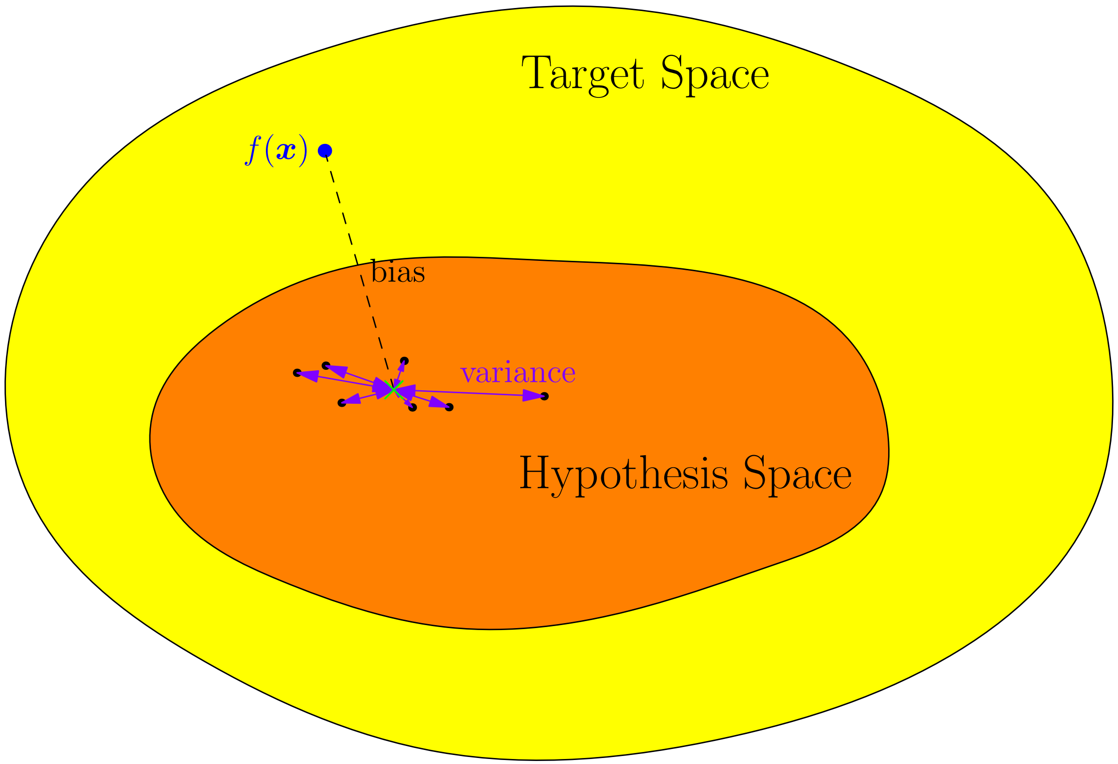
DISC-NET ML Workshop

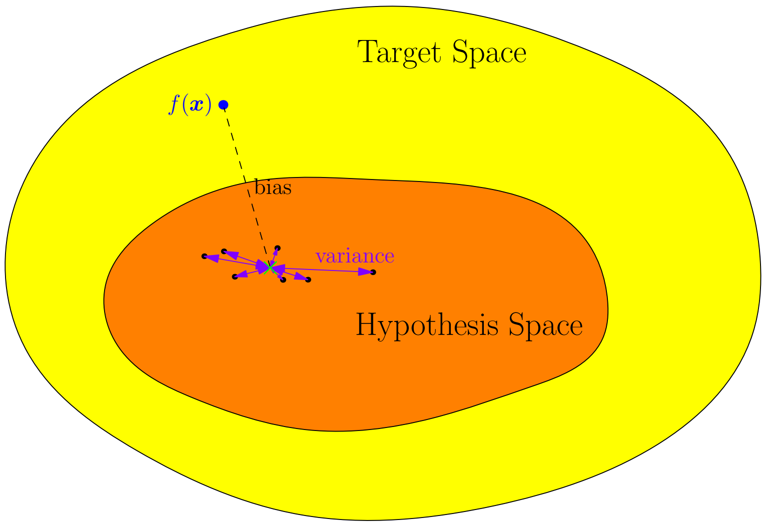
Advanced Machine Learning



When ML Works, SVMs, Decision Trees, Ensemble Methods, Bayesian Inference

Outline

1. **What Makes a Good Learning Machine?**
2. SVMs
3. Ensemble Methods
4. Bayesian Inference



What Makes a Good Learning Machine?

- We want to understand why some machine learning techniques work well and other don't
- To understand why these works we need to understand what makes a good learning machine
- For this we have to get conceptual and think about **generalisation** performance

  generalisation*: how well do we do on unseen data as opposed to the training data*

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What Makes Machine Learning Hard?

- Typically work in high dimensions (i.e. have many features)
- The problem can be over-constrained (i.e. we have conflicting data to deal with)
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Least Squared Errors

- Suppose we want to learn some function $f(\boldsymbol{x})$
- We construct a learning machine that makes a prediction $\hat{f}(\boldsymbol{x})$
- We typically choose the machine that minimise a *training error*

$$E_T(\mathcal{D}) = \sum_{\boldsymbol{x} \in \mathcal{D}} \left(\hat{f}(\boldsymbol{x}) - f(\boldsymbol{x}) \right)^2$$

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where $\mathcal{D} = \{(\boldsymbol{x}_i, y_i = f(\boldsymbol{x}_i))\}_{i=1}^{m}$ is a set of size m, sampled from the set of all inputs, $\mathcal{X}$, according to a probability distribution $p(\boldsymbol{x})$ describing where our data is

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- Choose machine with smallest training error $\hat{f}(\boldsymbol{x}|\mathcal{D})$

Generalisation Error

- We want to minimise the *generalisation error* which in this case is

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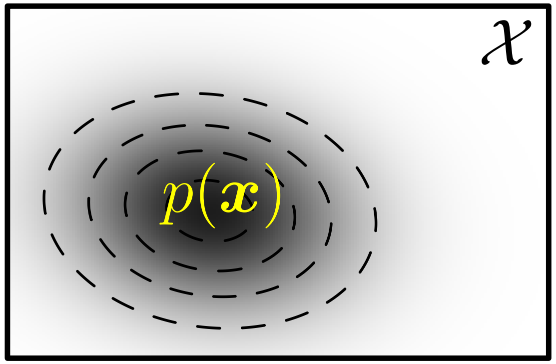

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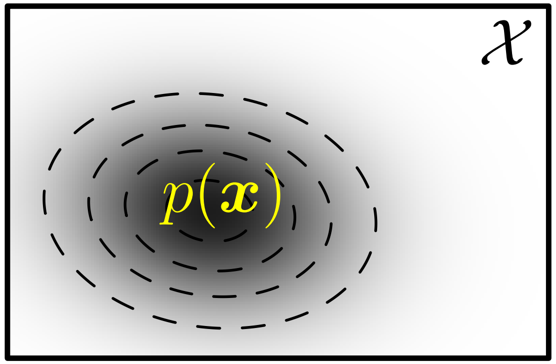

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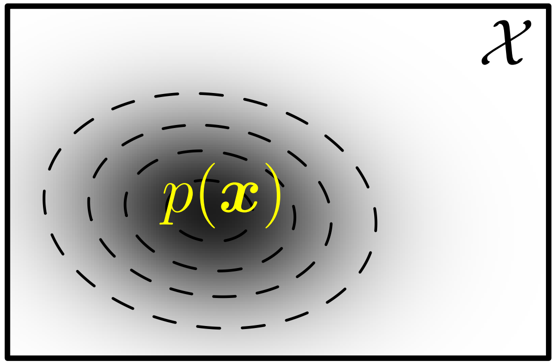

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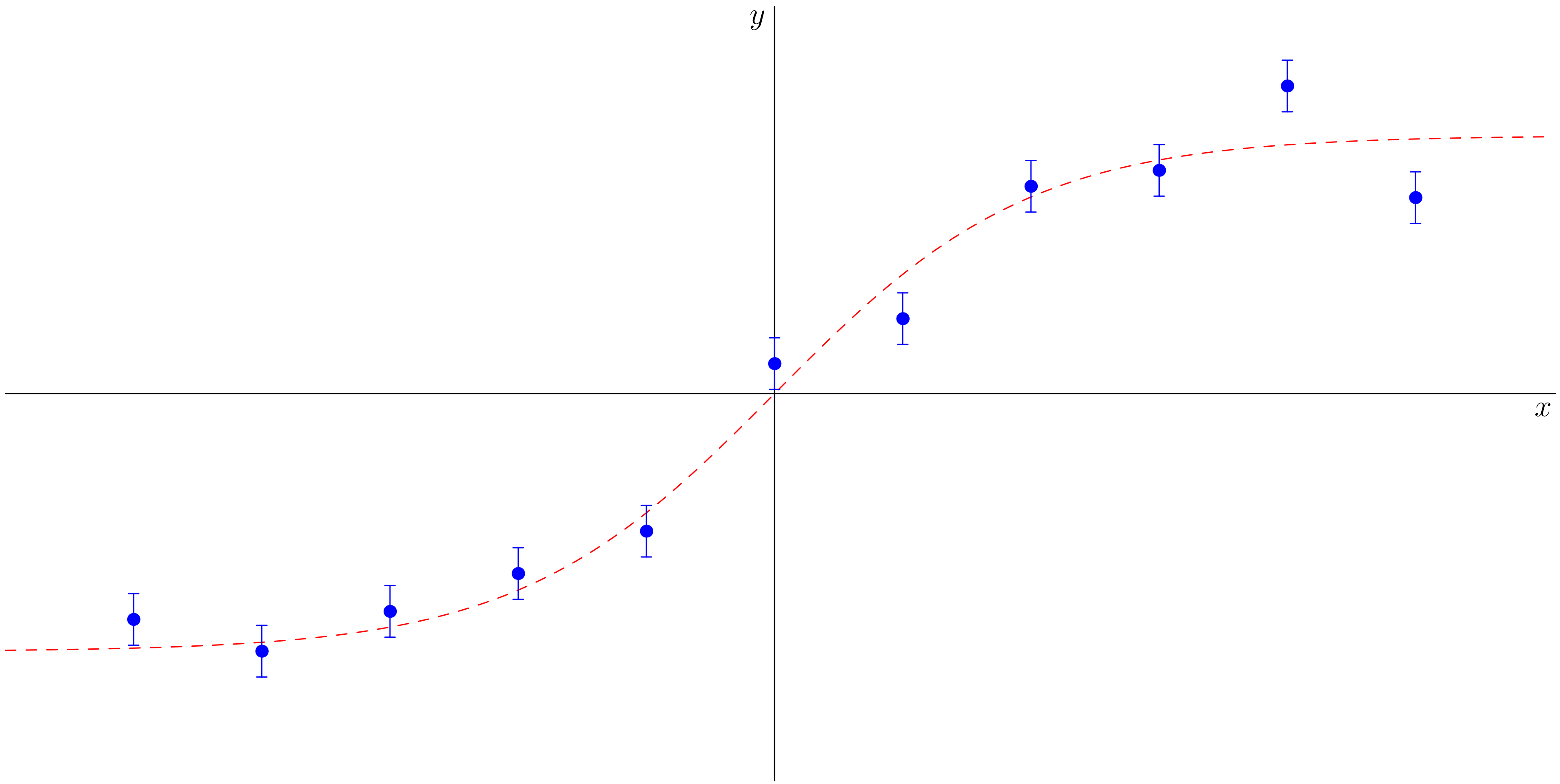

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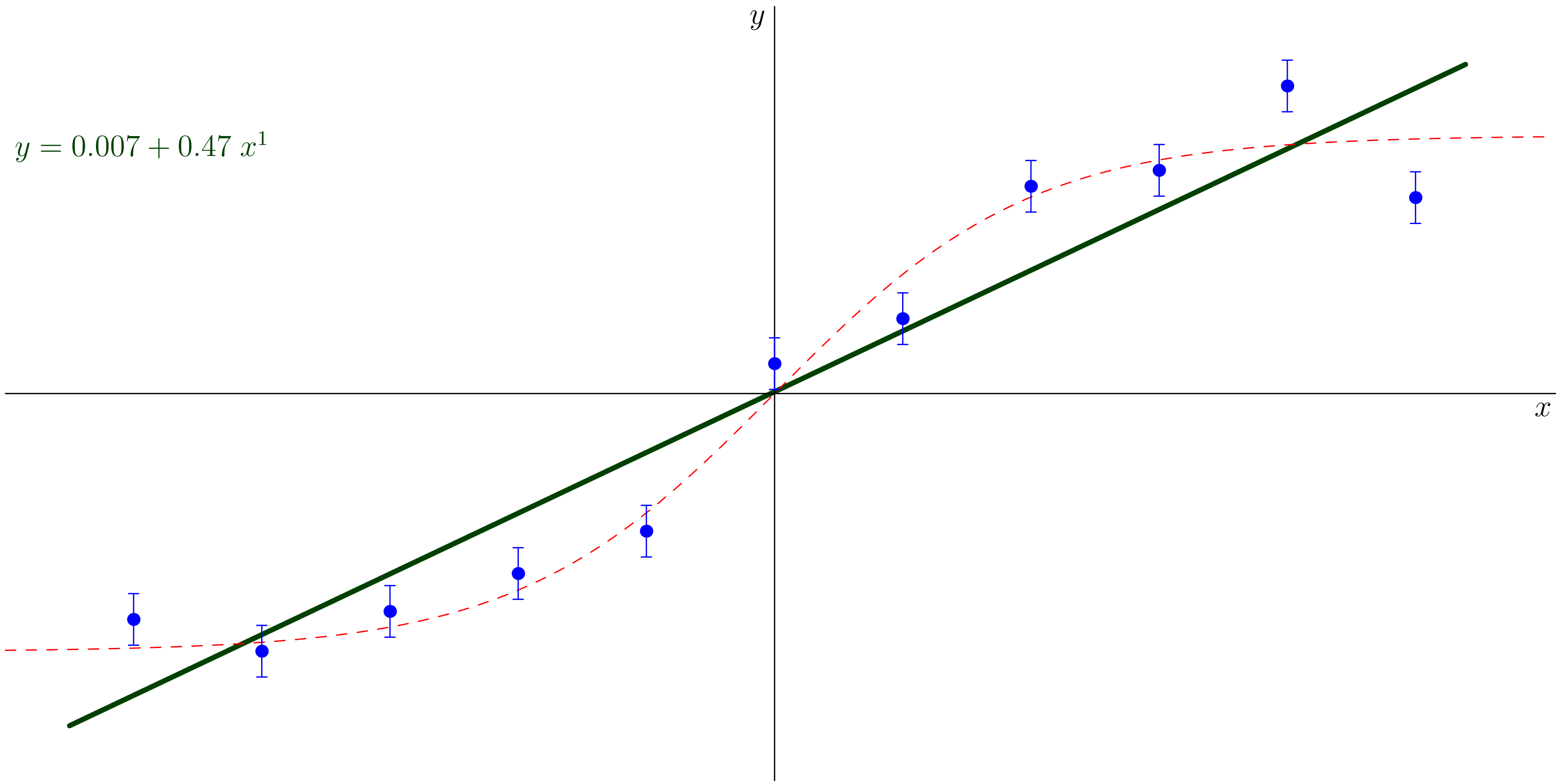

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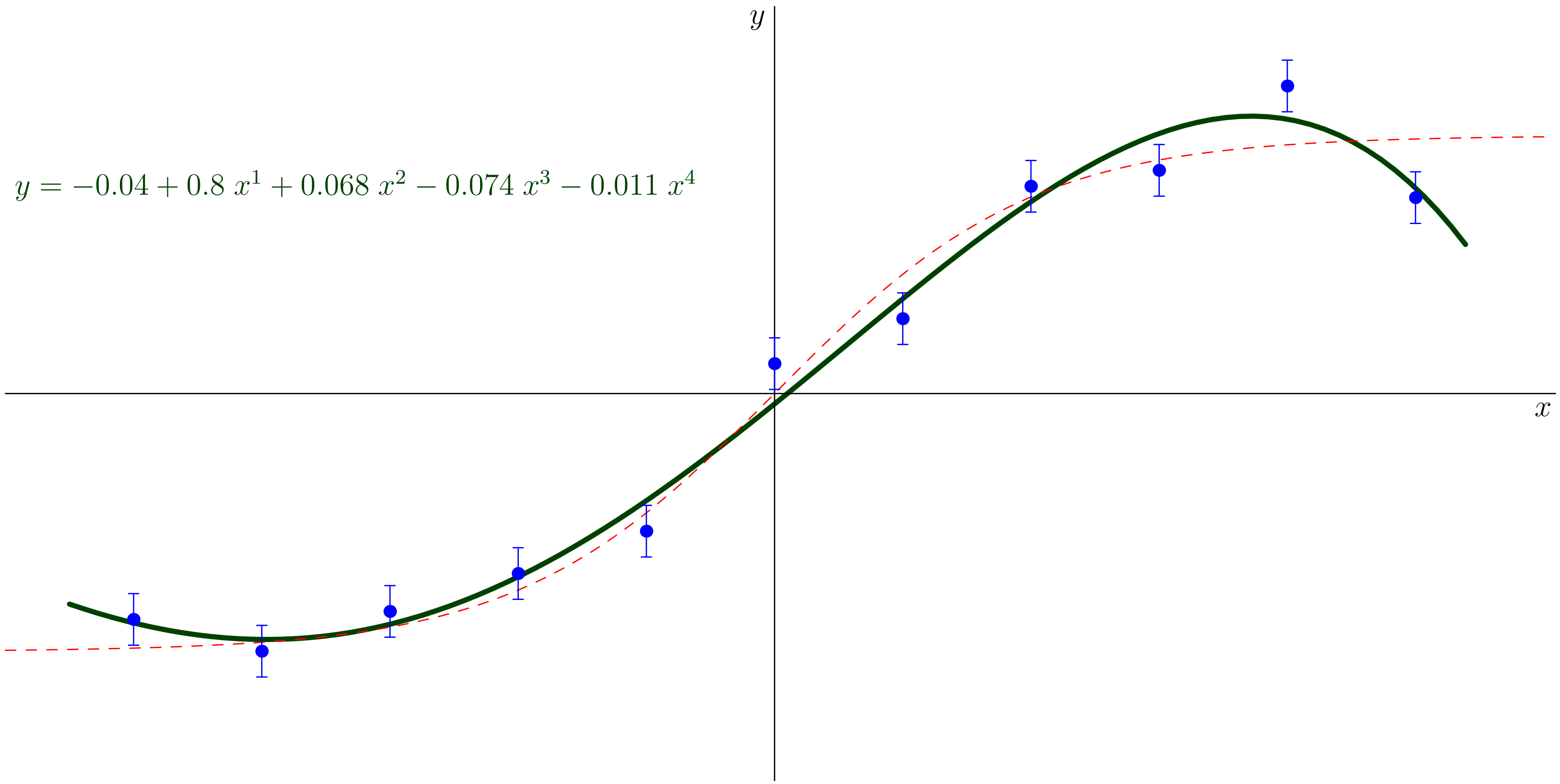

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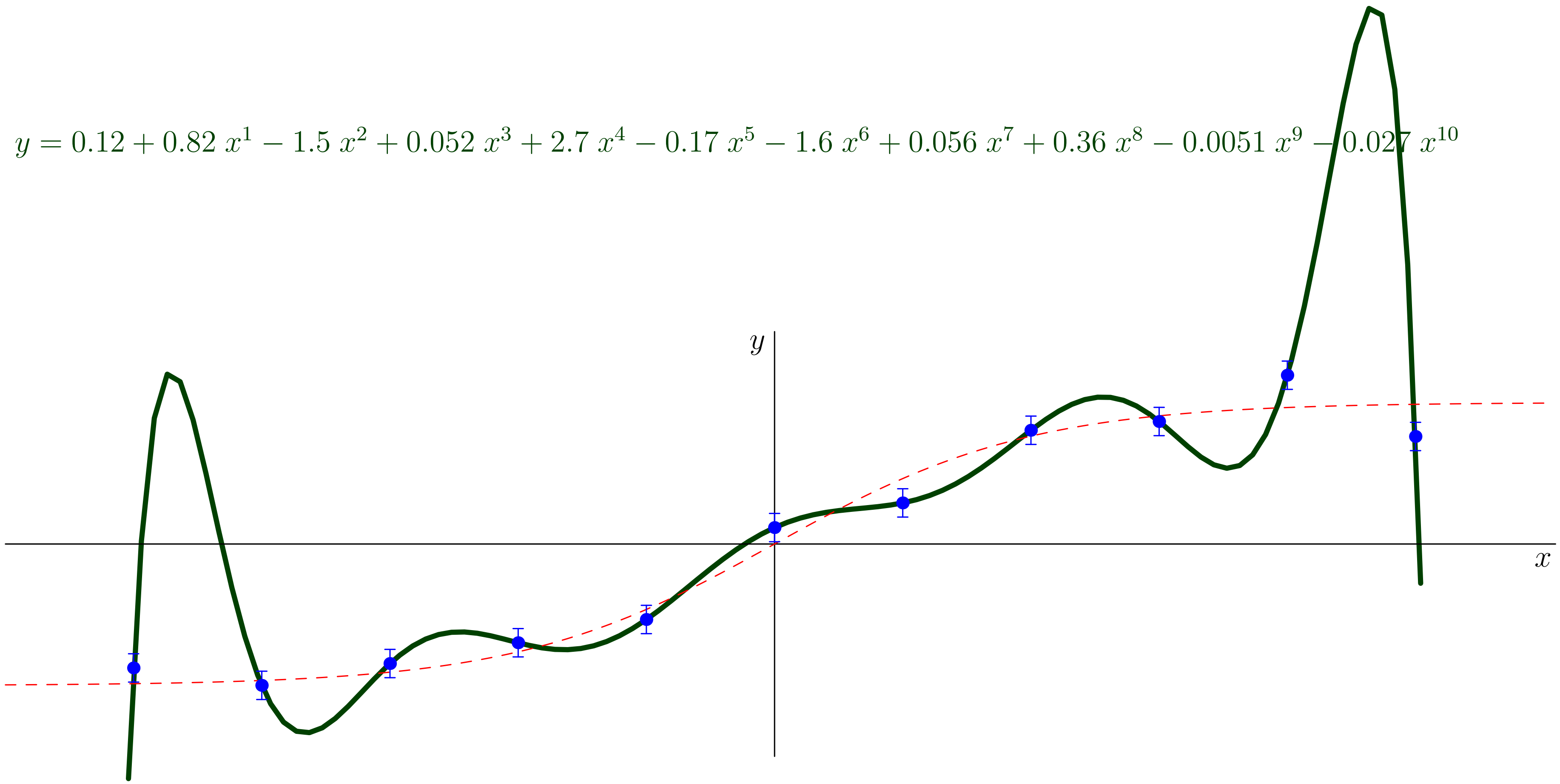
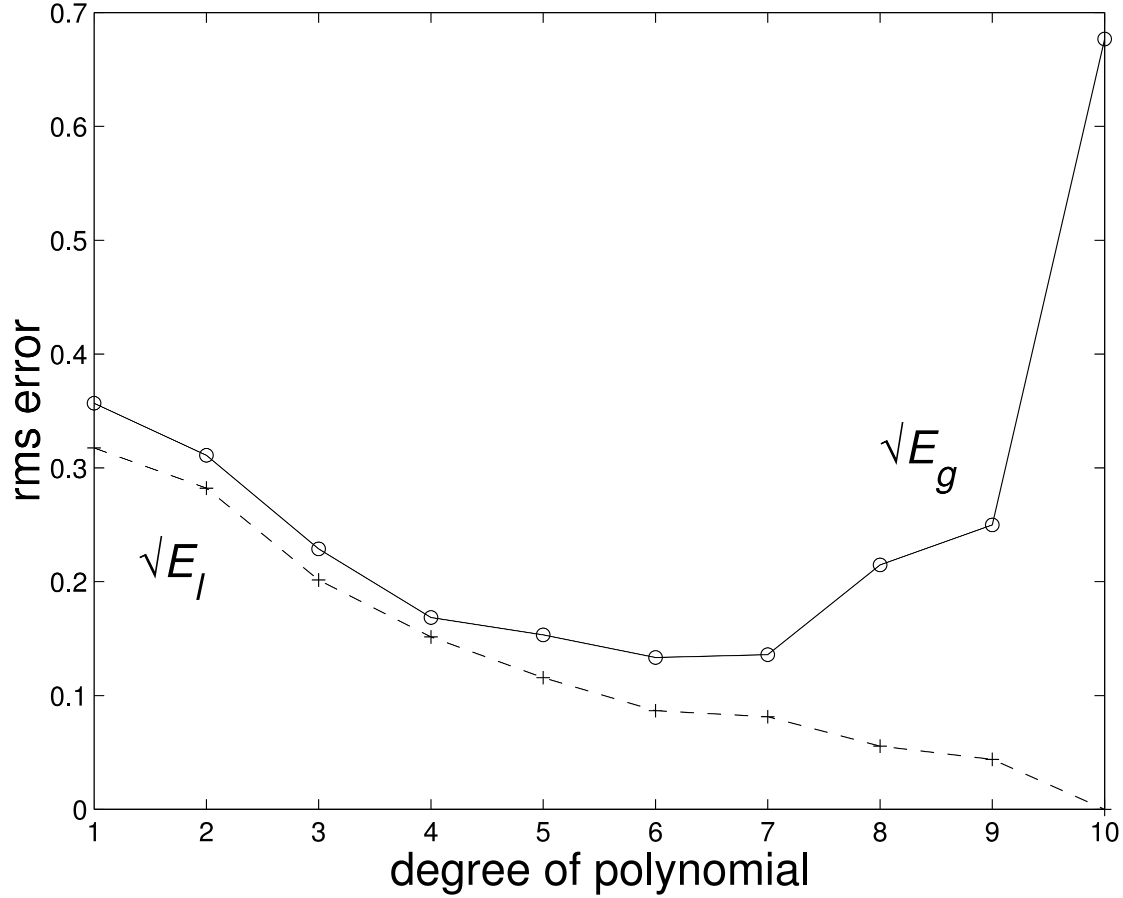


Measuring Generalisation Error for Regression

- Consider the regression example. The root mean squared error is



Expected Generalisation Performance

- Our generalisation performance will depend on our training set, $\mathcal{D}$
- To reason about generalisation we can ask what is the *expected generalisation*, that is, when we average over all different data sets of size m drawn independently from $p(\boldsymbol{x})$
- For each data set, $\mathcal{D}$, we would learn a different approximator $\hat{f}(\boldsymbol{x}|\mathcal{D})$ (usually through weights $\boldsymbol{w}_{\mathcal{D}}$)
- Note that in practice we only get one data set. We might be lucky and do better than the expected generalisation or we might be unlucky and do worse

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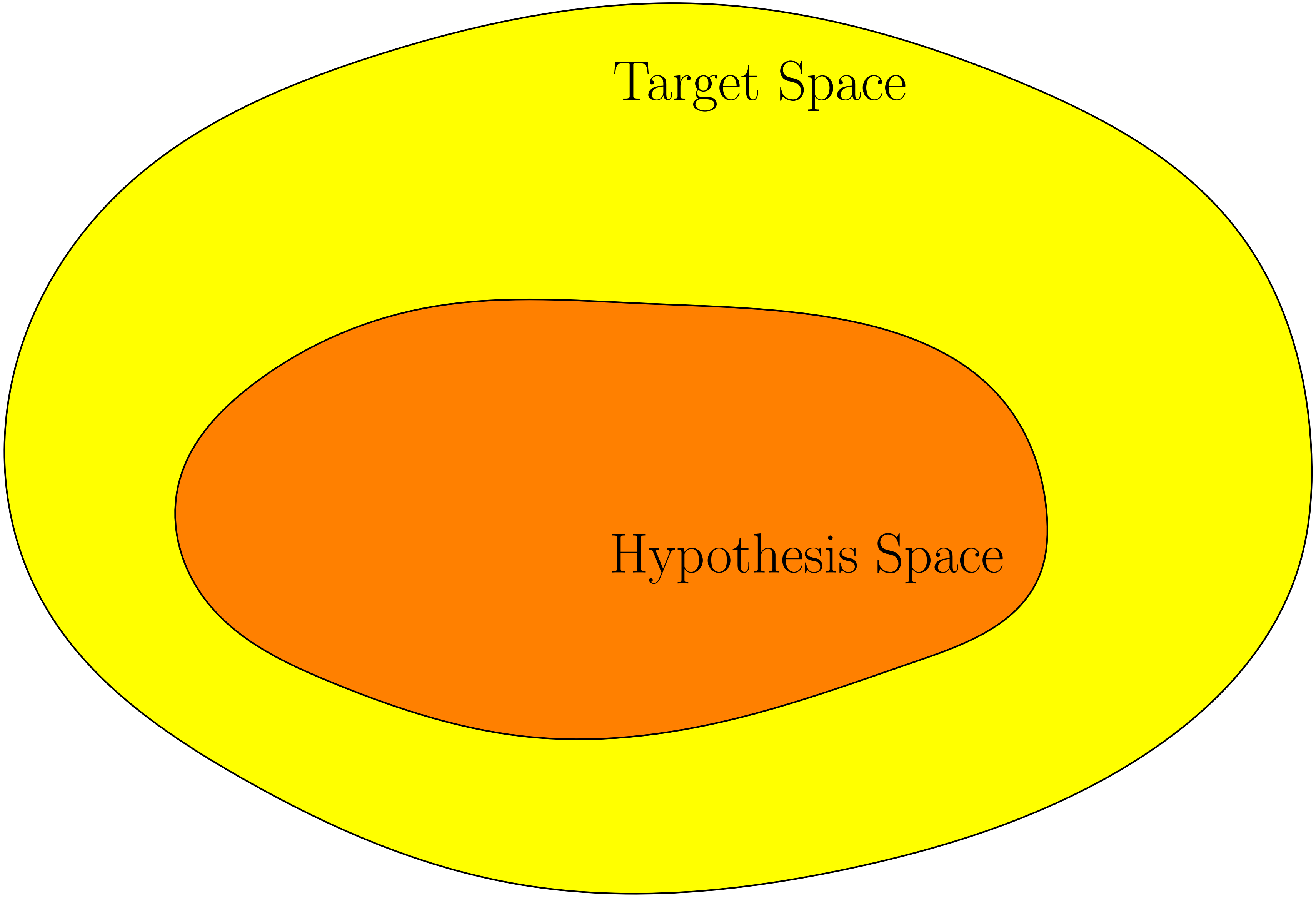

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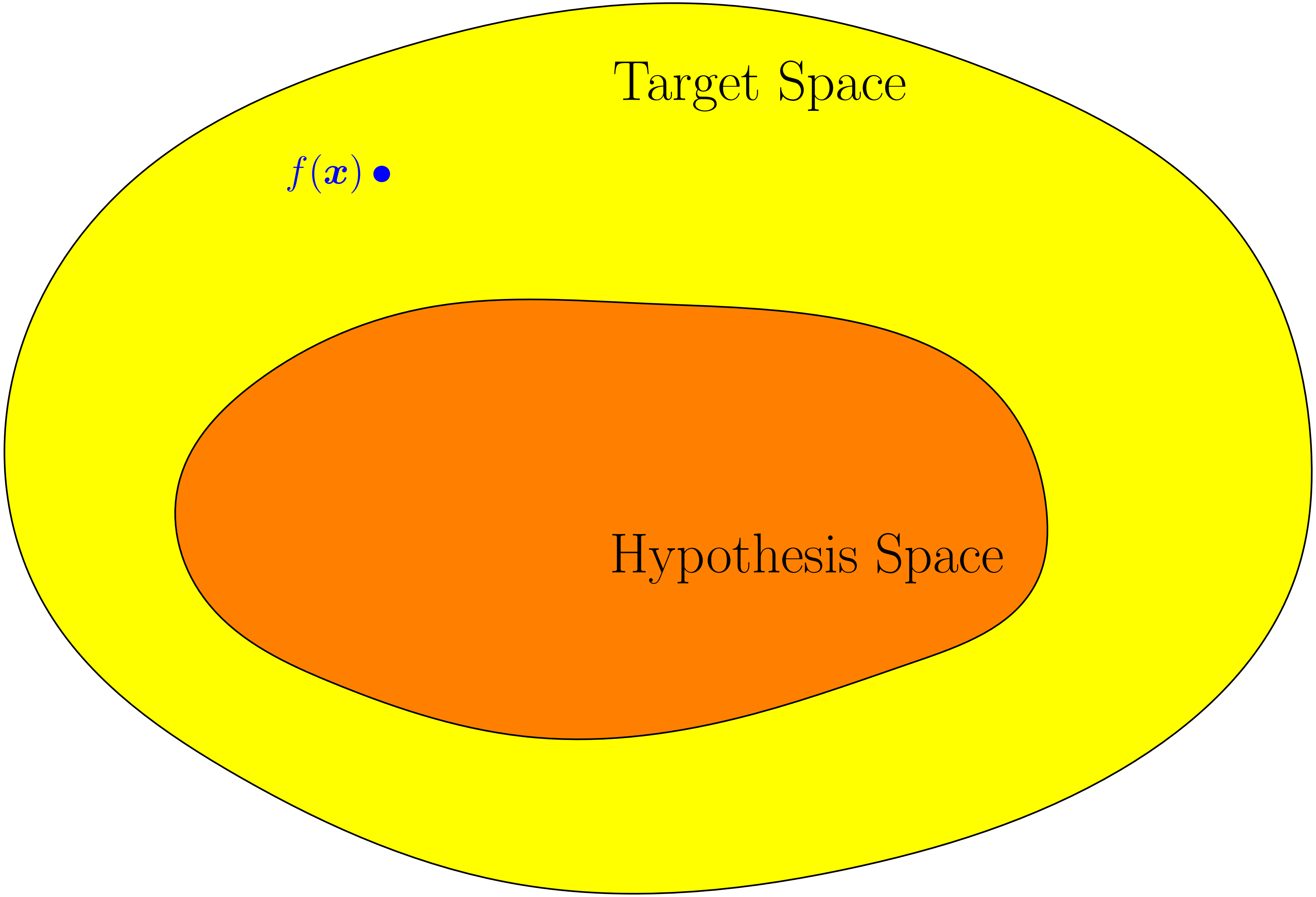

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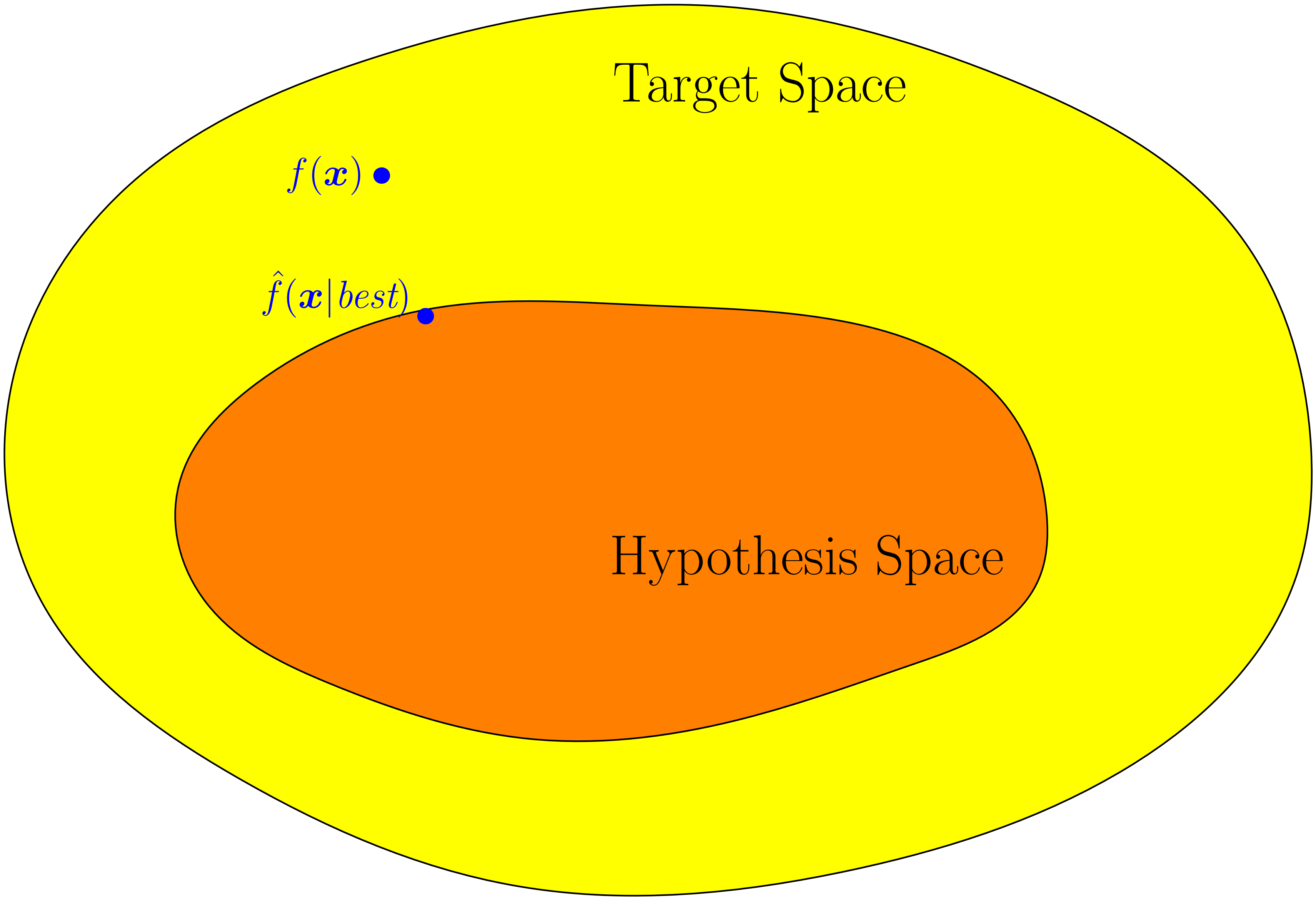

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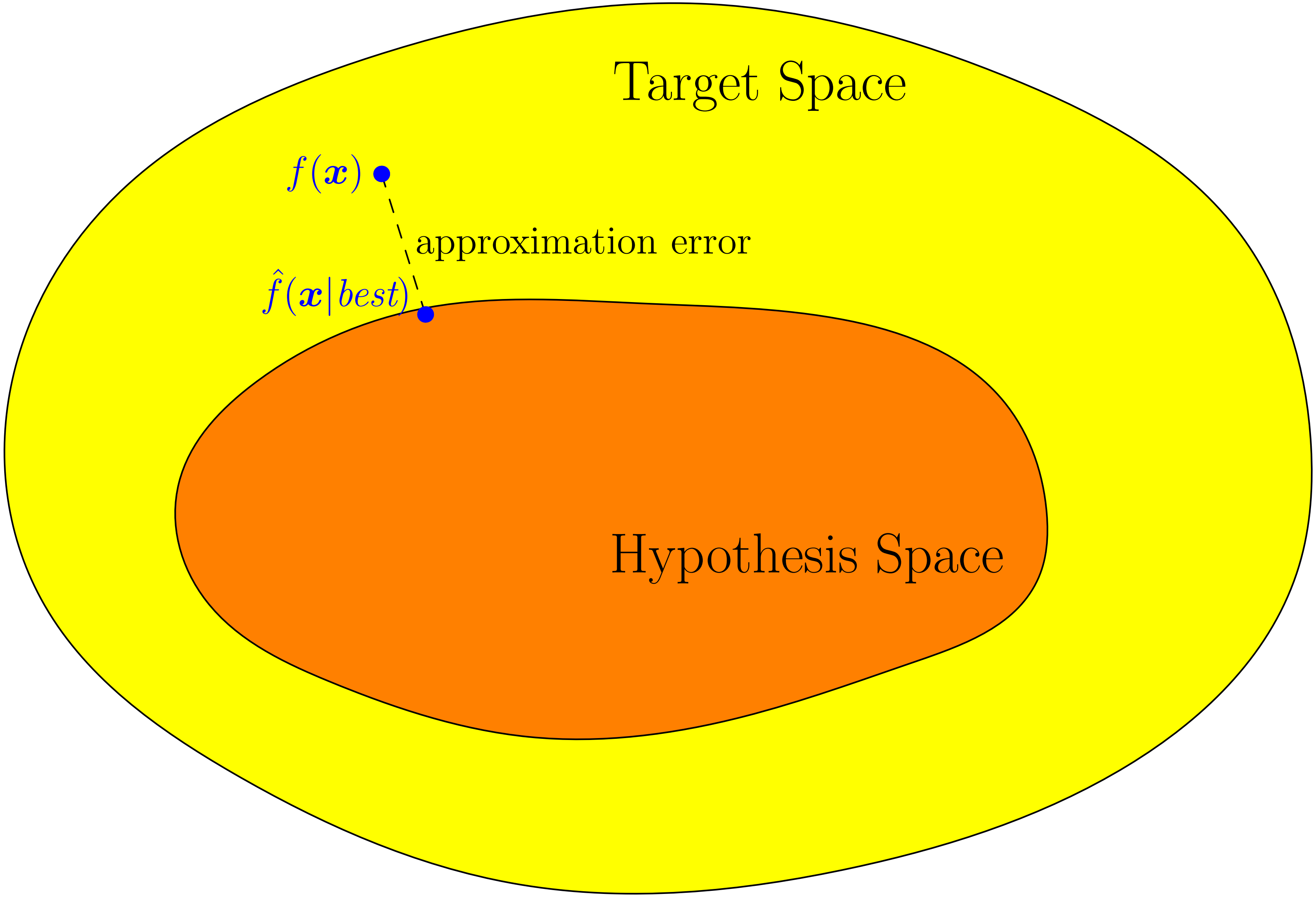

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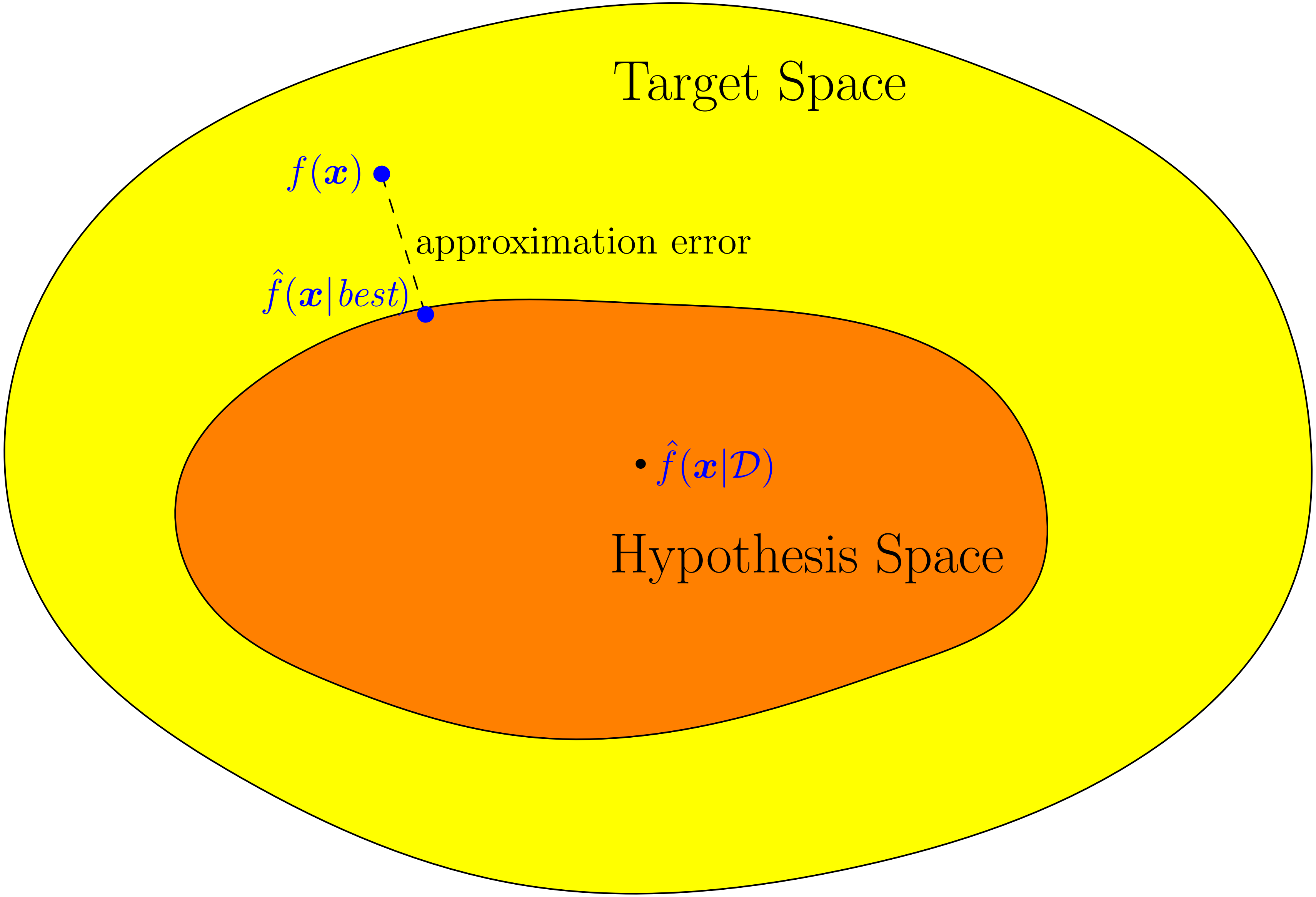

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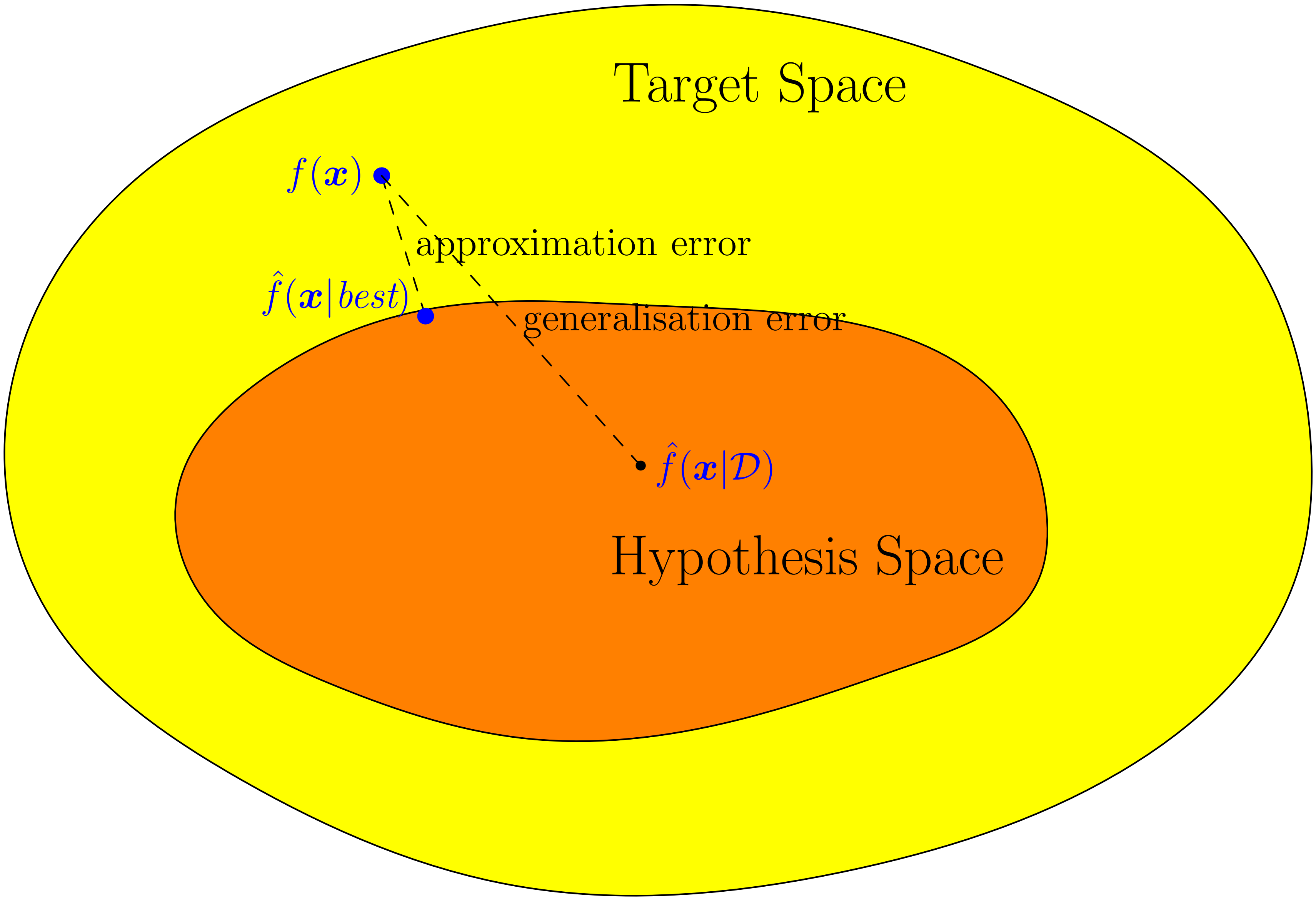

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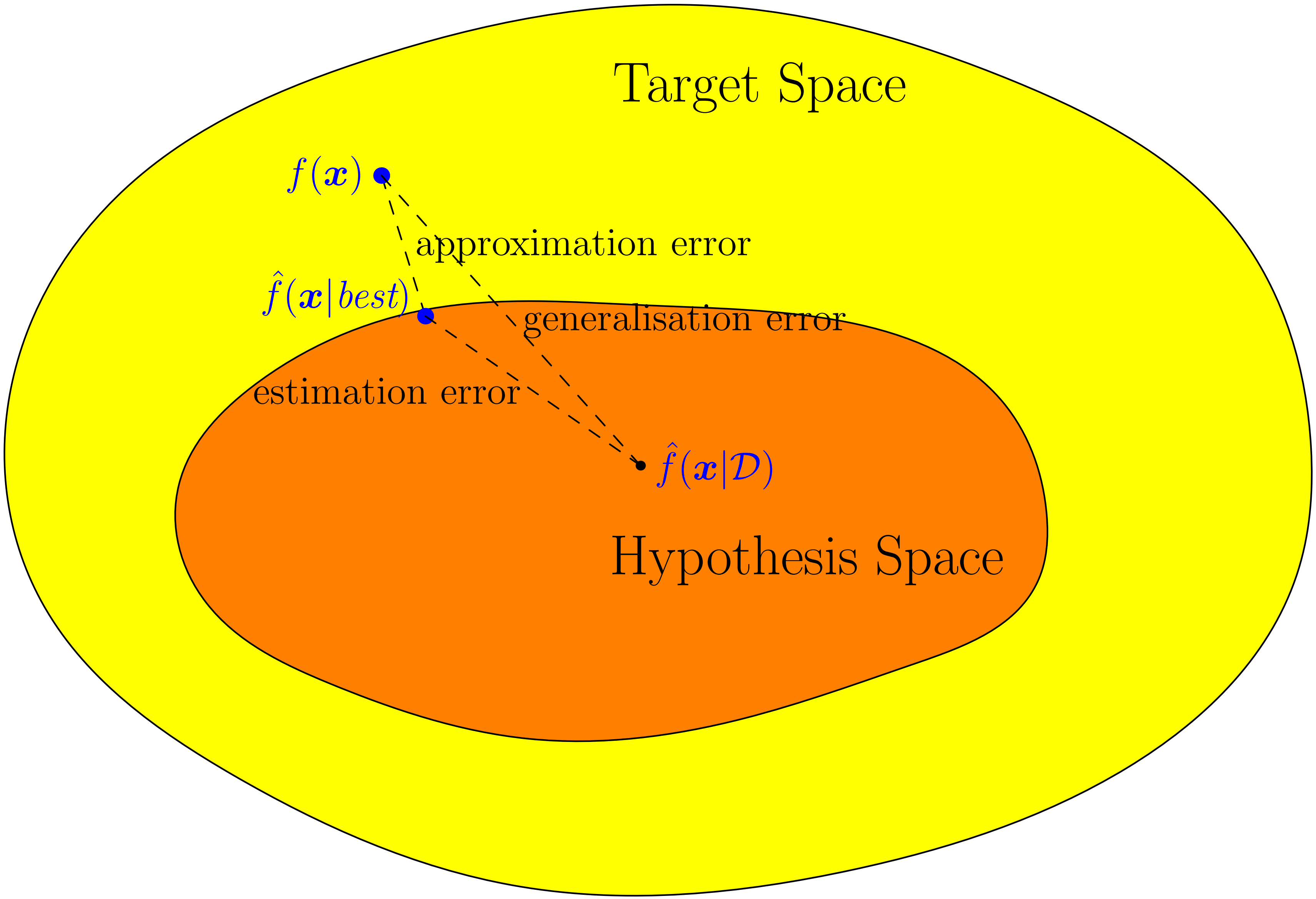

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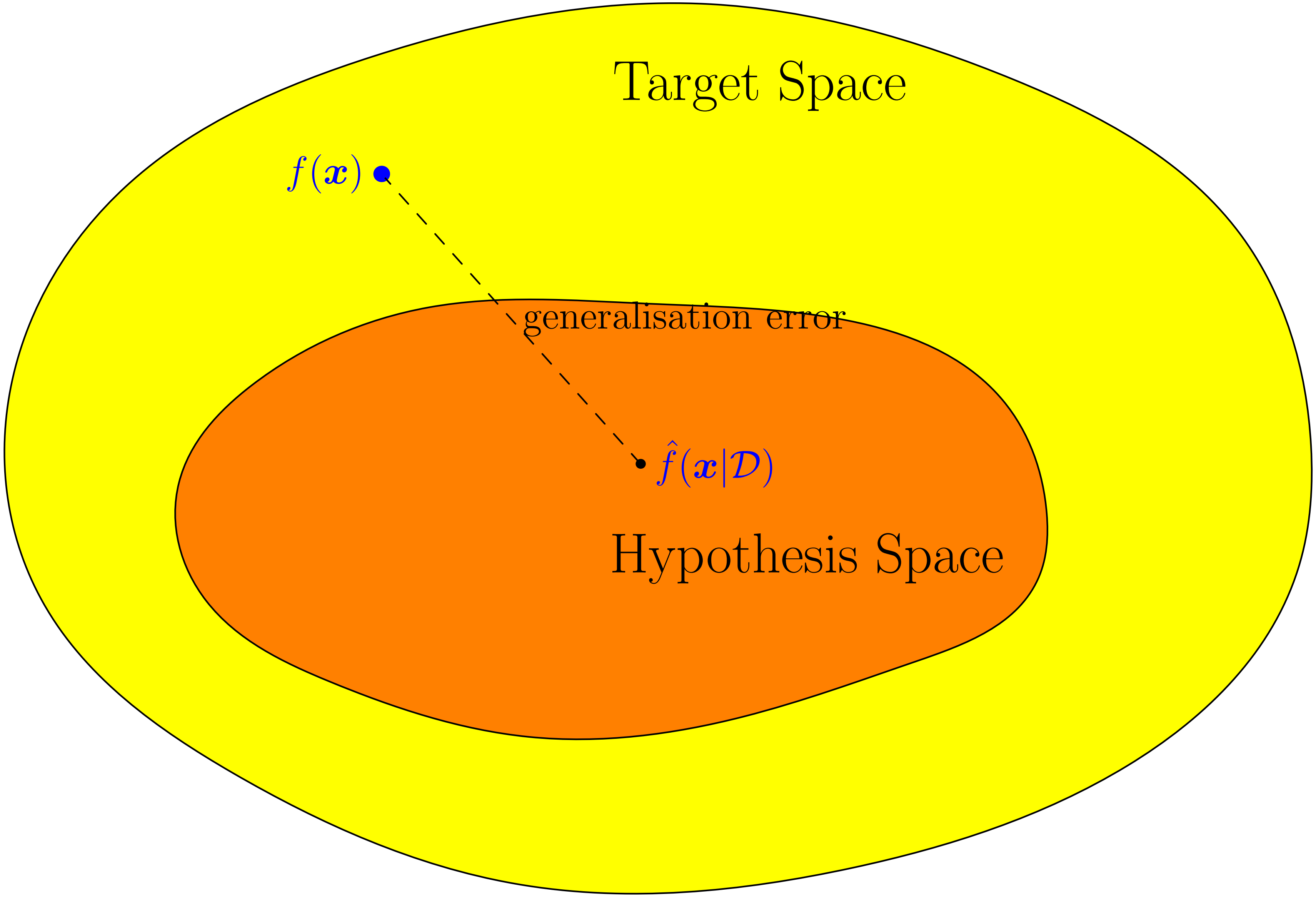

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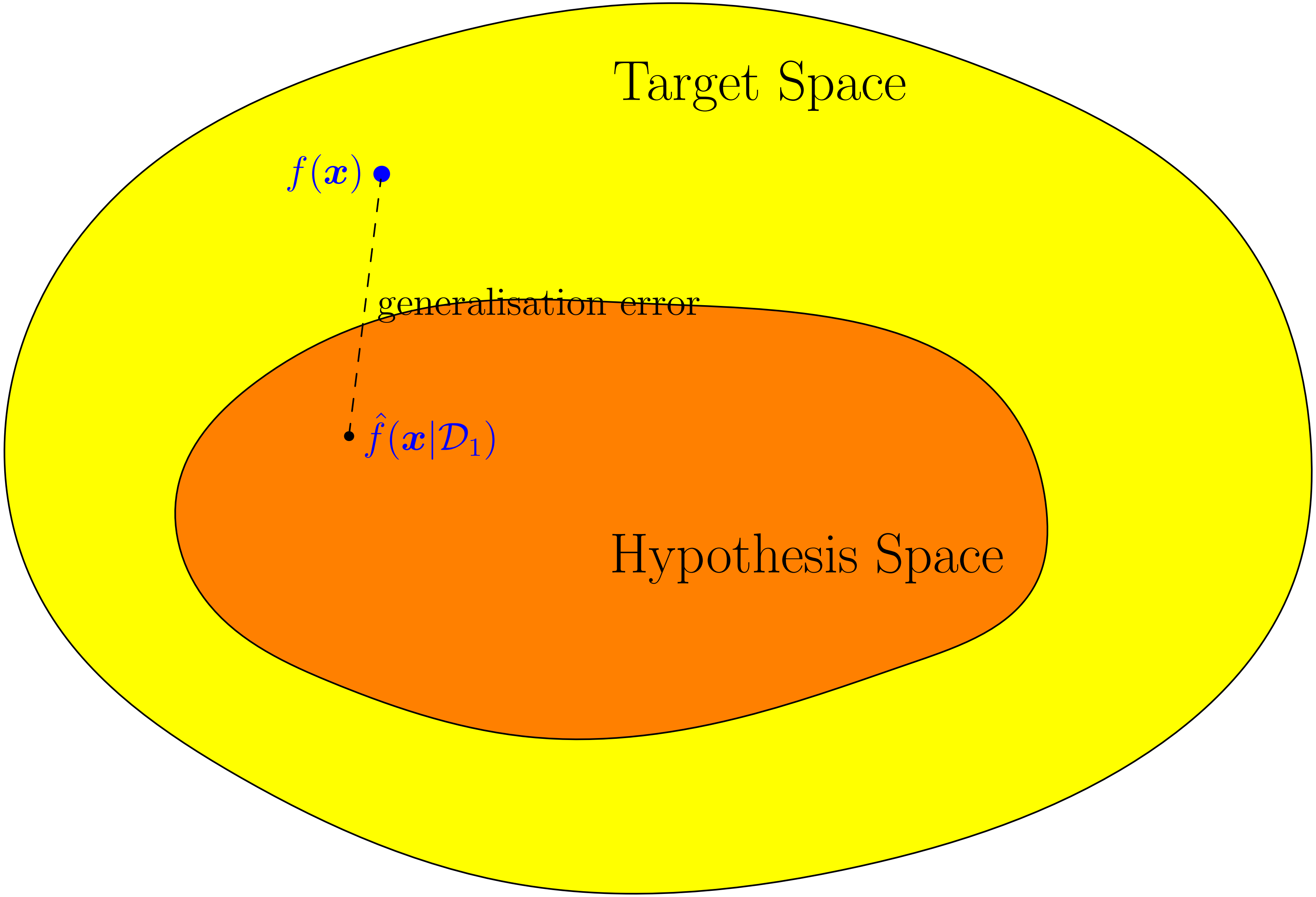

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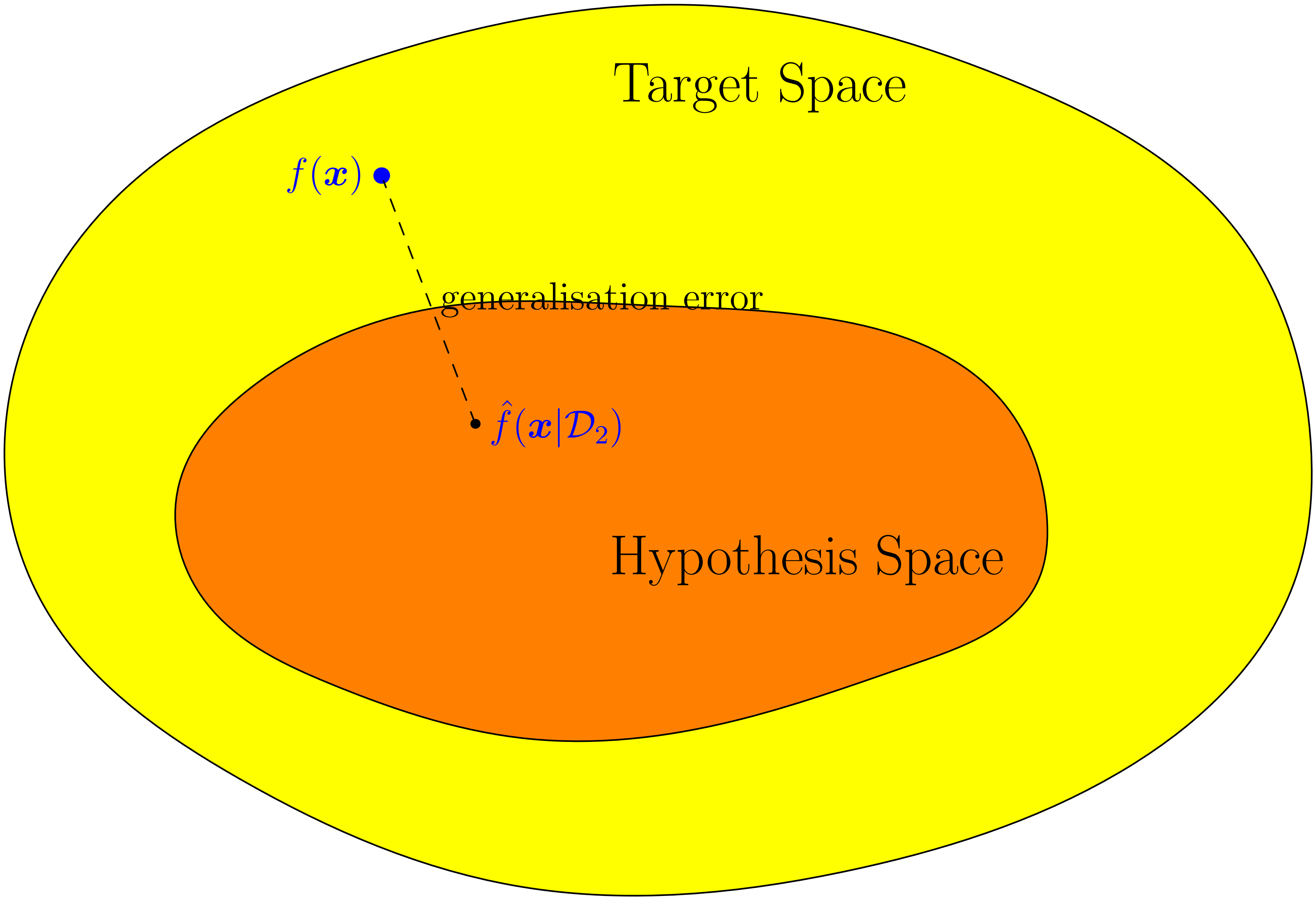

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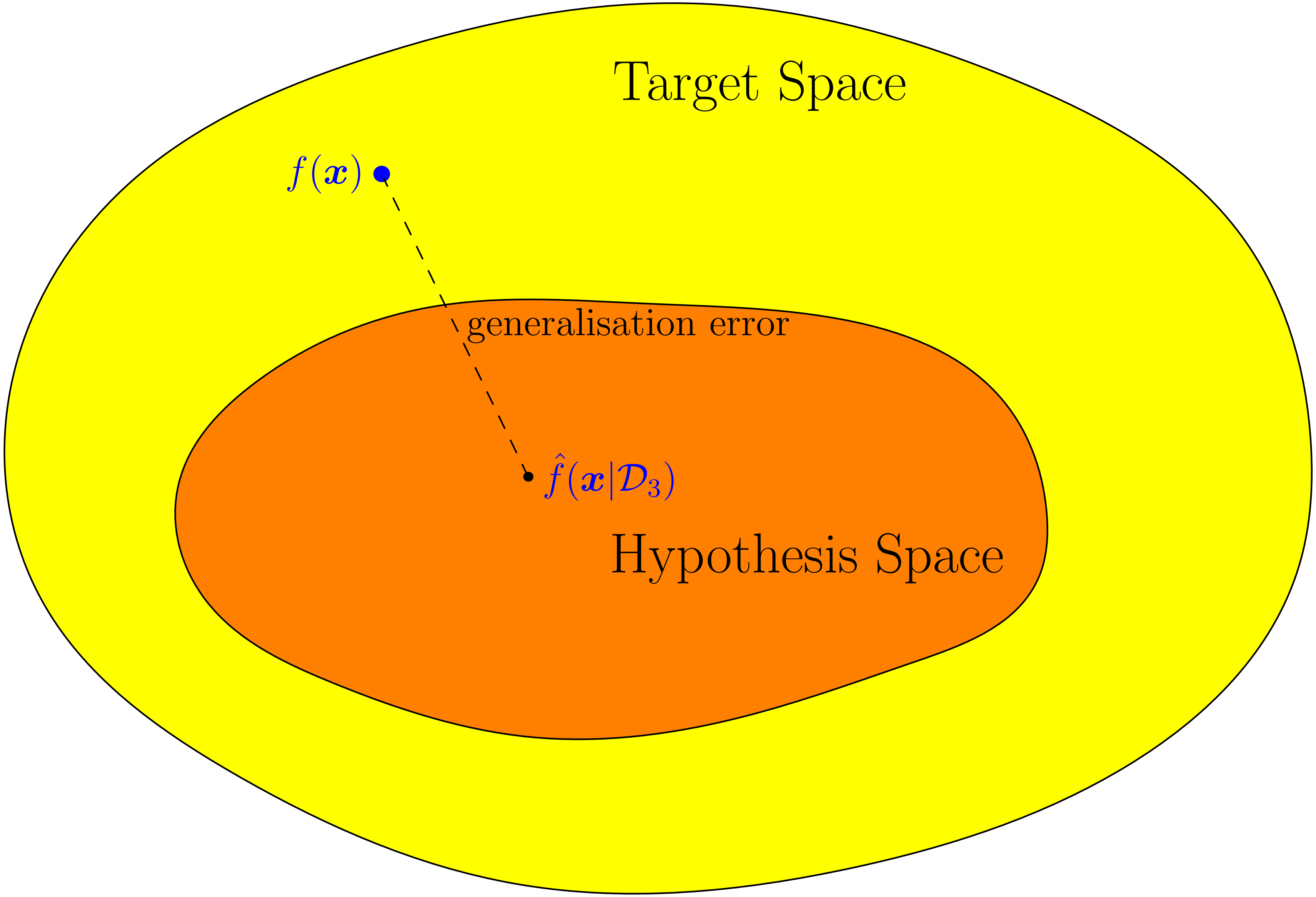

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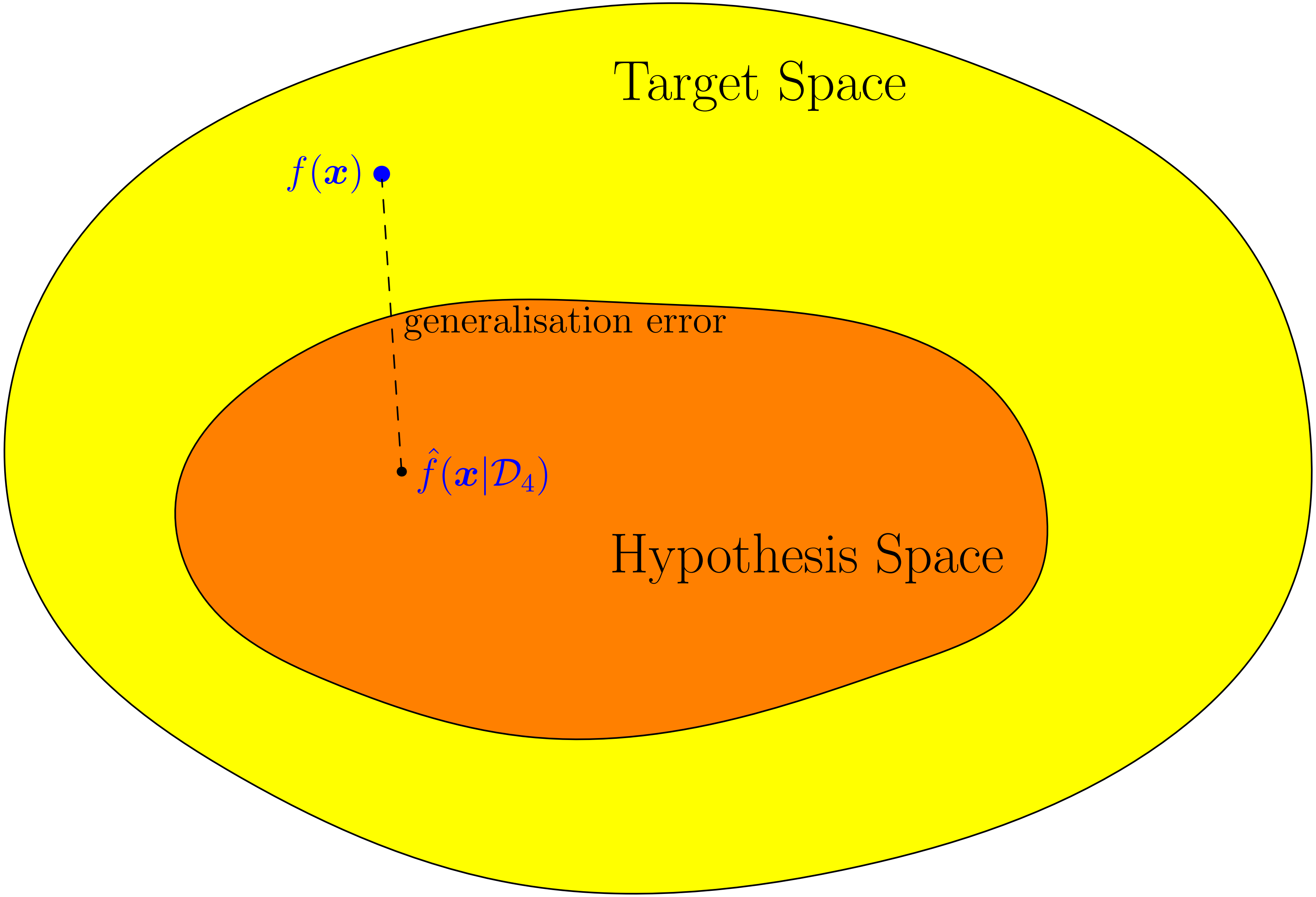

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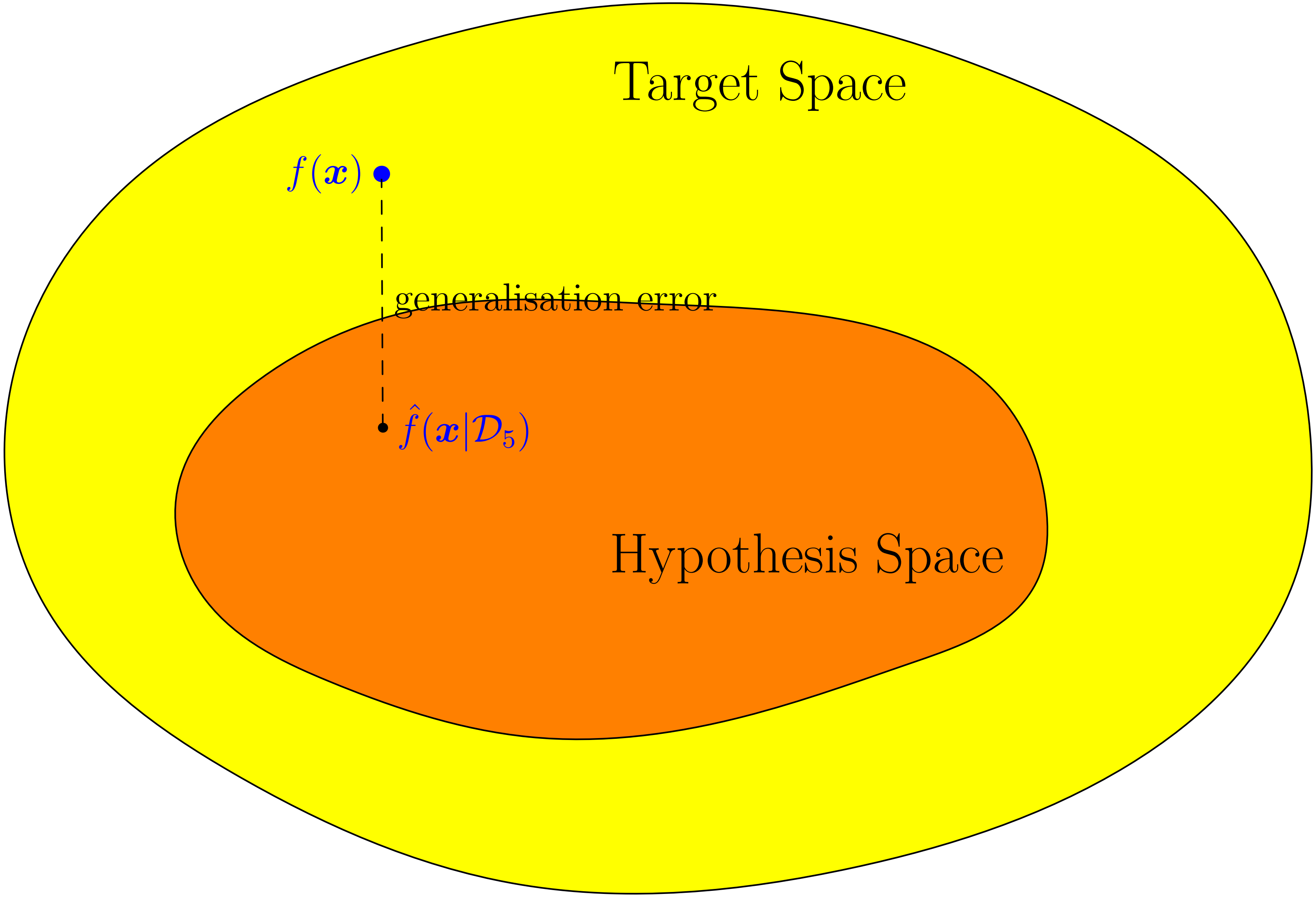

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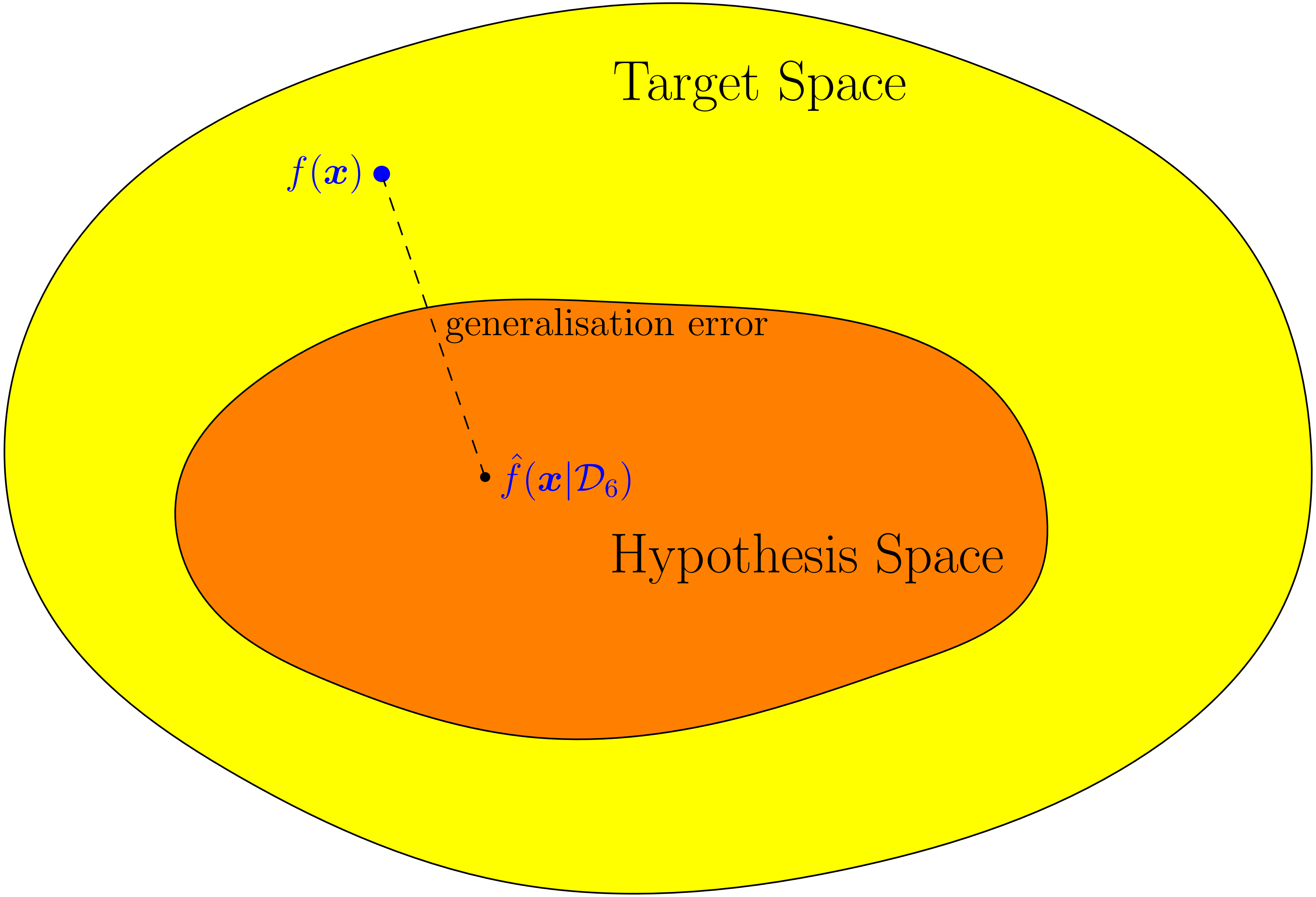

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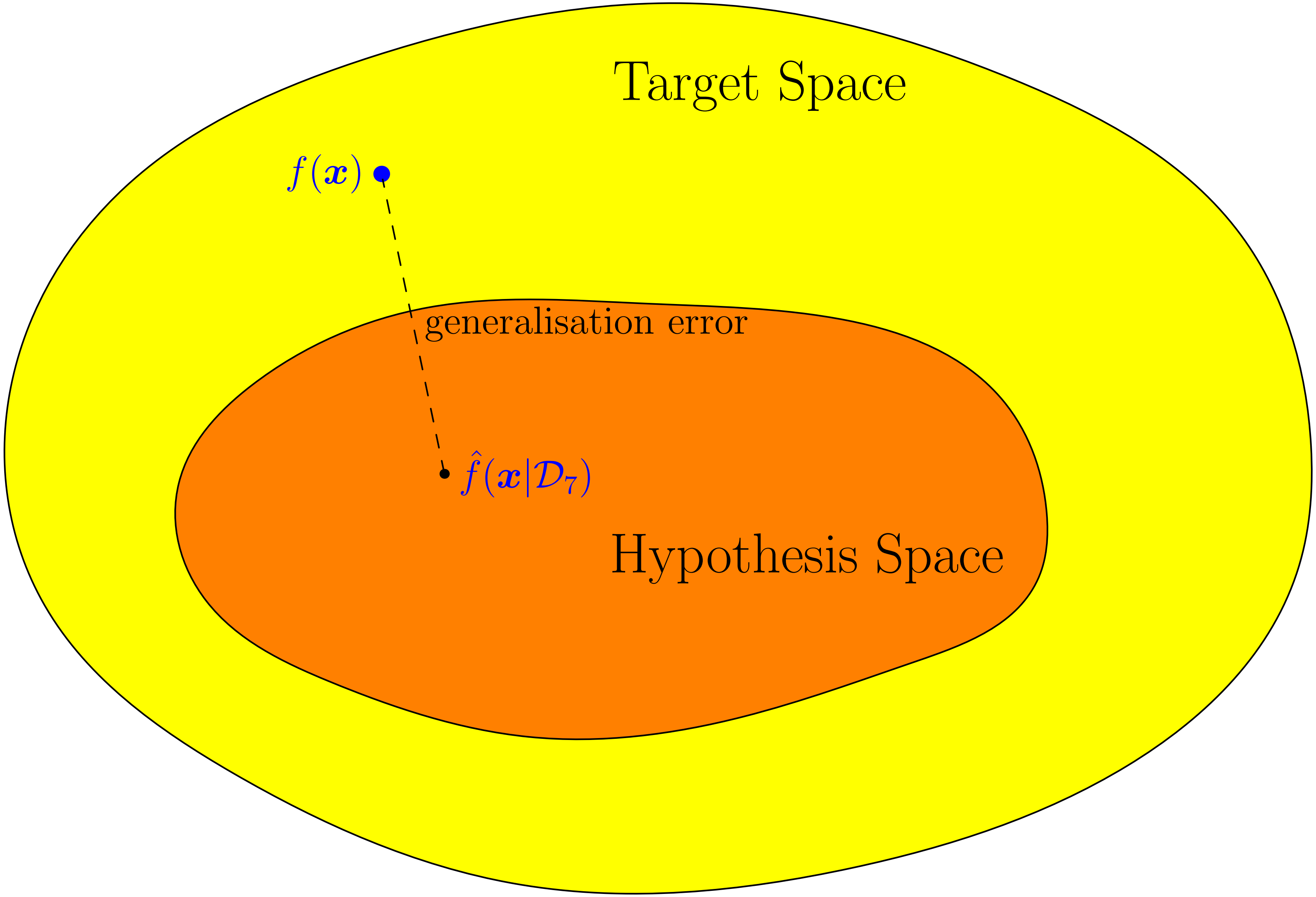

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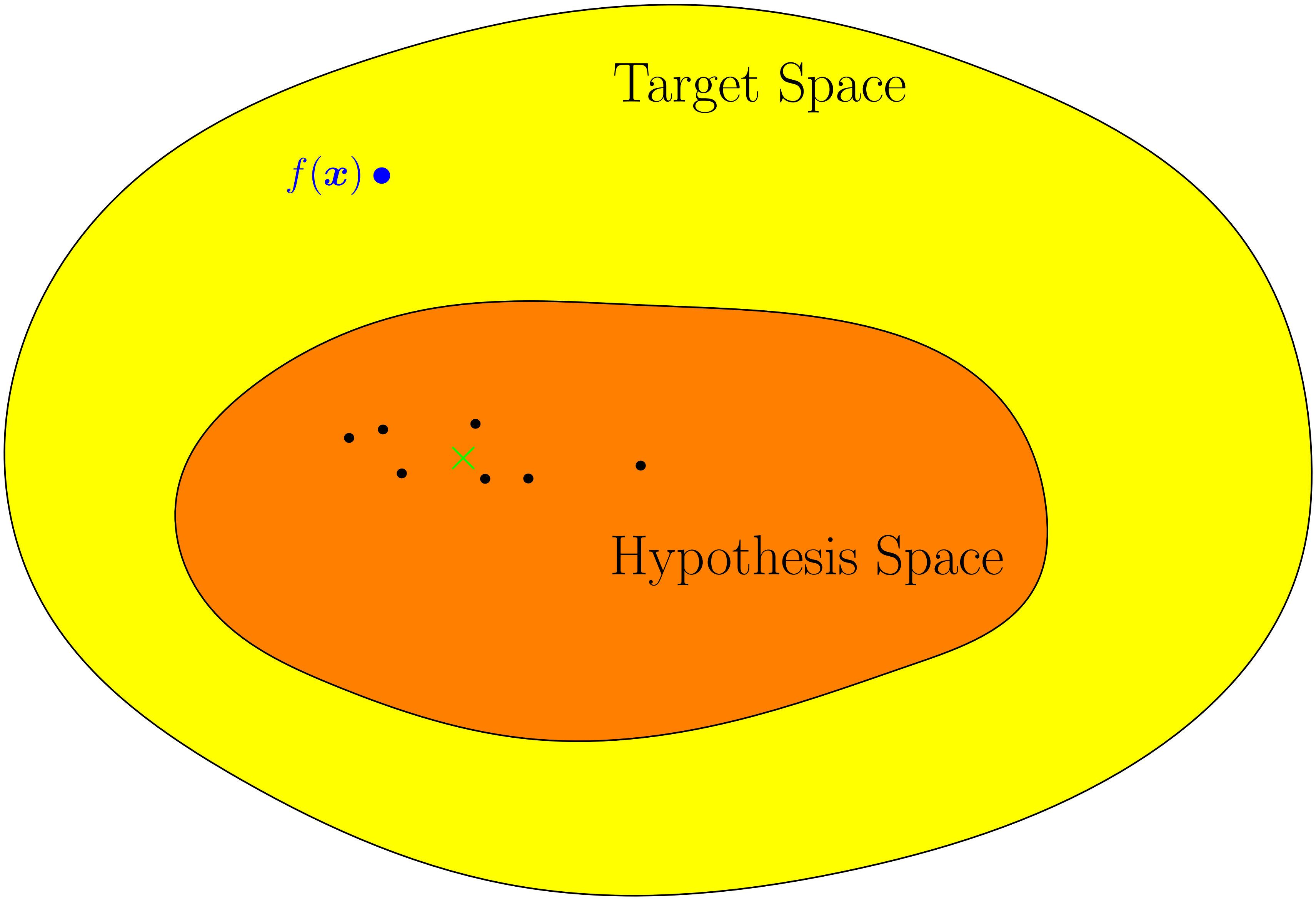

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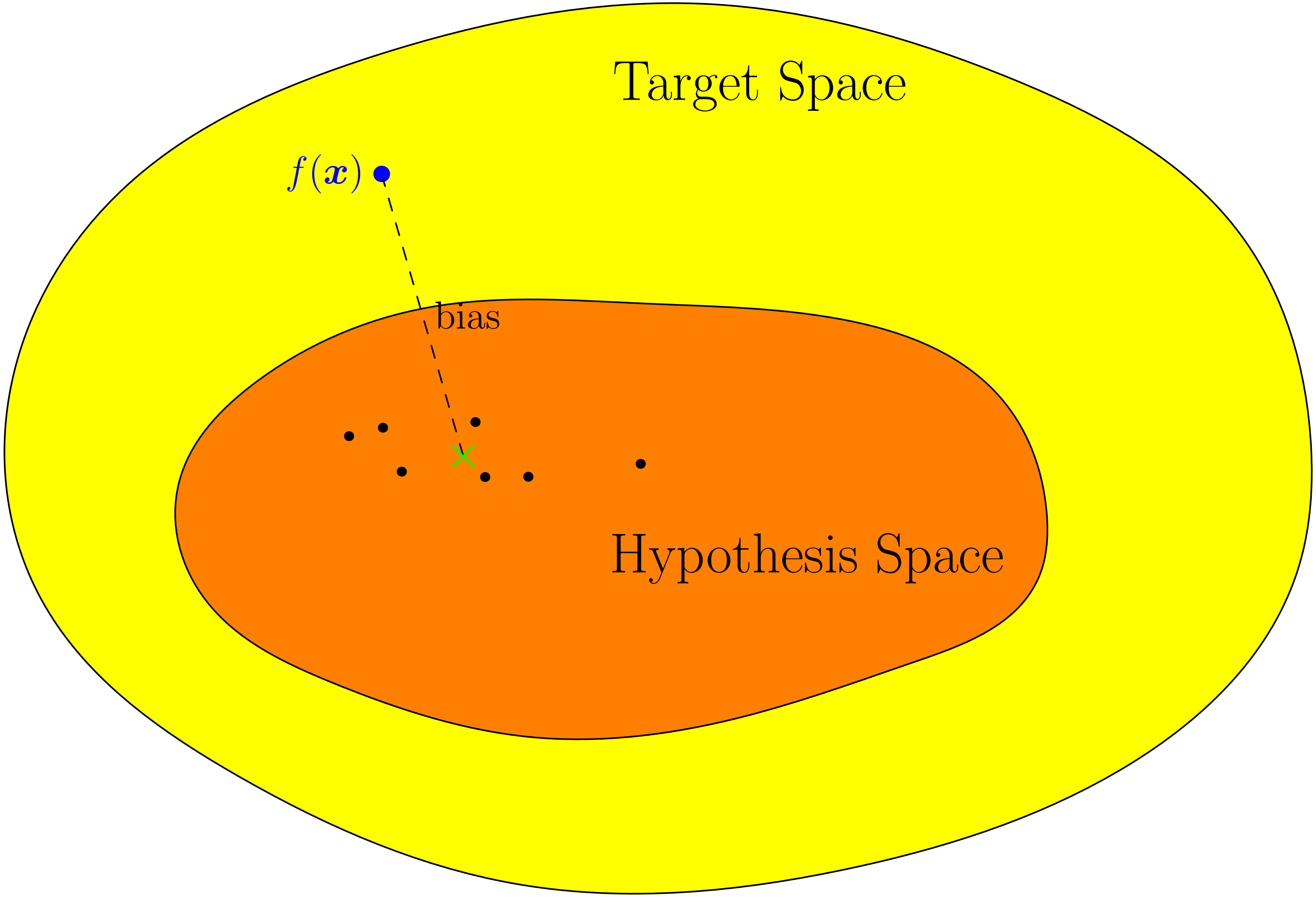

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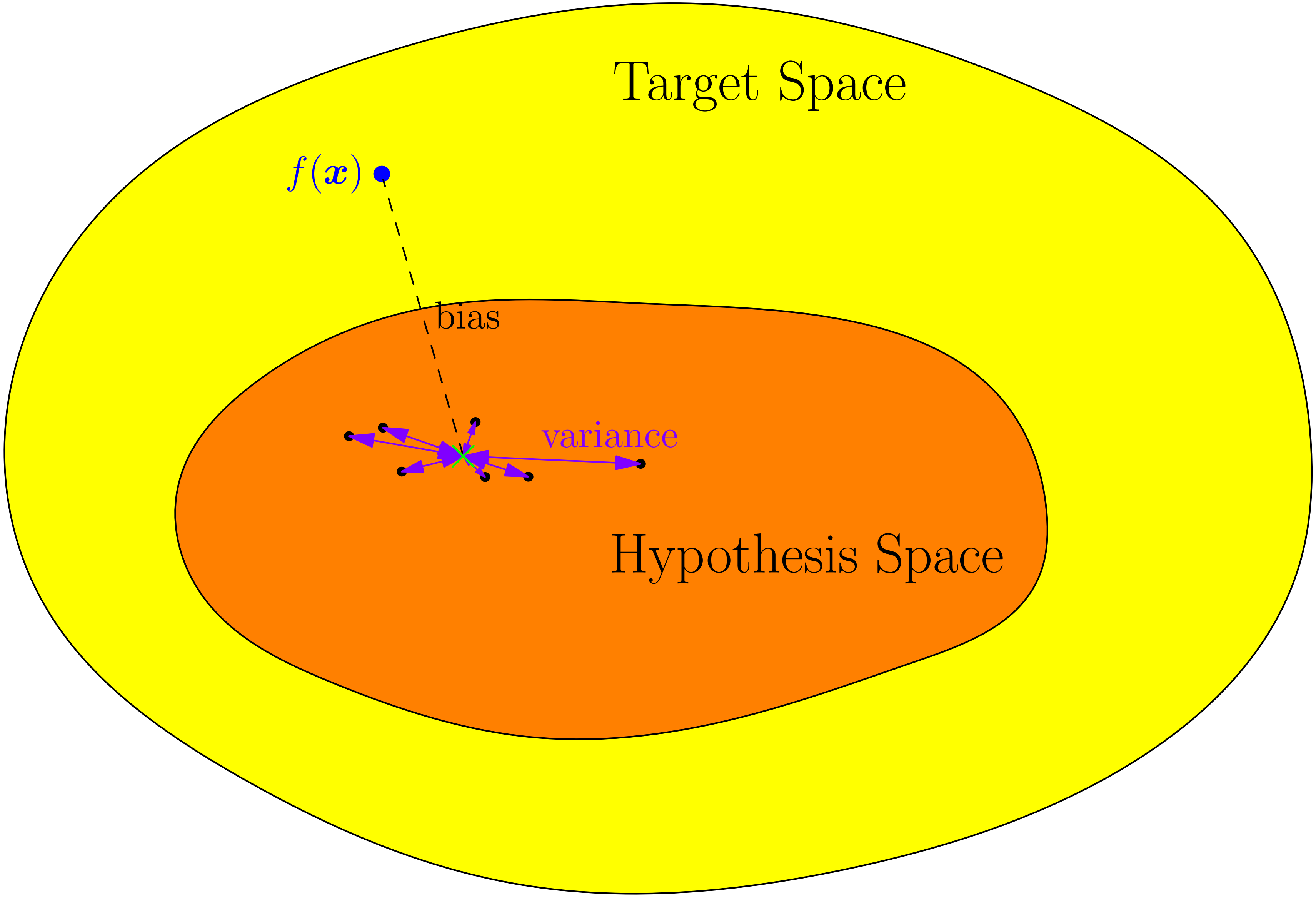

Mean Machine

- To help understand generalisation we can consider the mean prediction with respect to machines trained with all data sets of size m

$$\hat{f}_m(\boldsymbol{x}) = \mathbb{E}_{\mathcal{D}}\left[\hat{f}\left(\boldsymbol{x}|\mathcal{D}\right)\right]$$

- We can define the **bias** to be generalisation performance of the mean machine

$$B = \sum_{\boldsymbol{x} \in \mathcal{X}} p(\boldsymbol{x}) \left(\hat{f}_m(\boldsymbol{x}) - f\left(\boldsymbol{x}\right)\right)^2$$

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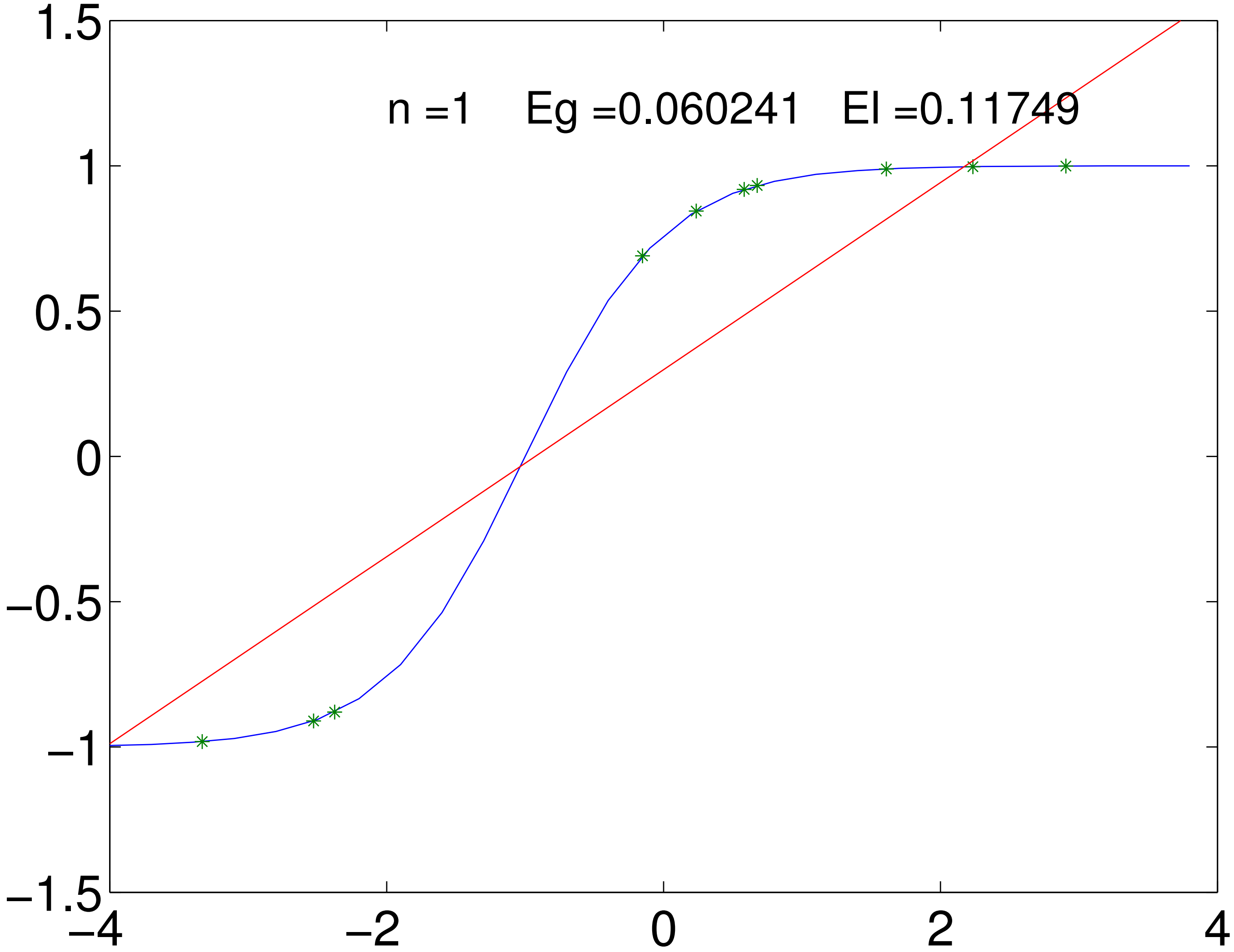

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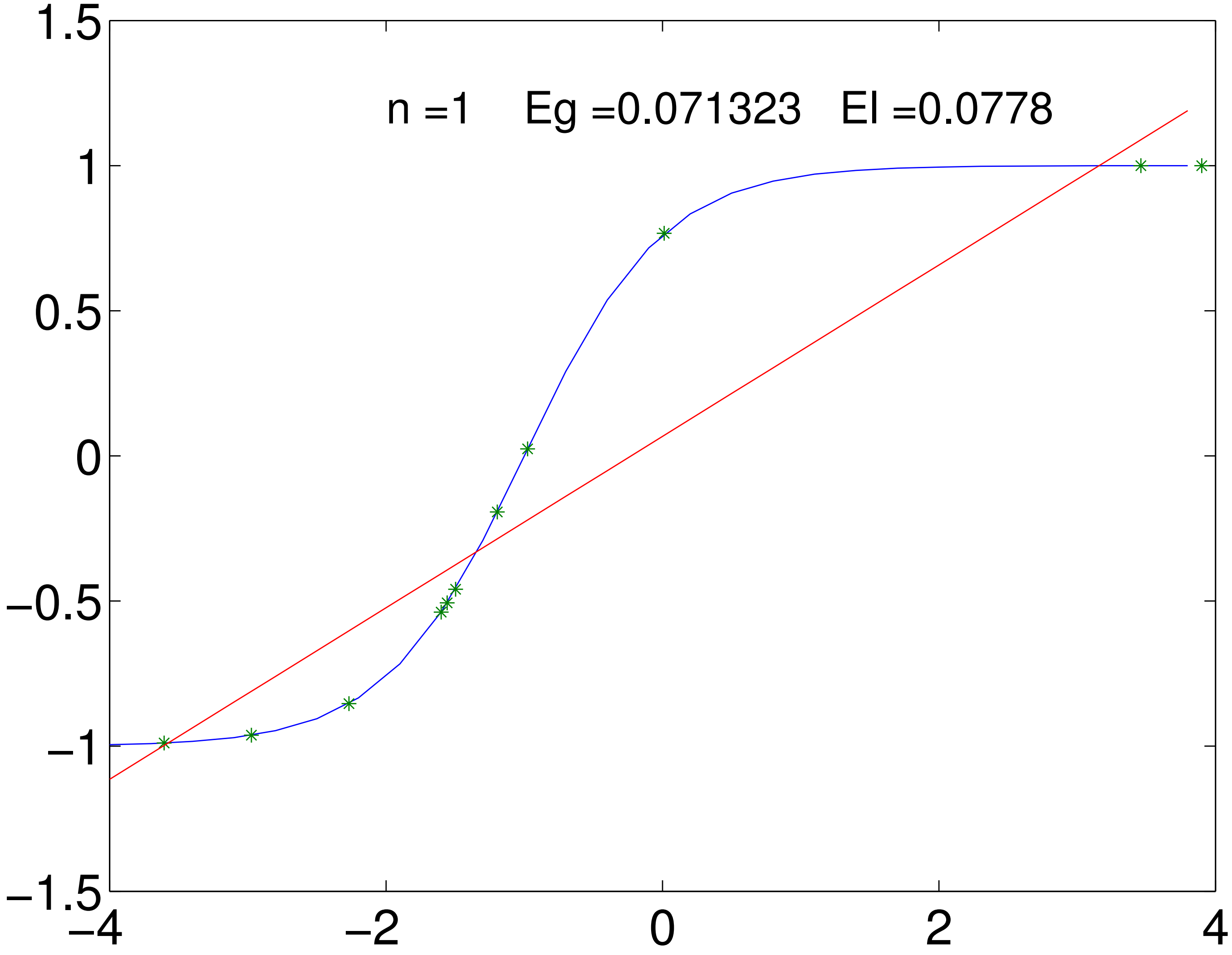

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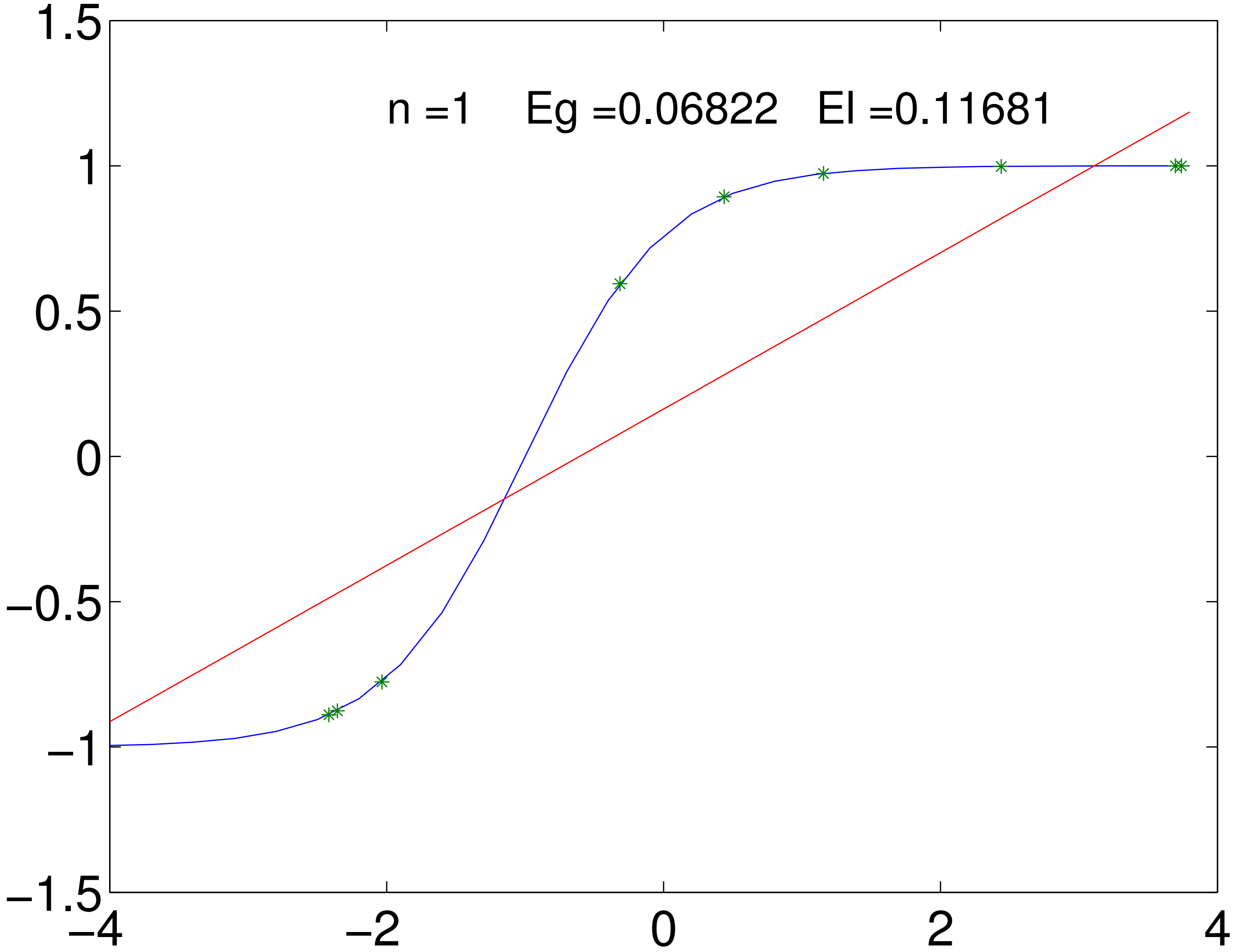

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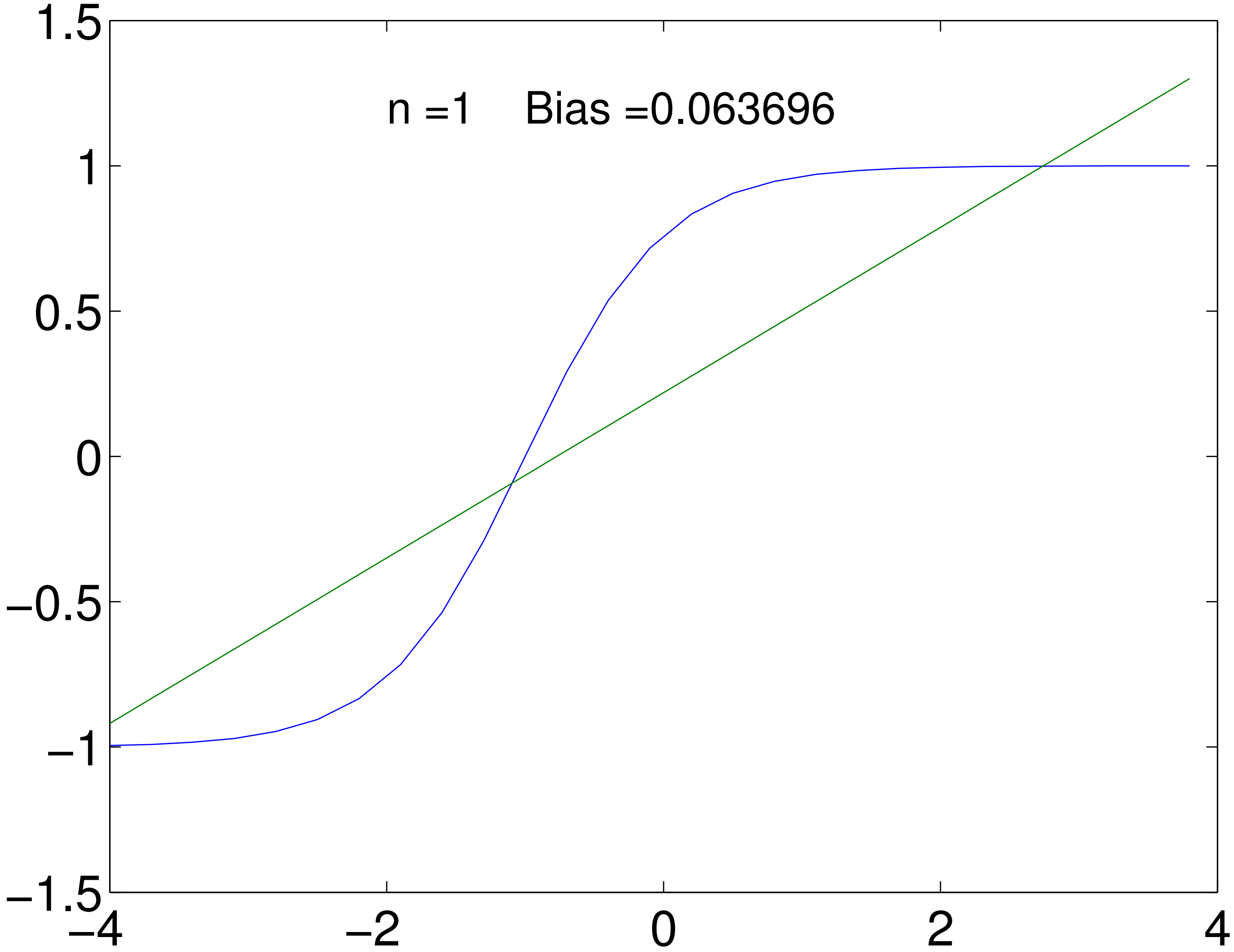

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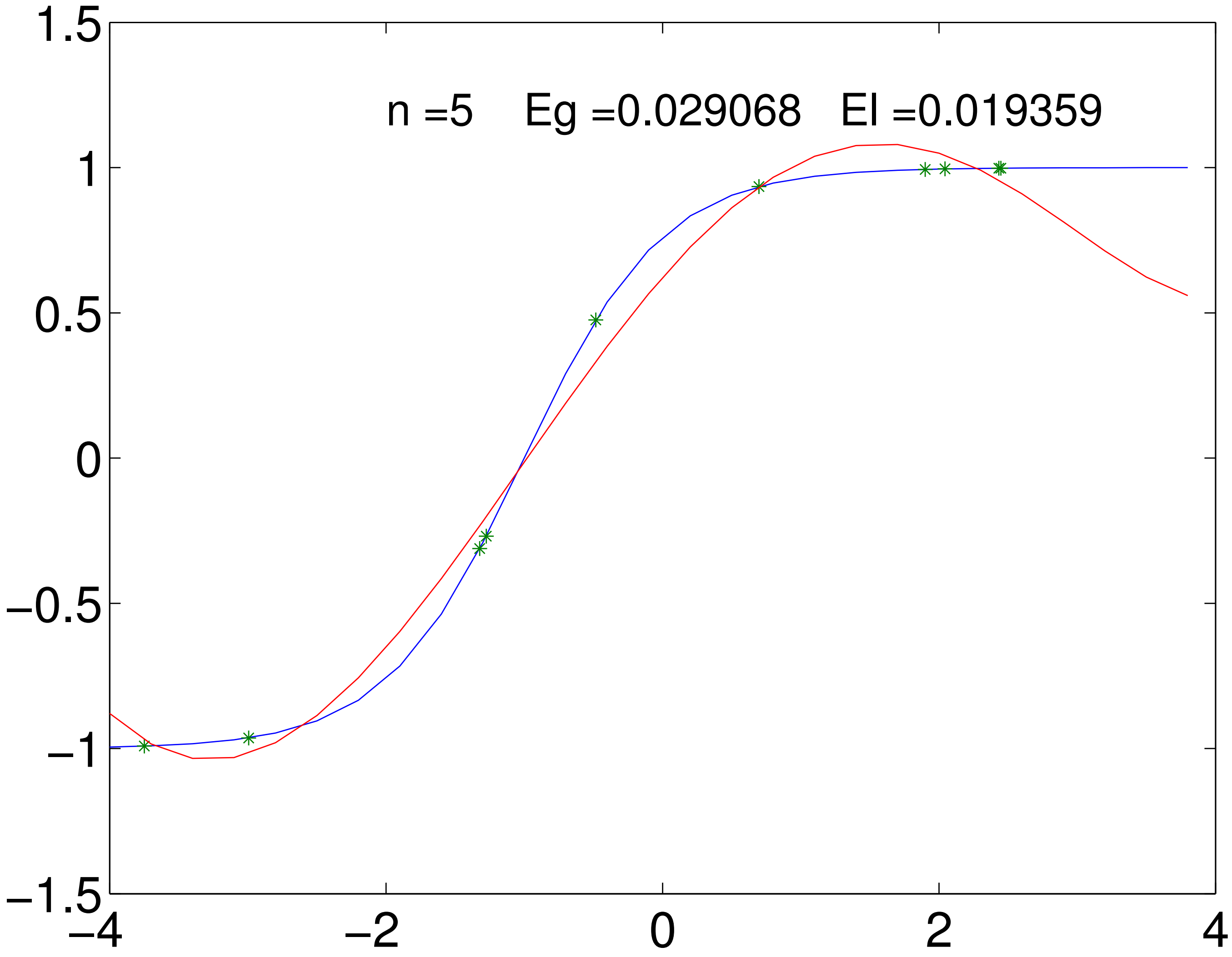

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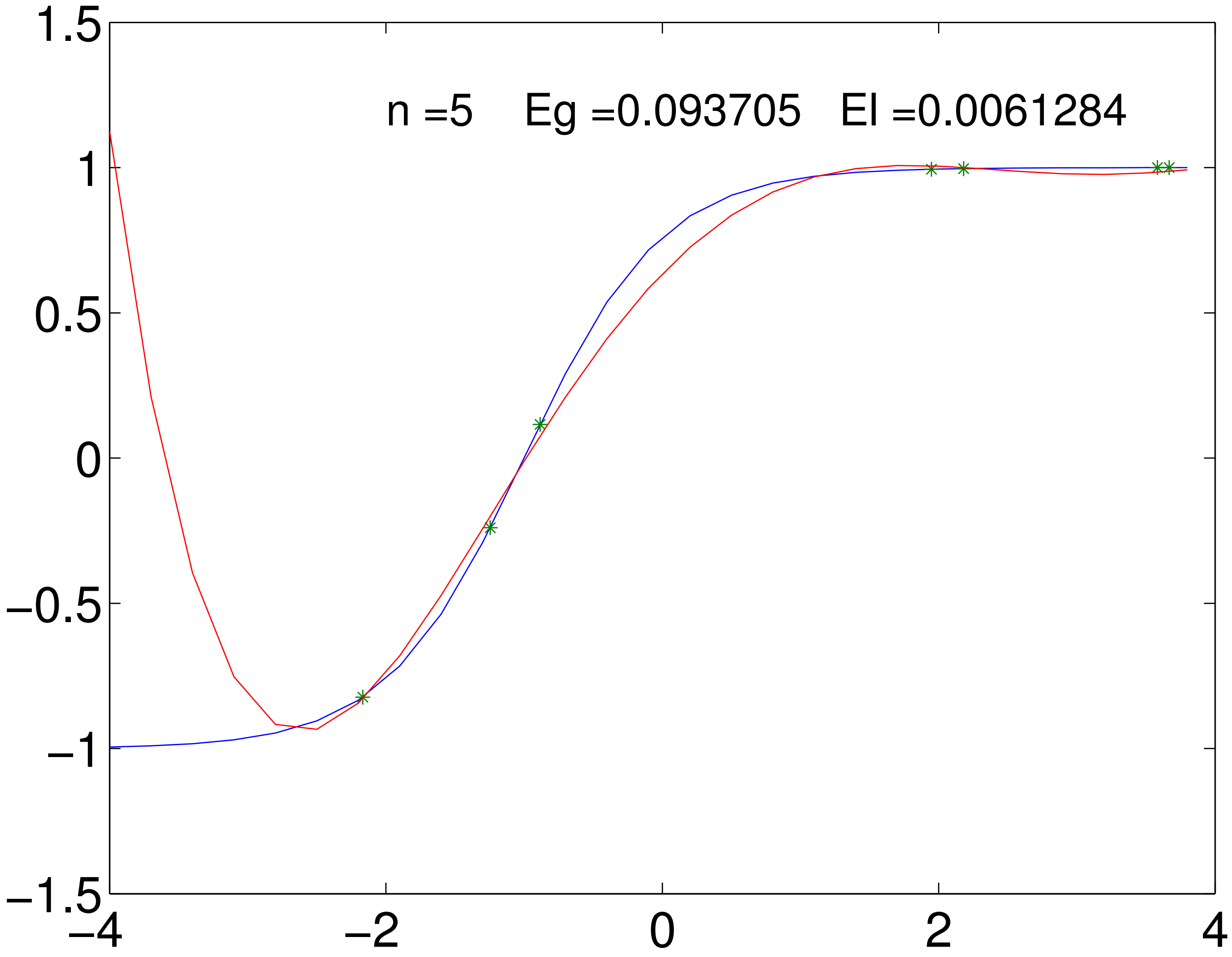

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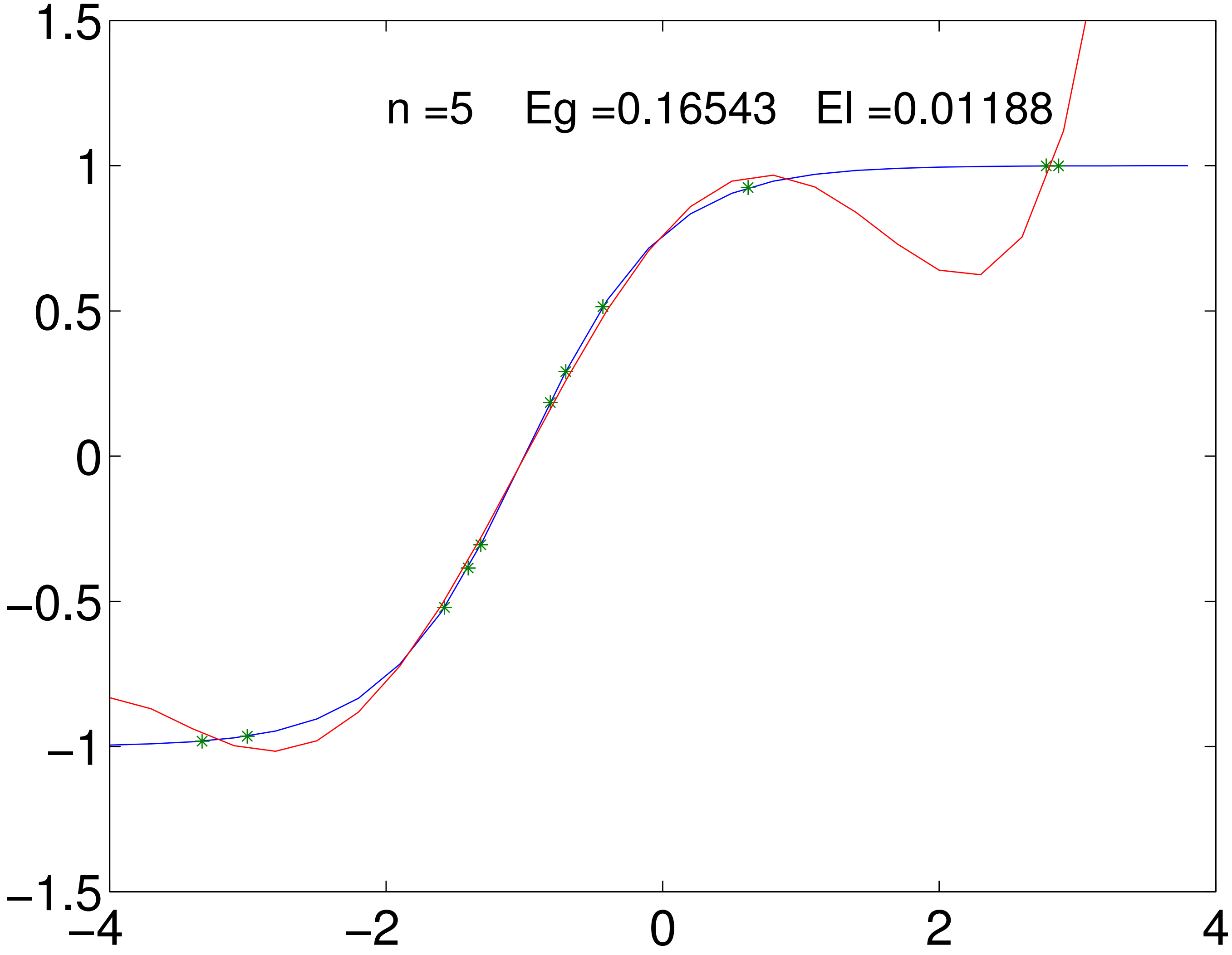

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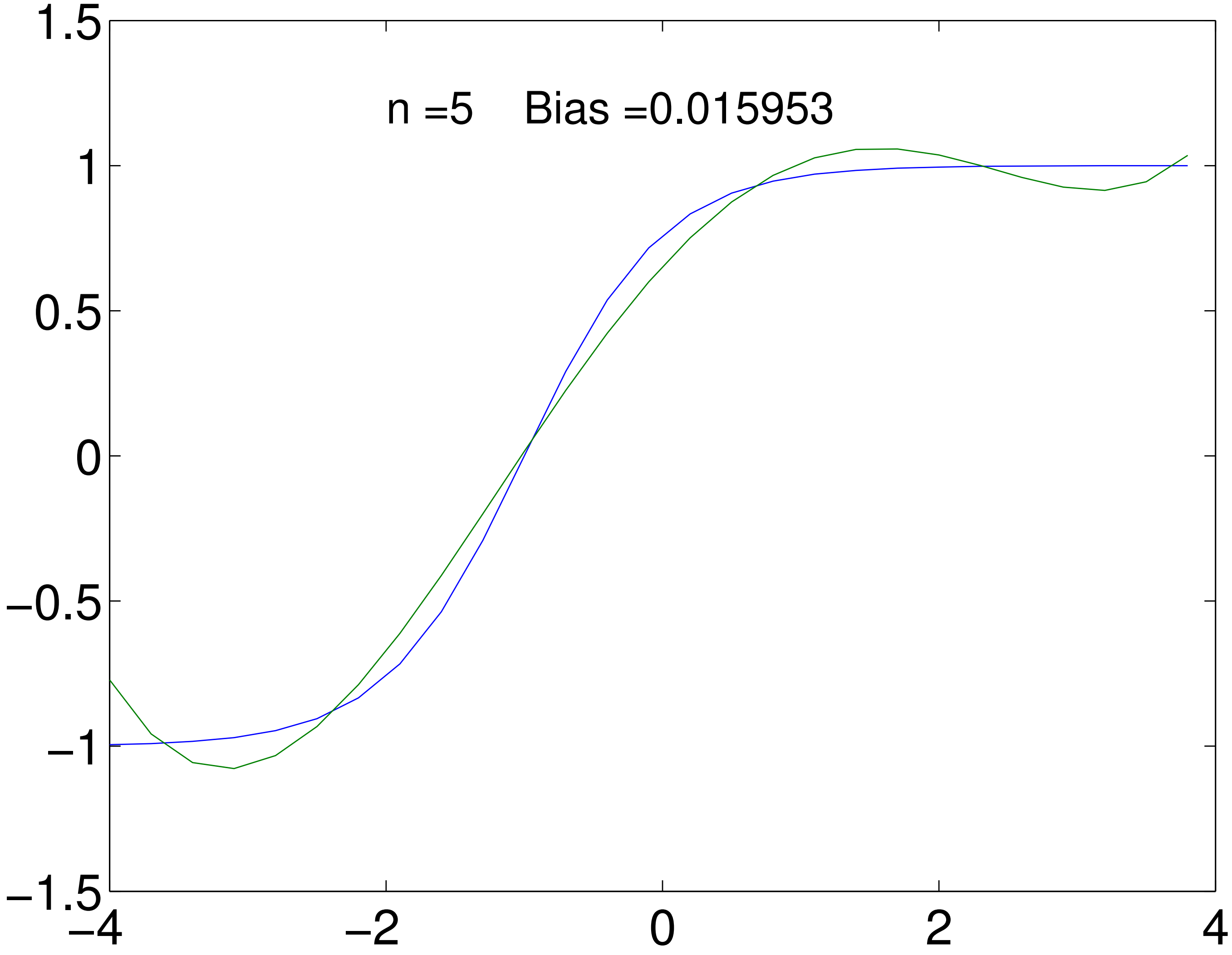

Bias and Variance

Consider the expected generalisation for data sets of size $|\mathcal{D}| = m$

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$$= \sum_{\boldsymbol{x}\in\mathcal{X}} p(\boldsymbol{x})\, \mathbb{E}_{\mathcal{D}}\left[\left(\hat{f}(\boldsymbol{x}|\mathcal{D}) - \hat{f}_m(\boldsymbol{x}) + \hat{f}_m(\boldsymbol{x}) - f(\boldsymbol{x}) \right)^2\right]$$

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$$\bar{E}_G = \mathbb{E}_{\mathcal{D}}[E_G(\mathcal{D})] = \mathbb{E}_{\mathcal{D}}\left[\sum_{\boldsymbol{x}\in\mathcal{X}} p(\boldsymbol{x}) \left(\hat{f}(\boldsymbol{x}|\mathcal{D}) - f(\boldsymbol{x})\right)^2\right]$$

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Cross Term

- The cross term vanishes

$$C = \mathbb{E}_{\mathcal{D}}\left[\left(\hat{f}(\boldsymbol{x}|\mathcal{D}) - \hat{f}_m(\boldsymbol{x})\right)\left(\hat{f}_m(\boldsymbol{x}) - f(\boldsymbol{x})\right)\right]$$

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\bar{E}_G = \sum_{\boldsymbol{x}\in\mathcal{X}} p(\boldsymbol{x})\mathbb{E}_{\mathcal{D}}\left[\left(\hat{f}(\boldsymbol{x}|\mathcal{D}) - \hat{f}_m(\boldsymbol{x})\right)^2 + \left(\hat{f}_m(\boldsymbol{x}) - f(\boldsymbol{x})\right)^2\right]
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Bias and Variance

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$$+ \sum_{\boldsymbol{x} \in \mathcal{X}} p(\boldsymbol{x}) \left(\hat{f}_m(\boldsymbol{x}) - f(\boldsymbol{x})\right)^2 = V + B$$

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Bias-Variance Dilemma

- The bias measure the generalisation performance of the *mean machine* and is large if the machine is too simple to capture the changes in the function we want to learn

- The variance measures the variation in the prediction of the machine as we change the data set we train on

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Balancing Bias and Variance

- We want to choose a learning machine that is complex enough to capture the underlying function we are trying to learn, but otherwise as simple as possible
- There are a number of tricks to achieve this balance
- Some require us to preprocess the data to reduce the number of inputs
- Some machines cleverly adjust their own complexity
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Over-fitting

- Complex machine can **over-fitting**

  ***over-fitting**: fitting the training data well at the cost of getting poorer generalisation performance*

- Three red cars. . .

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Binary Classification Task for You

Class 1

Class 2

Which Category?

- Which category does the following image belong to?

Spurious Rules

- You ask a learning machine to solve a task based on data
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- Infinitely flexible machines have an infinity of spurious rules they can learn—they are useless

All Binary Functions

$$\boldsymbol{x}_0 = 0\,0\,0 \quad y_0 = \left\{ \begin{array}{l} 0 \\ 1 \end{array} \right.$$

$$\boldsymbol{x}_1 = 1\,0\,0 \quad y_1 = \left\{ \begin{array}{l} 0 \\ 1 \end{array} \right.$$

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Controlling Complexity

- Infinitely flexible machine don't generalise

- **Machine learning only works because there is some structure in the data**

- A successful machine should capture this structure

- Even deep learning machines with millions of parameters only work because they successfully capture the structure of images or text

- Different learning machines have different performance on different problems because the data has different structure

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Training Examples

- As we increase the number of training examples, we make it hard to find a spurious rule
- Bigger data sets allow us to use more complicated machines
- Part of the success of deep learning is because they use huge training sets
- (Labelled) data is often expensive to collect so we sometimes have no choice but to use a small training set
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Dimensionality Reduction

- We can simplify our machines by using less features
- We can project our data onto a lower dimensional sub-space (e.g. one with the maximum variation in the data PCA)
- We can use clustering to find exemplars and recode our data in terms of differences from the exemplars (radial basis functions)
- Whether this helps depends on whether the information we discard is pertinent to the task we are trying to perform

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- We can try different combinations of features to find the best set, although it rapidly becomes intractable to do this in all ways
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Explicit Regularisation

- As Niranjan showed us we can modify our error function to choose smoother functions

$$E = \sum_{n=1}^{N} \left(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n - y_n \right)^2$$

- Second term is minimised when $w_i = 0$

- If w_i is large then

$$f(\boldsymbol{x}|\boldsymbol{w}) = \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n$$

varies rapidly as we change x_i

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Lasso

- We can us other regularisers

$$E = \sum_{n=1}^{N} \left(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n - y_n \right)^2$$

- Spurious features (e.g. shoe size) will give us a small improvement in training error

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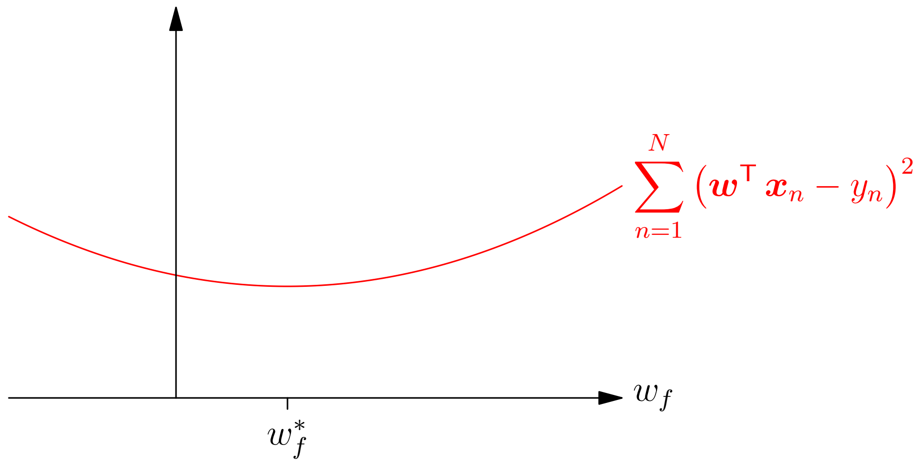

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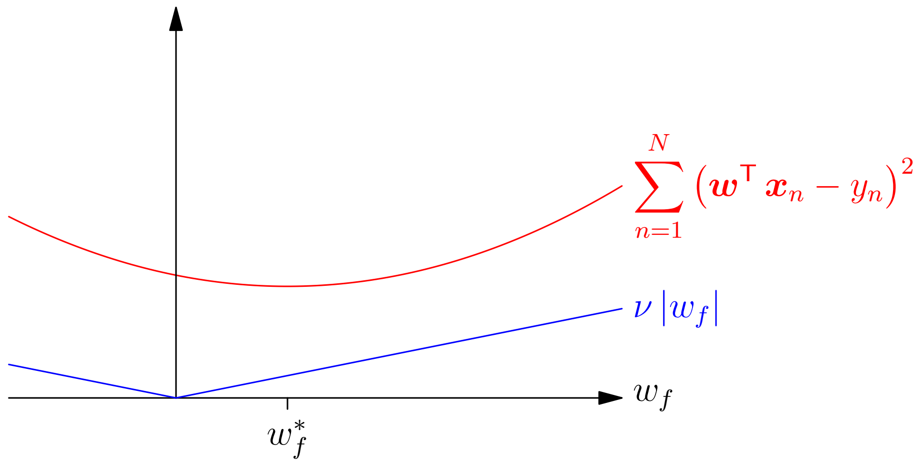

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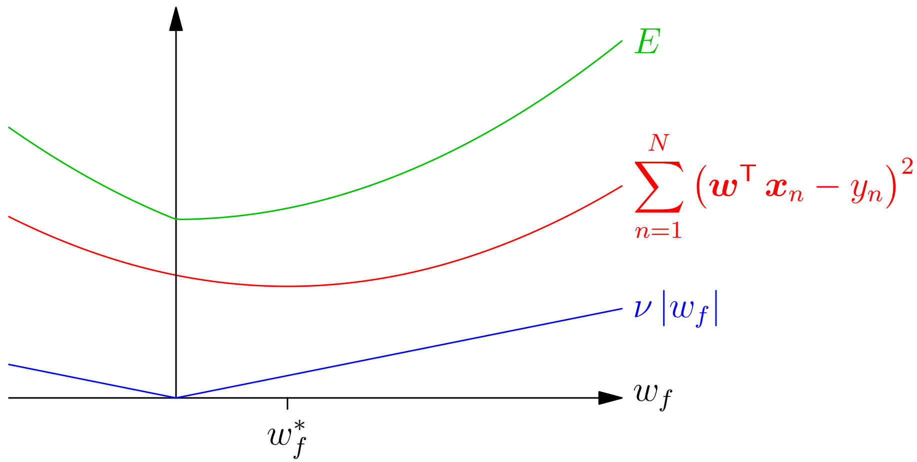

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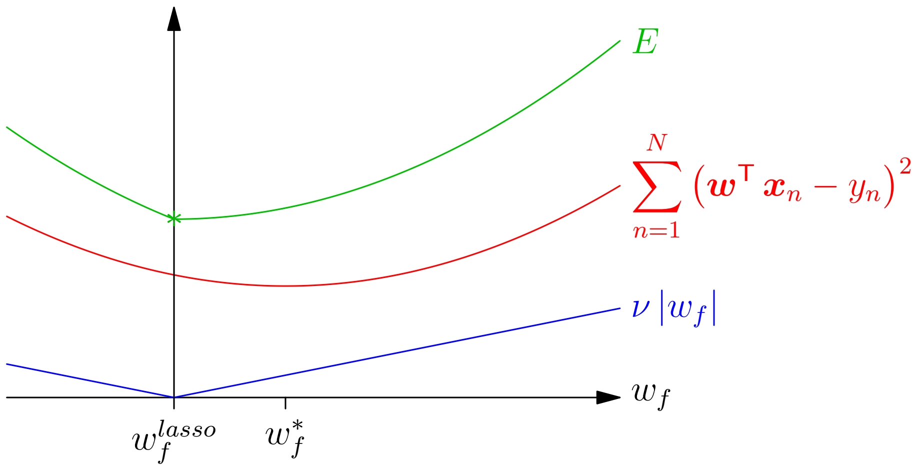

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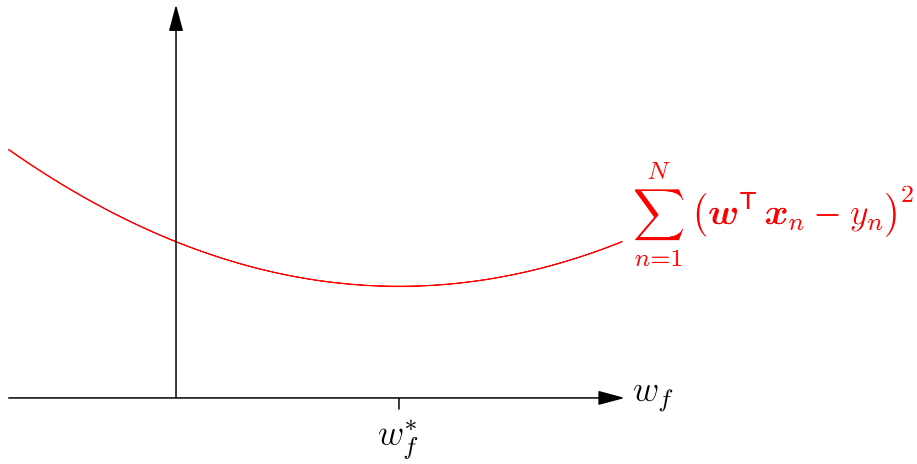

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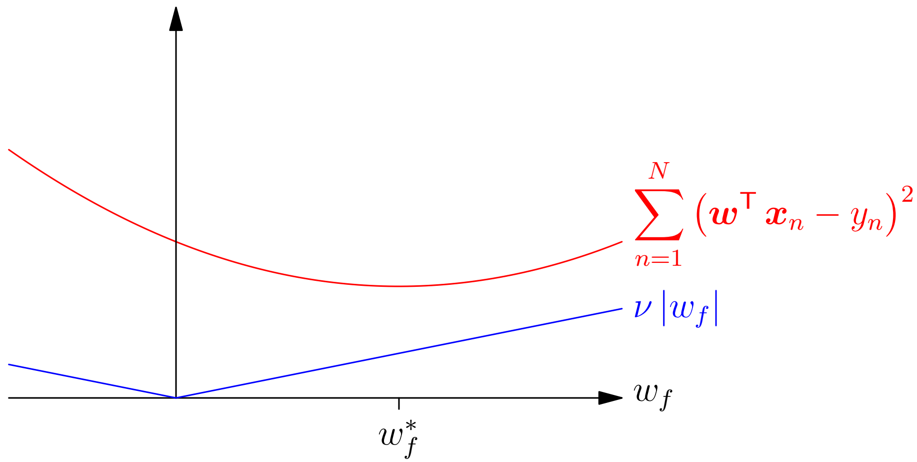

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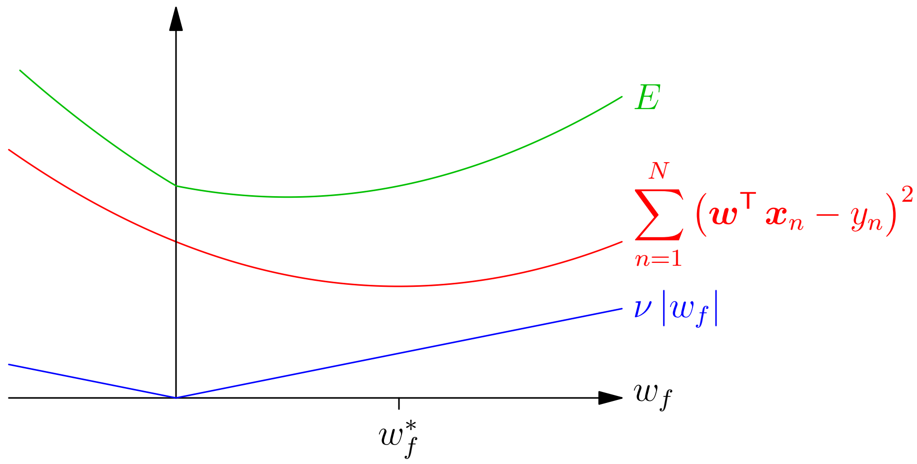

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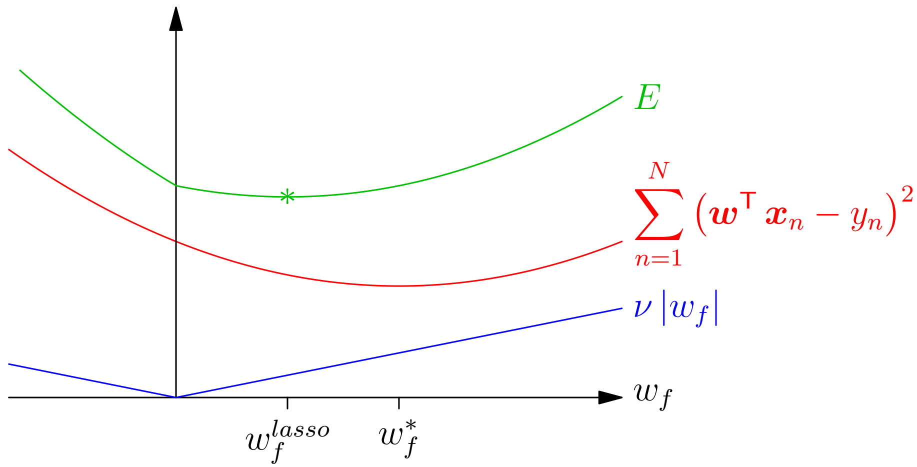

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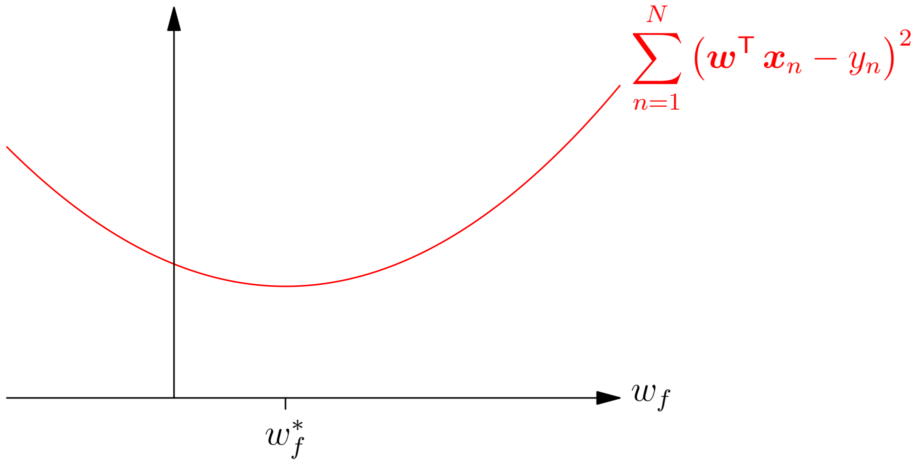

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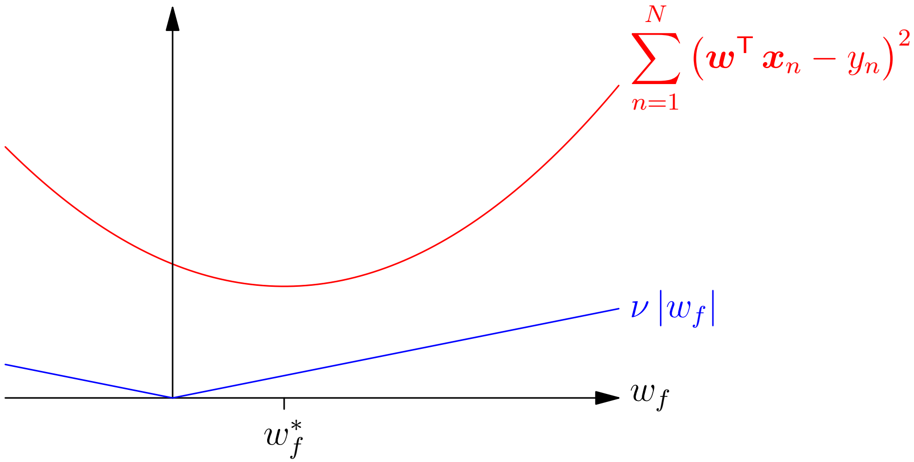

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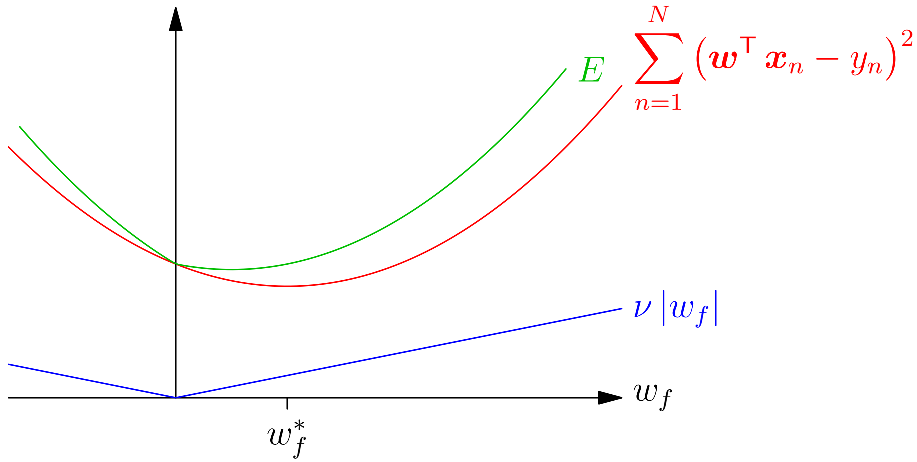

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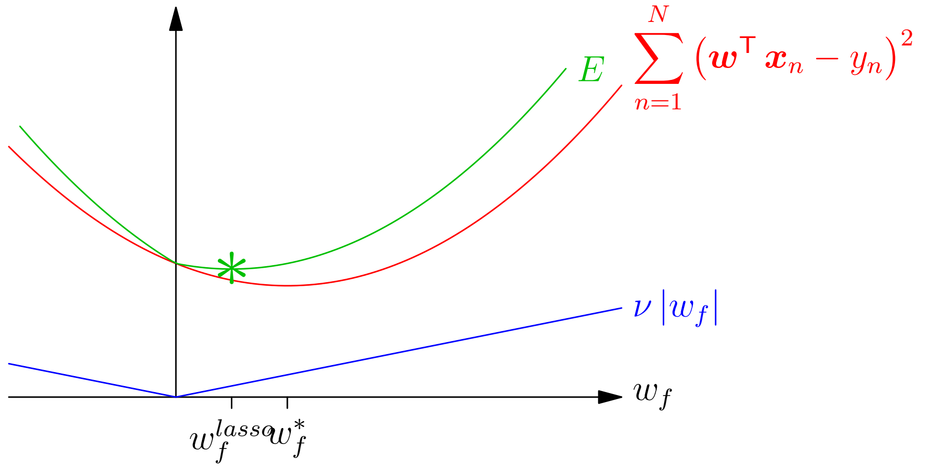

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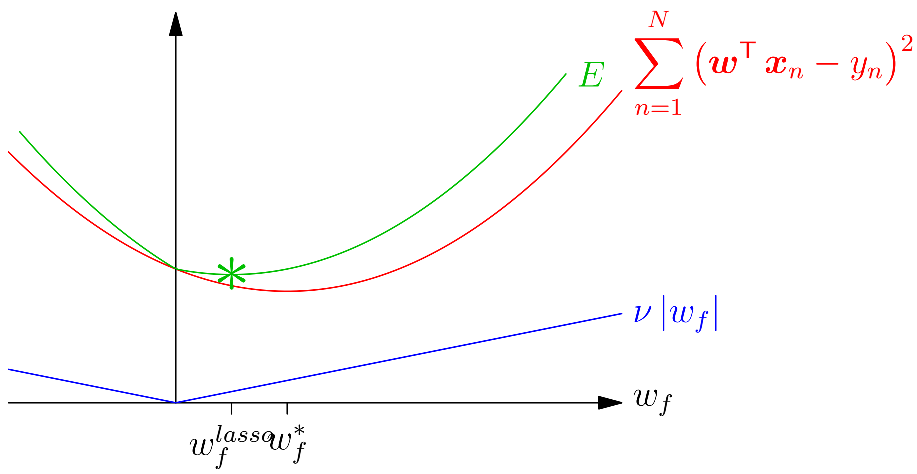

- Does automatic feature selection

Implicit Regularisation

- In the last two examples we added an explicit regularisation term that made the function we learnt simpler
- Some learning machines do this less explicitly
- Some deep learning architectures do subtle averaging
- Sometimes the architecture biases the machine to find a simple solution
- We will see this in support vector machines shortly

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Choosing Machines

- We often have to choose between learning machines
- Or select "*hyper-parameters*"
- Decide what features to use
- We don't want to choose a model that over-fits the training data
- Need an unbiased estimate of the generalisation performance

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- Recall, we want to predict **unseen** data
- **You cannot use data that you have trained on!**
- Need to split your data up into training and validation set
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Cross Validation

- If you want to use more data for training then you can use cross validation

- K-fold cross validation splits the data into K groups

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Test Set   Training Set

5-fold cross-validation

$$E_g = \qquad 5.1$$

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Training Set   Test Set   Training Set

5-fold cross-validation

$$E_g = \qquad 3.7$$

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Training Set — Test Set — Training Set

5-fold cross-validation

$$E_g = \qquad 4.6$$

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Training Set Test Set Training Set

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Training Set Test Set

5-fold cross-validation

$E_g =$ 3.3

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$$\langle E_g \rangle = \frac{5.1 + 3.7 + 4.6 + 4.6 + 3.3}{5} = 4.3$$

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Test Set

Training Set

10-fold cross-validation

$$E_g = \quad 5.4$$

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Test Set

Training Set

10-fold cross-validation

$$E_g = \qquad 1.4$$

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Training Set Test Set Training Set

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Training Set — Test Set — Training Set

10-fold cross-validation

$$E_g = \qquad 3.2$$

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Training Set Test Set Training Set

10-fold cross-validation

$E_g =$

7

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Training Set Test Set Training Set

10-fold cross-validation

$$E_g = \quad 0.59$$

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Training Set   Test Set   Training Set

10-fold cross-validation

$$E_g = \qquad 4.1$$

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Training Set Test Set Training Set

10-fold cross-validation

$E_g =$ 5

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D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}

Training Set Test Set

10-fold cross-validation

$E_g =$ 5.8

Cross Validation

- If you want to use more data for training then you can use cross validation
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Training Set

Test Set

10-fold cross-validation

$$E_g = \qquad\qquad 2.3$$

Cross Validation

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$$\langle E_g \rangle = \frac{5.4 + 1.4 + 4.4 + 3.2 + 7 + 0.59 + 4.1 + 5 + 5.8 + 2.3}{10} = 3.9$$

Cross Validation

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Test

Leave-one-out cross-validation

$E_g = {}^{4.2}$

Cross Validation

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	Test																		

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$$E_g = \quad 2.9$$

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			Test																

Leave-one-out cross-validation

$$E_g = \qquad 1.4$$

Cross Validation

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				Test															

Leave-one-out cross-validation

$$E_g = \qquad 3$$

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					Test														

Leave-one-out cross-validation

$$E_g = \quad 3.7$$

Cross Validation

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$$\langle E_g \rangle = 3.98$$

- Leave-one-out cross-validation is extreme case

Testing and Validation

- The *validation set* is usually used for choosing hyper-parameters
- This also can include ways of preprocessing, how long you train for, different ways of handling missing data, etc.
- Having chosen your best machine you now have a **biased** estimate of your generalisation performance
- You need a third independent set, *the test set*, to obtain an unbiased estimate of the generalisation error

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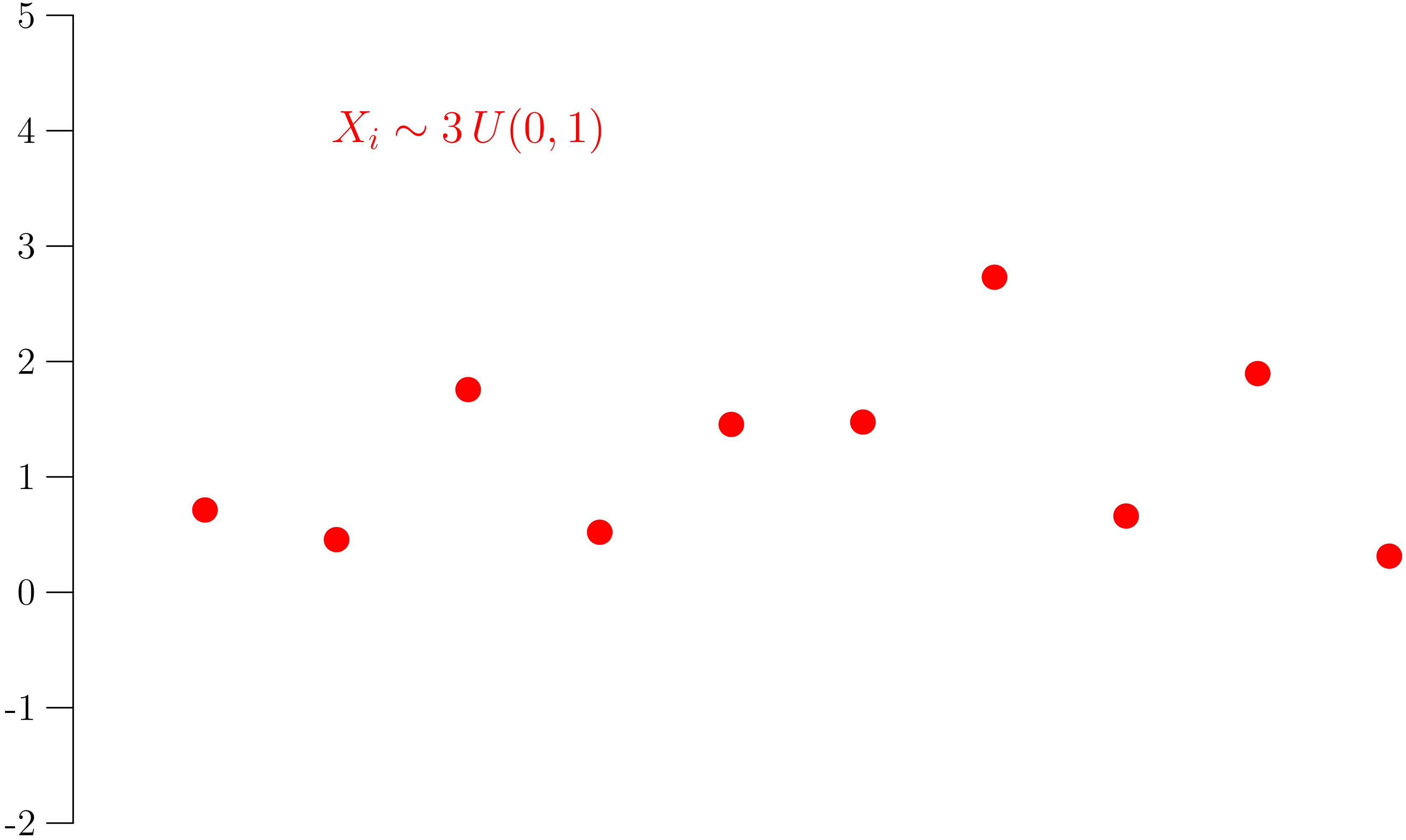
The Over-fitting Game



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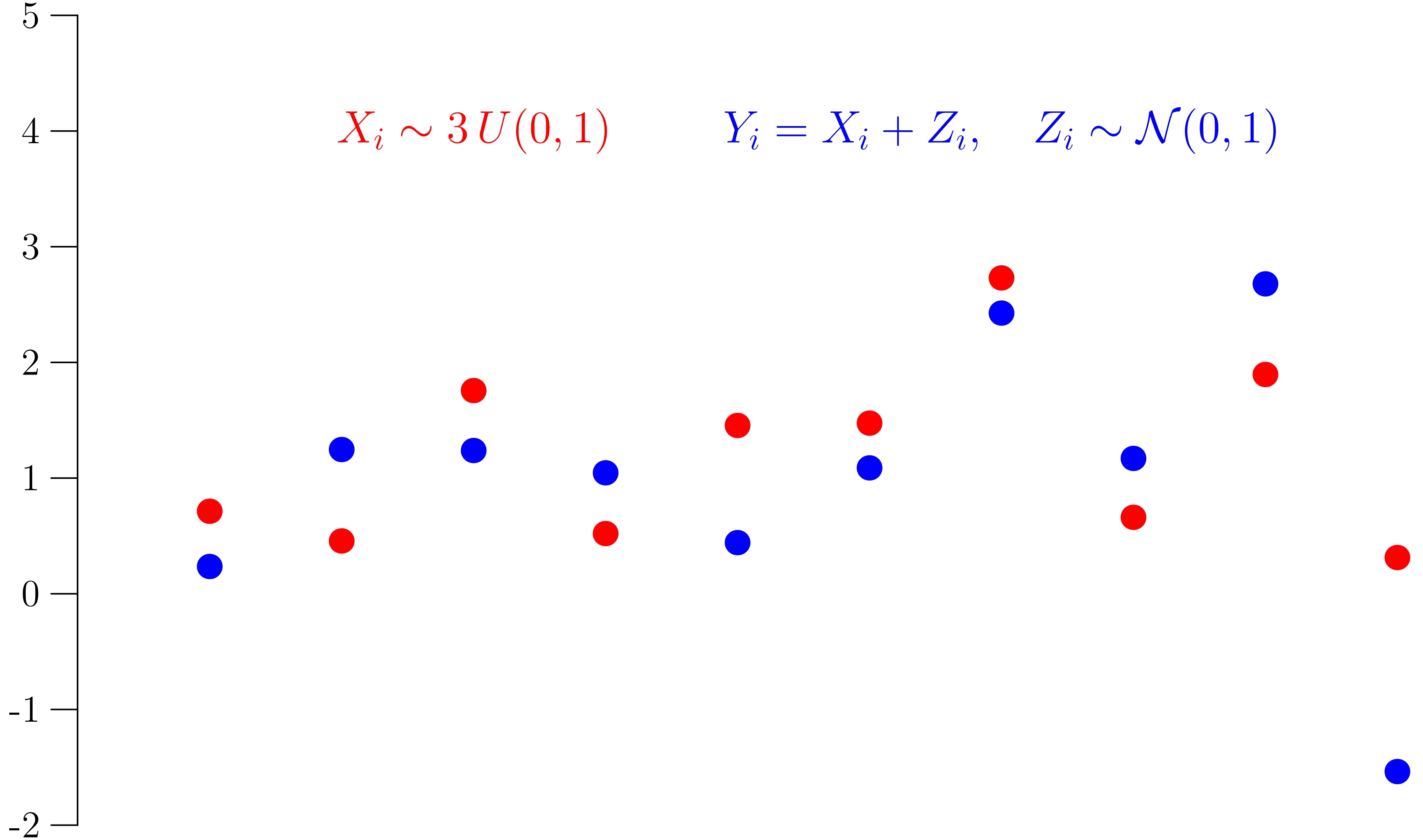

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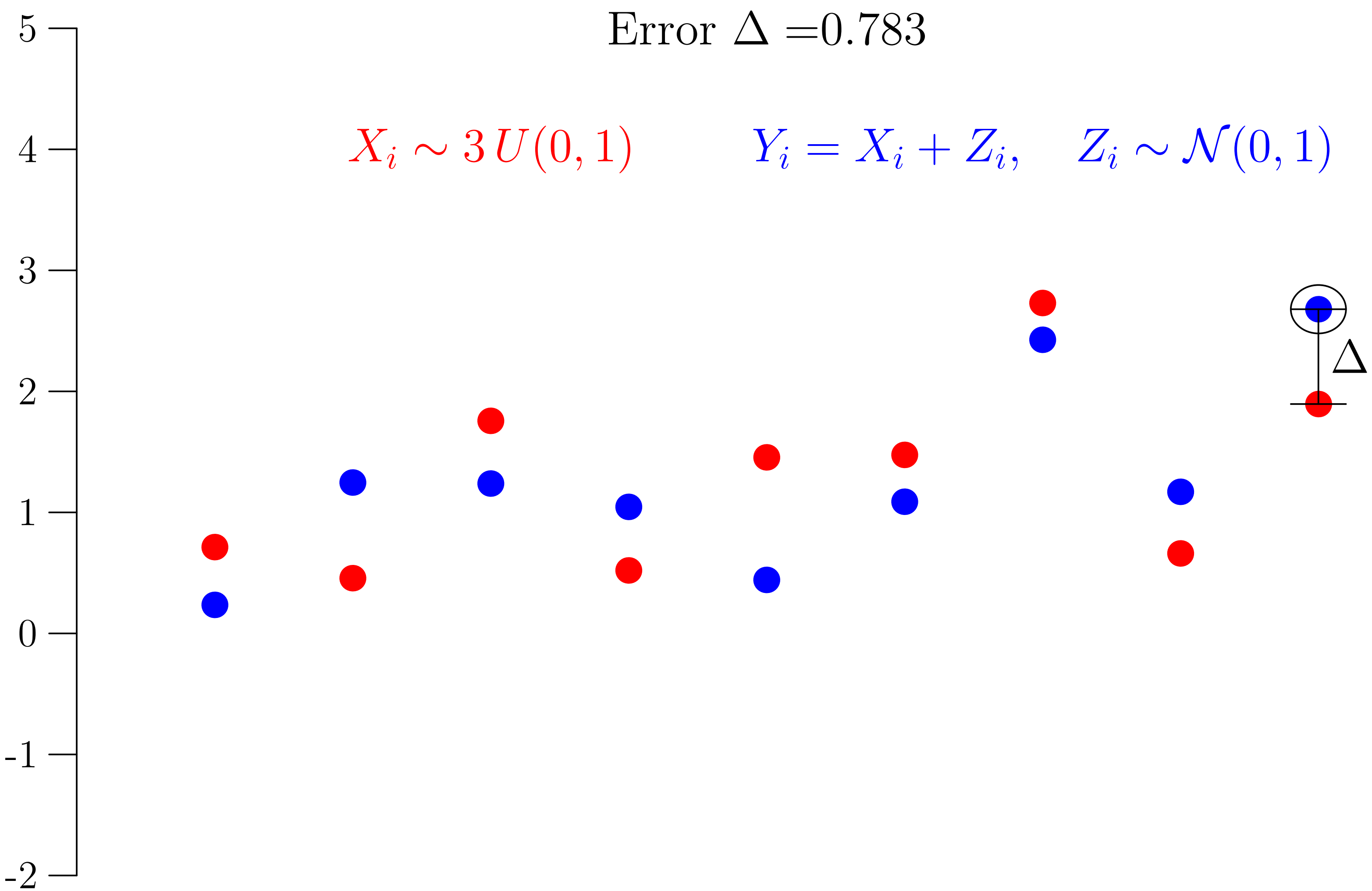

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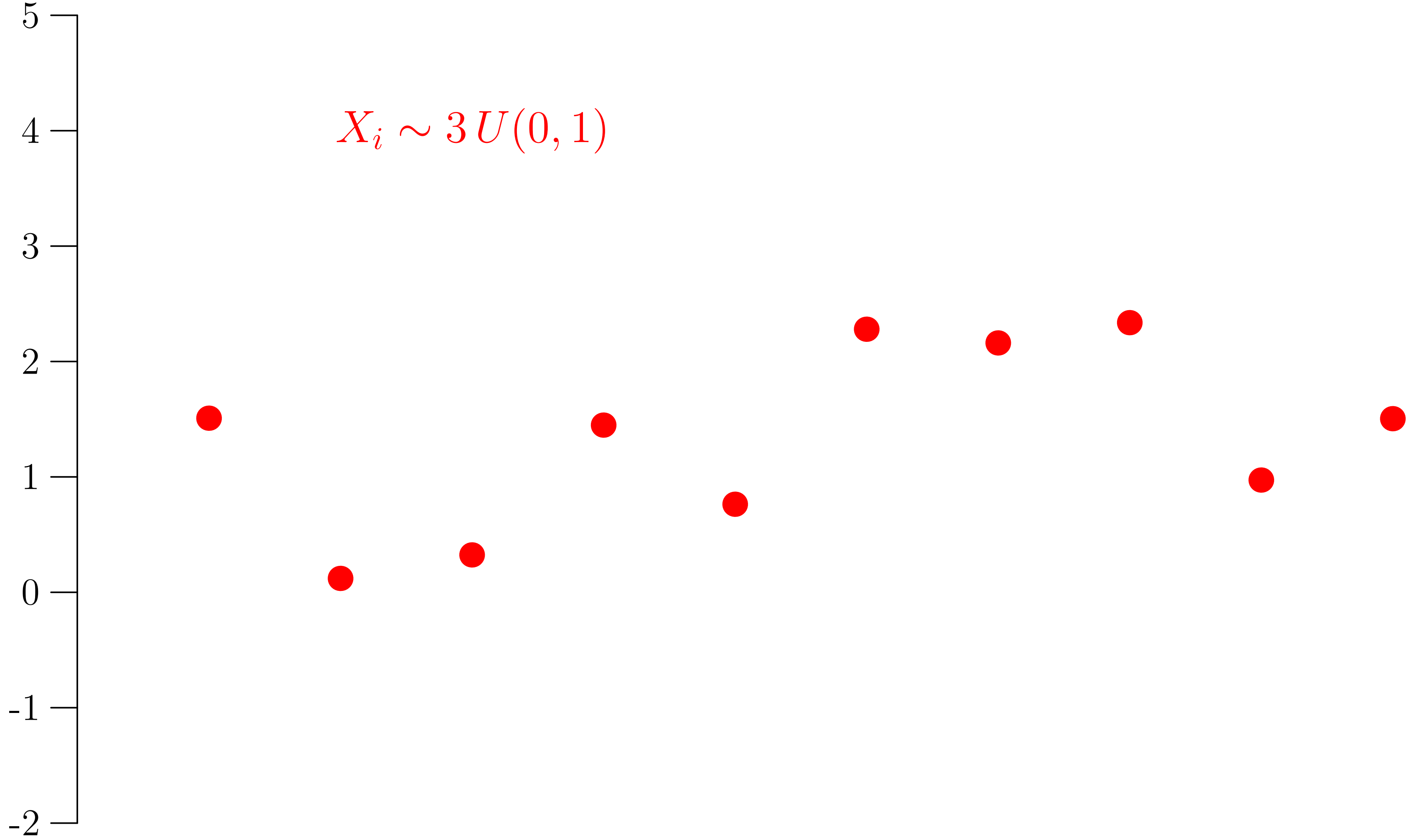

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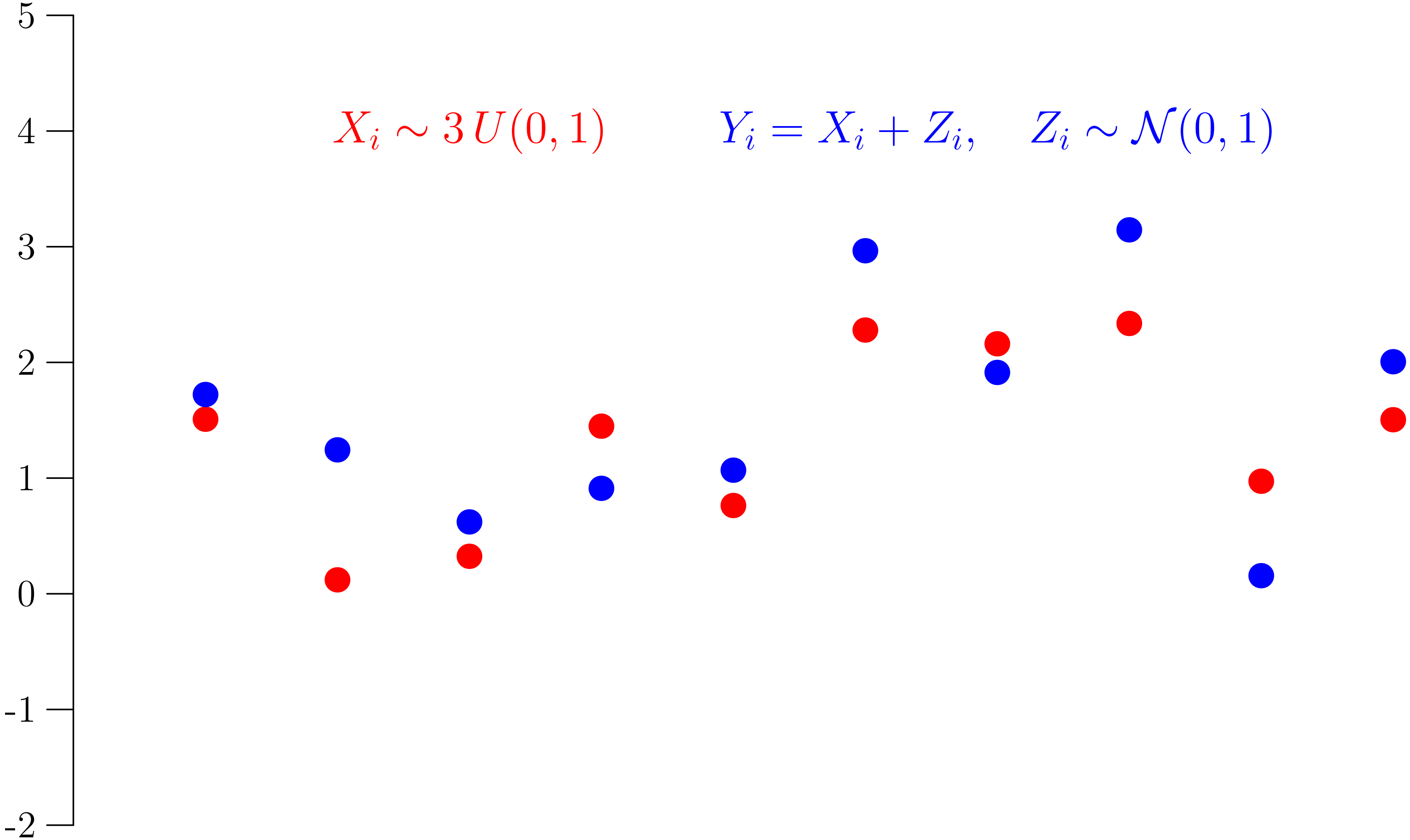

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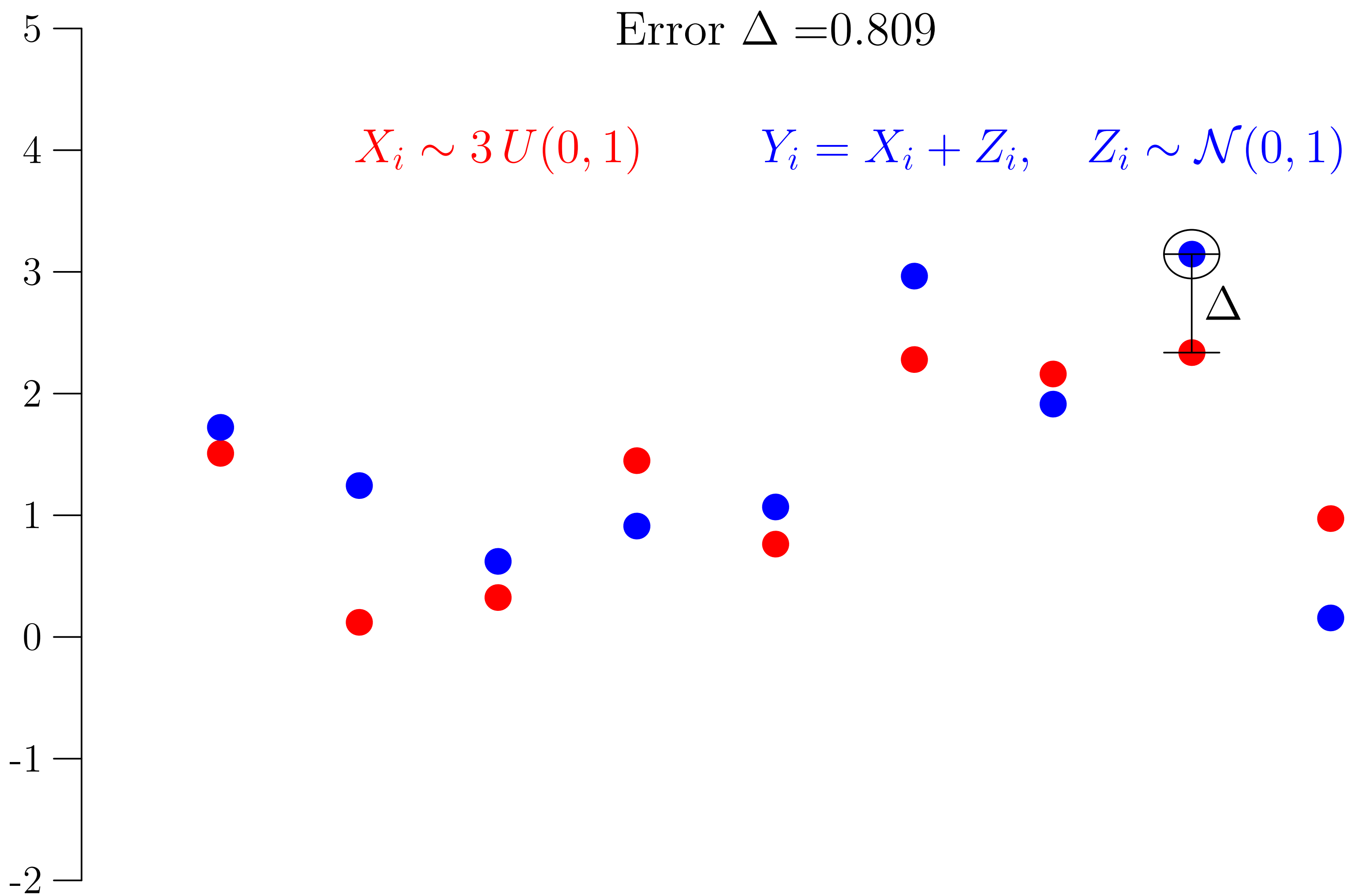

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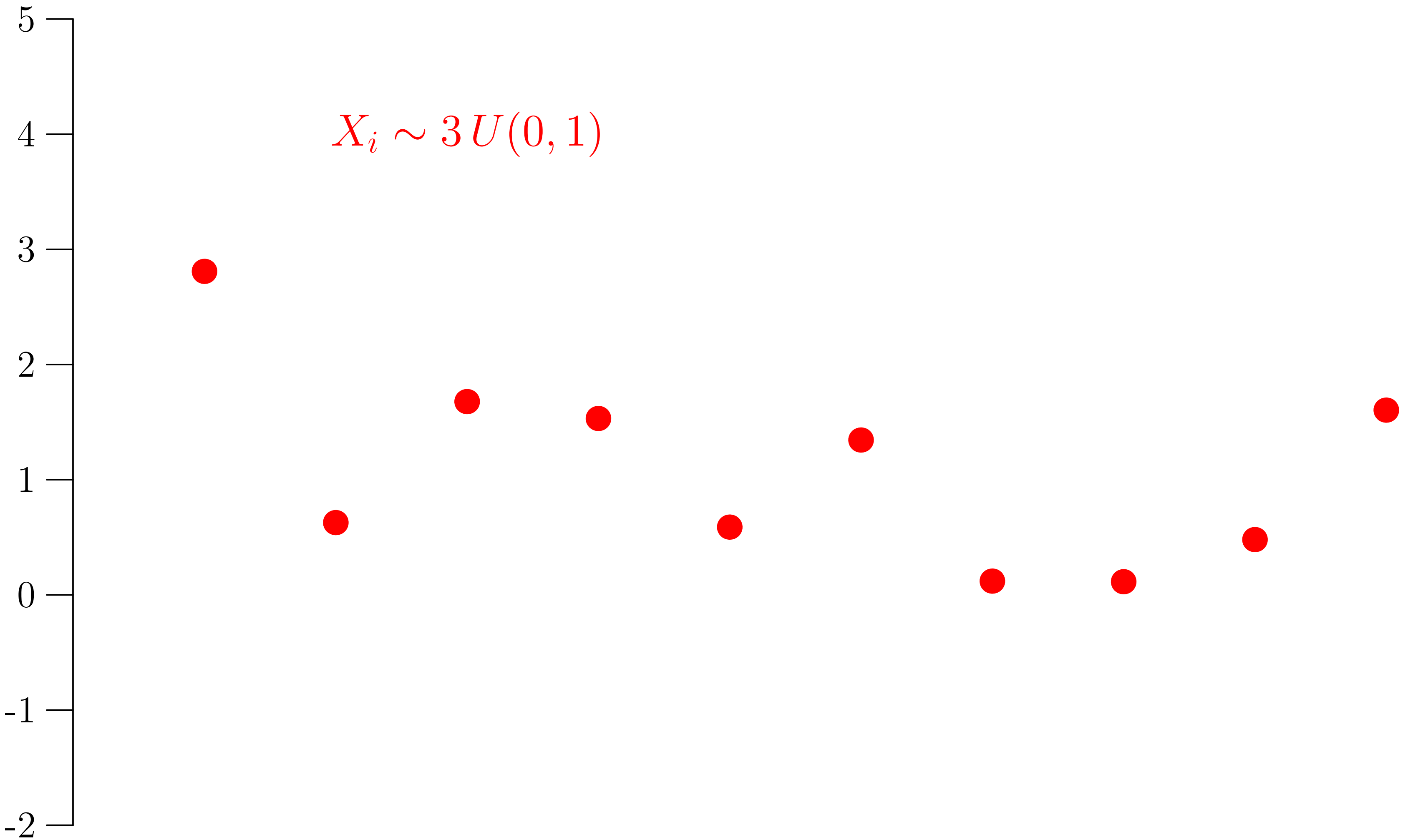

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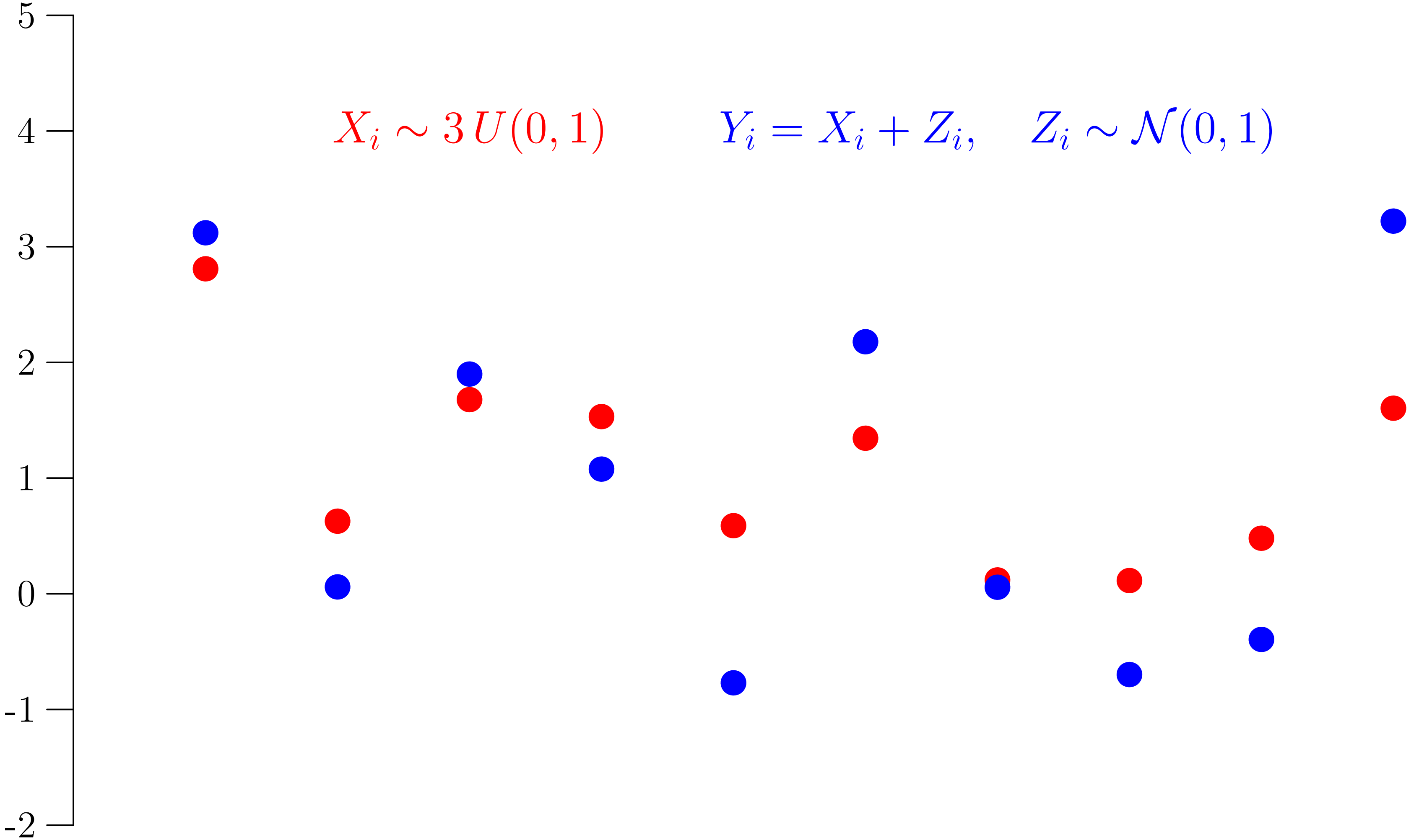

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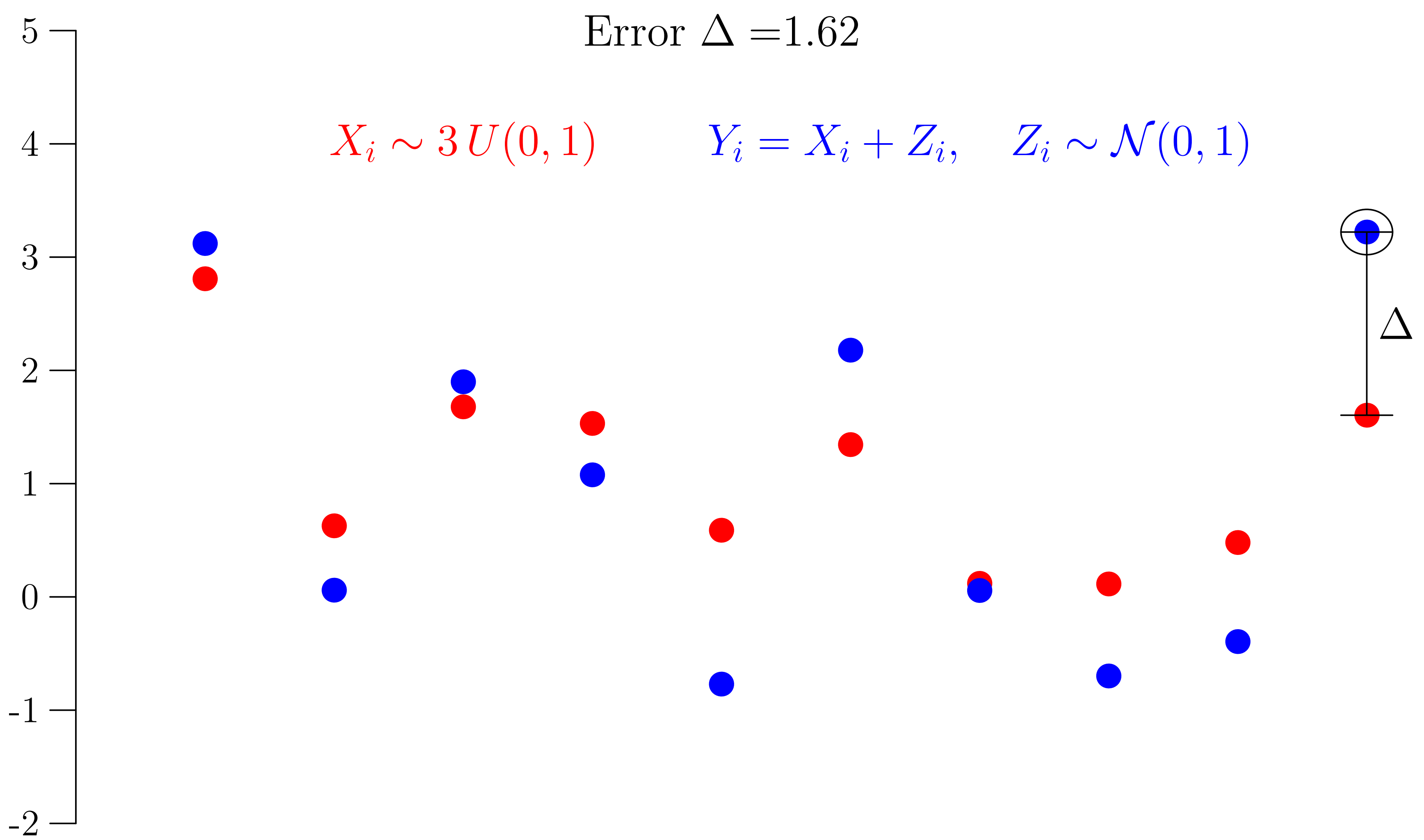

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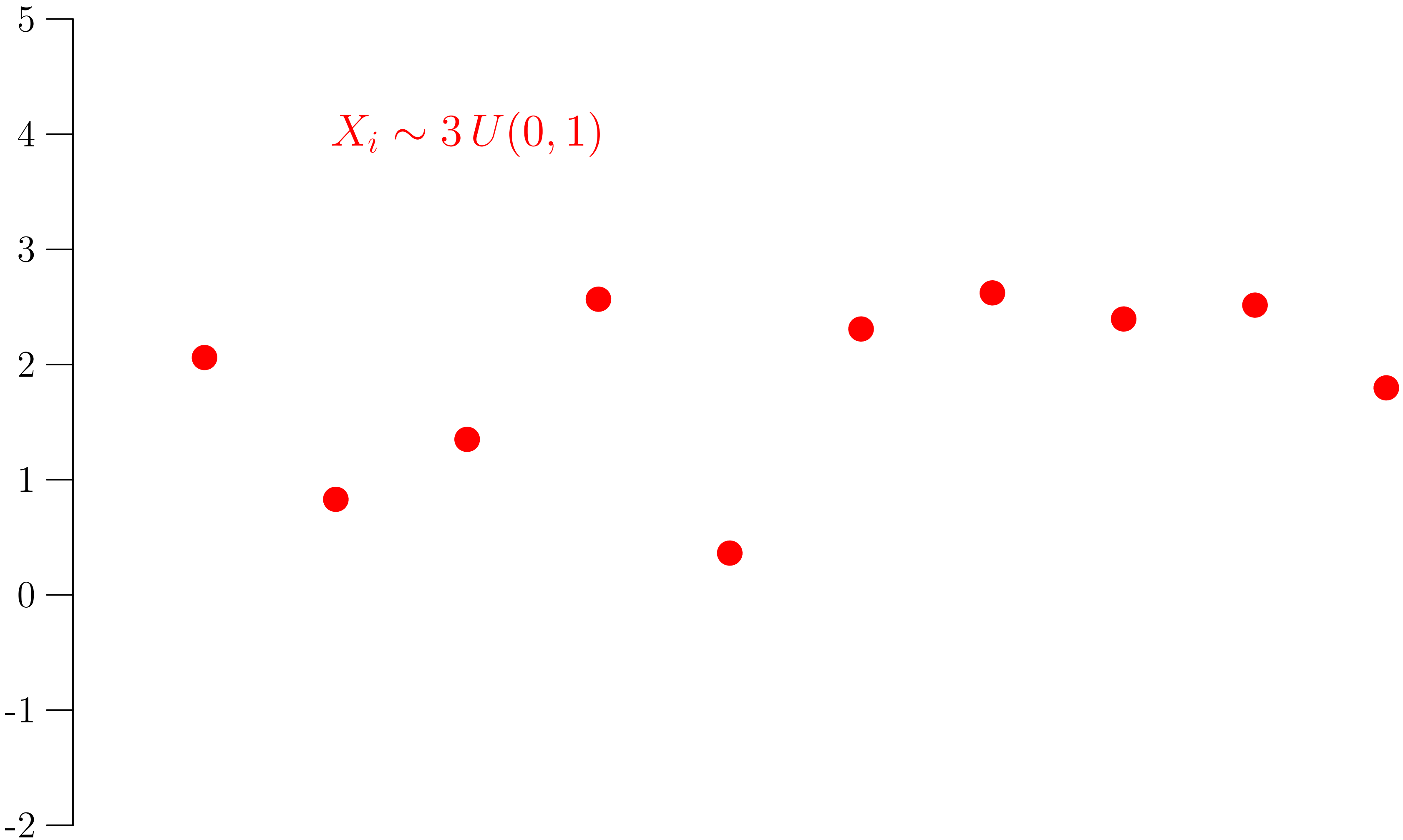

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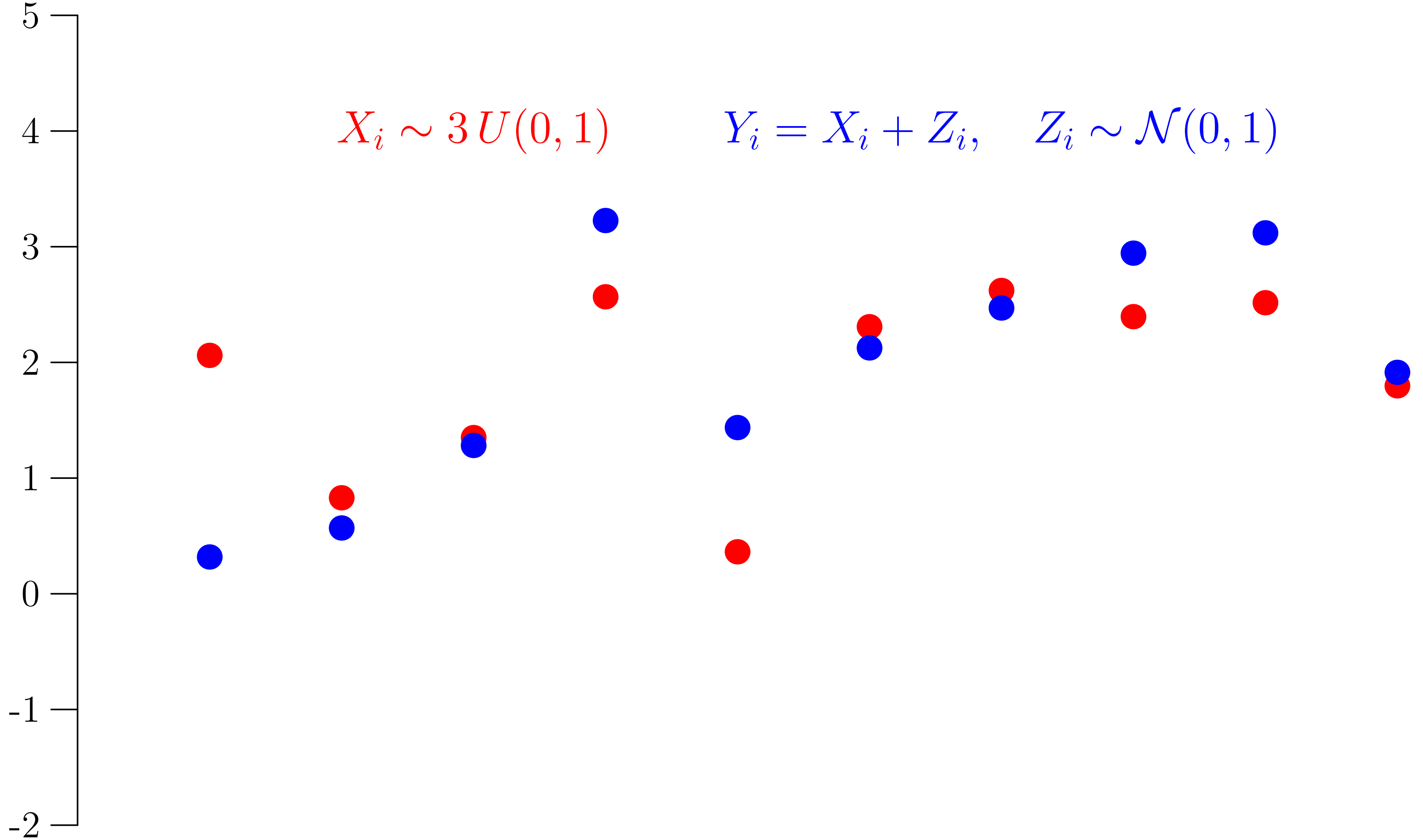

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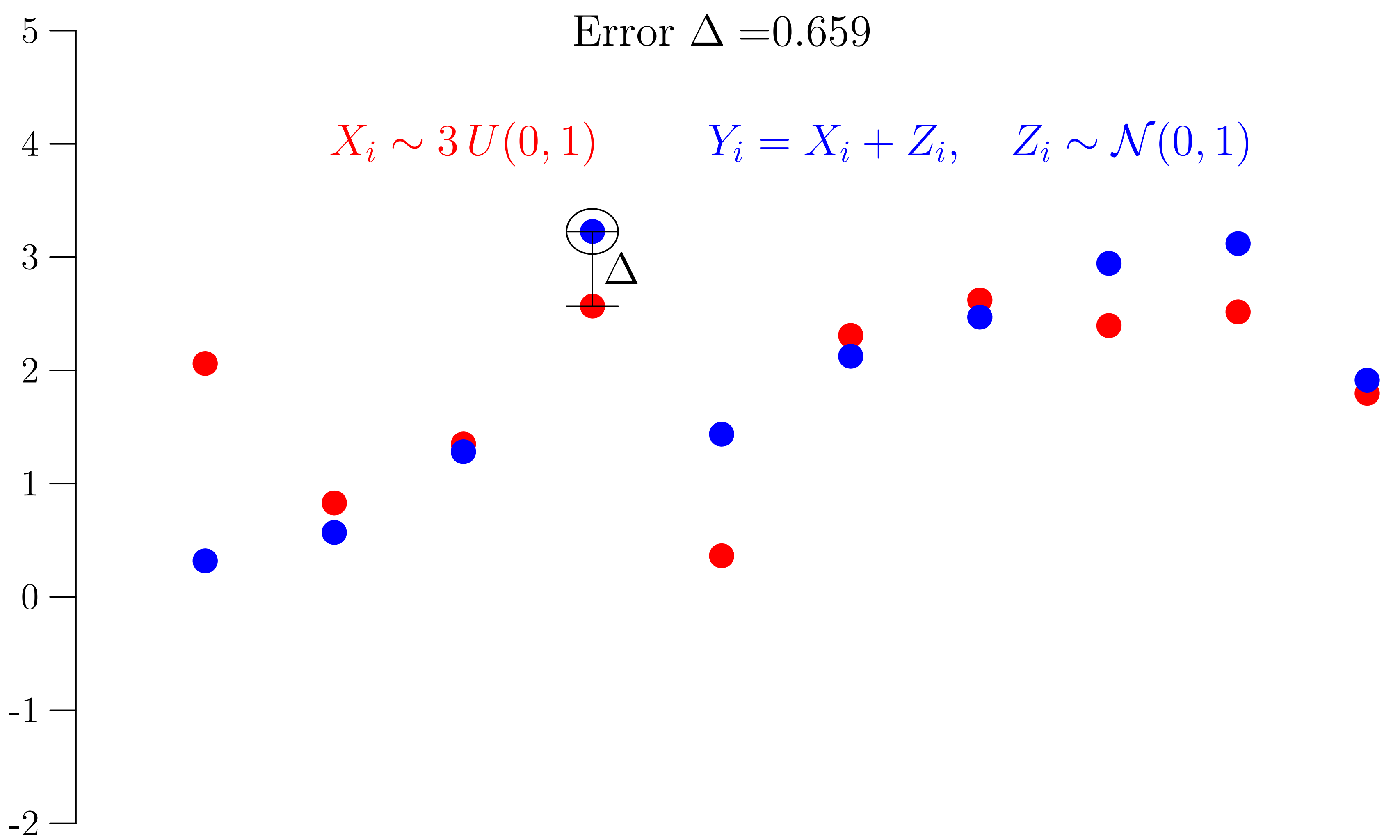

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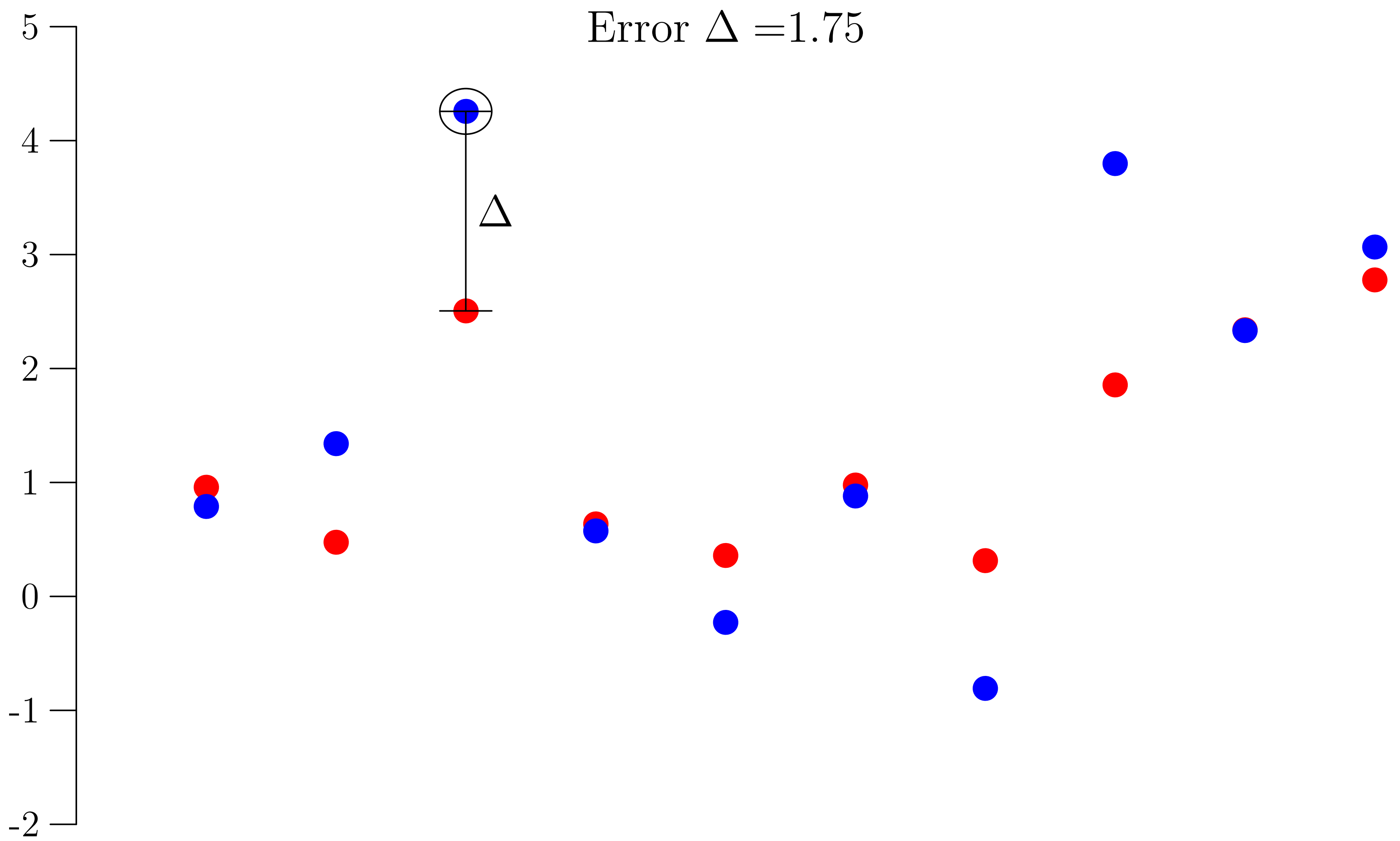

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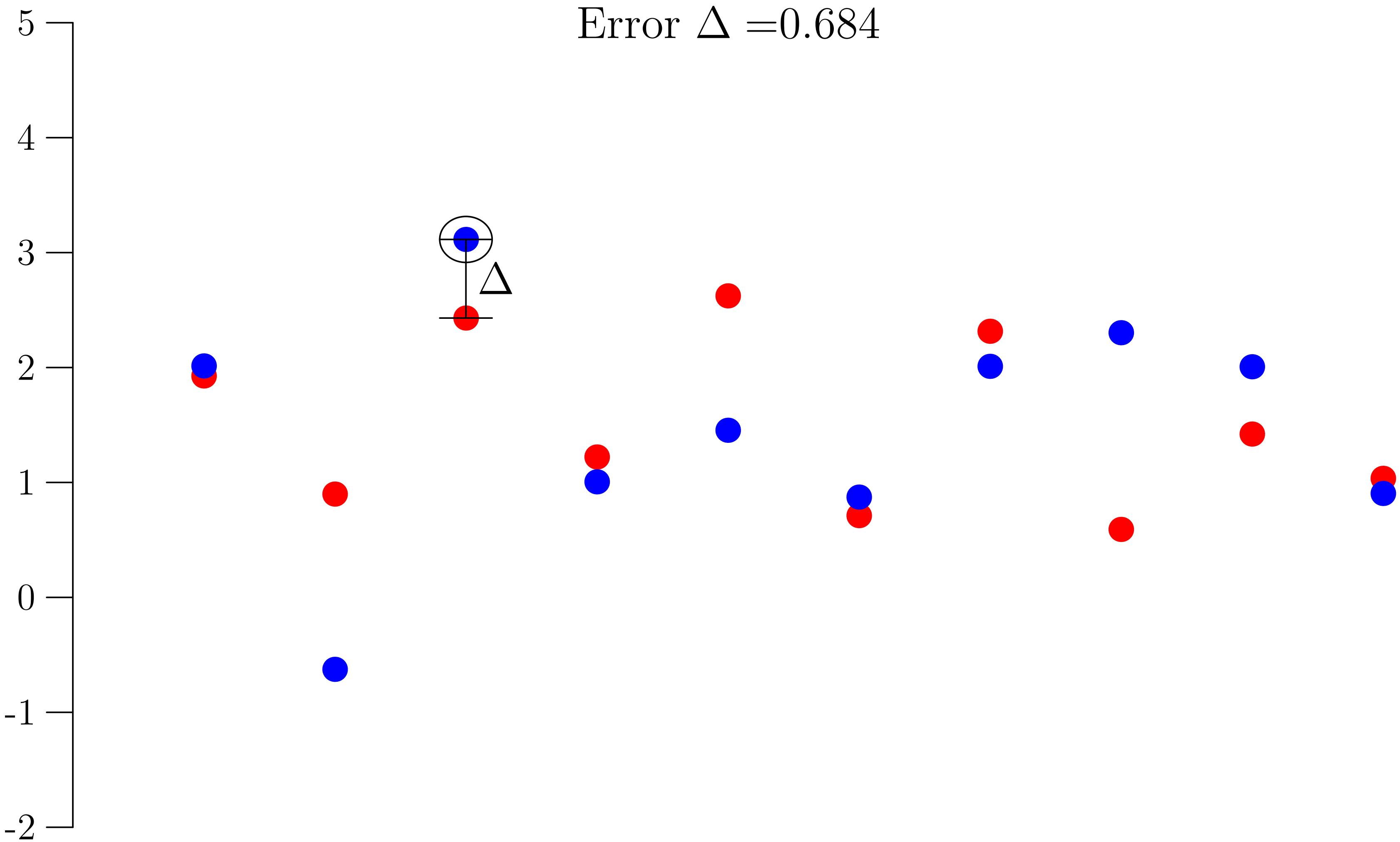

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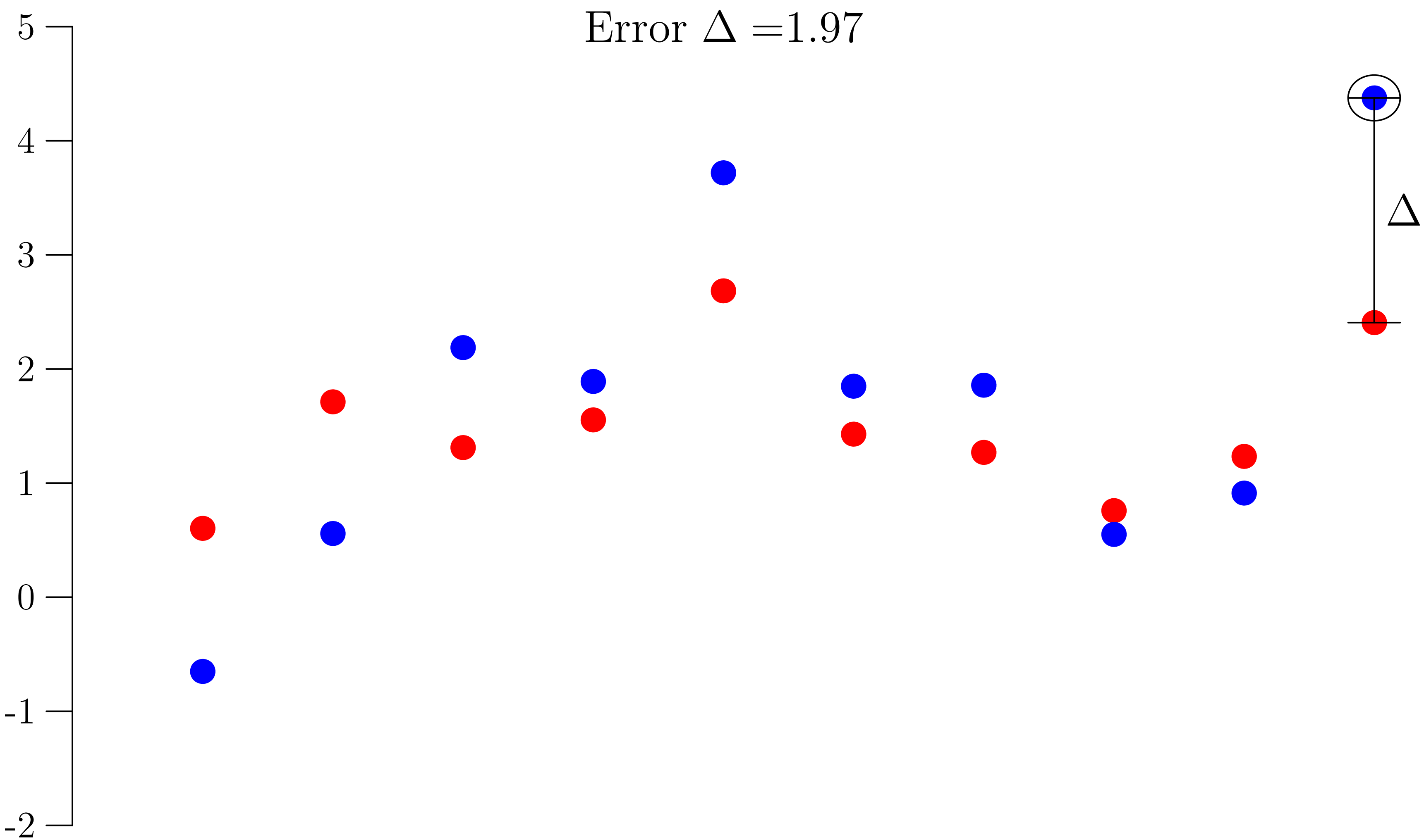

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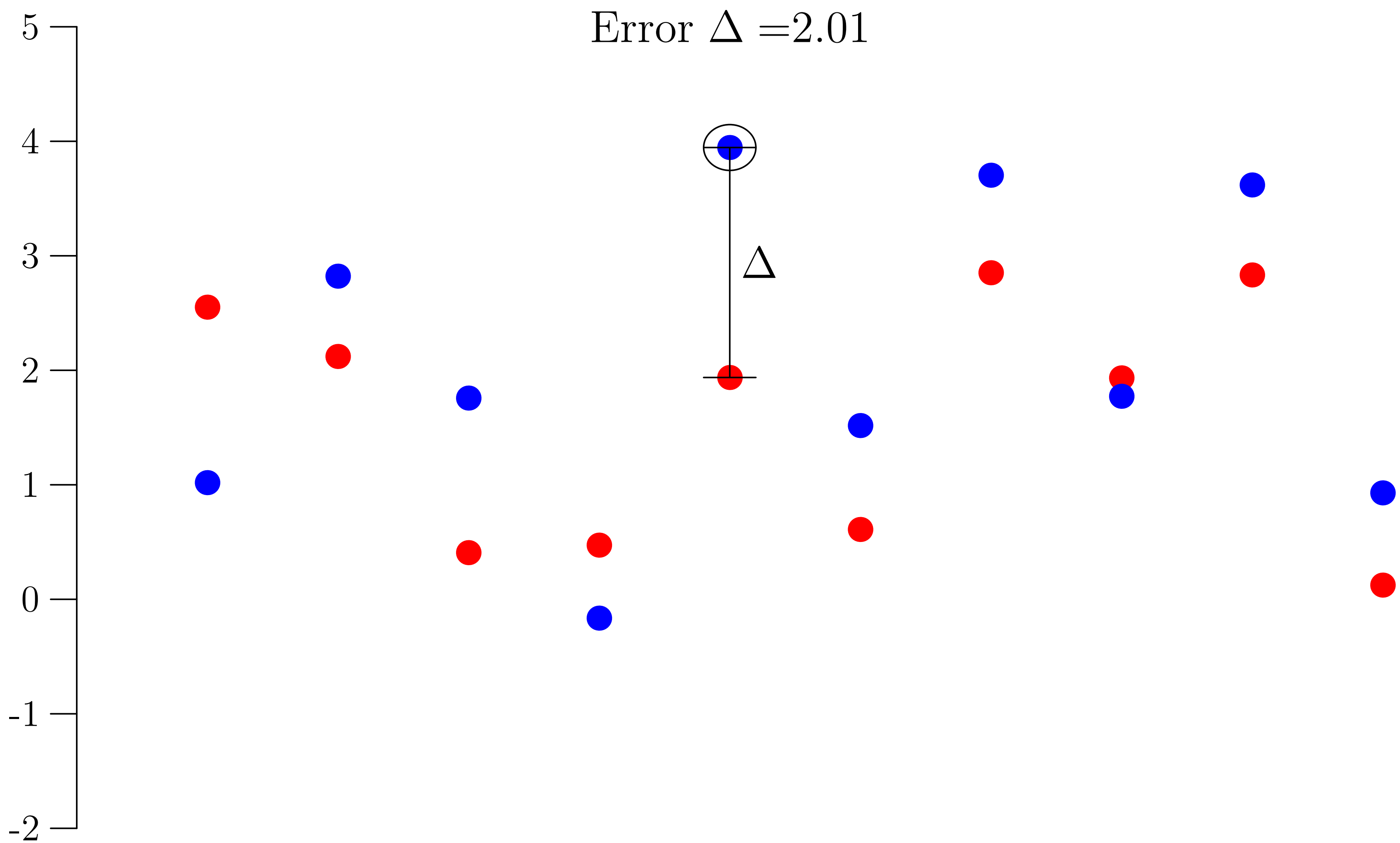

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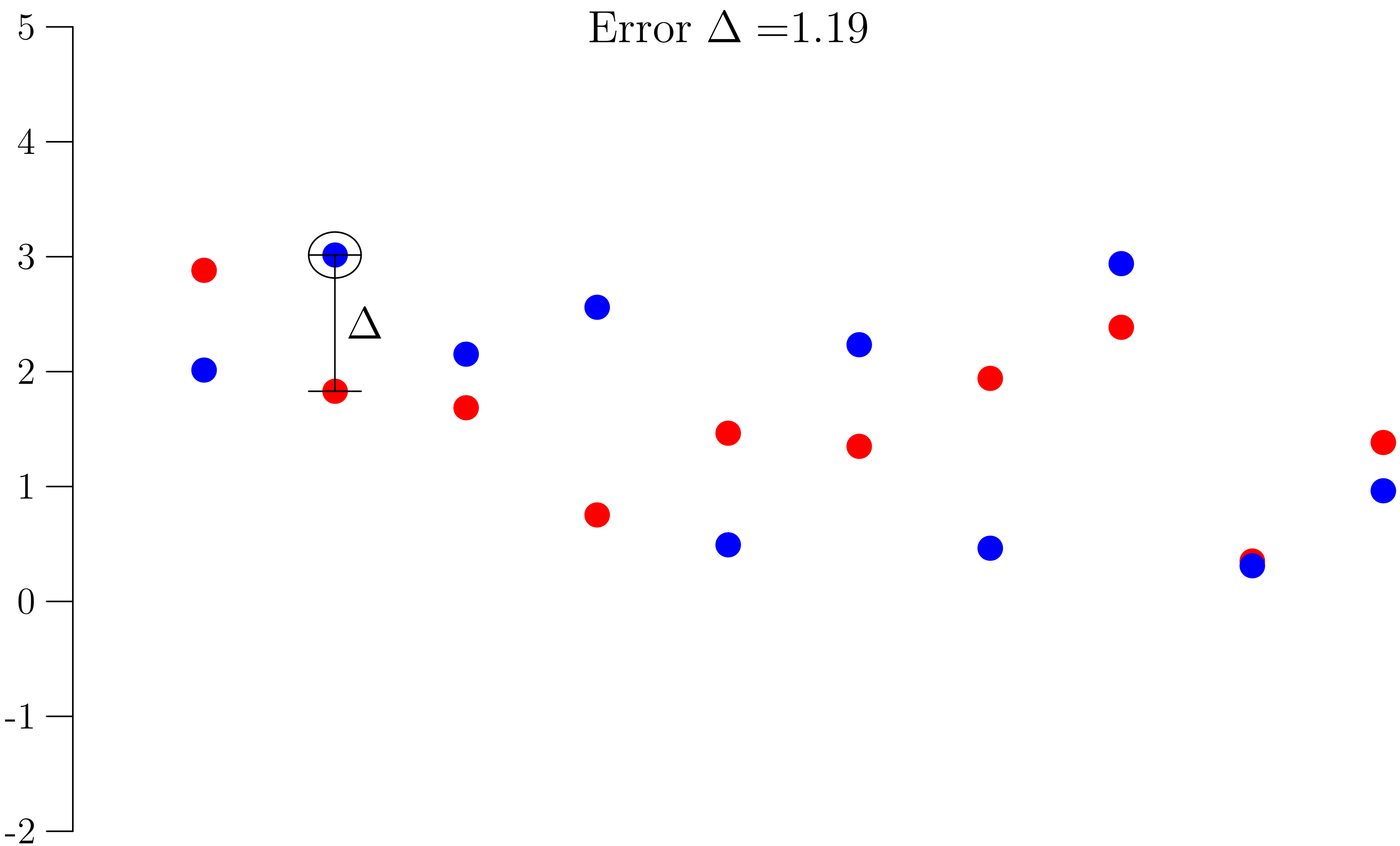

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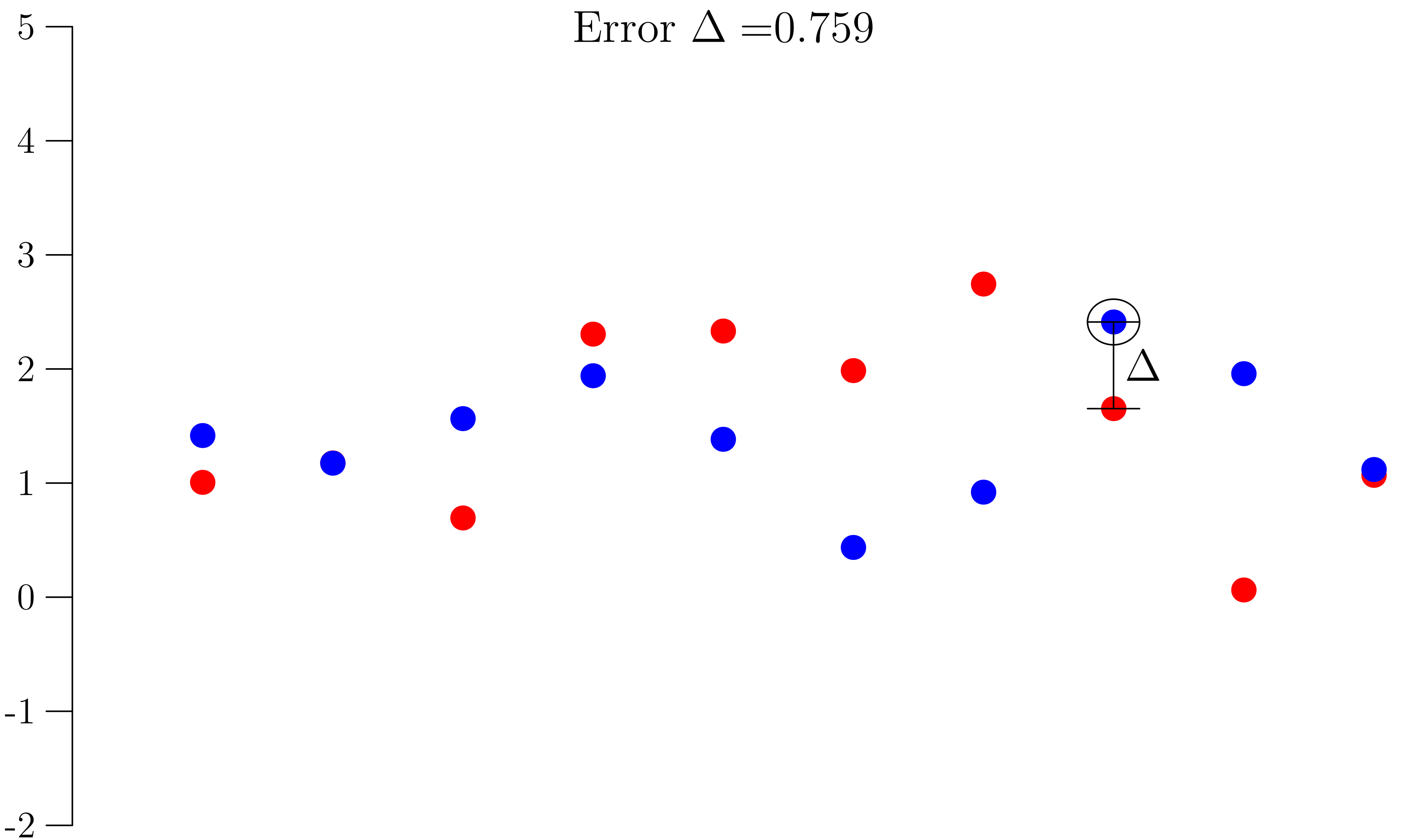

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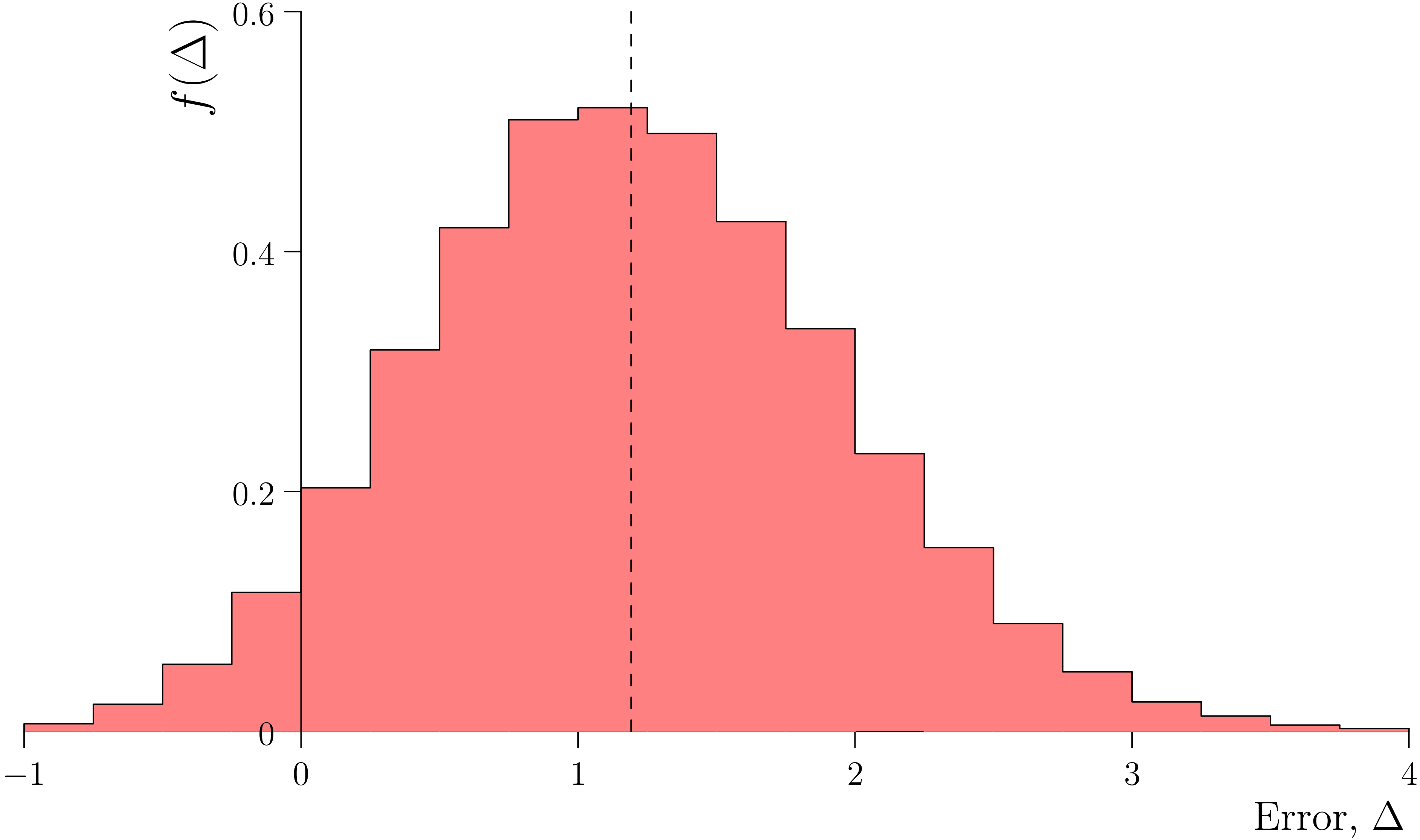

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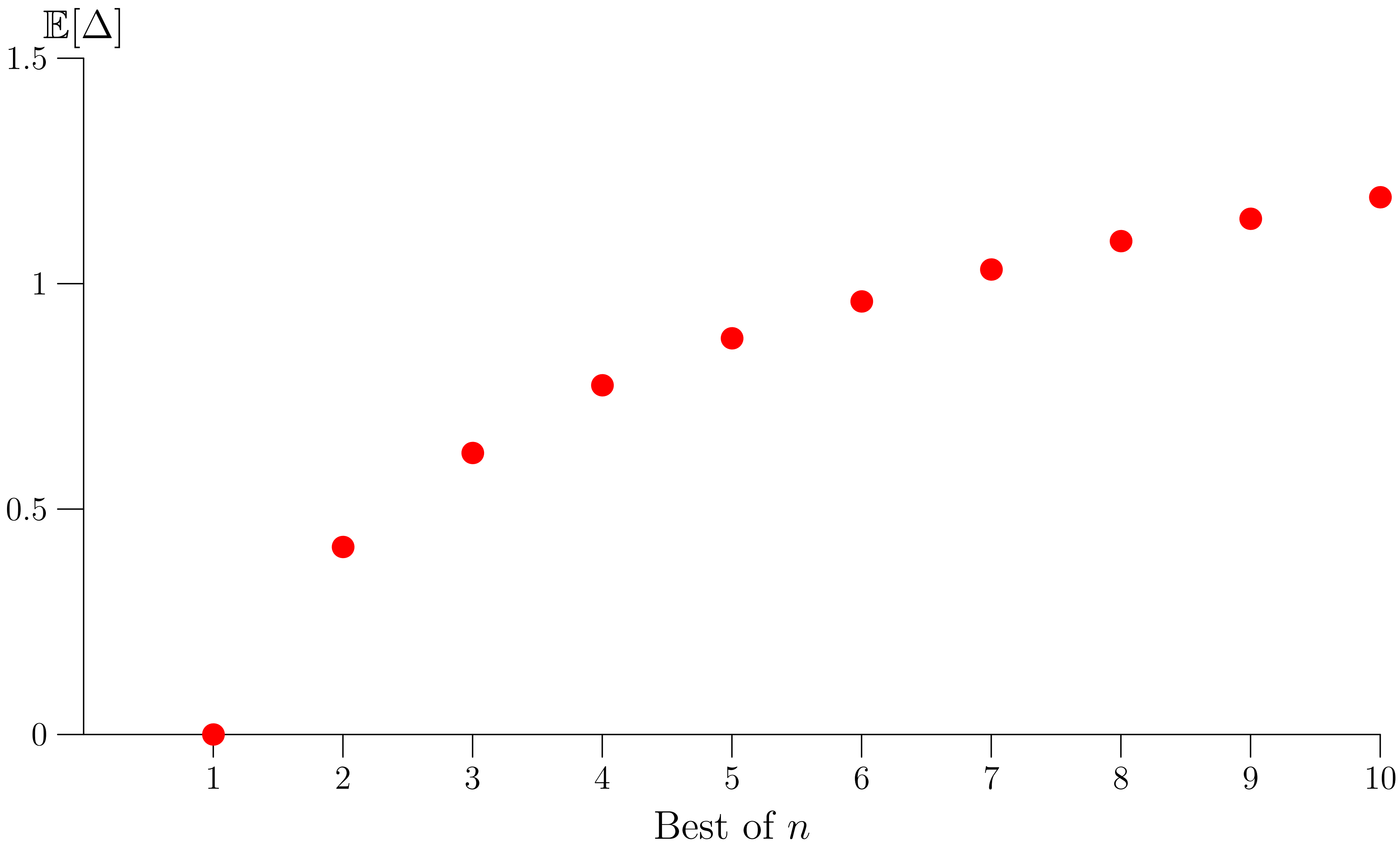
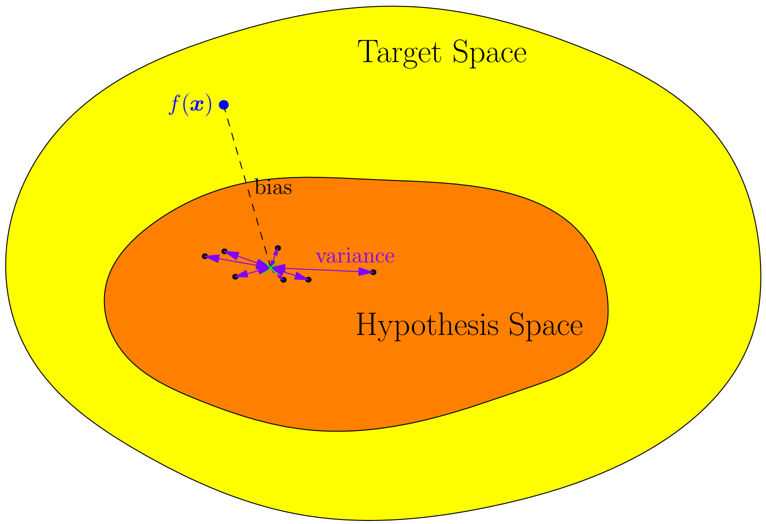


Outline

1. What Makes a Good Learning Machine?
2. **SVMs**
3. Ensemble Methods
4. Bayesian Inference



Support Vector Machines

- Support vector machines, when used right, often have the best generalisation results
- They are typically used on numerical data, but can and have been adapted to text, sequences, etc.
- Although not as trendy as deep learning, they will often be the method of choice on small data sets
- They subtly regularise themselves, choosing a solution that generalises well from a host of different solutions

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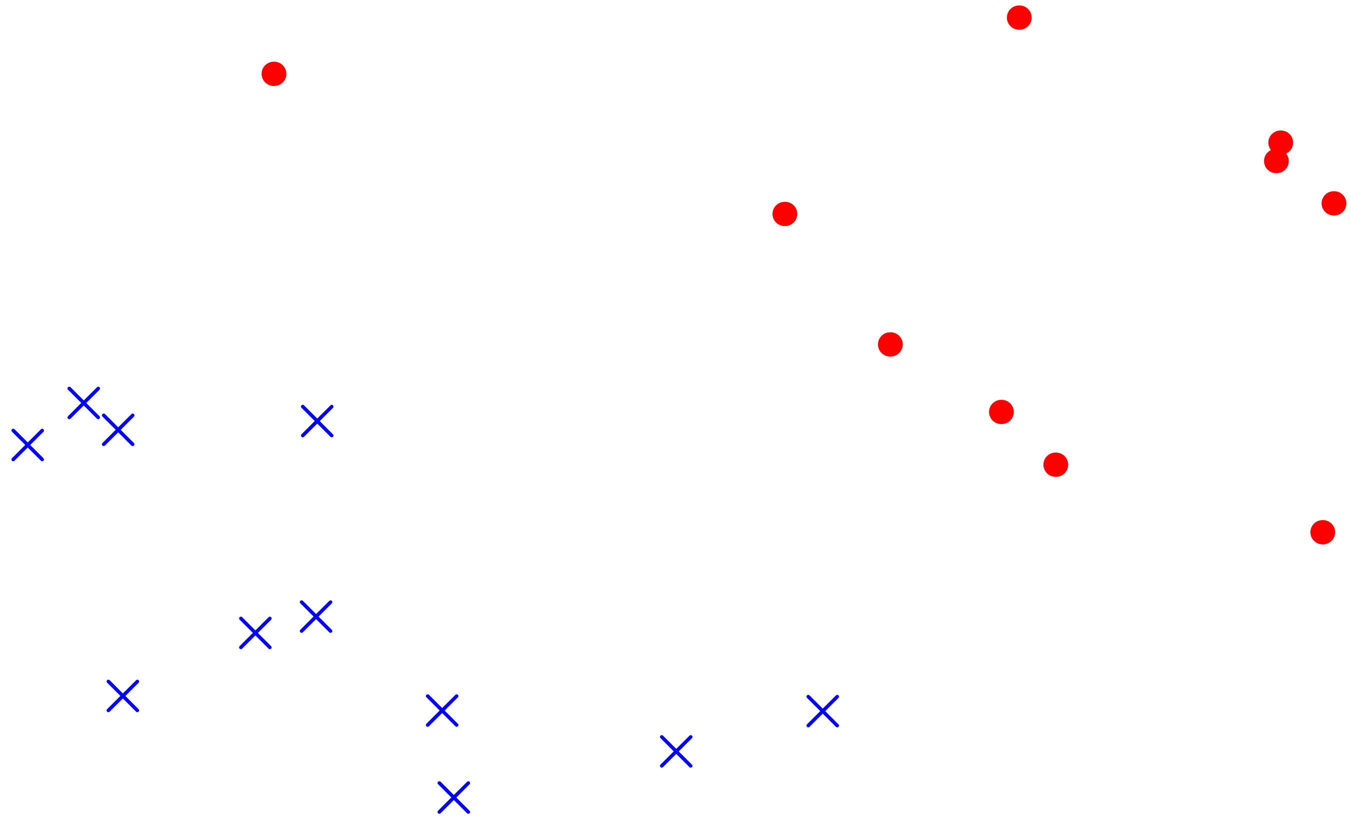
Linear Separation of Data

- SVMs classify linearly separable data



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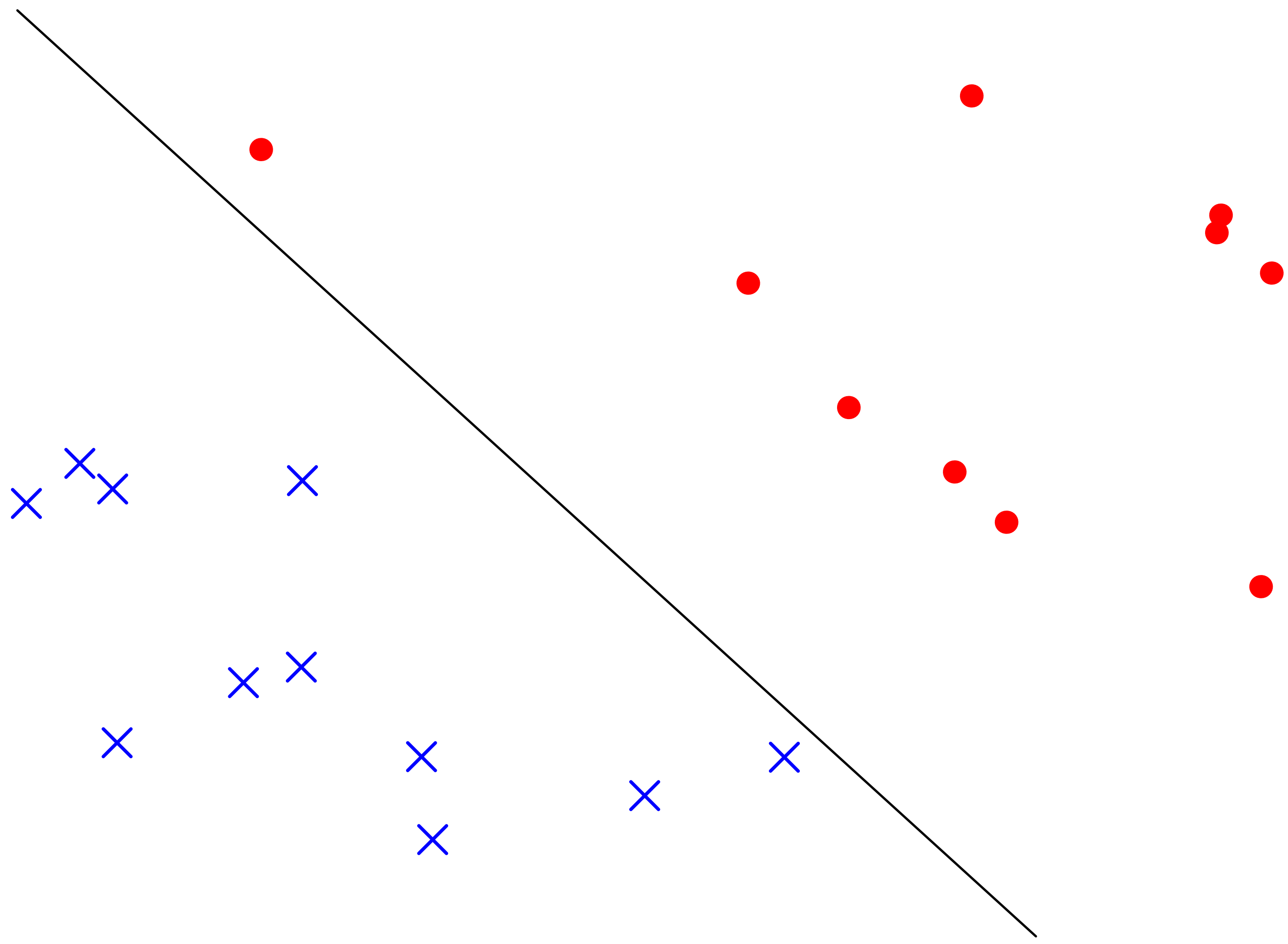

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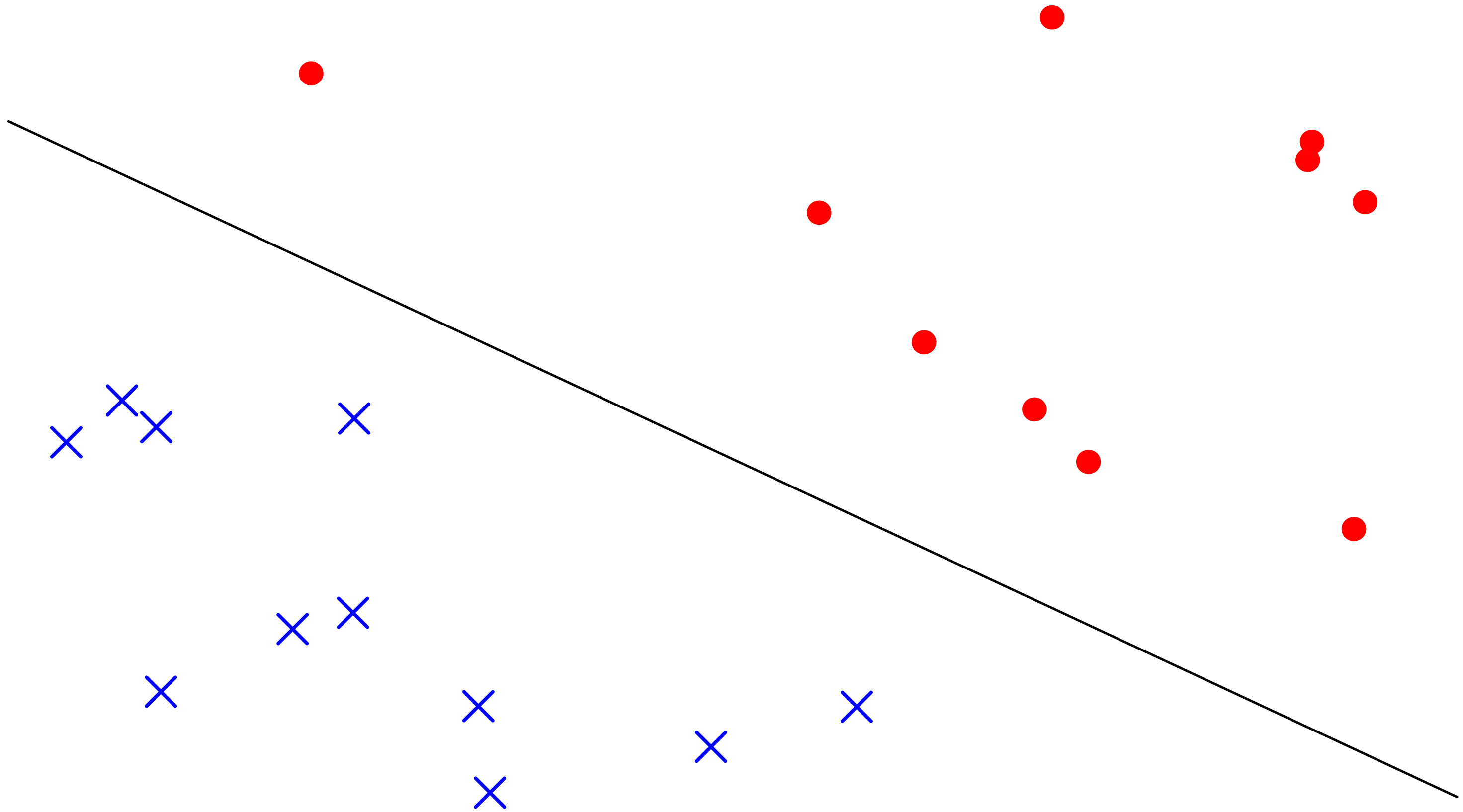

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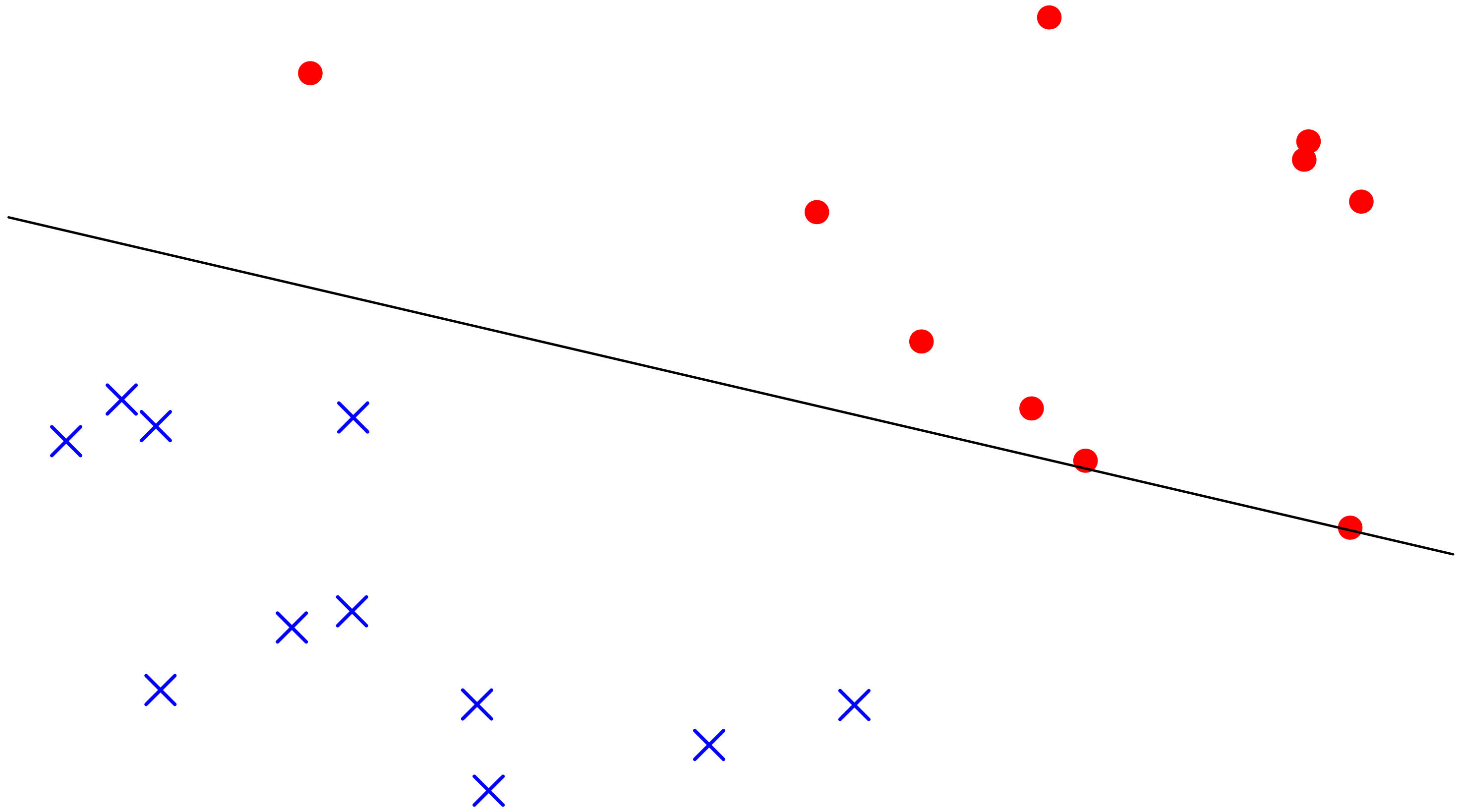

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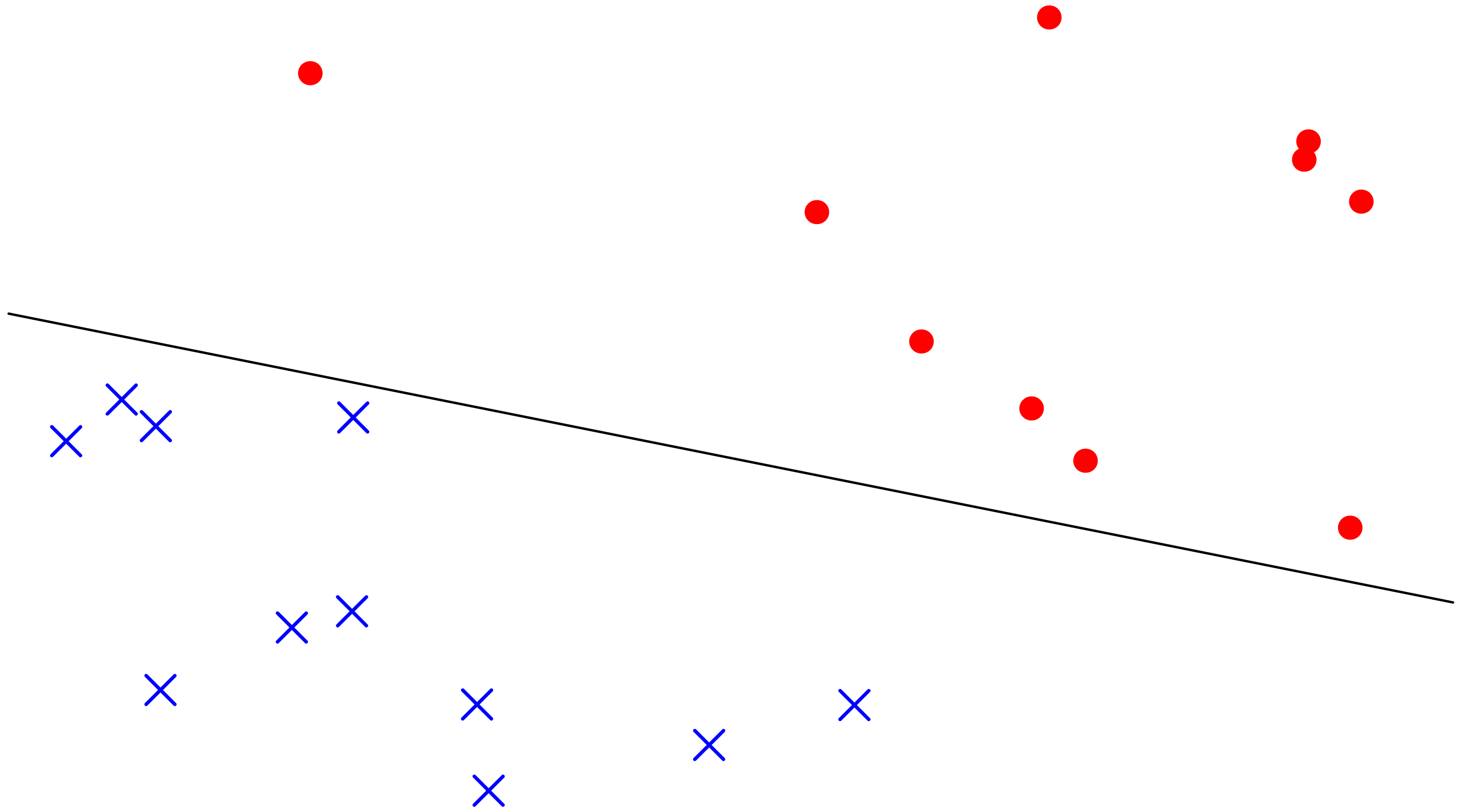

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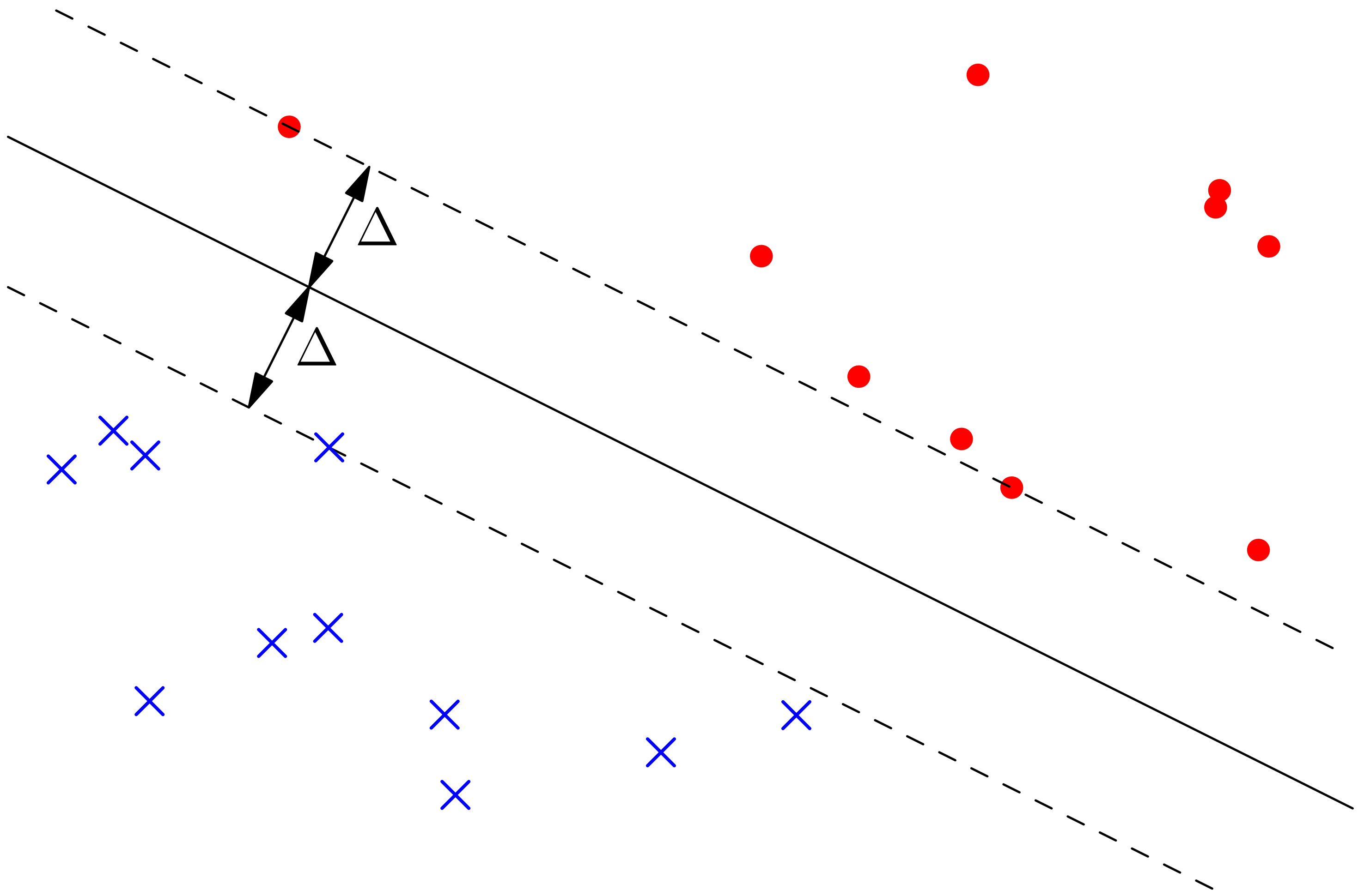

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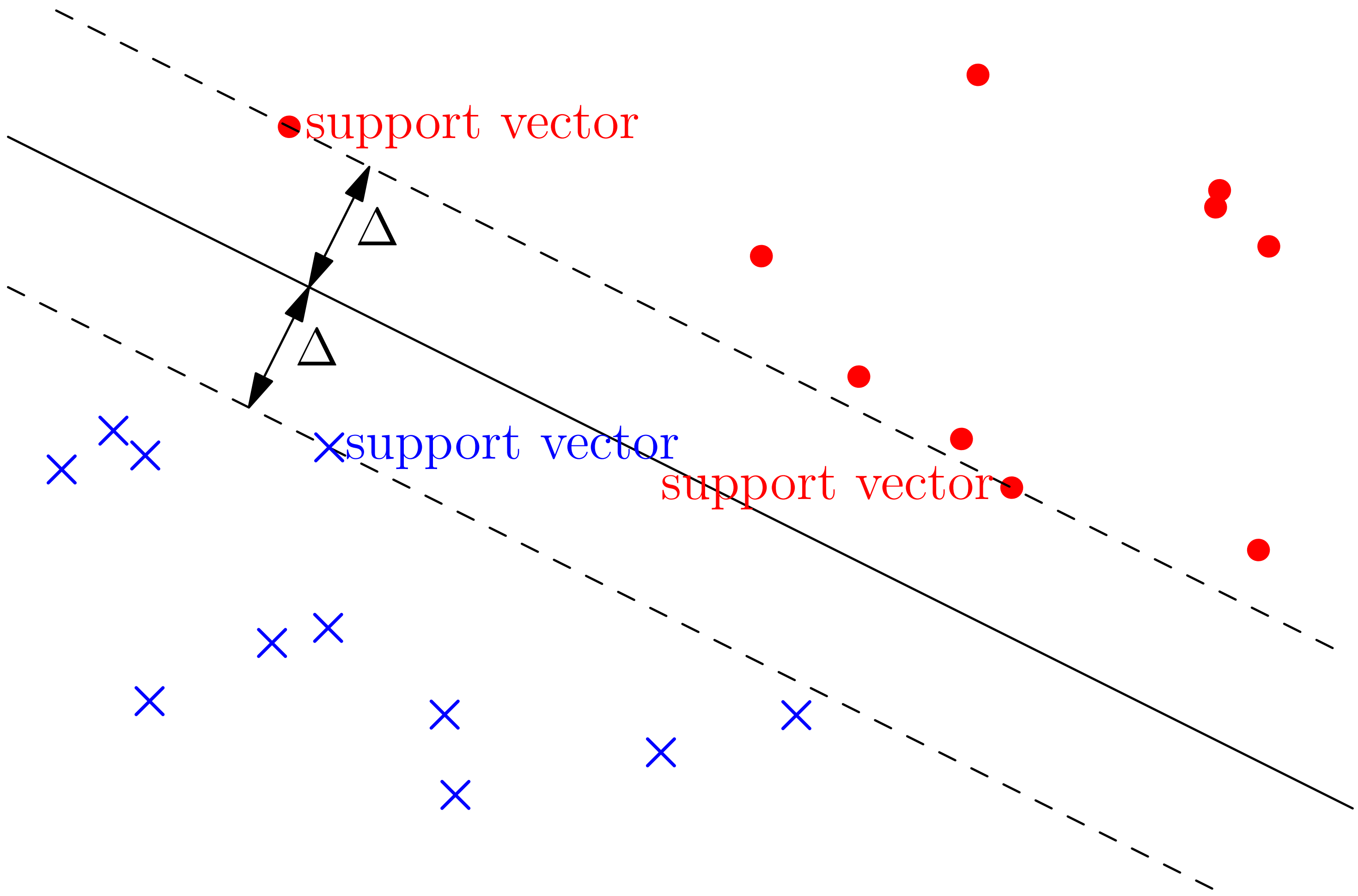

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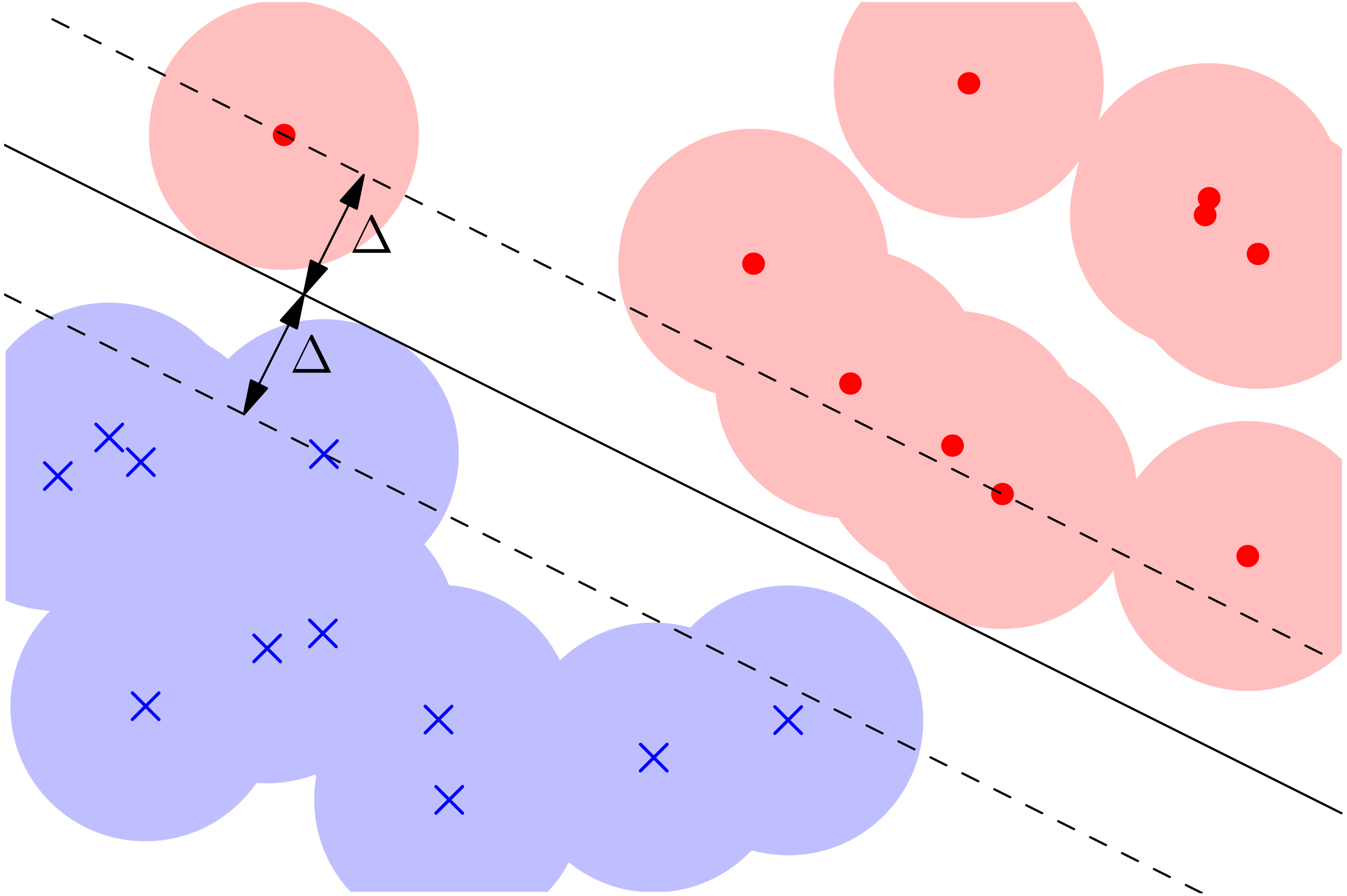

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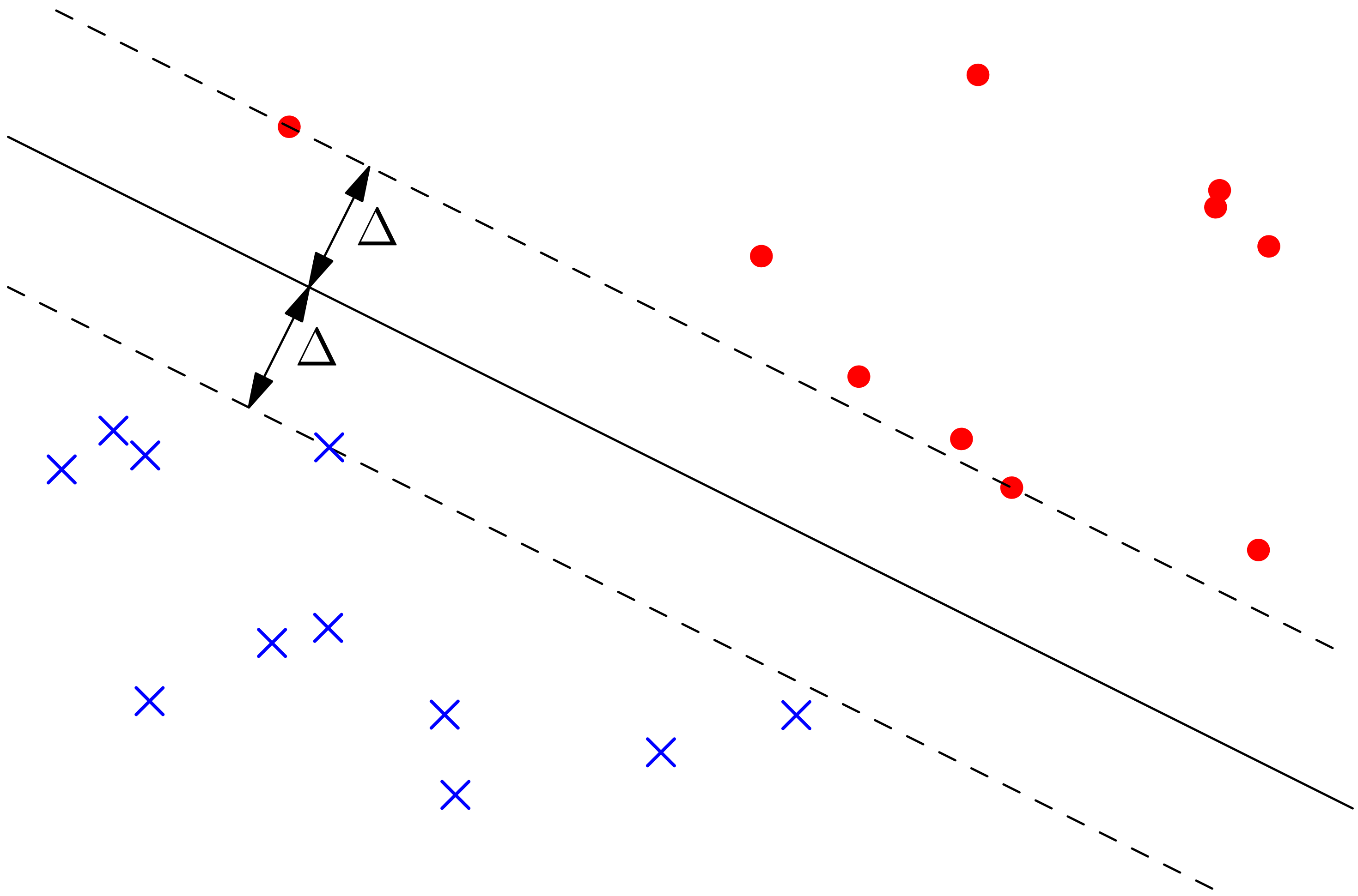

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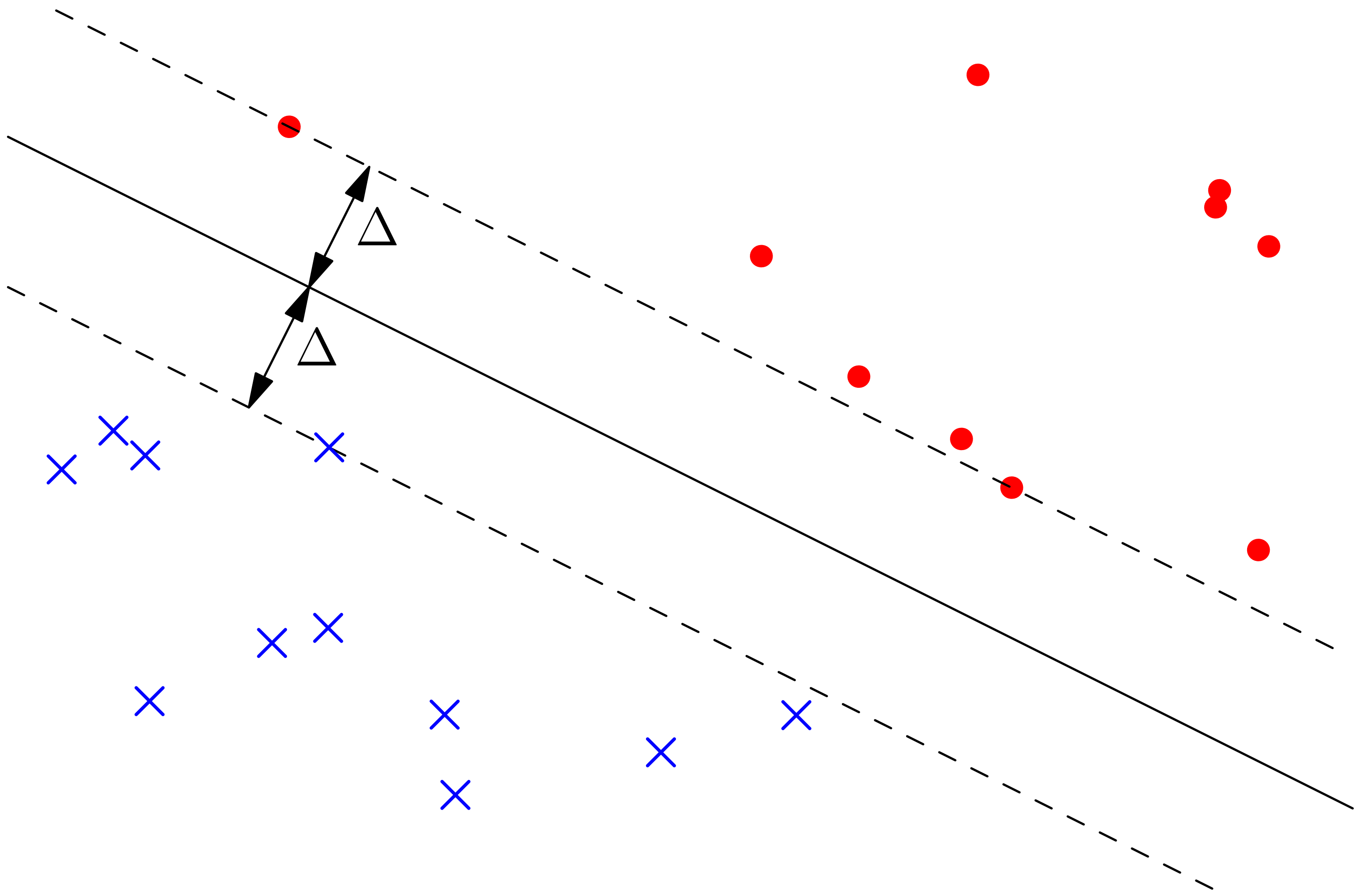

- Finds maximum-margin separating plane

Extended Feature Space

- To increase the likelihood of linear-separability we often use a high-dimensional mapping

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_p) \to \boldsymbol{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots, \phi_{p'}(\boldsymbol{x}))$$

$p' \gg p$

- Finding the maximum margin hyper-plane is time consuming in "primal" form if p' is large

- We can work in the "dual" space of patterns, then we only need to compute dot products

$$\boldsymbol{\phi}(\boldsymbol{x}_i) \cdot \boldsymbol{\phi}(\boldsymbol{x}_j)$$

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$$\boldsymbol{\phi}(\boldsymbol{x}_i) \cdot \boldsymbol{\phi}(\boldsymbol{x}_j) = \sum_{k=1}^{p'} \phi_k(\boldsymbol{x}_i)\, \phi_k(\boldsymbol{x}_j)$$

Kernel Trick

- If we choose a **positive semi-definite** kernel function $K(\boldsymbol{x},\boldsymbol{y})$ then there exists functions $\phi_k(\boldsymbol{x})$, such that

$$K(\boldsymbol{x}_i,\boldsymbol{x}_j) = \boldsymbol{\phi}(\boldsymbol{x}_i)\cdot\boldsymbol{\phi}(\boldsymbol{x}_j)$$

  (like an eigenvector decomposition of a matrix)

- Never need to compute $\phi_k(\boldsymbol{x}_i)$ explicitly as we only need the dot-product $\boldsymbol{\phi}(\boldsymbol{x}_i)\cdot\boldsymbol{\phi}(\boldsymbol{x}_j) = K(\boldsymbol{x}_i,\boldsymbol{x}_j)$ to compute maximum margin separating hyper-plane

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Kernel Functions

- Kernel functions are symmetric functions of two variable
- Strong restriction: *positive semi-definite*
- Examples

$$\text{Quadratic kernel:} \qquad K(\boldsymbol{x}_1, \boldsymbol{x}_2) = \left(\boldsymbol{x}_1^\top \boldsymbol{x}_2\right)^2$$

$$\text{Gaussian (RBF) kernel:} \qquad K(\boldsymbol{x}_1, \boldsymbol{x}_2) = \mathrm{e}^{-\gamma \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}$$

- Consider the mapping

$$\boldsymbol{x}_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix} \to \boldsymbol{\phi}(\boldsymbol{x}_i) = \begin{pmatrix} x_i^2 \\ y_i^2 \\ \sqrt{2}\, x_i\, y_i \end{pmatrix}$$

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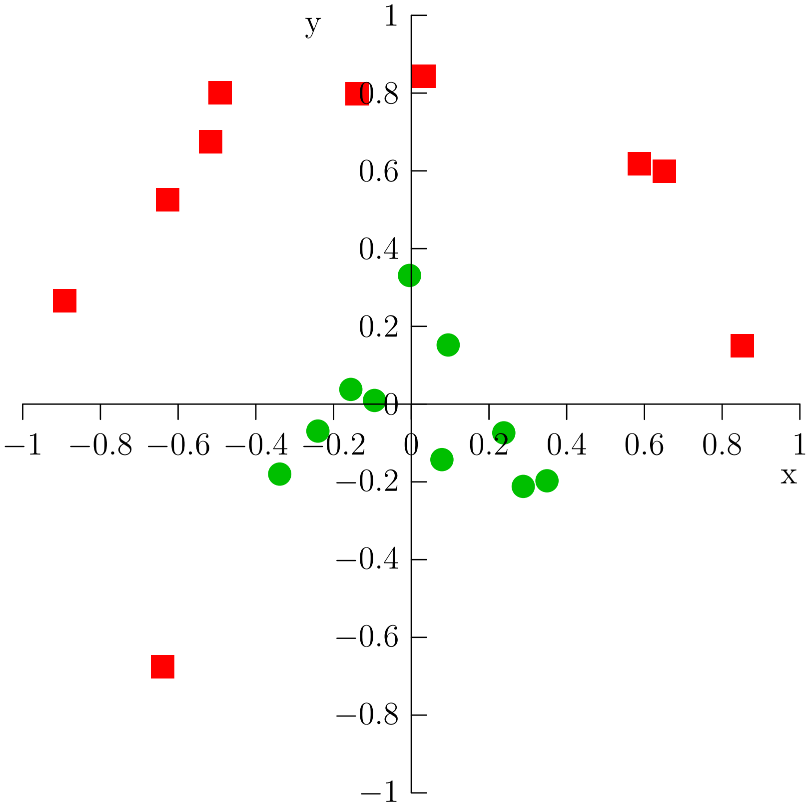

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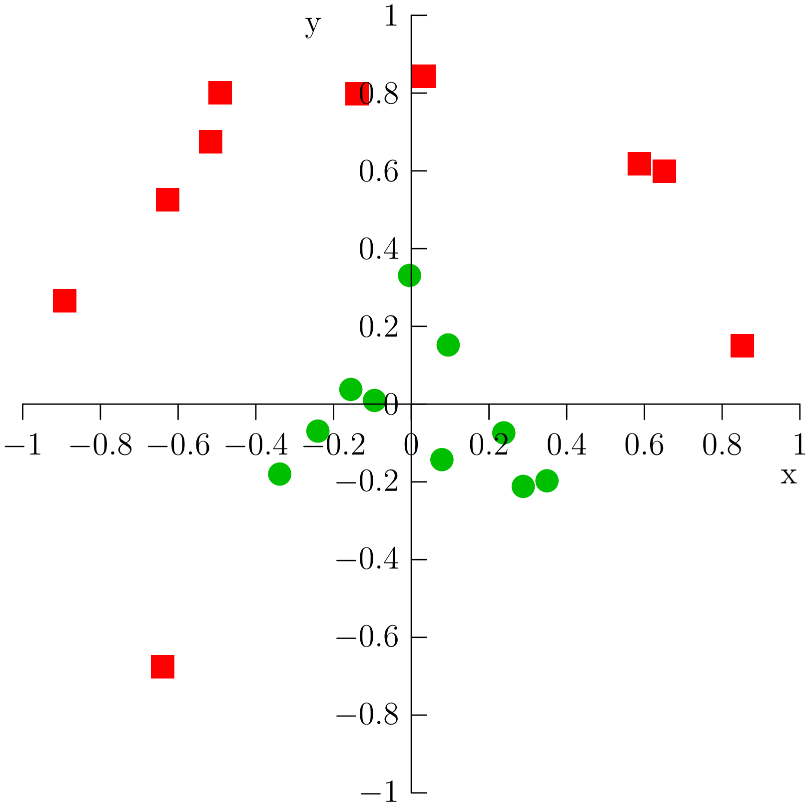

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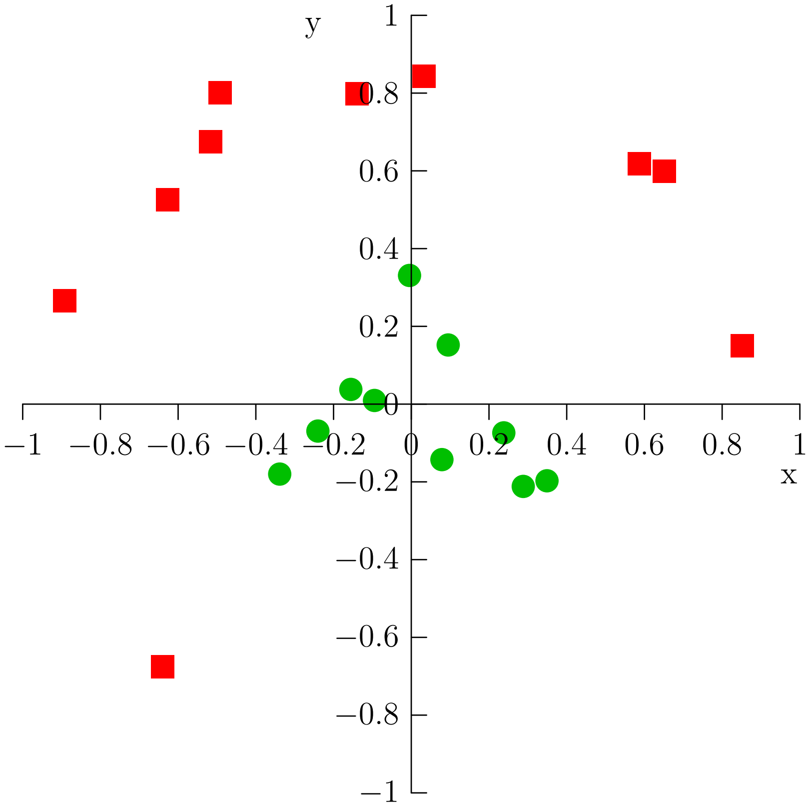

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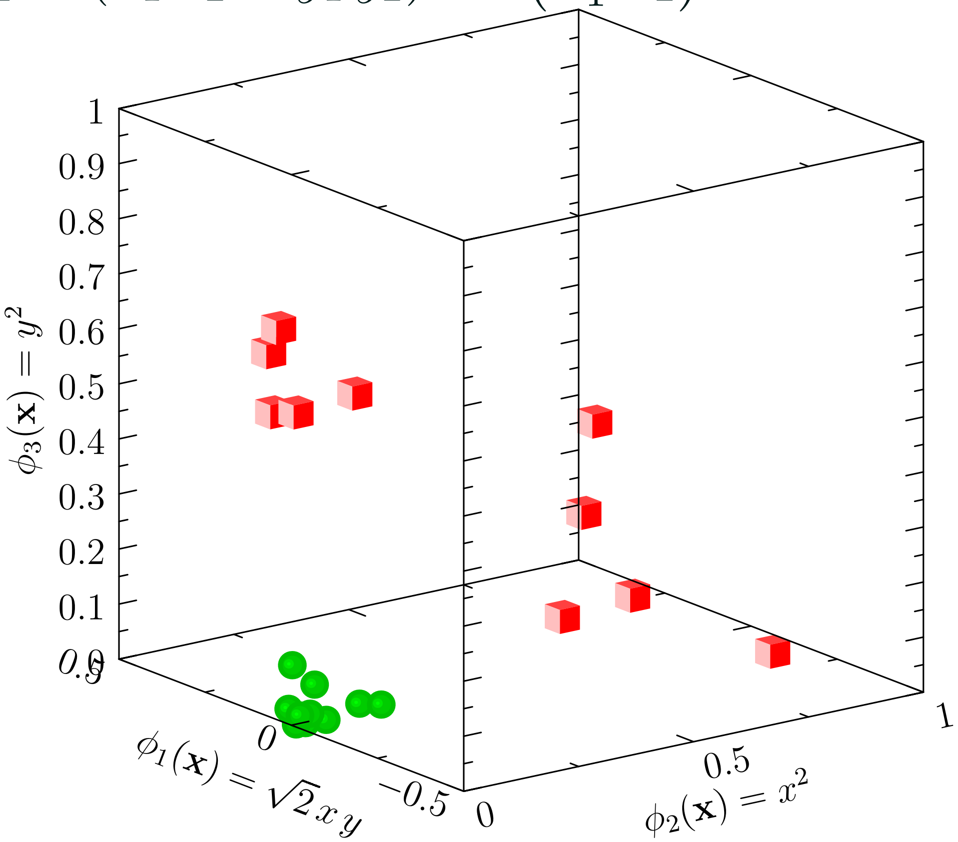

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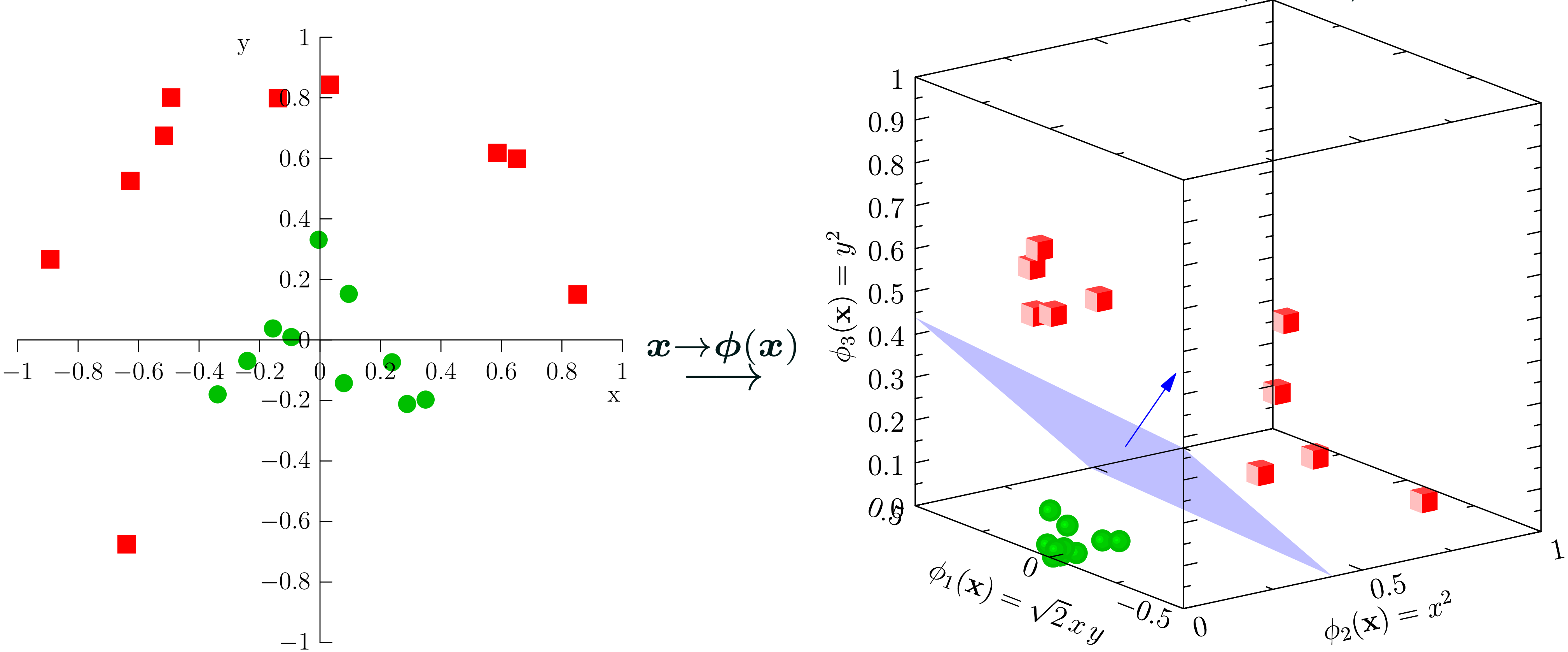

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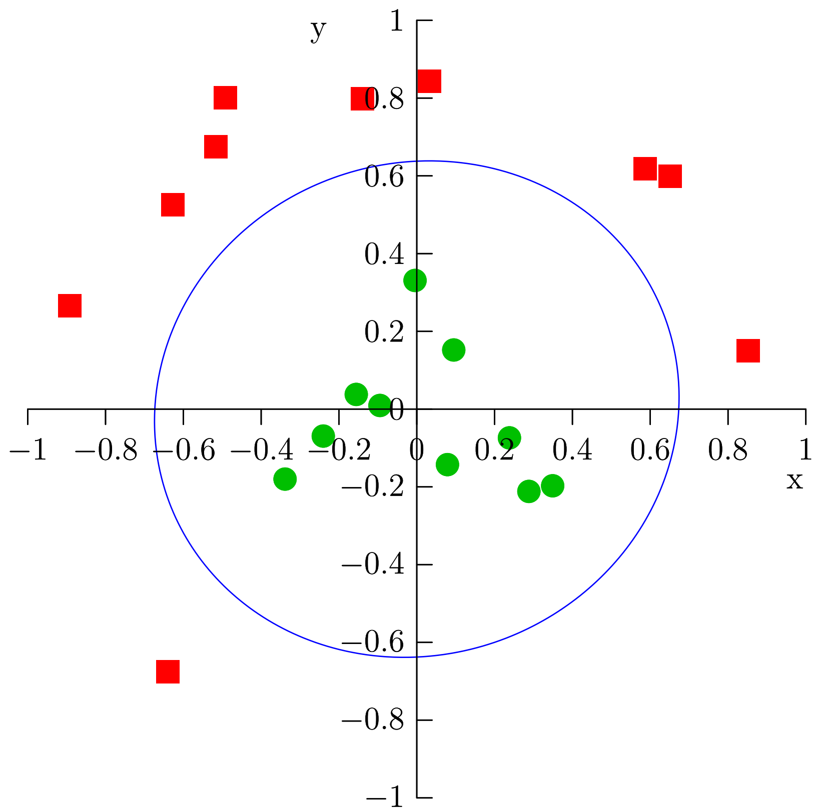

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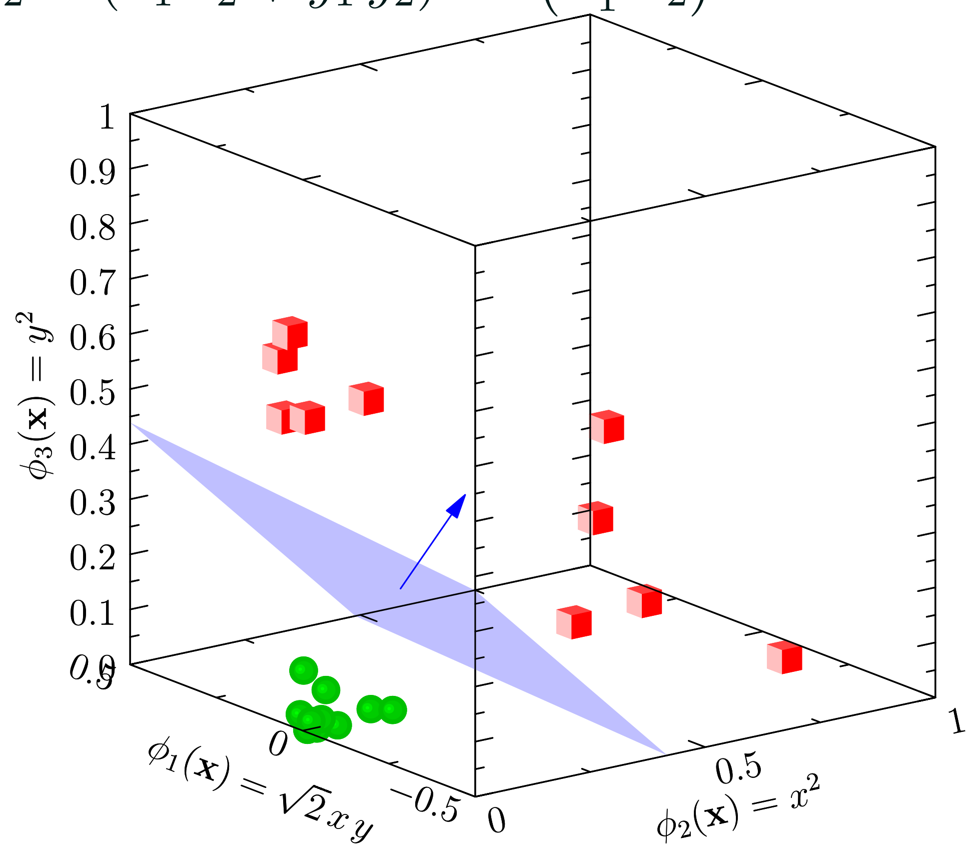

Computing the Maximum-Margin Hyper-plane

- Although it is not hugely difficult to derive the equations for finding the maximum-margin hyper-plane it is not that illuminating (although very elegant)

- Never need to compute $\phi_i(\boldsymbol{x})$ only need to compute $\boldsymbol{\phi}^{\mathsf{T}}(\boldsymbol{x}_i)\boldsymbol{\phi}(\boldsymbol{x}_j)$

- We end up with a quadratic programming problem, which requires some sophisticated algorithms to solve

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Getting SVMs to Work Well

- SVMs rely on distances between data points

- These will change relative to each other if we rescale some features but not other—giving different maximum-margin hyper-planes

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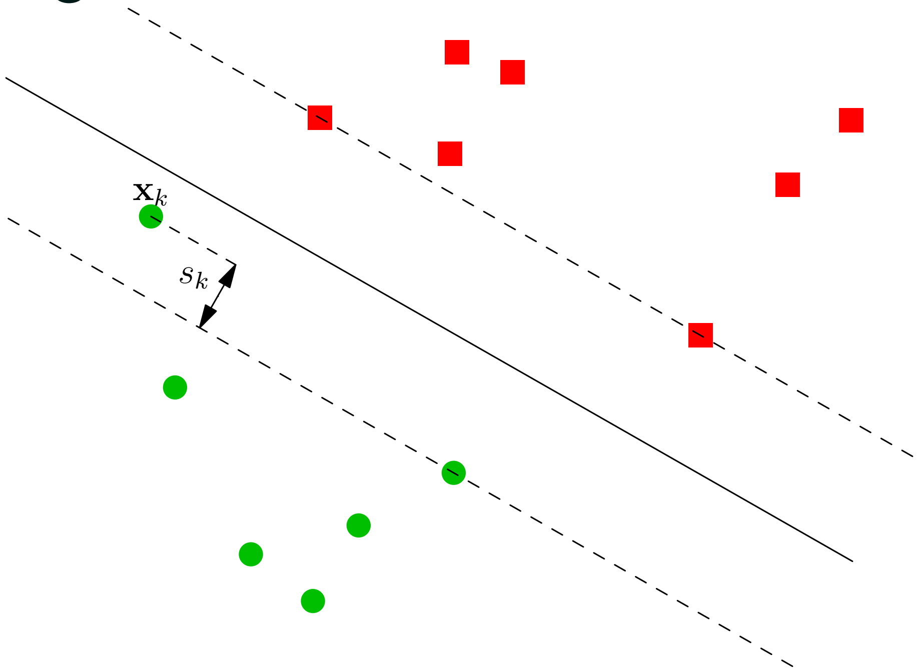
- Relax constraints by introducing *slack variables*, $s_k \geq 0$

$$y_k(\boldsymbol{x}_k^\mathsf{T}\boldsymbol{w} - b) \geq 1 - s_k$$



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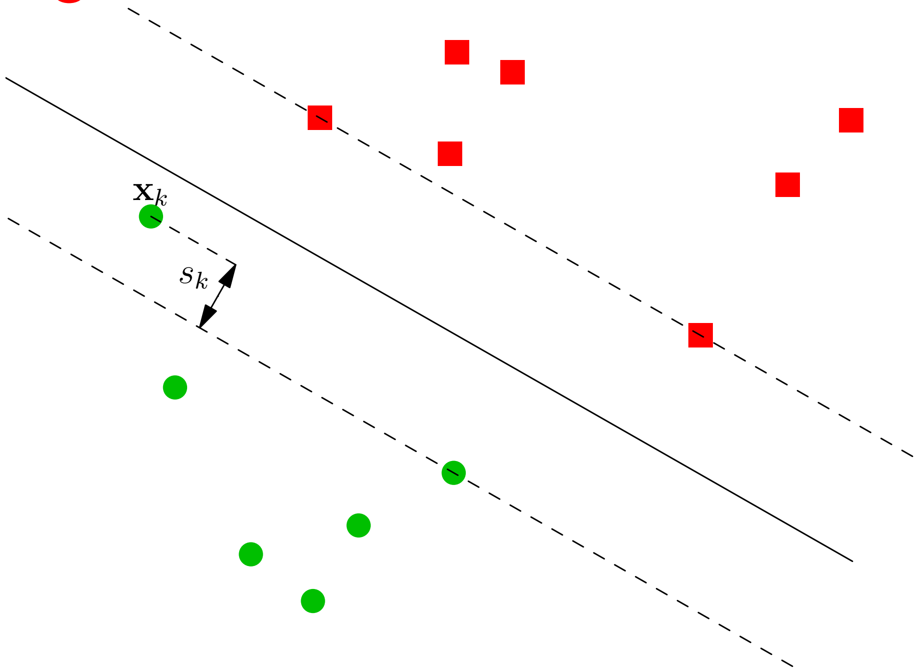

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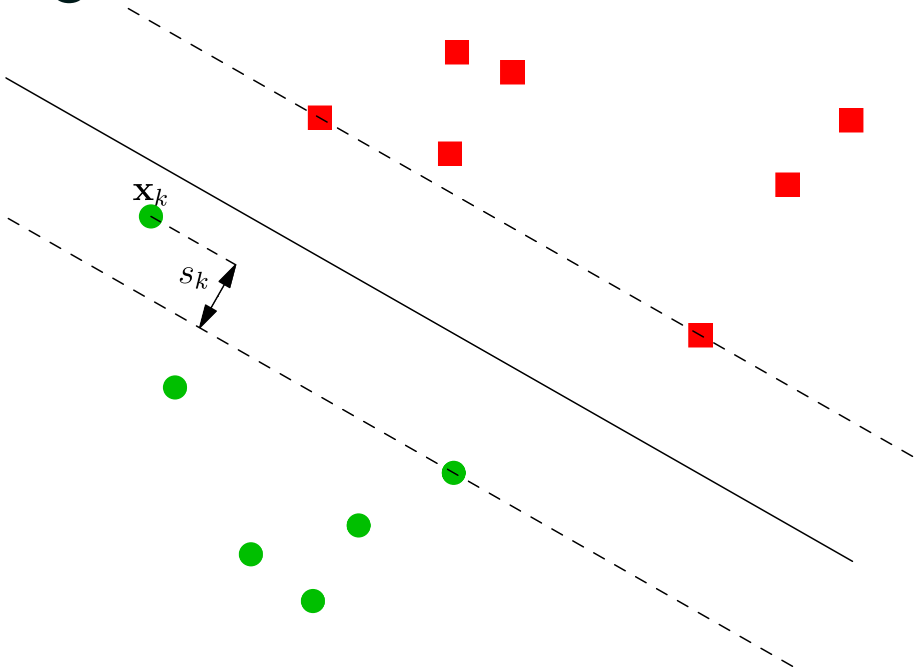

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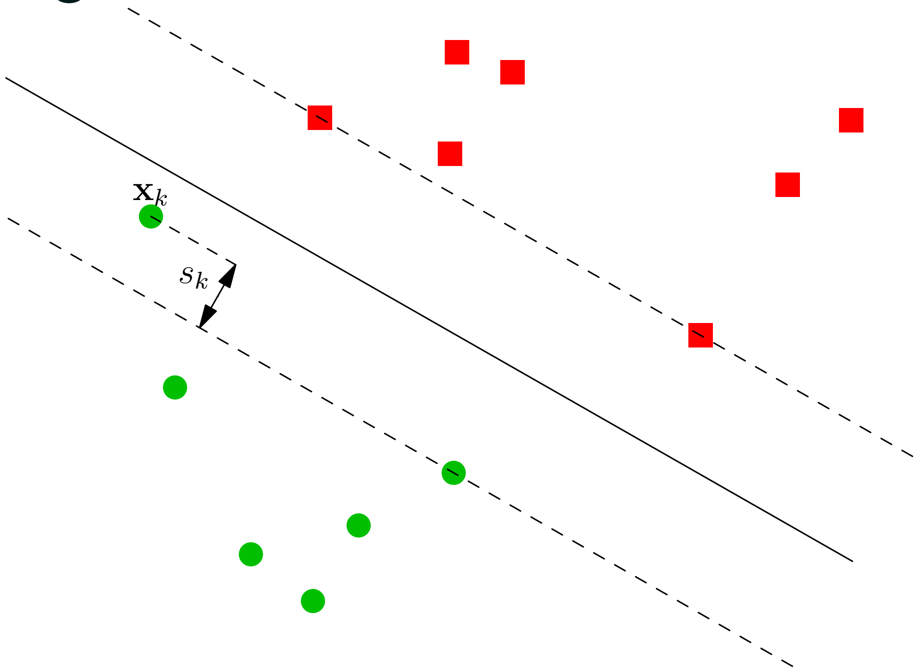

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- There are kernels designed for particular data types (e.g. string kernels for text or biological sequences)
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Outline

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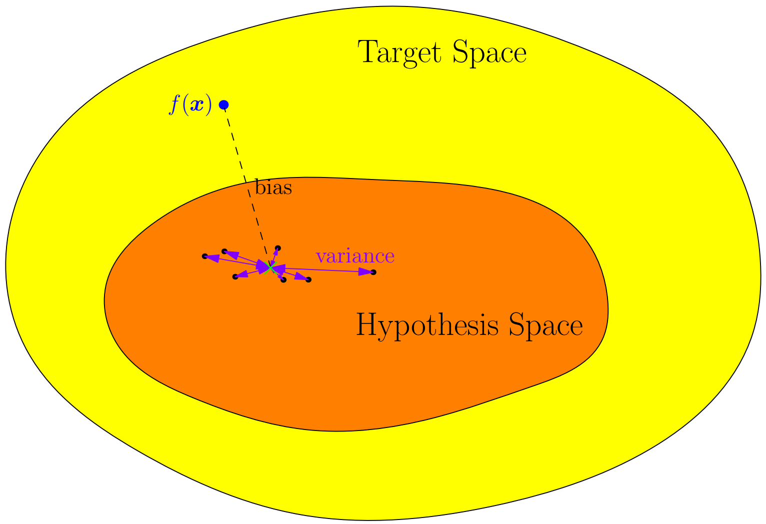
2. SVMs
3. **Ensemble Methods**
4. Bayesian Inference



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- One set of algorithms where ensembling are common place are decision trees

- These are particularly good for handling messy data
  - ⋆ categorical data
  - ⋆ mixture of data types
  - ⋆ missing data
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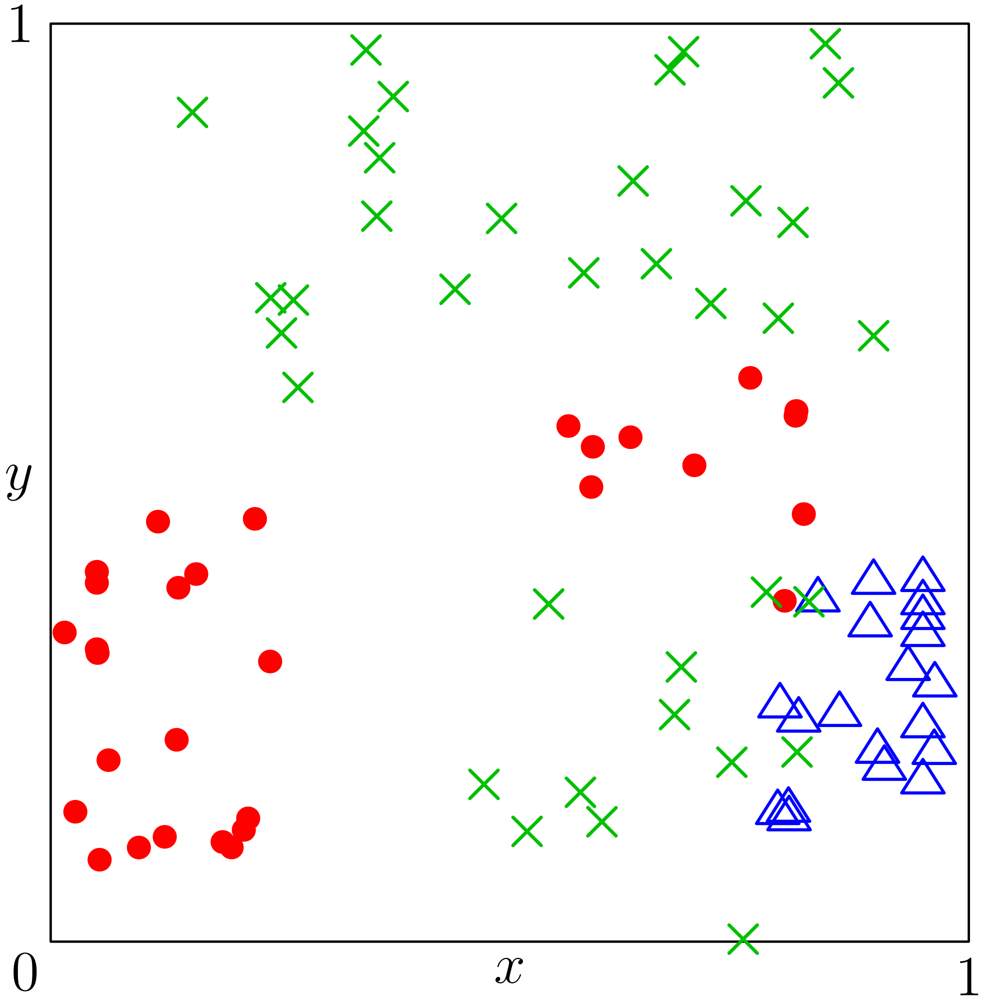

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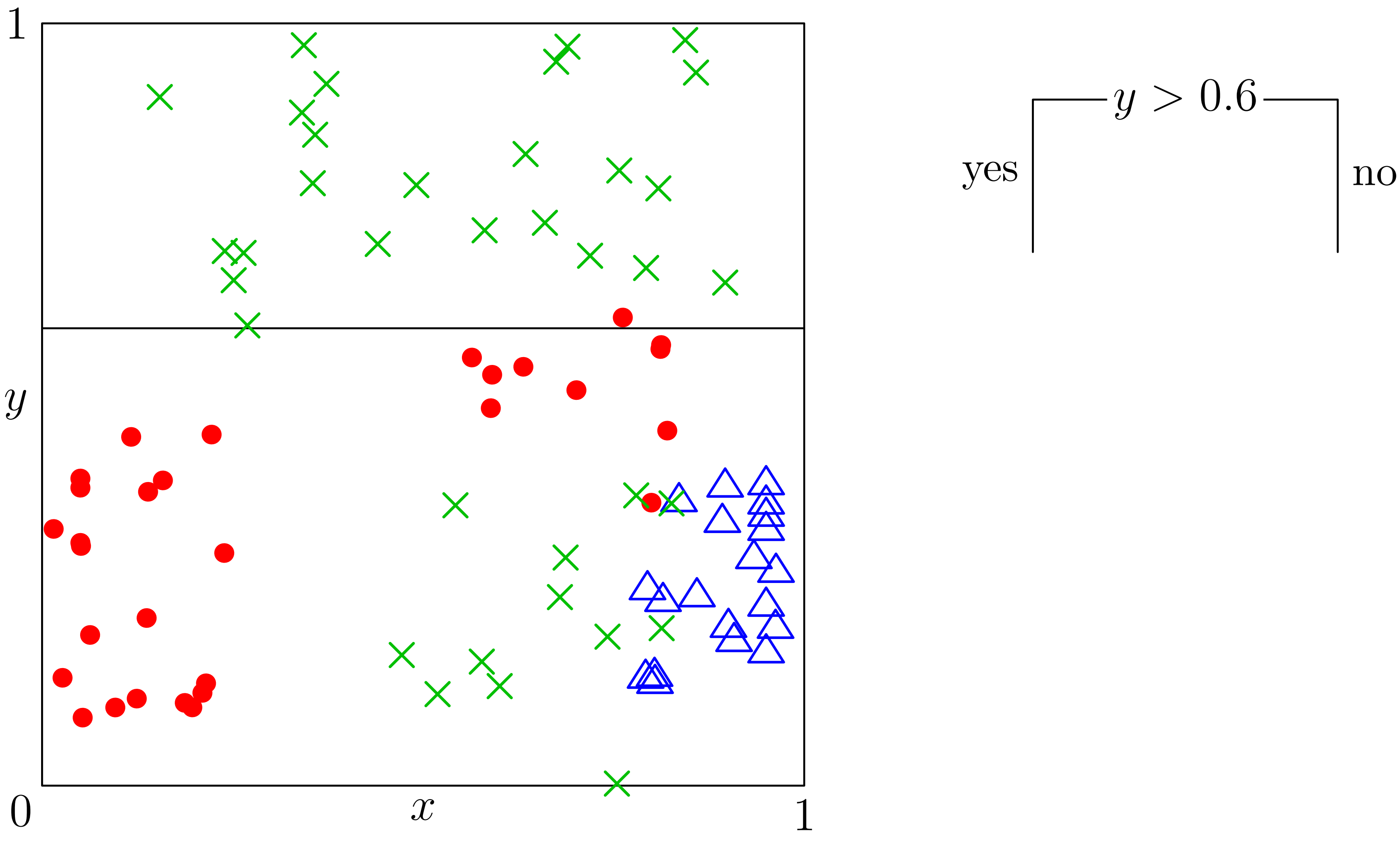

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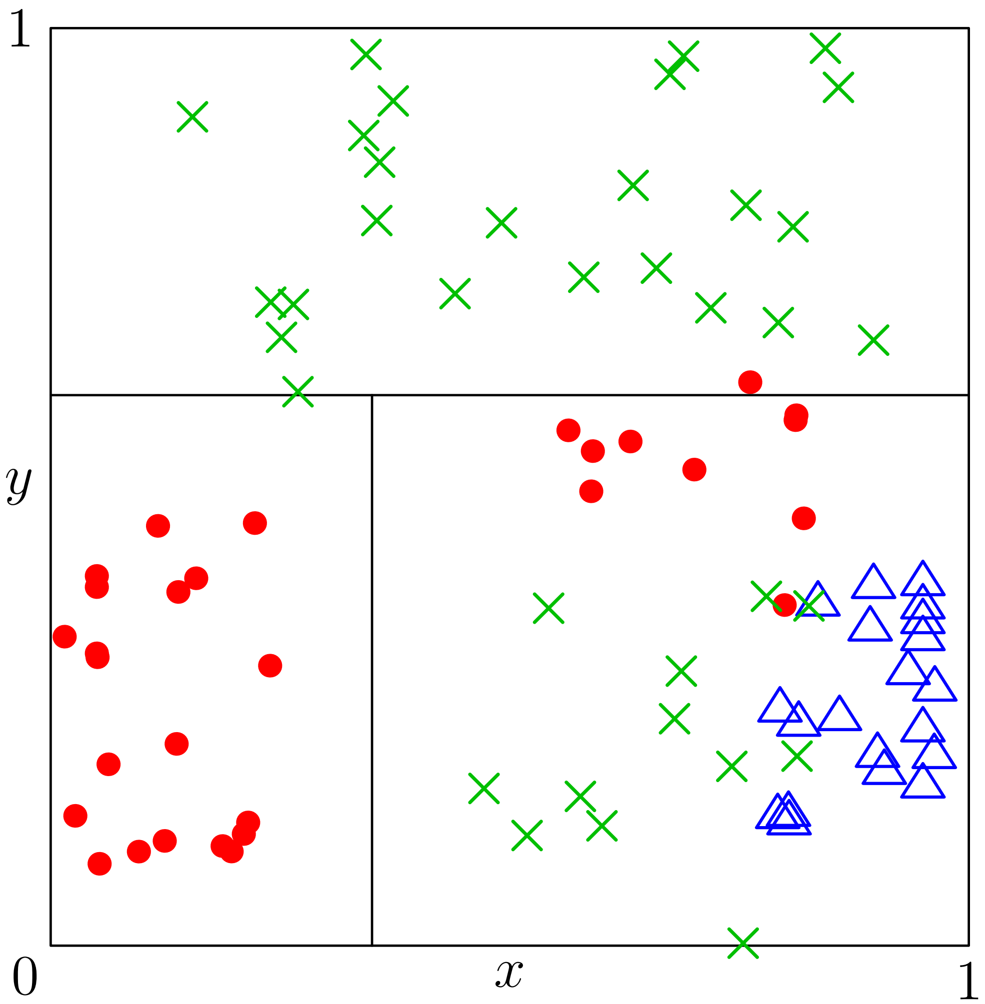

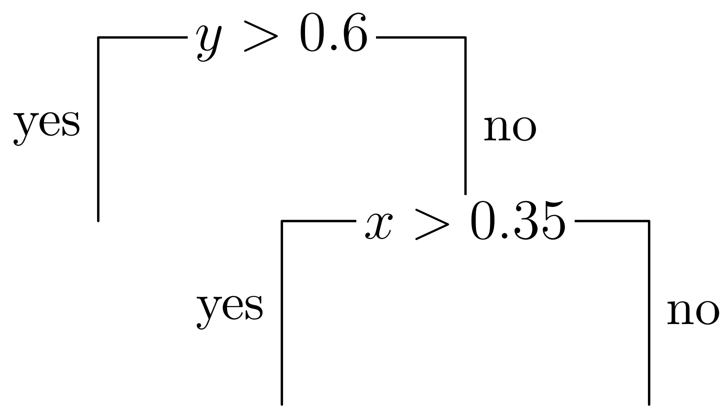

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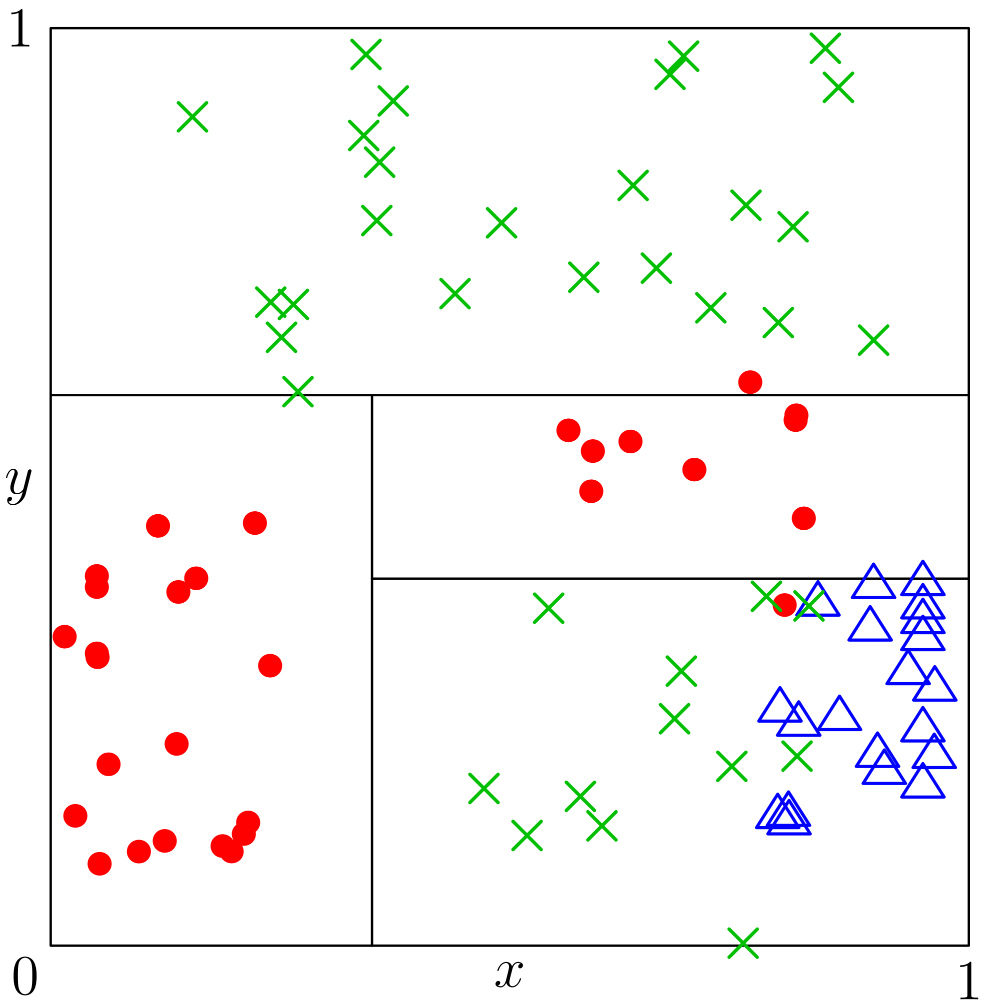

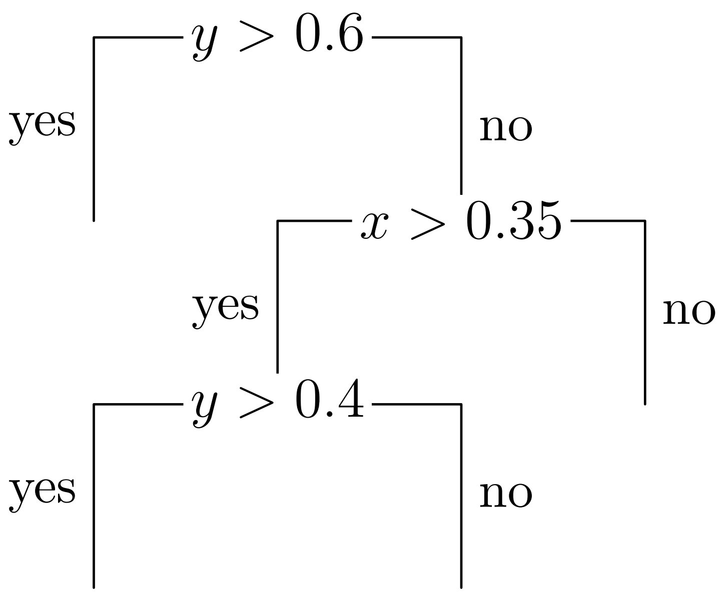

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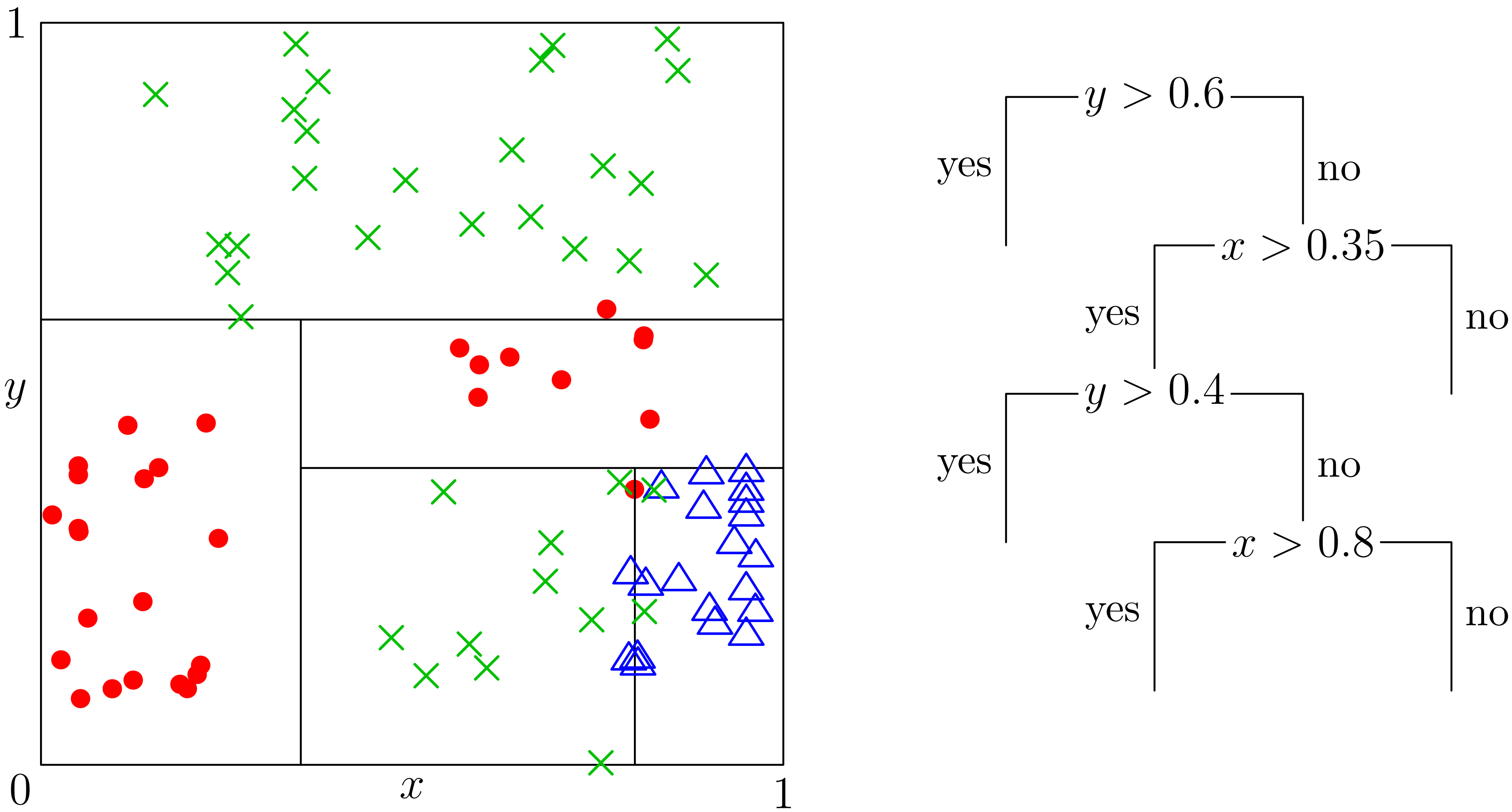

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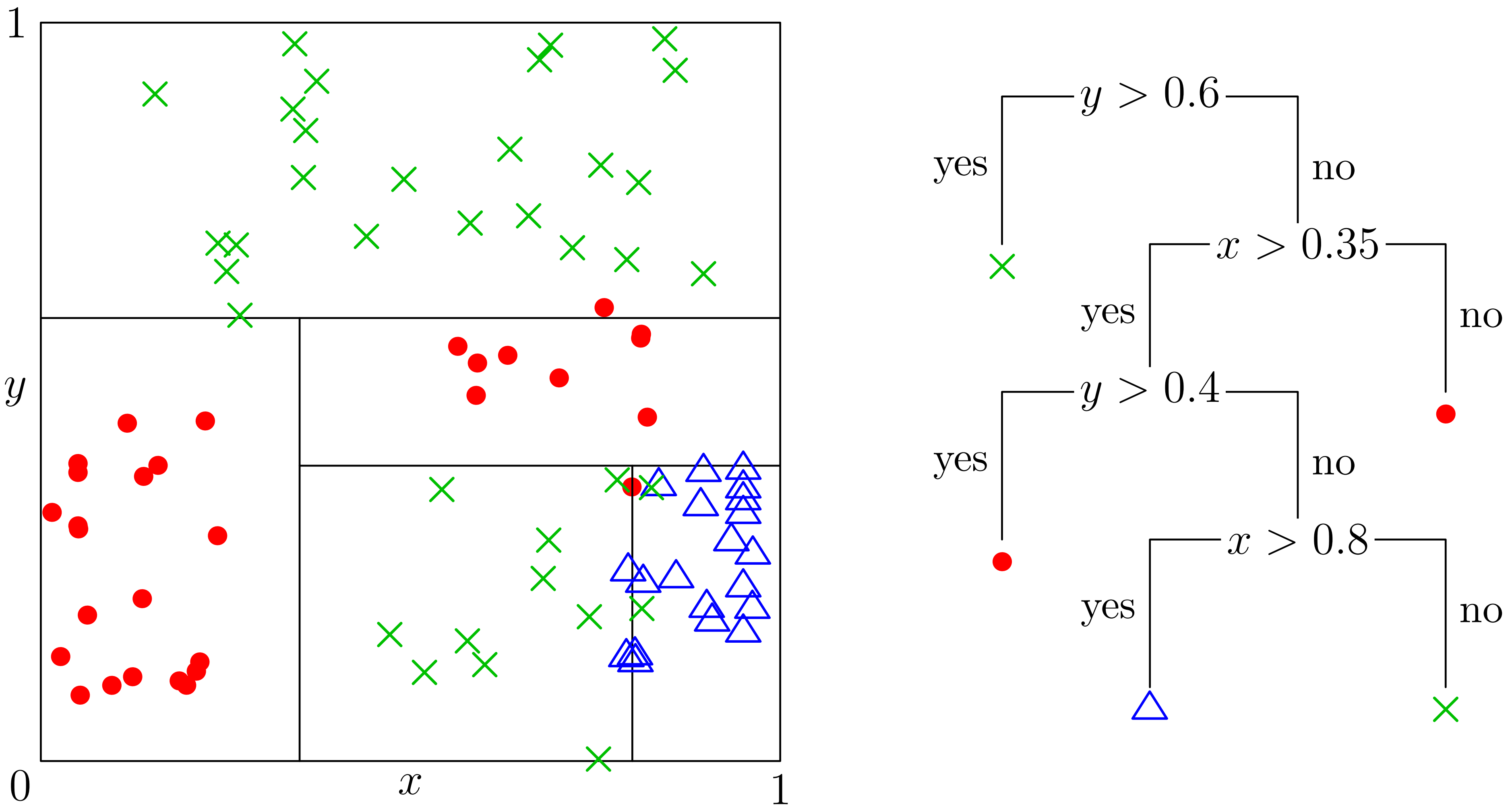

Using Decision Trees

- Decision trees are very dependent on the first few splits of data
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- Nevertheless they can be very useful for quickly exploring data
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- In boosting we make a **strong learner** by using a weighted sum of **weak learners**

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{n} w_i \, \hat{h}_i(\boldsymbol{x})$$

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Shallow Trees

- One of the most effective type of weak learner are very shallow trees, (e.g. $\sqrt{p}$)
- Use at most only small number of random variables, (e.g. $\sqrt{p}$)
- There are different algorithms for choosing the weights
  - ⋆ adaboost
  - ⋆ gradient boosting
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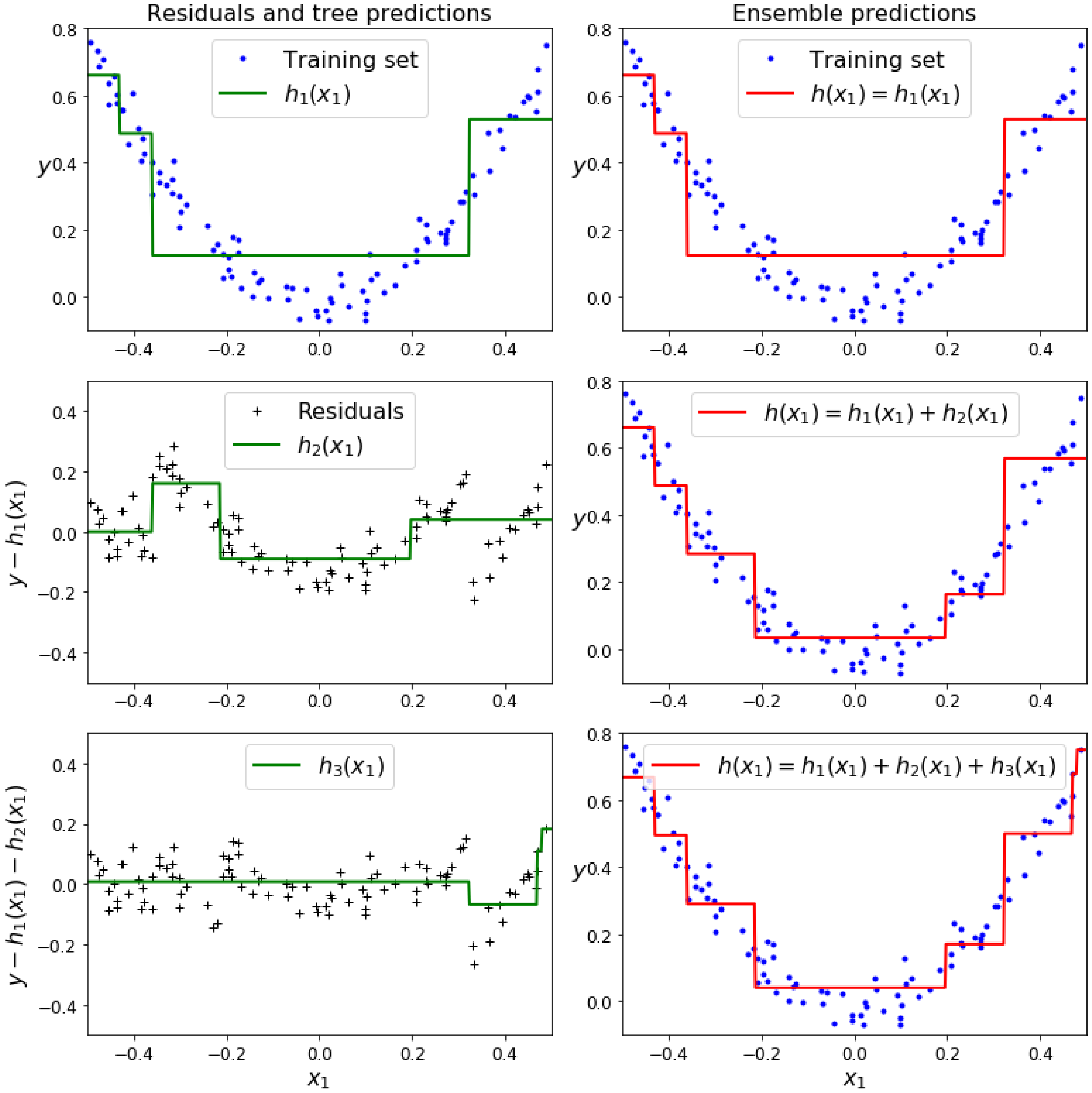

Residuals and tree predictions
Ensemble predictions
Training set
$h_1(x_1)$
$h(x_1) = h_1(x_1)$
Residuals
$h_2(x_1)$
$h(x_1) = h_1(x_1) + h_2(x_1)$
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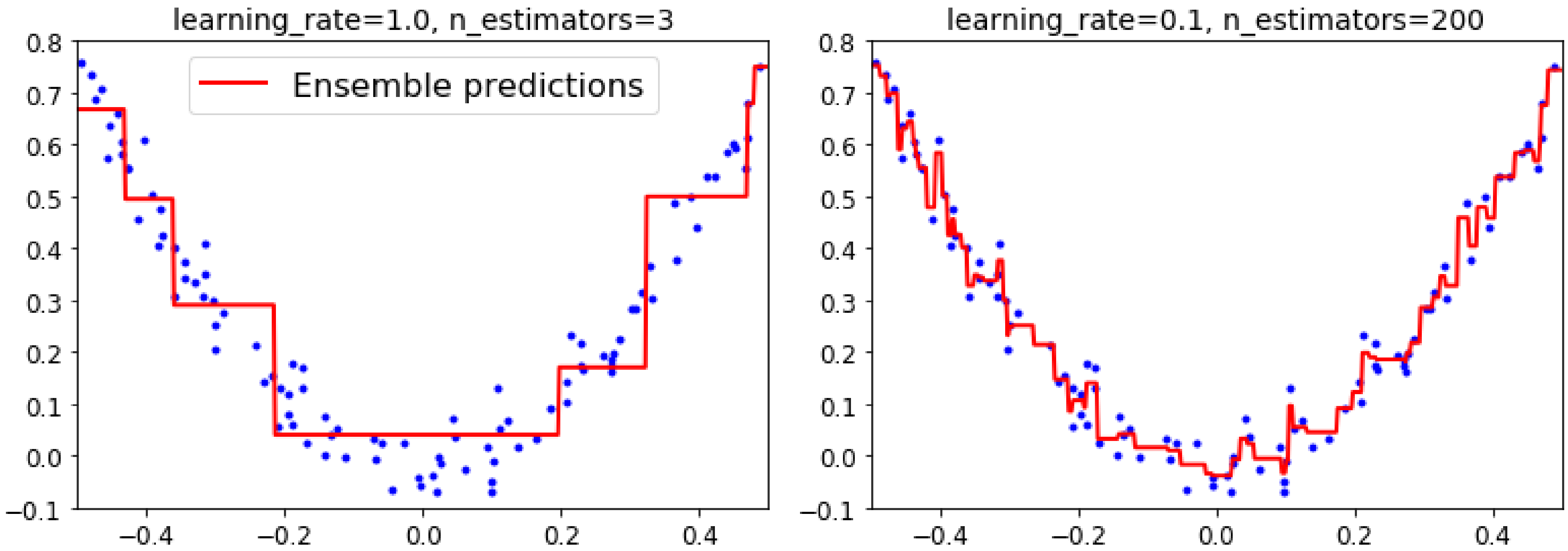
$y - h_1(x_1) - h_2(x_1)$
x_1

Keep On Going

- We can keep on going



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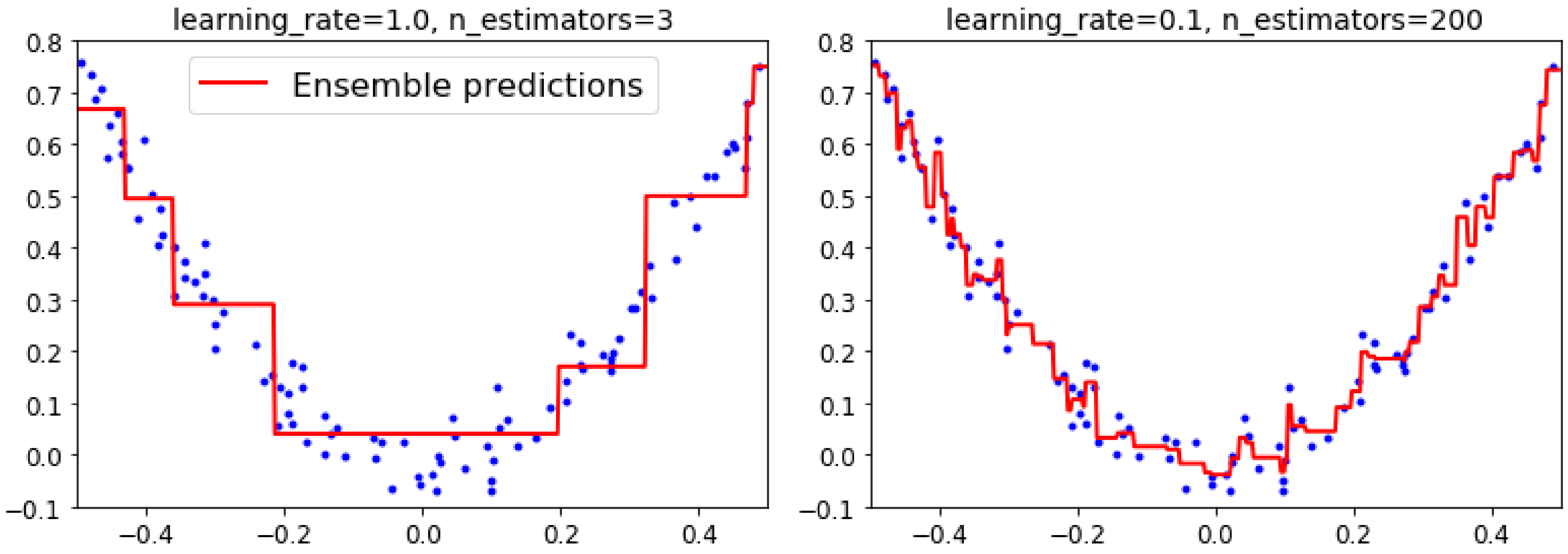
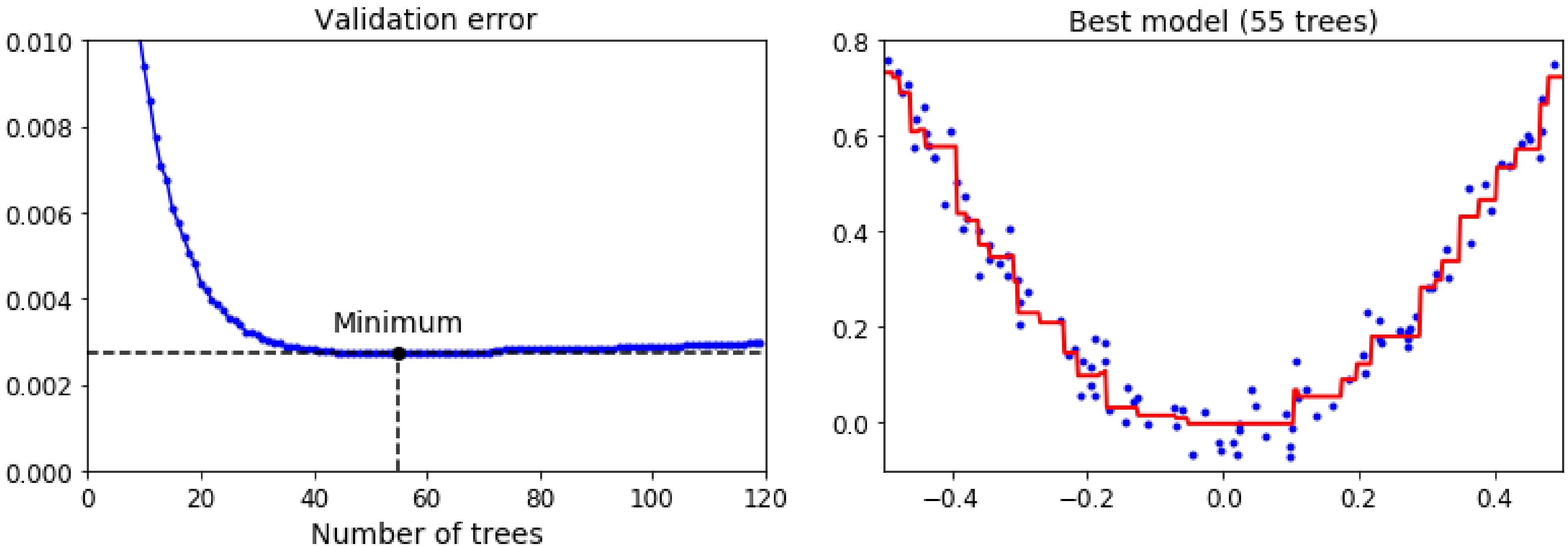


- But we will over-fit eventually

Early Stopping

- Like many algorithms we often get better results by early stopping



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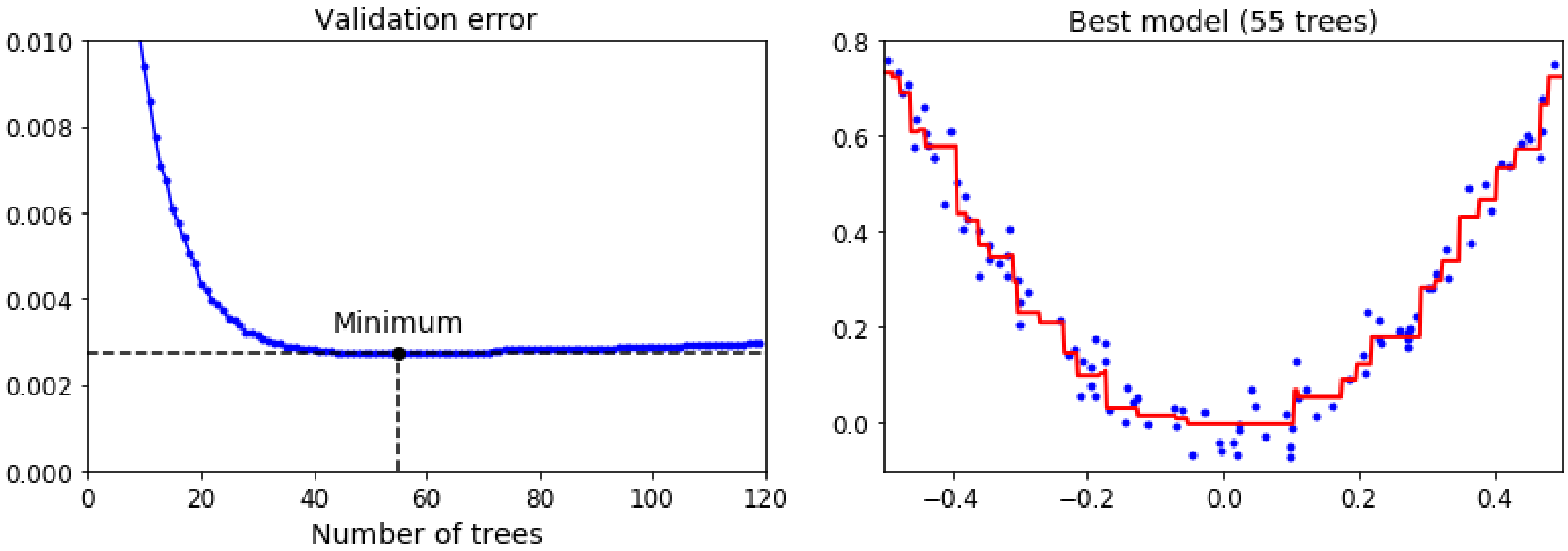

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- XGBoost stands for eXtreme Gradient Boosting
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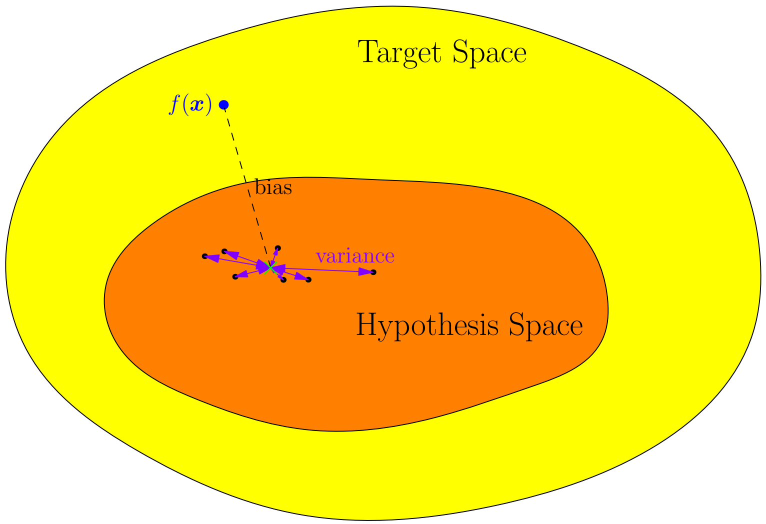
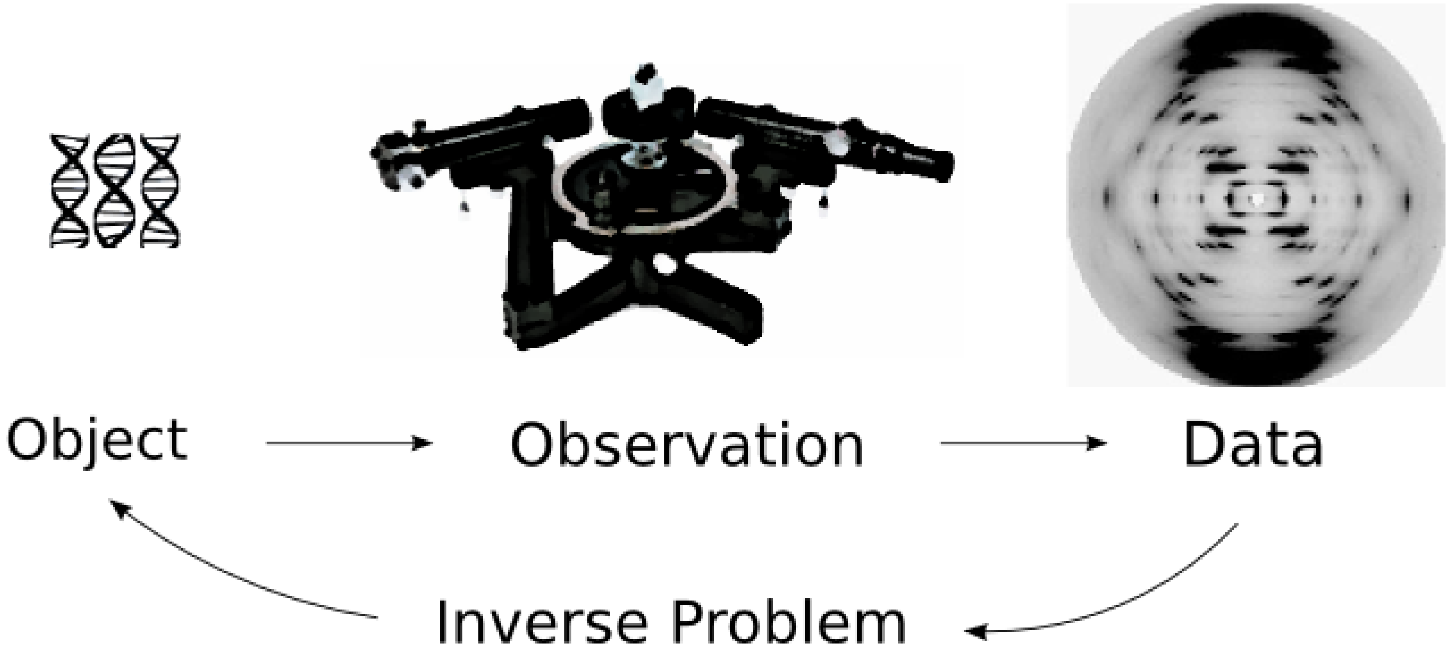
Outline

1. What Makes a Good Learning Machine?
2. SVMs
3. Ensemble Methods
4. **Bayesian Inference**



Inverse Problems



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- We are given some data generated by the world and we want to infer something about the world

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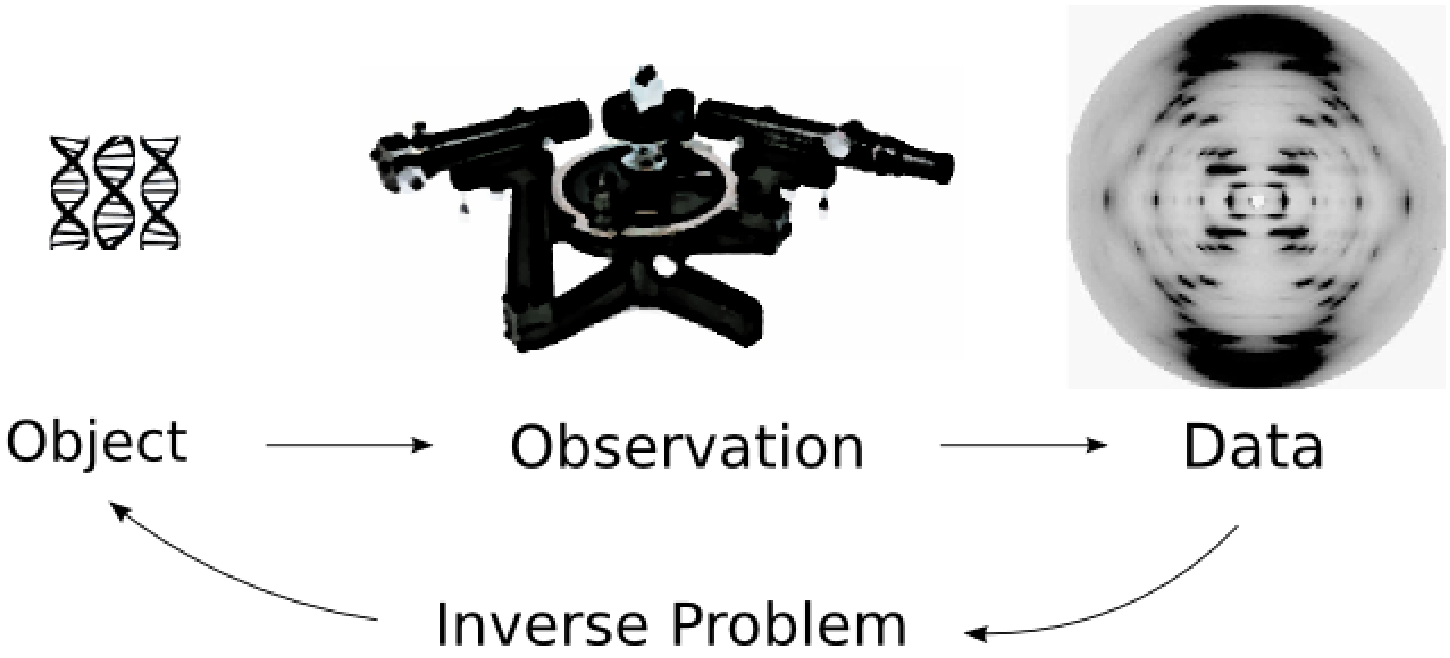

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Bayes' Rule

- A trivial identity in probability known as Bayes' rules tells you how to solve inverse problems

$$\mathbb{P}\left(W|\mathcal{D}\right) = \frac{\mathbb{P}\left(\mathcal{D}|W\right)\,\mathbb{P}\left(W\right)}{\mathbb{P}\left(D\right)}$$

- What we want is to know the probability of the world, W, given the data, $\mathcal{D}$ we have observered—this is known as the **posteriori** probability

- This depends on the **likelihood** of the data given the world $\mathbb{P}\left(\mathcal{D}|W\right)$

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- W is some model of the world—technically they are parameters of the likelihood function

- If we trying to infer the length of rod then it would be a length

- If we are trying to infer the DNA sequence given a set of short reads then W would be a DNA sequence

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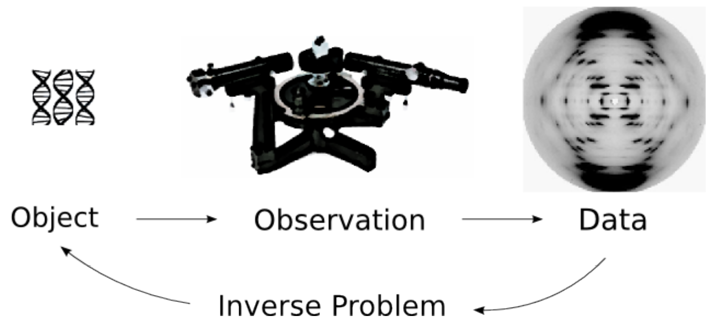
Advantages of Bayesian Inference

- Its optimal (follows from a simple probabilistic identity)
- It is relatively easy to model the likelihood (this is a forward process not an inverse process)



- No problem with missing data—we just calculate the likelihood of the data we see
- Won't over-fit
- Provides a full probabilistic description of the inference

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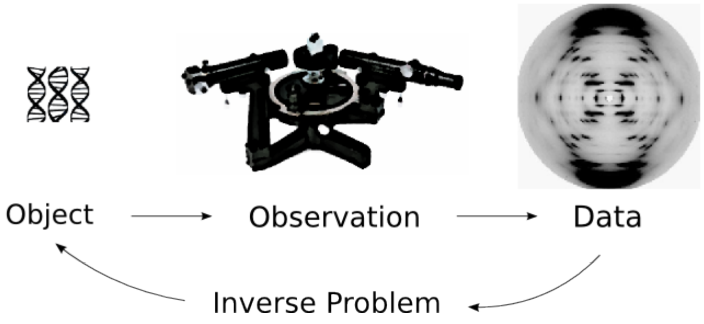

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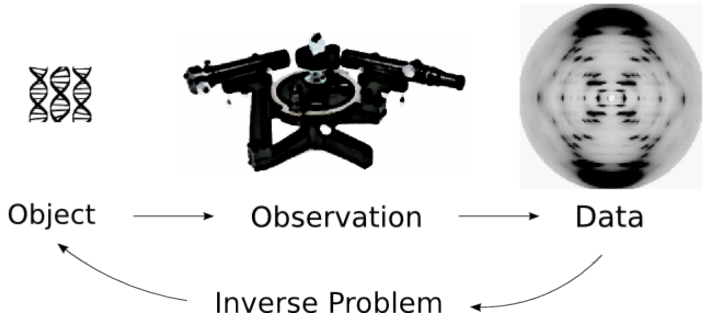

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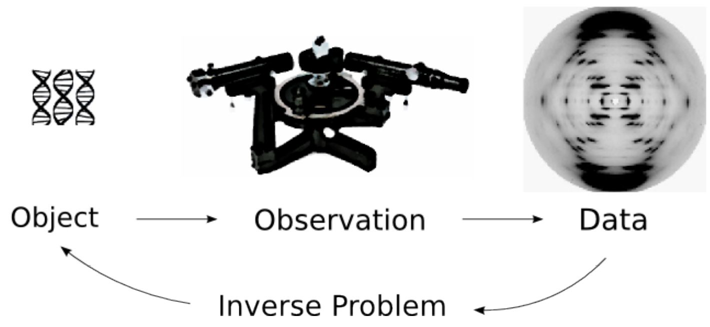

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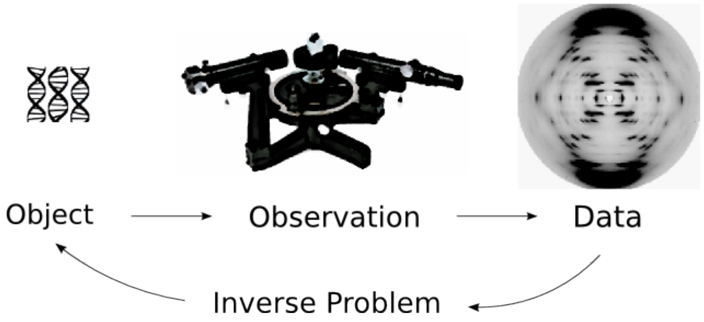

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- Need to be able to sum over all possible worlds

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Simple Bayes

- There are a few cases where Bayesian Inference is relatively simple
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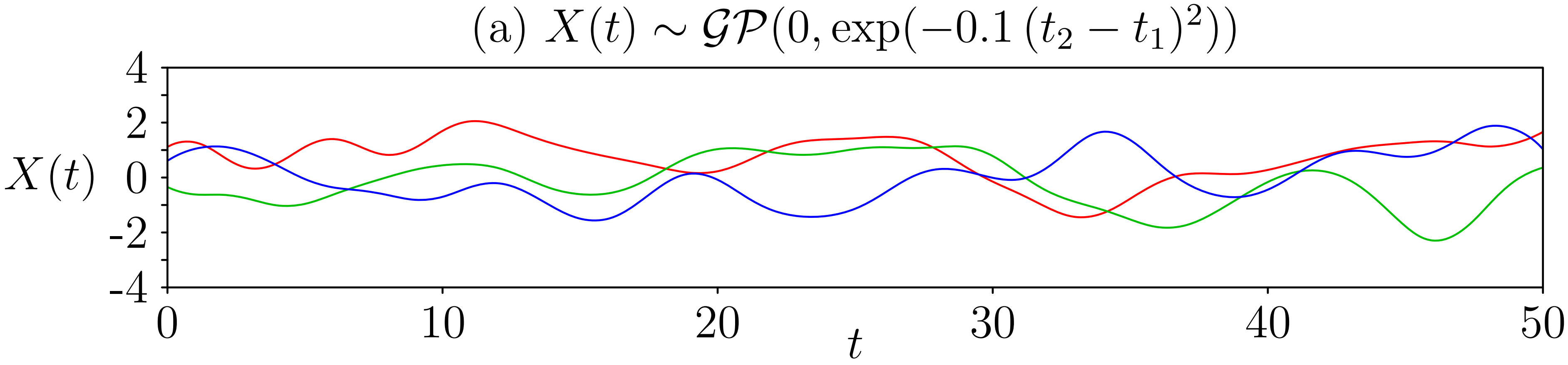

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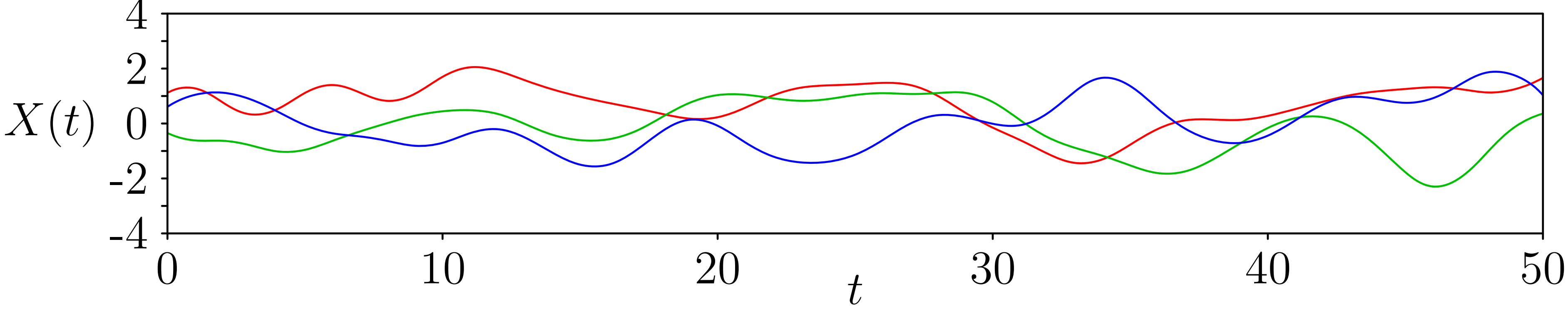
(a) $X(t) \sim \mathcal{GP}(0, \exp(-0.1\,(t_2 - t_1)^2))$



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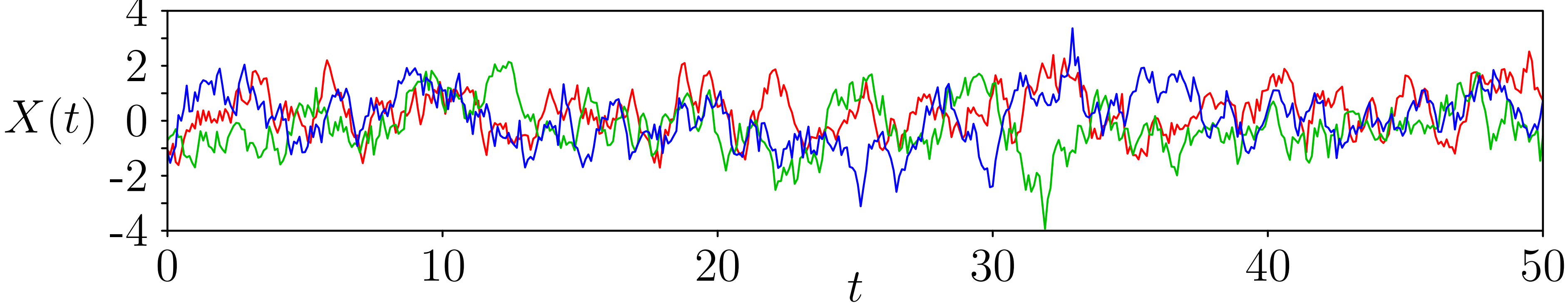
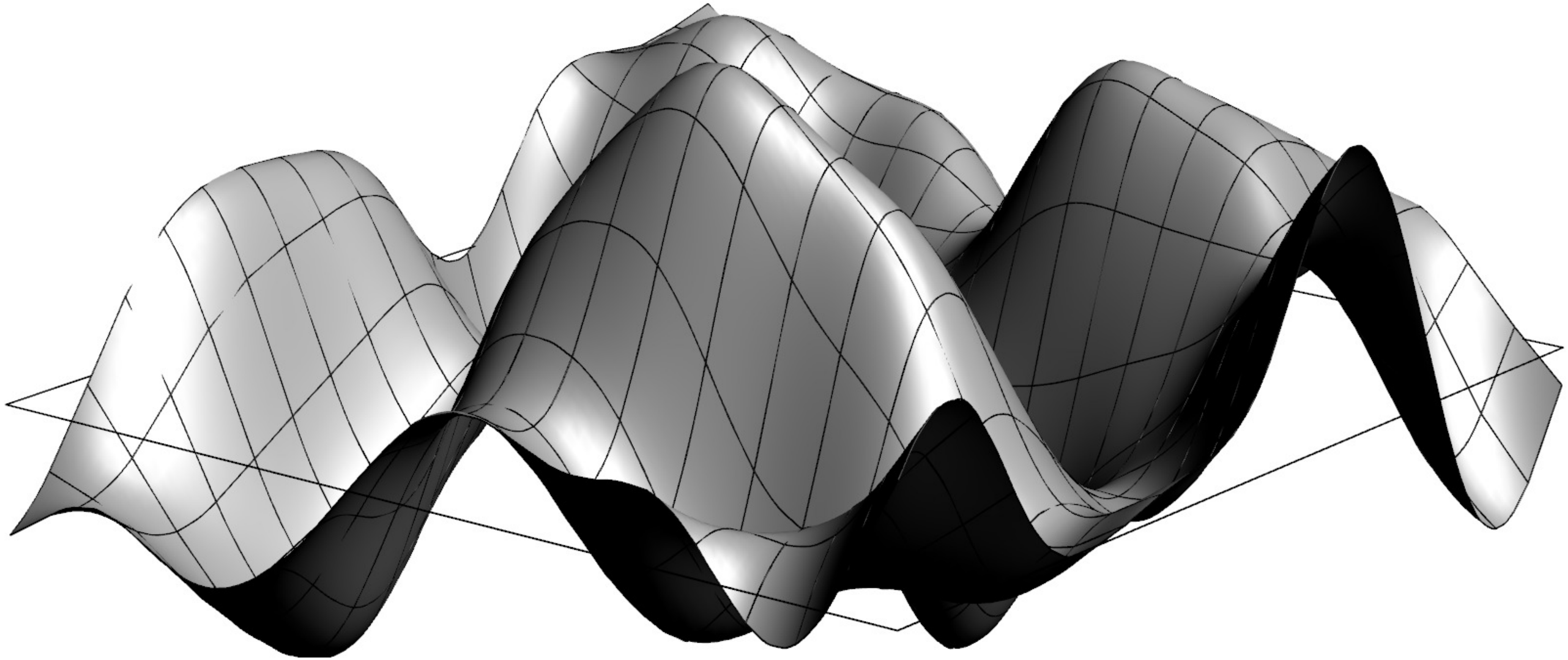
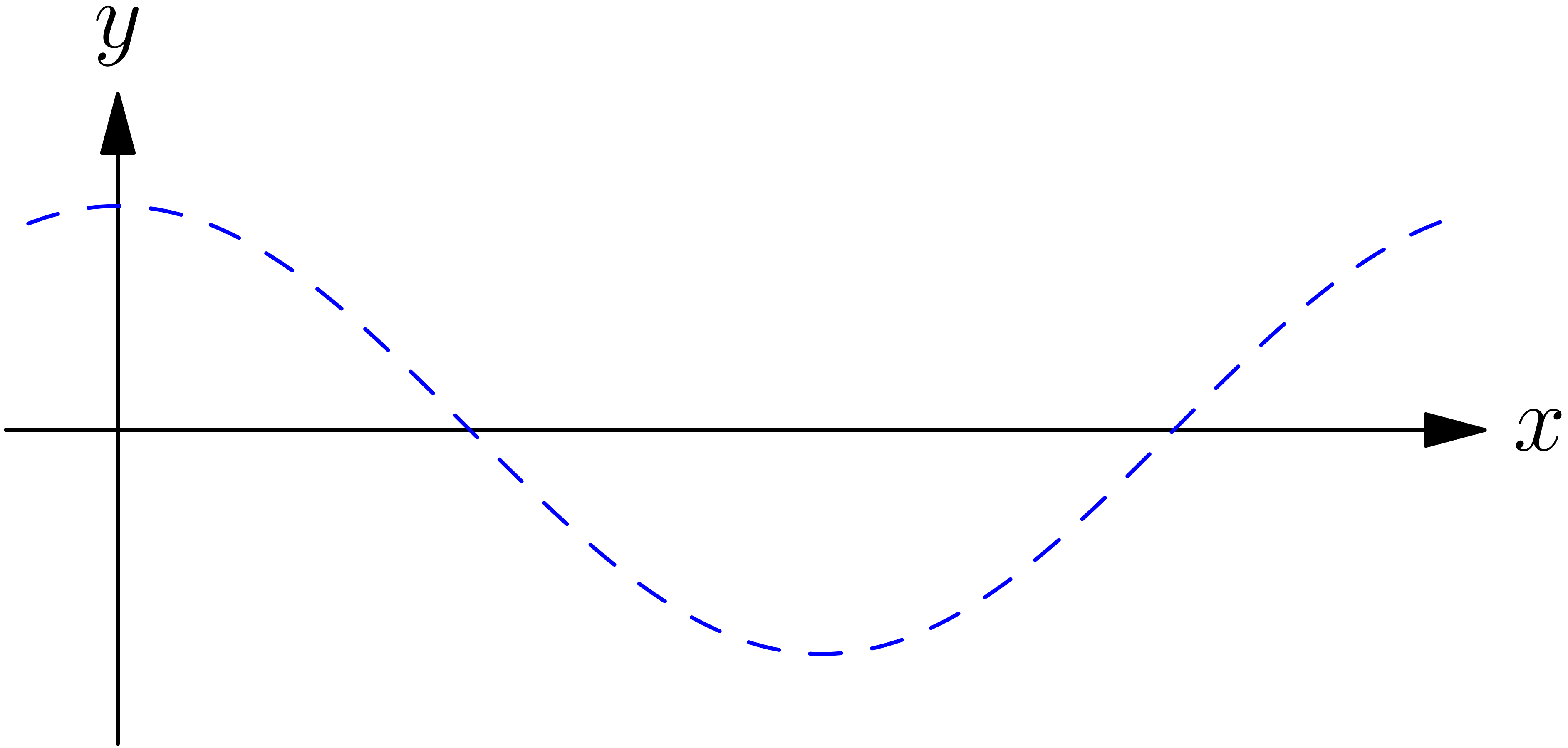


2-D Gaussian Processes



$$K(x, x') = \exp(-(x - x')^2/(2\,\ell^2))$$



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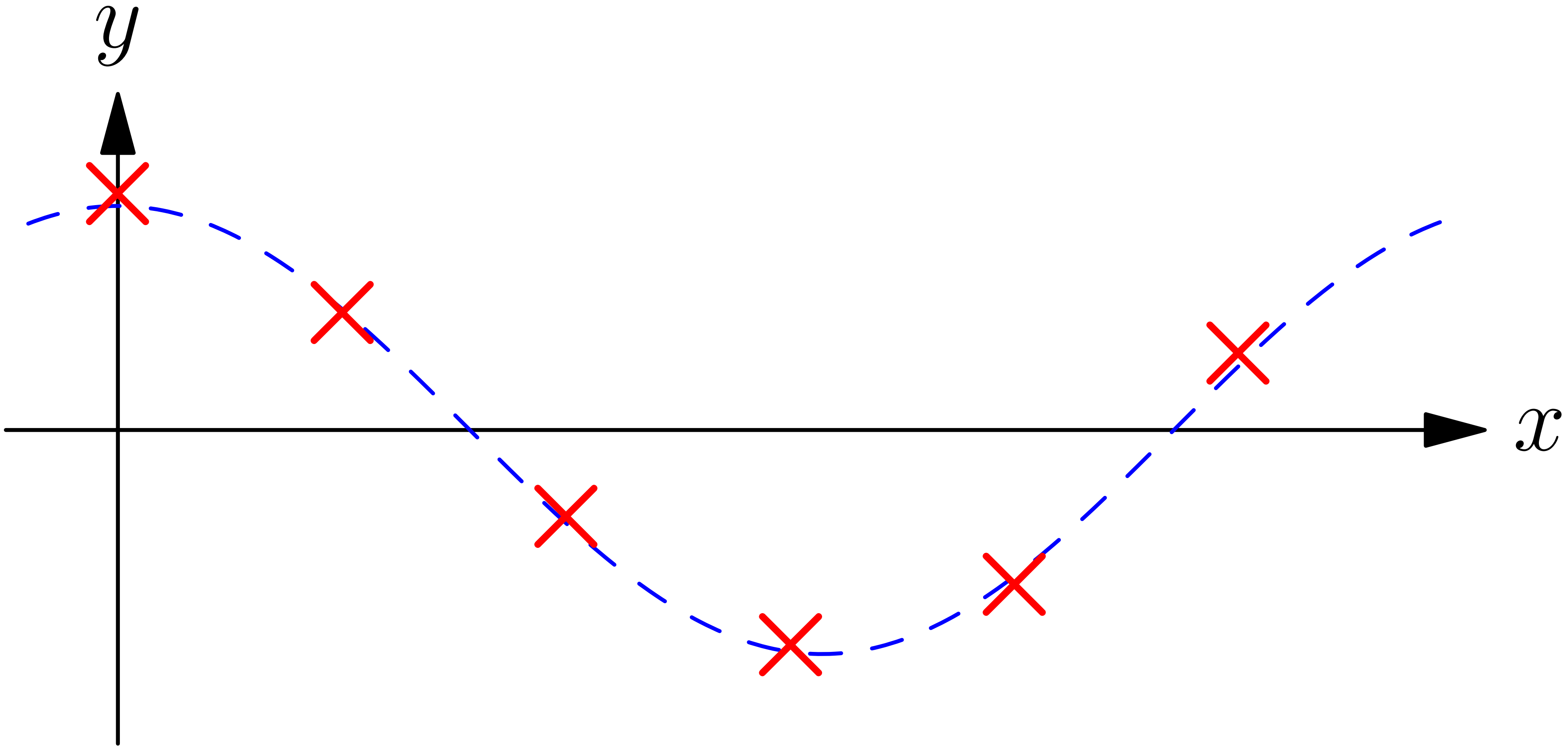

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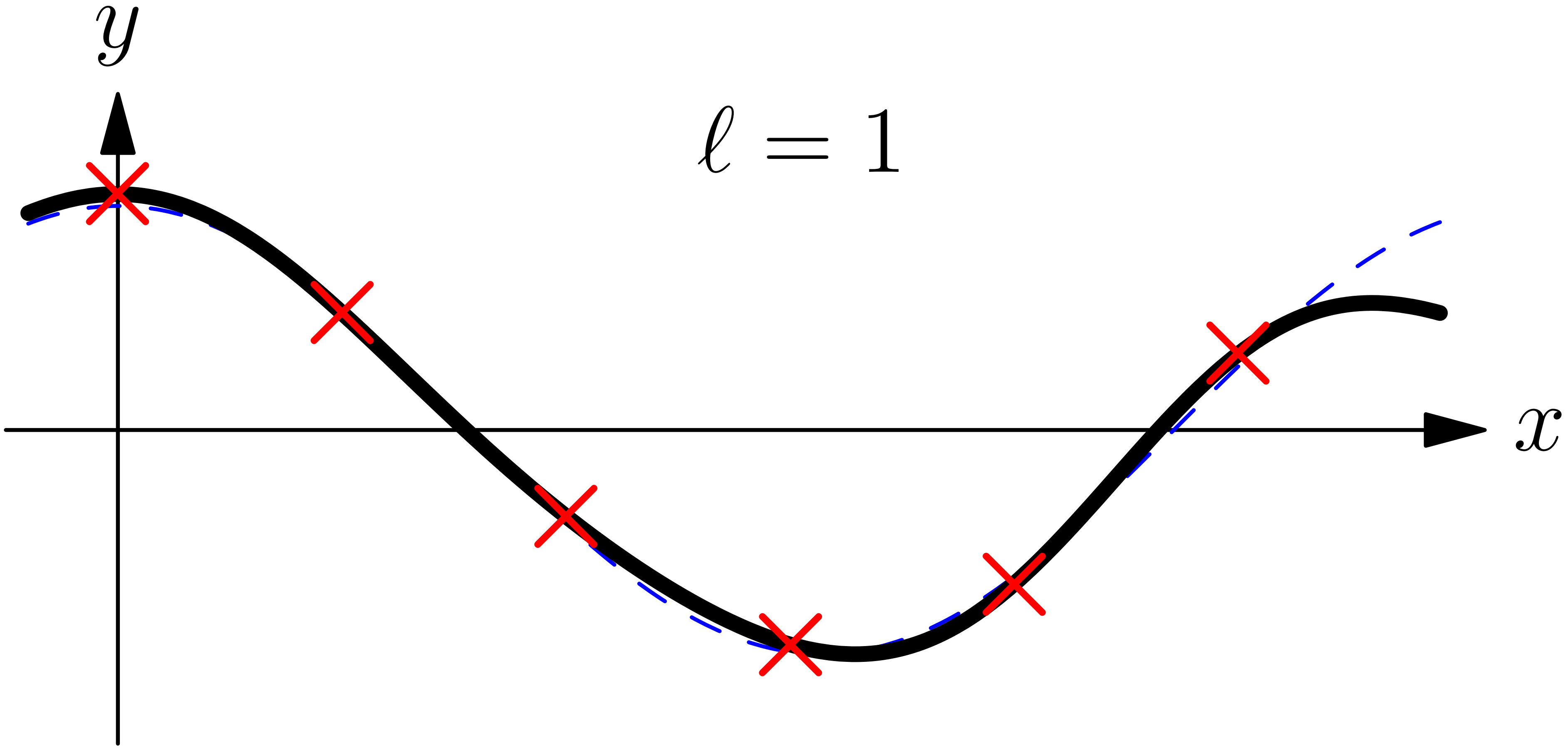

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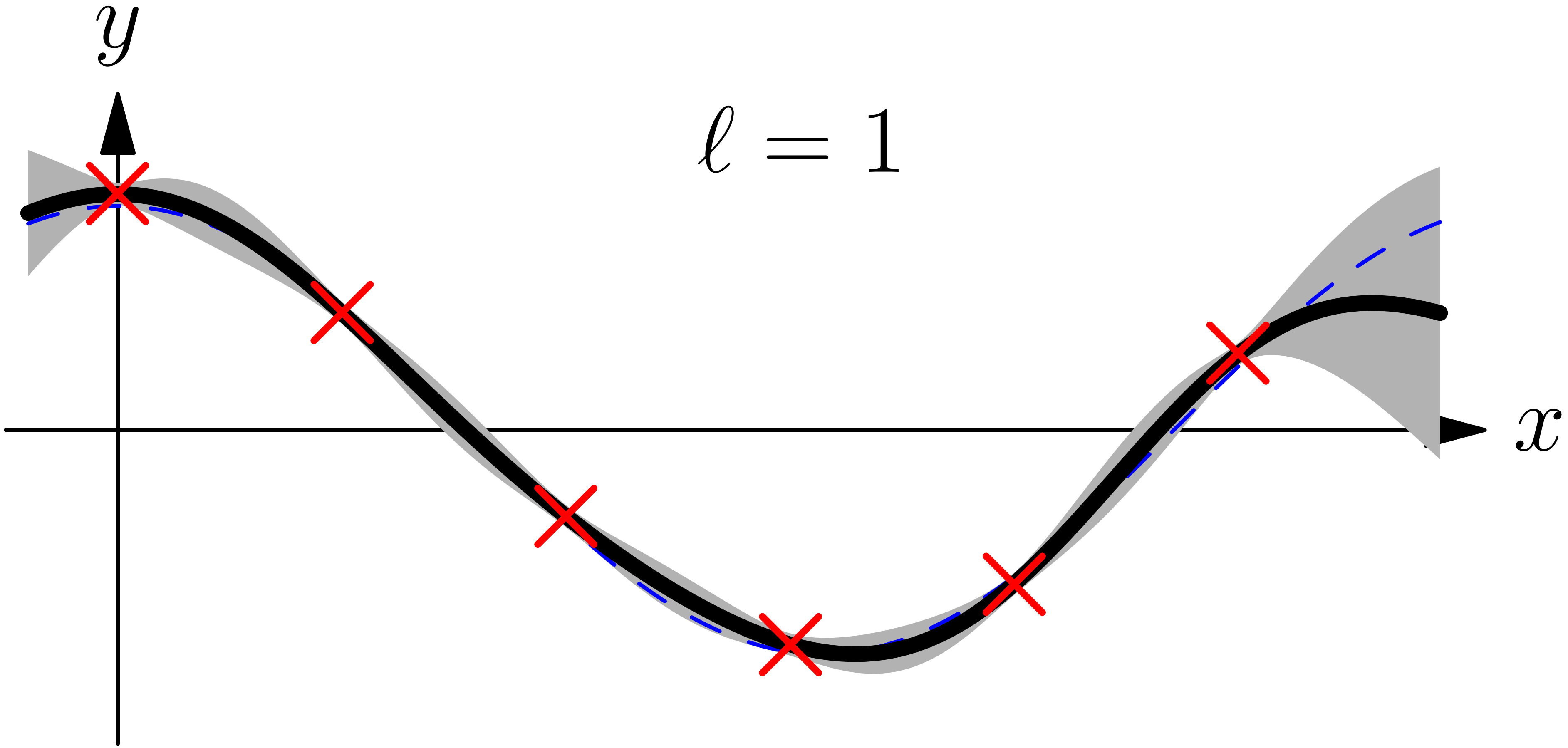

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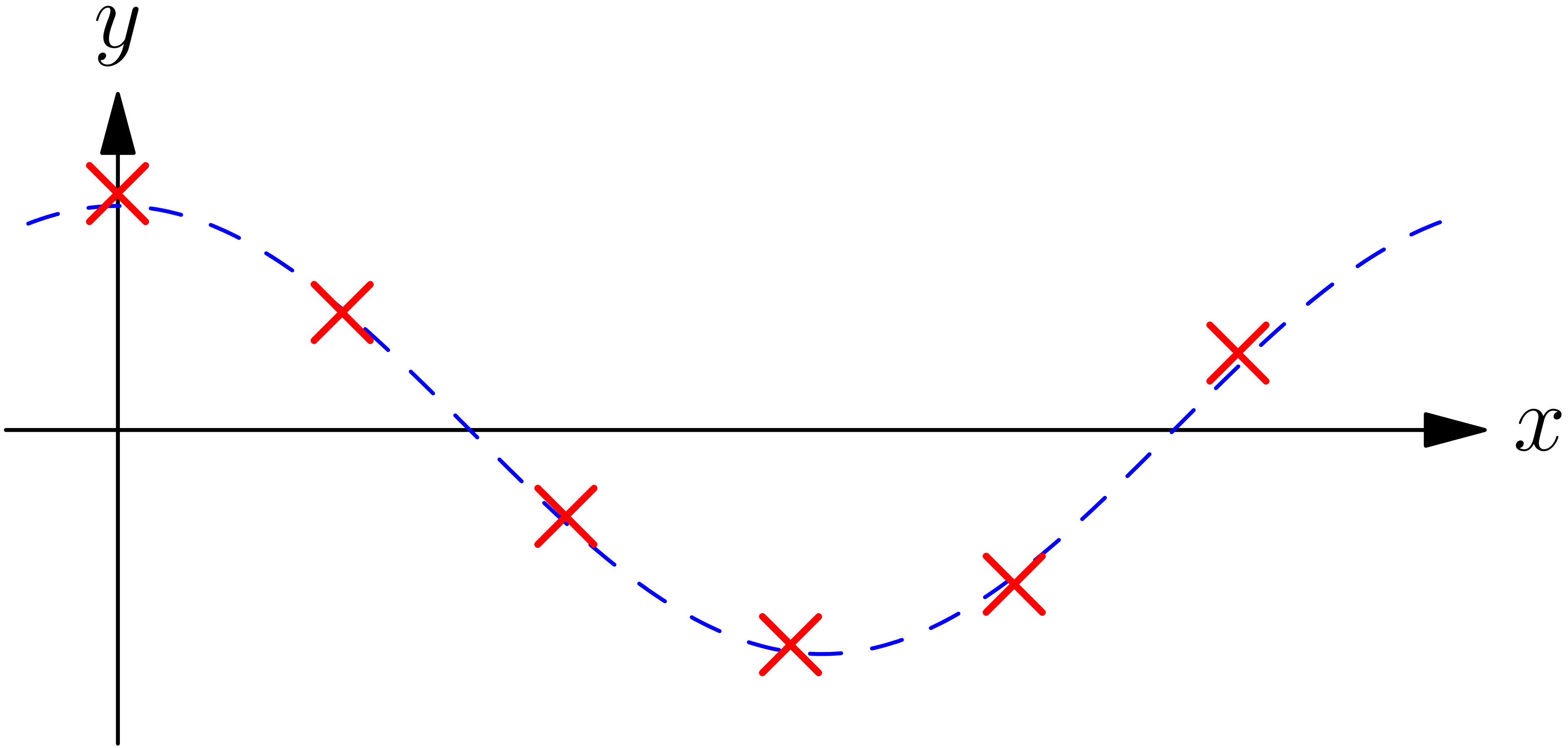

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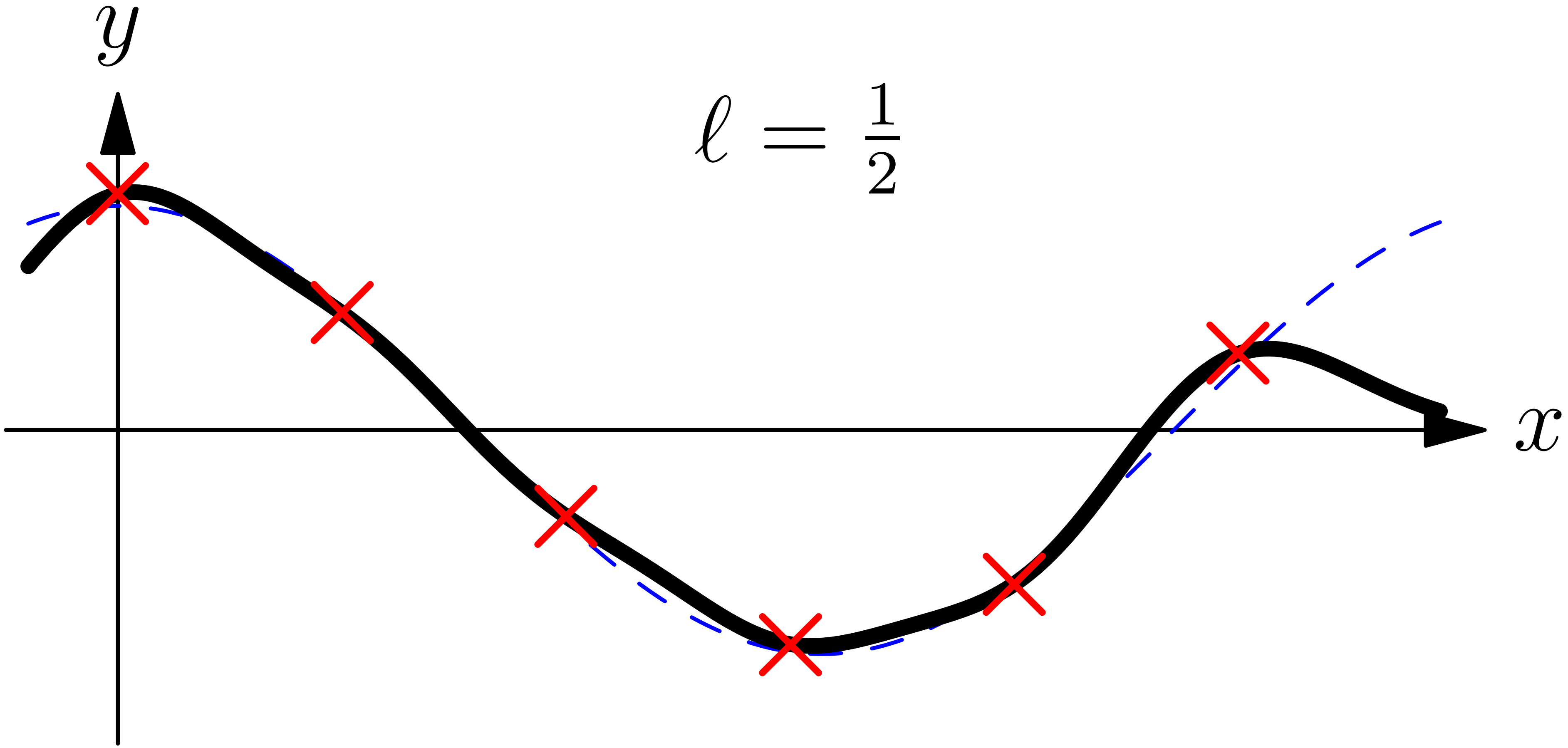

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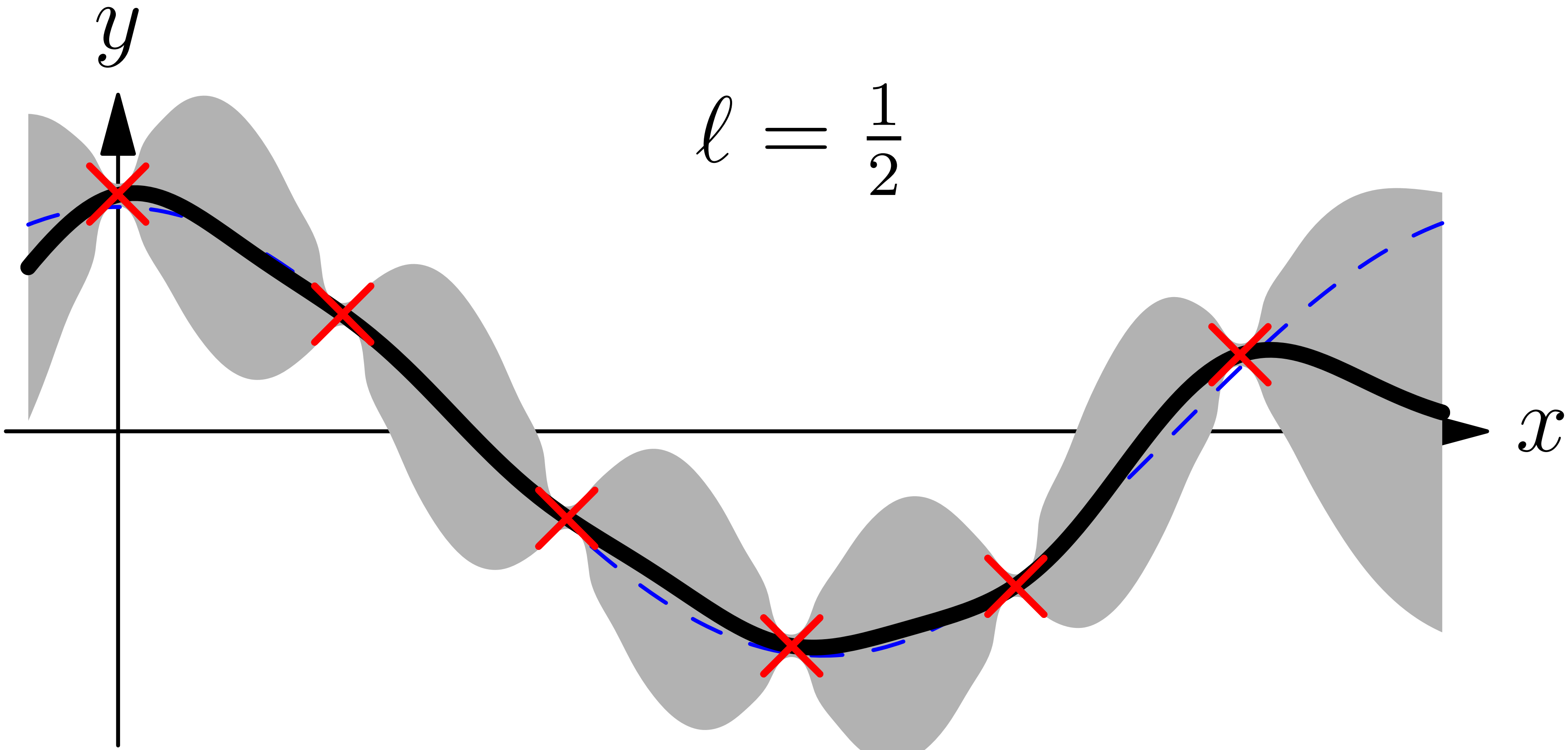

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