Local Methods

CS771: Introduction to Machine Learning

Purushottam Kar

Announcements

Registered students would have received a Piazza invitation on their CC email IDs – please activate your account and join discussions

Please do not forget to form groups of 5 registered students – will be asked to submit group names next week itself

Code repository - https://tinyurl.com/ml19-20ac

Will contain lecture code as well as lecture notes

Tip: do not download individual file from repository – instead, do a git pull operation so that all updates (to old files as well) are received

Recap of Last Lecture

What are features – their types and how are they used in ML

Storing features as vectors – common ML operations on vectors

Learning with Prototypes (LwP) – an extremely simple method that gives lightweight models (just one prototype per class)

When LwP fails – when data points in class are very diverse, or else oddly distributed

One solution – make every training data point a prototype – 1NN

Learning with the 1-NN Classifier

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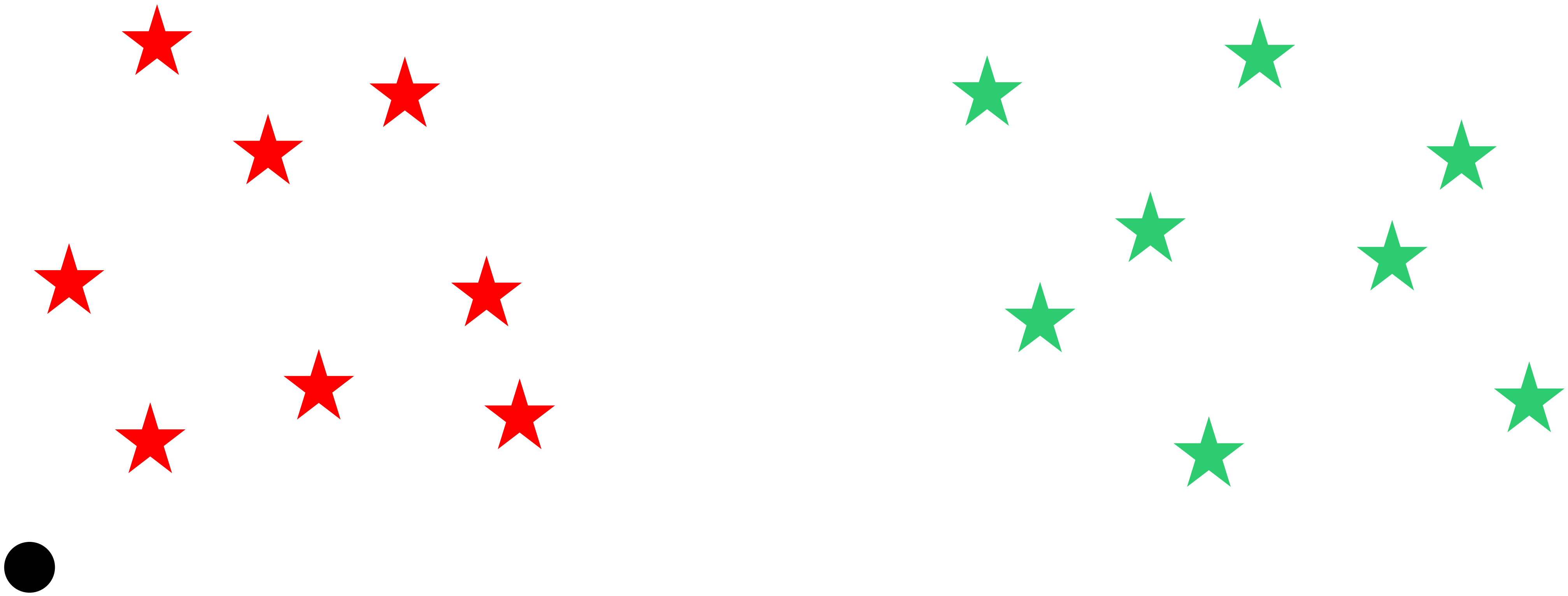

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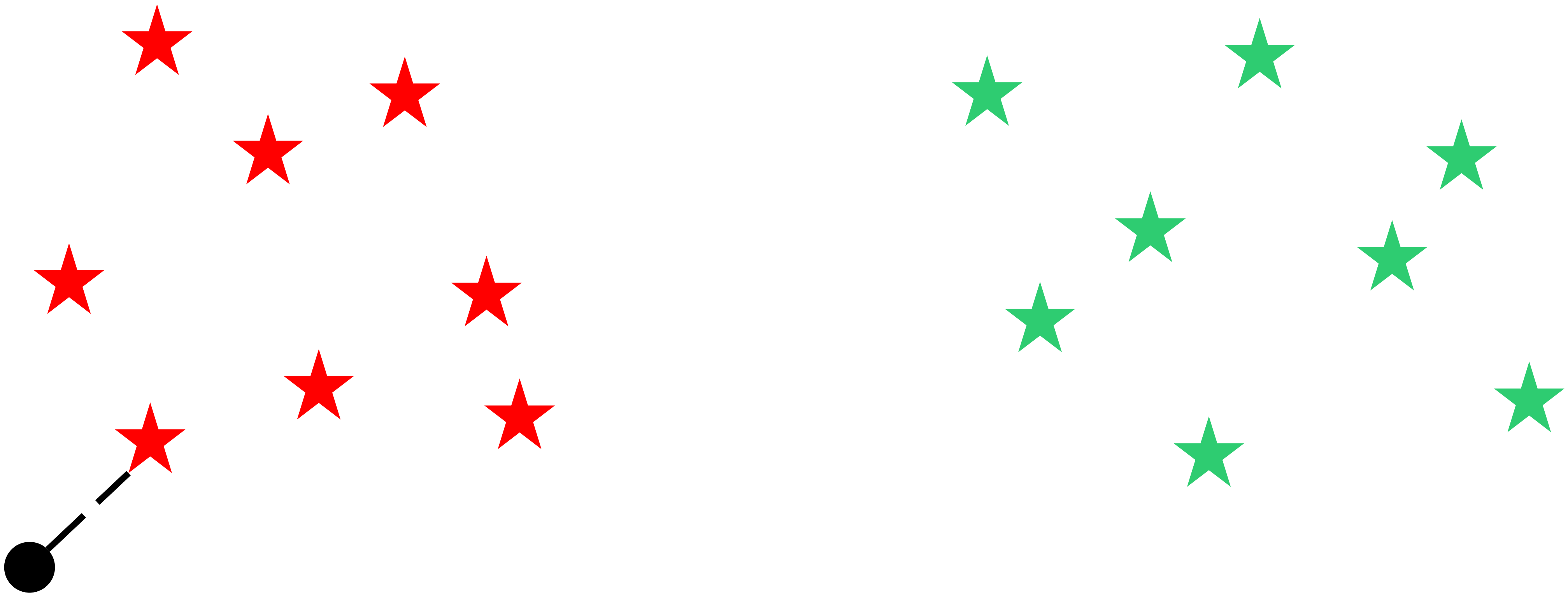

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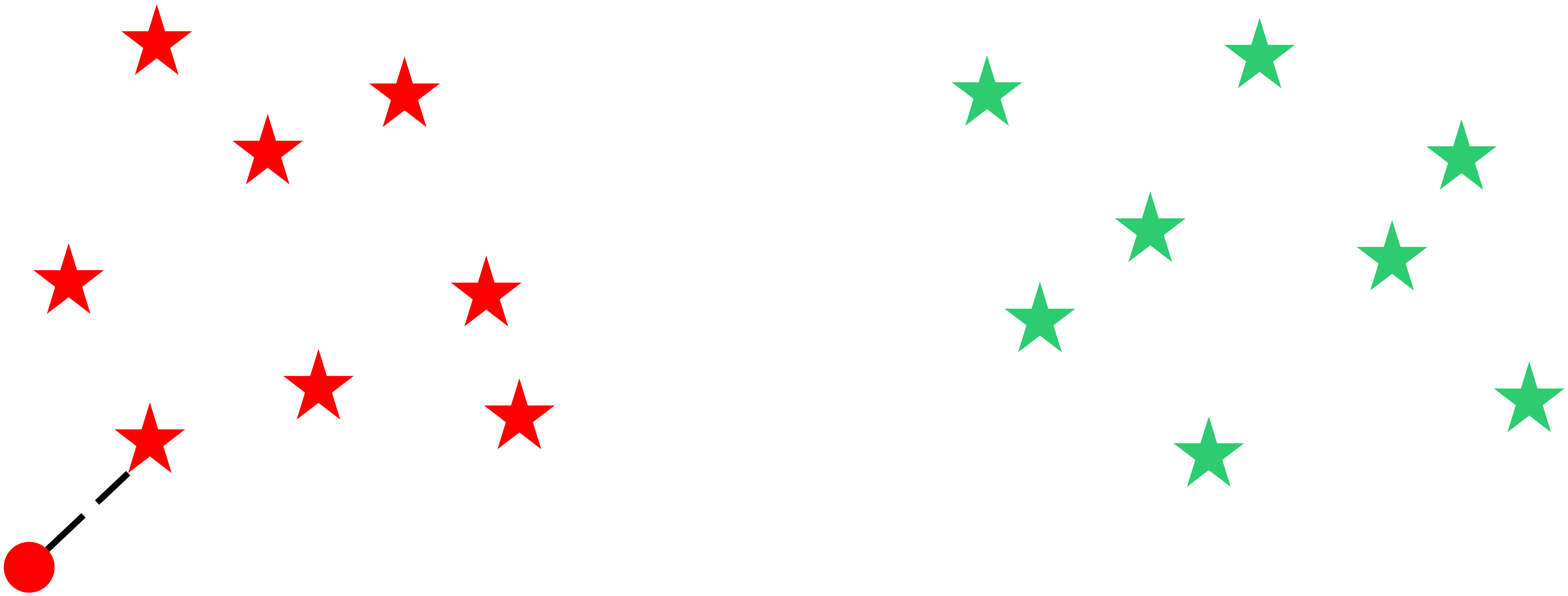

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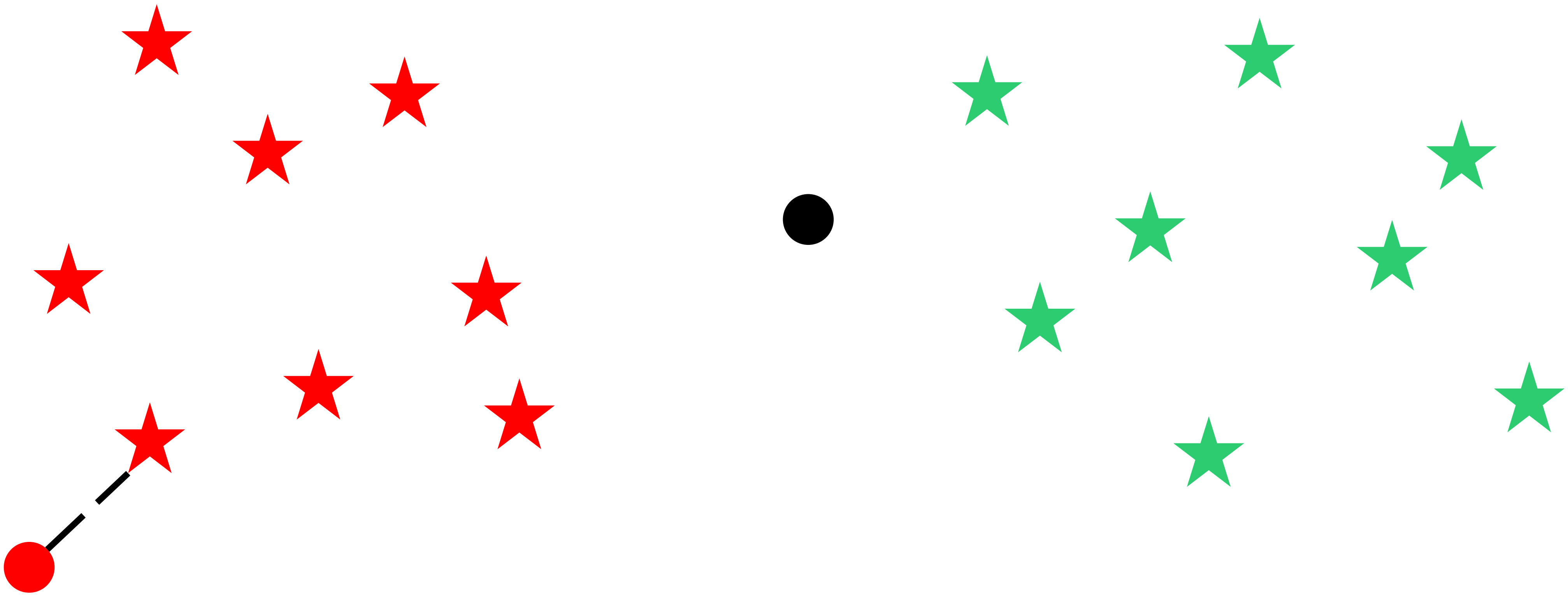

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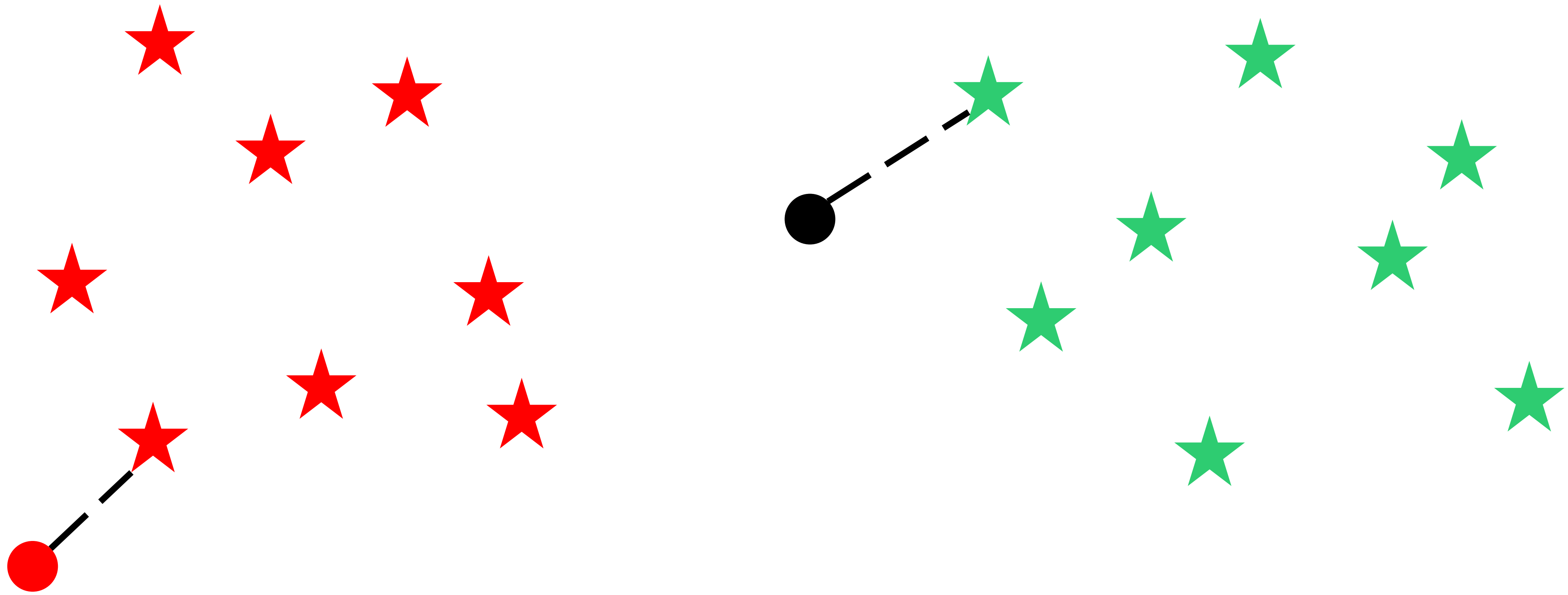

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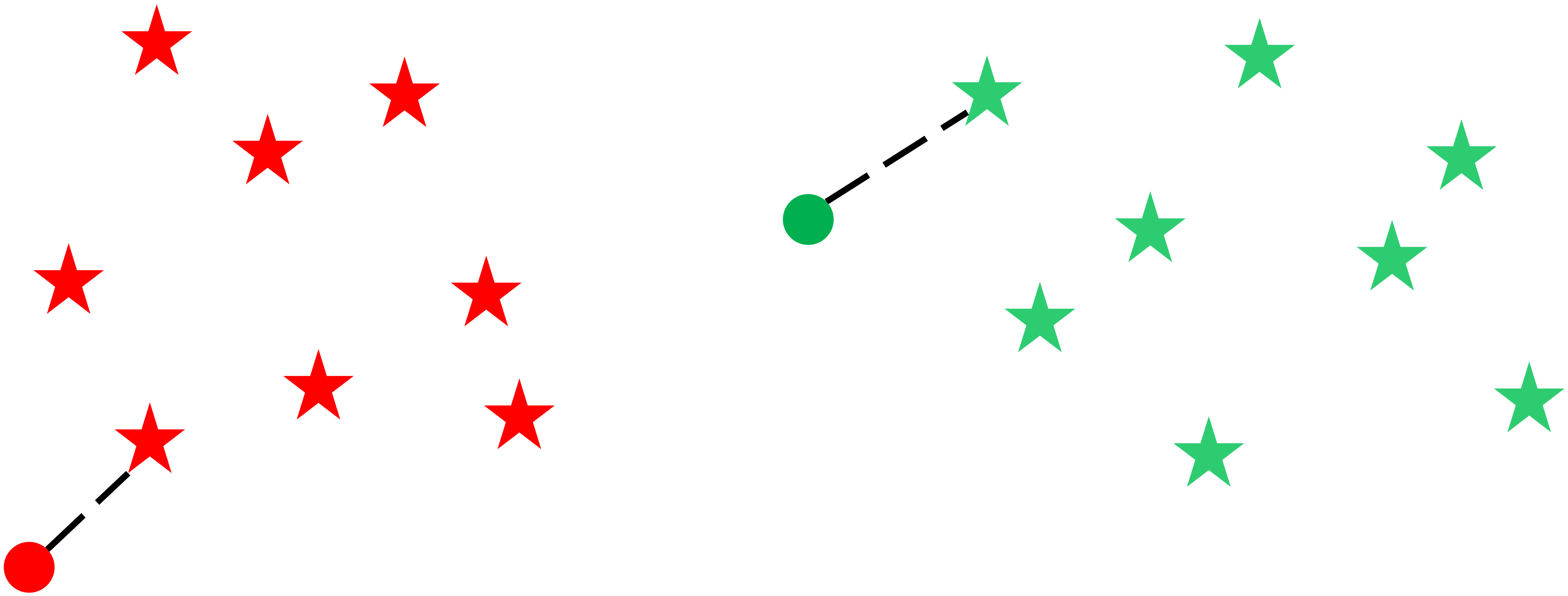

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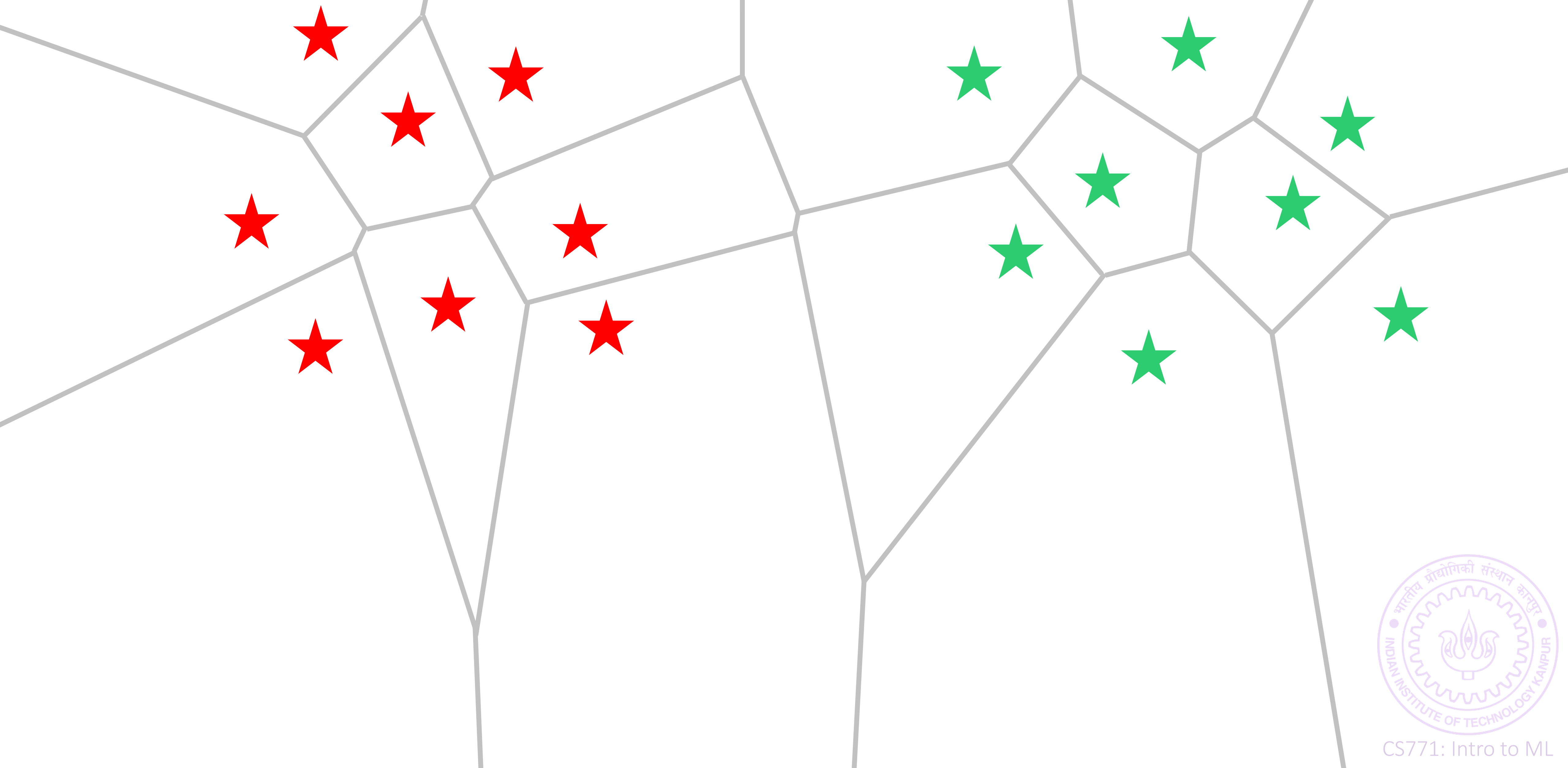

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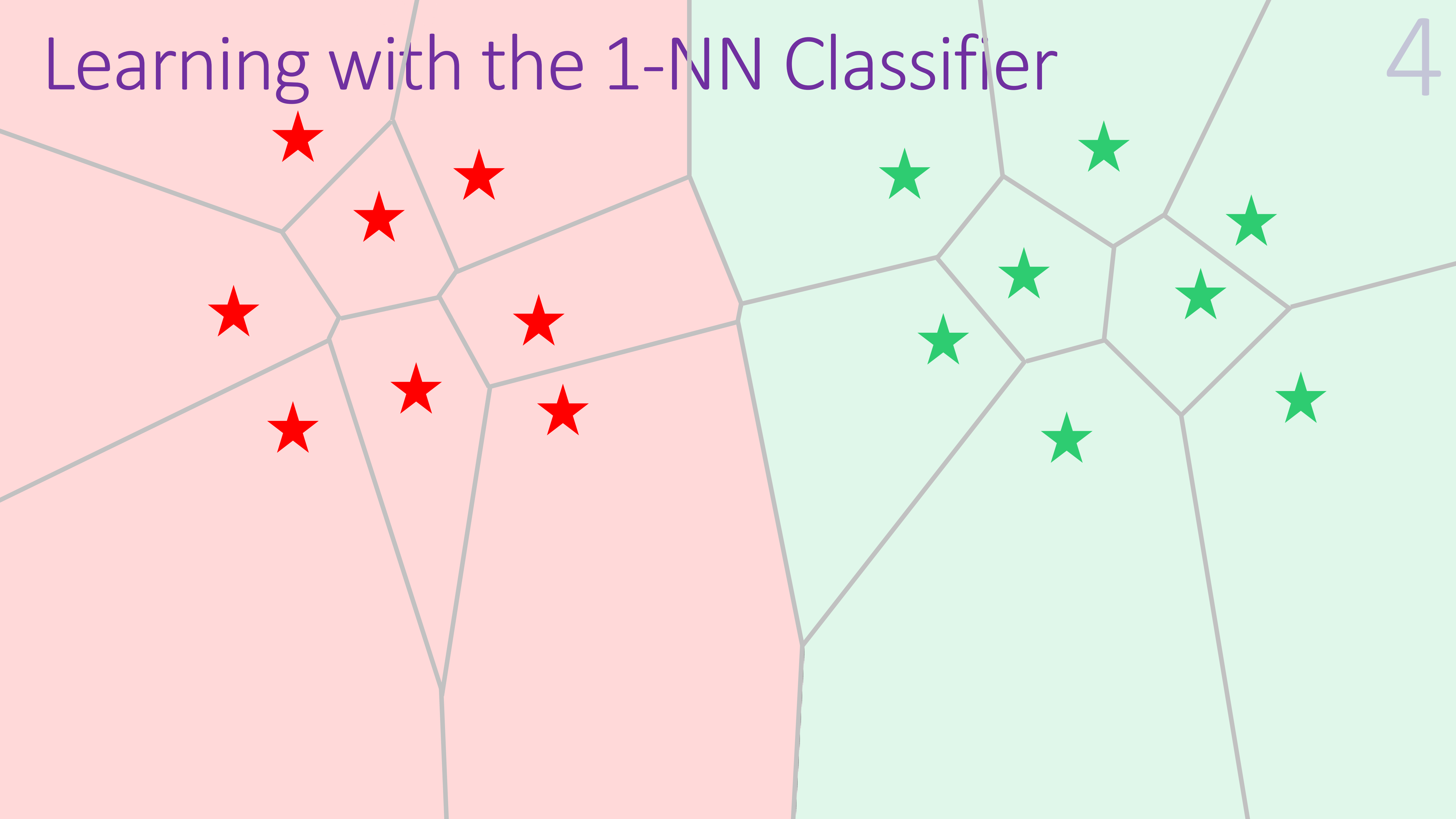

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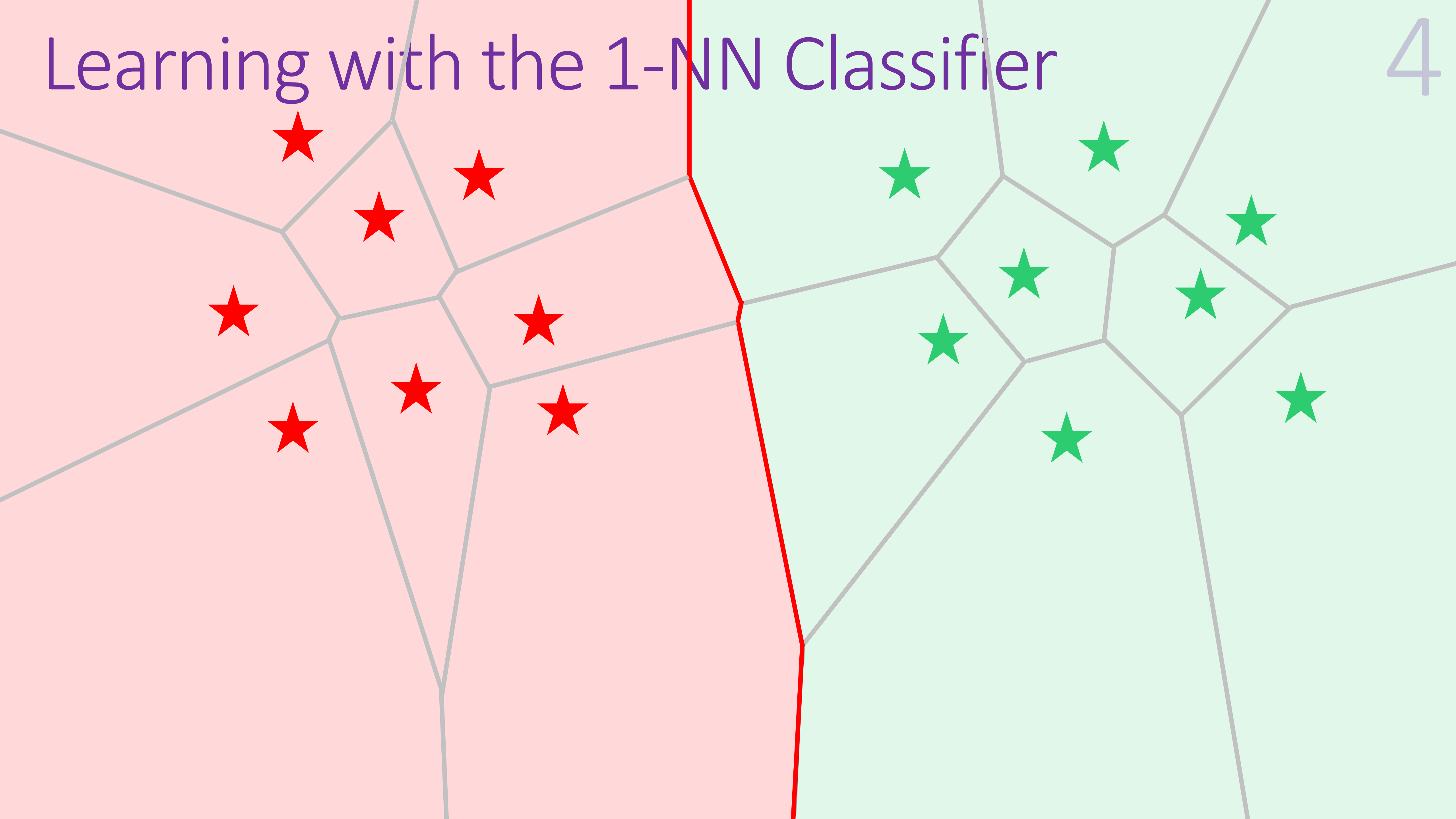

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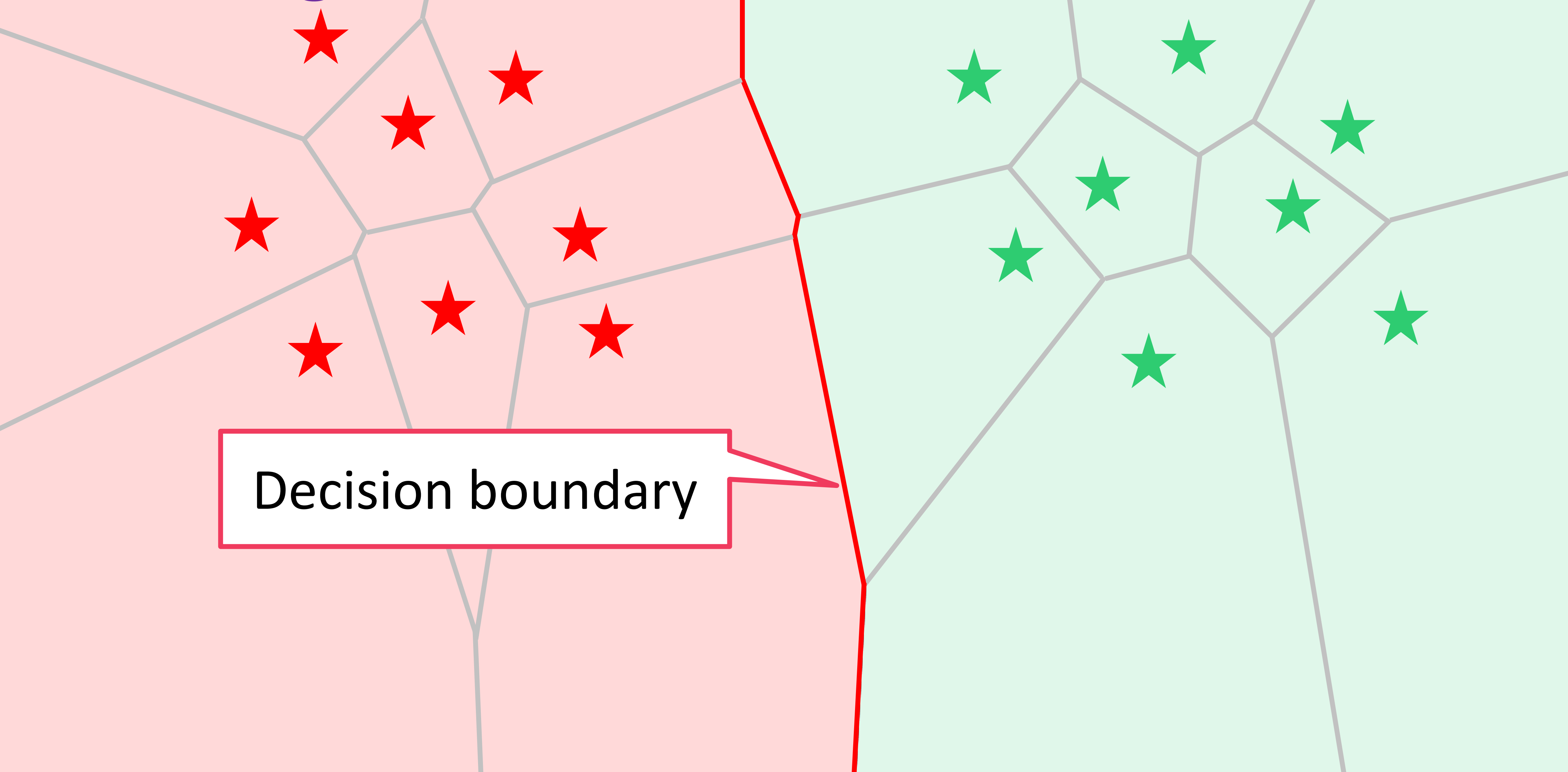

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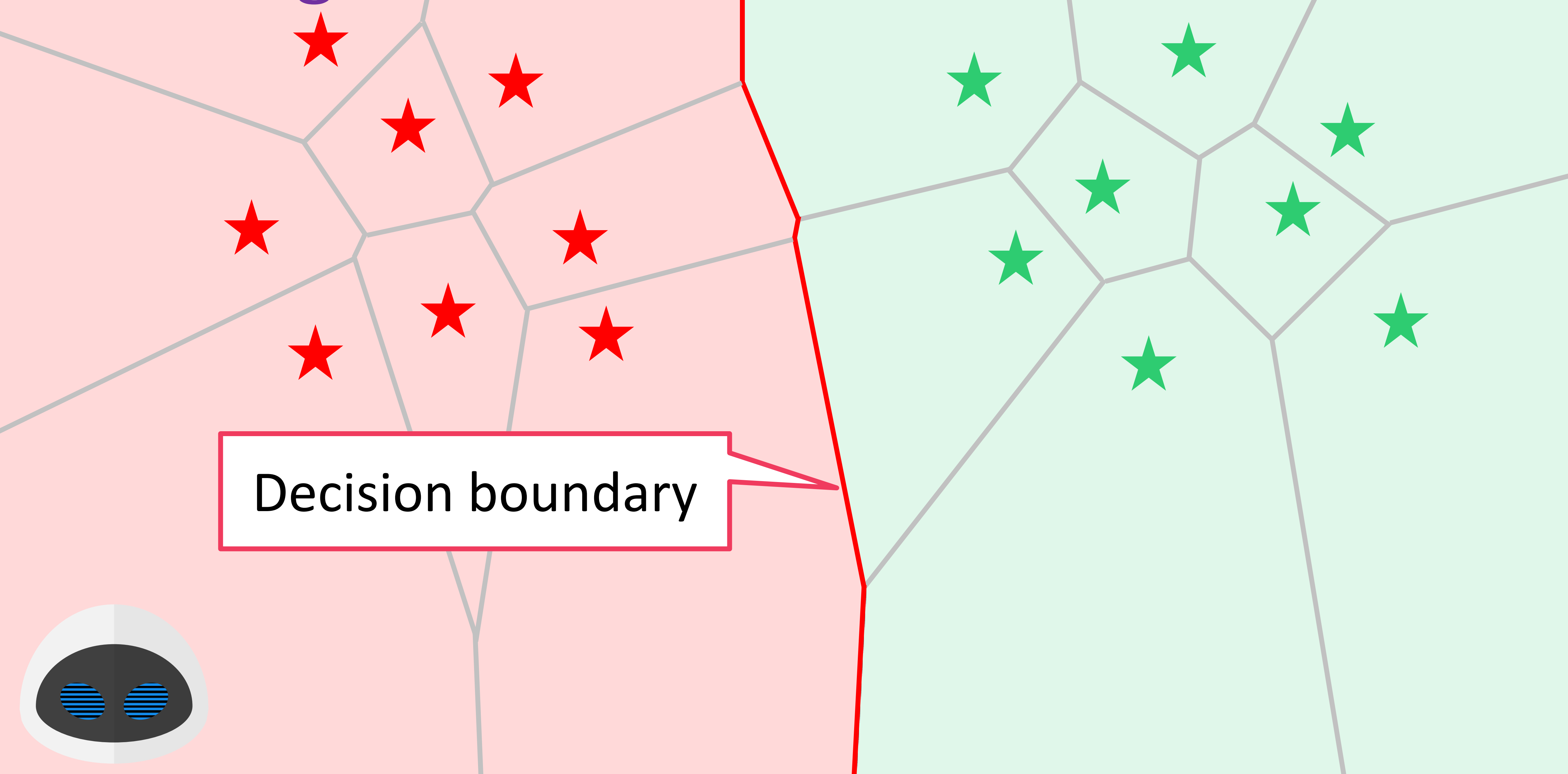

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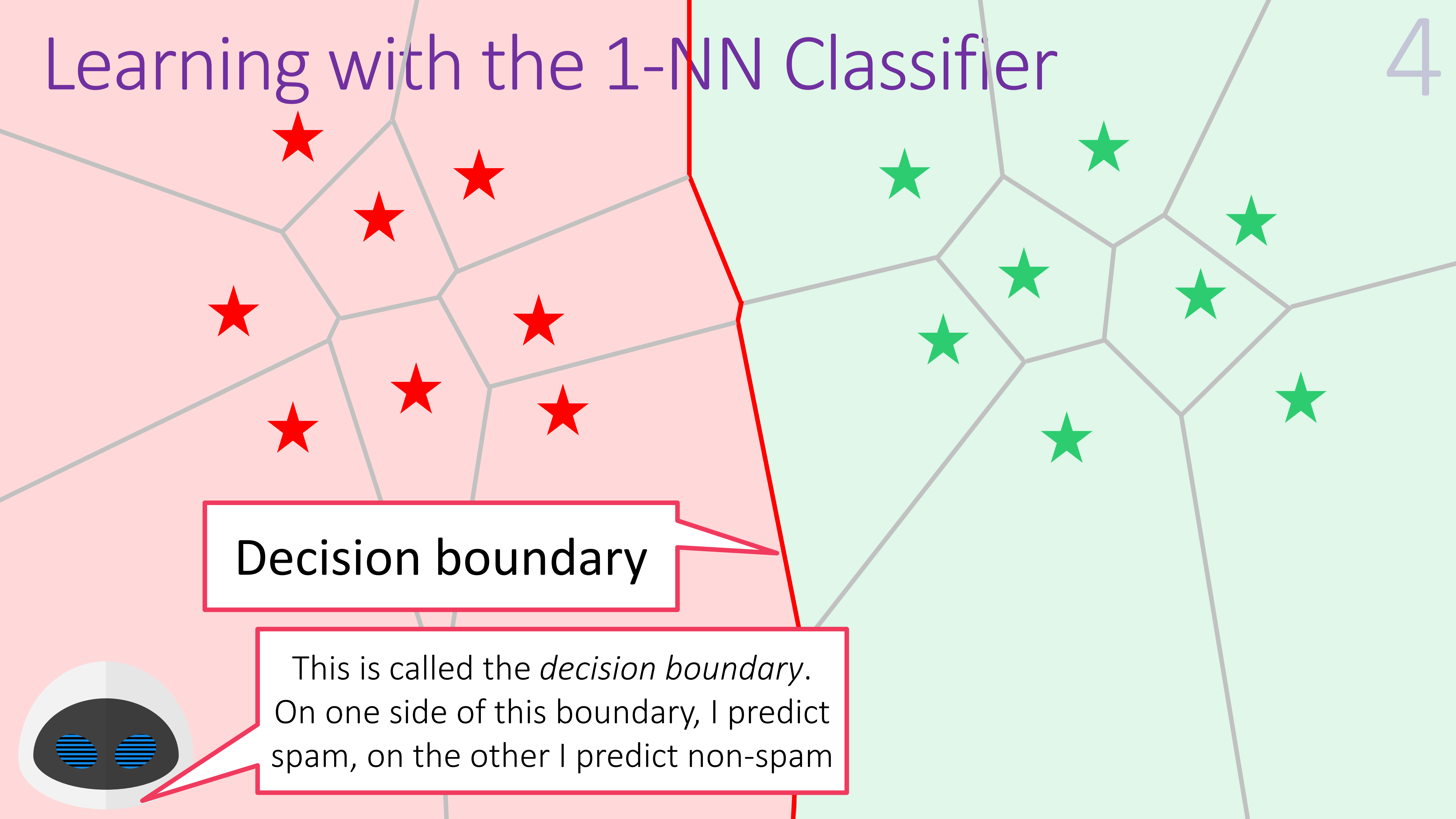

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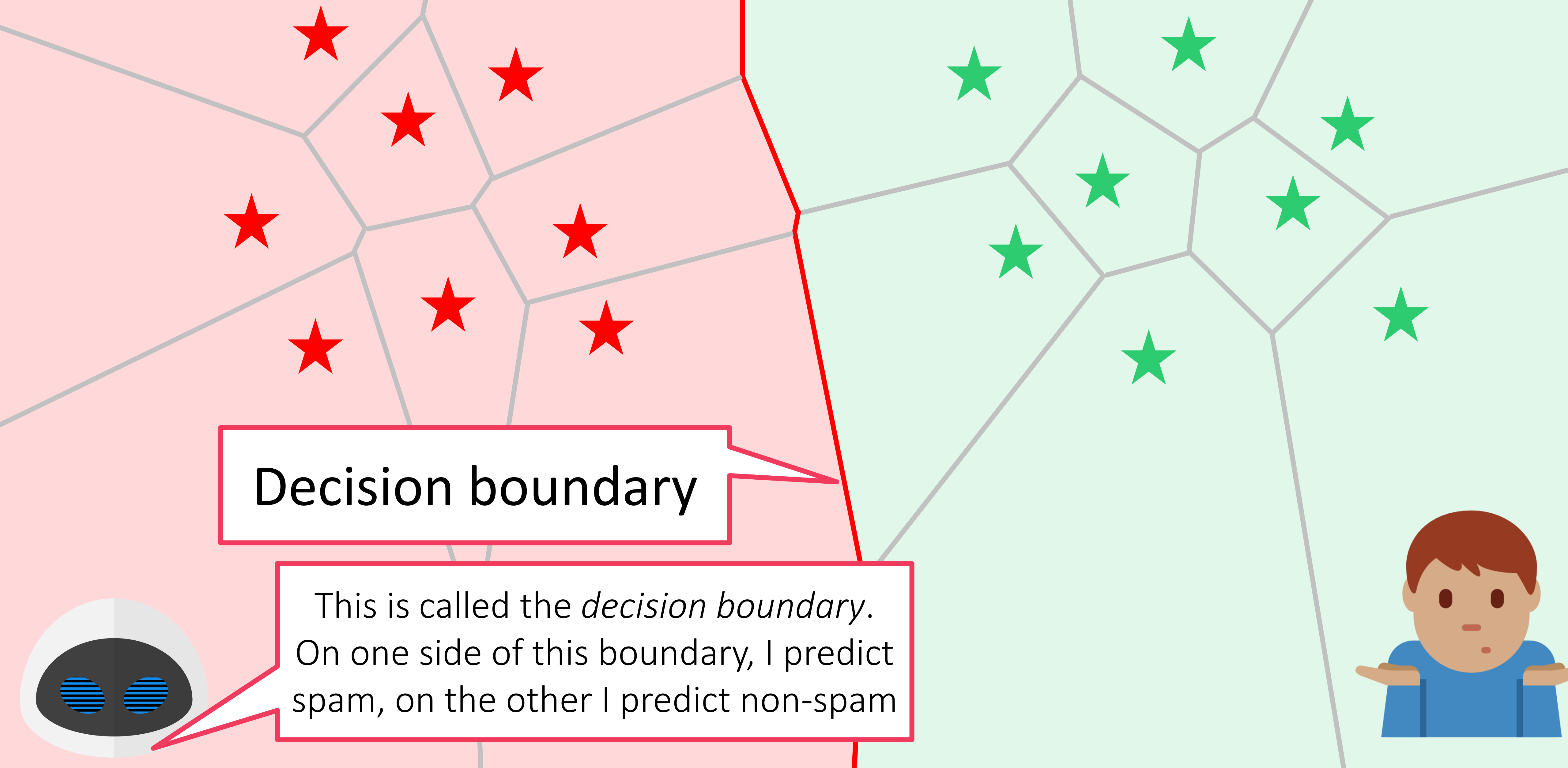

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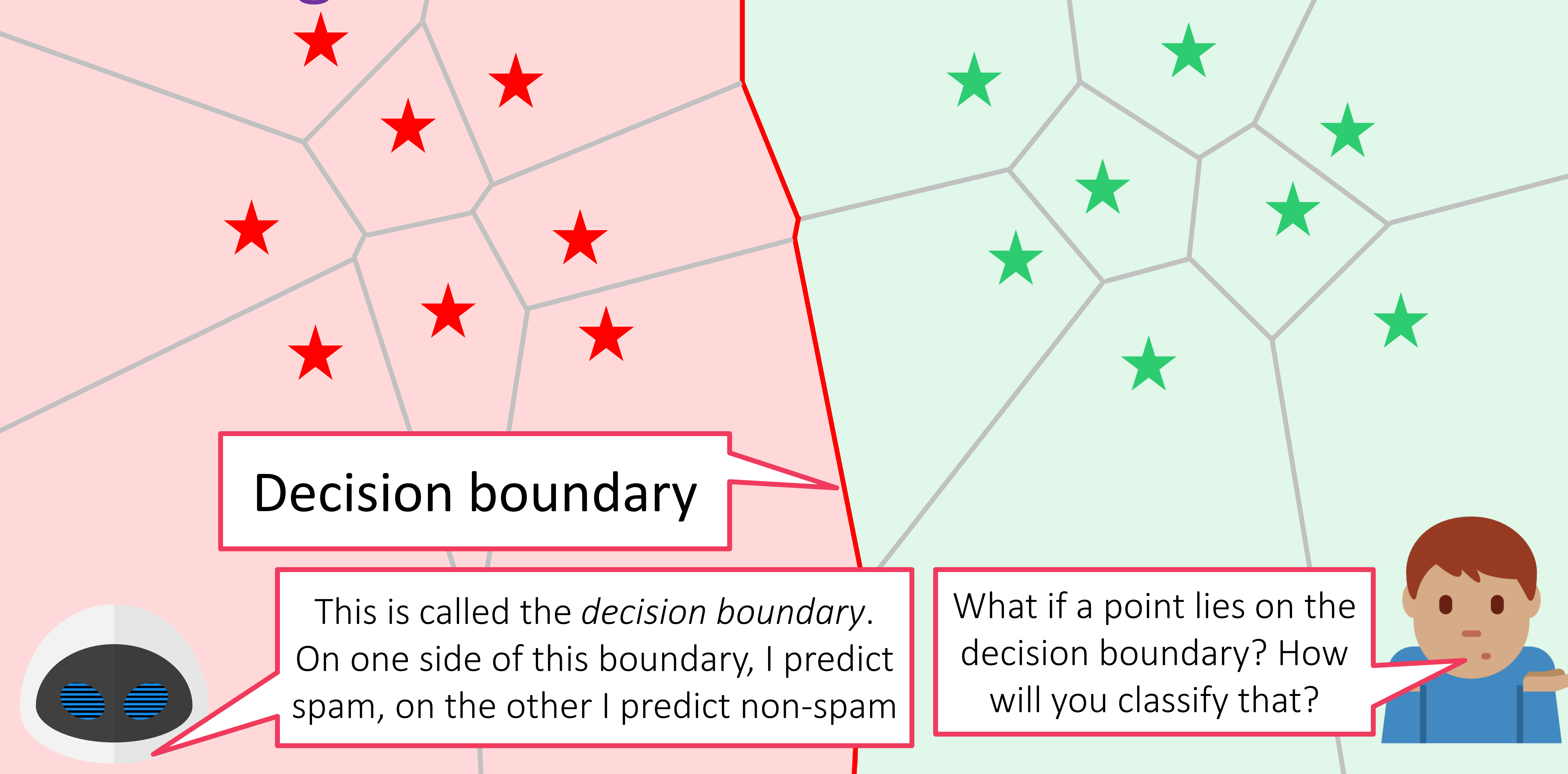
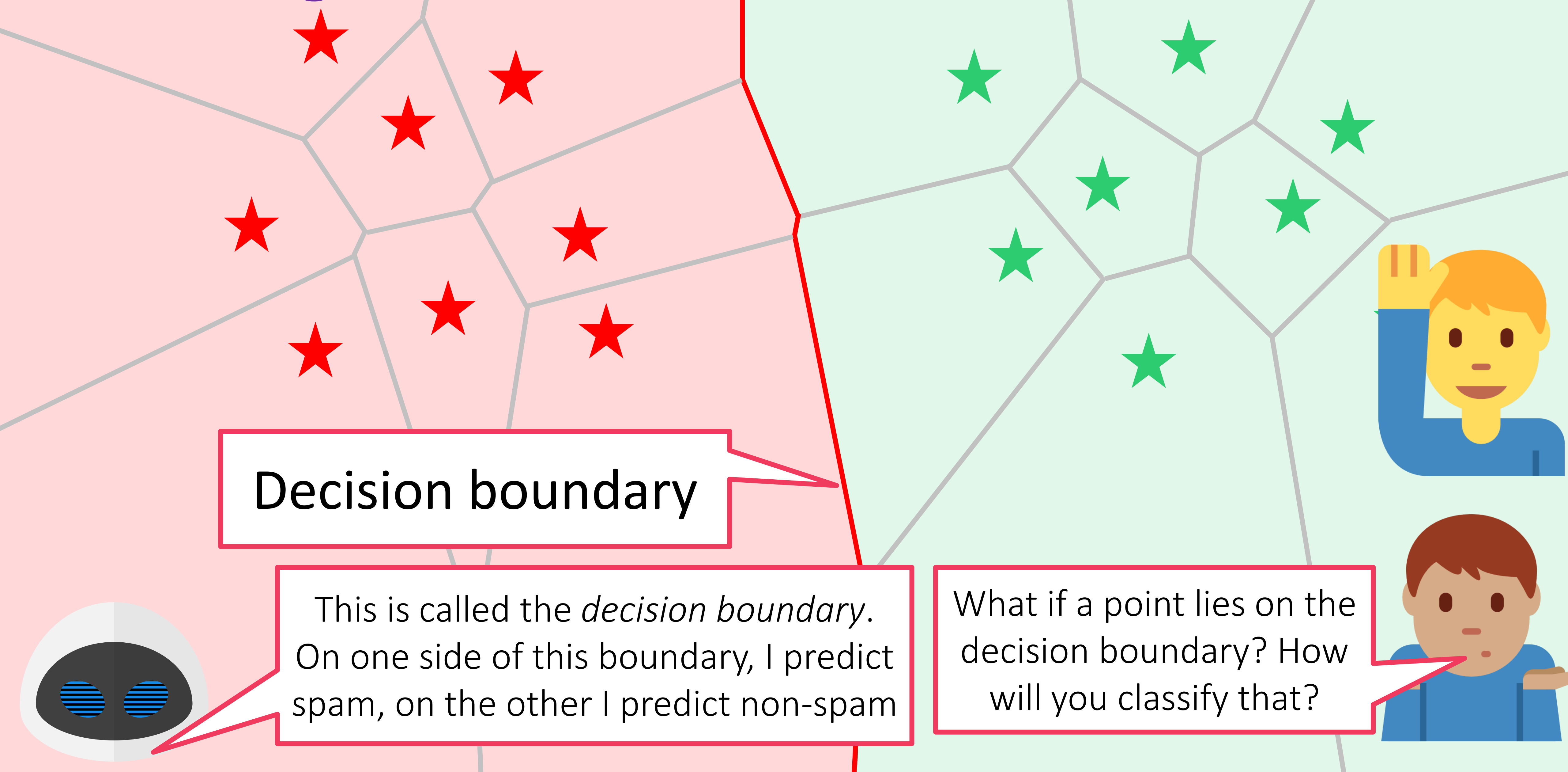


Decision boundary

This is called the *decision boundary*. On one side of this boundary, I predict spam, on the other I predict non-spam

What if a point lies on the decision boundary? How will you classify that?

Learning with the 1-NN Classifier



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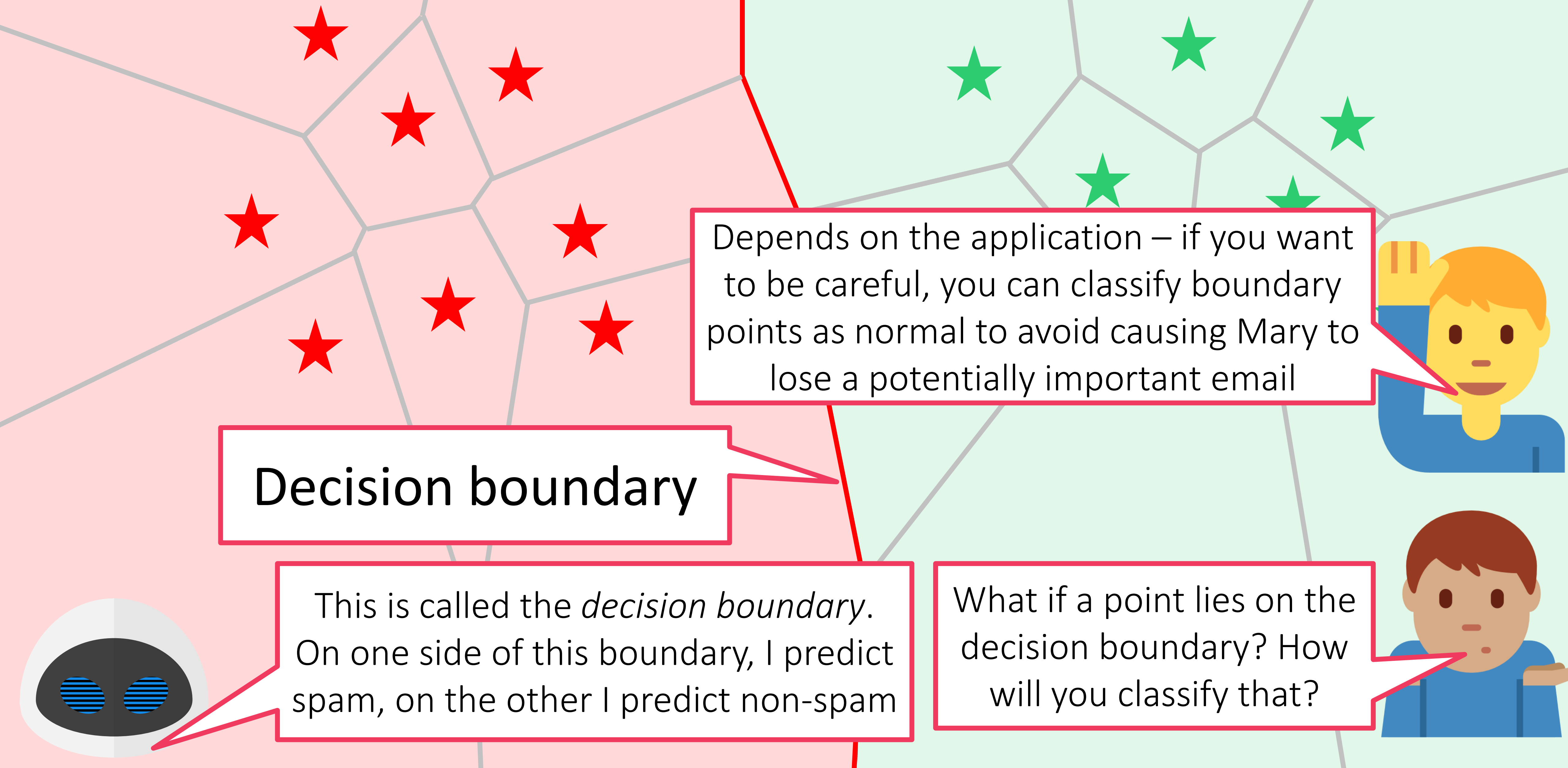

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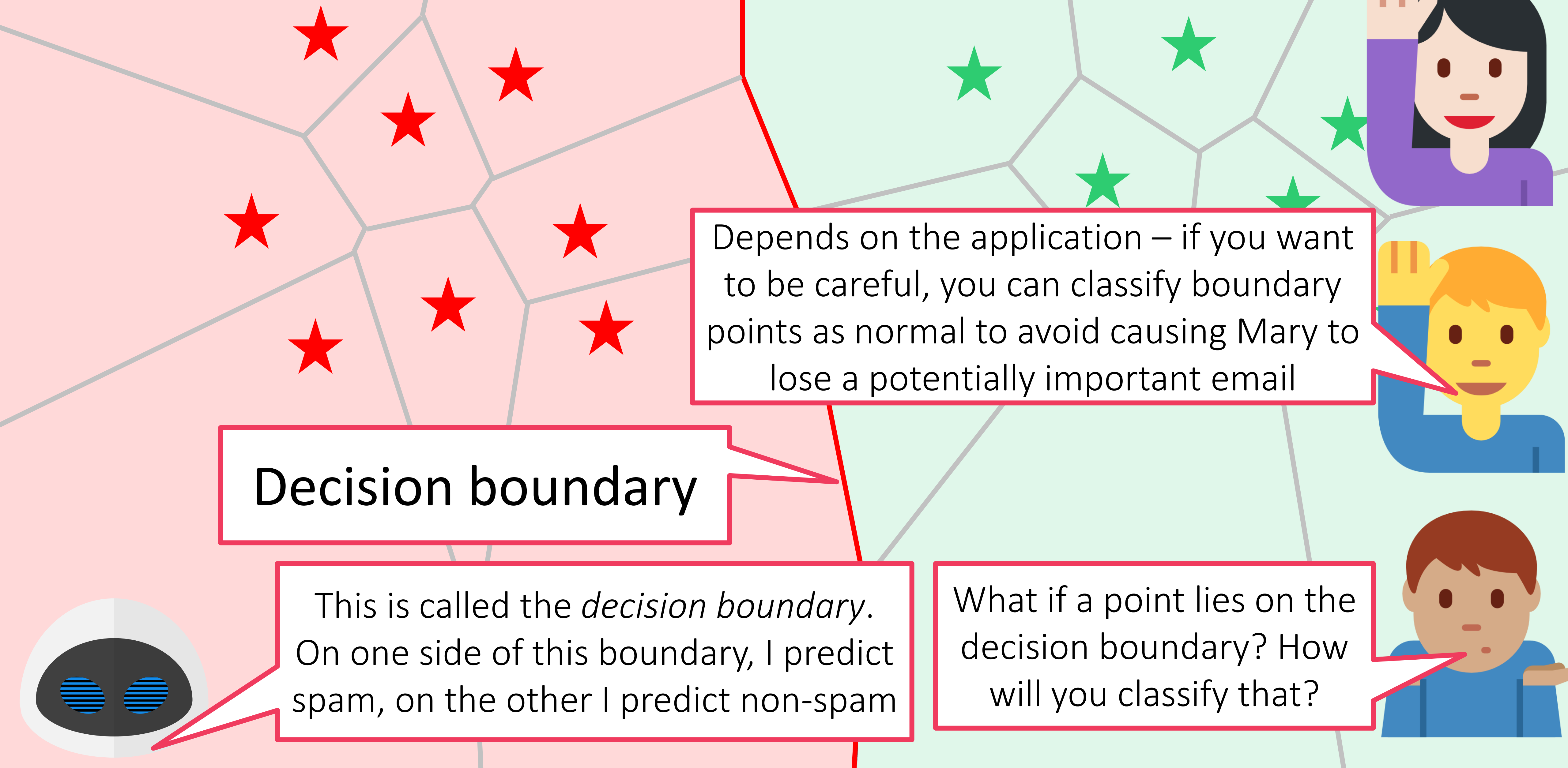

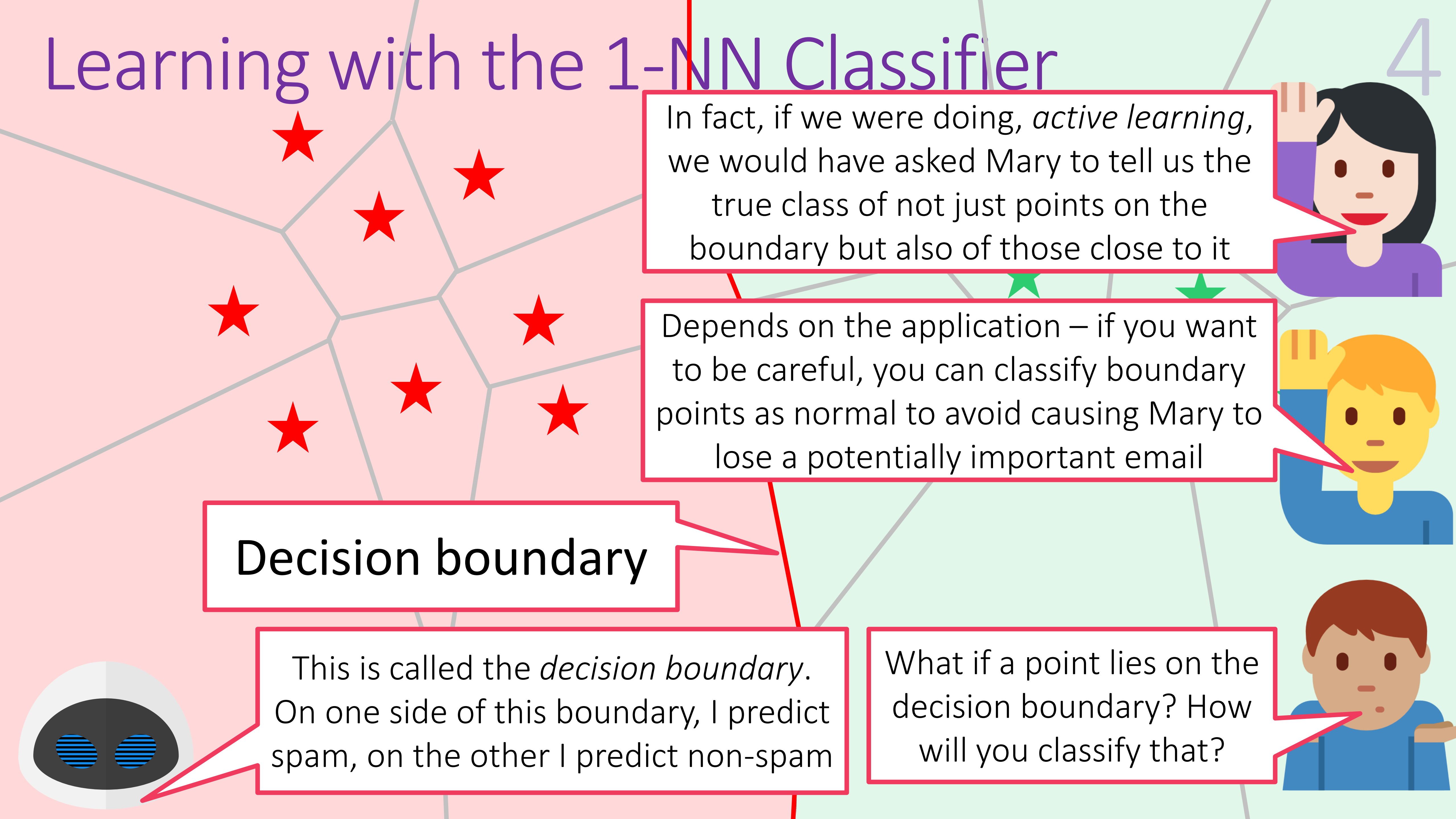
Learning with the 1-NN Classifier
4
In fact, if we were doing, *active learning*, we would have asked Mary to tell us the true class of not just points on the boundary but also of those close to it
Depends on the application – if you want to be careful, you can classify boundary points as normal to avoid causing Mary to lose a potentially important email
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Decision boundary

What is the decision boundary of LwP classifier?

This is called the *decision boundary*. On one side of this boundary, I predict spam, on the other I predict non-spam

What if a point lies on the decision boundary? How will you classify that?

LwP – behind the scenes

Let $\boldsymbol{\mu}^+, \boldsymbol{\mu}^-$ be the prototypes of the spam, non-spam classes resp.

Recall that we classify an email with feature vector $\mathbf{x}$ as spam if

$$\|\mathbf{x} - \boldsymbol{\mu}^+\|_2 < \|\mathbf{x} - \boldsymbol{\mu}^-\|_2$$

$$\Leftrightarrow \|\mathbf{x} - \boldsymbol{\mu}^+\|_2^2 < \|\mathbf{x} - \boldsymbol{\mu}^-\|_2^2$$

$$\Leftrightarrow \|\mathbf{x}\|_2^2 + \|\boldsymbol{\mu}^+\|_2^2 - 2\langle \mathbf{x}, \boldsymbol{\mu}^+ \rangle < \|\mathbf{x}\|_2^2 + \|\boldsymbol{\mu}^-\|_2^2 - 2\langle \mathbf{x}, \boldsymbol{\mu}^- \rangle$$

$$\Leftrightarrow \|\boldsymbol{\mu}^+\|_2^2 - 2\langle \mathbf{x}, \boldsymbol{\mu}^+ \rangle < \|\boldsymbol{\mu}^-\|_2^2 - 2\langle \mathbf{x}, \boldsymbol{\mu}^- \rangle$$

$$\Leftrightarrow \langle \mathbf{x}, 2(\boldsymbol{\mu}^+ - \boldsymbol{\mu}^-) \rangle + \|\boldsymbol{\mu}^-\|_2^2 - \|\boldsymbol{\mu}^+\|_2^2 > 0$$

$$\equiv \ \langle \mathbf{x}, \mathbf{w} \rangle + b > 0 \text{ with } \mathbf{w} = 2(\boldsymbol{\mu}^+ - \boldsymbol{\mu}^-), \mathrm{b} = \|\boldsymbol{\mu}^-\|_2^2 - \|\boldsymbol{\mu}^+\|_2^2$$

LwP – behind the scenes

Let $\boldsymbol{\mu}^+, \boldsymbol{\mu}^-$ be the prototypes of the spa

Recall that we classify an email with feat

$$\|\mathbf{x} - \boldsymbol{\mu}^+\|_2 < \|\mathbf{x} - \boldsymbol{\mu}^-\|_2$$

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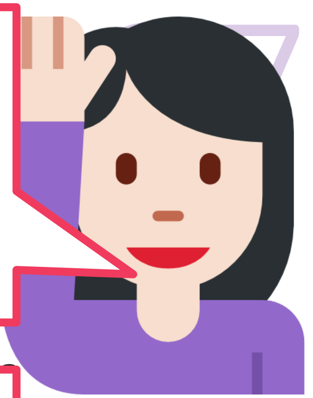
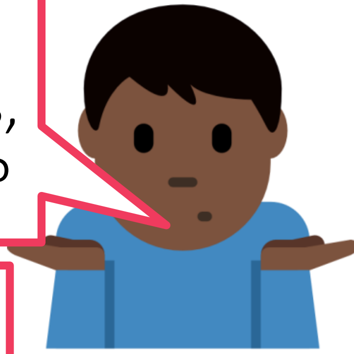
$$\Leftrightarrow \langle \mathbf{x}, 2(\boldsymbol{\mu}^+ - \boldsymbol{\mu}^-)\rangle + \|\boldsymbol{\mu}^-\|_2^2 - \|\boldsymbol{\mu}^+\|_2^2 >$$

$$\equiv \langle \mathbf{x}, \mathbf{w} \rangle + b > 0 \text{ with } \mathbf{w} = 2($$

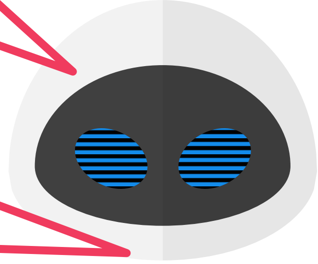
Classifiers with linear decision boundaries are called *linear classifiers*. Thus, LwP is a linear classifier



What happens if there are 2 or more prototypes per class, or else if there are 3 classes?

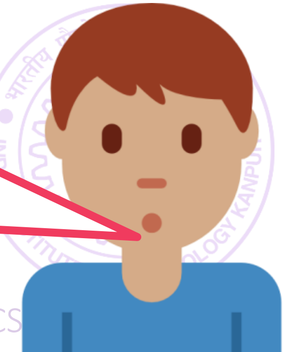


Think about this on your own – will discuss later



Yes, this is known as a *linear decision boundary*.

So the decision boundary of the LwP classifier is always a line or a hyperplane if the distance function is Euclidean!!



Linear/hyperplane Classifiers

The model is a single vector $\mathbf{w}$ of dimension d (features are also d-dim), and an optional scalar term (called *bias*) b

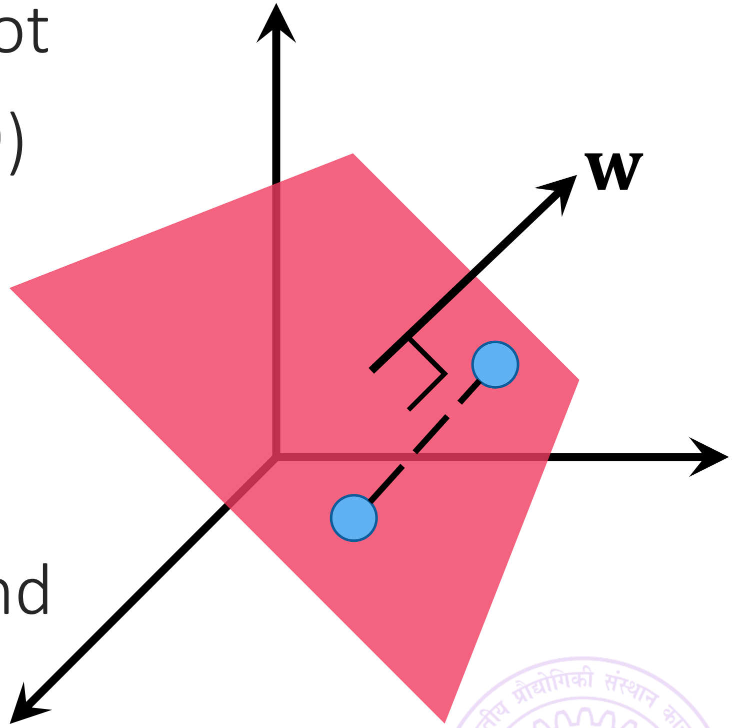
Predict on a test point $\mathbf{x}$ by checking if $\mathbf{w}^\top \mathbf{x} + b > 0$ or not

Decision boundary: line/hyperplane (where $\mathbf{w}^\top \mathbf{x} + b = 0$)

The vector w is called the *normal* or *perpendicular* vector of the hyperplane – why?

Consider any two vectors $\mathbf{x}, \mathbf{y}$ on the hyperplane i.e. $\mathbf{w}^\top \mathbf{x} + b = 0 = \mathbf{w}^\top \mathbf{y} + b$. This means $\mathbf{w}^\top (\mathbf{x} - \mathbf{y}) = 0$. Note that the vector $\mathbf{x} - \mathbf{y}$ is parallel to the hyperplane and $\mathbf{w}$ perpendicular to all such vectors

The bias term b if changed, shifts the plane – it can be thought of as a threshold as well – how large does $\mathbf{w}^\top \mathbf{x}$ have to be in order for us to classify $\mathbf{x}$ as spam etc!



To b or not to b – that is the question!

Trivia: the closest point (Euclidean distance) on the hyperplane to the origin is at a distance $|b|/\|\mathbf{w}\|_2$ from the origin – can you show why?

Sometimes, it is convenient to not have a separate bias term

Create another dim in feature vector and fill it with 1 i.e. $\tilde{\mathbf{x}} = [\mathbf{x}, 1]$

So now features (and model) are $d + 1$-dimensional

However, note that if we have a model $\tilde{\mathbf{w}} = [w_0, w_1, \ldots, w_d] \in \mathbb{R}^{d+1}$ over the new features and if we denote $w = [w_0, \ldots w_{d-1}] \in \mathbb{R}^d$, then

$$\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}} = \mathbf{w}^\top \mathbf{x} + w_d$$

Thus, w_d effectively acts as a bias term for us ☺

Making LwP more Powerful

The Euclidean distance is nice but gives all features equal weight

Also does not allow features to talk to each other

E.g. $\|\mathbf{x}\|_2 = \sqrt{\sum_{j=1}^{d} \mathbf{x}_j^2}$ has no $\mathbf{x}_j \mathbf{x}_k$ term for $j \neq k$

Using a different distance function really helps

Metric learning: learn this distance function as well

A very popular family of metrics – Mahalanobis metrics

Given a symmetric $d \times d$ matrix $A \in \mathbb{R}^{d \times d}$, we define a distance

$$d_A(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^\top A (\mathbf{x} - \mathbf{y})}$$

Taking $A = I_d$ i.e. identity matrix, gives us the usual Euclidean distance

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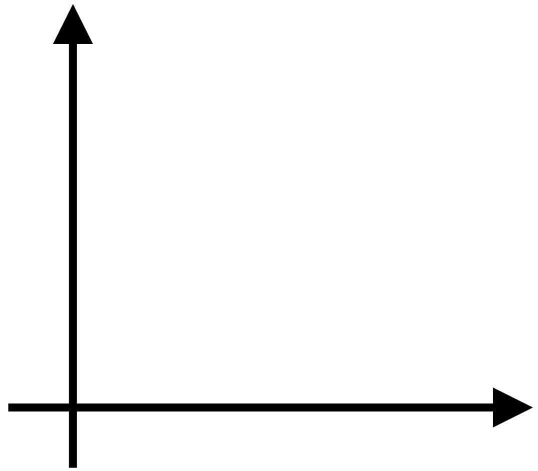

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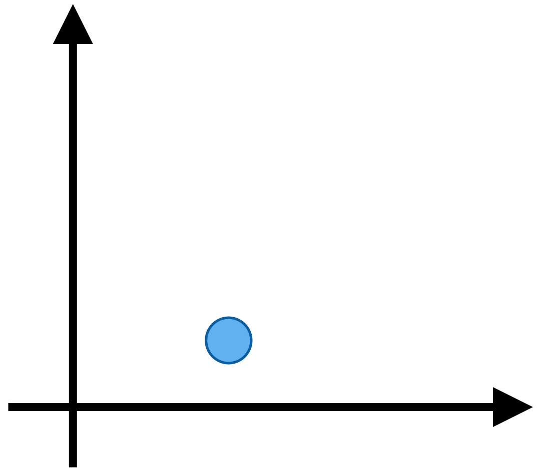

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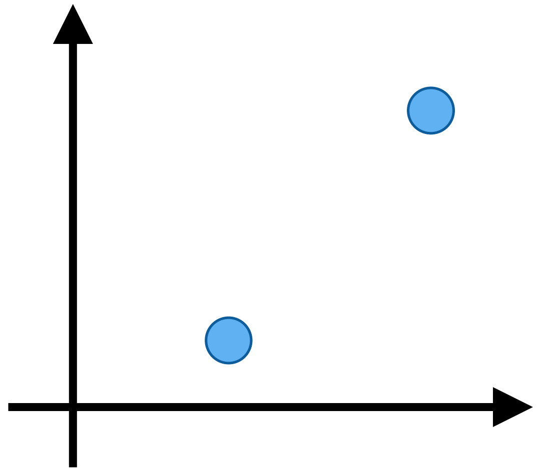

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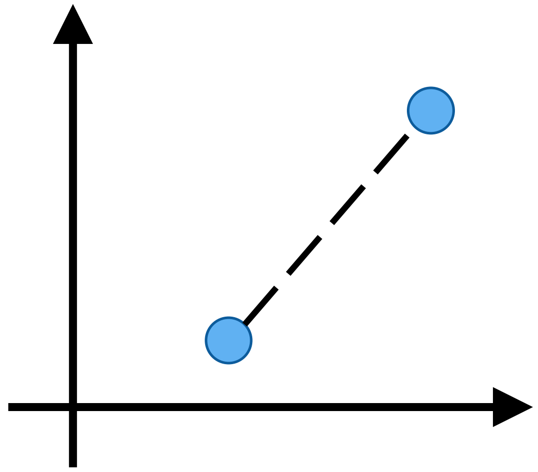

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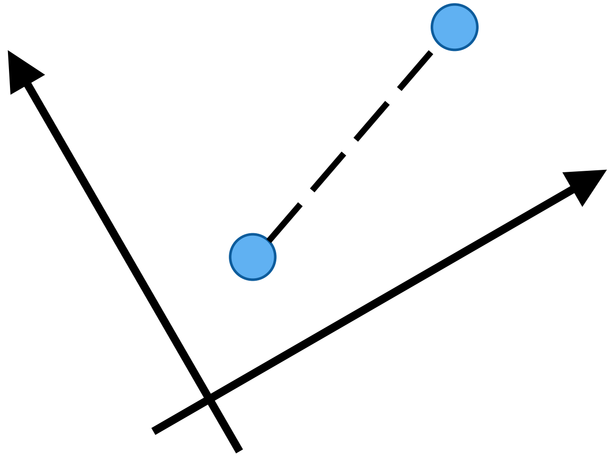

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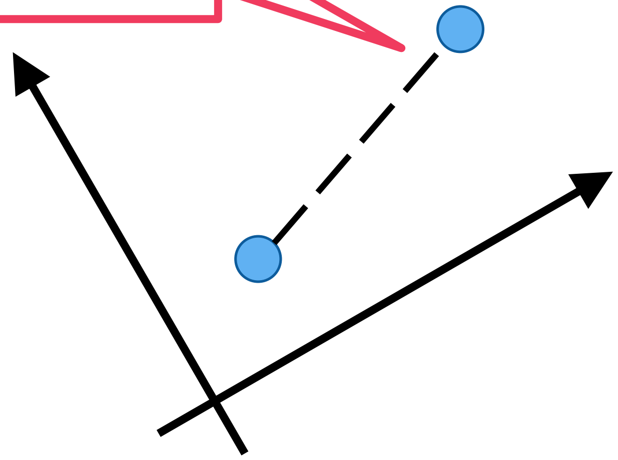
Making LwP more Powerful

The Euclidean distance is nice but … eight

Also does not allow features to tal…

Euclidean distance does not change even if axes are rotated



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LwP with Mahalanobis metric still linear!!

A matrix A that satisfies a property called *positive semi-definiteness* (PSD has several other nice properties too

For all vectors $\mathbf{x}$, we must have $\mathbf{x}^\top A\mathbf{x} \geq 0$

$$d_A(\mathbf{x}, \boldsymbol{\mu}^+) < d_A(\mathbf{x}, \boldsymbol{\mu}^-) \Leftrightarrow 2\mathbf{x}^\top A(\boldsymbol{\mu}^+ - \boldsymbol{\mu}^-) + {\boldsymbol{\mu}^-}^\top A\boldsymbol{\mu}^- - {\boldsymbol{\mu}^+}^\top A\boldsymbol{\mu}^+ > 0$$

$$\equiv \langle \mathbf{x}, \mathbf{w} \rangle + b > 0 \text{ where } \mathbf{w} = 2A(\boldsymbol{\mu}^+ - \boldsymbol{\mu}^-), b = {\boldsymbol{\mu}^-}^\top A\boldsymbol{\mu}^- - {\boldsymbol{\mu}^+}^\top A\boldsymbol{\mu}^+$$

We can write $A = LL^\top$ where $L \in \mathbb{R}^{d\times d}$ (L need not be sym or PSD)

$$d_A(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x}-\mathbf{y})^\top A(\mathbf{x}-\mathbf{y})} = \sqrt{(\mathbf{x}-\mathbf{y})^\top LL^\top(\mathbf{x}-\mathbf{y})}$$

$$= \|L^\top\mathbf{x} - L^\top\mathbf{y}\|_2$$

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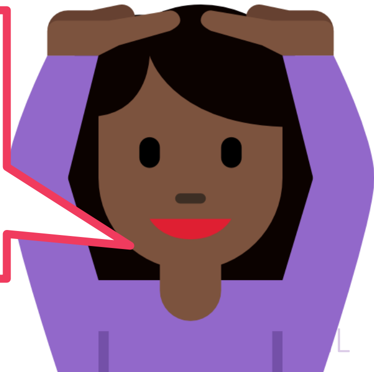
$$= \|L^\top \mathbf{x} - L^\top \mathbf{y}\|$$

Nice! This means that $d_A(\mathbf{x}, \mathbf{y}) \geq 0$ for all $\mathbf{x}, \mathbf{y}$ i.e. this will never give us negative distances which don't make sense



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$$\equiv \langle \mathbf{x}, \mathbf{w} \rangle + b > 0 \text{ where } \mathbf{w} = 2A(\boldsymbol{\mu}^+ - \boldsymbol{\mu}^-), b = {\boldsymbol{\mu}^-}^\top A\boldsymbol{\mu}^- - {\boldsymbol{\mu}^+}^\top A\boldsymbol{\mu}^+$$

We can write $A = LL^\top$ where $L \in \mathbb{R}^{d\times d}$ (L need not be sym or PSD)

$$d_A(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x}-\mathbf{y})^\top A(\mathbf{x}-\mathbf{y})} = \sqrt{(\mathbf{x}-\mathbf{y})^\top LL^\top(\mathbf{x}-\mathbf{y})}$$

$$= \|L^\top\mathbf{x} - L^\top\mathbf{y}\|_2$$

LwP with Mahalanobis metric still linear!!

A matrix A that satisfies a property called *positive semi-definiteness* (PSD has several other nice properties too

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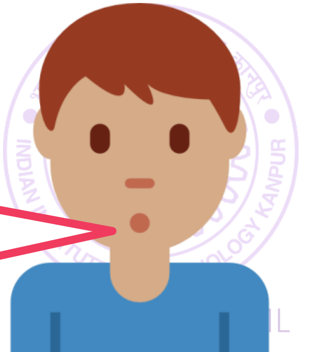
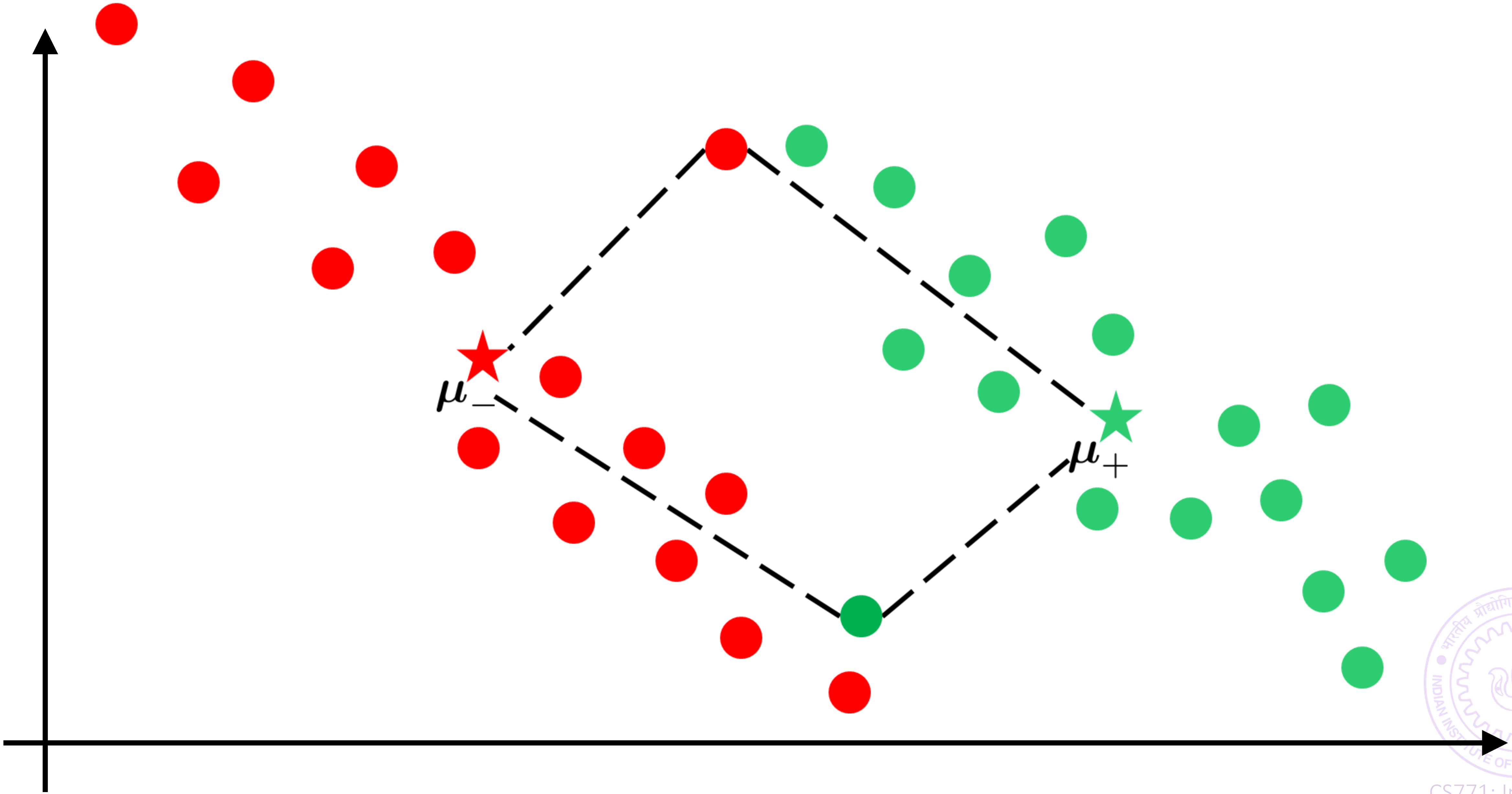
Oh! So the Mahalanobis distance is just Euclidean distance if we transform the vectors as $\mathbf{x} \mapsto L\mathbf{x}$



Why metric learning works



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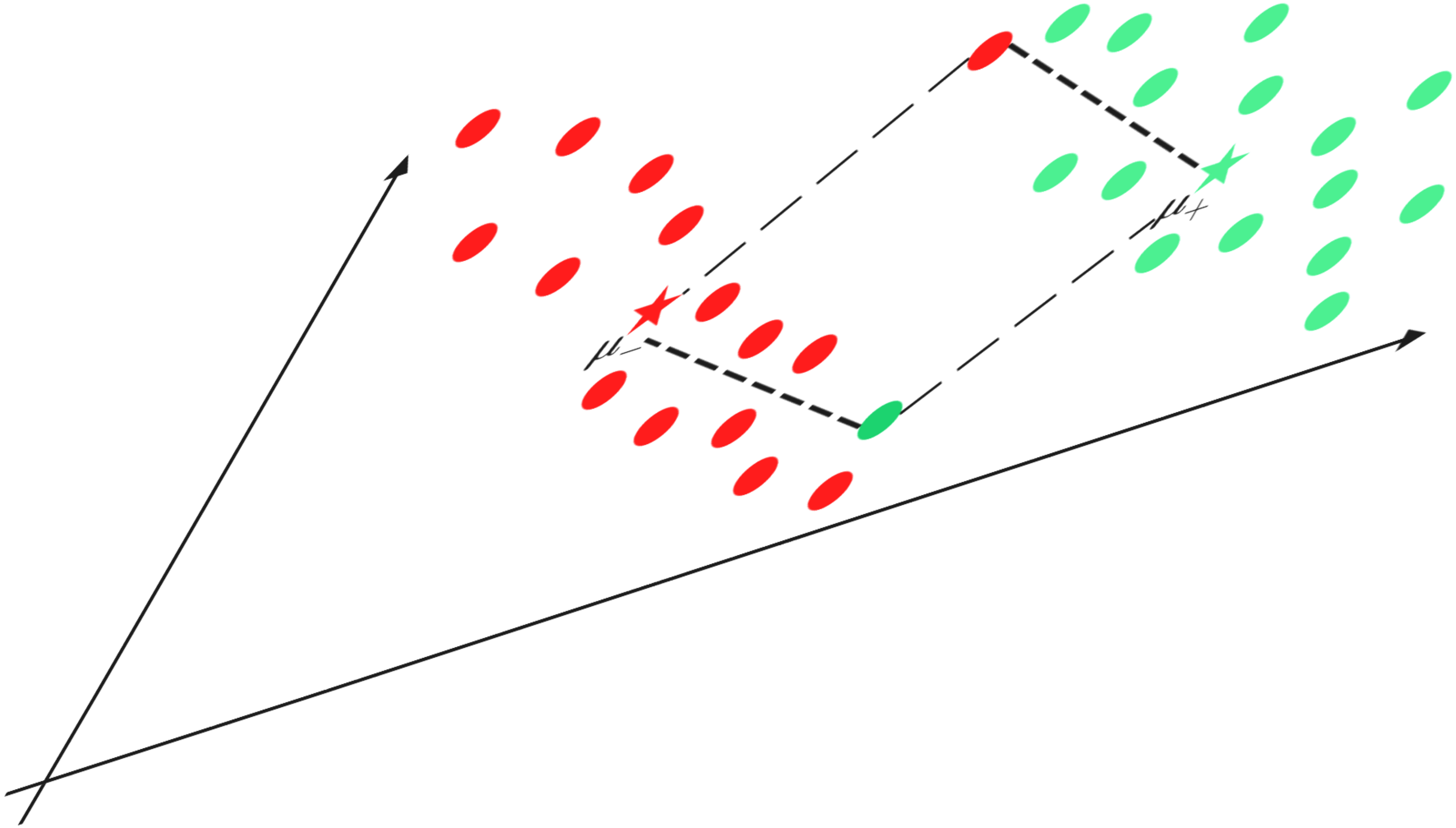

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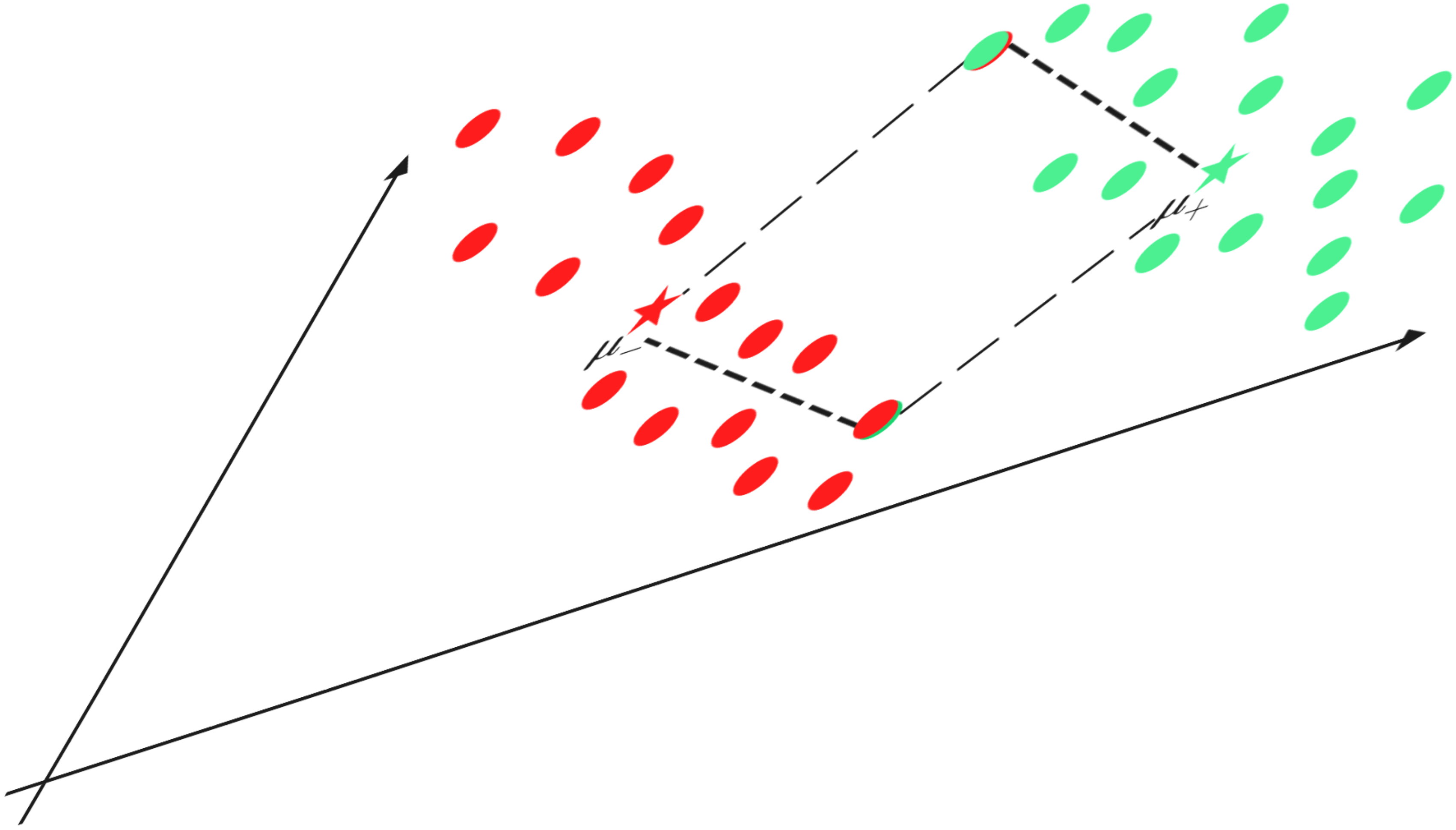

Back to Nearest Neighbors - kNN

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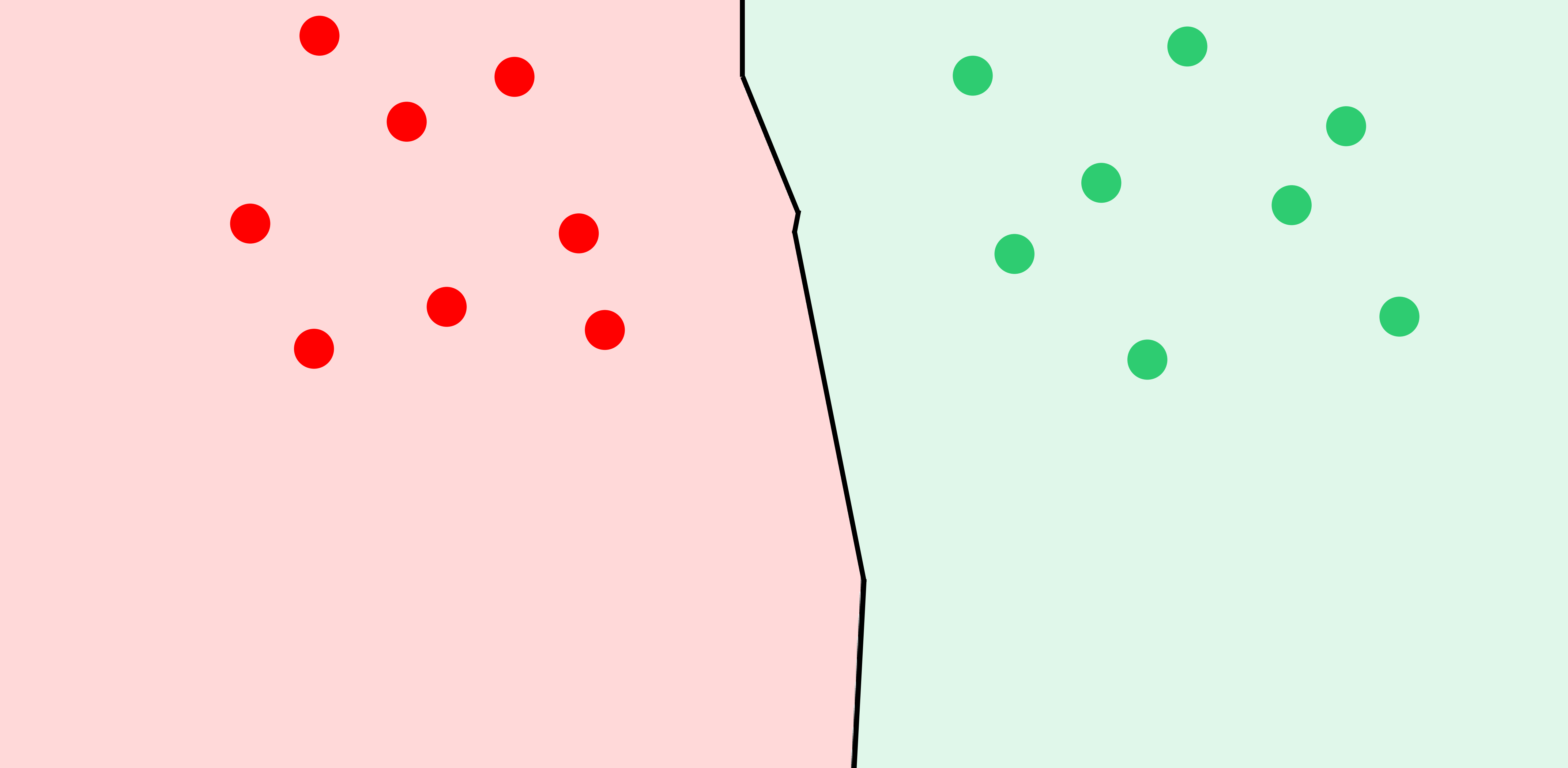

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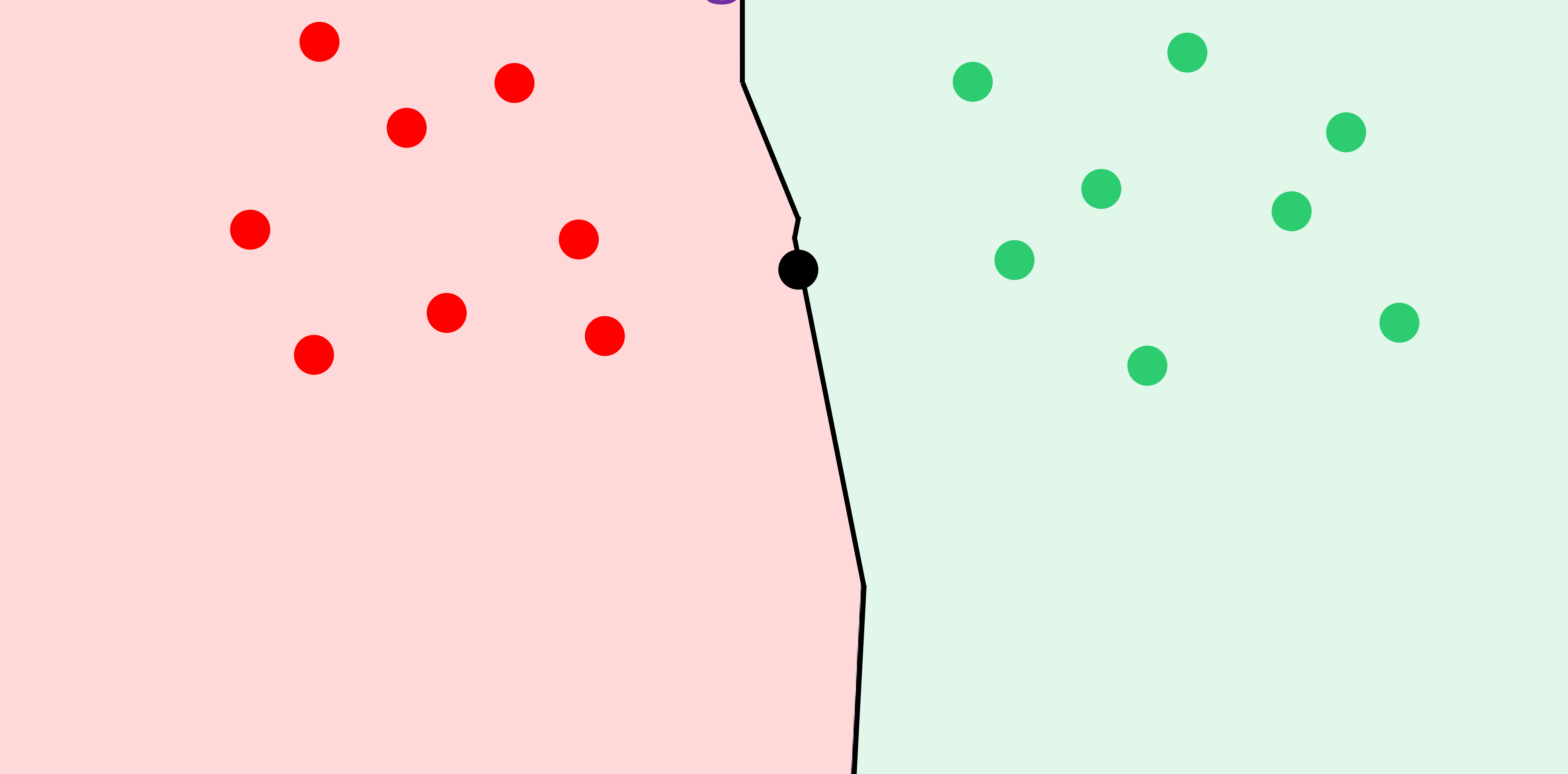

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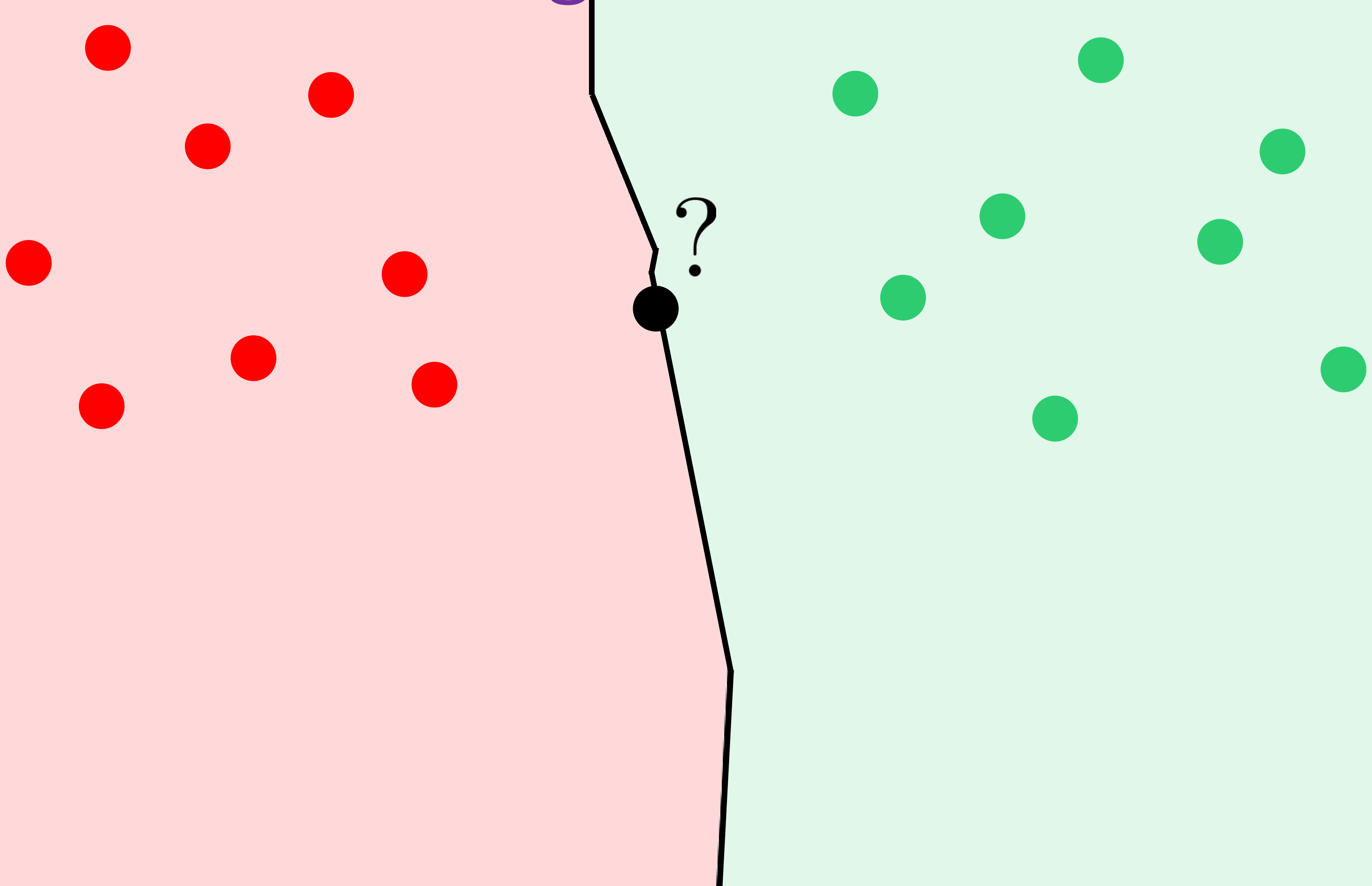

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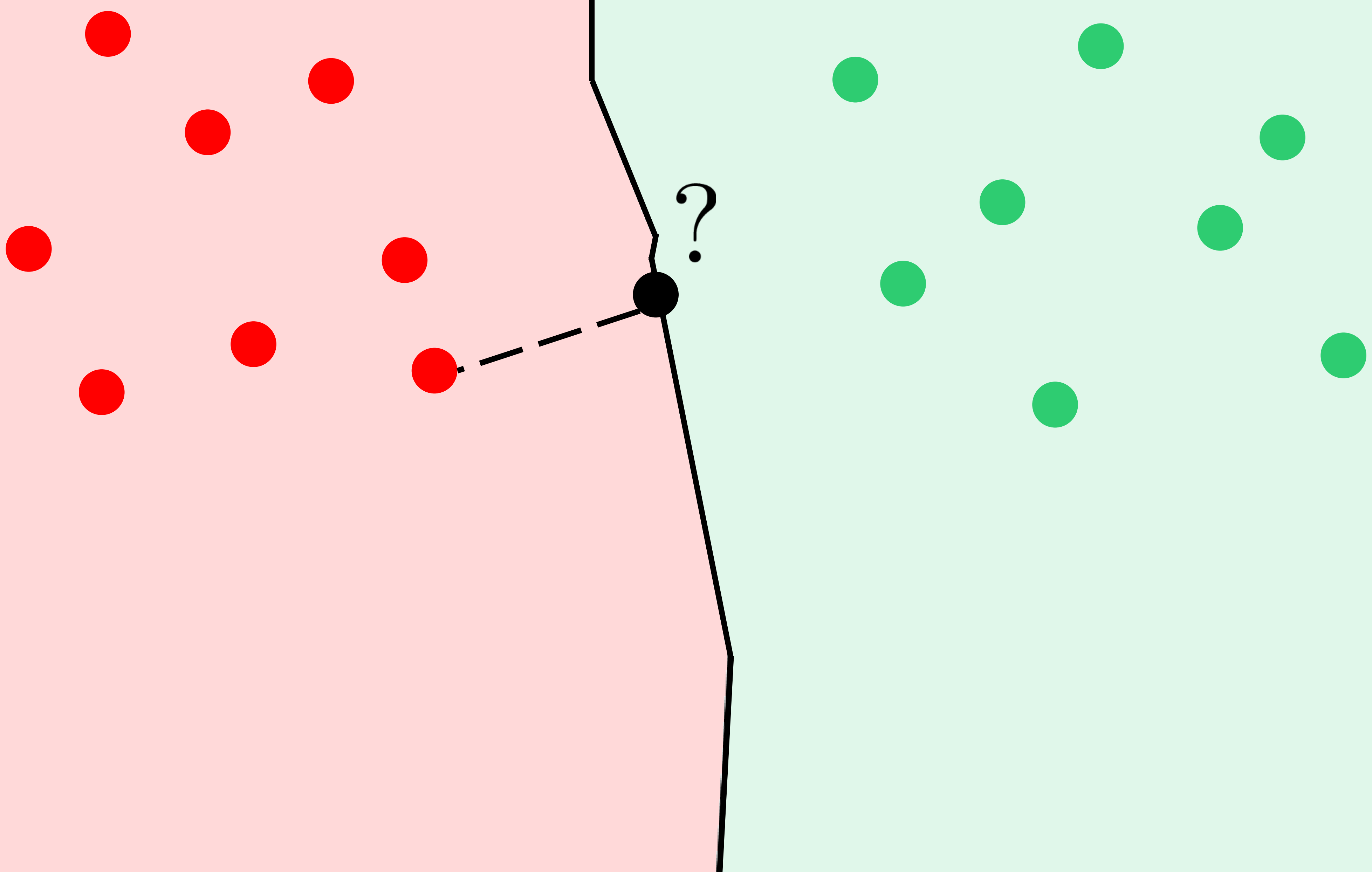

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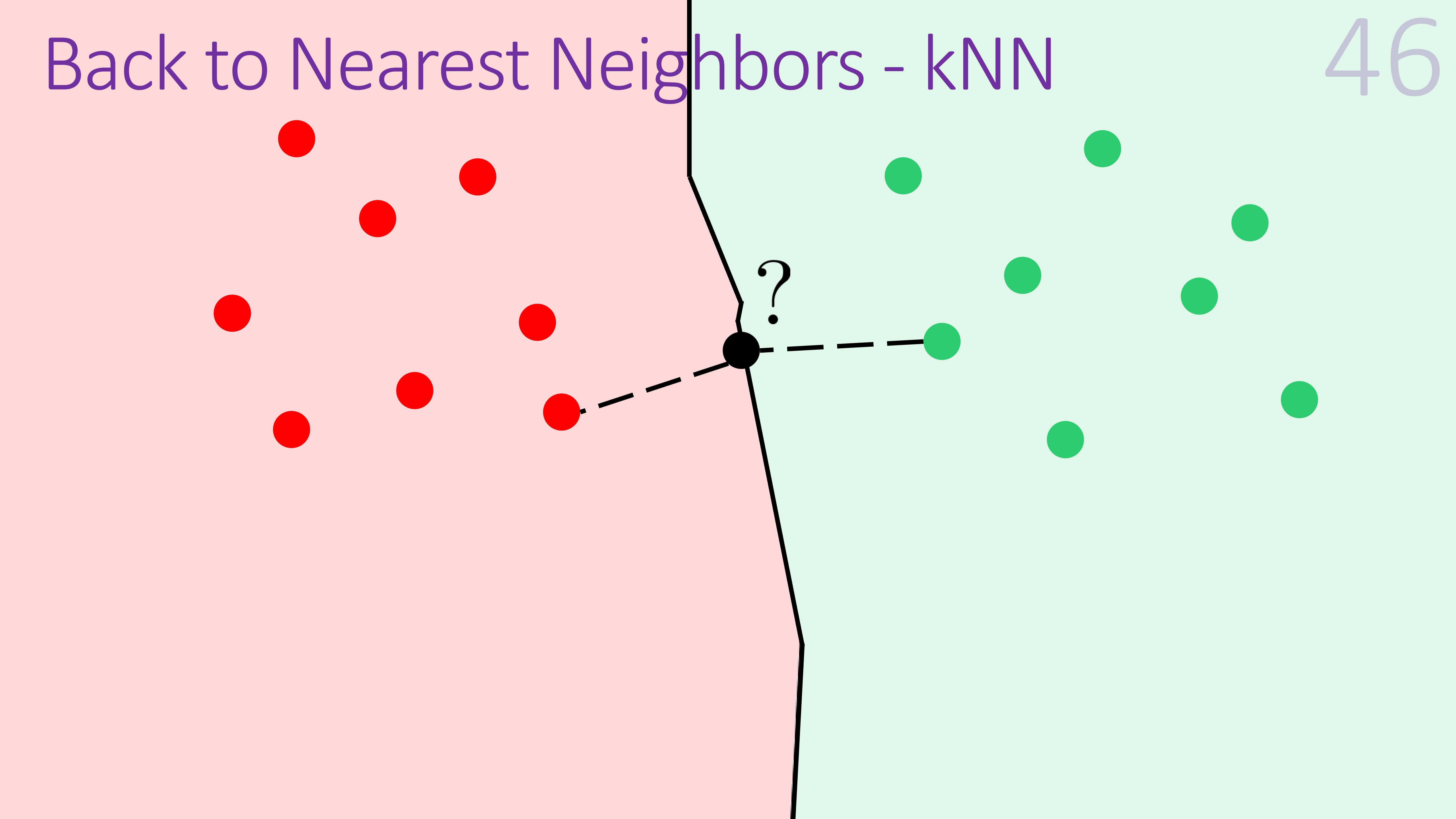

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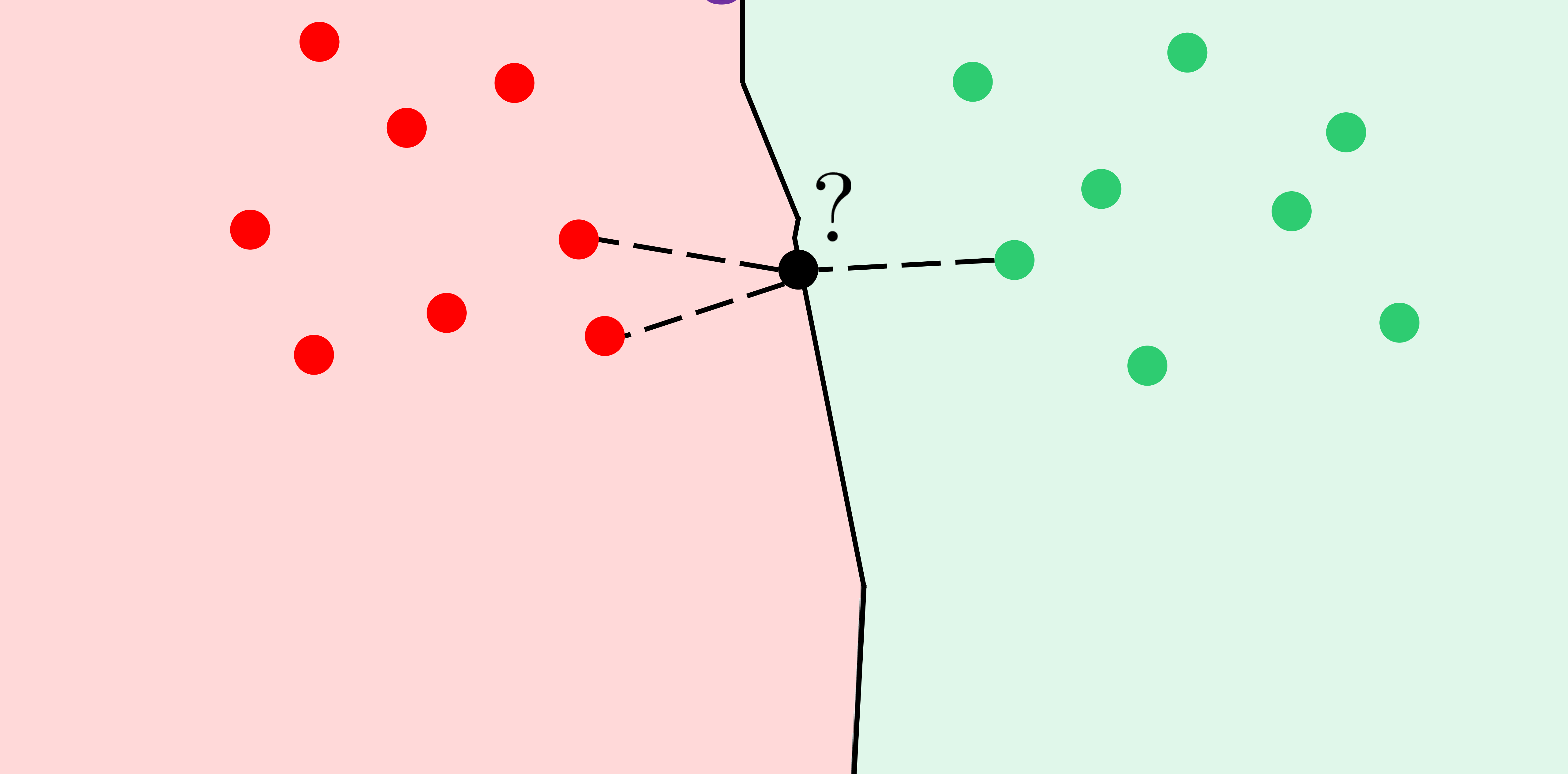

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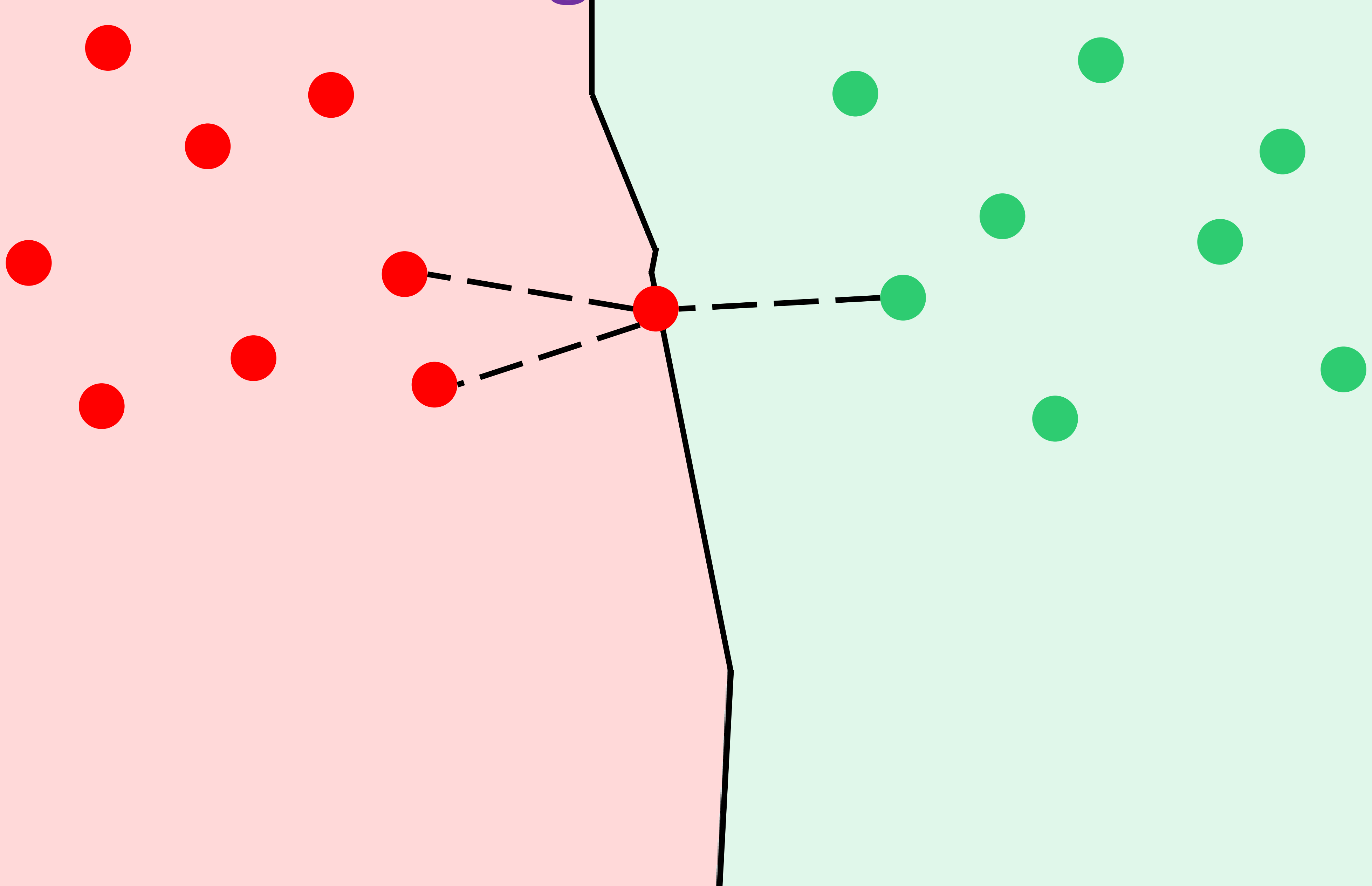

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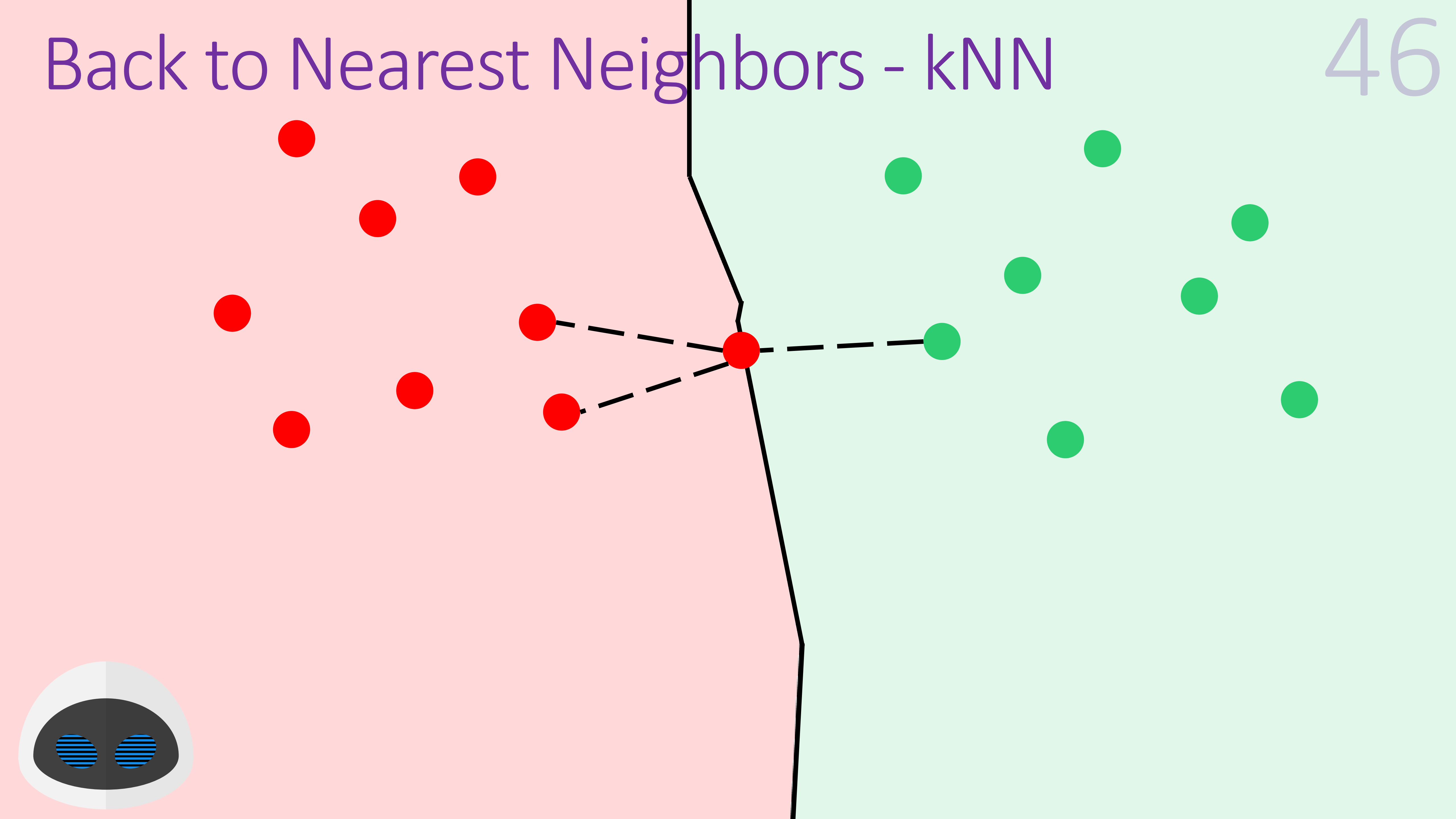

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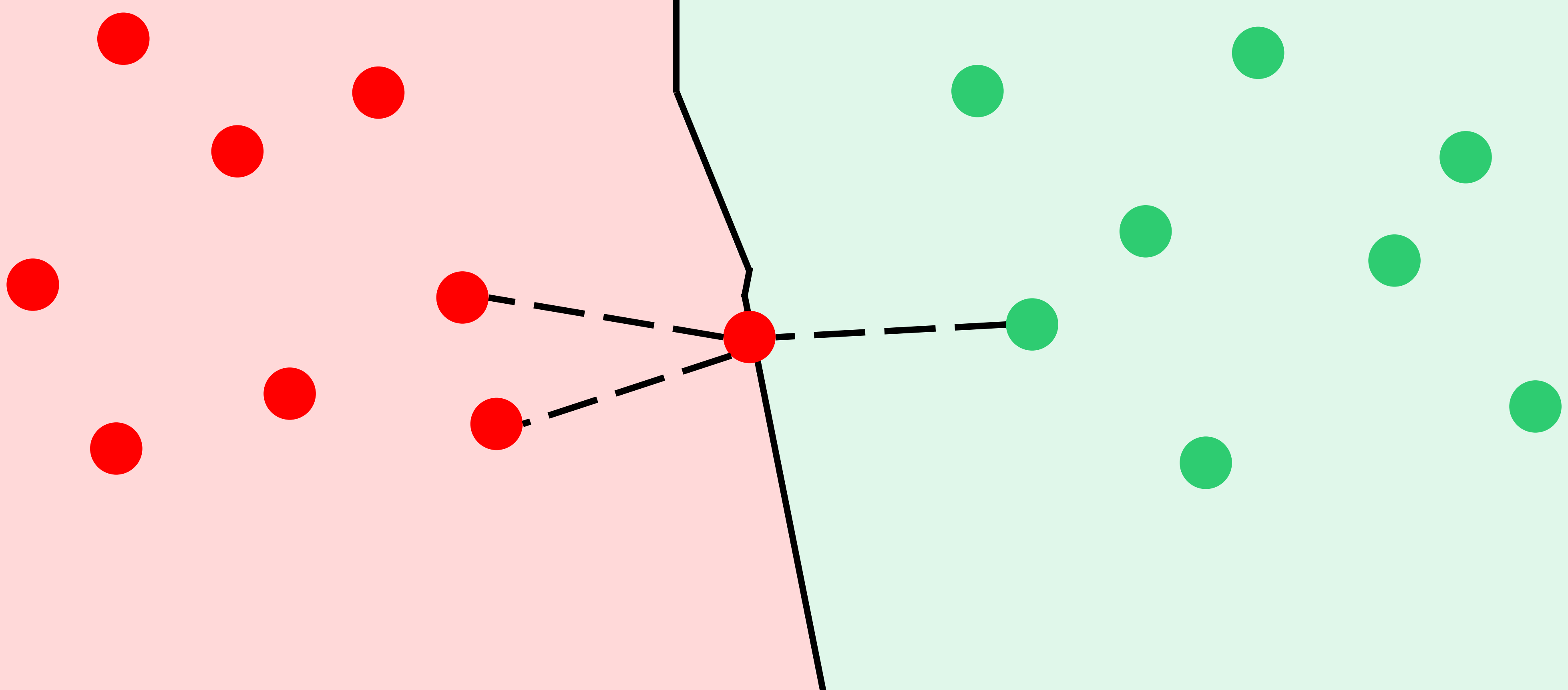

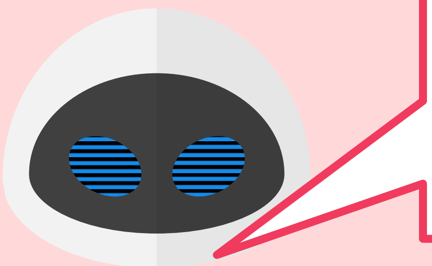

Instead of looking at just the label of the nearest neighbour, look at the labels of the k nearest neighbors and choose the one that is most popular

Back to Nearest Neighbors - rNN

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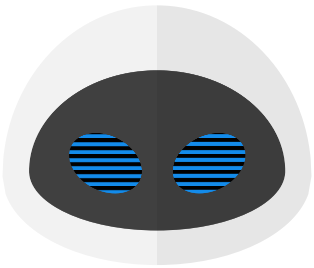

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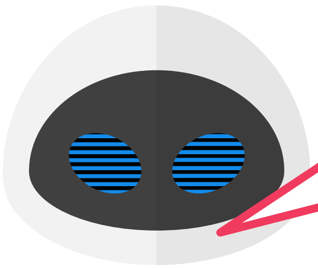
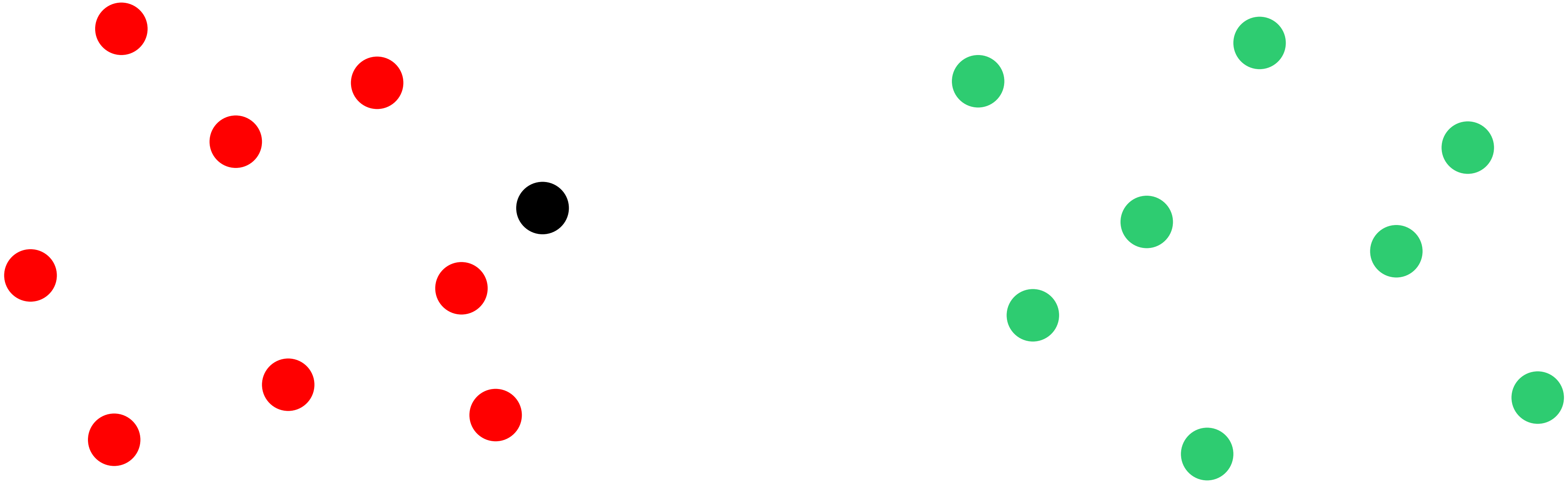
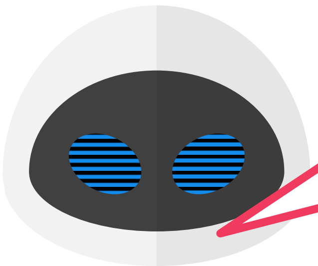


Look at all neighbors who are within an r radius of the test point and choose the label most popular among the neighbors

Back to Nearest Neighbors - rNN





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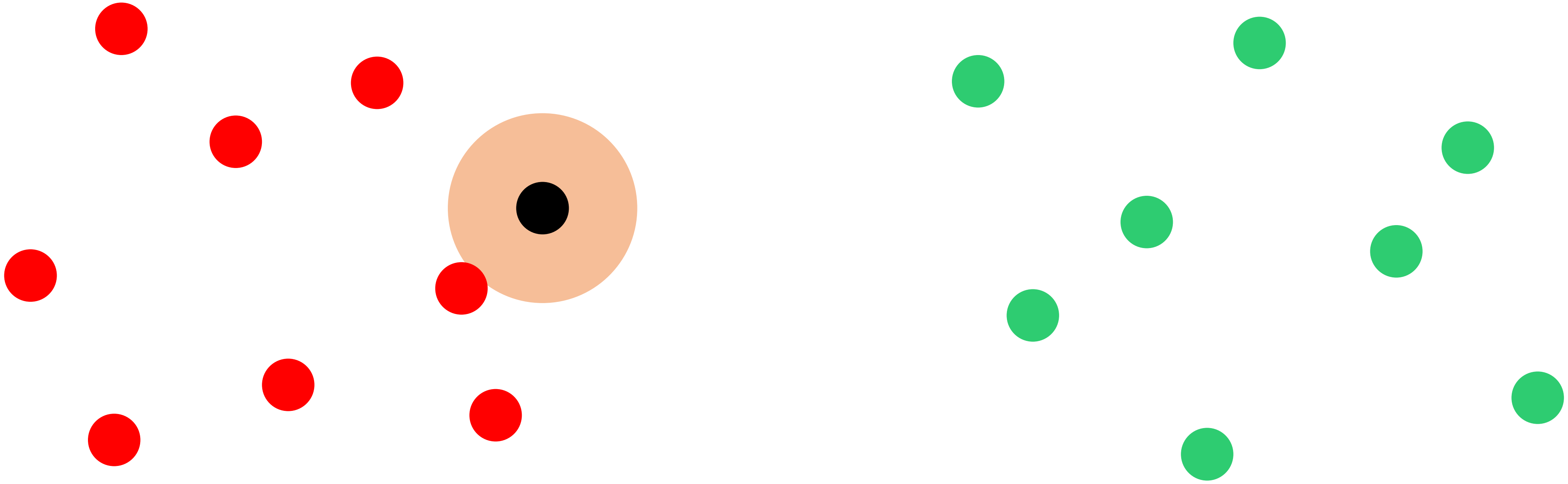

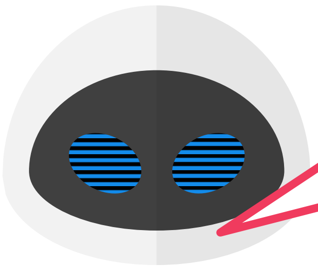

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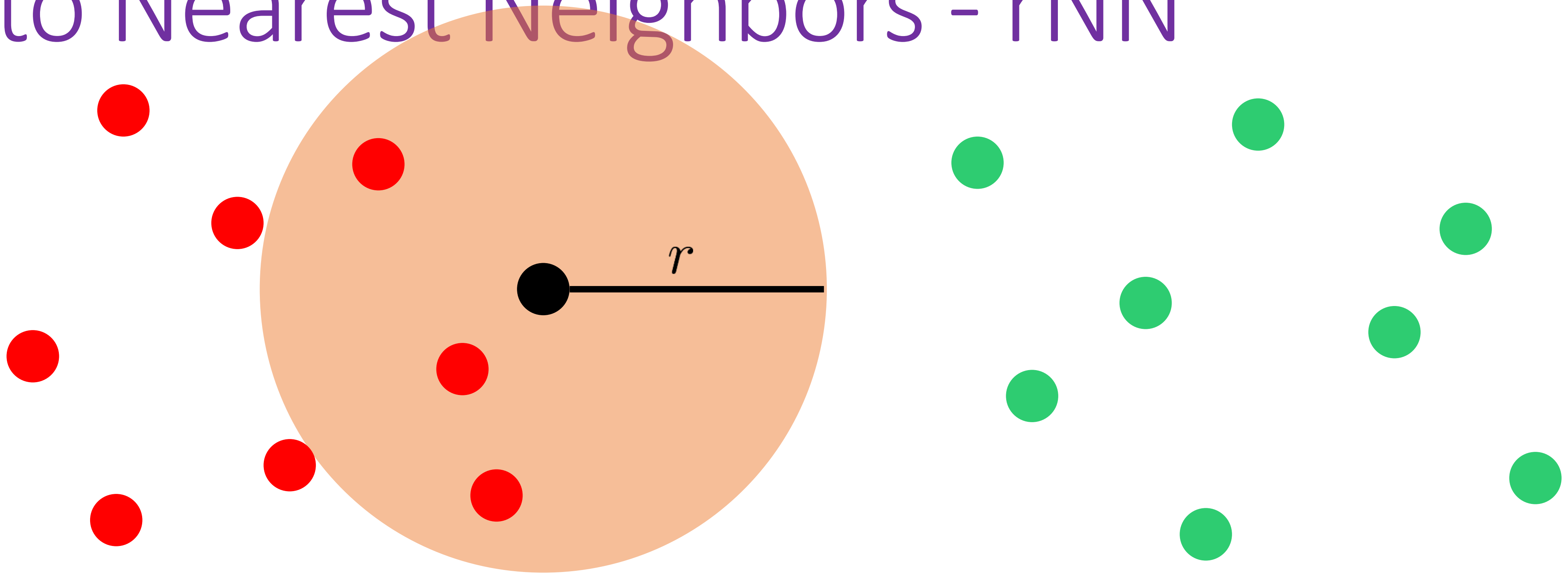

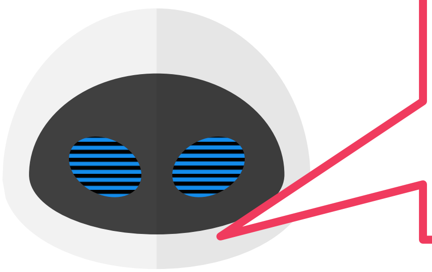

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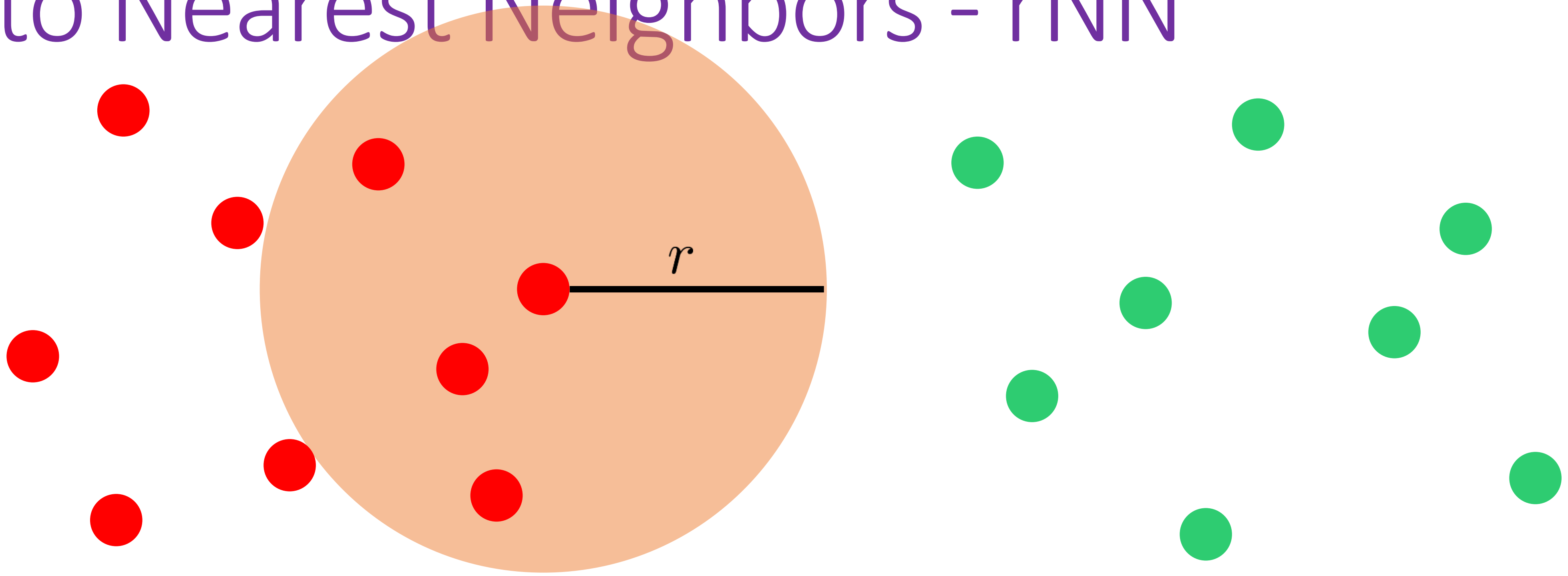

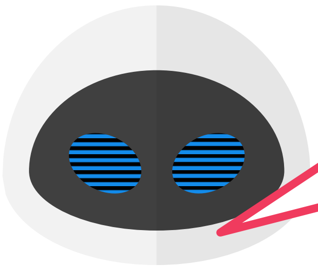

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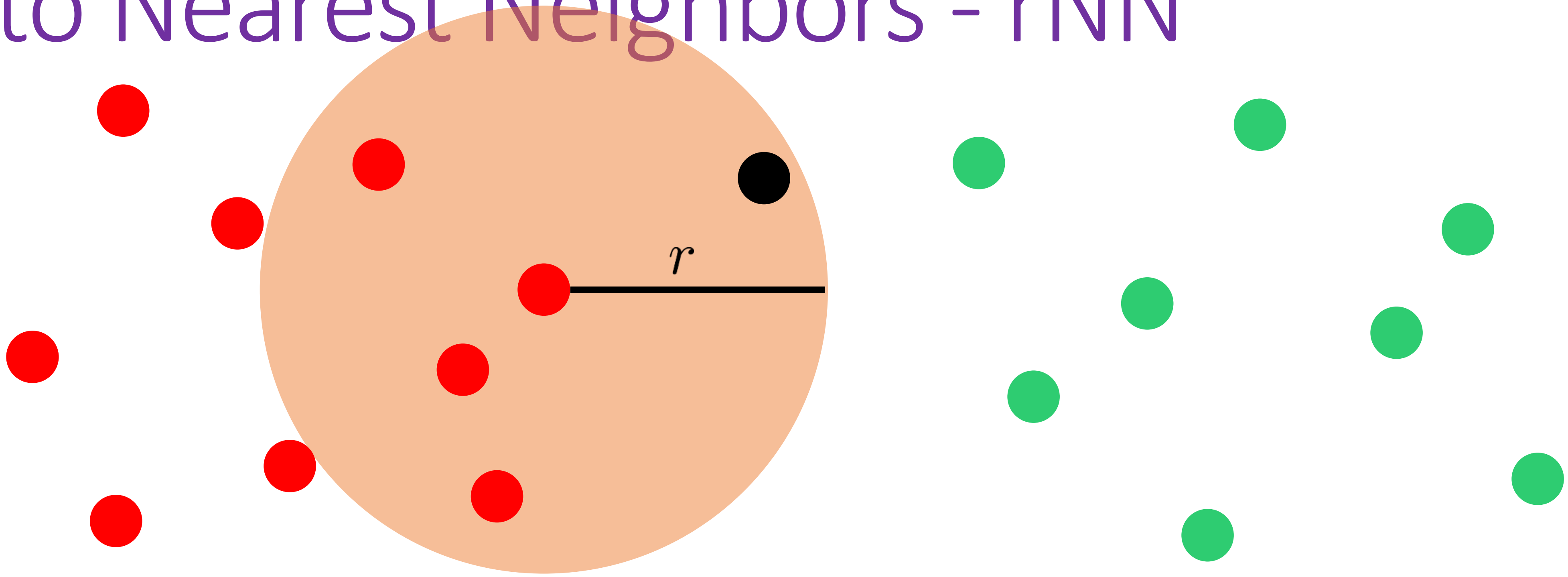

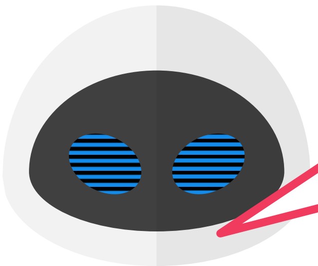

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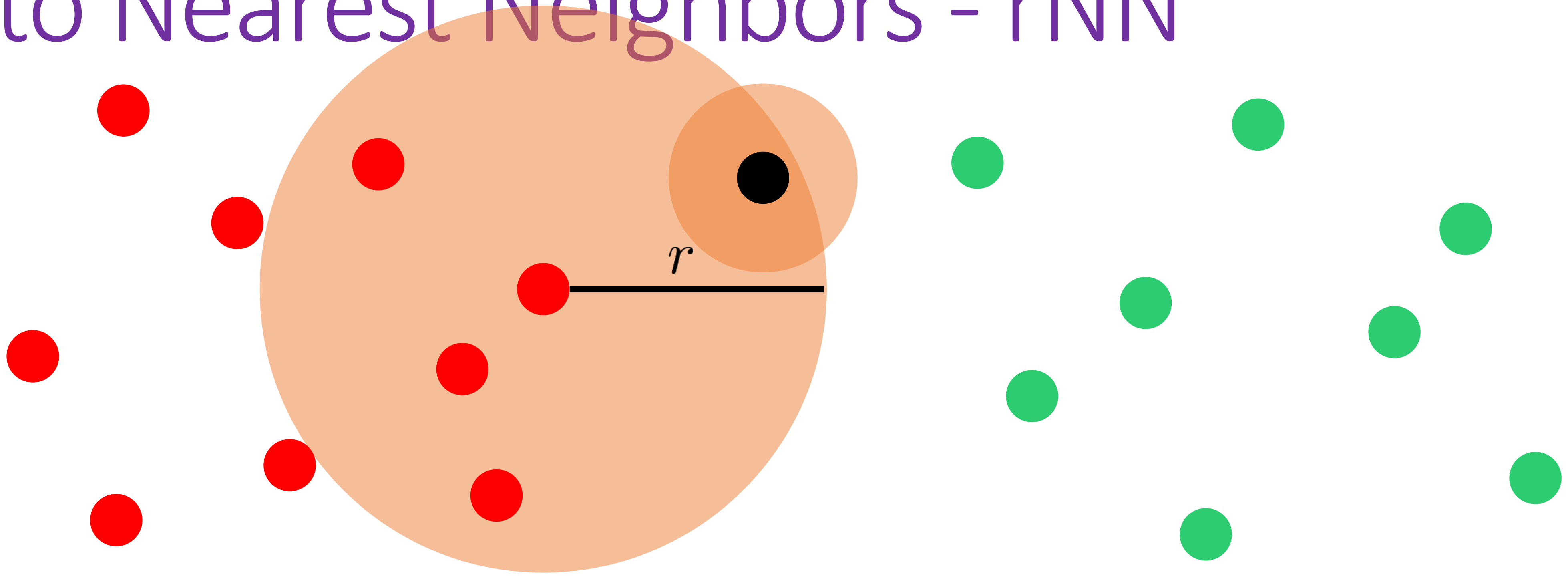

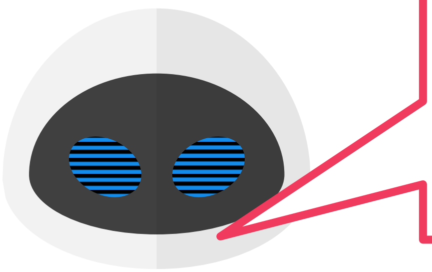

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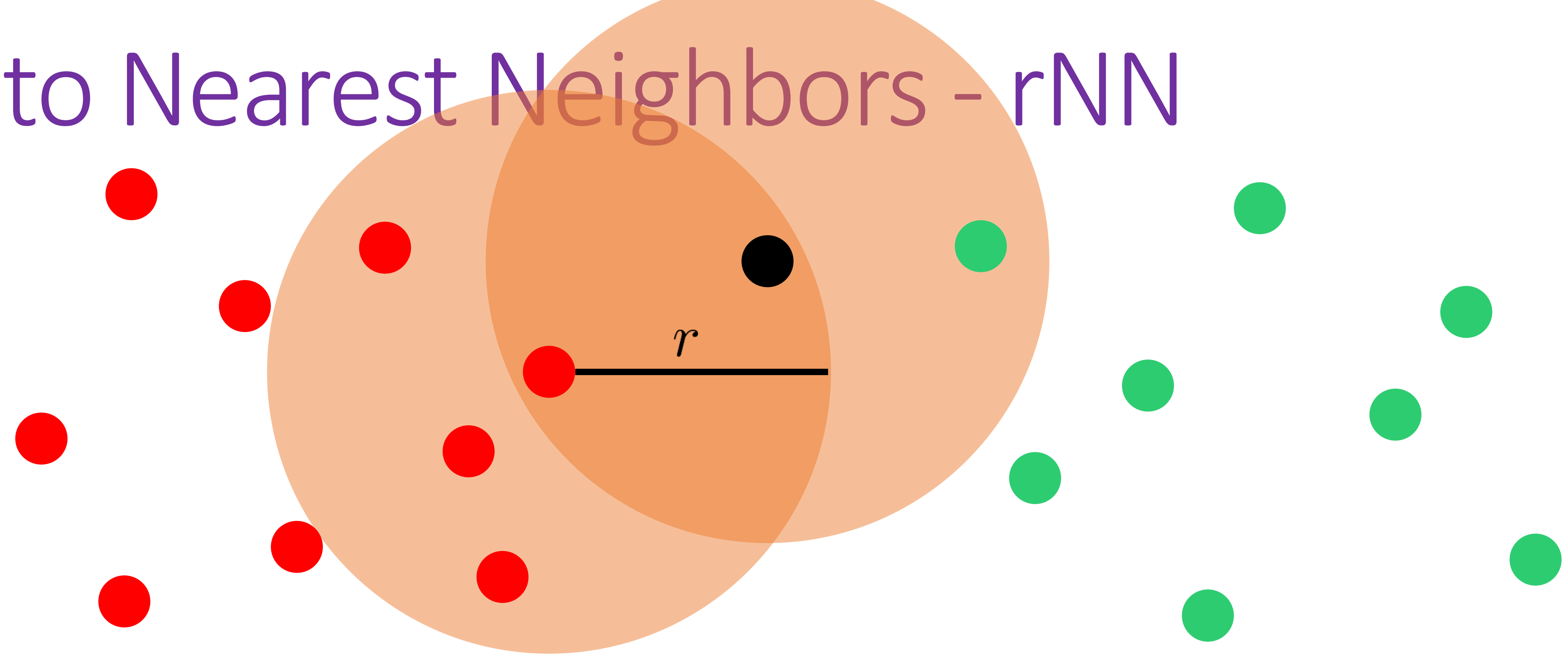

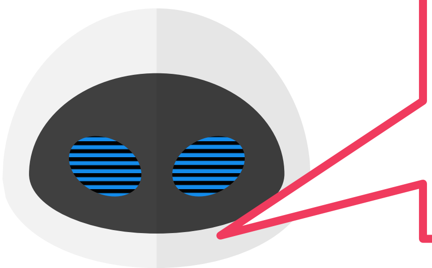

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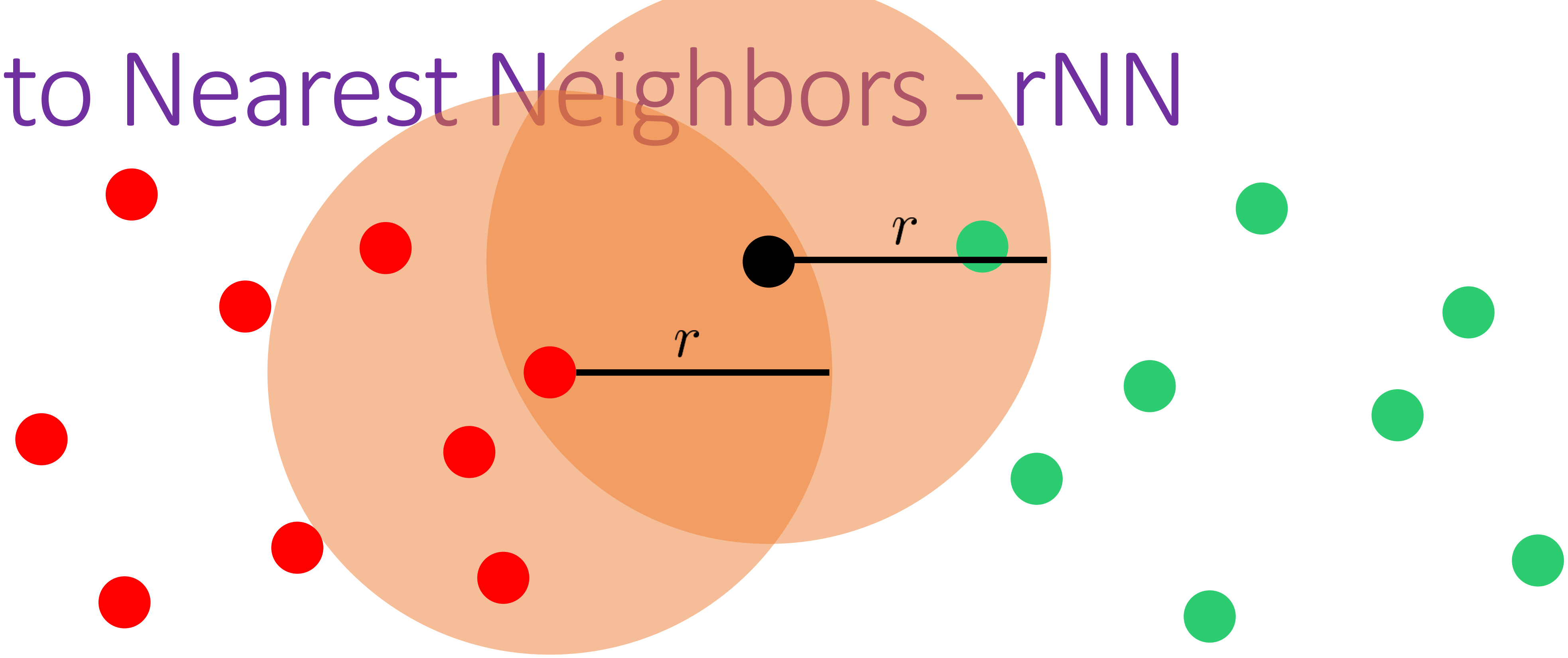

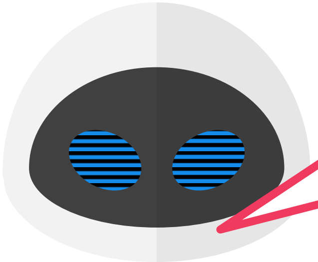

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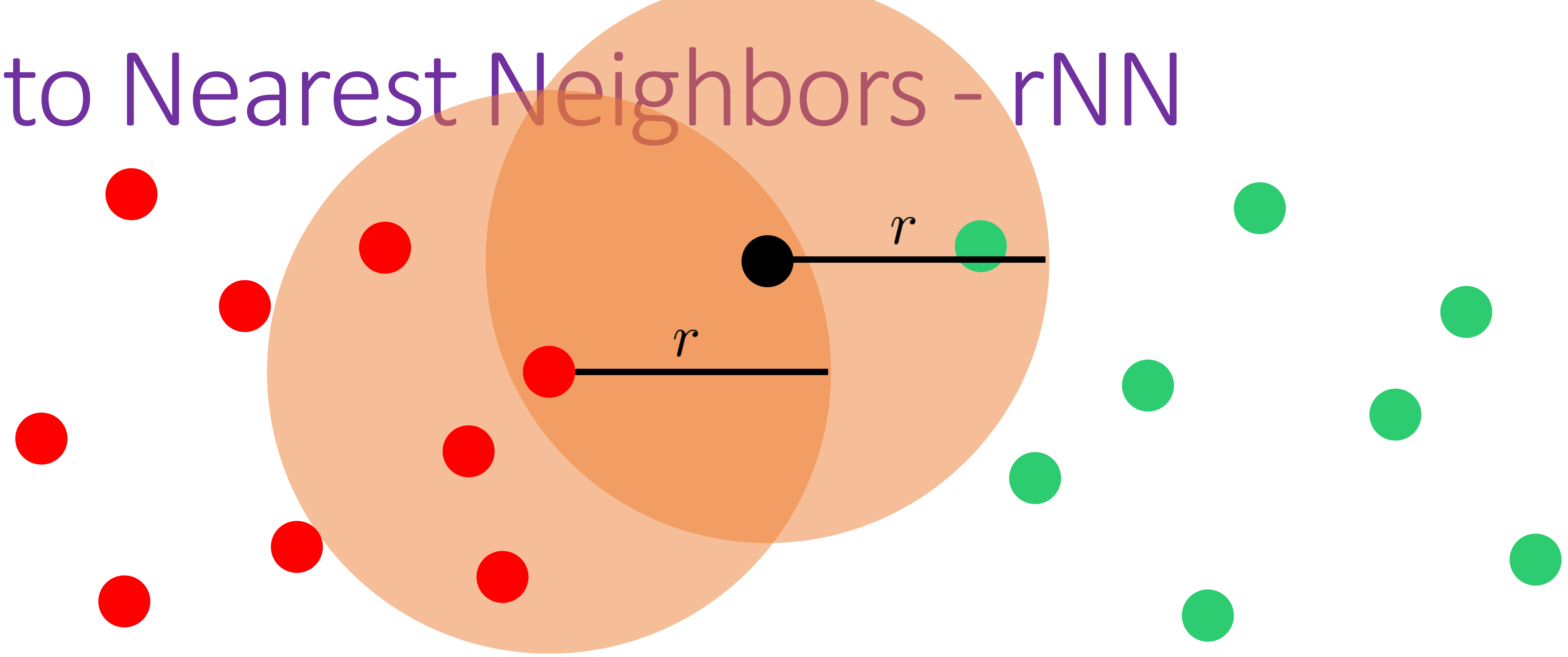

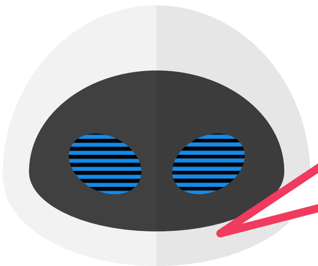

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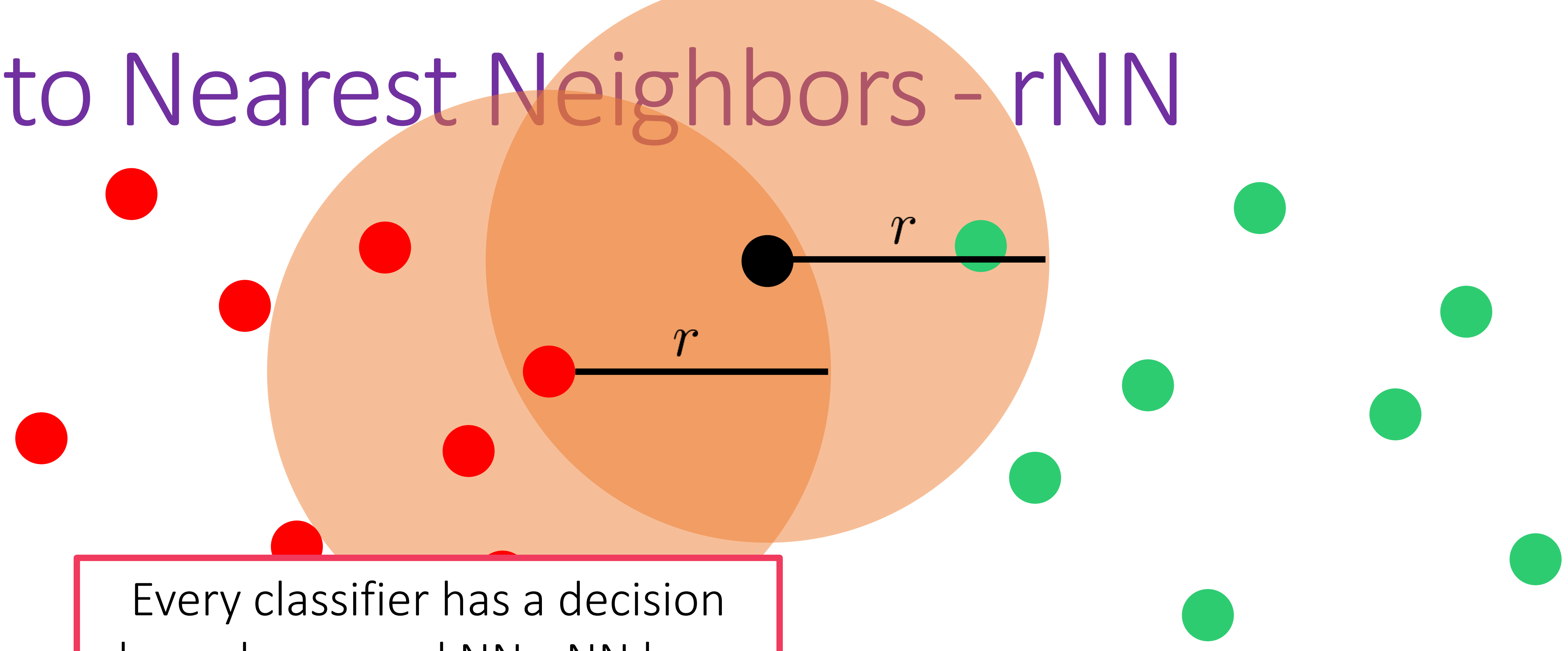

Every classifier has a decision boundary even kNN, rNN have some decision boundary (which we hope are better than 1NN's)

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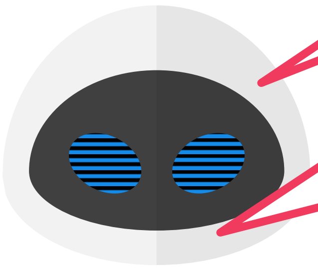
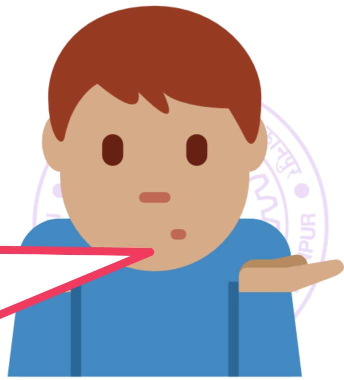


How should I decide which value of k or r to use? Also, should I use kNN or rNN?



Hyperparameter Tuning in ML

Constants like k in kNN, r in rNN, or even the metric to use in LwP are called *hyperparameters* of an ML algorithm

Just a fancy name (model vectors like $\mathbf{w}$ are called *parameters*)

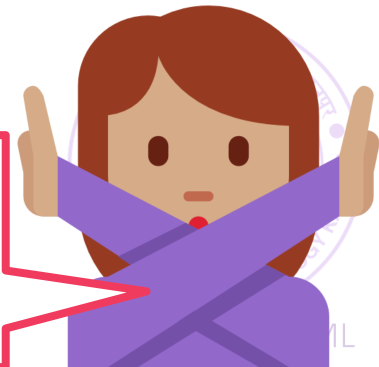
We usually tune these hyperparameters by setting them to a value that gives us highest test accuracy

Take out a part of the training data and pretend it is test data for the purpose of hyperparameter tuning ☺

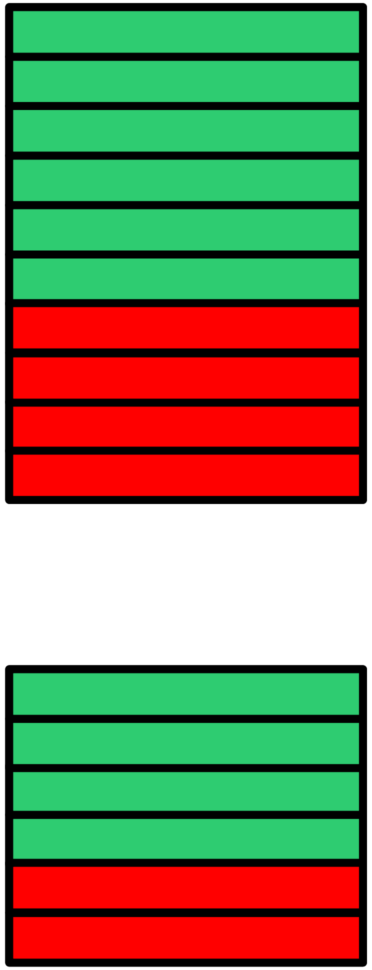
This part of data that is a mock test for us is called *validation data*

Let us look at the two most popular ways of creating such validation datasets

Looking at test data during training is an execution-worthy crime!



Held-out Validation



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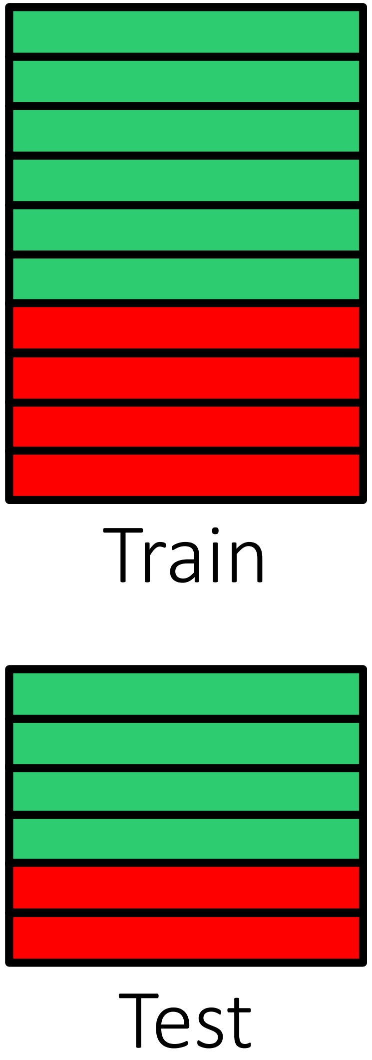

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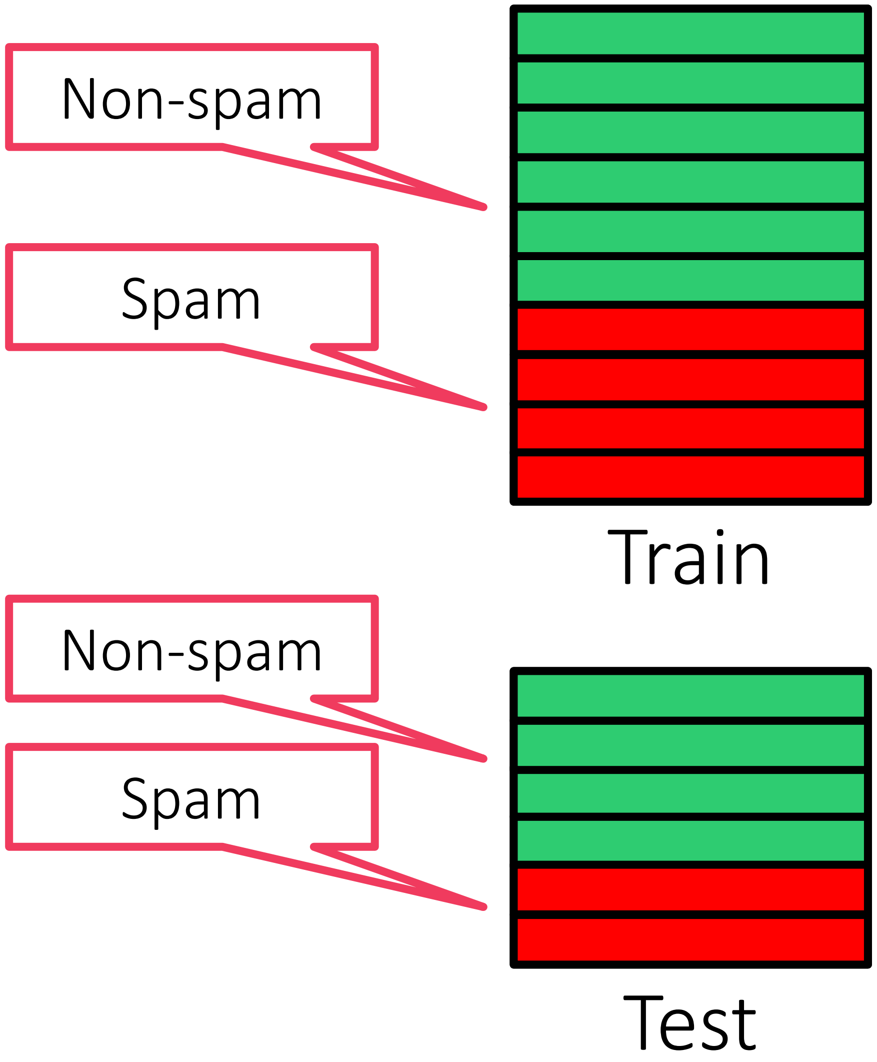

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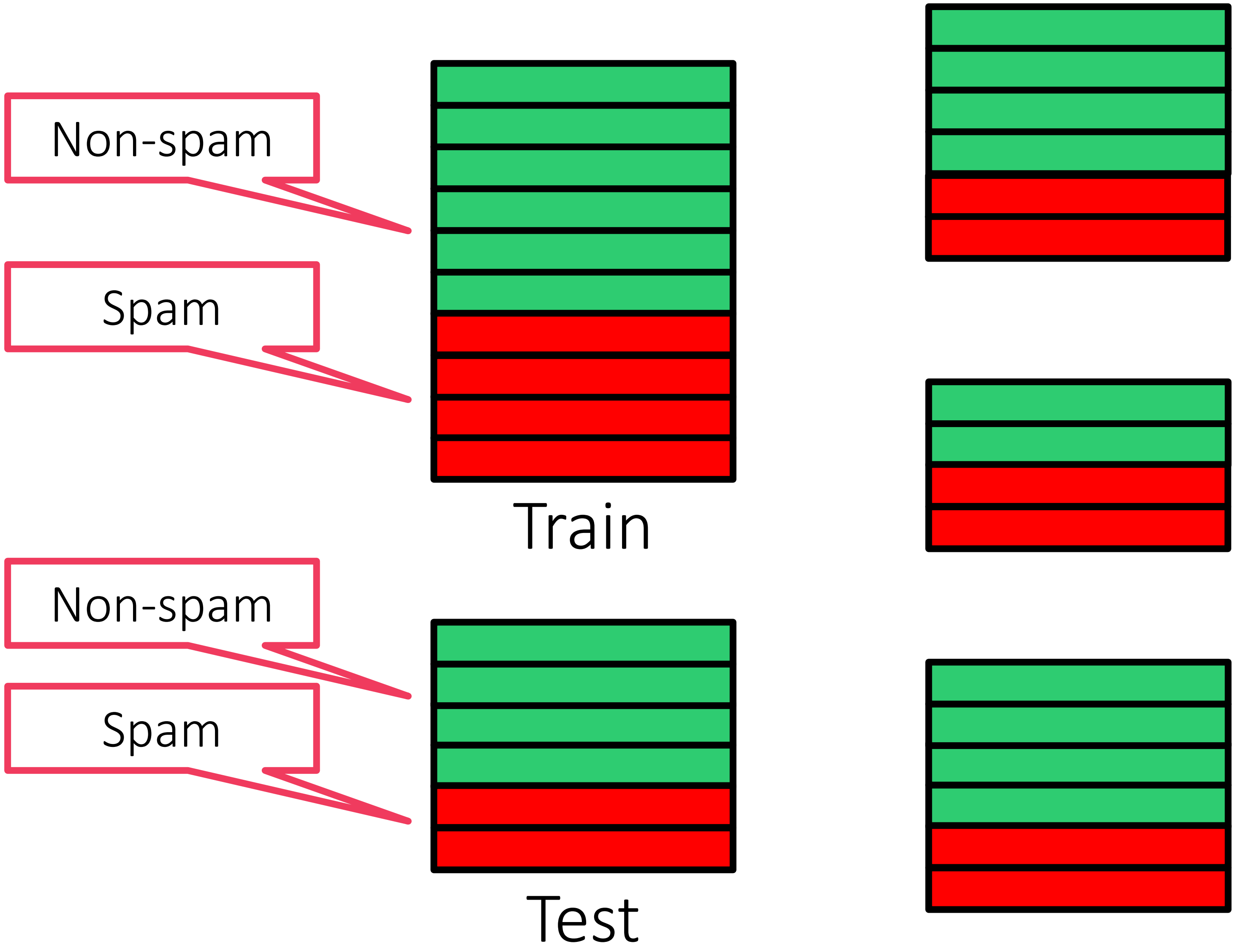

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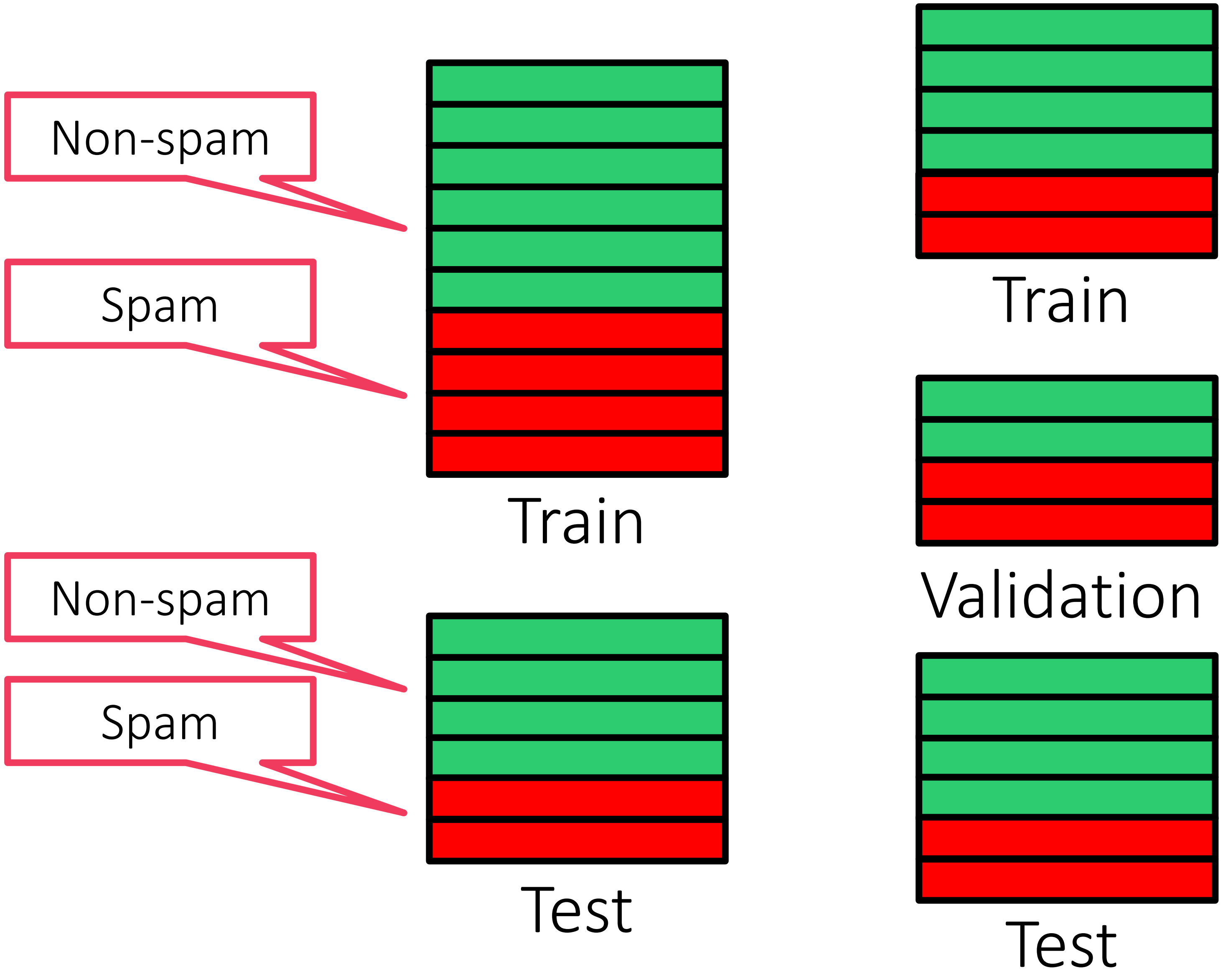

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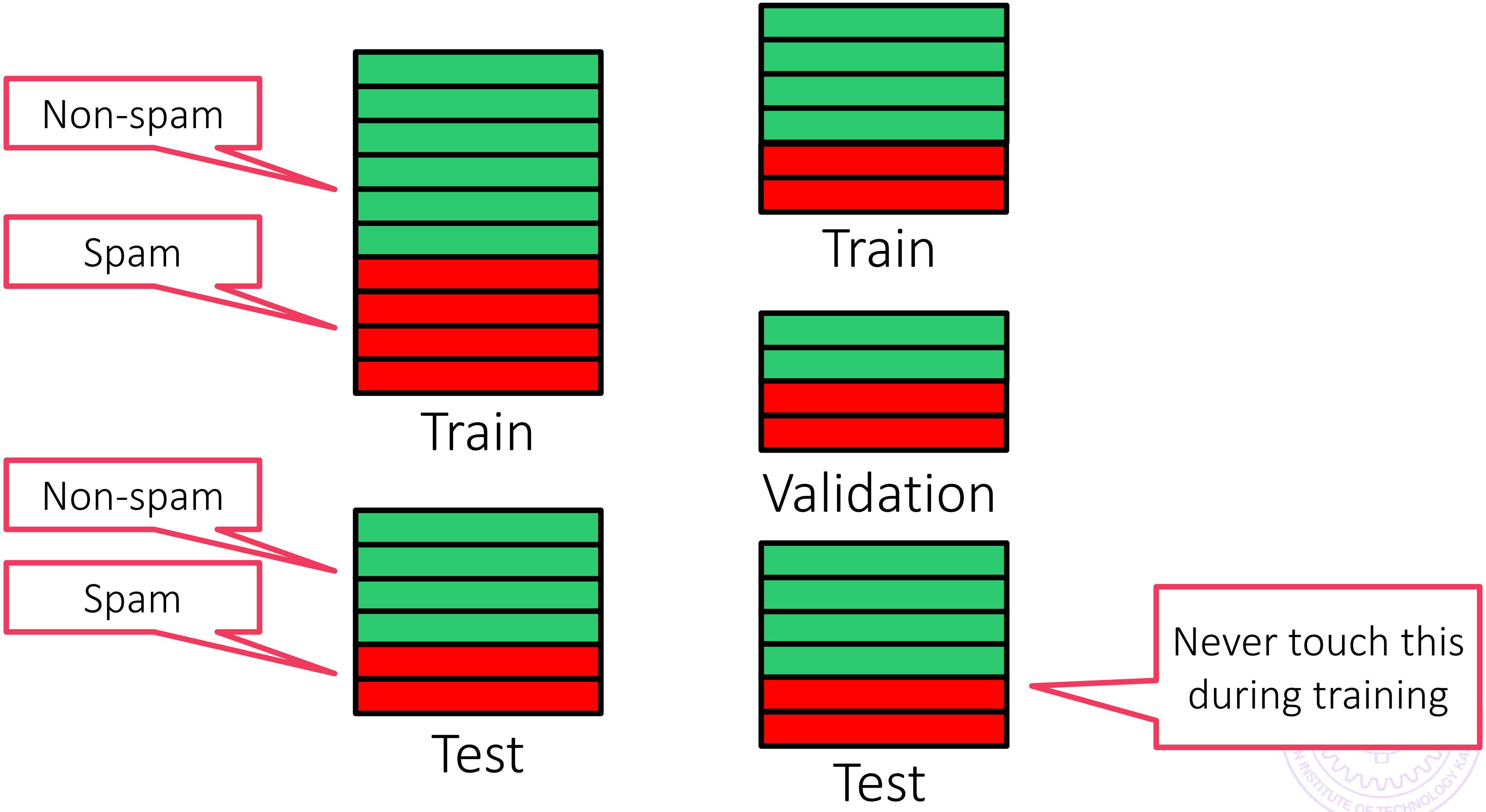

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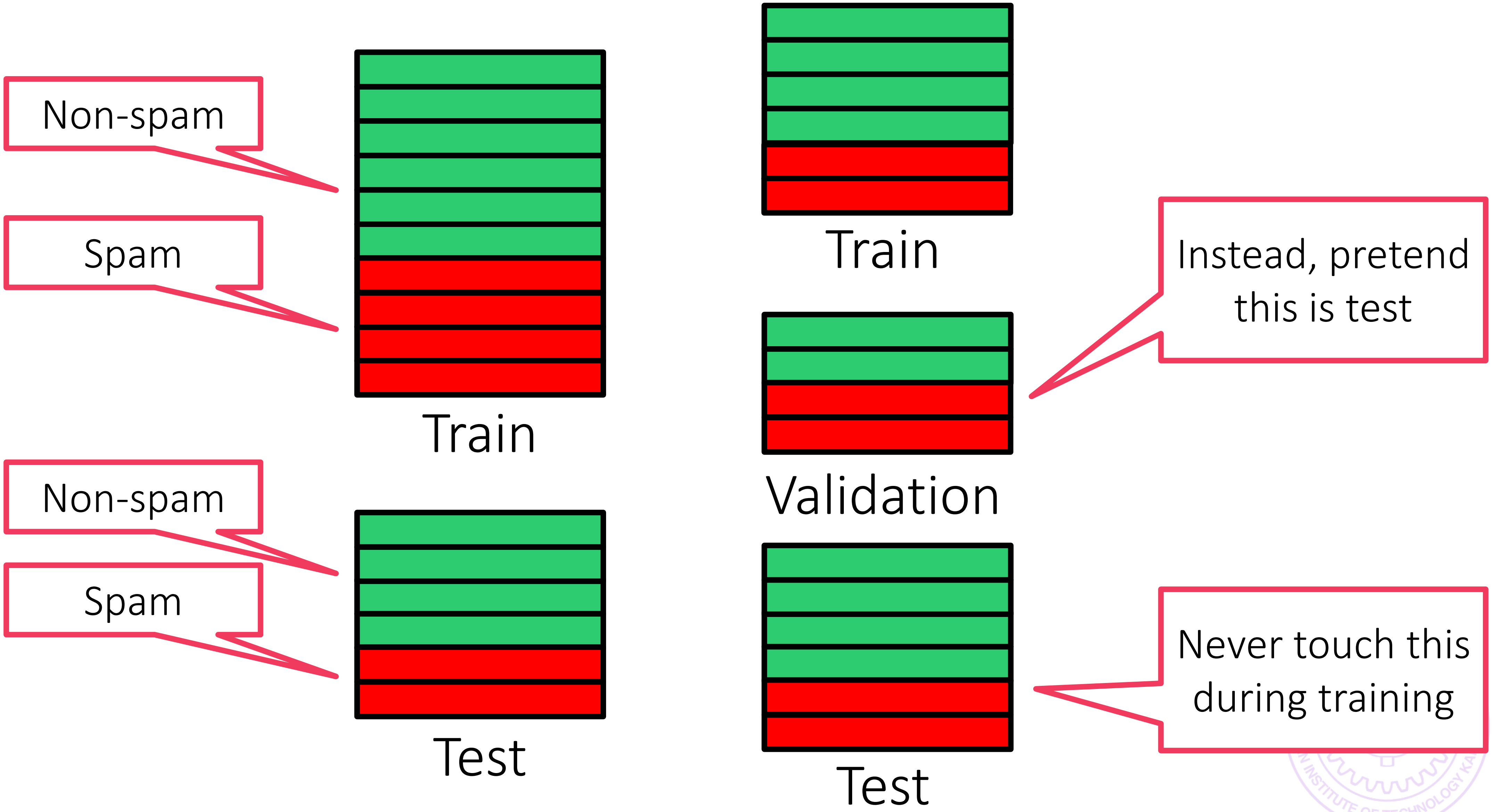
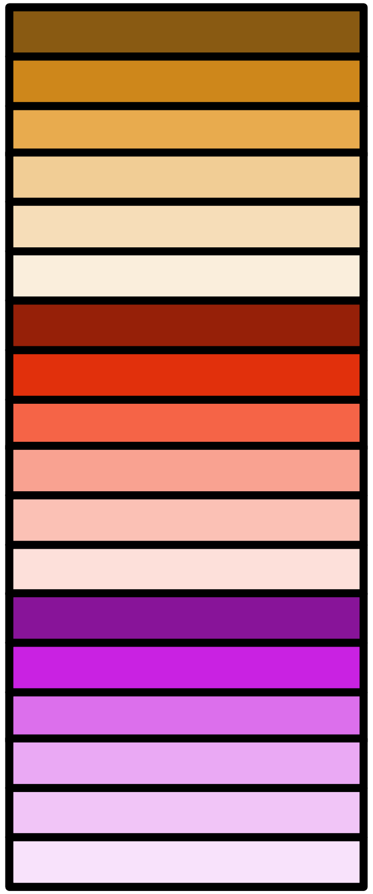


Multi-*fold* Cross Validation



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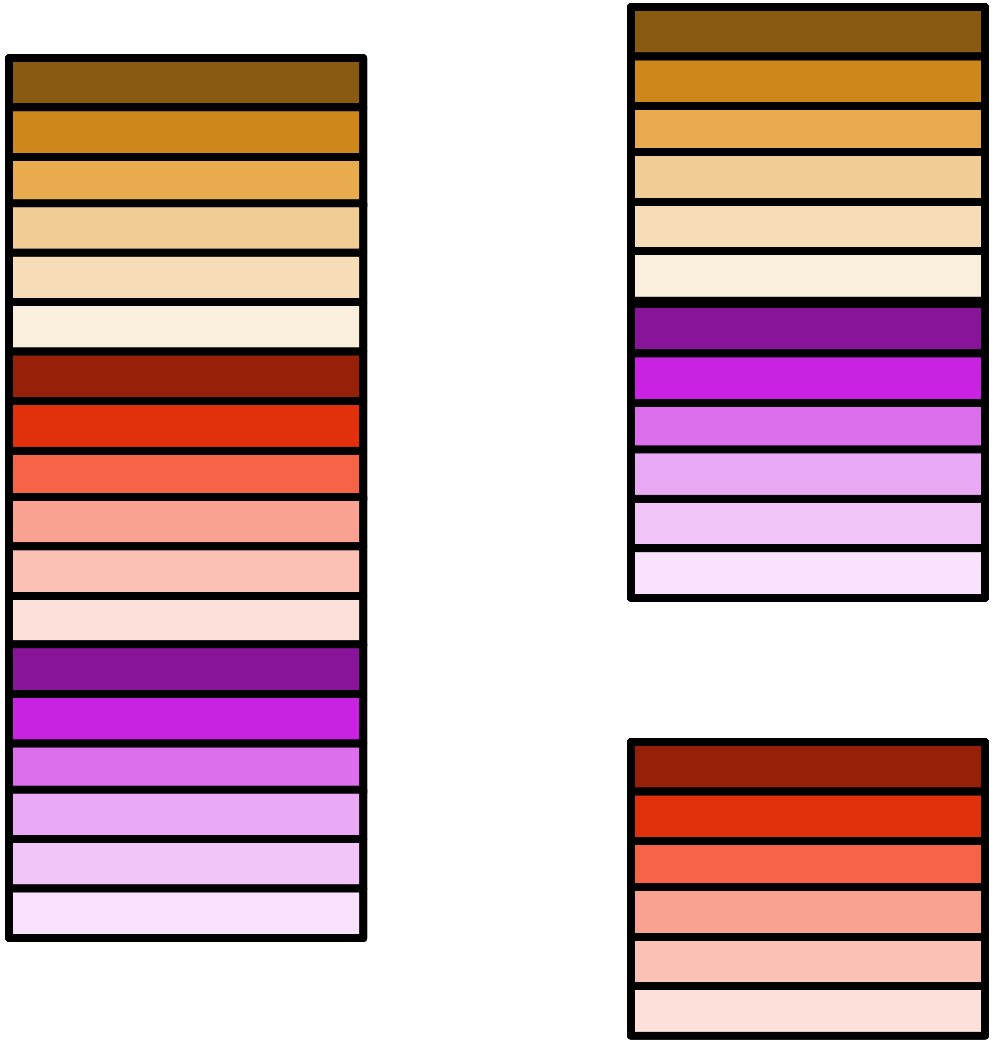

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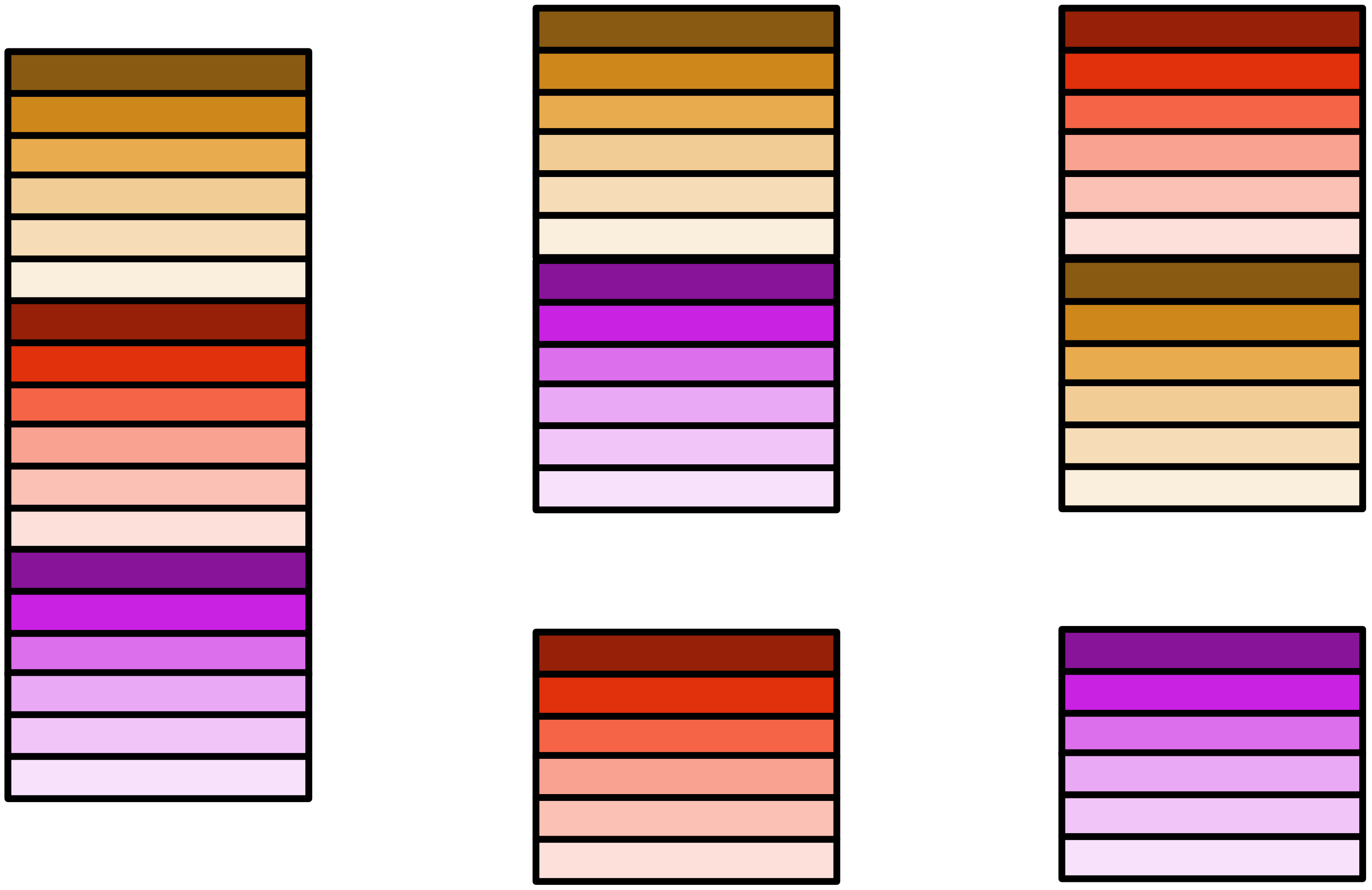

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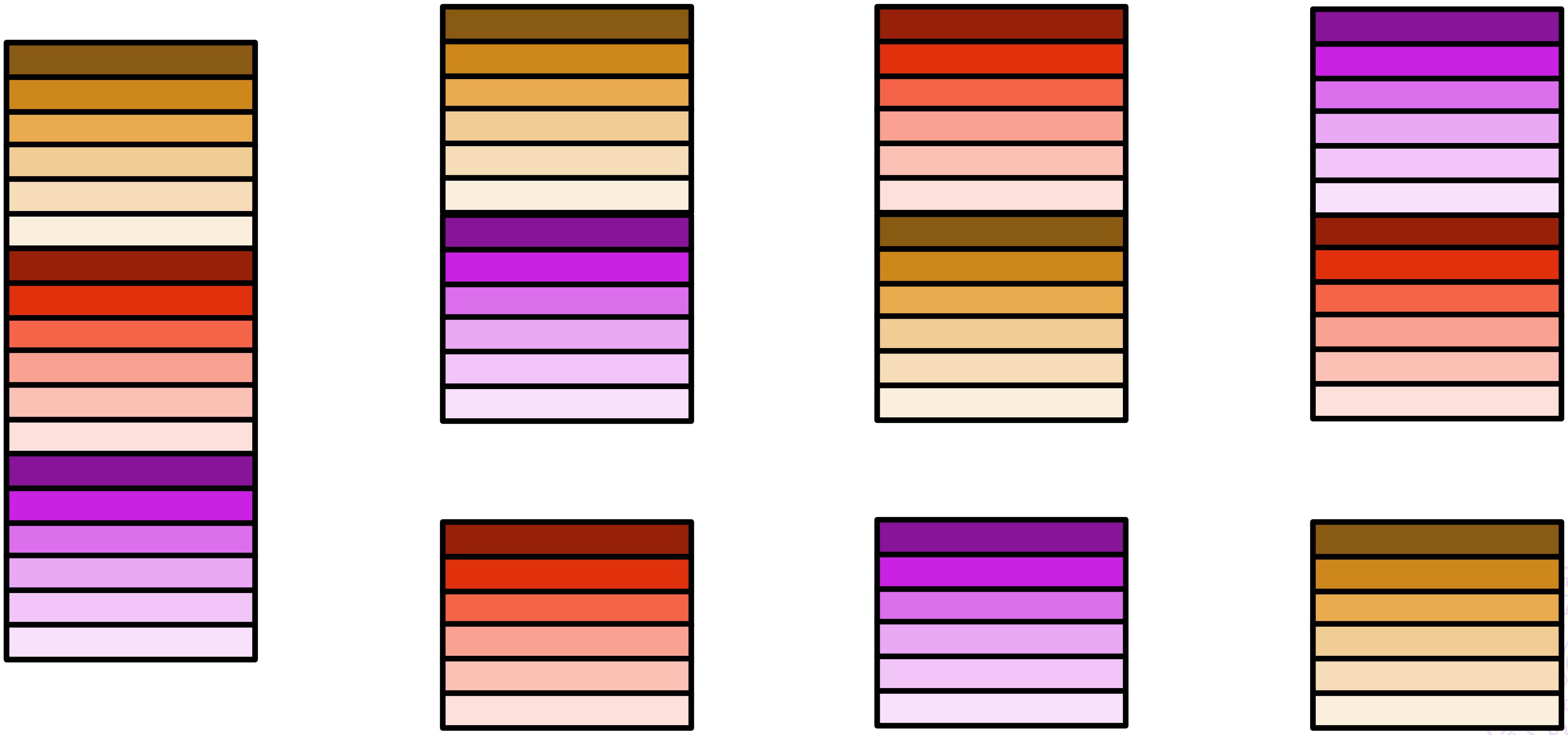

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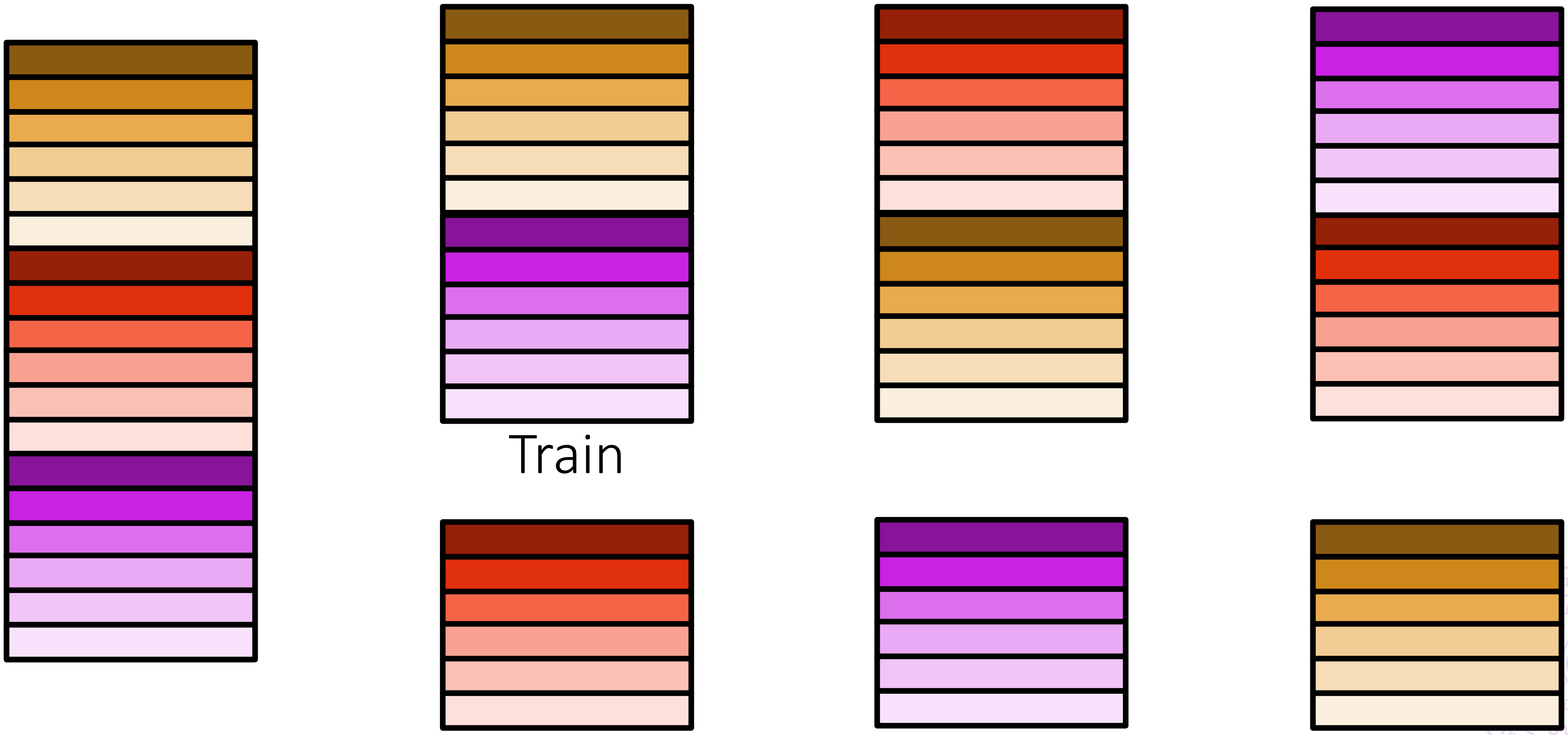

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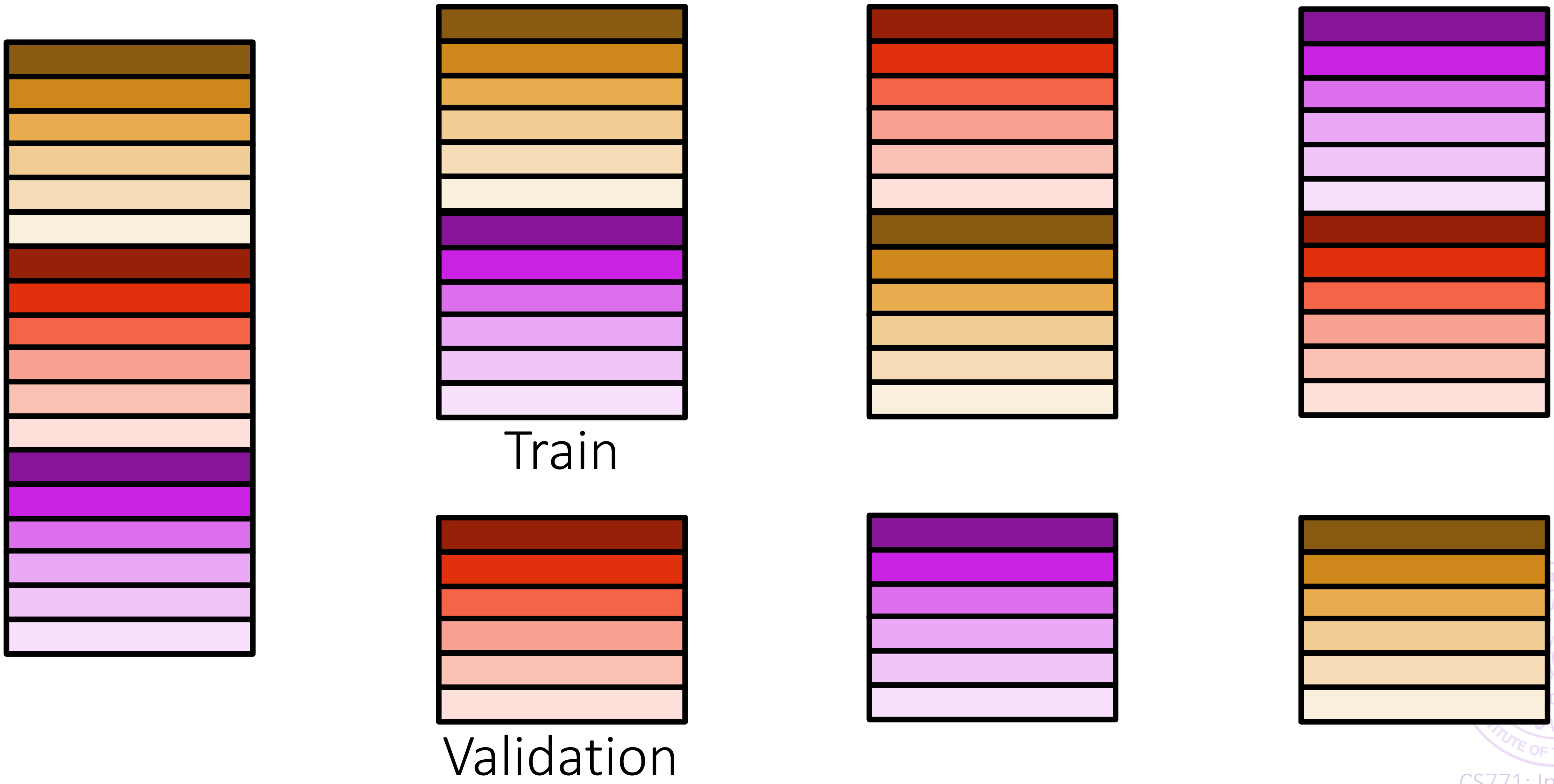

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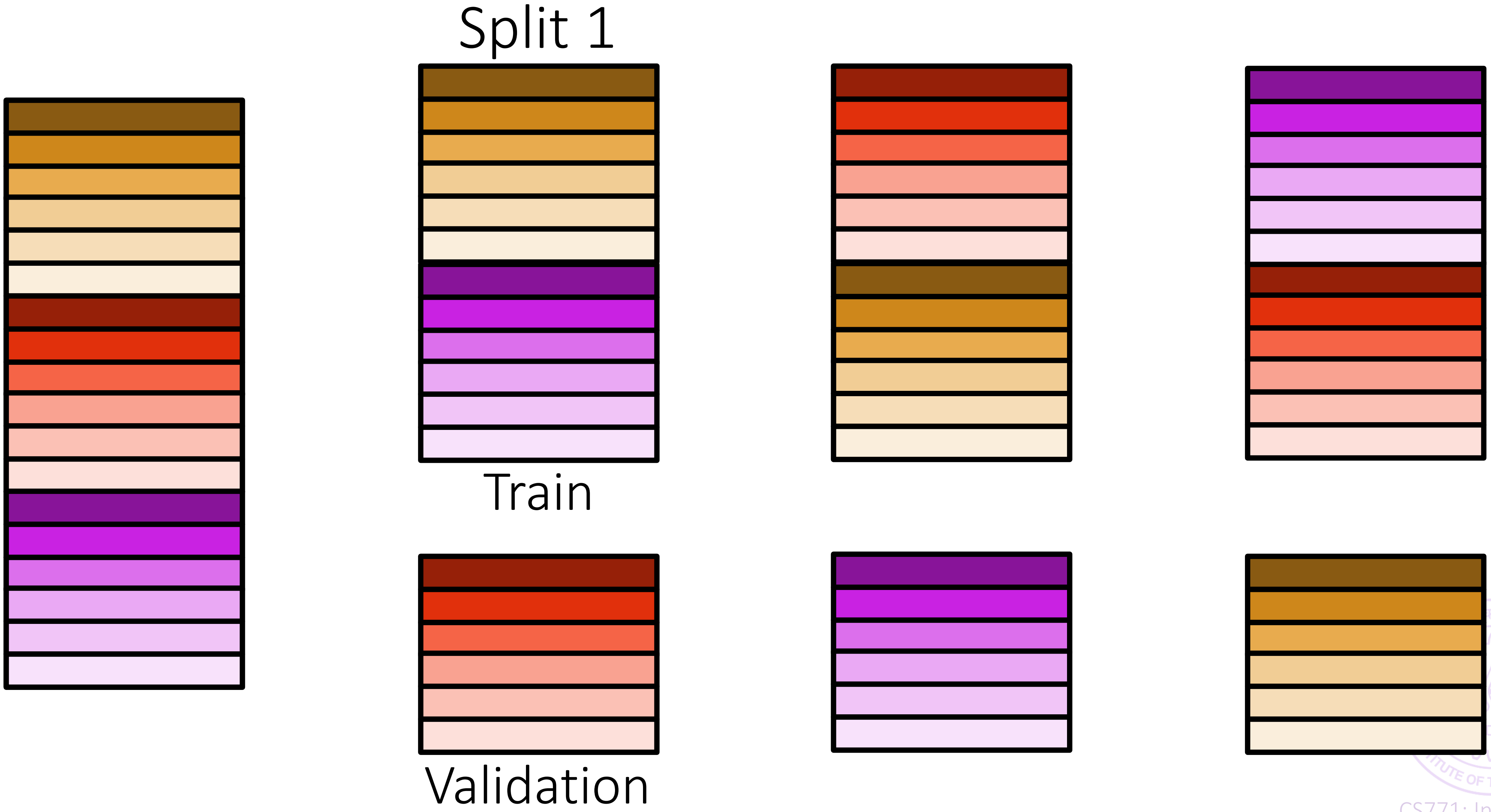

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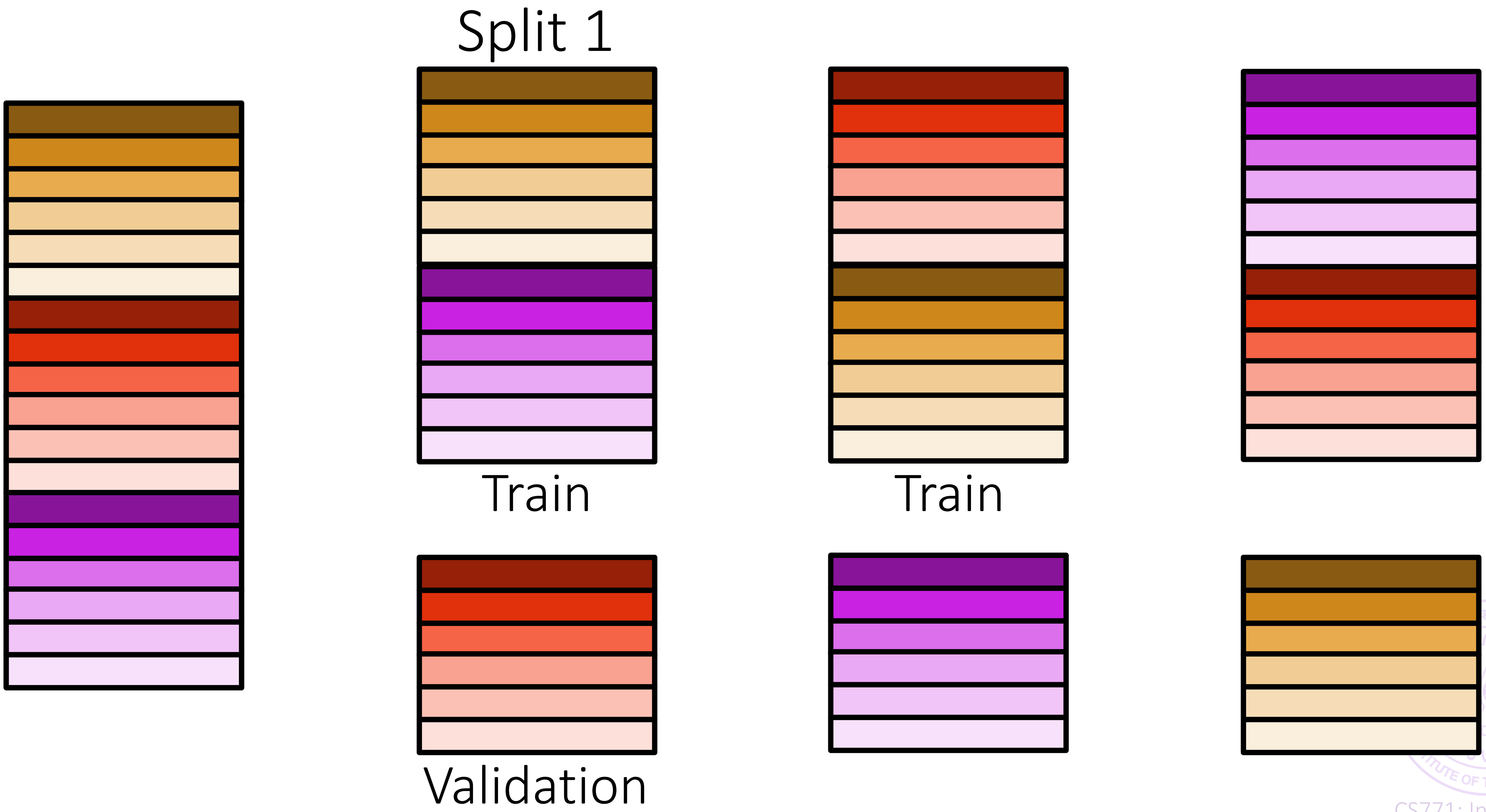

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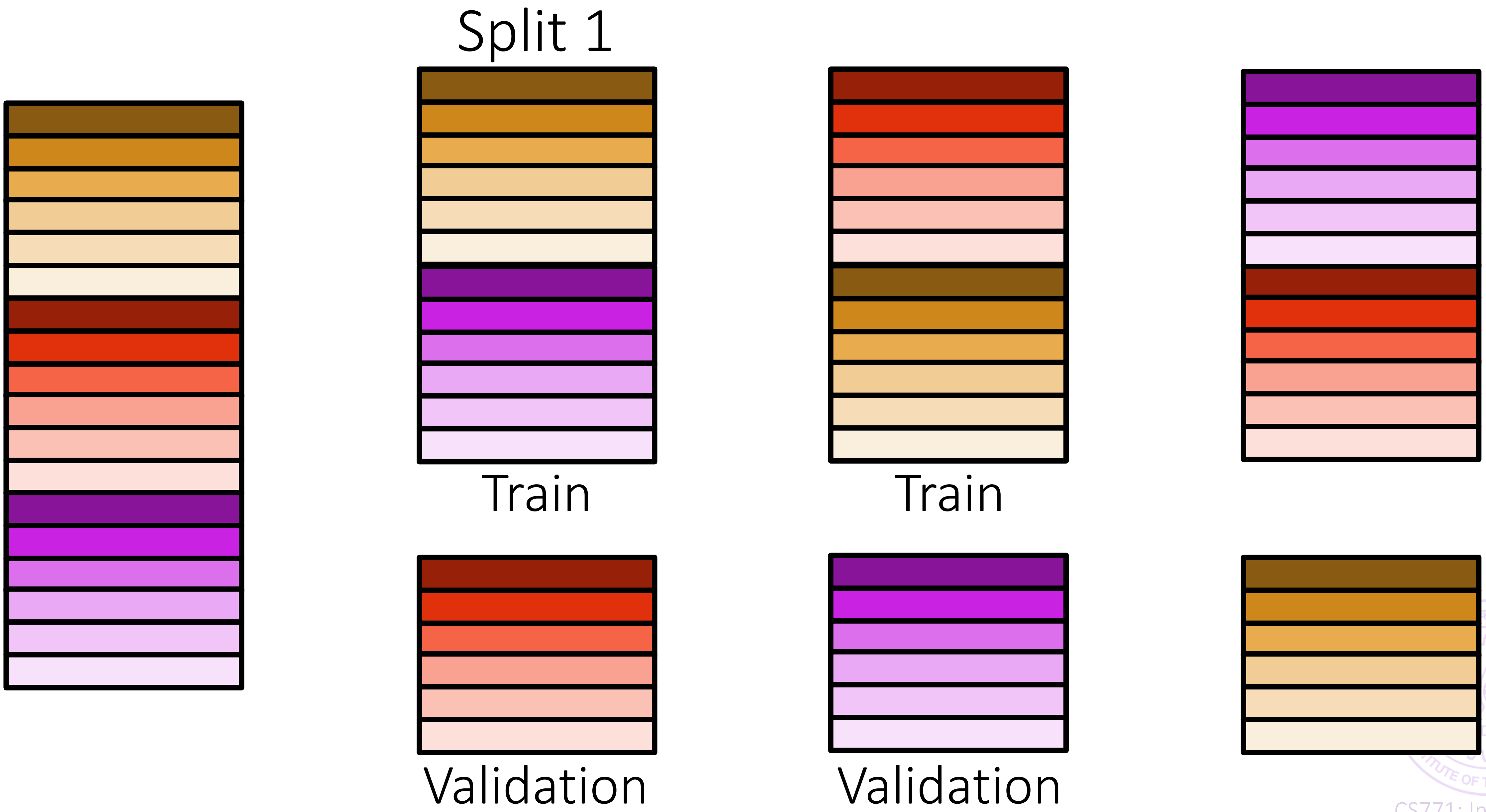

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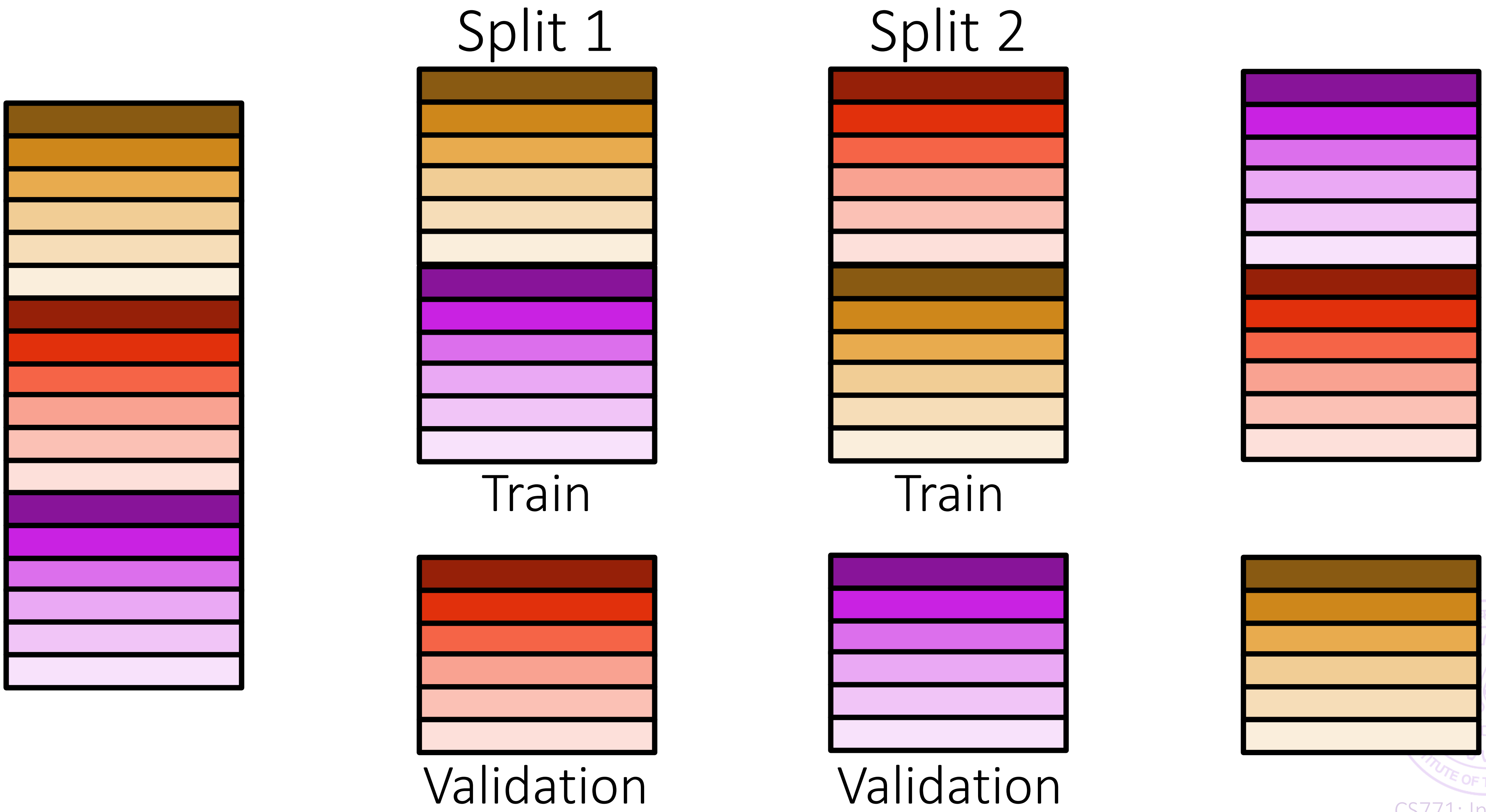

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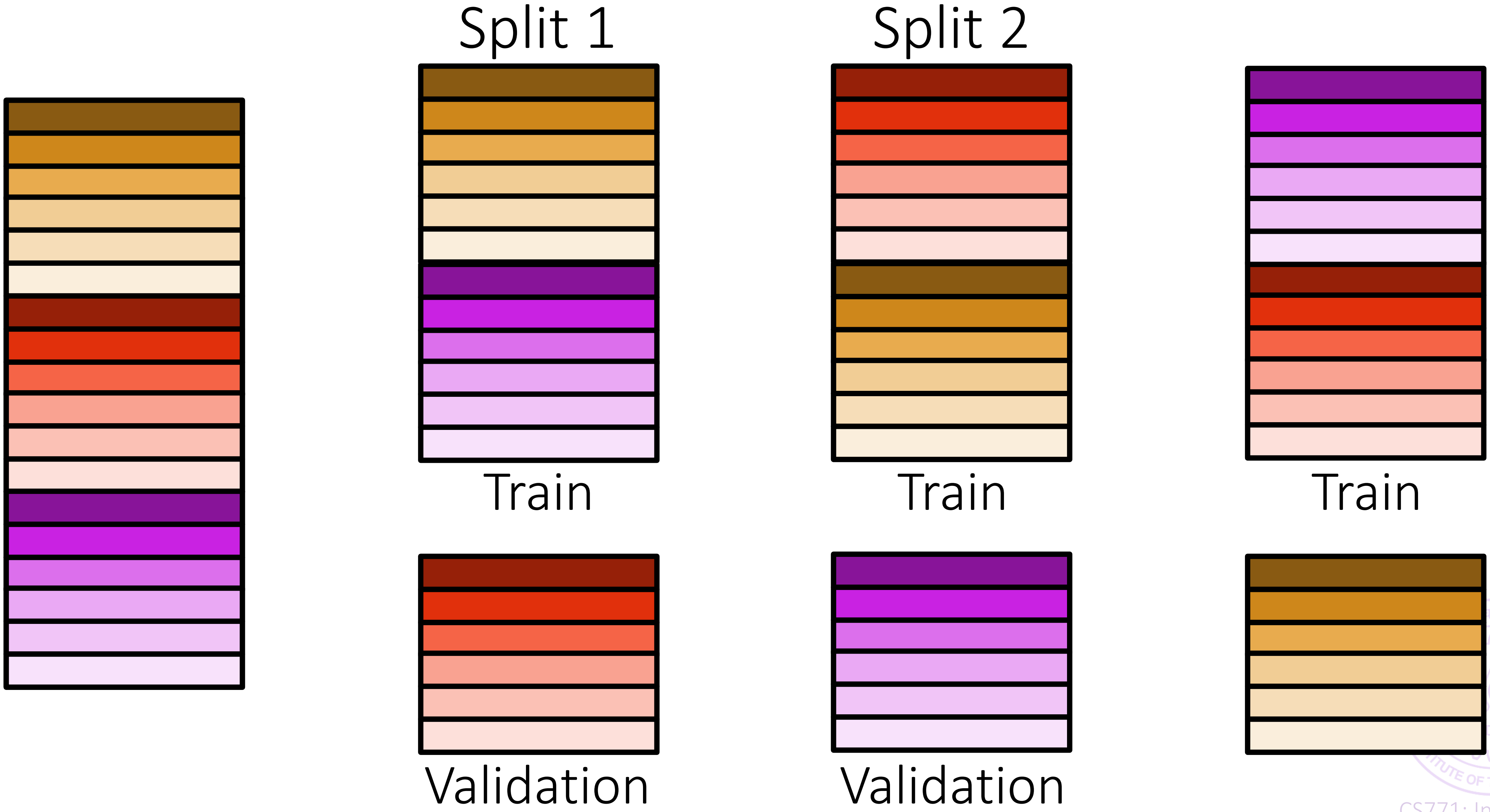

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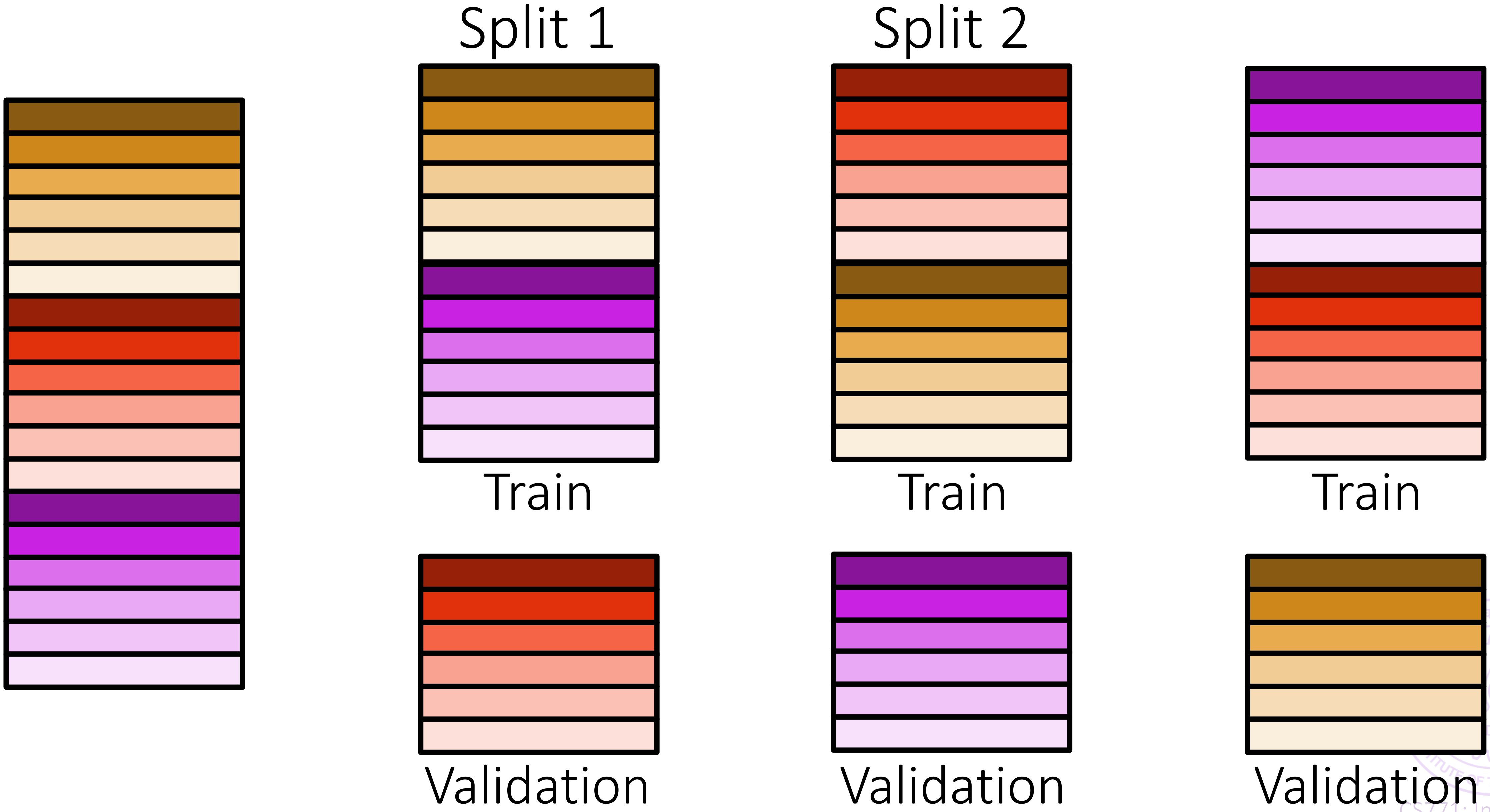

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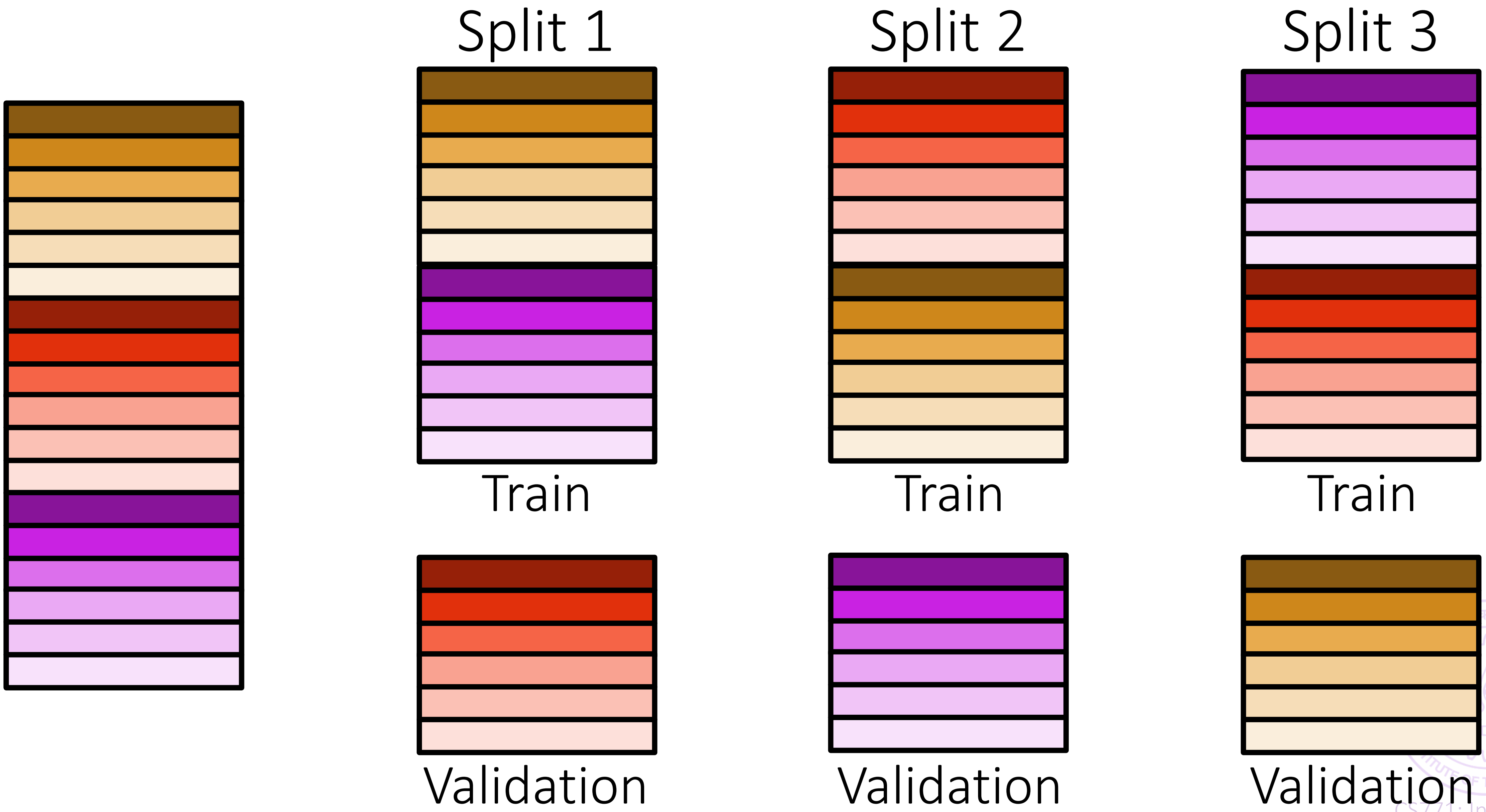

Learning with NN – Lessons

One of the oldest learning algorithms - Fix and Hodges (1951)

Very intuitive, in fact – theoretically, it is the best algorithm possible

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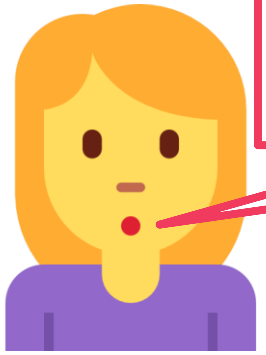

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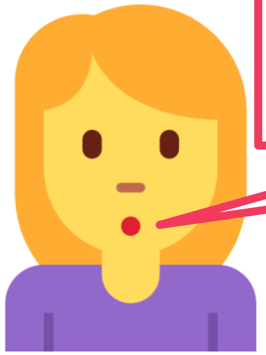

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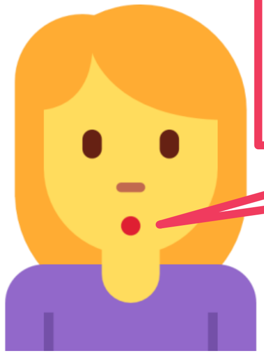

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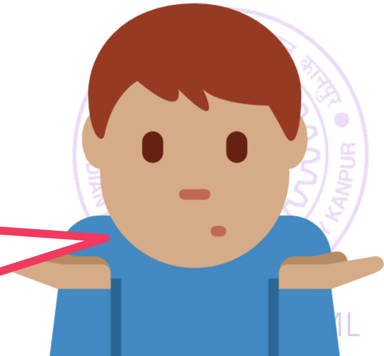

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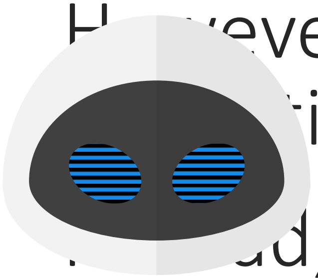

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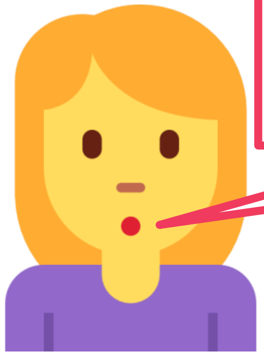

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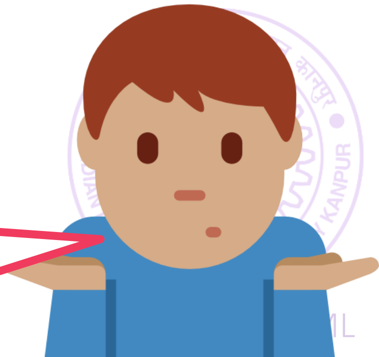

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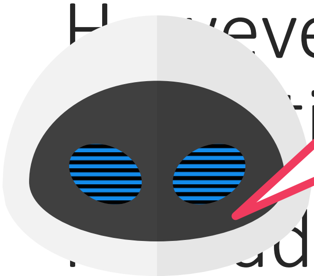

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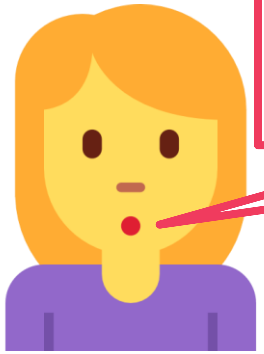

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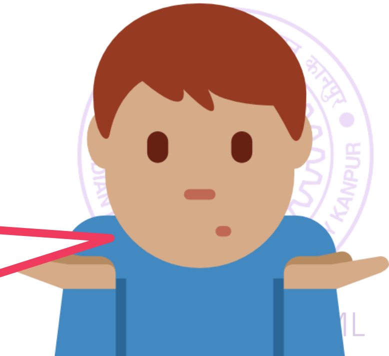

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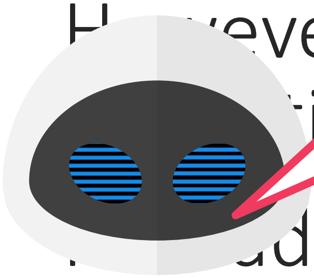

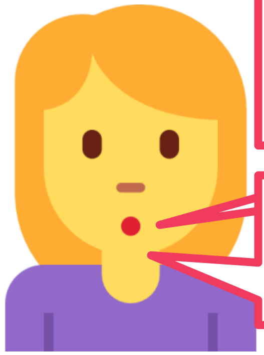

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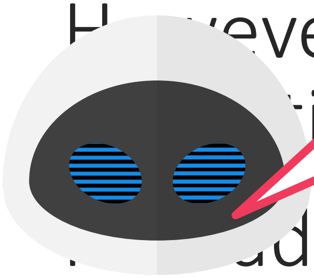

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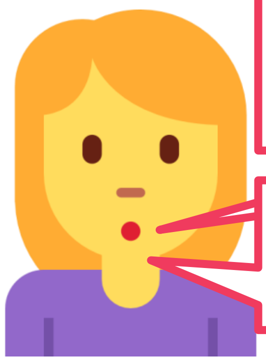

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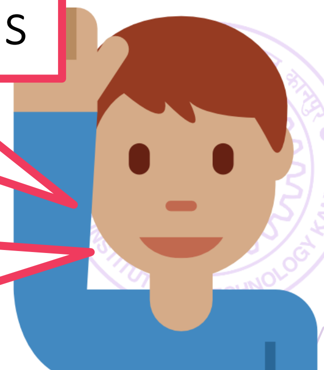

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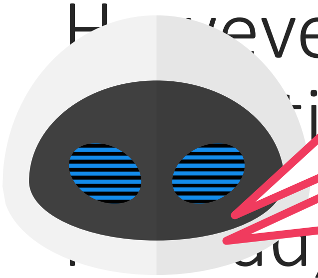

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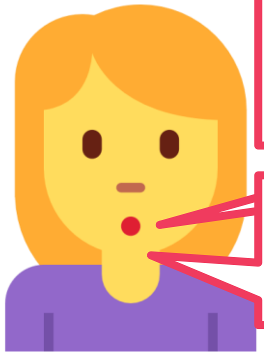

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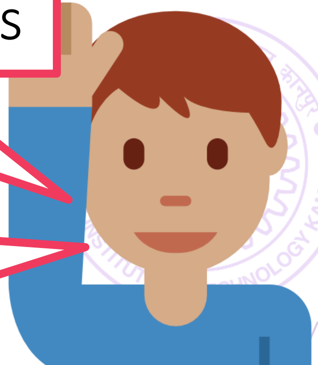

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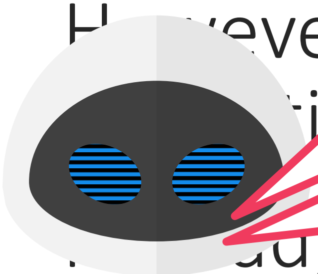

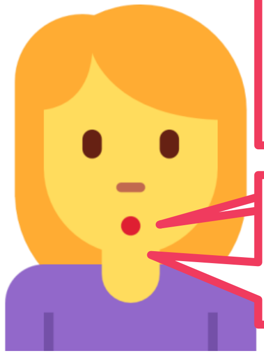

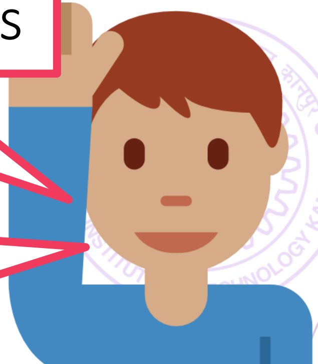

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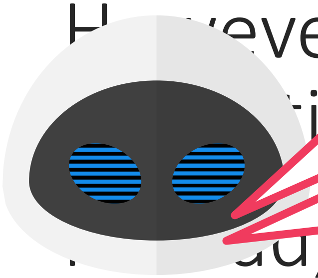
Compare this to LwP where model had 2 vectors no matter how many training points – such models are called *parametric models*



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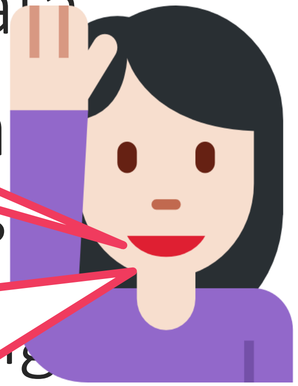

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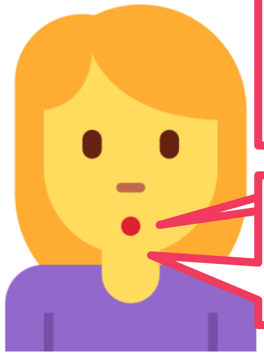

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