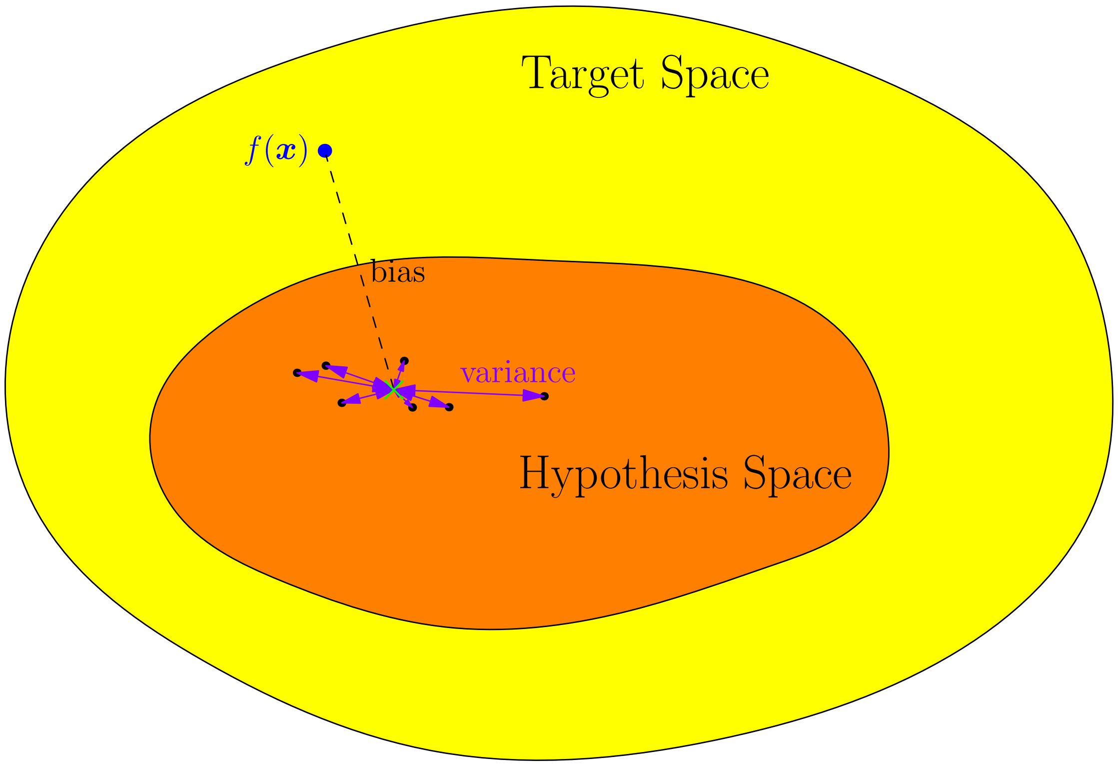
NGCM ML Workshop

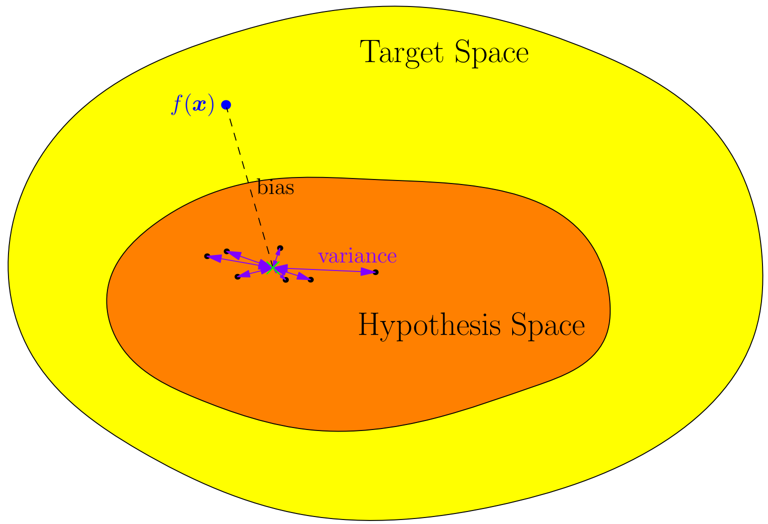
Advanced Machine Learning



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

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

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 $p(\boldsymbol{x})$ describing where our data is

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- We want to minimise the *generalisation error* which in this case we can measure as

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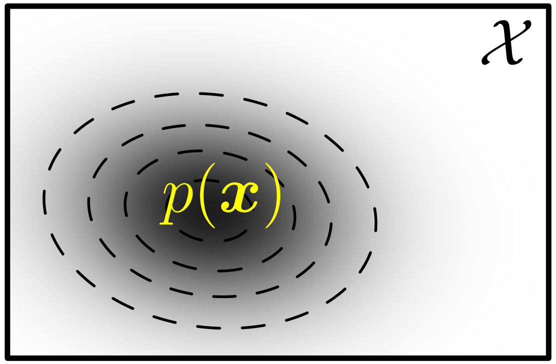

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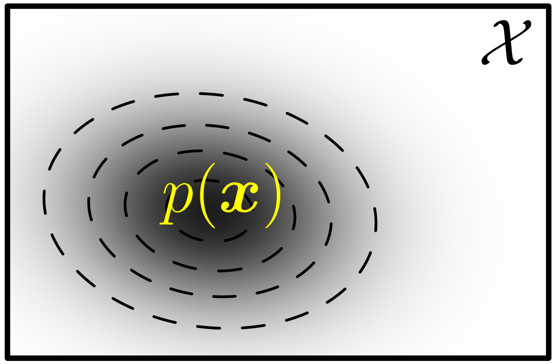

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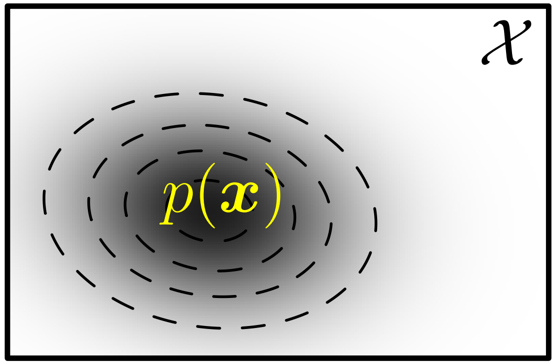

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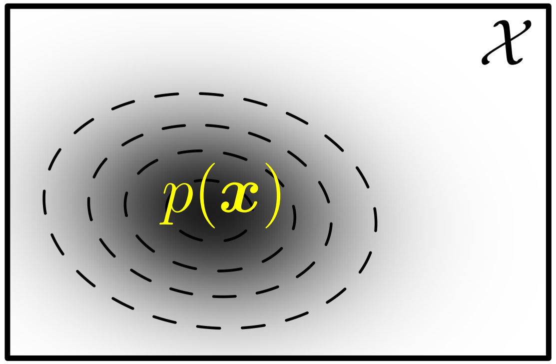

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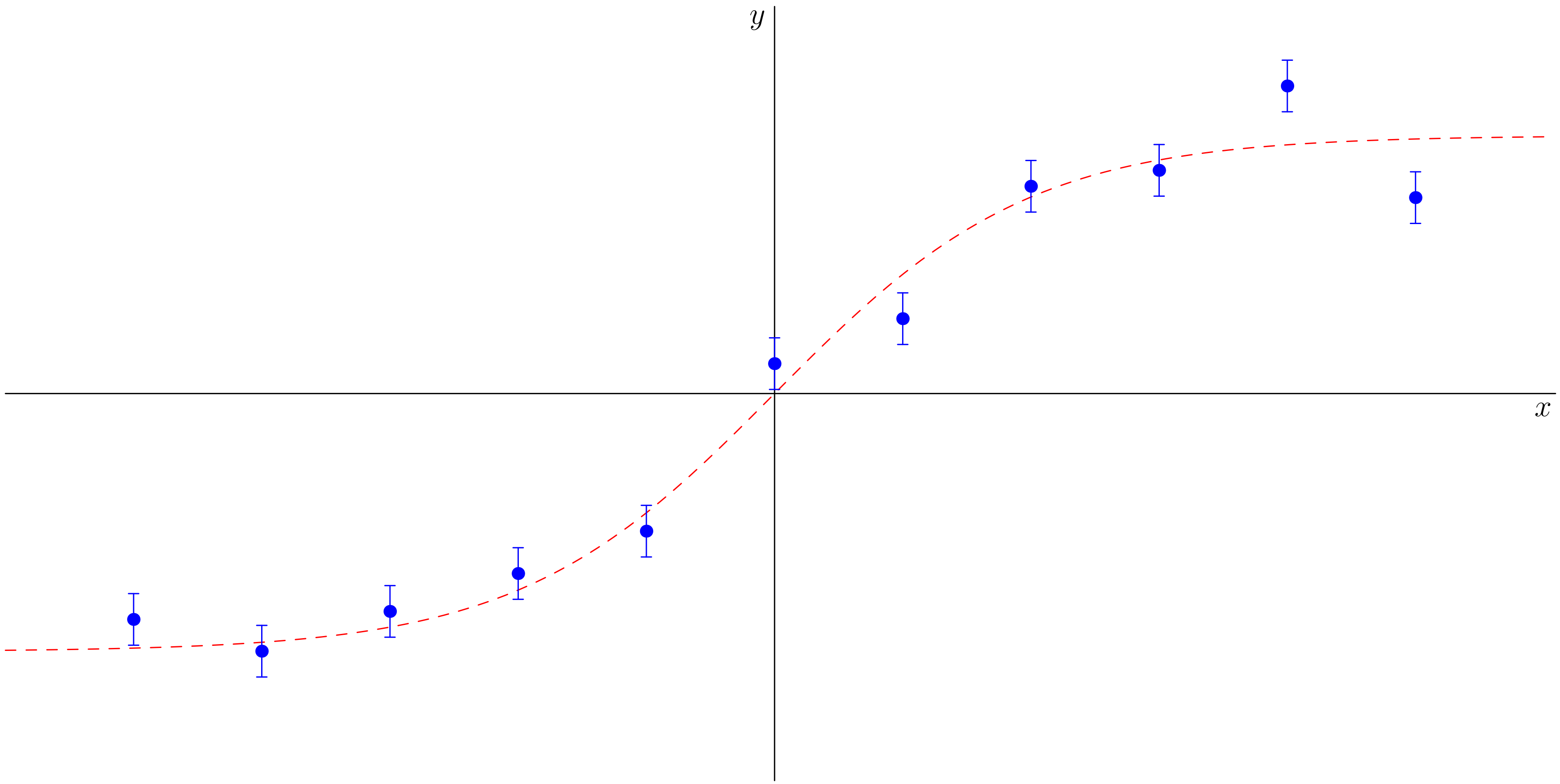
- We want to minimise $E_G(\boldsymbol{w})$ but in practice we are minimising $E_T(\boldsymbol{w})$, *what could possibly go wrong?*

Too Simple or Too Complex?

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



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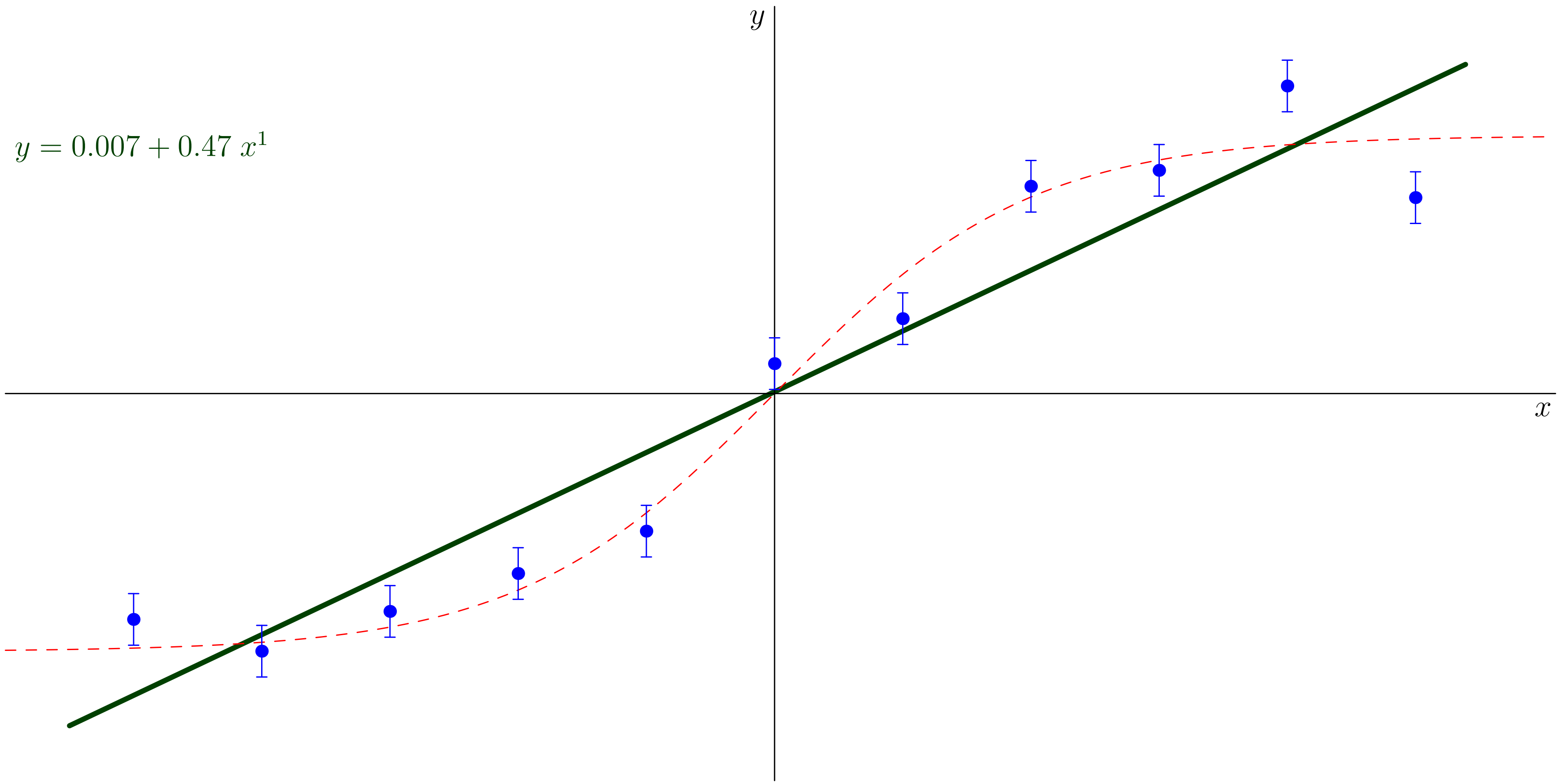

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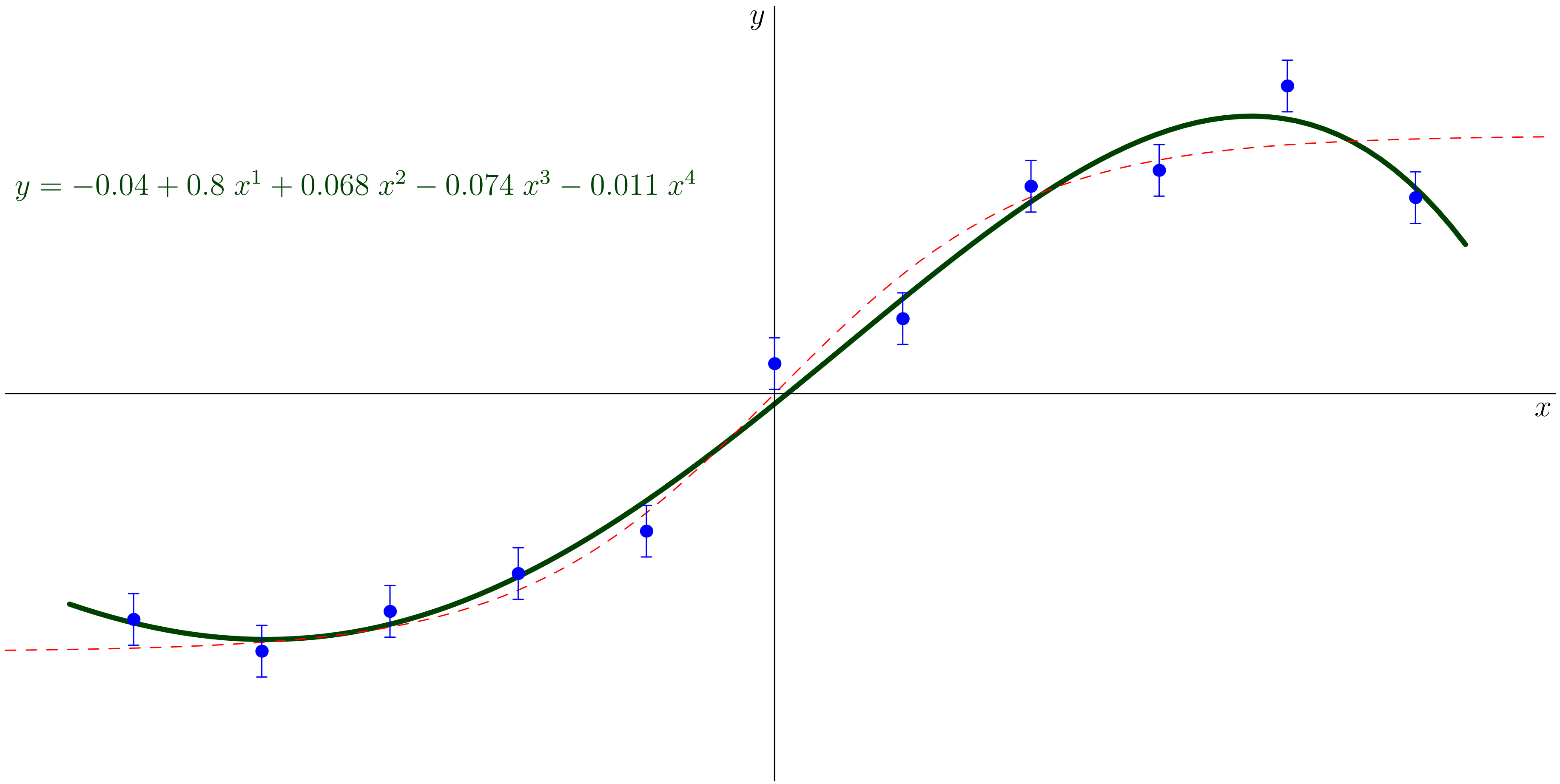

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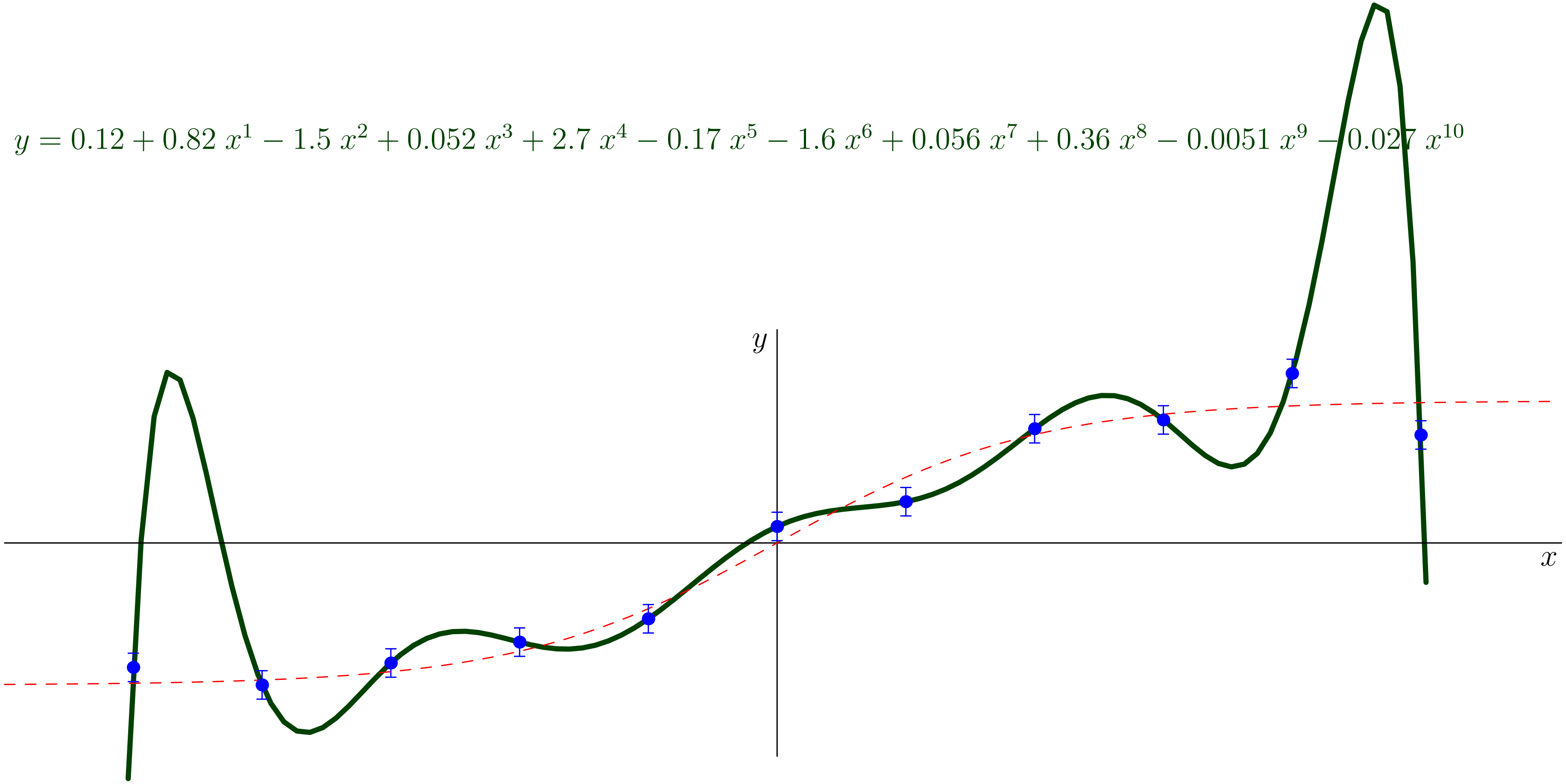
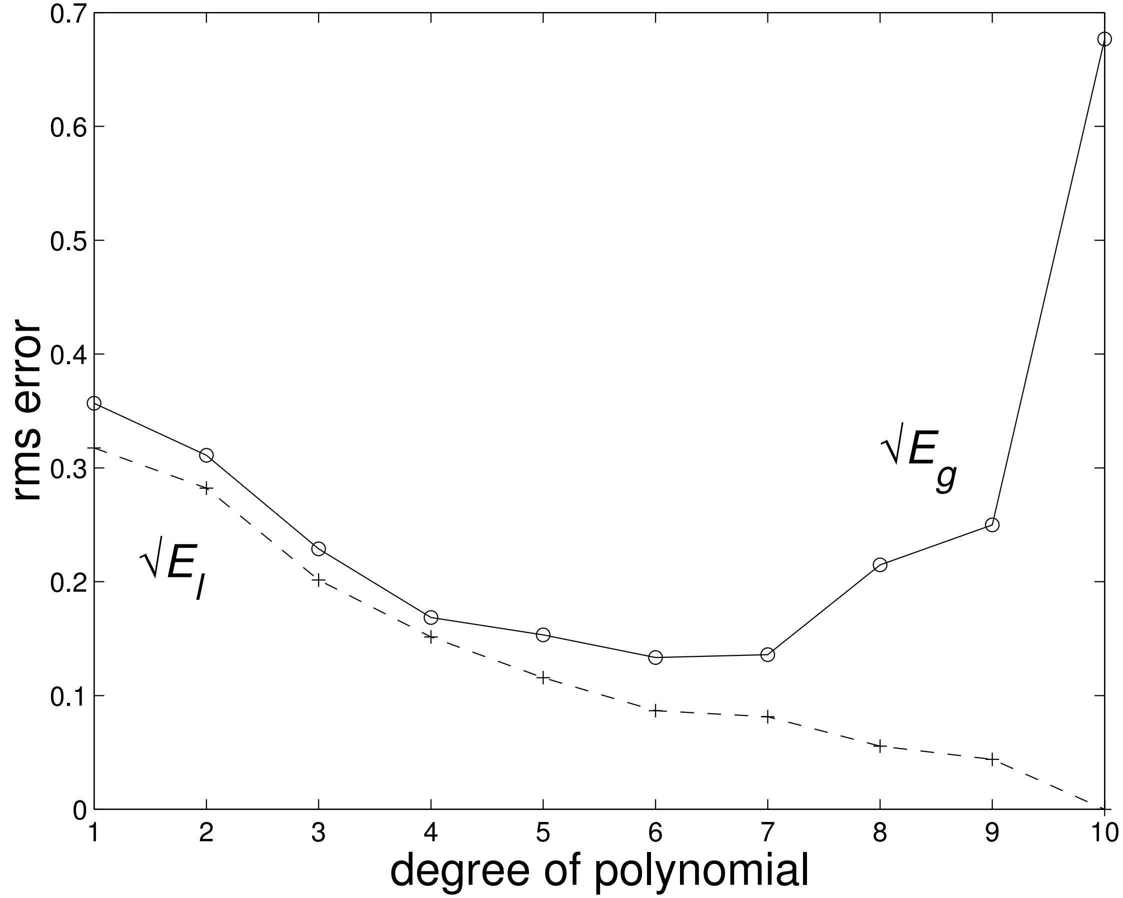


Measuring Generalisation Error for Regression

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



Expected Generalisation Performance

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

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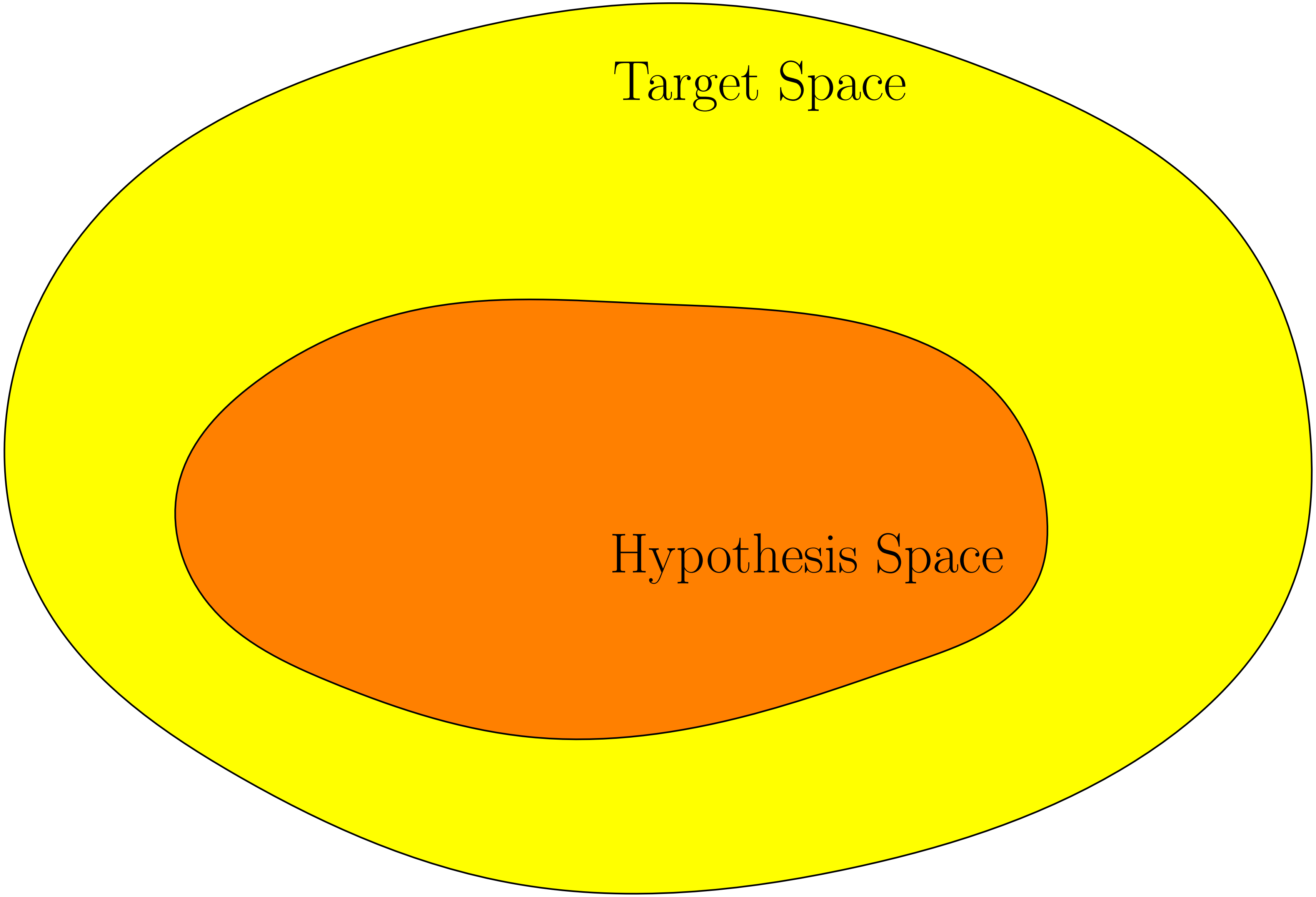

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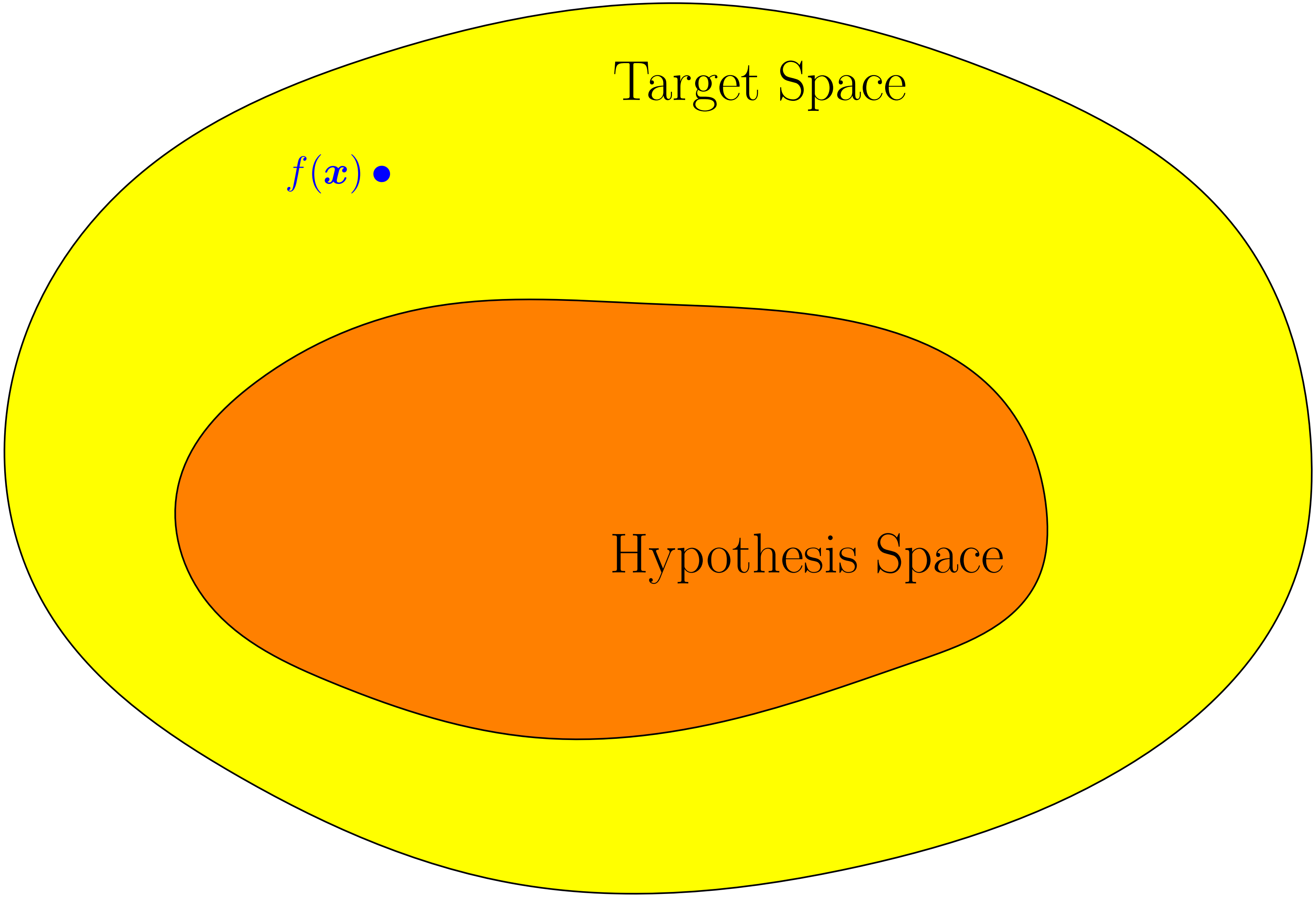

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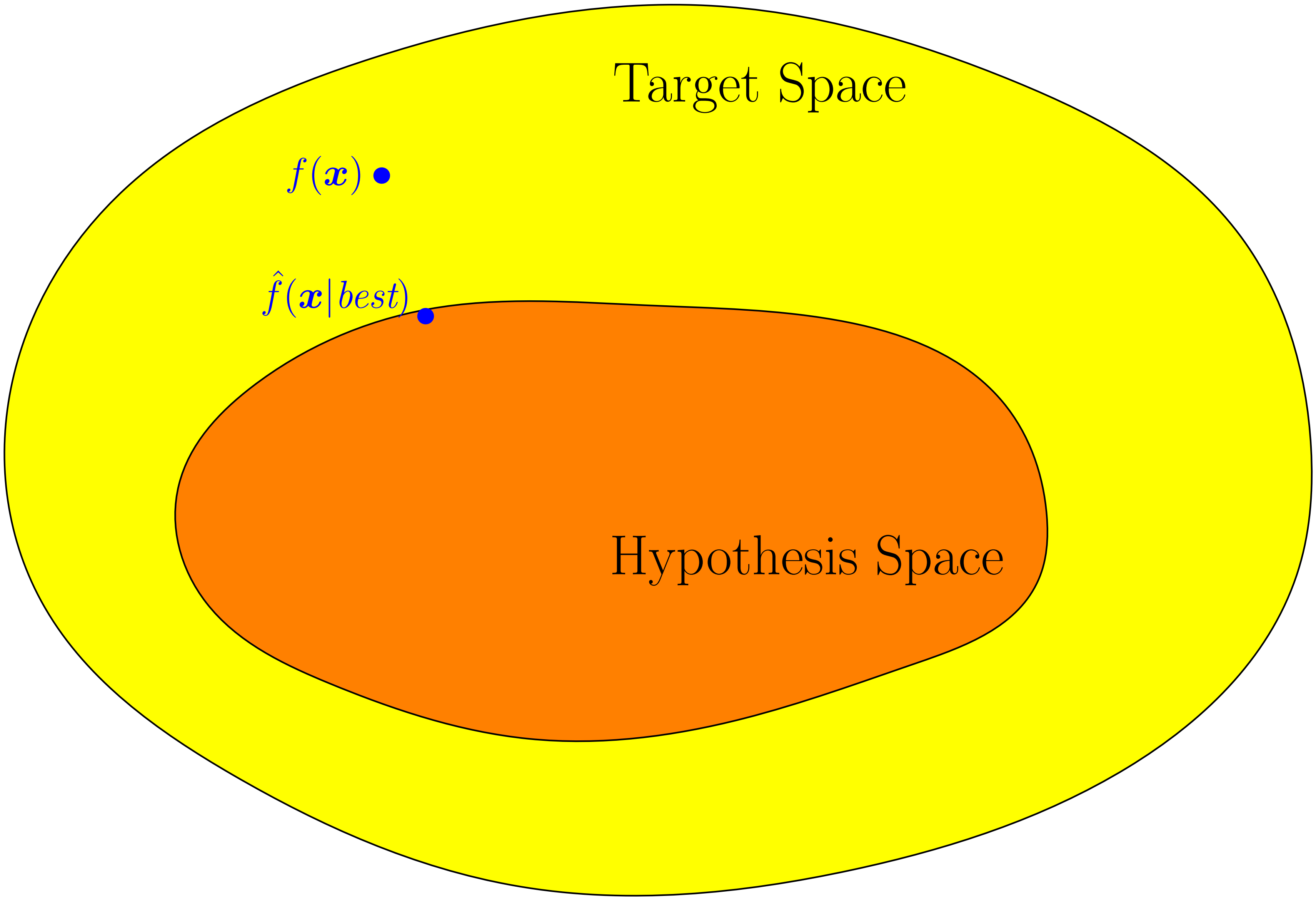

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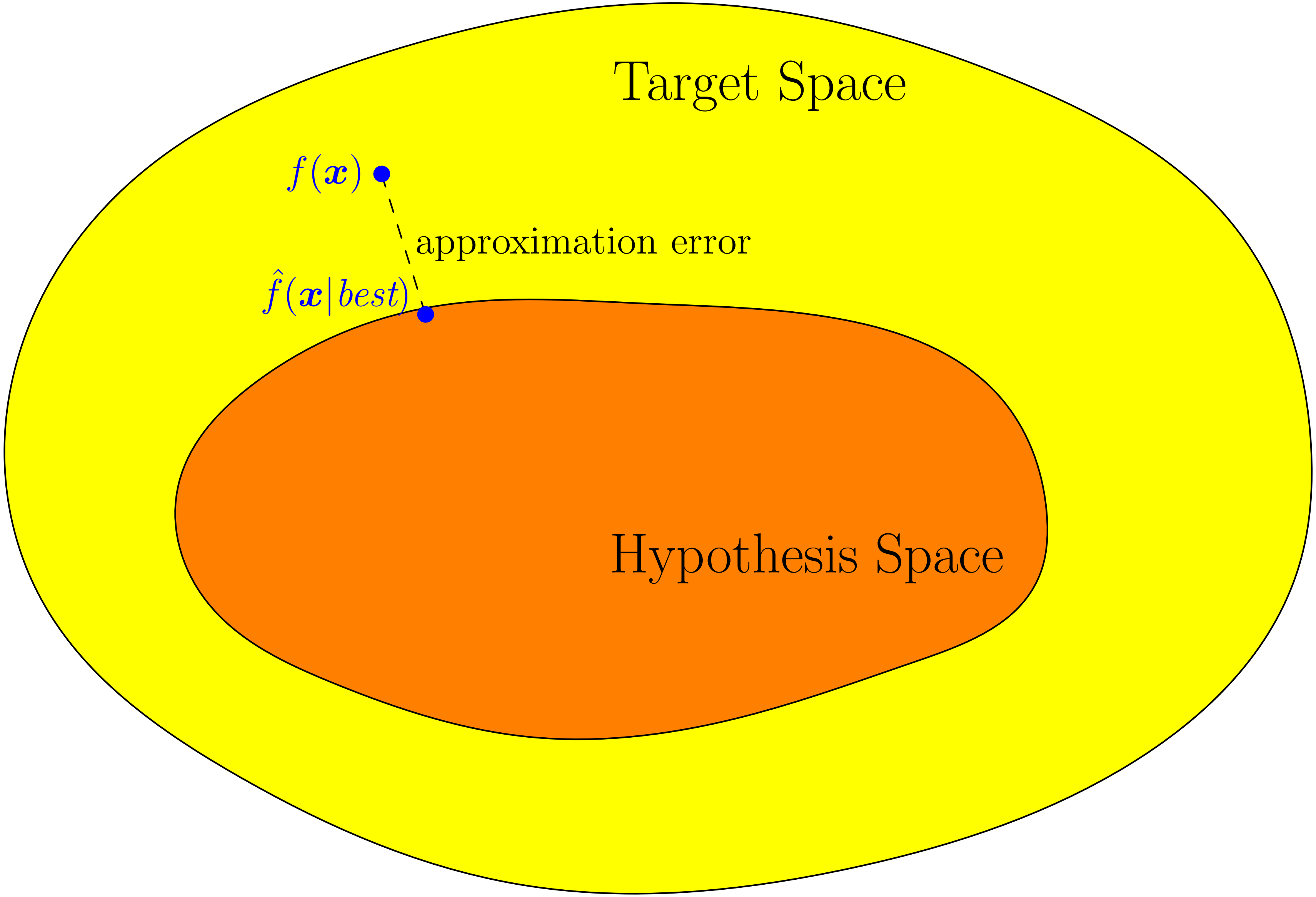

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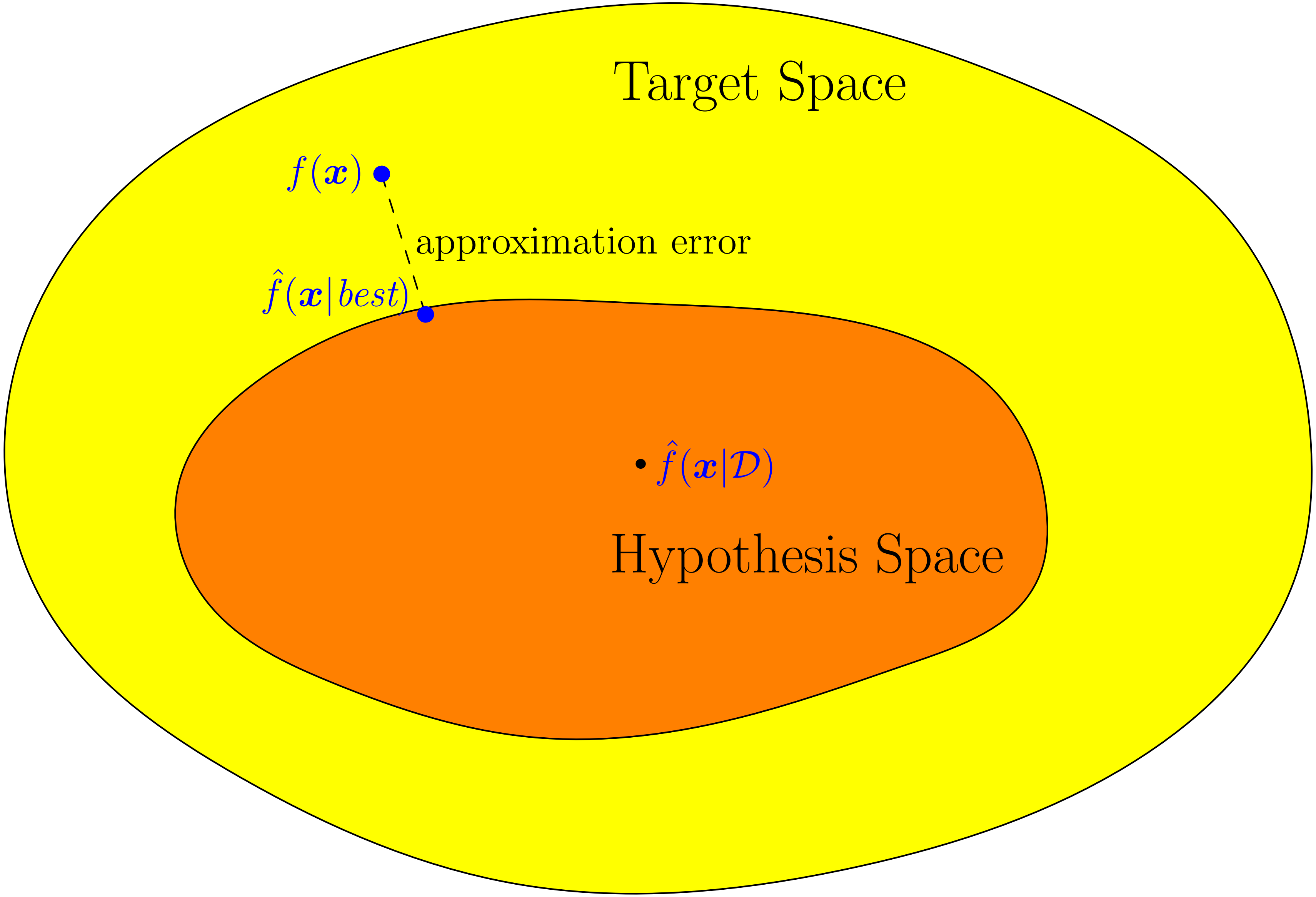

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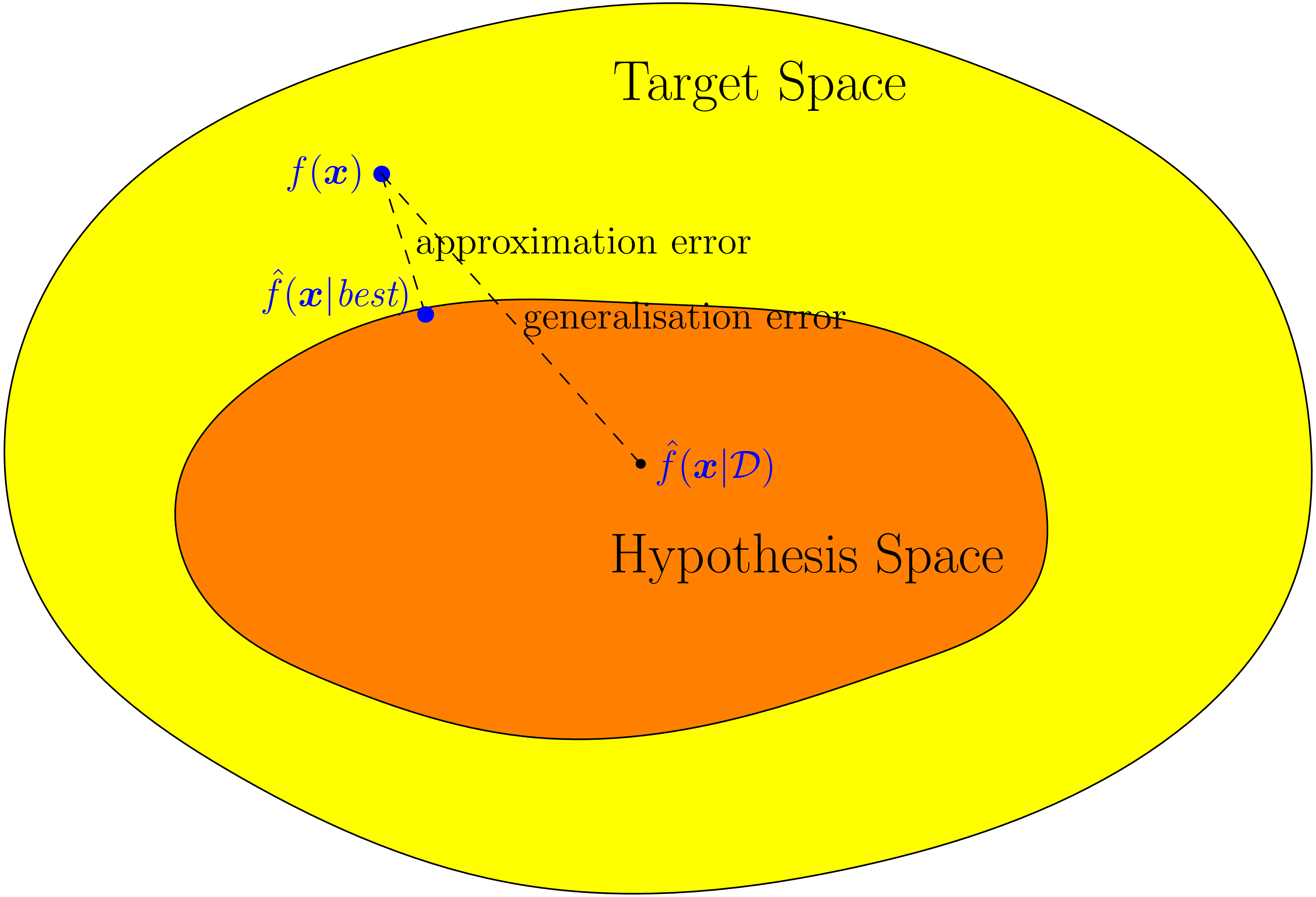

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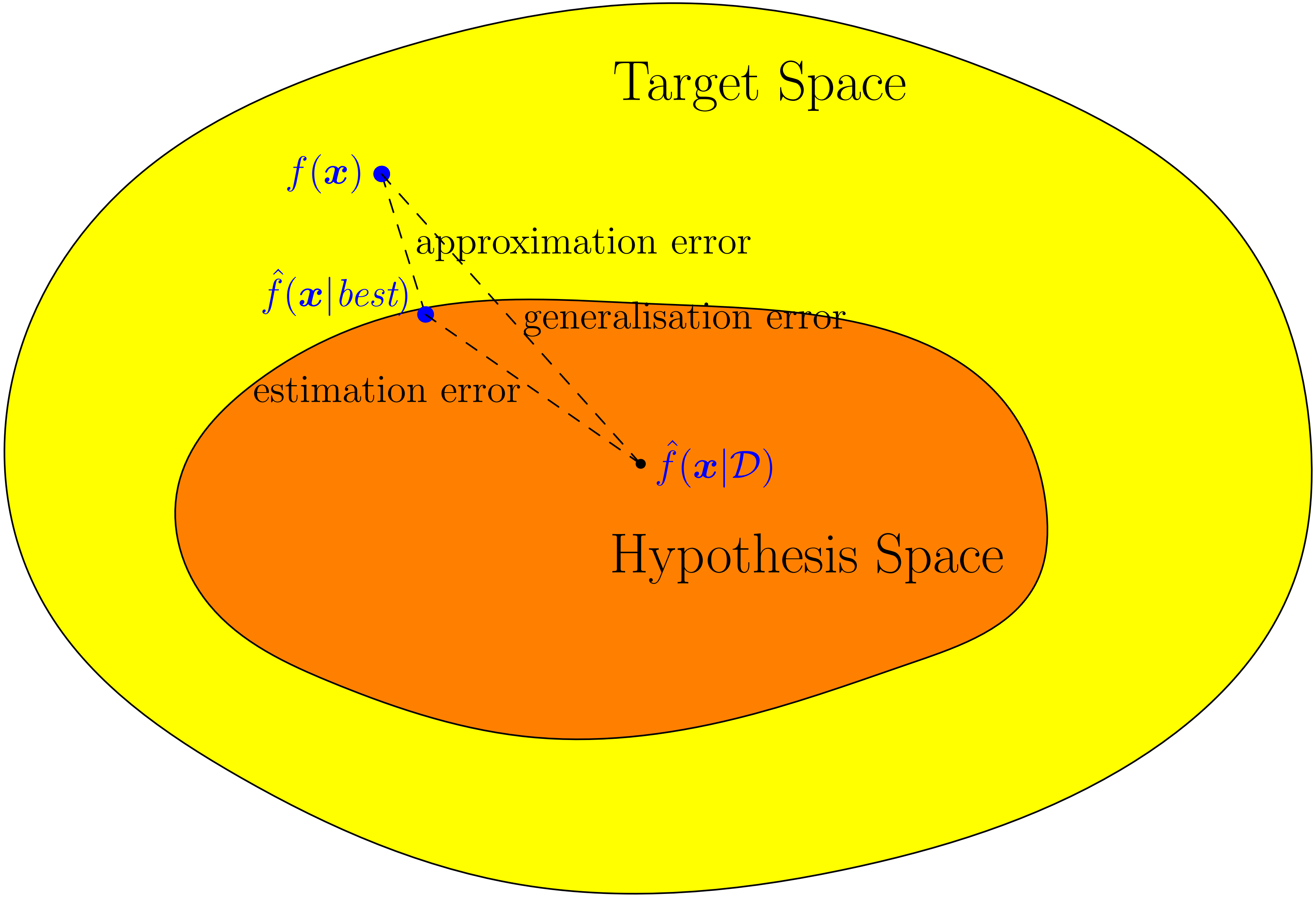

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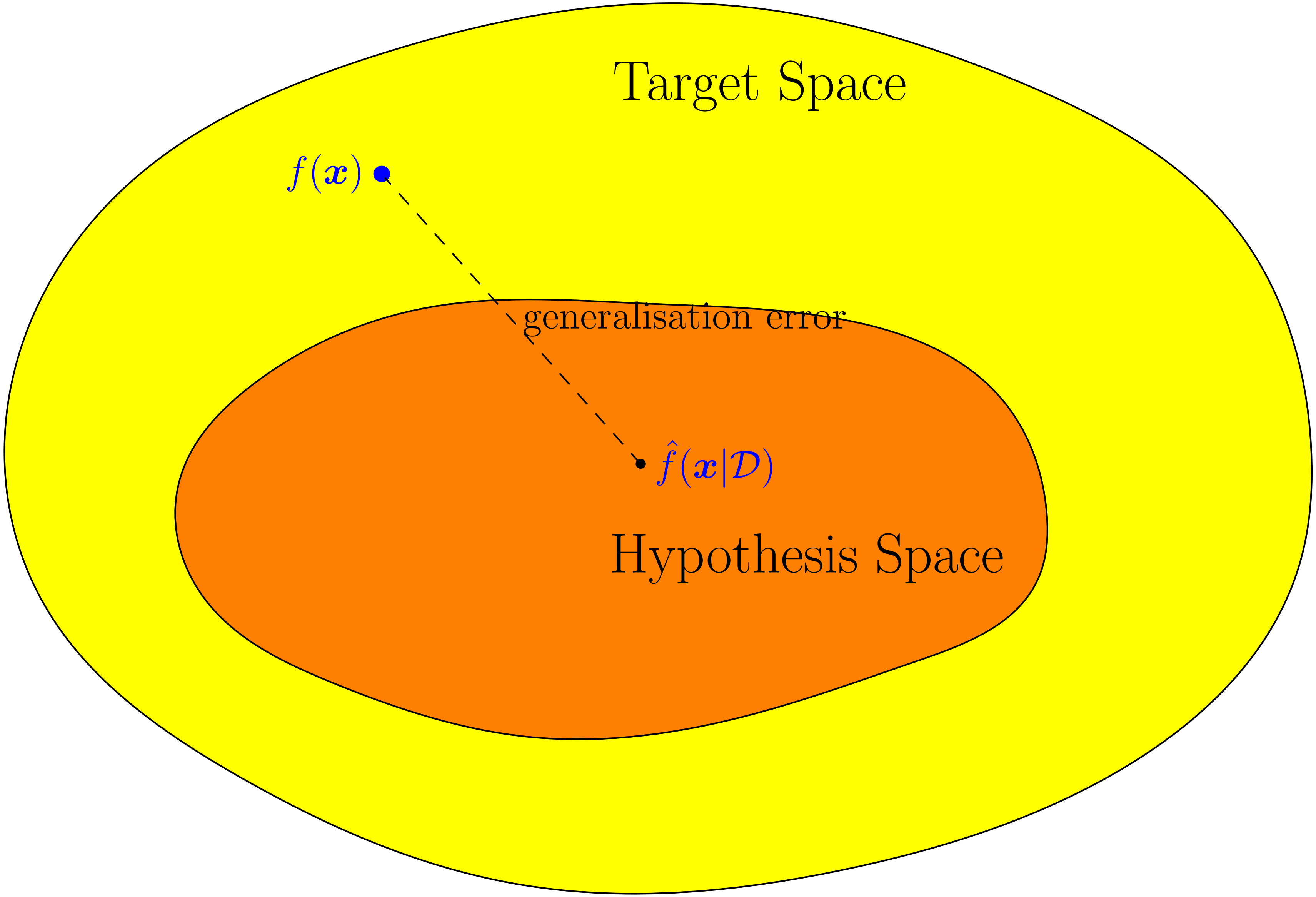

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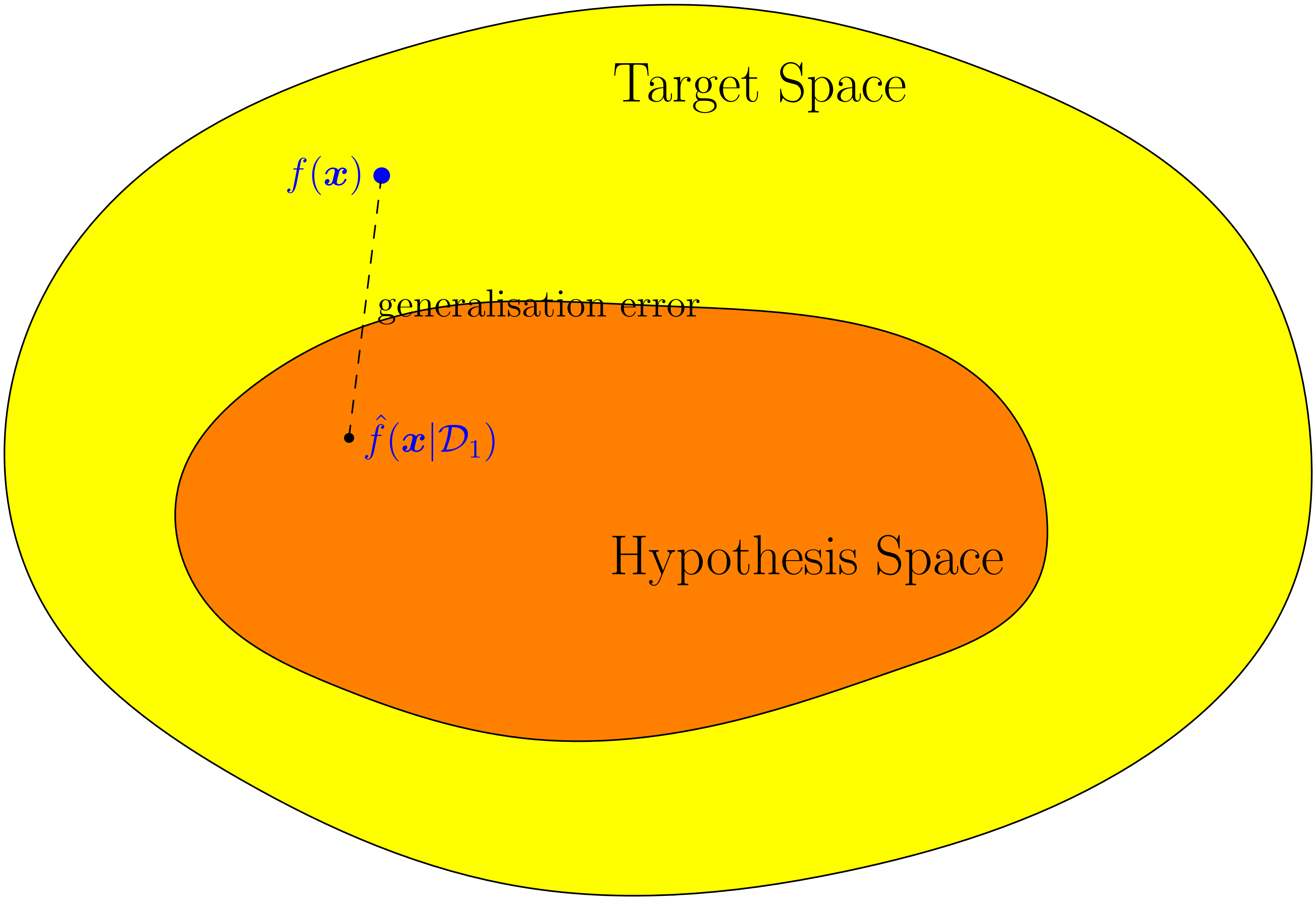

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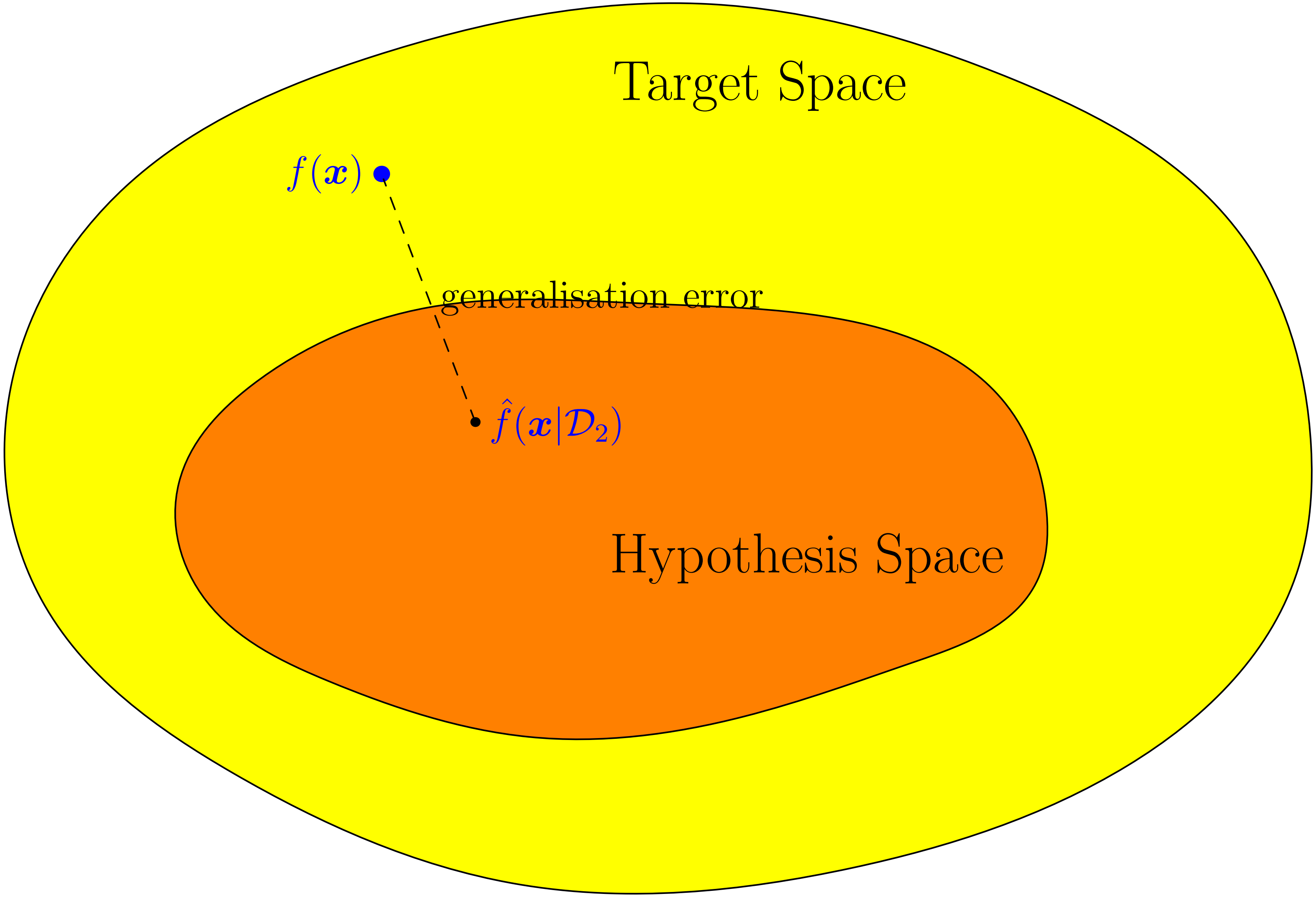

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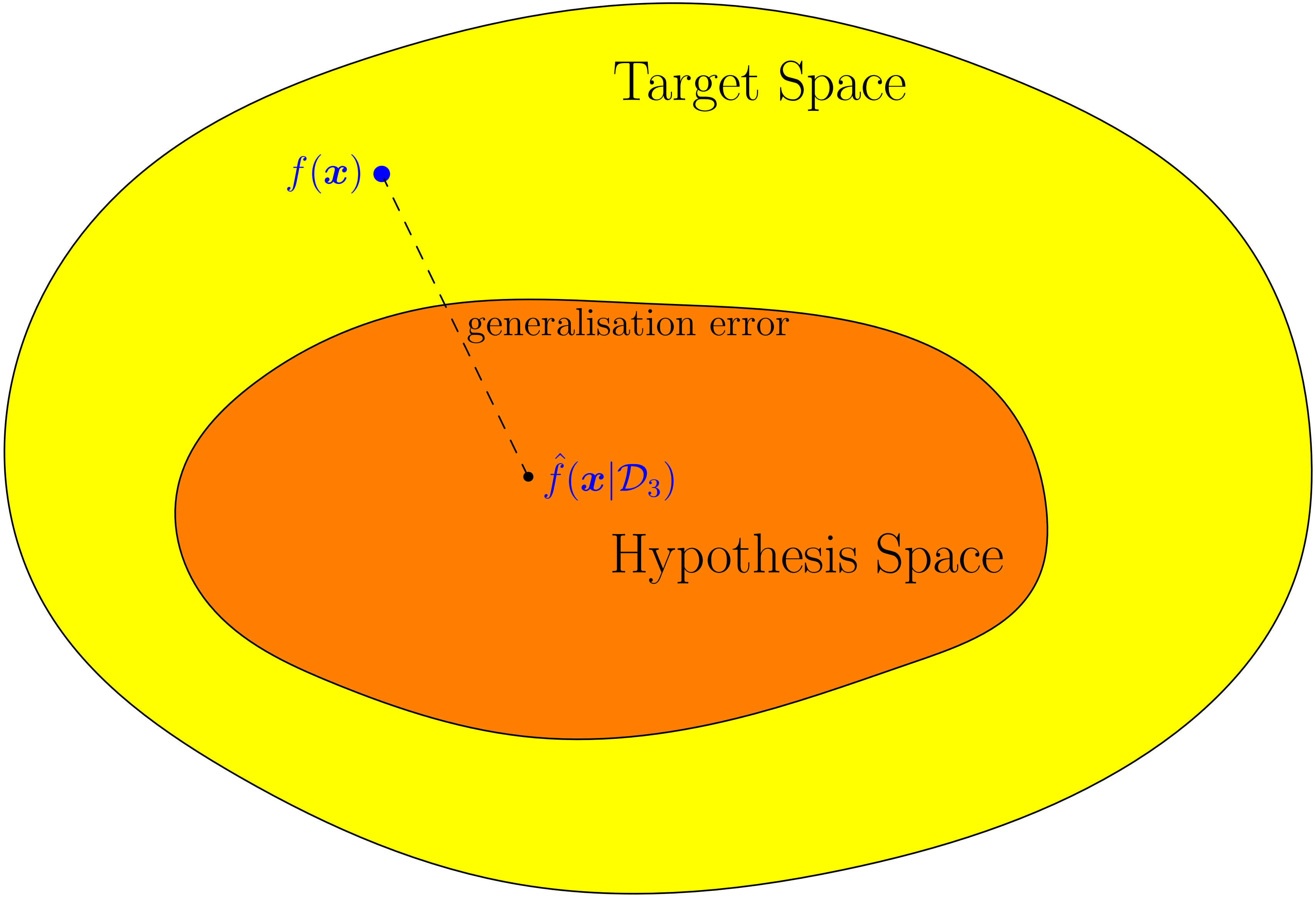

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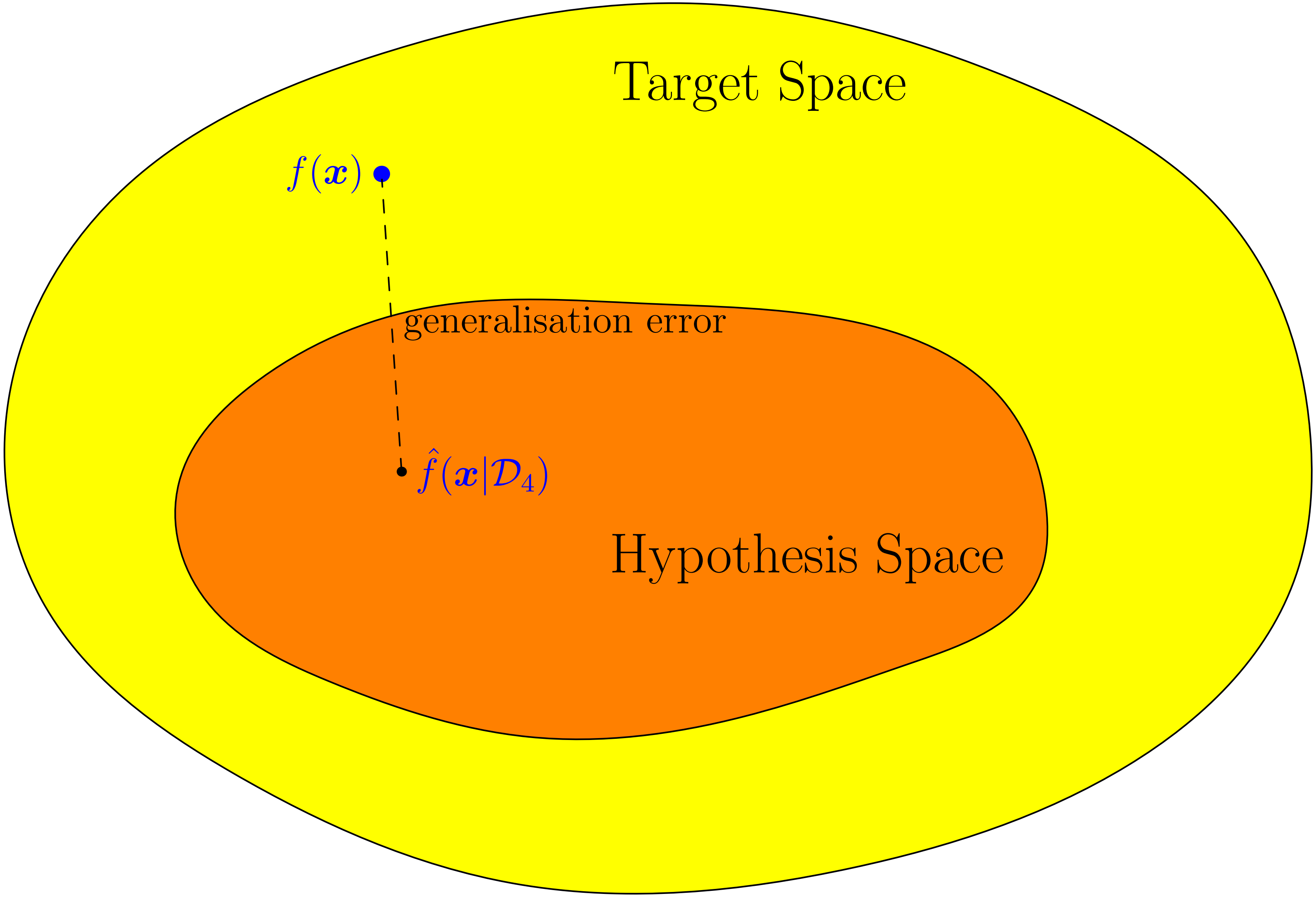

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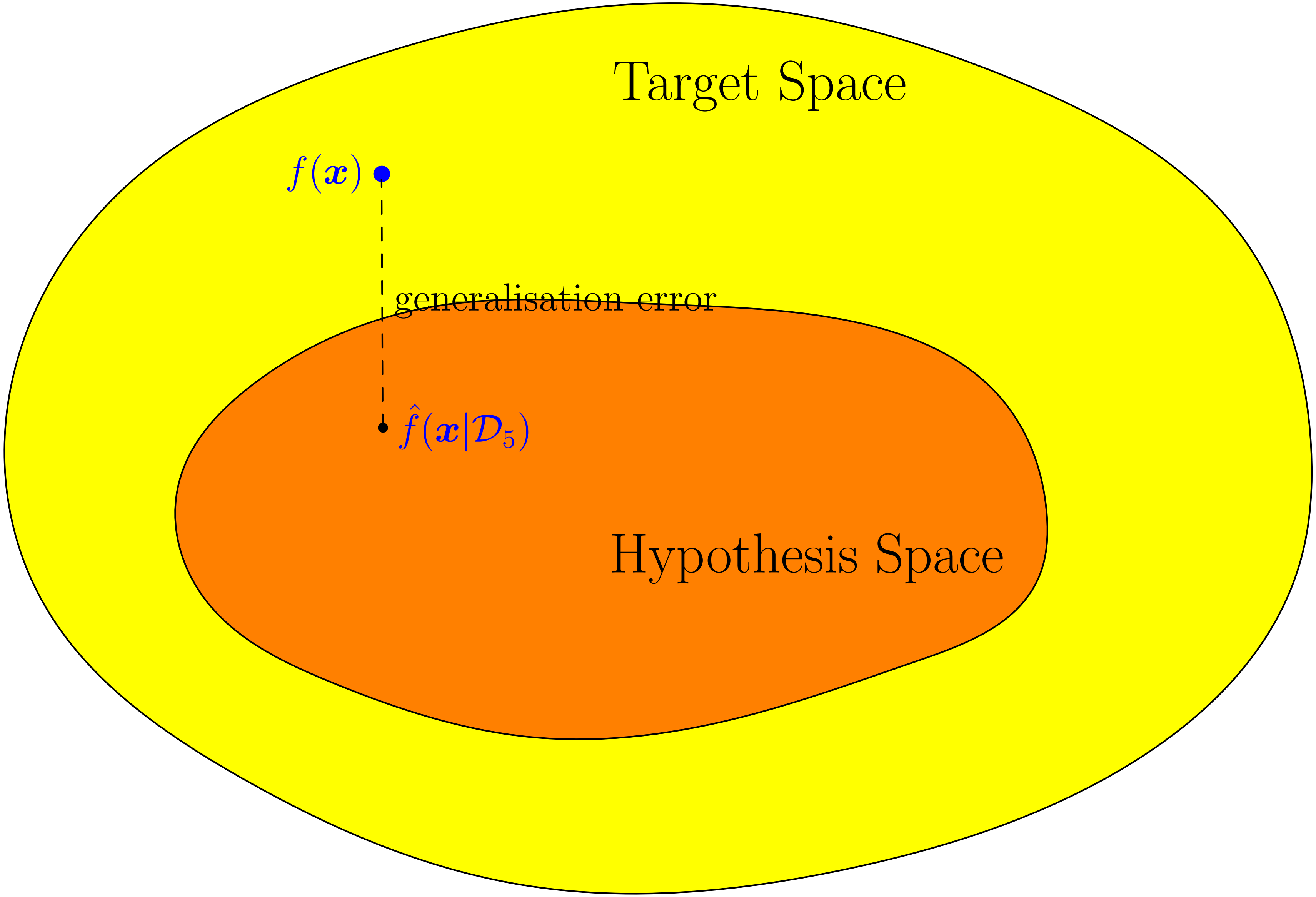

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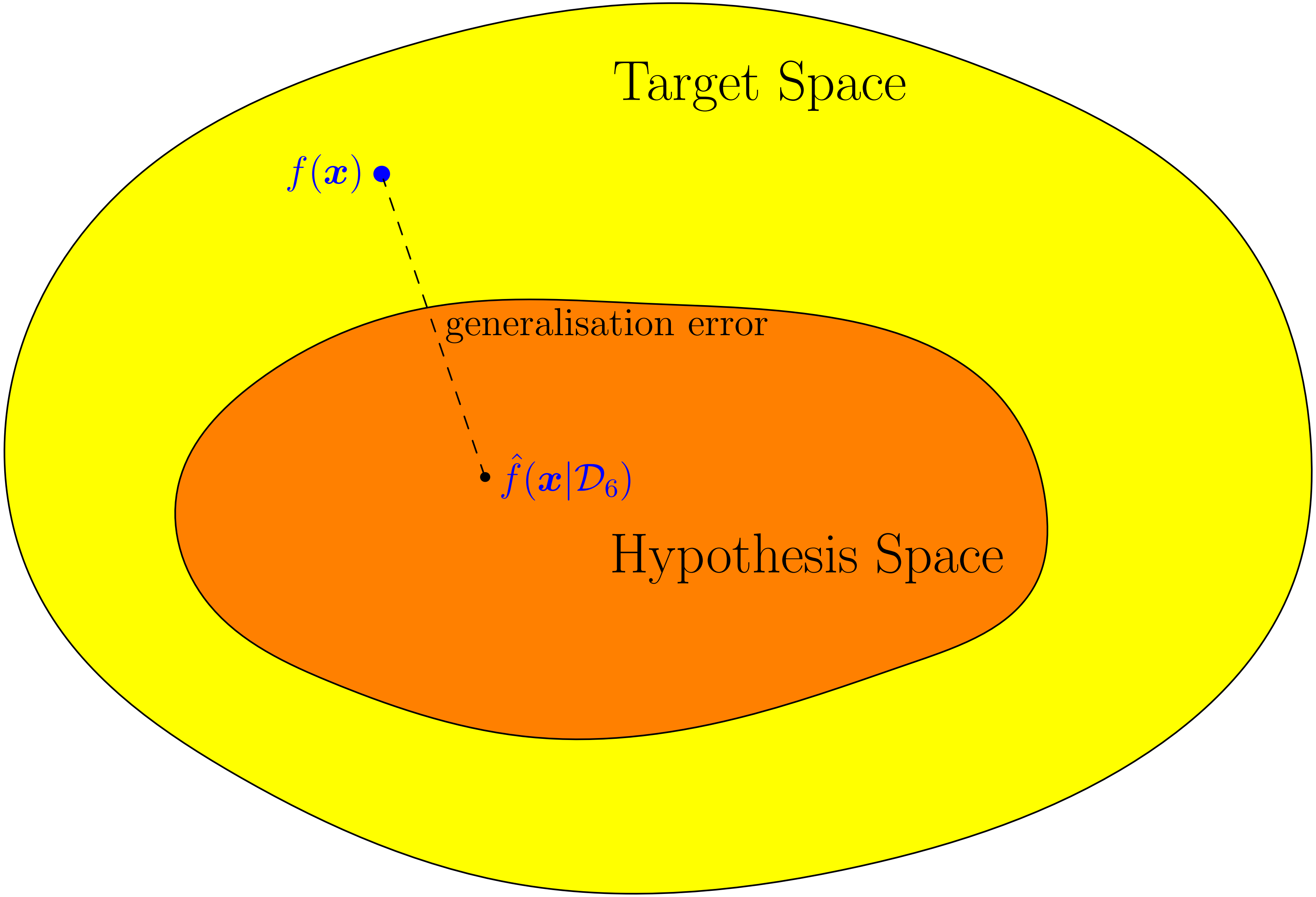

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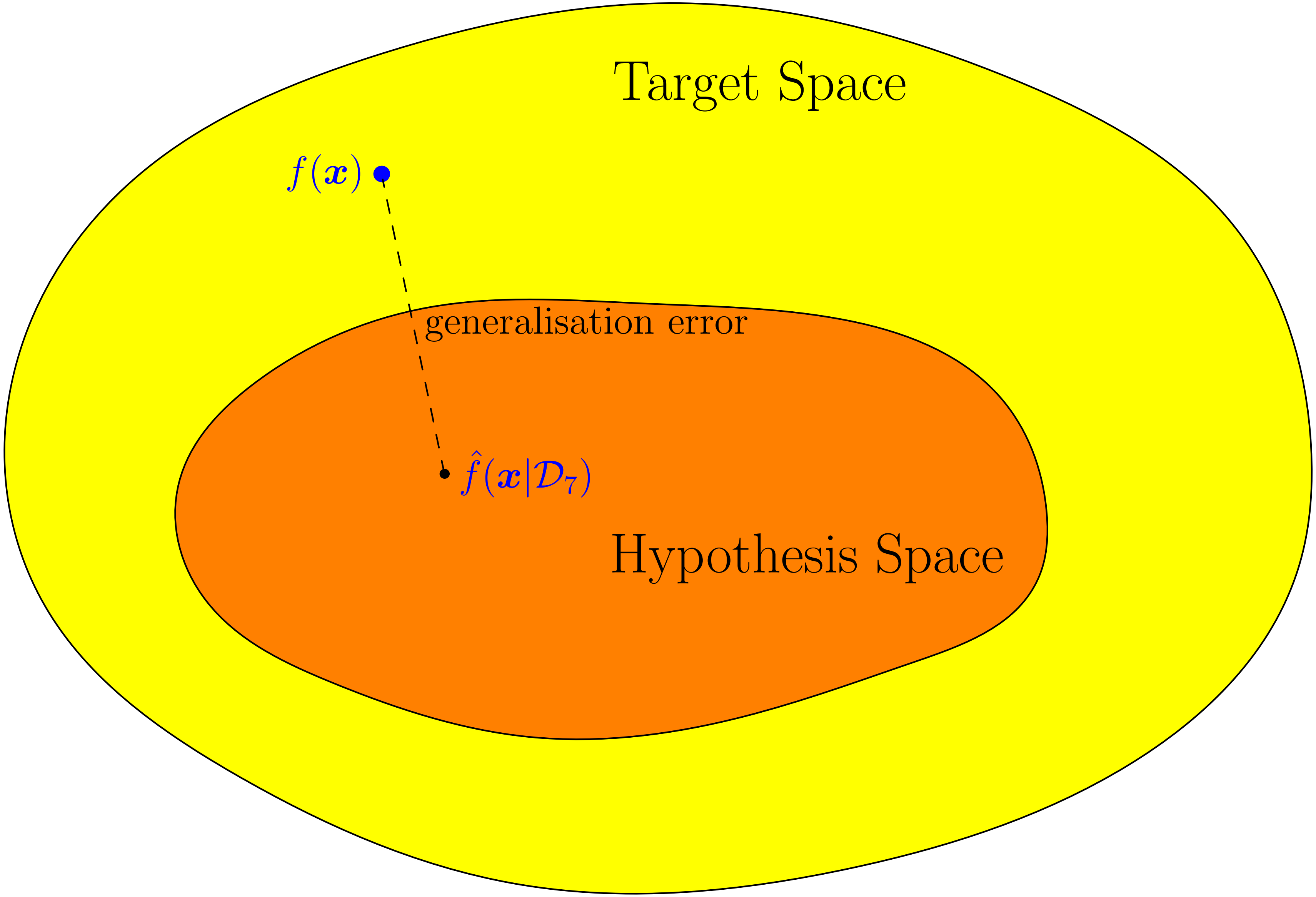

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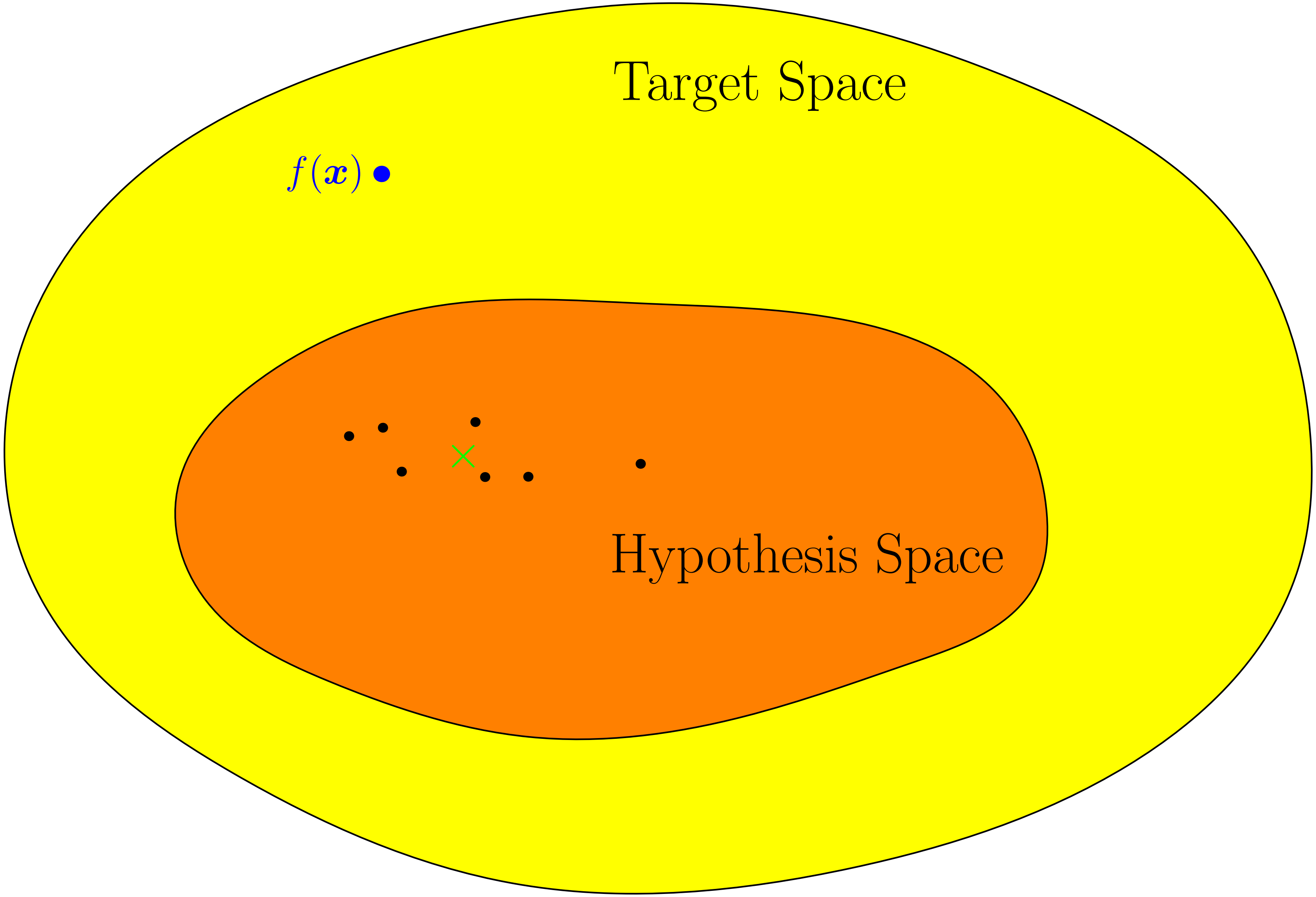

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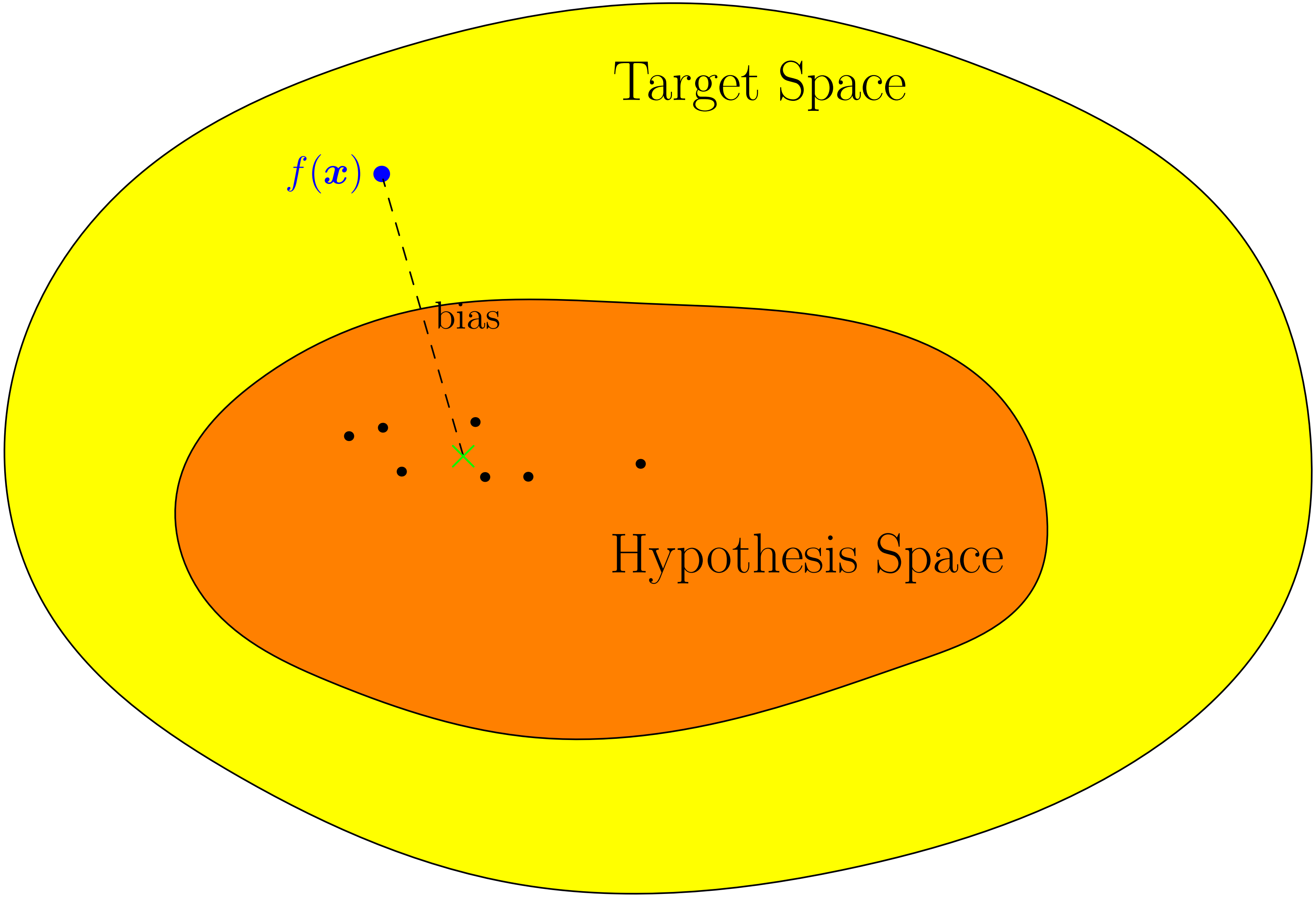

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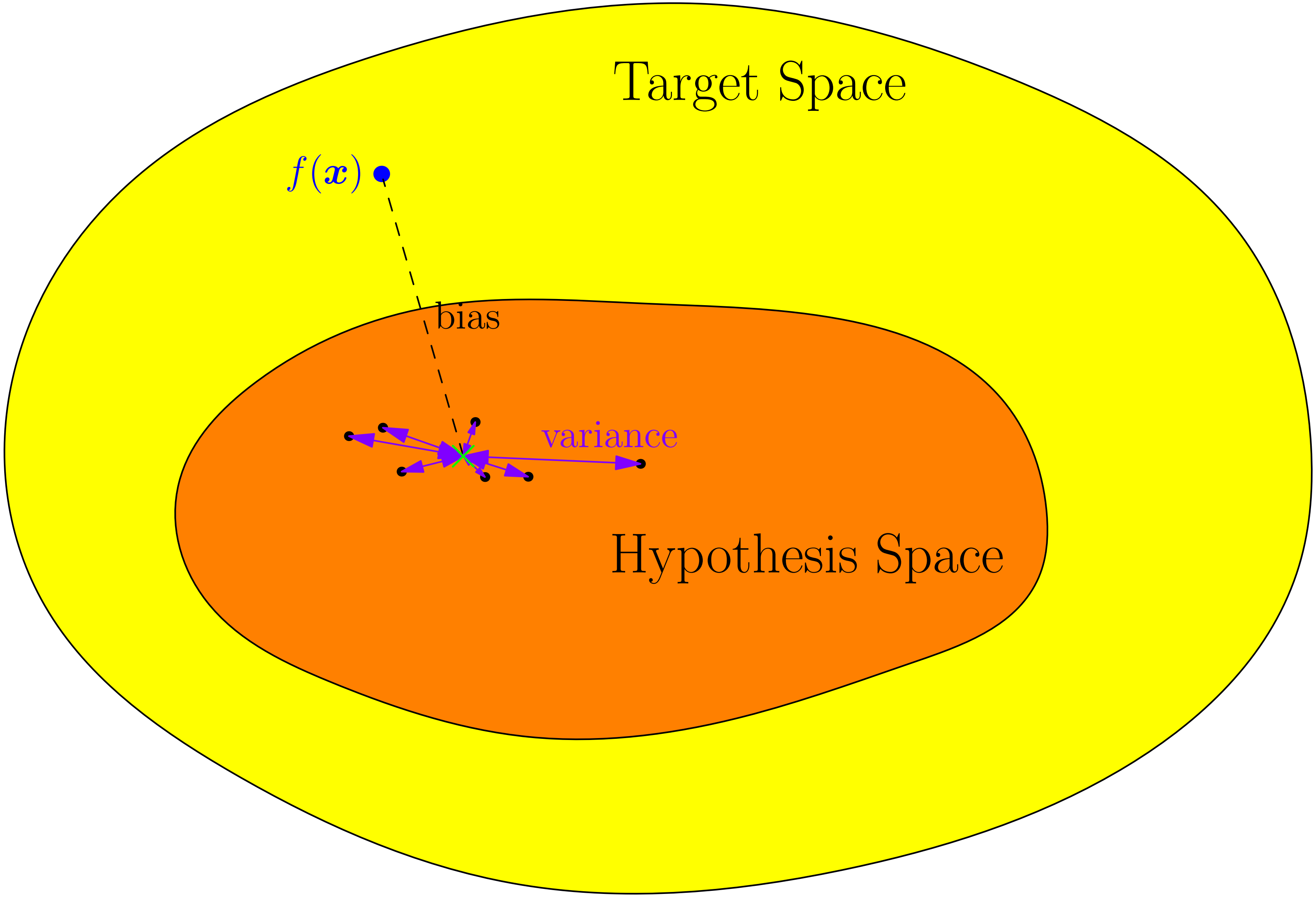

Mean Machine

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

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

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

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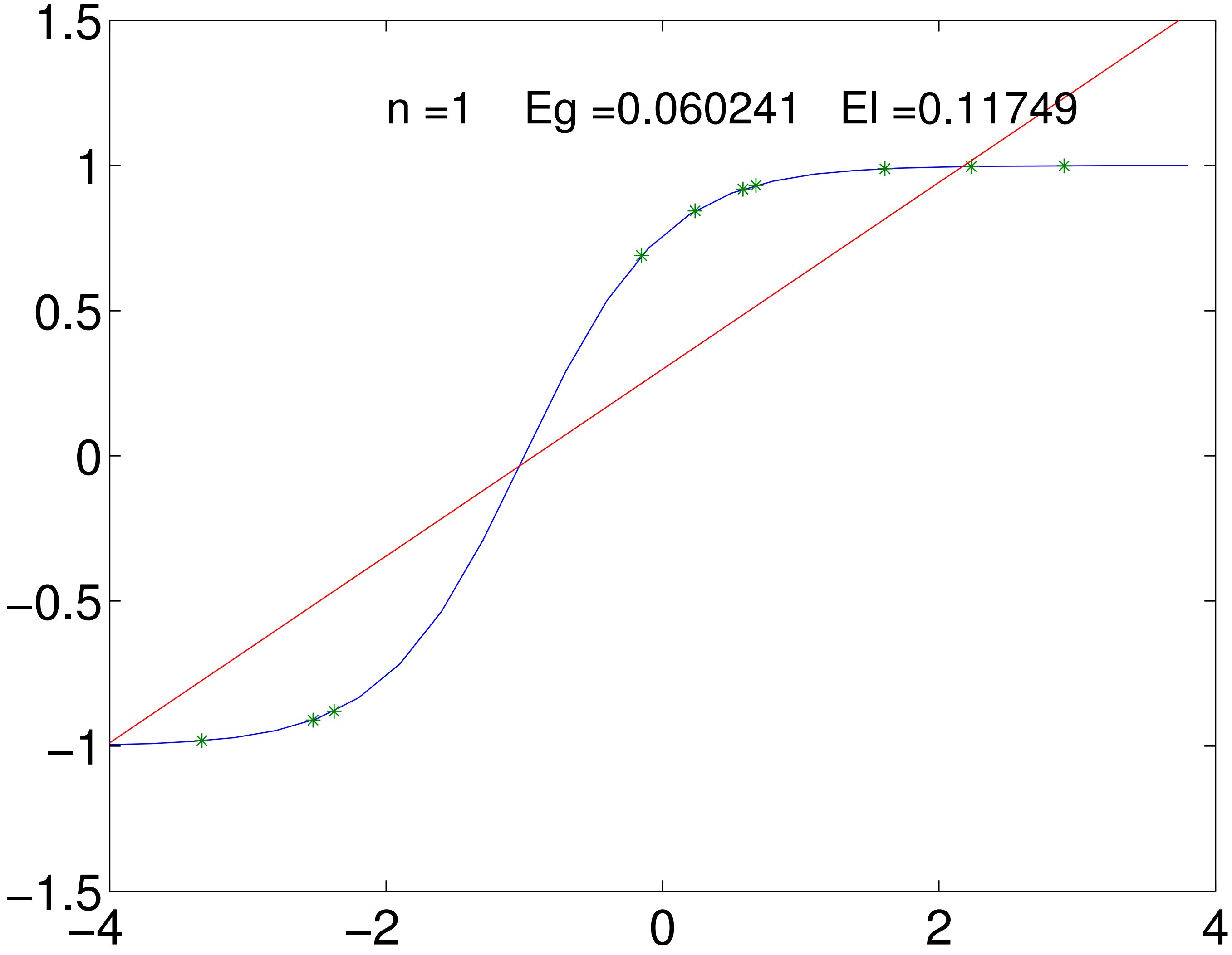

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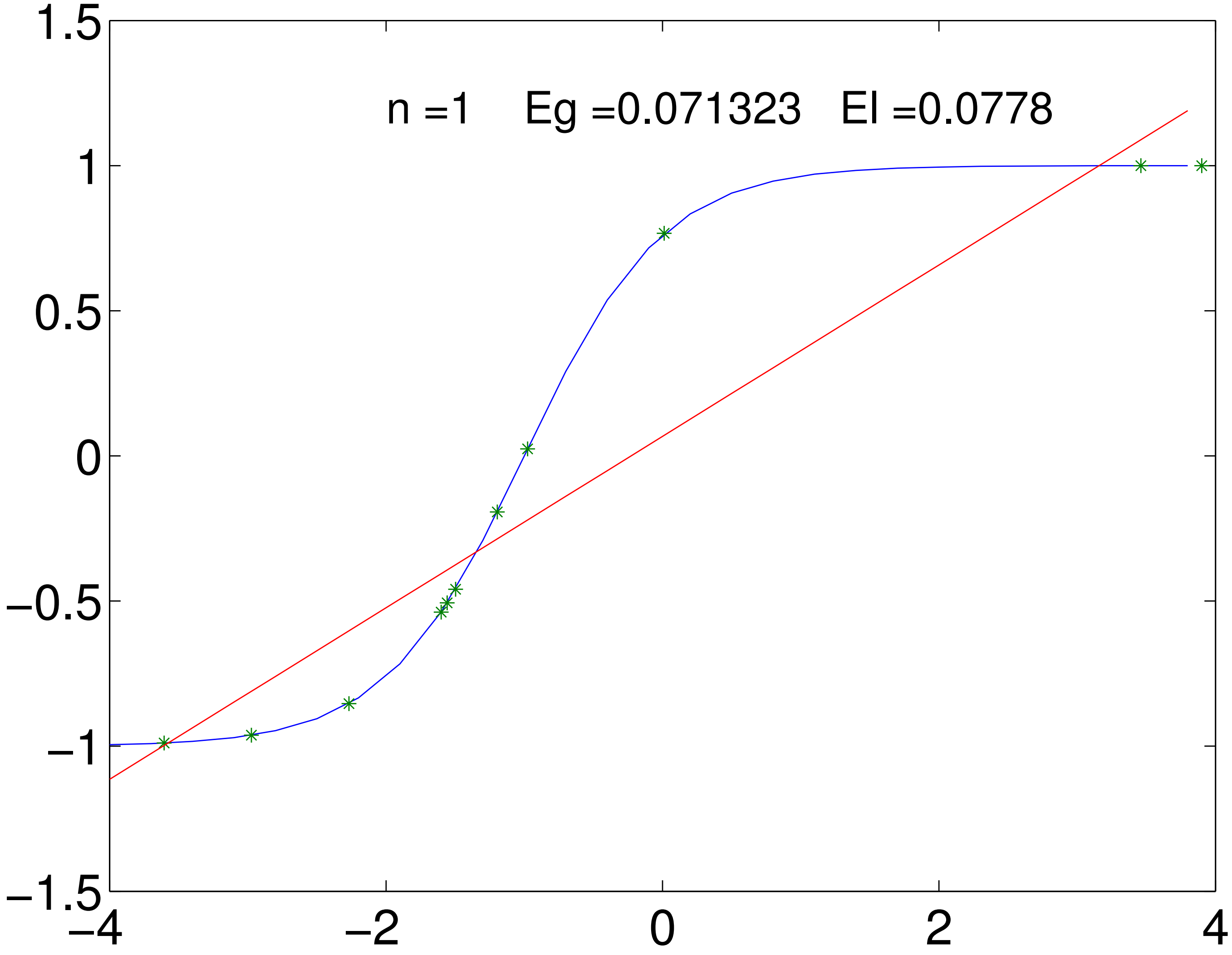

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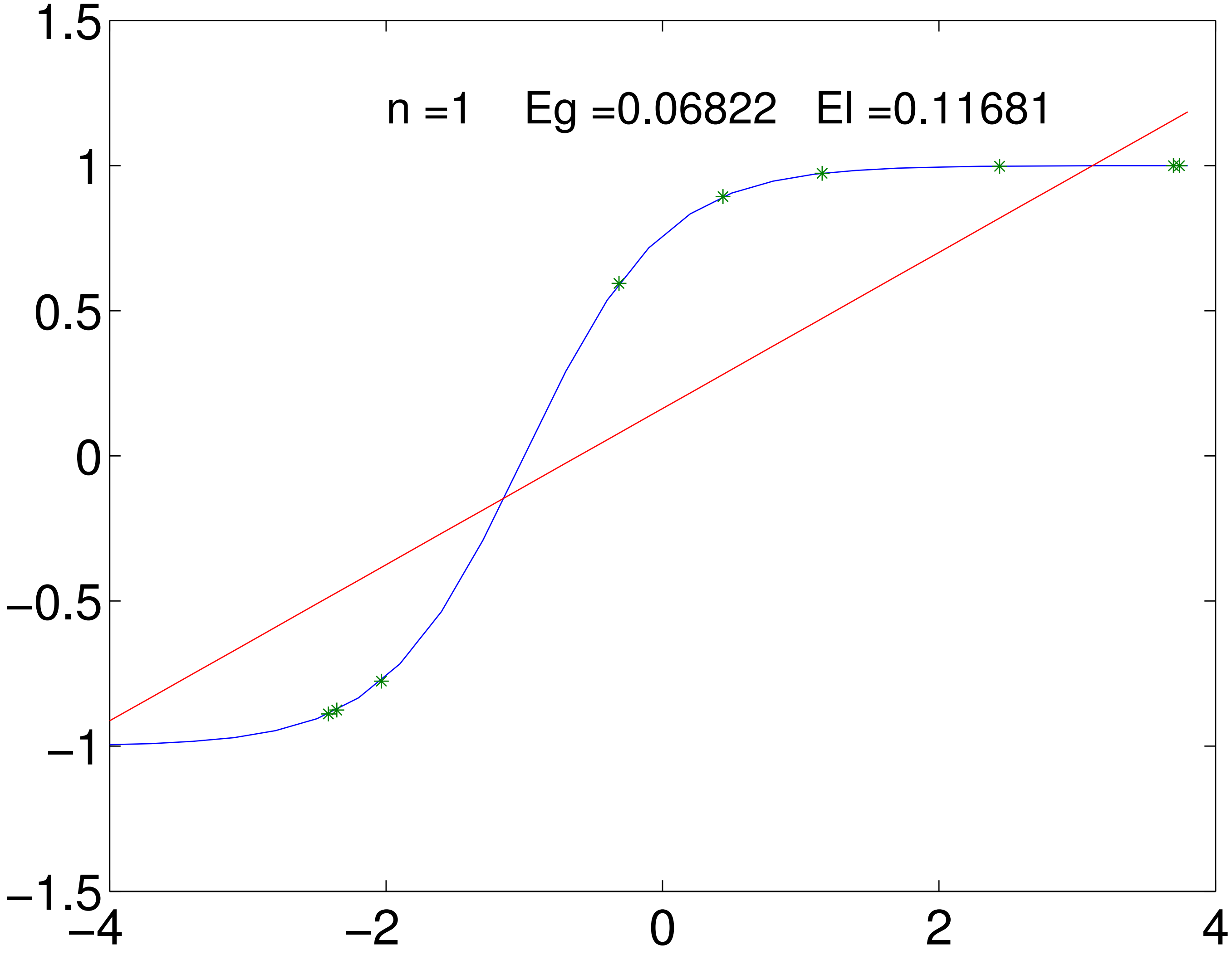

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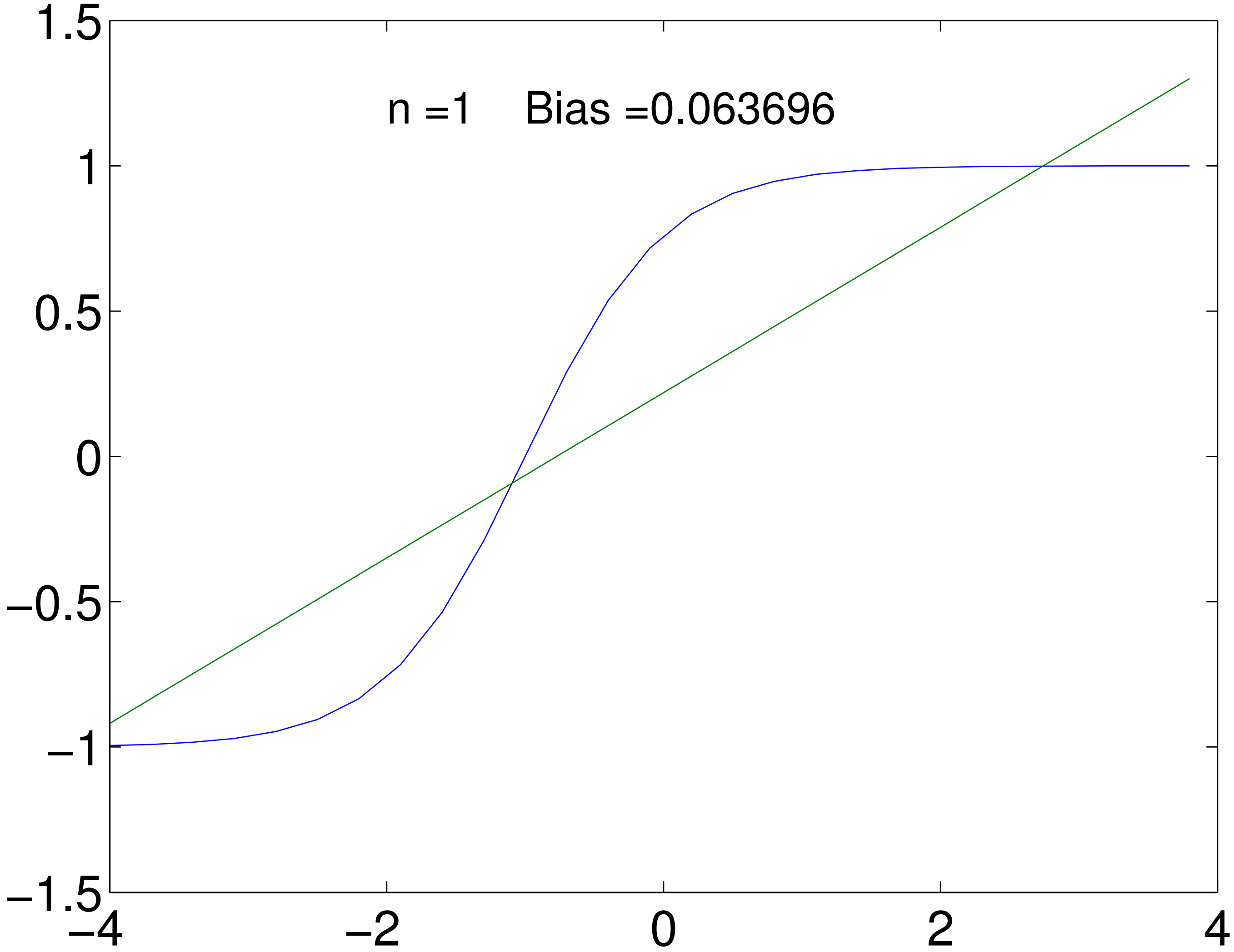

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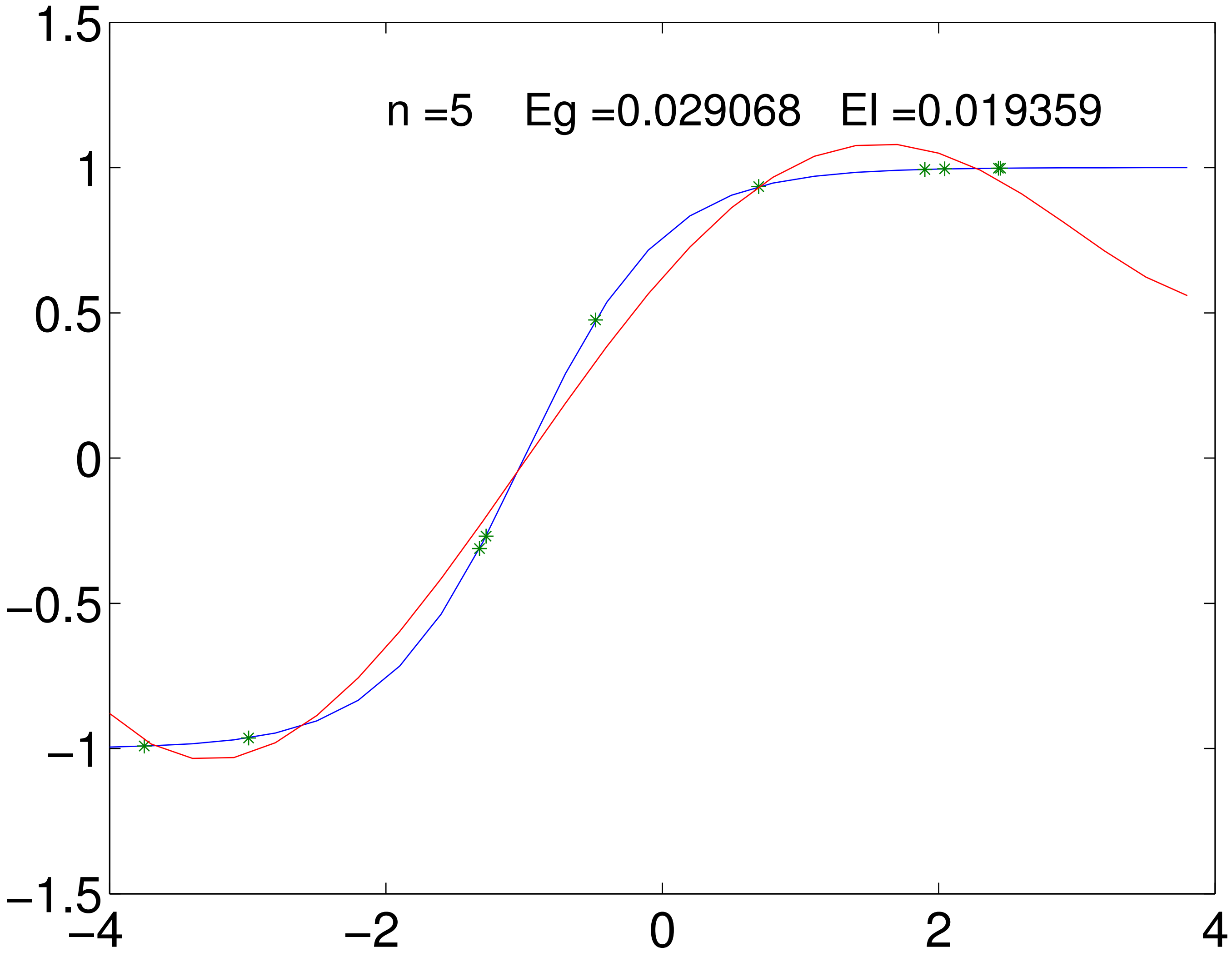

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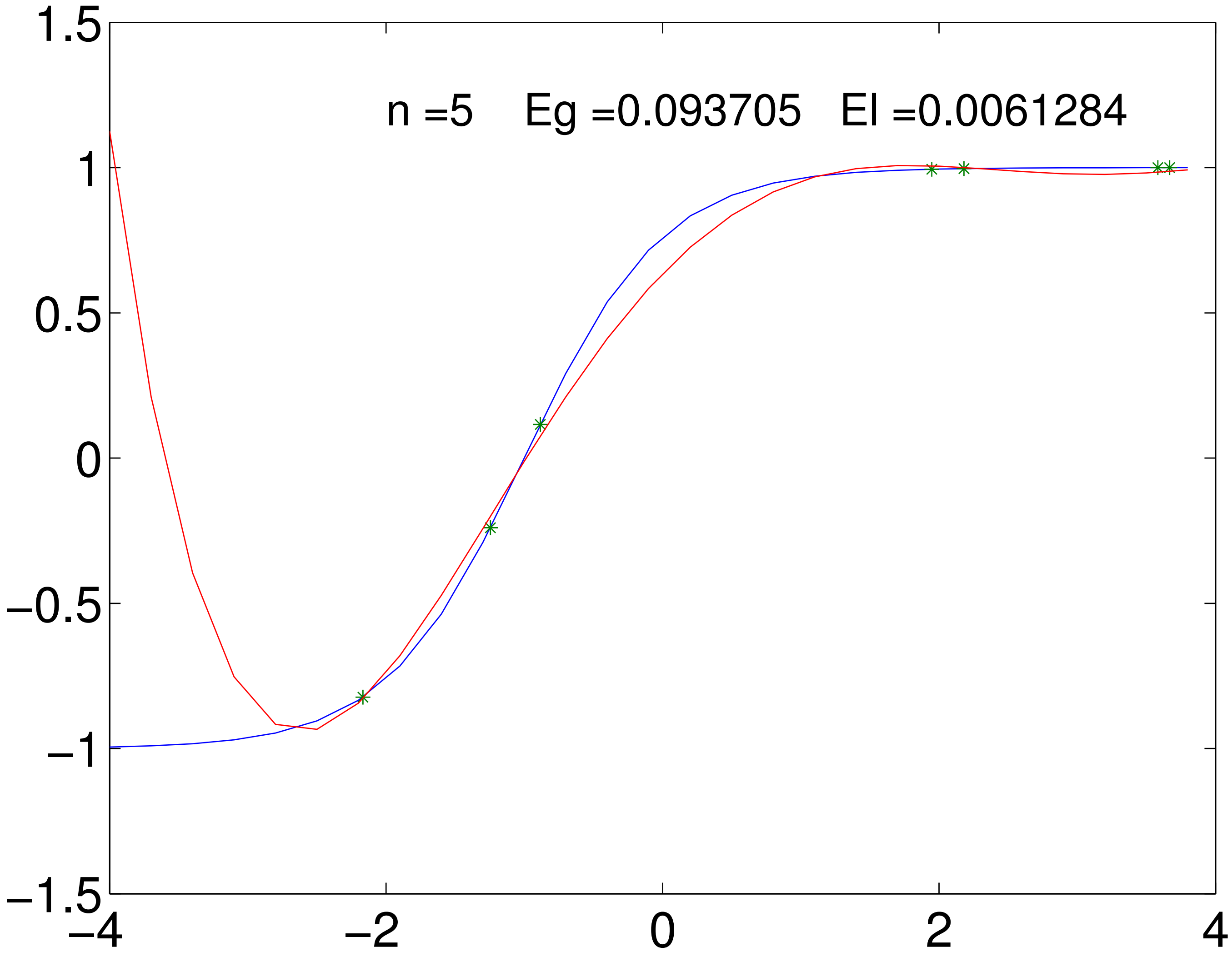

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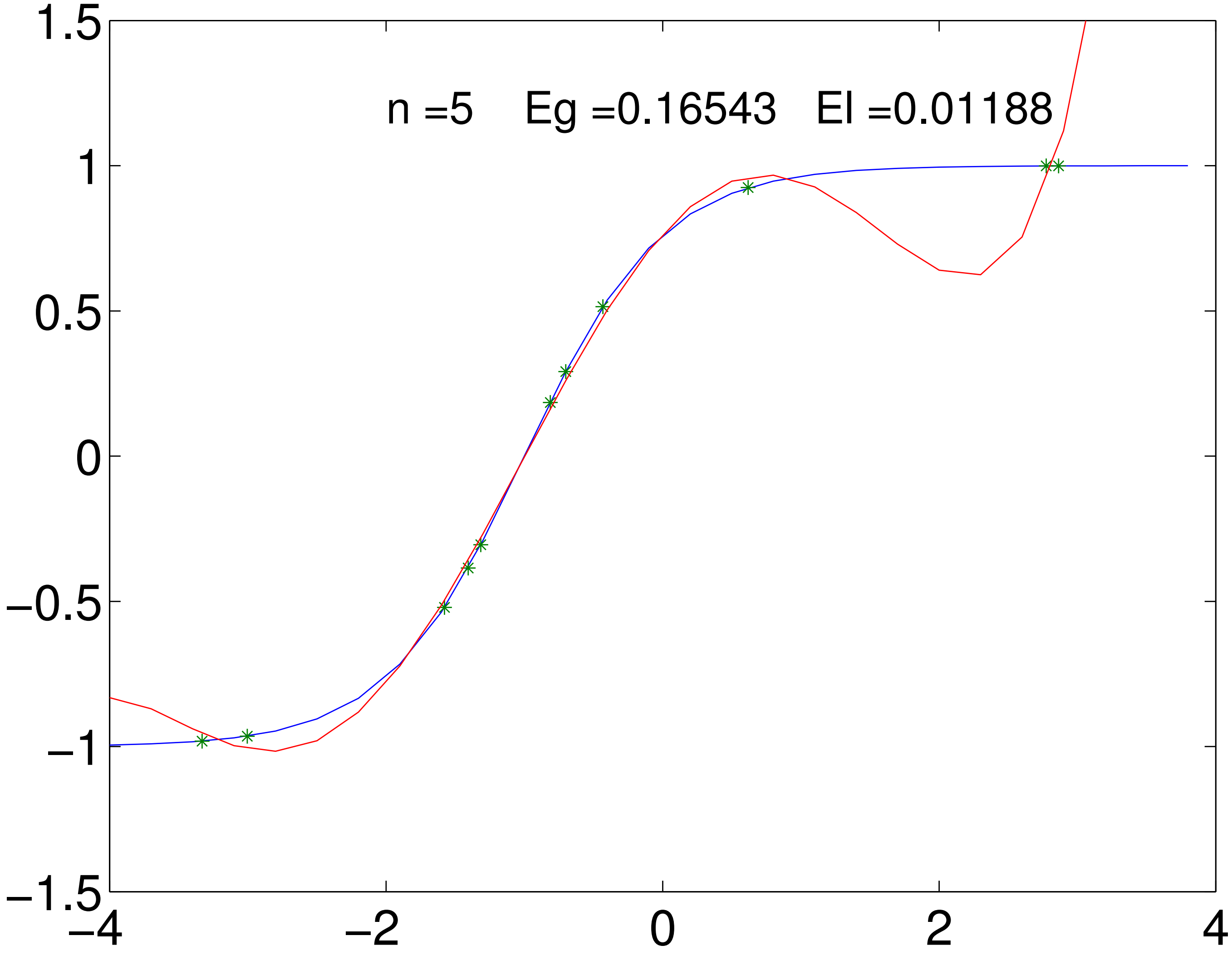

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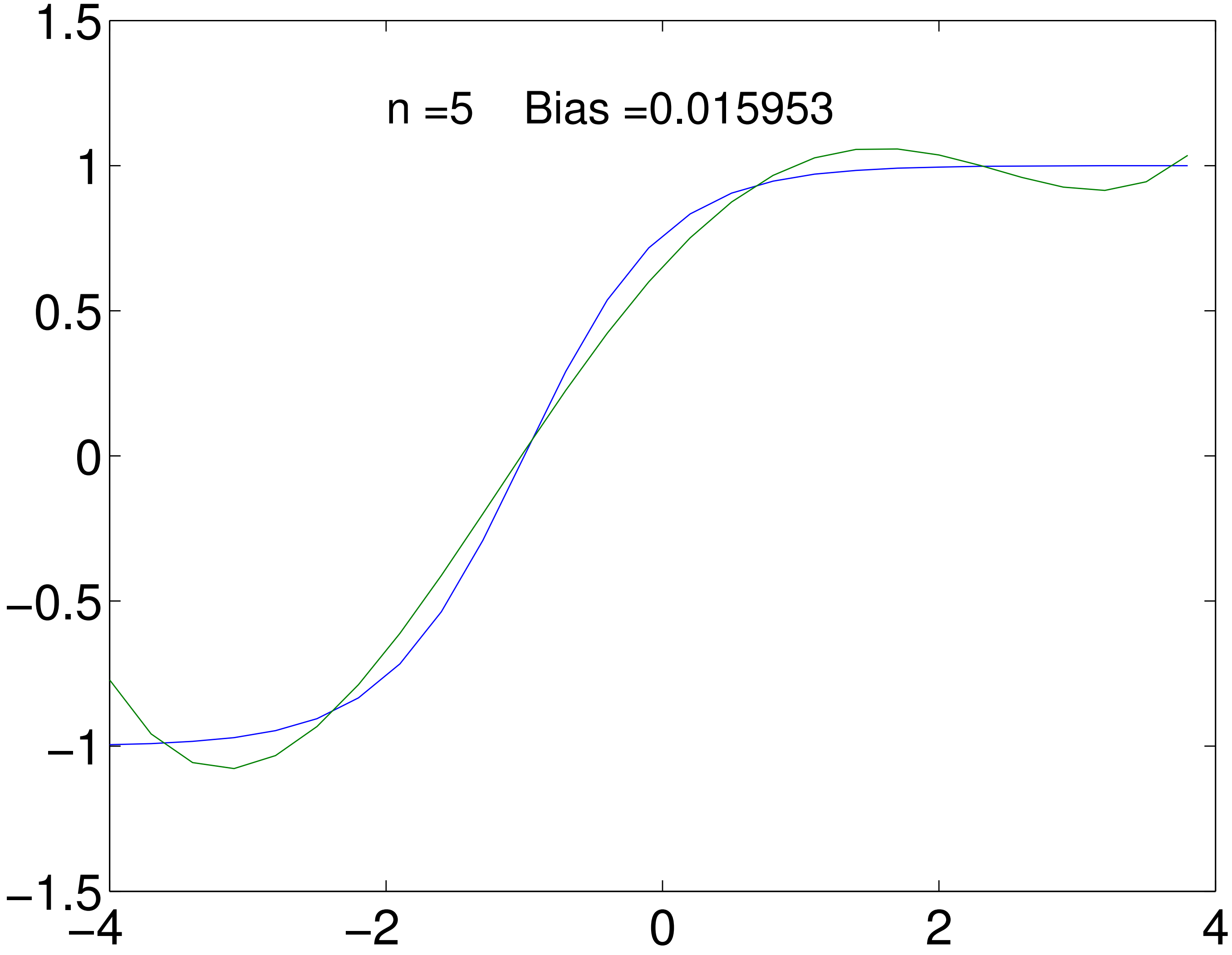

Bias and Variance

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

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

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

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Bias and Variance

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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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- 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
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- 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
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Dimensionality Reduction

- We can simplify our machines by using less features
- We can project our data onto a lower dimensional sub-space (e.g. one with the maximum variation in the data PCA)
- We can use clustering to find exemplars and recode our data in terms of differences from the exemplars (radial basis functions)
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Feature Selection

- Spurious features will allow us to find spurious rules (**over-fitting**)
- We can try different combinations of features to find the best set, although it rapidly becomes intractable to do this in all ways
- We can use various heuristics to decide which features to keep, but no heuristic is fail-safe
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Explicit Regularisation

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

- Second term is minimised when $w_i = 0$
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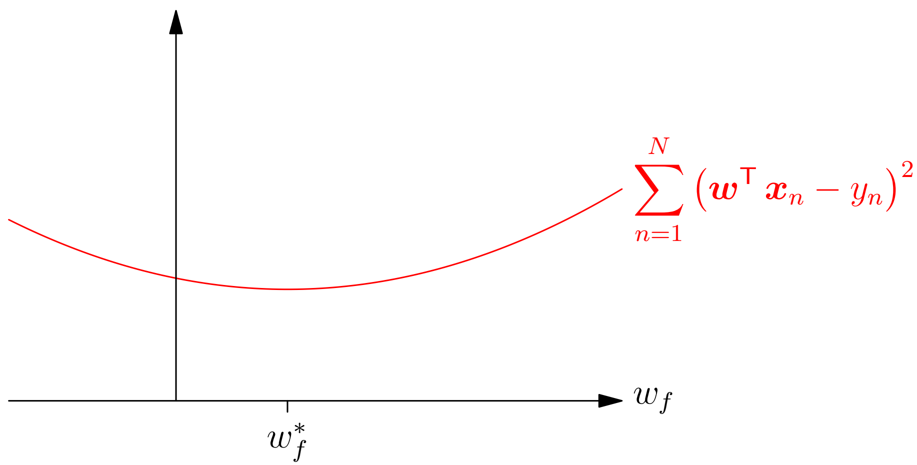

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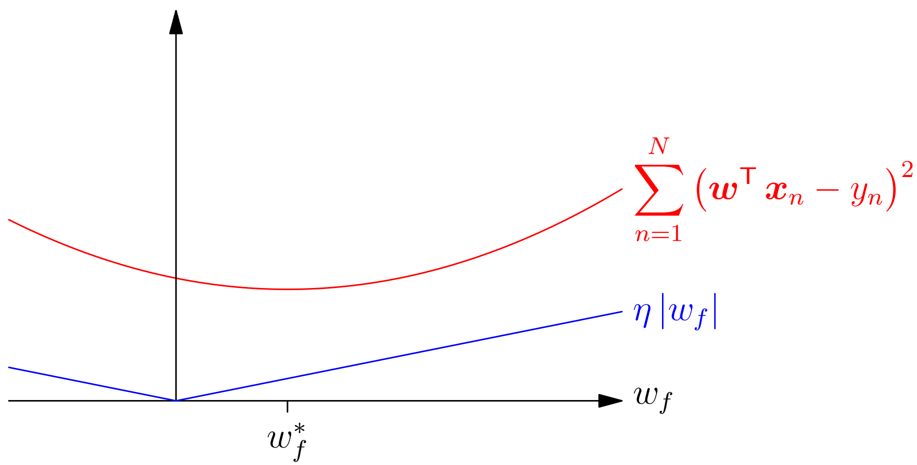

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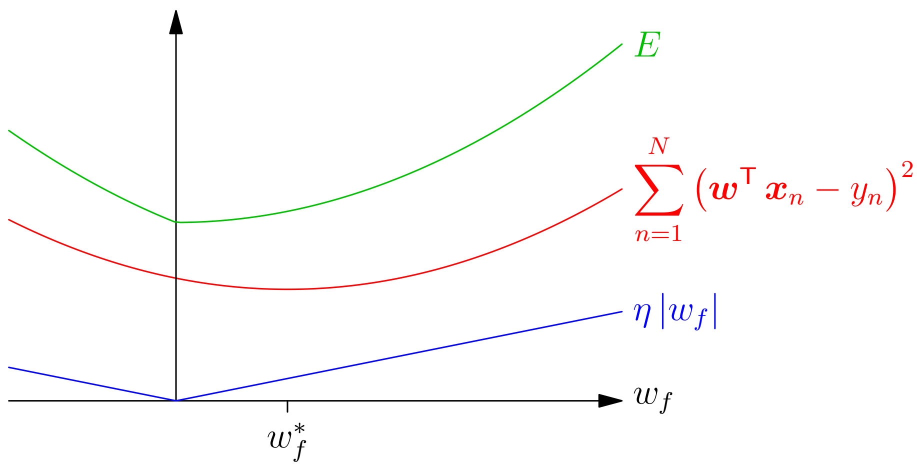

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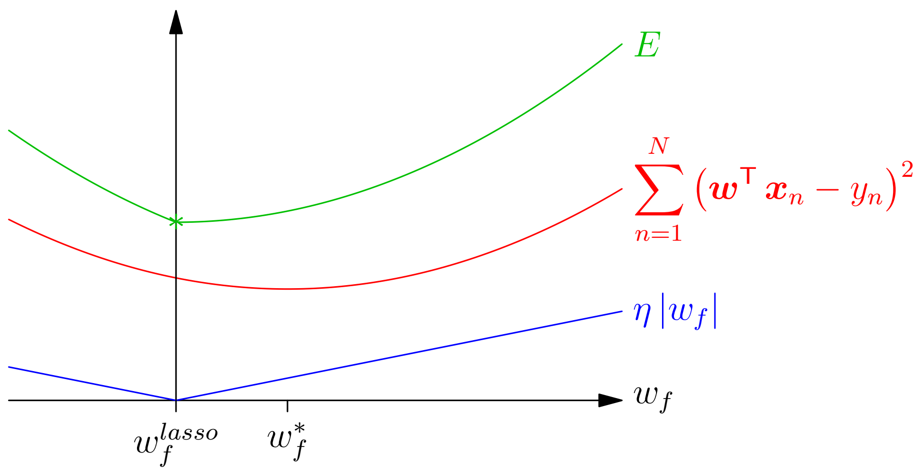

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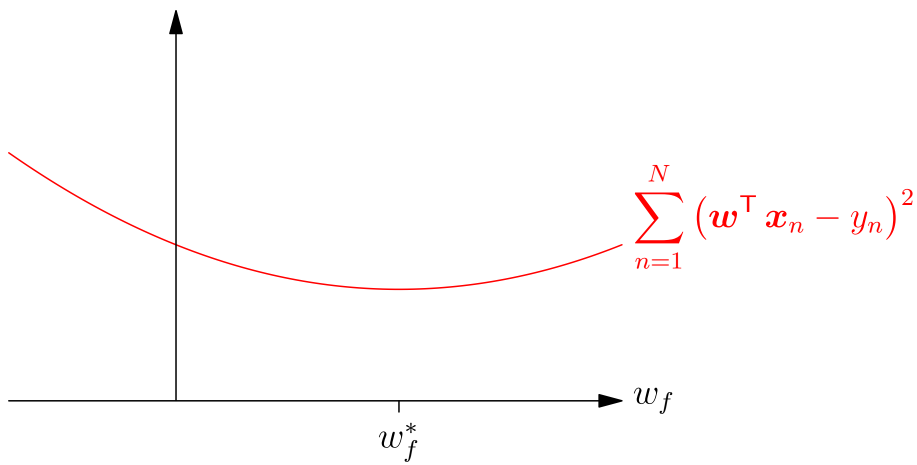

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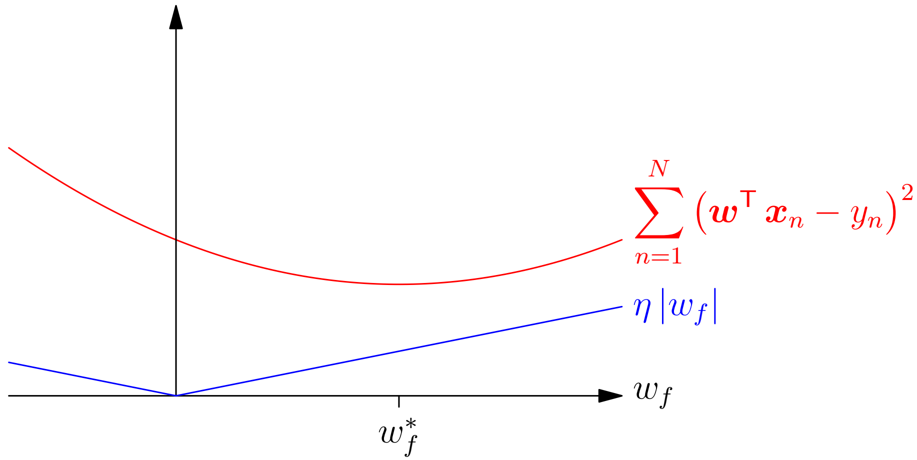

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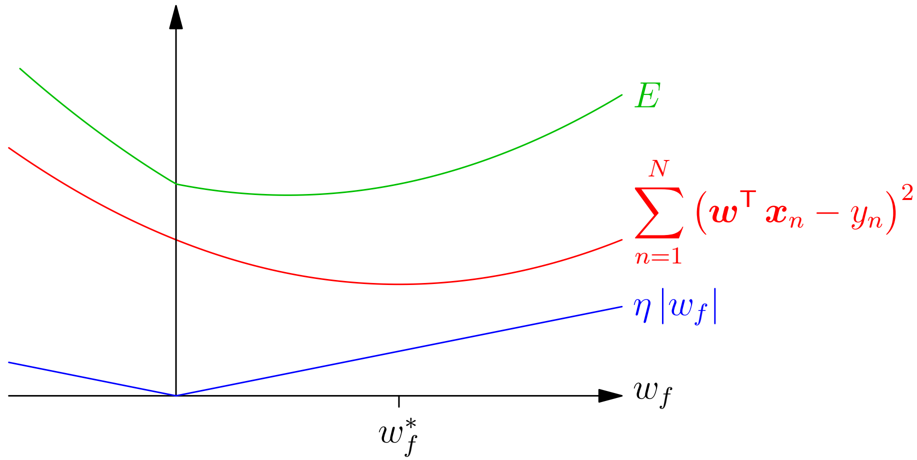

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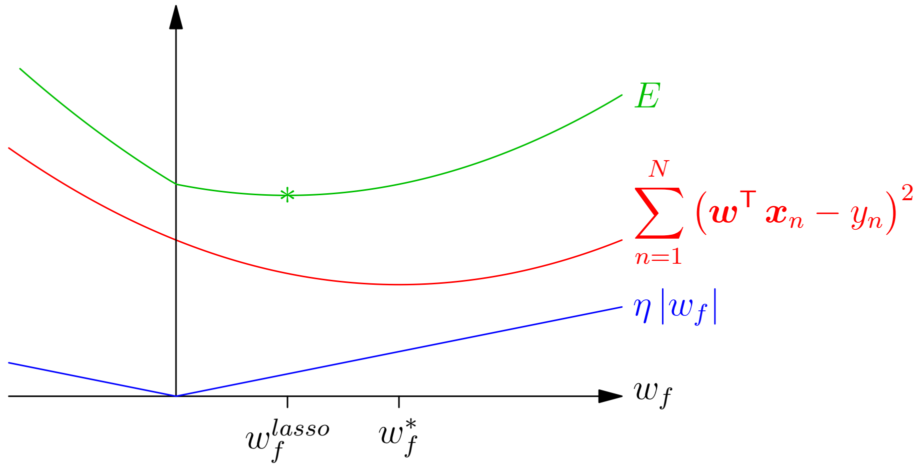

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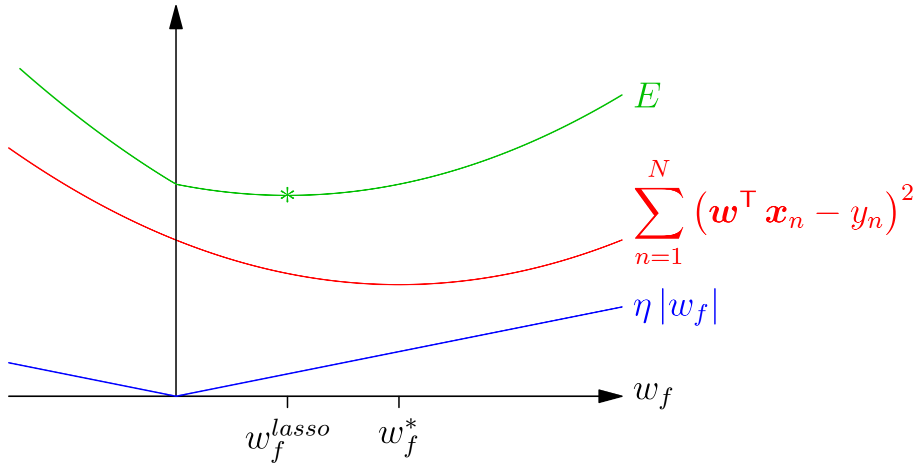

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- In the last two examples we added an explicit regularisation term that made the function we learnt simpler
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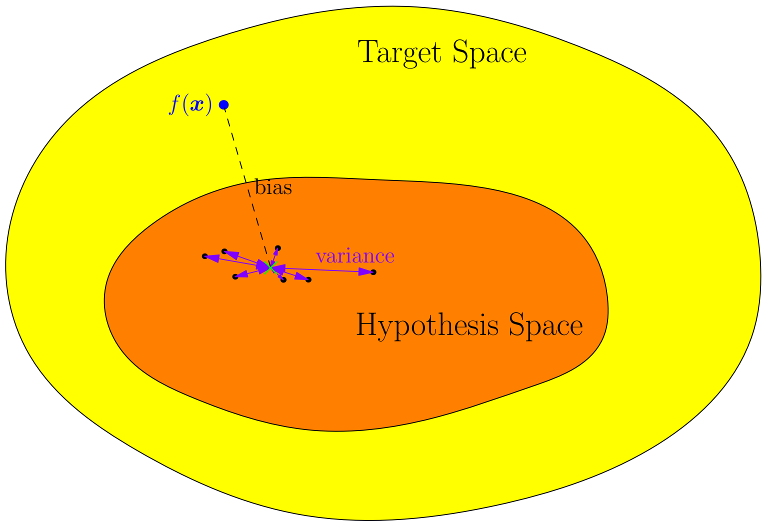
Outline

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



Support Vector Machines

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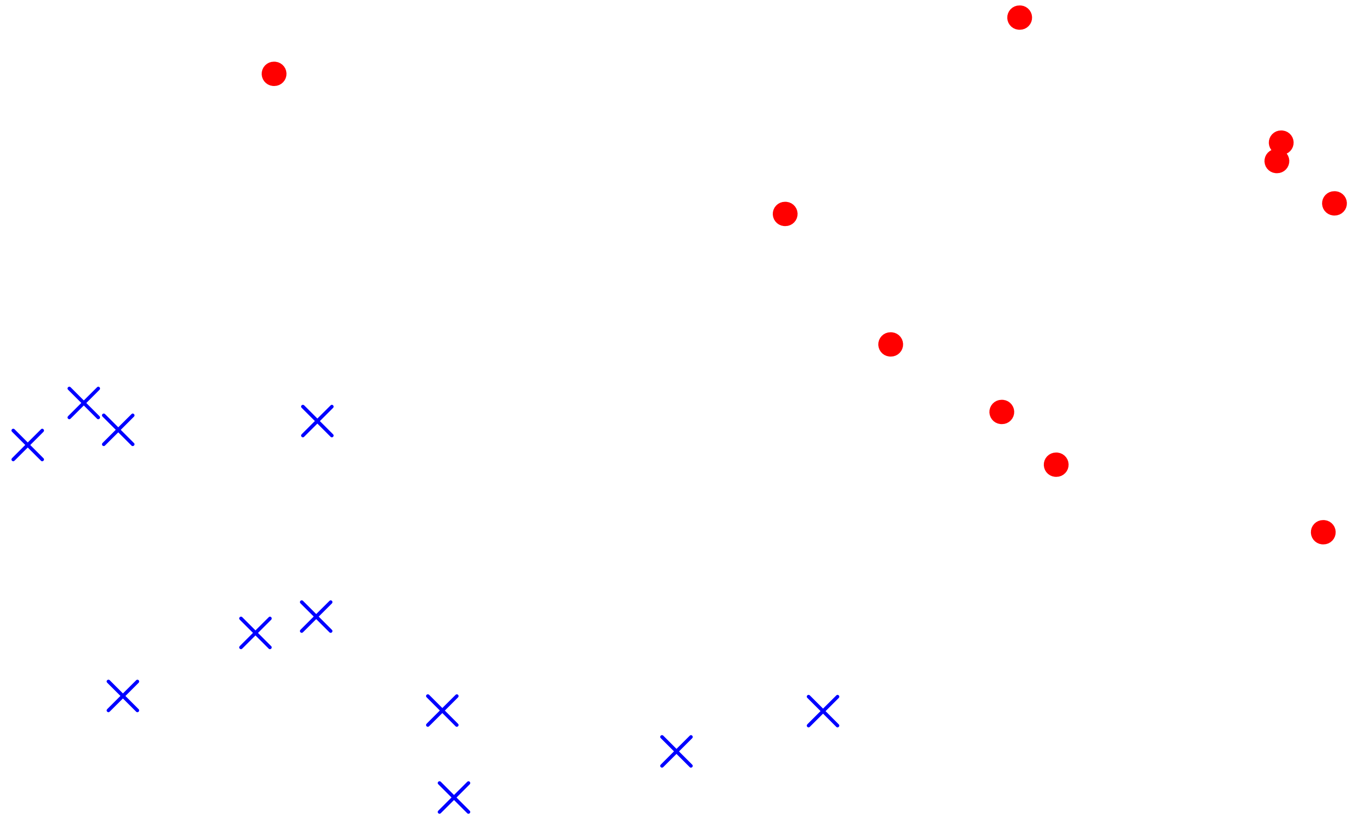
Linear Separation of Data

- SVMs classify linearly separable data



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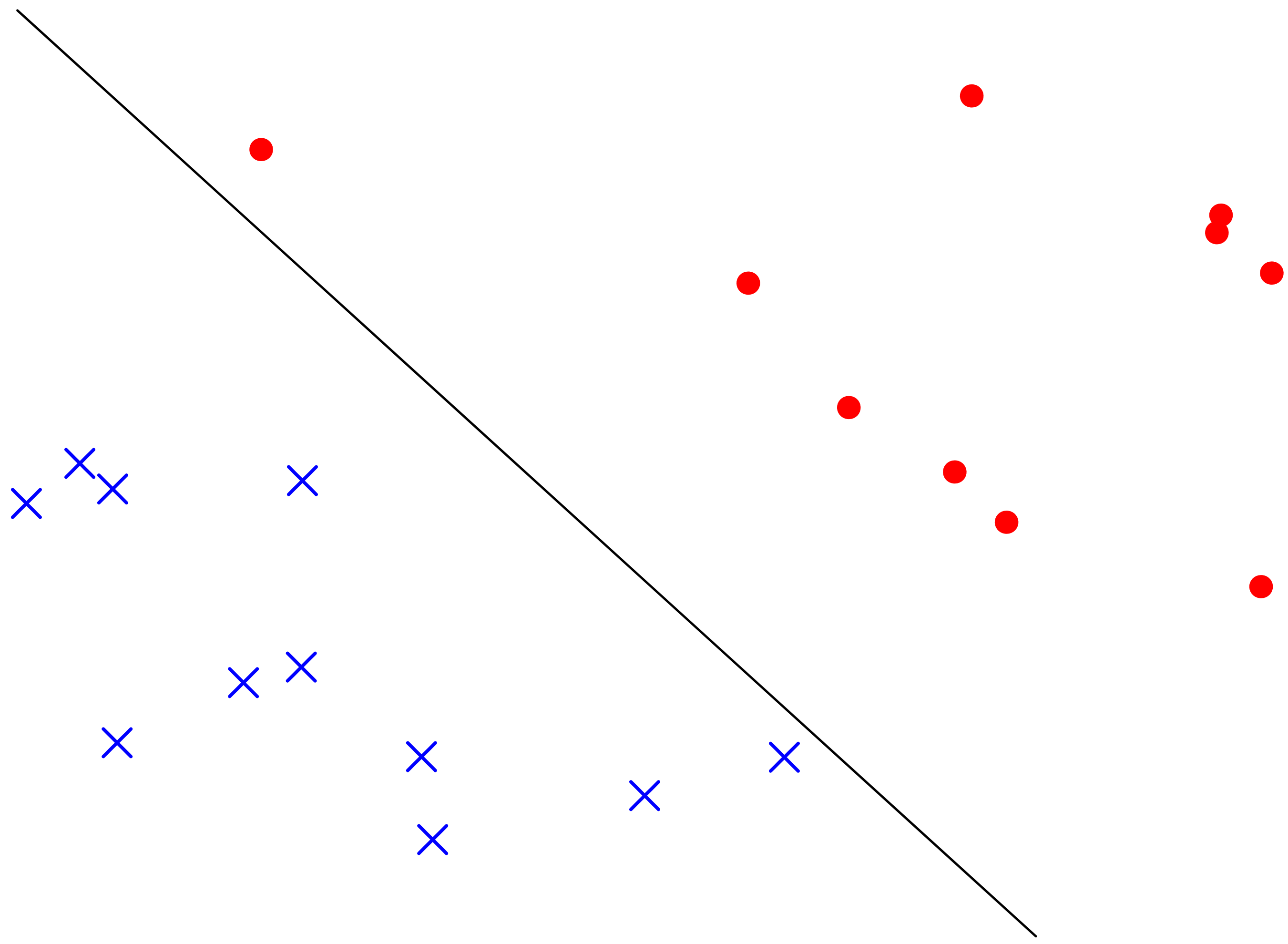

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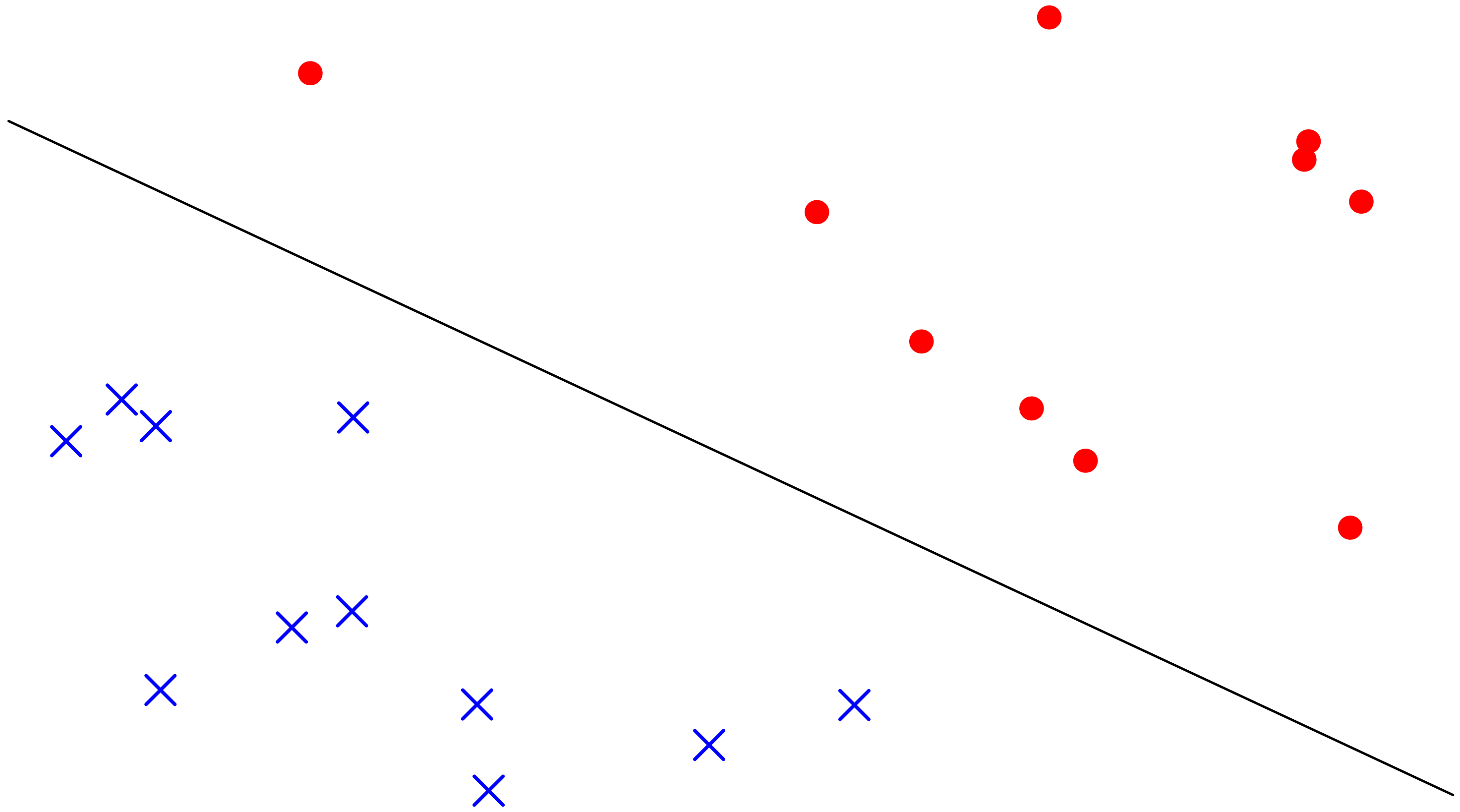

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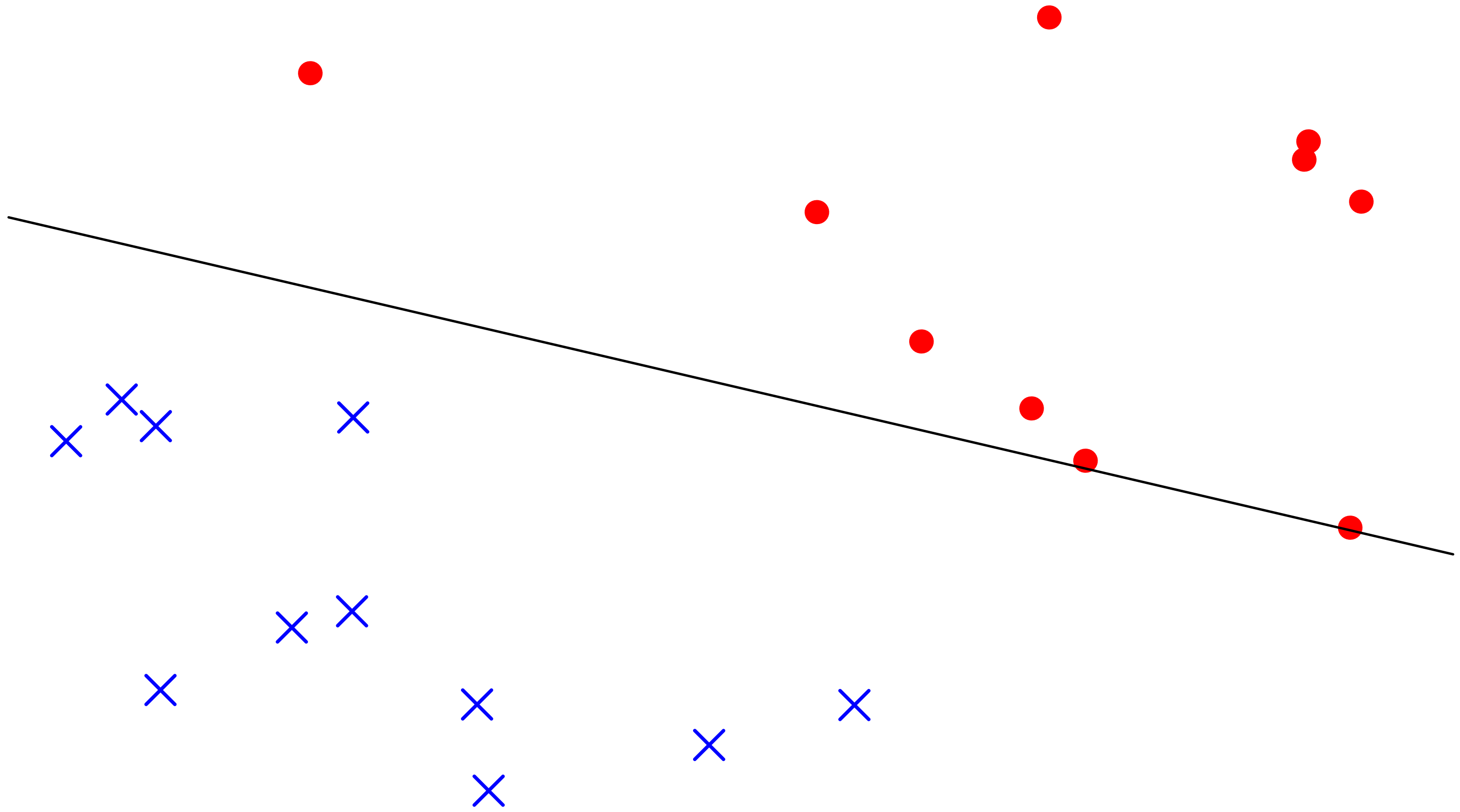

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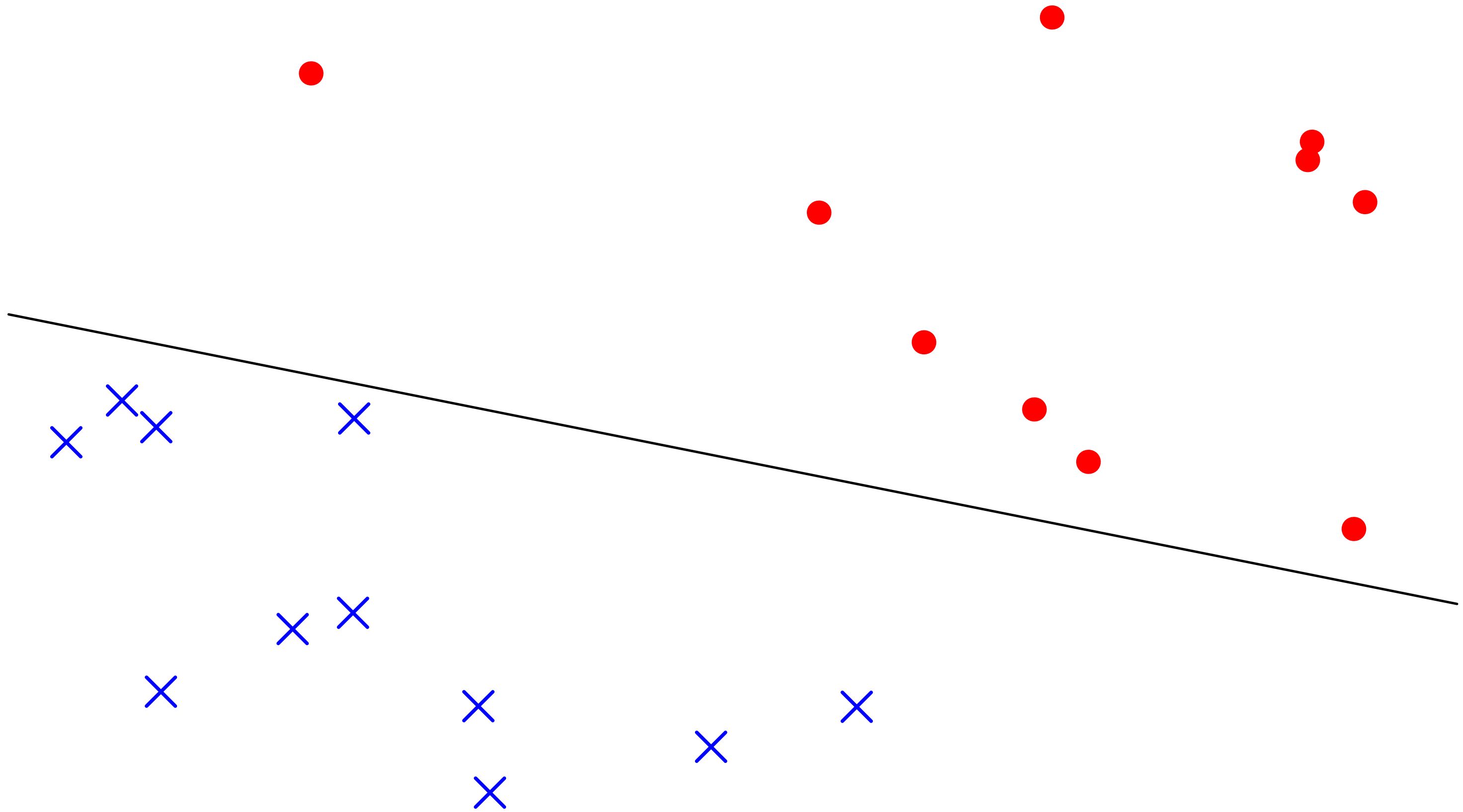

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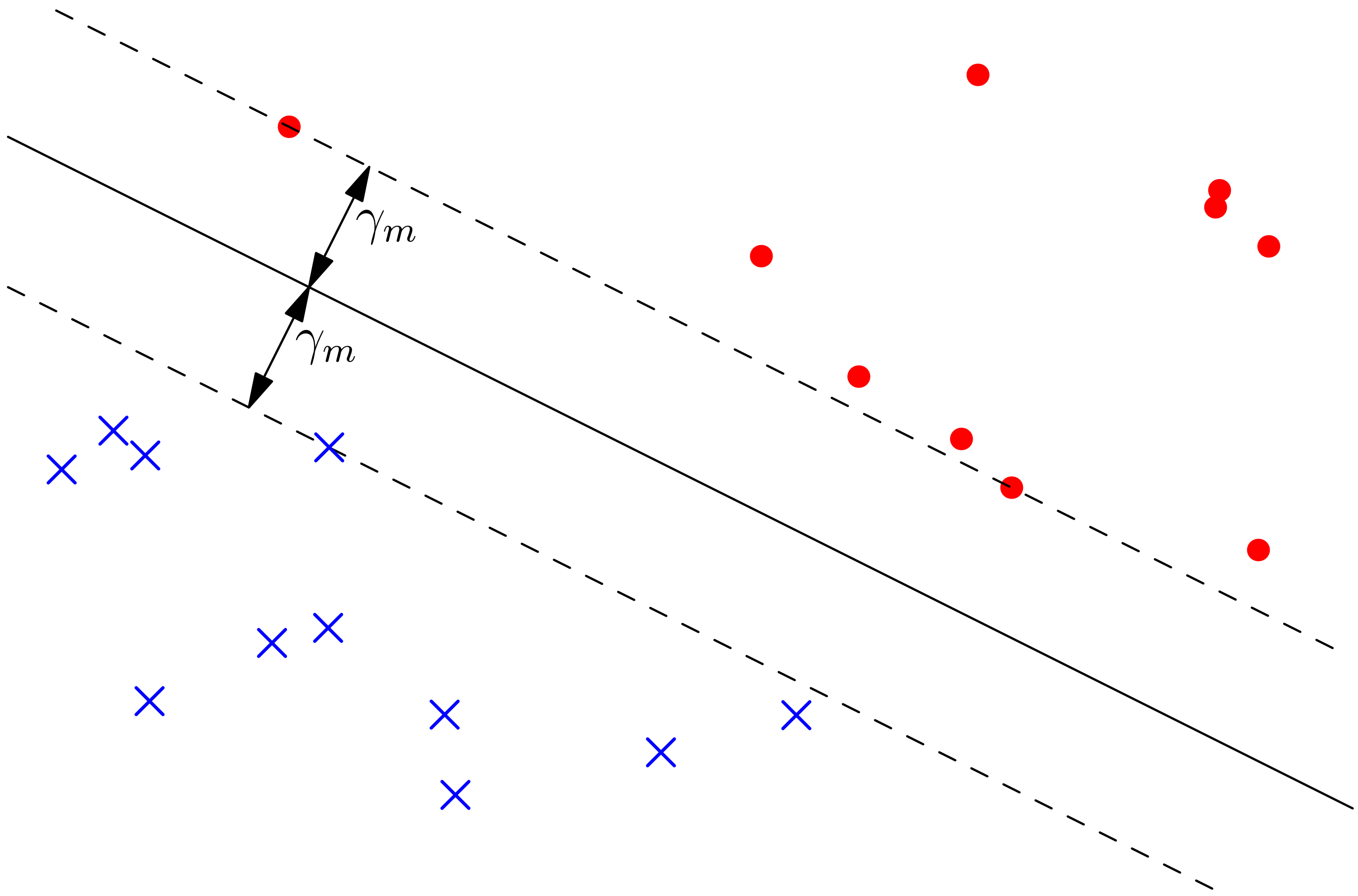

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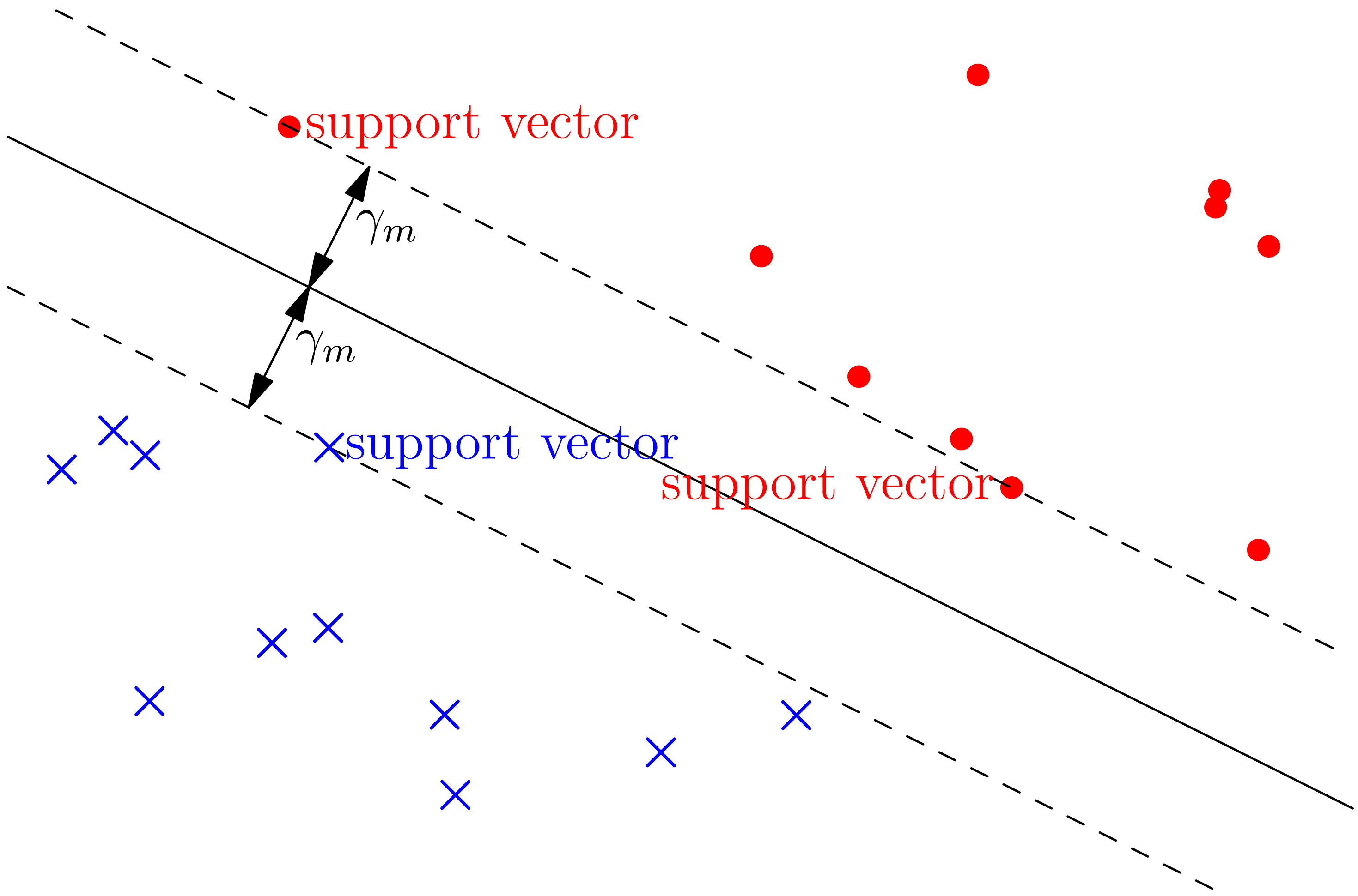

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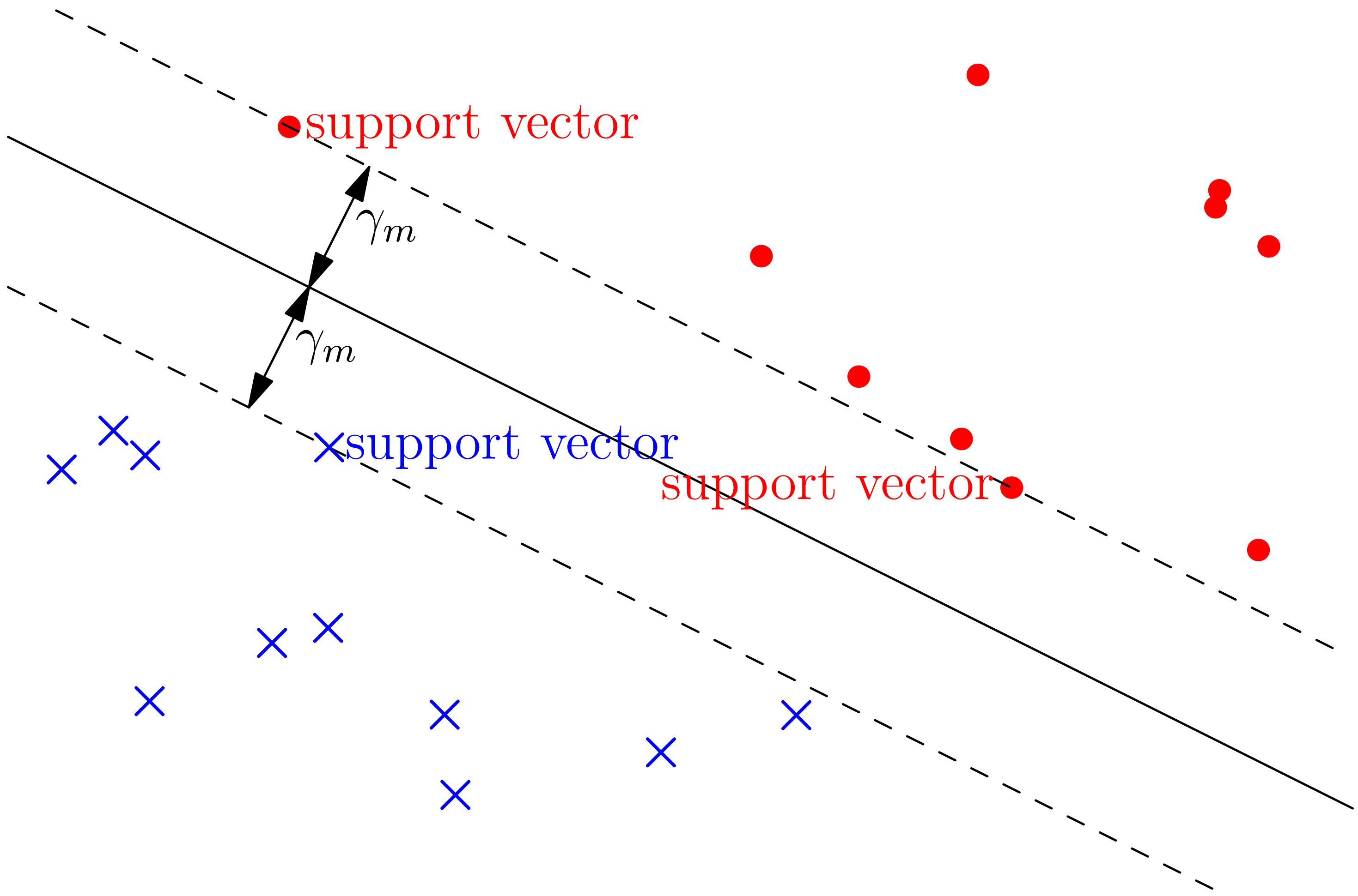

- Finds maximum-margin separating plane

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

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Kernel Functions

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

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

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

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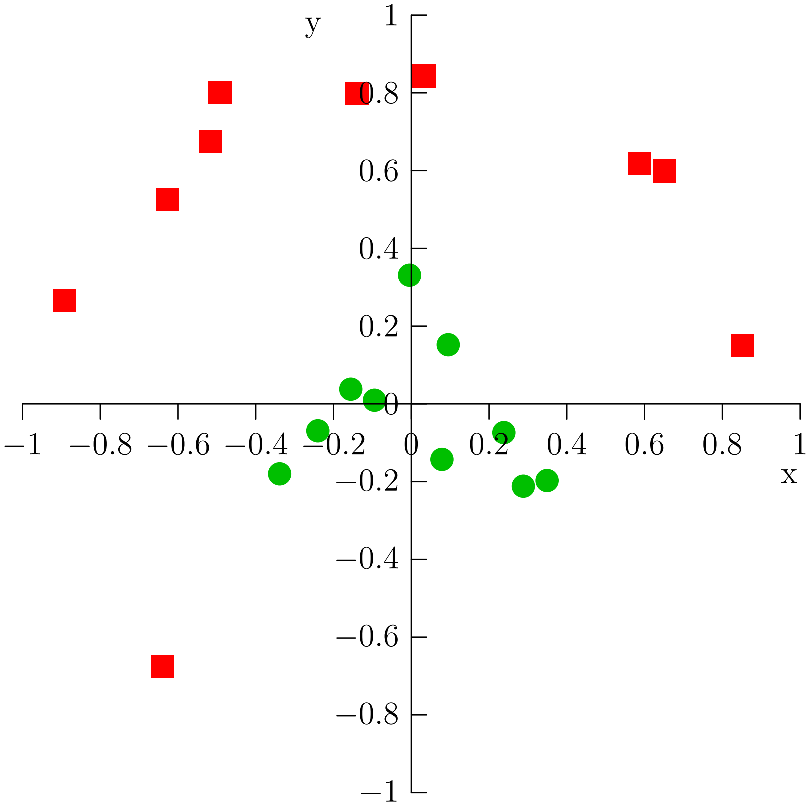

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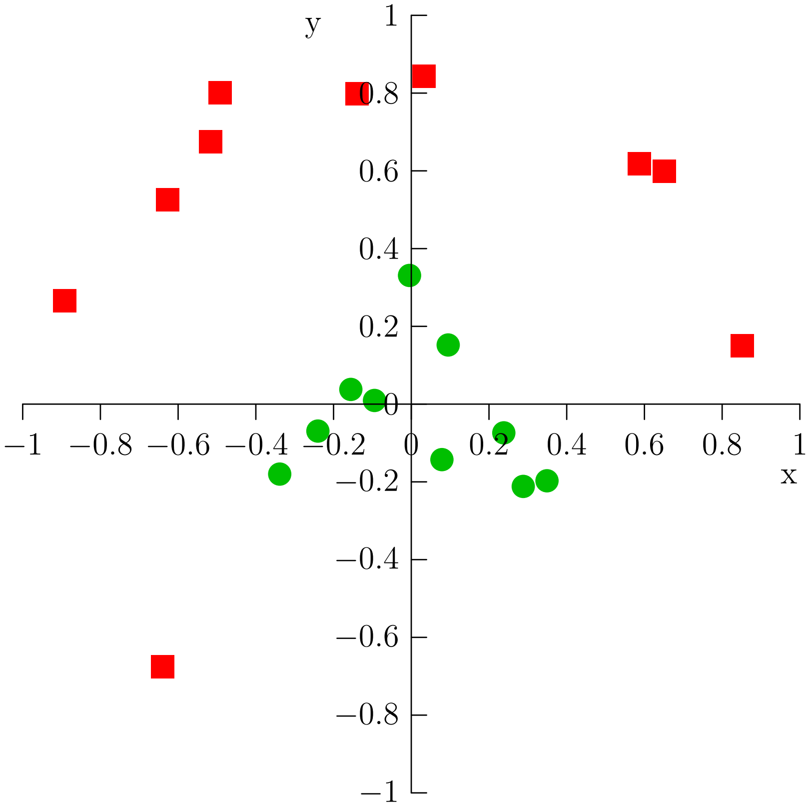

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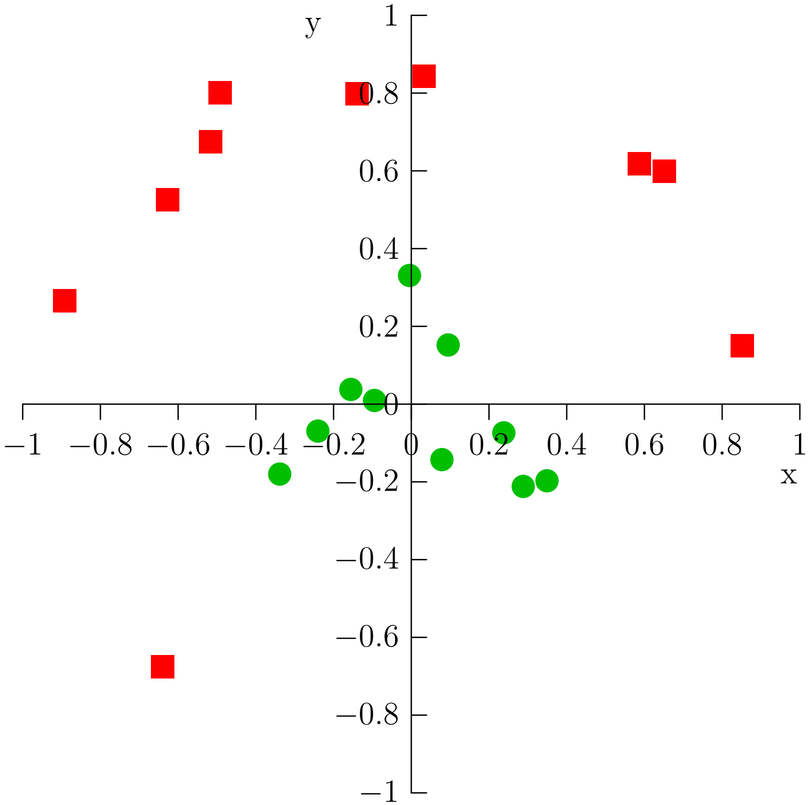

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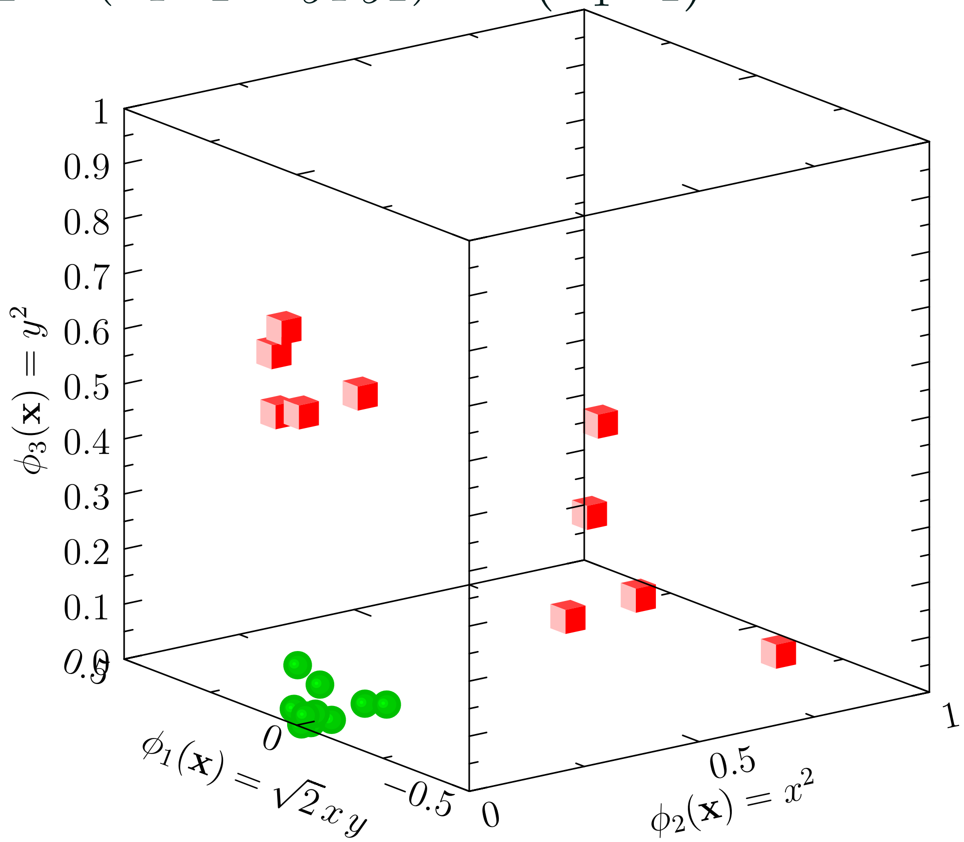

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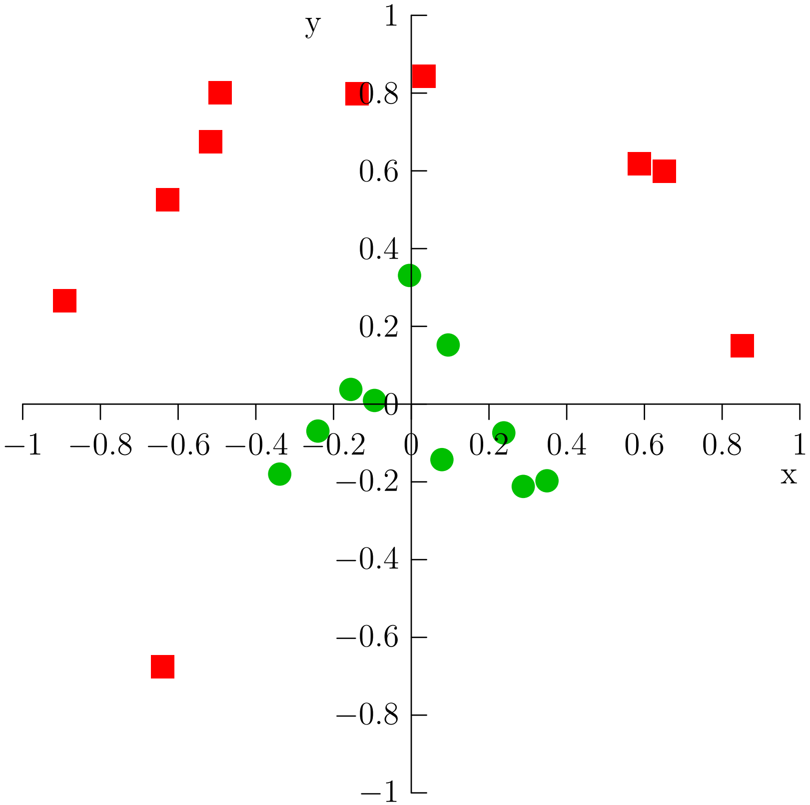

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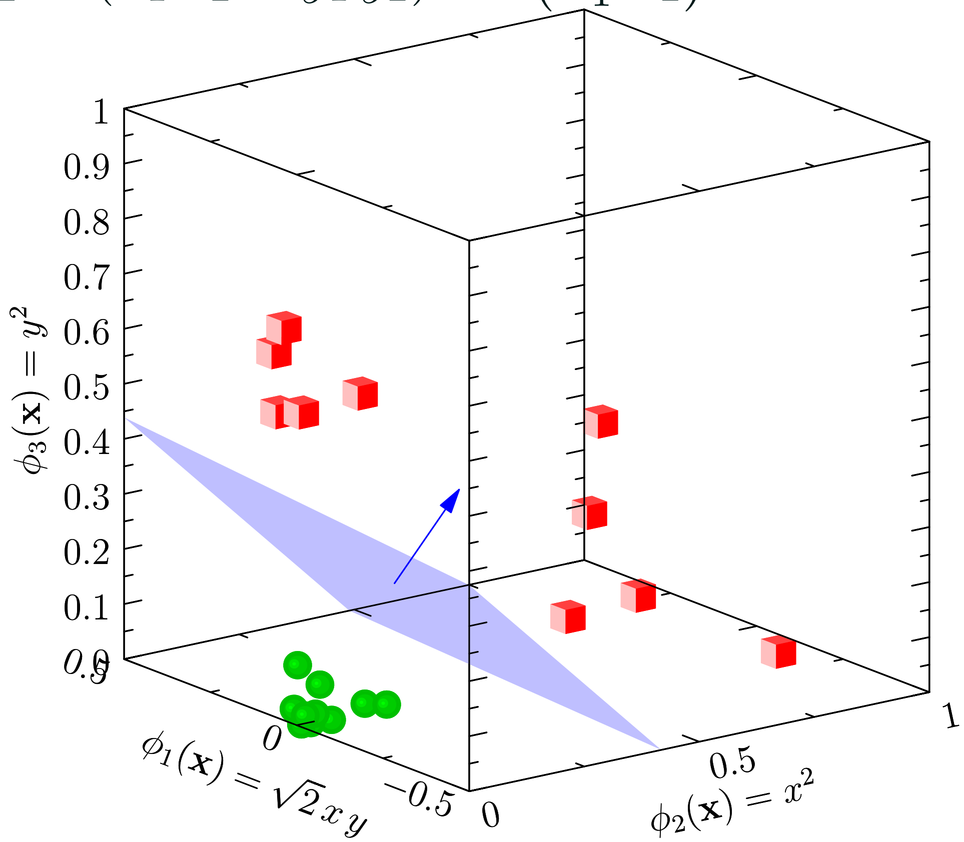

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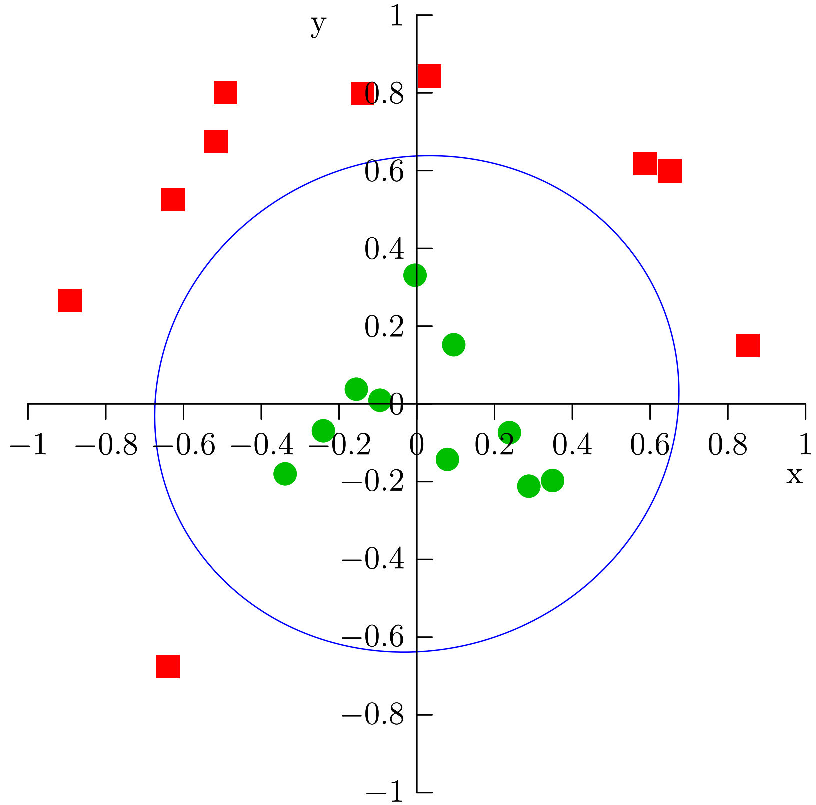

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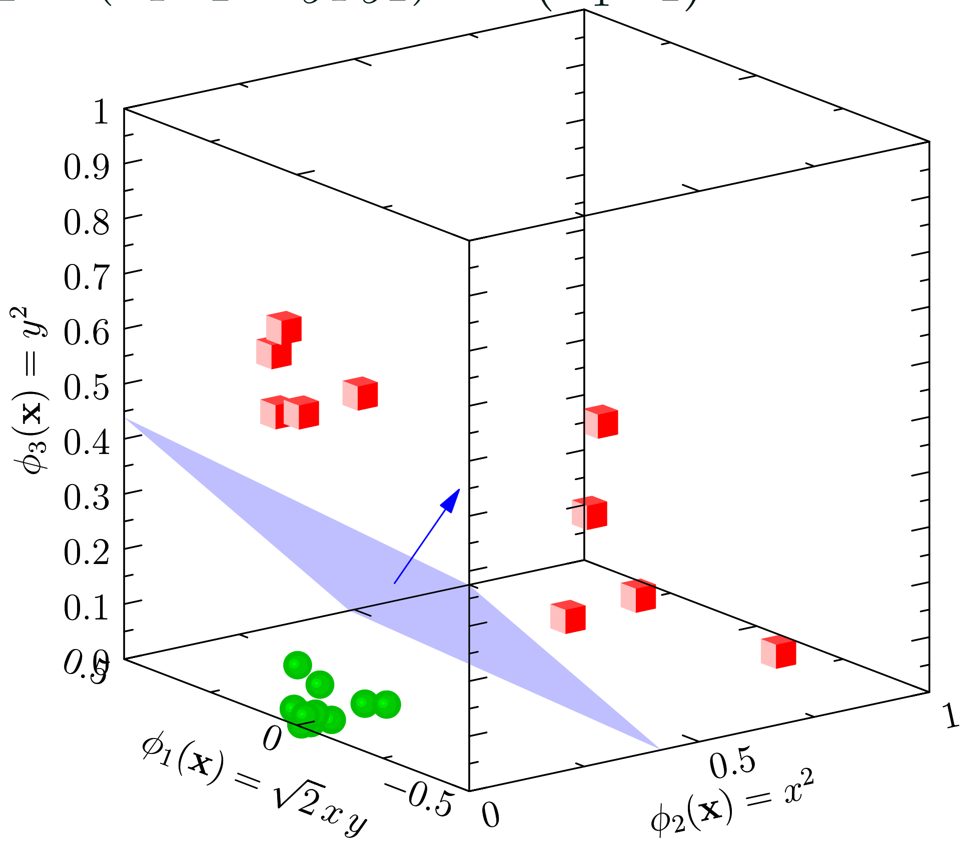

Computing the Maximum-Margin Hyper-plane

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

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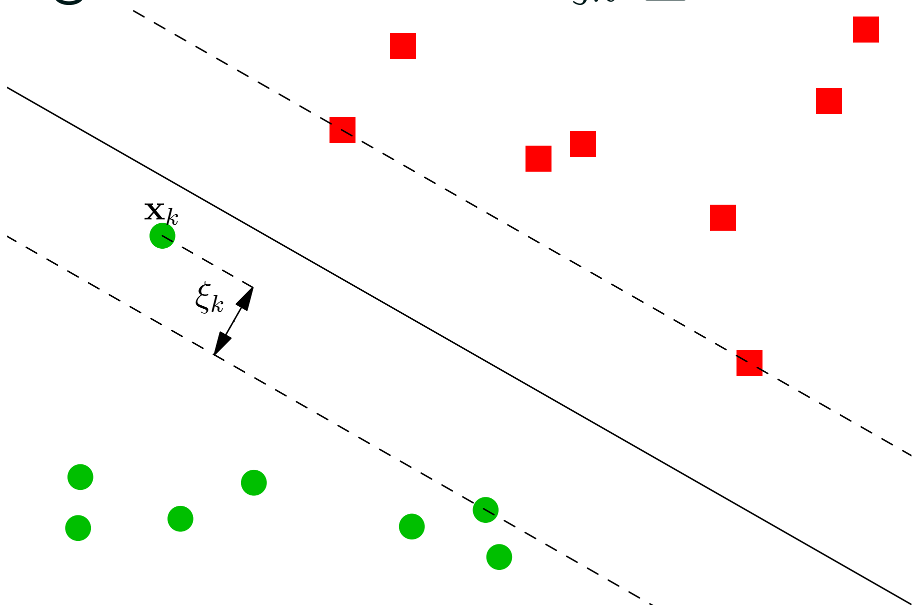
- Sometimes the margin constraint is too severe
- Relax constraints by introducing *slack variables*, $\xi_k \geq 0$

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



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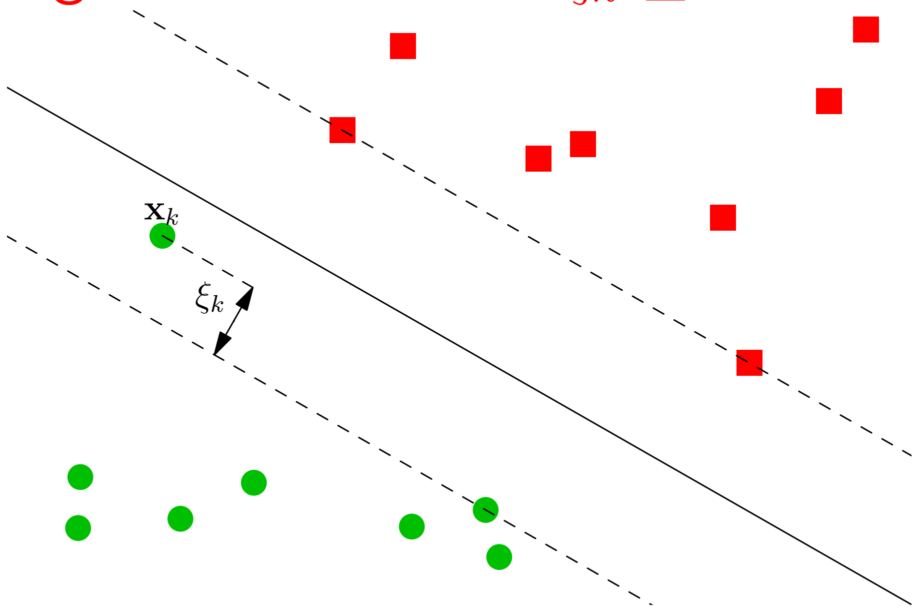

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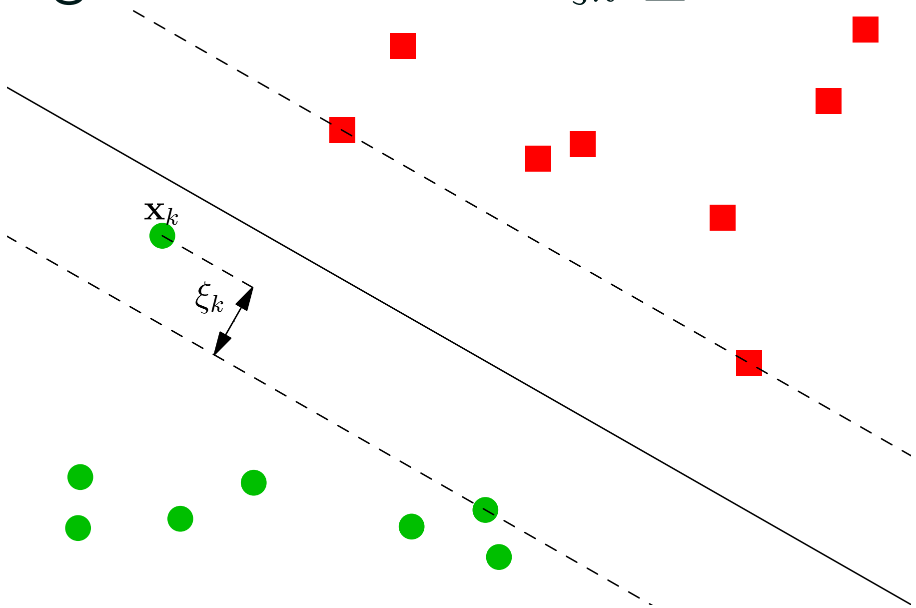

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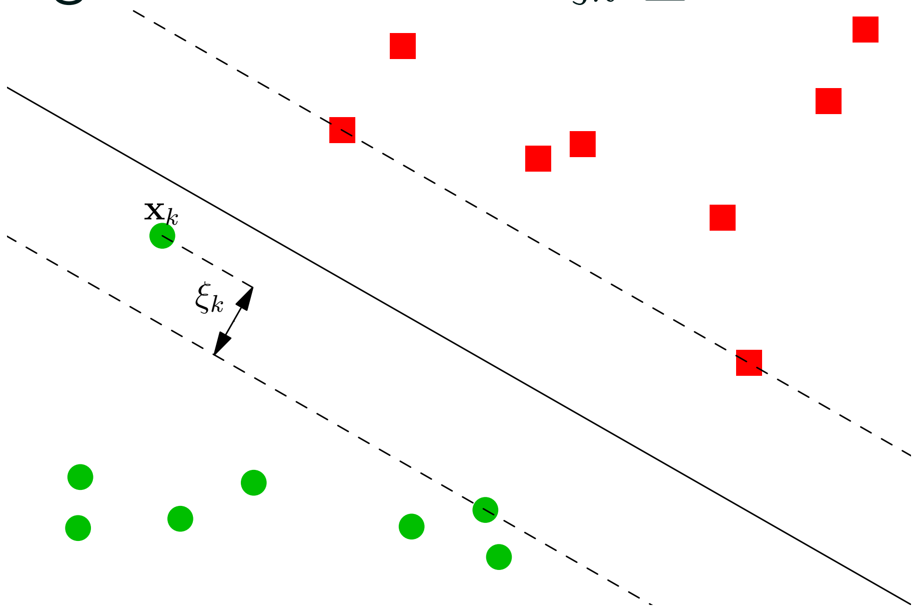

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Choosing the Right Kernel Function

- 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

$$K(\boldsymbol{x}, \boldsymbol{y}) = \mathrm{e}^{-\gamma \|\boldsymbol{x}-\boldsymbol{y}\|^2}$$

- Optimal γ values range over 2^{-15}–2^{3}

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SVM Libraries

- Although SVMs have unique solutions, they require very well written optimisers
- If you have a large data set they can be very slow
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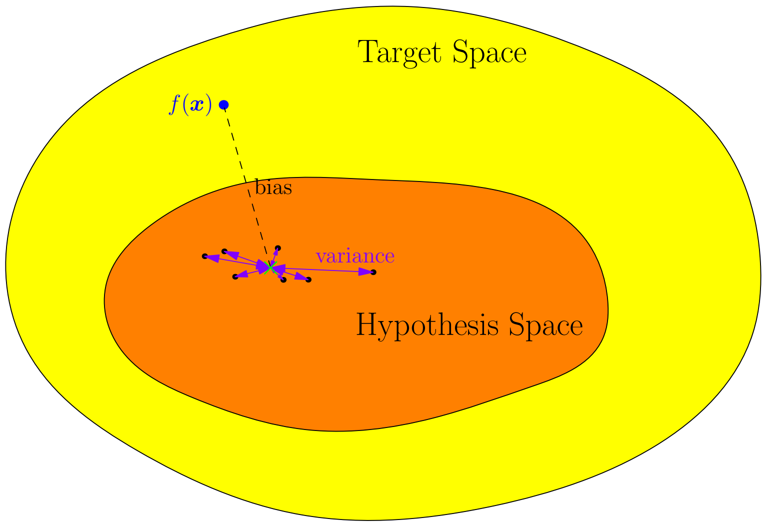
Outline

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

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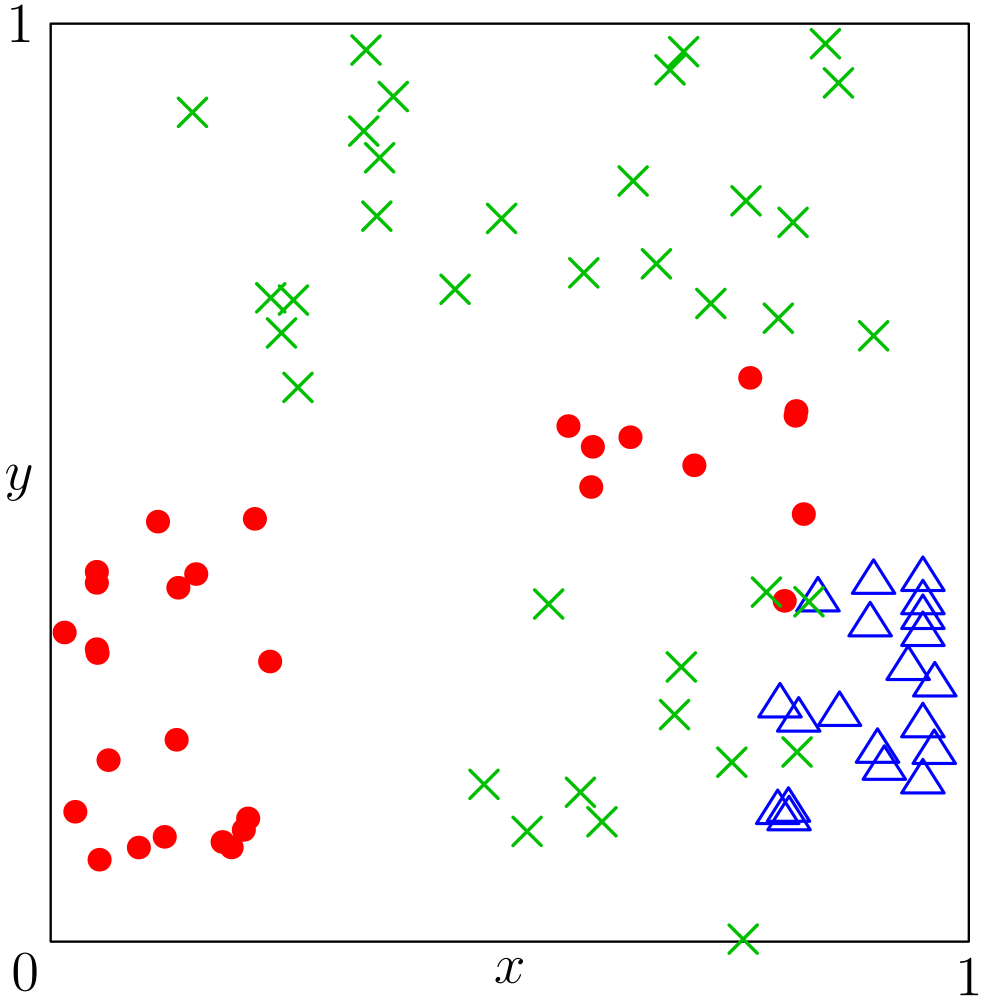

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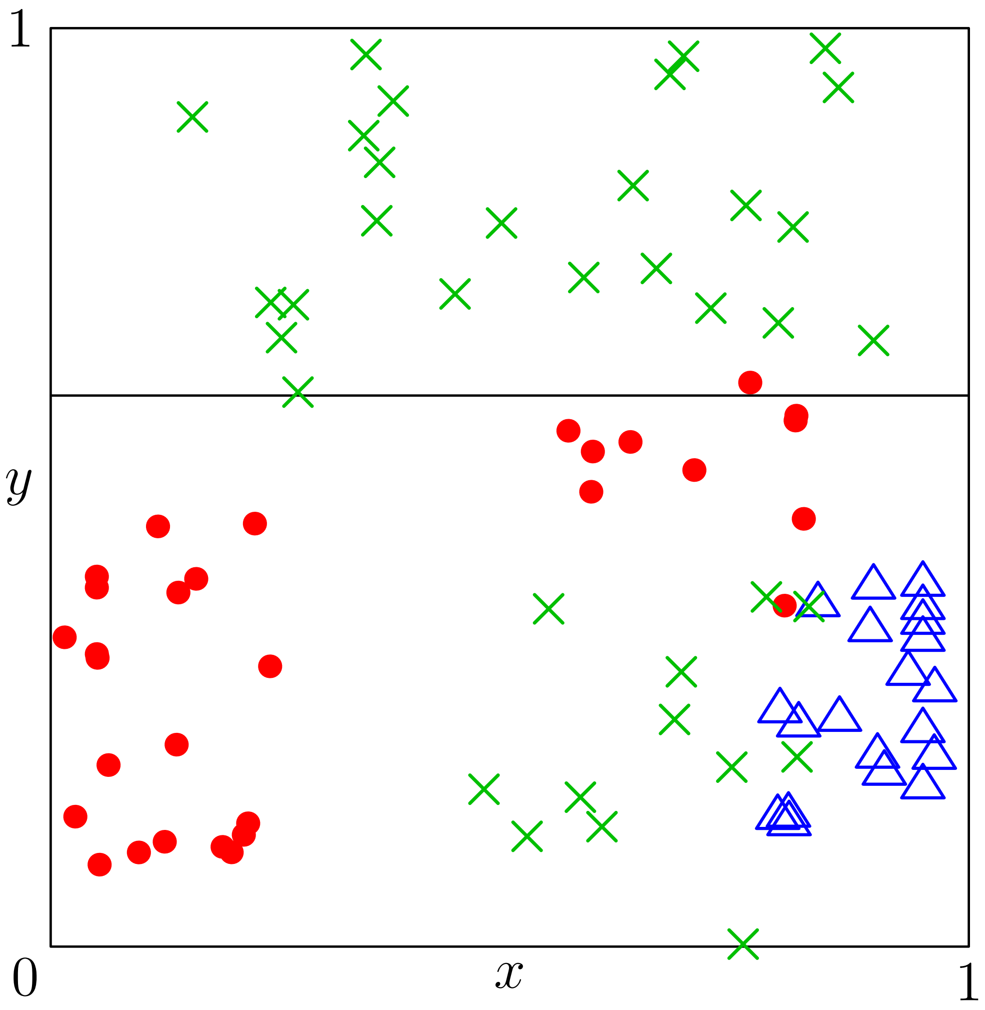

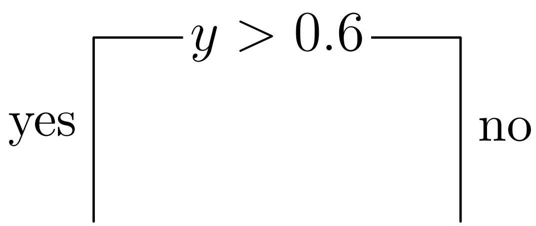

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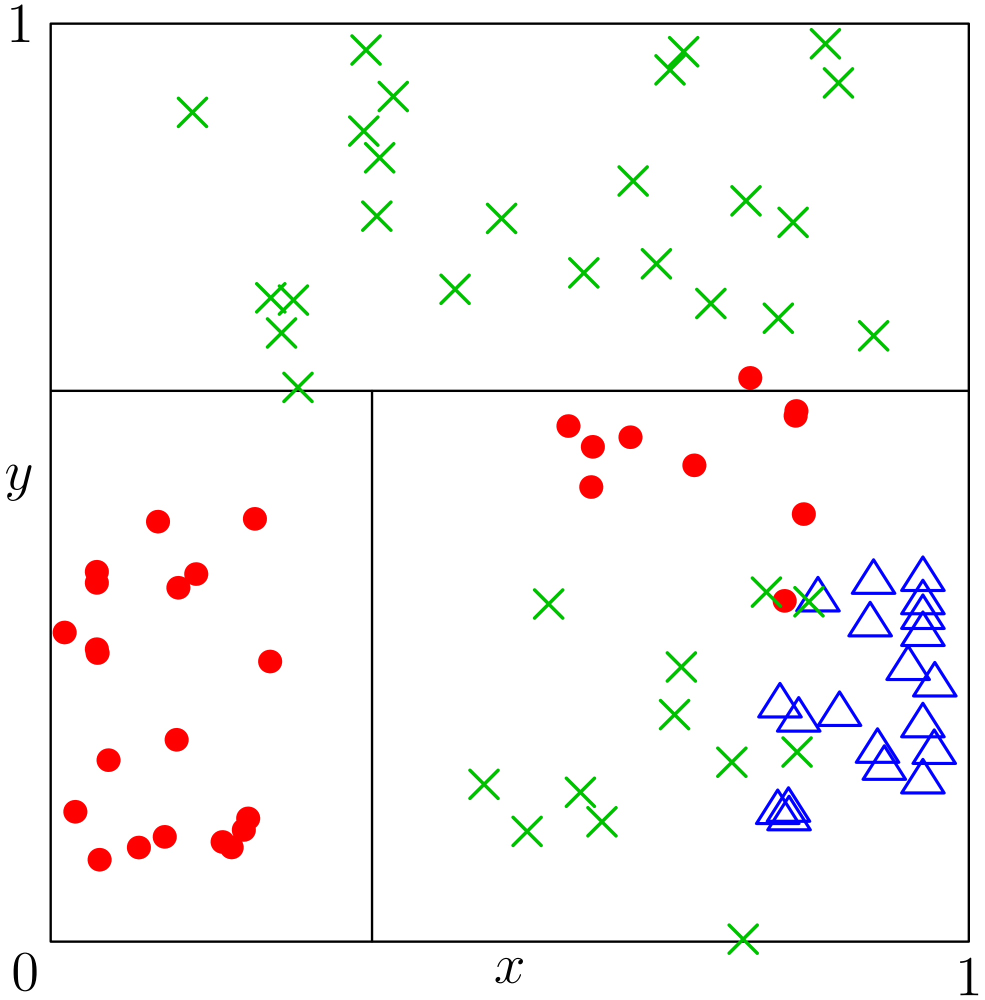

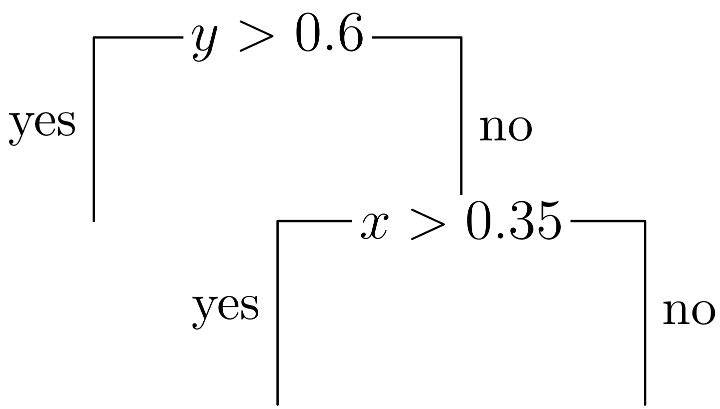

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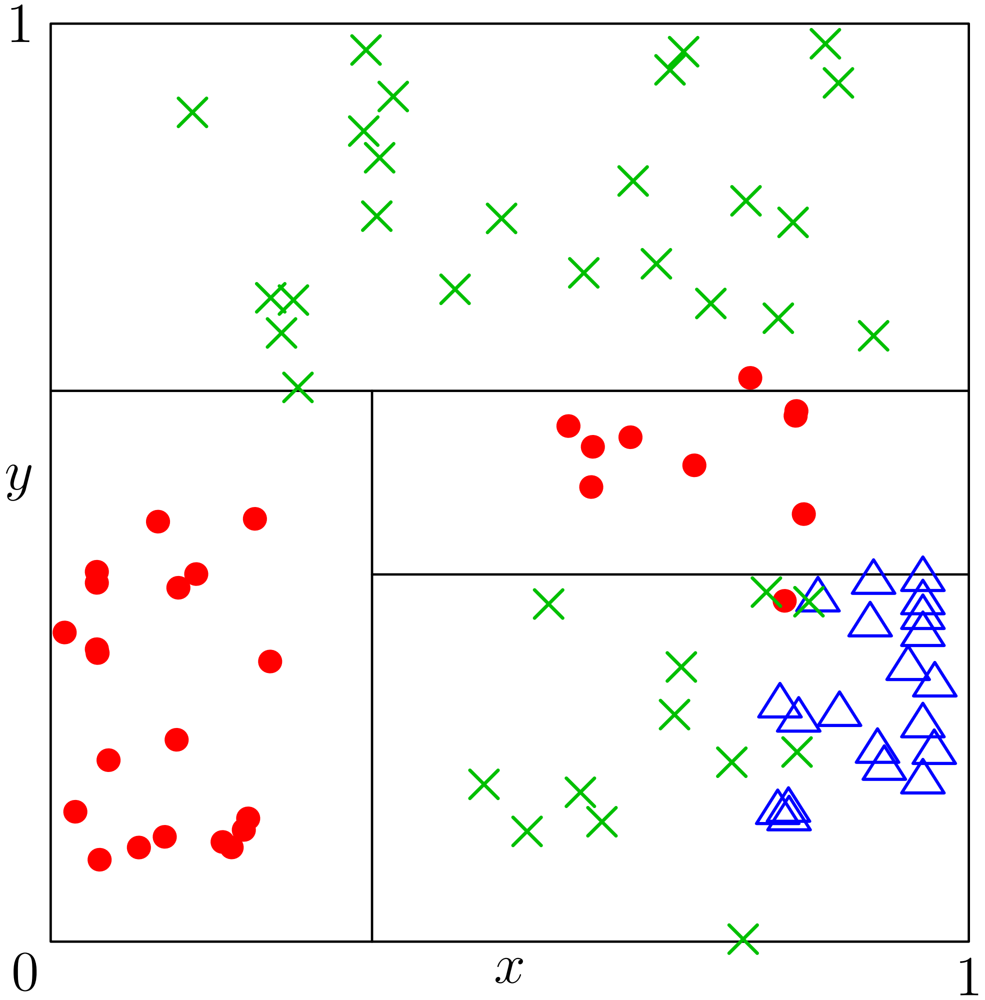

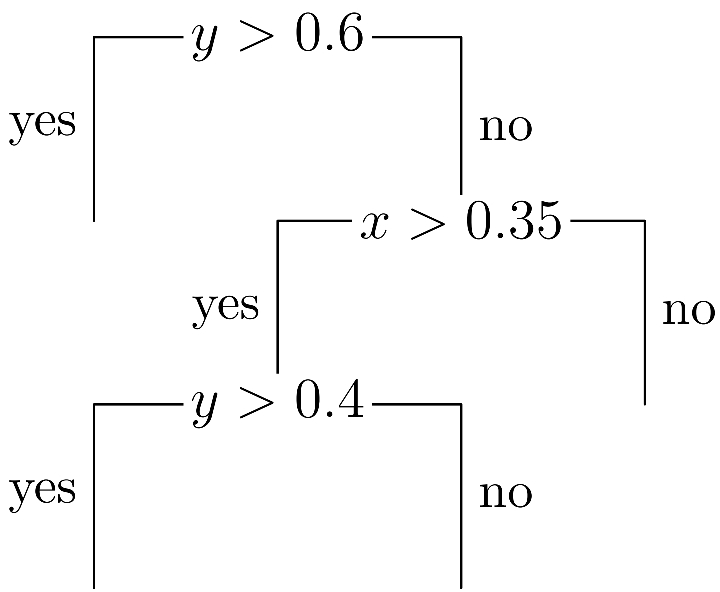

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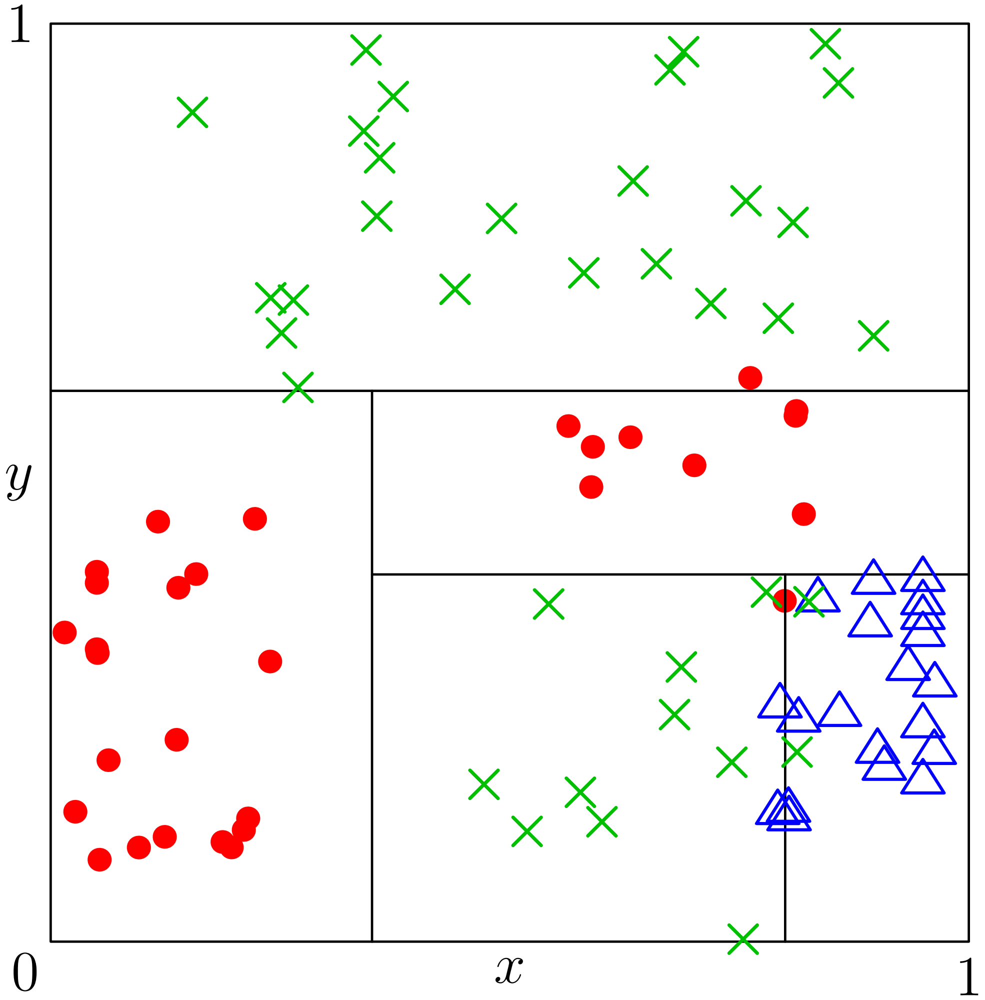

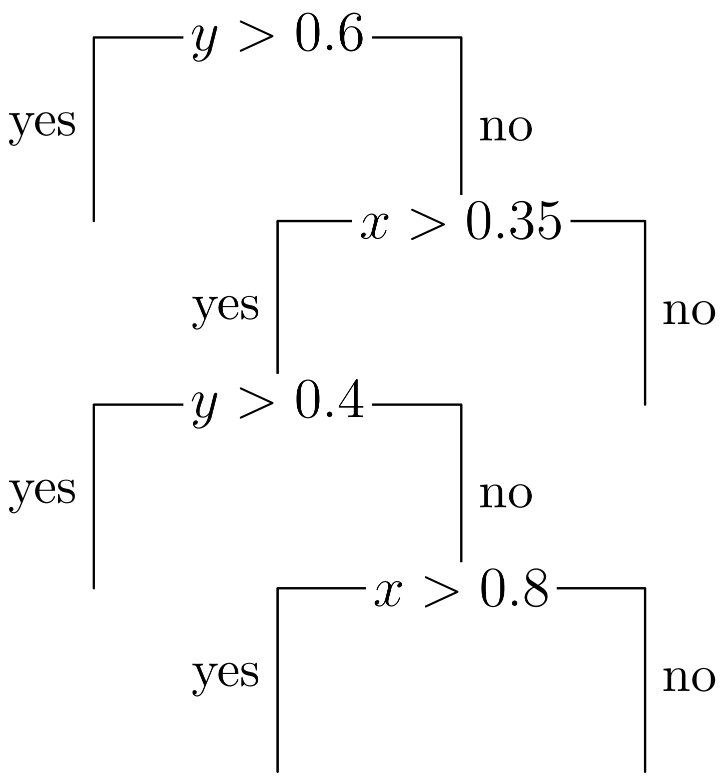

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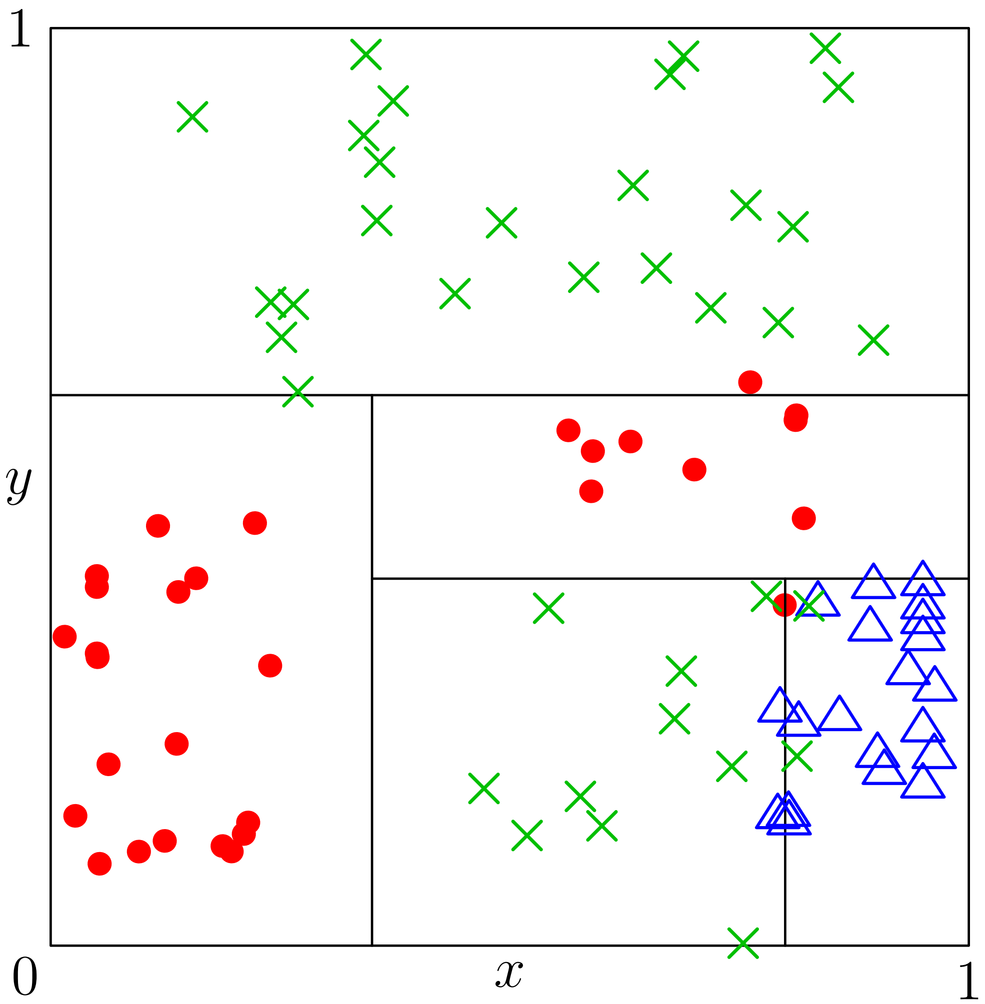

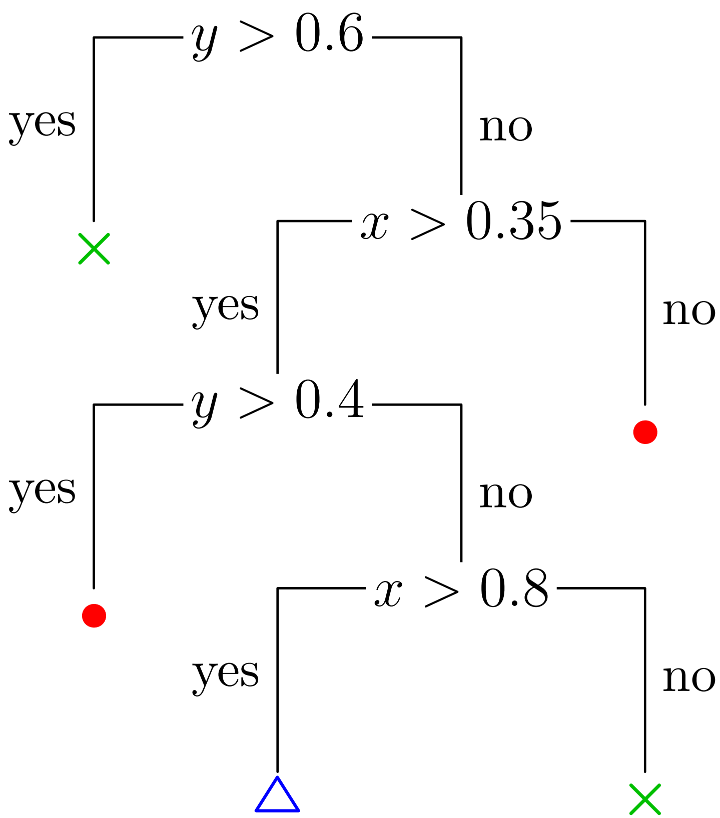

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- In order to average machine they must learn something different

- We only have one data set, but we can resample from the data set to make them look a bit different—this is known a **bootstrapping**

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- In boosting we make a **strong learner** by using a weighted sum of **weak learners**

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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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  - ⋆ adaboost
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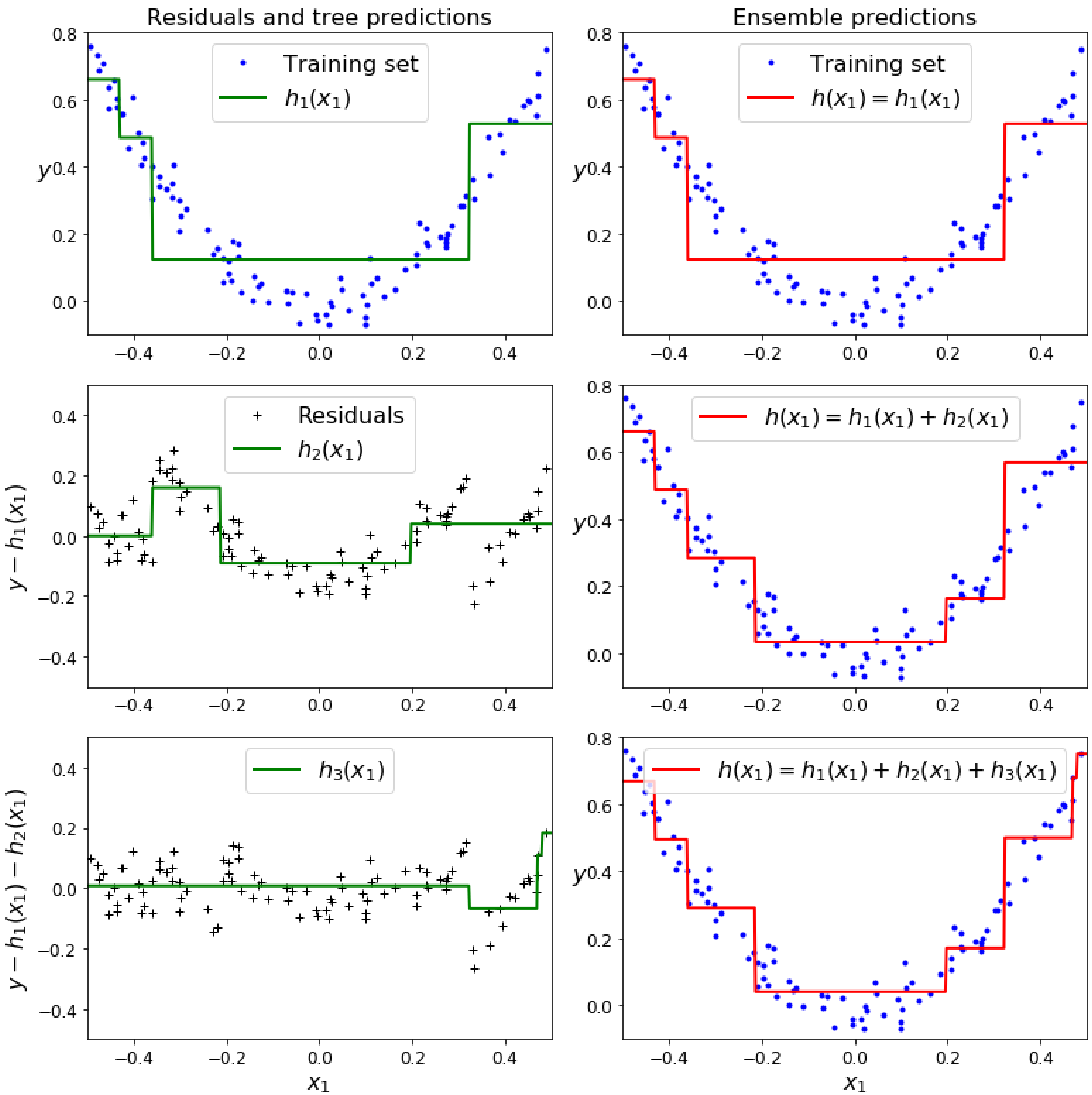

Residuals and tree predictions
Ensemble predictions
Training set
$h_1(x_1)$
$h(x_1) = h_1(x_1)$
Residuals
$h_2(x_1)$
$h(x_1) = h_1(x_1) + h_2(x_1)$
$h_3(x_1)$
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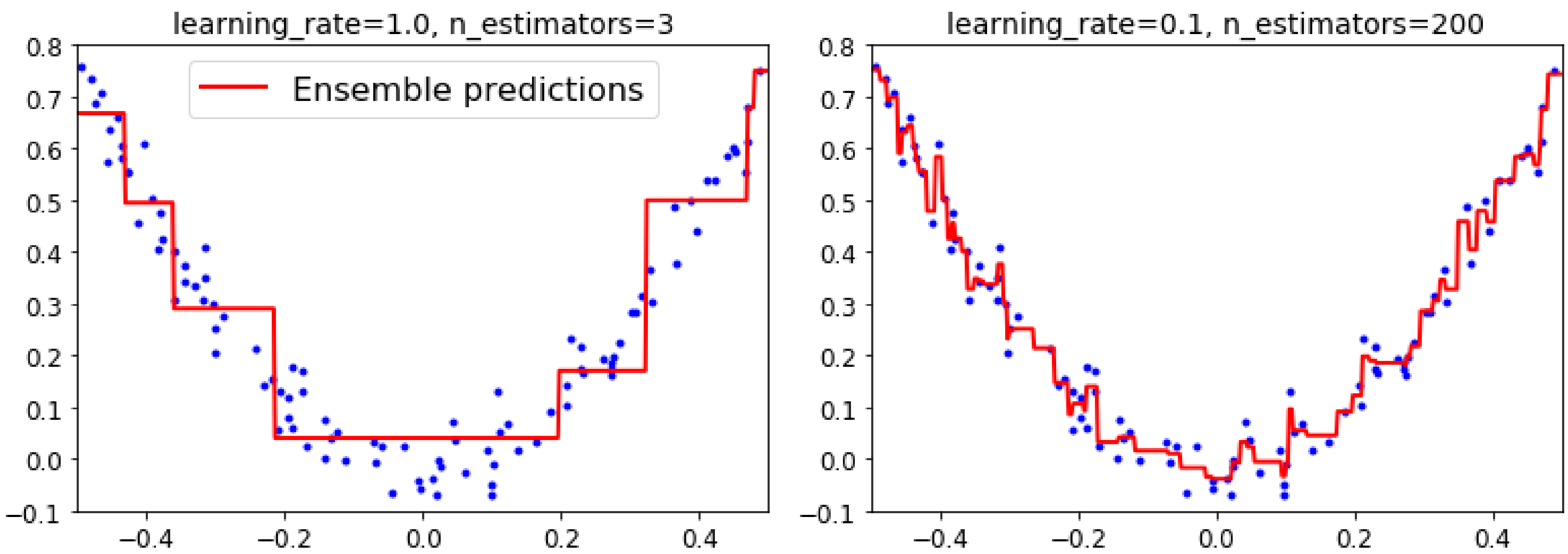
y
$y - h_1(x_1)$
$y - h_1(x_1) - h_2(x_1)$
x_1

Keep On Going

- We can keep on going



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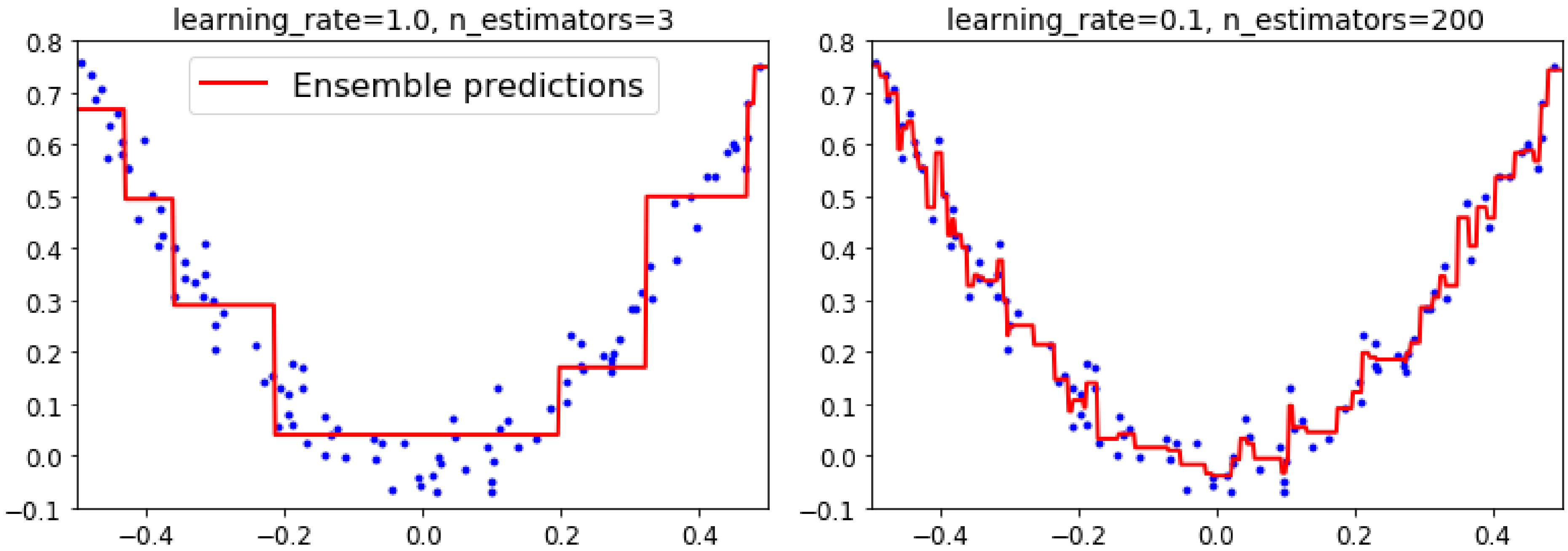

- But we will over-fit eventually

Early Stopping

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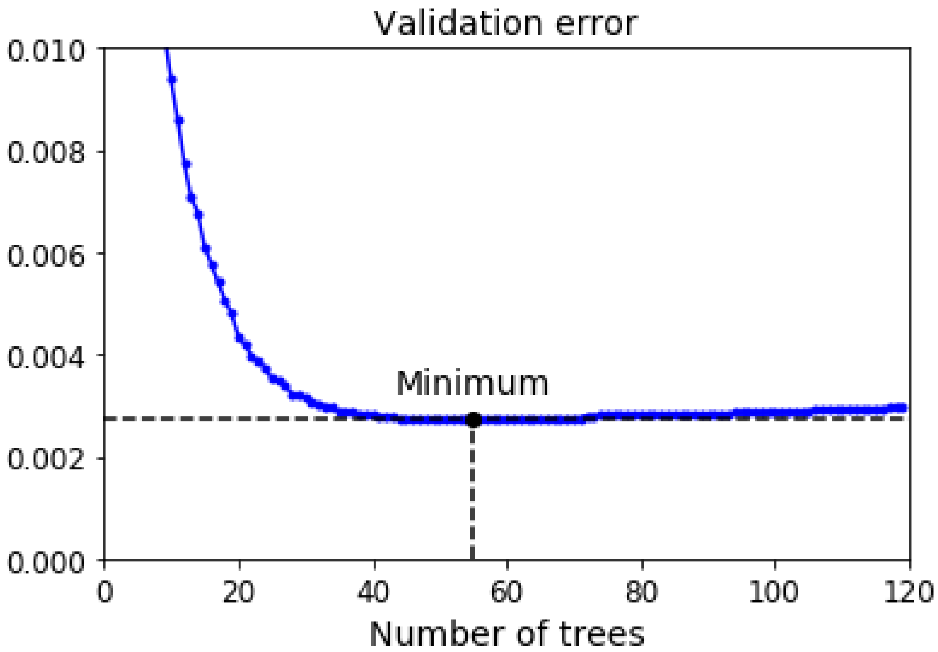

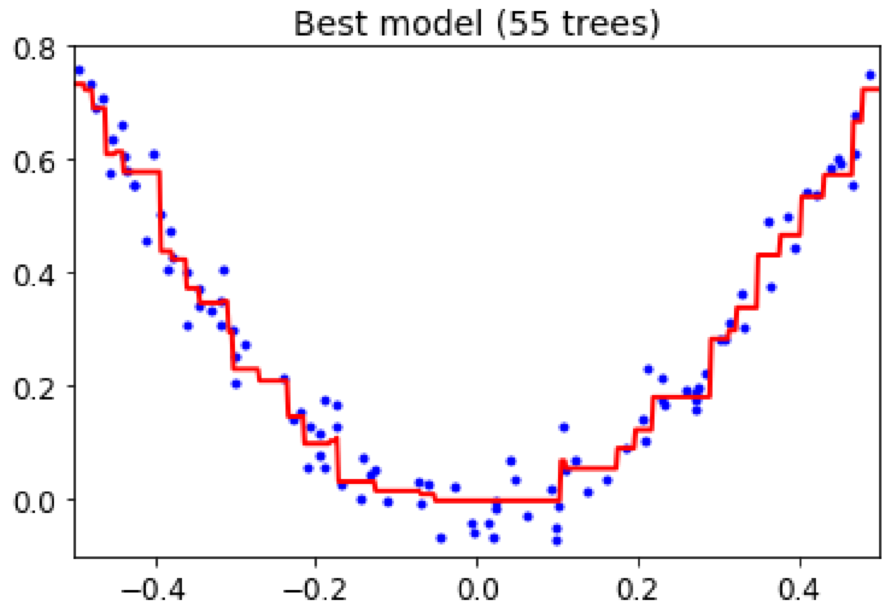

- Use cross-validation against a validation set to decide when to stop

Early Stopping

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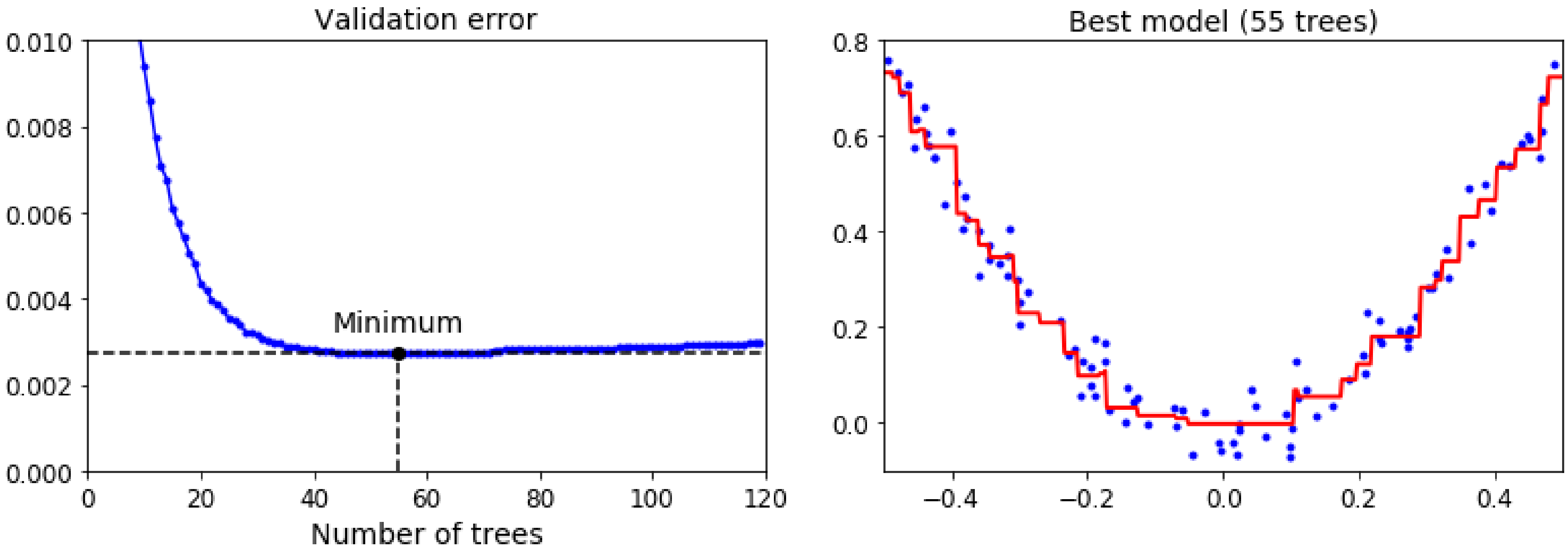

- Use cross-validation against a validation set to decide when to stop

XGBoost

- 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

- It is much faster than most gradient boosting algorithms and scales to billions of training data points

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- Finds a clever way to approximately minimise error plus regulariser very fast

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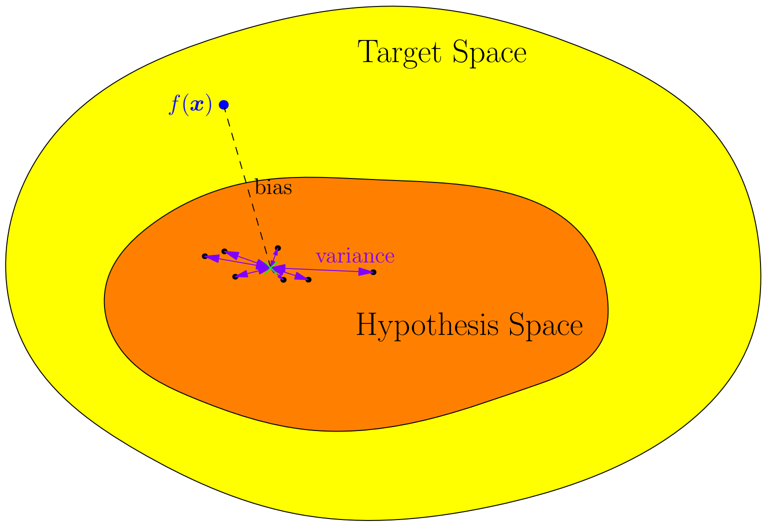
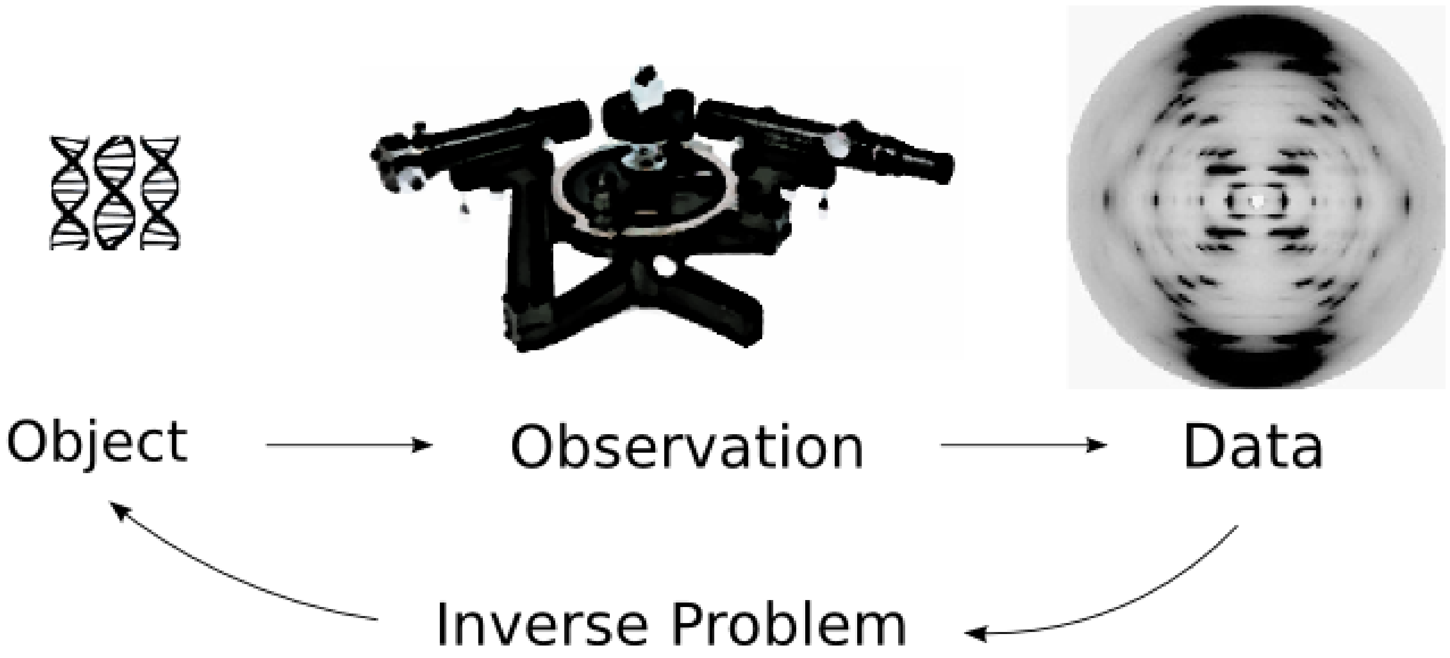
Outline

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



Inverse Problems



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

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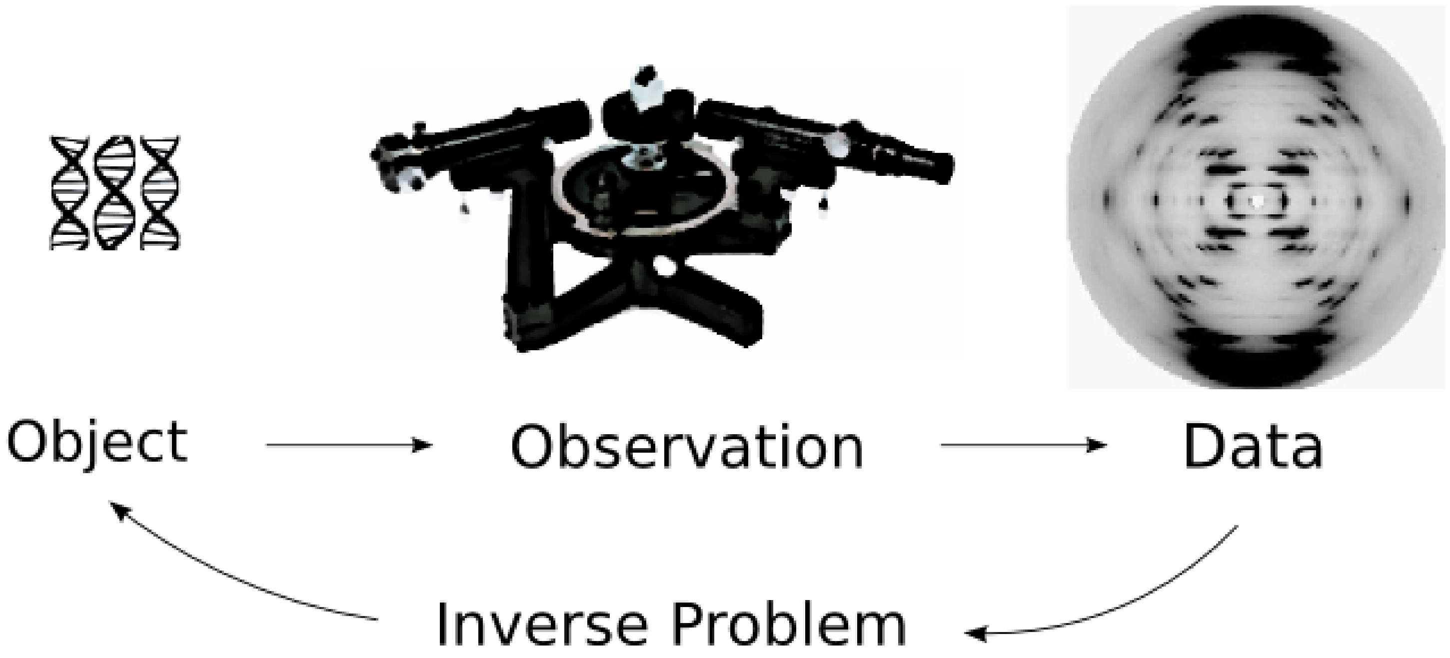

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Bayes' Rule

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

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

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

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

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- The denumerator is a normalisation constant

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Worlds

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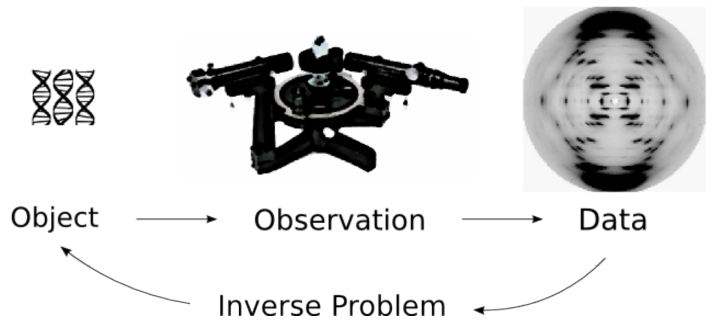
- It is relatively easy to model the likelihood (this is a forward process not an inverse process)



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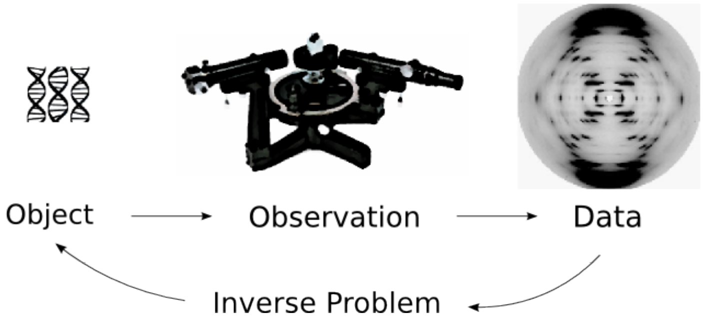

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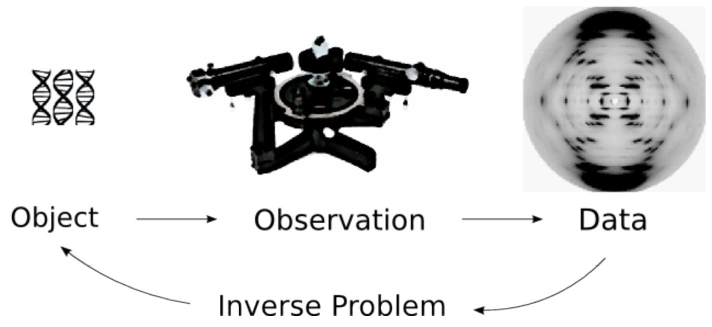

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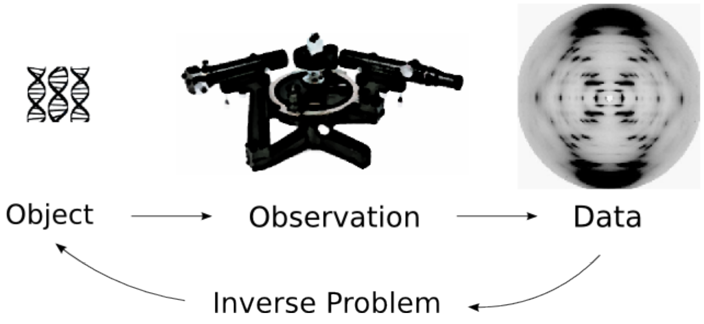

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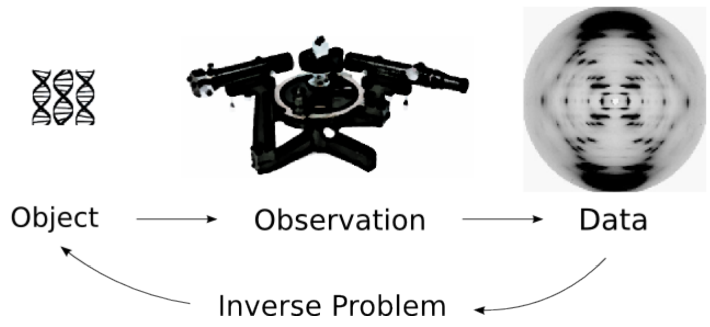

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Disadvantages of Bayesian Inference

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- This is technically challenging and/or computationally slow
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  - ⋆ There exist mature libraries
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Simple Bayes

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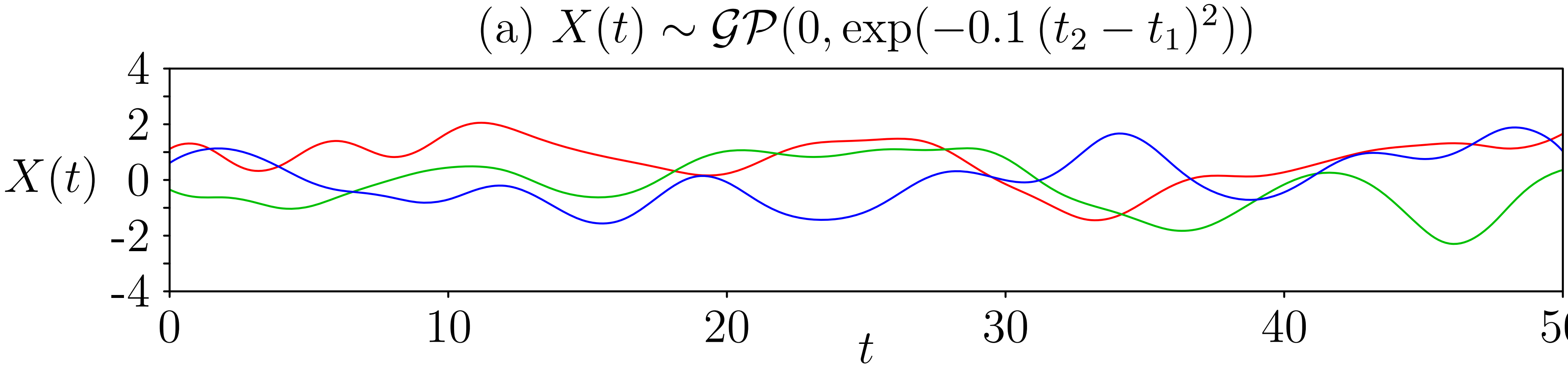
Gaussian Process Worlds



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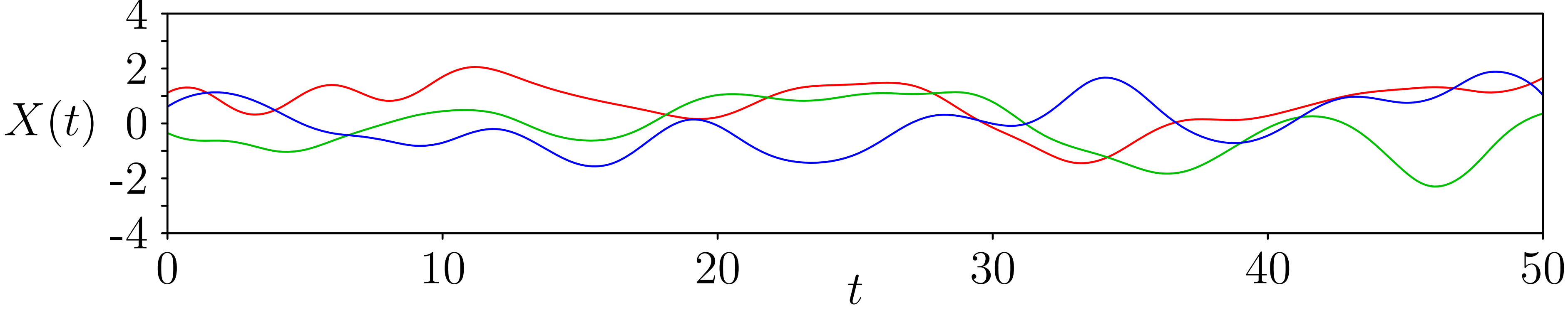
(a) $X(t) \sim \mathcal{GP}(0, \exp(-0.1\,(t_2 - t_1)^2))$



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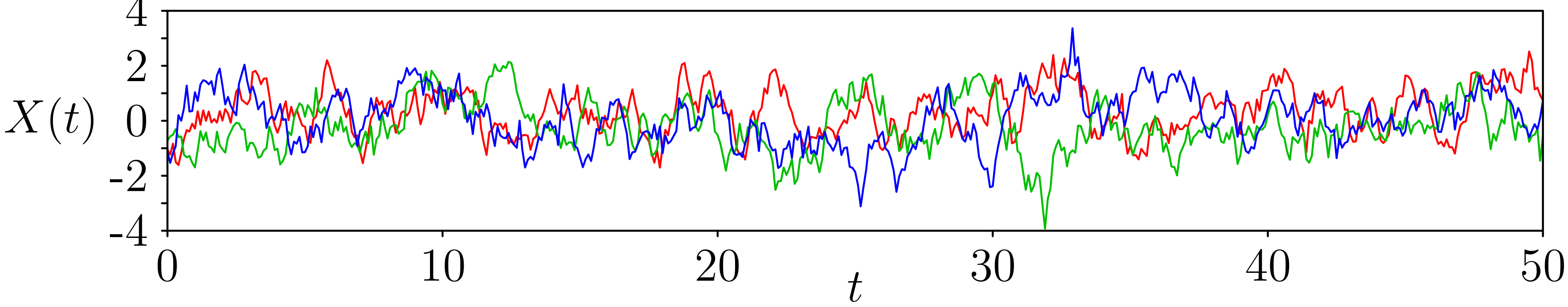
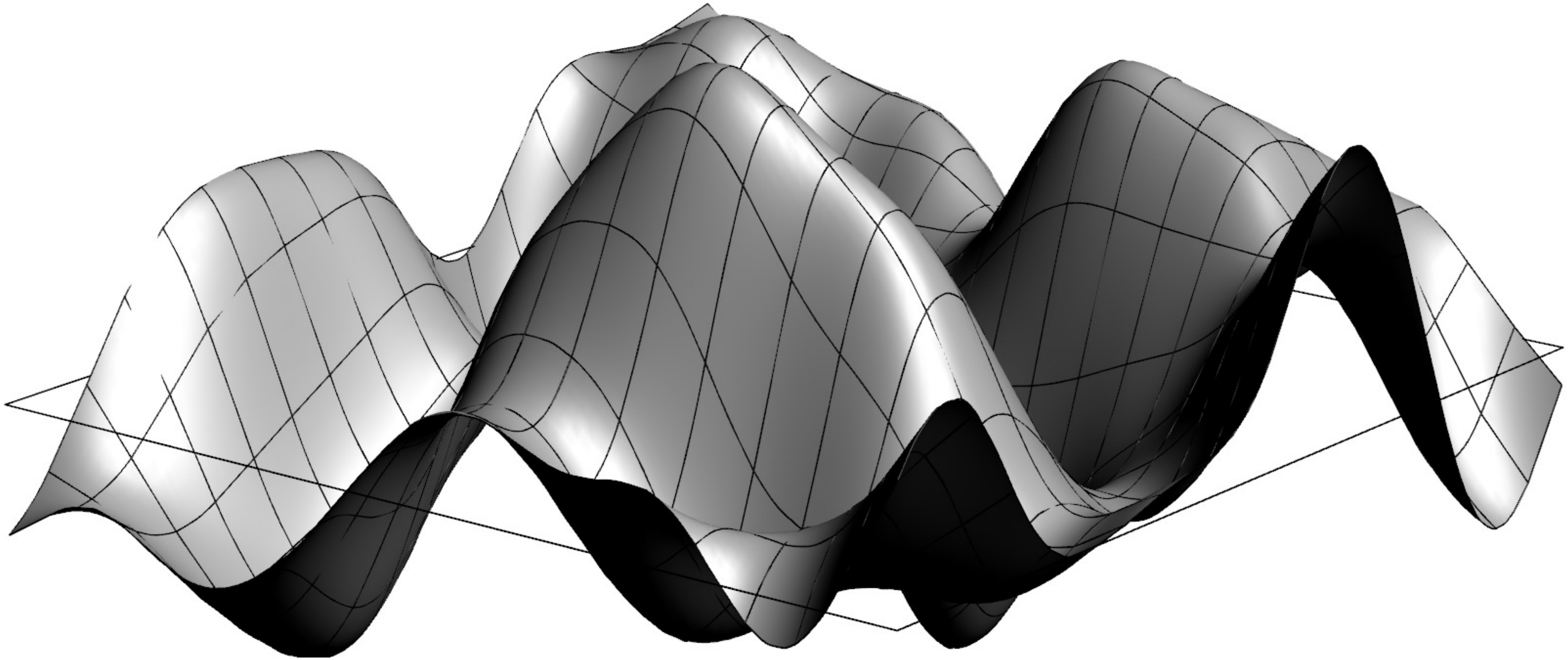
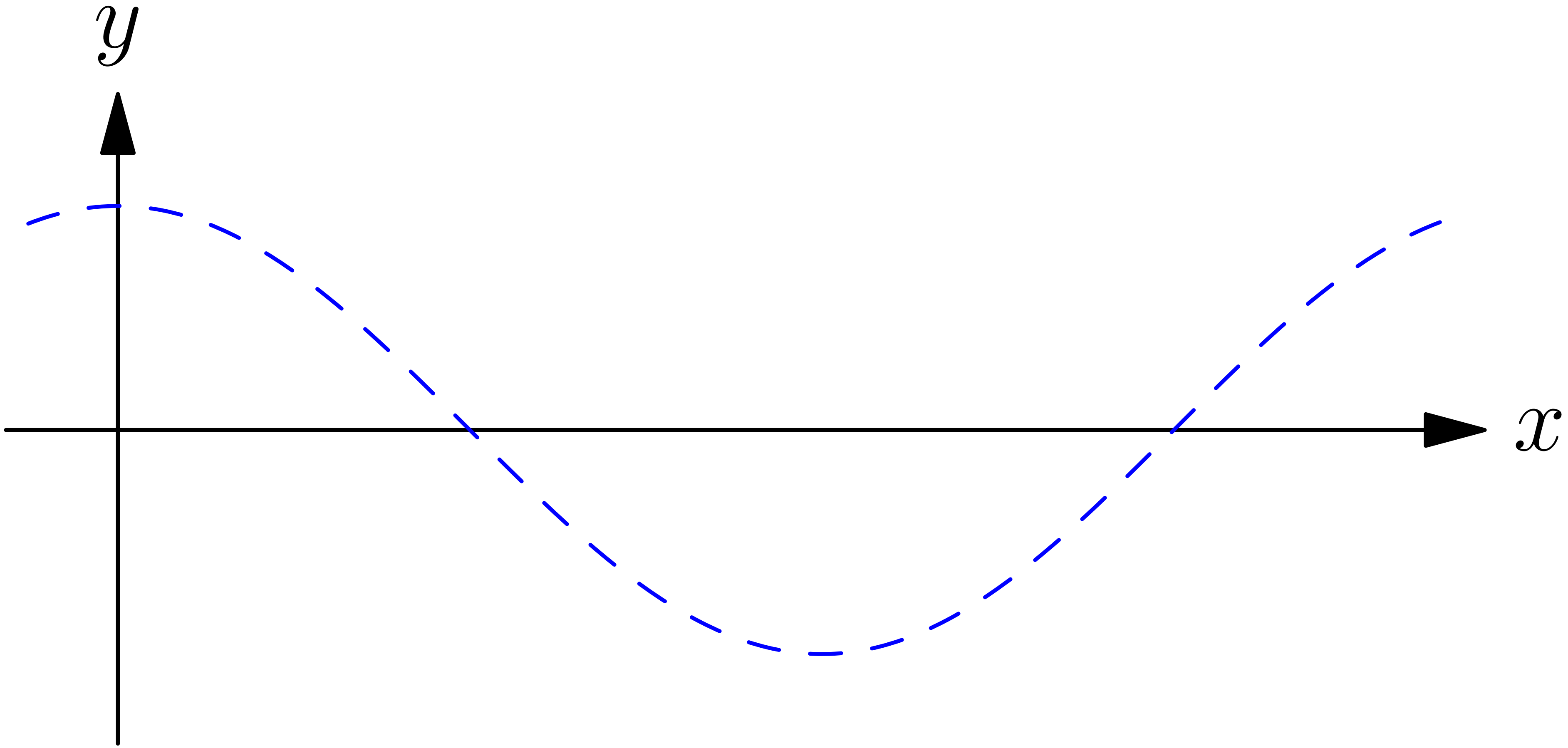


2-D Gaussian Processes



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



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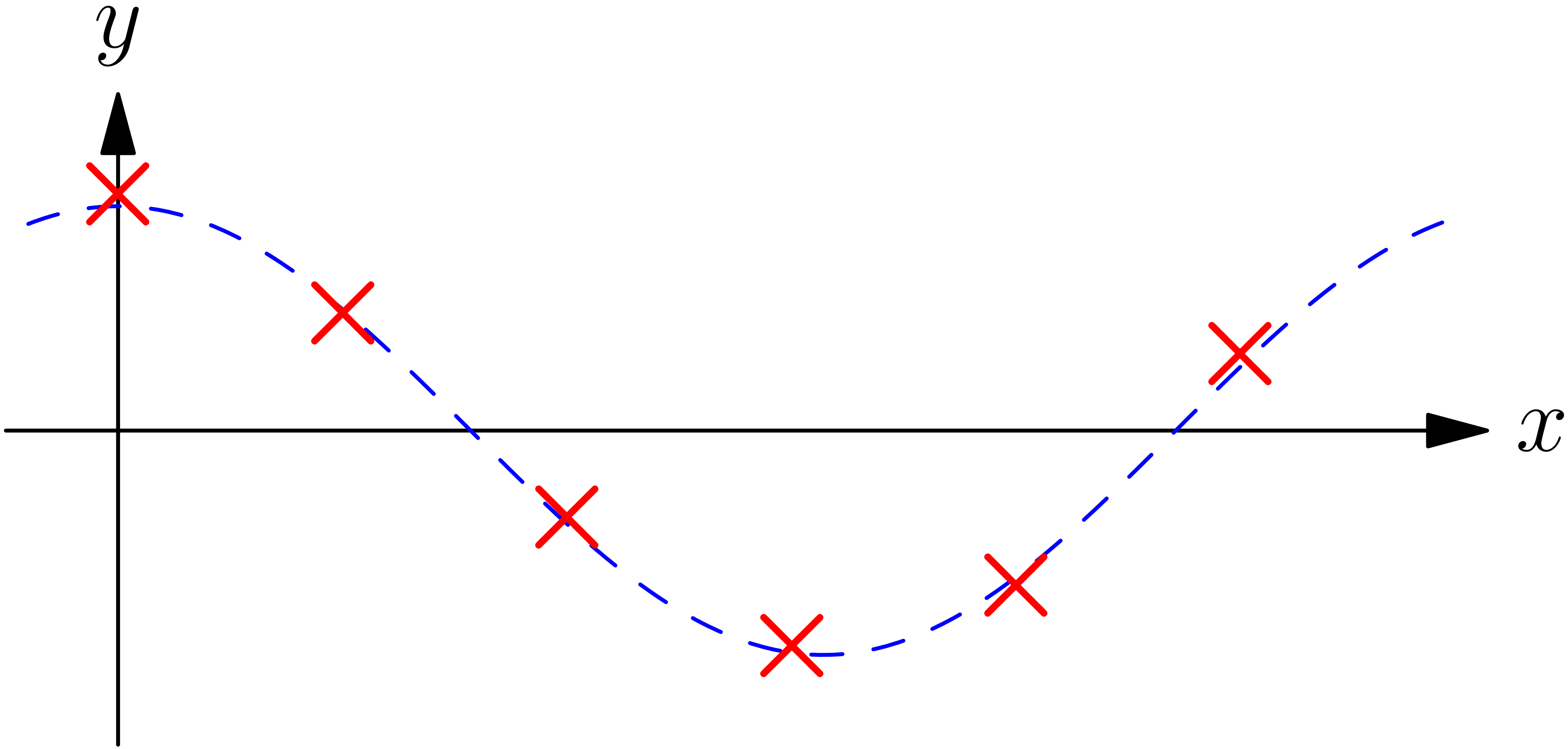

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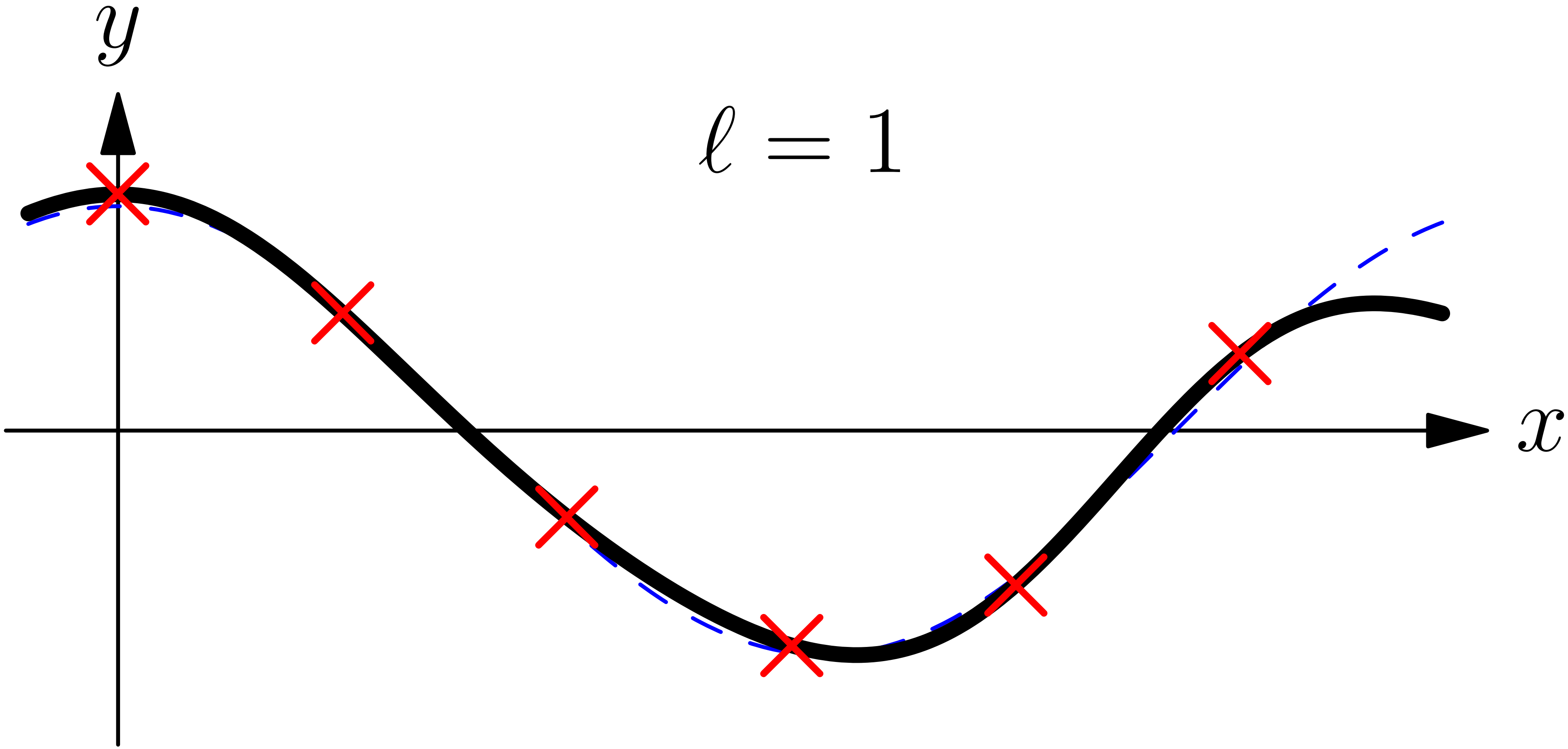

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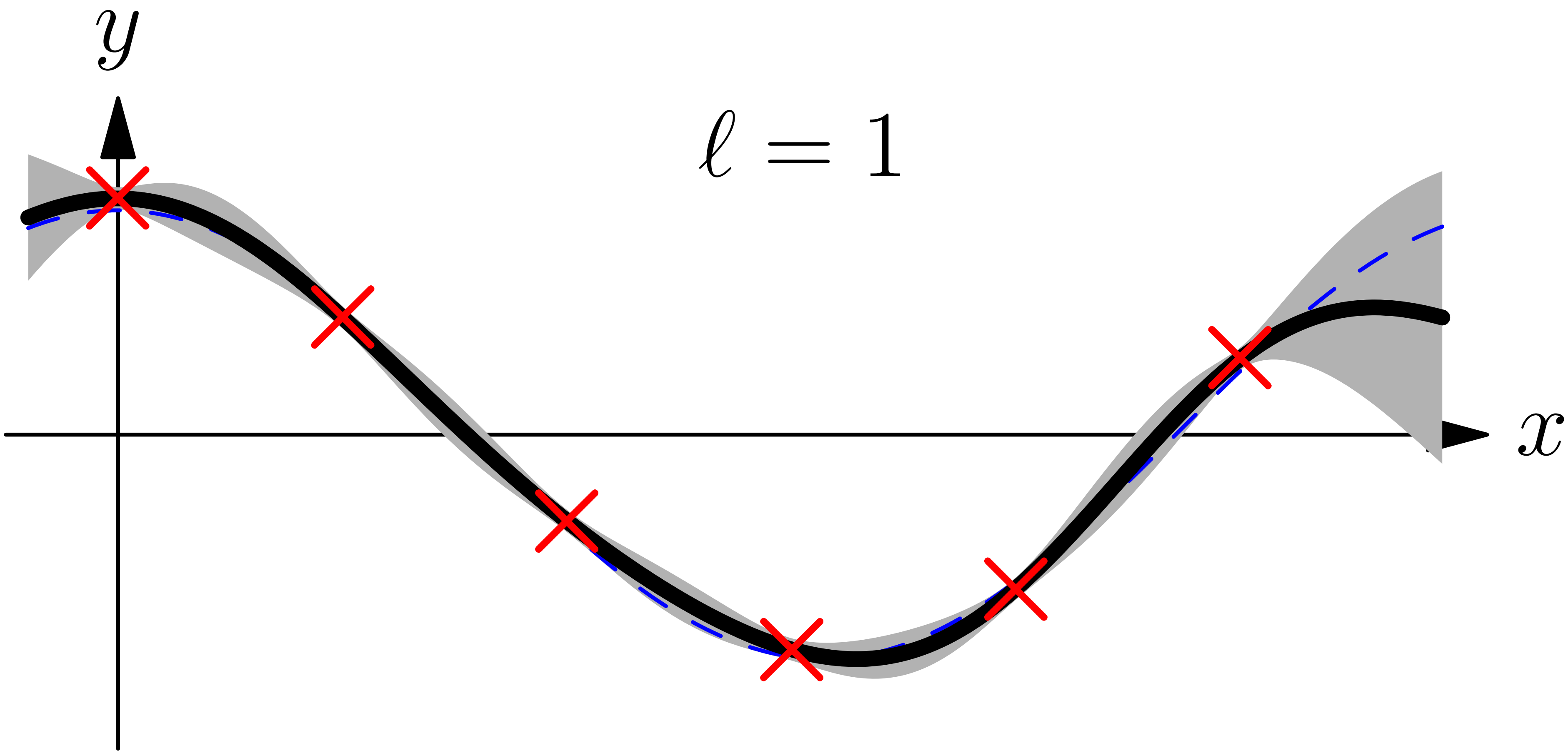

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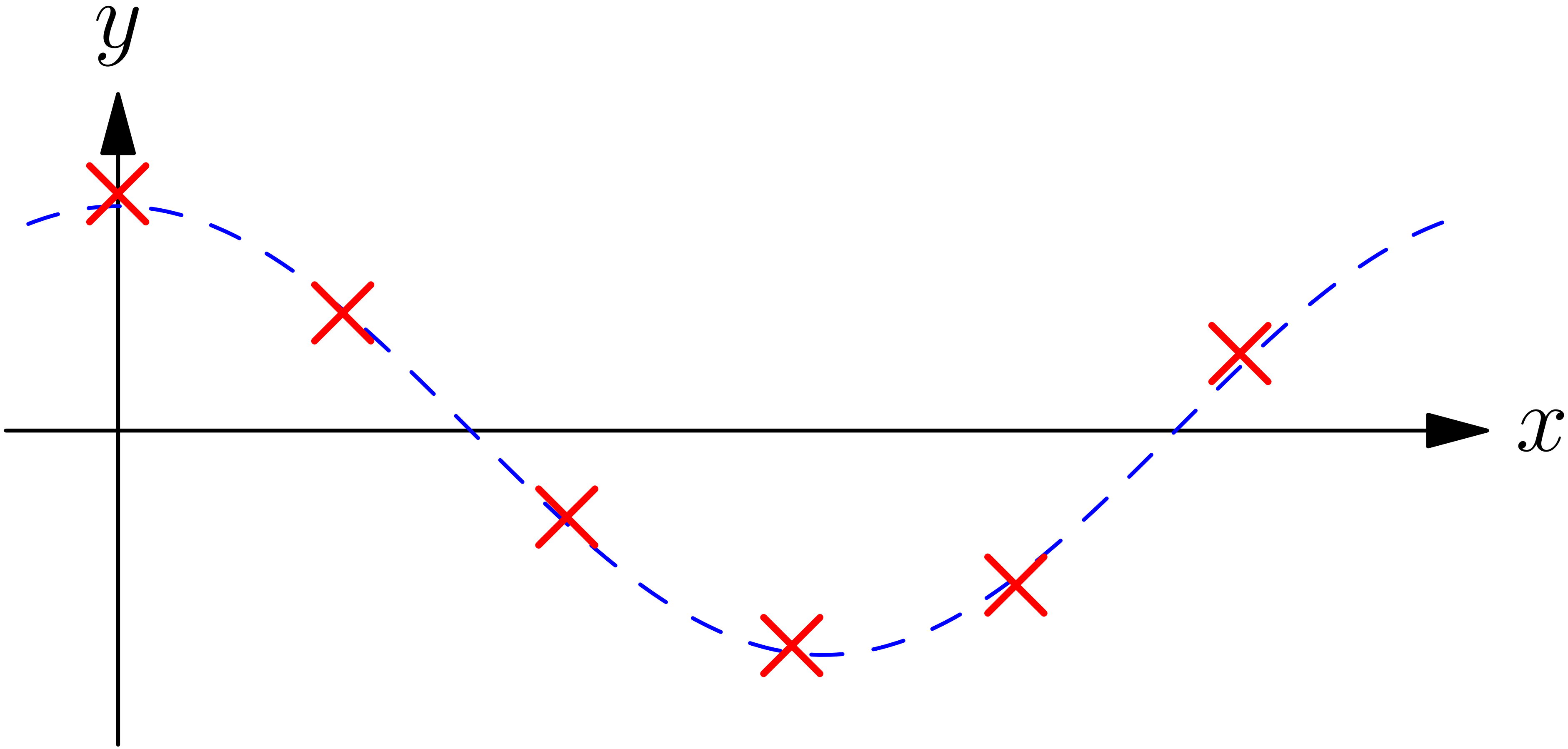

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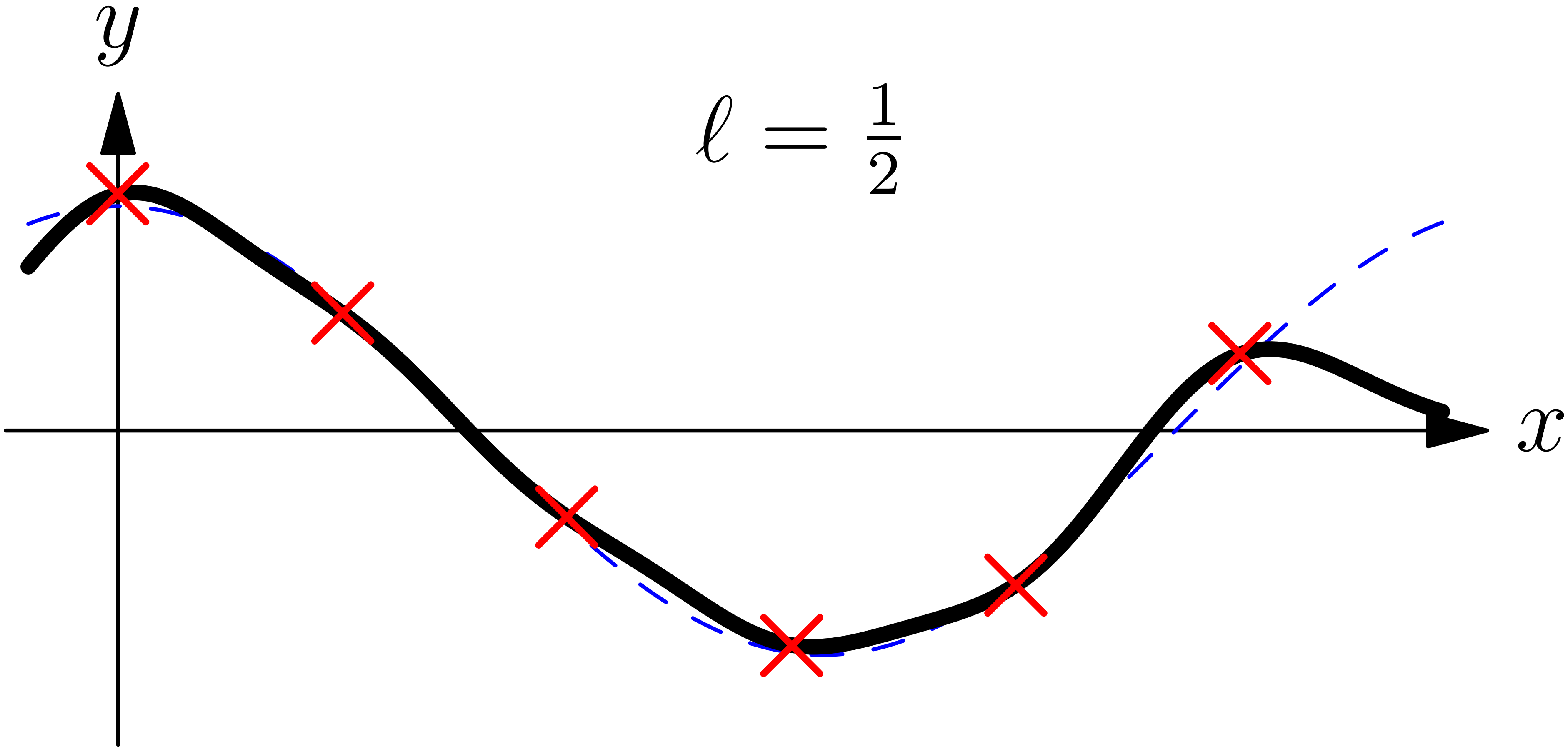

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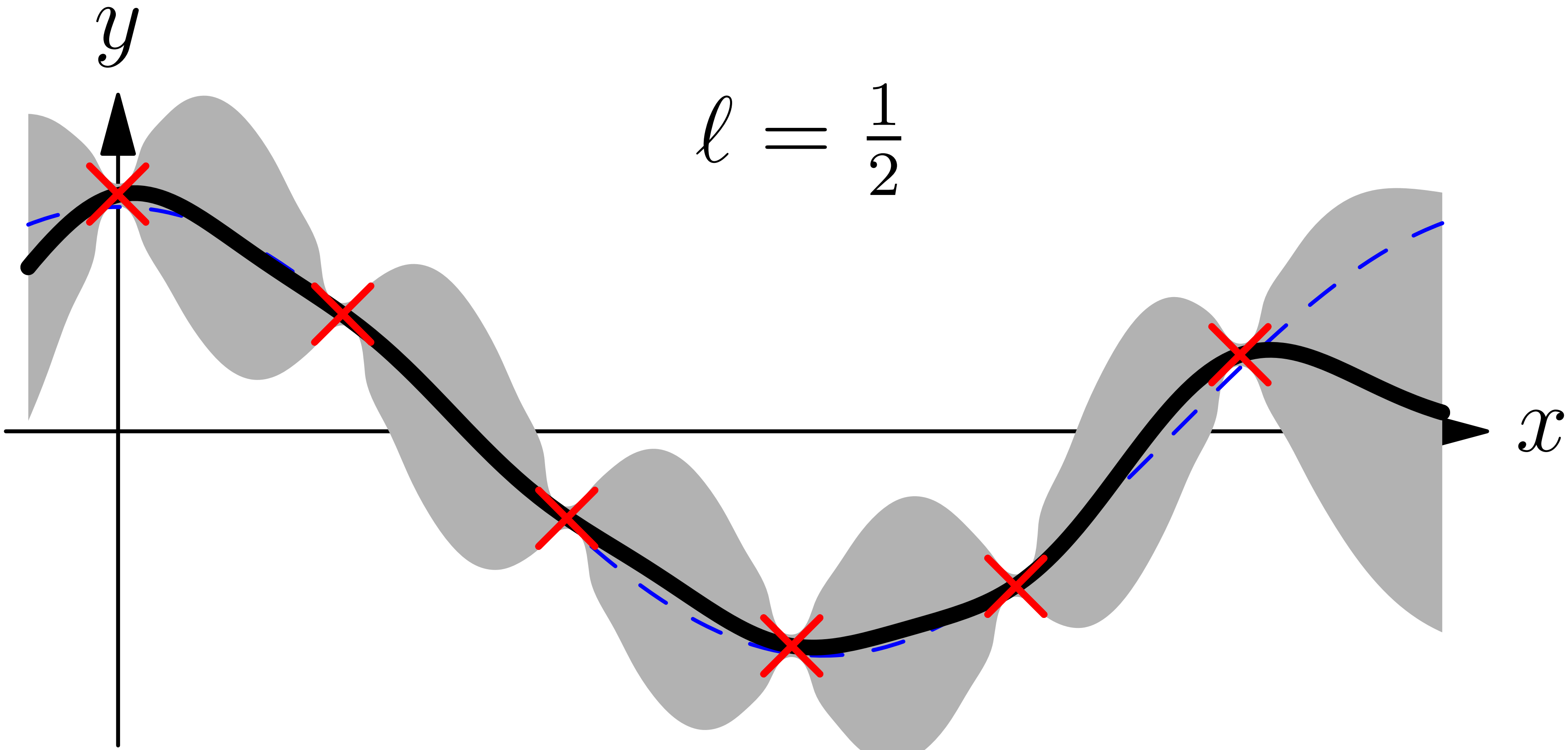

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- We finish with *Naive Bayes* which is unreasonably successful at many text problems
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- It makes the crude approximation that the probability of a document depends only on the words, with all words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

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- We've looked at many of the machine learning methods that are currently state-of-the-art
- They nearly all try to address the bias-variance dilemma one way or another
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