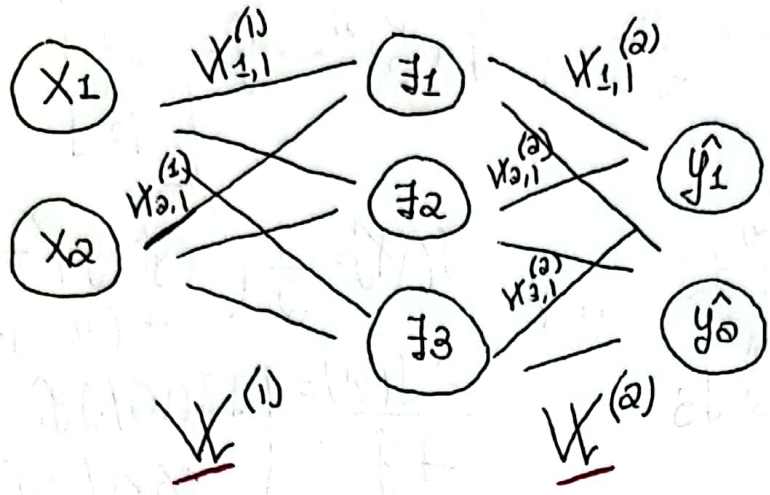
Anar Rzayev — MA8473: Homework Set 4 — ID: 20190188

4)



Fully-connected network

$$z_j = \sigma\left(\sum_{i=1}^{2} W_{i,j}^{(1)} x_i + b_j\right)$$

$$\hat{y}_k = \sum_{i=1}^{2} W_{i,k}^{(2)} z_i + b_k$$

$$J(W) = \frac{1}{2}\|y-\hat{y}\|_2^2$$

Vectorizing the above implementation, we can write the followings:

$$J(W) = \frac{1}{2}\|\hat{y}-y\|_2^2$$

$$z = \sigma\left(W^{(1)}x + b^{(1)}\right)$$

$$\hat{y} = W^{(2)}z + b^{(2)}$$

Now, it's time to proceed with backward propagation using correspondent gradients

$$\frac{\partial J(W)}{\partial W^{(2)}} = \frac{\partial J(W)}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial W^{(2)}}$$

Since $J(W) = \frac{1}{2}\|\hat{y}-y\|_2^2 \Rightarrow \boxed{\frac{\partial J(W)}{\partial \hat{y}} = \hat{y}-y}$ and $\hat{y} = W^{(2)}z + b^{(2)}$, it's easily seen that from matrix differentiation

$\boxed{\frac{\partial \hat{y}}{\partial W^{(2)}} = z^T}$ Thus, $\boxed{\frac{\partial J(W)}{\partial W^{(2)}} = (\hat{y}-y)z^T}$ ☆ Now, we proceed to evaluate gradient with respect to $b^{(2)}$. Using the chain Rule $\Rightarrow$

$$\frac{\partial J(W)}{\partial b^{(2)}} = \frac{\partial J(W)}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial b^{(2)}}$$

where $\frac{\partial J(W)}{\partial \hat{y}} = \hat{y}-y$ and $\frac{\partial \hat{y}}{\partial b^{(2)}} = 1^T$ using the formula

$\hat{y} = W^{(2)}z + b^{(2)}$ $\left(\frac{\partial \hat{y}}{\partial b^{(2)}} = \begin{bmatrix} \partial \hat{y}_1/\partial b_1^{(2)} \\ \partial \hat{y}_2/\partial b_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}\right)$ More specifically, if we evaluate $\frac{\partial \hat{y}}{\partial b^{(2)}}$ explicitly

$$\frac{\partial \hat{y}}{\partial b^{(2)}} = \begin{bmatrix} \partial \hat{y}_1/\partial b_1^{(2)} & \partial \hat{y}_1/\partial b_2^{(2)} \\ \partial \hat{y}_2/\partial b_1^{(2)} & \partial \hat{y}_2/\partial b_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I \Rightarrow \boxed{\frac{\partial J(W)}{\partial b^{(2)}} = \hat{y}-y}$$ ☆ Now

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Our aim is to evaluate gradient wrt vector-z $\Rightarrow$ Using the chain-rule,

$$\frac{\partial J(W)}{\partial z} = \frac{\partial J(W)}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} \quad \text{where } \hat{y} = W^{(2)} z + b^{(2)} \rightsquigarrow \hat{y} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \end{bmatrix}$$

$$\hat{y}_1 = W^{(2)}_{1,1} z_1 + W^{(2)}_{2,1} z_2 + W^{(2)}_{3,1} z_3$$

$$\hat{y}_2 = W^{(2)}_{1,2} z_1 + W^{(2)}_{2,2} z_2 + W^{(2)}_{3,2} z_3$$

and

$$J(W) = \frac{1}{2}\left((\hat{y}_1 - y_1)^2 + (\hat{y}_2 - y_2)^2 \right)$$

$$\frac{\partial J(W)}{\partial \hat{y}} = \begin{bmatrix} \partial J(W)/\partial \hat{y}_1 \\ \partial J(W)/\partial \hat{y}_2 \end{bmatrix}$$

$$\frac{\partial J(W)}{\partial \hat{y}} = \begin{bmatrix} \hat{y}_1 - y_1 \\ \hat{y}_2 - y_2 \end{bmatrix} \in \mathbb{R}^{2\times 1} \quad \text{and} \quad \hat{y} = \begin{bmatrix} W^{(2)}_{1,1} z_1 + W^{(2)}_{2,1} z_2 + W^{(2)}_{3,1} z_3 \\ W^{(2)}_{1,2} z_1 + W^{(2)}_{2,2} z_2 + W^{(2)}_{3,2} z_3 \end{bmatrix}$$

$$\frac{\partial \hat{y}}{\partial z} = \begin{bmatrix} \partial \hat{y}_1/\partial z_1 & \partial \hat{y}_1/\partial z_2 & \partial \hat{y}_1/\partial z_3 \\ \partial \hat{y}_2/\partial z_1 & \partial \hat{y}_2/\partial z_2 & \partial \hat{y}_2/\partial z_3 \end{bmatrix} = \begin{bmatrix} W^{(2)}_{1,1} & W^{(2)}_{2,1} & W^{(2)}_{3,1} \\ W^{(2)}_{1,2} & W^{(2)}_{2,2} & W^{(2)}_{3,2} \end{bmatrix}$$

where we know that

$$W^{(2)} = \begin{bmatrix} W^{(2)}_{1,1} & W^{(2)}_{1,2} \\ W^{(2)}_{2,1} & W^{(2)}_{2,2} \\ W^{(2)}_{3,1} & W^{(2)}_{3,2} \end{bmatrix}^T \rightsquigarrow \boxed{\frac{\partial \hat{y}}{\partial z} = W^{(2)}}$$

$W^{(2)} \in \mathbb{R}^{2\times 3}$, $\hat{y} - y \in \mathbb{R}^{2\times 1}$ — using the dimensions matching,

one can obtain that $\frac{\partial J(W)}{\partial z} = \frac{\partial J(W)}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} = (W^{(2)})^T (\hat{y} - y) \in \mathbb{R}^{3\times 1}$

$$\boxed{\frac{\partial J(W)}{\partial z} = (W^{(2)})^T (\hat{y} - y)}$$

Now, we have to move with the gradient wrt $W^{(1)}$

$$\frac{\partial J(W)}{\partial W^{(1)}} = \frac{\partial J(W)}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} \frac{\partial z}{\partial W^{(1)}}$$

where we had

$$\frac{\partial J(W)}{\partial \hat{y}} = \hat{y} - y \in \mathbb{R}^{2\times 1}$$

$$\frac{\partial \hat{y}}{\partial z} = W^{(2)} \in \mathbb{R}^{2\times 3}$$

$z = \sigma(W^{(1)} x + b^{(1)})$ More equivalently, we can rewrite

$$\frac{\partial J(W)}{\partial W^{(1)}} = \frac{\partial J(W)}{\partial z} \cdot \frac{\partial z}{\partial W^{(1)}} \quad \text{with} \quad \frac{\partial J(W)}{\partial z} = (W^{(2)})^T (\hat{y} - y) \in \mathbb{R}^{3\times 1}$$

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Before tackling the gradient wrt $W^{(1)}$, it's important to define necessary terminologies so that we could obtain important results related to the gradient for $W^{(1)}$:

$\delta :=$ column-vector consisting of only zeros and ones in which

$$\delta_i = \begin{cases} 0, & \text{if } (W^{(1)}x + b^{(1)})_i \leq 0 \\ 1, & \text{otherwise} \end{cases}$$ (gradient of RELU giving effect of 1)

Leveraging the potential of those column-vectors, we'll find the gradient in which $z = \mathrm{ReLU}(\underbrace{W^{(1)}x + b^{(1)}}_{z'}) = \mathrm{ReLU}(z') \rightsquigarrow \frac{\partial J(W)}{\partial W^{(1)}} =$

$$= \frac{\partial J(W)}{\partial z} \cdot \frac{\partial z}{\partial W^{(1)}} = \frac{\partial J(W)}{\partial z} \frac{\partial z}{\partial z'} \frac{\partial z'}{\partial W^{(1)}}, \text{ considering } \frac{\partial J(W)}{\partial z} =$$

$$= (W^{(2)})^T(\hat{y} - y) \in \mathbb{R}^{3\times 1}, \quad \boxed{\frac{\partial z}{\partial z'} = \delta \in \mathbb{R}^{3\times 1}}$$ $\rightsquigarrow$ gradients wrt ReLU giving only 1's and 0's (aforementioned column-vector)

Since $z' = W^{(1)}x + b^{(1)} \Rightarrow \frac{\partial z'}{\partial W^{(1)}} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T = [x_1 \; x_2] \in \mathbb{R}^{1\times 2}$, therefore

$$\boxed{\frac{\partial z'}{\partial W^{(1)}} = x^T \in \mathbb{R}^{1\times 2}}$$

If we take into account the Hadamard operation (piecewise multiplication) for $(W^{(2)})^T(\hat{y} - y)$ and δ, where dimensions match as $\mathbb{R}^{3\times 1}$, we obtain

$$\boxed{\frac{\partial J(W)}{\partial W^{(1)}} = \left((W^{(2)})^T(\hat{y} - y) \odot \delta\right) x^T \in \mathbb{R}^{3\times 2}}$$

Using exactly similar gradients wrt $b^{(1)}$, chain-rule reveals that

$$\frac{\partial J(W)}{\partial b^{(1)}} = \frac{\partial J(W)}{\partial z} \frac{\partial z}{\partial b^{(1)}} = \frac{\partial J(W)}{\partial z} \frac{\partial z}{\partial z'} \frac{\partial z'}{\partial b^{(1)}} = (W^{(2)})^T(\hat{y} - y) \odot \delta$$

and since we also know considering $\frac{\partial z}{\partial z'} = \delta \in \mathbb{R}^{3\times 1}$, $(W^{(2)})^T(\hat{y} - y) \in \mathbb{R}^{3\times 1}$ (Hadamard operation giving correct calculation)

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$z^1 = W^{(1)}x + b^{(1)} \Rightarrow$ We conclude that gradient of $J(W)$ wrt $b^{(1)}$, is equal

$$\boxed{\frac{\partial J(W)}{\partial b^{(1)}} = (W^{(2)})^T(\hat{y}-y)\odot \delta}$$

In conclusion, the followings are final gradients to be calculated:

$$\frac{\partial J(W)}{\partial W^{(2)}} = (\hat{y}-y)z^T$$

$$\frac{\partial J(W)}{\partial W^{(1)}} = \left((W^{(2)})^T(\hat{y}-y)\odot\delta\right)x^T$$

$$\frac{\partial J(W)}{\partial b^{(2)}} = \hat{y}-y$$

$$\frac{\partial J(W)}{\partial b^{(1)}} = (W^{(2)})^T(\hat{y}-y)\odot\delta$$

Now, we will use the gradient descent approach with learning rate $\eta=1$

The gradient descent method illustrates the following updates (learning rate=1)

$$W^{(2)} := W^{(2)} - \frac{\partial J(W)}{\partial W^{(2)}} \qquad W^{(1)} := W^{(1)} - \frac{\partial J(W)}{\partial W^{(1)}}$$

$$b^{(2)} := b^{(2)} - \frac{\partial J(W)}{\partial b^{(2)}} \qquad b^{(1)} := b^{(1)} - \frac{\partial J(W)}{\partial b^{(1)}}$$

Given the dataset $D = \left\{ \begin{bmatrix} 2 \\ -3 \end{bmatrix}, \begin{bmatrix} -4 \\ 0 \end{bmatrix} \right\}$ with input $\begin{bmatrix} 2 \\ -3 \end{bmatrix}$ and target variable $\begin{bmatrix} -4 \\ 0 \end{bmatrix}$

our aim is to iterate forward-backward procedures for twice processes:

i) Plugging in $x = \begin{bmatrix} 2 \\ -3 \end{bmatrix}$, $W^{(1)}x + b^{(1)} = \begin{bmatrix} 1 & -1 \\ 0 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 2 \\ -3 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} =$

$= \begin{bmatrix} 5 \\ 3 \\ -5 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \\ -4 \end{bmatrix}$, applying ReLU $\rightsquigarrow \begin{bmatrix} 5 \\ 3 \\ 0 \end{bmatrix}$ and $W^{(2)}x' + b^{(2)}$

$= \begin{bmatrix} 0 & -2 & 1 \\ 1 & -1 & -1 \end{bmatrix}\begin{bmatrix} 5 \\ 3 \\ [illegible] \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -6 \\ 2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -5 \\ 2 \end{bmatrix}$ where

we used $\delta = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$ during the process of forward-propagation $\left(y = \begin{bmatrix} -4 \\ 0 \end{bmatrix}\right)$

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$\underline{1^{st}\text{ iteration:}}$ $W^{(2)} := W^{(2)} - \frac{\partial J(W)}{\partial W^{(2)}}$ where $\frac{\partial J(W)}{\partial W^{(2)}} = (\hat{y}-y)\, f^T =$

$$= \left(\begin{bmatrix} -5 \\ 2 \end{bmatrix} - \begin{bmatrix} -4 \\ 0 \end{bmatrix} \right) \begin{bmatrix} 5 \\ 3 \\ 0 \end{bmatrix}^T = \begin{bmatrix} -1 \\ 2 \end{bmatrix} \begin{bmatrix} 5 & 3 & 0 \end{bmatrix} = \begin{bmatrix} -5 & -3 & 0 \\ 10 & 6 & 0 \end{bmatrix}$$

Thus, $W^{(2)} \rightsquigarrow \begin{bmatrix} 0 & -2 & 1 \\ 1 & -1 & -1 \end{bmatrix} - \begin{bmatrix} -5 & -3 & 0 \\ 10 & 6 & 0 \end{bmatrix} = \underbrace{\begin{bmatrix} 5 & 1 & 1 \\ -9 & -7 & -1 \end{bmatrix}}$

$b^{(2)} := b^{(2)} - \frac{\partial J(W)}{\partial b^{(2)}}$, where $\frac{\partial J(W)}{\partial b^{(2)}} = \hat{y} - y = \begin{bmatrix} -5 \\ 2 \end{bmatrix} - \begin{bmatrix} -4 \\ 0 \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$

$b^{(2)} \rightsquigarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} -1 \\ 2 \end{bmatrix} = \underbrace{\begin{bmatrix} 2 \\ -2 \end{bmatrix}}$

$W^{(1)} := W^{(1)} - \frac{\partial J(W)}{\partial W^{(1)}}$ in which $\frac{\partial J(W)}{\partial W^{(1)}} = \left((W^{(2)})^T (\hat{y}-y) \odot f \right) x^T$

Since $W^{(1)}x + b^{(1)} = \begin{bmatrix} 5 \\ 3 \\ -4 \end{bmatrix} \Rightarrow f = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$ and thus, $(W^{(2)})^T(\hat{y}-y) =$

$$= \begin{bmatrix} 0 & 1 \\ -2 & -1 \\ 1 & -1 \end{bmatrix} \left(\begin{bmatrix} -5 \\ 2 \end{bmatrix} - \begin{bmatrix} -4 \\ 0 \end{bmatrix} \right) = \begin{bmatrix} 0 & 1 \\ -2 & -1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} -1 \\ 2 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ -3 \end{bmatrix}, \; f = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

So, $\frac{\partial J(W)}{\partial W^{(1)}} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 2 & -3 \end{bmatrix} = \begin{bmatrix} 4 & -6 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$, $W^{(1)} - \frac{\partial J(W)}{\partial W^{(1)}} =$

$$= \begin{bmatrix} 1 & -1 \\ 0 & -1 \\ -1 & 1 \end{bmatrix} - \begin{bmatrix} 4 & -6 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = \underbrace{\begin{bmatrix} -3 & 5 \\ 0 & -1 \\ -1 & 1 \end{bmatrix}} \rightsquigarrow W^{(1)} \text{ is updated as follows}$$

$b^{(1)} := b^{(1)} - \frac{\partial J(W)}{\partial b^{(1)}}$ where $\frac{\partial J(W)}{\partial b^{(1)}} = (W^{(2)})^T(\hat{y}-y) \odot f = \begin{bmatrix} 2 \\ 0 \\ -3 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} =$

$= [2\ 0\ 0]^T$, thus $b^{(1)} \rightsquigarrow [0\ 0\ 1]^T - [2\ 0\ 0]^T = \underbrace{\begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix}}$

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ii) Plugging in $x = \begin{bmatrix} 2 \\ -3 \end{bmatrix}$ with new updated values $W^{(2)}, b^{(2)}, W^{(1)}, b^{(1)}$

$$W^{(1)}x + b^{(1)} = \begin{bmatrix} -3 & 5 \\ 0 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ -3 \end{bmatrix} + \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -21 \\ 3 \\ -5 \end{bmatrix} + \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} =$$

$$= \begin{bmatrix} -23 \\ 3 \\ -4 \end{bmatrix} \text{ with ReLU} \rightsquigarrow \begin{bmatrix} 0 \\ 3 \\ 0 \end{bmatrix} \text{ and } f = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \text{ - gradient effect}$$

$$W^{(2)} \begin{bmatrix} 0 \\ 3 \\ 0 \end{bmatrix} + b^{(2)} = \begin{bmatrix} 5 & 1 & 1 \\ -9 & -7 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 3 \\ 0 \end{bmatrix} + \begin{bmatrix} 2 \\ -2 \end{bmatrix} = \begin{bmatrix} 3 \\ -21 \end{bmatrix} + \begin{bmatrix} 2 \\ -2 \end{bmatrix} =$$

$$= \underbrace{\begin{bmatrix} 5 \\ -23 \end{bmatrix}}_{} \rightsquigarrow \hat{y} \text{ and } \begin{bmatrix} -4 \\ 0 \end{bmatrix} \rightsquigarrow y$$

<u>2nd iteration:</u> $W^{(2)} := W^{(2)} - \dfrac{\partial J(W)}{\partial W^{(2)}}$ with $\dfrac{\partial J(W)}{\partial W^{(2)}} = (\hat{y} - y) z^T =$

$$= \left(\begin{bmatrix} 5 \\ -23 \end{bmatrix} - \begin{bmatrix} -4 \\ 0 \end{bmatrix} \right) \begin{bmatrix} 0 & 3 & 0 \end{bmatrix} = \begin{bmatrix} 9 \\ -23 \end{bmatrix} \begin{bmatrix} 0 & 3 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 27 & 0 \\ 0 & -69 & 0 \end{bmatrix}$$

$$W^{(2)} \rightsquigarrow \begin{bmatrix} 5 & 1 & 1 \\ -9 & -7 & -1 \end{bmatrix} - \begin{bmatrix} 0 & 27 & 0 \\ 0 & -69 & 0 \end{bmatrix} = \underbrace{\begin{bmatrix} 5 & -26 & 1 \\ -9 & 62 & -1 \end{bmatrix}}_{}$$

$b^{(2)} := b^{(2)} - \dfrac{\partial J(W)}{\partial b^{(2)}}$ in which $\dfrac{\partial J(W)}{\partial b^{(2)}} = \hat{y} - y = \begin{bmatrix} 5 \\ -23 \end{bmatrix} - \begin{bmatrix} -4 \\ 0 \end{bmatrix} = \begin{bmatrix} 9 \\ -23 \end{bmatrix}$

$$b^{(2)} \rightsquigarrow \begin{bmatrix} 2 \\ -2 \end{bmatrix} - \begin{bmatrix} 9 \\ -23 \end{bmatrix} = \underbrace{\begin{bmatrix} -7 \\ 21 \end{bmatrix}}_{}$$

$W^{(1)} := W^{(1)} - \dfrac{\partial J(W)}{\partial W^{(1)}}$ where $\dfrac{\partial J(W)}{\partial W^{(1)}} = \left((W^{(2)})^T (\hat{y} - y) \circ f \right) x^T$

$$(W^{(2)})^T (\hat{y} - y) = \begin{bmatrix} 5 & -9 \\ 1 & -7 \\ 1 & -1 \end{bmatrix} \left(\begin{bmatrix} 5 \\ -23 \end{bmatrix} - \begin{bmatrix} -4 \\ 0 \end{bmatrix} \right) = \begin{bmatrix} 5 & -9 \\ 1 & -7 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 9 \\ -23 \end{bmatrix}$$

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$$(W^{(2)})^T(\hat{y}-y) = \begin{bmatrix} 45+207 \\ 9+161 \\ 9+23 \end{bmatrix} = \begin{bmatrix} 252 \\ 170 \\ 32 \end{bmatrix}, \text{ since } f = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \Rightarrow$$

$$(W^{(2)})^T(\hat{y}-y) \circ f = \begin{bmatrix} 0 \\ 170 \\ 0 \end{bmatrix} \text{ with } \frac{\partial J(W)}{\partial W^{(1)}} = \begin{bmatrix} 0 \\ 170 \\ 0 \end{bmatrix} \begin{bmatrix} 2 & -3 \end{bmatrix} =$$

$$= \begin{bmatrix} 0 & 0 \\ 340 & -510 \\ 0 & 0 \end{bmatrix}, \quad W^{(1)} \rightsquigarrow \begin{bmatrix} -3 & 5 \\ 0 & -1 \\ -1 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 340 & -510 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} -3 & 5 \\ -340 & 509 \\ -1 & 1 \end{bmatrix}$$

$$b^{(1)} := b^{(1)} - \frac{\partial J(W)}{\partial b^{(1)}} \text{ where } \frac{\partial J(W)}{\partial b^{(1)}} = (W^{(2)})^T(\hat{y}-y) \circ f = \begin{bmatrix} 252 \\ 170 \\ 32 \end{bmatrix} \circ \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ 170 \\ 0 \end{bmatrix}, \quad b^{(1)} \rightsquigarrow \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 170 \\ 0 \end{bmatrix} = \begin{bmatrix} -2 \\ -170 \\ 1 \end{bmatrix}$$

In conclusion, after two iterations of optimization during the training data, we obtained (H) parameters $\longrightarrow$

$$W^{(1)} = \begin{bmatrix} -3 & 5 \\ -340 & 509 \\ -1 & 1 \end{bmatrix} \quad \boxed{V} \quad \boxed{\star}$$

$$b^{(1)} = \begin{bmatrix} -2 \\ -170 \\ 1 \end{bmatrix} \quad \boxed{\star}$$

$$\oplus$$

$$W^{(2)} = \begin{bmatrix} 5 & -26 & 1 \\ -9 & 62 & -1 \end{bmatrix} \quad \boxed{\star}$$

and

$$b^{(2)} = \begin{bmatrix} -7 \\ 21 \end{bmatrix} \quad \boxed{\star}$$

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1) a) Setting the initial state as $X_0=1$, we have to first construct Markov chains for <u>proposal distributions of q</u>. Since $X_0=1$, there exist two possible cases for $X_1 \rightsquigarrow$ <u>$X_1=2,4$</u>

Taking into account $\alpha_{ij}=\min\left\{\frac{\pi_j q_{ji}}{\pi_i q_{ij}}, 1\right\}$ measurement, we can find that

$q_{41}=q_{14}=\frac{1}{2}$ with $\pi_4=3$, $\pi_1=4 \Rightarrow \alpha_{14}=\min\left\{1, \frac{\pi_4 q_{41}}{\pi_1 q_{14}}\right\}=$

$=\min\left\{1, \frac{3}{4}\right\}=\frac{3}{4}$, $\boxed{\alpha_{14}=\frac{3}{4}}$ Similarly, $q_{12}=q_{21}=\frac{1}{2}$ where $\pi_1=4$, $\pi_2=2$

$\alpha_{12}=\min\left\{\frac{\pi_2 q_{21}}{\pi_1 q_{12}}, 1\right\}=\min\left\{1, \frac{2}{4}\right\}=\frac{1}{2}$, $\boxed{\alpha_{12}=\frac{1}{2}}$ It is well-known that the transition probability p_{ij} from state i to state j of the Markov chain is again

$p_{ij}=q_{ij}\alpha_{ij}$, $p_{12}=q_{12}\alpha_{12}=\frac{1}{2}\alpha_{12}=\frac{1}{4}$ and $p_{14}=q_{14}\alpha_{14}=\frac{1}{2}\frac{3}{4}=\frac{3}{8}$

$\boxed{p_{12}=\frac{1}{4}}$ $\boxed{p_{14}=\frac{3}{8}}$ Taking into account that the row sums should be 1, $\boxed{p_{13}=0}$ since $q_{13}=0$ and thus, $p_{11}=1-\frac{1}{4}-\frac{3}{8}=$

$=1-\frac{5}{8}=\frac{3}{8}$, $\boxed{p_{11}=\frac{3}{8},\ p_{12}=\frac{1}{4},\ p_{13}=0,\ p_{14}=\frac{3}{8}}$ ★ Now, moving to the second X_1

<u>$X_1=4$ will yield $X_2=3,1$</u> From the properties written above, it's clear

$\alpha_{43}=\min\left\{\frac{\pi_3 q_{34}}{\pi_4 q_{43}}, 1\right\}$ where $q_{34}=q_{43}=\frac{1}{2}$ and $\pi_3=\pi_4=3$

Thus, $\boxed{\alpha_{43}=1}$ and $p_{43}=q_{43}\alpha_{43}=\frac{1}{2}$

$\boxed{p_{43}=\frac{1}{2}}$ $\pi_1=4$, $\pi_4=3$, and $q_{14}=q_{41}=\frac{1}{2} \Rightarrow \frac{\pi_1 q_{14}}{\pi_4 q_{41}}=\frac{4}{3}>1$, so

$\alpha_{41}=1$ with $p_{41}=q_{41}\alpha_{41}=\frac{1}{2} \Rightarrow \boxed{p_{41}=\frac{1}{2}}$ Since $p_{42}=q_{42}\alpha_{42}=0$,

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$\boxed{p_{42}=0}$ Sum of rows are equal to 1, thus $p_{41}+p_{42}+p_{43}+p_{44}=1$ and

$p_{44}=1-\frac{1}{2}-\frac{1}{2}=0$, $\boxed{p_{41}=\frac{1}{2},\ p_{42}=0,\ p_{43}=\frac{1}{2},\ p_{44}=0}$ ☆ In the sub-sequent phase, it's clear that

by choosing $X_2=3 \Rightarrow$ we can declare $X_3=2$ and 4

$\pi_3=\pi_4=3$, $q_{34}=q_{43}=\frac{1}{2} \Rightarrow \pi_4 q_{43}=\pi_3 q_{34}$ meaning that $\boxed{\alpha_{34}=1}$

$q_{23}=q_{32}=\frac{1}{2}$, $\pi_2=2$, $\pi_3=3 \Rightarrow \frac{\pi_2 q_{23}}{\pi_3 q_{32}}=\frac{2}{3}<1$, thus $\boxed{\alpha_{32}=\frac{2}{3}}$

$\alpha_{34} q_{34}=q_{34}=\boxed{\frac{1}{2}=p_{34}}$ $\alpha_{32} q_{32}=\frac{2}{3}\frac{1}{2}=\frac{1}{3} \Rightarrow \boxed{p_{32}=\frac{1}{3}}$ Since we know $p_{31}=\alpha_{31}q_{31}=0$

$\boxed{p_{31}=0}$ Summation of row elements $=1 \Rightarrow p_{33}=1-\frac{1}{2}-\frac{1}{3}=\frac{1}{6}$, yielding that

$\boxed{p_{31}=0,\ p_{32}=\frac{1}{3},\ p_{33}=\frac{1}{6},\ p_{34}=\frac{1}{2}}$ ☆ In the last phase, choosing $X_3=2$

$\pi_1=4$, $\pi_2=2$, $q_{12}=q_{21}=\frac{1}{2} \Rightarrow$

$\frac{\pi_1 q_{12}}{\pi_2 q_{21}}=2>1$, so $\boxed{\alpha_{21}=1}$ $\pi_2=2$, $\pi_3=3$, $q_{23}=q_{32}=\frac{1}{2} \Rightarrow$

$p_{21}=\alpha_{21}q_{21}=q_{21}=\frac{1}{2}$

$\frac{\pi_3 q_{32}}{\pi_2 q_{23}}=\frac{3}{2}>1 \Rightarrow \boxed{\alpha_{23}=1}$ $p_{23}=\alpha_{23}q_{23}=\frac{1}{2}$ $\Big\}$ $\boxed{p_{21}=p_{23}=\frac{1}{2}}$

$p_{24}=\alpha_{24}q_{24}=$ should be 1

$=0$, therefore $p_{22}=1-p_{21}-p_{23}-p_{24}=0$ since sum of row elements

$\boxed{p_{21}=\frac{1}{2},\ p_{22}=0,\ p_{23}=\frac{1}{2},\ p_{24}=0}$ ☆ In conclusion, the desired transition matrix for q will be

$$P=\begin{bmatrix} \frac{3}{8} & \frac{1}{4} & 0 & \frac{3}{8} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{3} & \frac{1}{6} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{bmatrix}$$ ☆ ☆ $\boxed{Y}$

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Now, setting the initial state as $X_0=1$, we will construct Markov chains for proposal distribution of $\tilde{q}$. Since $X_0=1$, we will set $X_1=2$ and

$\pi_4=3$, $\pi_1=4$, $\tilde{q}_{14}=\frac{1}{3}$, $\tilde{q}_{41}=\frac{2}{3} \Rightarrow \frac{\pi_4 \tilde{q}_{41}}{\pi_1 \tilde{q}_{14}} = \frac{2}{4/3} = \frac{3}{2} > 1$ with

$\alpha_{14}=\min\left\{1, \frac{\pi_4 \tilde{q}_{41}}{\pi_1 \tilde{q}_{14}}\right\}=1$ where $p_{14}=\alpha_{14}\tilde{q}_{14}=\frac{1}{3} \Rightarrow \boxed{p_{14}=\frac{1}{3}}$

$\pi_2=2$, $\pi_1=4$, $\tilde{q}_{12}=\frac{2}{3}$, $\tilde{q}_{21}=\frac{1}{3} \Rightarrow \frac{\pi_2 \tilde{q}_{21}}{\pi_1 \tilde{q}_{12}} = \frac{2/3}{8/3} = \frac{1}{4} < 1$, so

$\alpha_{12}=\min\left\{1, \frac{\pi_2 \tilde{q}_{21}}{\pi_1 \tilde{q}_{12}}\right\}=\frac{1}{4}$, where $p_{12}=\alpha_{12}\tilde{q}_{12}=\frac{1}{4}\cdot\frac{2}{3}=\frac{1}{6}$

in the row should be equal to 1

$\boxed{p_{12}=\frac{1}{6}}$ $p_{13}=\alpha_{13}\tilde{q}_{13}=0 \Rightarrow p_{11}=1-\frac{1}{3}-\frac{1}{6}=1-\frac{1}{2}=\frac{1}{2}$ since sum of elems

$\boxed{p_{11}=\frac{1}{2},\ p_{12}=\frac{1}{6},\ p_{13}=0,\ p_{14}=\frac{1}{3}}$ ☆ Subsequently, having $X_1=4$, we set $X_2=3$ and 1:

$\frac{\pi_3 \tilde{q}_{34}}{\pi_4 \tilde{q}_{43}} = \frac{3\times\frac{2}{3}}{3\times\frac{1}{3}} = 2 > 1 \Rightarrow \alpha_{43}=\min\left\{1, \frac{\pi_3 \tilde{q}_{34}}{\pi_4 \tilde{q}_{43}}\right\}=1$ and

similarly, $p_{43}=\alpha_{43}\tilde{q}_{43}=1\times\frac{1}{3}=\frac{1}{3}$ $\boxed{p_{43}=\frac{1}{3}}$

$\frac{\pi_1 \tilde{q}_{14}}{\pi_4 \tilde{q}_{41}} = \frac{4\times\frac{1}{3}}{3\times\frac{2}{3}} = \frac{2}{3} < 1 \Rightarrow \alpha_{41}=\frac{2}{3}$ and $p_{41}=\alpha_{41}\tilde{q}_{41}=\frac{2}{3}\times\frac{2}{3}=\frac{4}{9}$

$\boxed{p_{41}=\frac{4}{9}}$

Since $p_{42}=\alpha_{42}\tilde{q}_{42}=0$, and sum of elem's in the row should be 1, therefore

$p_{44}=1-\frac{4}{9}-\frac{1}{3}=1-\frac{7}{9}=\frac{2}{9}$, $\boxed{p_{41}=\frac{4}{9},\ p_{42}=0,\ p_{43}=\frac{1}{3},\ p_{44}=\frac{2}{9}}$ ☆ Now, after

setting $X_2=3 \Rightarrow X_3=2$ and 4 $\frac{\pi_2 \tilde{q}_{23}}{\pi_3 \tilde{q}_{32}} = \frac{2\times 2/3}{3\times 1/3} = \frac{4}{3} > 1$, meaning

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$\alpha_{32}=1$ and $p_{32}=\alpha_{32}\tilde{q}_{32}=\tilde{q}_{32}=\frac{1}{3} \Rightarrow \boxed{p_{32}=\frac{1}{3}}$ $p_{34}=\alpha_{34}\tilde{q}_{34}=$

$$=\min\left\{\frac{\pi_4\tilde{q}_{43}}{\pi_3\tilde{q}_{34}},1\right\}\frac{2}{3}=\min\left\{1,\frac{\tilde{q}_{43}}{\tilde{q}_{34}}\right\}\frac{2}{3}=\min\left\{1,\frac{1/3}{2/3}\right\}\frac{2}{3}=$$

$=\frac{1}{\cancel{2}}\times\frac{\cancel{2}}{3}=\frac{1}{3}$, so $\boxed{p_{34}=\frac{1}{3}}$ $p_{31}=\alpha_{31}\tilde{q}_{31}=0$, and since the summation of row elements $=1$, we ensure

$p_{33}=1-\frac{1}{3}-\frac{1}{3}=\frac{1}{3} \Rightarrow \boxed{p_{31}=0,\ p_{32}=\frac{1}{3},\ p_{33}=\frac{1}{3},\ p_{34}=\frac{1}{3}}$ ☆ In the final phase, setting $X_3=2$ yields

$\frac{\pi_1\tilde{q}_{12}}{\pi_2\tilde{q}_{21}}=\frac{4\times\frac{2}{3}}{2\times\frac{1}{3}}=4>1$, which shows $\alpha_{21}=1$ and $p_{21}=\alpha_{21}\tilde{q}_{21}=$ $=\frac{1}{3}$, $\boxed{p_{21}=\frac{1}{3}}$ Similarly,

$\frac{\pi_3\tilde{q}_{32}}{\pi_2\tilde{q}_{23}}=\frac{3\times 1/3}{2\times 2/3}=\frac{3}{4}<1$, yielding $\alpha_{23}=\frac{3}{4}$ and $p_{23}=\alpha_{23}\tilde{q}_{23}=$ $=\frac{3}{4}\times\frac{2}{3}=\frac{1}{2}$

$\boxed{p_{23}=\frac{1}{2}}$ Since $p_{24}=\alpha_{24}\tilde{q}_{24}=0$ where summation of row elements is equal to 1, $p_{22}=1-\frac{1}{2}-\frac{1}{3}=\frac{1}{6}$. $\boxed{p_{21}=\frac{1}{3},\ p_{22}=\frac{1}{6},\ p_{23}=\frac{1}{2},\ p_{24}=0}$ ☆

In conclusion, transition matrix for $\tilde{q}$ will be

$$\tilde{P}=\begin{bmatrix}\frac{1}{2} & \frac{1}{6} & 0 & \frac{1}{3}\\ \frac{1}{3} & \frac{1}{6} & \frac{1}{2} & 0\\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3}\\ \frac{4}{9} & 0 & \frac{1}{3} & \frac{2}{9}\end{bmatrix}$$ ☆ ☆

6) Now, we'll calculate the exact $E[f(X)] \Rightarrow$ Since from the given statements and definition, $E[f(X)]=$

$$=E[X^2-3]=\sum_{j=0}^{\infty}(j^2-3)P(X=j)=$$ since given is PMF prop problem

$$\Rightarrow E[f(X)]=(1^2-3)P(X=1)+(2^2-3)P(X=2)+(3^2-3)P(X=3)+(4^2-3)P(X=4)$$

Since we have to normalize probabilities given the fact that $\tilde{p}(X=1)=4$, $\tilde{p}(X=2)=2$, $\tilde{p}(X=3)=3$, $\tilde{p}(X=4)=3 \Rightarrow$ the followings are normalized:

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$$P(X=1) = \frac{4}{4+2+3+3} = \frac{4}{12} = \frac{1}{3}$$

$$P(X=2) = \frac{2}{4+2+3+3} = \frac{2}{12} = \frac{1}{6}$$

$$P(X=3) = \frac{3}{4+2+3+3} = \frac{3}{12} = \frac{1}{4}$$

$$P(X=4) = \frac{3}{4+2+3+3} = \frac{3}{12} = \frac{1}{4}$$

$$E[f(x)] = (-2)\frac{1}{3} + \frac{1}{6} + 6 \times \frac{1}{4} + 13 \times \frac{1}{4} = \frac{-2}{3} + \frac{1}{6} + \frac{3}{2} + \frac{13}{4} = -\frac{4}{6} + \frac{1}{6} + \frac{3}{2} + \frac{13}{4} = -\frac{1}{2} + \frac{3}{2} + \frac{13}{4} = \frac{17}{4}$$

Thus, $\boxed{E[f(x)] = \frac{17}{4}}$ ☆

Theoreticoppy, q and $\tilde{q}$ will definitely converge the expected value $\frac{17}{4}$ after some iterations, but it should be noted after plotting the errors along during programming $h=1, \dots, 1000$, $\tilde{q}$-proposal distribution will converge faster in the expected sense ☑ ⊕ as it could be observed over there (for $\tilde{q}$-proposed distribution, less # of iterations could be enough to converge)

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2) a) Since we know that $P(a_0|s_0) = \frac{1}{2}$ ①

$P(a_1|s_1) = \frac{1}{2}$ ②

$P(a_2|s_2) = \frac{1}{2}$ ③

$P(a_3|s_3) = \frac{3}{10}$ ④

are satisfied, meanwhile it's also clear that according to given statements

$P(\overbrace{(s_0+2)\%5}^{s_1} | s_0, a^1) = \frac{1}{3}$ ①

$P((s_1+3)\%5 | s_1, a^2) = \frac{1}{2}$ ②

$P((s_2+3)\%5 | s_2, a^2) = \frac{1}{2}$ ③

$P(\underbrace{(s_3+1)\%5}_{s_4} | s_3, a^2) = \frac{1}{2}$ ④

and moreover, we have to take into account that $P(r_1 = 1) = \frac{1}{2}$ holds true

Therefore, using all these results, we can measure the probability that trajectory is sampled:

$$P(\tau) = P(\tau = (s_0=0, a_0=a^1, r_0=0, s_1=2, a_1=a^2, r_1=1, s_2=0, a_2=a^2, r_2=0, s_3=3, a_3=a^2, r_3=0, s_4=4))$$

$$= \frac{1}{2} \times 1 \times \frac{1}{3} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times 1 \times \frac{1}{2} \times \frac{3}{10} \times 1 \times \frac{1}{2} =$$

$$= \frac{\frac{1}{24} \times \frac{3}{80}}{2} = \frac{1}{640} \cdot \frac{1}{2} = \boxed{\frac{1}{1280}}$$

b) We can use the Bellman Equation iteratively starting with a value function zero everywhere. This method converges usually very quickly. But since we have a very small state and action space, the Bellman Equation is only a small set of linear equations that can be obtained in an explicit manner. After that, we can solve them using matrix methods (basic LA)

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The Bellman equation for this problem is given as a system of $|S|$ equations: $V^{\pi}(s) = \sum_{\text{actions } a} \pi(a|s) \sum_{\text{states } s'} P(s'|s,a)\left(R(s',a,s) + \gamma \cdot V^{\pi}(s')\right)$

The trick is to rewrite this in matrix form and solve the achieved equation wrt V^{π}:

$V^{\pi} = \pi^1 P_1 (R_1 \mathbf{1}^T + \gamma V^{\pi}) + \pi^2 P_2 (R_2 \mathbf{1}^T + \gamma V^{\pi})$, or just

$V^{\pi} = \pi^1 P_1 (R_1 \mathbf{1}^T + \gamma V^{\pi}) + \pi^2 P_2 (R_2 \mathbf{1}^T + \gamma V^{\pi})$ where

$\pi^i = (\pi(a^i|0), \dots, \pi(a^i|4))$

$$R_i = \begin{pmatrix} R(0,a^i,0) & \dots & R(4,a^i,0) \\ \vdots & \ddots & \vdots \\ R(0,a^i,4) & \dots & R(4,a^i,4) \end{pmatrix}$$

$\mathbf{1} = (1, \dots, 1)$

Then, we can regroup and obtain the following:

$V^{\pi} = (\pi^1 P_1 R_1 + \pi^2 P_2 R_2)\mathbf{1}^T + (\pi^1 P_1 + \pi^2 P_2) V^{\pi}$

which finally results in

$V^{\pi} = (Id - \gamma(\pi^1 P_1 + \pi^2 P_2))^{-1} (\pi^1 P_1 R_1 + \pi^2 P_2 R_2)\mathbf{1}^T$

It should be noted that the inverse exists only for $\gamma < 1$, where the rewards are randomized and depend on state transition, too.

The below recursion also indicates how the computations are implemented correctly:

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We set initially $V^{\pi}(0)=(0,0,0,0,0)$ and

$$V^{\pi}(k+1,s) \leftarrow \sum_{\text{actions } a} \pi(a|s) \sum_{\text{states } s'} P(s'|s,a)\left(R(s',a,s) + \gamma \cdot V^{\pi}(k,s')\right)$$

c) <u>Policy Iteration:</u>

Setting $n=0$ and selecting an arbitrary policy $d_0 \in D^{MD}$ (1)

(policy evaluation) (2)

→ obtaining $v^{(n)}$ by solving $(I-\lambda P_{d_n})v^{(n)} = r_{d_n}$

(policy improvement) (3)

→ Choosing d_{n+1} to satisfy

$$d_{n+1} \in \operatorname{argmax}_{d \in D^{MD}} \{ r_d + \lambda P_d v^{(n)} \}$$

setting $d_{n+1} = d_n$ if possible

If $d_{n+1} = d_n$, stop and set $d^* = d_n$. Otherwise, increasing n by 1 and returning to step 2 (4)

$$d_0 = [a^1\ a^1\ a^1\ a^1\ a^1]^T$$

$$P_a^2 = \begin{bmatrix} 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \\ 1/2 & 0 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 0 & 1/2 \\ 1/2 & 0 & 1/2 & 0 & 0 \end{bmatrix}$$

$$P_{d_0} = P_a^1 = \begin{bmatrix} 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 1/3 & 0 & 1/3 & 1/3 & 0 \\ 0 & 1/3 & 0 & 1/3 & 1/3 \\ 1/3 & 0 & 1/3 & 0 & 1/3 \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 \end{bmatrix} \Rightarrow r_{d_0} = \begin{bmatrix} 0 \\ 1/3 \\ 0 \\ 1/3 \\ 1/3 \end{bmatrix} \cdot \frac{1}{2} = \begin{bmatrix} 0 \\ 1/6 \\ 0 \\ 1/6 \\ 1/6 \end{bmatrix}$$

Taking into account the equation $(I-\lambda P_{d_0})v^{(0)} = r_{d_0}$, and plugging in those matrices (and λ-variable) with solving in numpy algorithms will yield $v^{(0)} = (I-\lambda P_{d_0})^{-1} r_{d_0} =$

$$= \begin{bmatrix} 0.913182 \\ 1.036418 \\ 0.943111 \\ 1.042877 \\ 1.064410 \end{bmatrix}$$

Now, if we take into account policy improvement stage in which $d_1 = \operatorname{argmax}\{ r_{a_1} + \lambda P_{a_1} v^{(0)}, r_{a_2} + \lambda P_{a_2} v^{(0)} \}$

$r_{a_1} \to 1/2$ of the 1st column of P_{a_1} → similar for a_2

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