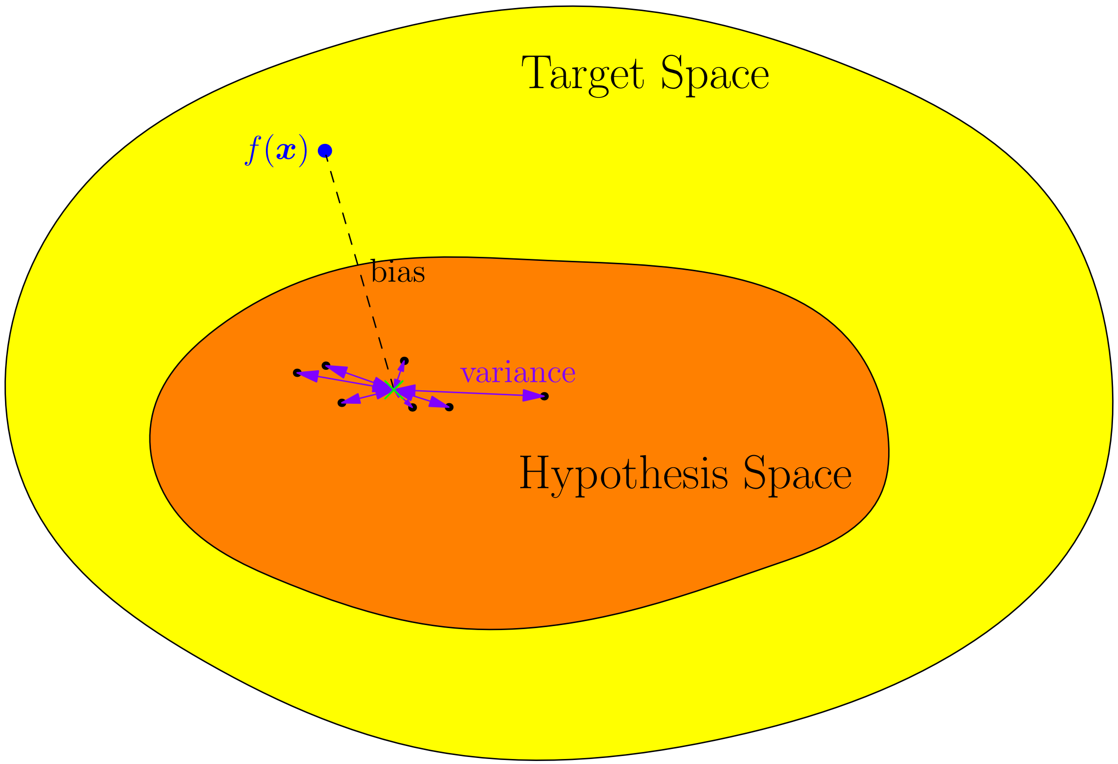
DISC-NET ML Workshop

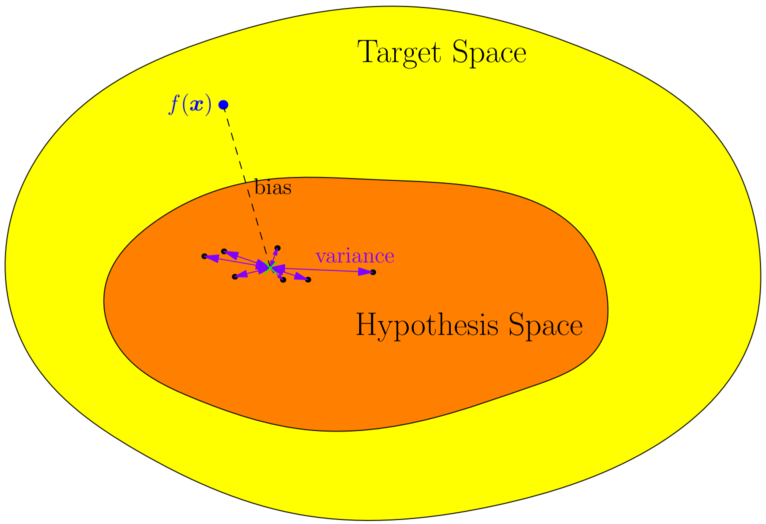
Advanced Machine Learning



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)
- The problem can be under-constrained (i.e. there are many possible solutions that are consistent with the data)

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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 $\hat{f}(\boldsymbol{x}|\mathcal{D})$
- We typically choose the weights to minimise a *training error*

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

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$$E_T(\mathcal{D}) = \sum_{\boldsymbol{x} \in \mathcal{D}} \left(\hat{f}(\boldsymbol{x}|\mathcal{D}) - f(\boldsymbol{x}) \right)^2 = \sum_{i=1}^{m} \left(\hat{f}(\boldsymbol{x}_i|\mathcal{D}) - y_i \right)^2$$

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

Generalisation Error

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

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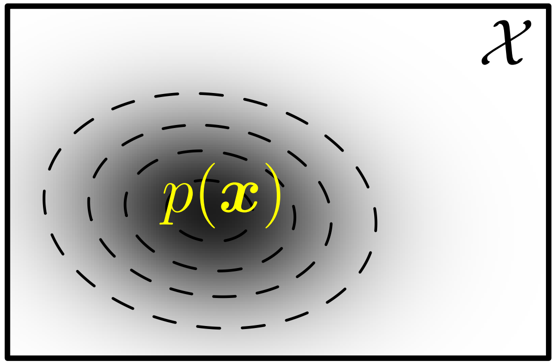

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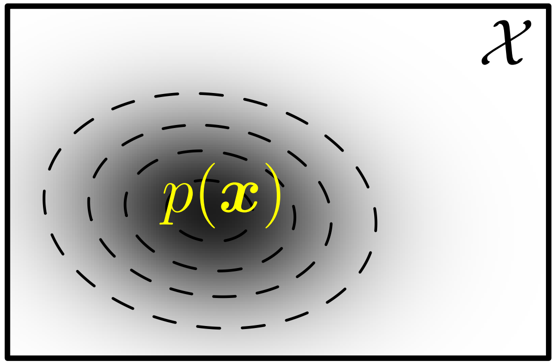

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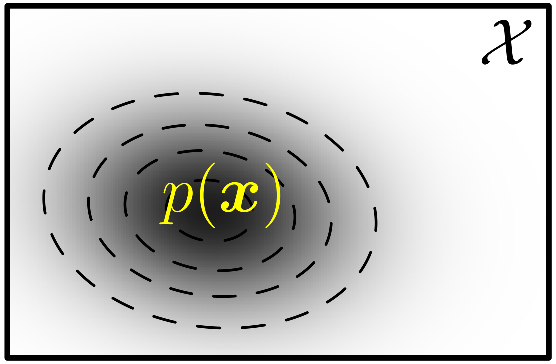

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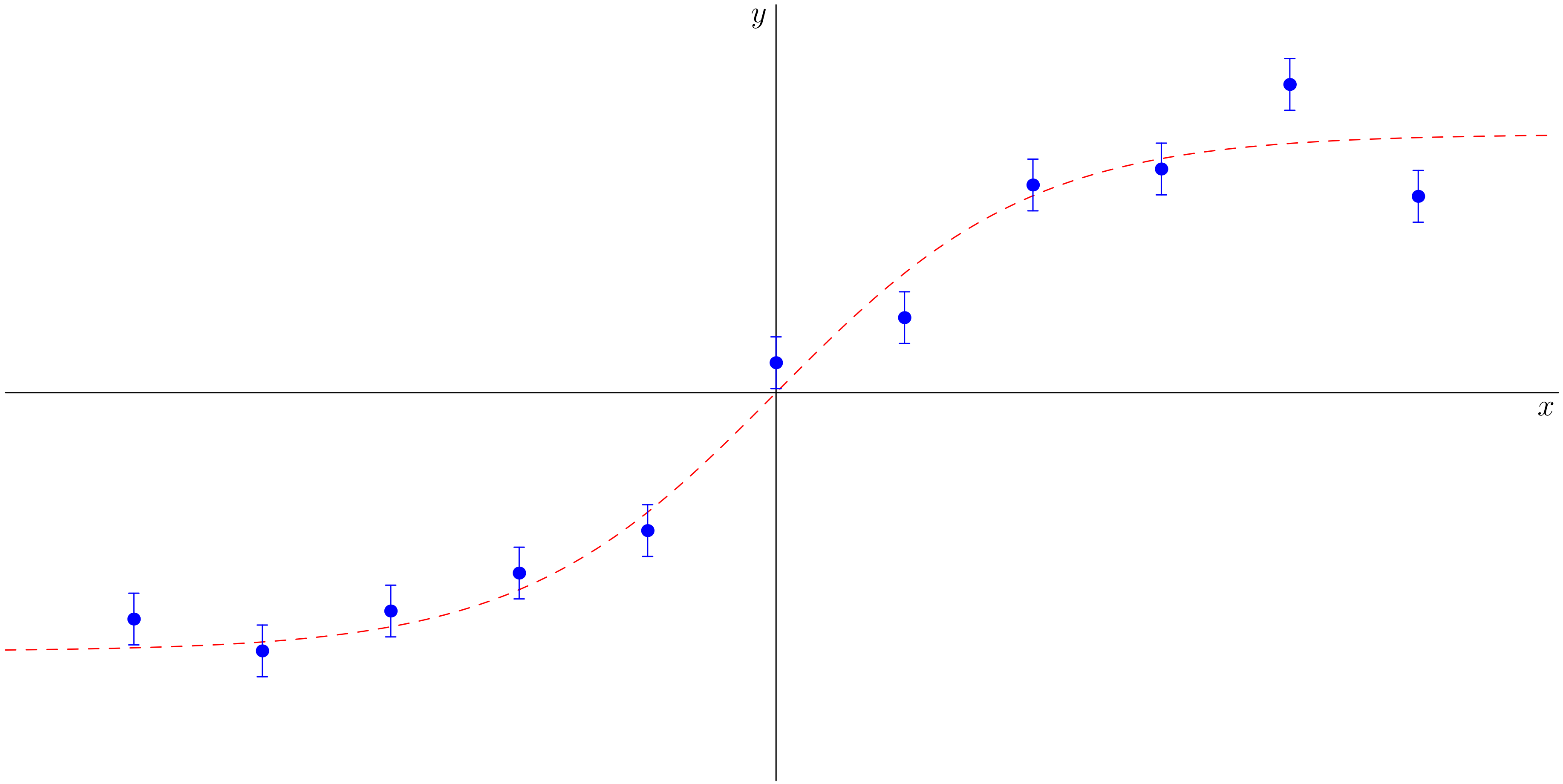

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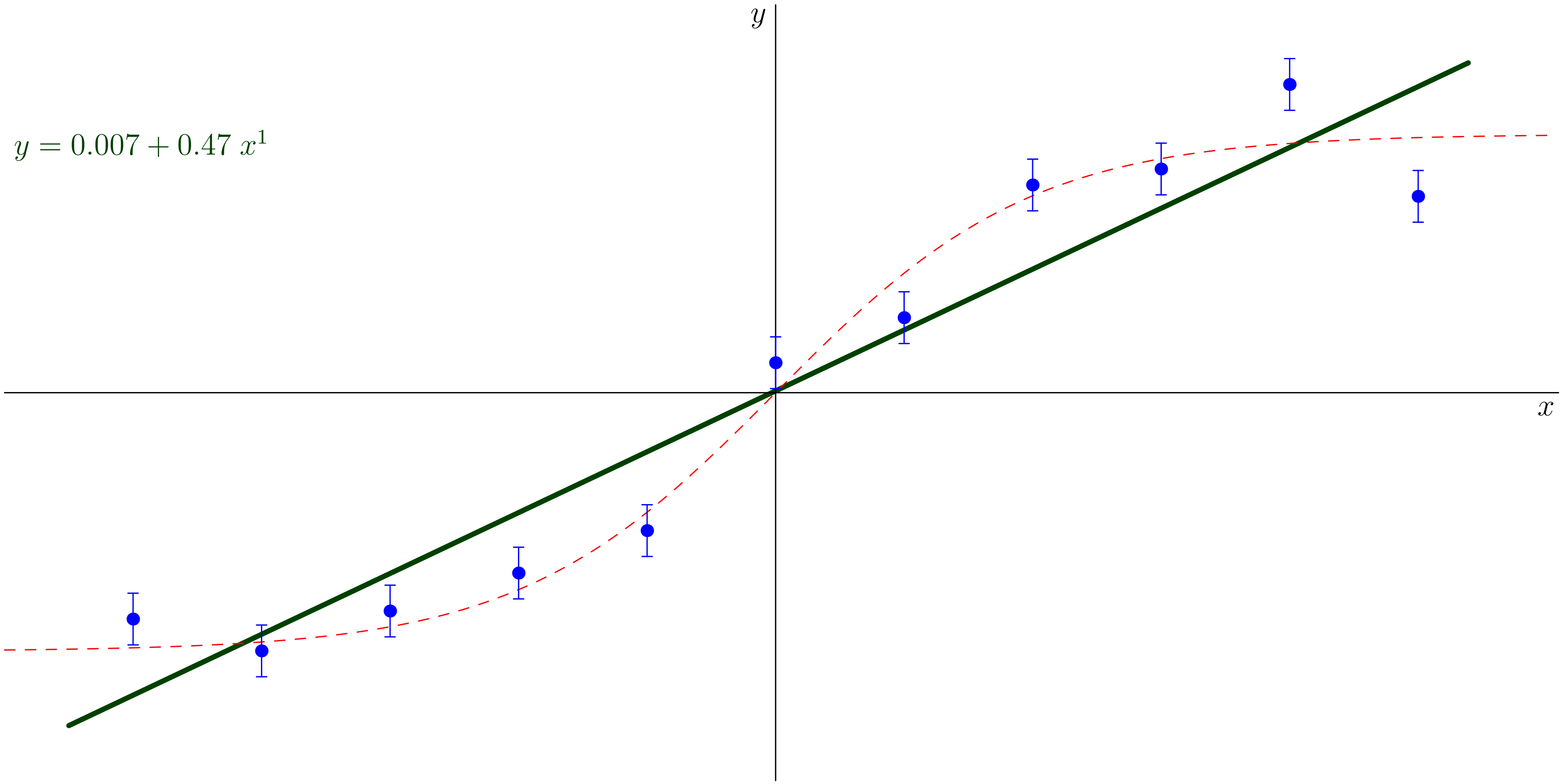

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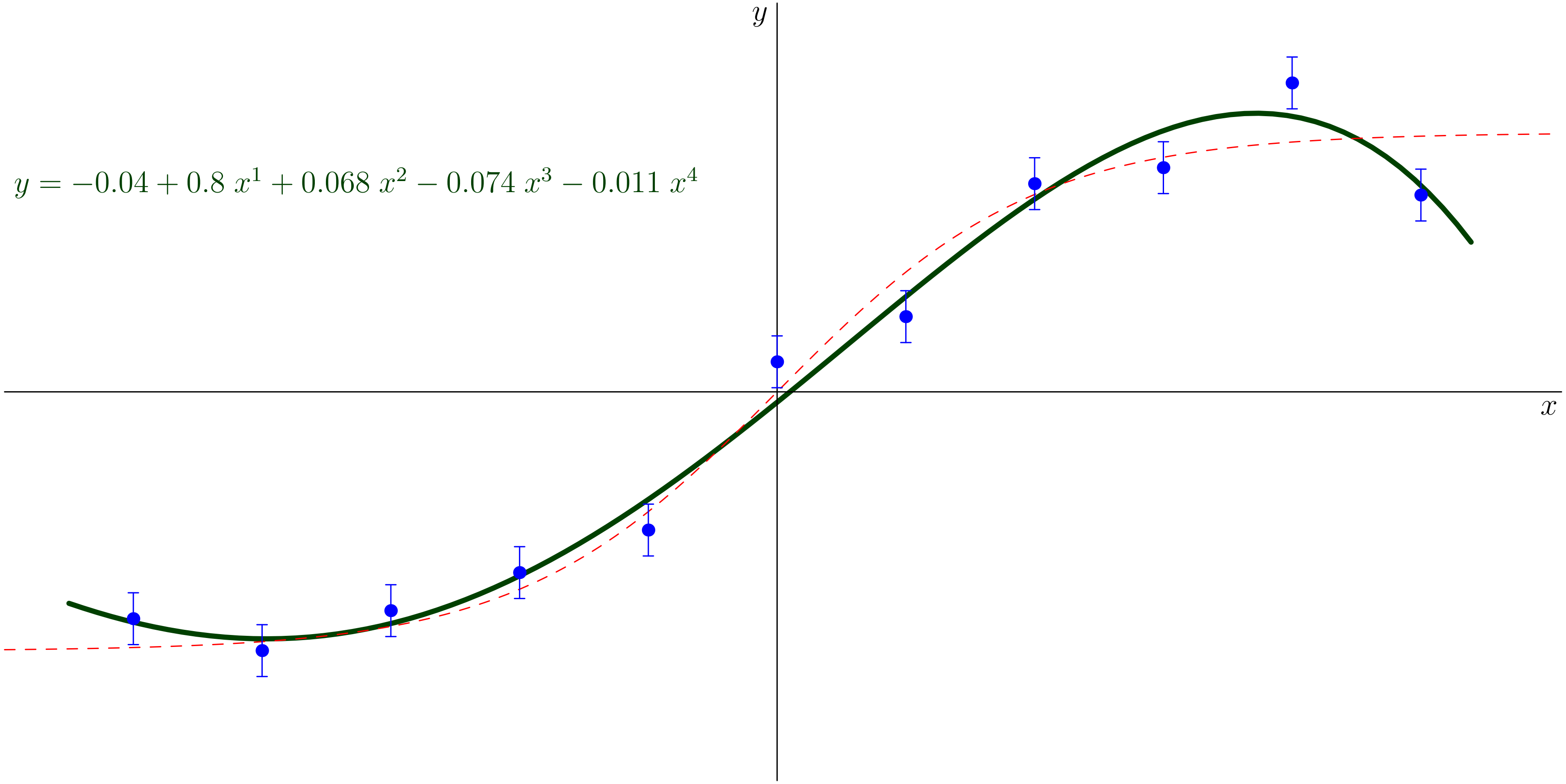

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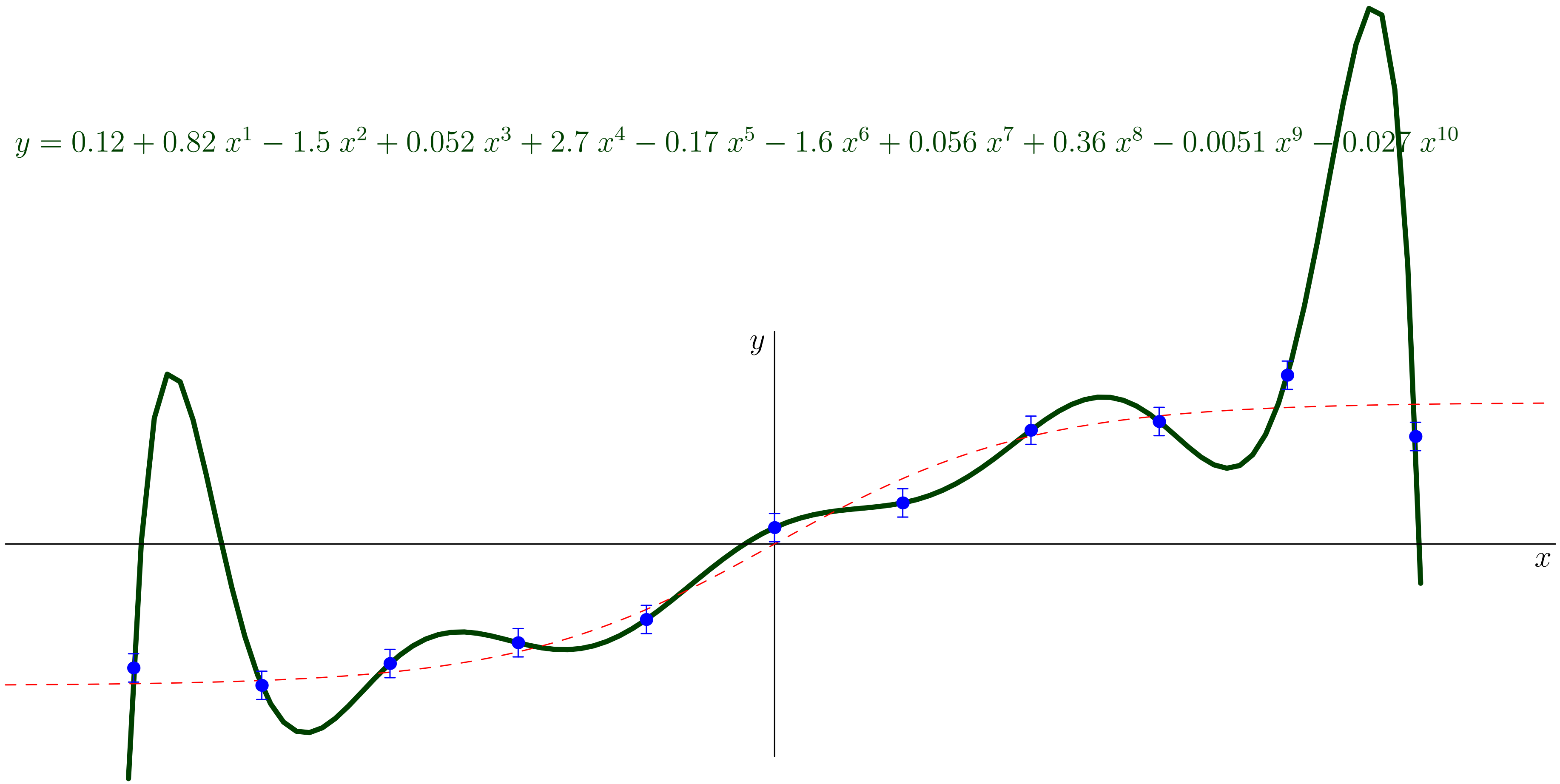
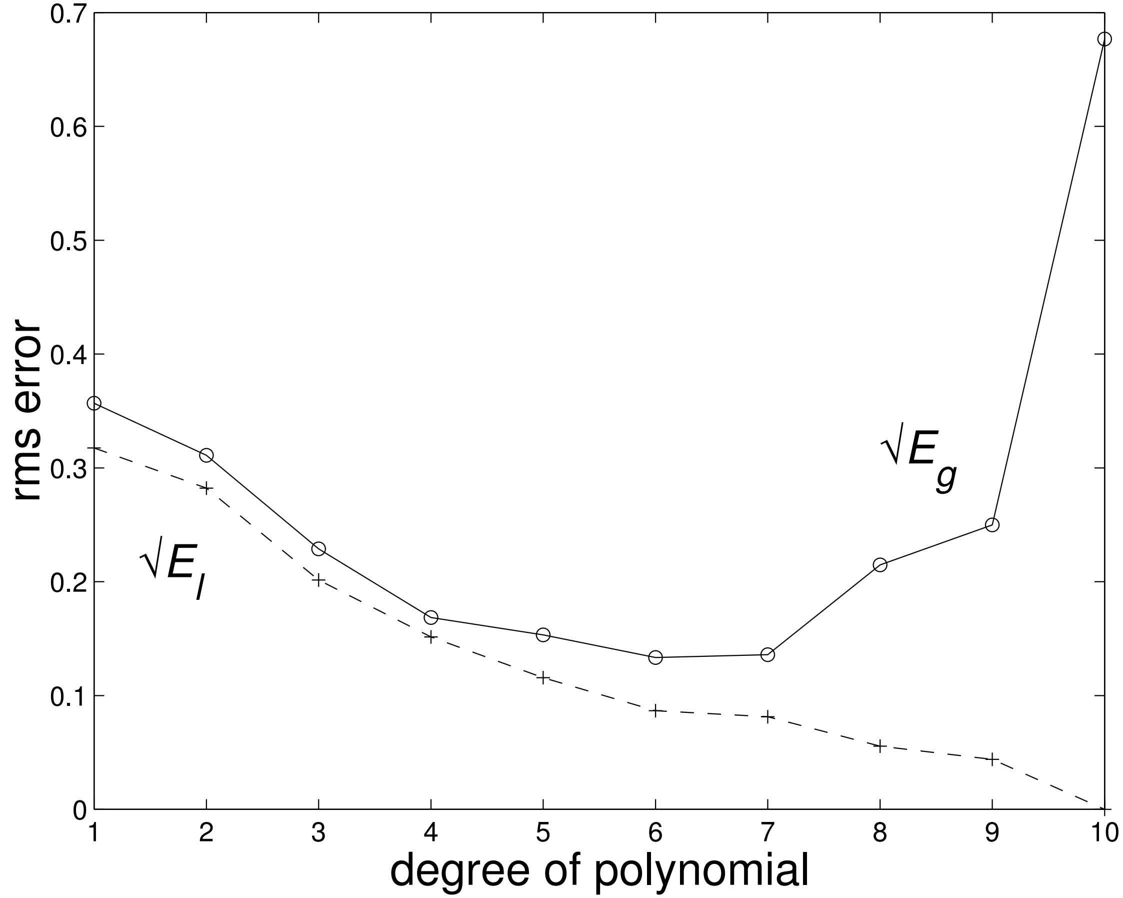


Measuring Generalisation Error for Regression

- 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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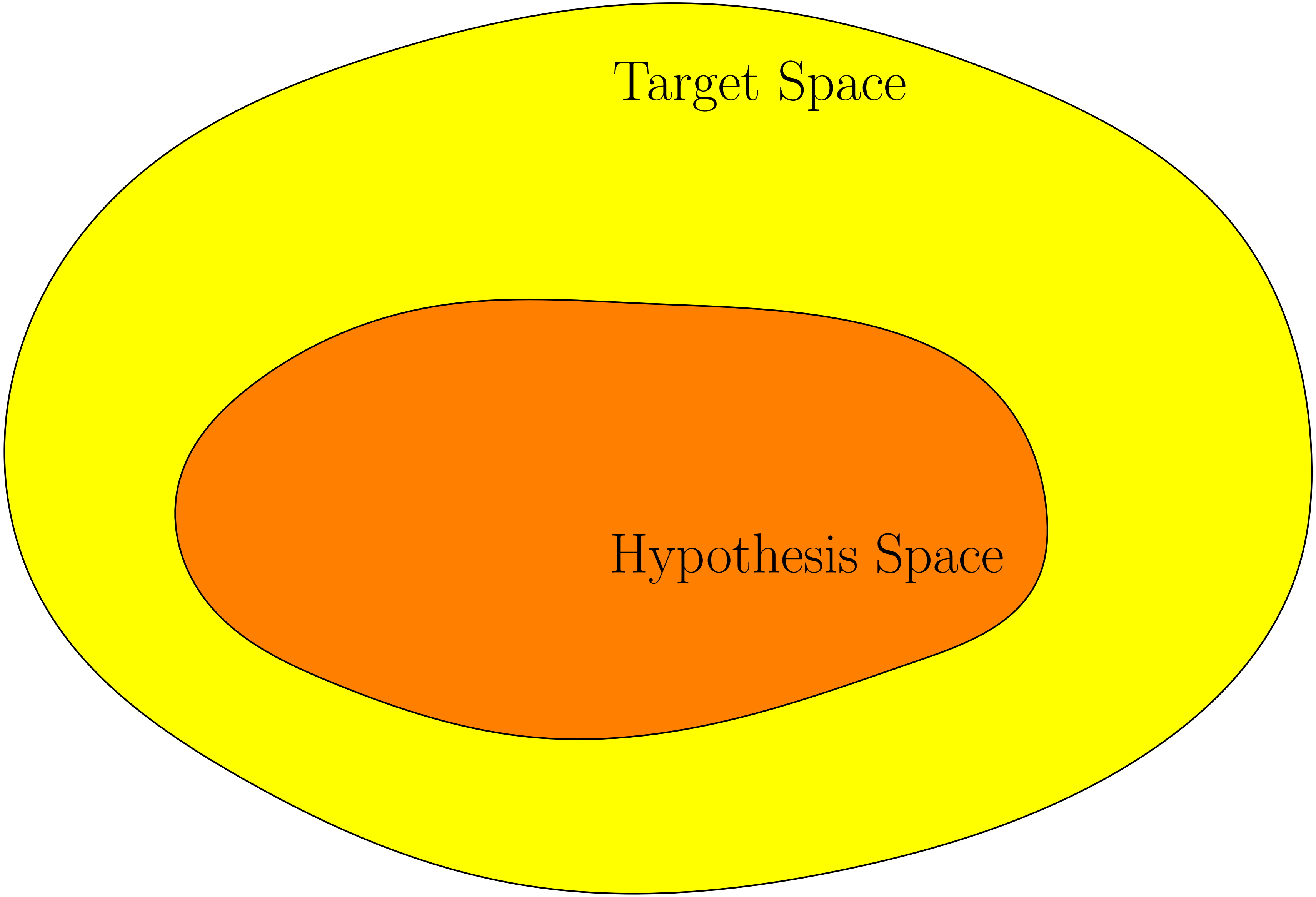

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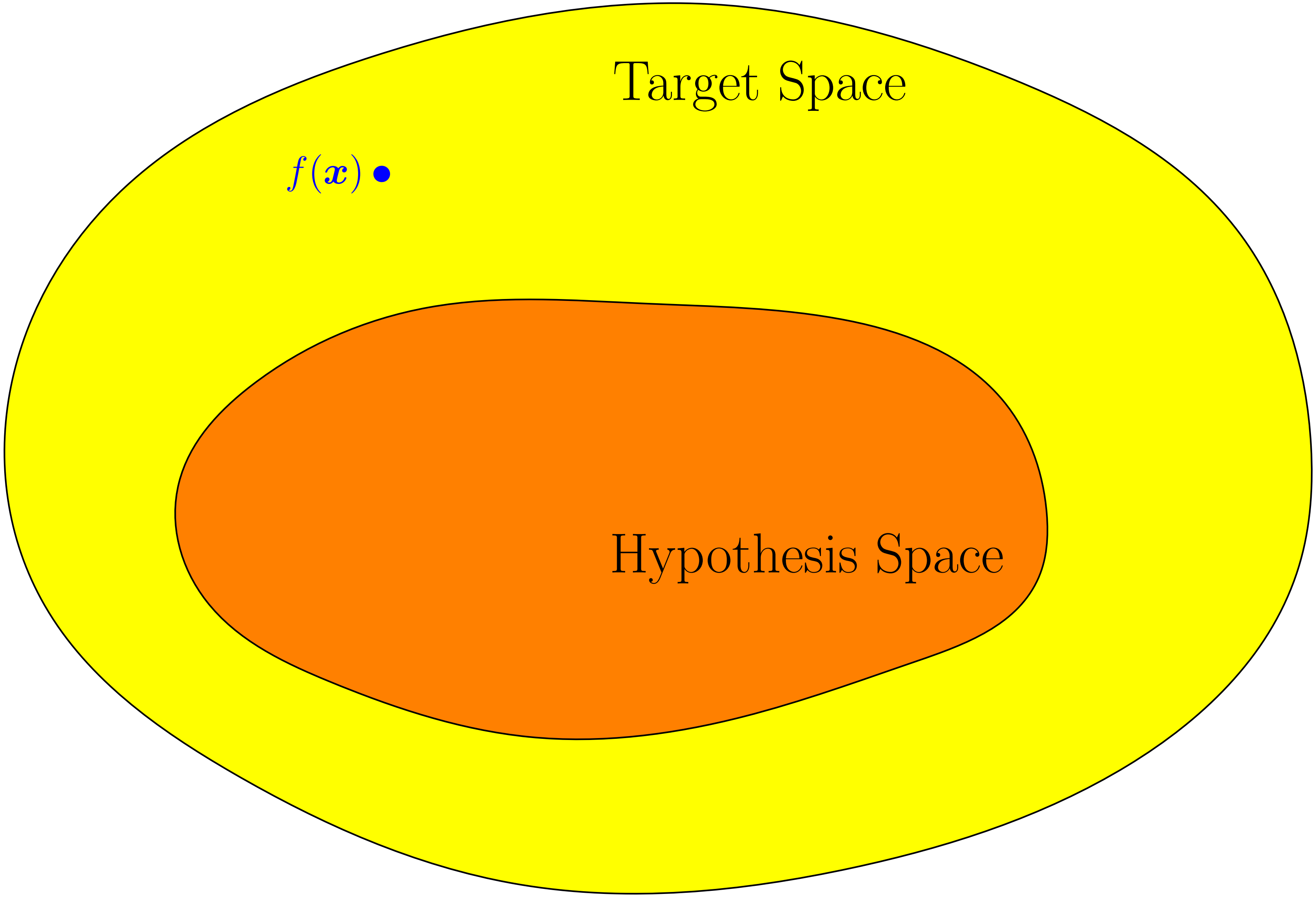

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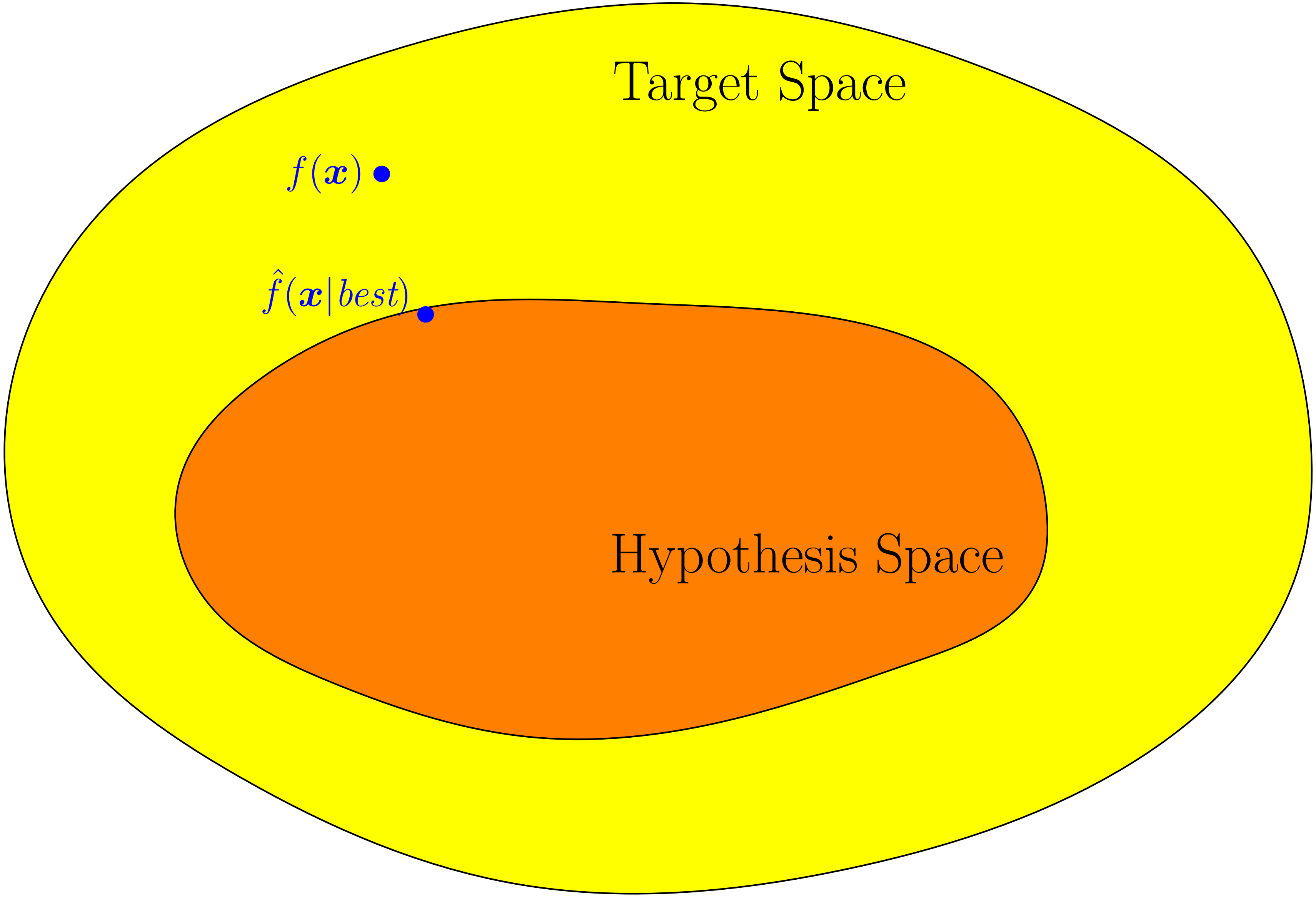

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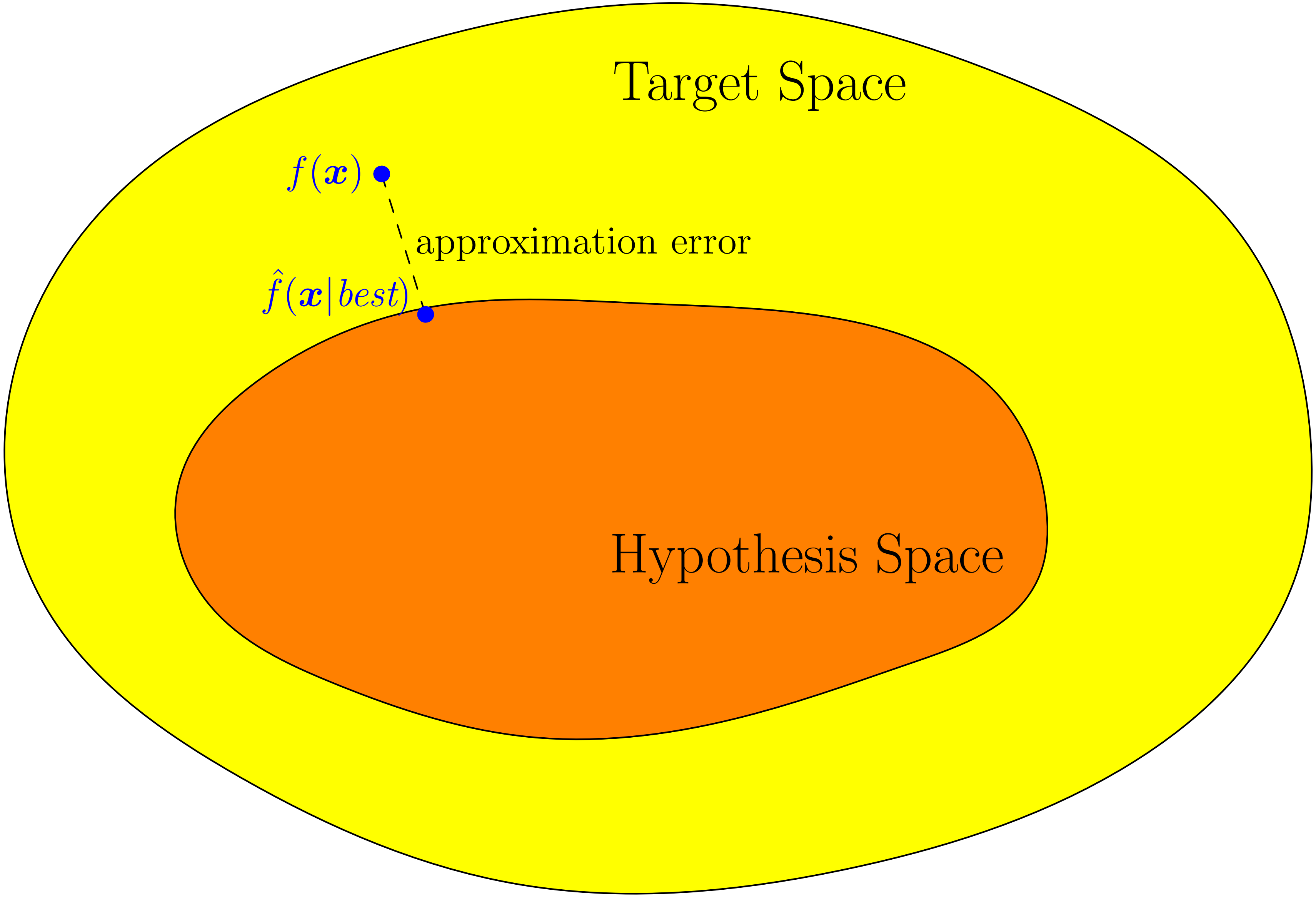

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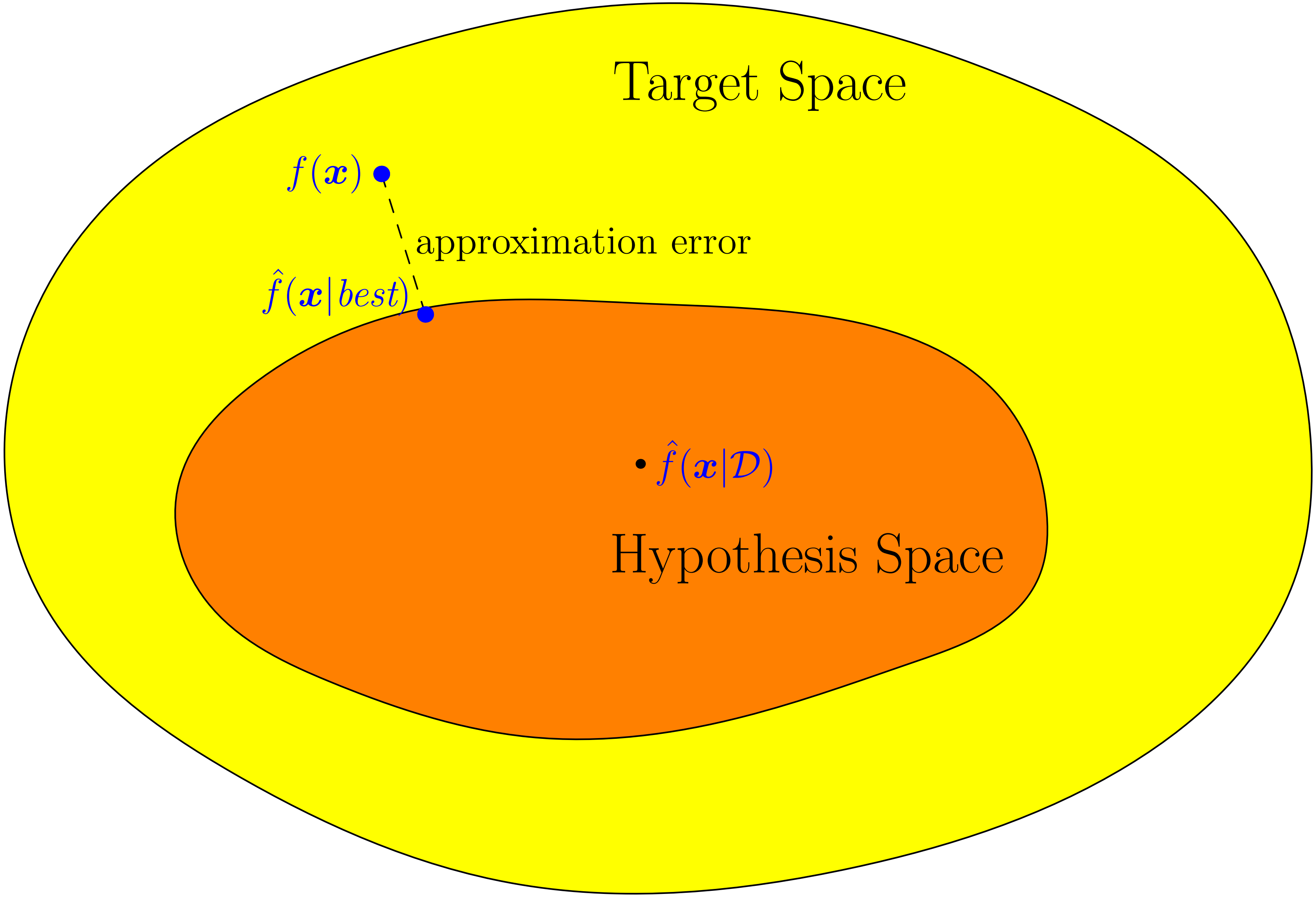

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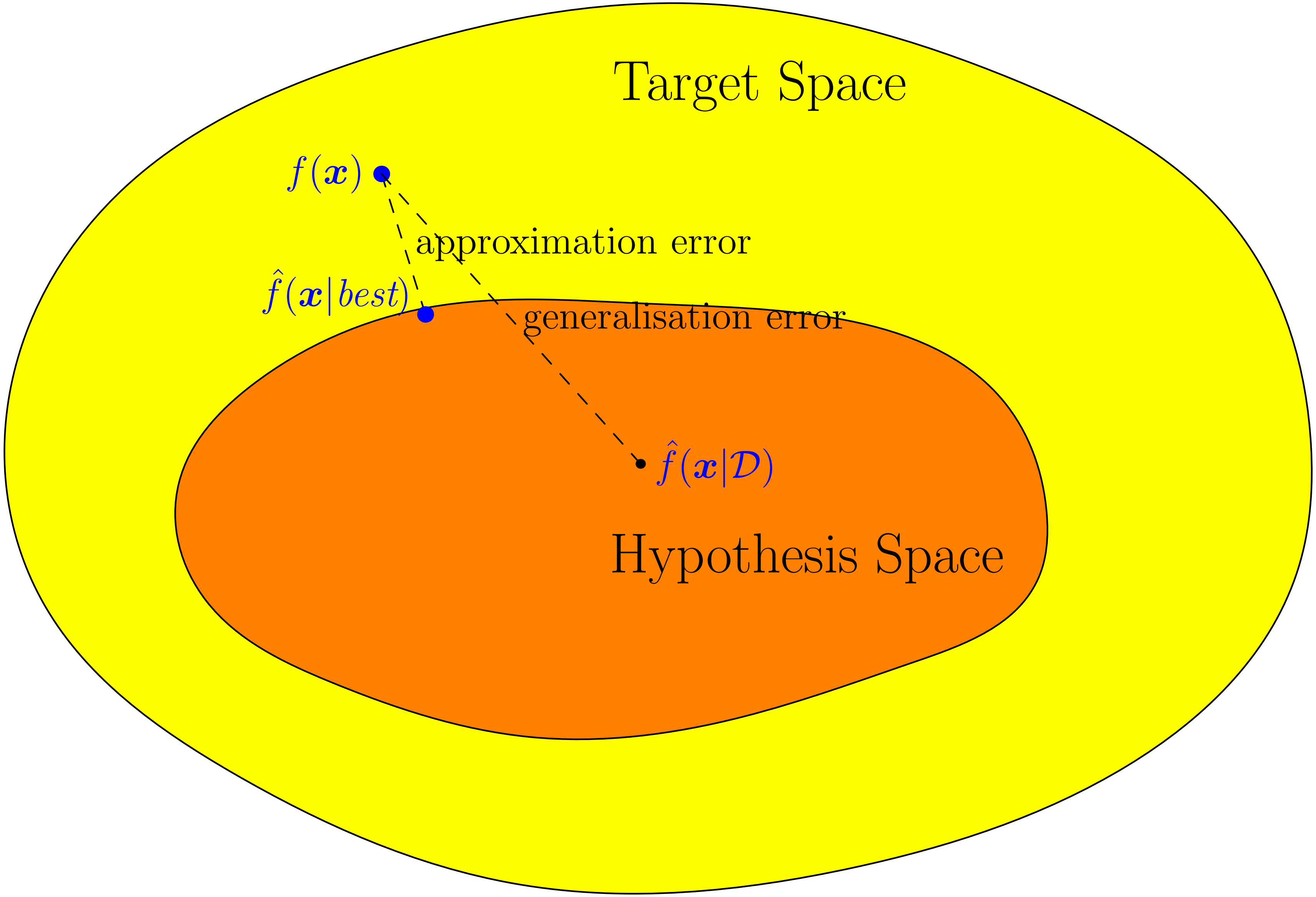

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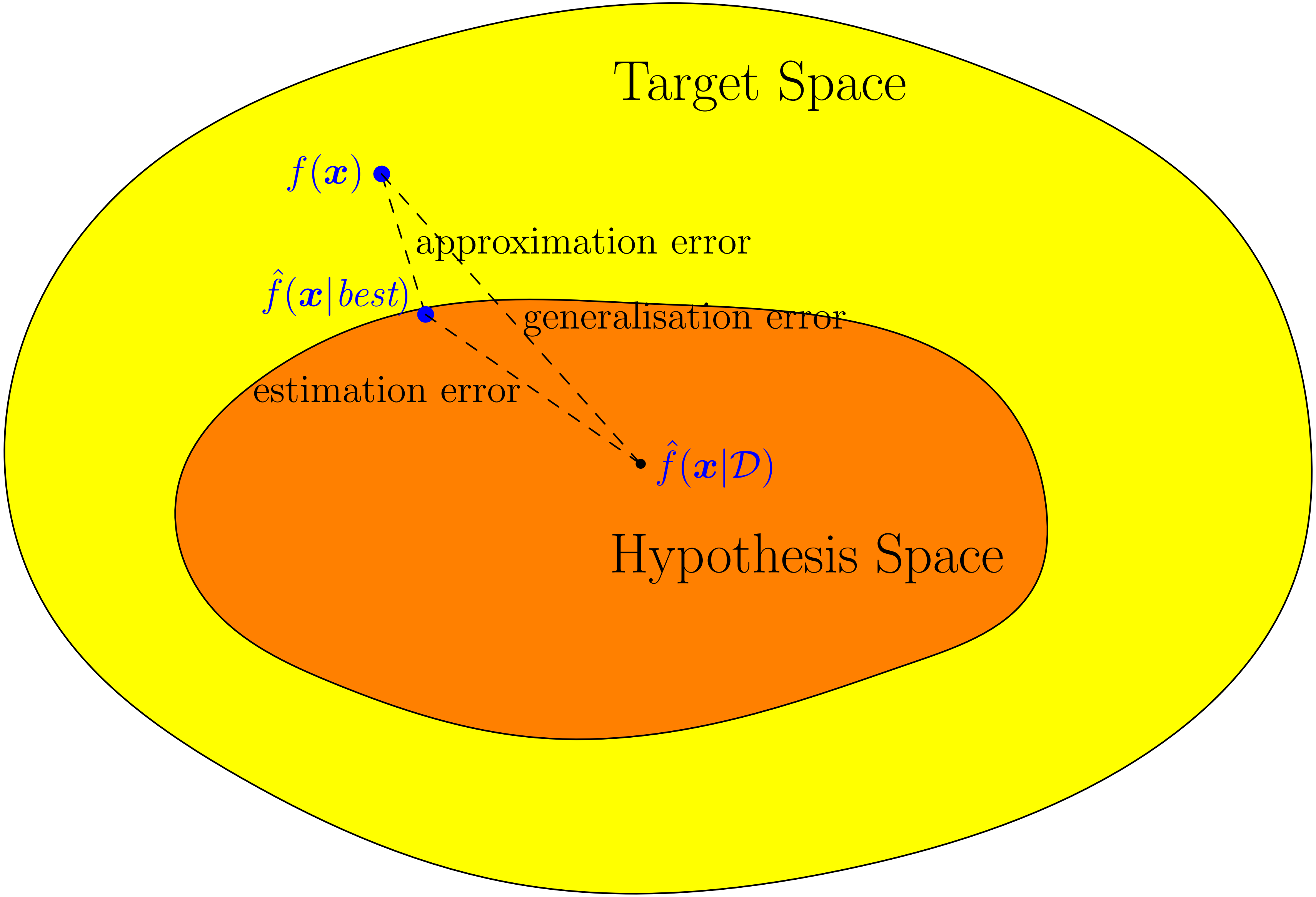

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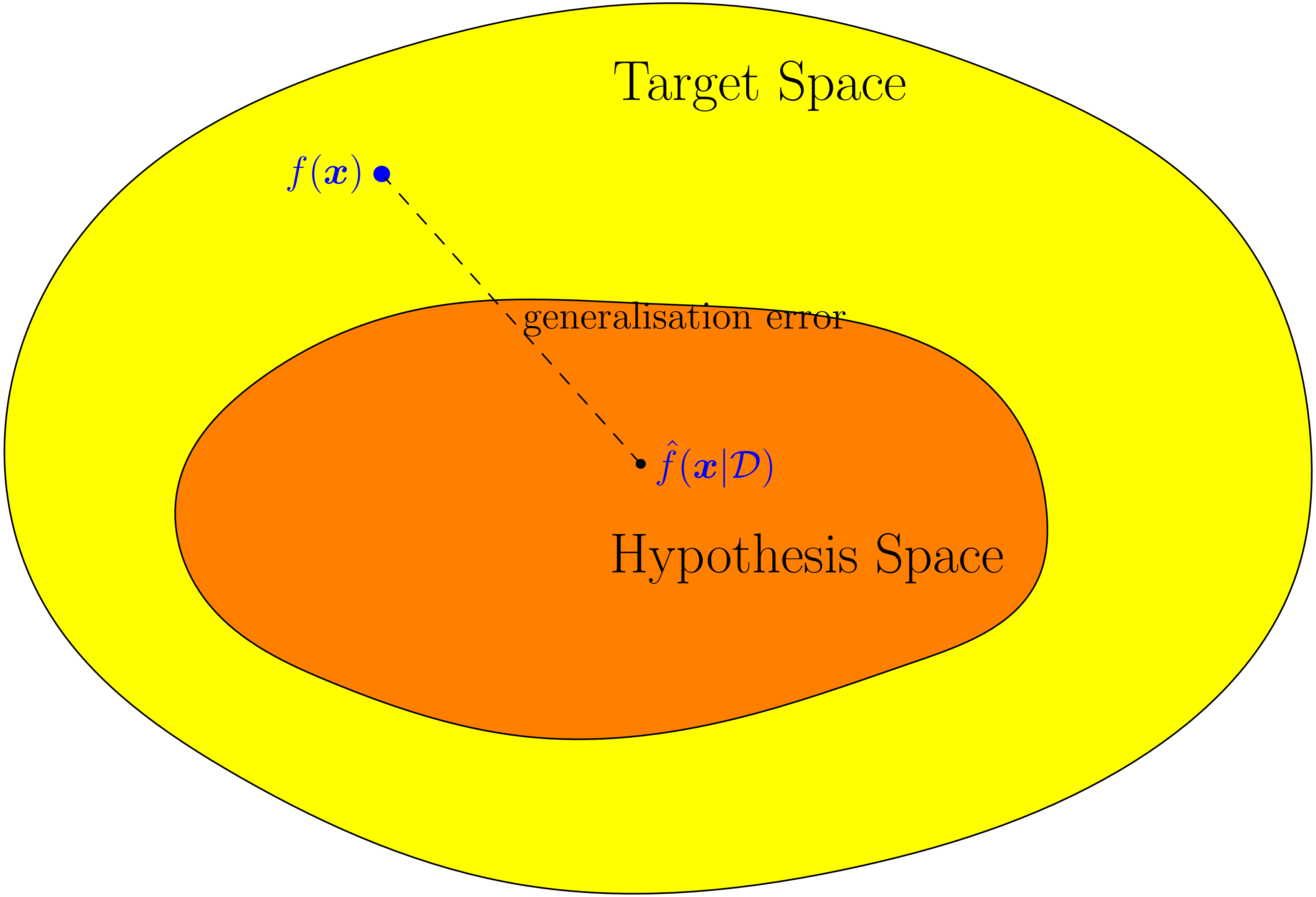

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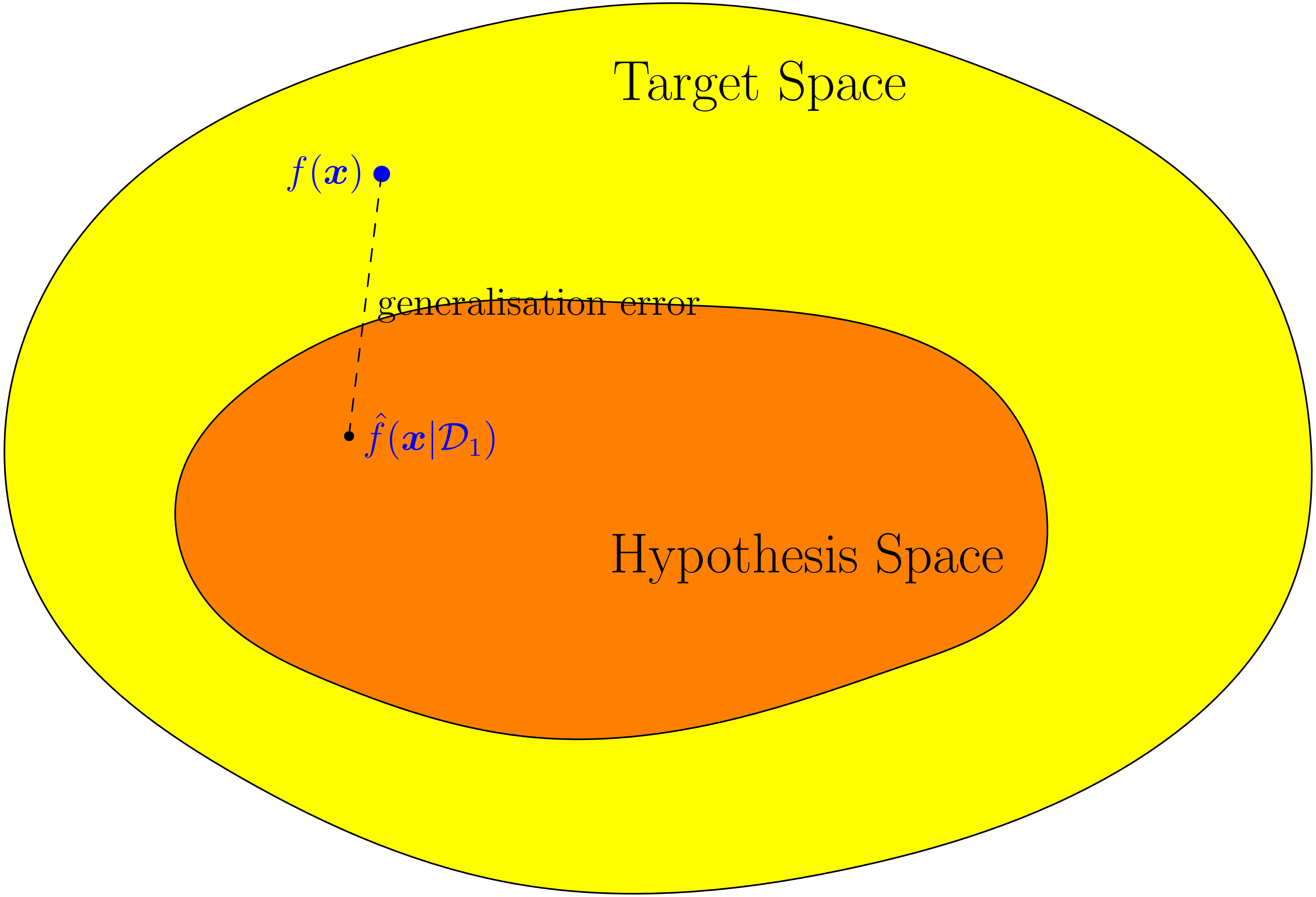

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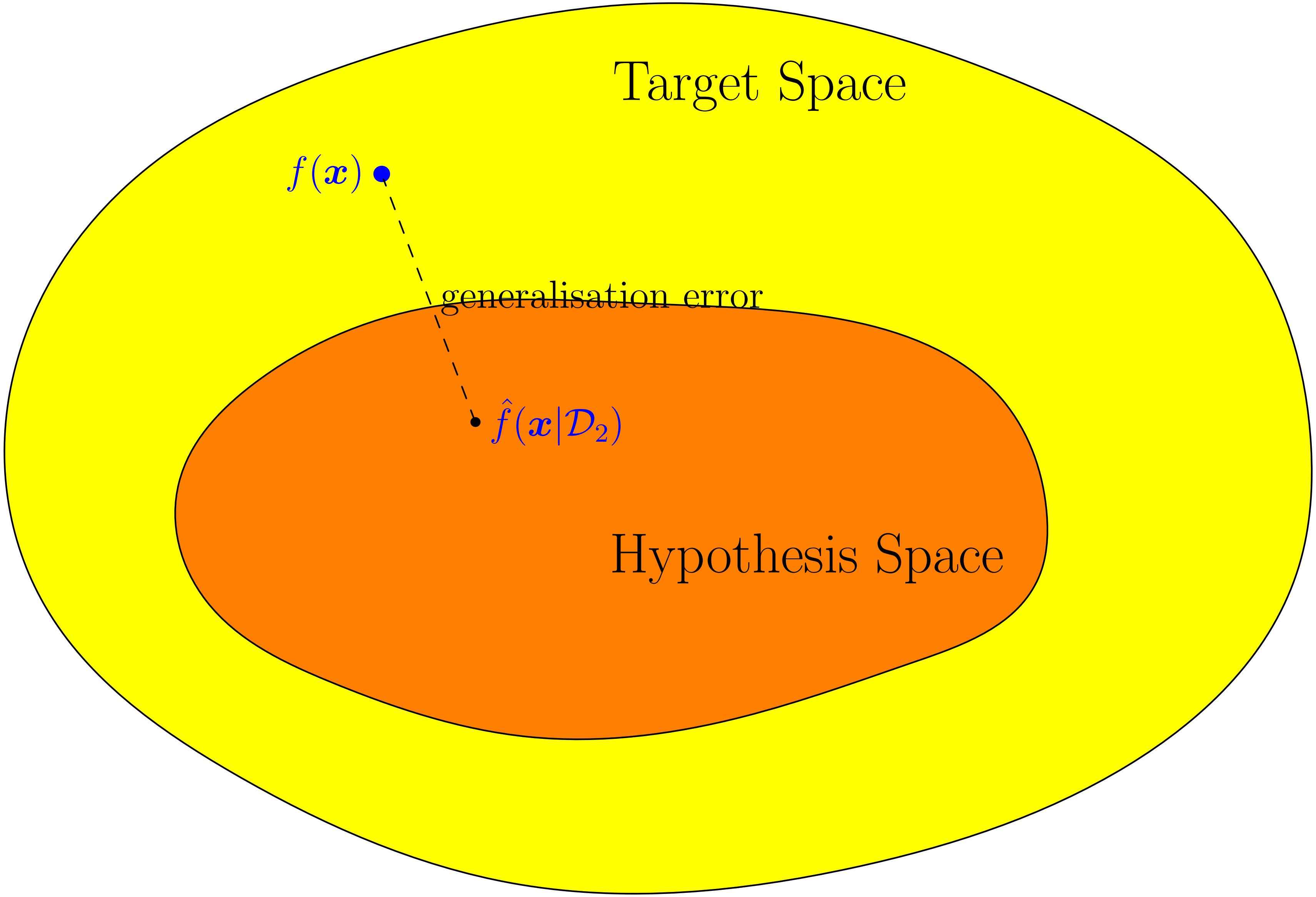

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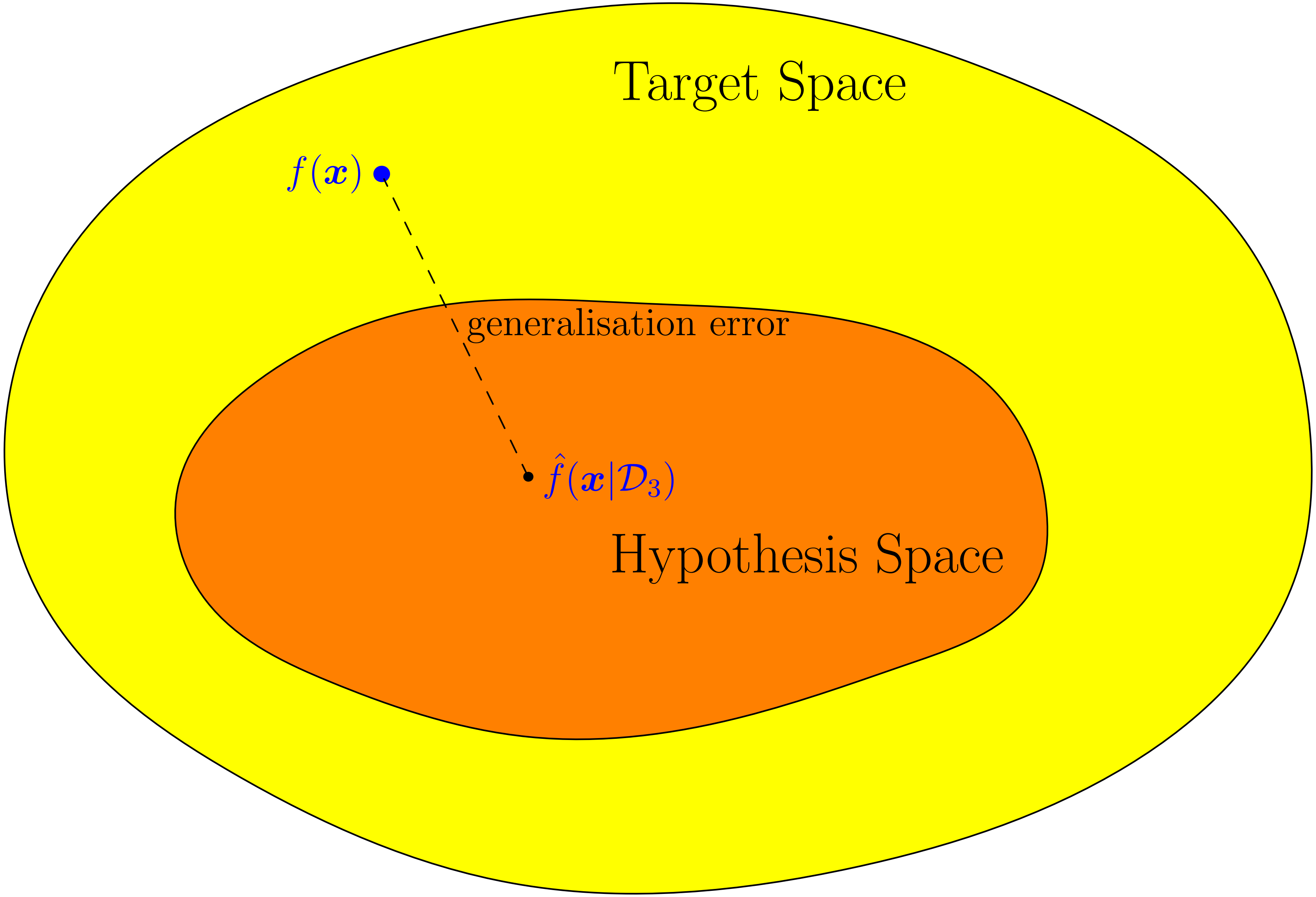

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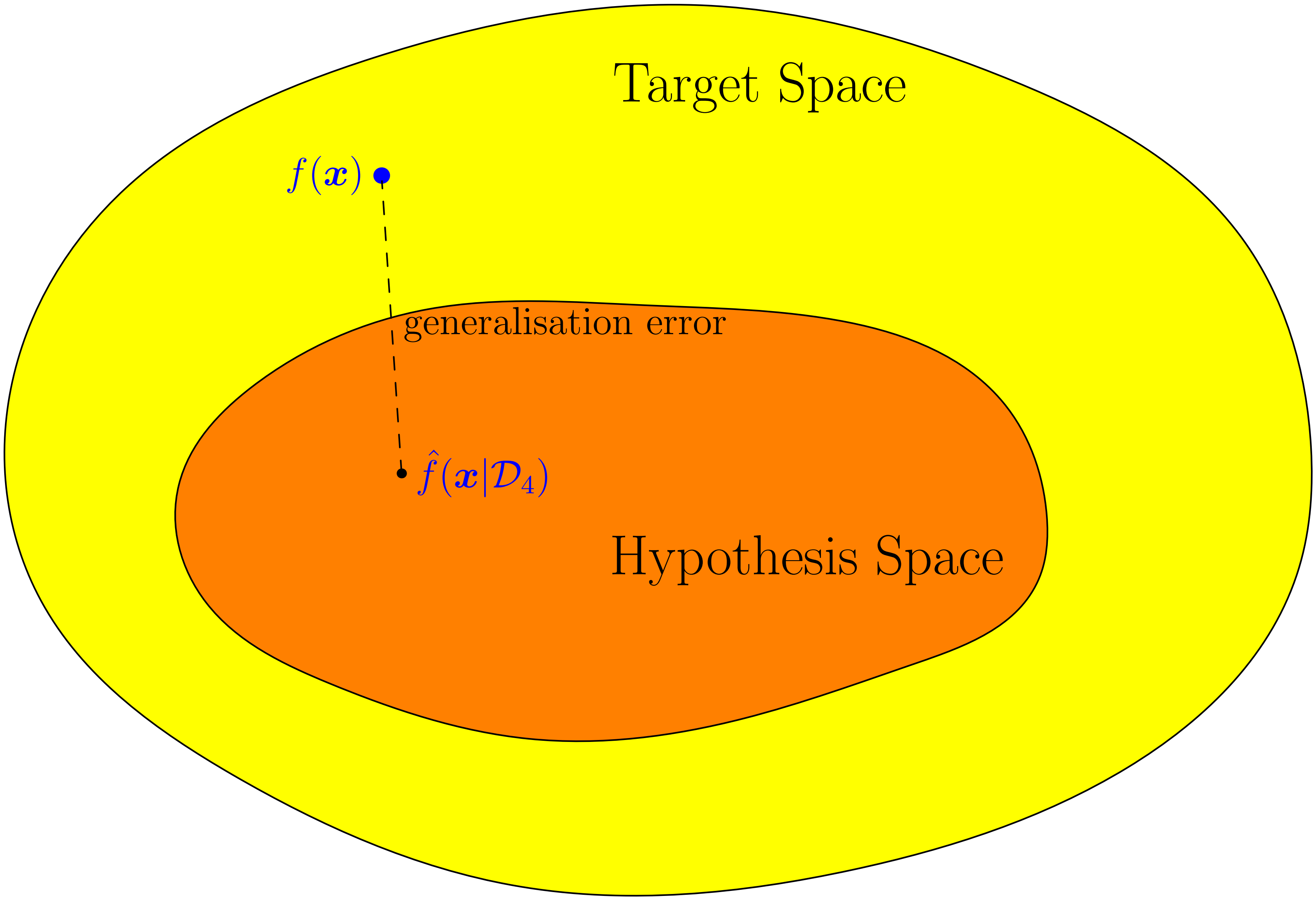

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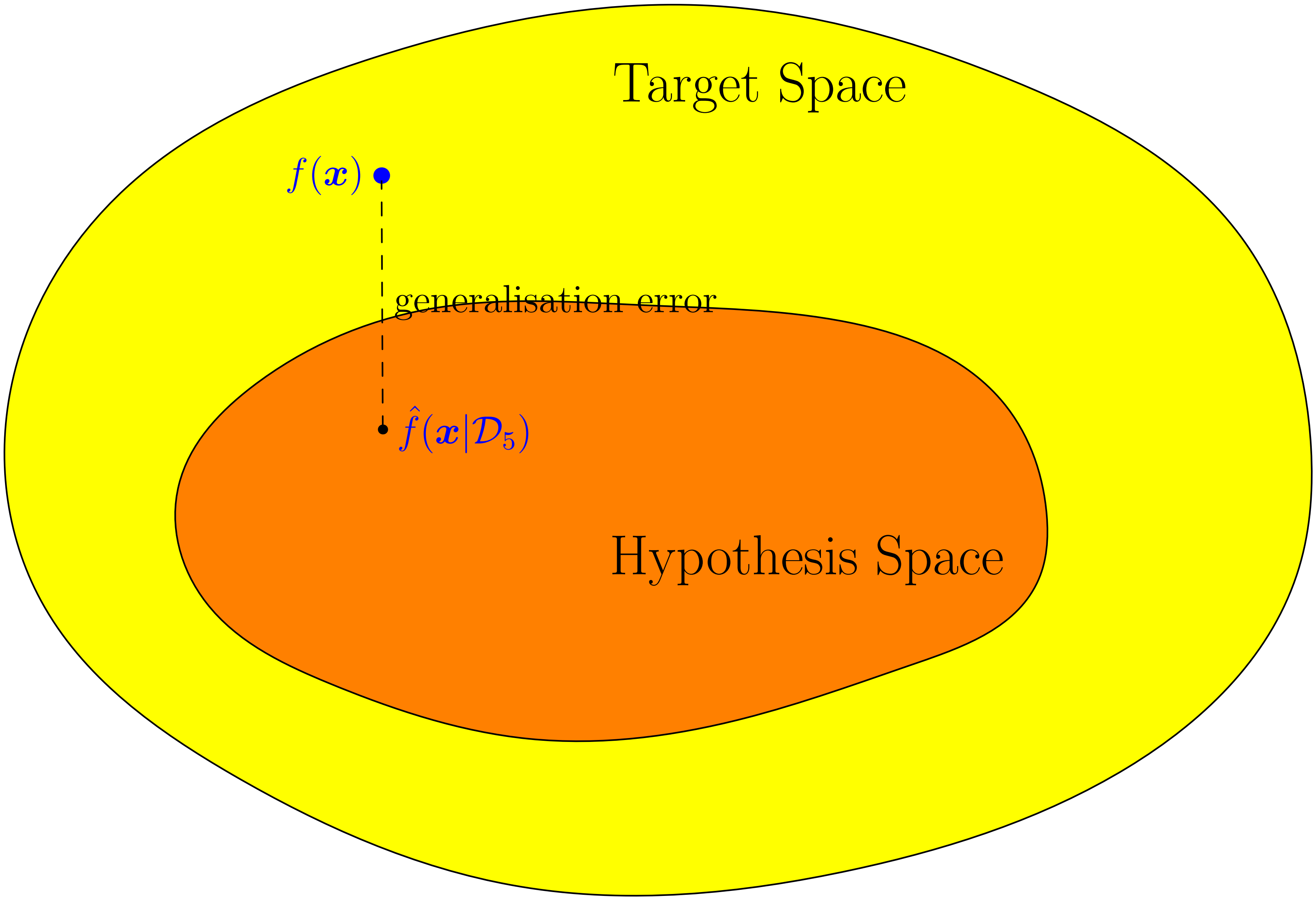

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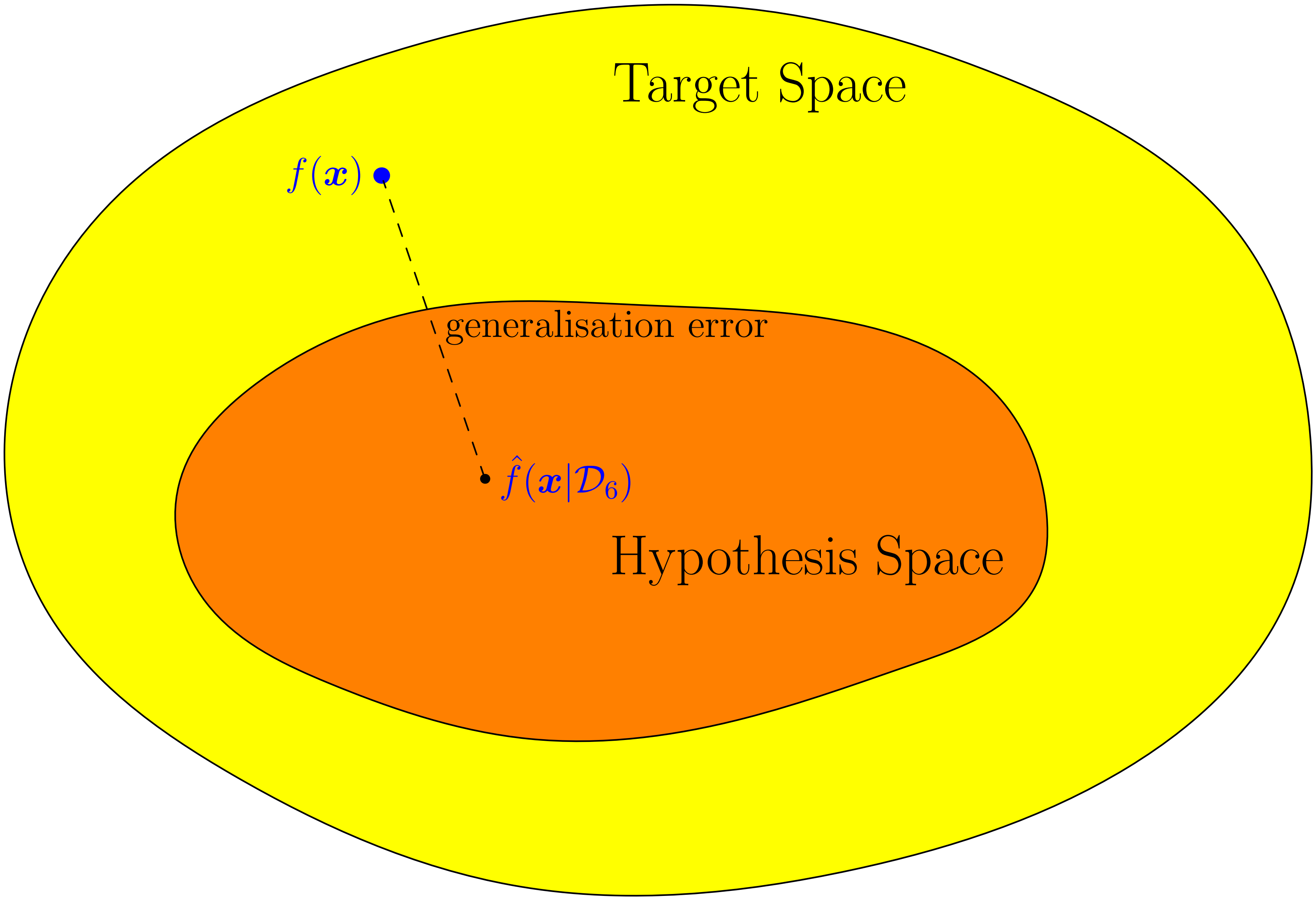

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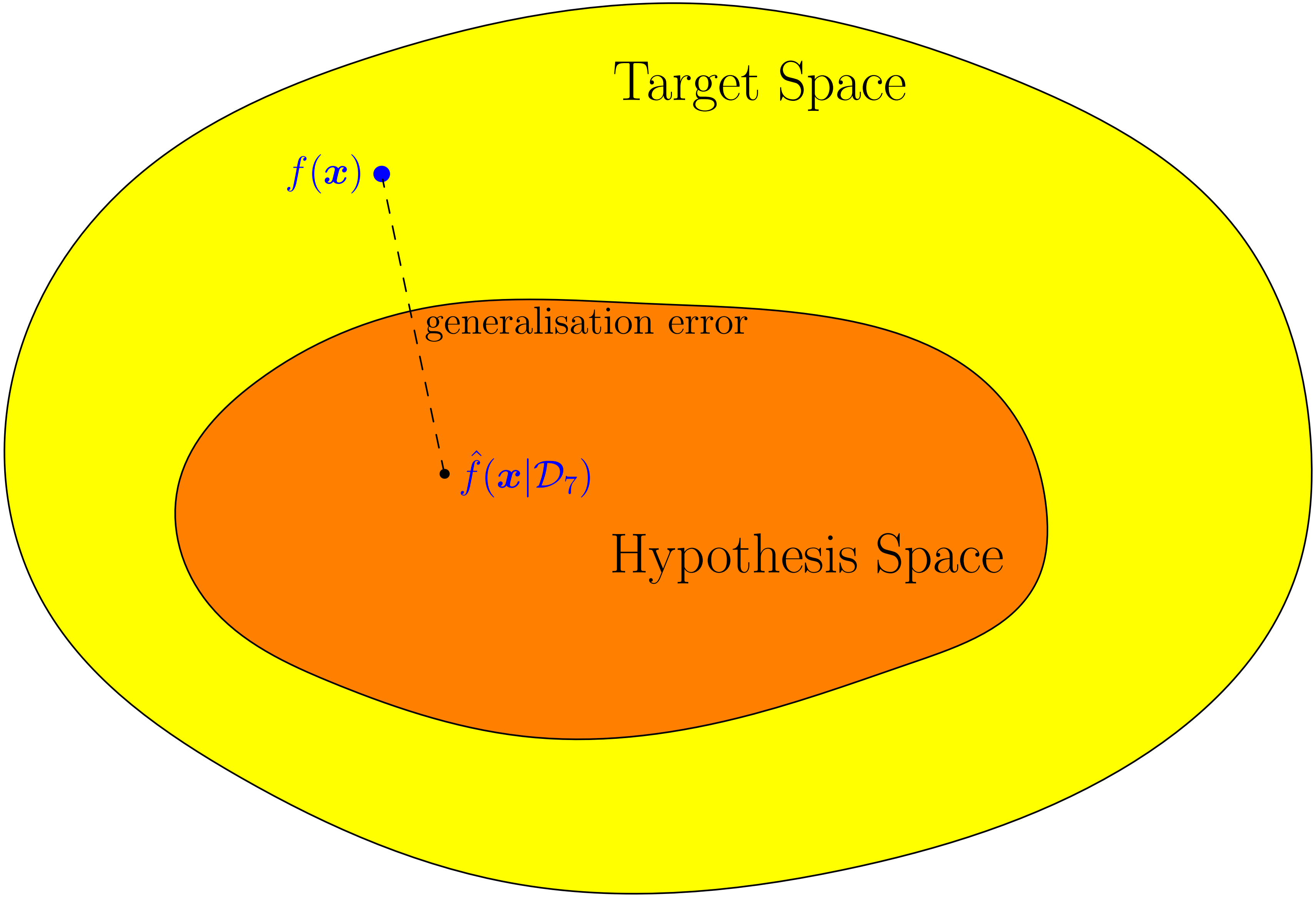

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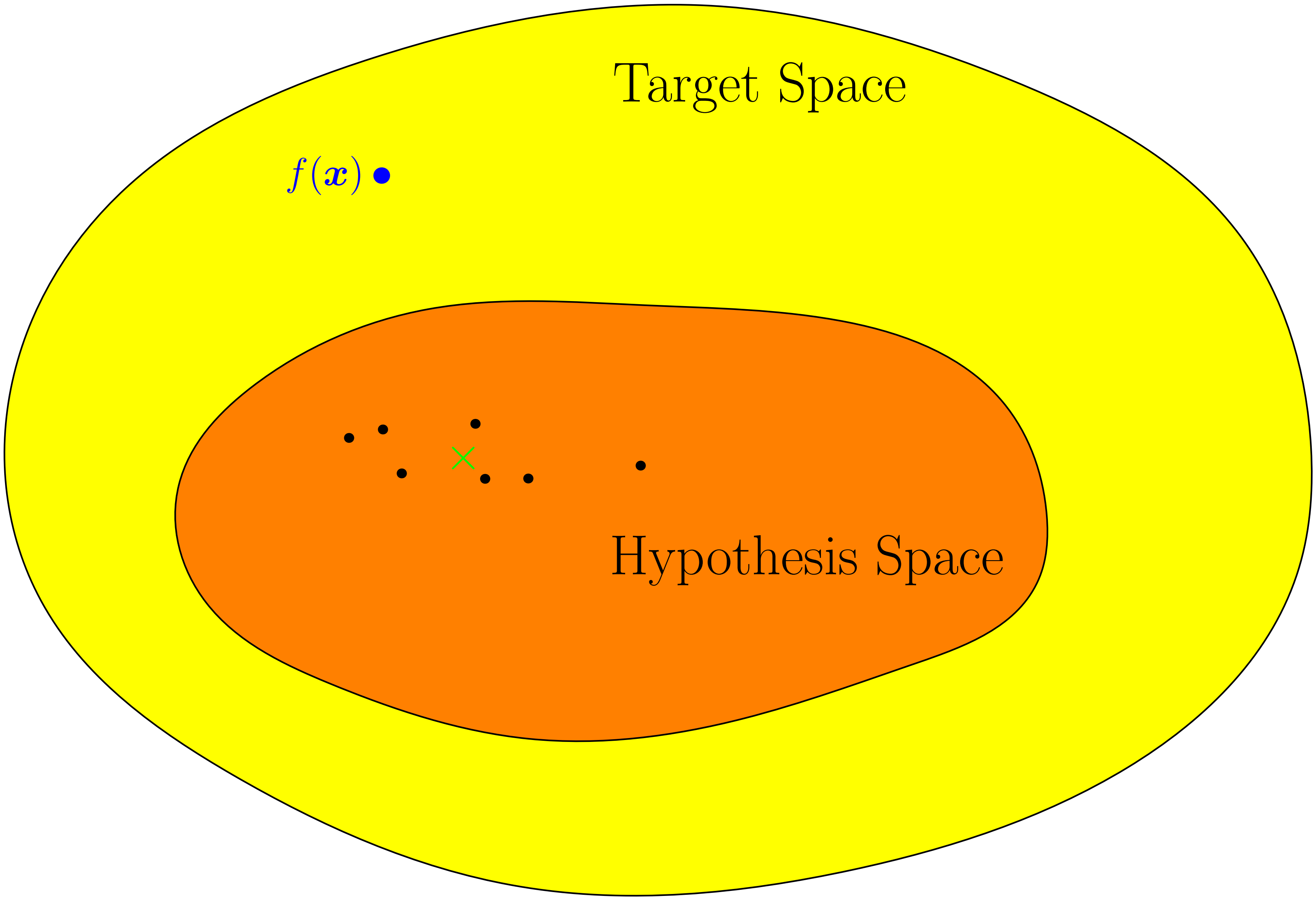

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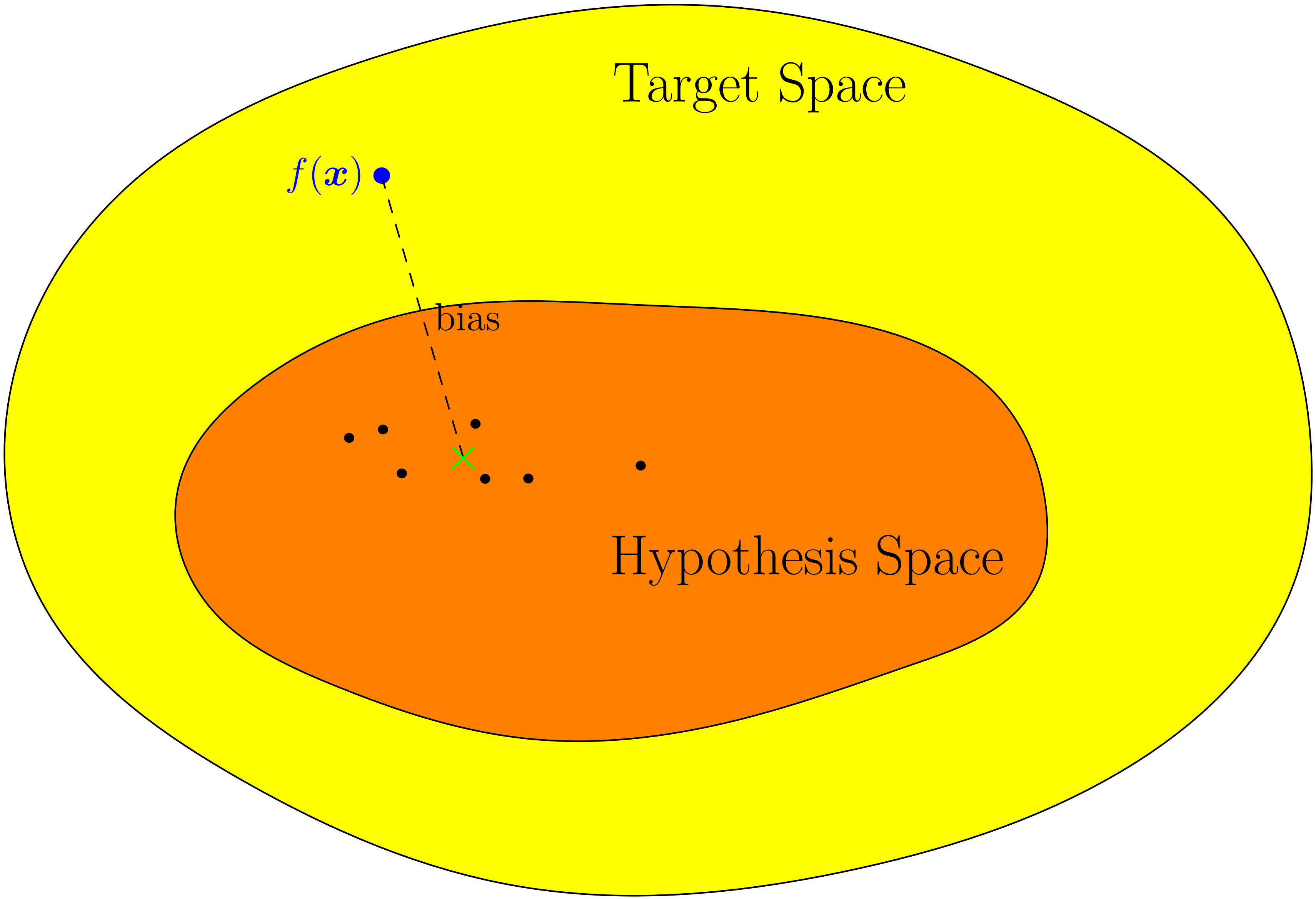

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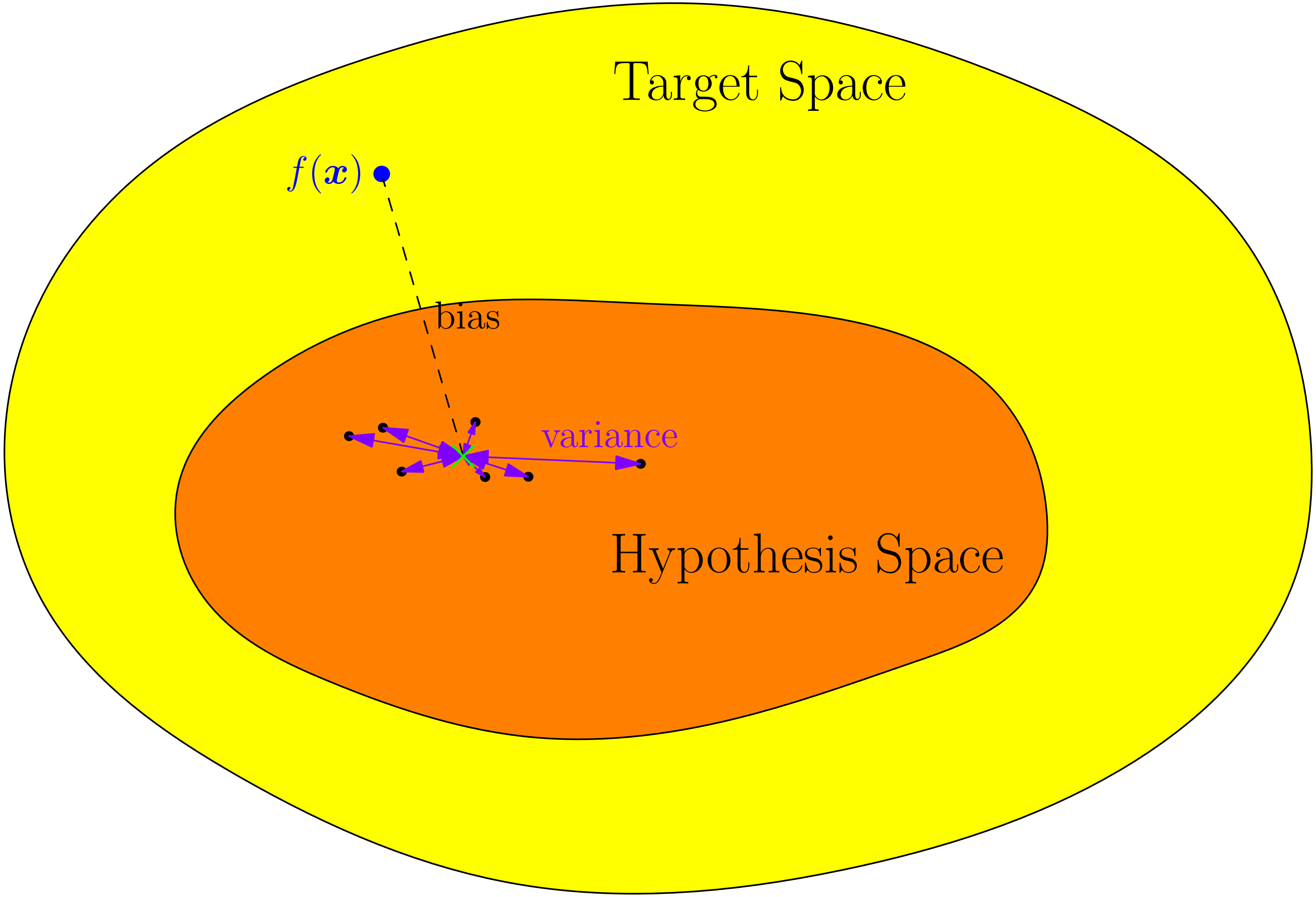

Mean Machine

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

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

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

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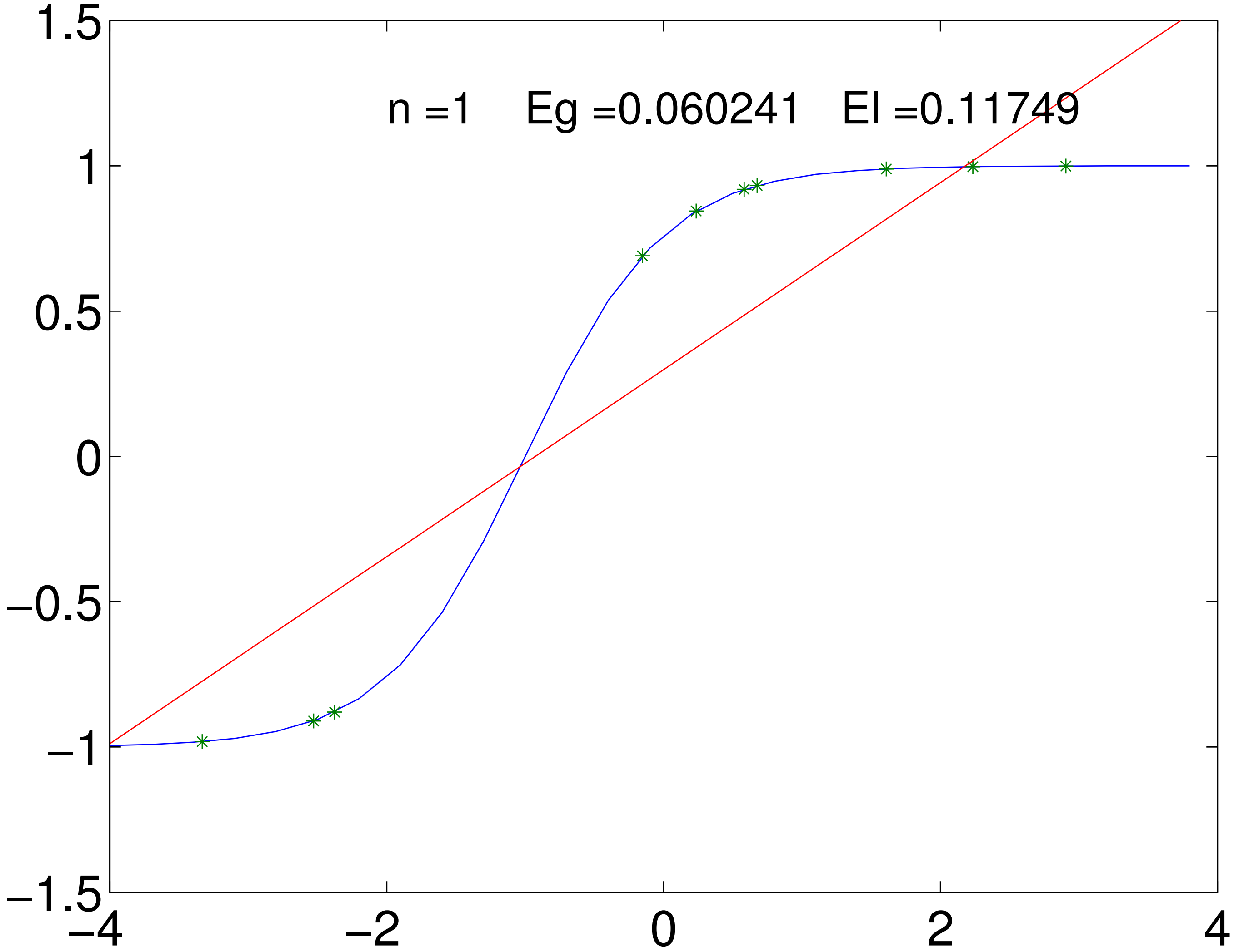

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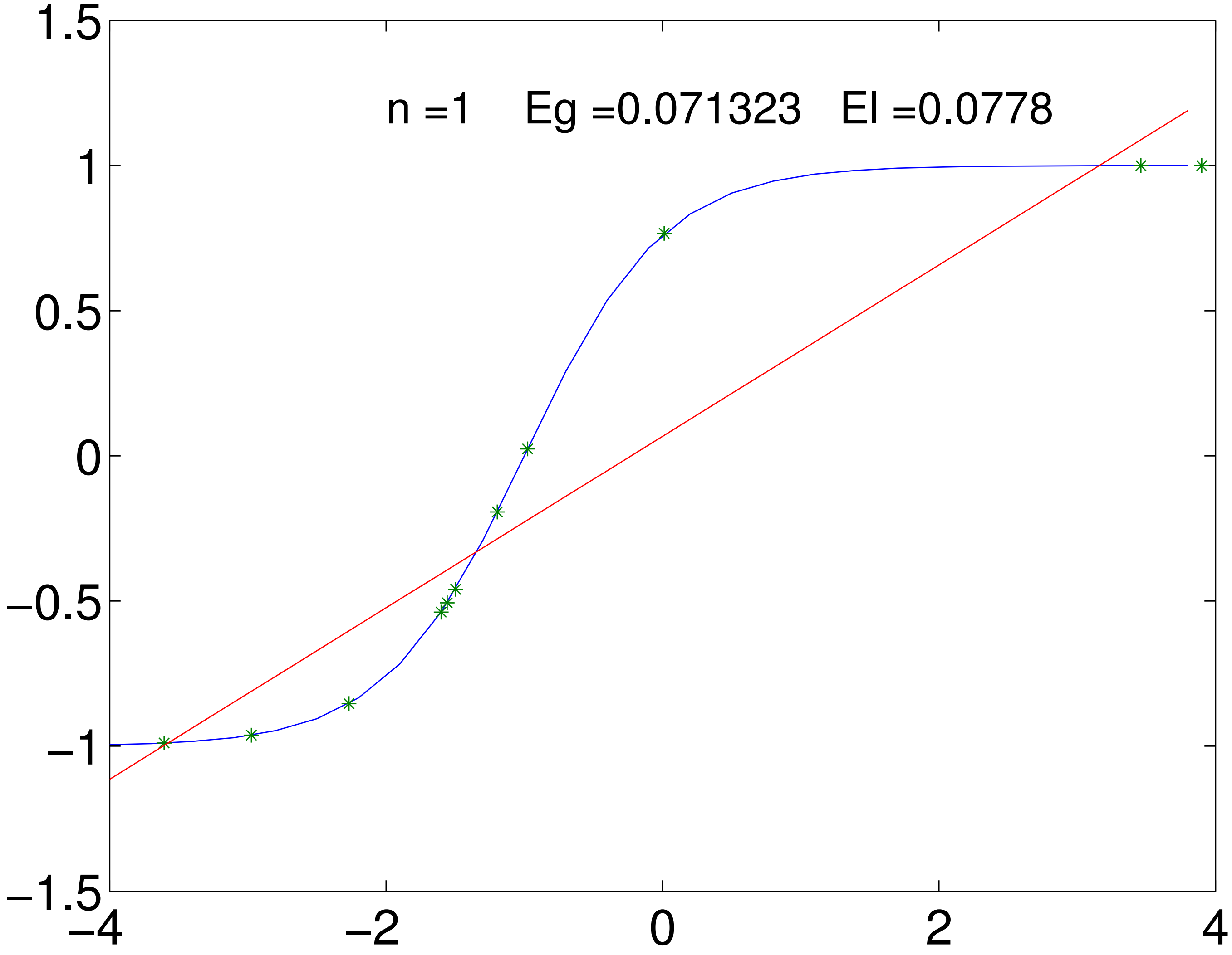

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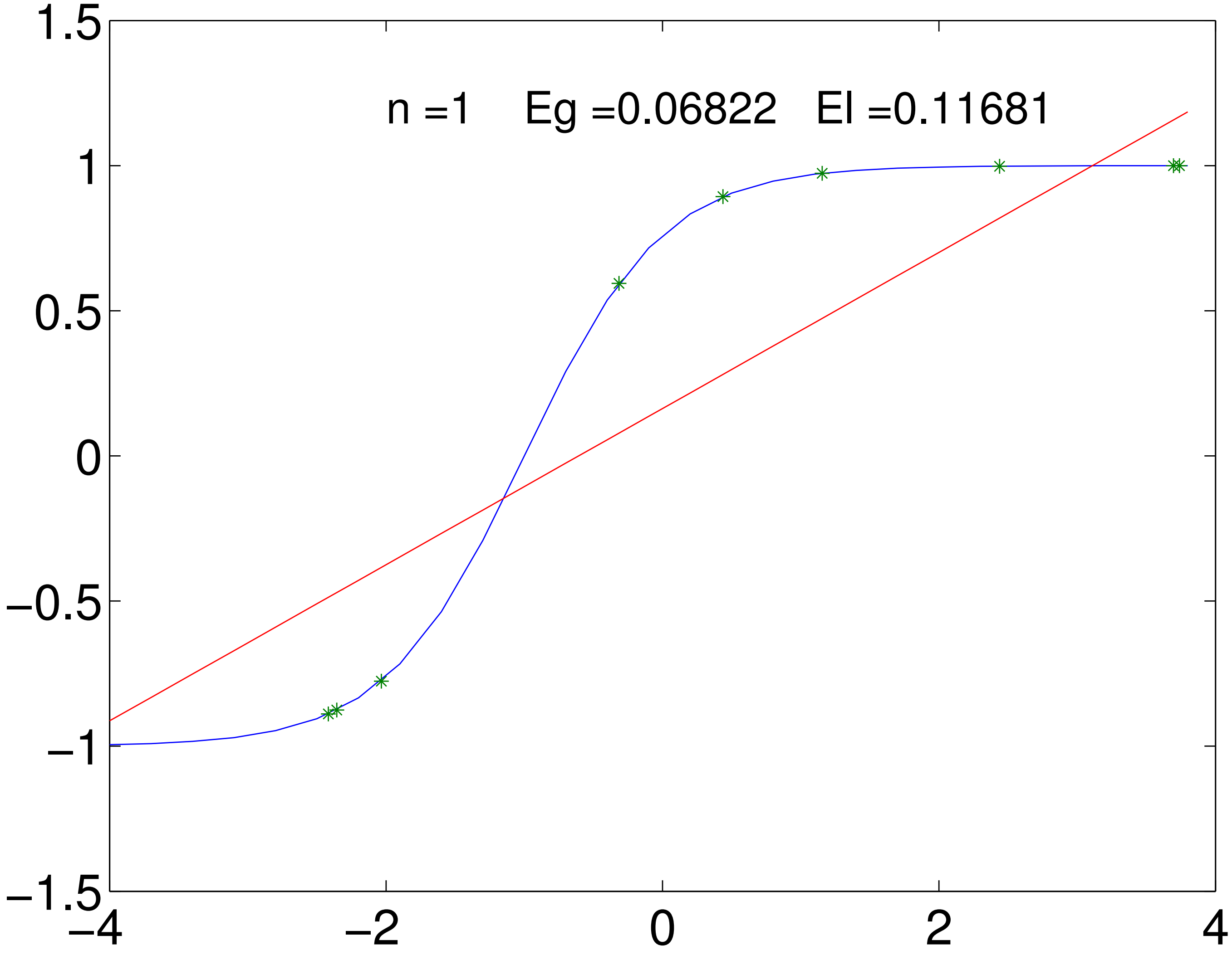

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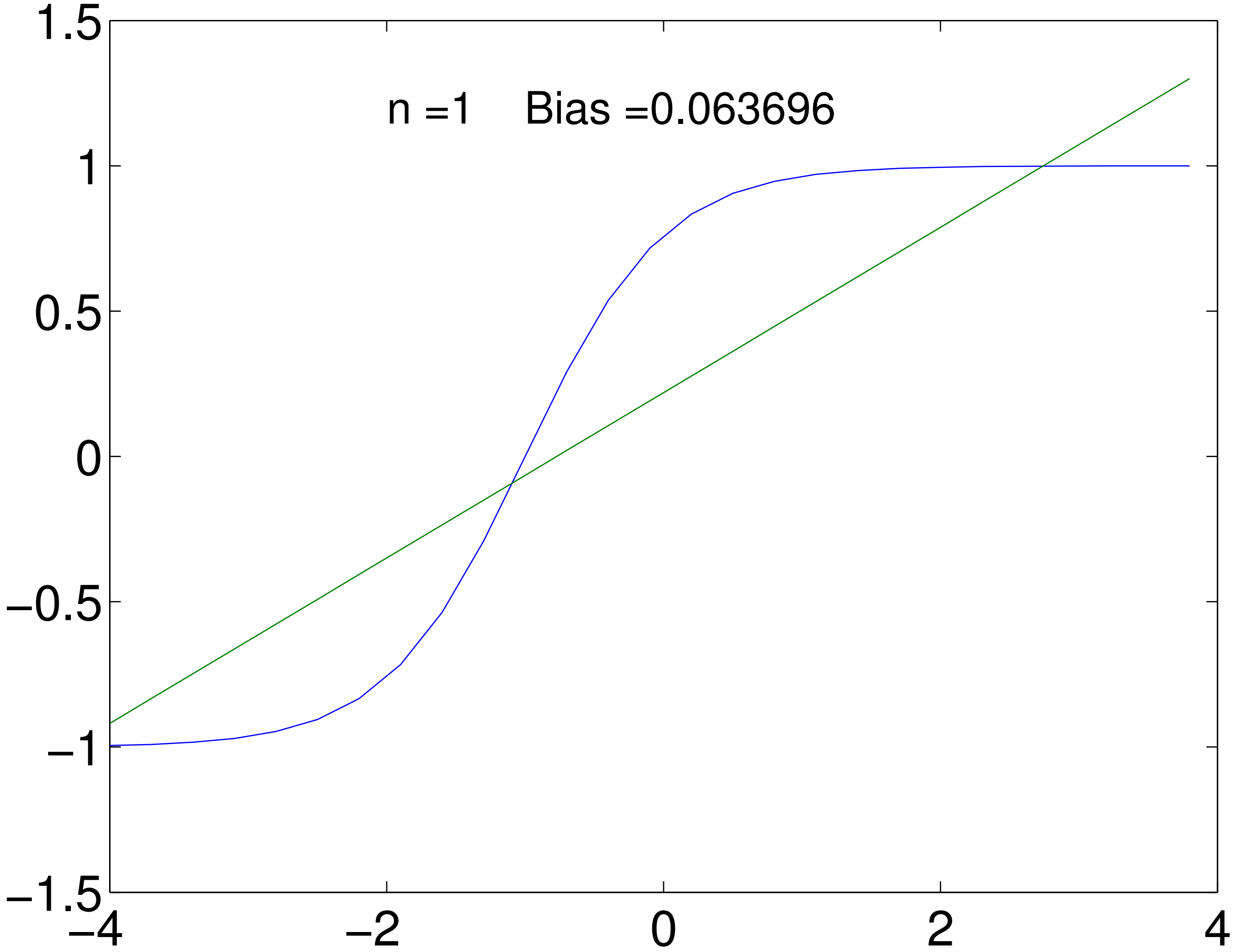

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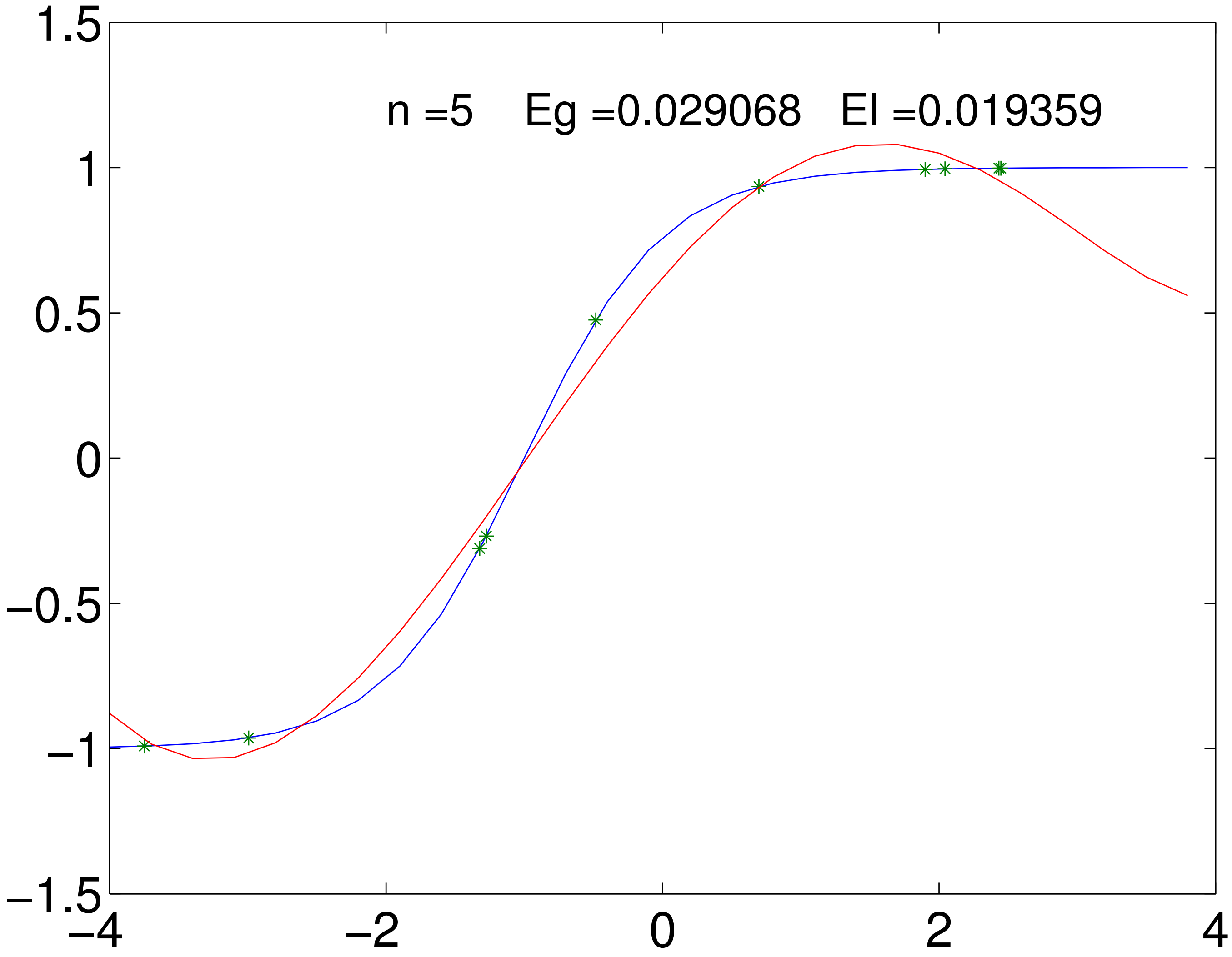

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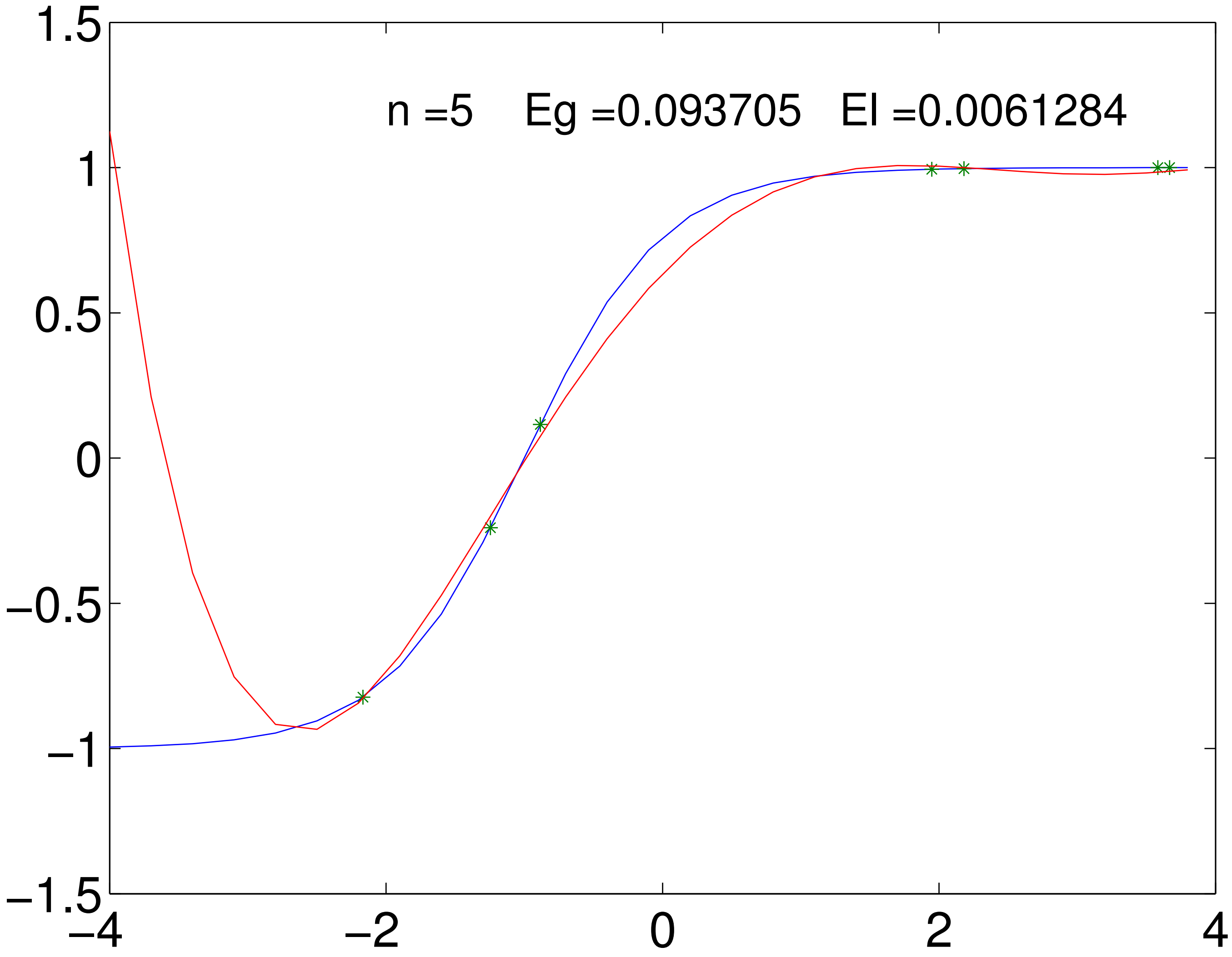

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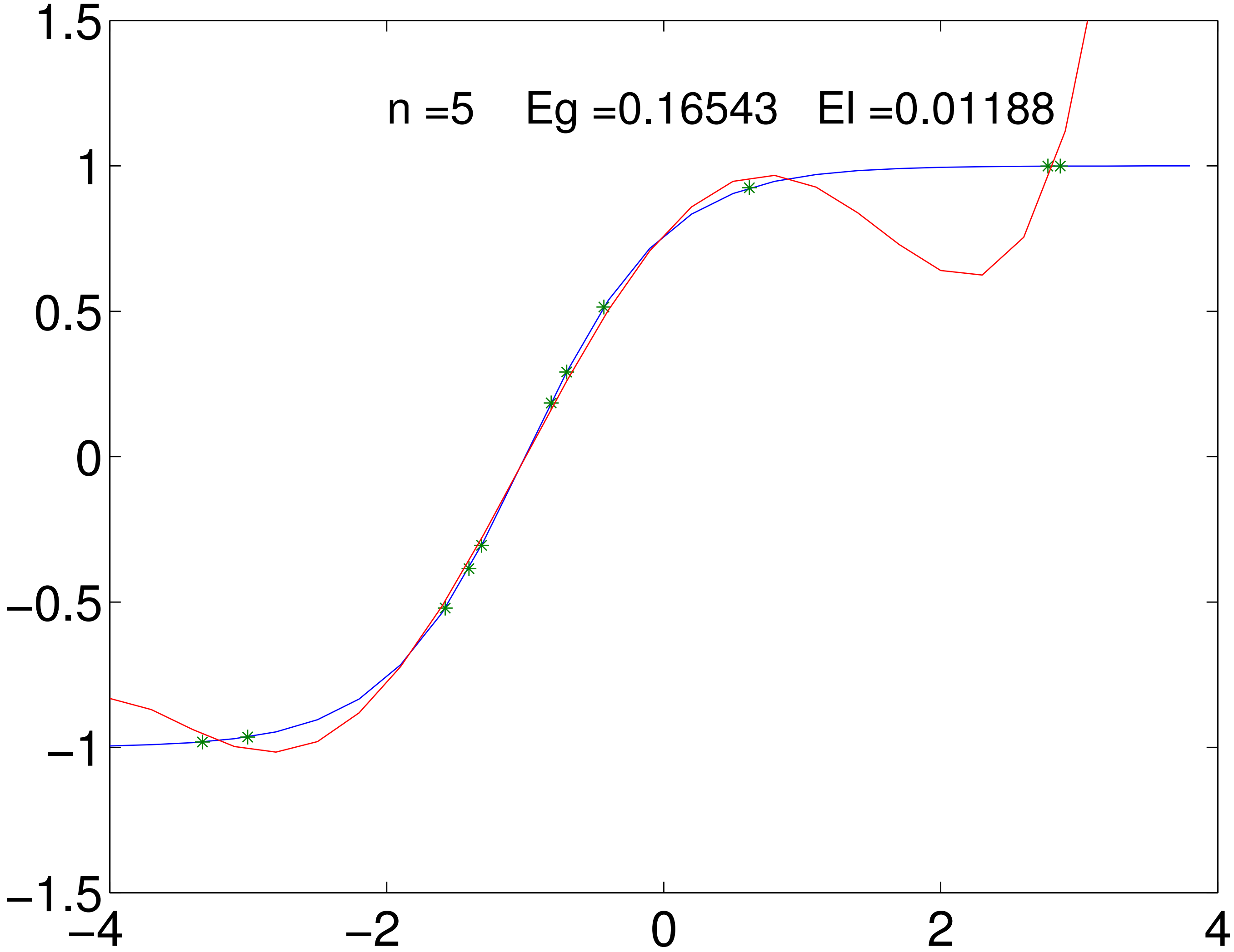

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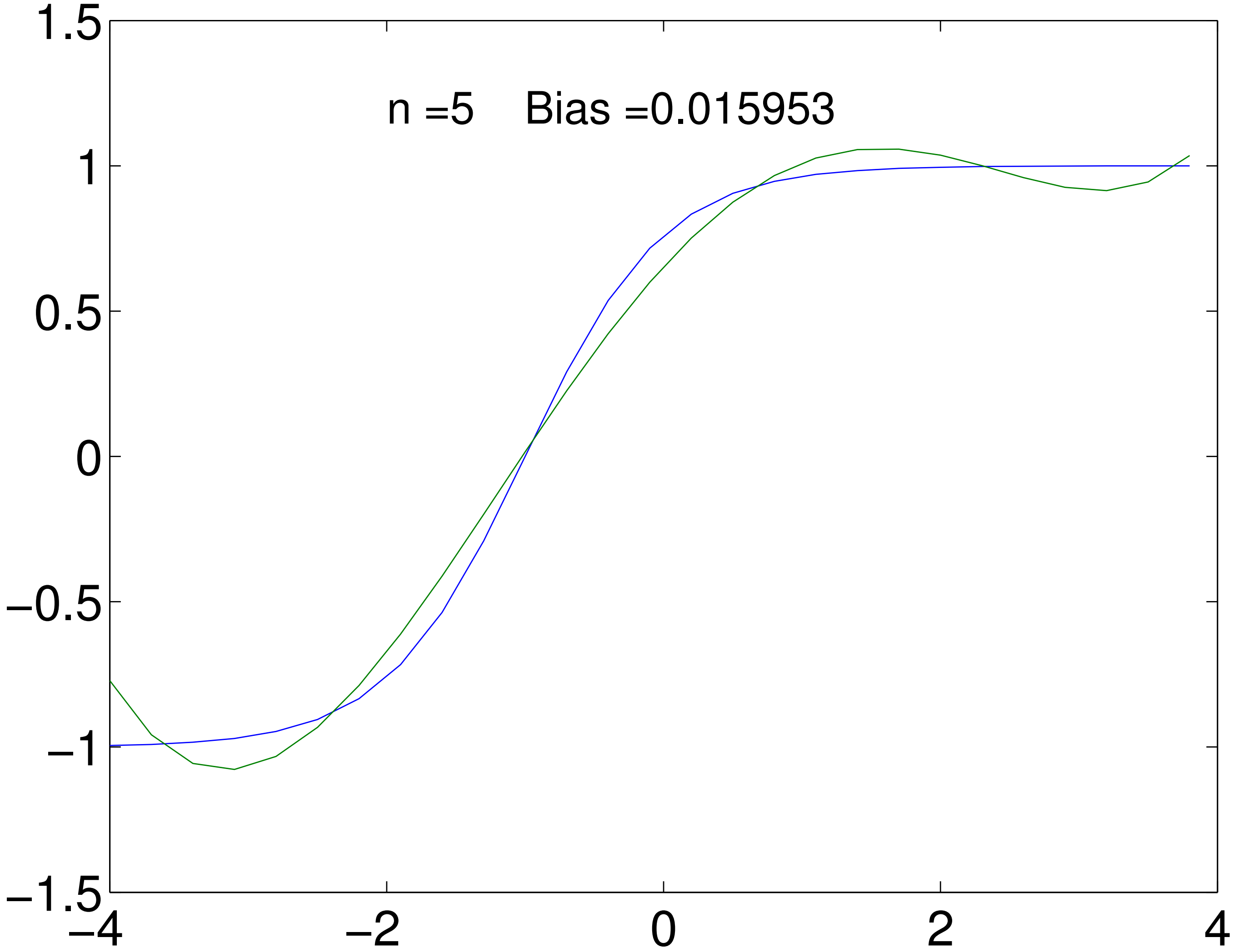

Bias and Variance

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

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Bias and Variance

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

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$$\left. + 2\,\mathbb{E}_{\mathcal{D}}\left[\left(\hat{f}(\boldsymbol{x}|\mathcal{D}) - \hat{f}_m(\boldsymbol{x})\right)\left(\hat{f}_m(\boldsymbol{x}) - f(\boldsymbol{x})\right)\right]\right)$$

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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$$
\begin{aligned}
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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Bias and Variance

- We can write the expected generalisation as

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

- Where B is the bias and V is the variance defined by

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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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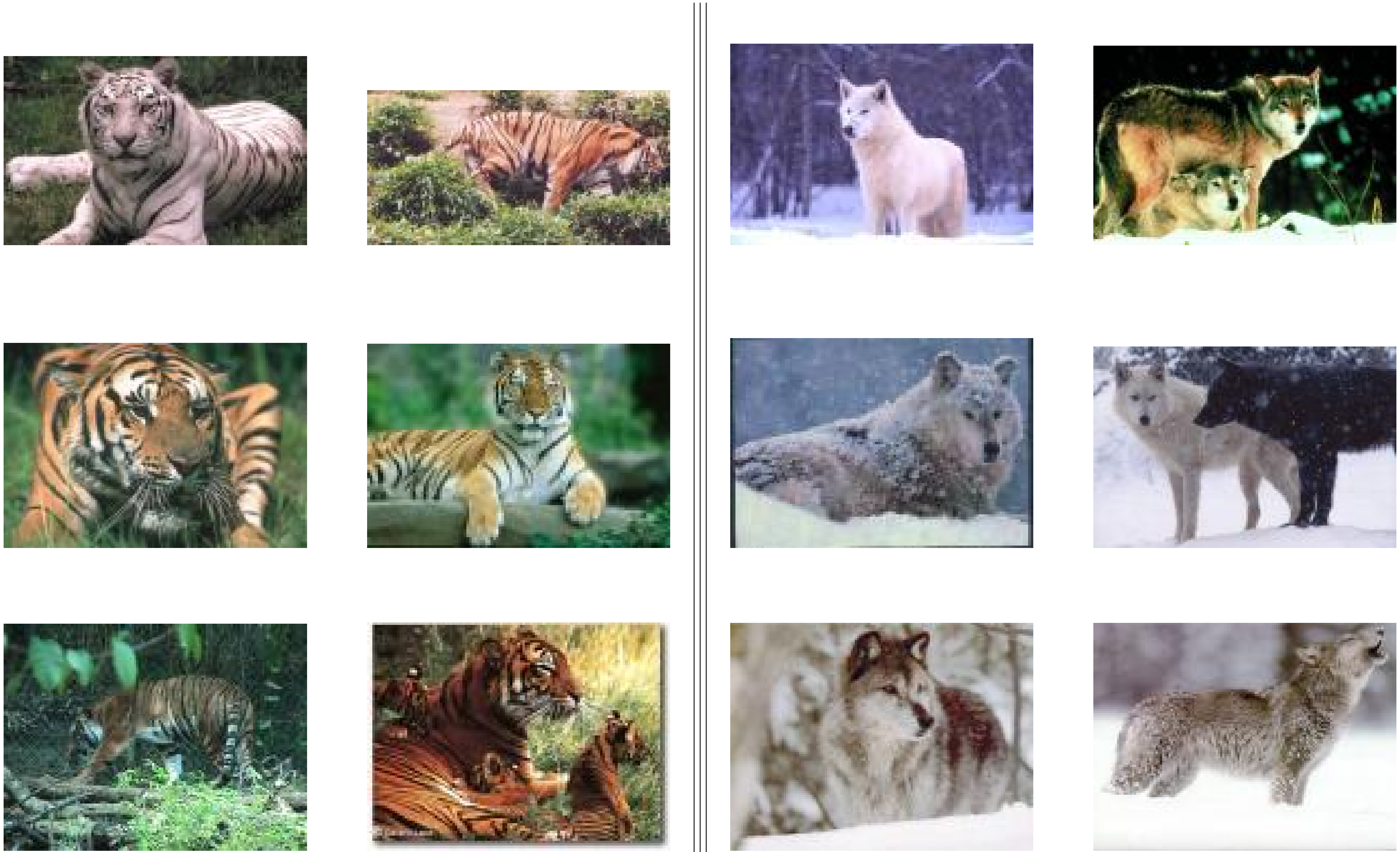
Binary Classification Task for You



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
- It will find a rule that does this, but not necessary the rule you had in mind
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All Binary Functions

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

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

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$$\mathcal{D} = \big\{(0\,0\,0\,,\,0),\,(0\,1\,0\,,\,1),\,(1\,1\,0\,,\,1),\,(0\,0\,1\,,\,0),\,(1\,0\,1\,,\,0)\big\}$$

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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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- 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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- We can use various heuristics to decide which features to keep, but no heuristic is fail-safe
- Feature selection however can be powerful, often we can get very good results by keeping only a few variables
- As well as possibly improving generalisation we also get a more **interpretable** rule

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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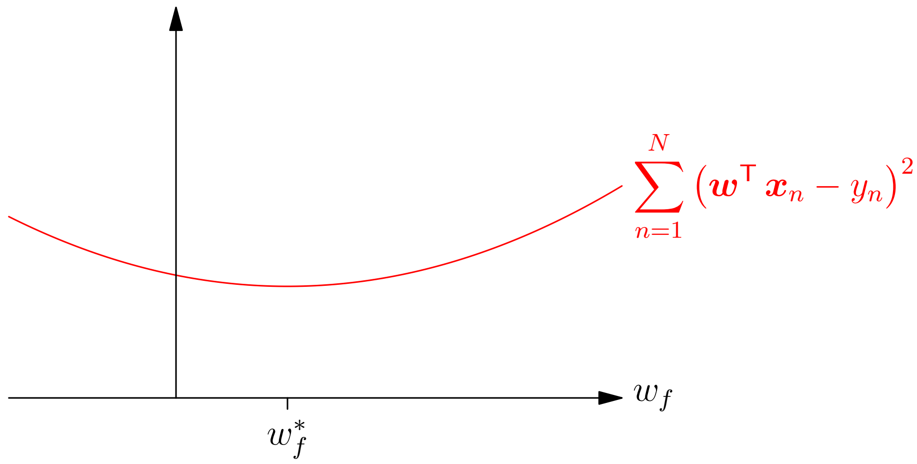

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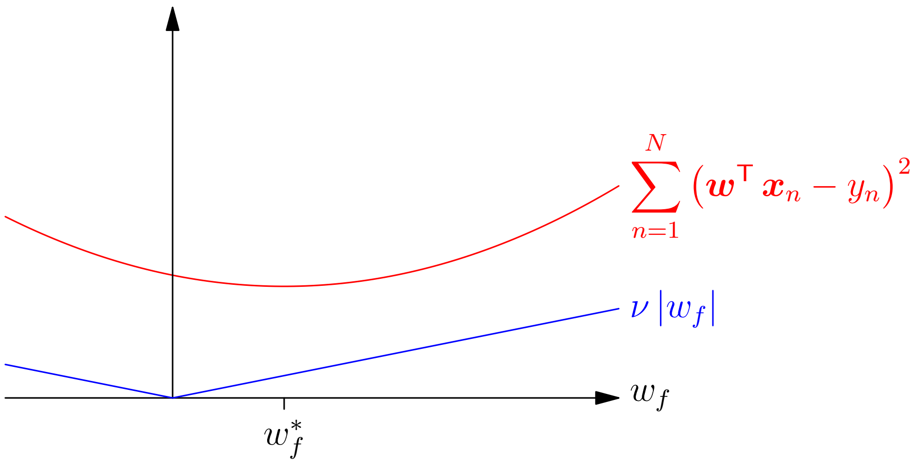

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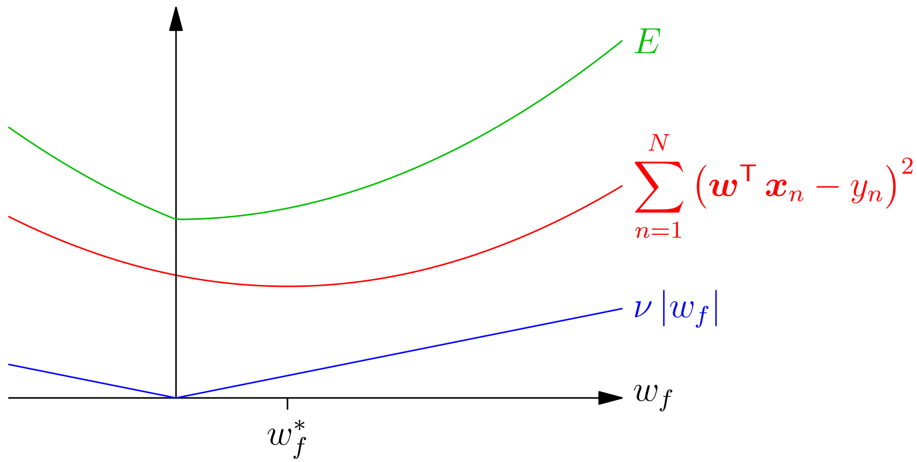

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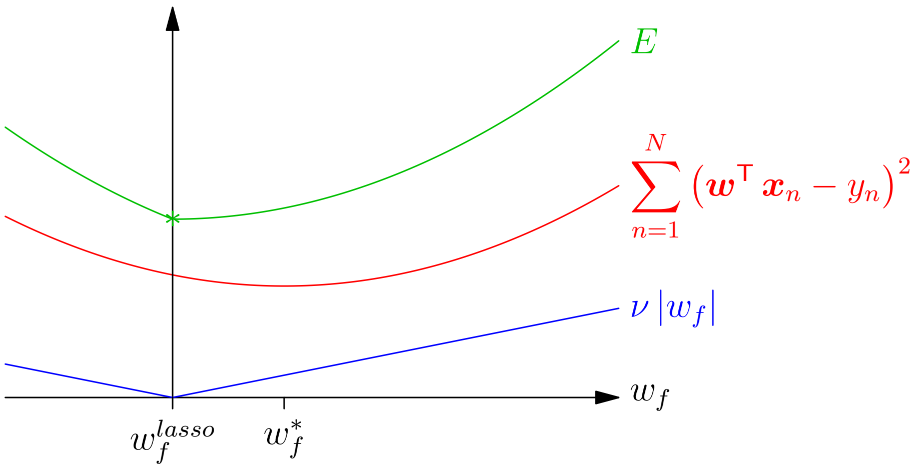

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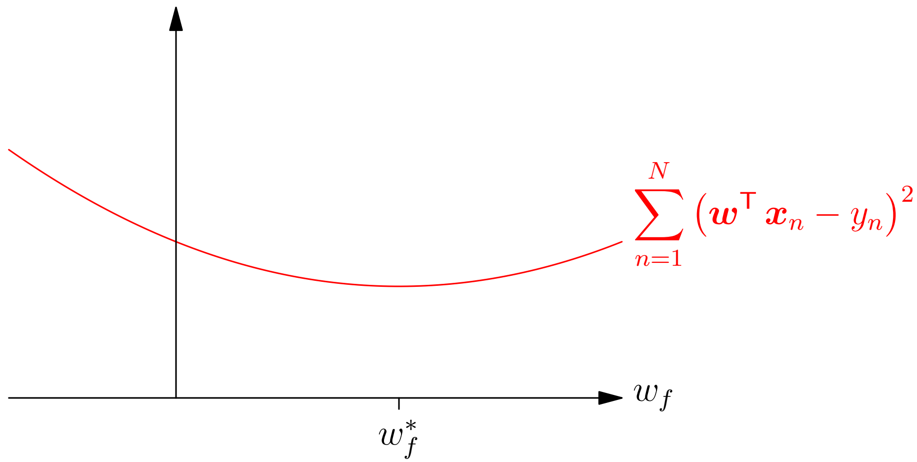

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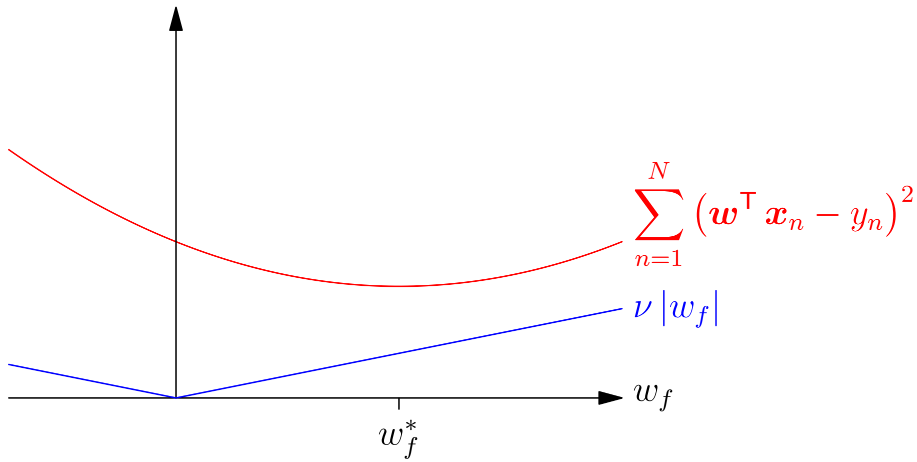

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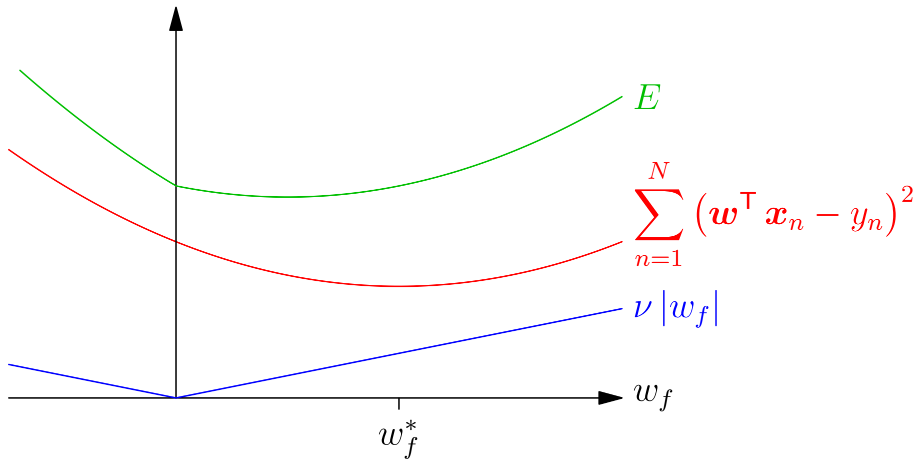

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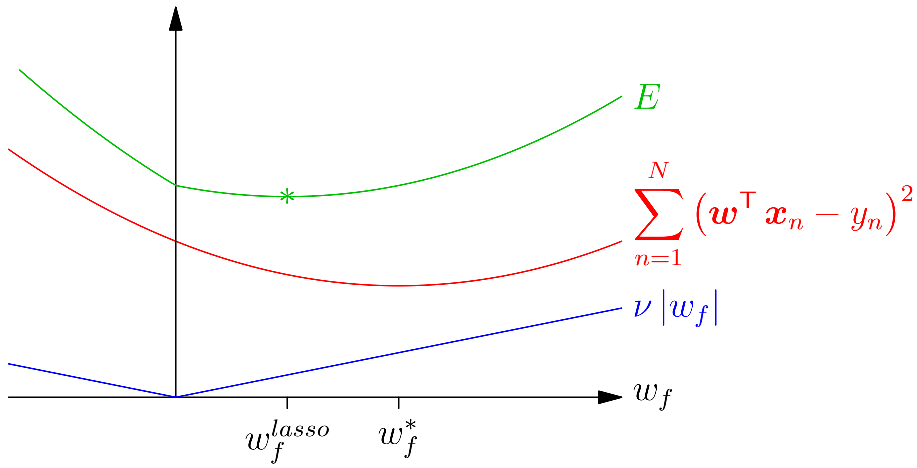

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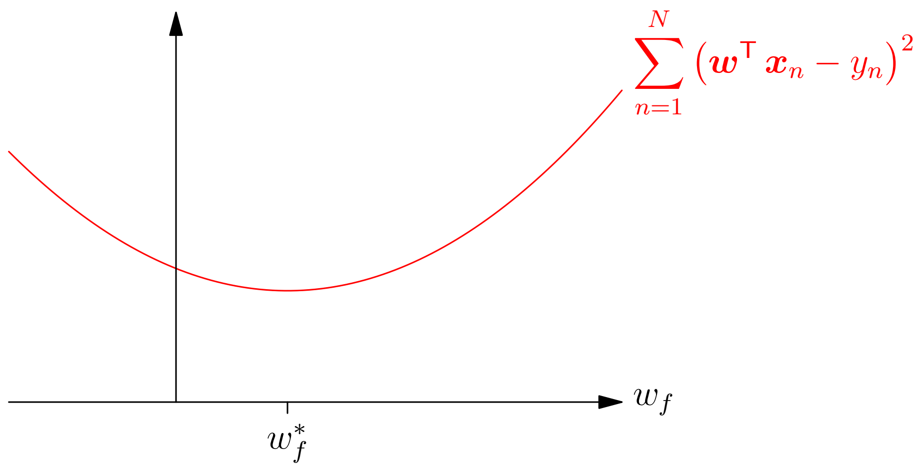

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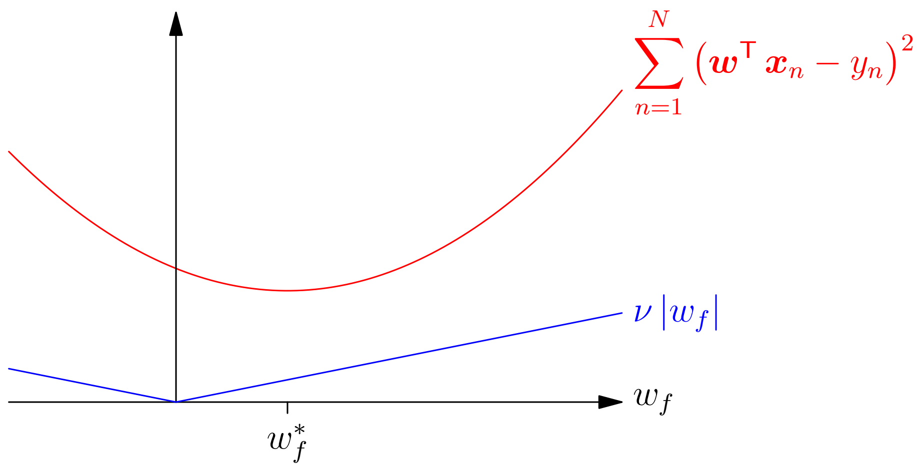

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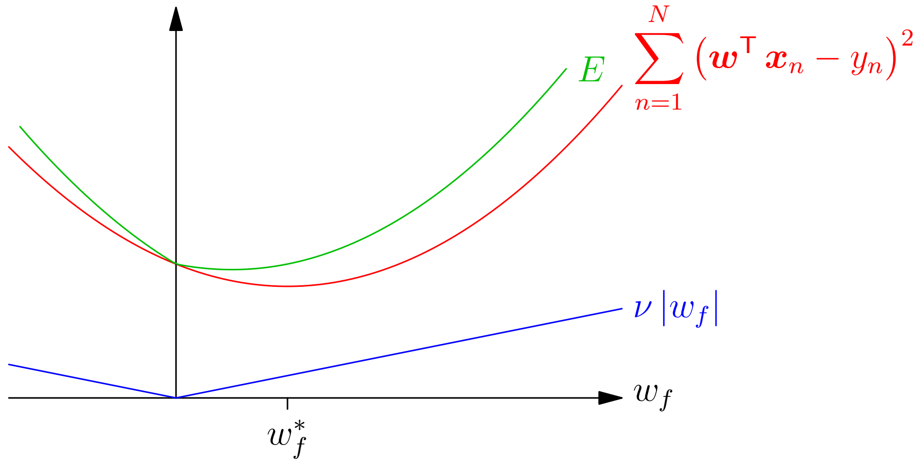

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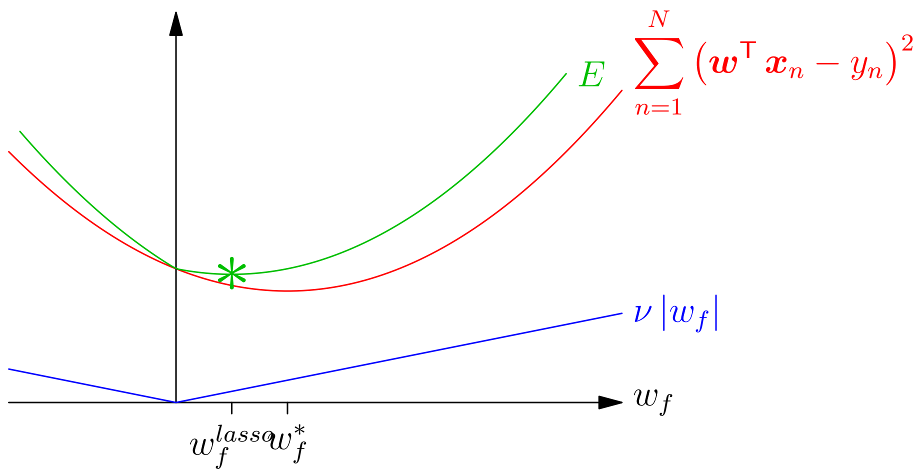

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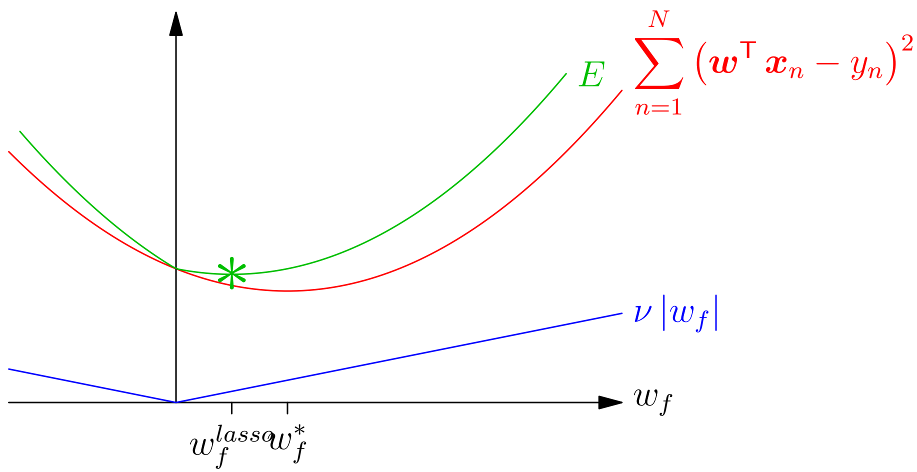

- Does automatic feature selection

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
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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
- Use the validation set to choose the hyper-parameters
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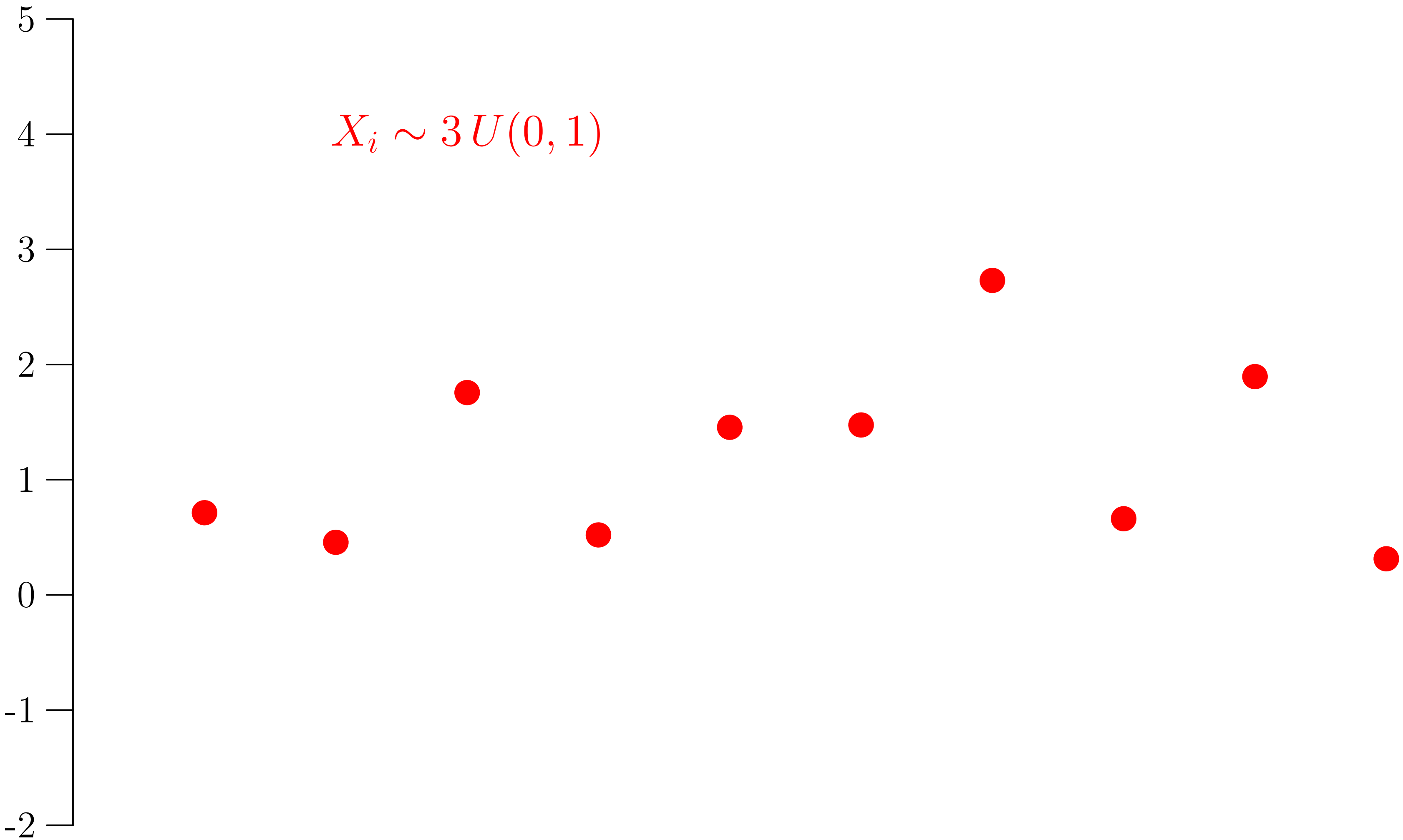

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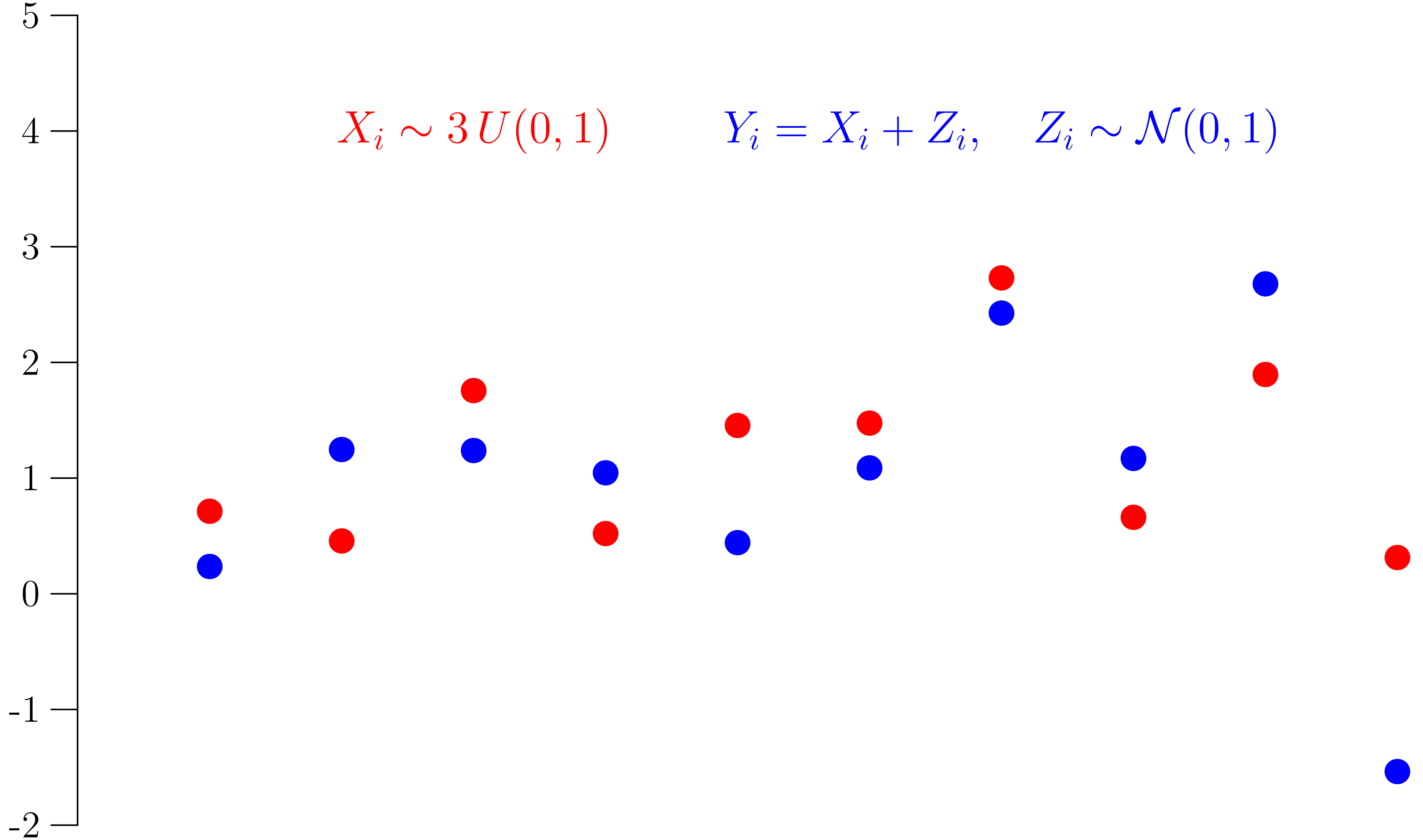

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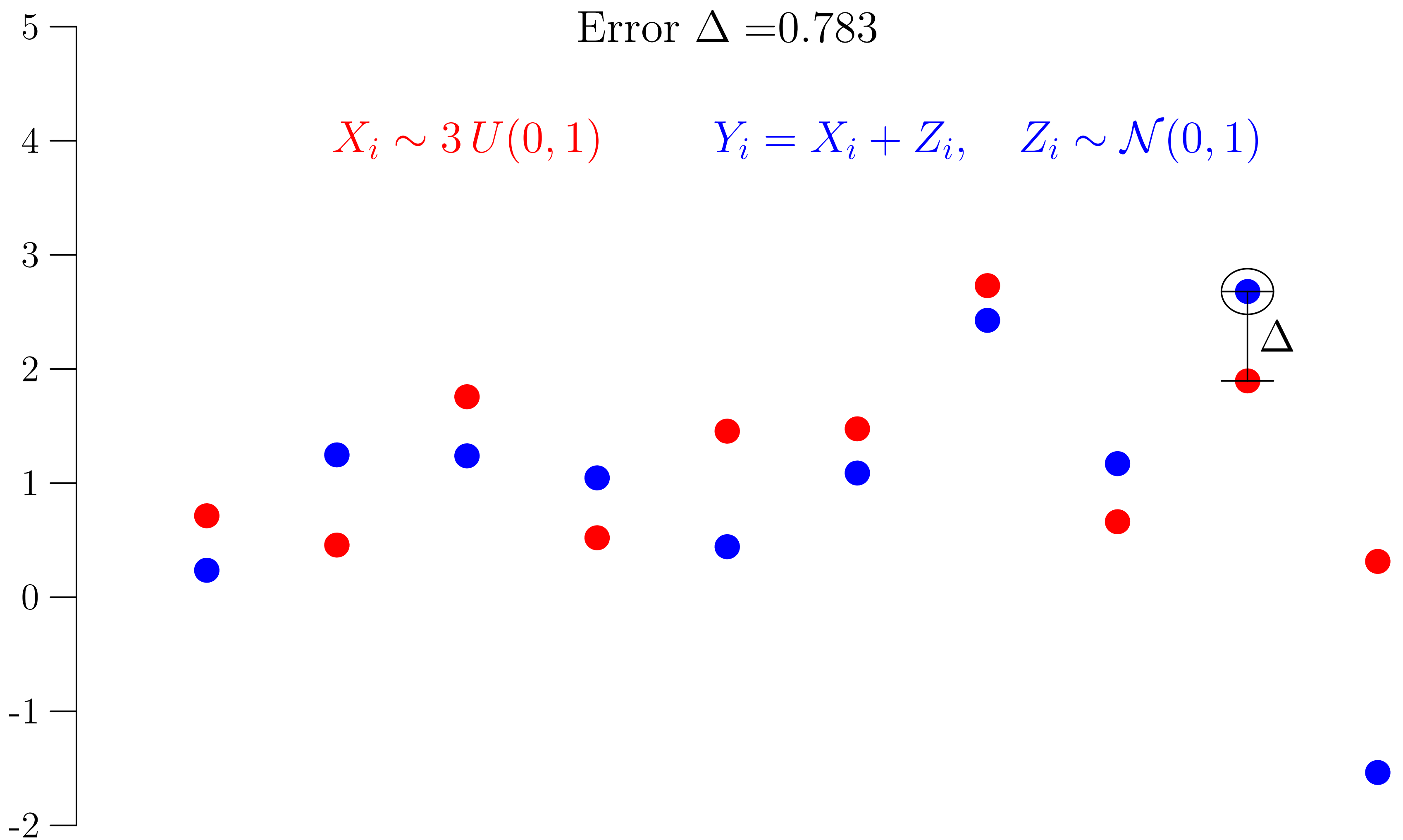

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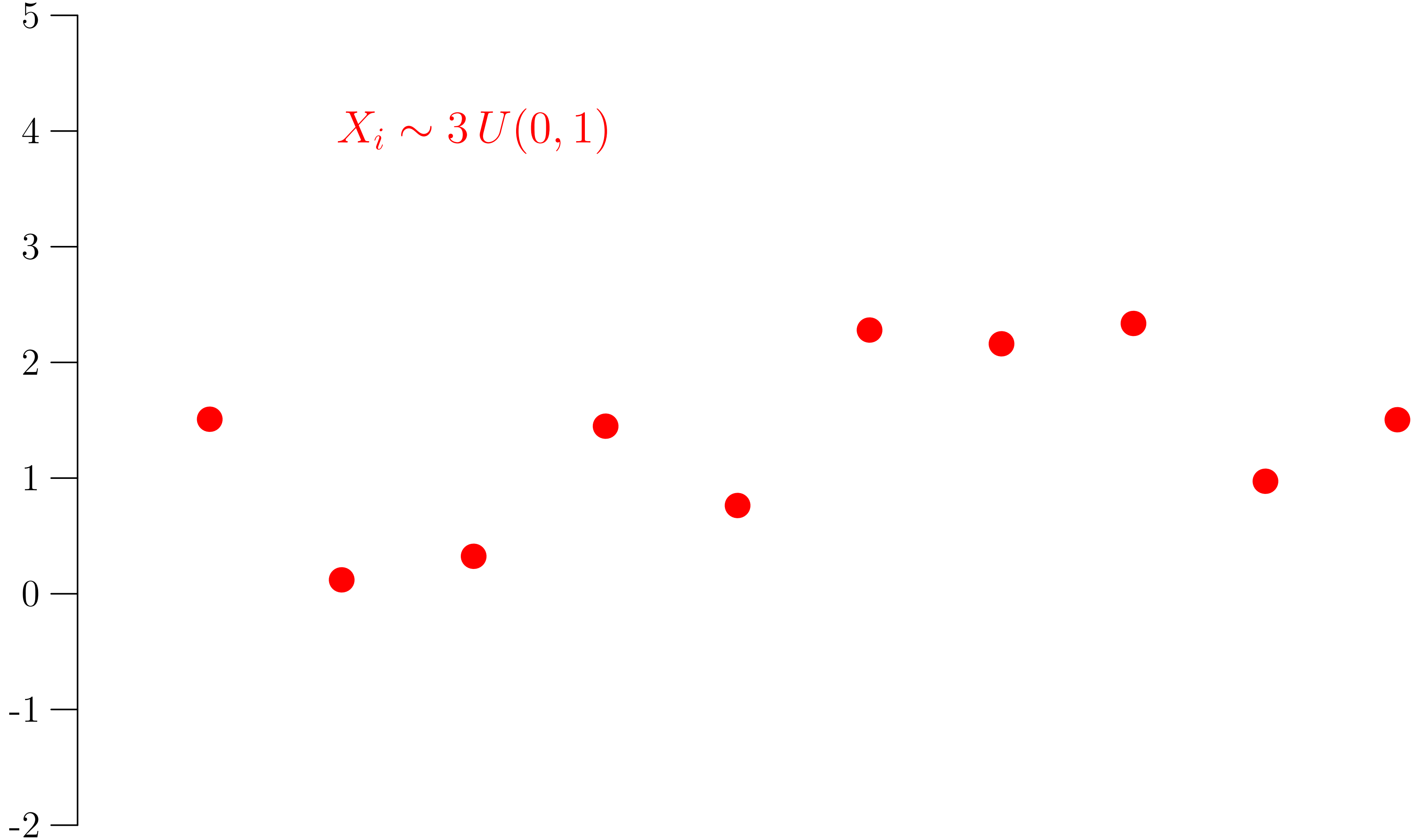

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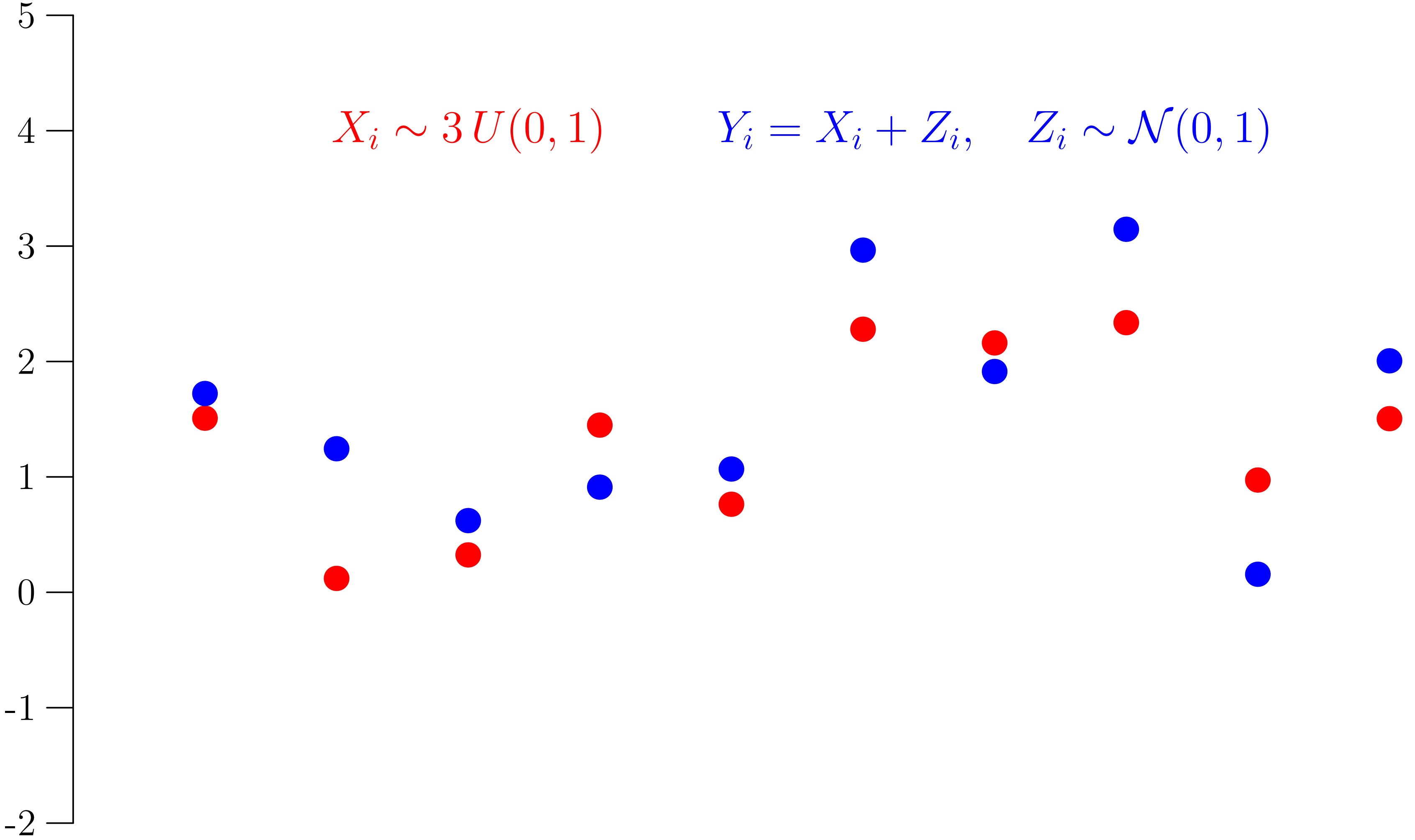

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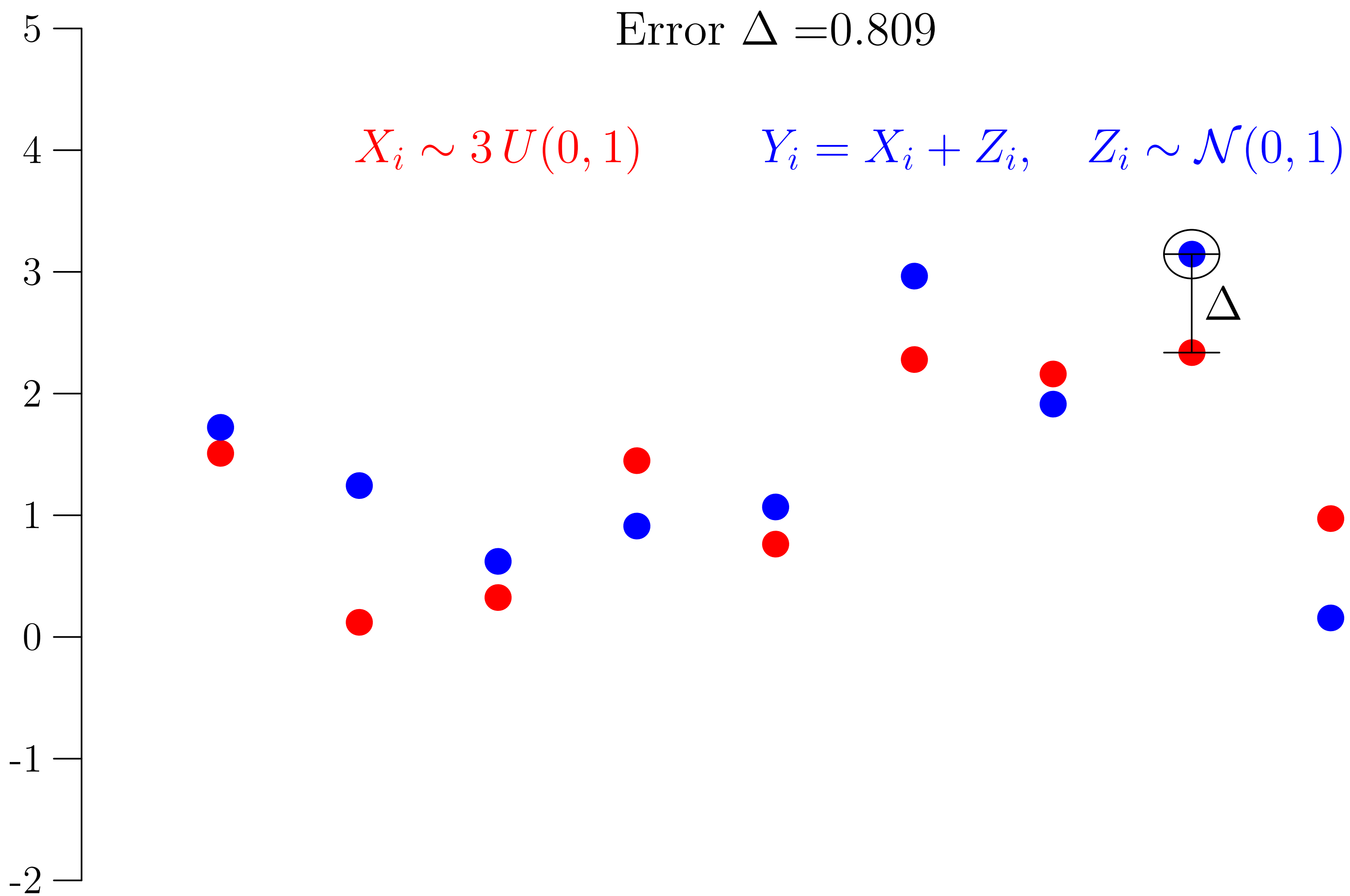

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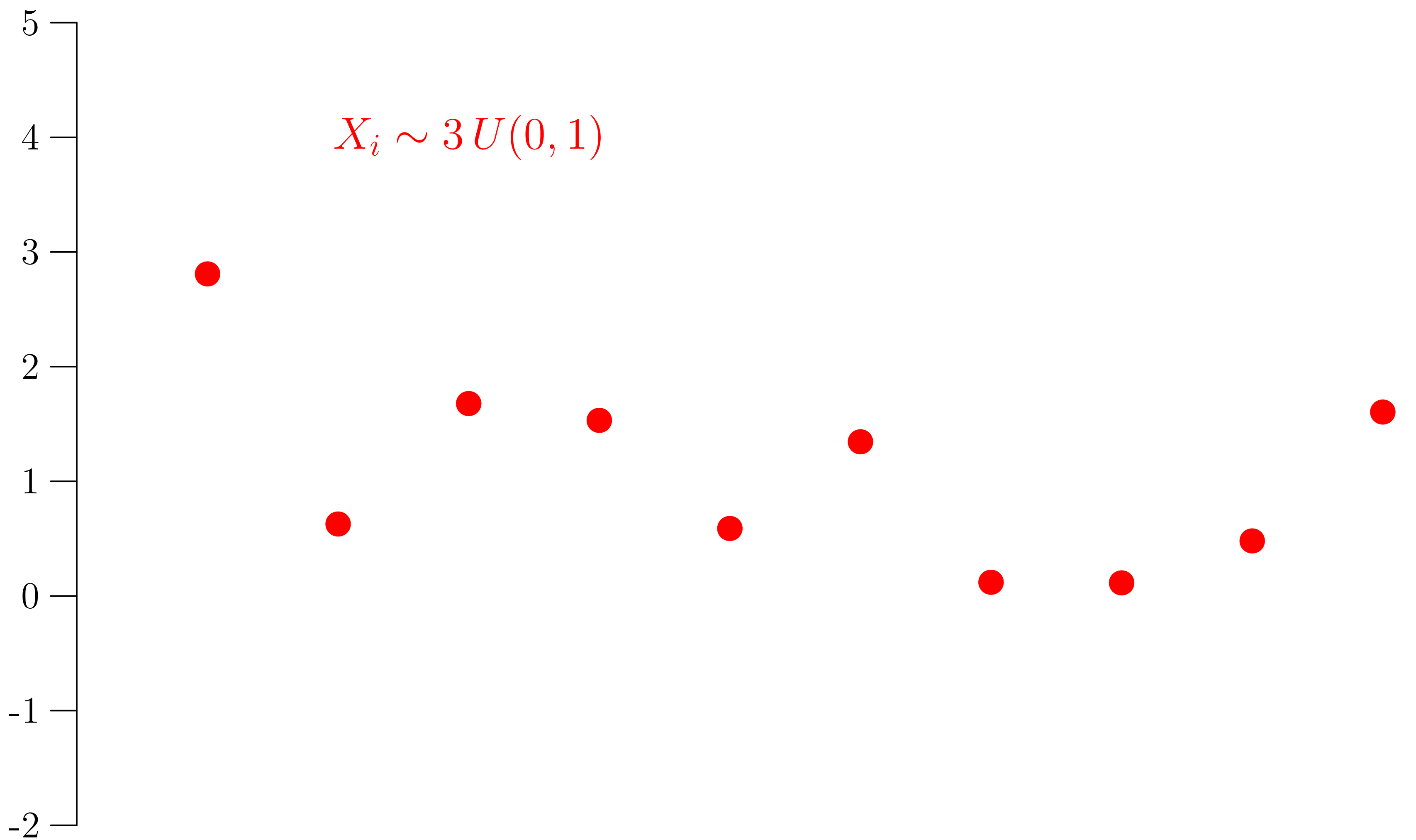

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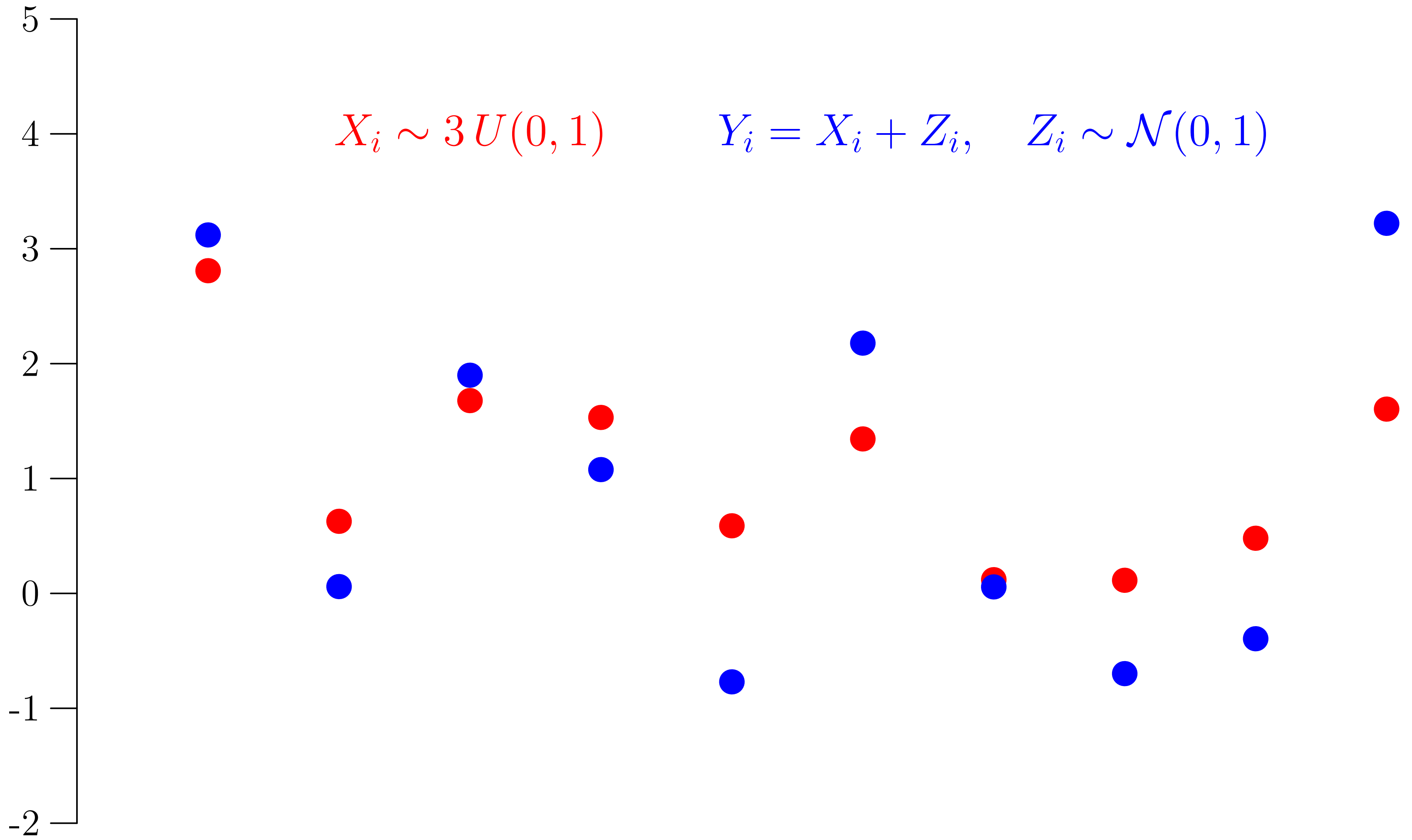

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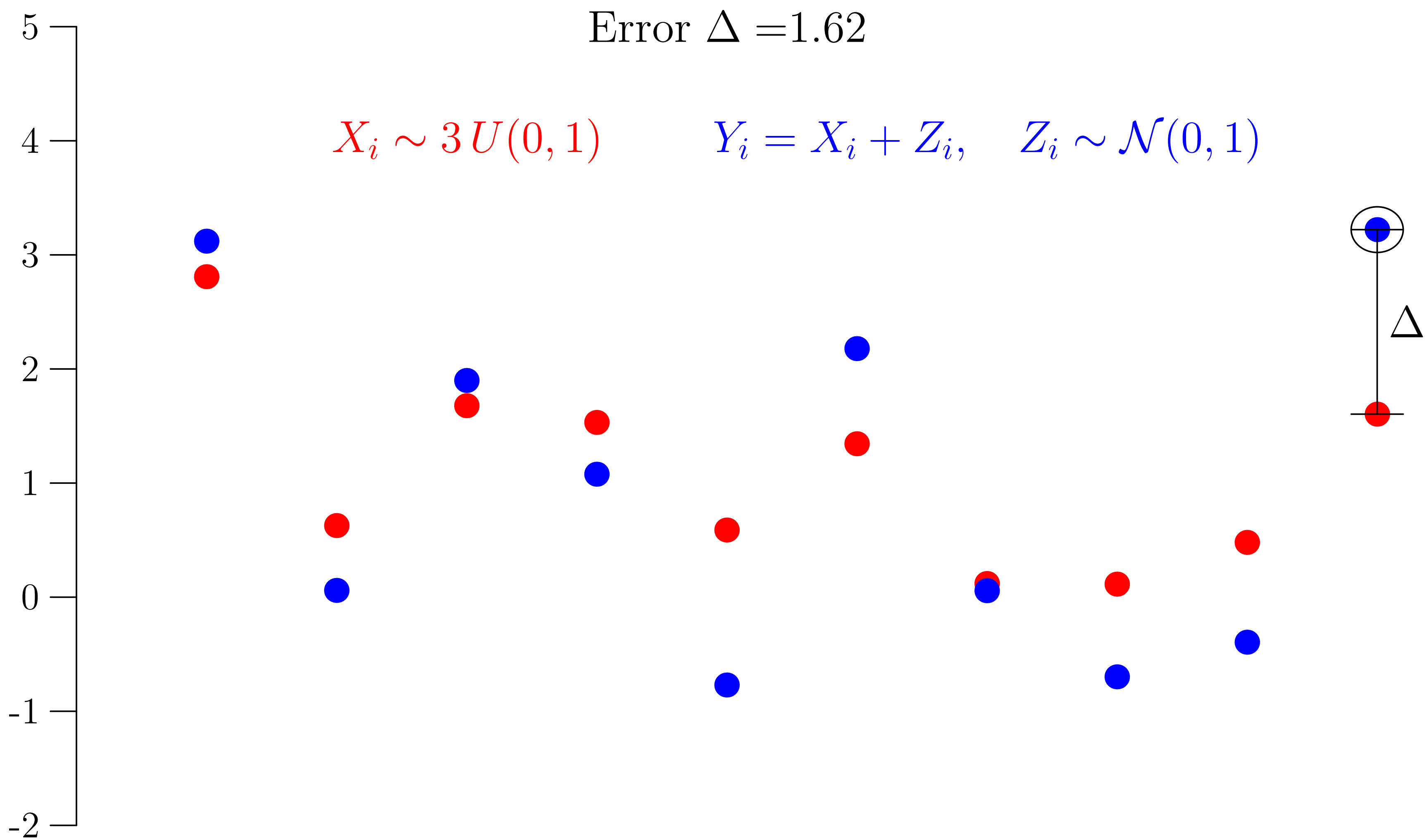

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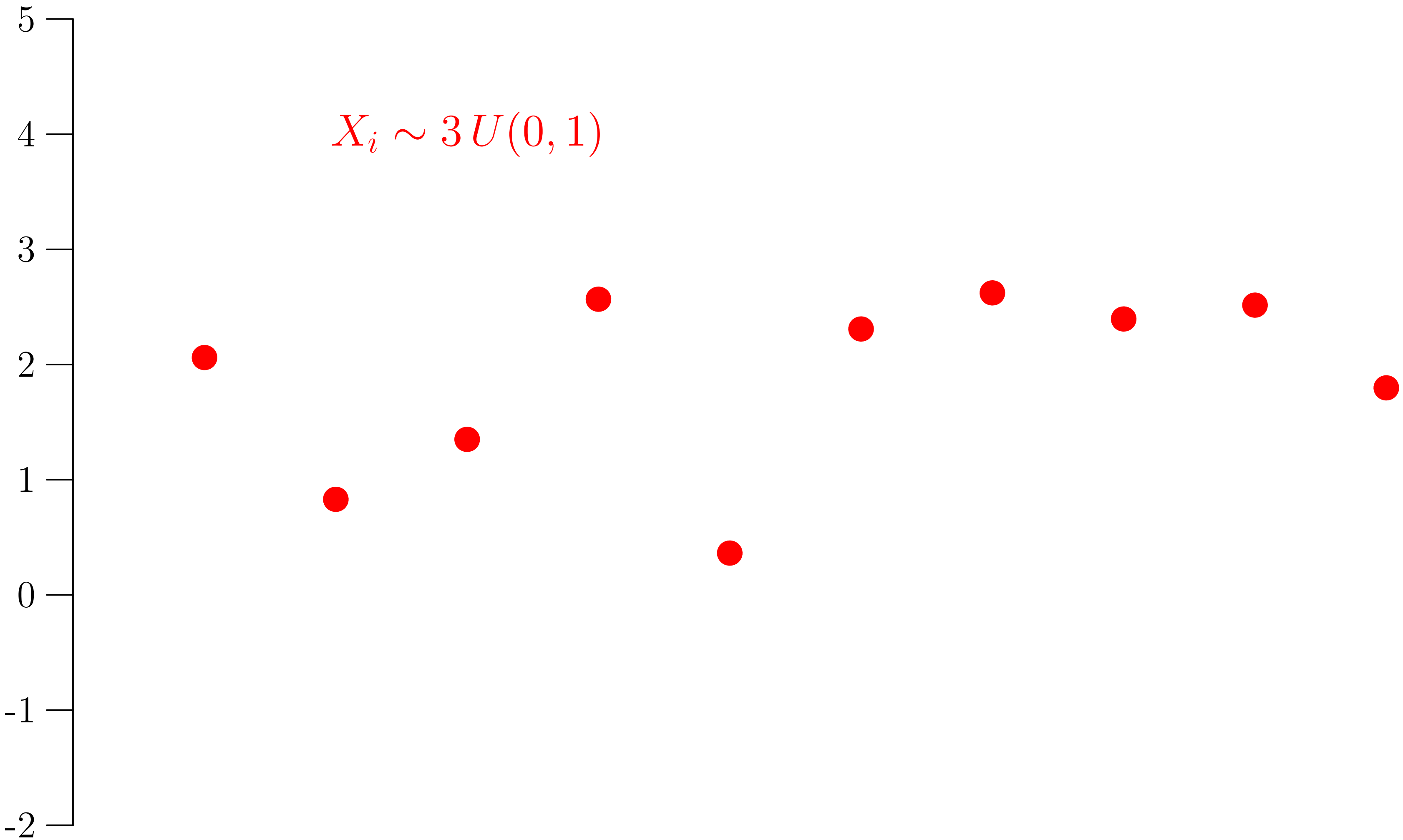

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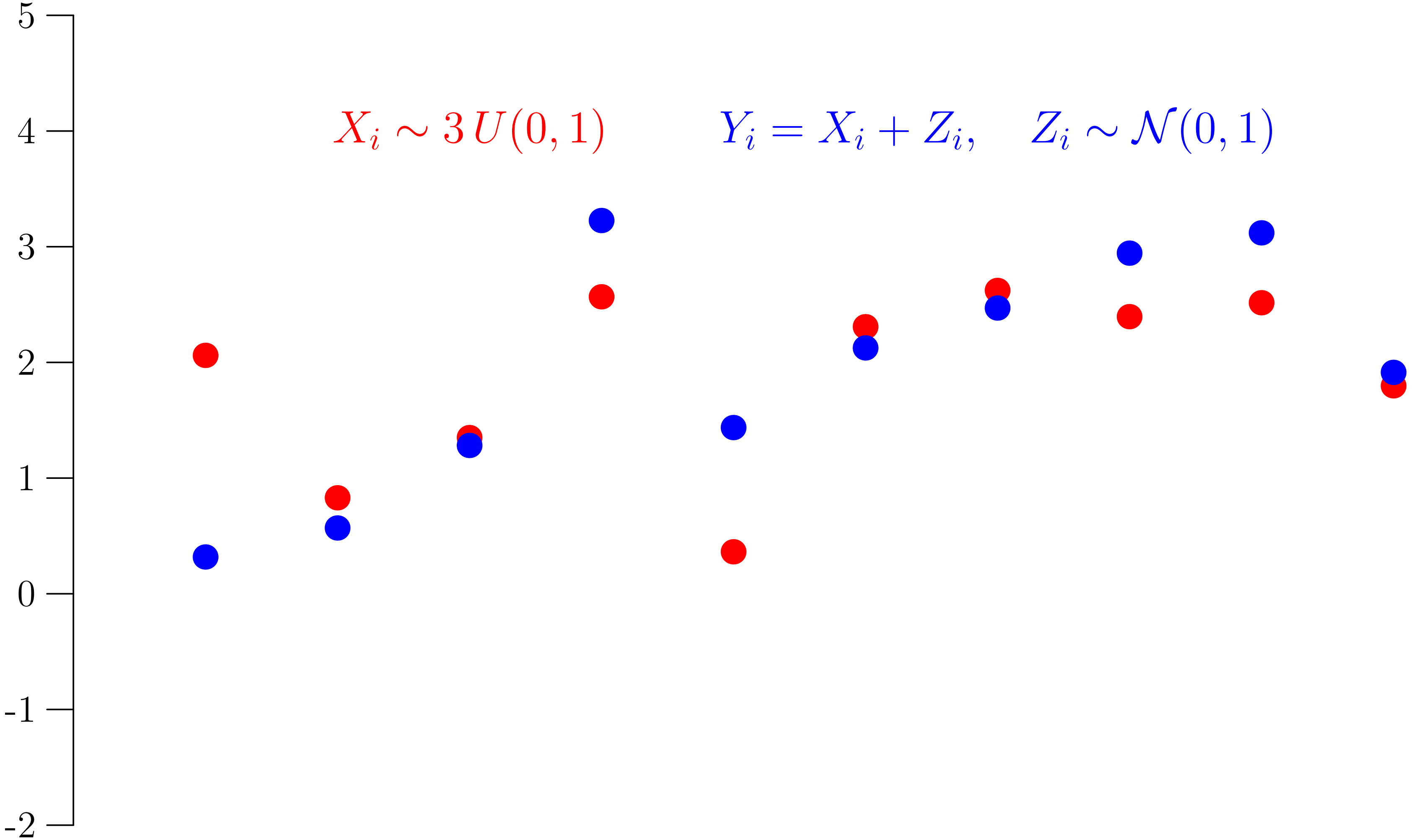

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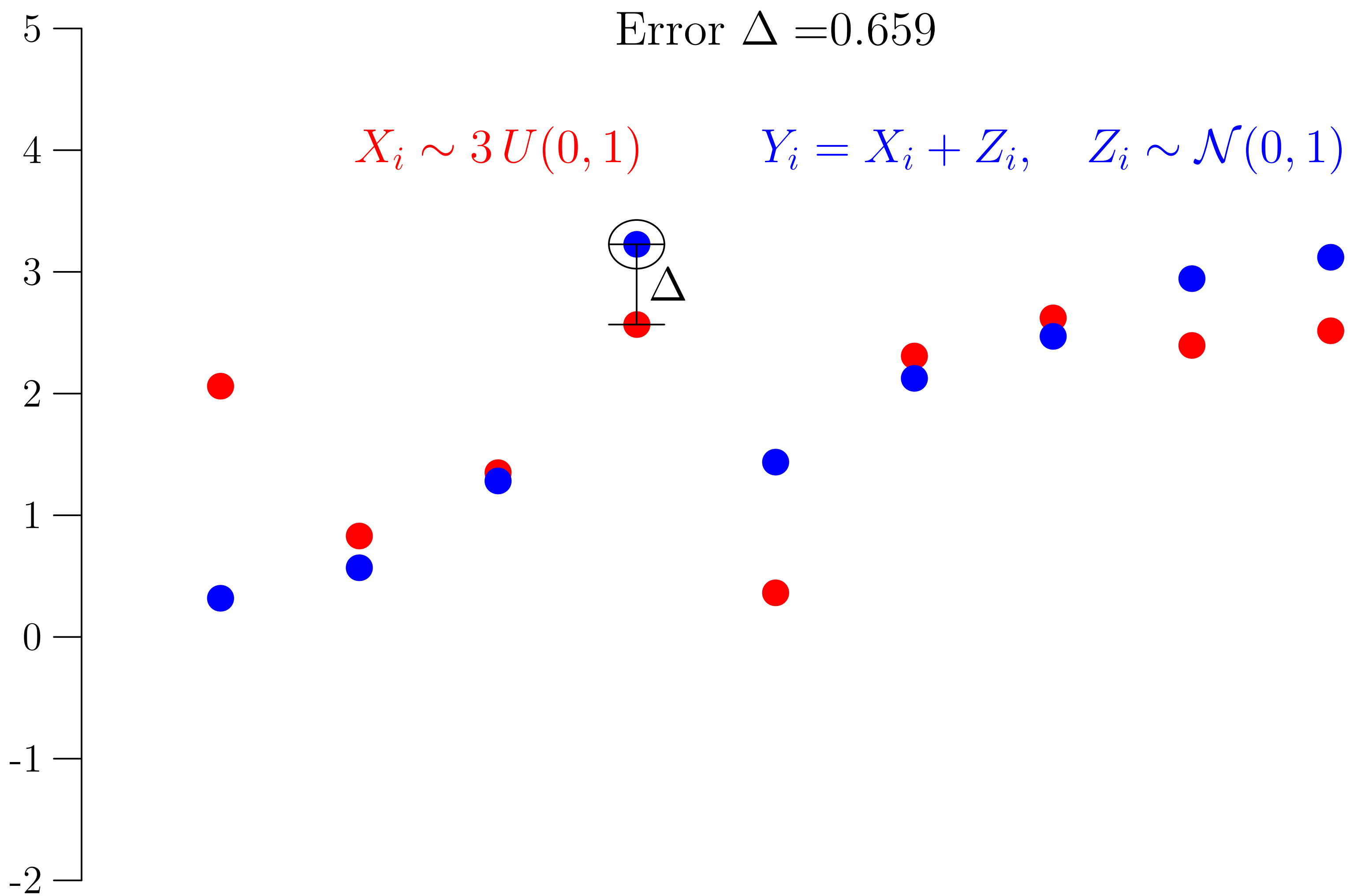

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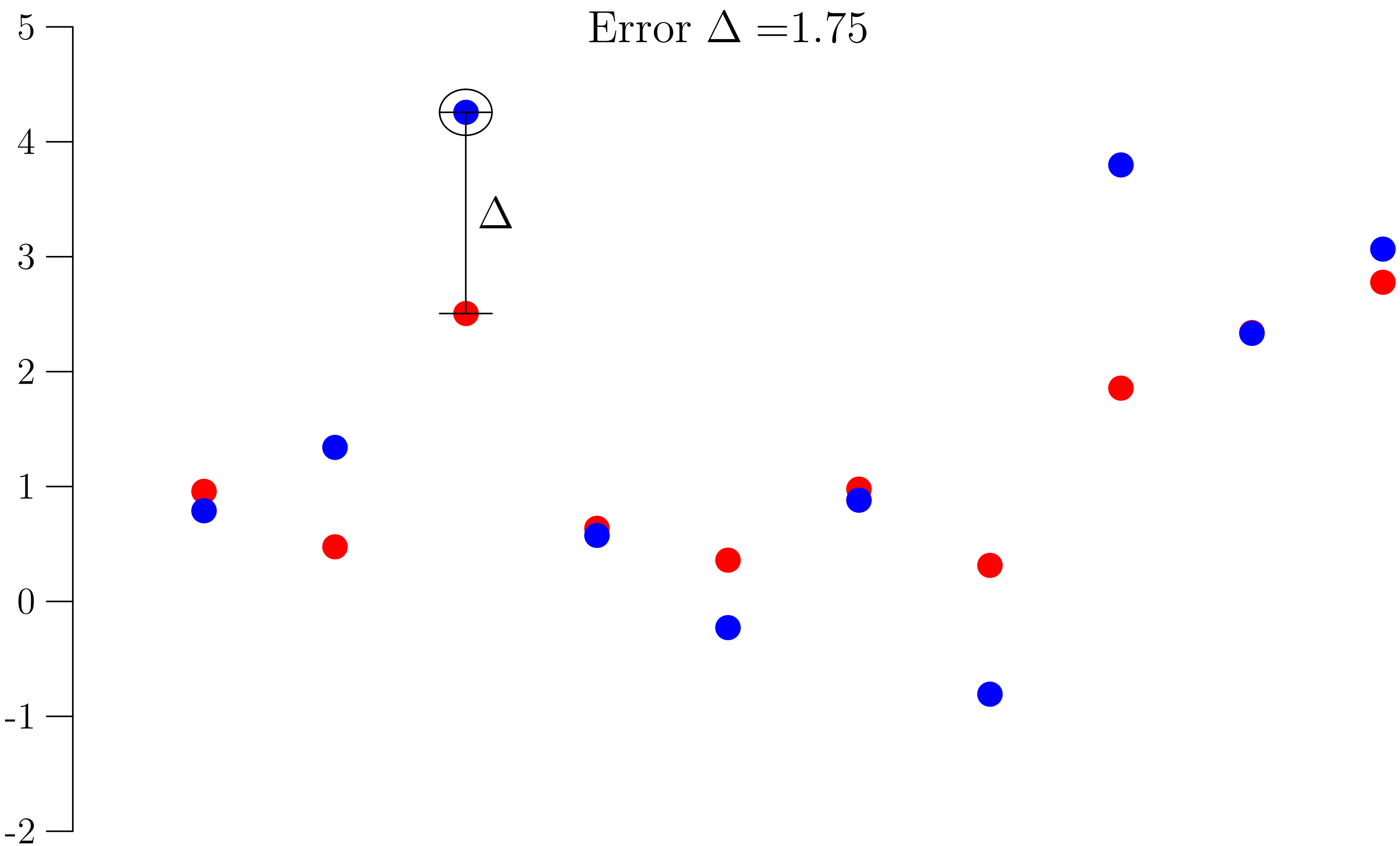

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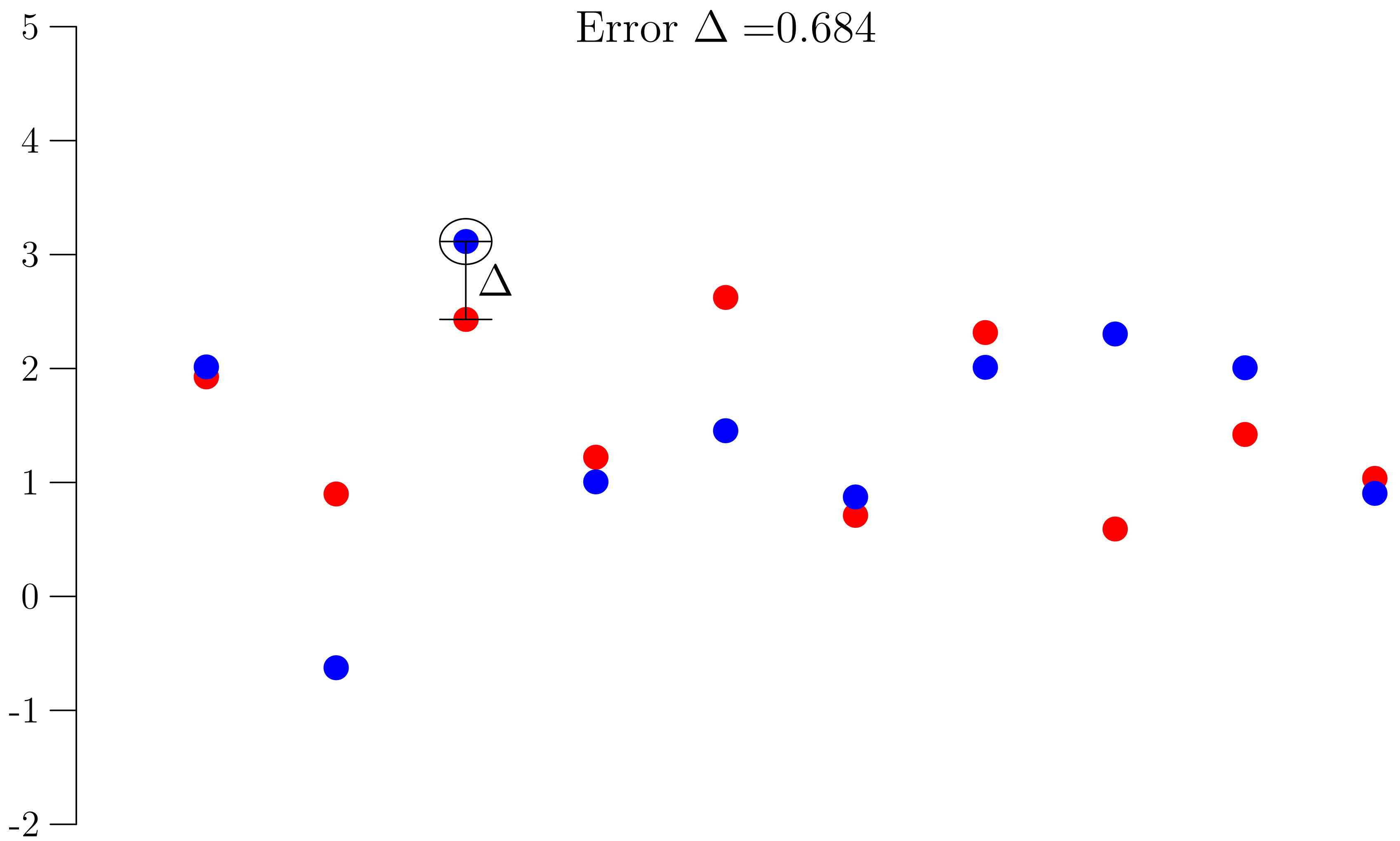

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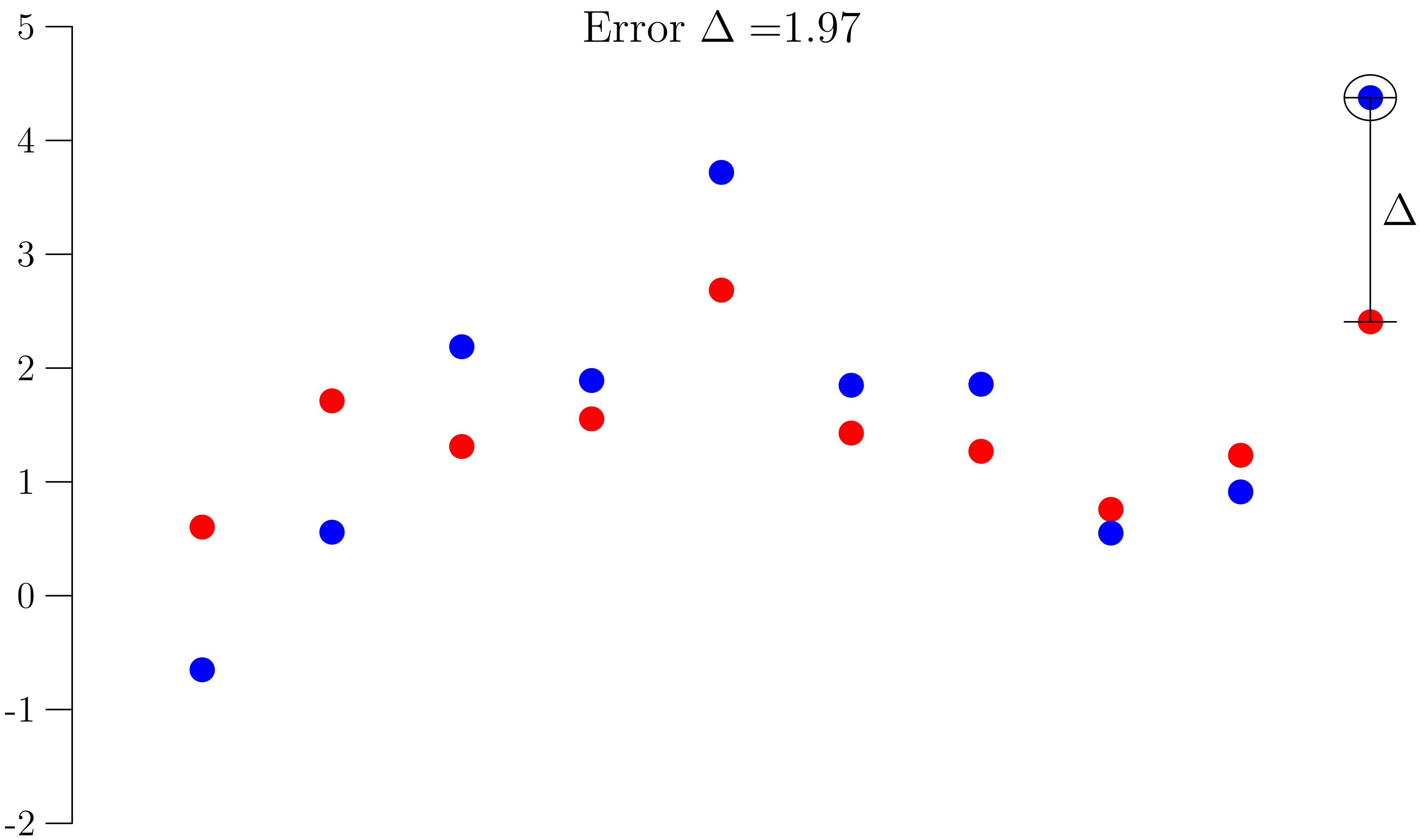

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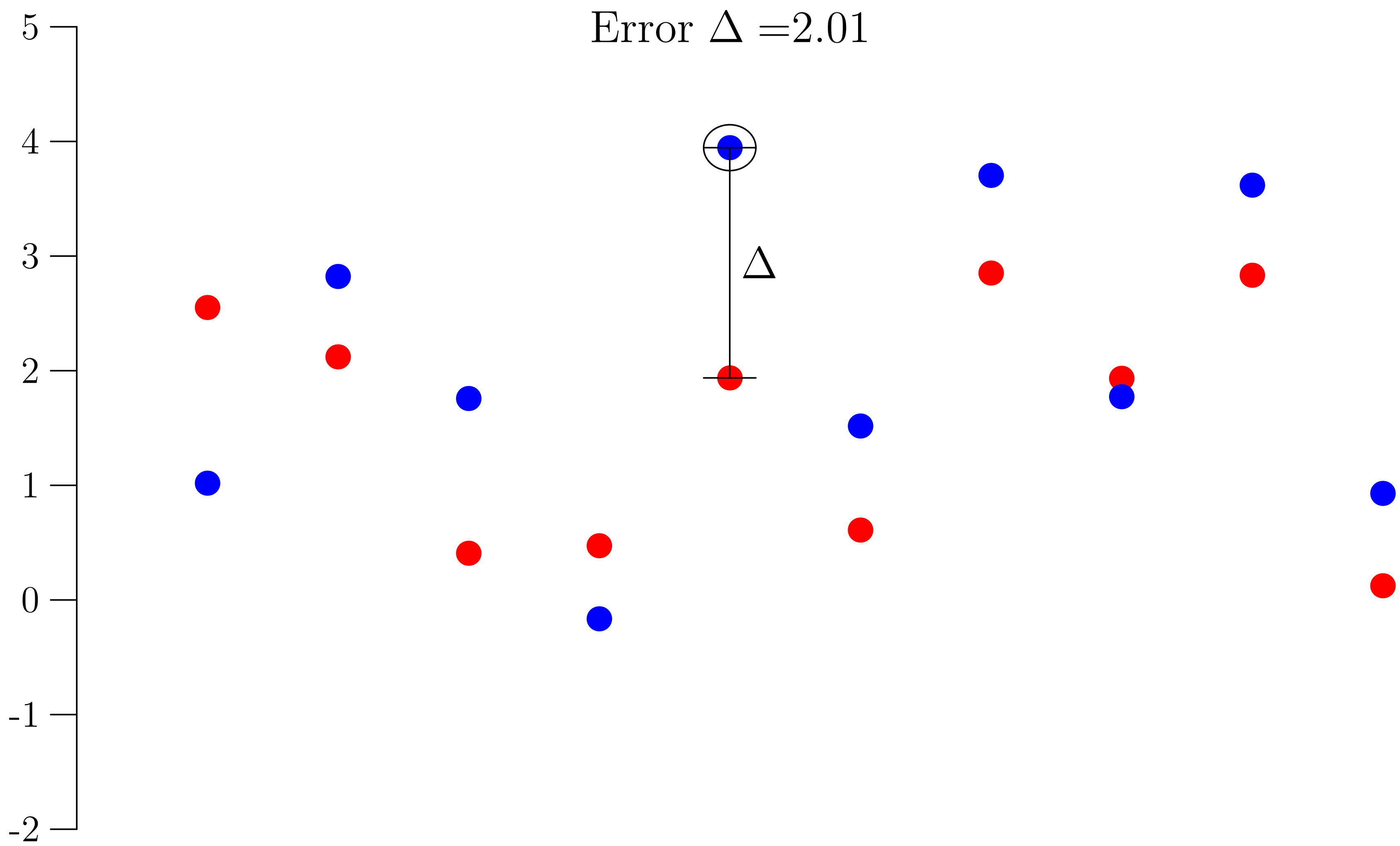

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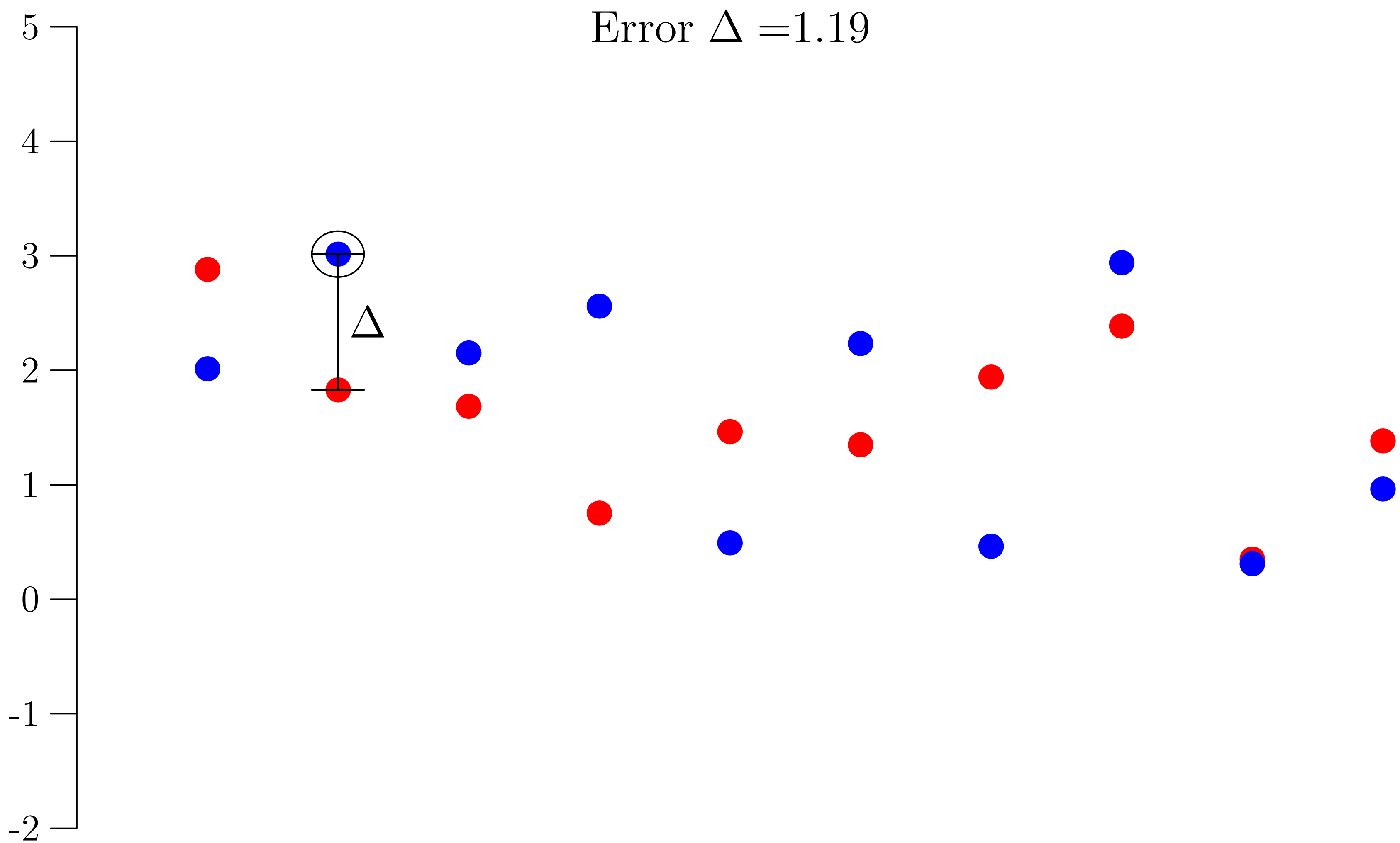

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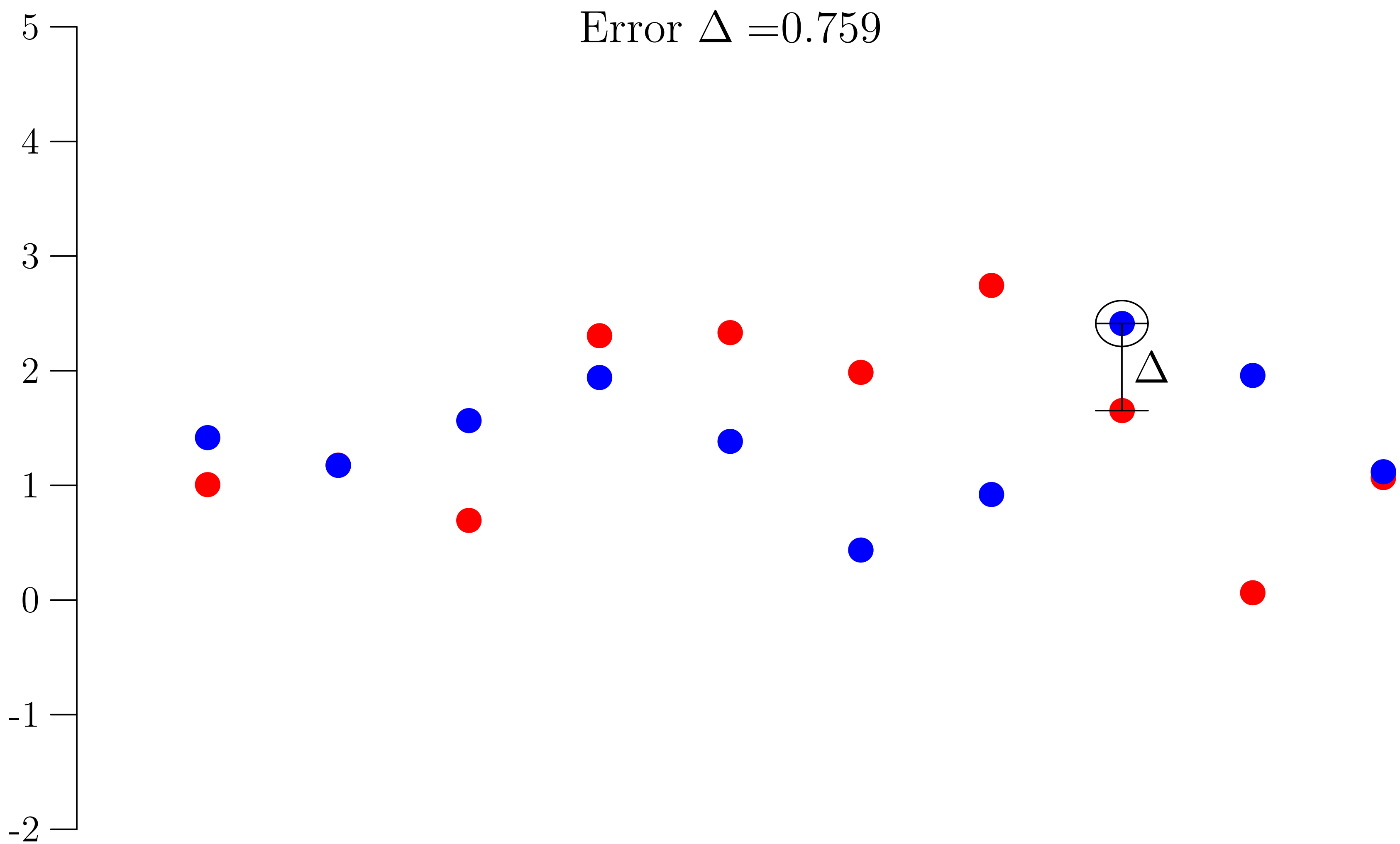

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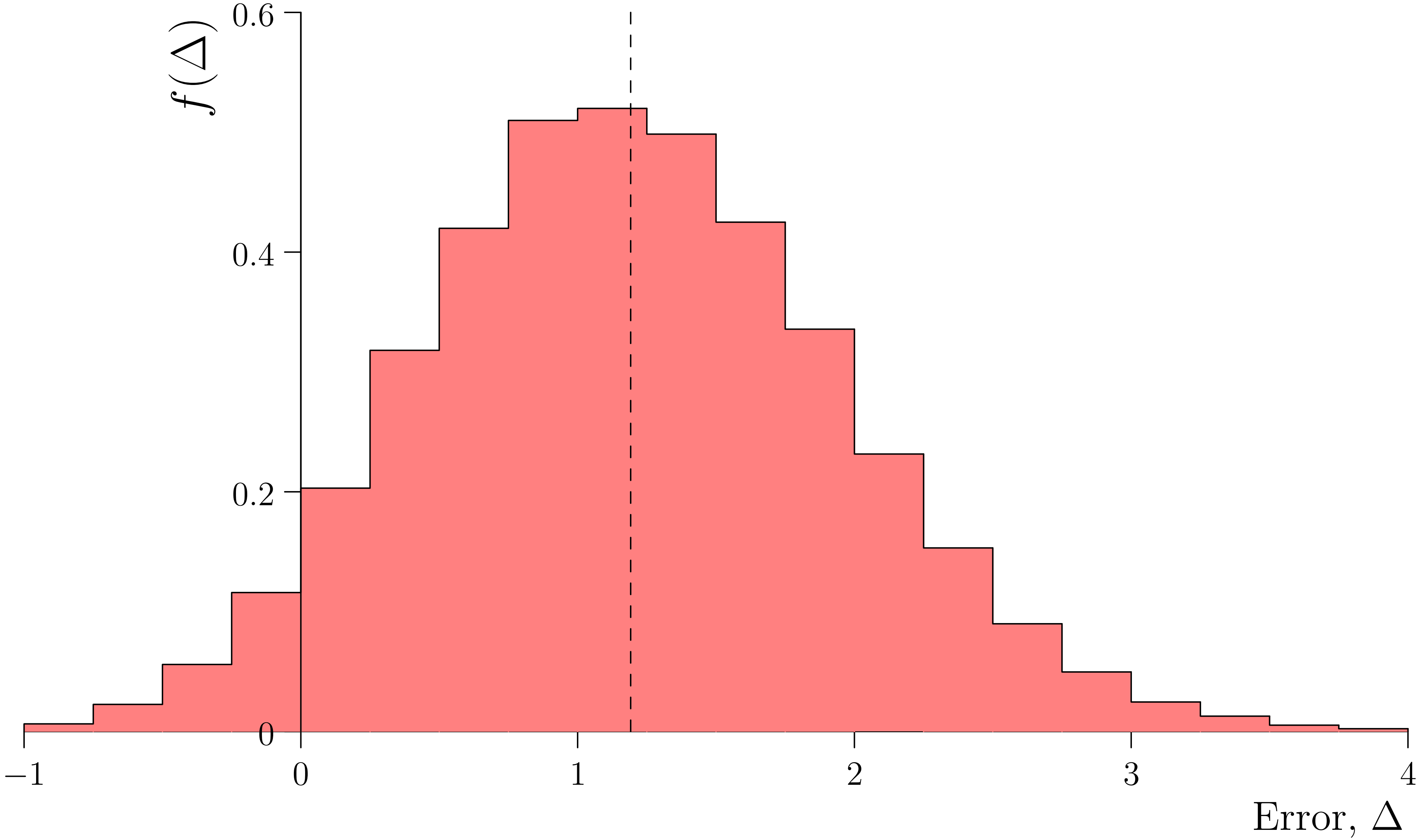

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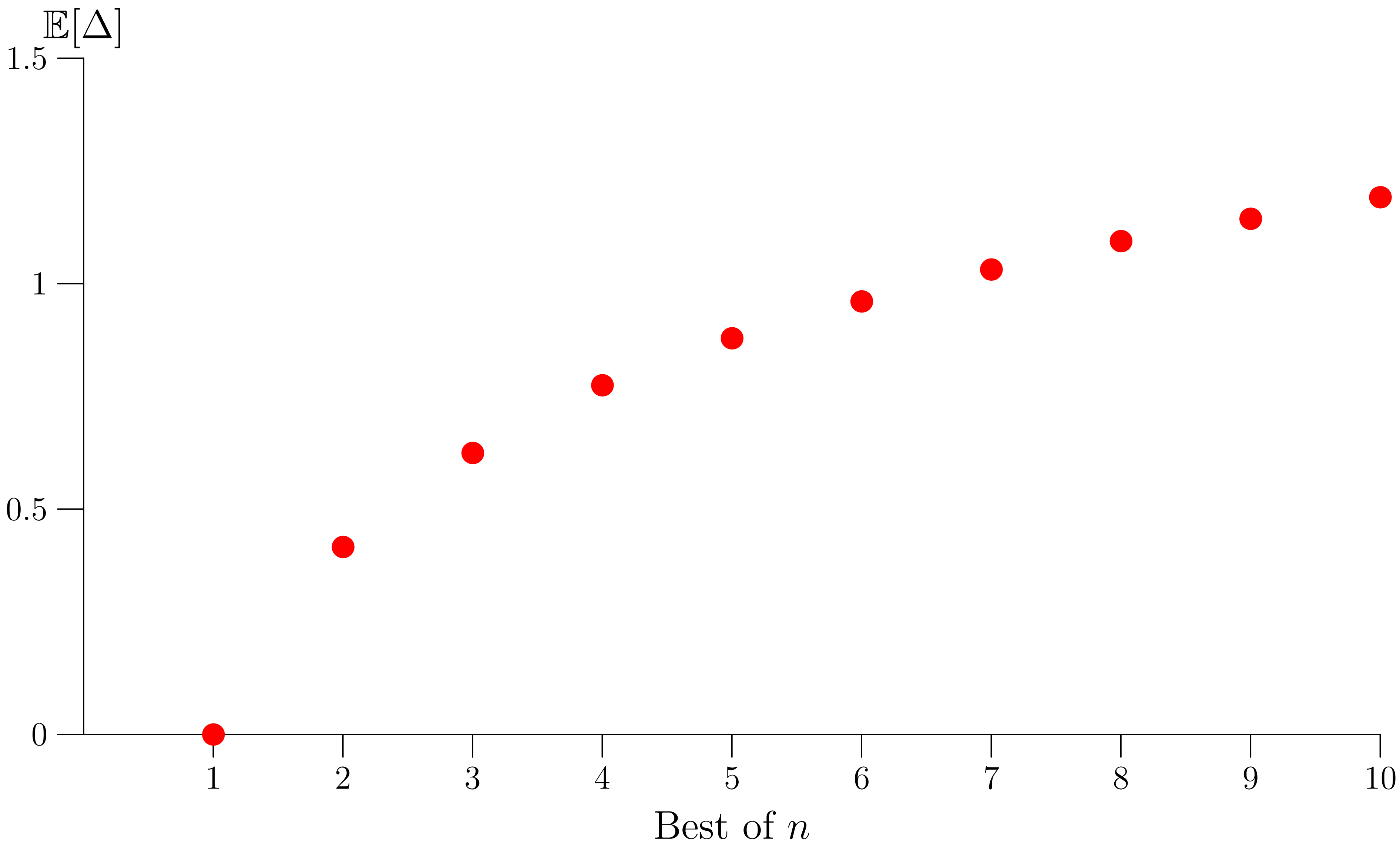

Cross Validation

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

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Test Set Training Set

5-fold cross-validation

$E_g =$ 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

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$$E_g = \qquad 4.6$$

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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

5-fold cross-validation

$E_g =$ 3.3

Cross Validation

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

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

Cross Validation

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Test Set Training Set

10-fold cross-validation

$$E_g = \quad 5.4$$

Cross Validation

- If you want to use more data for training then you can use cross validation
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$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

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Test Set   Training Set

10-fold cross-validation

$$E_g = \quad 1.4$$

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 Training Set

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Training Set Test Set Training Set

10-fold cross-validation

3.2

$$E_g =$$

Cross Validation

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Training Set Test Set Training Set

10-fold cross-validation

$$E_g = \qquad 7$$

Cross Validation

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Training Set Test Set Training Set

10-fold cross-validation

$$E_g = \qquad 0.59$$

Cross Validation

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Training Set — Test Set — Training Set

10-fold cross-validation

4.1

$$E_g =$$

Cross Validation

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Training Set   Test Set   Training Set

10-fold cross-validation

$E_g =$

5

Cross Validation

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Training Set Test Set

10-fold cross-validation

$E_g =$ 5.8

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																		

Leave-one-out cross-validation

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Leave-one-out cross-validation

$$E_g = \quad 1.4$$

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Leave-one-out cross-validation

$$E_g = \qquad 3$$

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Leave-one-out cross-validation

$E_g =$ 3.7

Cross Validation

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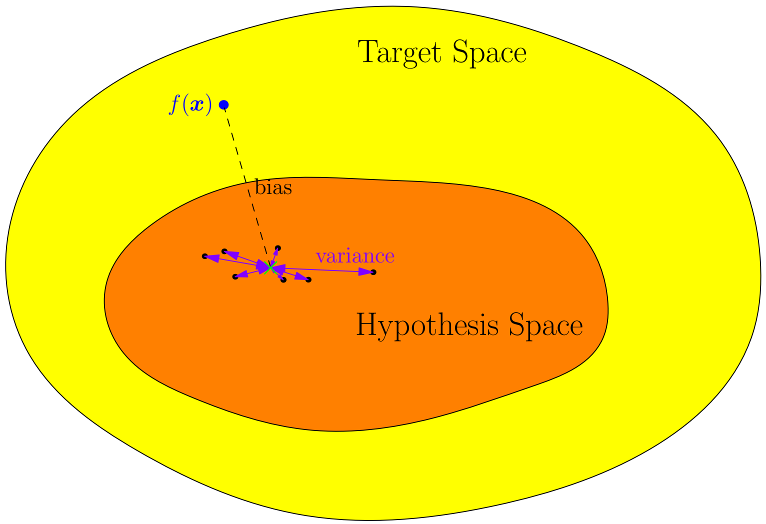
$$\langle E_g \rangle = 3.98$$

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

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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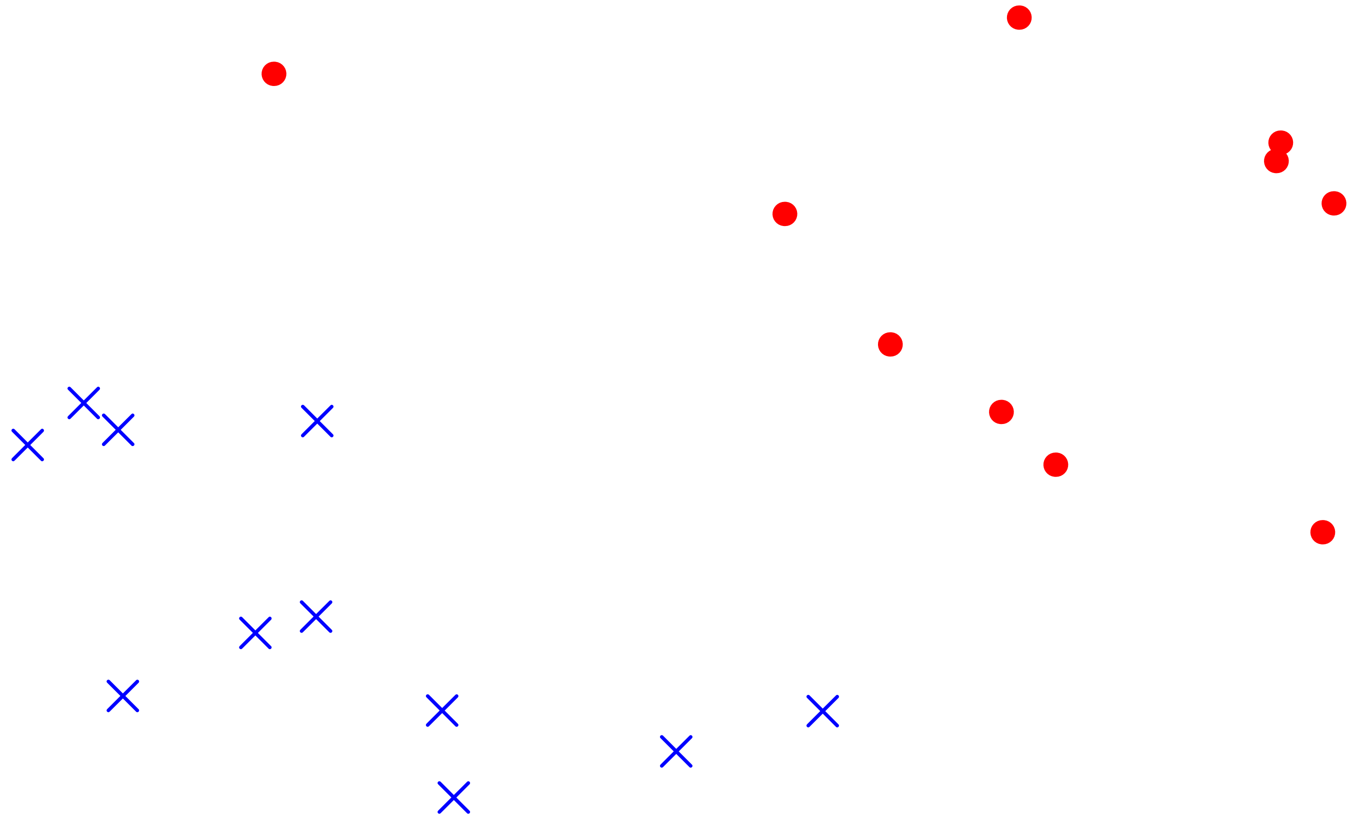
Linear Separation of Data

- SVMs classify linearly separable data



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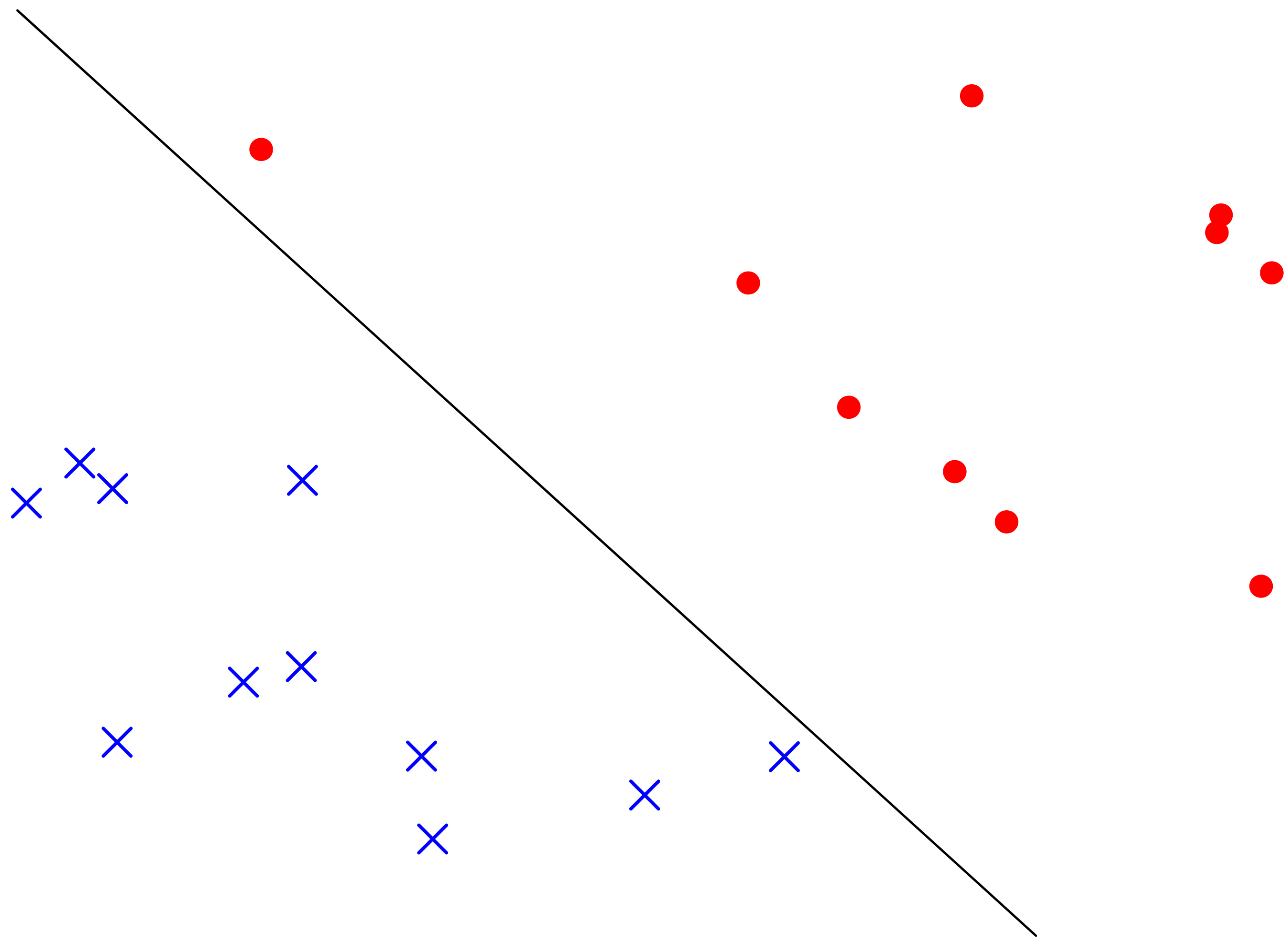

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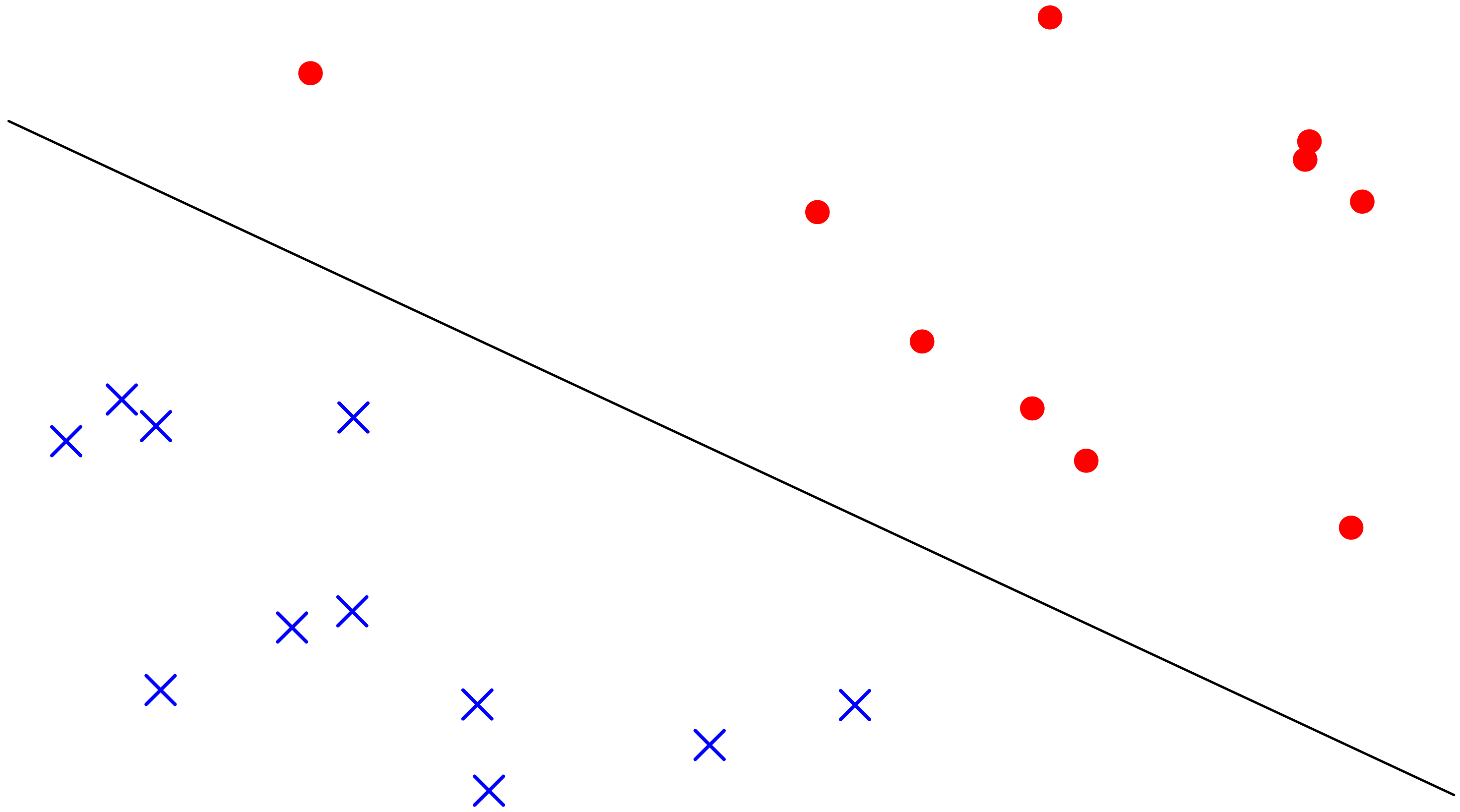

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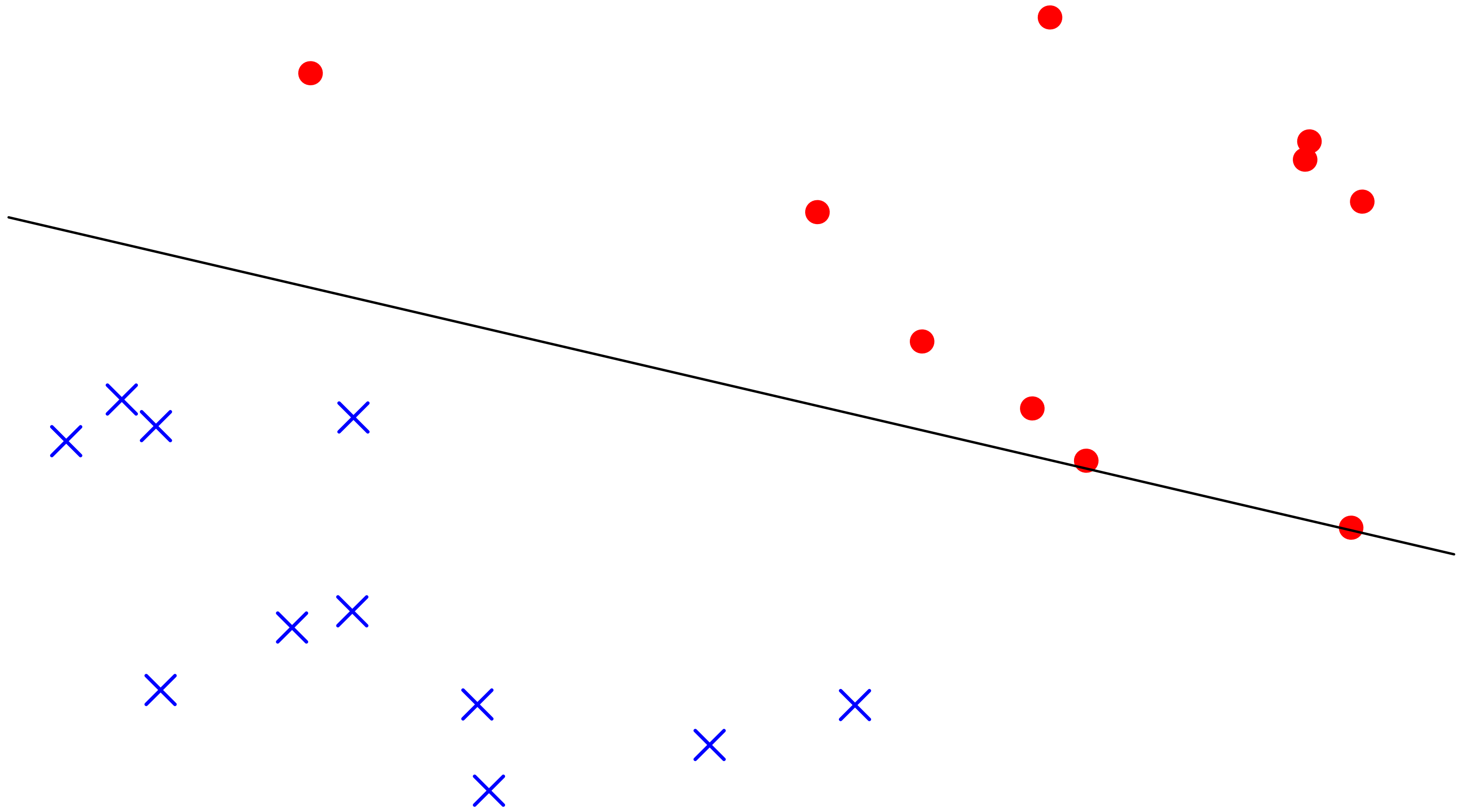

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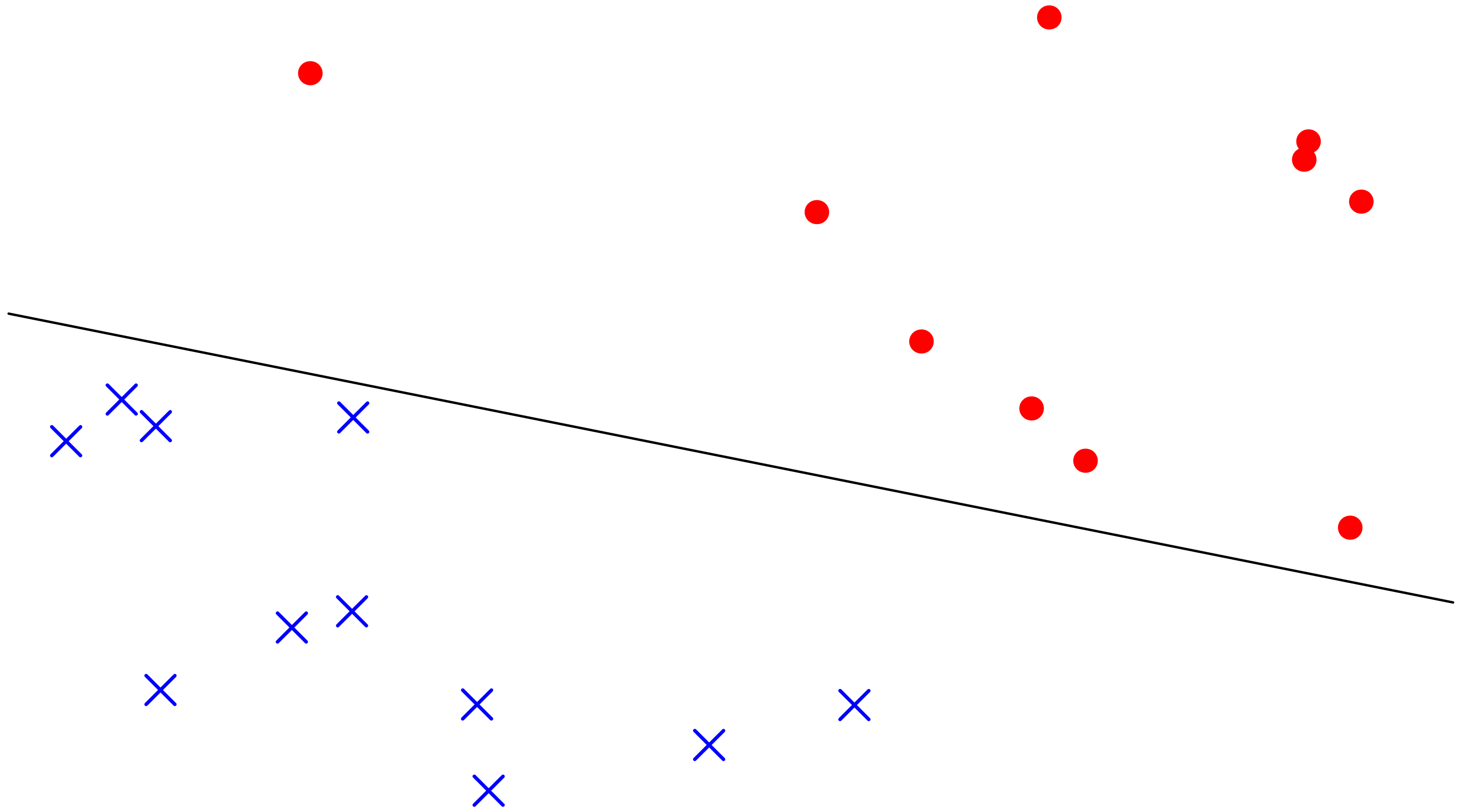

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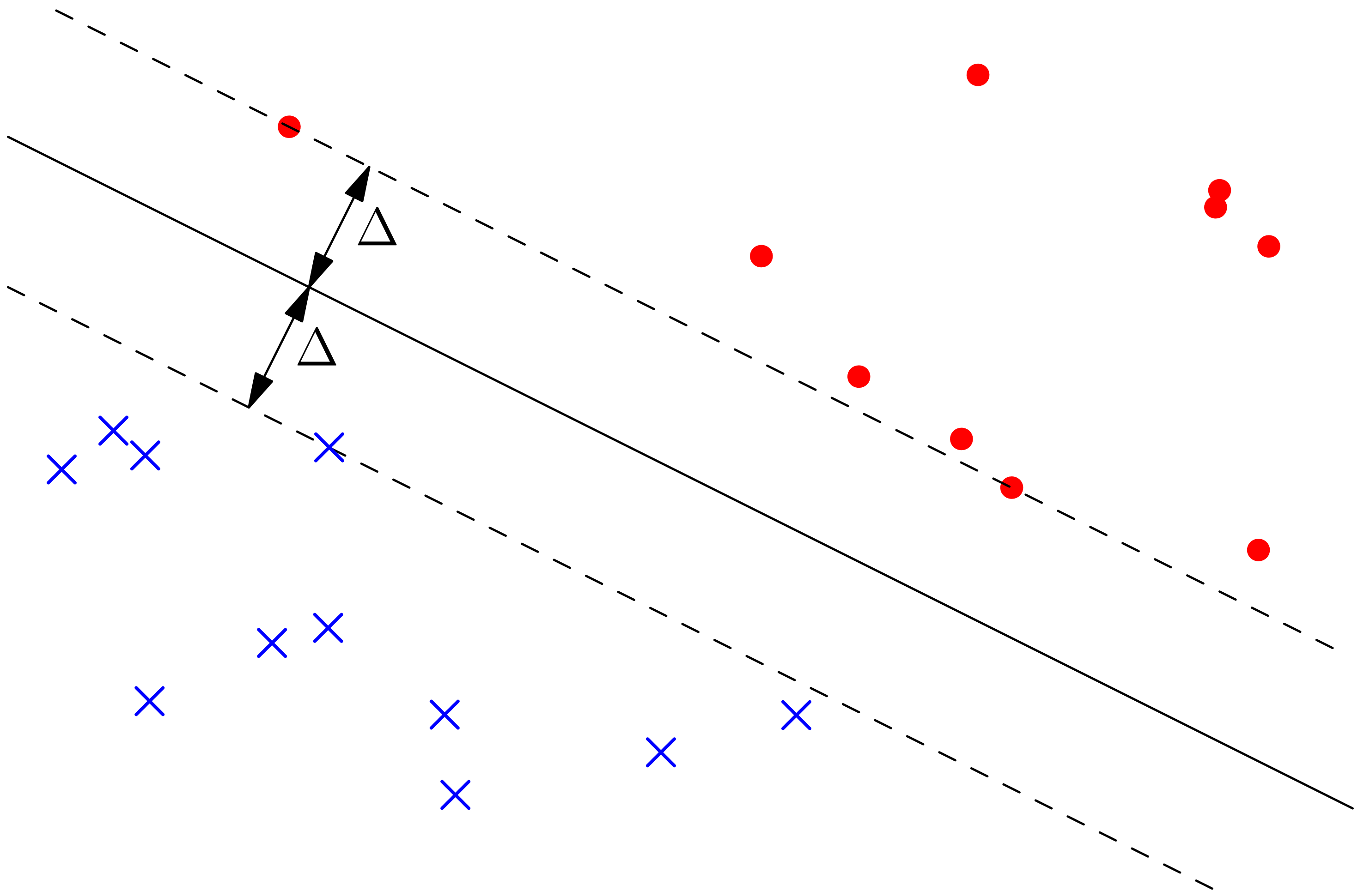

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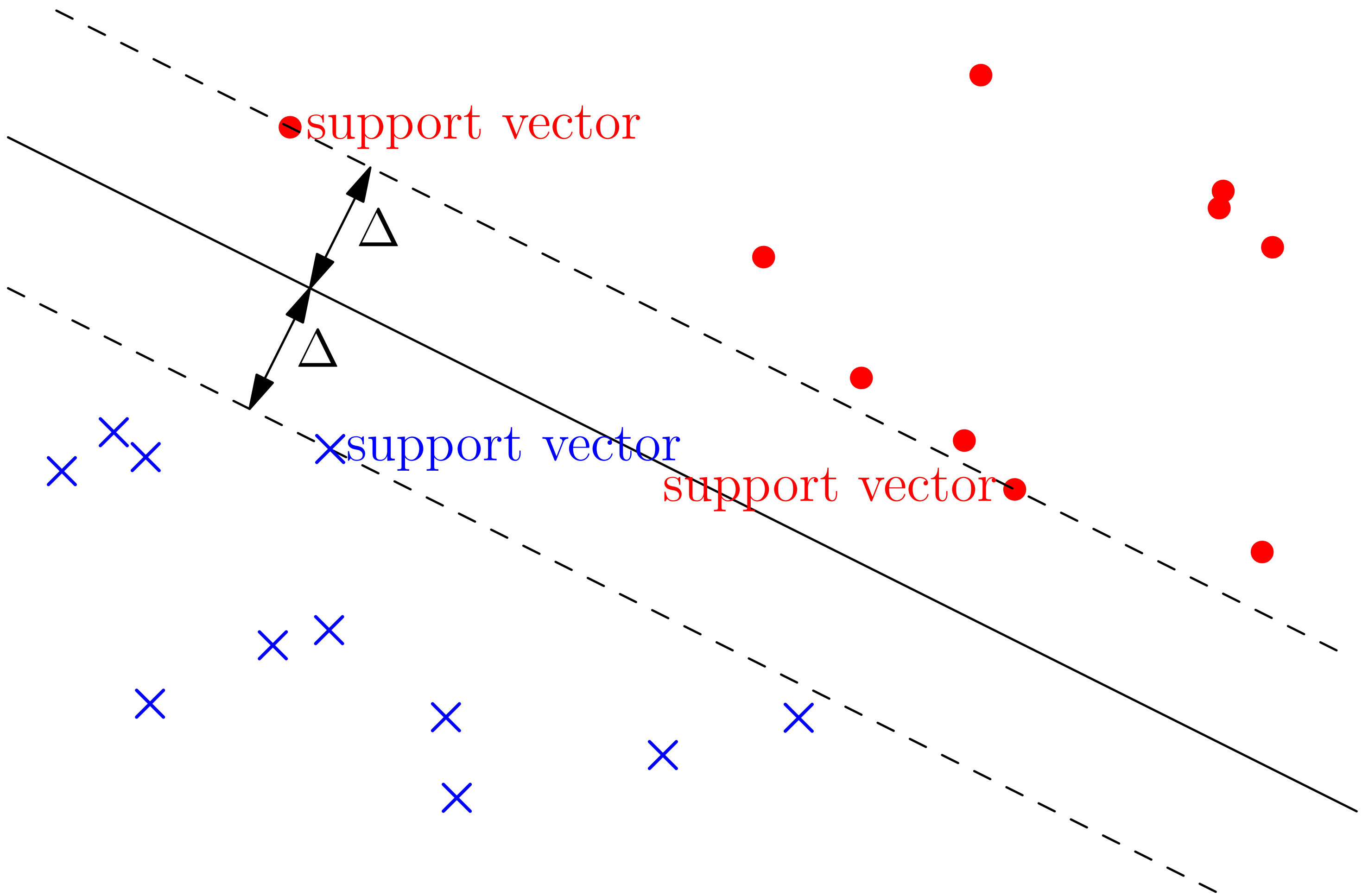

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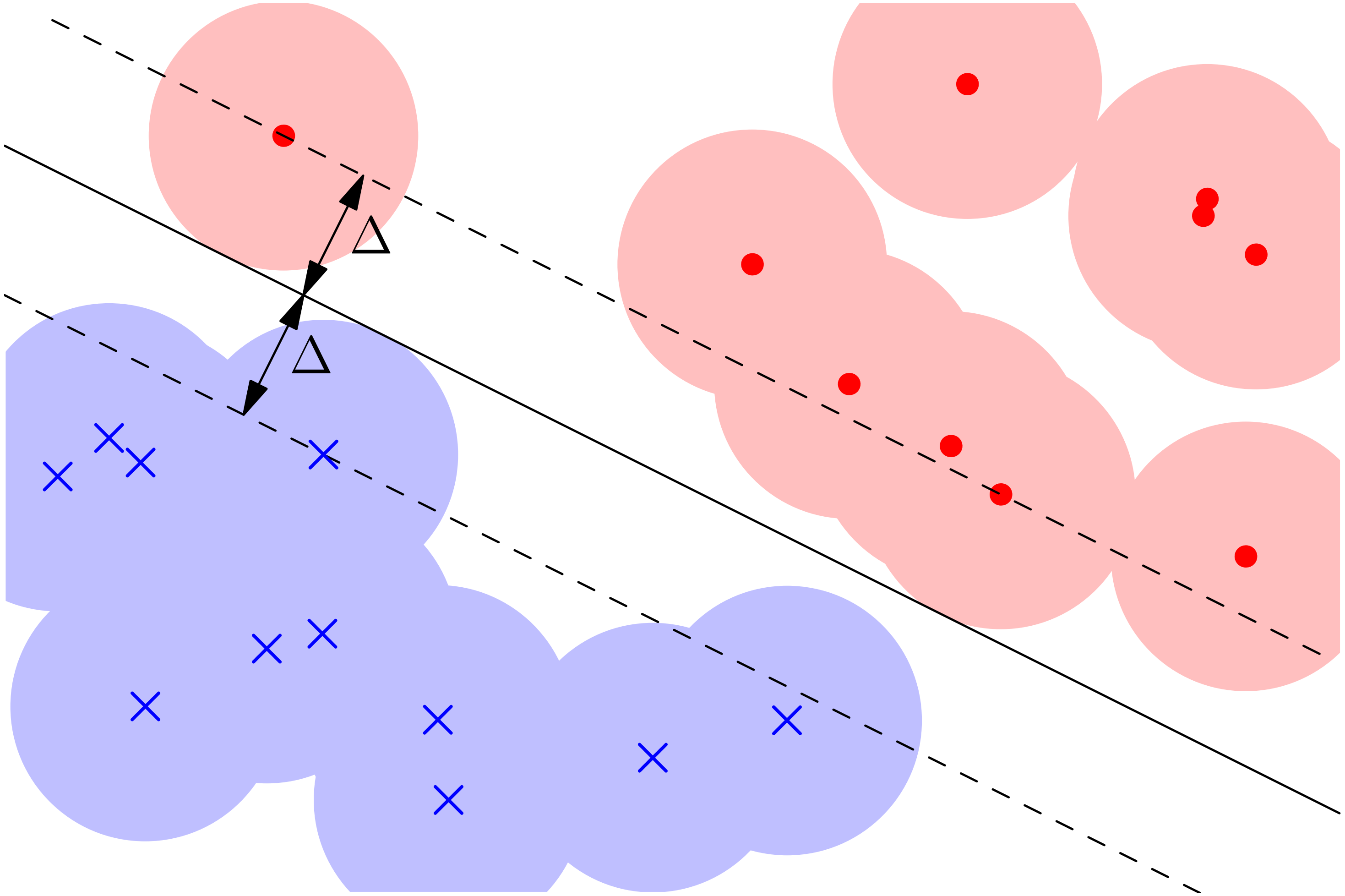

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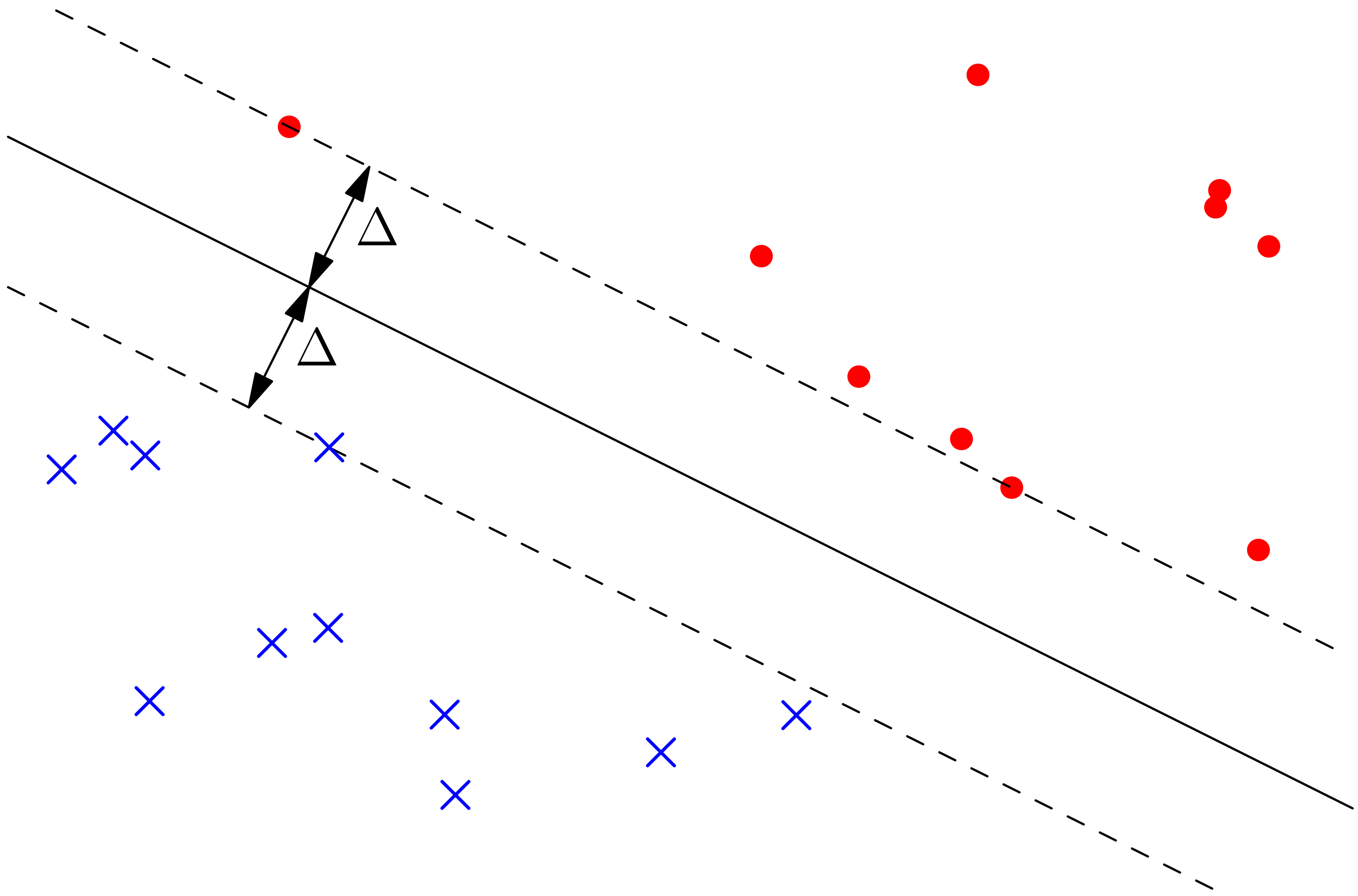

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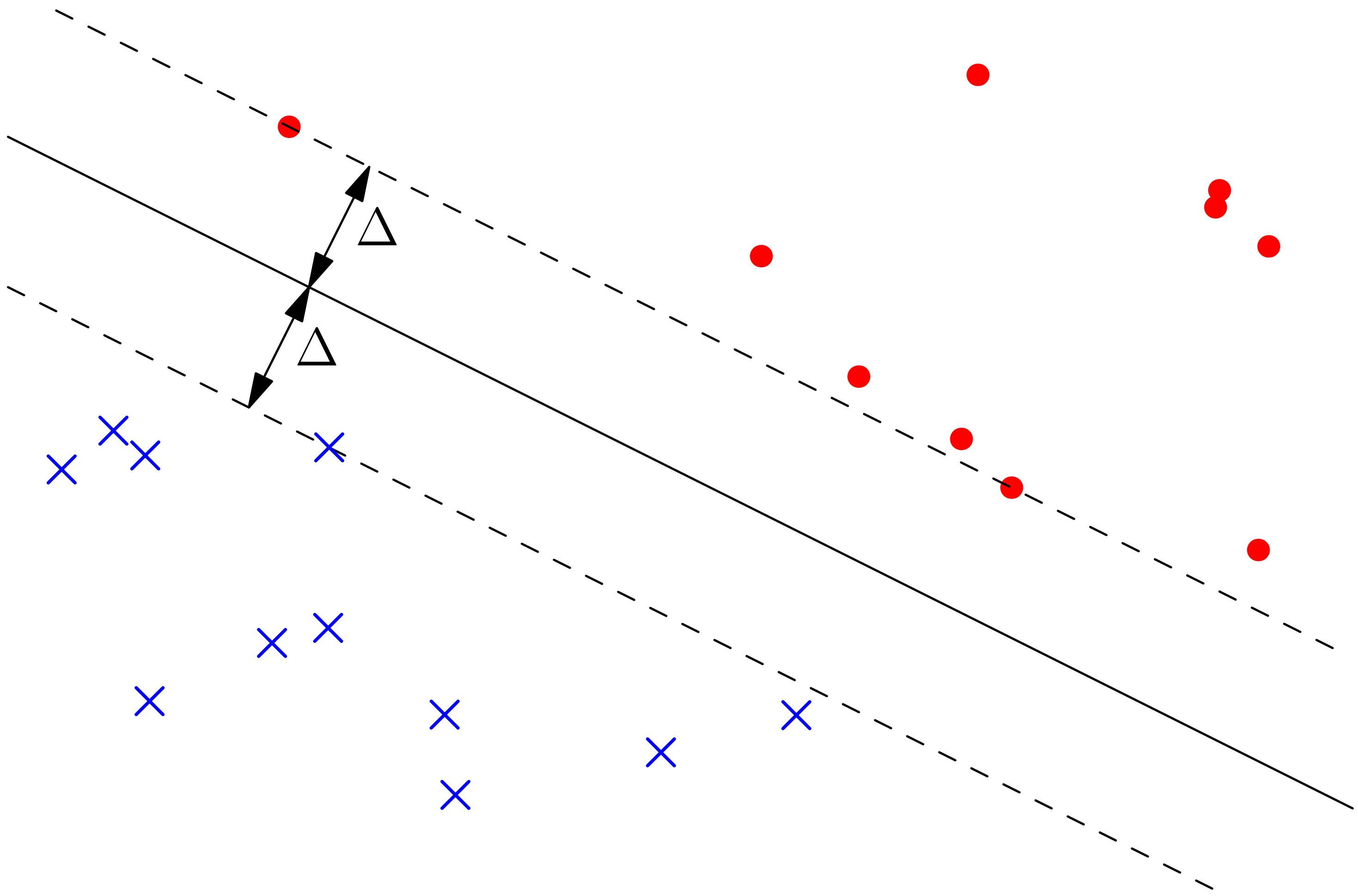

- Finds maximum-margin separating plane

Extended Feature Space

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

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

$m \gg p$

- Finding the maximum margin hyper-plane is time consuming in "primal" form if m 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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$$\boldsymbol{\phi}(\boldsymbol{x}_i) \cdot \boldsymbol{\phi}(\boldsymbol{x}_j) = \sum_{k=1}^{m} \phi_k(\boldsymbol{x}_i)\, \phi_k(\boldsymbol{x}_j)$$

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

- Sometimes $\boldsymbol{\phi}(\boldsymbol{x}_i)$ is an infinite dimensional vector so its good we don't have to compute it!

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Kernel Functions

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

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

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

- 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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Non-linearly Separation of Data

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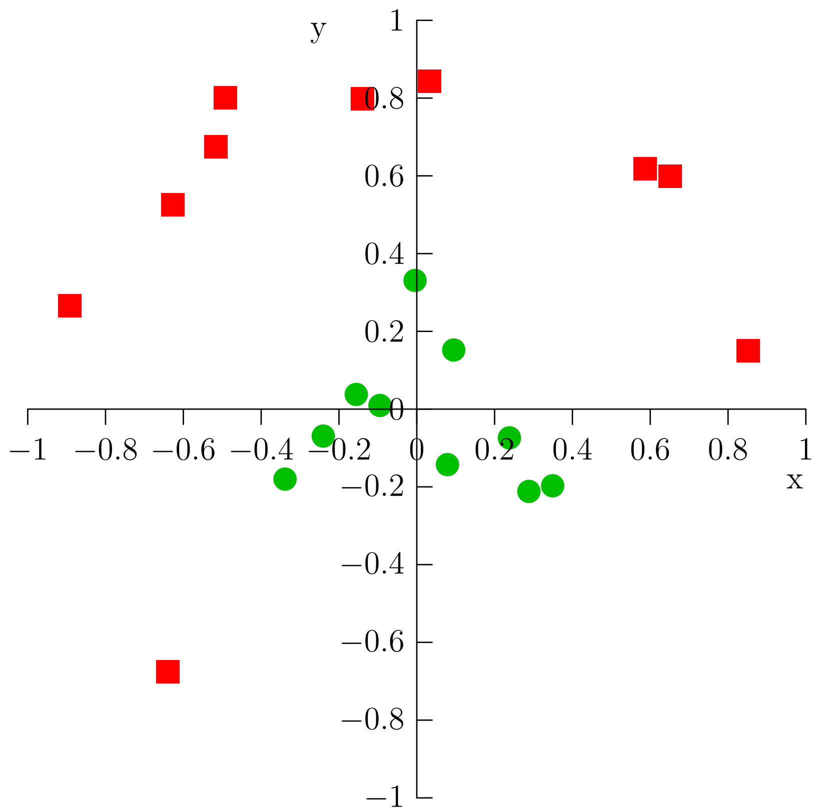

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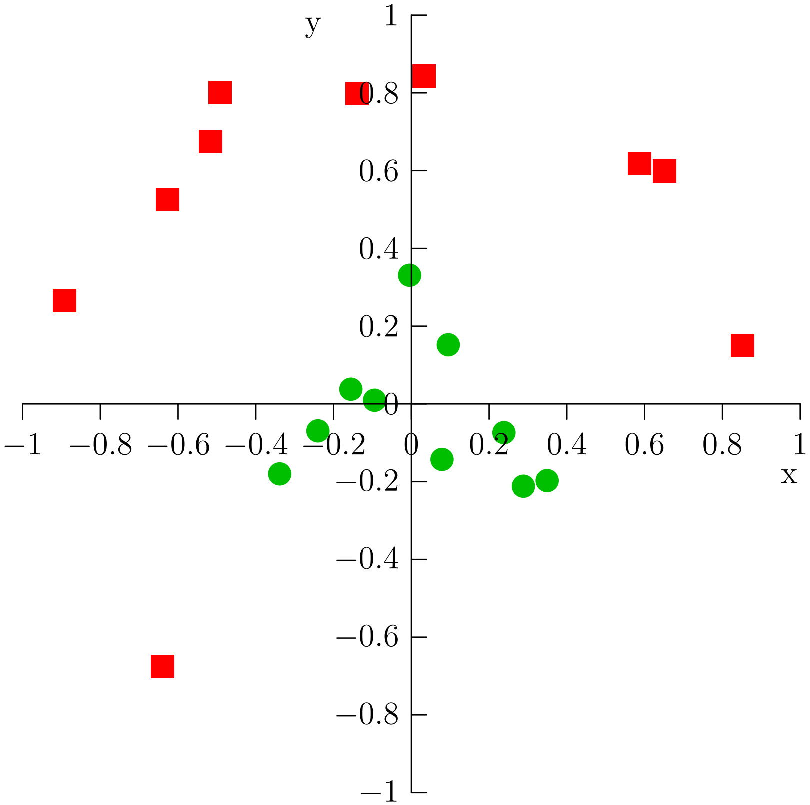

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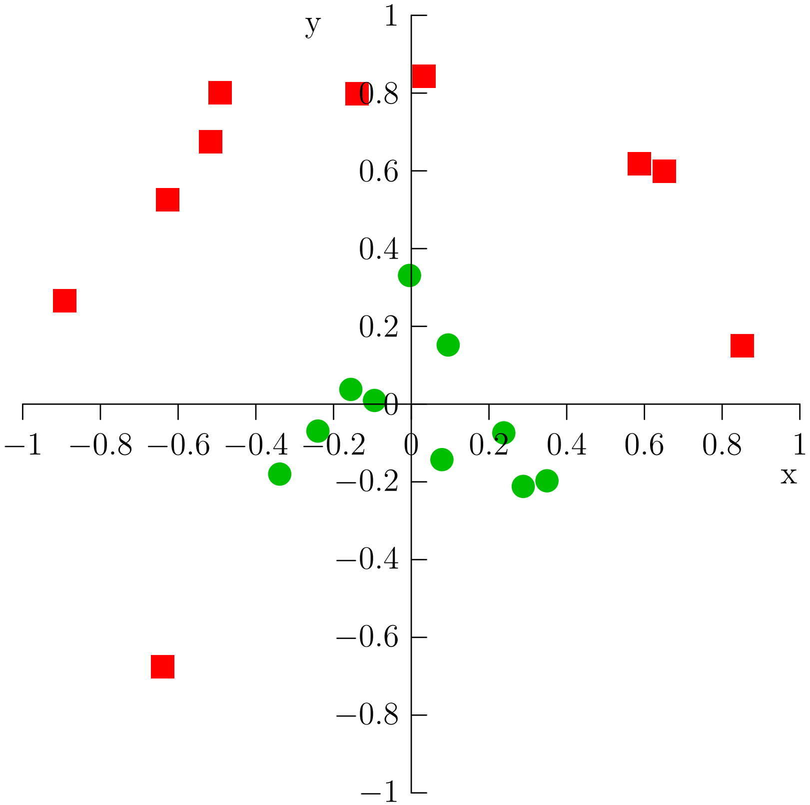

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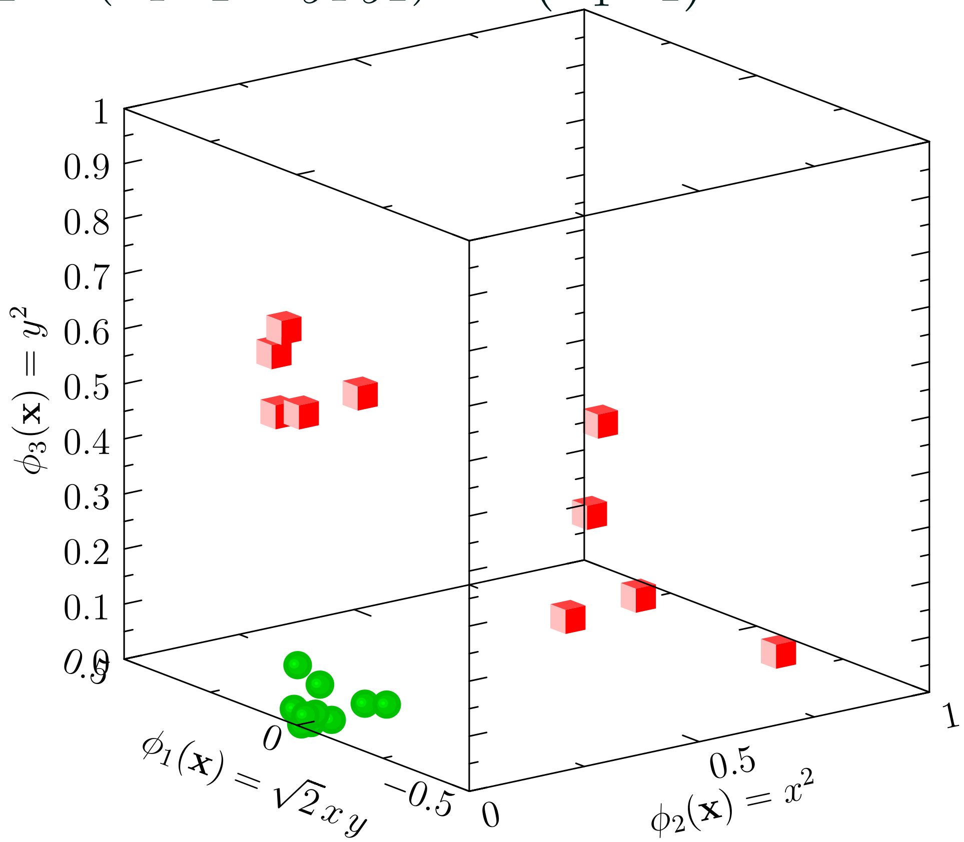

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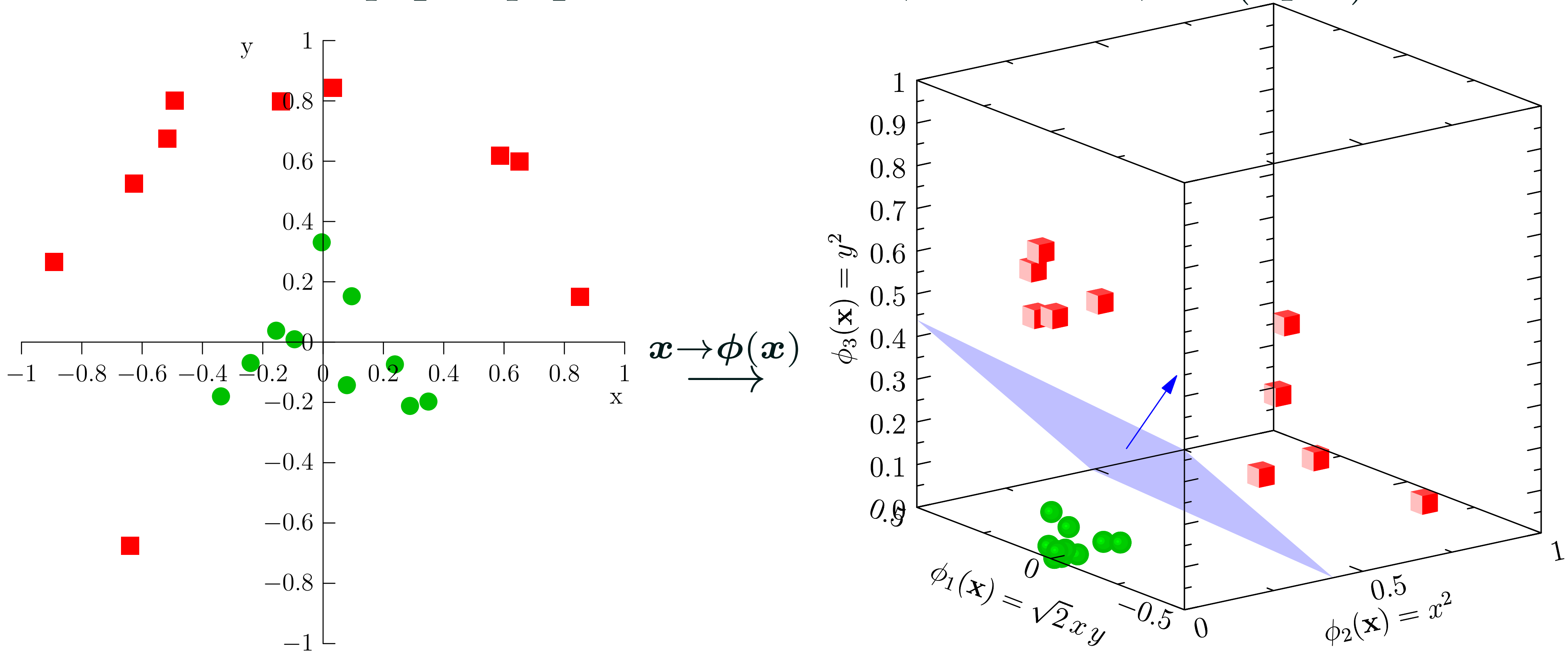

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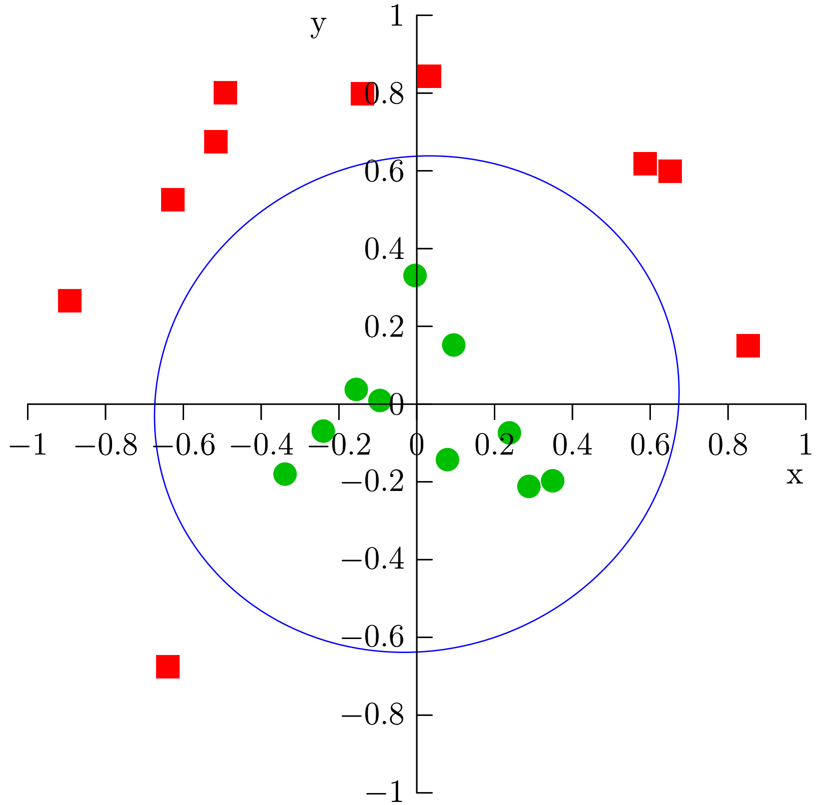

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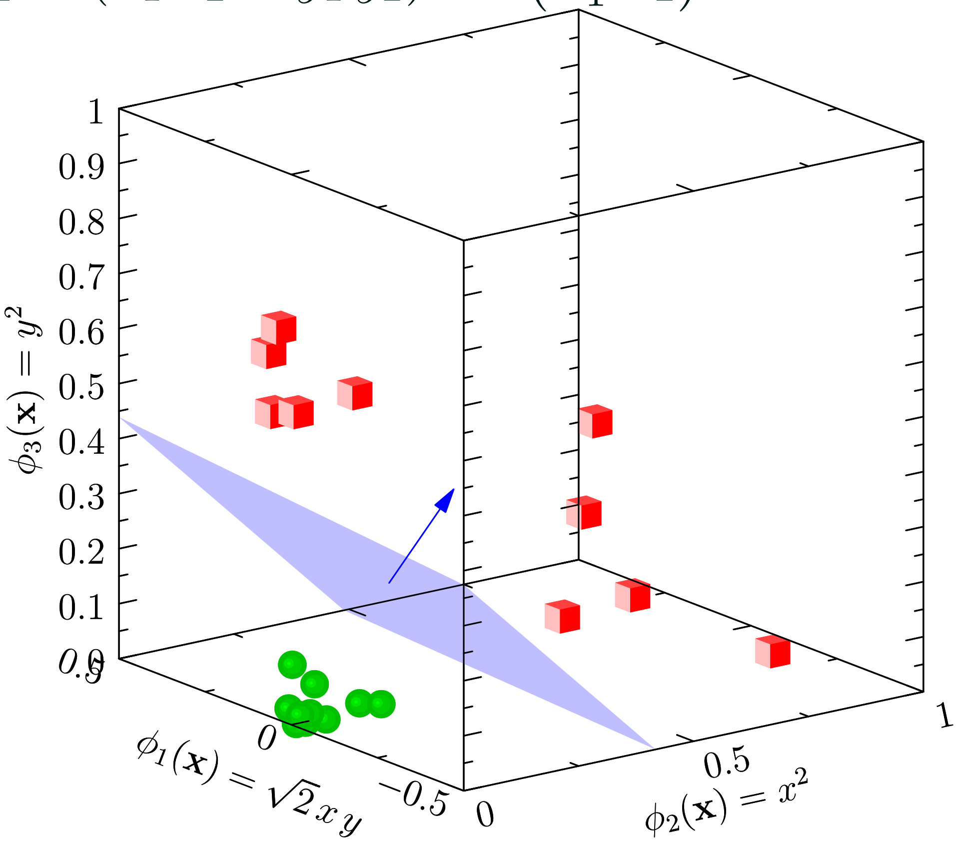

Computing the Maximum-Margin Hyper-plane

- 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)
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Getting SVMs to Work Well

- SVMs rely on distances between data points
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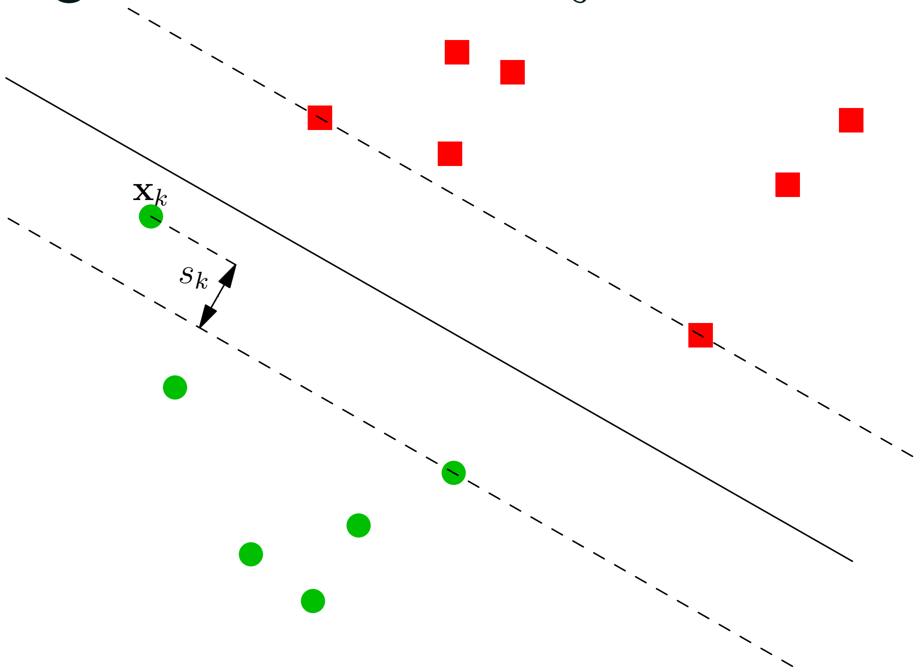

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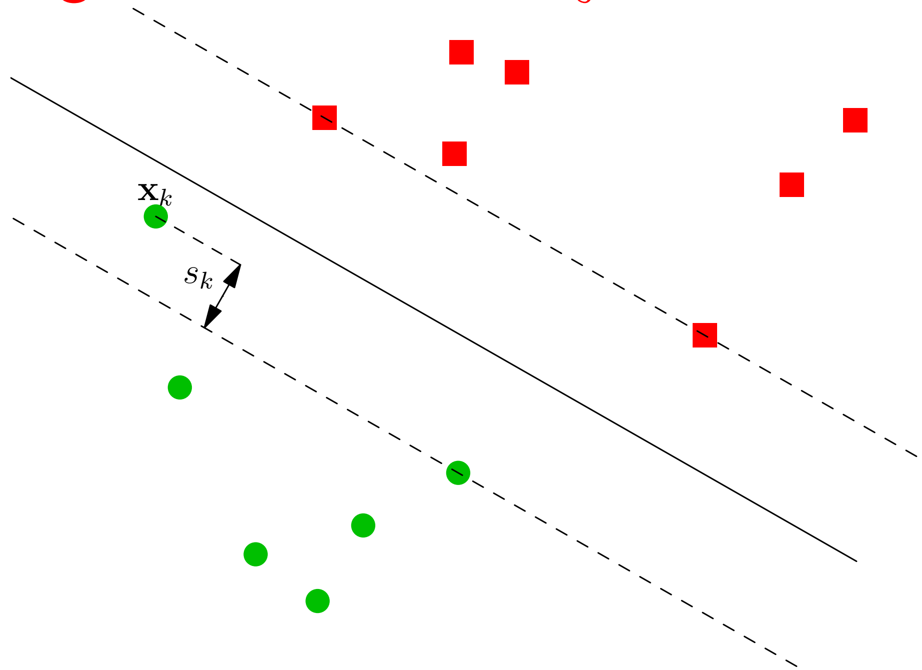

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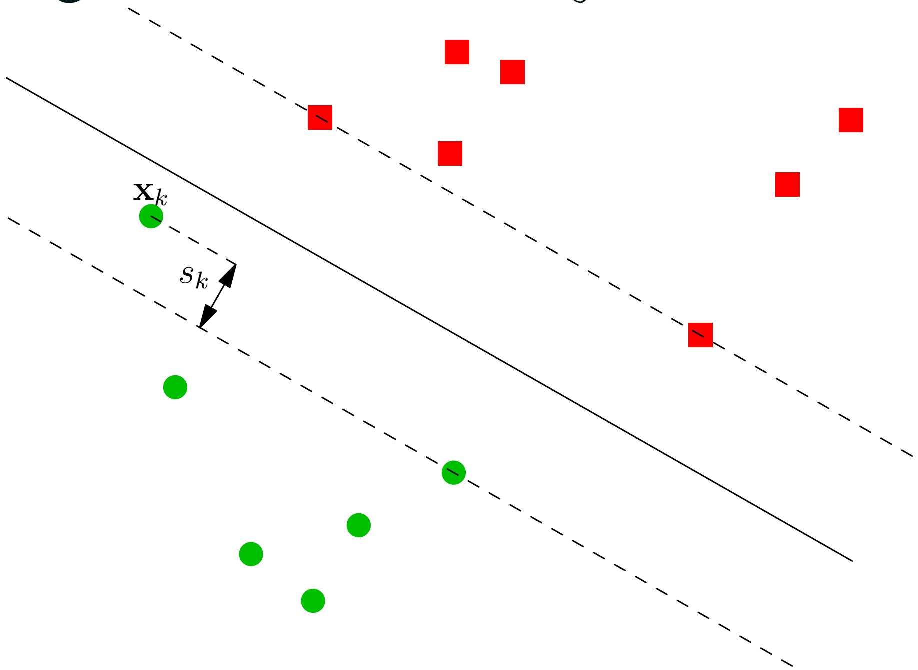

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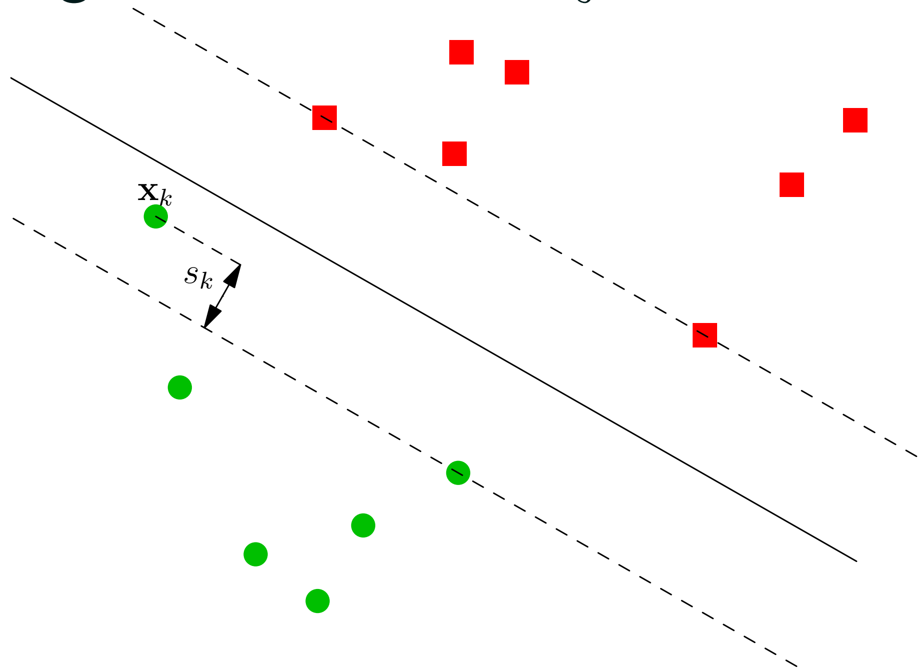

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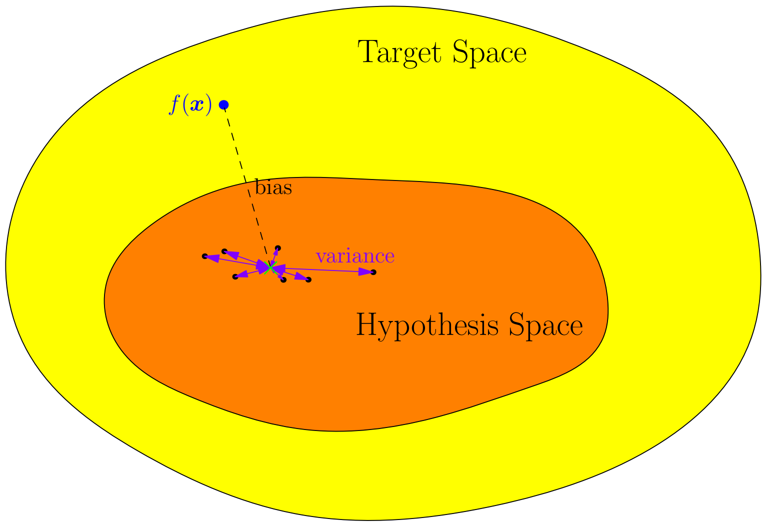
Outline

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



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- These are particularly good for handling messy data
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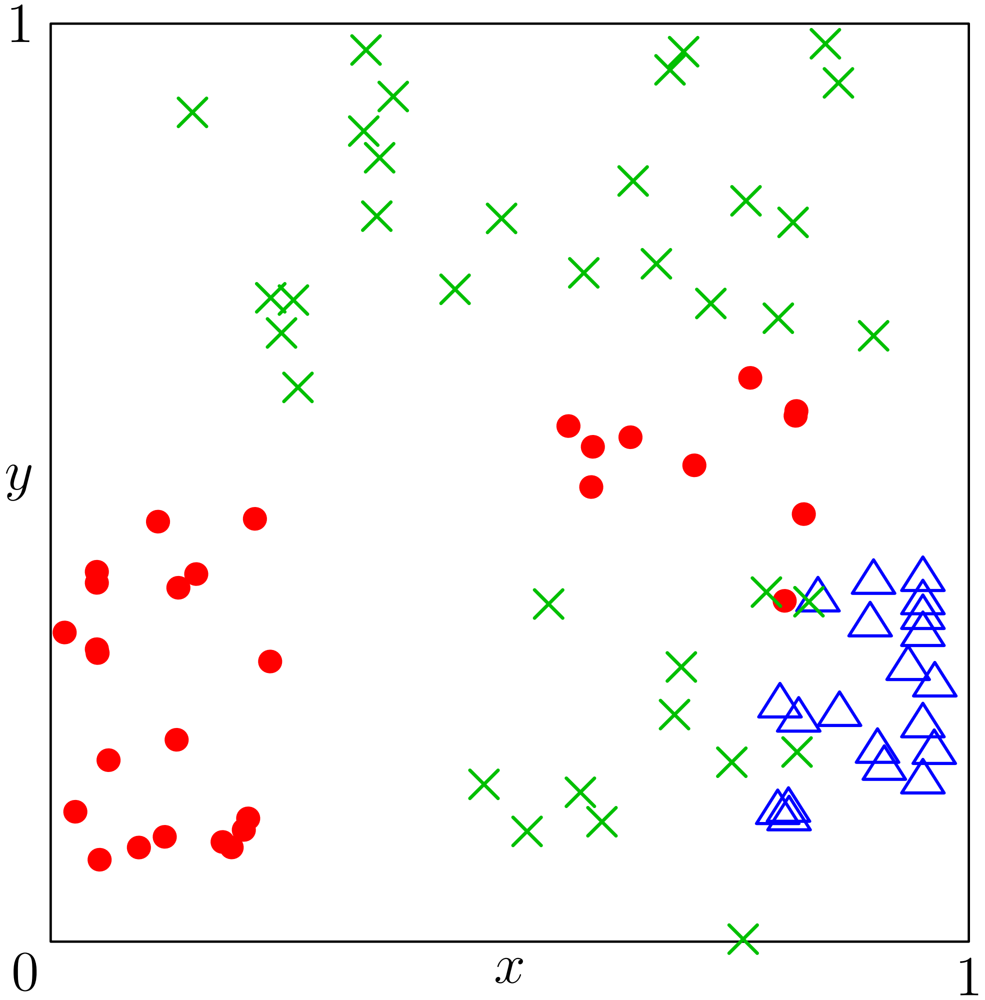

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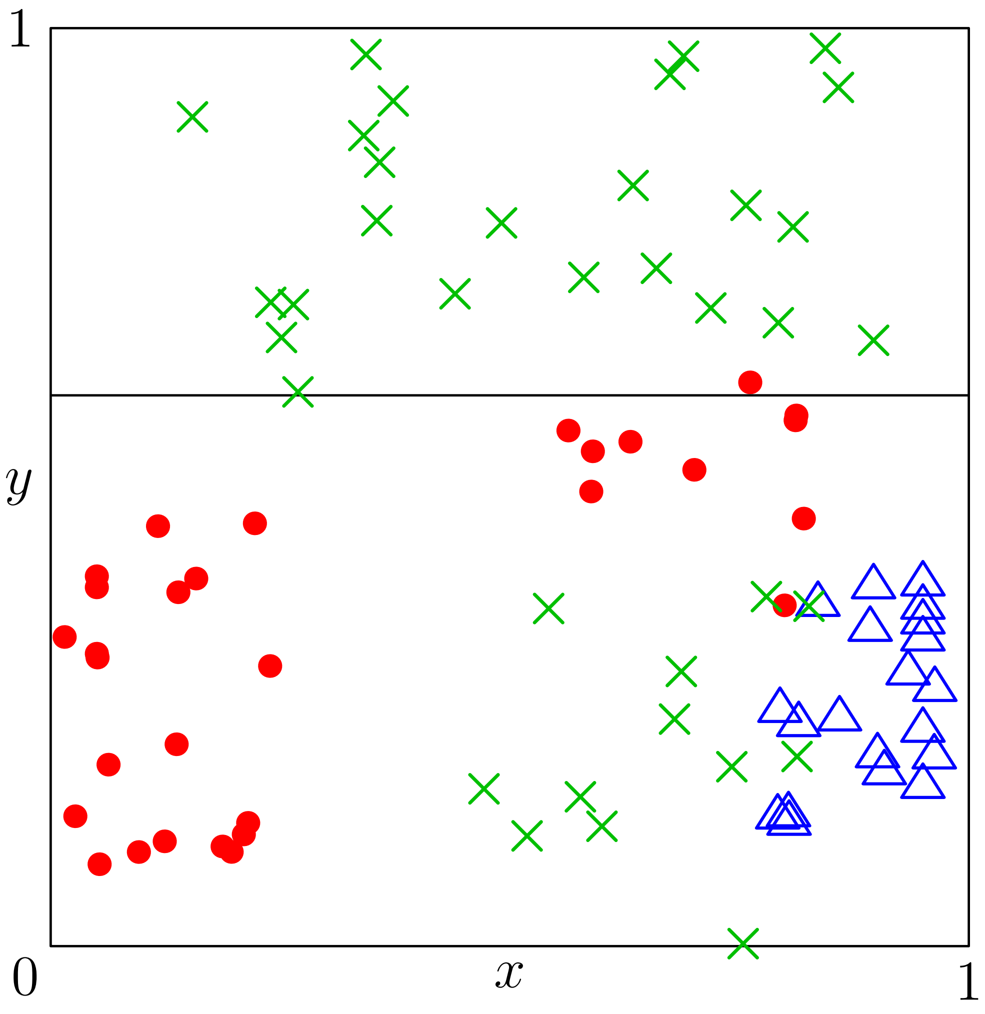

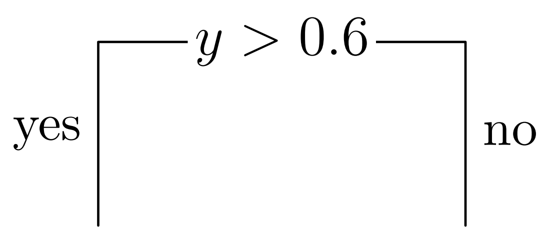

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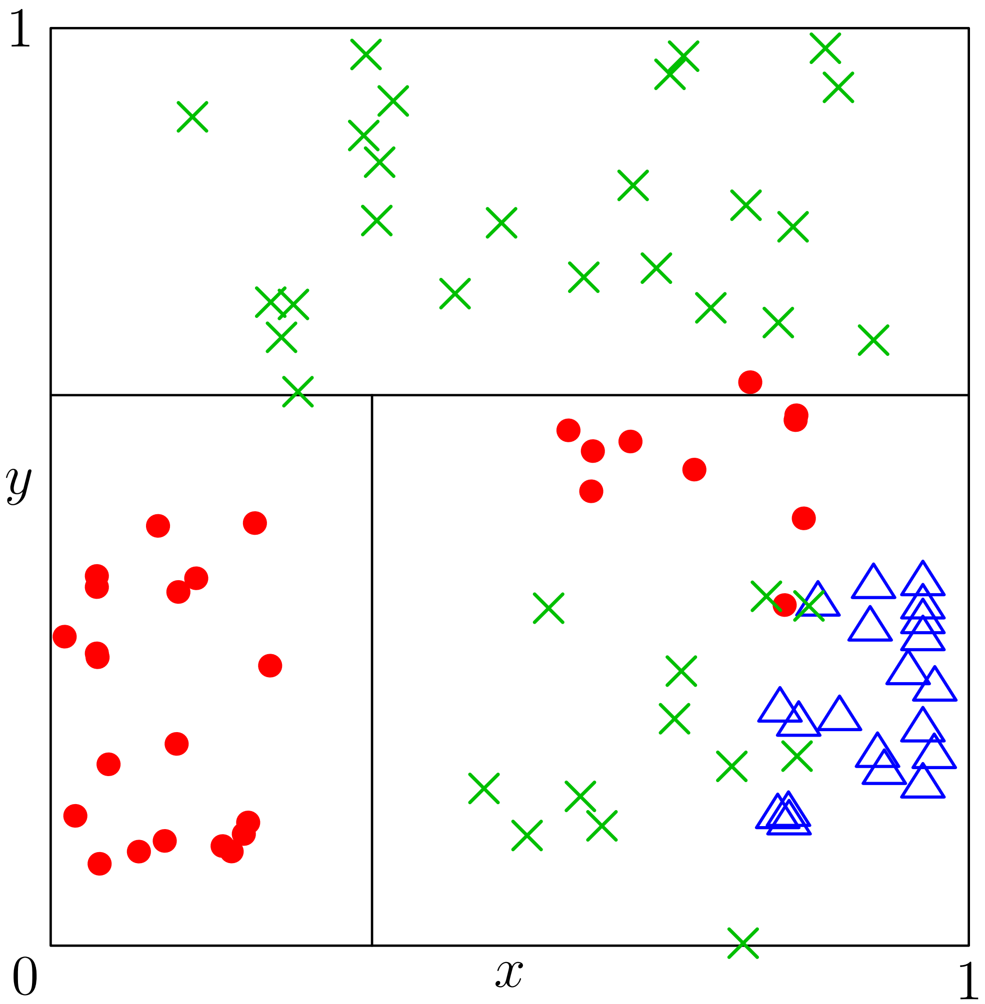

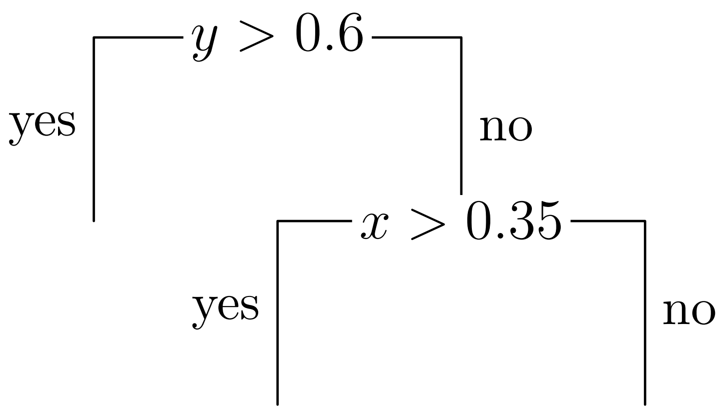

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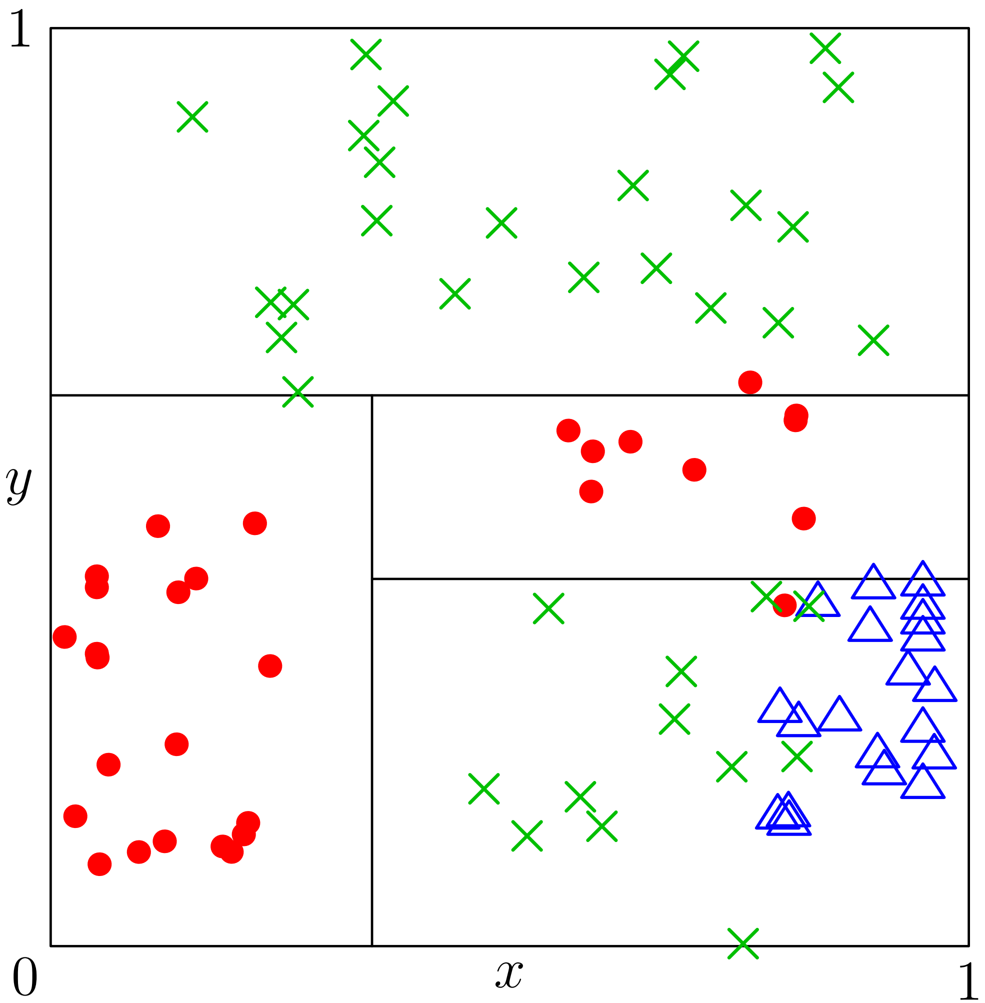

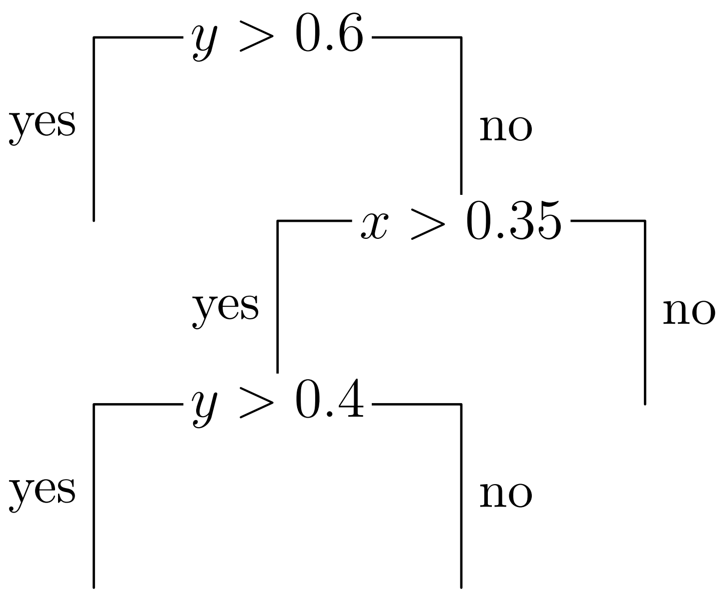

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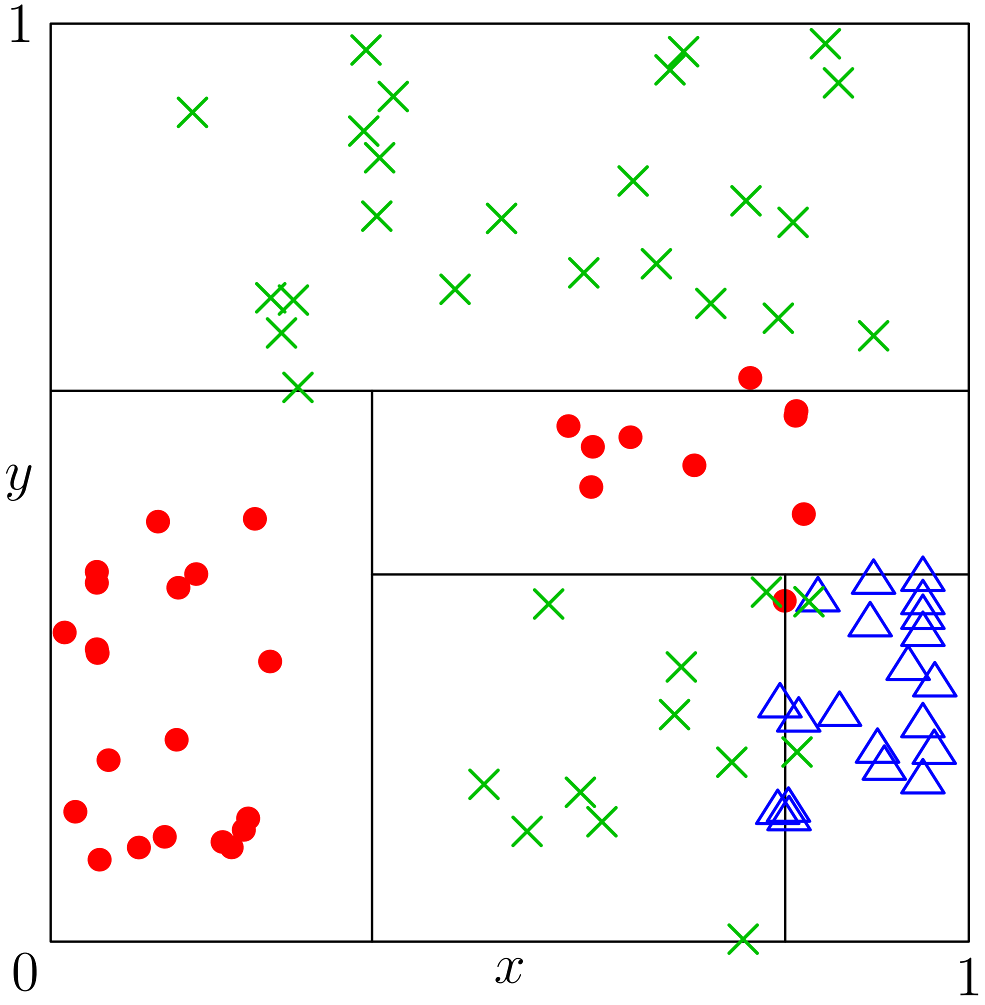

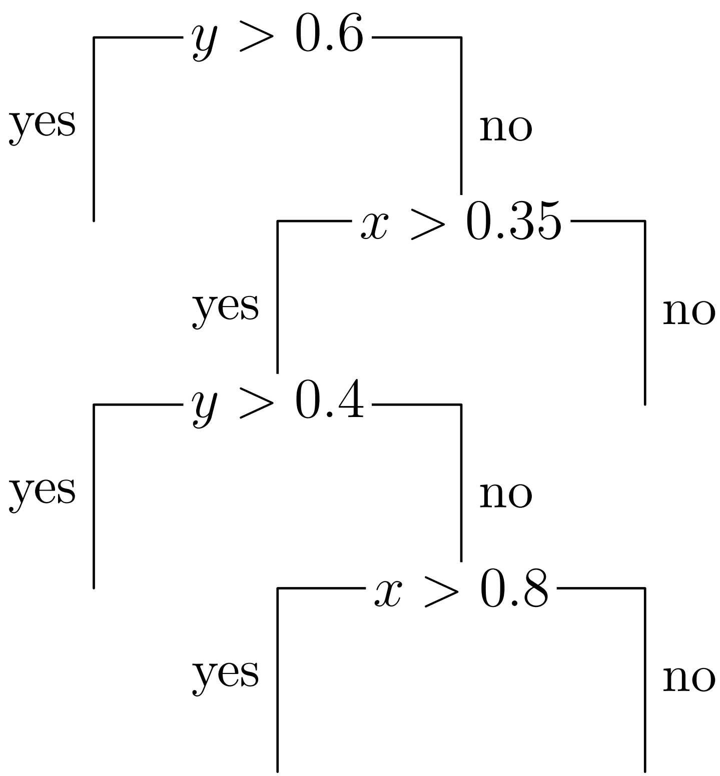

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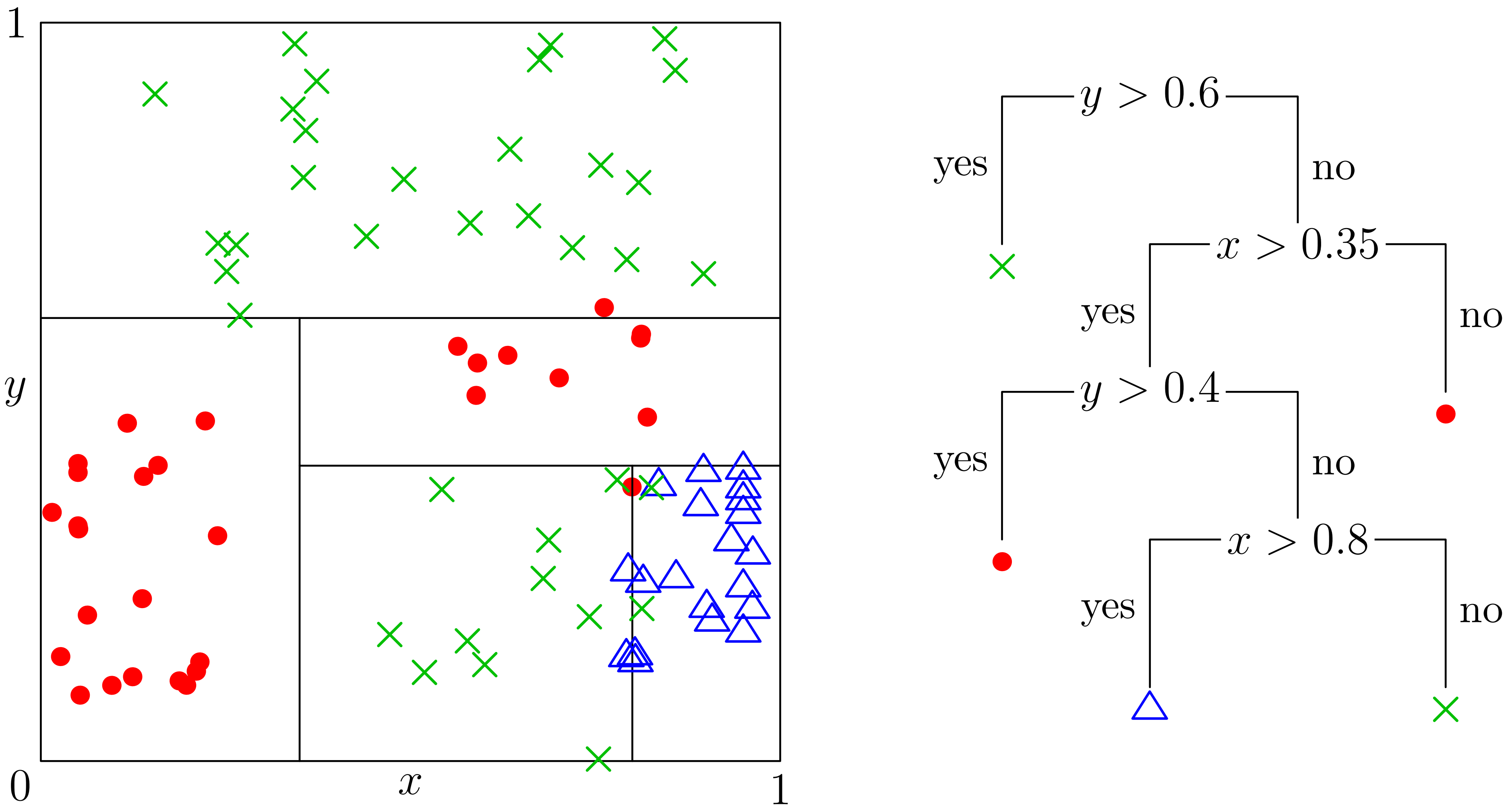

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Shallow Trees

- 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. $\sqrt{p}$)
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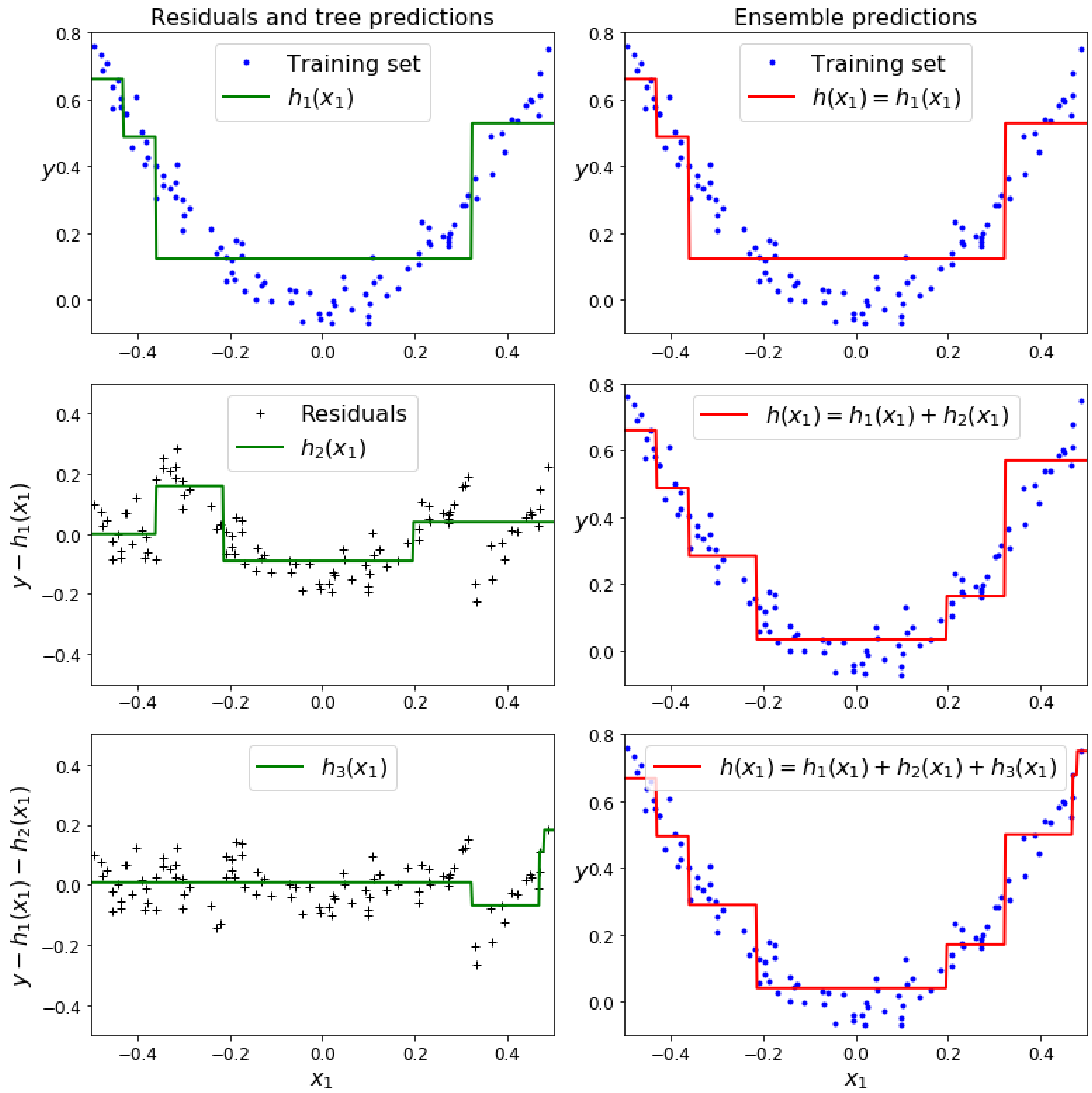
Residuals and tree predictions
Ensemble predictions
Training set
$h_1(x_1)$
$h(x_1) = h_1(x_1)$
Residuals
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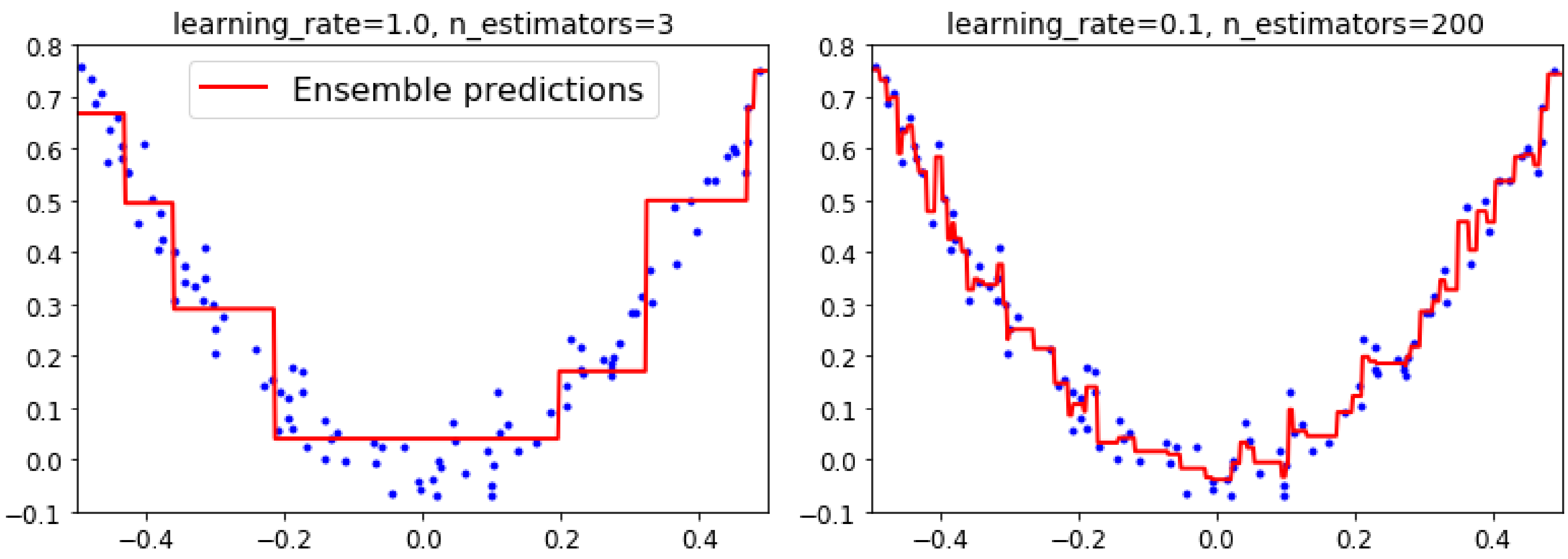
x_1

Keep On Going

- We can keep on going



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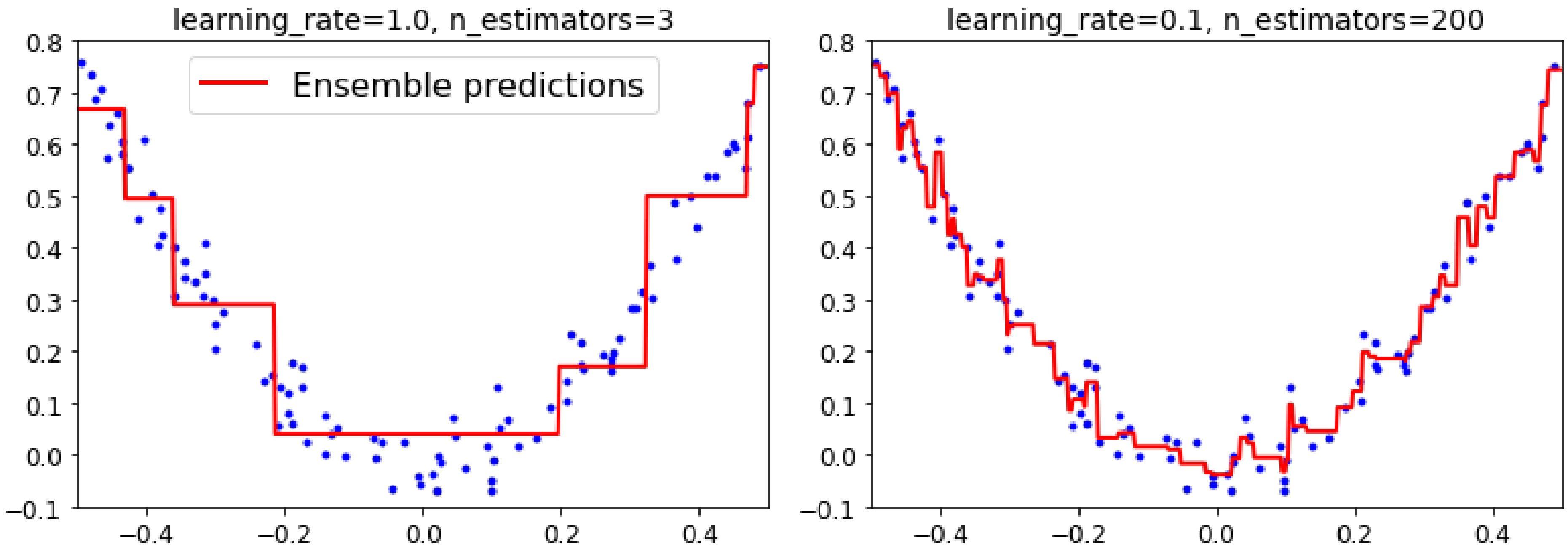
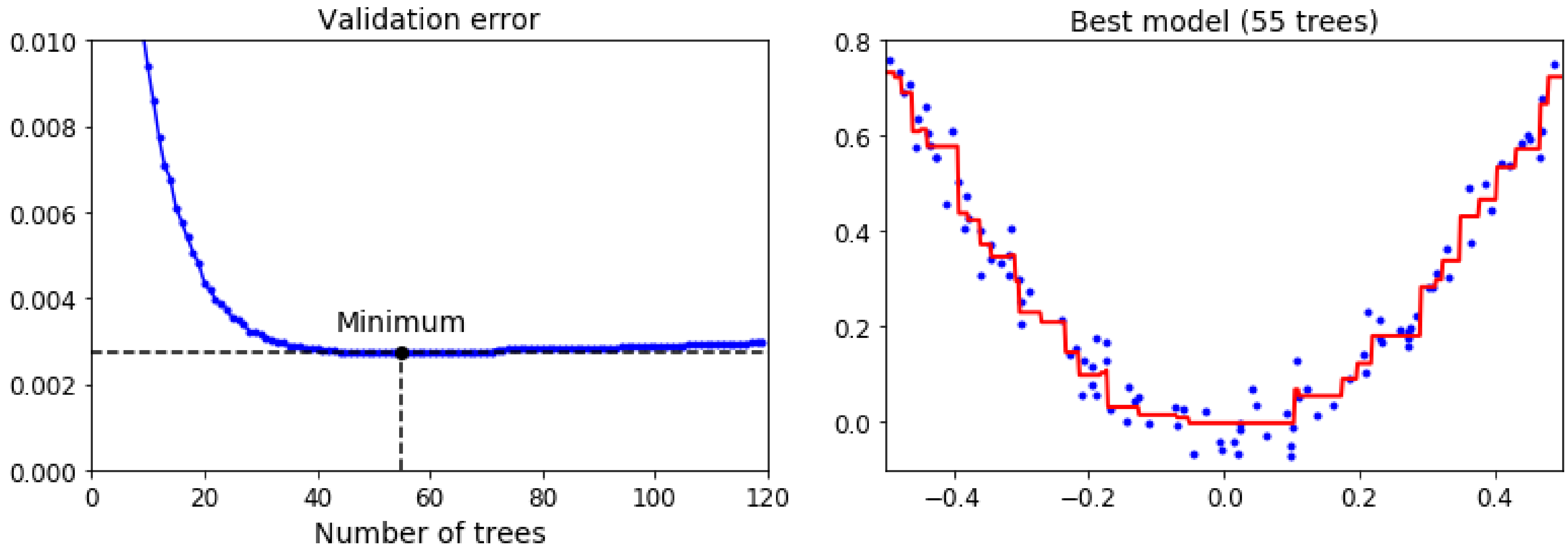


- But we will over-fit eventually

Early Stopping

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



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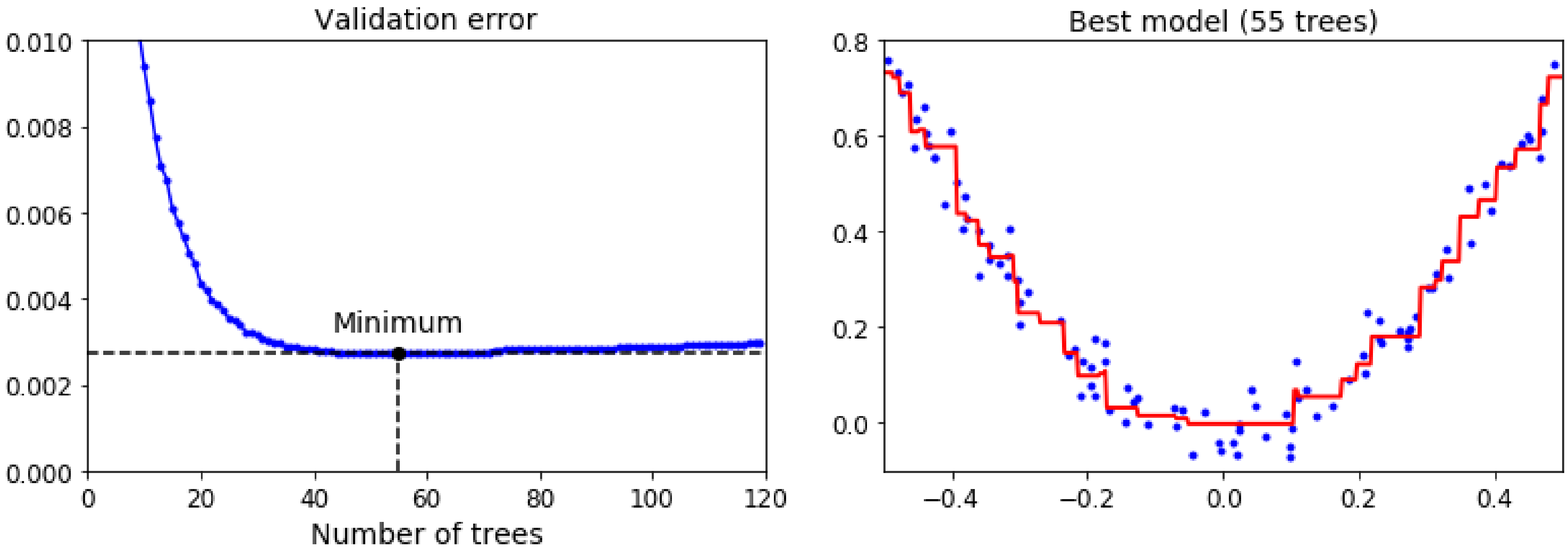

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- XGBoost is an implementation of gradient boosting that won the Higg's Boson challenge and regularly wins Kaggle competitions
- XGBoost stands for eXtreme Gradient Boosting
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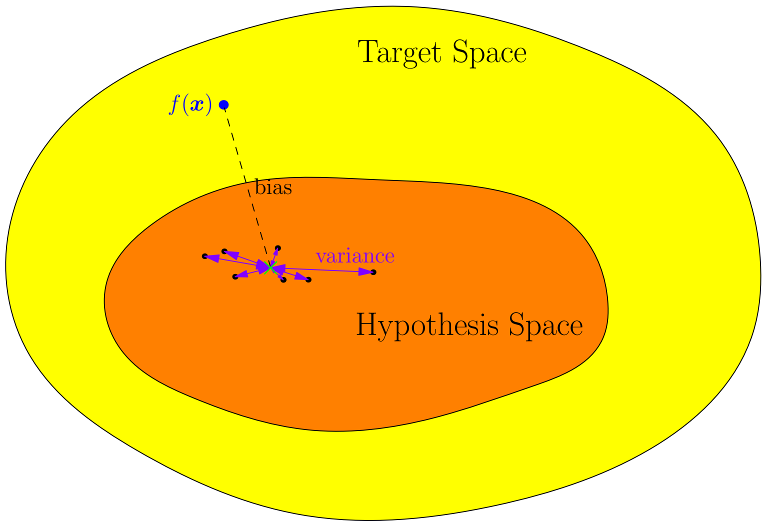
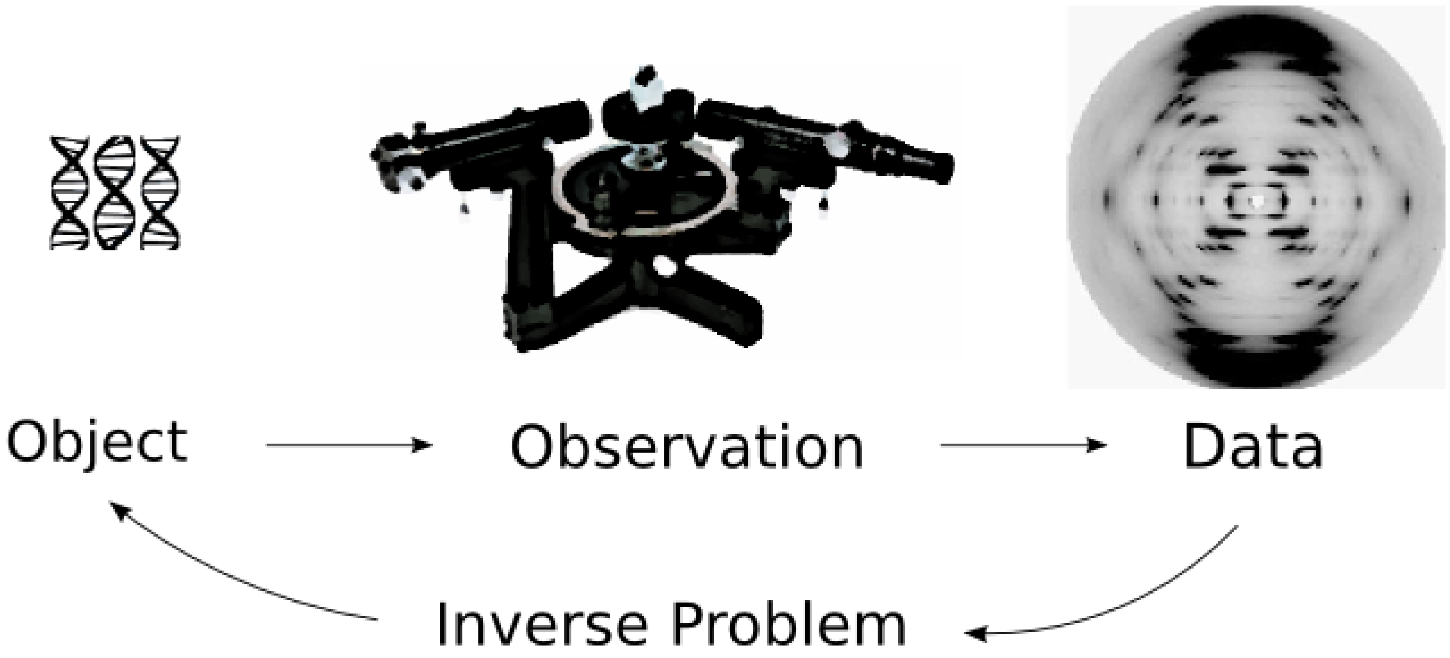
Outline

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



Inverse Problems



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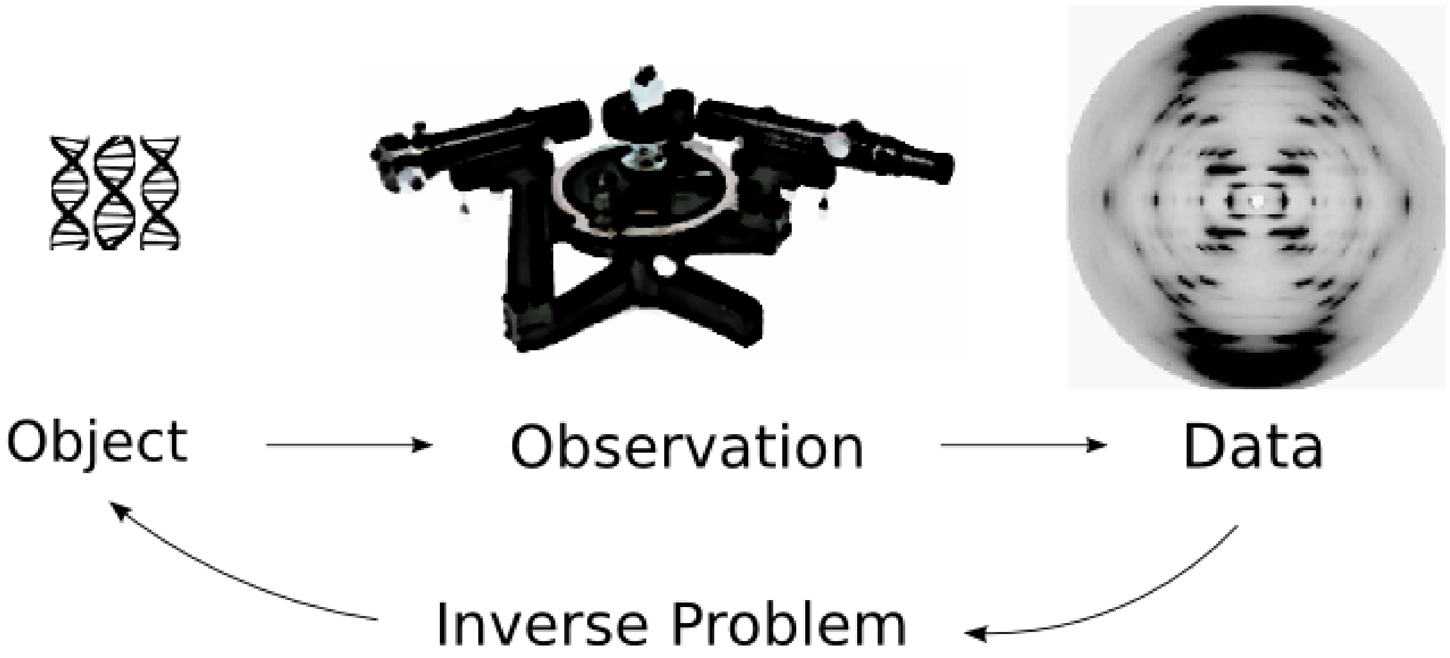

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Bayes' Rule

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

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

- 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 $\mathbb{P}(\mathcal{D}|W)$

- Multiplied by the **prior probability** of the world, $\mathbb{P}(W)$

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Worlds

- 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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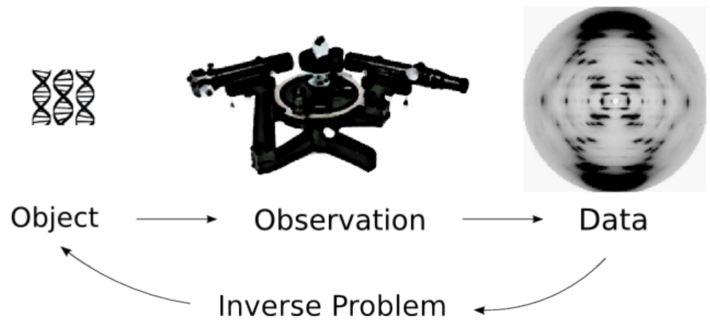
- Its optimal (follows from a simple probabilistic identity)

- It is relatively easy to model the likelihood (this is a forward process not an inverse process)



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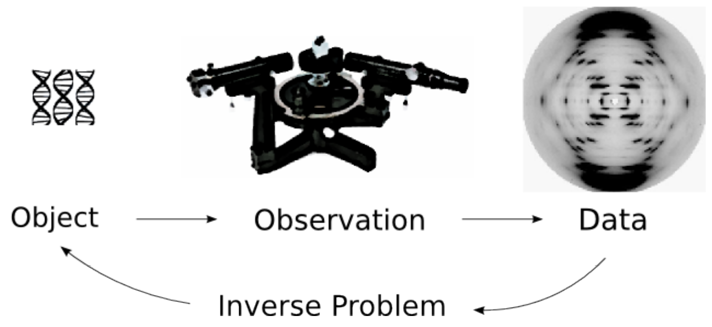

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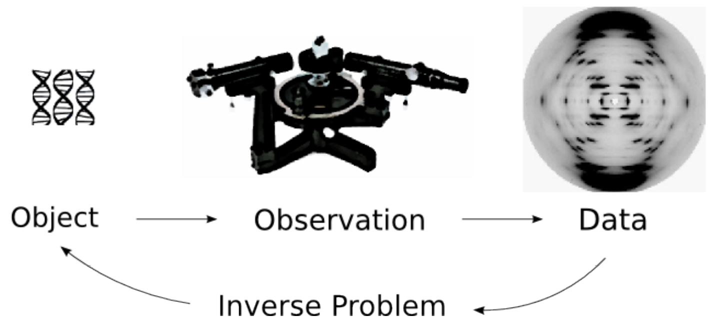

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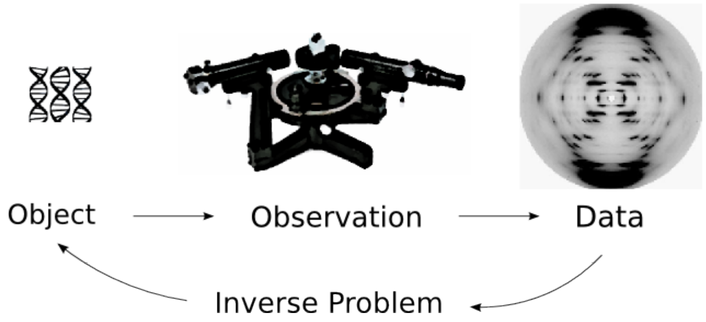

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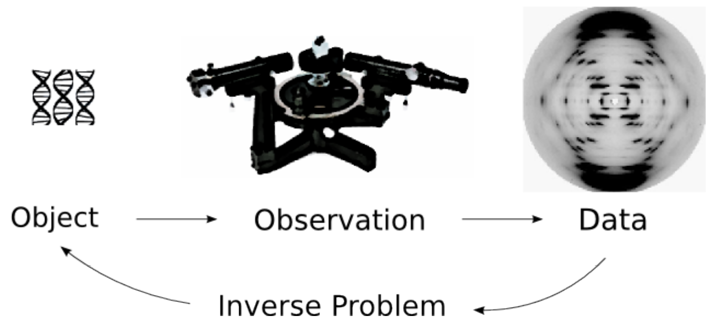

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- Need to be able to sum over all possible worlds

- This is technically challenging and/or computationally slow

- Markov Chain Monte Carlo (MCMC) is a very established framework for suming over worlds
  - ⋆ There exist mature libraries
  - ⋆ Large number of tricks to speed things up

- Various approximations also exist for averaging over worlds

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Simple Bayes

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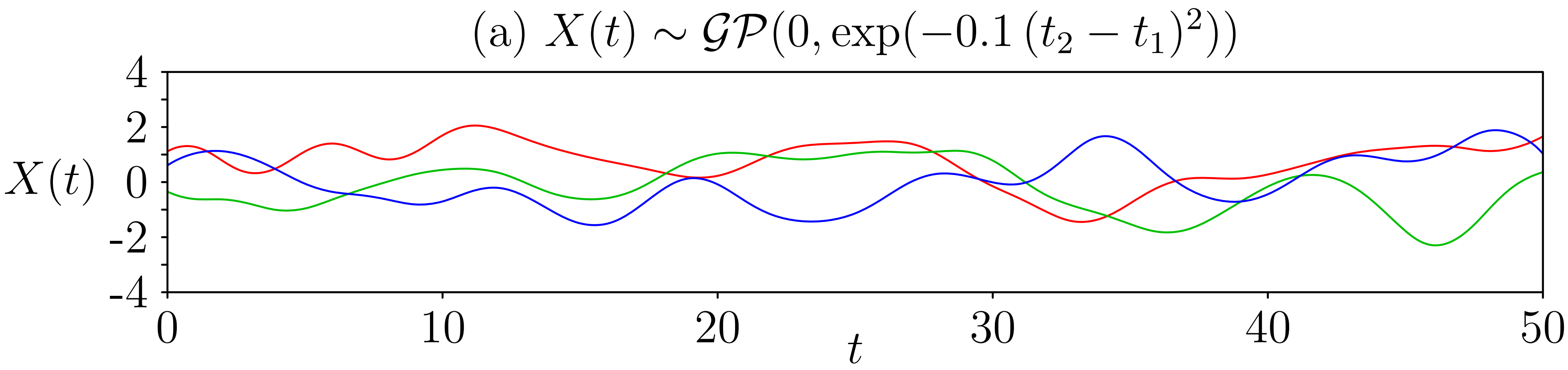

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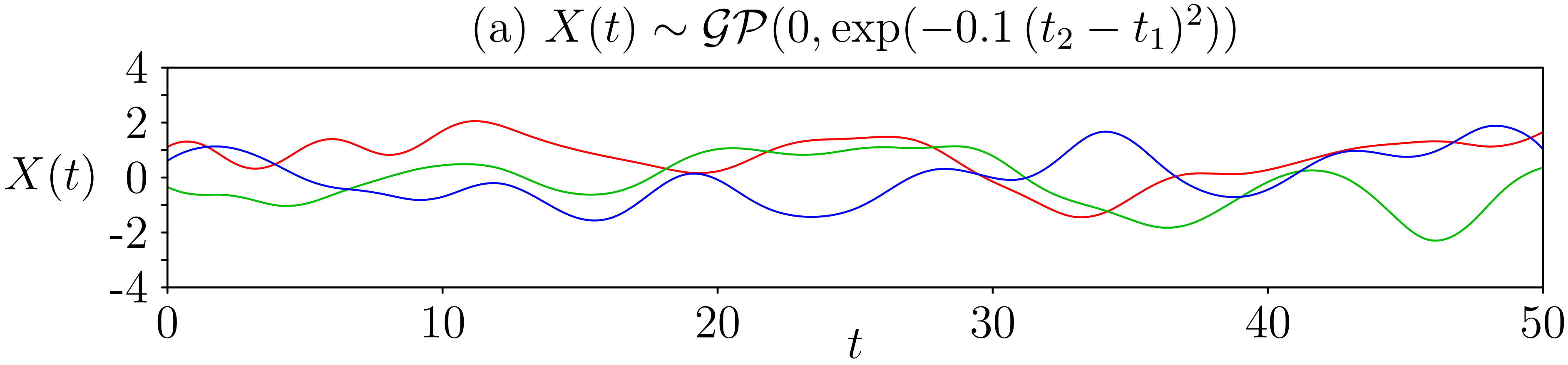
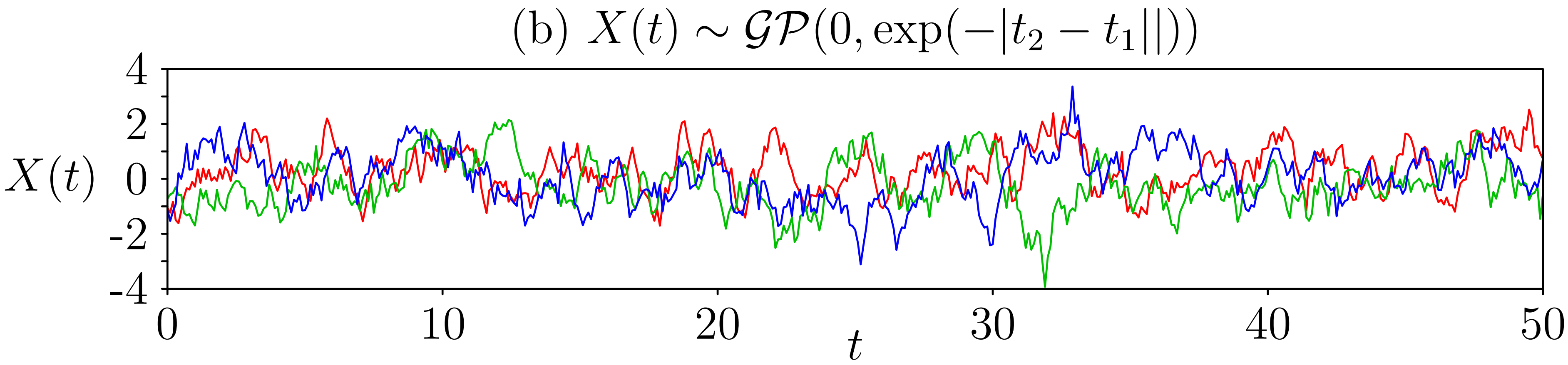
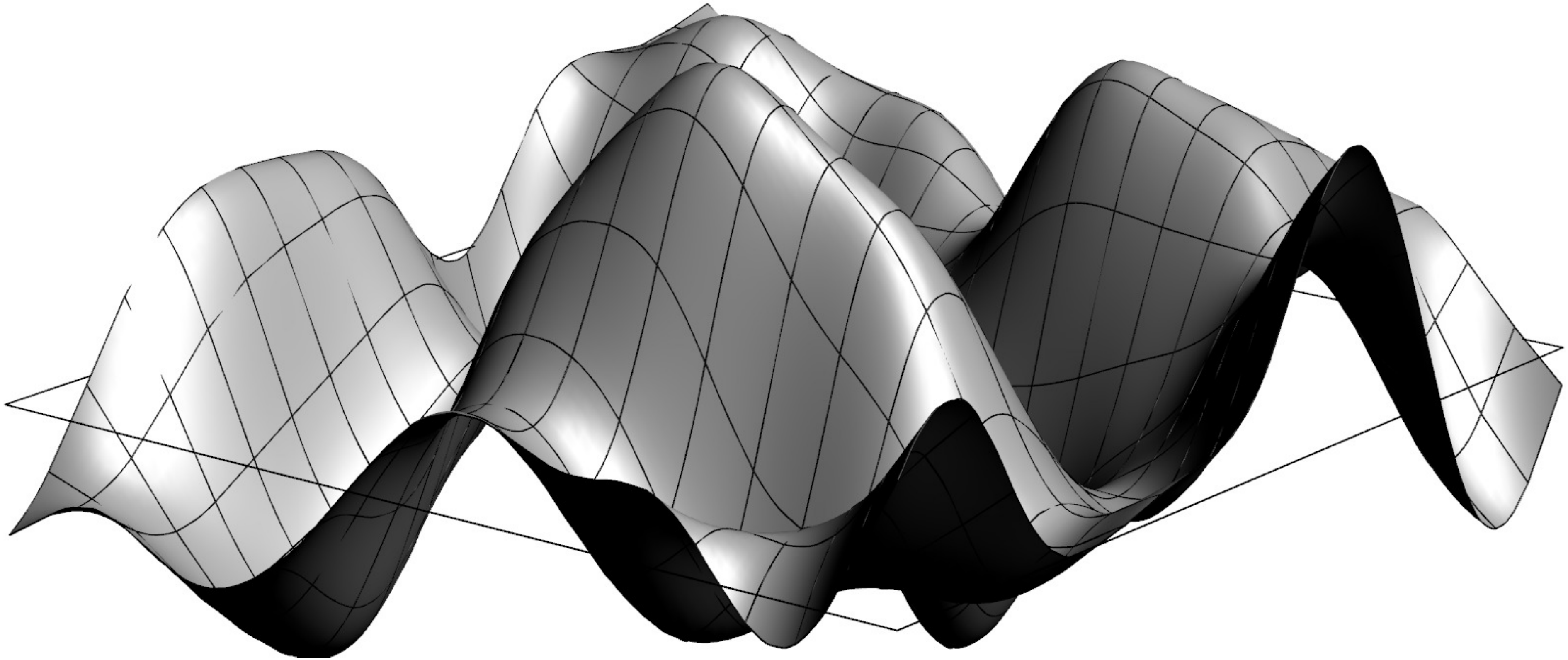




2-D Gaussian Processes



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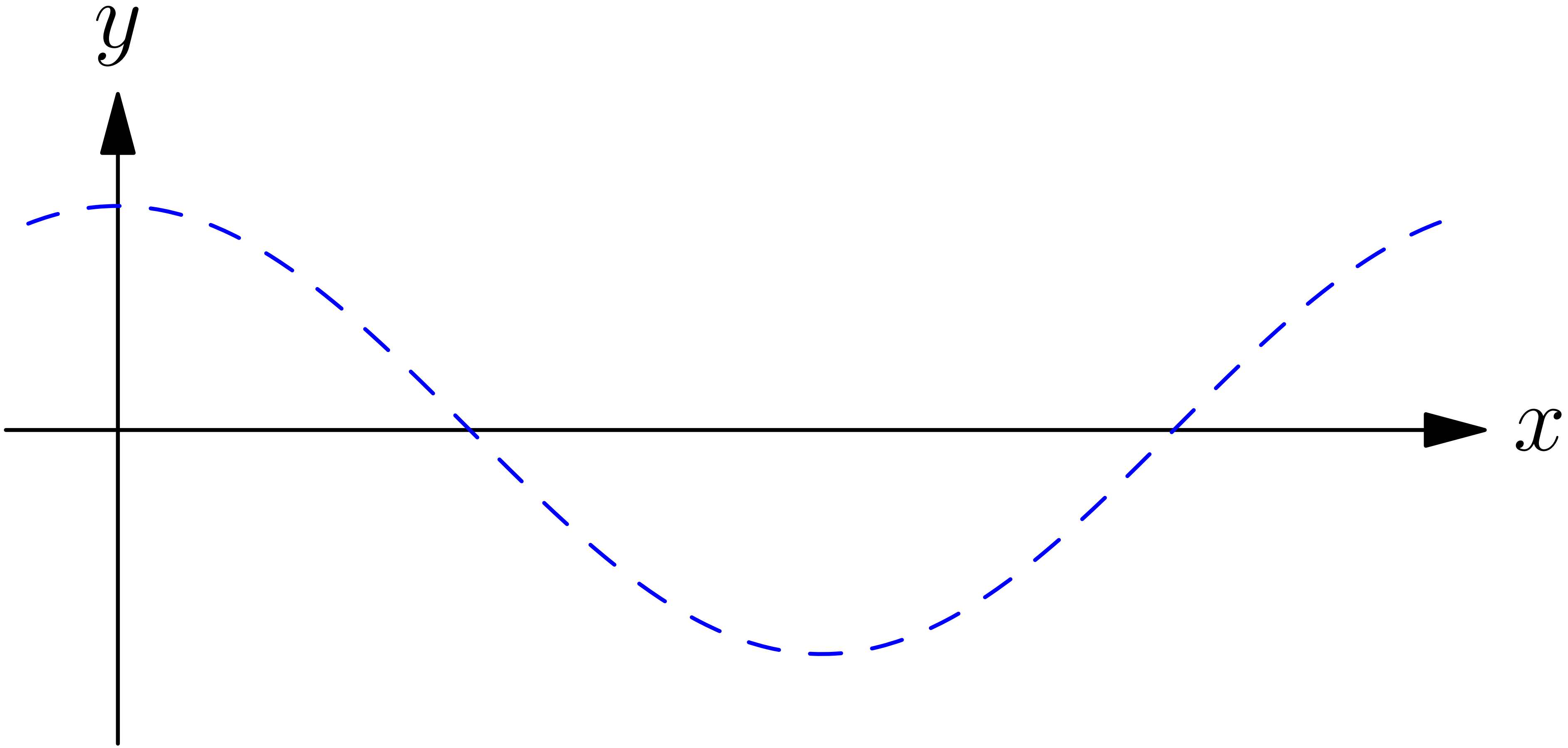

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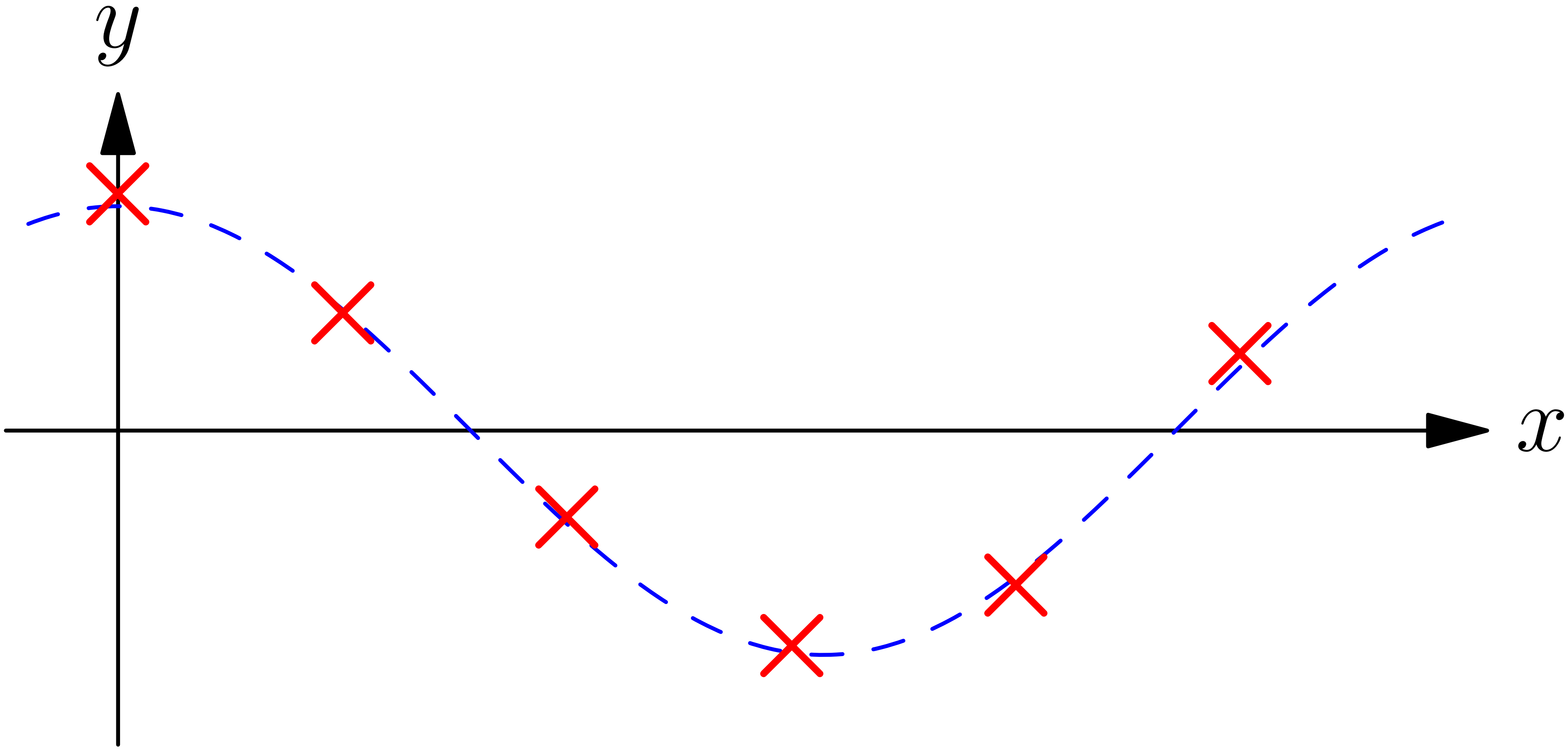

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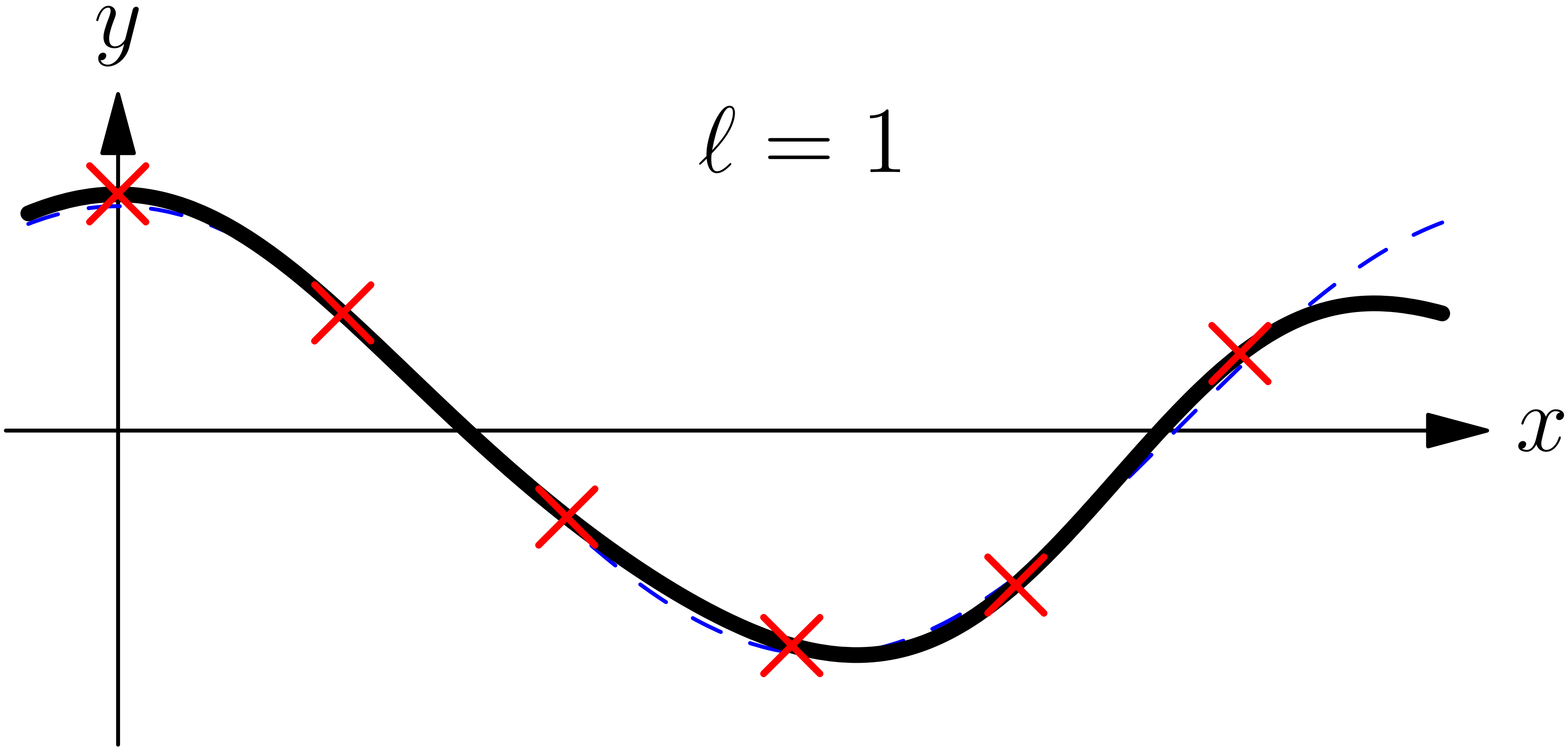

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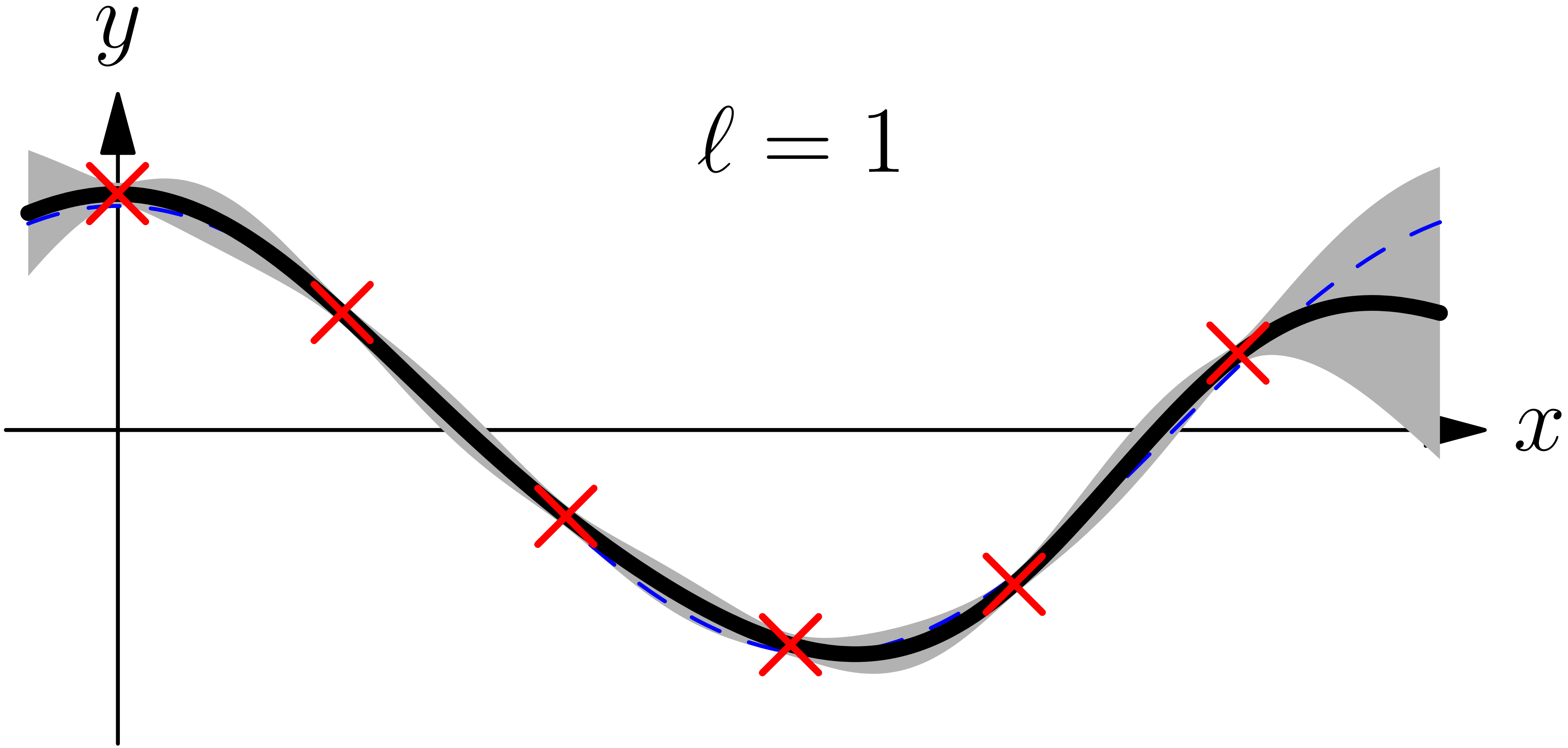

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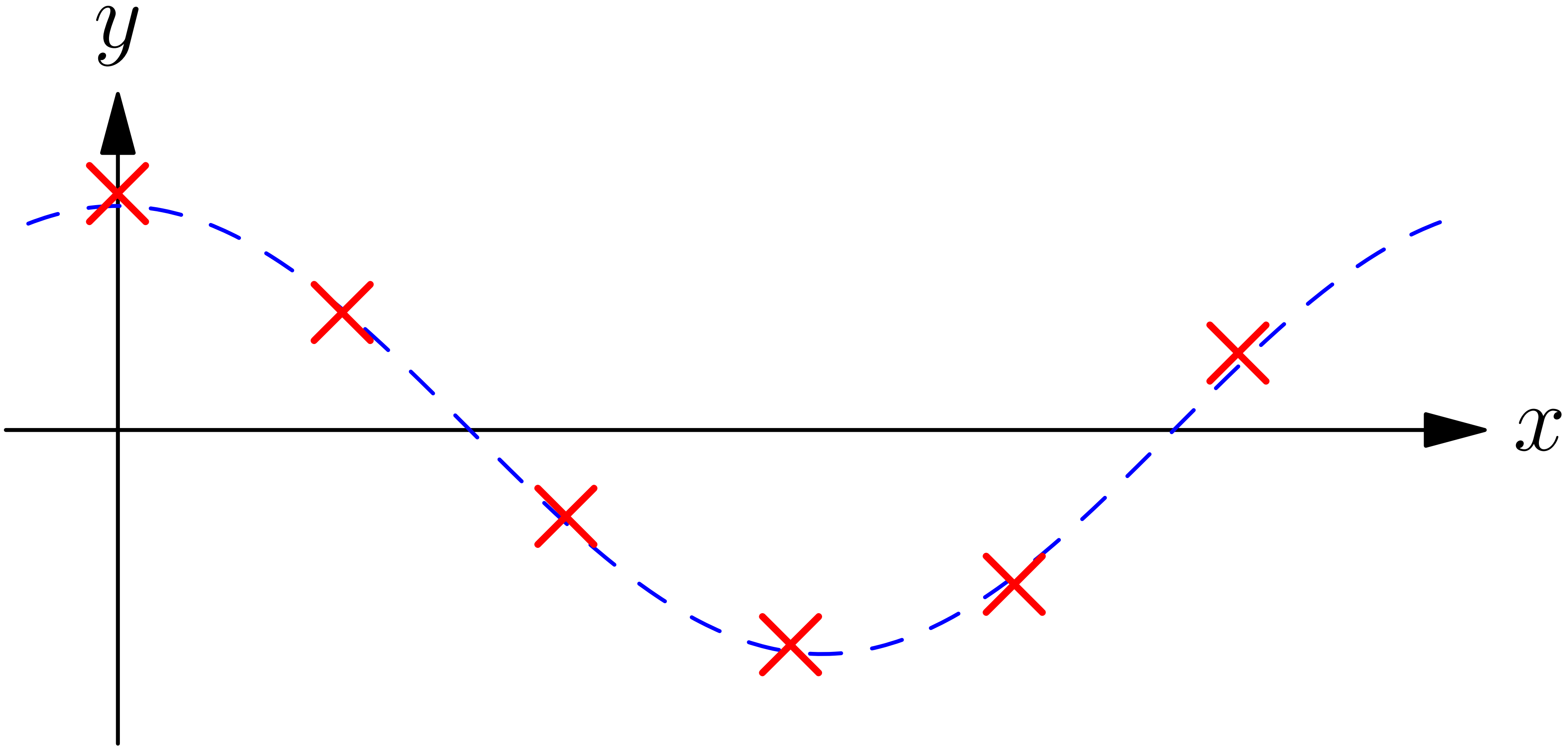

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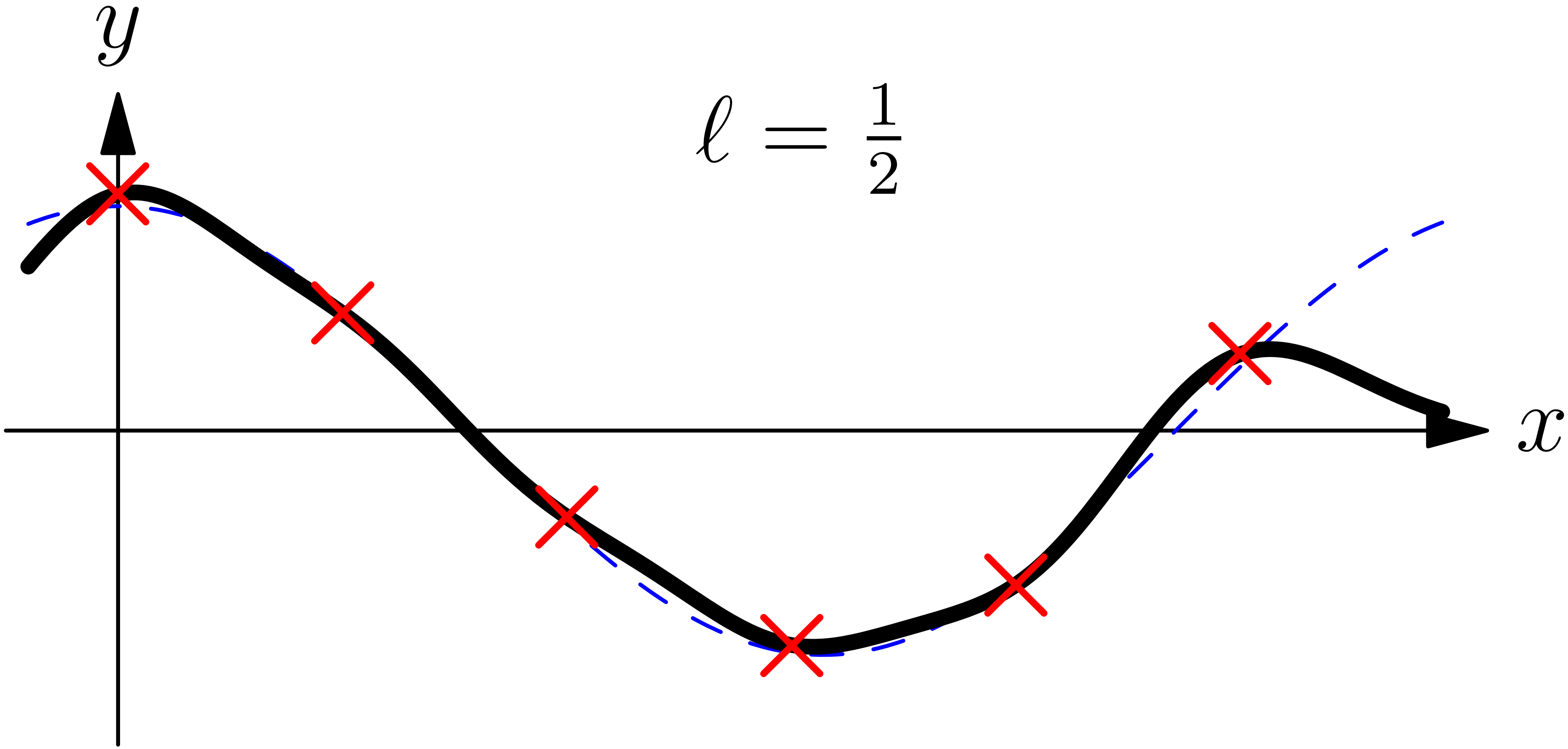

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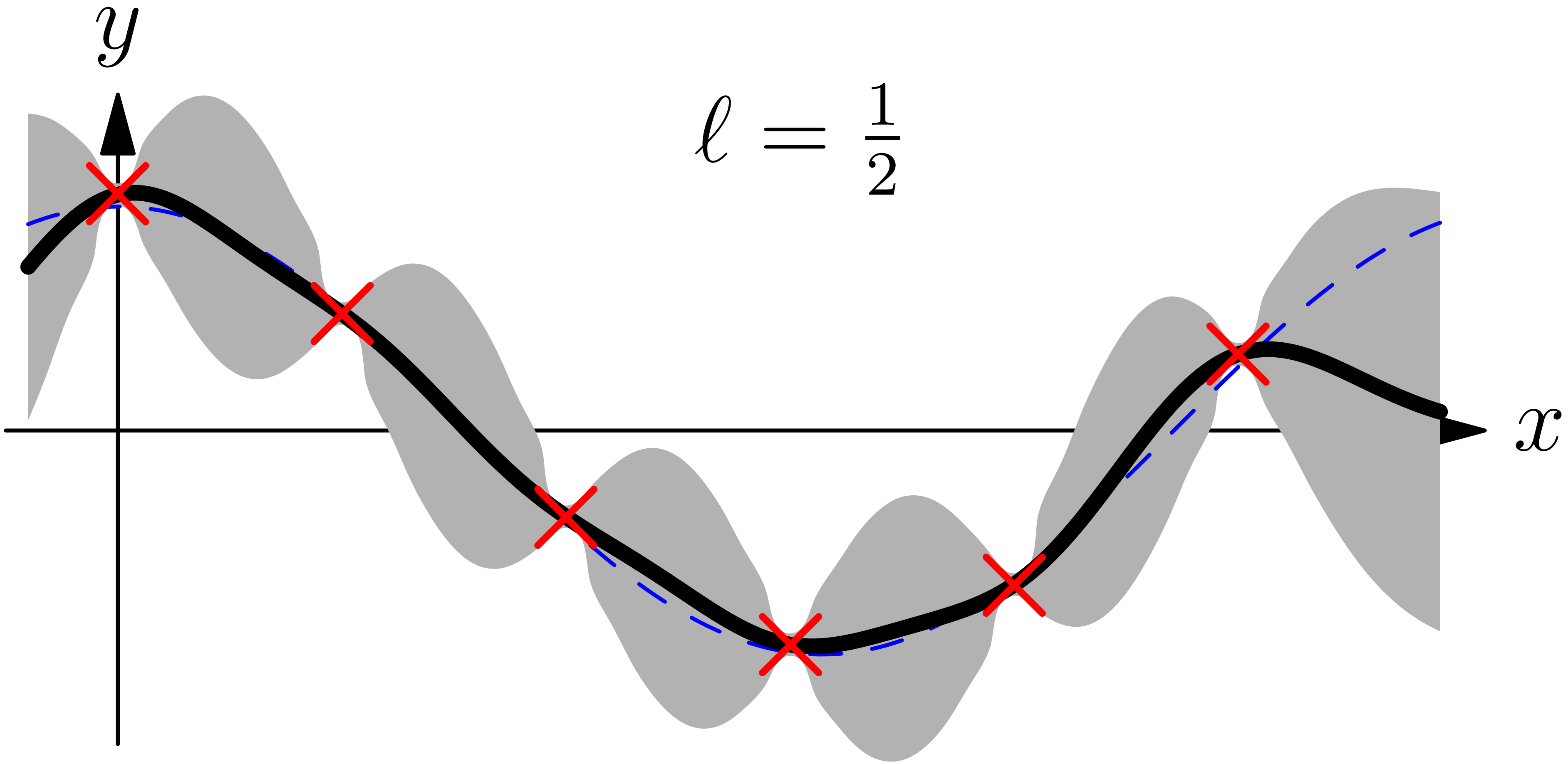

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- We finish with *Naive Bayes* which is unreasonably successful at many text problems
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- It makes the crude approximation that the probability of a document depends only on the words, with all words being independent

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