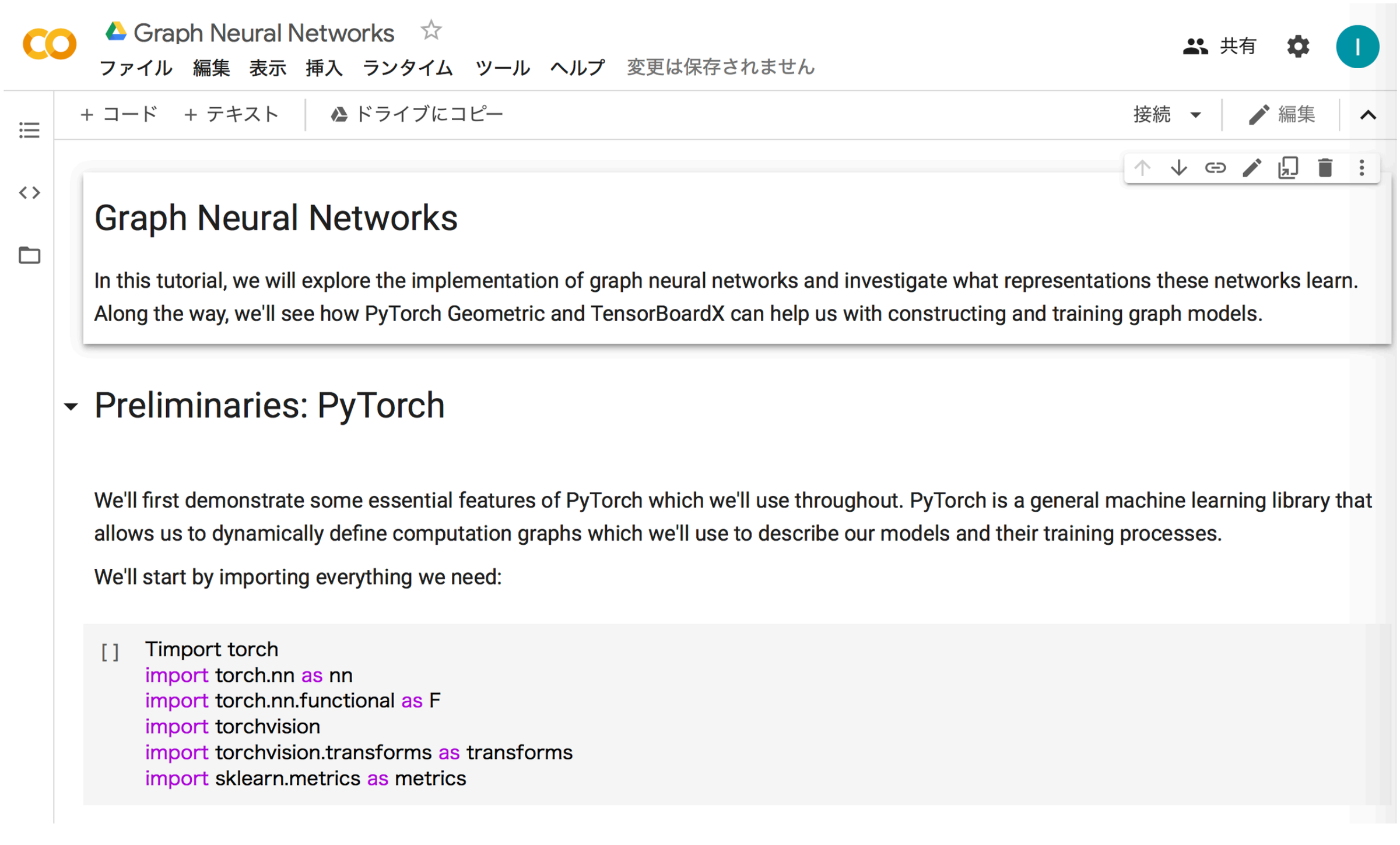
  https://ai.tencent.com/ailab/ml/KDD-Deep-Graph-Learning.html

- **Book "Deep Learning on Graphs"**

  http://cse.msu.edu/~mayao4/dlg_book/index.html

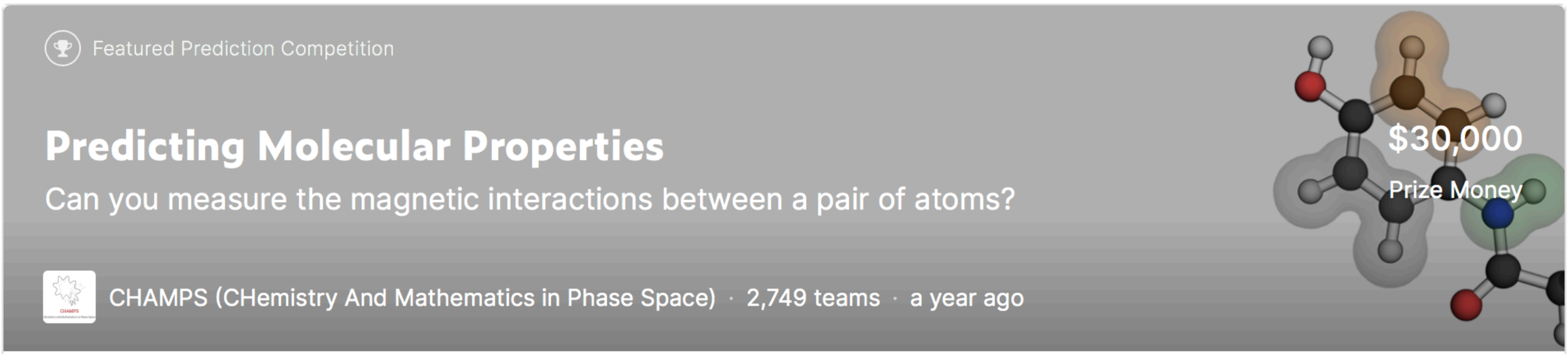
Pytorch Geometricを使ったハンズオン (CS224W)

https://colab.research.google.com/drive/1DIQm9rOx2mT1bZETEeVUThxcrP1RKqAn



Kaggle CHAMPS (xyzが要るタスク)

https://www.kaggle.com/c/champs-scalar-coupling/discussion/93972



Overview Data Notebooks Discussion Leaderboard Rules New Topic

255th place

Which graph CNN is the best (with starter kit at LB -1.469)?

219

Posted in champs-scalar-coupling a year ago

This post is for information and results using graph CNN. For a start:

useful Graph CNN lib:

- https://github.com/rusty1s/pytorch_geometric
- https://github.com/pfnet-research/chainer-chemistry
- https://github.com/jparkhill/TensorMol

ICLR2020: A Fair Comparisons of GNNs

https://github.com/diningphil/gnn-comparison

A FAIR COMPARISON OF GRAPH NEURAL NETWORKS FOR GRAPH CLASSIFICATION

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Table 3: Results on chemical datasets with mean accuracy and standard deviation are reported. Best performances are highlighted in bold.

	D&D	**NCI1**	**PROTEINS**	**ENZYMES**
Baseline	**78.4** ± 4.5	69.8 ± 2.2	**75.8** ± 3.7	**65.2** ± 6.4
DGCNN	76.6 ± 4.3	76.4 ± 1.7	72.9 ± 3.5	38.9 ± 5.7
DiffPool	75.0 ± 3.5	76.9 ± 1.9	73.7 ± 3.5	59.5 ± 5.6
ECC	72.6 ± 4.1	76.2 ± 1.4	72.3 ± 3.4	29.5 ± 8.2
GIN	75.3 ± 2.9	**80.0** ± 1.4	73.3 ± 4.0	59.6 ± 4.5
GraphSAGE	72.9 ± 2.0	76.0 ± 1.8	73.0 ± 4.5	58.2 ± 6.0

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GNNは発展途上の技術で現在進行形で研究されている

- 学習できる表現に限界がある？

  Generalization and Representational Limits of Graph Neural Networks
  Garg, Jegelka, Jaakkola (ICML2020)

- Deepにできない？

  DeepGCNs: Can GCNs Go as Deep as CNNs?
  Li, Müller, Thabet, Ghanem (ICCV2019)

  PairNorm: Tackling Oversmoothing in GNNs
  Zhao, Akoglu (ICLR2020)

  Towards Deeper Graph Neural Networks with Differentiable Group Normalization
  Zhou, Huang, Li, Zha, Chen, Hu (NeurIPS2020)

- 事前学習ができない？

  Strategies for Pre-training Graph Neural Networks
  Hu, Liu, Gomes, Zitnik, Liang, Pande, Leskovec (ICLR2020)

  GROVER: Self-Supervised Message Passing Transformer on Large-scale Molecular Graphs Rong, Bian, Xu, Xie, Wei, Huang, Huang (NeurIPS2020)

今日の話の応用・発展

- **Graph Pooling**

  Rethinking Pooling in Graph Neural Networks
  Mesquita, Souza, Kaski (NeurIPS2020)

  Path Integral Based Convolution and Pooling for Graph Neural Networks
  Ma, Xuan, Guang Wang, Li, Liò (NeurIPS2020)

- **分子の生成**

  GraphAF: a Flow-based Autoregressive Model for Molecular Graph Generation
  Jin, Barzilay, Jaakkola (ICML2020)

  Generalization and Representational Limits of Graph Neural Networks
  Shi, Xu, Zhu, Zhang, Zhang, Tang (ICLR2020)

- **化学反応の予測・逆合成**

  RetroXpert: Decompose Retrosynthesis Prediction like A Chemist
  Yan, Ding, Zhao, Zheng, Yang, Yu, Huang (NeurIPS2020)

  A Graph to Graphs Framework for Retrosynthesis Prediction
  Shi, Xu, Guo, Zhang, Tang (ICML2020)

まとめ

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