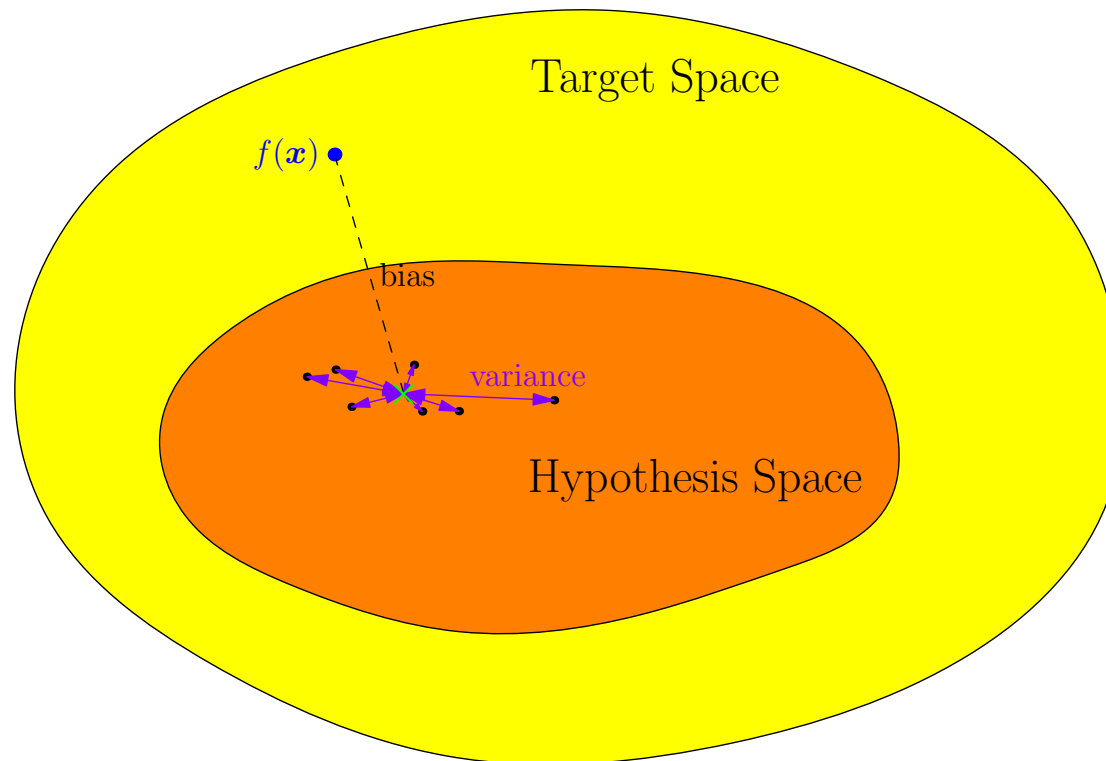


NGCM ML Workshop

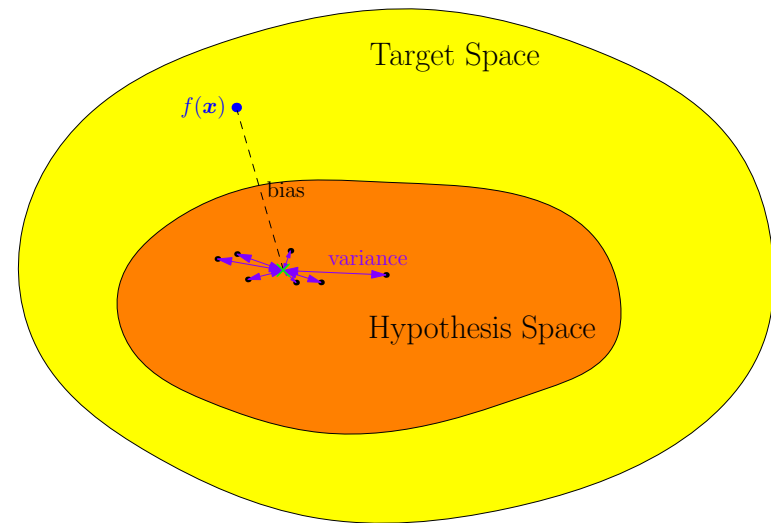
Advanced Machine Learning



*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 are going to cover some advanced machine learning techniques
- 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 $f(\mathbf{x})$
- We construct a learning machine that makes a prediction $\hat{f}(\mathbf{x}|\mathbf{w})$, where \mathbf{w} are weights we want to learn
- We typically choose the weights to minimise a *training error*

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

where \mathcal{D} is a finite data set of size N , sampled from the set of all inputs, \mathcal{X} , according to a probability distribution $p(\mathbf{x})$ describing where our data is

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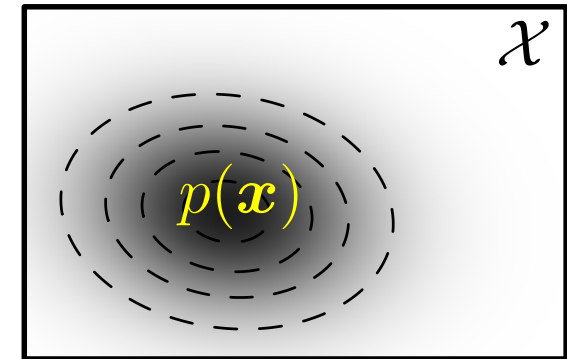
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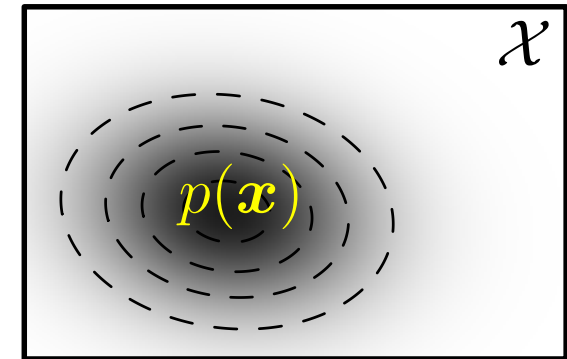
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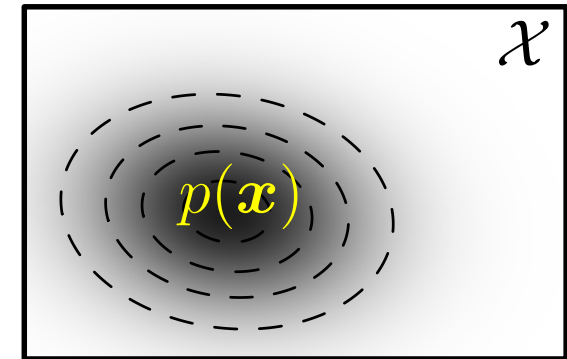
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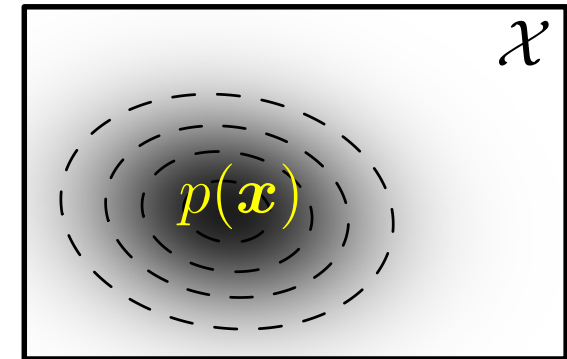
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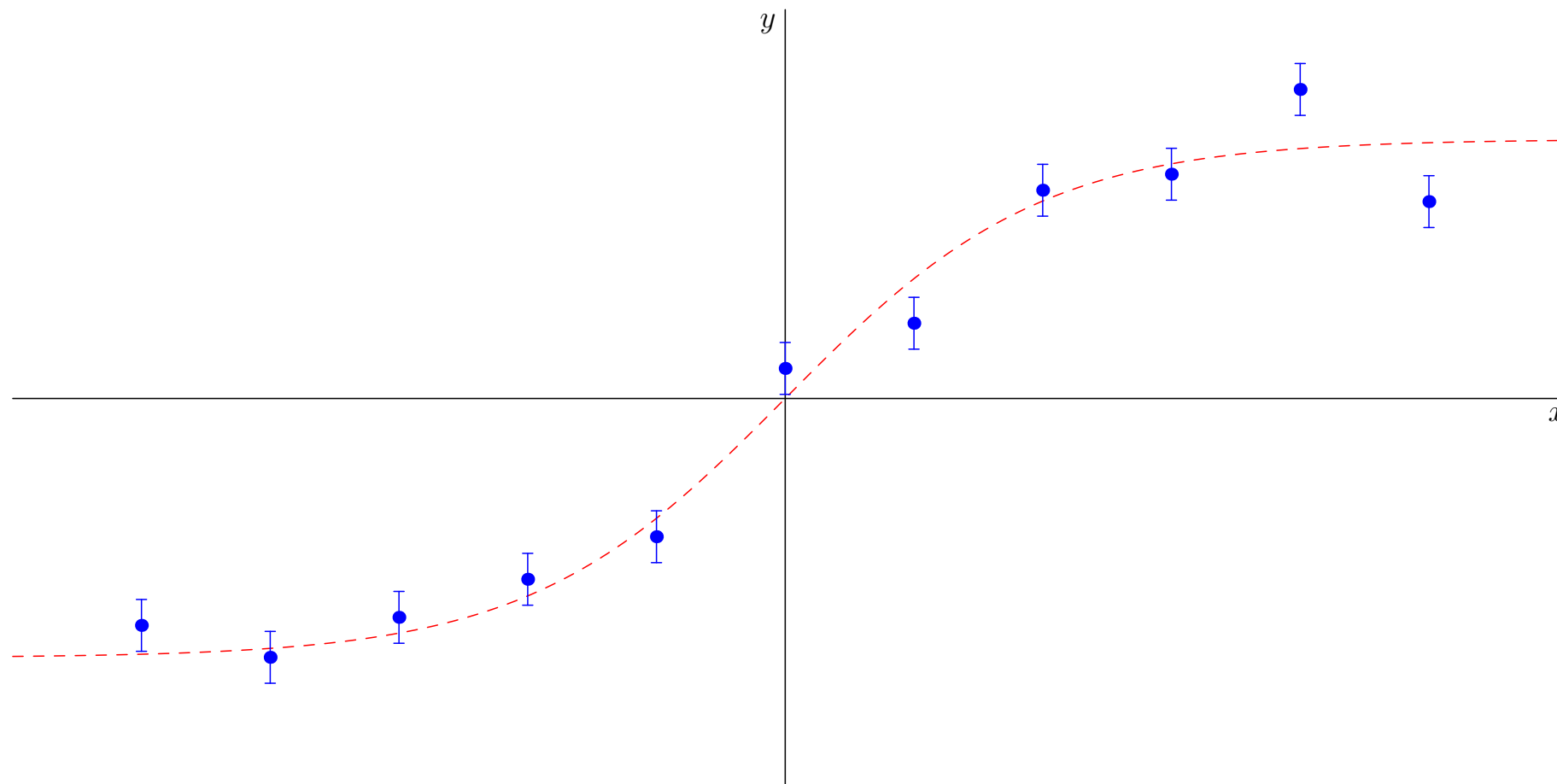


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- We want to minimise $E_G(\mathbf{w})$ but in practice we are minimising $E_T(\mathbf{w})$, *what could possibly go wrong?*

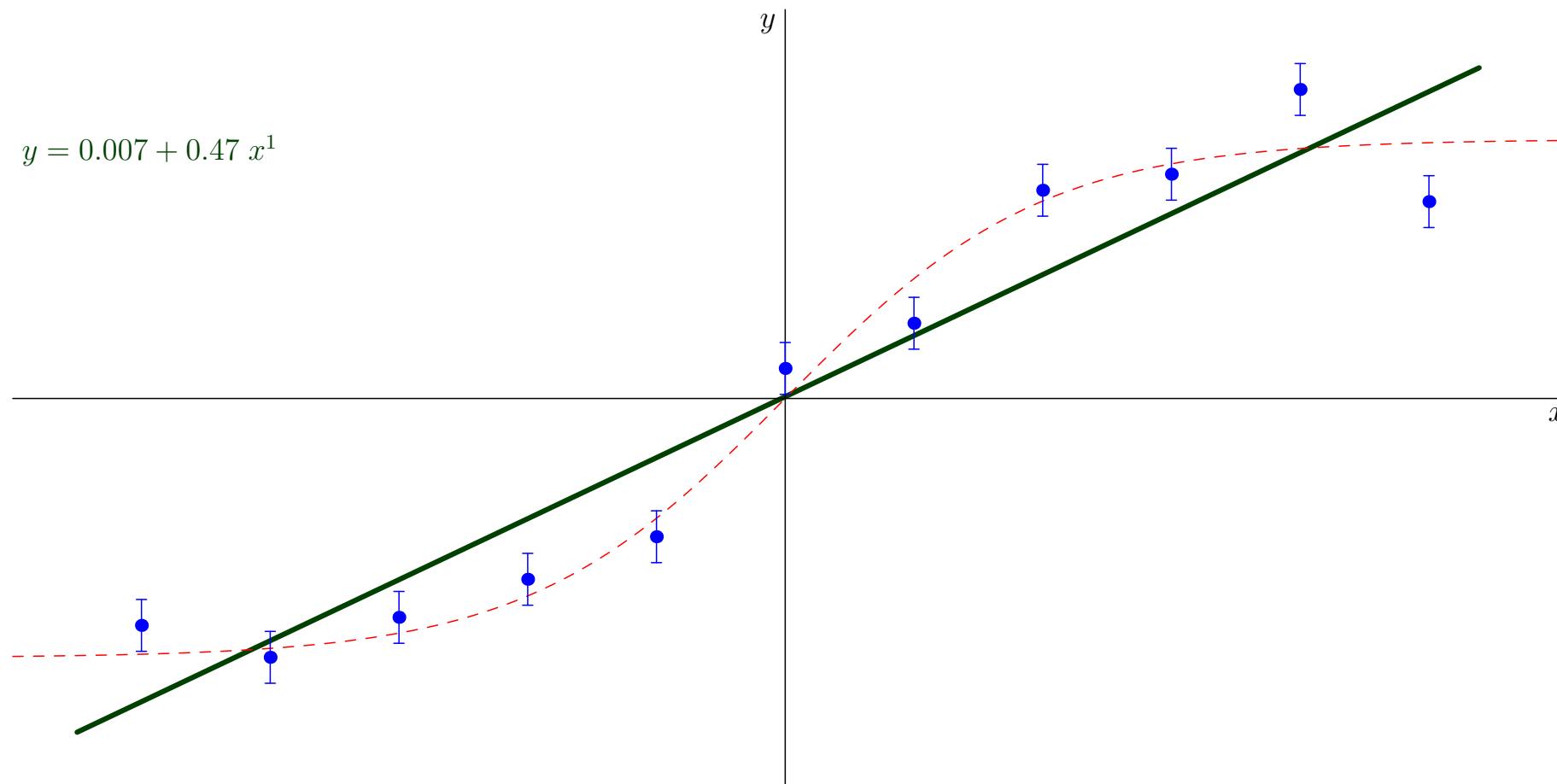
Too Simple or Too Complex?

- Fit $\hat{f}(x, w)$ to data



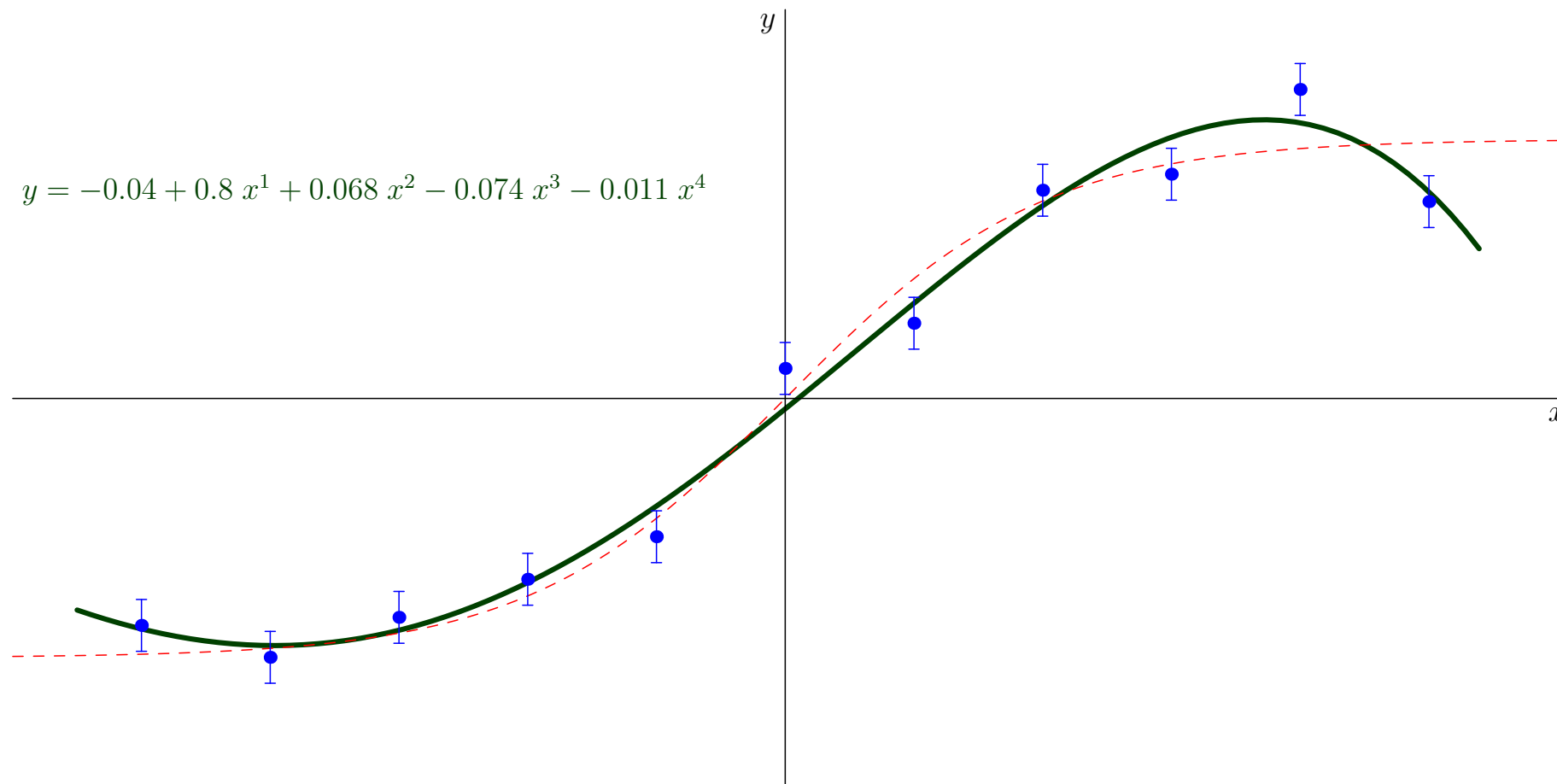
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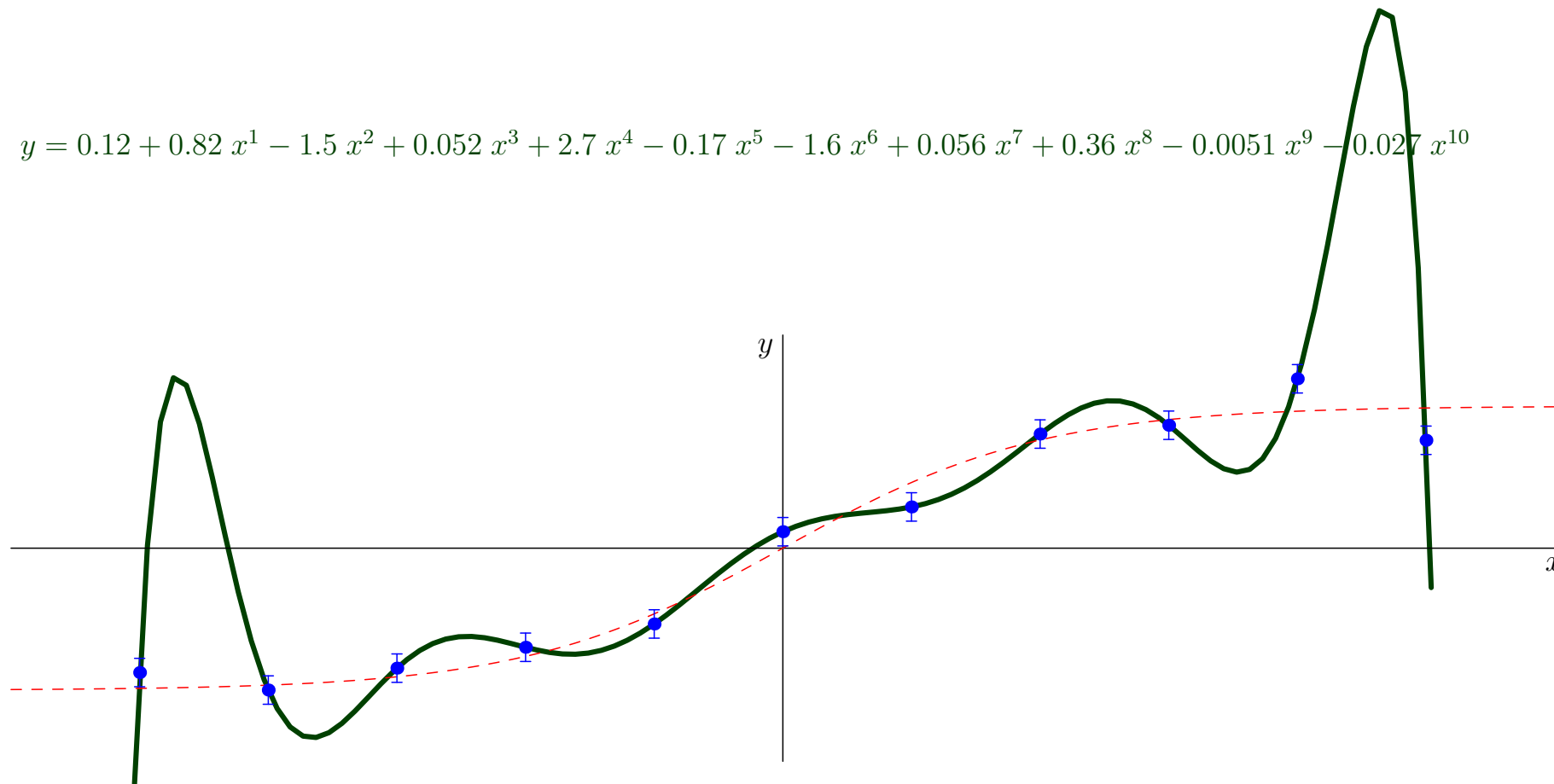
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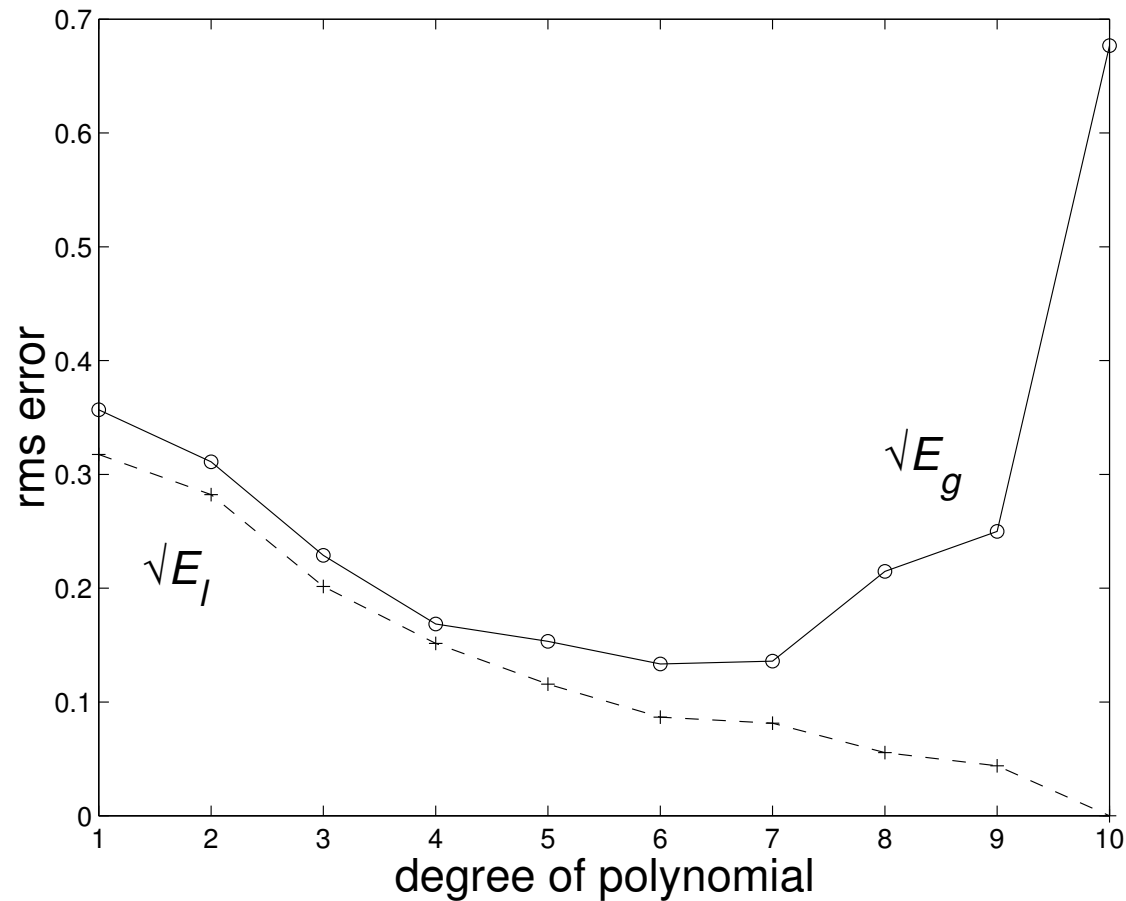
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$$y = 0.12 + 0.82 x^1 - 1.5 x^2 + 0.052 x^3 + 2.7 x^4 - 0.17 x^5 - 1.6 x^6 + 0.056 x^7 + 0.36 x^8 - 0.0051 x^9 - 0.027 x^{10}$$



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 $p(\mathbf{x})$
- For each data set, \mathcal{D} , we would learn a different approximator $\hat{f}(\mathbf{x}|\mathcal{D})$ (usually through weights $\mathbf{w}_{\mathcal{D}}$)
- 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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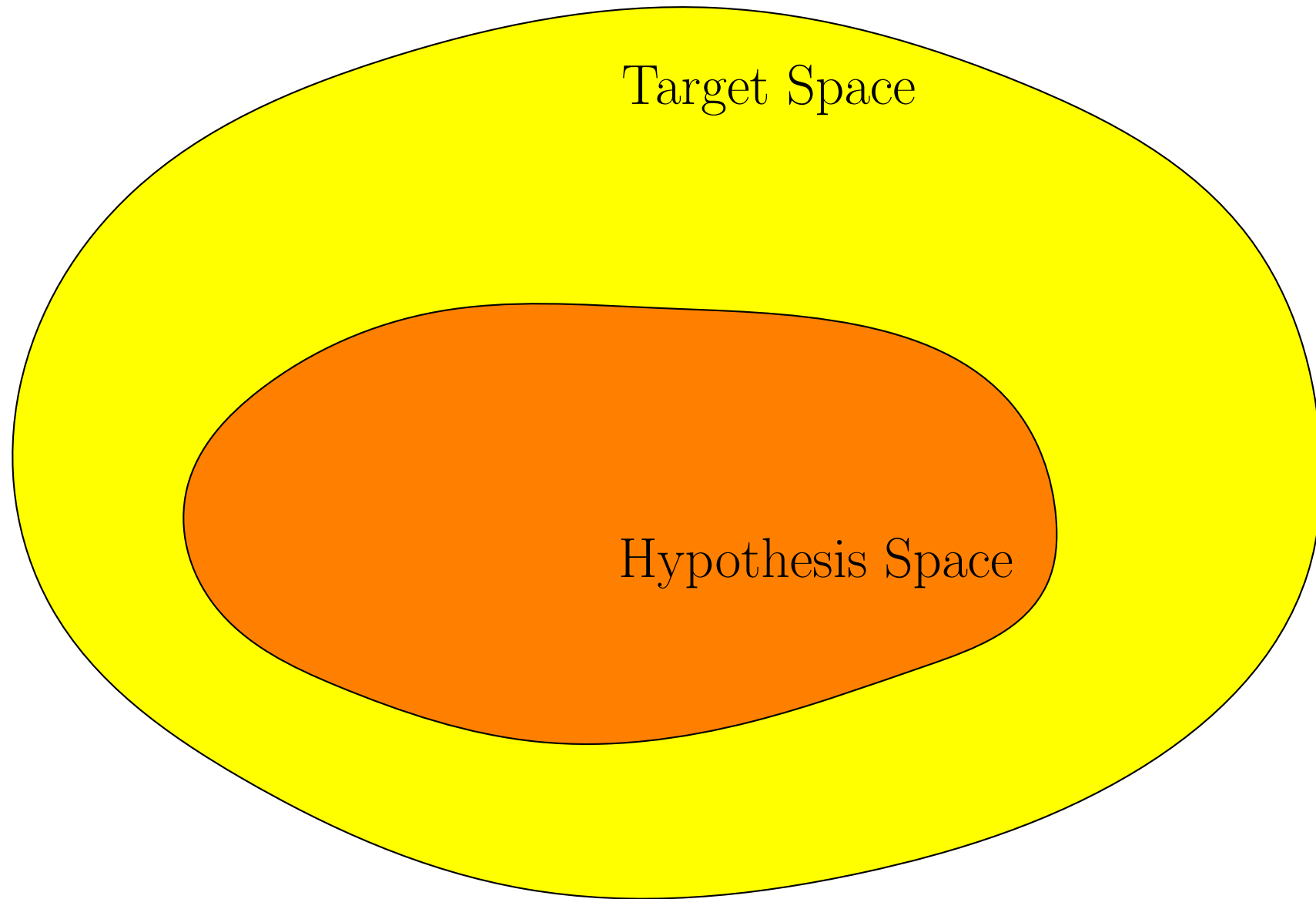
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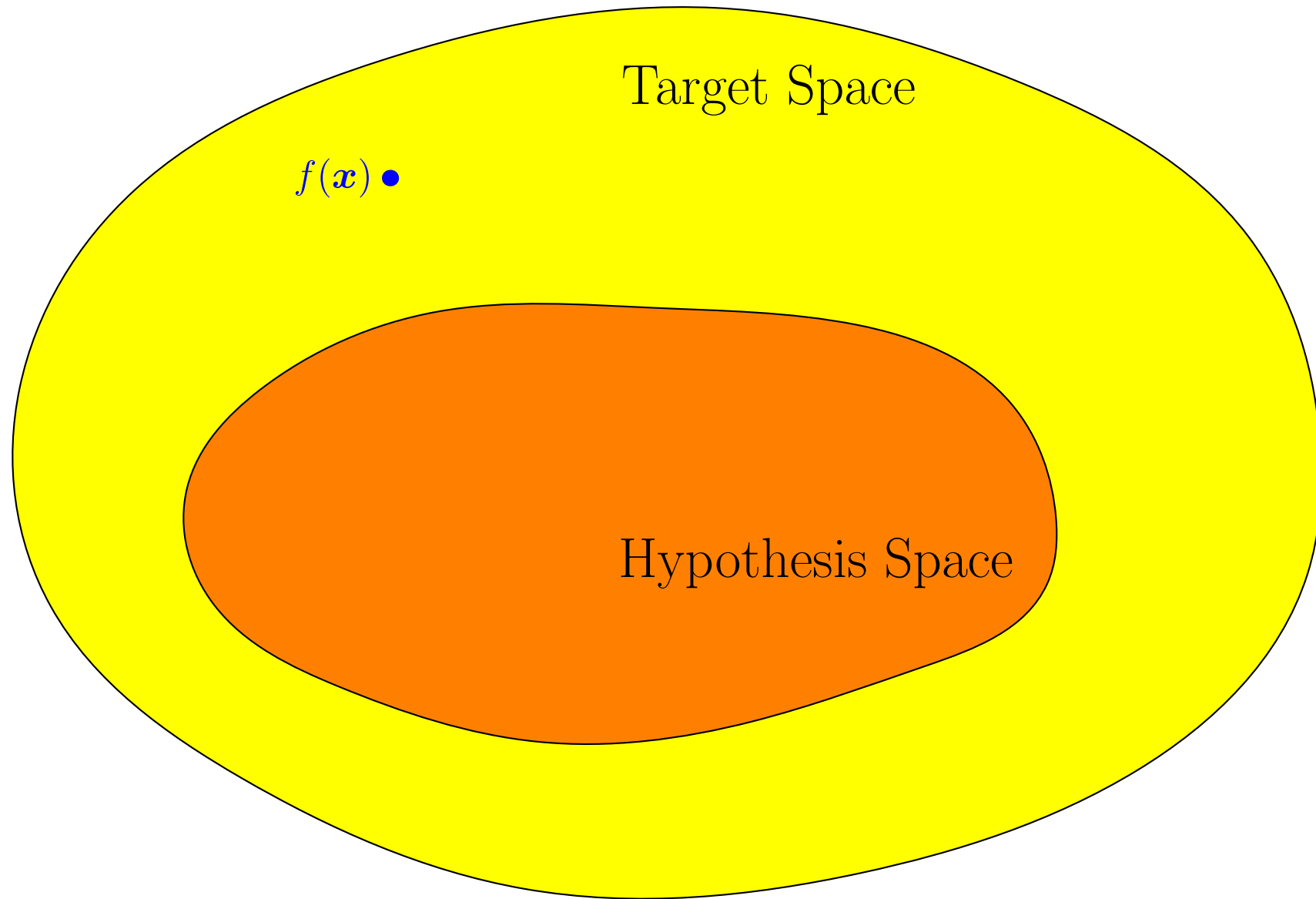
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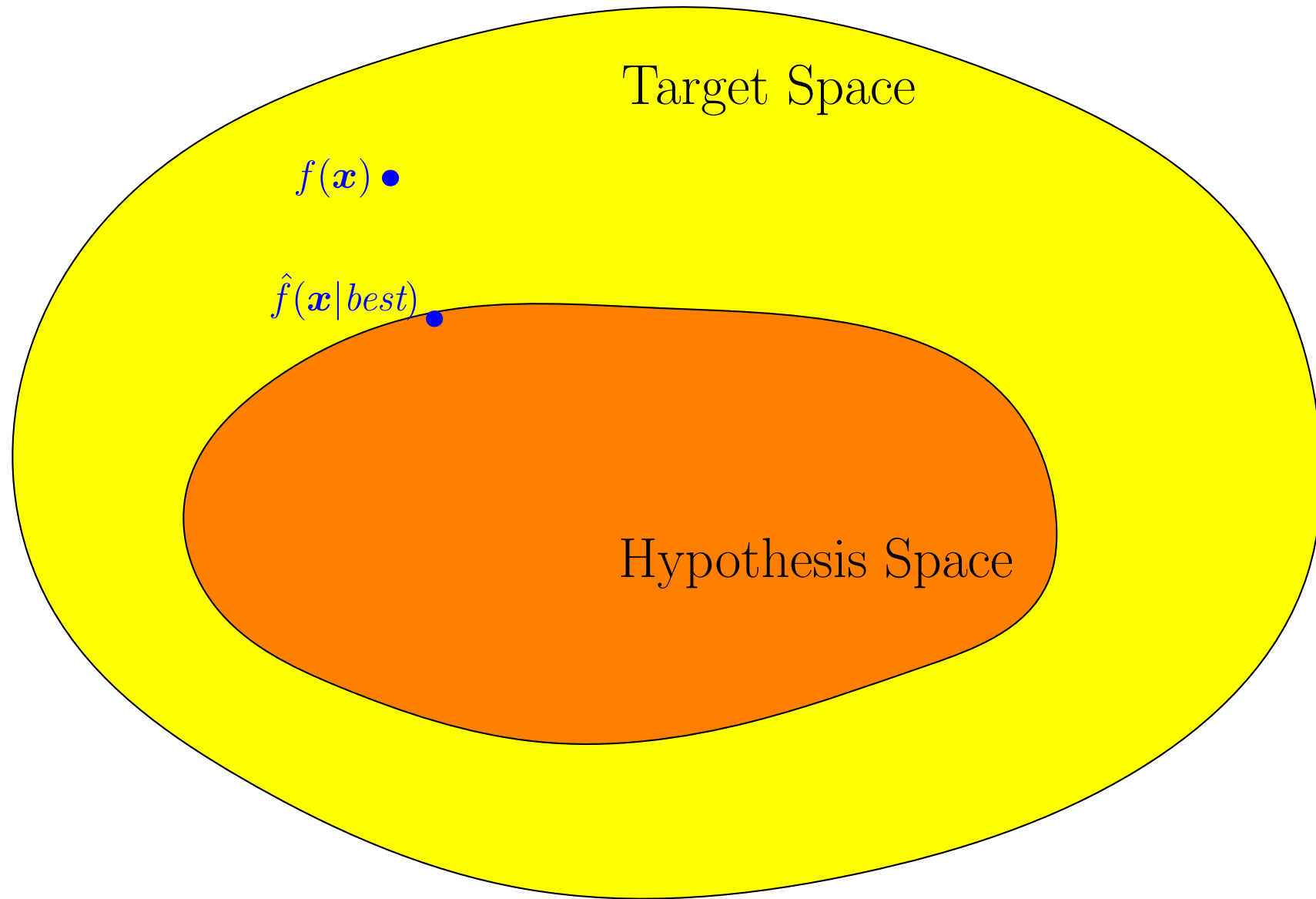
Approximation and Estimation Errors



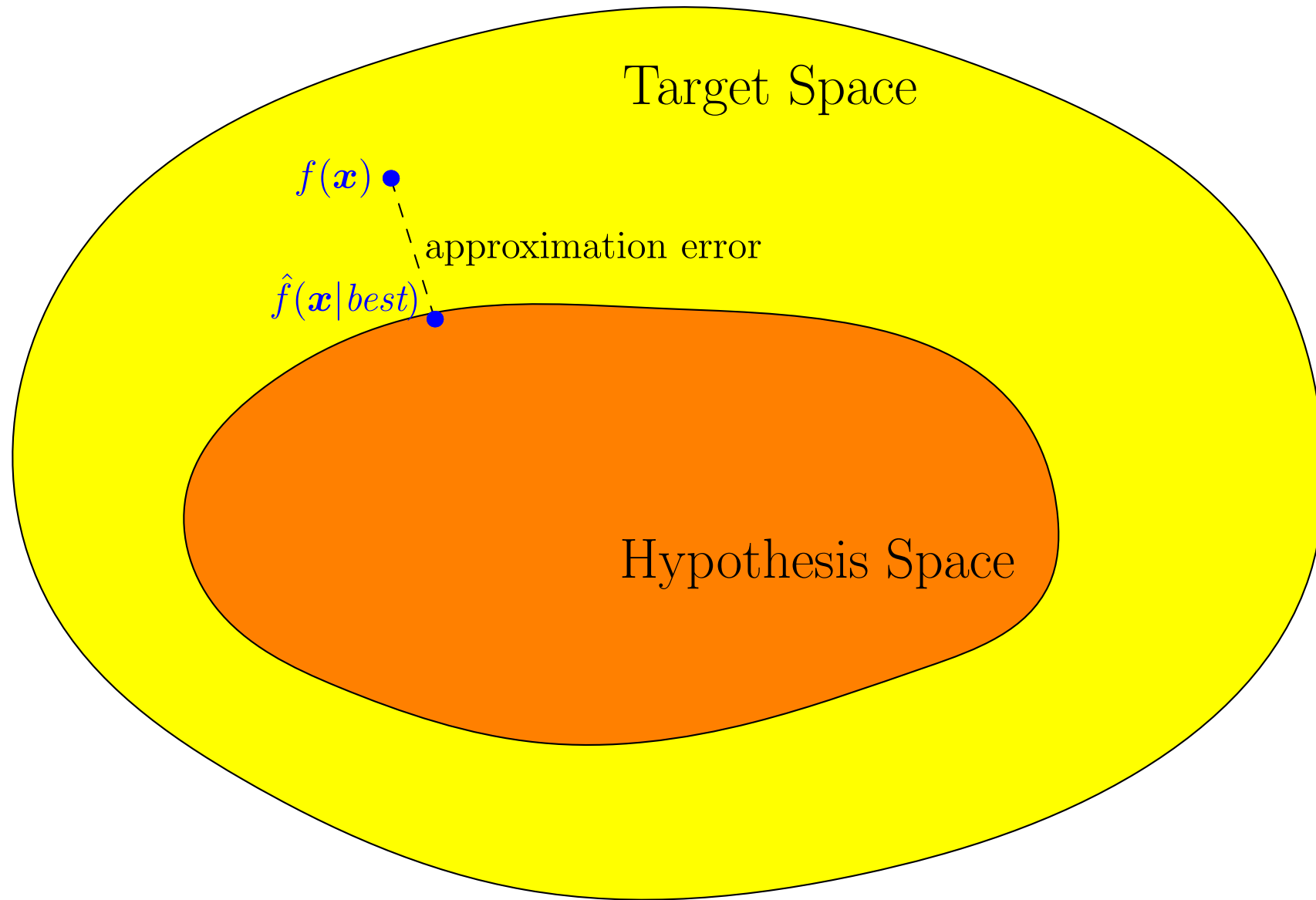
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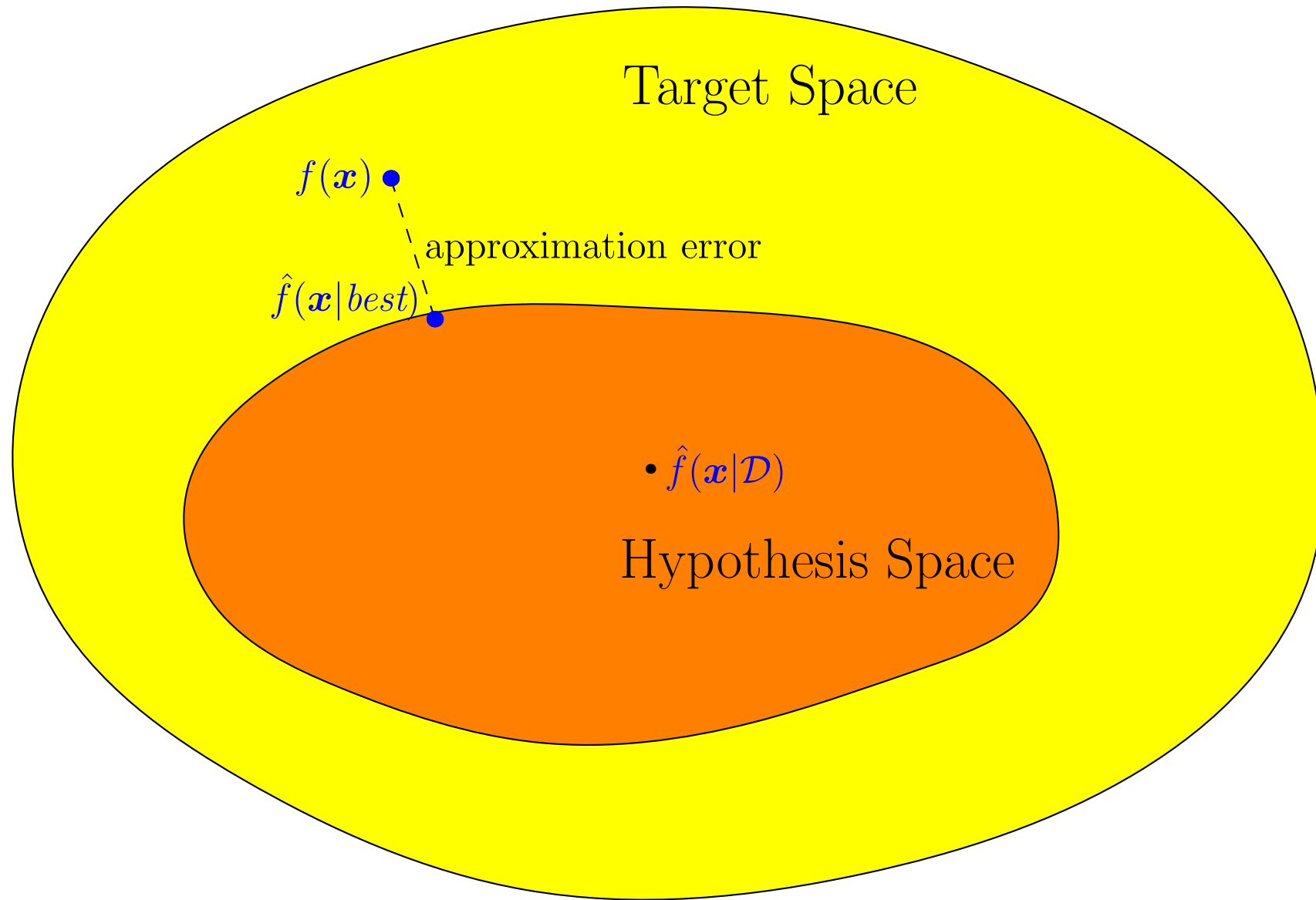
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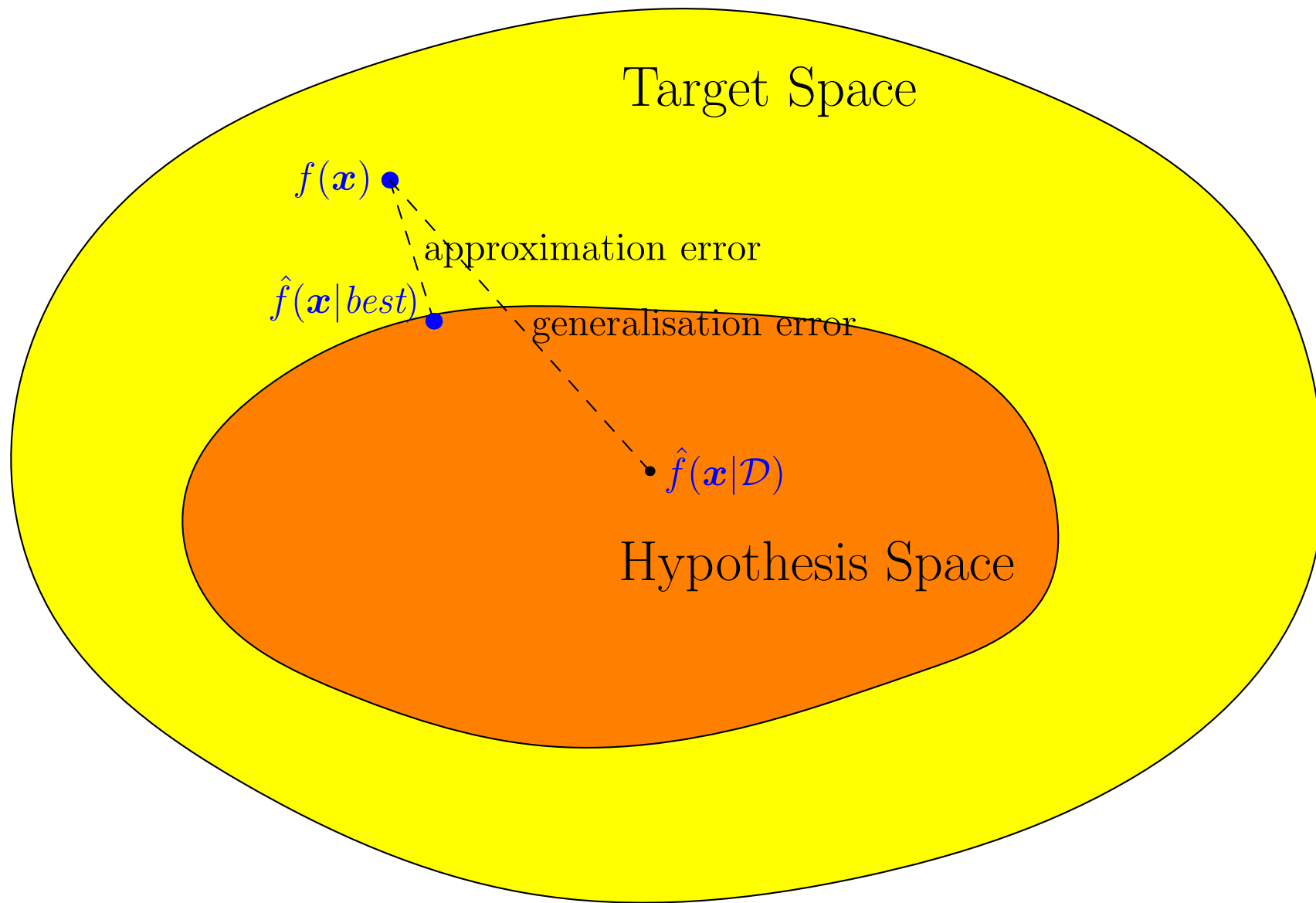
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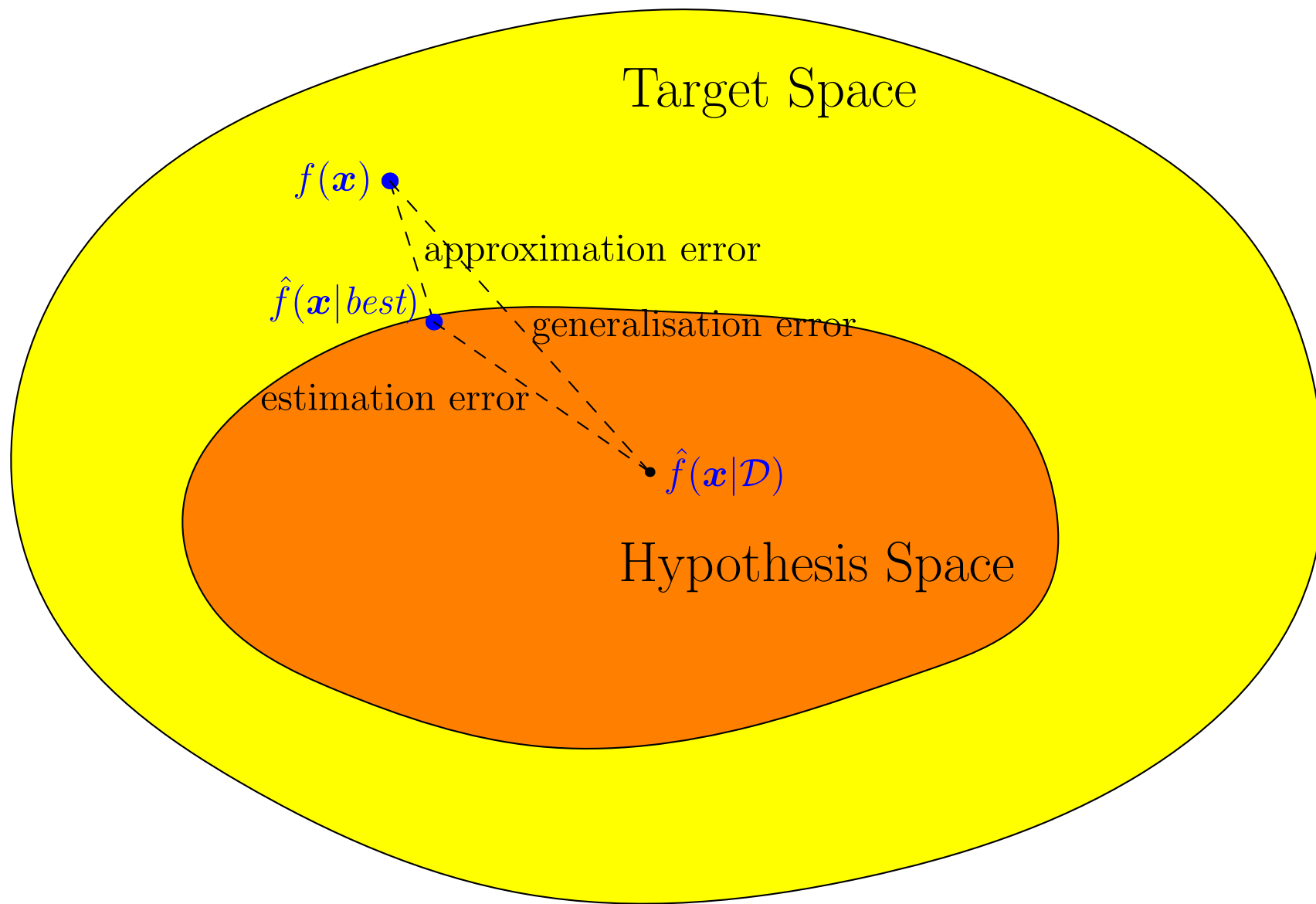
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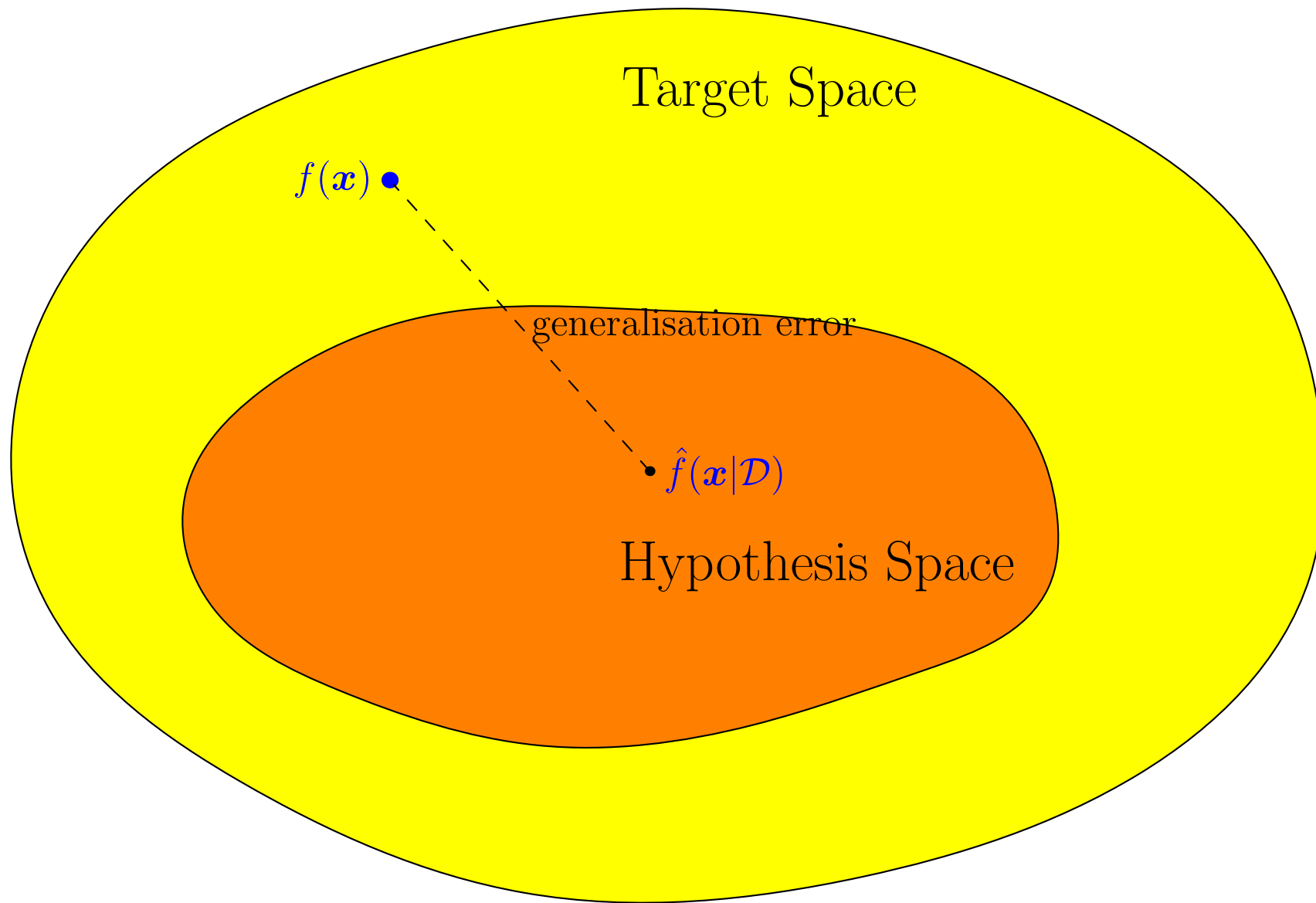
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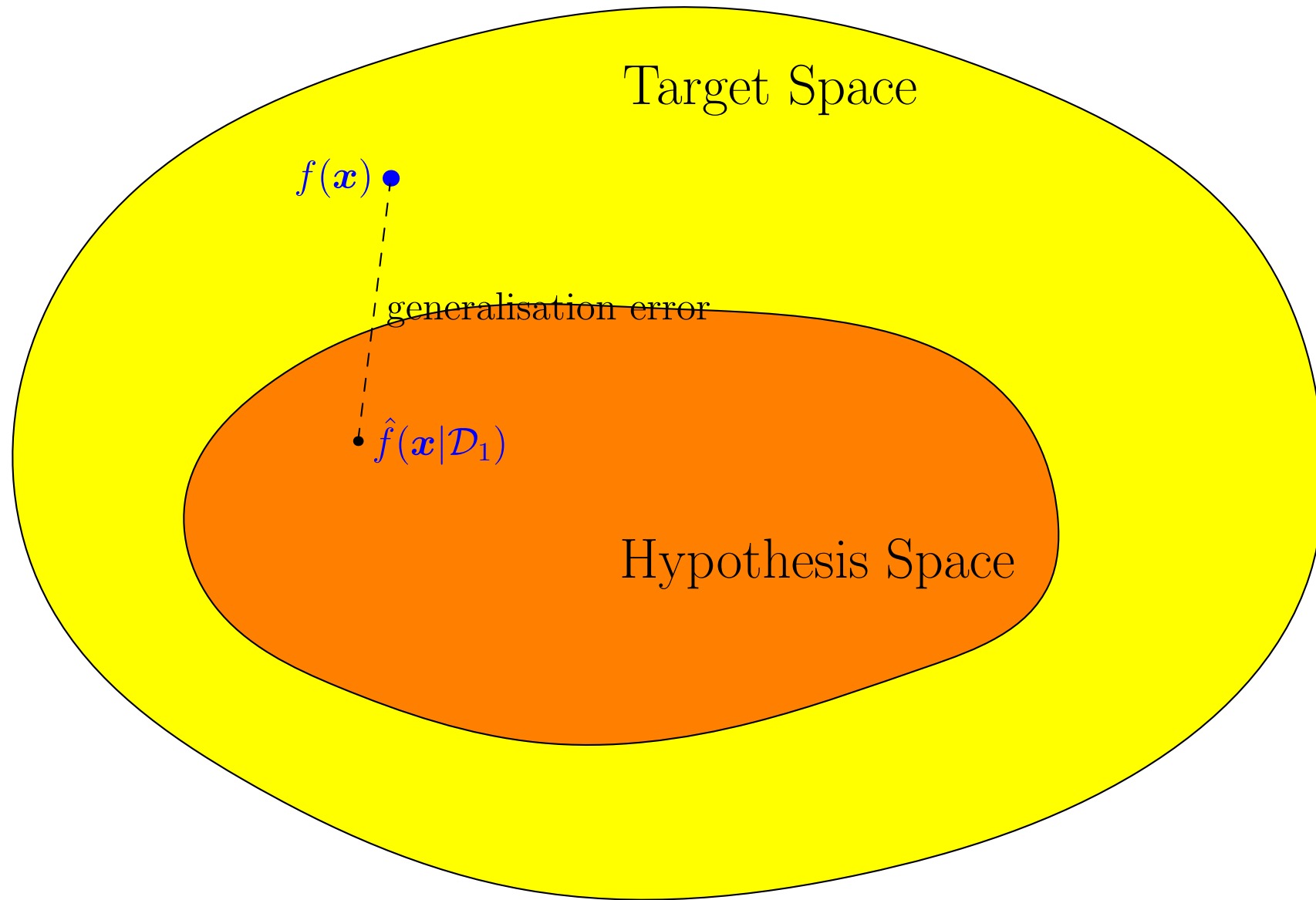
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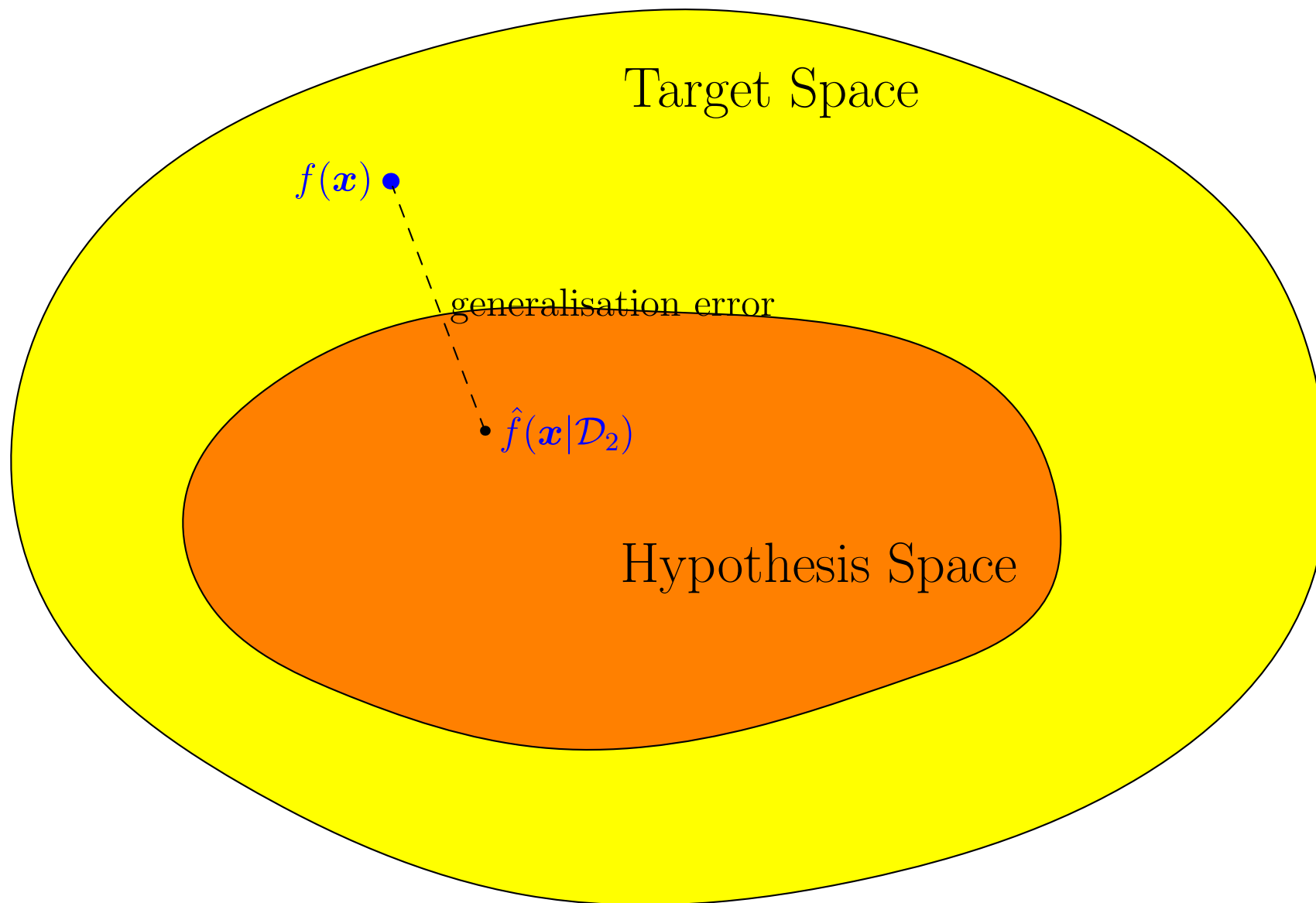
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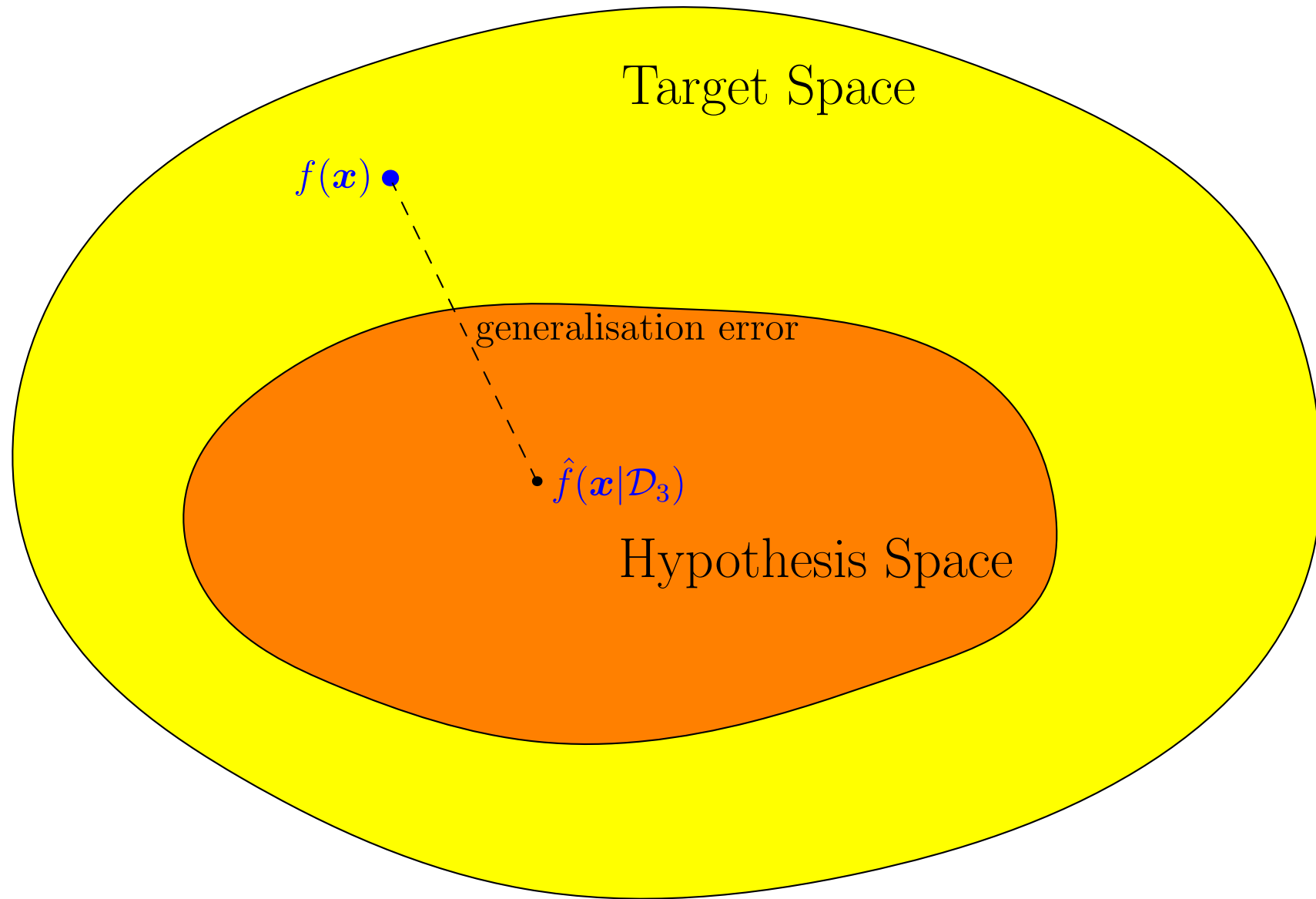
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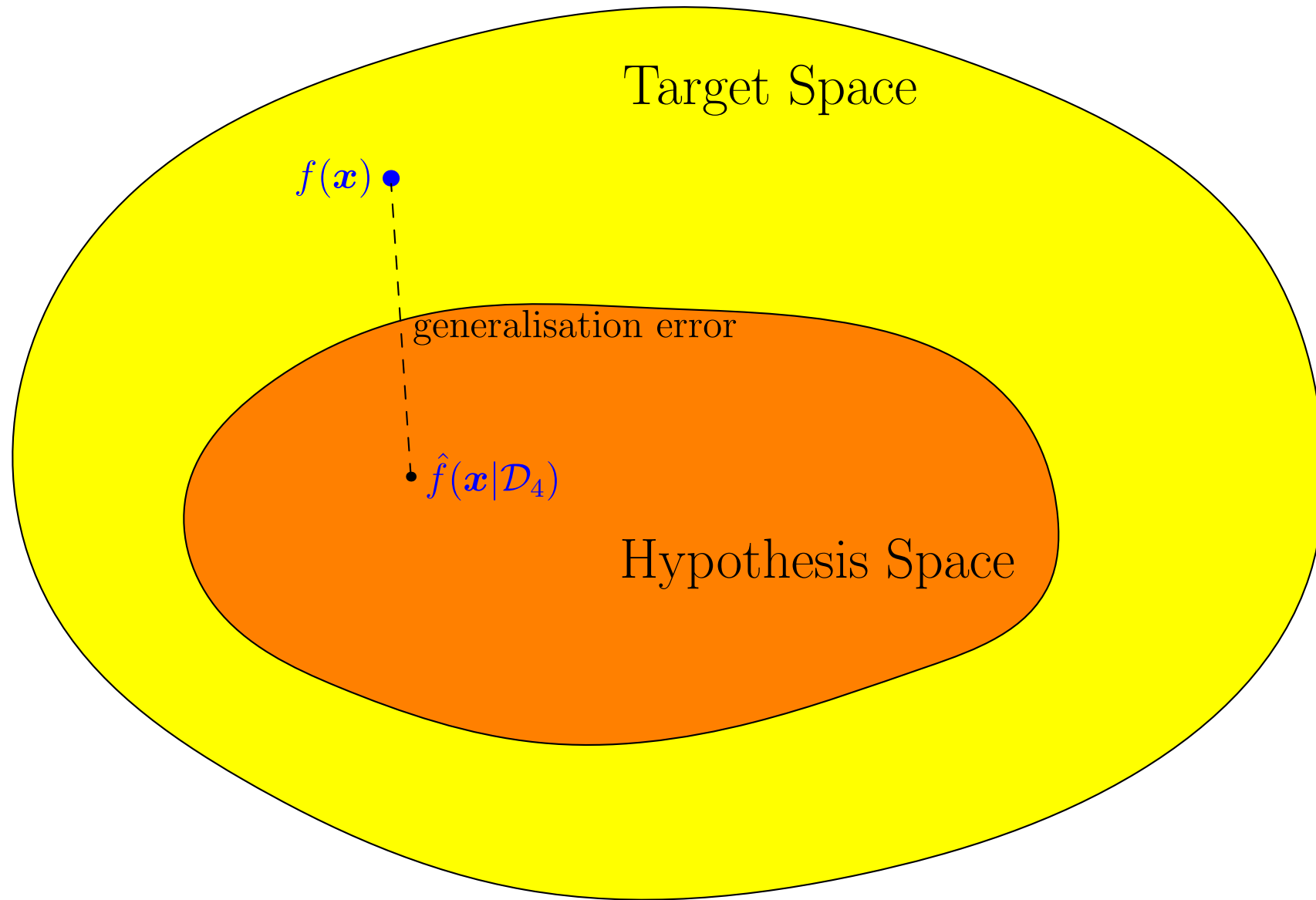
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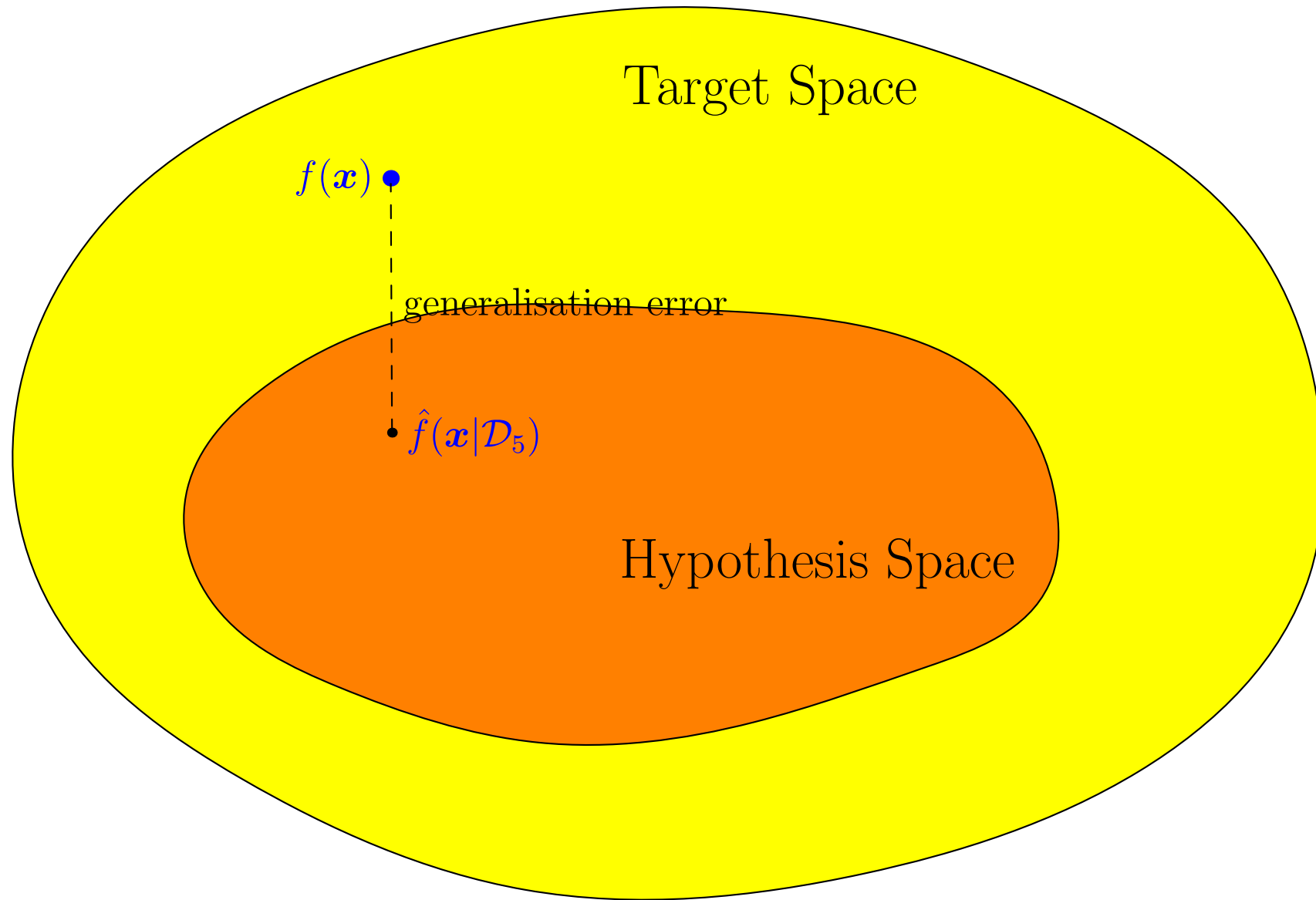
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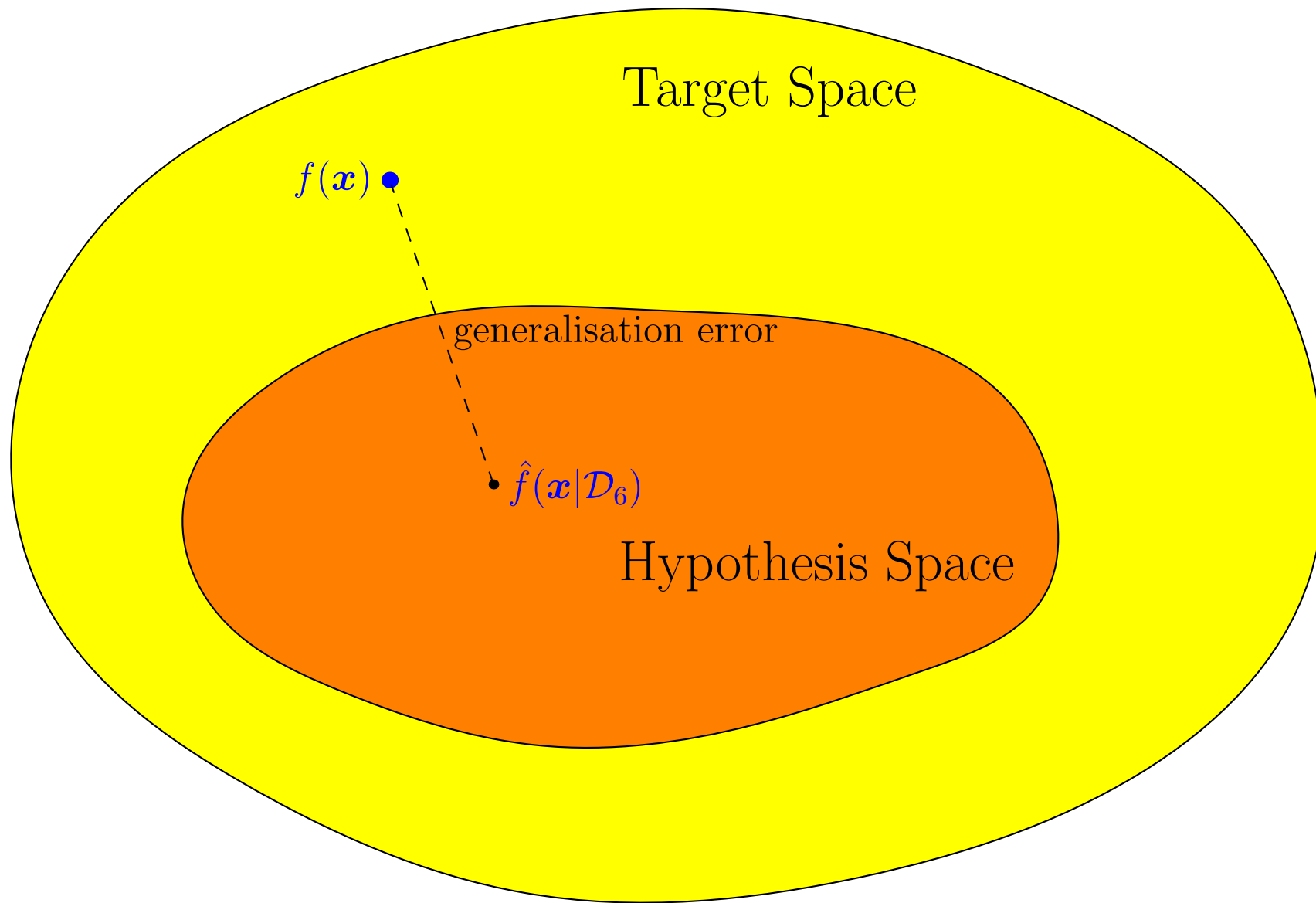
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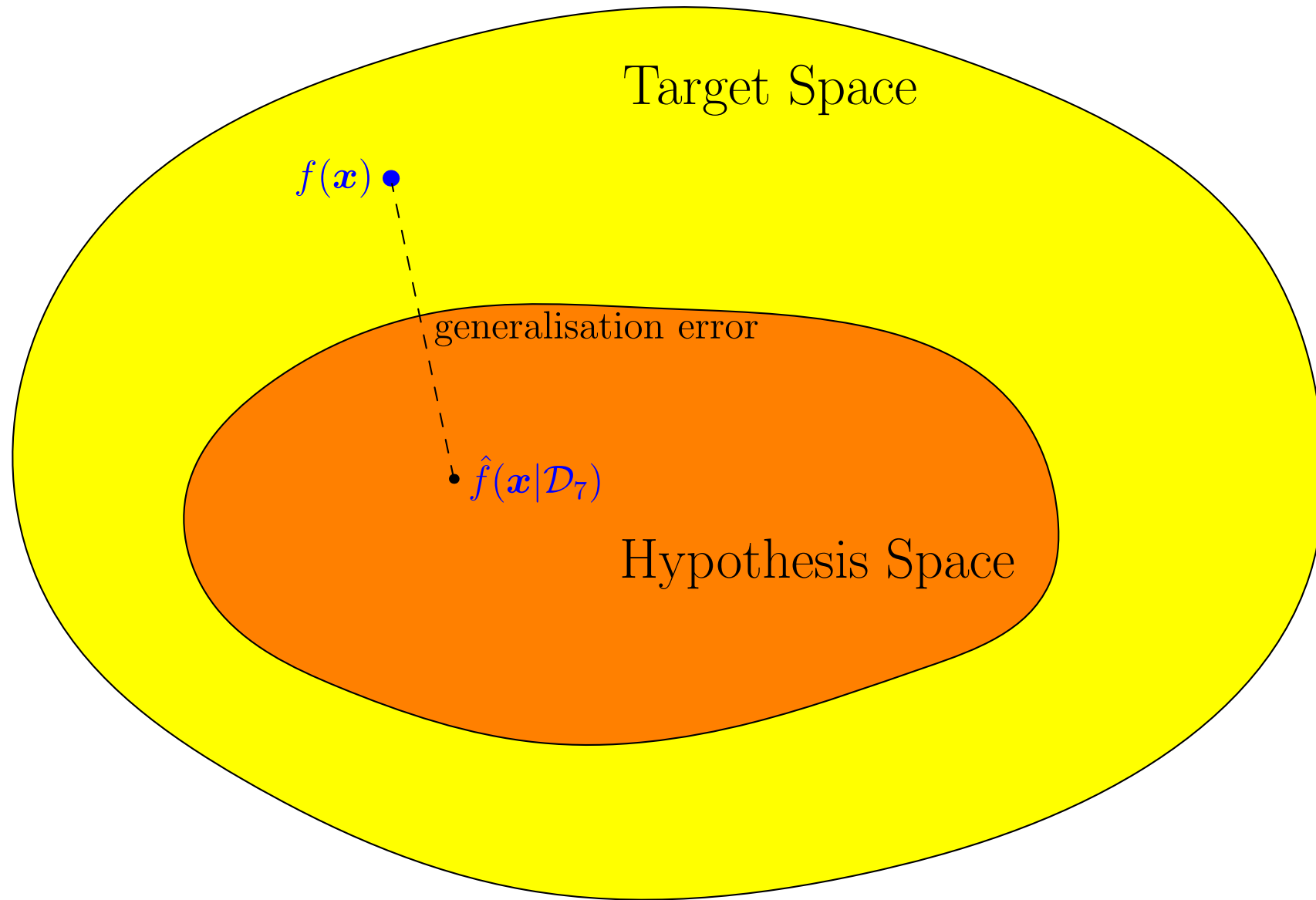
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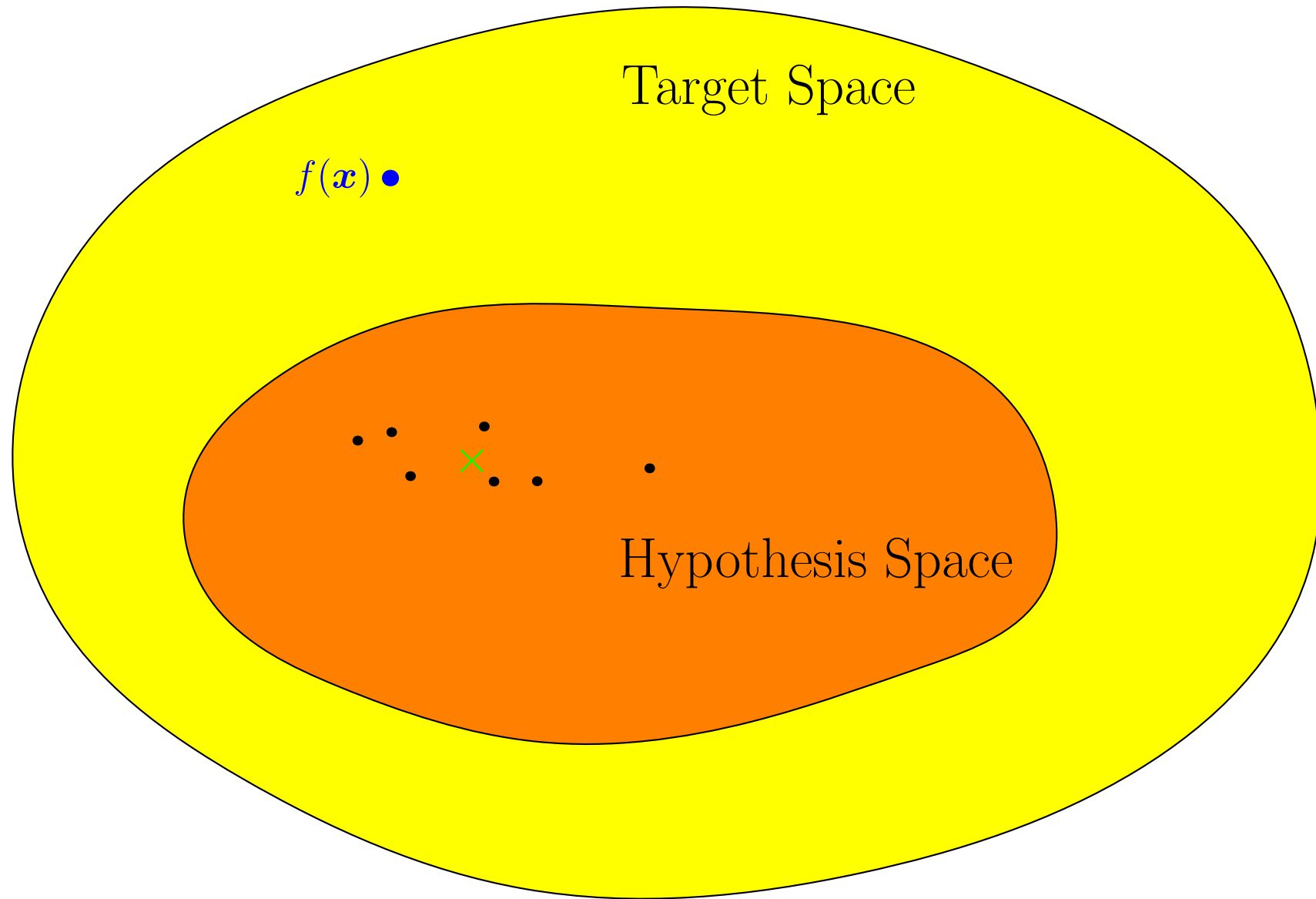
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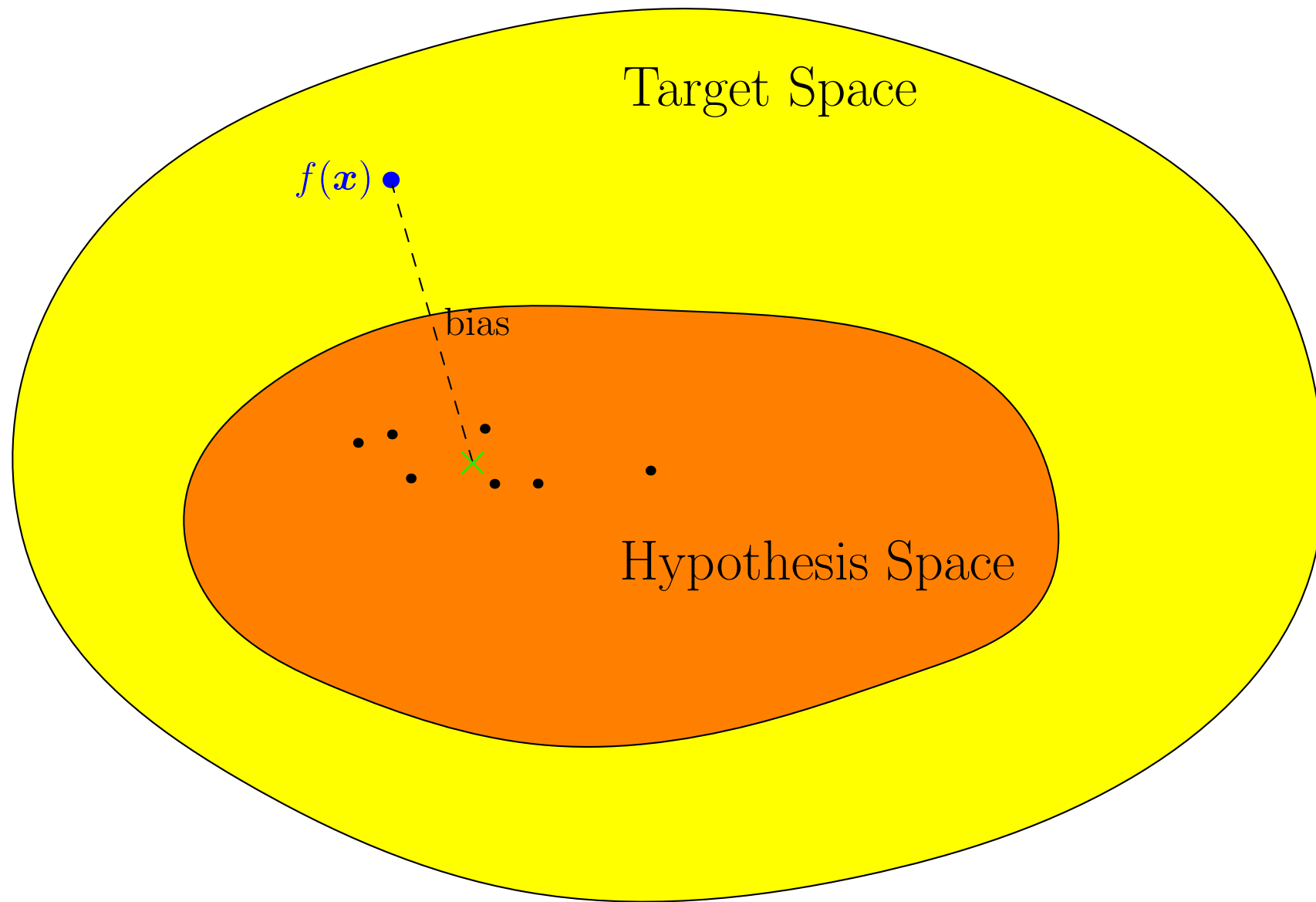
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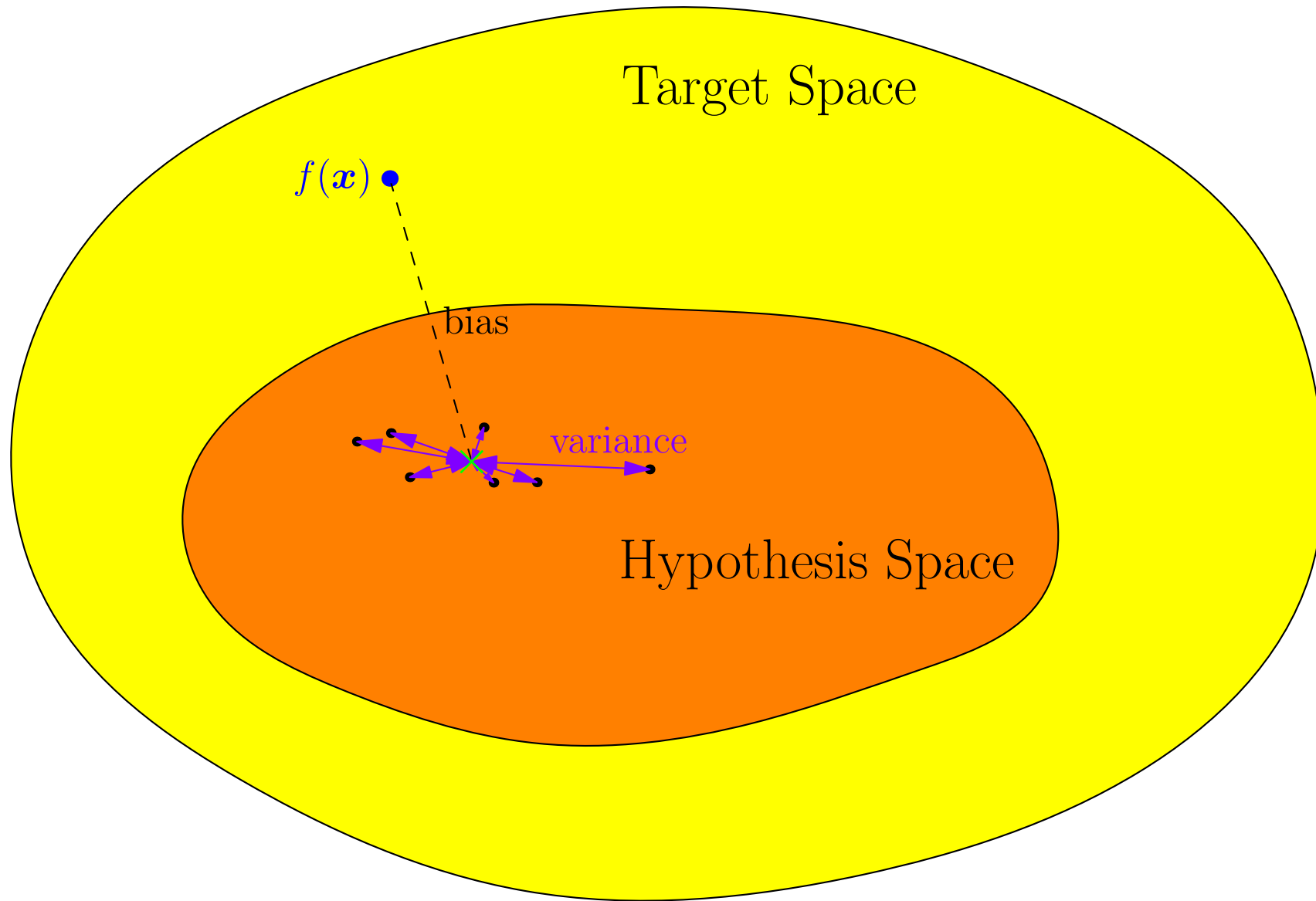
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Mean Machine

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

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

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

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

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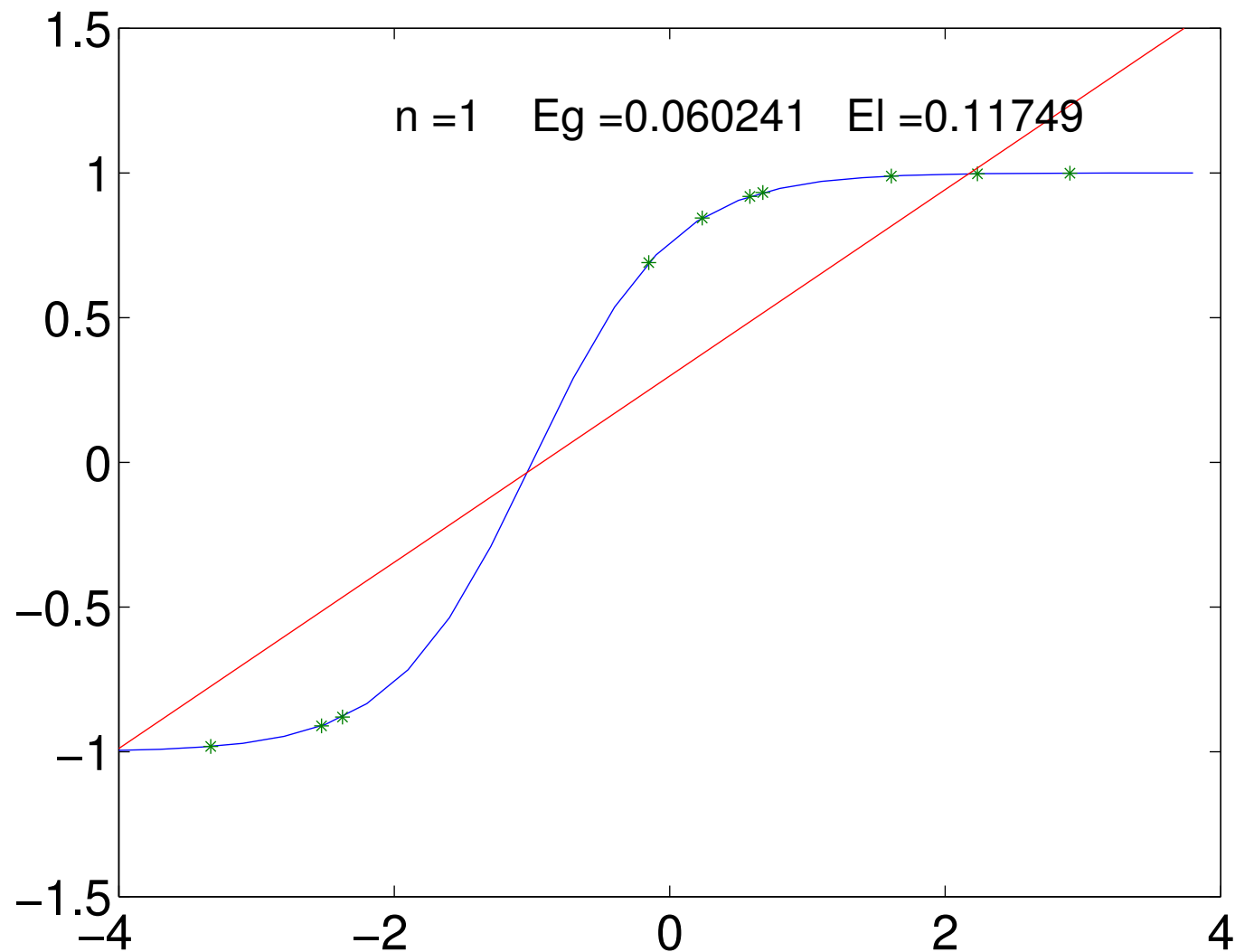
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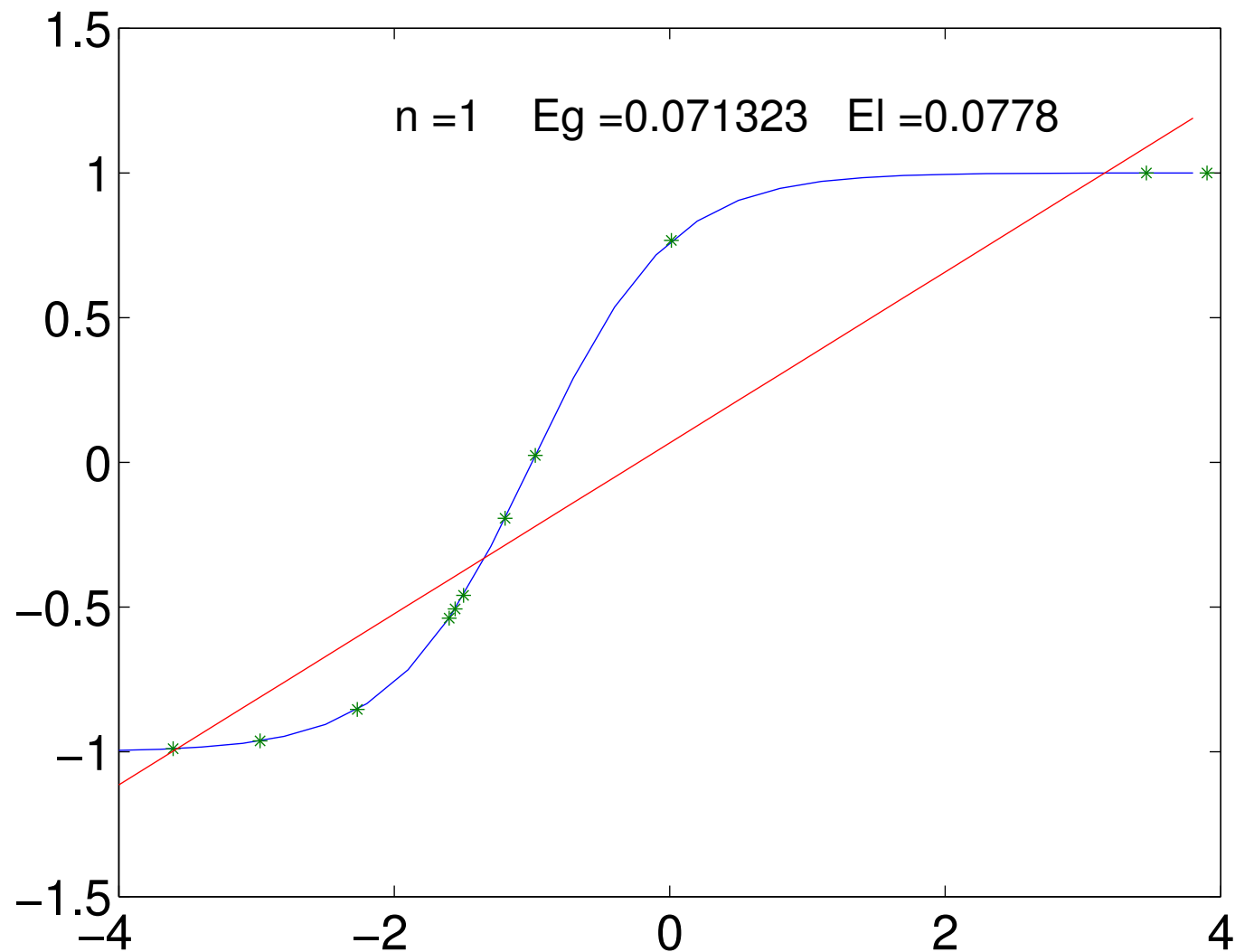
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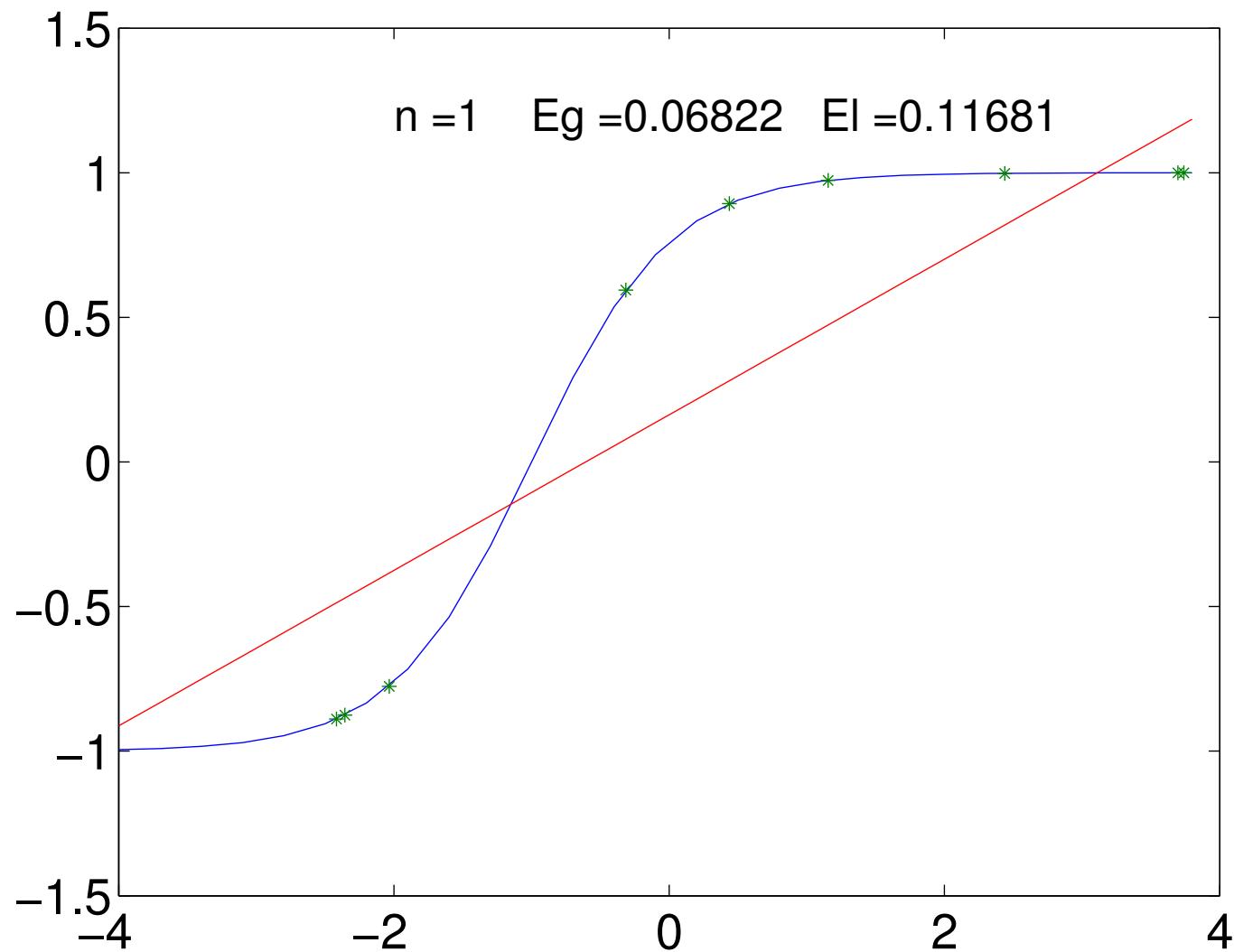
Regression Example $n = 1$



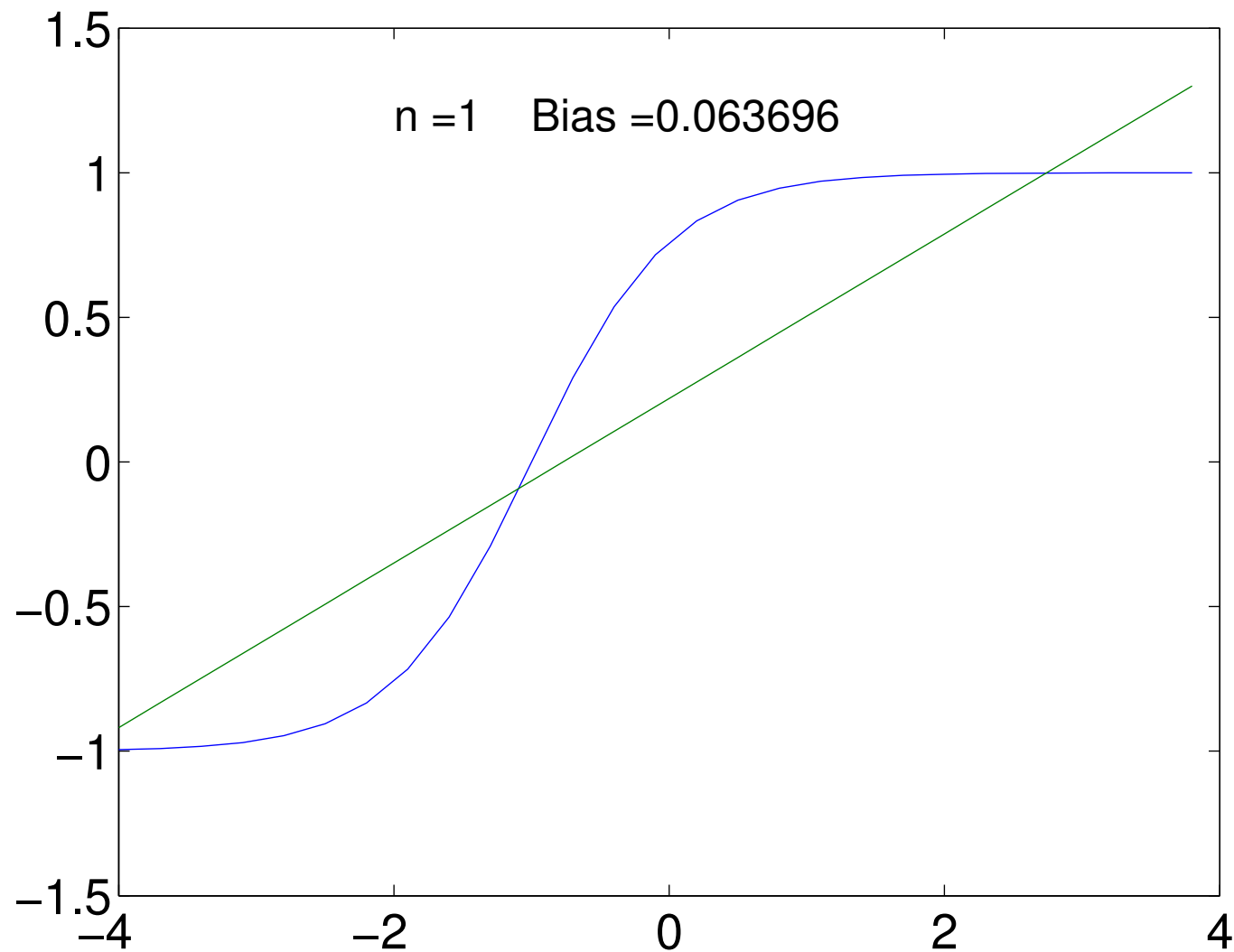
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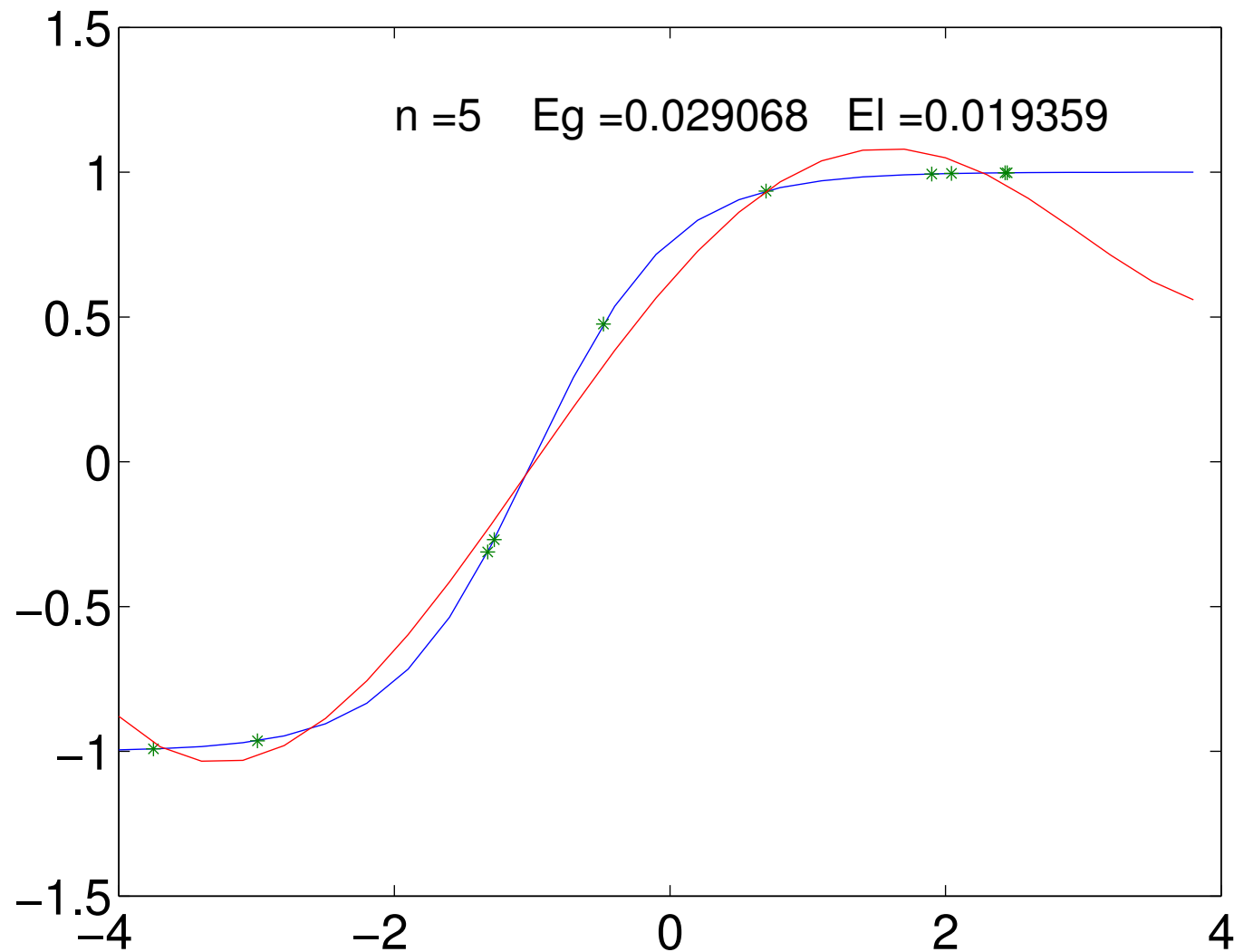
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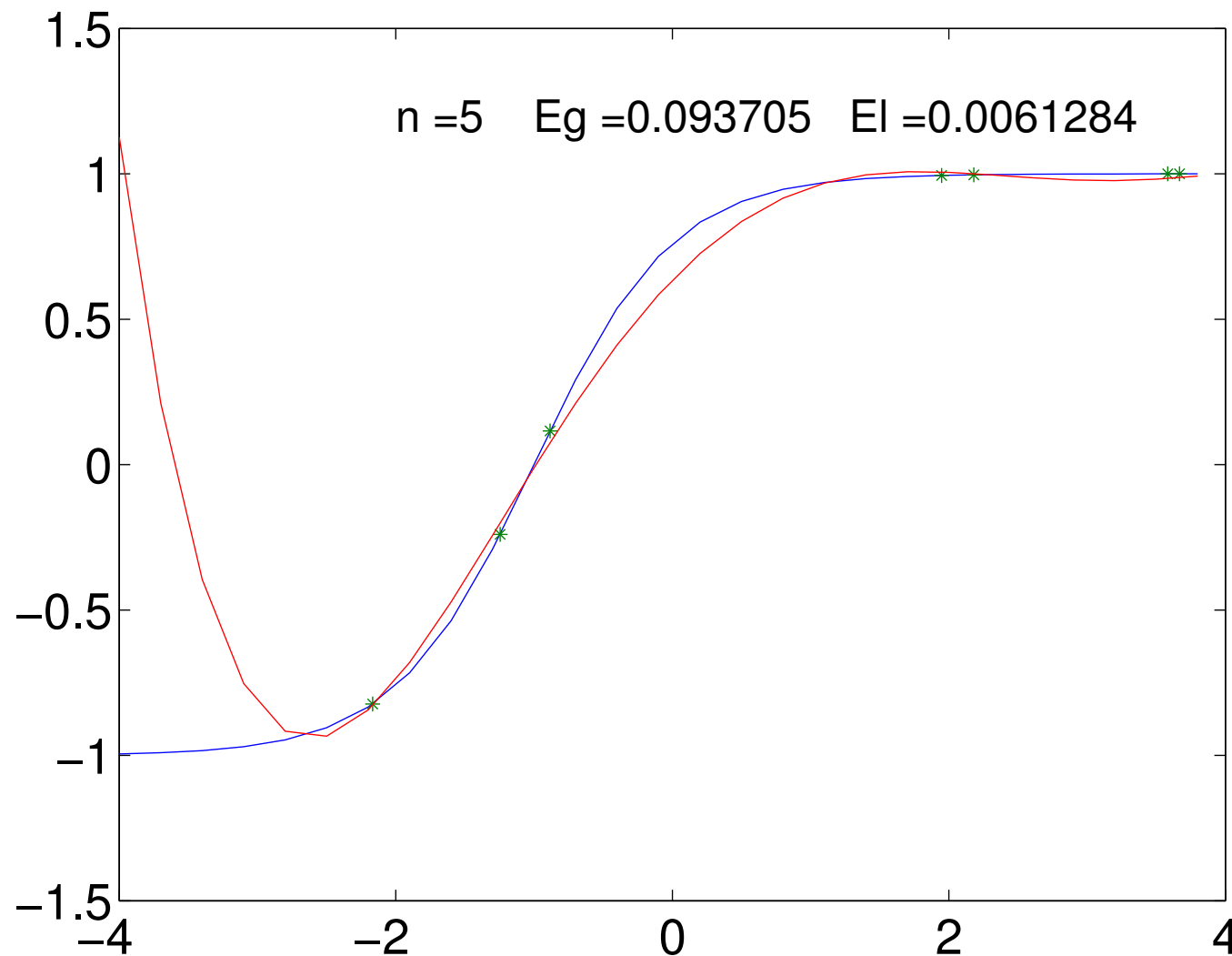
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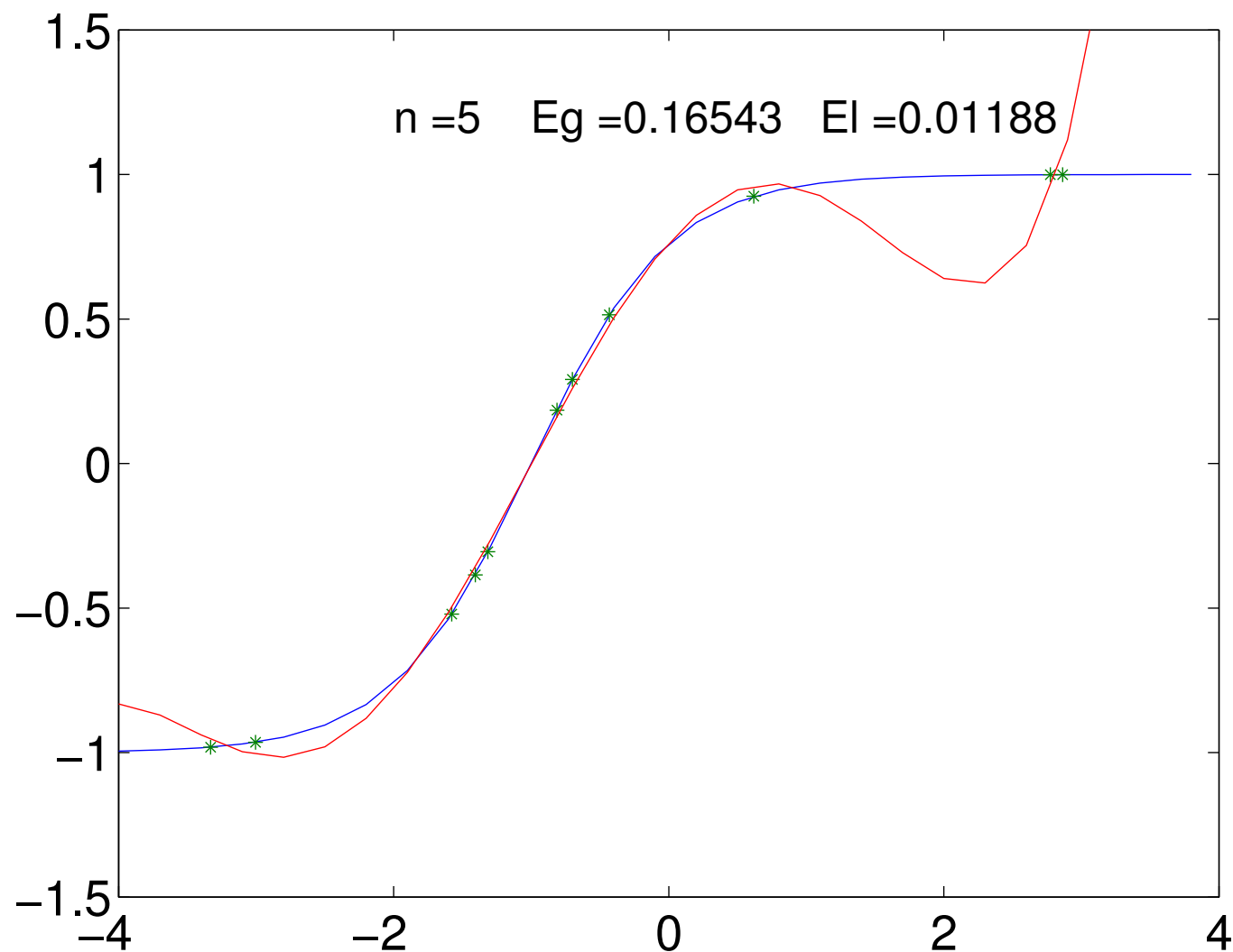
Regression Example $n = 5$



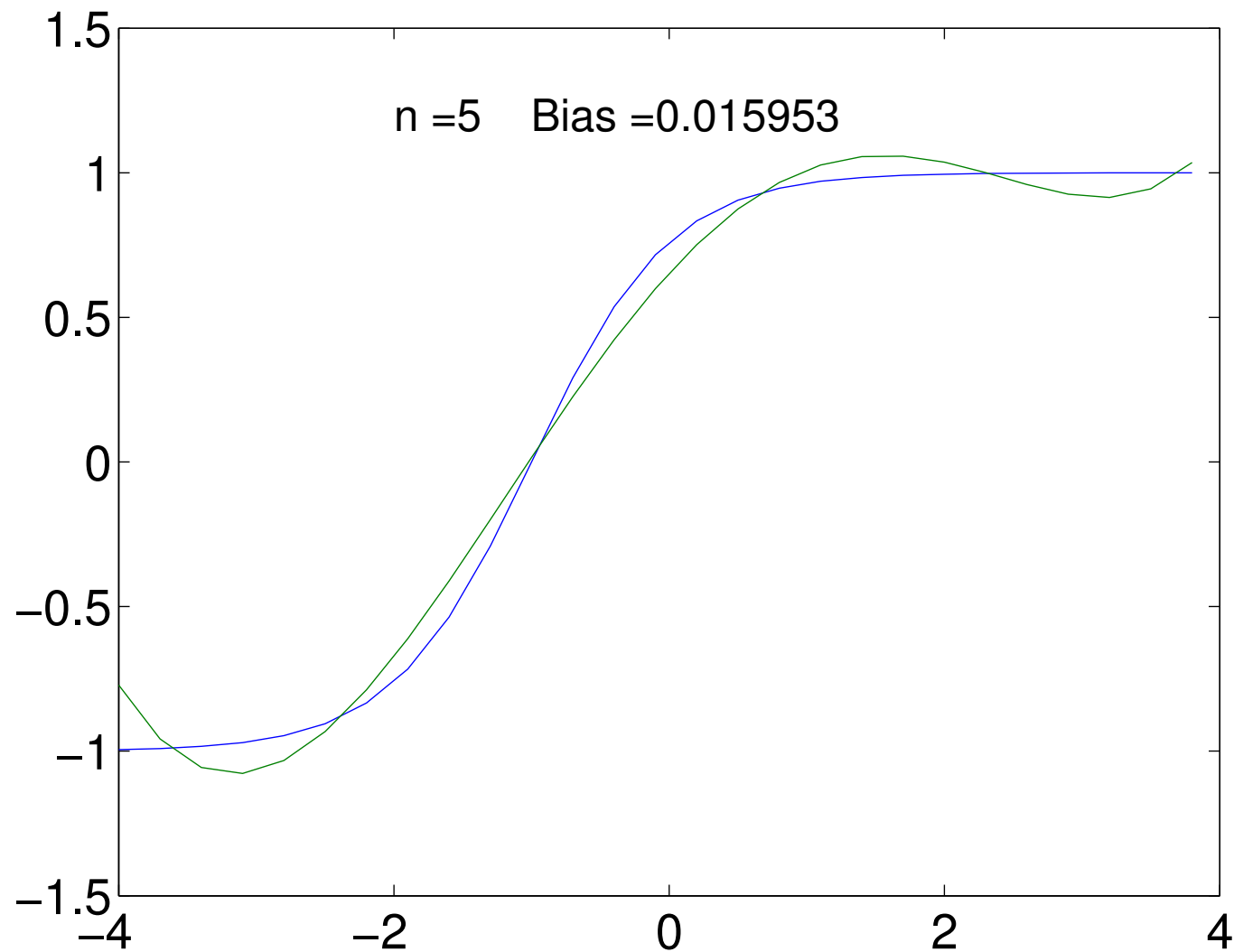
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Bias and Variance

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

$$\begin{aligned}\bar{E}_G &= \mathbb{E}_{\mathcal{D}}[E_G(\mathcal{D})] = \mathbb{E}_{\mathcal{D}} \left[\sum_{\mathbf{x} \in \mathcal{X}} p(\mathbf{x}) \left(\hat{f}(\mathbf{x}|\mathcal{D}) - f(\mathbf{x}) \right)^2 \right] \\&= \sum_{\mathbf{x} \in \mathcal{X}} p(\mathbf{x}) \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x}|\mathcal{D}) - f(\mathbf{x}) \right)^2 \right] \\&= \sum_{\mathbf{x} \in \mathcal{X}} p(\mathbf{x}) \mathbb{E}_{\mathcal{D}} \left[\left(\left(\hat{f}(\mathbf{x}|\mathcal{D}) - \hat{f}_m(\mathbf{x}) \right) + \left(\hat{f}_m(\mathbf{x}) - f(\mathbf{x}) \right) \right)^2 \right] \\&= \sum_{\mathbf{x} \in \mathcal{X}} p(\mathbf{x}) \left(\mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x}|\mathcal{D}) - \hat{f}_m(\mathbf{x}) \right)^2 \right] + \left(\hat{f}_m(\mathbf{x}) - f(\mathbf{x}) \right)^2 \right. \\&\quad \left. + \mathbb{E}_{\mathcal{D}} \left[2 \left(\hat{f}(\mathbf{x}|\mathcal{D}) - \hat{f}_m(\mathbf{x}) \right) \left(\hat{f}_m(\mathbf{x}) - f(\mathbf{x}) \right) \right] \right)\end{aligned}$$

Bias and Variance

- We can write the expected generalisation as

$$\begin{aligned}\mathbb{E}_{\mathcal{D}}[E_G(\mathcal{D})] &= \mathbb{E}_{\mathcal{D}} \left[\sum_{\mathbf{x} \in \mathcal{X}} p(\mathbf{x}) \left(\hat{f}(\mathbf{x}|\mathcal{D}) - \hat{f}_m(\mathbf{x}) \right)^2 \right] \\ &\quad + \sum_{\mathbf{x} \in \mathcal{X}} p(\mathbf{x}) \left(\hat{f}_m(\mathbf{x}) - f(\mathbf{x}) \right)^2 = V + B\end{aligned}$$

- 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
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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?



Training Examples

- As we increase the number of training examples, we make it hard to find a spurious rule
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- (Labelled) data is often expensive to collect so we sometimes have no choice
- Need to control the complexity of our learning machine

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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)
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Feature Selection

- Spurious features will allow us to find spurious rules (**over-fitting**)
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- We can use various heuristics to decide which features to keep, but no heuristic is fail-safe
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- As Niranjan showed us we can modify our error function to choose smoother functions

$$E = \sum_{n=1}^N (\mathbf{w}^\top \mathbf{x}_n - y_n)^2$$

- Second term is minimised when $w_i = 0$
- If w_i is large then

$$f(\mathbf{x}|\mathbf{w}) = \mathbf{w}^\top \mathbf{x}_n$$

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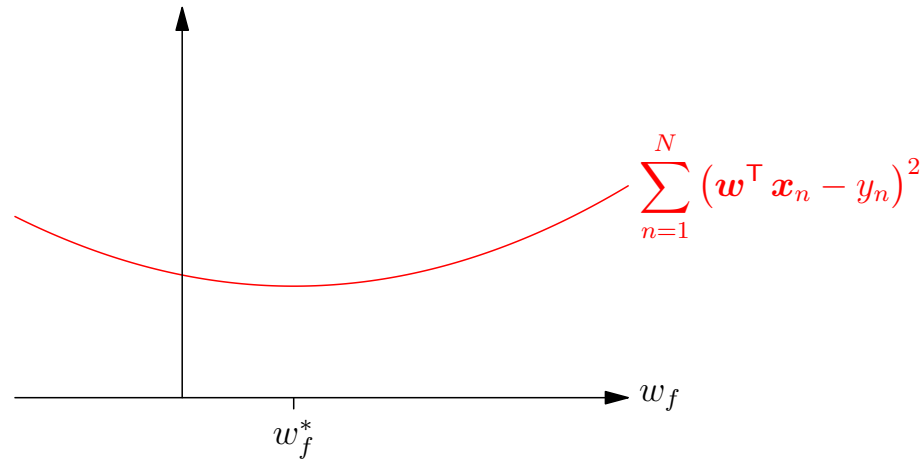
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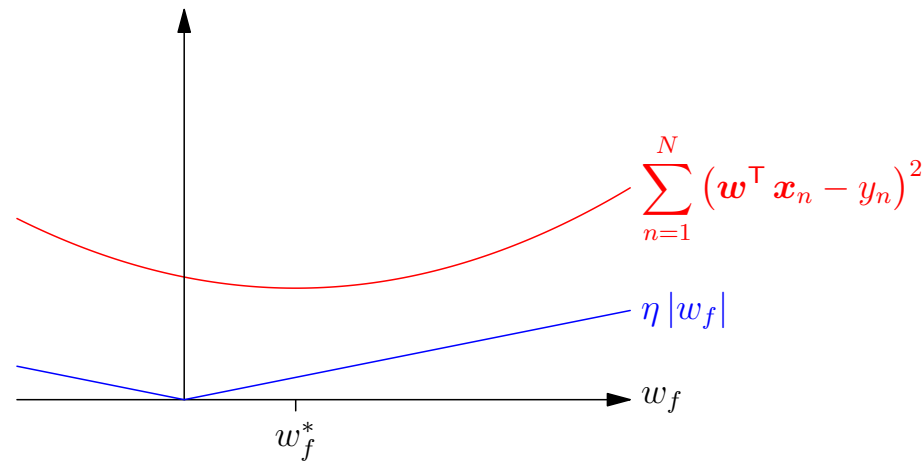


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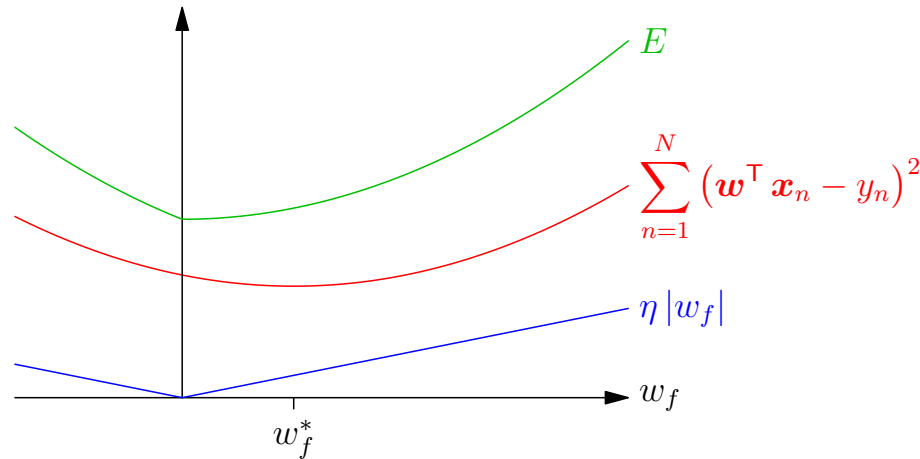


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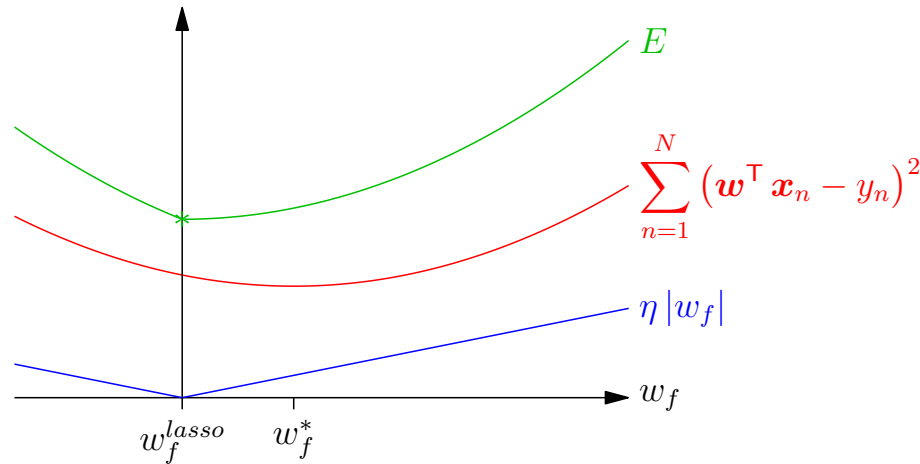


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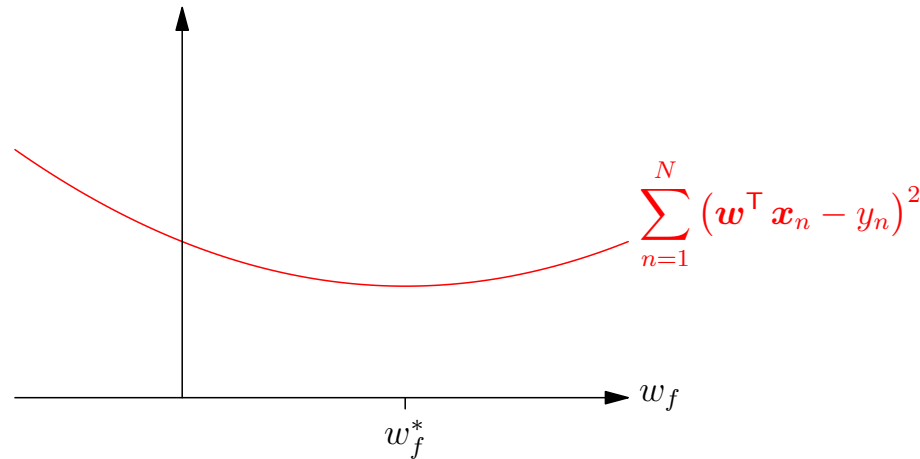


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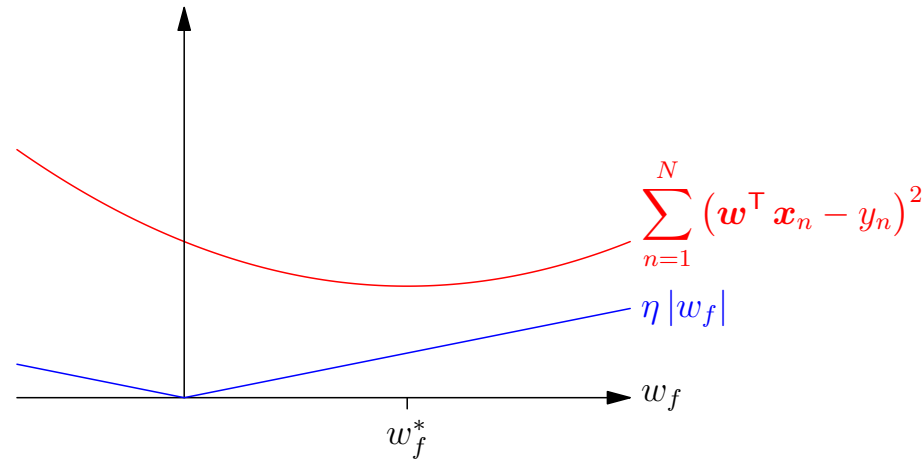


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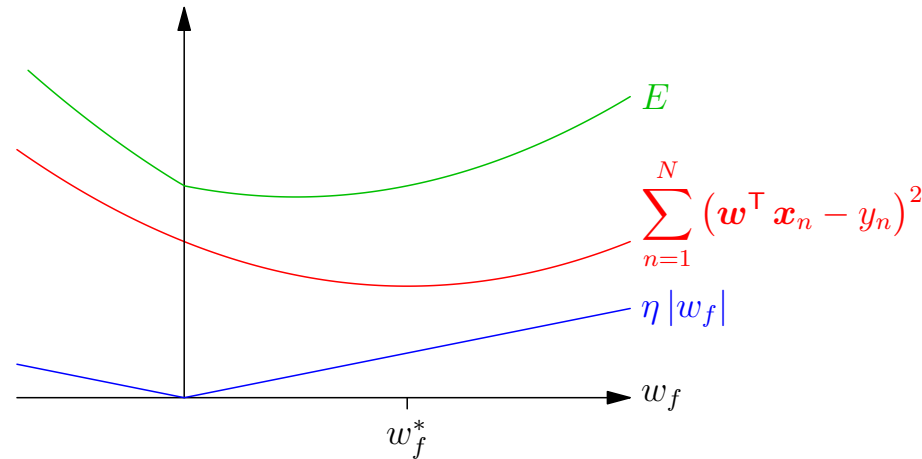


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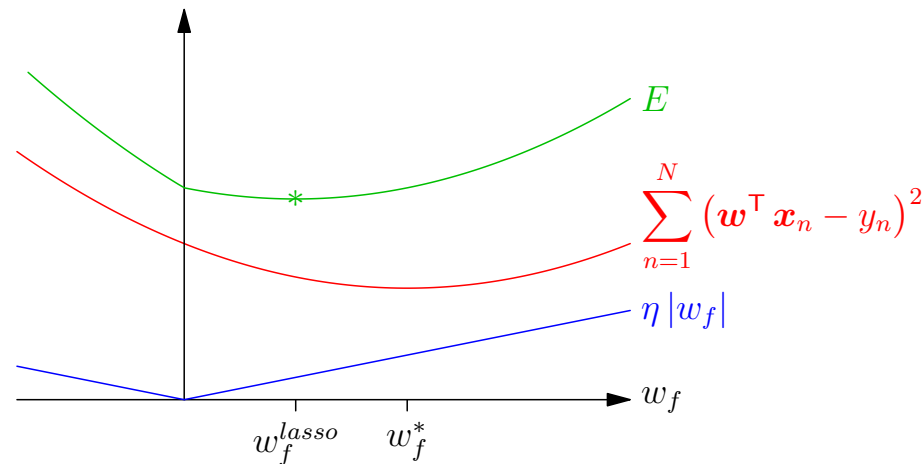


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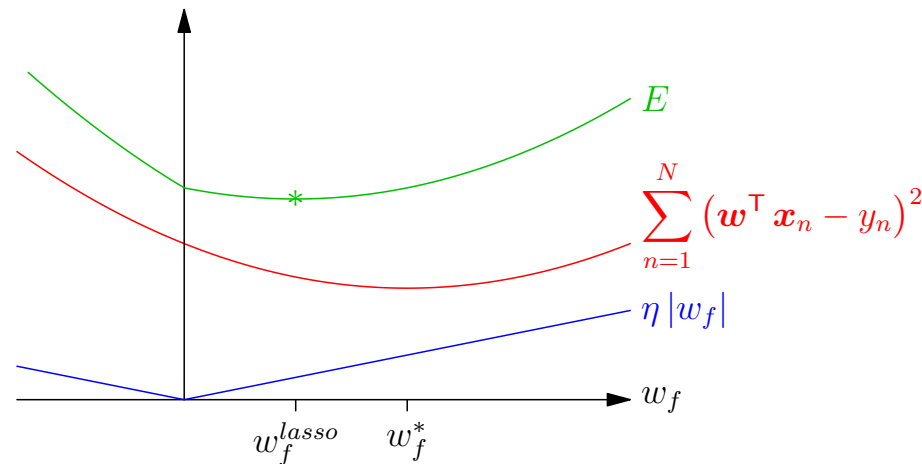


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- Does automatic feature selection

Implicit Regularisation

- In the last two examples we added an explicit regularisation term that made the function we learnt simpler
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- 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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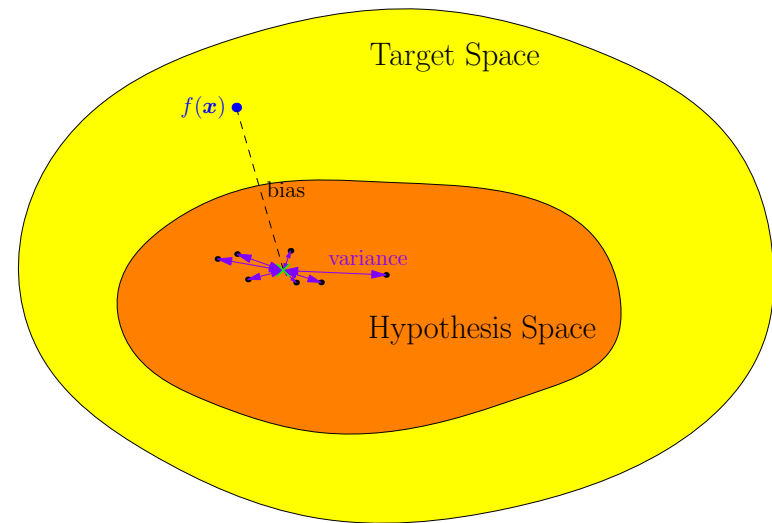
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Outline

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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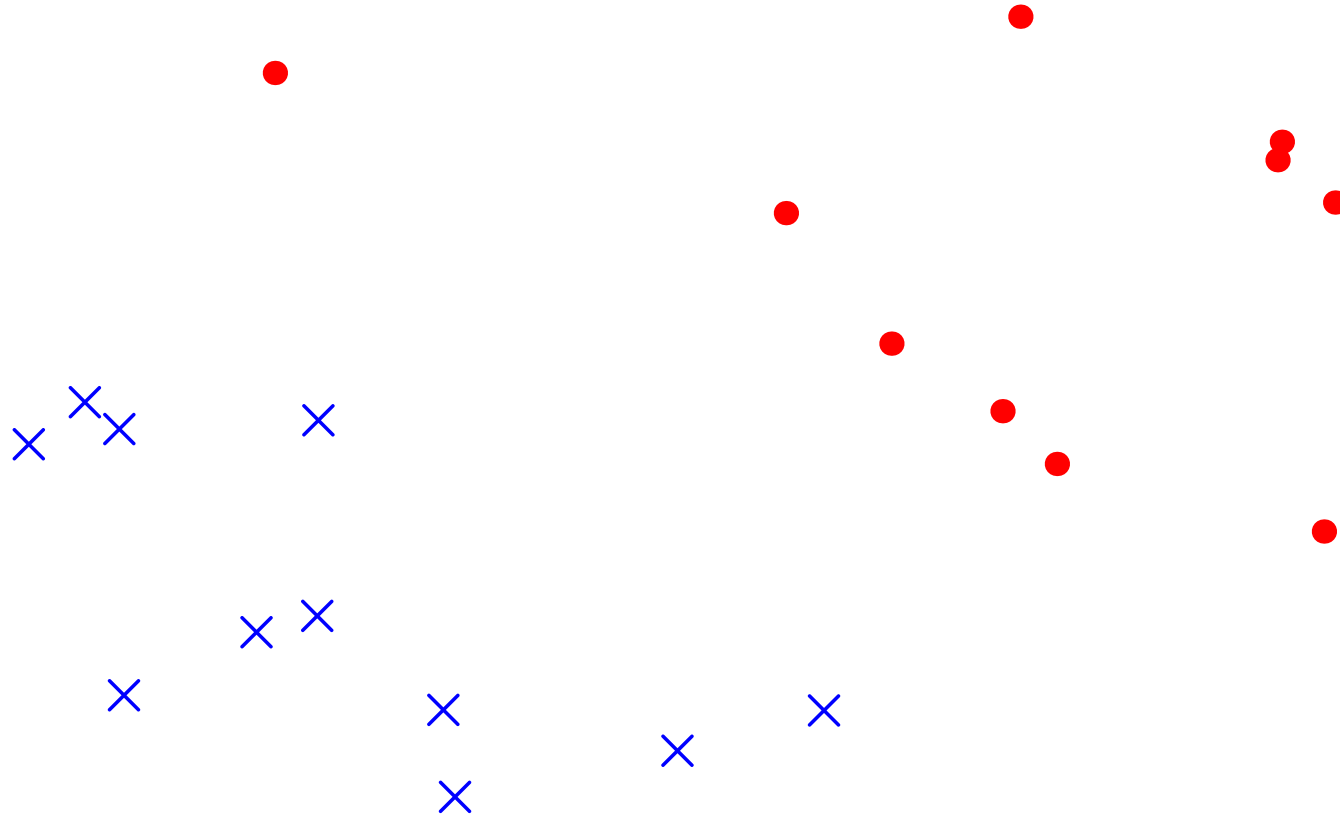
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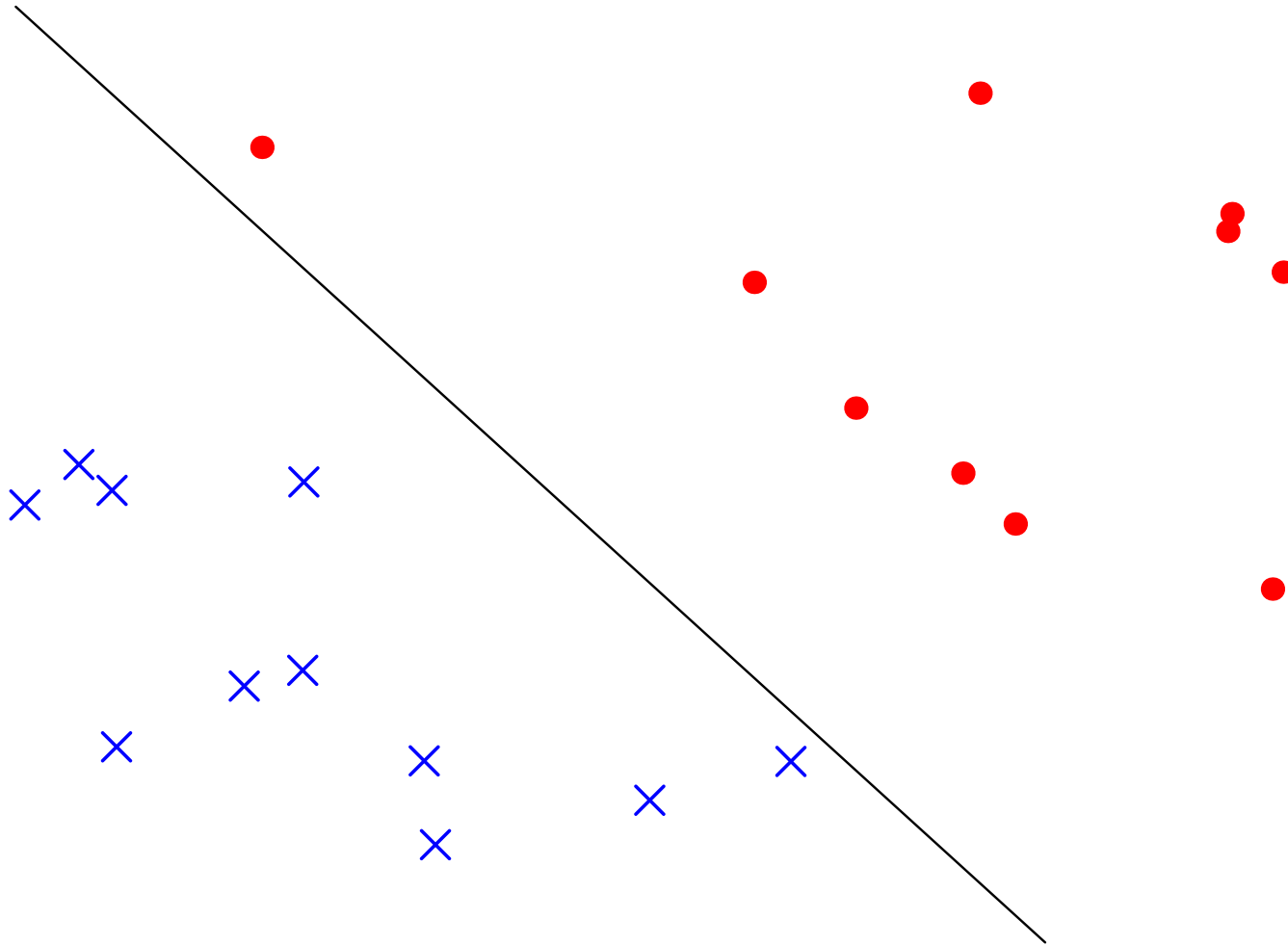
Linear Separation of Data

- SVMs classify linearly separable data



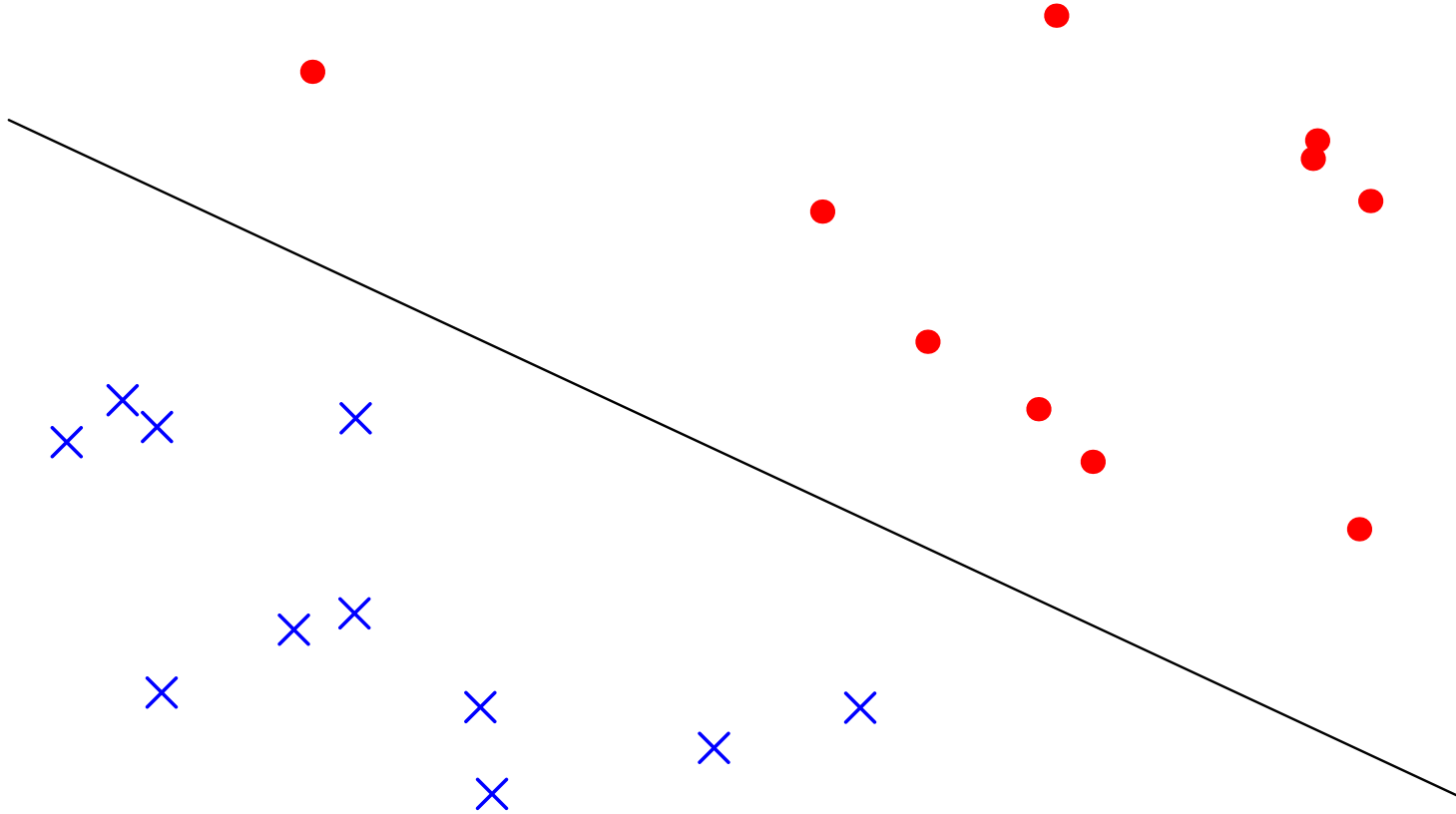
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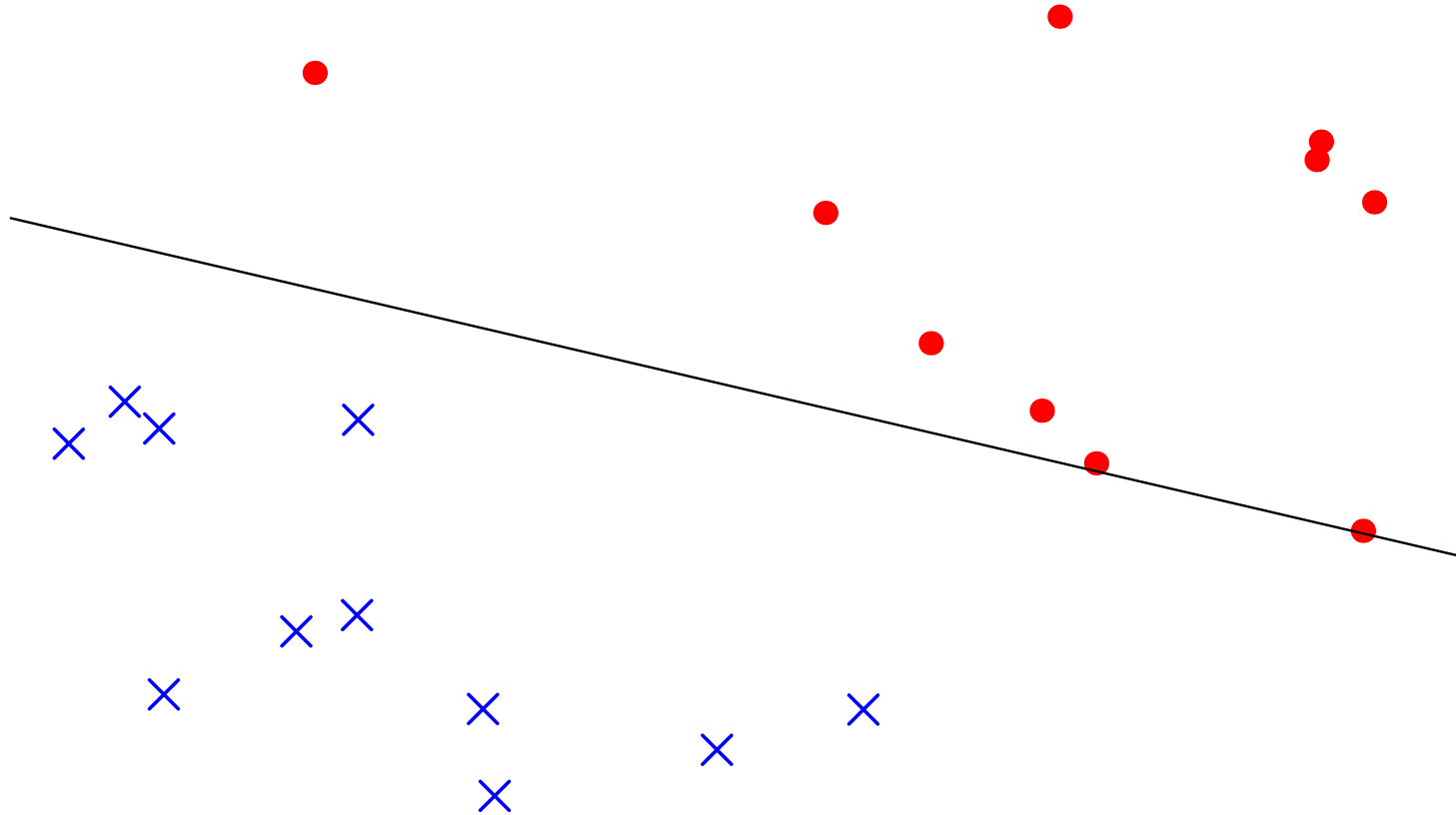
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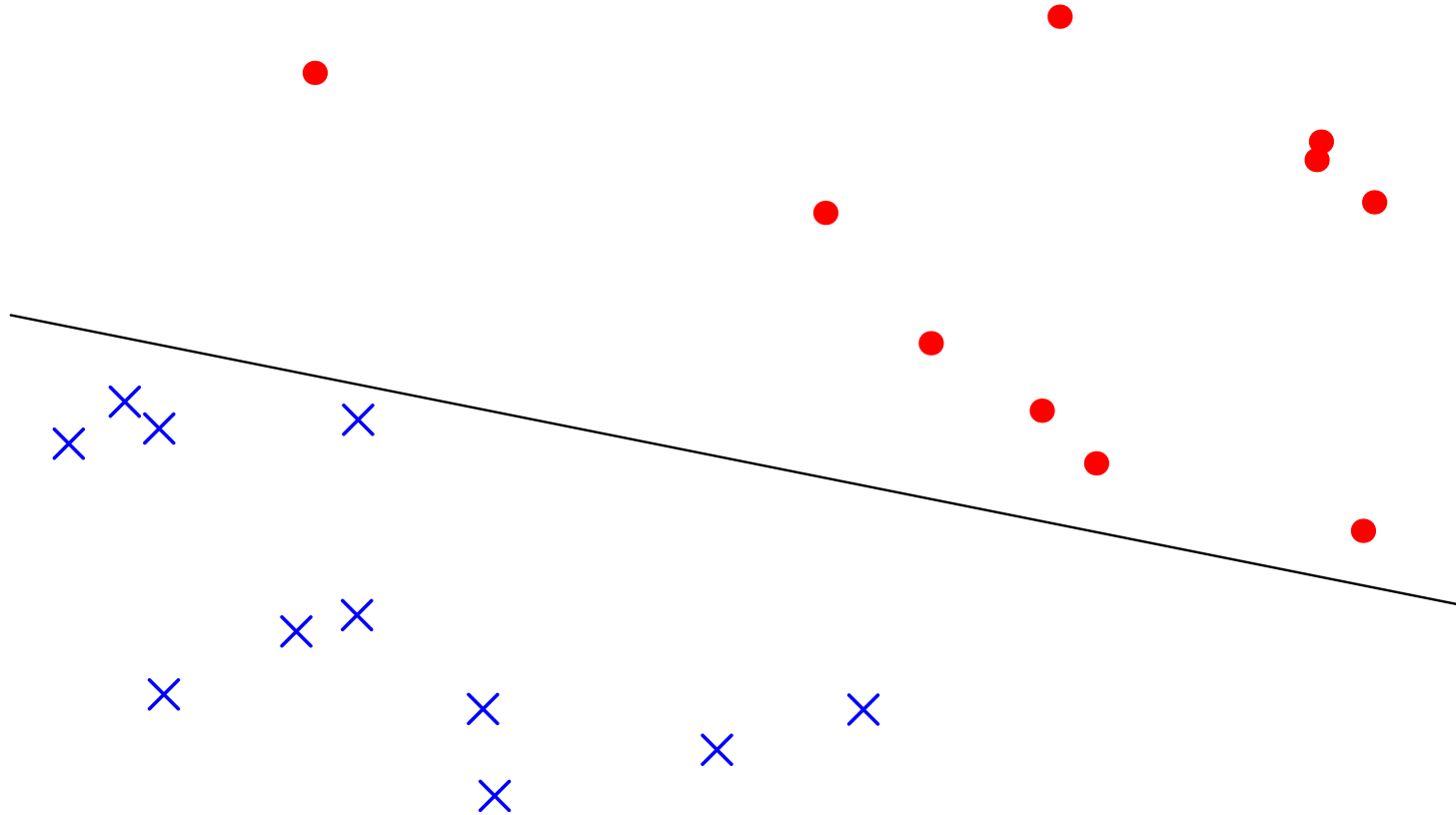
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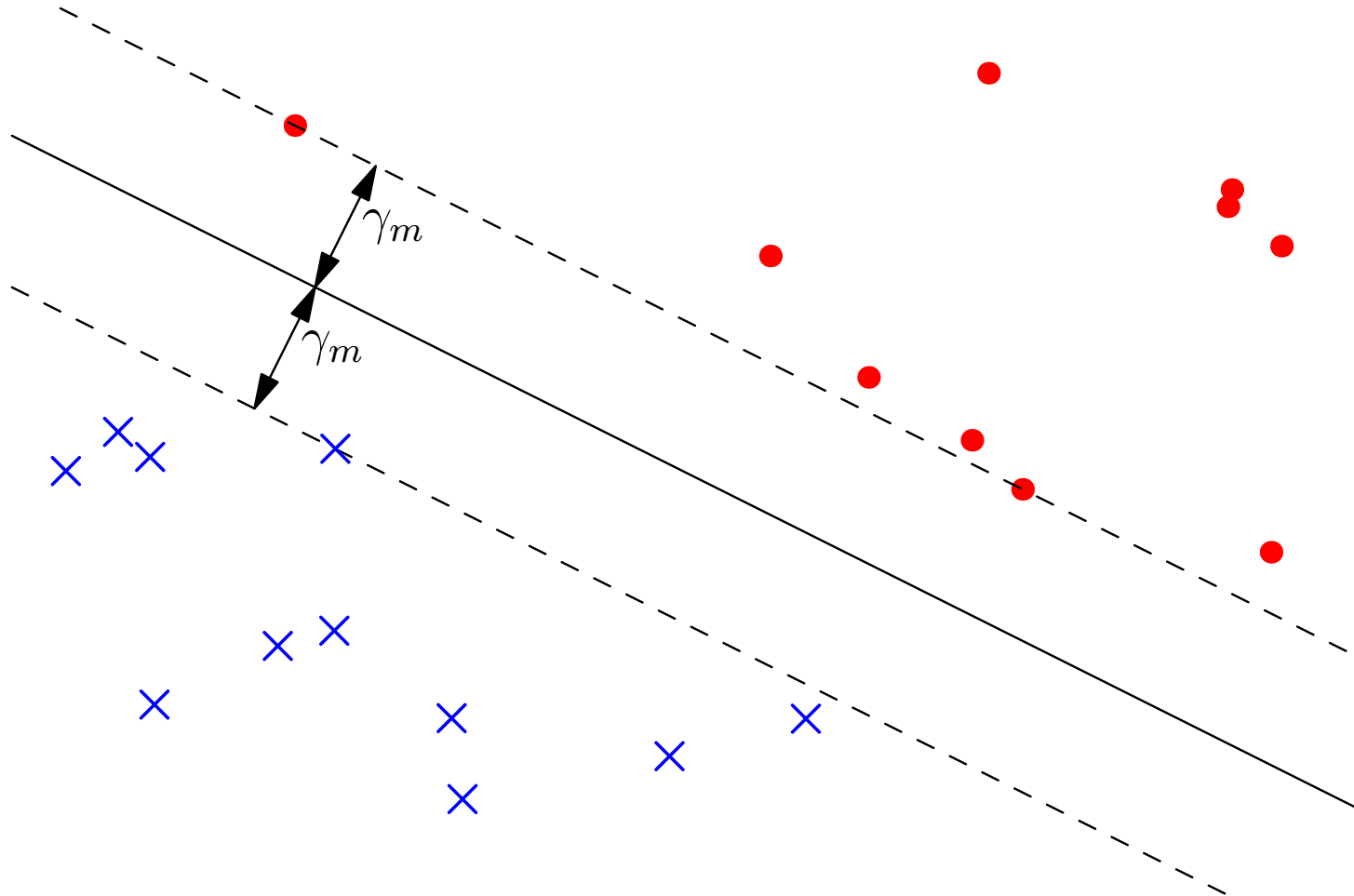
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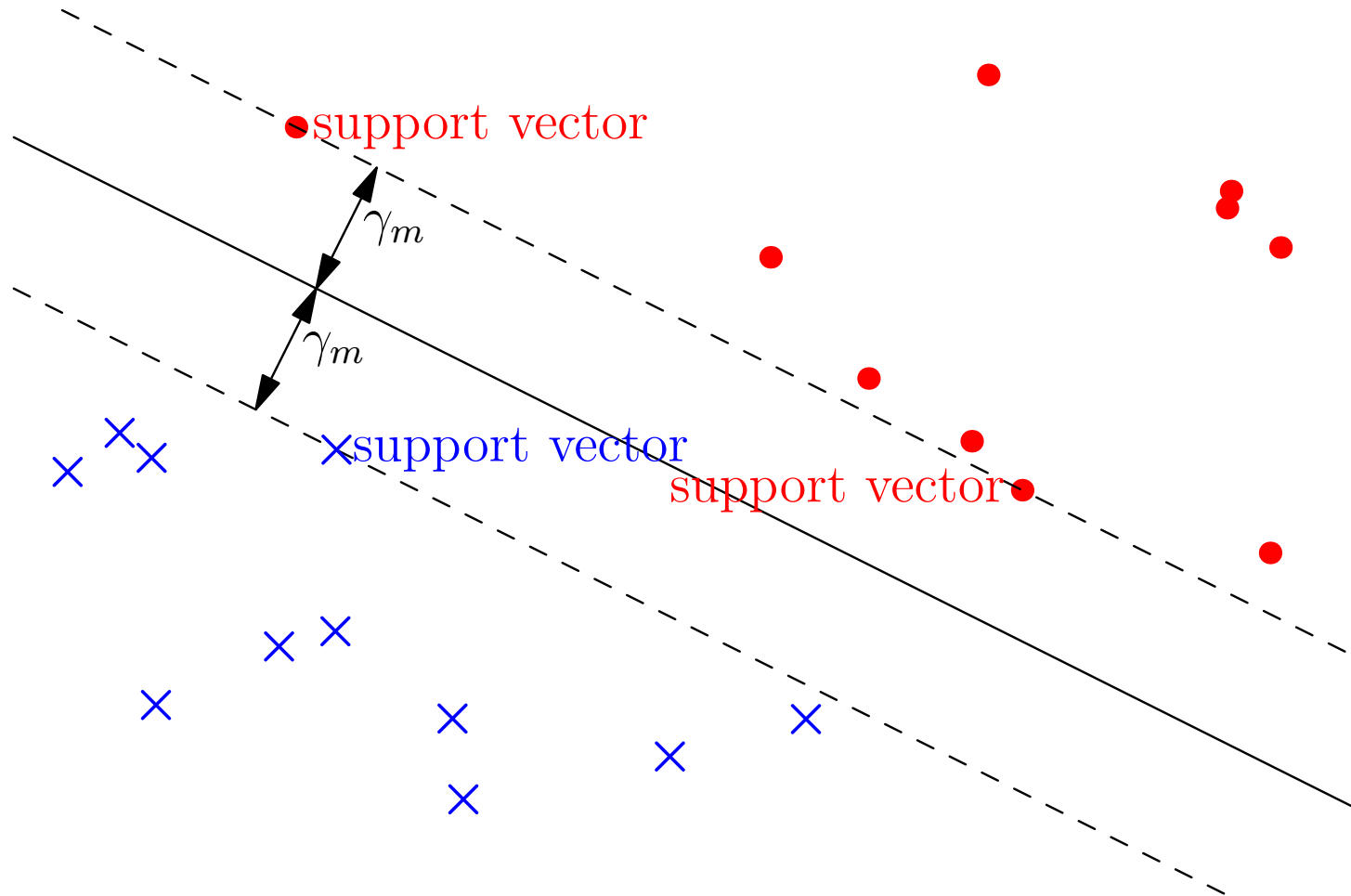
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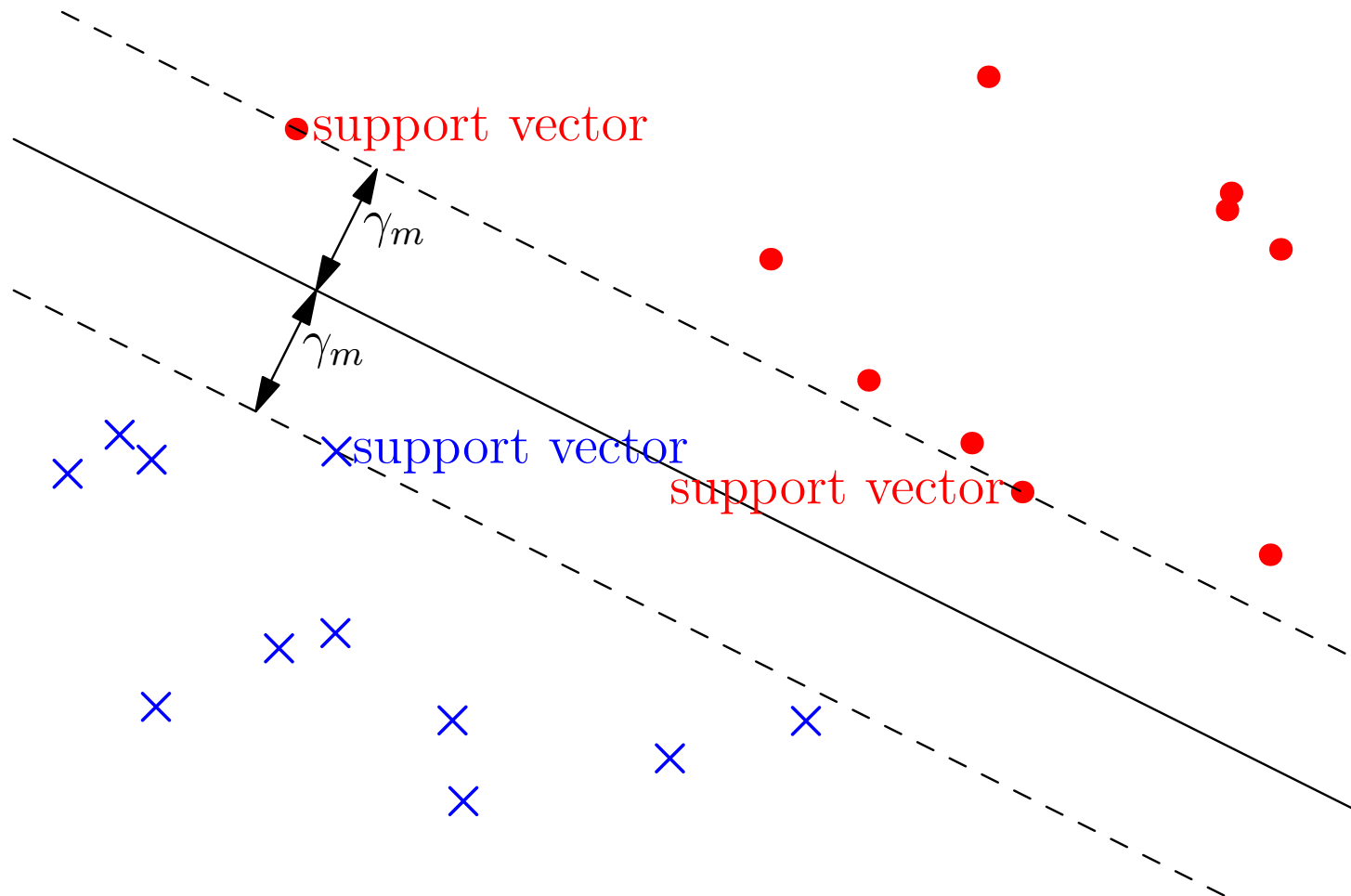
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- Finds maximum-margin separating plane

Extended Feature Space

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

$$\mathbf{x} = (x_1, x_2, \dots, x_p) \rightarrow \phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \dots, \phi_m(\mathbf{x}))$$

$$m \gg p$$

- 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

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

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Kernel Trick

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

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(like an eigenvector decomposition of a matrix)

- Never need to compute $\phi_k(\mathbf{x}_i)$ explicitly as we only need the dot-product $\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j)$ 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

Quadratic kernel: $K(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1^\top \mathbf{x}_2)^2$

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

- Consider the mapping

$$\mathbf{x}_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix} \rightarrow \phi(\mathbf{x}_i) = \begin{pmatrix} x_i^2 \\ y_i^2 \\ \sqrt{2} x_i y_i \end{pmatrix}$$

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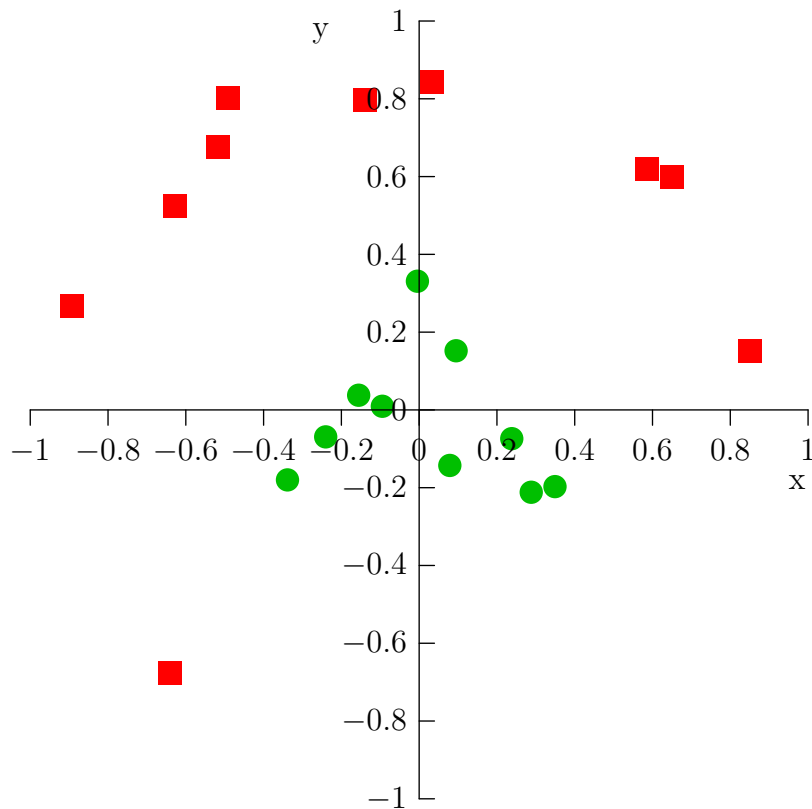
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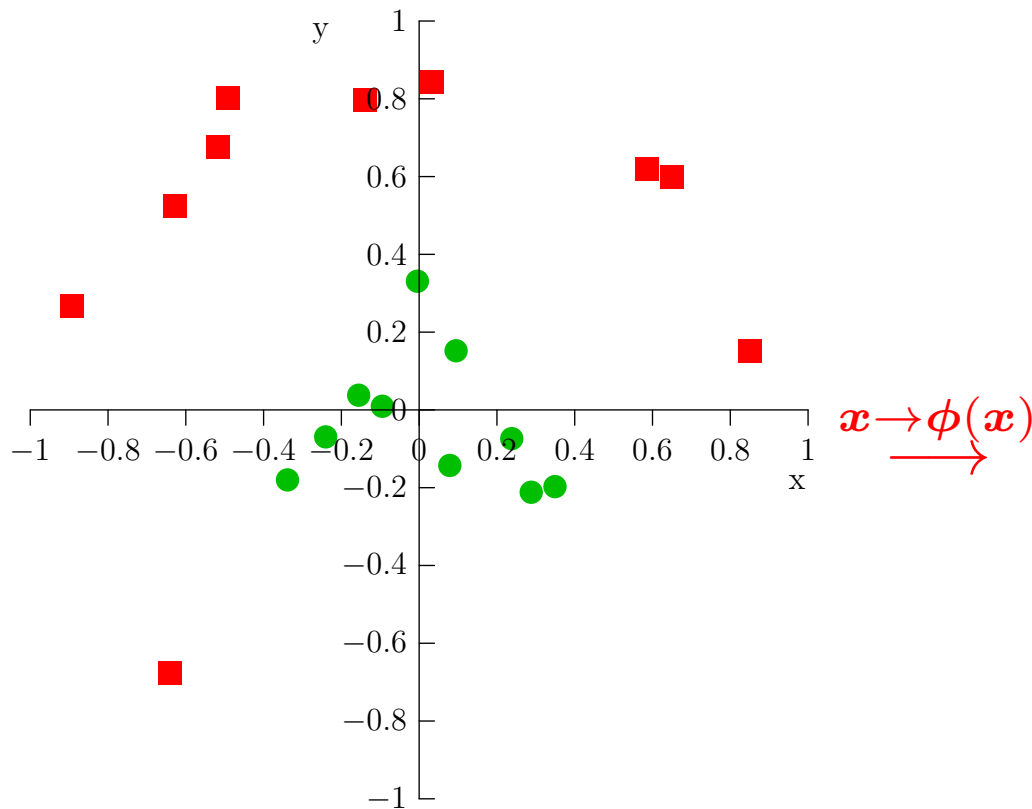
Non-linearly Separable Data

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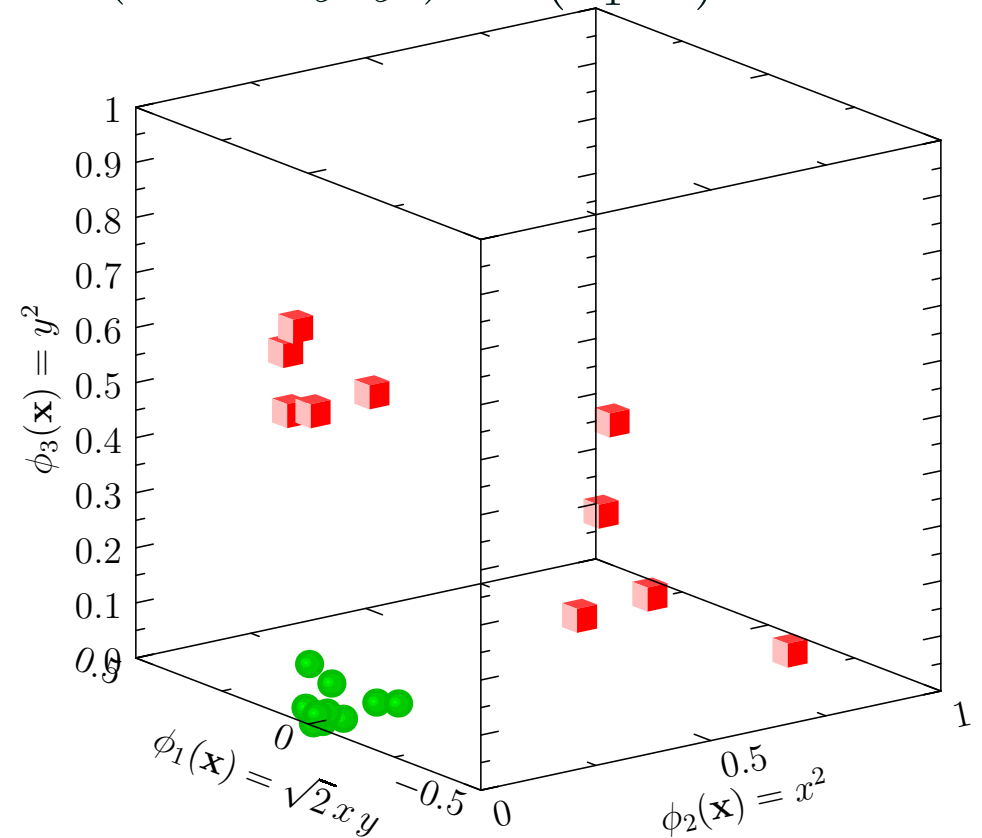
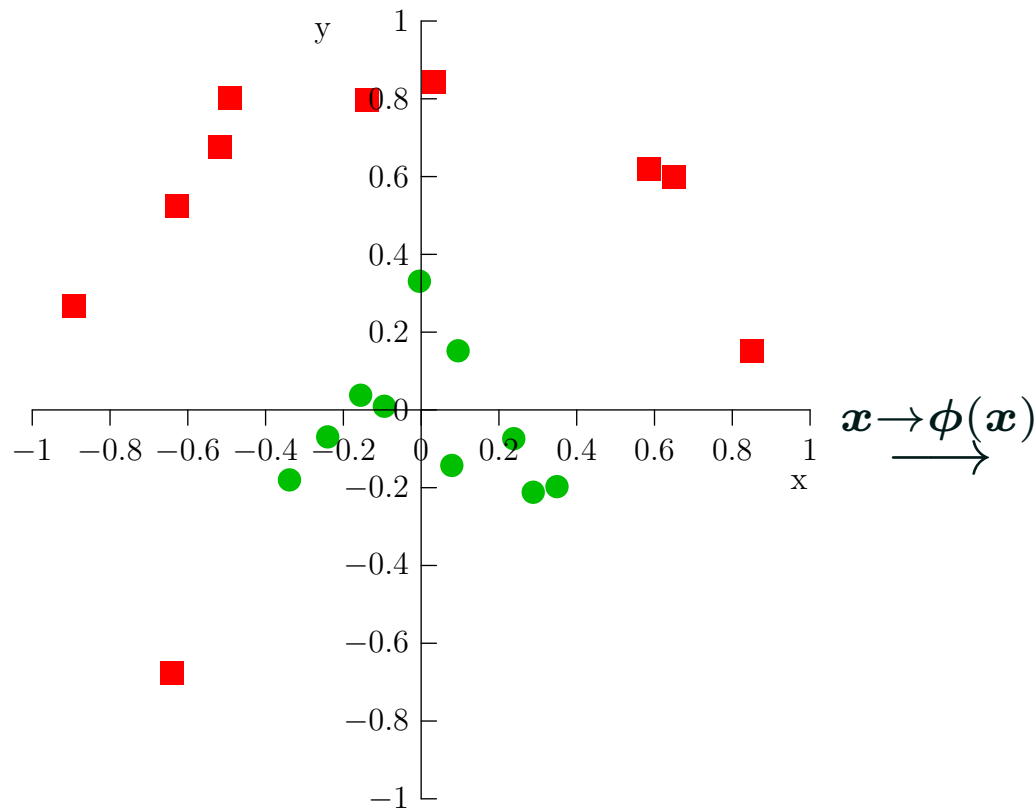
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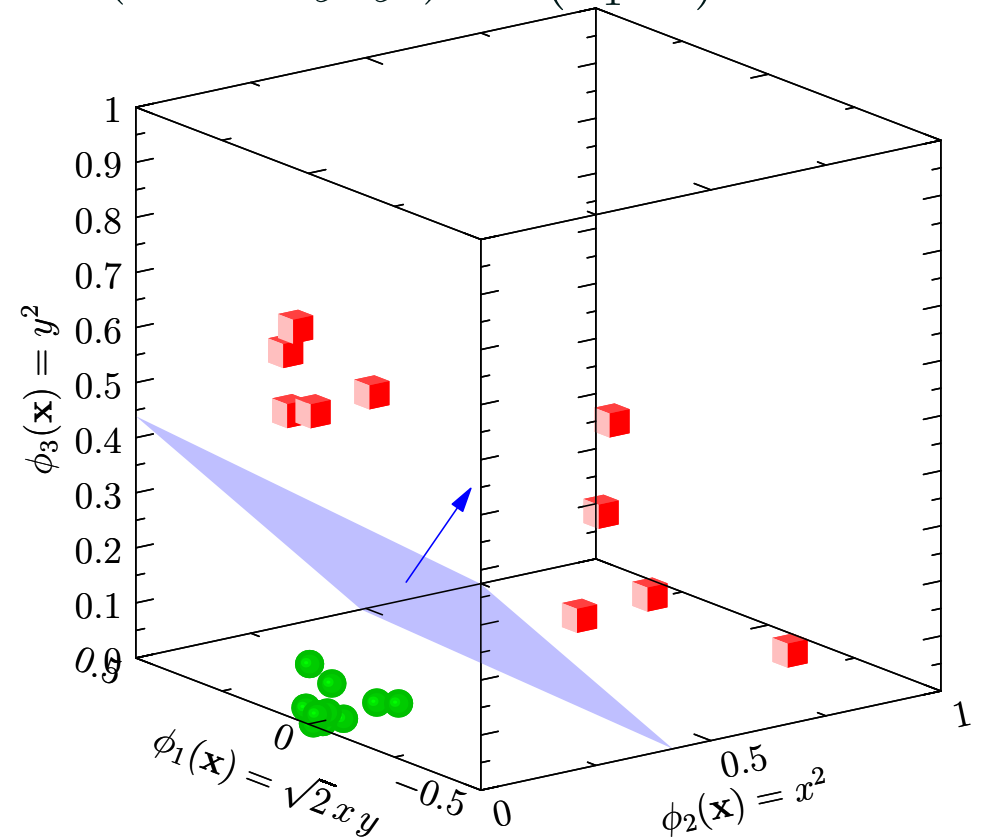
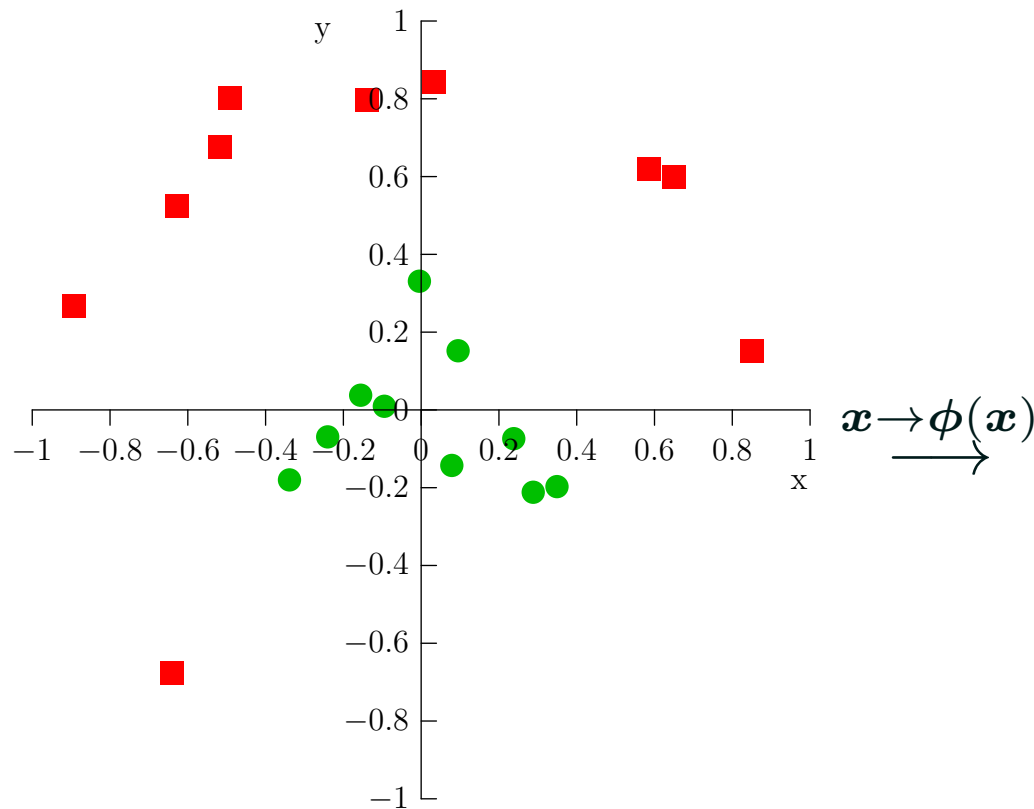
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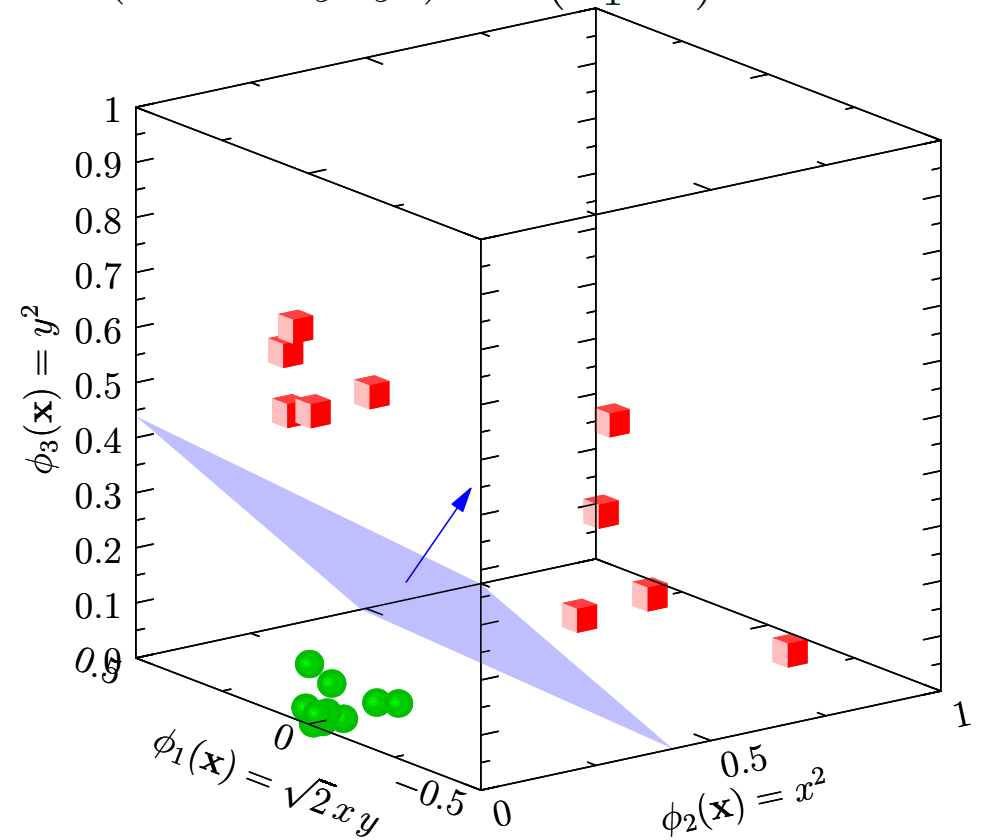
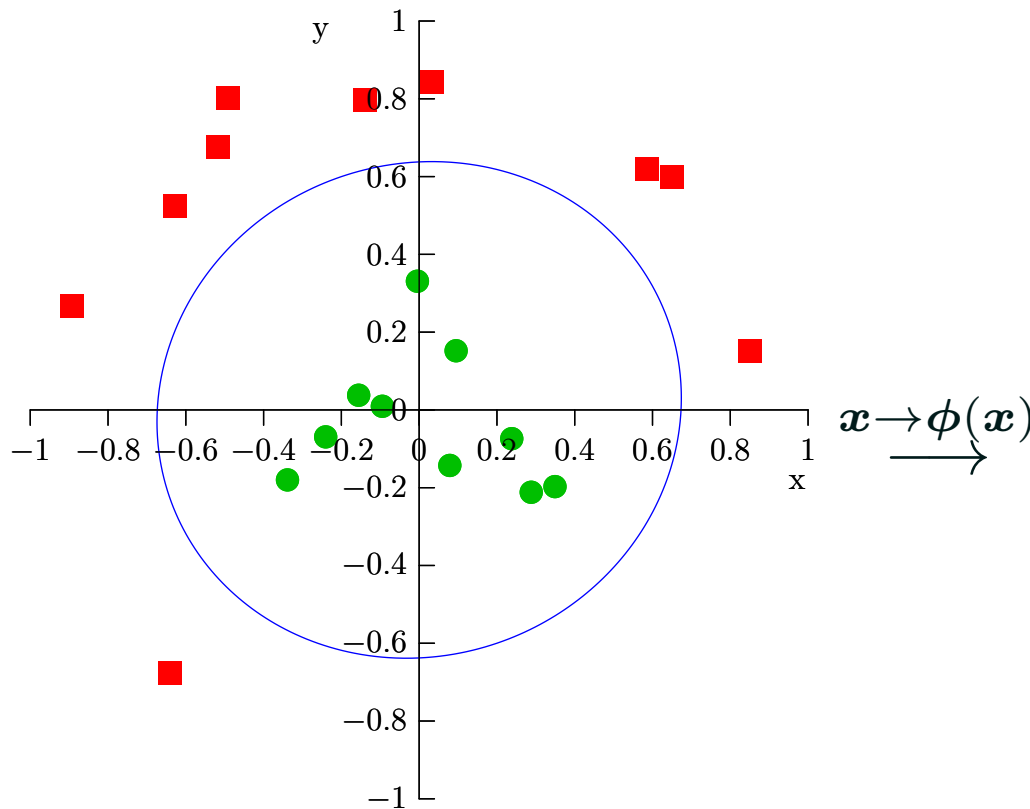
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Computing the Maximum-Margin Hyper-plane

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- Never need to compute $\phi_i(\mathbf{x})$ only need to compute $\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$
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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
- If we don't know what features are important (most often the case), then it is worth scaling each feature (for example, so their range is between 0 and 1 or their variance is 1)

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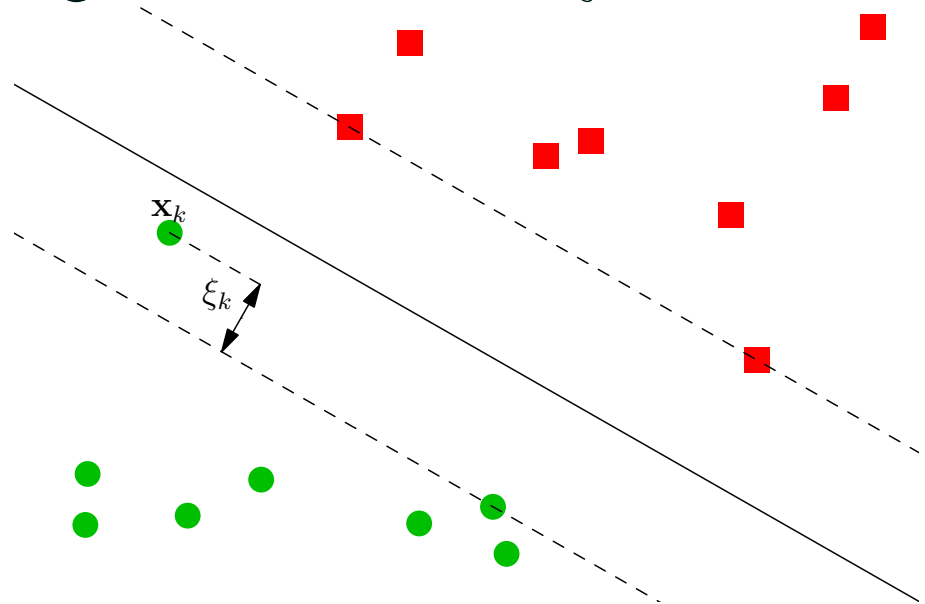
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Soft Margins

- Sometimes the margin constraint is too severe
- Relax constraints by introducing *slack variables*, $\xi_k \geq 0$

$$y_k(\mathbf{x}_k^\top \mathbf{w} - b) \geq 1 - \xi_k$$

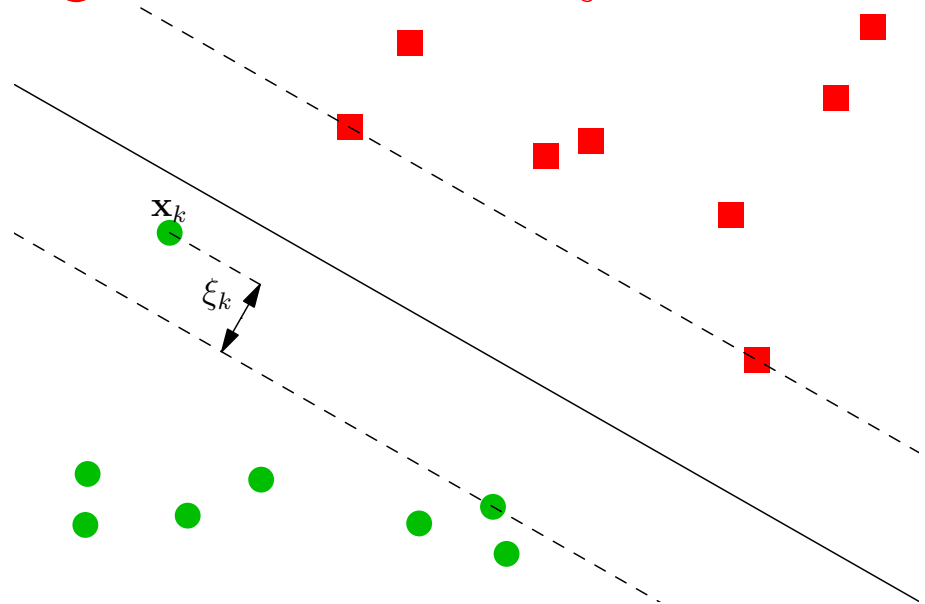


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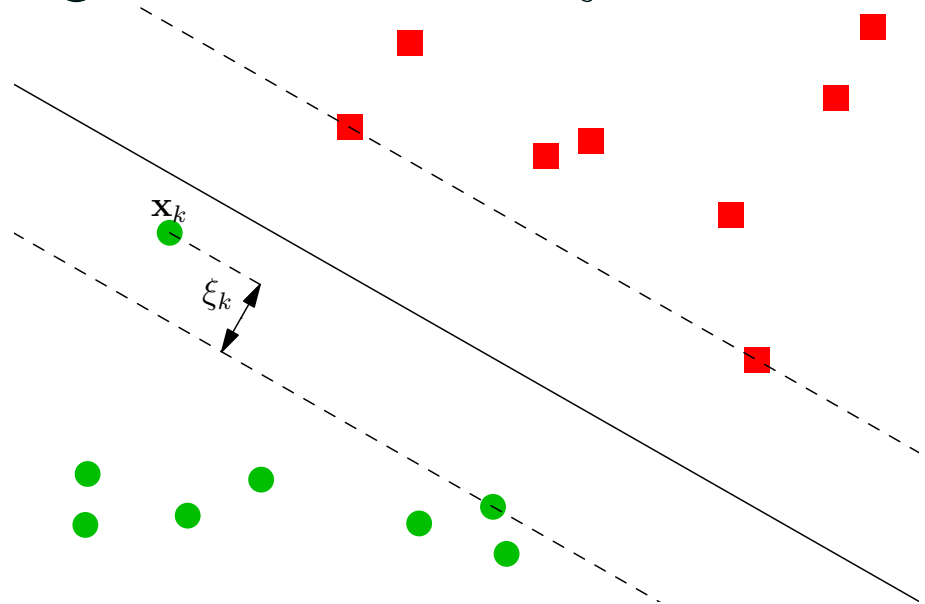


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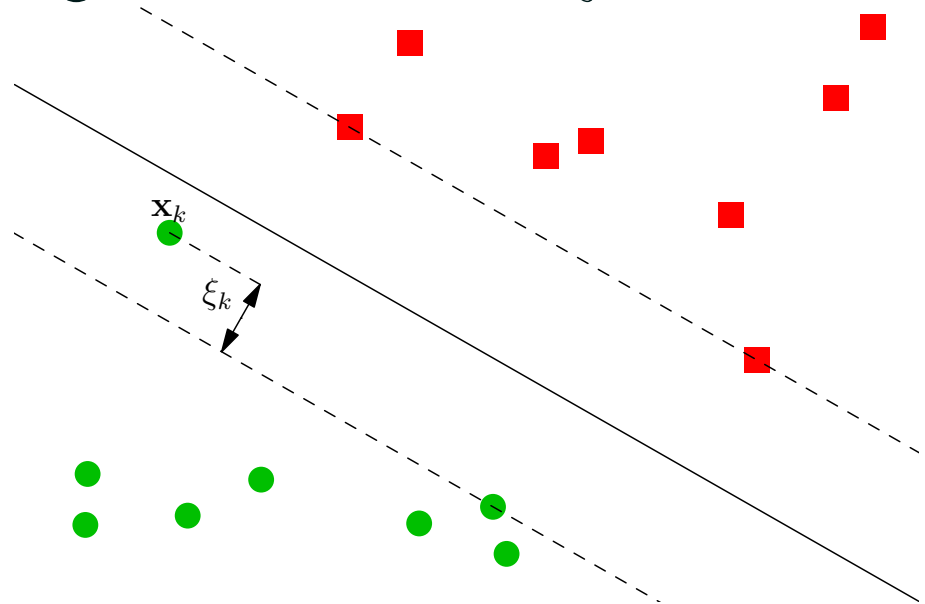


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Choosing the Right Kernel Function

- There are kernels design for particular data types (e.g. string kernels for text or biological sequences)
- For numerical data people tend to look at using no kernel (linear SVM), a radial basis function (Gaussian) kernel or polynomial kernels
- Kernel's often come with parameters, e.g. the popular radial basis function kernel

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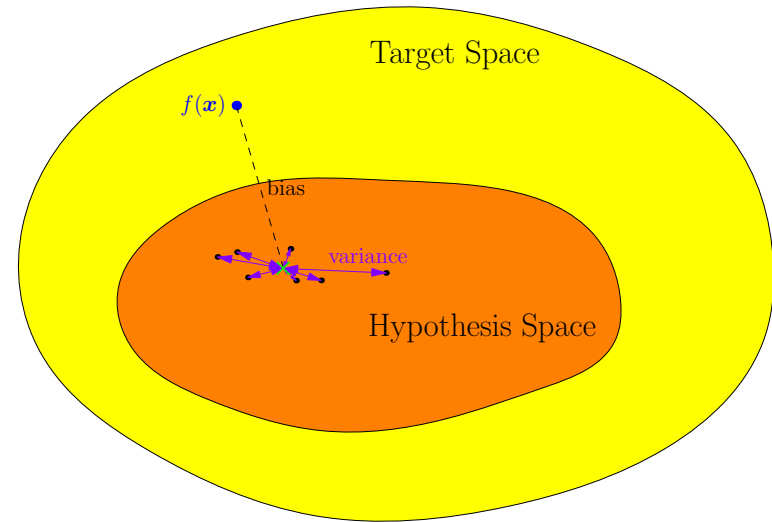
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Outline

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



Removing Variance By Averaging

- We can reduce the variance and hence improve our generalisation error by averaging over different learning machines
- There are a number of different techniques for doing this that go by the name of **ensemble methods** or **ensemble learning**
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 - ★ mixture of data types
 - ★ missing data
 - ★ large data sets
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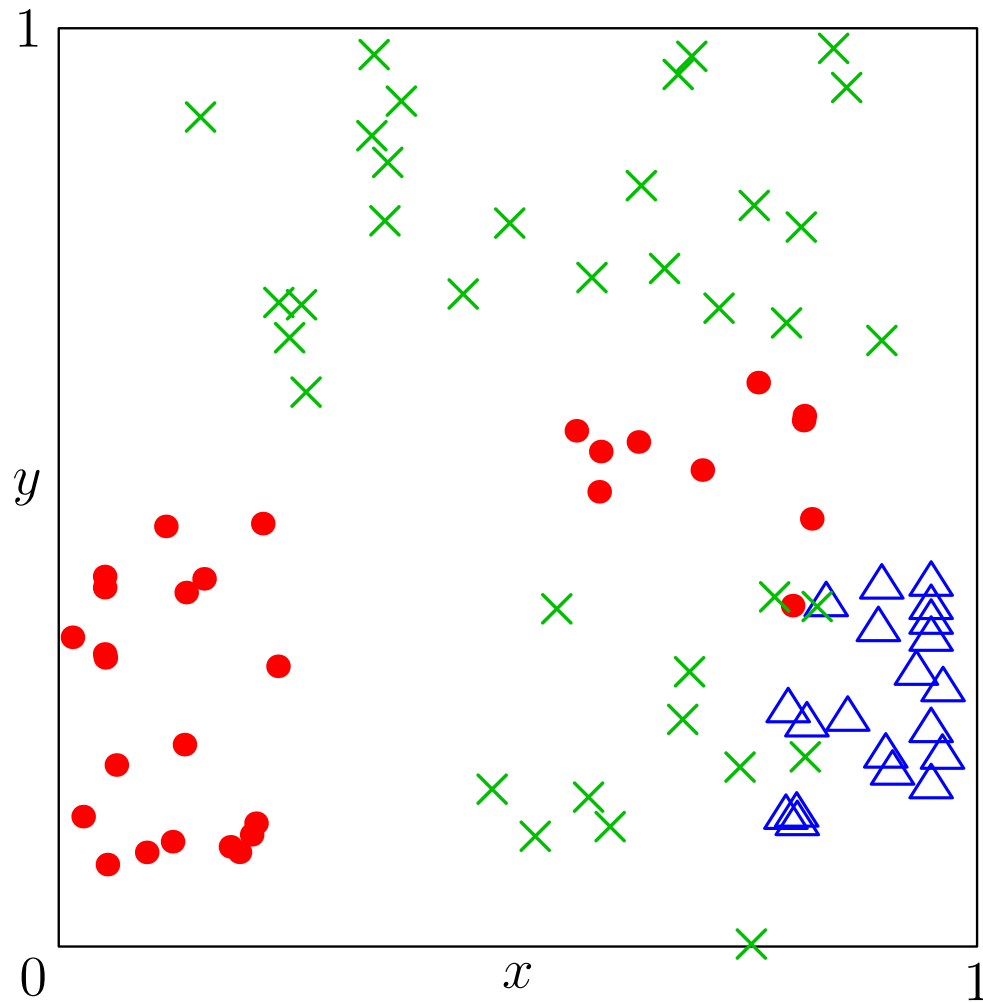
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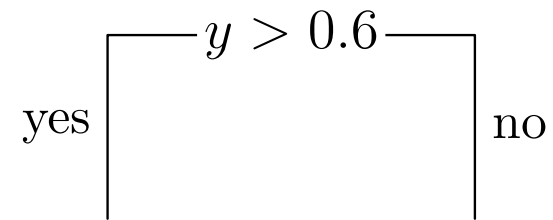
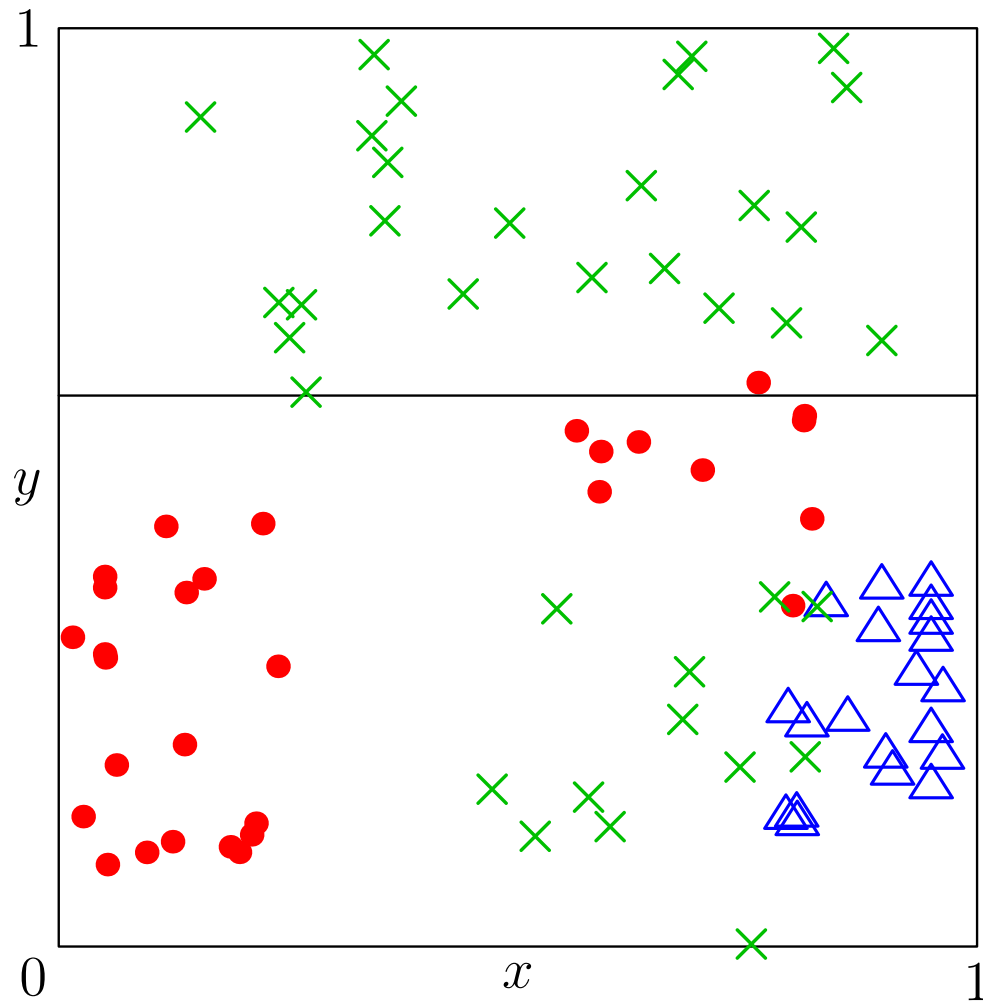
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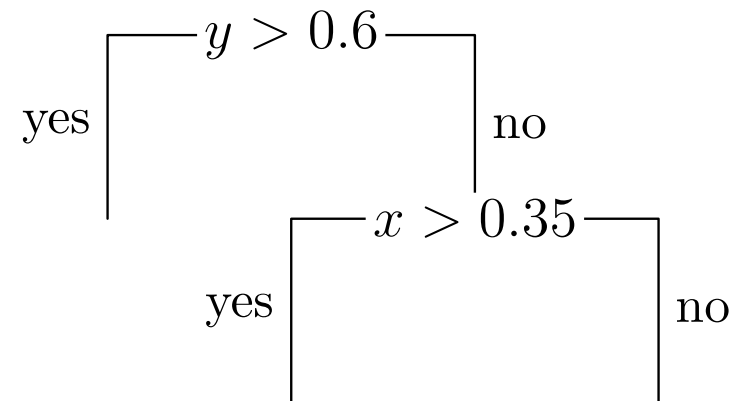
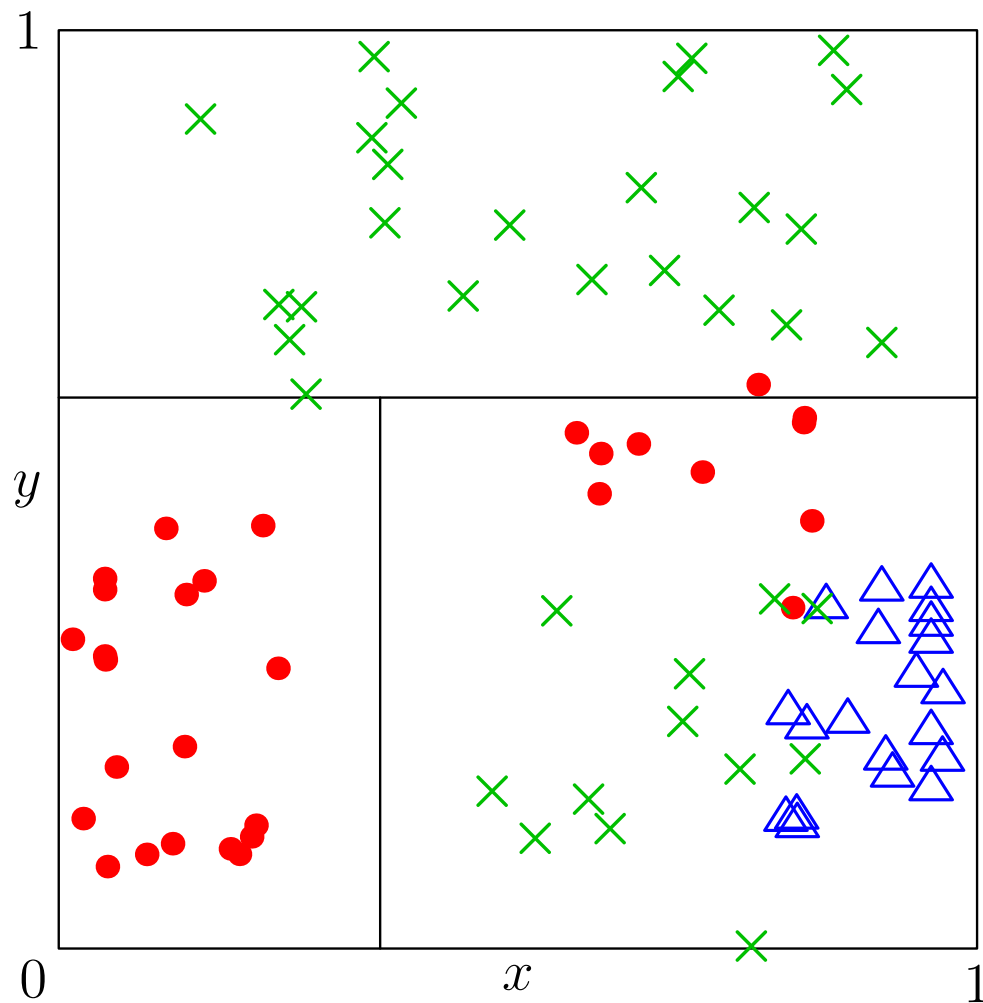
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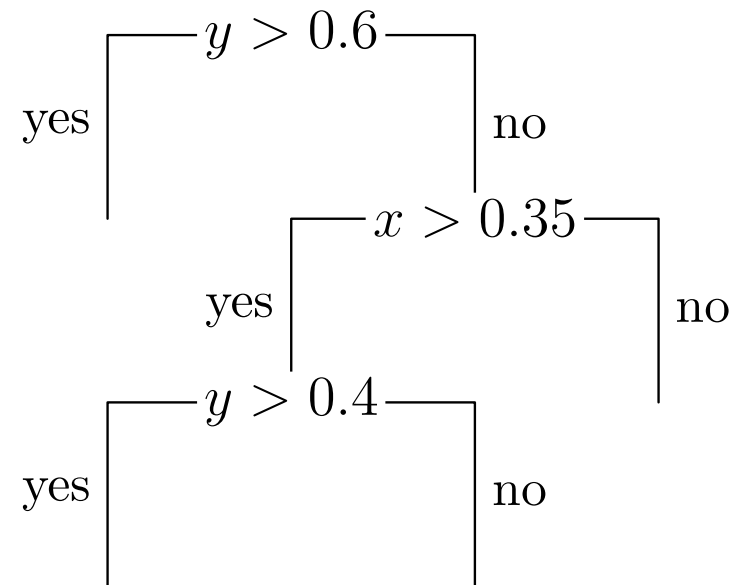
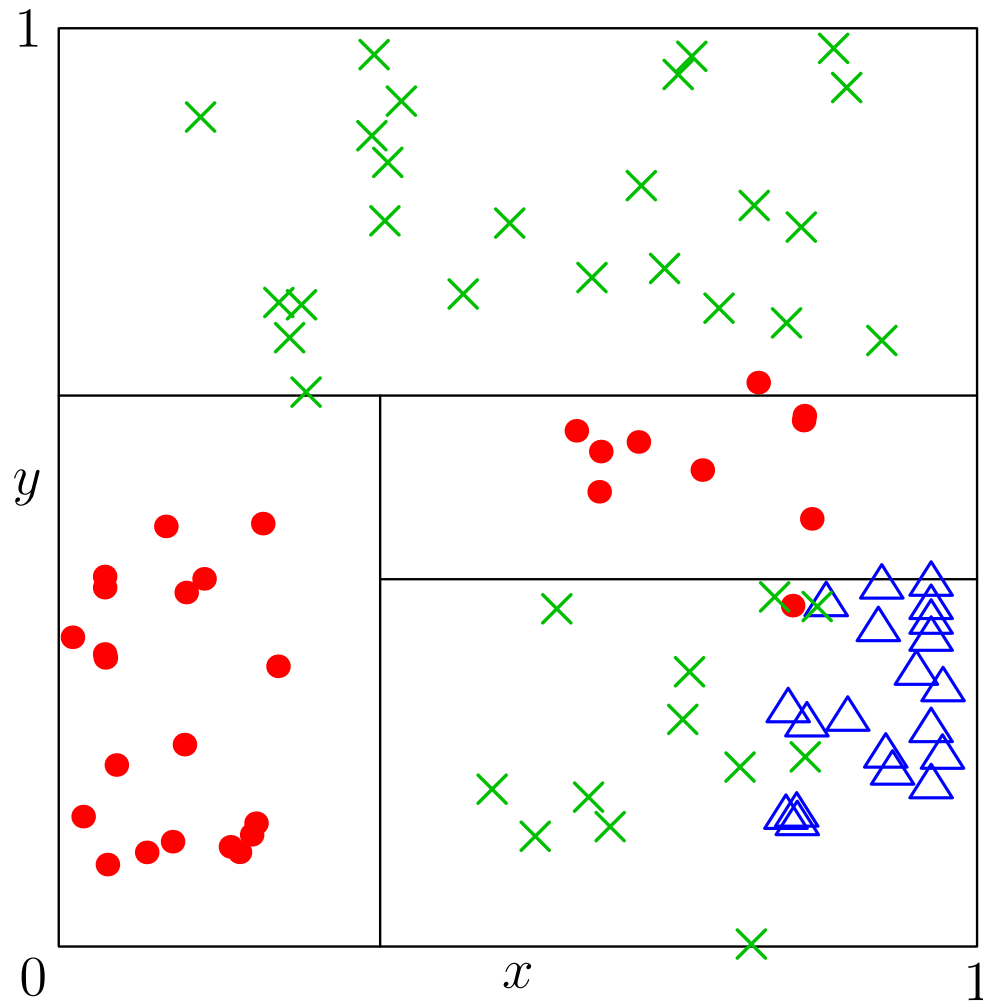
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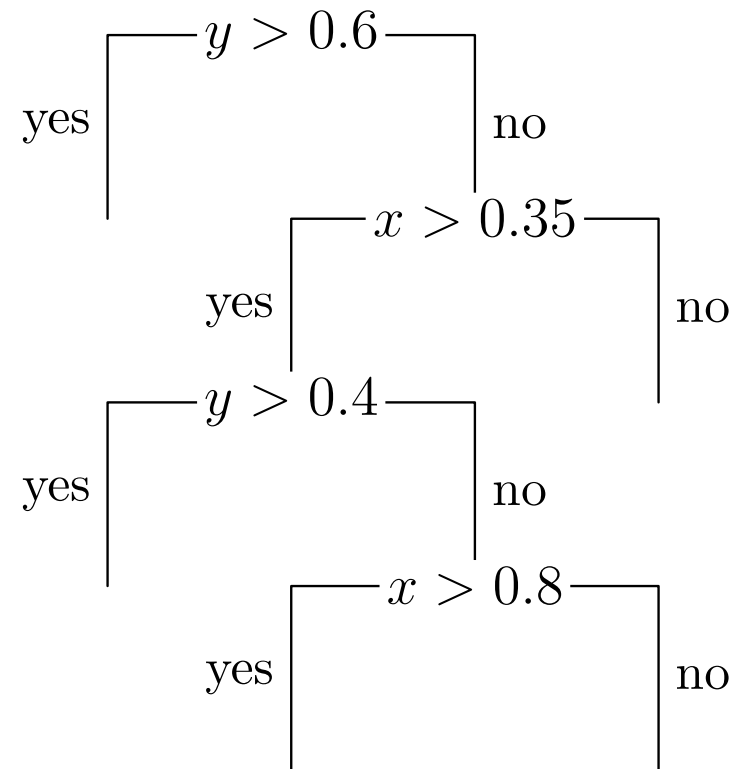
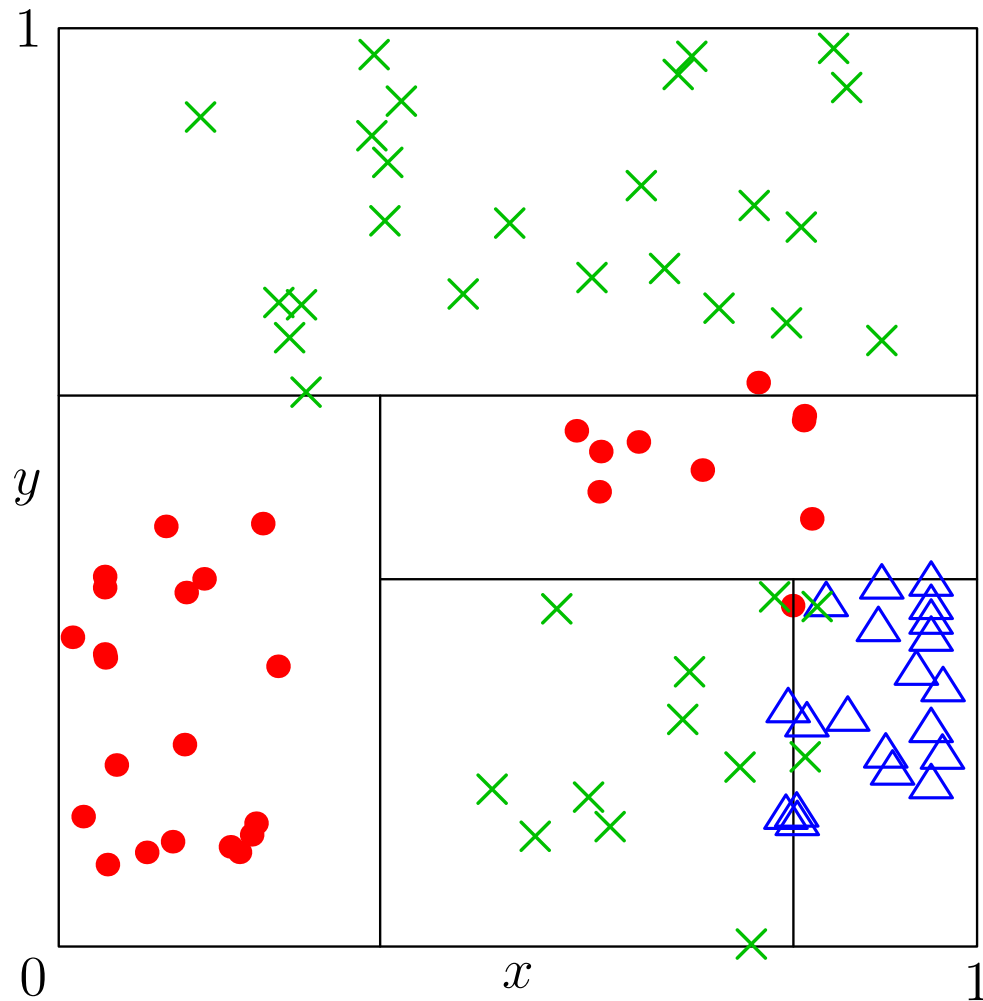
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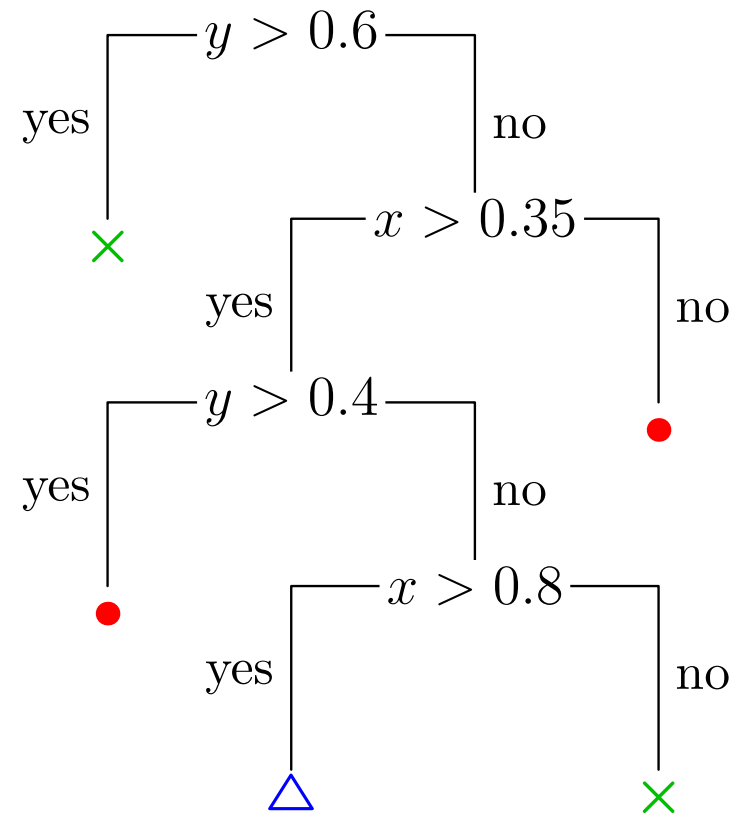
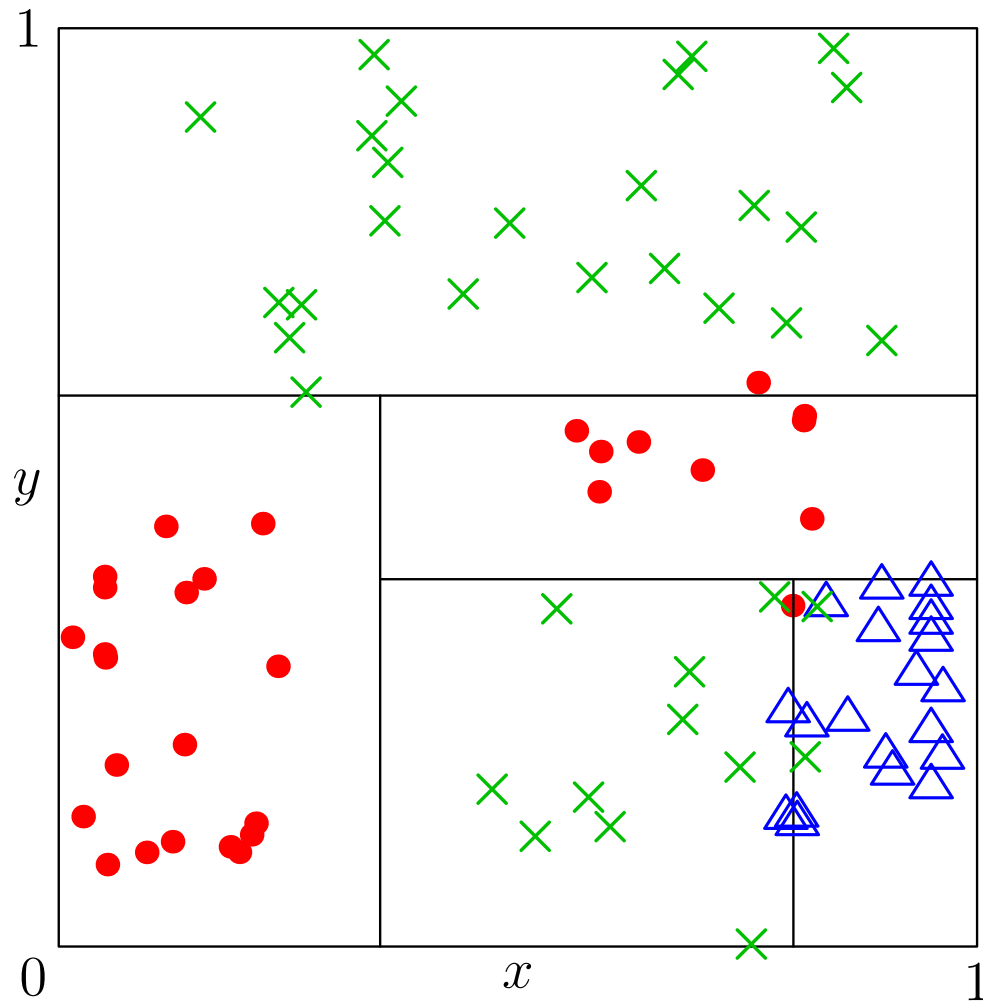
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Building Decision Trees



Bootstrap Aggregation (Bagging)

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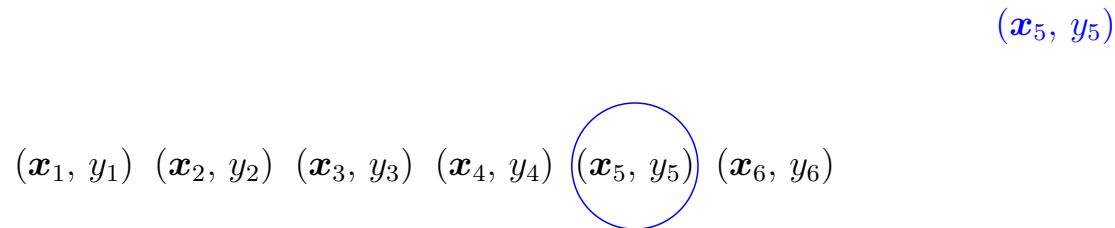
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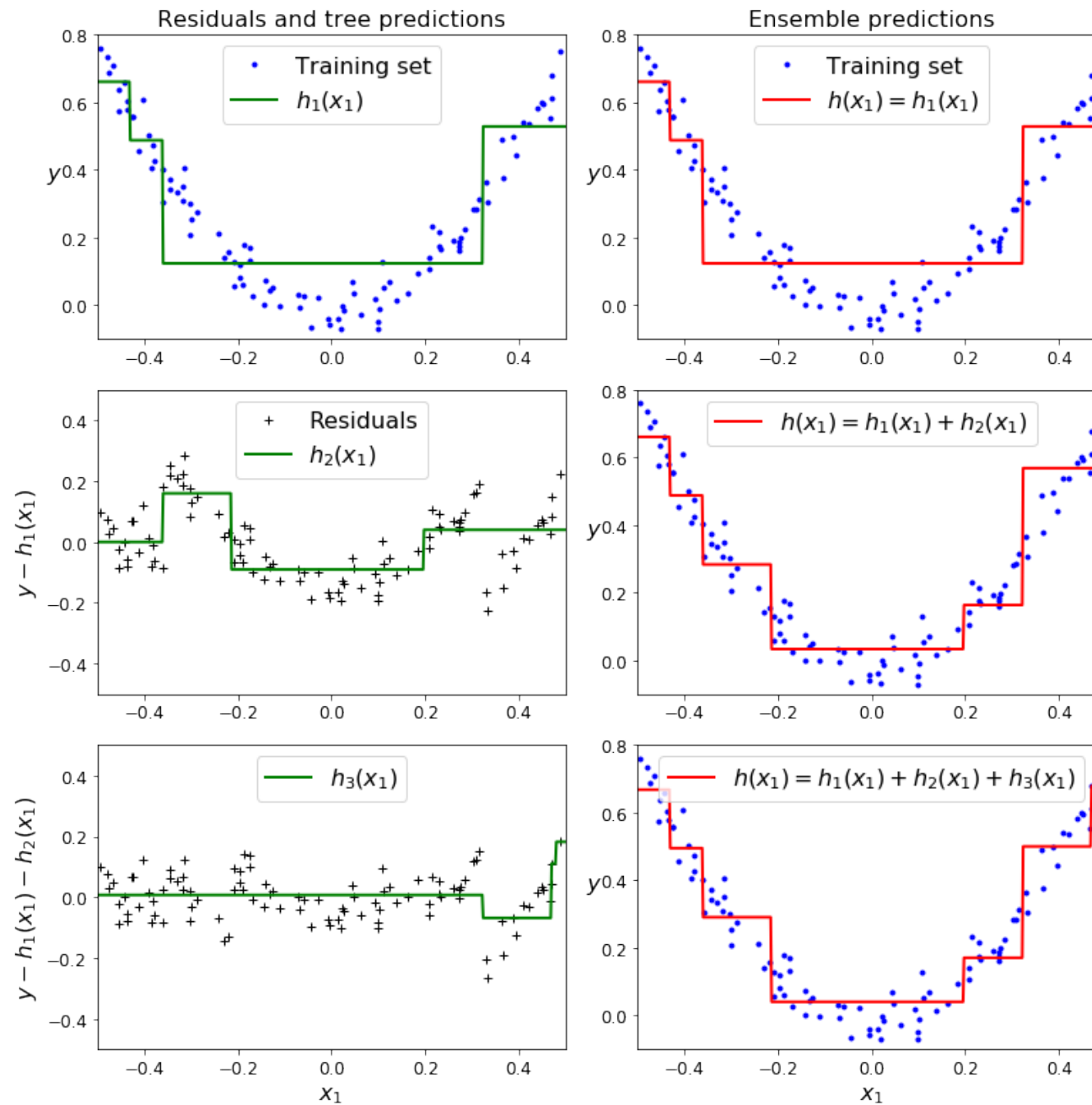
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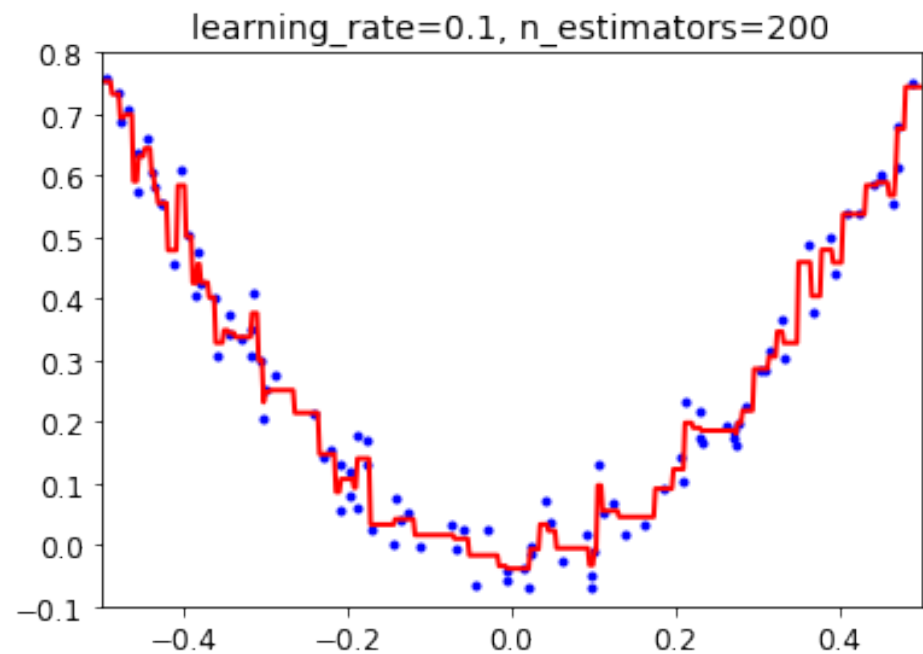
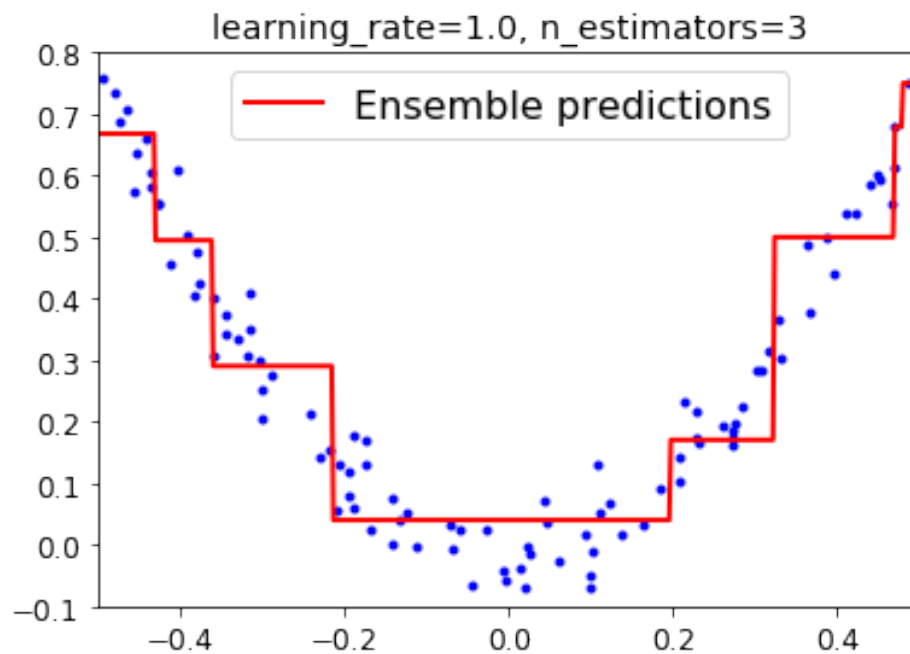
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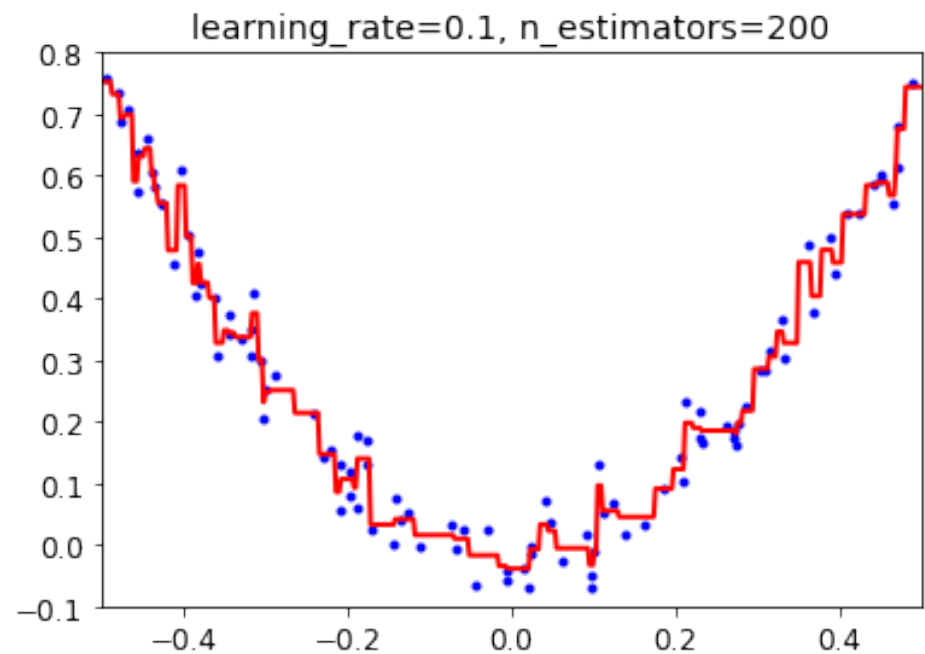
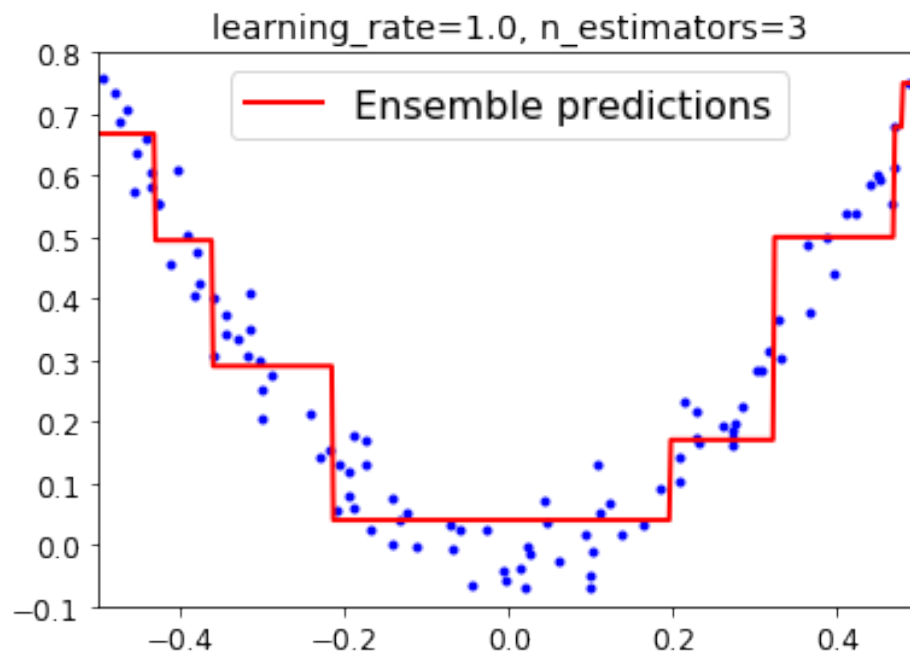
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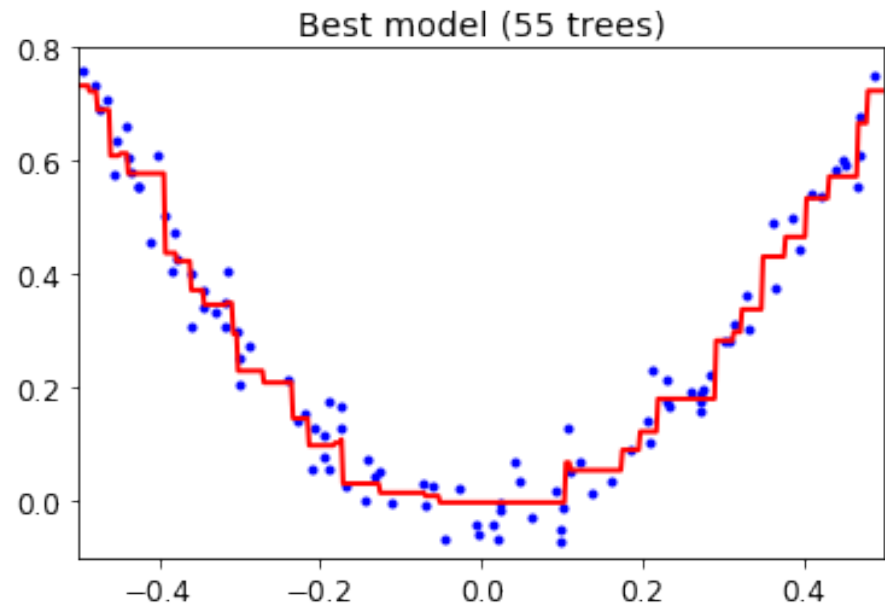
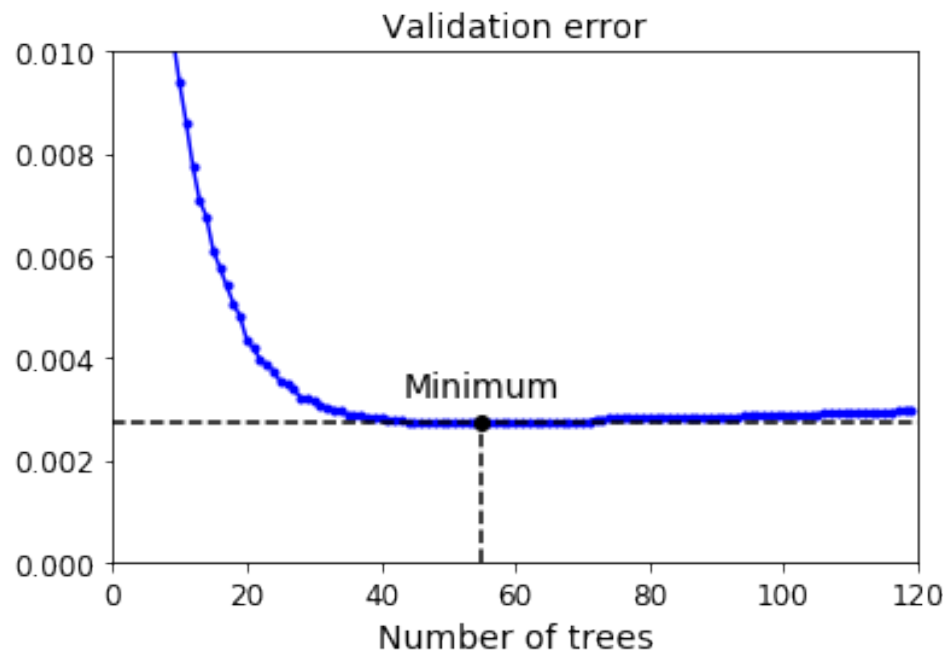
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- But we will over-fit eventually

Early Stopping

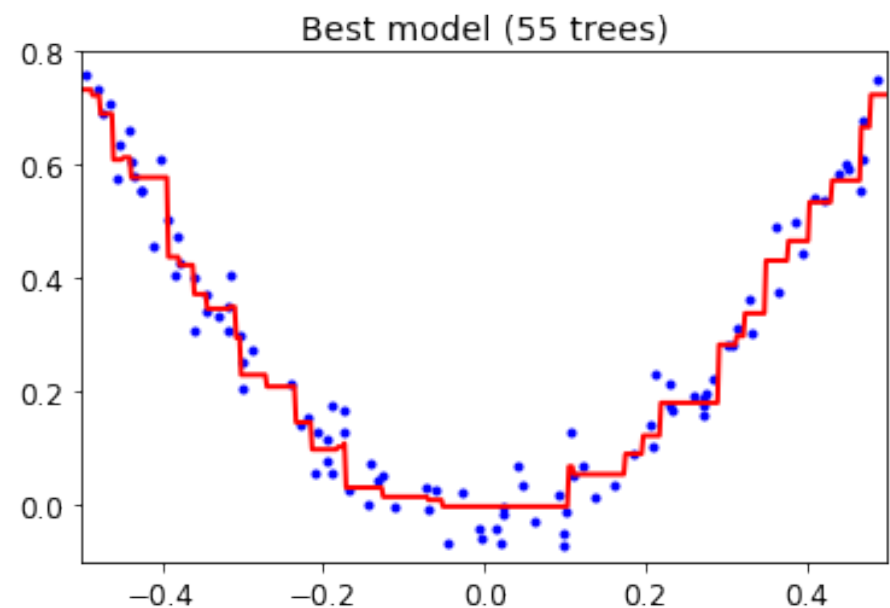
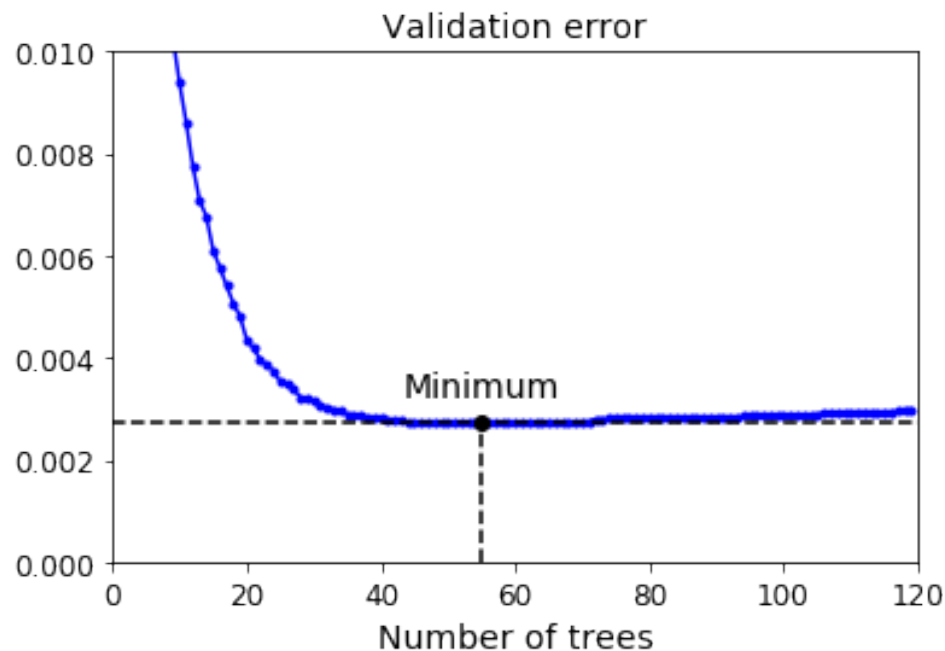
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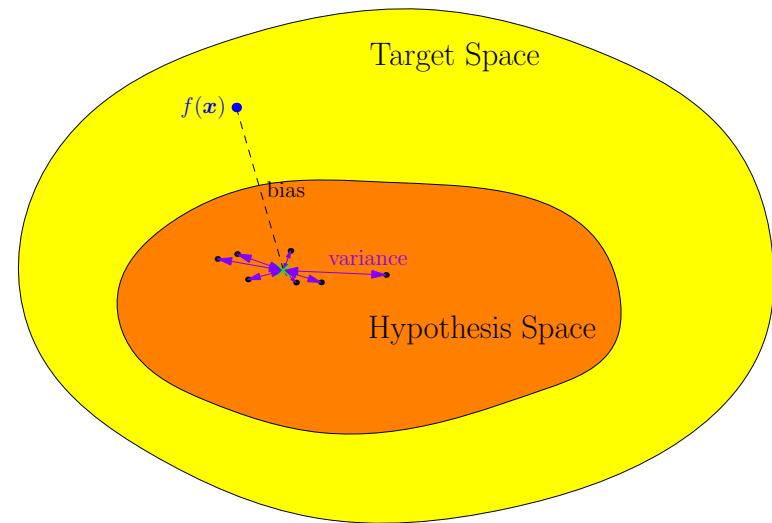
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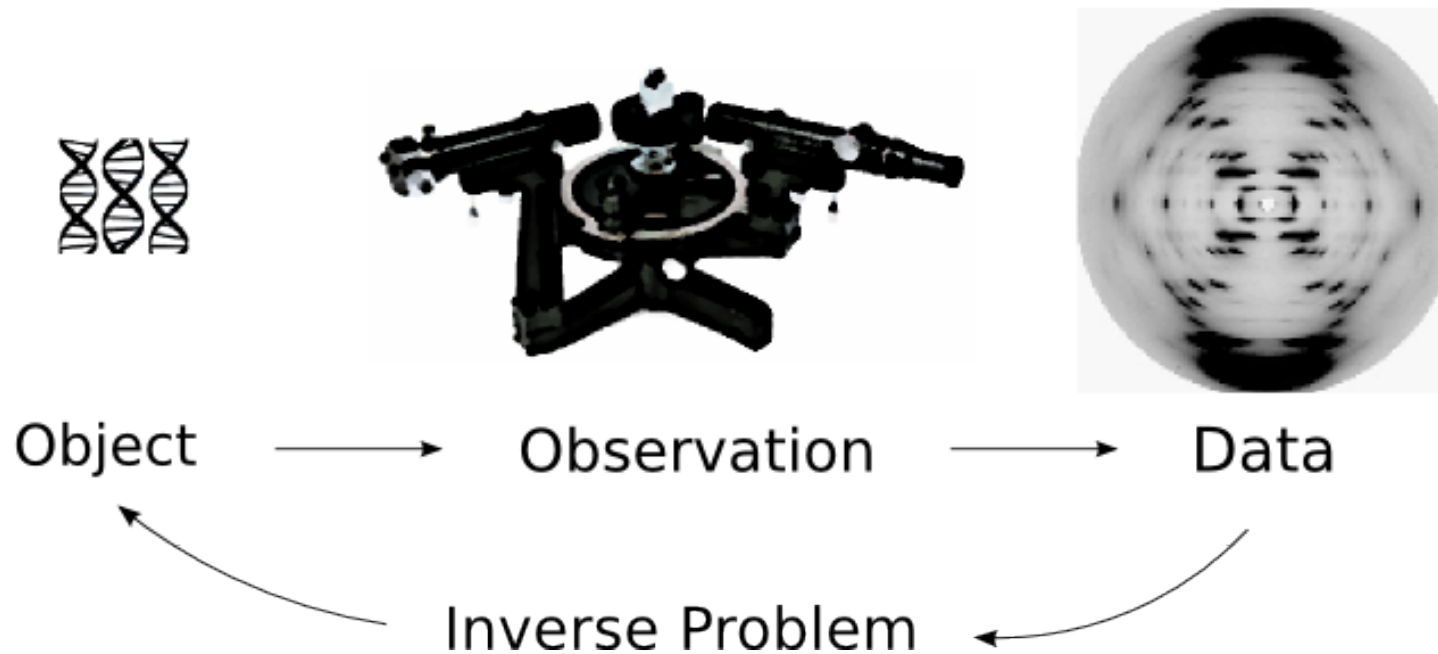
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Outline

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

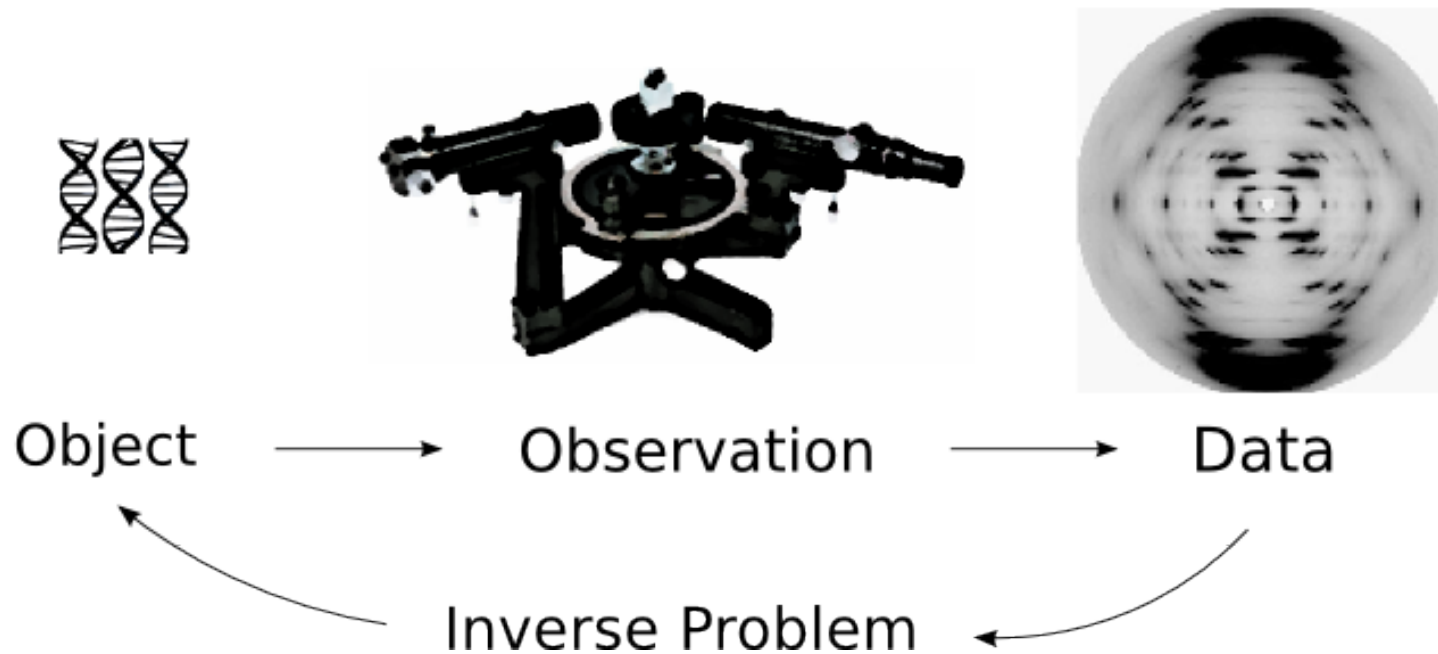


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Bayes' Rule

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

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

- What we want is to know the probability of the world, W , given the data, \mathcal{D} we have observed—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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Normalisation

- The denominator is a normalisation constant

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

- It is useful for comparing between different models of the world, W , and is sometimes called the **evidence**
- The model with the largest evidence is the most likely model to be correct

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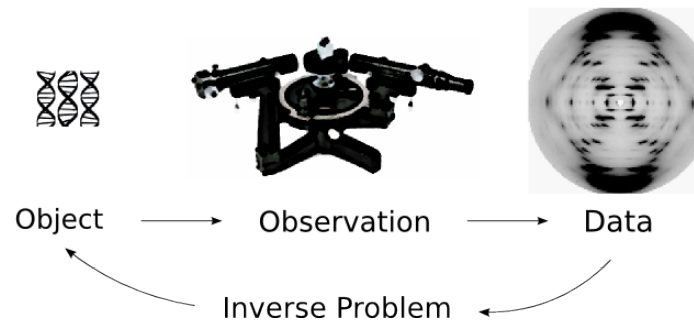
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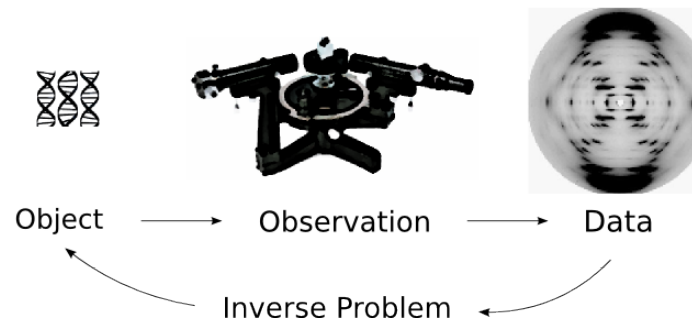
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- It is relatively easy to model the likelihood (this is a forward process not an inverse process)



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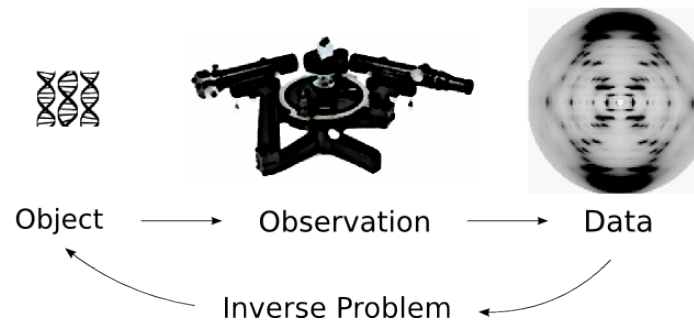
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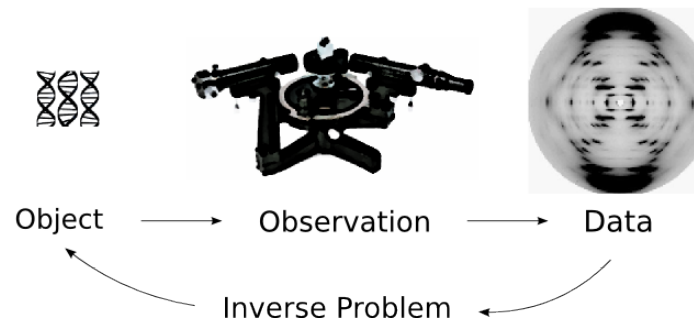
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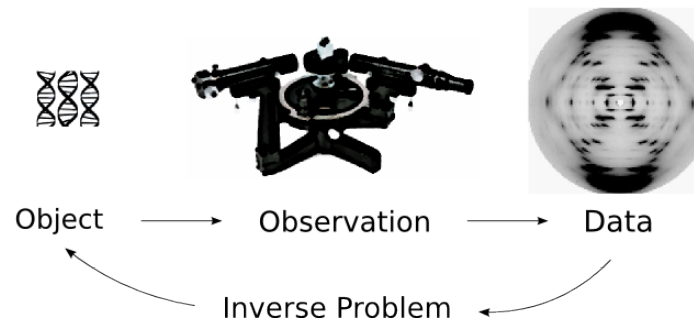
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Simple Bayes

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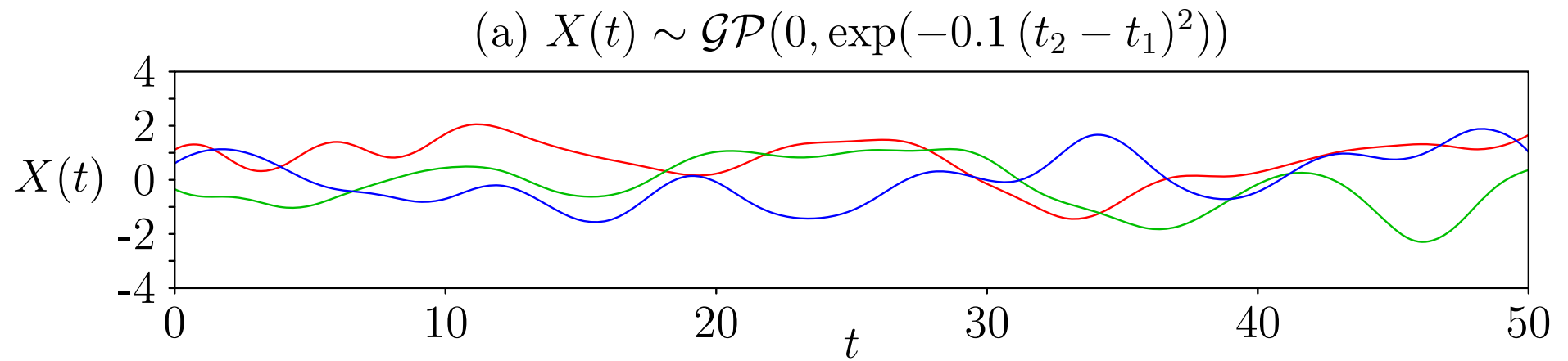
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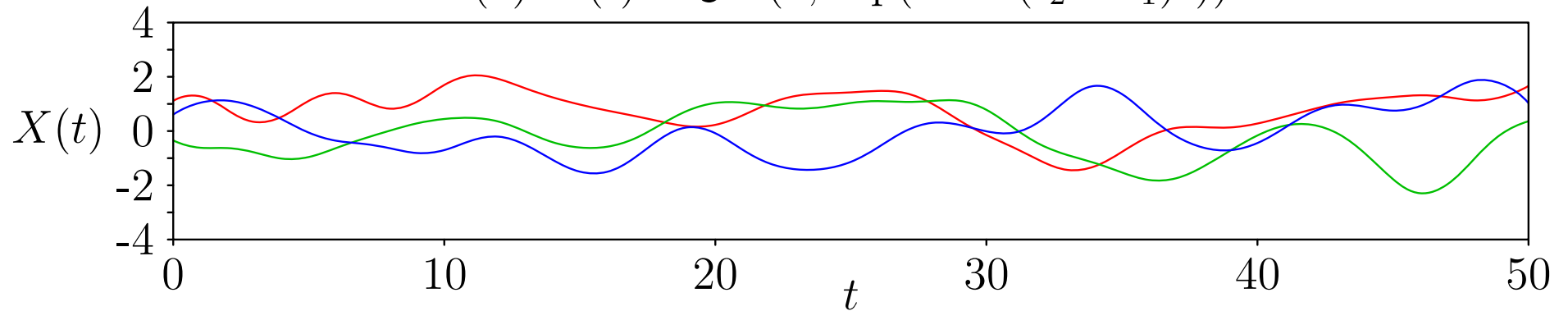
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Gaussian Process Worlds

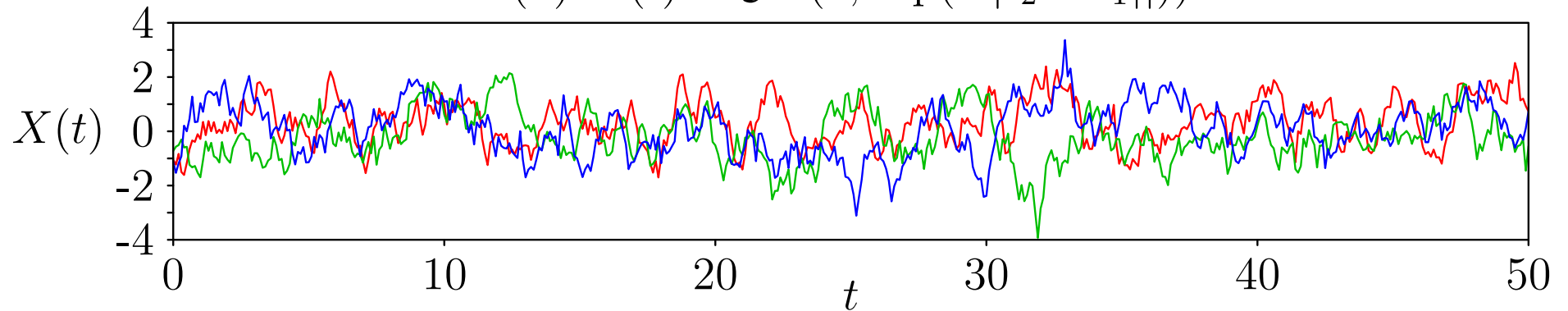


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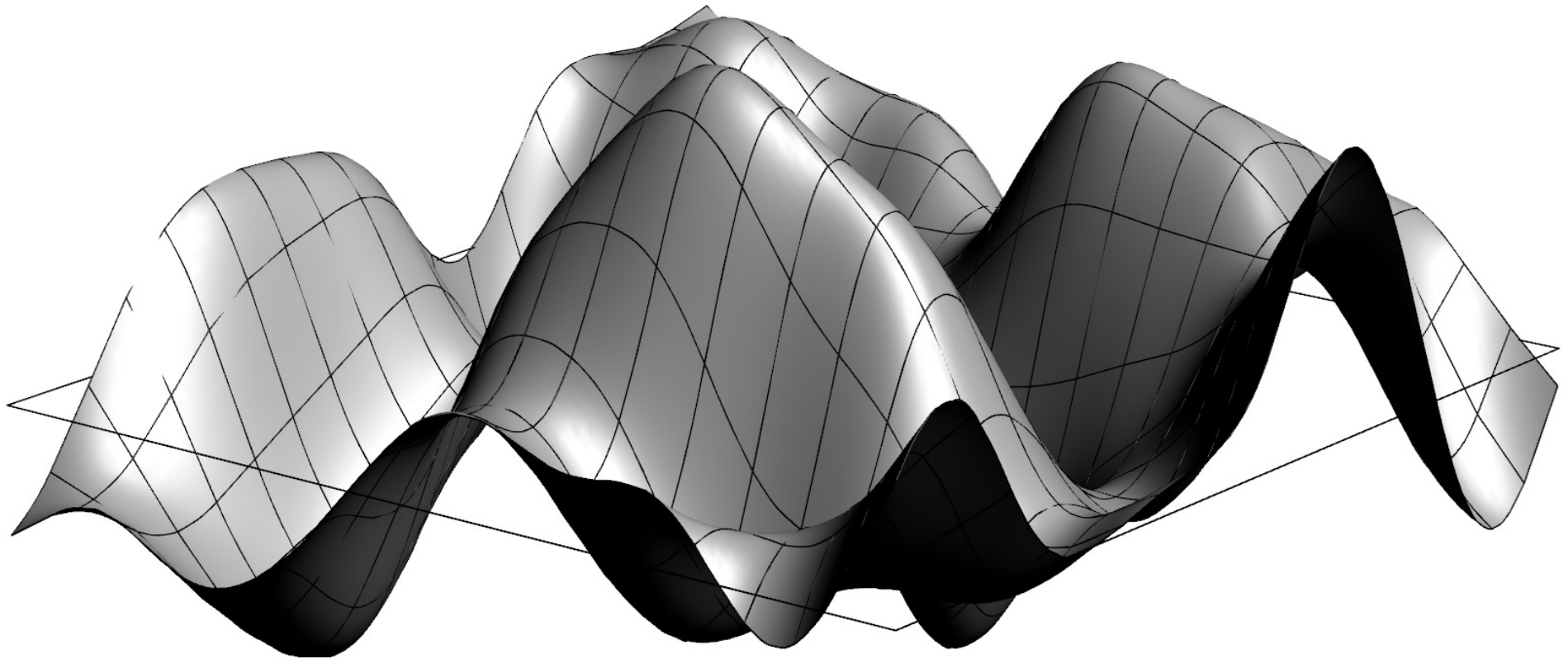
(a) $X(t) \sim \mathcal{GP}(0, \exp(-0.1(t_2 - t_1)^2))$



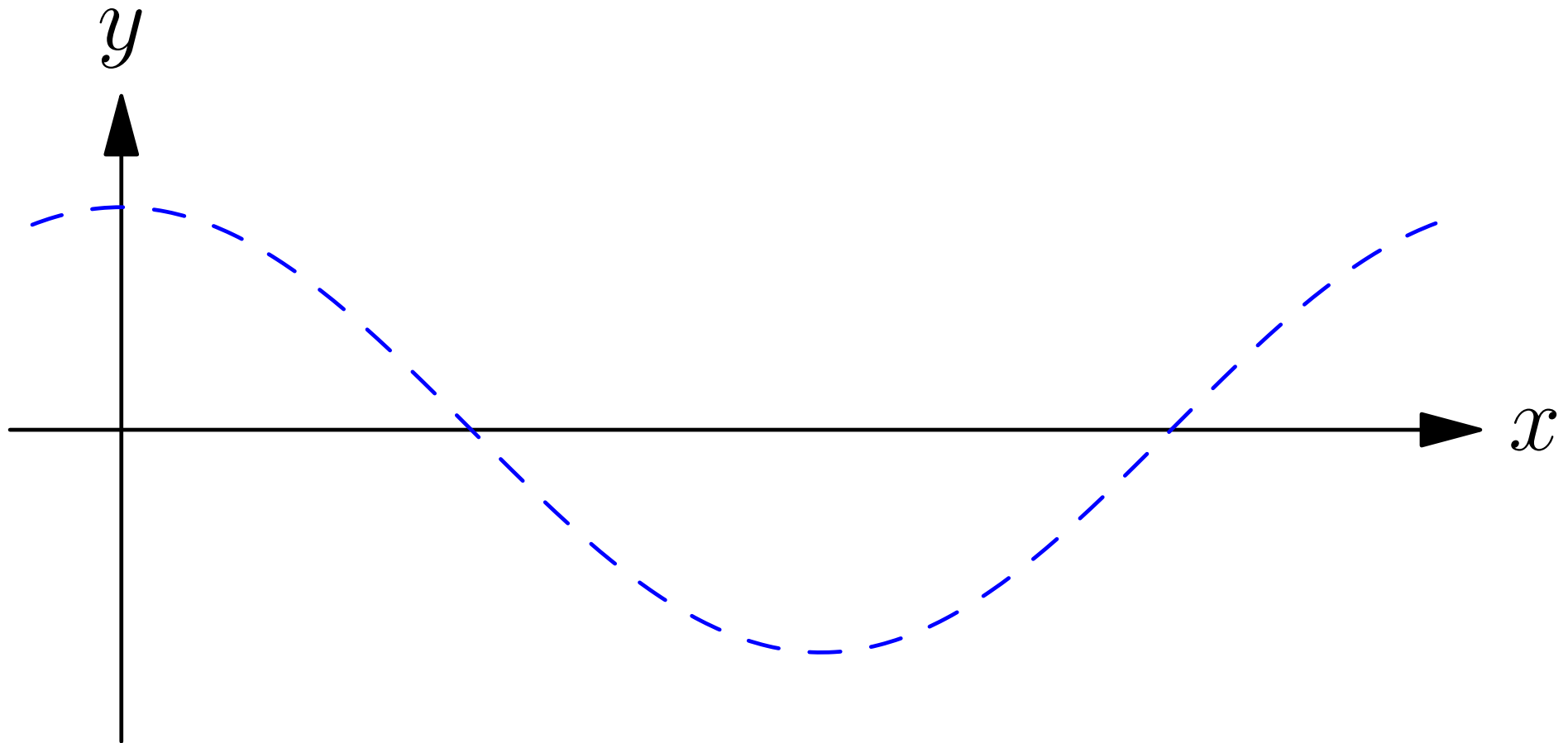
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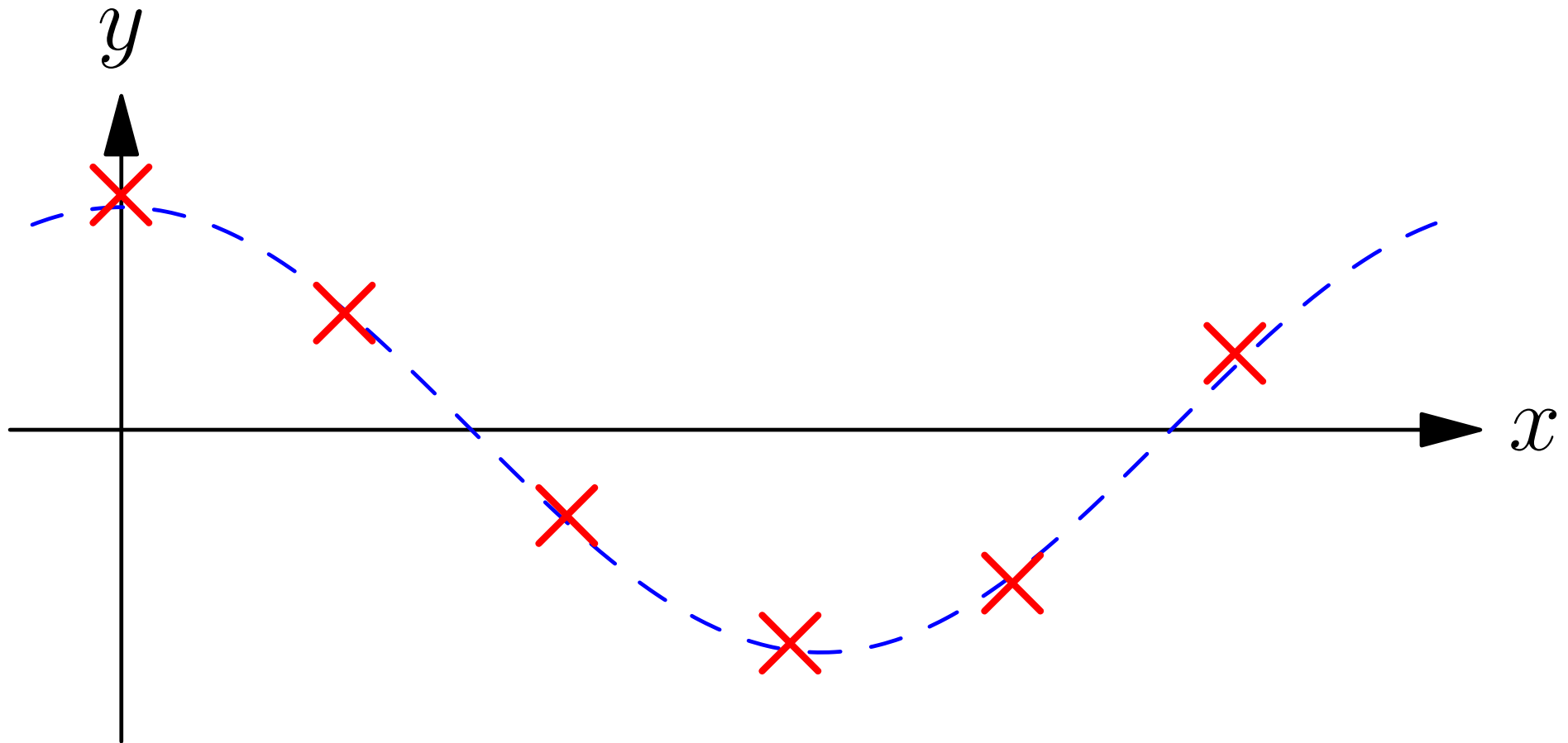
2-D Gaussian Processes



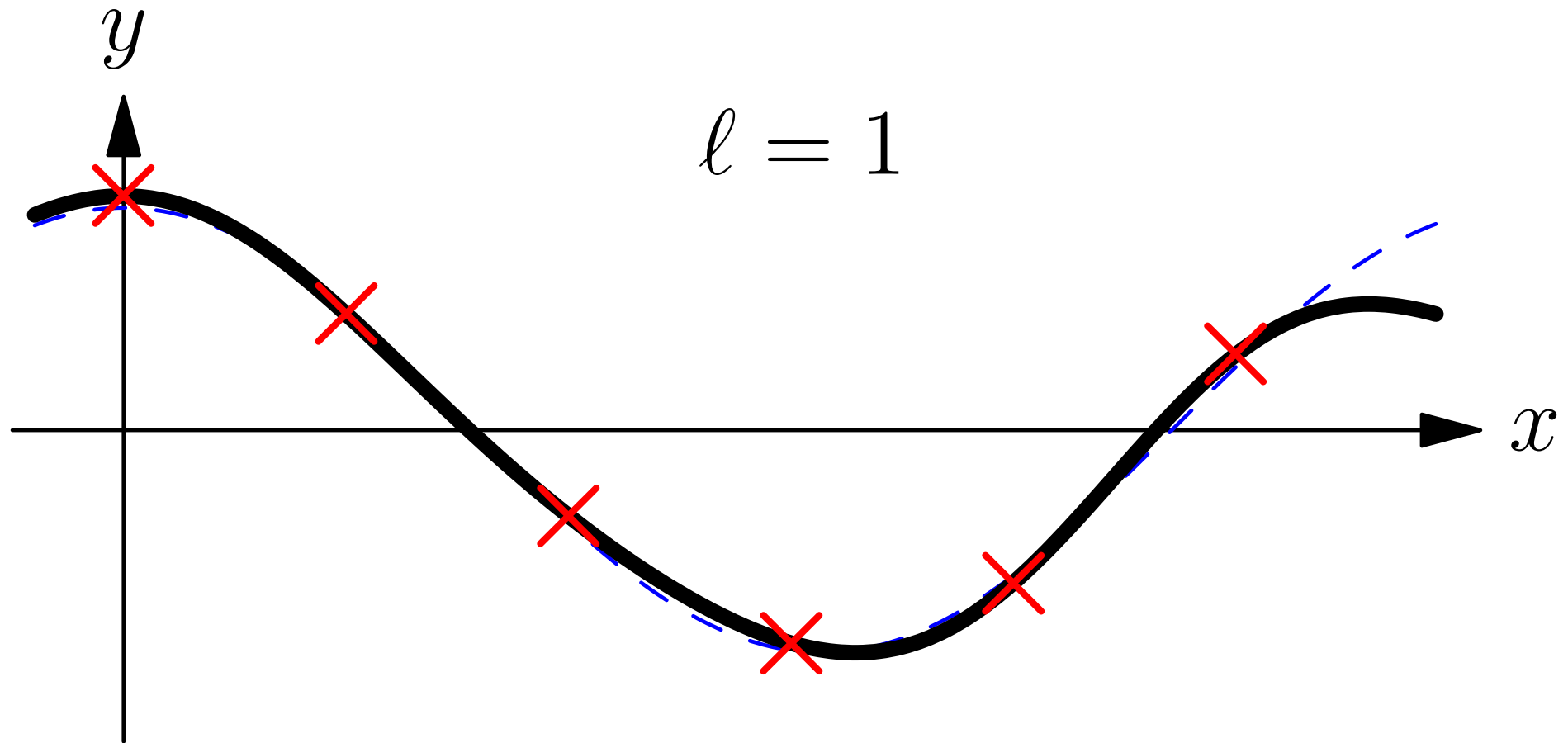
$$K(x, x') = \exp(-(x - x')^2 / (2 \ell^2))$$



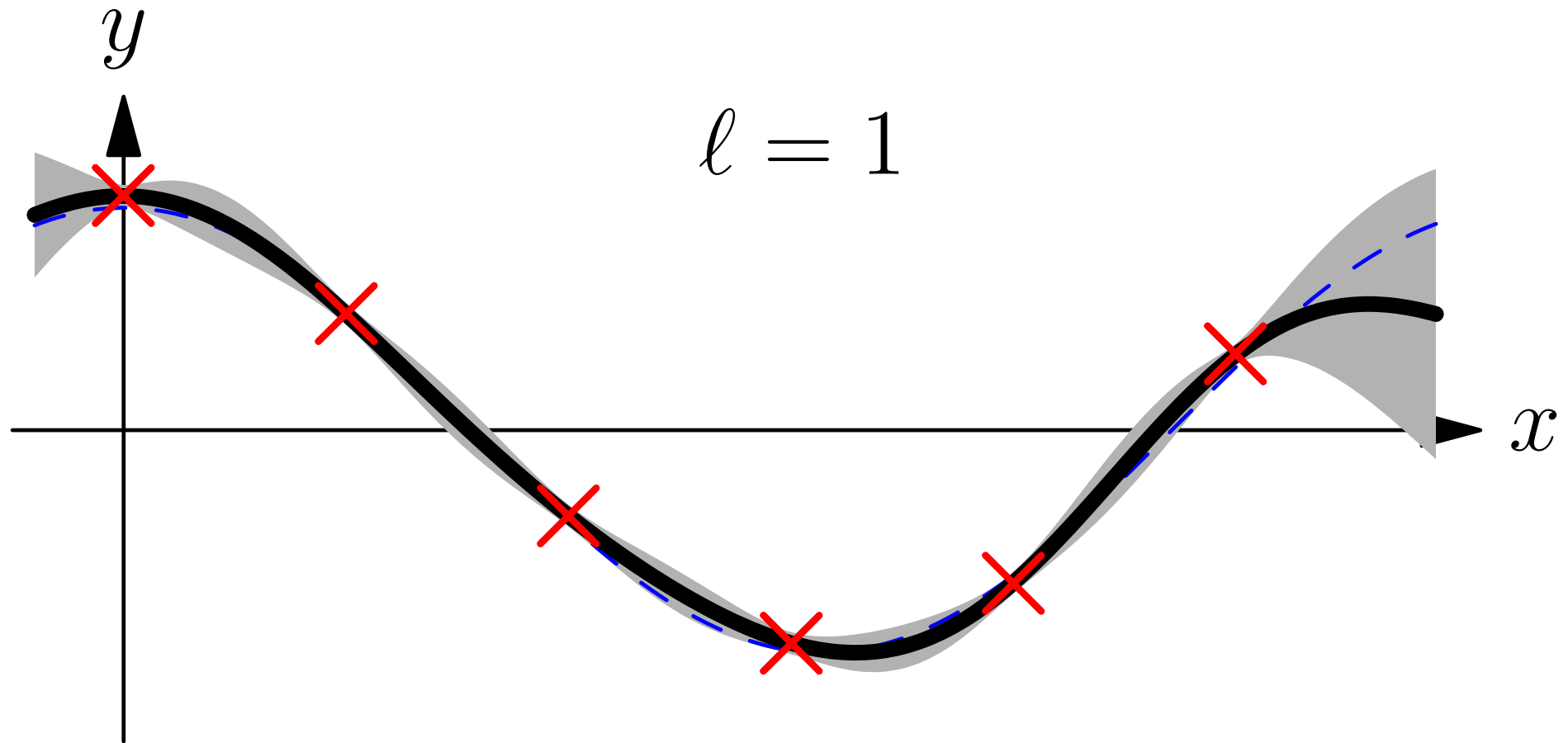
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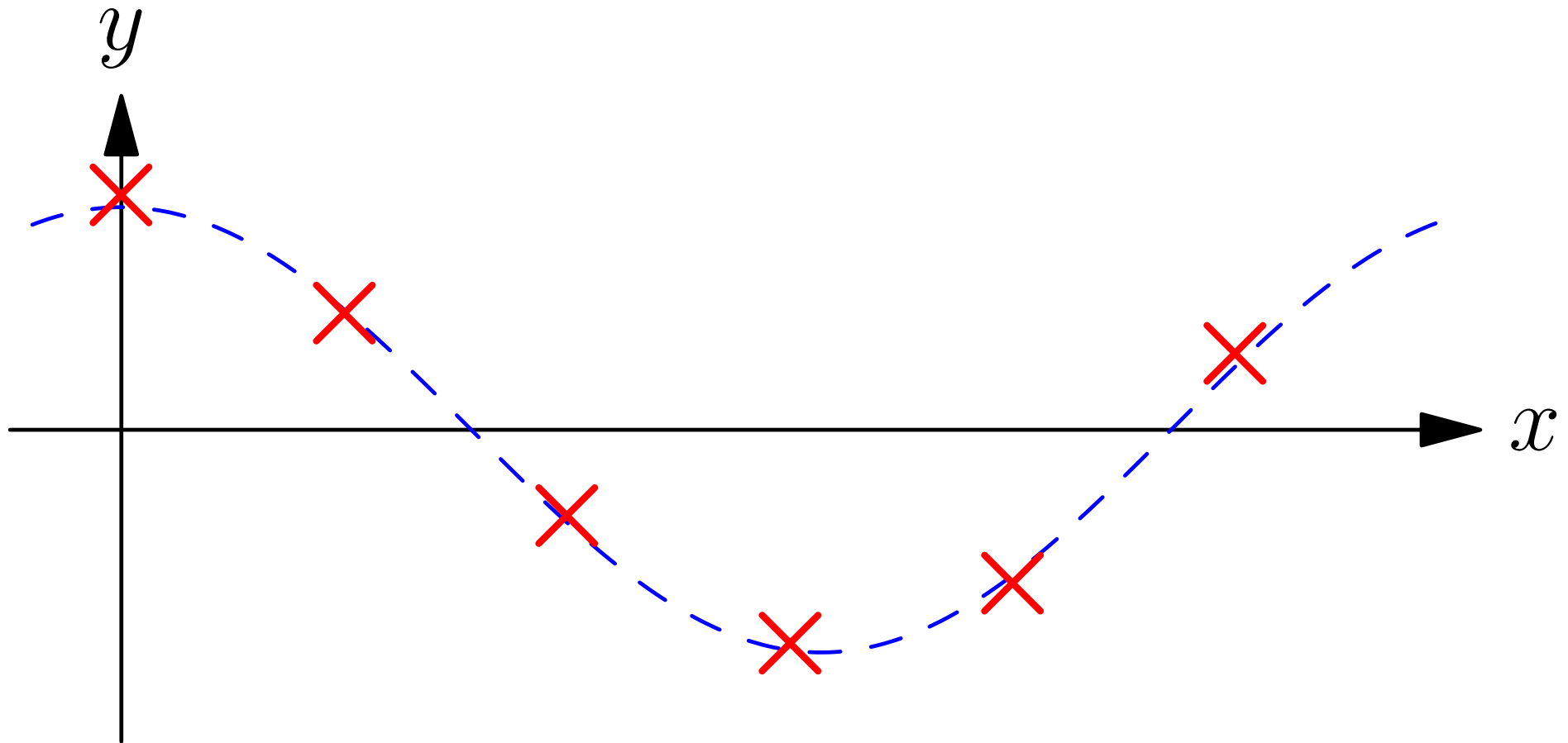
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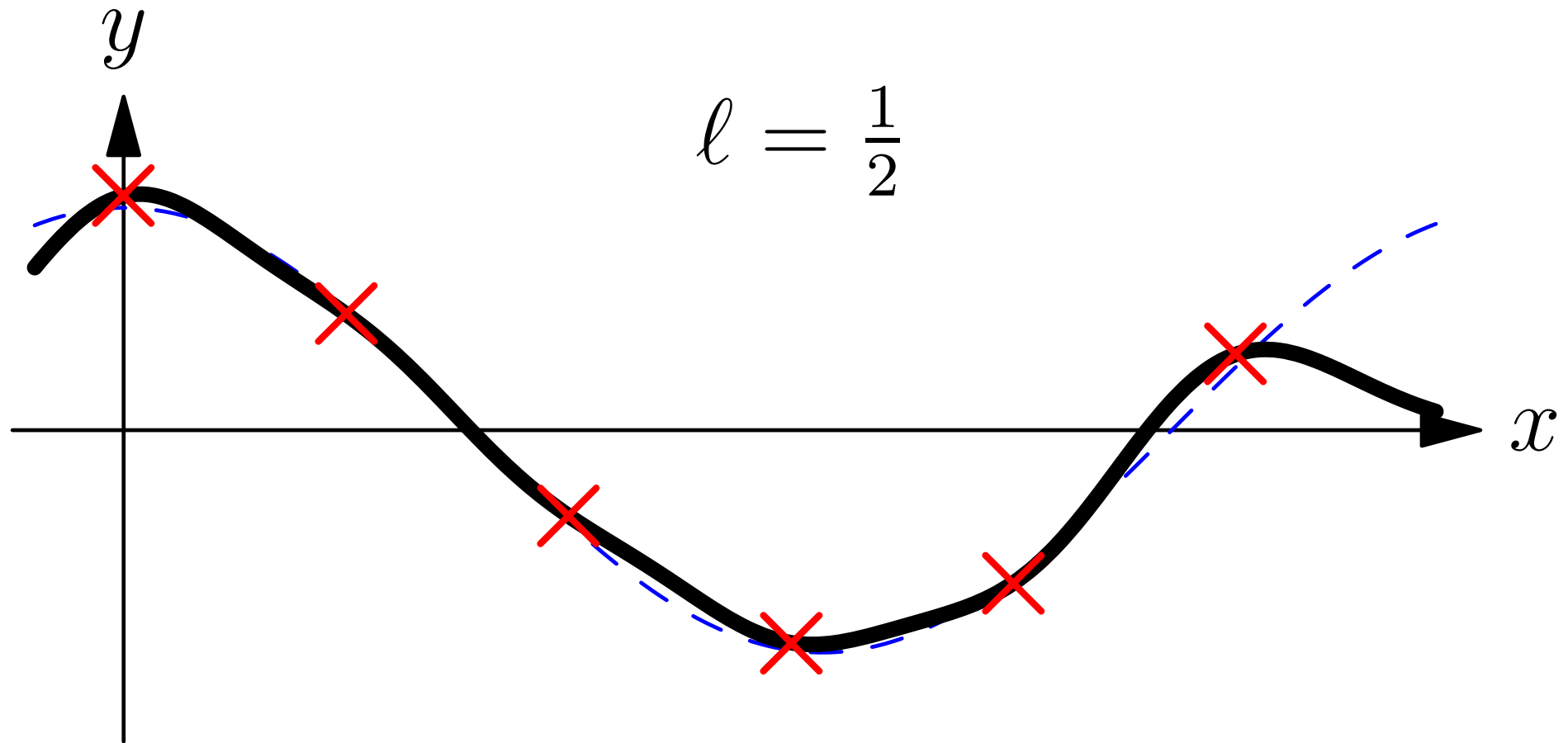
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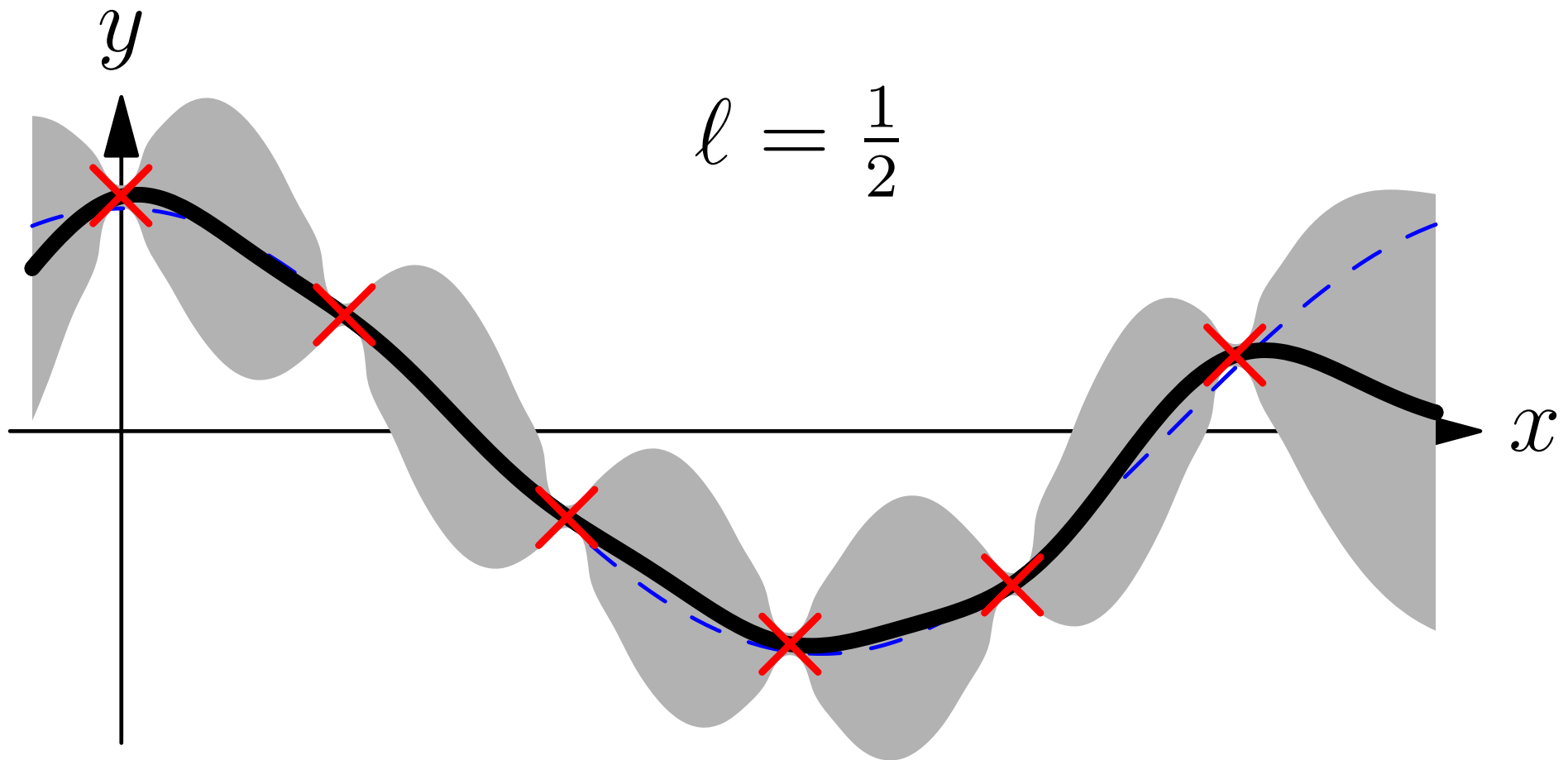
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