

On Classification of Noiseless and Noisy Pattern Orientations

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Presentation Outline



- Preamble / Motivation
- Noiseless Data (Tasks 1-3)
- Noisy Data (Task 4)
- Likelihood Models (Task 5)
- Noisy Sparse Data (Task 6)
- The Master Image (Task 7)



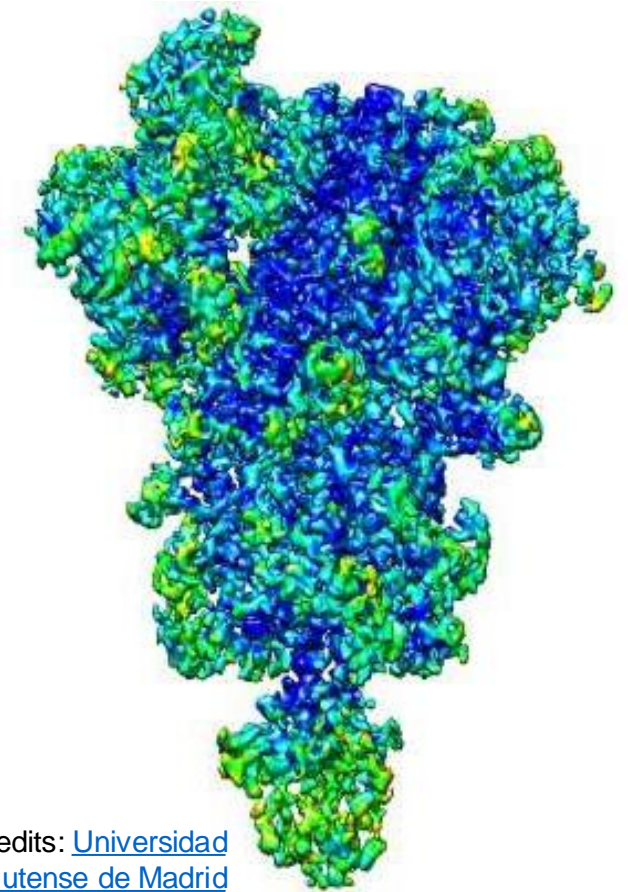
Part 0: Preamble

Motivation



Understanding involves seeing. This is especially true for complex biological systems, such as proteins.

Techniques such as single particle imaging (SPI) can achieve this by computationally reconstructing structures from several measurements.



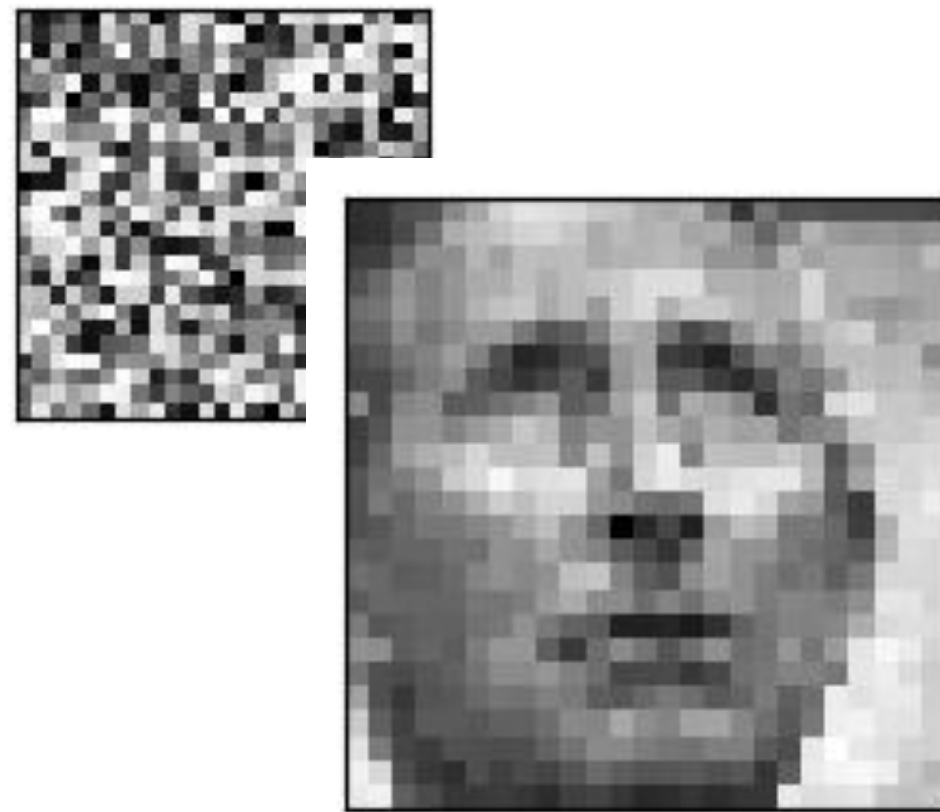
Credits: [Universidad Complutense de Madrid](#)

A Toy Model



SPI involves reconstructing 3D structures from 2D images in varying orientations.

Here we explore the simpler case of reconstructing 2D images from differently oriented 2D patterns.





Part 1: On Noiseless Data

Tasks 1-3: Noiseless Images

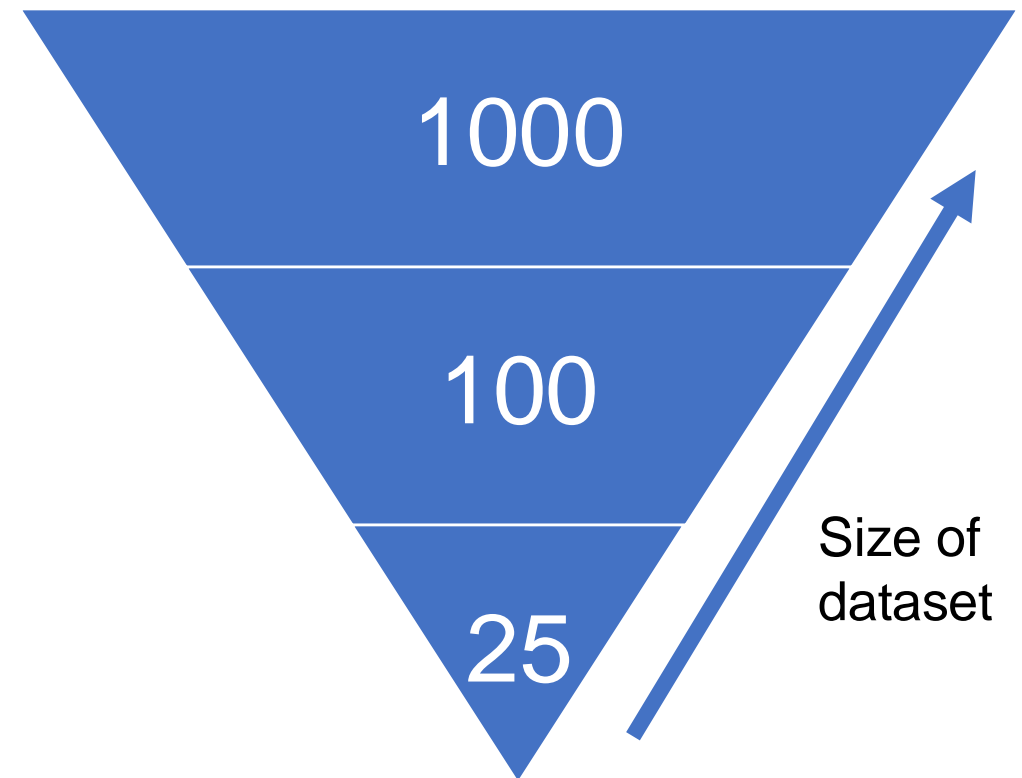


- In an idealized world, the image data we collect would be **noiseless**.
- This makes it **easy to classify in what orientation** each measurement is (i.e., measurements of the same orientation would have the same pixel values)

Profiling Tasks 1-3



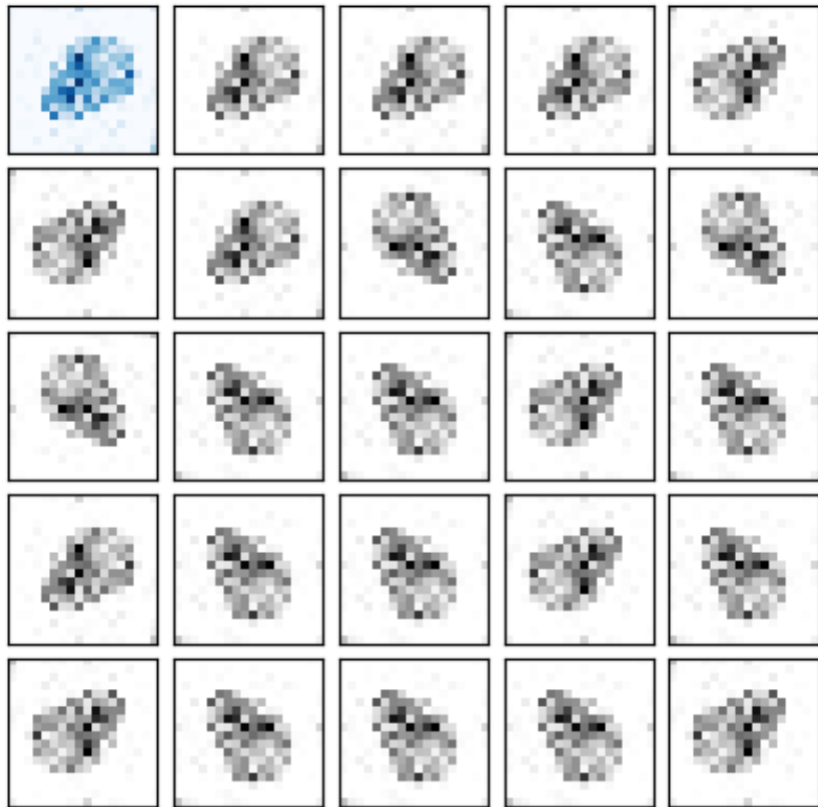
- Tasks 1 to 3 all deal with noiseless pattern data.
- The magnitude of the dataset size increases.
- **We were able to create one algorithm that can classify patterns into 4 orientation classes for all of Tasks 1 to 3.**



Task 1



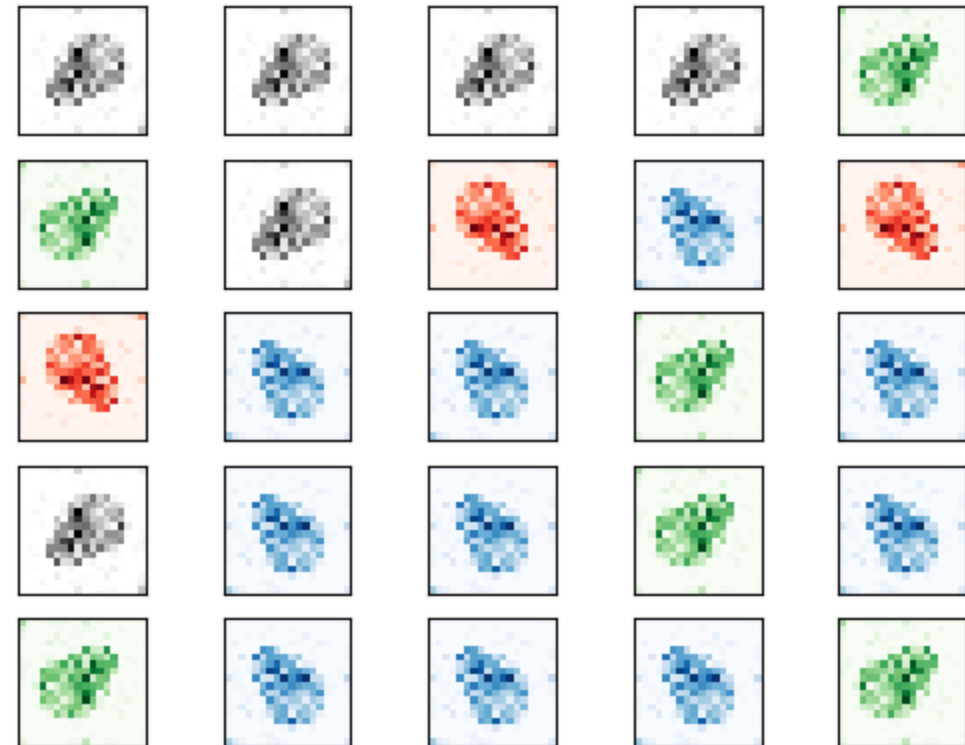
25 images (2D)



(from problem statement)



Classified into orientation classes

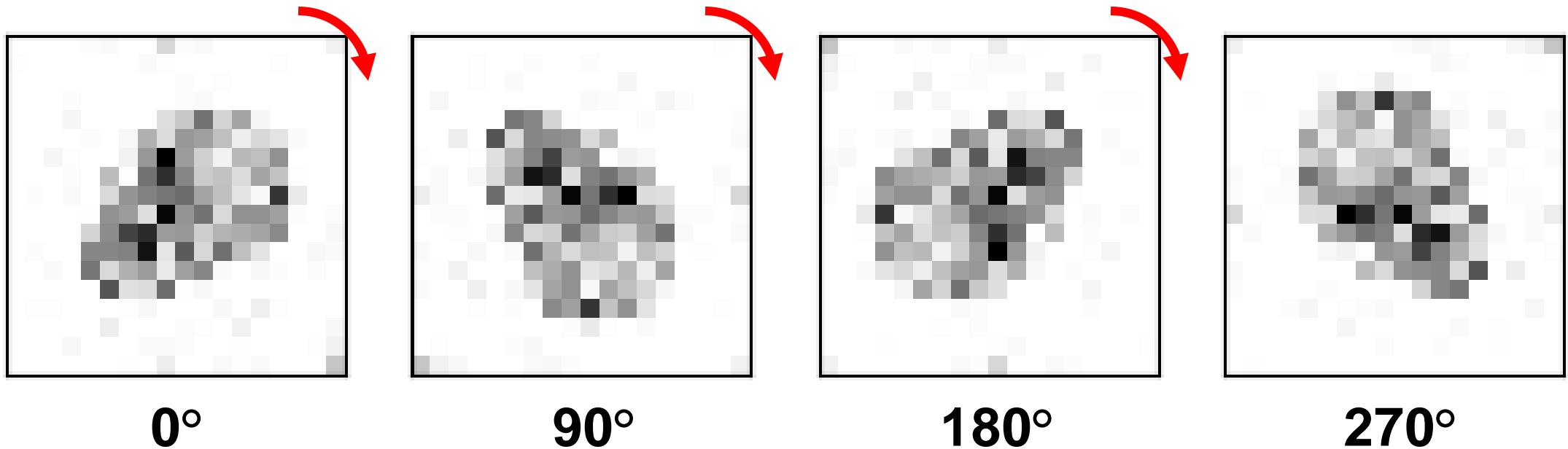


■ 0° ■ 90° ■ 180° ■ 270°

Task 1(a)



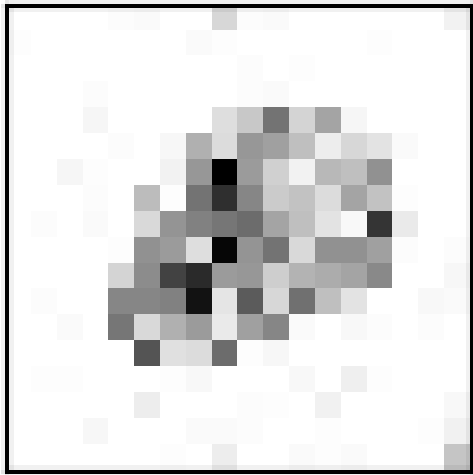
- We produced the rotations of the reference image.



Task 1(b)

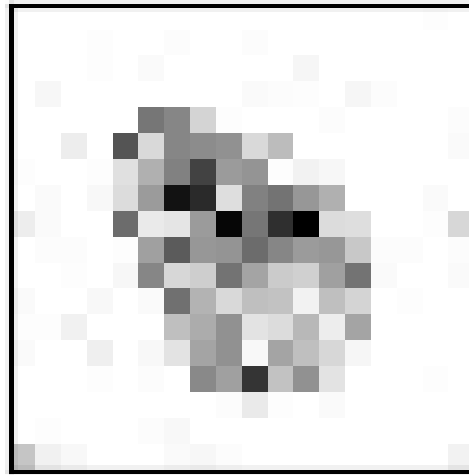


- We produced the rotations of the reference image.



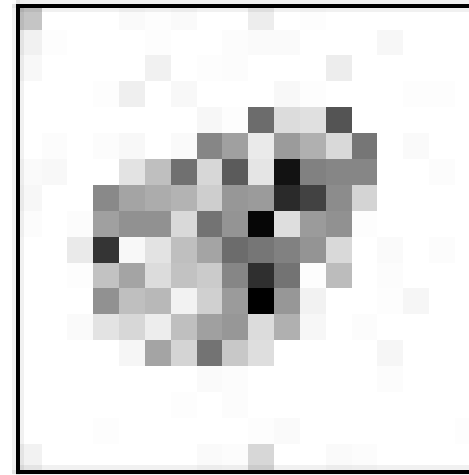
0°

6 patterns



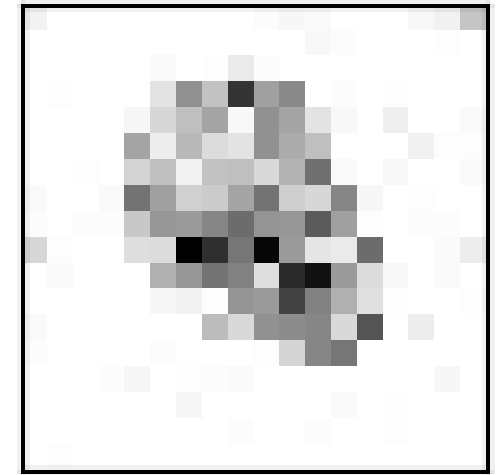
90°

10 patterns



180°

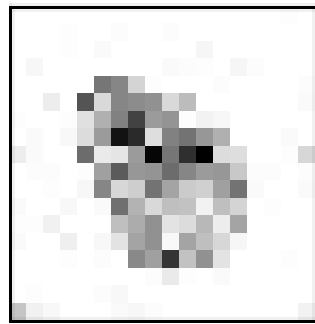
6 patterns



270°

3 patterns

Task 1(c)



Image

$$H = \sum a_i \cdot 2^i \pmod{p}$$

Prime Hash Function ($p = 10^9 + 7$)

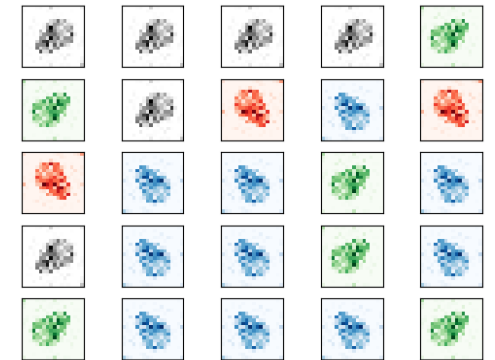
458621916

Hashed Value

0°: 240650399
90°: 458621916
180°: 967870281
270°: 747319434

Hash rotations of
the reference
image

Compare hashes
of each pattern to
reference hashes





Task 1(c)

Given

- We are given $A = 25$ patterns and $B = 625$ pixels in the image.

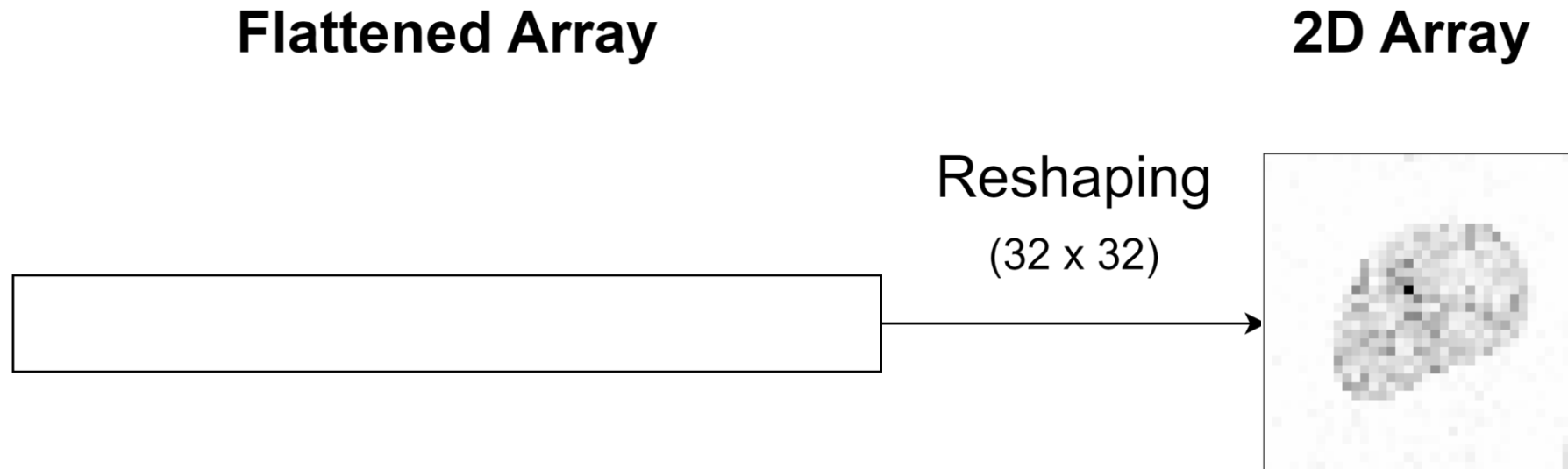
Time Complexity

- The time complexity of hashing is $O(B)$.
- The time complexity of all comparisons is $O(AB)$.
- The number of operations is $\sim 10^1 \times 10^2 = 10^3$.
- Non-hashing algorithms to compare patterns to reference images could probably be used (i.e., naïve searching or visual comparison).



Task 2(a)

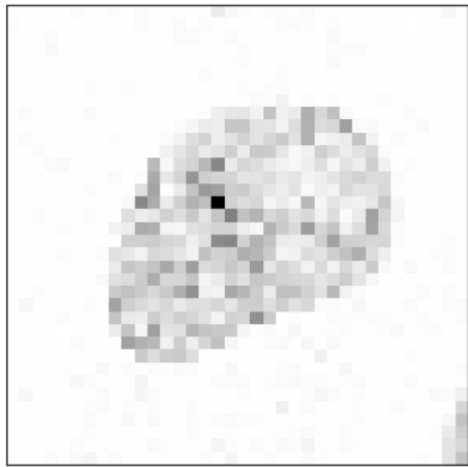
- The data was provided in a flattened format.
- We first rendered the reference image by reshaping a 1024-long flattened array into a 32 x 32 array.



Task 2(b)

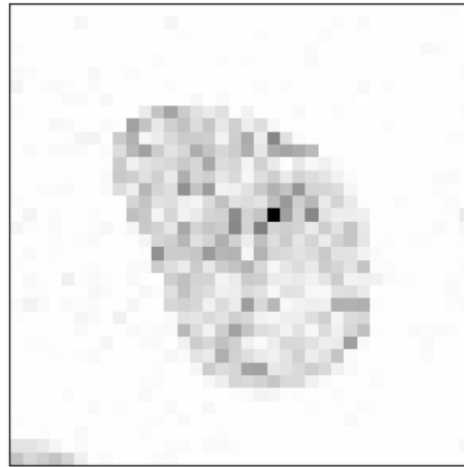


- We produced the **rotations of the reference image** and counted the number of such images:



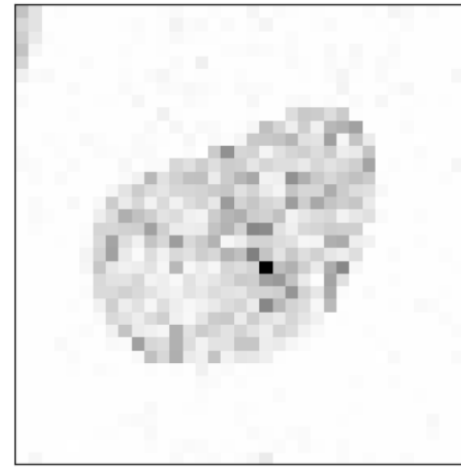
0°

22 patterns



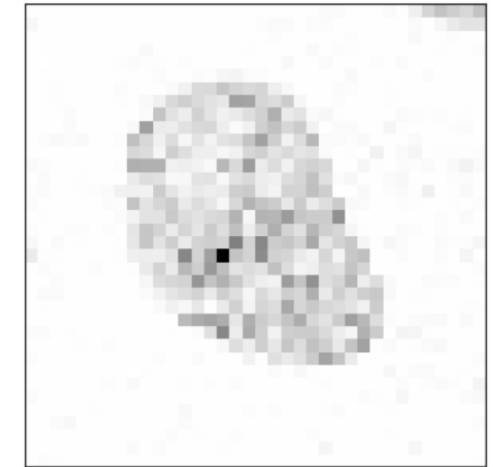
90°

32 patterns



180°

21 patterns



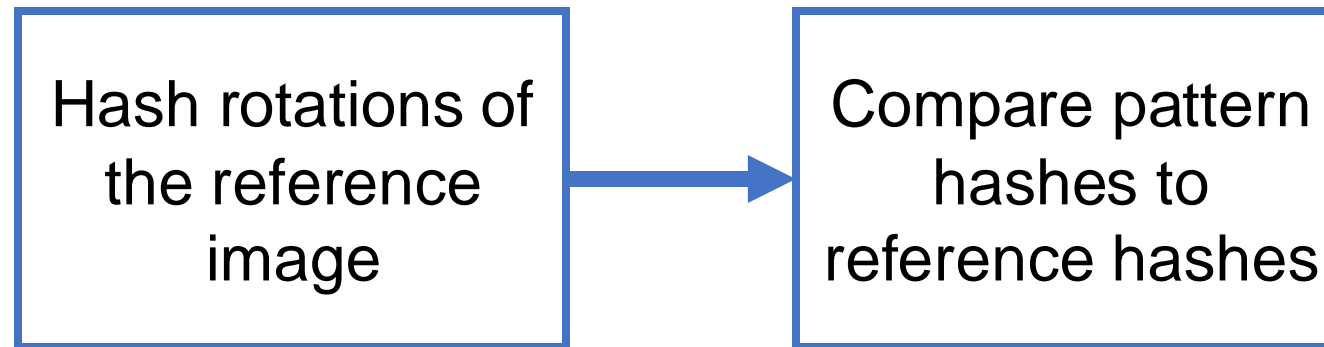
270°

25 patterns



Task 2(c)

- We use the same methodology to compare the images.



- However, we perform slightly more operations (with a magnitude change of $\sim 10^3$ to $\sim 10^4$). Yet, our algorithm remains resilient to this change in magnitude.

Task 3(a)



- The tasks revealed that the image has dimensions 33 x 33 pixels, since the total number of pixels in the flattened image is $1089 = 33^2$ pixels. This produces an image of a horse:



Task 3(b)



- We produced the **rotations of the reference image** and counted the number of such images:



0°

254 patterns



90°

236 patterns



180°

250 patterns



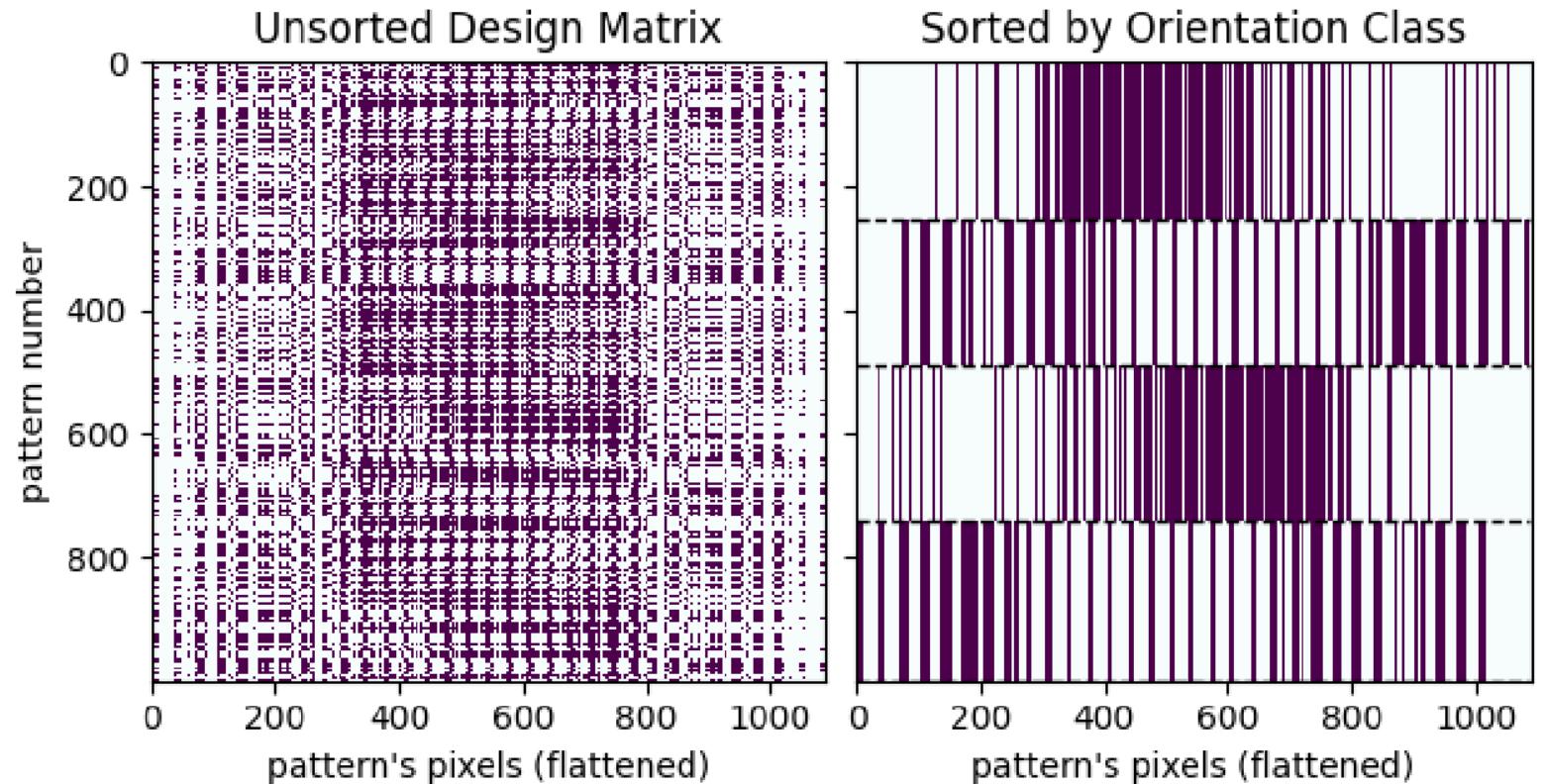
270°

260 patterns

Task 3(c)



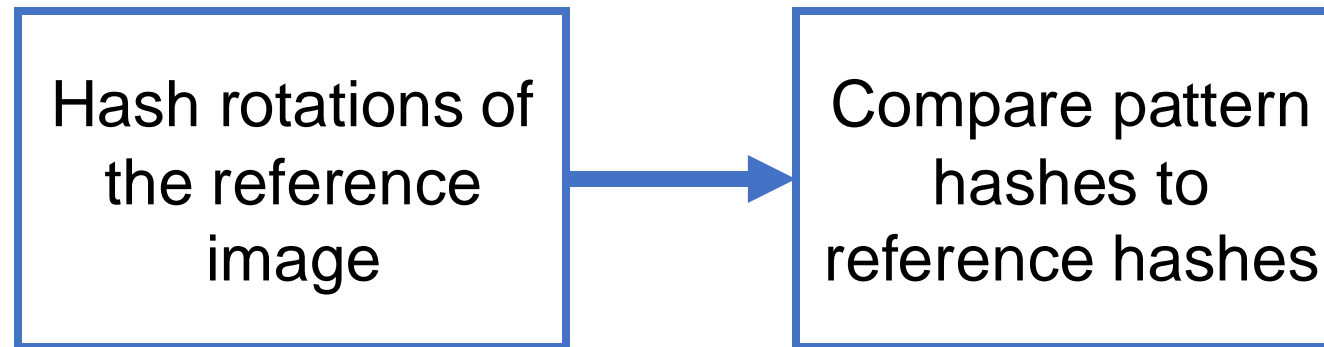
- We also show that we have classified the images based on the sorted design matrices:





Task 3(d)

- We use the same methodology to compare the images.



- However, we perform slightly more operations (with a magnitude change of $\sim 10^4$ to $\sim 10^6$). Yet, our algorithm remains resilient to this change in magnitude.



Part 2: On Noisy Data

Tasks 4-7: Noisy Images



- **Noise:** A simple comparison of each image to the representative images would no longer work.
- **Larger Datasets:** The number of combinations of the orientations can get drastically higher (as high as $10^{60,000}$).
- **Signal-to-Noise Ratios:** The cause of the difference between the two images is no longer obvious (i.e., noise or orientation). There is also no way to visually confirm the orientations.



Task 4 (Introduction of Noise)

- The dataset for Task 4 is similar to the dataset for Task 3, with a total of $A = 1,000$ images and $B = 50 \times 50 = 2,500$ pixels. However, noise is introduced in the dataset, which makes hashing useless.



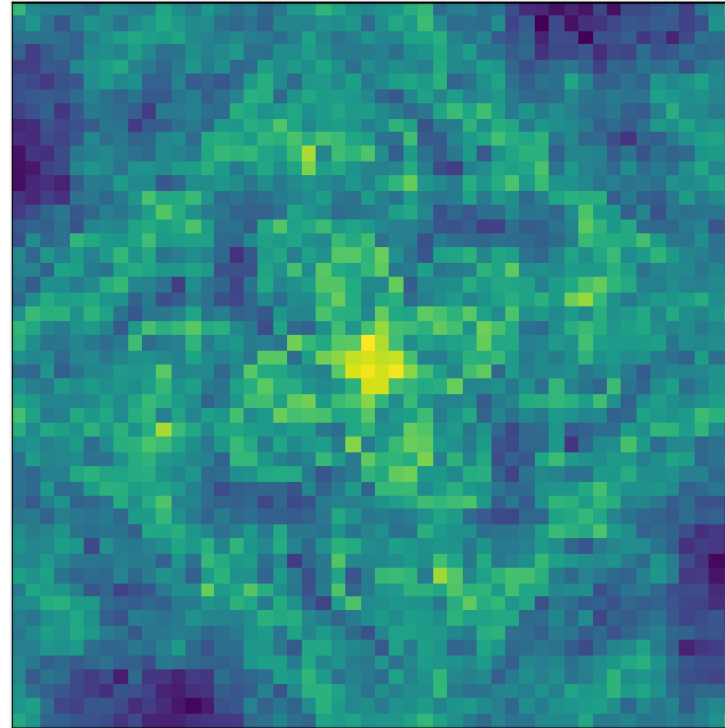
Task 4(a)

- Using native **numpy** implementations, we take the sum of all the values in the $B = 50 \times 50$ pattern (sum of the values in each row of the design matrix), and take its average over $A = 1,000$ patterns. This average is equal to 1251.047.

Task 4(b)



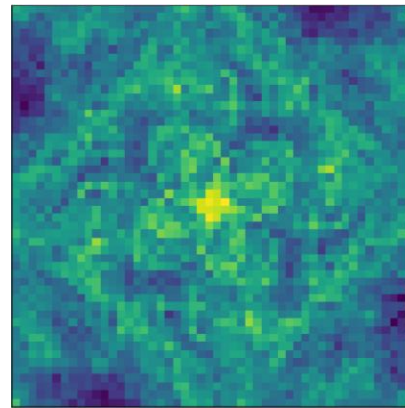
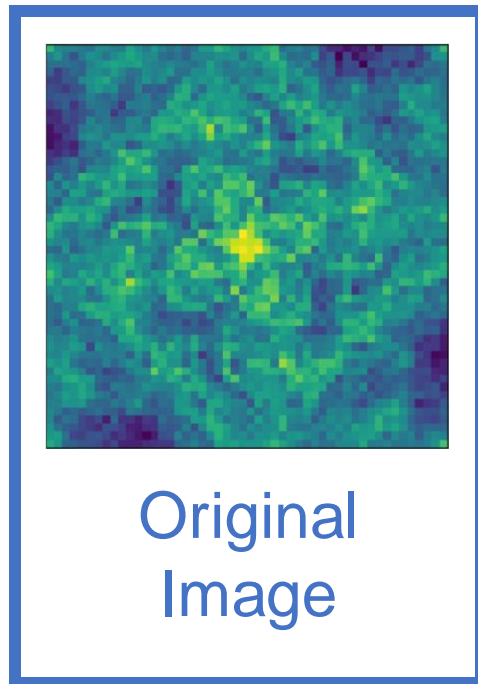
- Rendering the average value of each dataset, we arrive at this figure (the coloring scheme does not matter much):



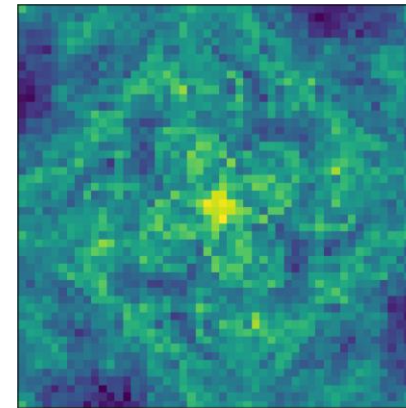
Task 4(b)



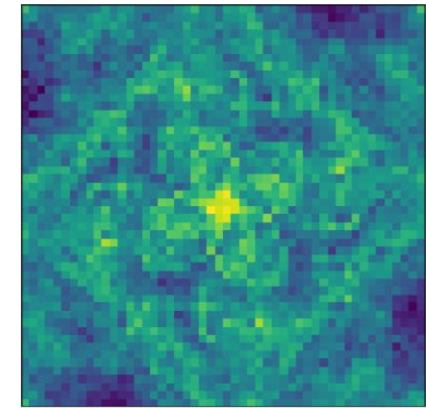
- This figure has an approximate 4-fold symmetry, which motivates us to use $K = 4$ means for our clustering algorithm:



90°



180°

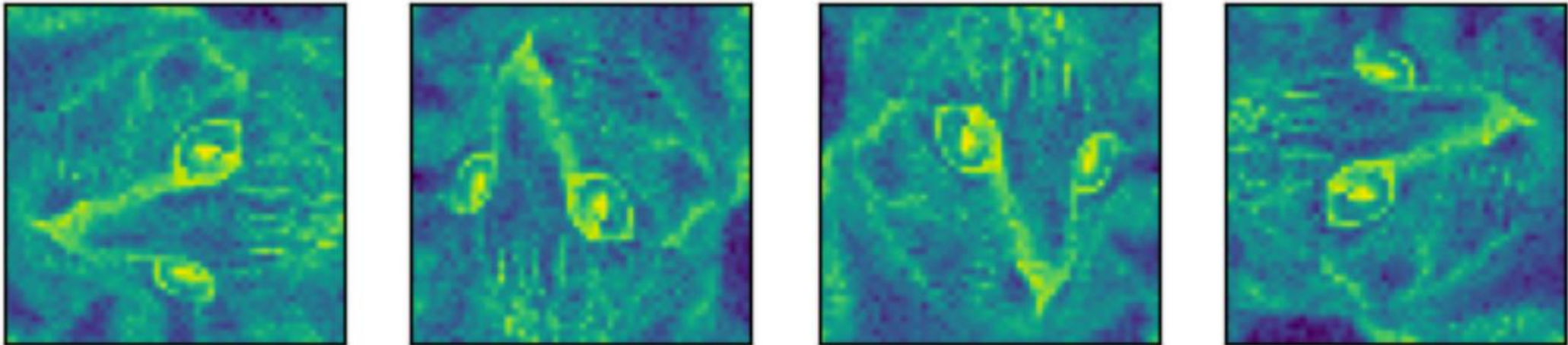


270°



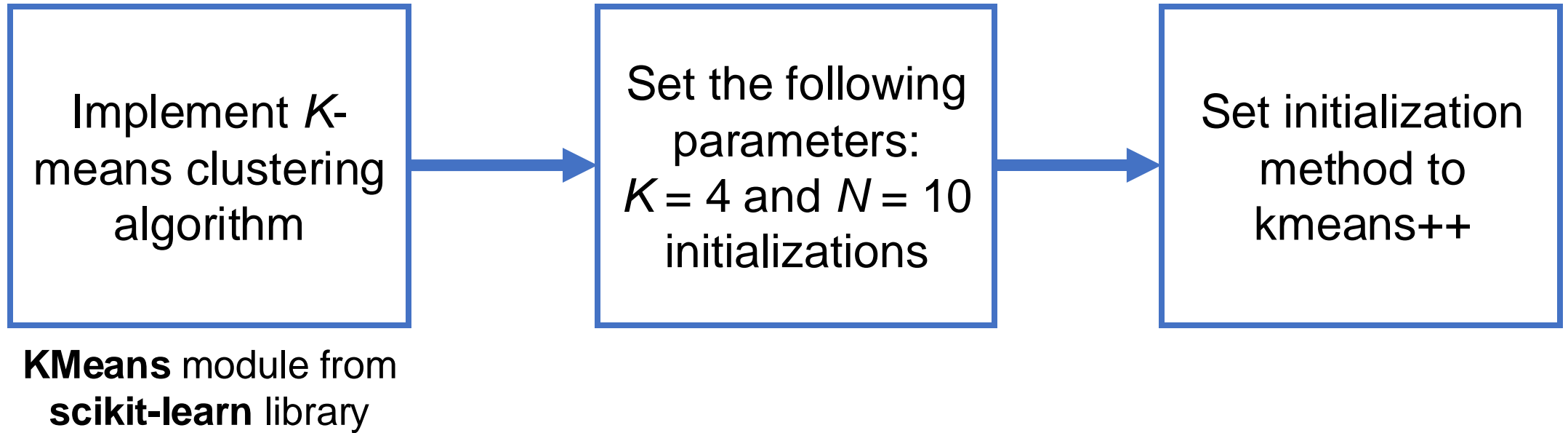
Task 4(c)

- After implementing the K -means clustering algorithm ($K = 4$), we arrive at the following images separated by orientation:



- This looks like a cat. Quite cute, actually.

Task 4(d)





Task 4(d)

- Here are the time complexities for the two tasks:

Algorithm	Time Complexity
<i>K</i> -means clustering	$O(NKI \times AB)$
Hashing algorithm	$O(AB)$

A = number of images
B = number of pixels per image
N = number of initializations
K = number of clusters
I = number of iterations

- The time is **linear with the size of the dataset**.
- Keeping the **hyperparameters *N*, *K*, and *I* constant**, the time complexity of *K*-means is **asymptotically optimal**, which performs about the same as hashing.



Part 4:

Likelihood Models



Task 5(a) (Success with Noise Distributions)

- We number the pixels from left to right and top to bottom:

μ	$\beta\lambda$	λ	$\beta\lambda$	$\beta\lambda$
K	1	0	0	0

$$\begin{aligned}\mathcal{L}(r = 90^\circ | K_{(4)}, \mu_{(4)}) &= \mathbf{Pr}(k_1 = 1 | \beta\lambda) \cdot \mathbf{Pr}(k_2 = 0 | \lambda) \cdot \mathbf{Pr}(k_3 = 0 | \beta\lambda) \cdot \mathbf{Pr}(k_4 = 0 | \beta\lambda) \\ &= \boxed{\beta\lambda(1 - \lambda)(1 - \beta\lambda)^2}\end{aligned}$$



Task 5(b)

- We use the expression from Task 5(a). Substituting the aligned likelihood from the Problem Statement and the misalignment likelihood from Task 5(a), the likelihood ratio is:

$$\frac{\mathcal{L}(r = 0^\circ | K_{(4)}, \mu_{(4)})}{\mathcal{L}(r = 90^\circ | K_{(4)}, \mu_{(4)})} = \frac{\lambda(1 - \beta\lambda)^3}{\beta\lambda(1 - \lambda)(1 - \beta\lambda)^2} = \boxed{\frac{1 - \beta\lambda}{\beta(1 - \lambda)}}$$



Task 5(c)

- We use the likelihood ratio from Task 5(b):

$$\frac{1 - \beta\lambda}{\beta(1 - \lambda)} = 1$$

$$1 - \beta\lambda = \beta(1 - \lambda)$$

$$\boxed{\beta = 1}$$

- When $\beta = 1$, all pixels have the same value.

Task 5(d)



aligned λ	λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$
measured K	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0

$$\begin{aligned}
 \frac{\mathcal{L}(r = 0^\circ | K_{(16)}, \mu_{(16)})}{\mathcal{L}(r = 90^\circ | K_{(16)}, \mu_{(16)})} &= \frac{\mathbf{Pr}(k = 1 | \lambda) \cdot \mathbf{Pr}(k = 0 | \beta\lambda)^{15}}{\mathbf{Pr}(k = 1 | \beta\lambda) \cdot \mathbf{Pr}(k = 0 | \lambda) \cdot \mathbf{Pr}(k = 0 | \beta\lambda)^{14}} \\
 &= \frac{\lambda(1 - \beta\lambda)^{15}}{\beta\lambda(1 - \lambda)(1 - \beta\lambda)^{14}} = \boxed{\frac{1 - \beta\lambda}{\beta(1 - \lambda)}}
 \end{aligned}$$

Task 5(d)



misaligned λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$
measured K	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0

$$\begin{aligned}
 \frac{\mathcal{L}(r = 0^\circ | K_{(16)}, \mu_{(16)})}{\mathcal{L}(r = 90^\circ | K_{(16)}, \mu_{(16)})} &= \frac{\mathbf{Pr}(k = 1 | \lambda) \cdot \mathbf{Pr}(k = 0 | \beta\lambda)^{15}}{\mathbf{Pr}(k = 1 | \beta\lambda) \cdot \mathbf{Pr}(k = 0 | \lambda) \cdot \mathbf{Pr}(k = 0 | \beta\lambda)^{14}} \\
 &= \frac{\lambda(1 - \beta\lambda)^{15}}{\beta\lambda(1 - \lambda)(1 - \beta\lambda)^{14}} = \frac{1 - \beta\lambda}{\beta(1 - \lambda)}
 \end{aligned}$$

Task 5(d)



aligned λ	λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$
misaligned λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$
measured K	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0

$$\begin{aligned}
 \frac{\mathcal{L}(r = 0^\circ | K_{(16)}, \mu_{(16)})}{\mathcal{L}(r = 90^\circ | K_{(16)}, \mu_{(16)})} &= \frac{\mathbf{Pr}(k = 1 | \lambda) \cdot \mathbf{Pr}(k = 0 | \beta\lambda)^{15}}{\mathbf{Pr}(k = 1 | \beta\lambda) \cdot \mathbf{Pr}(k = 0 | \lambda) \cdot \mathbf{Pr}(k = 0 | \beta\lambda)^{14}} \\
 &= \frac{\lambda(1 - \beta\lambda)^{15}}{\beta\lambda(1 - \lambda)(1 - \beta\lambda)^{14}} = \boxed{\frac{1 - \beta\lambda}{\beta(1 - \lambda)}}
 \end{aligned}$$



Task 5(e)

- The alignment table is:

master	1	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0° (aligned)	λ	$\beta\lambda$	λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$
90° (misaligned)	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	λ	$\beta\lambda$	λ	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	$\beta\lambda$	λ	$\beta\lambda$	$\beta\lambda$

- The likelihood ratio is:

$$\begin{aligned}
 \frac{\mathcal{L}(\text{aligned})}{\mathcal{L}(\text{misaligned})} &= \frac{\mathbf{Pr}(k = 1|\lambda)^3 \cdot \mathbf{Pr}(k = 0|\beta\lambda)^{13}}{\mathbf{Pr}(k = 0|\lambda)^3 \cdot \mathbf{Pr}(k = 1|\beta\lambda)^3 \cdot \mathbf{Pr}(k = 0|\beta\lambda)^{10}} \\
 &= \frac{\lambda^3(1 - \beta\lambda)^{13}}{(1 - \lambda)^3(\beta\lambda)^3(1 - \beta\lambda)^{10}} = \boxed{\frac{(1 - \beta\lambda)^3}{\beta^3(1 - \lambda)^3}} \quad (\text{Eq. 2.4})
 \end{aligned}$$



Task 5(f)

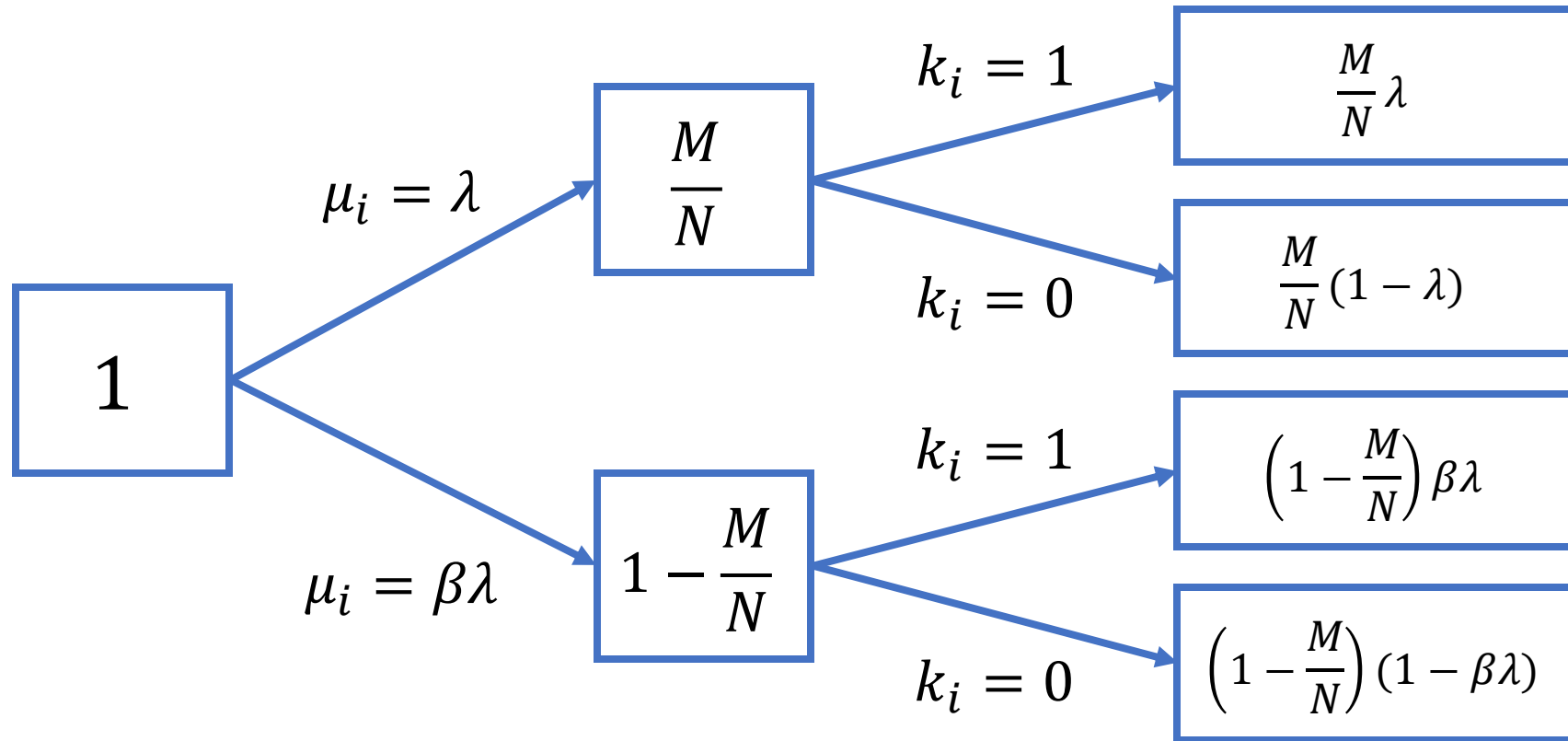
- We define a function $f(\mu_i, k_i)$ as in the problem statement:

$$f(\mu_i, k_i) = k_i \ln \mu_i + (1 - k_i) \ln(1 - \mu_i)$$

- Here are the pertinent values of $f(\mu_i, k_i)$:

μ_i	k_i	$f(\mu_i, k_i)$
λ	1	$\ln \lambda$
λ	0	$\ln(1 - \lambda)$
$\beta\lambda$	1	$\ln(\beta\lambda)$
$\beta\lambda$	0	$\ln(1 - \beta\lambda)$

Task 5(f)





Task 5(f)

- The expected value of the log-likelihood is:

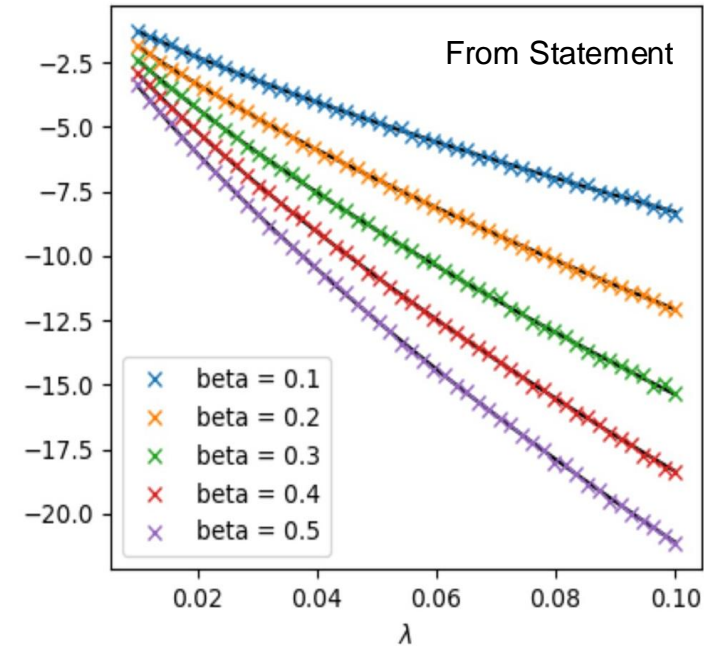
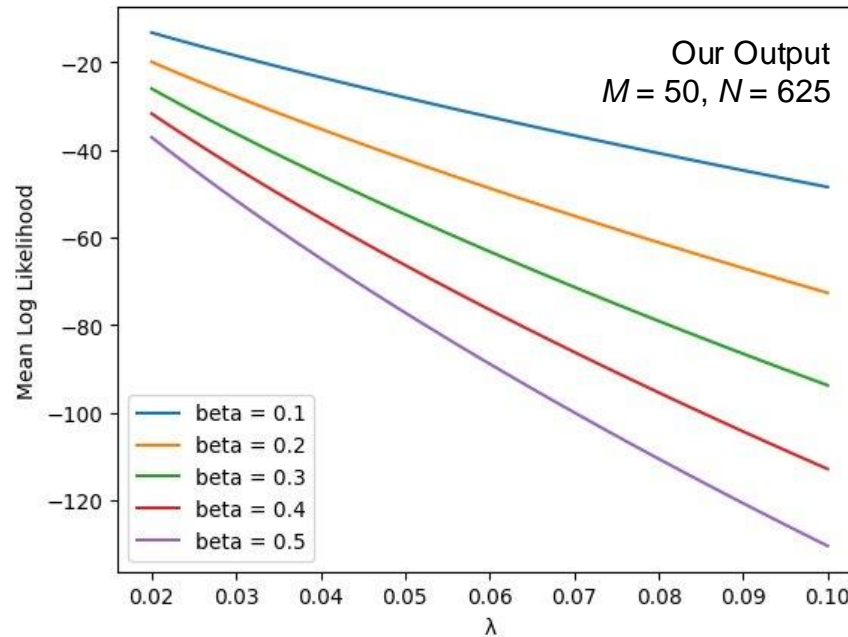
$$\begin{aligned}\mathbf{E}(\text{likelihood}) &= \mathbf{E}\left(\sum f(\mu_i, k_i)\right) = N \cdot \mathbf{E}(f(\mu_i, k_i)) \\ &= N \left[\frac{M}{N} \lambda \cdot \ln \lambda + \frac{M}{N} (1 - \lambda) \cdot \ln(1 - \lambda) + \left(1 - \frac{M}{N}\right) \beta \lambda \cdot \ln(\beta \lambda) + \left(1 - \frac{M}{N}\right) (1 - \beta \lambda) \cdot \ln(1 - \beta \lambda) \right] \\ &= \boxed{M(\lambda \ln \lambda + (1 - \lambda) \ln(1 - \lambda)) + (N - M)(\beta \lambda \ln(\beta \lambda) + (1 - \beta \lambda) \ln(1 - \beta \lambda))}\end{aligned}$$

- This looks similar to the **cross-entropy of a system**.

Task 5(f)



$$\begin{aligned}\mathbf{E}(\text{likelihood}) &= \mathbf{E}\left(\sum f(\mu_i, k_i)\right) = N \cdot \mathbf{E}(f(\mu_i, k_i)) \\ &= N \left[\frac{M}{N} \lambda \cdot \ln \lambda + \frac{M}{N} (1 - \lambda) \cdot \ln(1 - \lambda) + \left(1 - \frac{M}{N}\right) \beta \lambda \cdot \ln(\beta \lambda) + \left(1 - \frac{M}{N}\right) (1 - \beta \lambda) \cdot \ln(1 - \beta \lambda) \right] \\ &= \boxed{M(\lambda \ln \lambda + (1 - \lambda) \ln(1 - \lambda)) + (N - M)(\beta \lambda \ln(\beta \lambda) + (1 - \beta \lambda) \ln(1 - \beta \lambda))}\end{aligned}$$



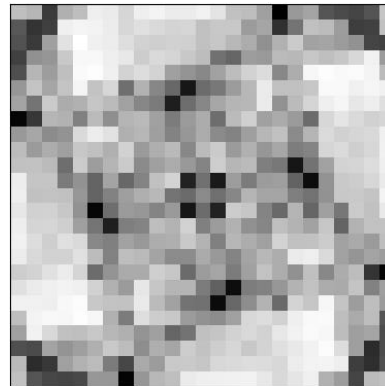
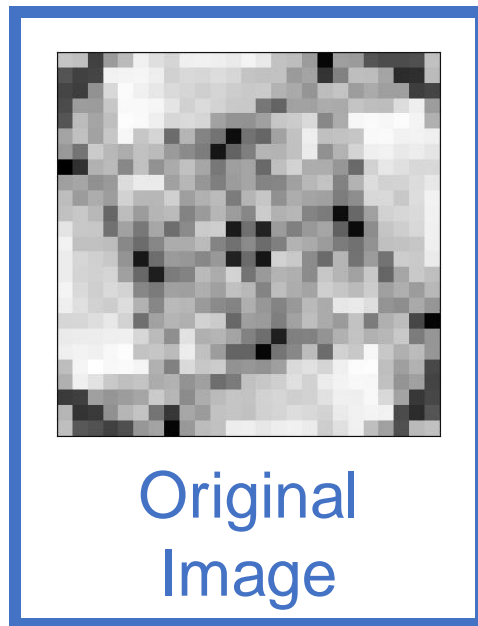


Part 5: Noisy Sparse Data

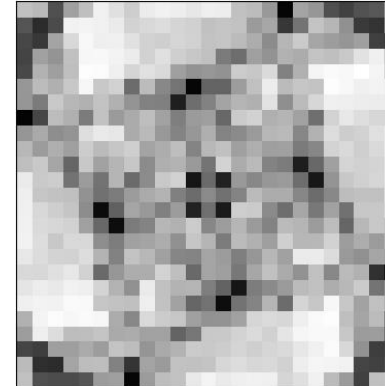


Task 6 (Initial Observations)

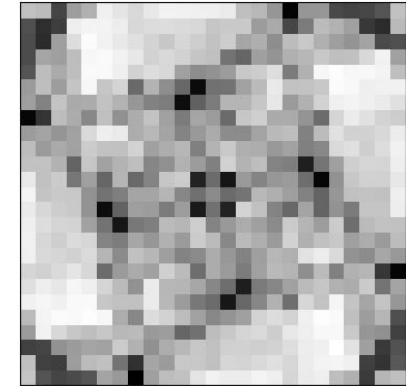
- The mean image for Task 6 has four-fold symmetry:



90°



180°



270°

Task 6 (Problems with Dense Representation)



- For Task 6, there are $A = 65,535$ images with each image having a size $B = 25 \times 25 = 625$ pixels.
- **Quick Computation:** How much memory would it take to store all images using 64-bit floating point numbers?

$$65,535 \times 625 \times 64 \text{ bits} \approx \mathbf{312.5 \text{ Mb}}$$

- This uses up a lot of memory. Also, K -means runs multiple iterations of cluster and mean assignments. Naïve K -means implementations will take too long to run on the dataset.



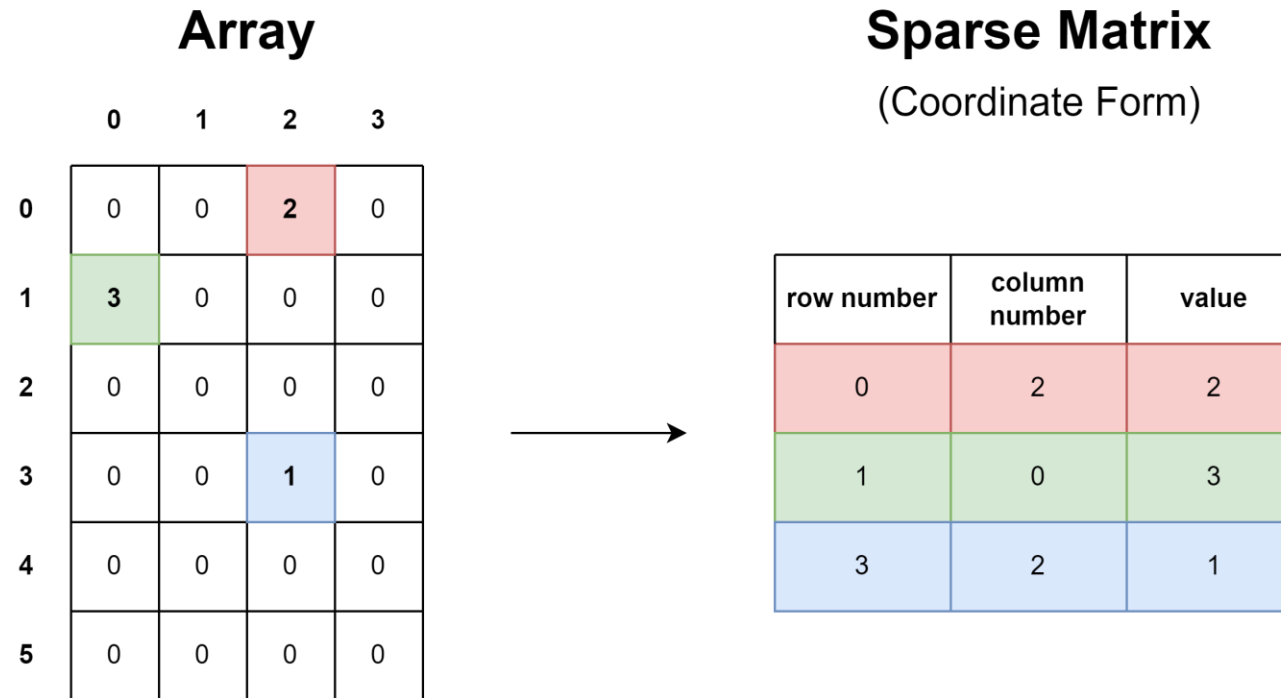
Task 6 (Observations about the Data)

- The average number of activated pixels per image is **23.745**, which is a **lot smaller** than the number of pixels per image (**625**).
- Majority of the pixels are set to a value of 0, so the activated pixels (i.e., pixels with a value of 1) are **sparsely distributed** within the image.



Task 6 (Sparse Representation)

- **Sparse matrices** work with sparse data (i.e., arrays with only a few nonzero values).





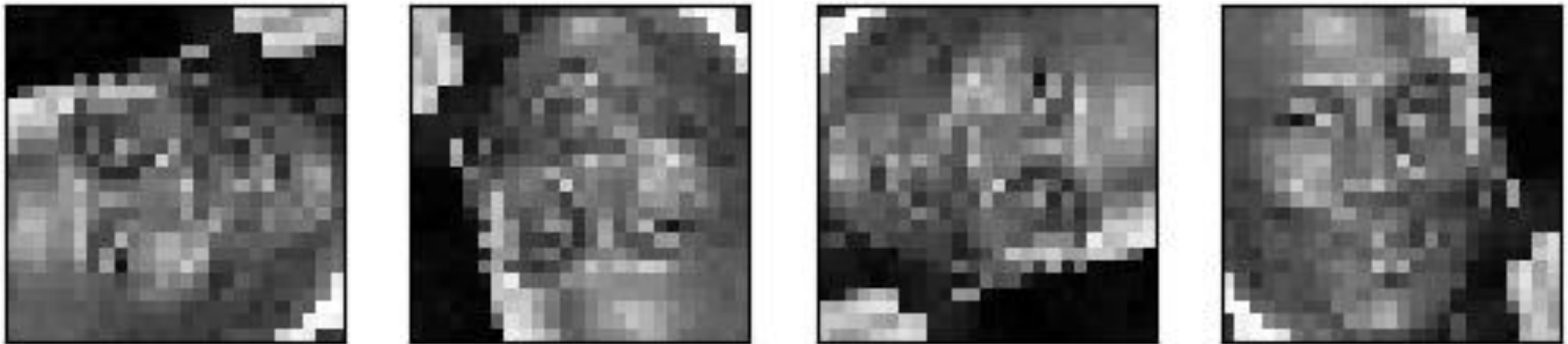
Task 6 (Sparse Representation)

- Sparse matrices have lower memory requirements:
 - Normal Array: $O(L)$, where L – elements in the array.
 - Sparse Matrix: $O(L')$, where L' – nonzero elements.
- If $L' \ll L$, sparse matrices use significantly less memory.
- For Task 6, $L = 40,959,375$, while $L' = 1,556,153$. Since $L' \ll L$, sparse matrices use significantly less memory for Task 6.
- We used K -means clustering with sparse matrices.



Task 6 (Results)

- After applying the K -means clustering algorithm on the Task 6 dataset, we obtain the following cluster means:



- This might be Michael Jordan? We are also not sure.



Part 6: The Master Image

Task 7 (Problems with Dense Representations^{2.0})

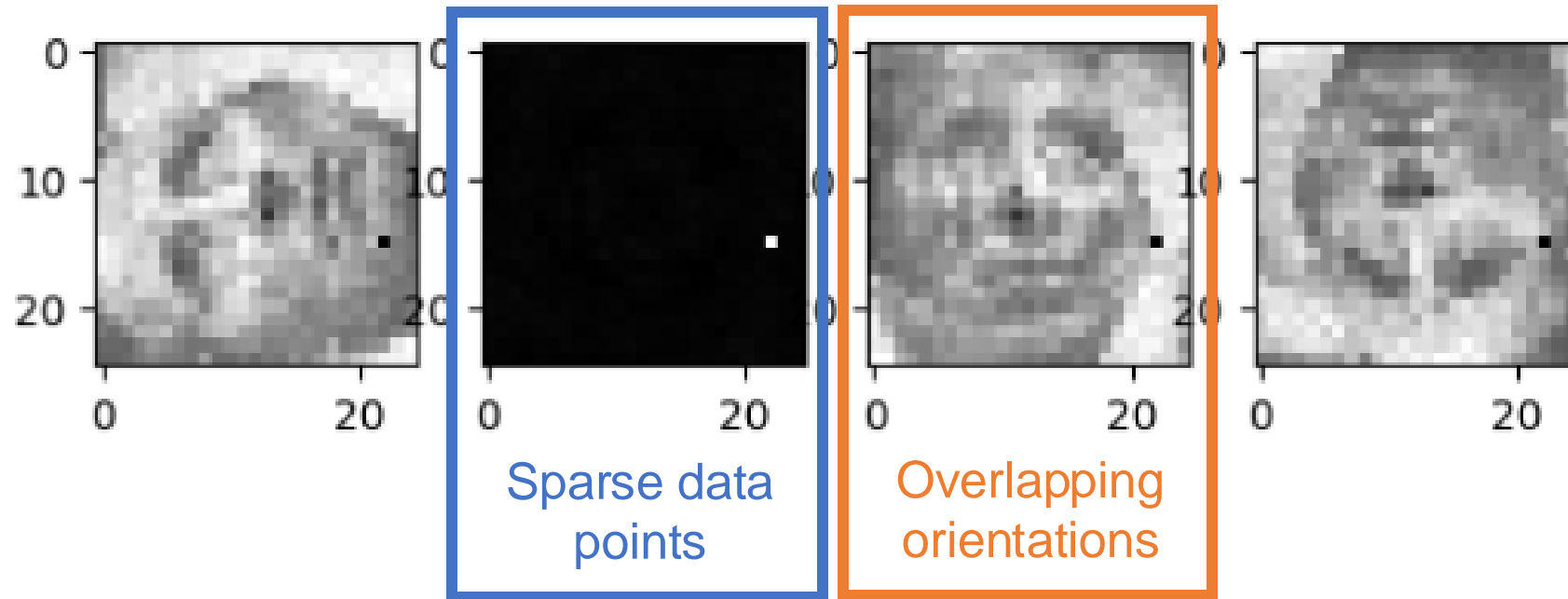


- In the dataset, there are a total of $A = 100,000$ images, each with a size $B = 25 \times 25 = 625$ pixels.
- The dataset is composed of **task7a** (with parameters x_i indicating the image number, $0 \leq x_i \leq A - 1$) and **task7b** (with parameters y_i indicating the pixel number in the design matrix, $0 \leq y_i \leq B - 1$).

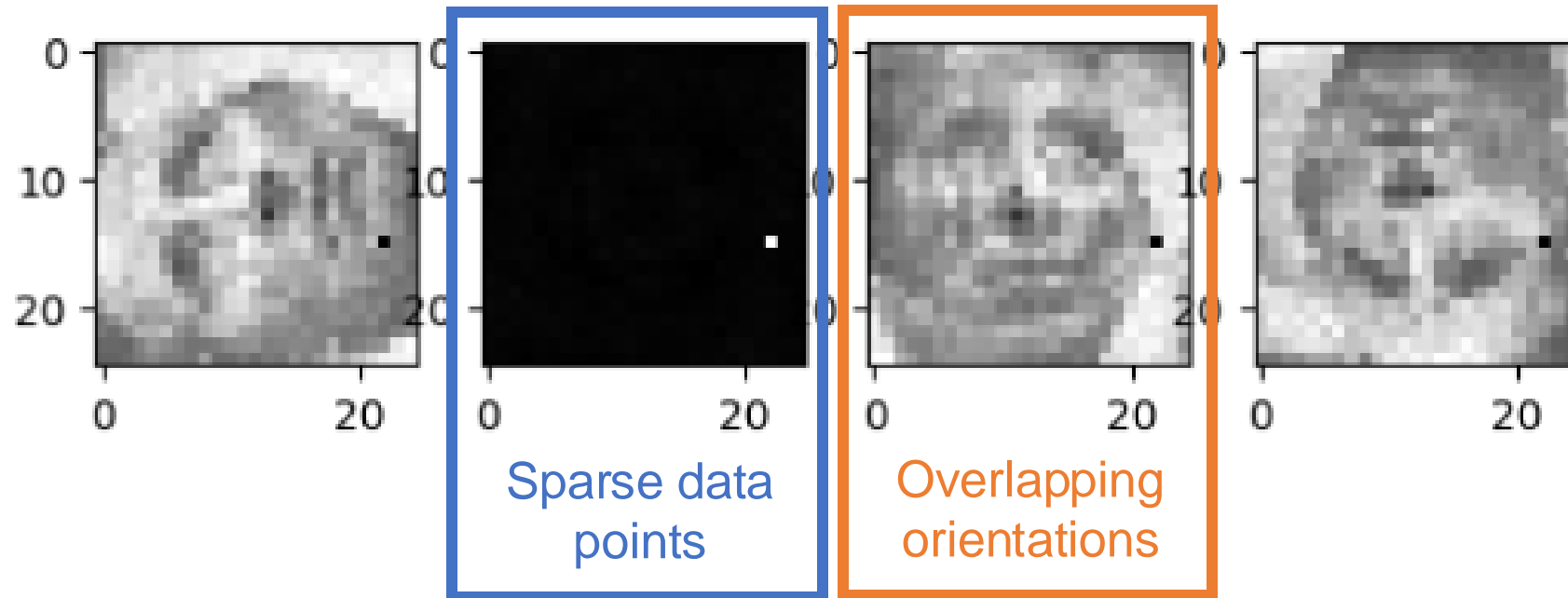
Task 7 (Problems with Dense Representations^{2.0})



- The implementation of *K*-means clustering algorithm in Task 6 came with a lot of failures:



Task 7 (Problems with Dense Representations^{2.0})



- These are both characterized by low entropy (same colors).
- This is a problem with **initial mean selection**.

Task 7 (Problems with Dense Representations^{2.0})



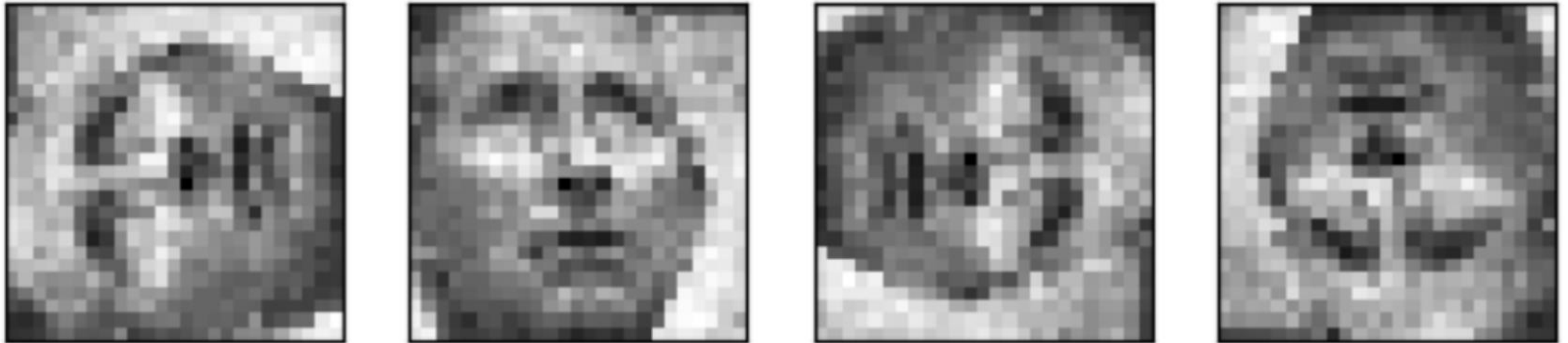
- We decided to characterize the “messiness” or the entropy of the function using a modified Shannon entropy:

$$S(\vec{p}) = - \sum [p_i \log_2 p_i + (1 - p_i) \log_2 p_i]$$

Task 7(a)



- The oriented images that result from a modified version of the K -means algorithm are as follows:

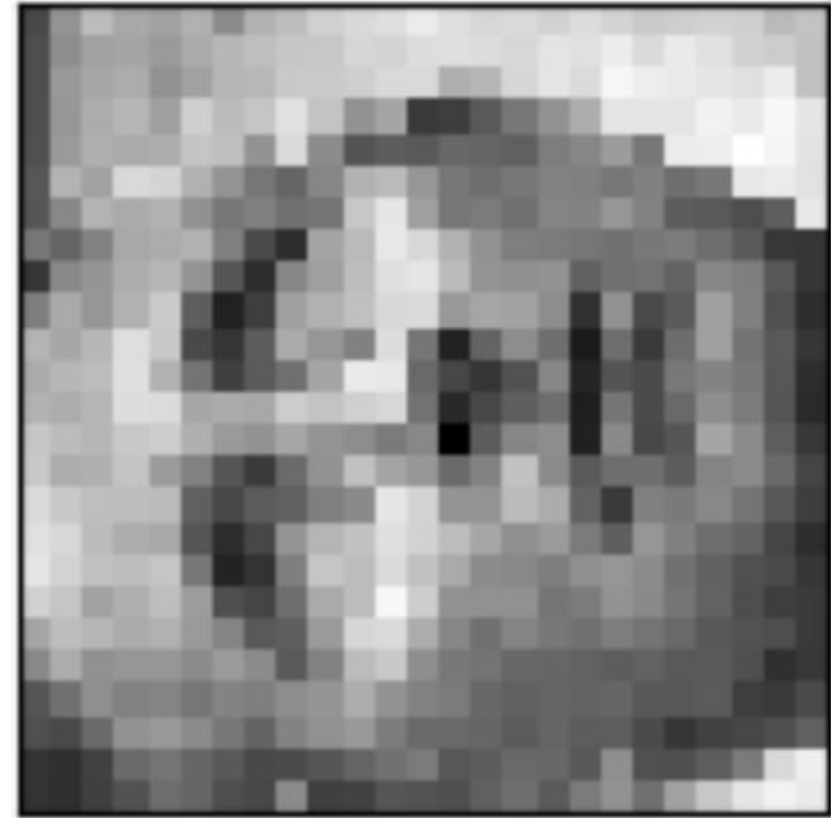


- Might be Vladimir Putin? Boris Johnson? King Charles? James Bond? We don't know, but it does look like a person.



Task 7(a)

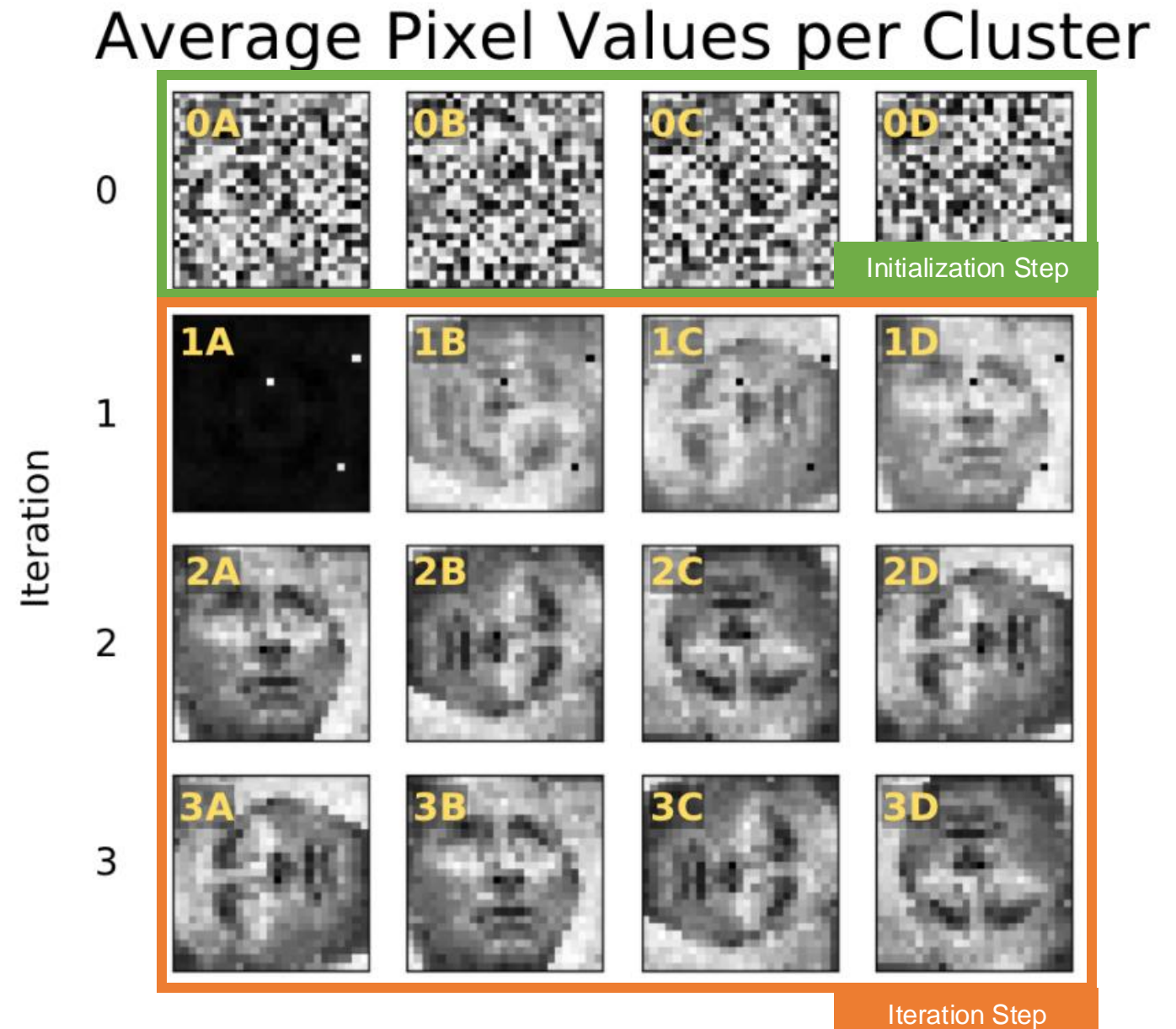
- We implemented a system that determines the orientation of each sample image, and takes the average of the aligned images to get a “correct” master image. (*Note: We assumed that the master image is orientation-agnostic.*)



“Correct” Master Image

Task 7(b)

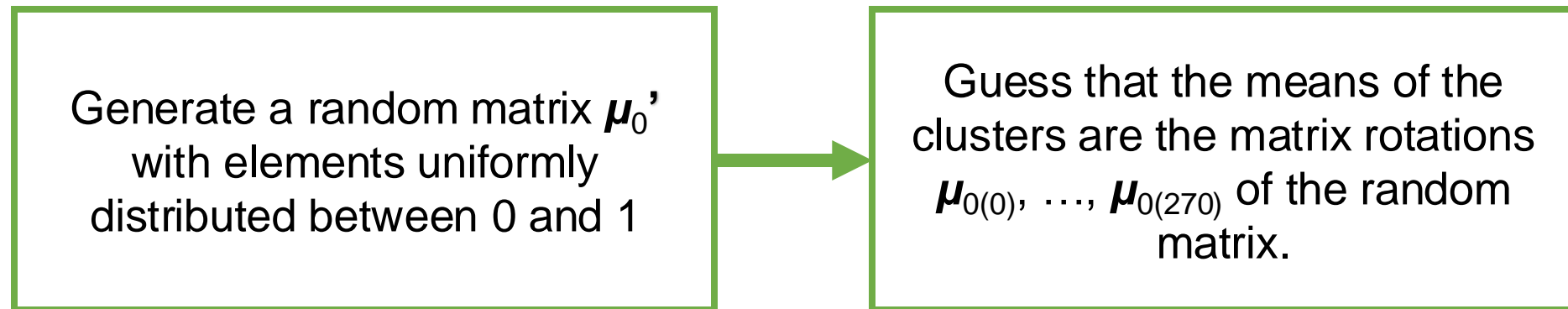
- There are two steps to the implementation of our modified K -means algorithm.



Task 7(b)



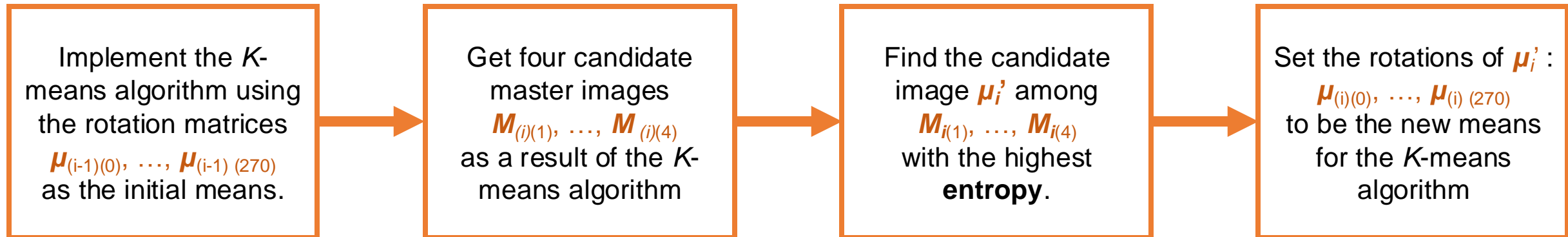
- There are two steps to our modified K -means algorithm. The first step is the mean initialization step:



Task 7(b)



- The second step is the mean iteration step. **For $i = 1, 2, \dots, T$, where T is the number of iterations steps, do the following:**

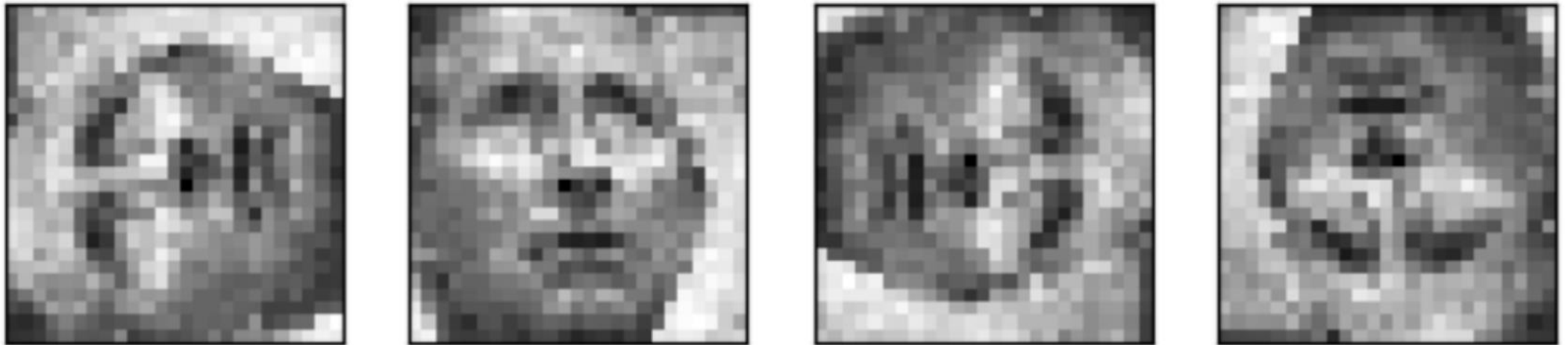


- After T iterations, the master images $M_{(T)(1)}, \dots, M_{(T)(4)}$ produce our candidate images.



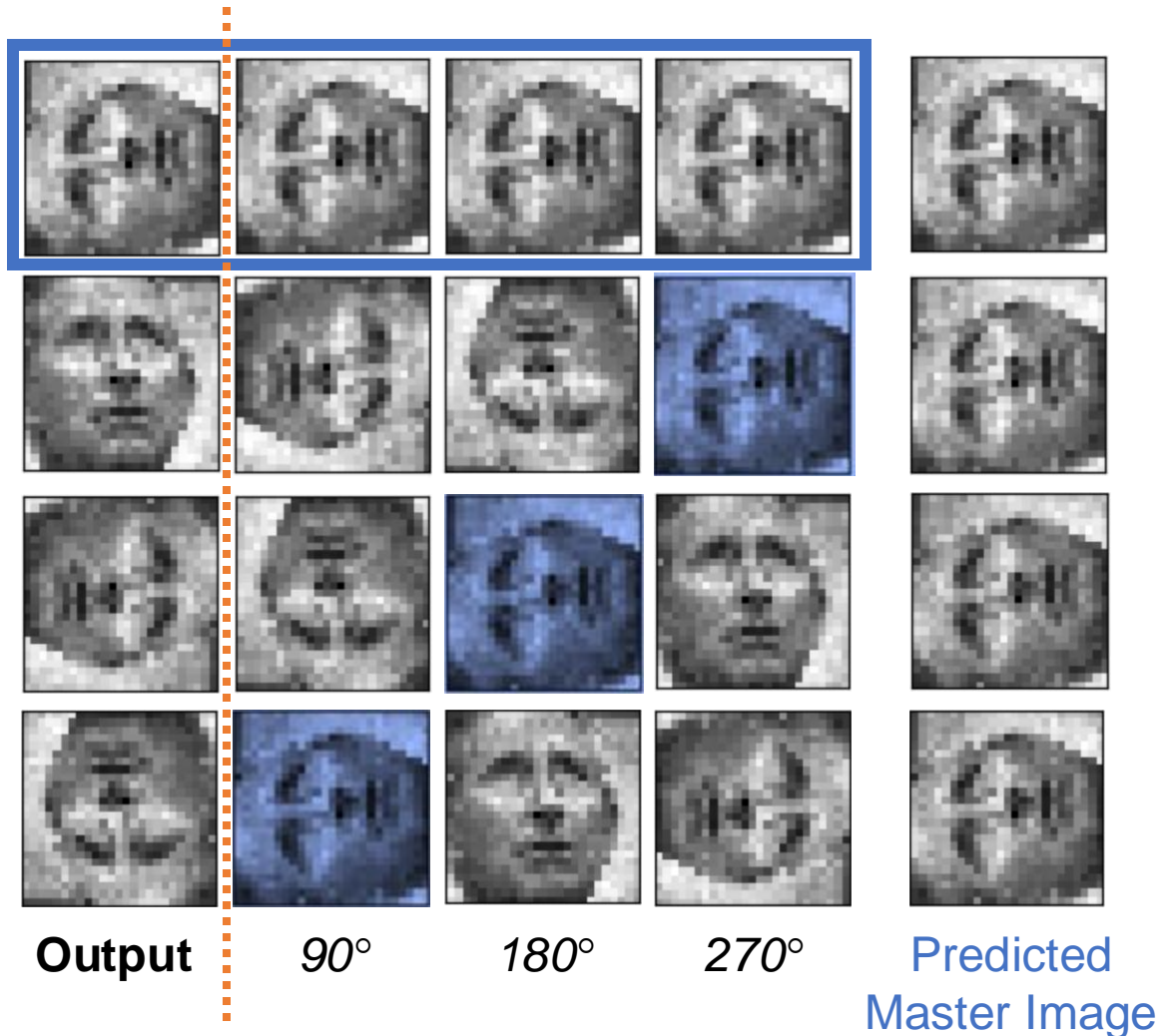
Task 7(b)

- We attempt to extract a master image from each of the orientations that was extracted after T iterations of our modified algorithm.



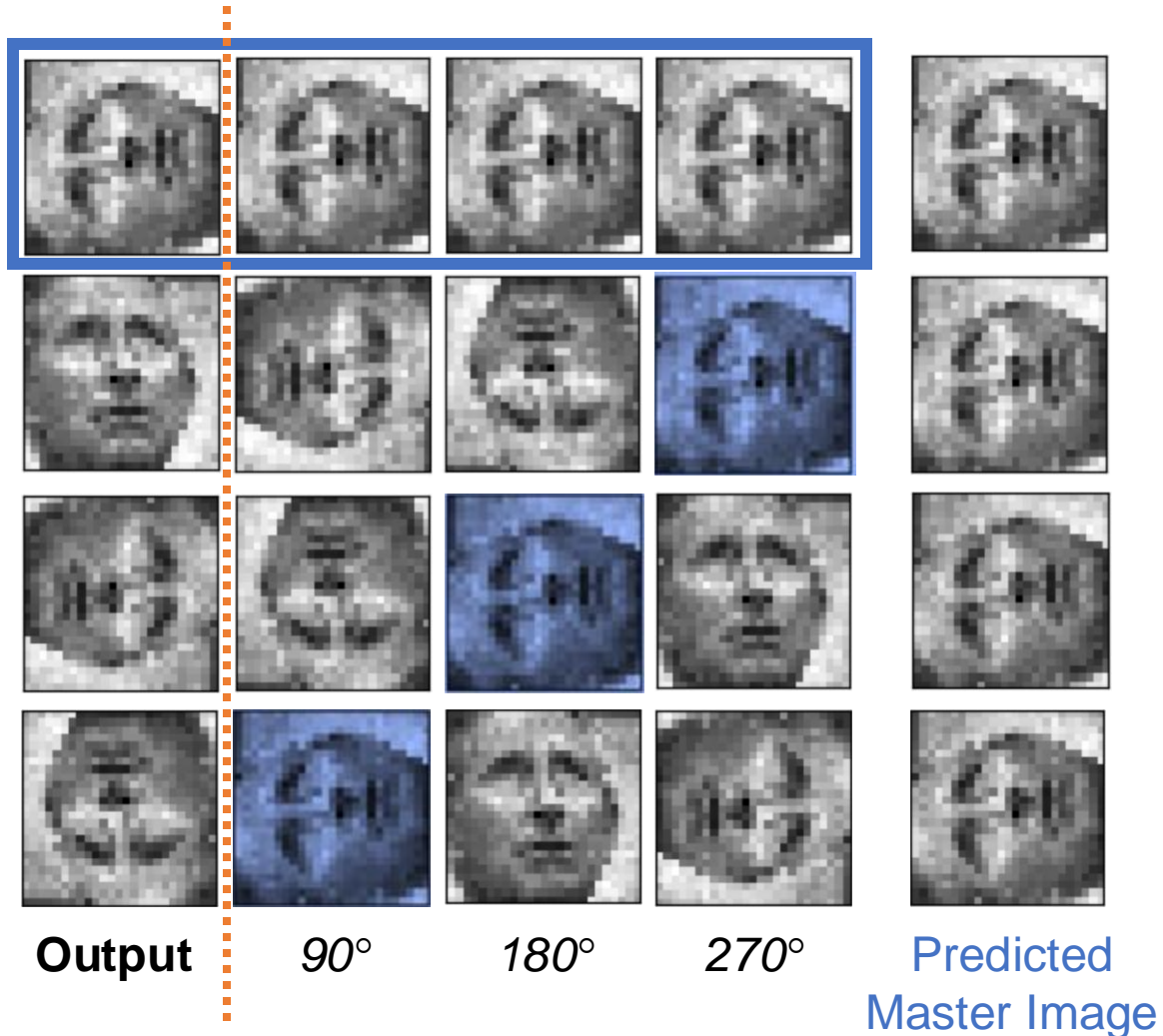


Task 7(b)



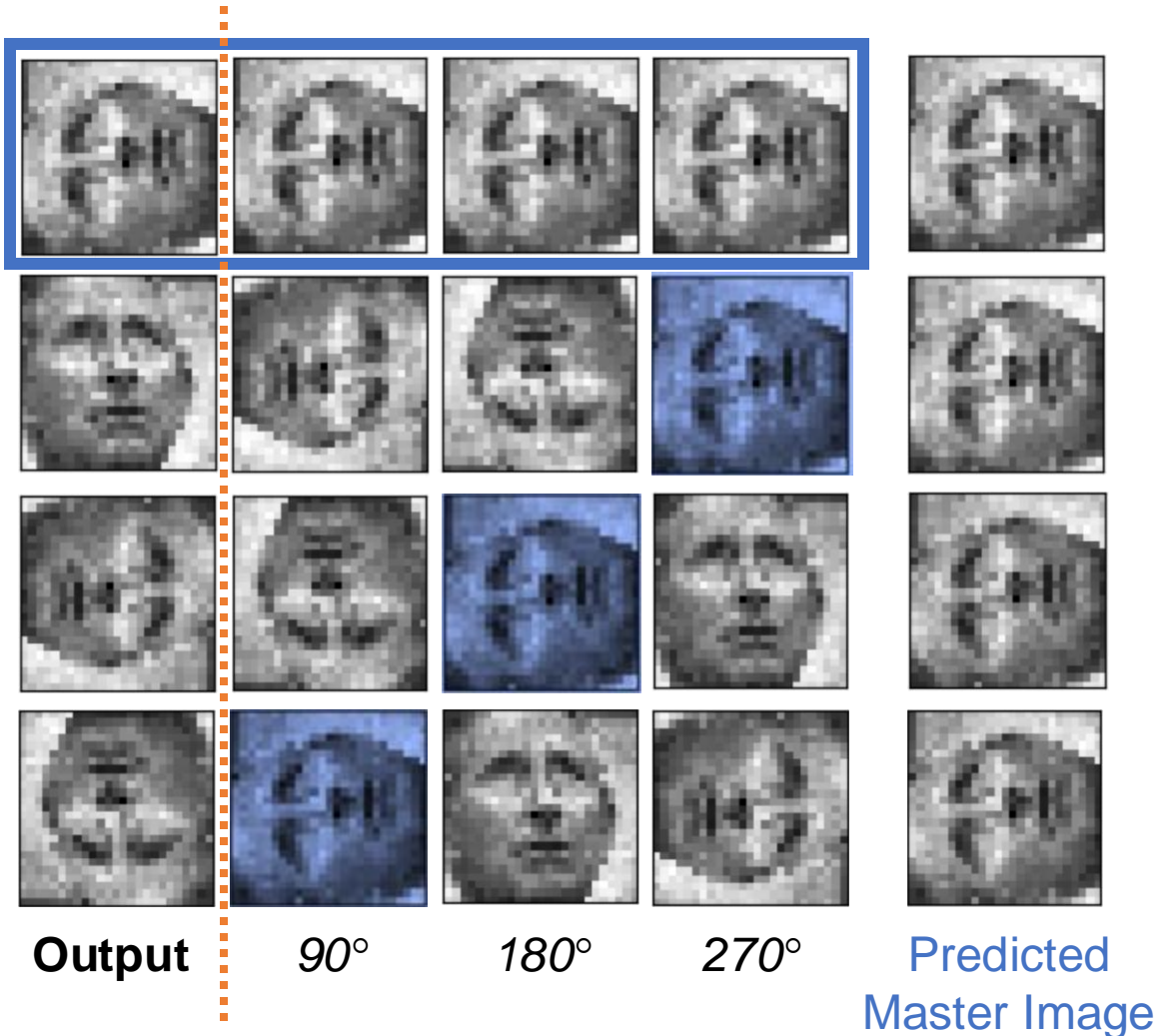
- First, we guess that the master image is in the orientation of the first master image $M_{(T)(1)}$ since K-means clustering cannot determine what an “upright” face looks like (i.e., master images are orientation-agnostic).

Task 7(b)



- Second, for each of the master images $M_{(T)(2)}, \dots, M_{(T)(4)}$, we determine the orientation with the closest similarity (cosine similarity) to master image $M_{(T)(1)}$. The closest image is highlighted in blue.

Task 7(b)



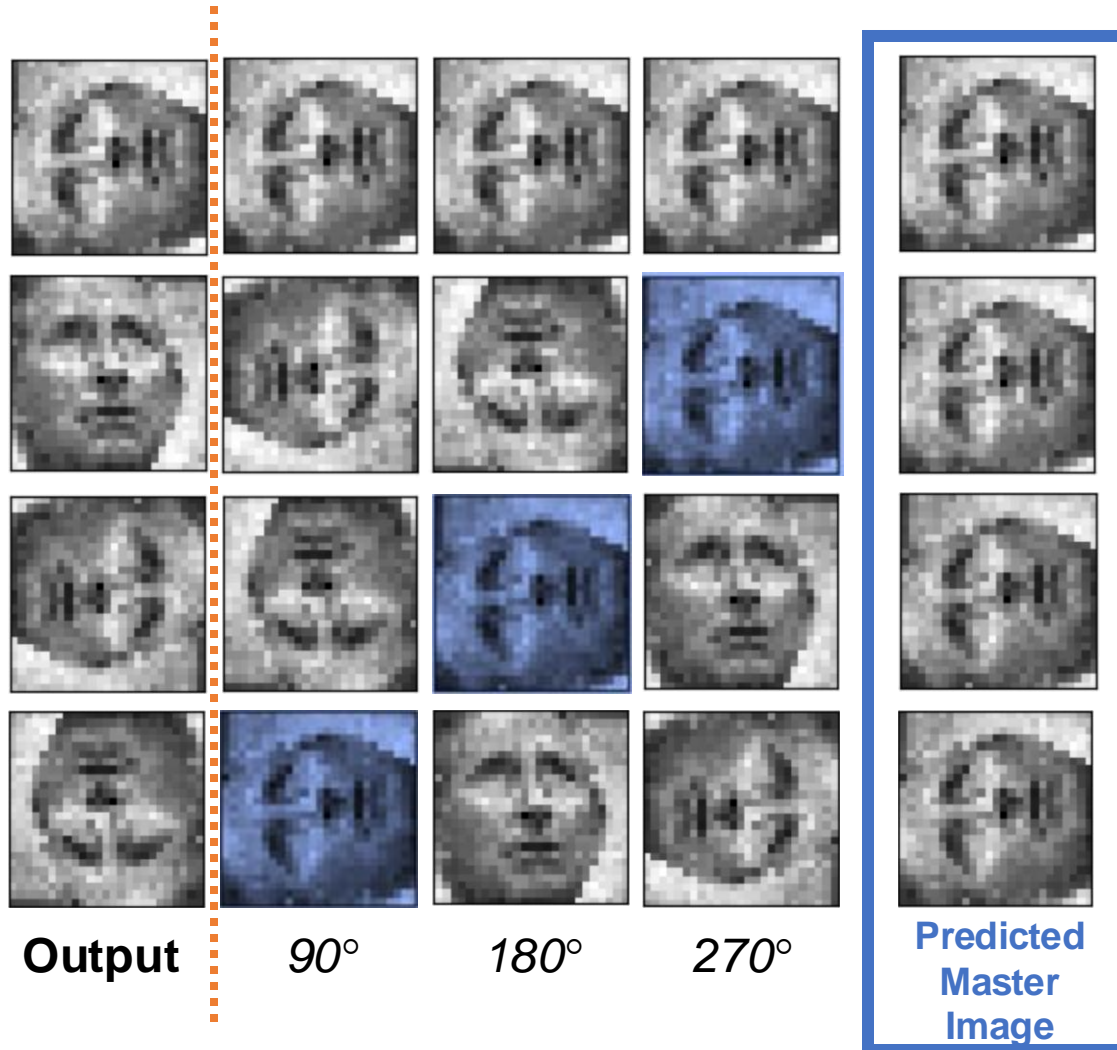
Cosine Similarity Formula

$$\cos \theta = \frac{\vec{\mu}_1 \cdot \vec{\mu}_2}{\|\vec{\mu}_1\| \|\vec{\mu}_2\|}$$

$\vec{\mu}$ = vector representation of an image

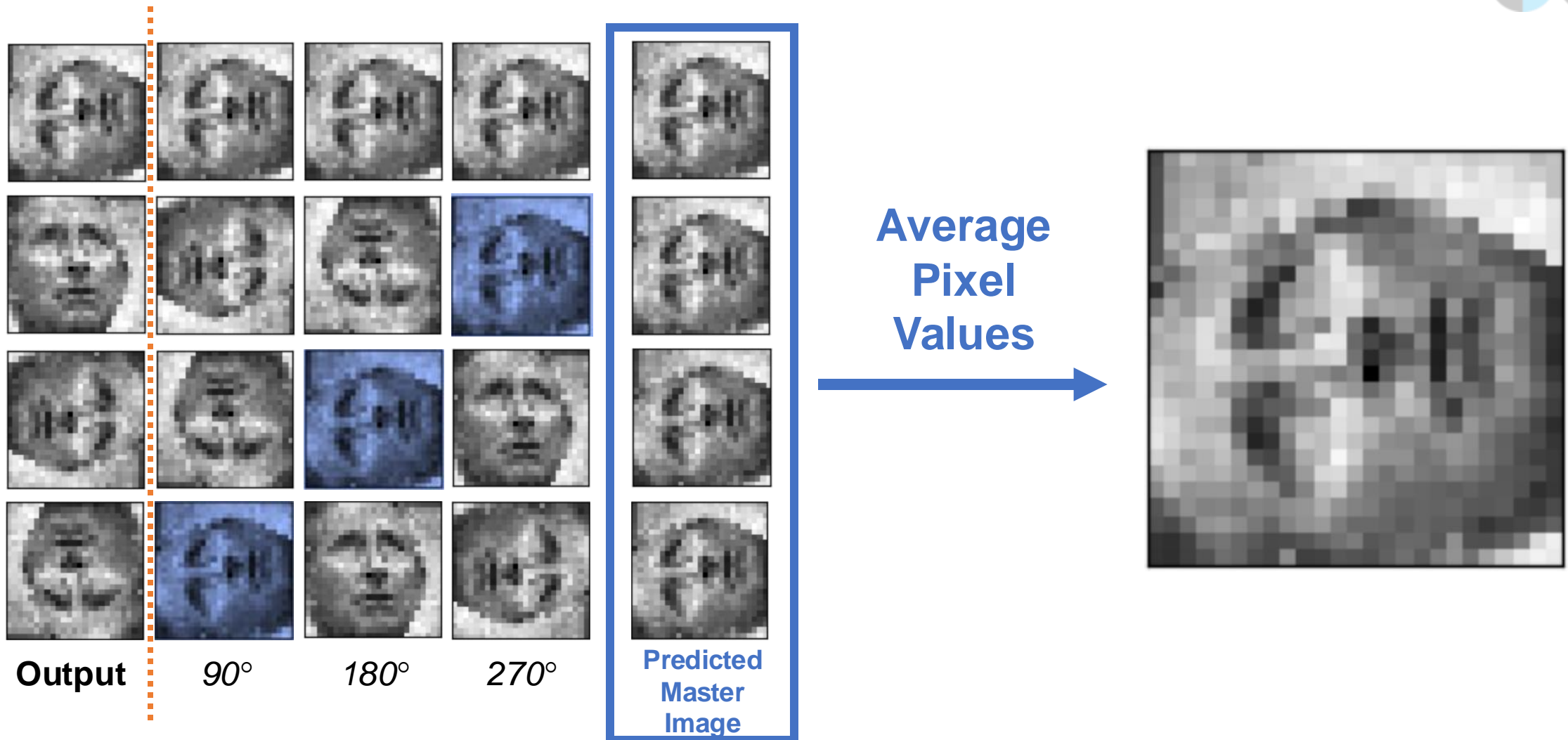


Task 7(b)



- Finally, we take the **average pixel values** of each the predicted master images for each orientation.

Task 7(b)





Part 7: Recommendations

Recommendations



- Implement K -means clustering with a **modification of the cluster-entropy** (since there is no way to change the distance function in **sklearn**, and cluster-entropy does not satisfy the conditions for a distance function).
- Implement a **measure of convergence** (similar to the Frobenius norm for K -means clustering) to determine how fast the means do not change (as seen in Task 7).

On Classification of Noiseless and Noisy Pattern Orientations

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Appendix

Modified K-means Algorithm



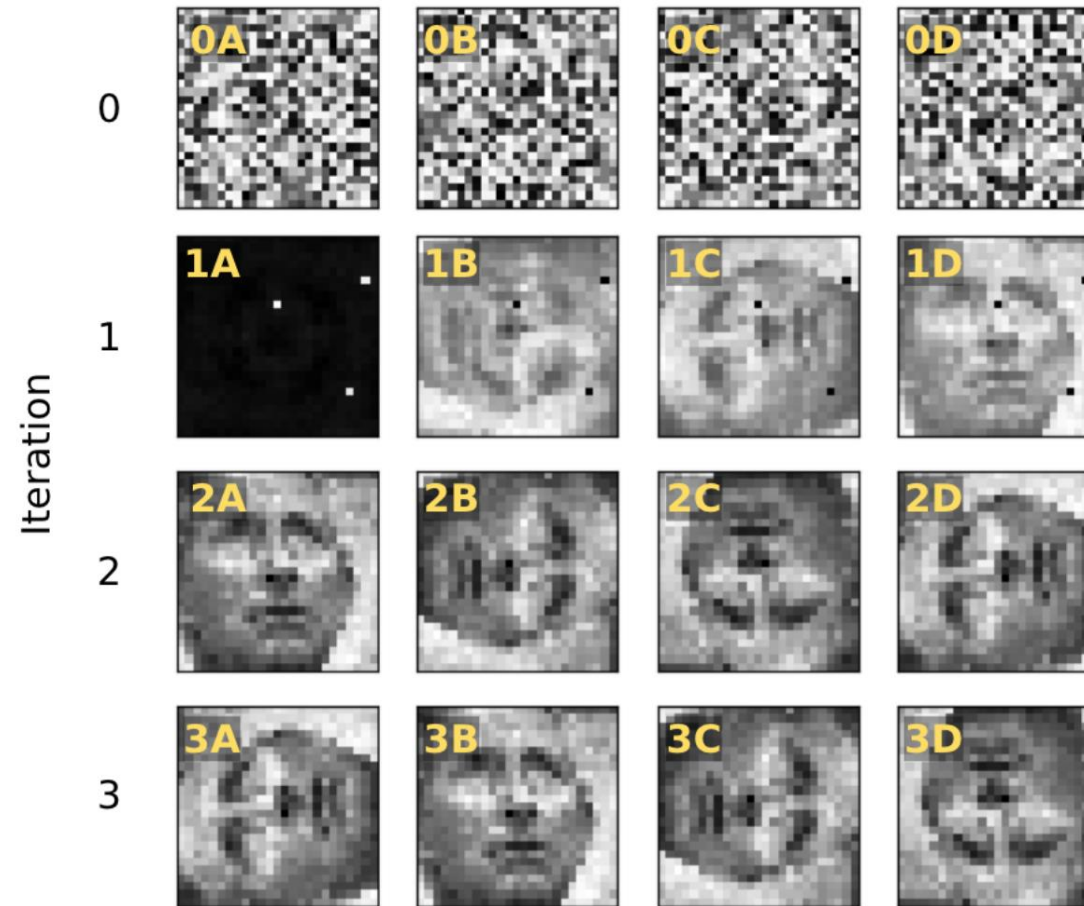
Algorithm 1 Modified K-means Algorithm for Task 7b. The number of iterations to run the algorithm for, T , is a hyperparameter.

```
1: procedure MODIFIEDKMEANS
2:   Initialize the master image  $\mu'_0$  with each entry uniformly sampled between 0 and 1.
3:   Predict the means of the cluster to be the four rotations  $\mu_{0(0^\circ)}, \dots, \mu_{0(270^\circ)}$  of  $\mu'_0$ .
4:   for iterations  $i = 1, 2, 3, \dots, T$ , do
5:     Implement the  $k$ -means algorithm using  $\mu_{(i-1)(0^\circ)}, \dots, \mu_{(i-1)(270^\circ)}$  as the initial means.
6:     Store the four master images  $\vec{M}_{i(1)}, \dots, \vec{M}_{i(4)}$  from the  $k$ -means algorithm.
7:     Select the cluster  $\mu'_i$  with the highest entropy  $S(\vec{\mu}')$  (Eq. 2.7) as the new master image.
8:     Set the new means  $\mu_i$  to be the  $90^\circ$  rotations of  $\mu'_i$ .
9:   end for
10:  for images  $j = 1, 2, 3, 4$  do
11:    Define  $\vec{A}_j$  to be a rotation of the vector  $\vec{M}_{T(j)}$  that maximizes the cosine similarity with  $\vec{M}_{T(1)}$ .
12:  end for
13:  Take the predicted master image to be  $\vec{M} = \frac{\vec{A}_1 + \vec{A}_2 + \vec{A}_3 + \vec{A}_4}{4}$ 
```



Visualizing the Clustering (Task 7)

Average Pixel Values per Cluster





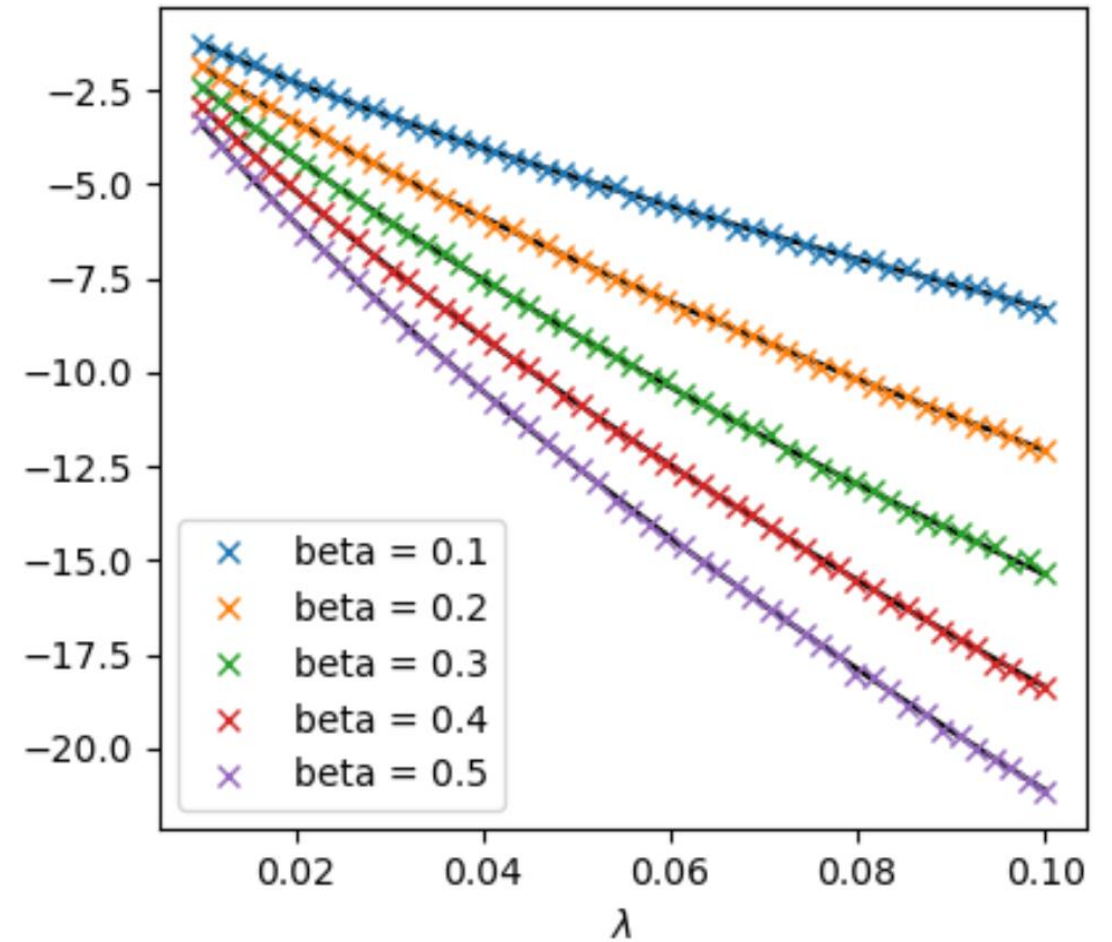
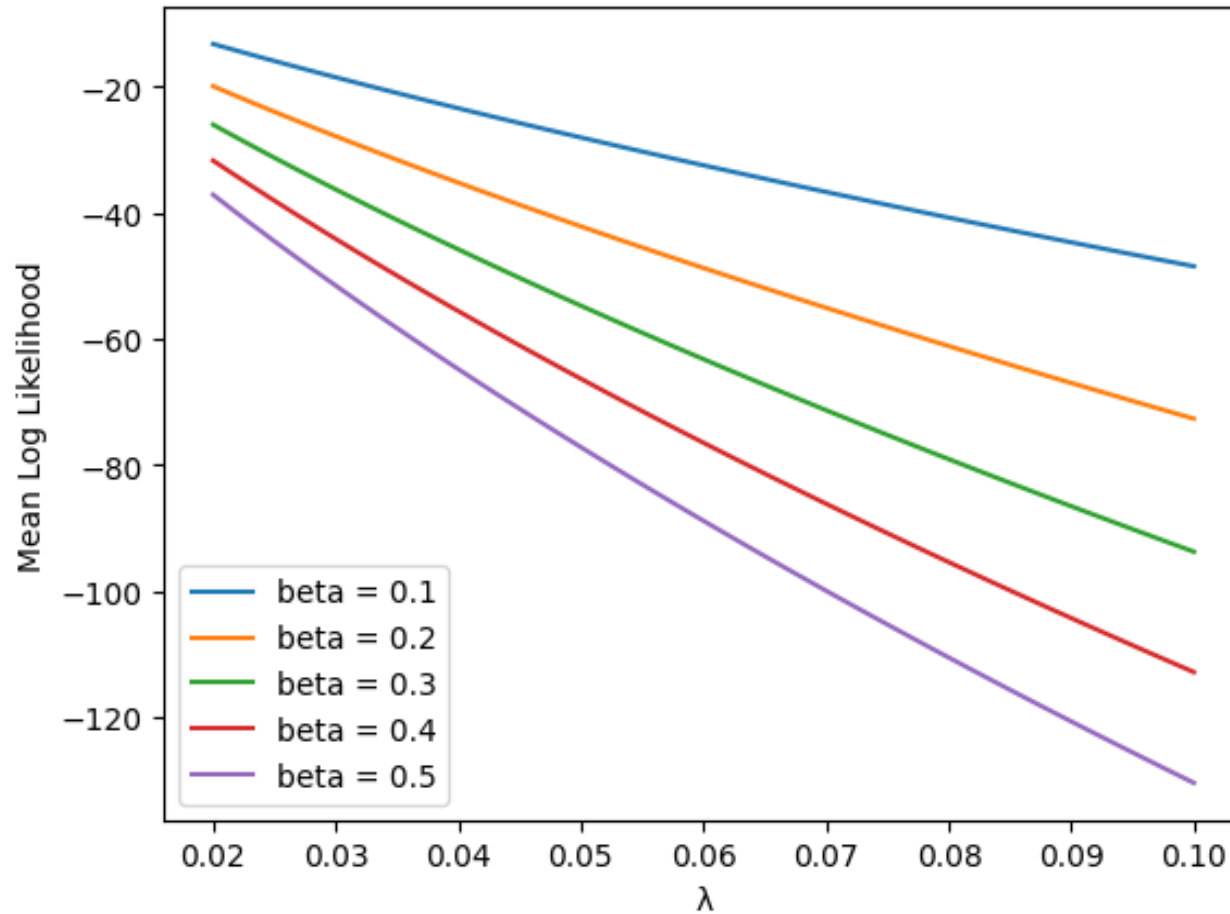
Hashing Function (Code)

```
### Precomputing powers of two for more efficient prime hashing
pow_2 = [1]
P_mod = (10 ** 9) + 7
for i in range(200000):
    pow_2.append((pow_2[-1] << 1) % P_mod)

### Hashing function for patterns ('img' is a multidimensional pattern,
### so passing the 2D representation or 1D flattened version would both work)
def hash_img(img):
    img_flattened = img.flatten()
    flat_len = img_flattened.shape[0]

    return np.dot(img_flattened, pow_2[:flat_len]) % P_mod
```

Task (5f) Trends



Task 2 Sorted Design Matrix

