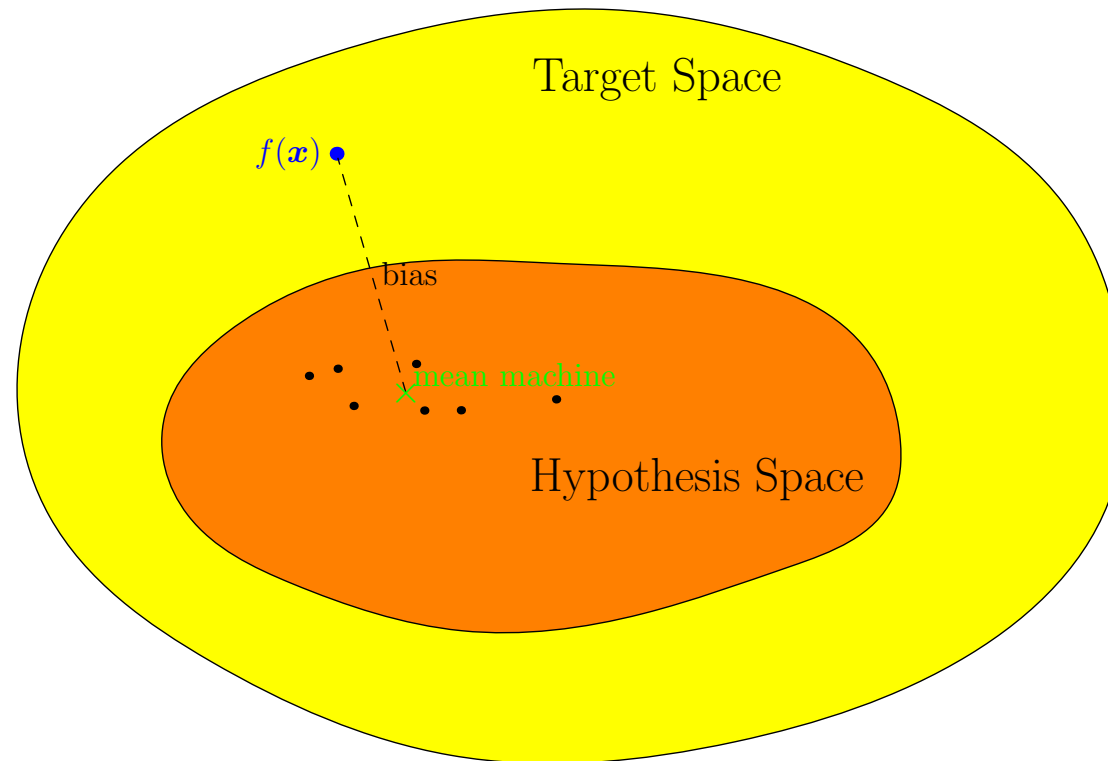


Advanced Machine Learning

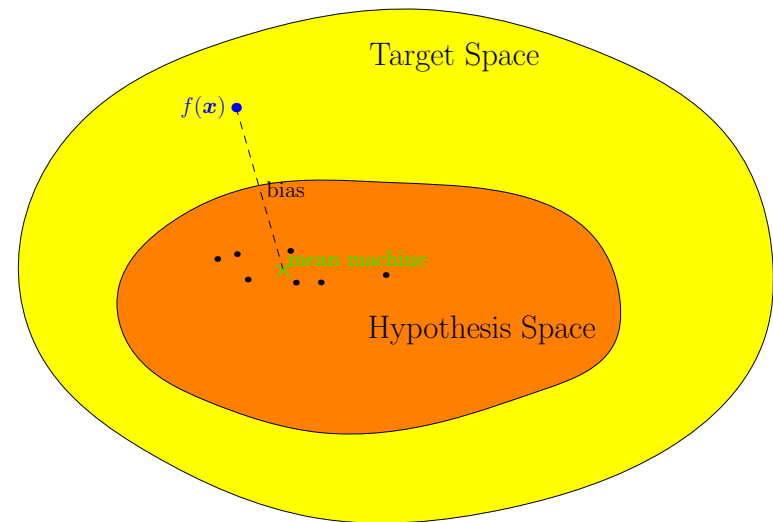
When Machine Learning Works



When ML Works, Bias Variance

Outline

1. **What Makes a Good Learning Machine?**
2. Bias-Variance Dilemma



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

- Suppose we want to learn some output y for a feature vector x
- We construct a learning machine that makes a prediction $\hat{f}(x|\theta)$
- We typically choose the machine to minimise a *training loss*

$$L_T(\mathcal{D}) = \sum_{(x,y) \in \mathcal{D}} \left(\hat{f}(x|\theta) - y \right)^2$$

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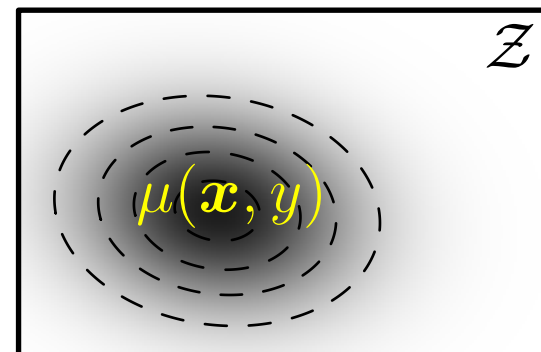
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- We call this machine $\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}})$

Generalisation Error

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

$$L_G(\boldsymbol{\theta}_{\mathcal{D}}) = \sum_{(\mathbf{x}, y) \in \mathcal{Z}} \mu(\mathbf{x}, y) \left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - y \right)^2$$



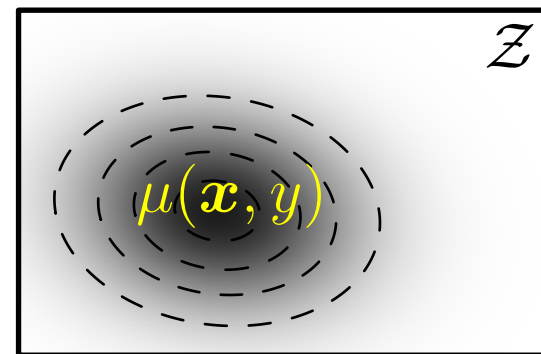
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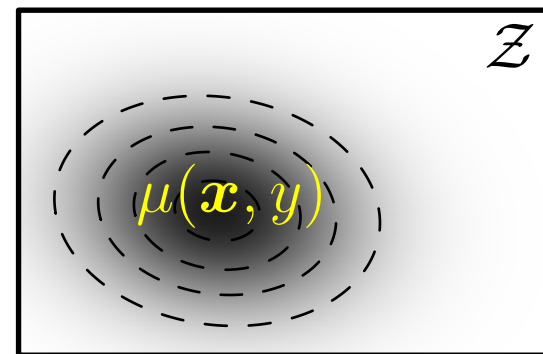
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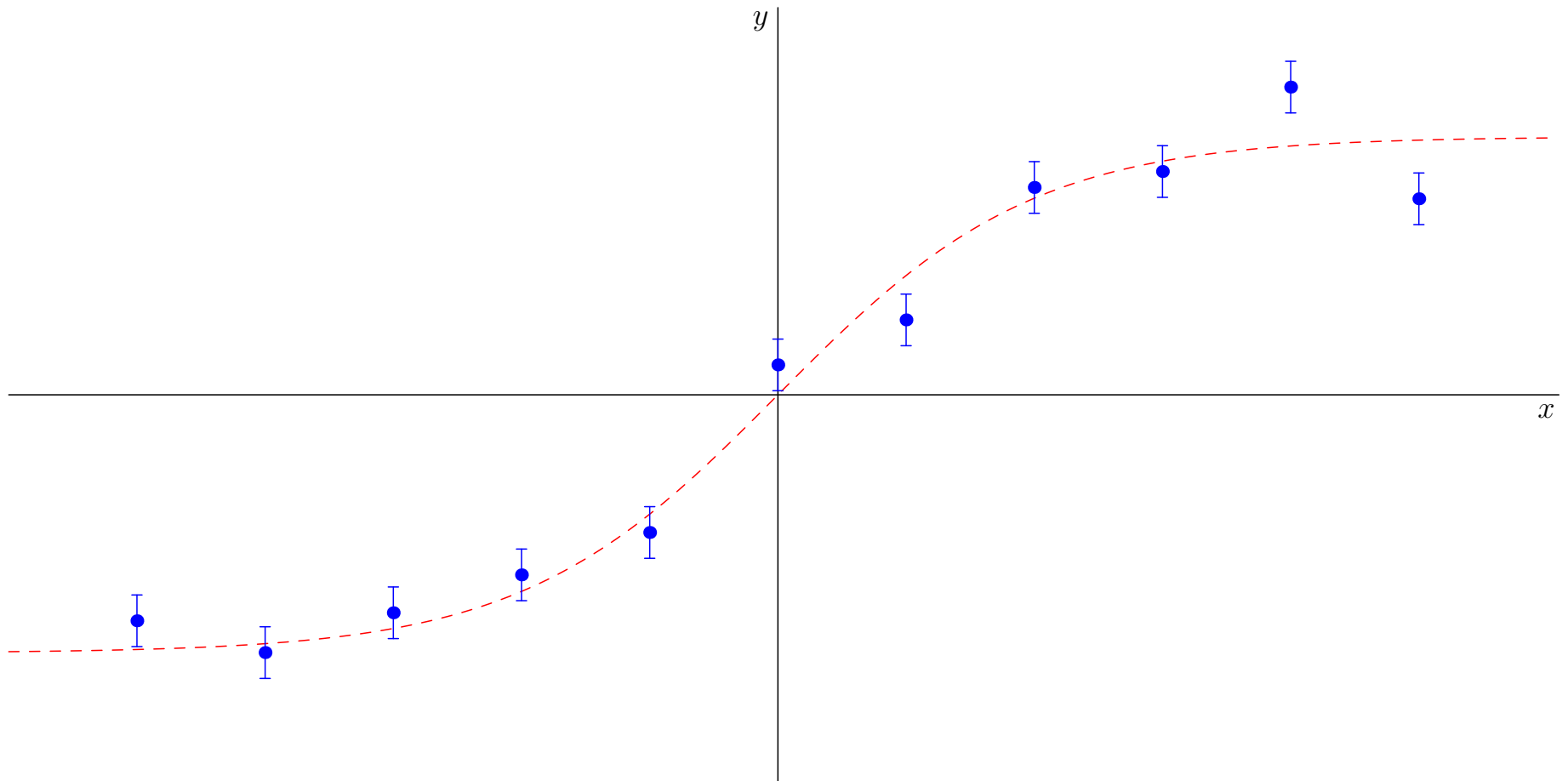
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Too Simple or Too Complex?

- Fit $\hat{f}(x|\boldsymbol{\theta}_{\mathcal{D}})$ to data

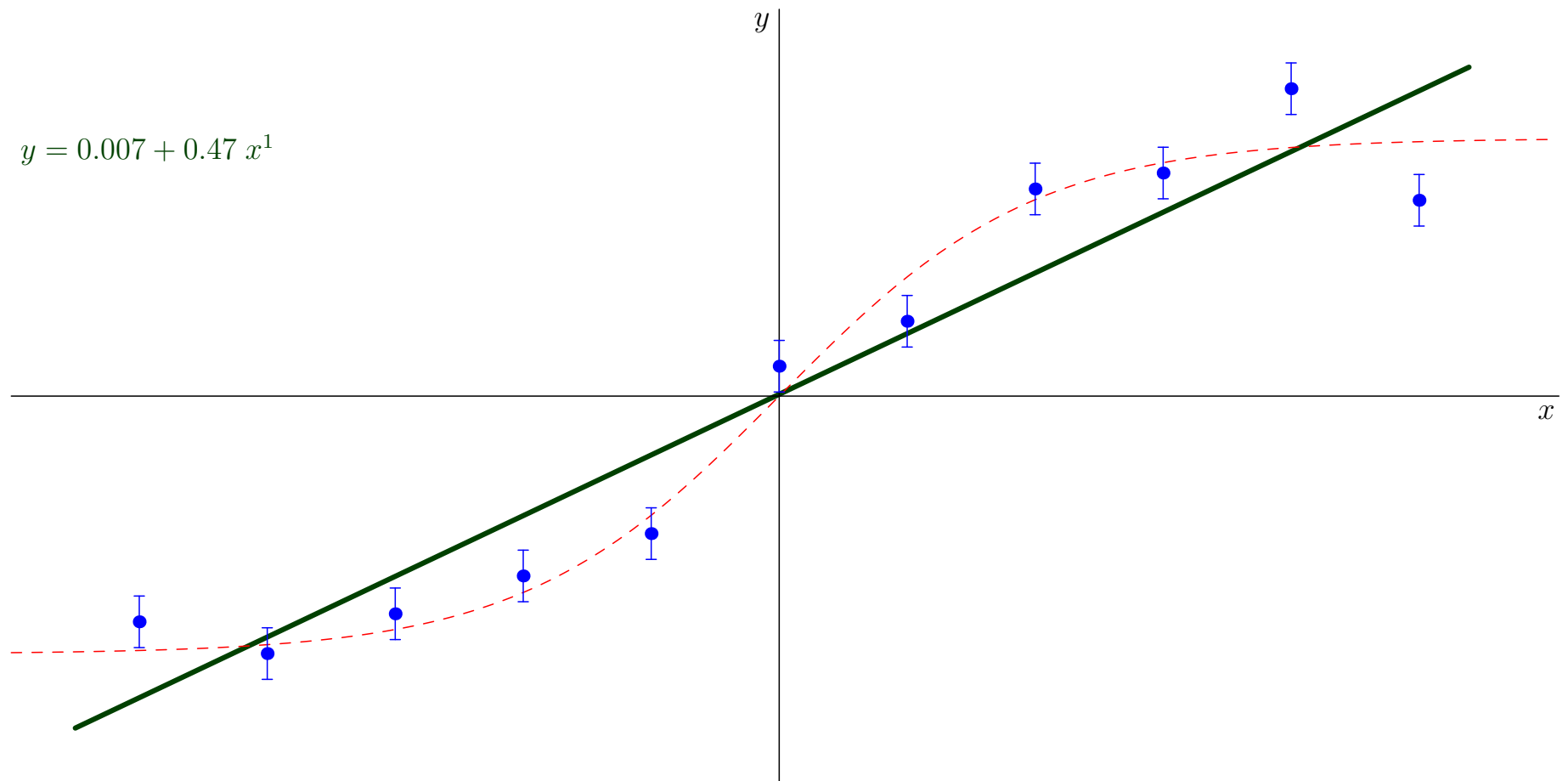
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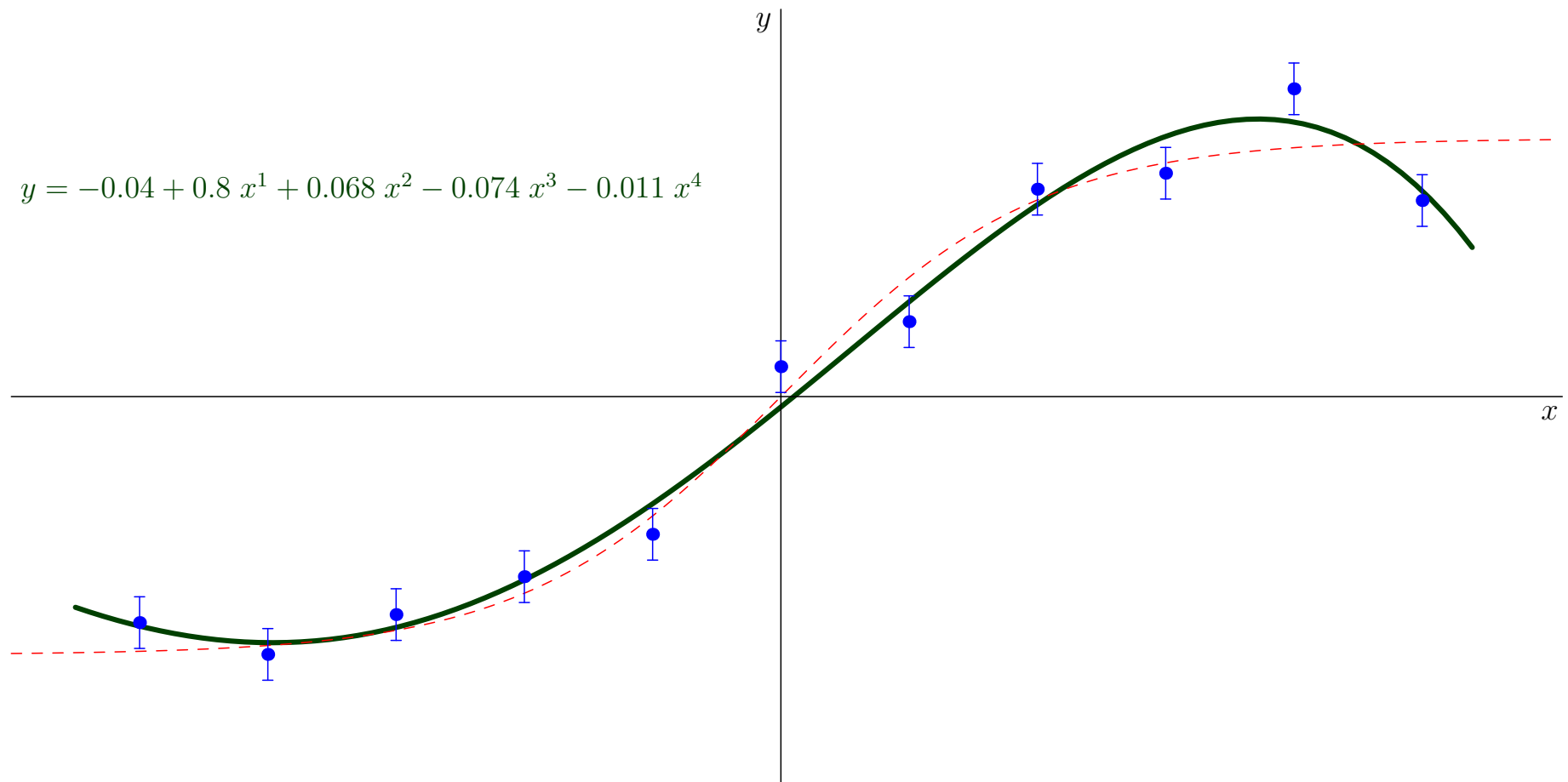
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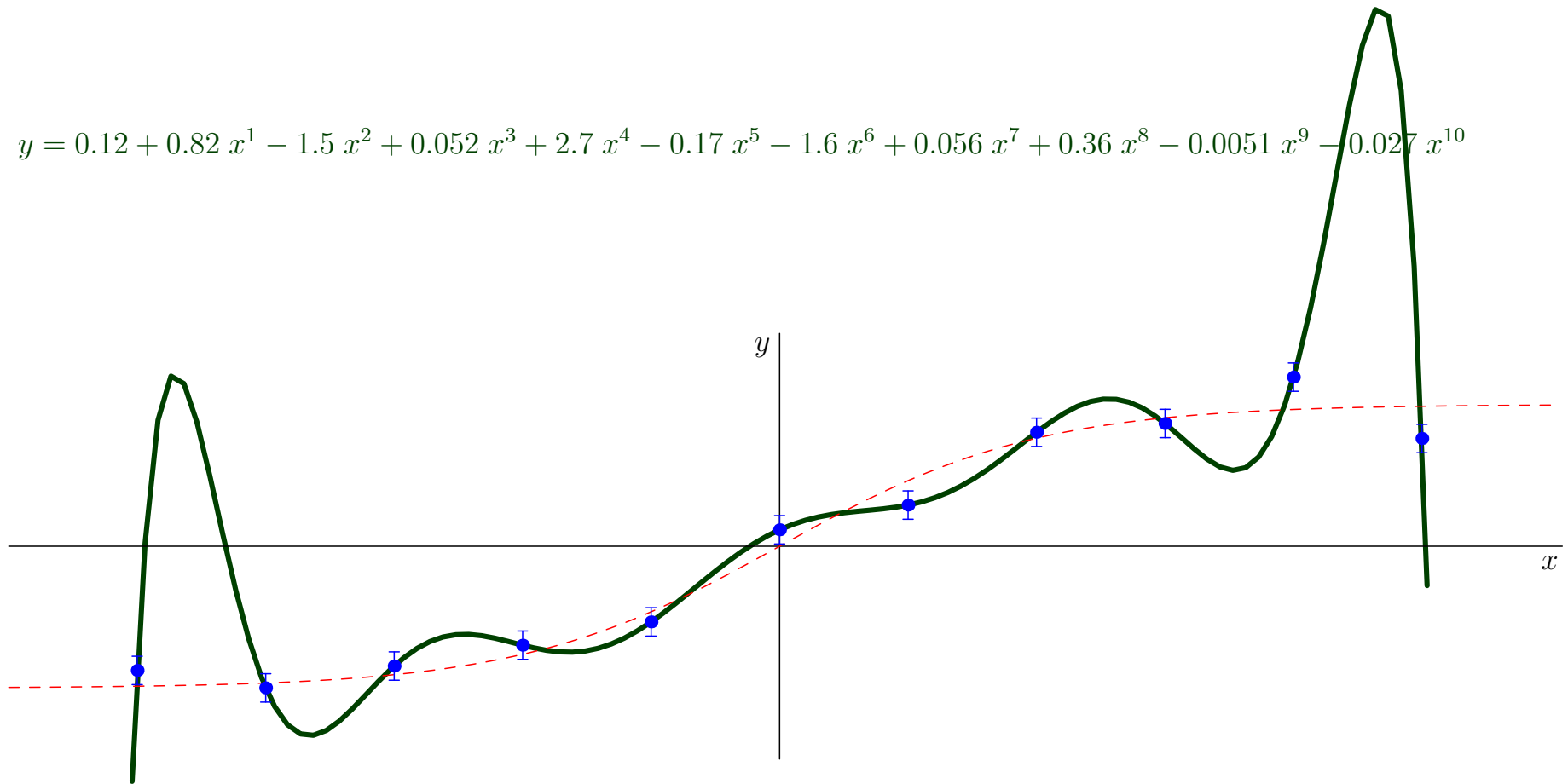
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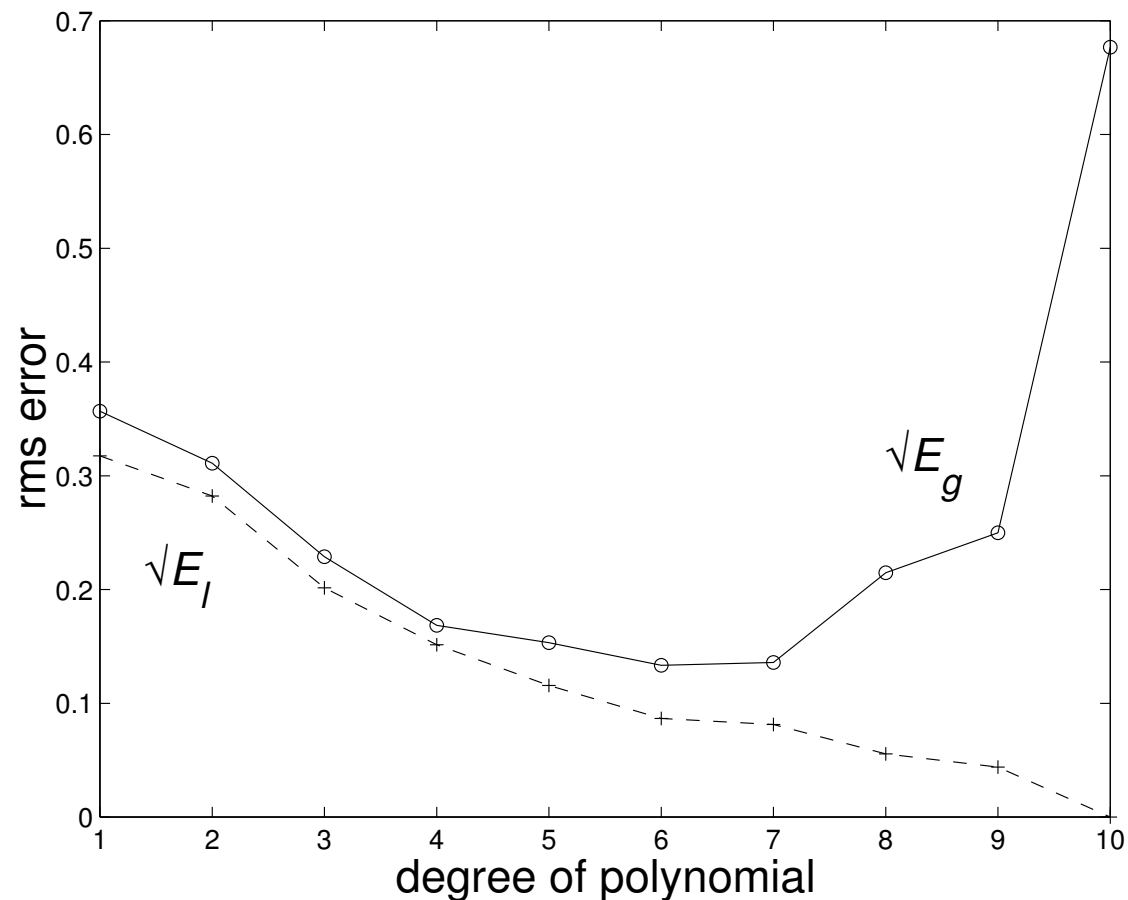
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$$y = 0.12 + 0.82 x^1 - 1.5 x^2 + 0.052 x^3 + 2.7 x^4 - 0.17 x^5 - 1.6 x^6 + 0.056 x^7 + 0.36 x^8 - 0.0051 x^9 - 0.027 x^{10}$$



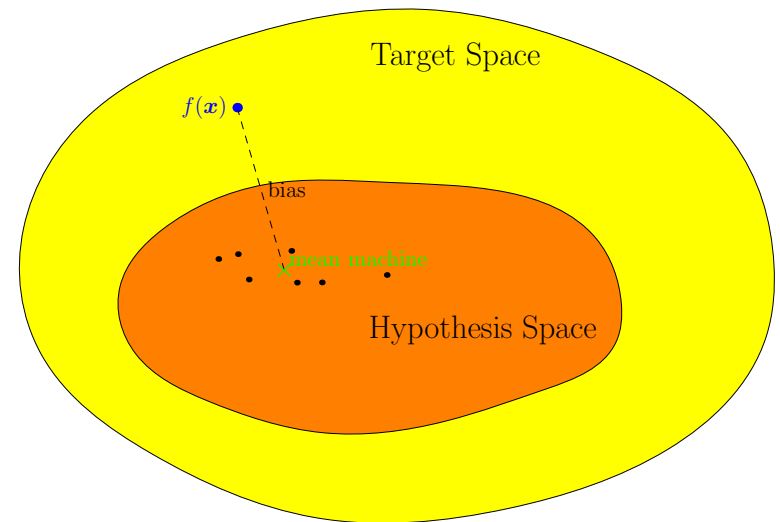
Measuring Generalisation Error for Regression

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



Outline

1. What Makes a Good Learning Machine?
2. **Bias-Variance Dilemma**



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 loss*, when we average over all different data sets of size m drawn independently from $\mu(\mathbf{x}, y)$
- For each data set, \mathcal{D} , we would learn a different approximator $\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}})$
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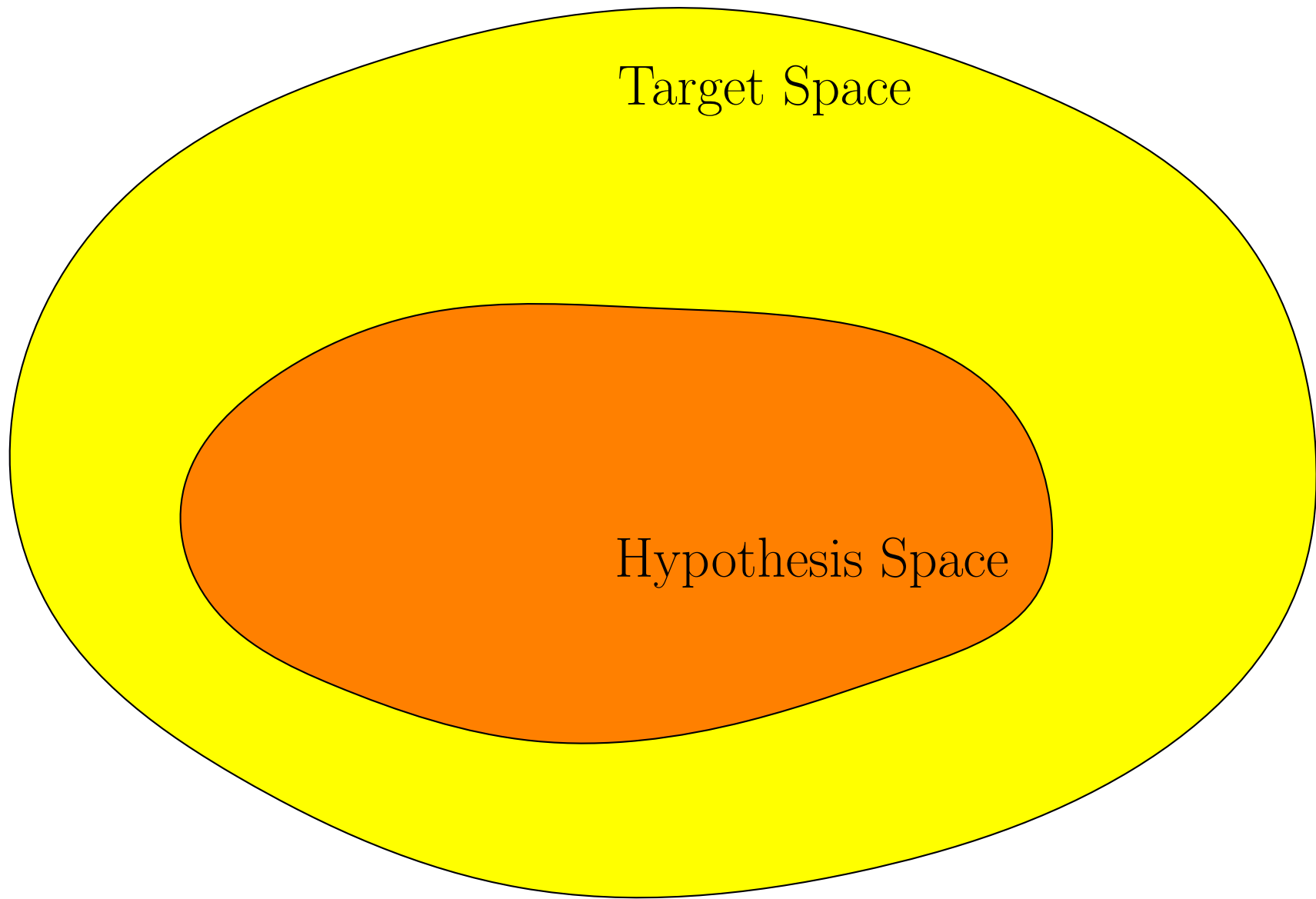
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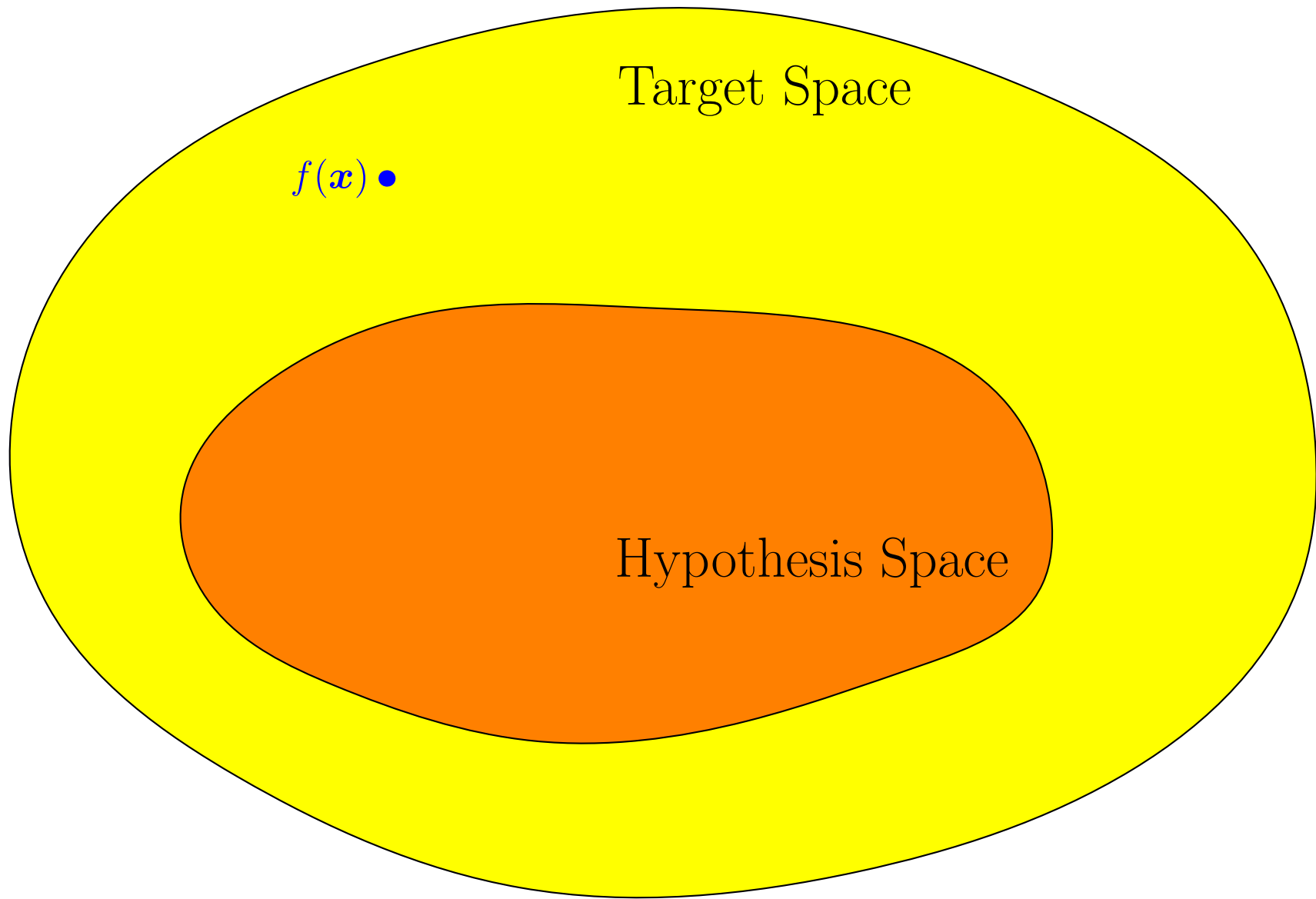
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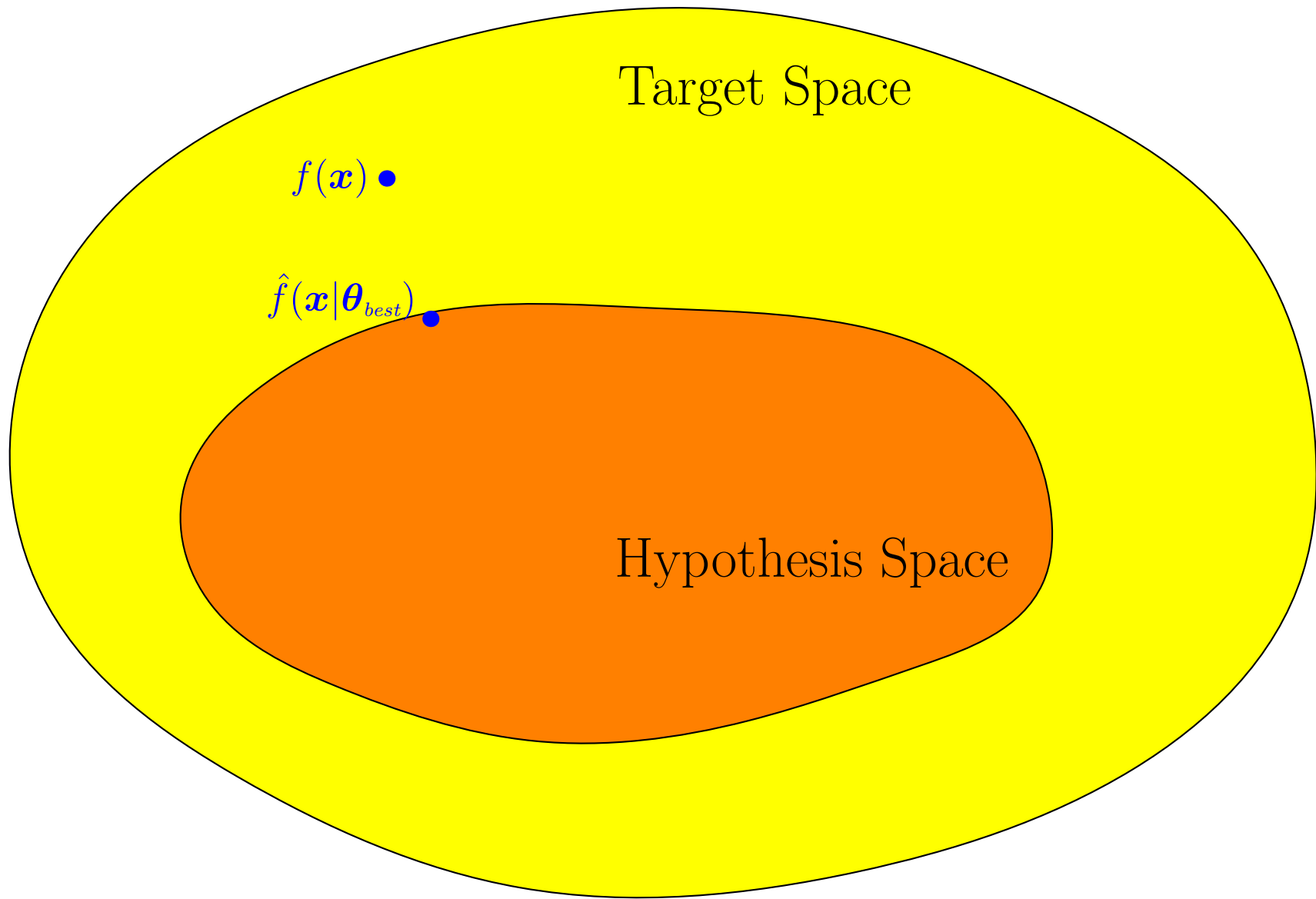
Approximation and Estimation Errors



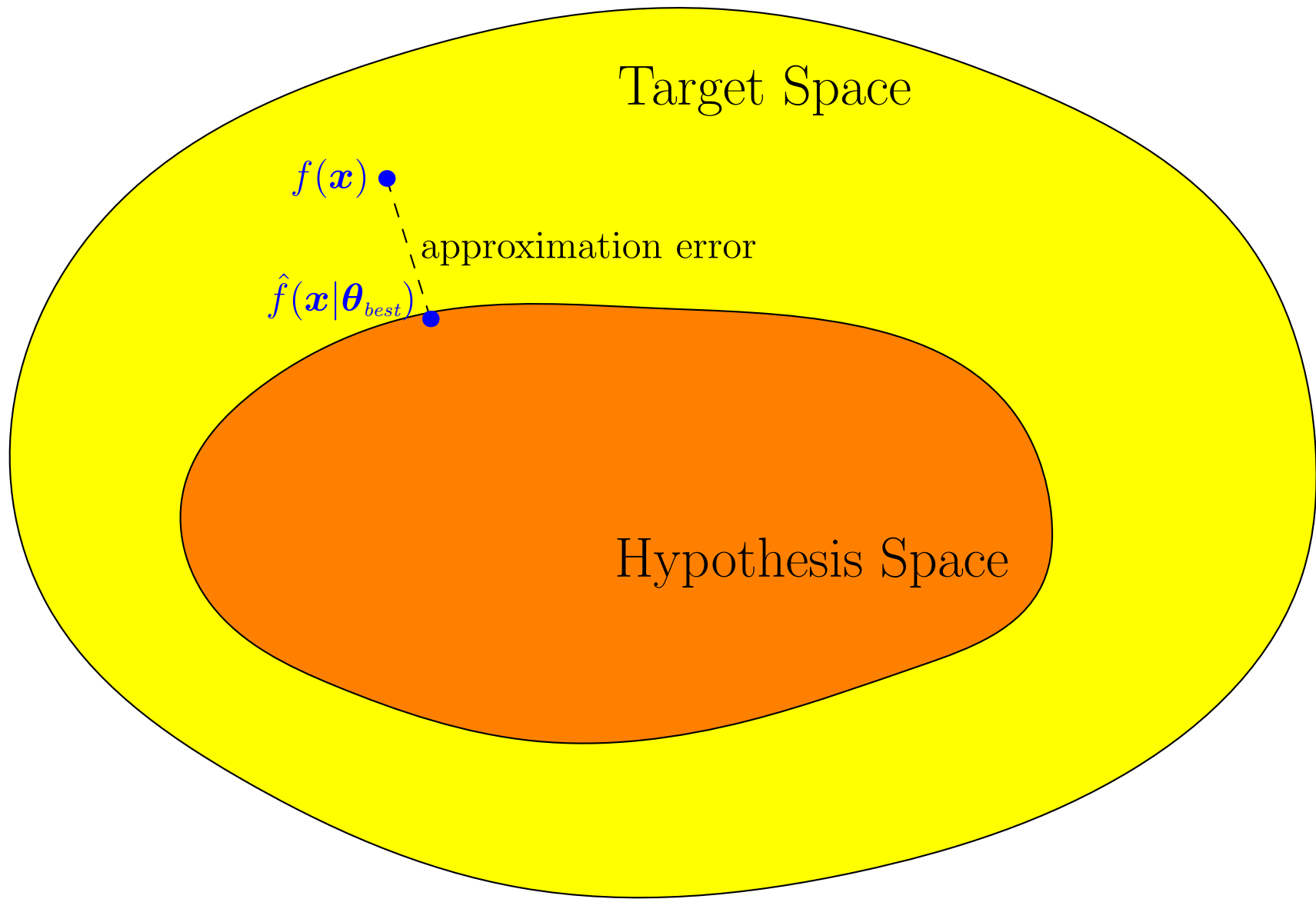
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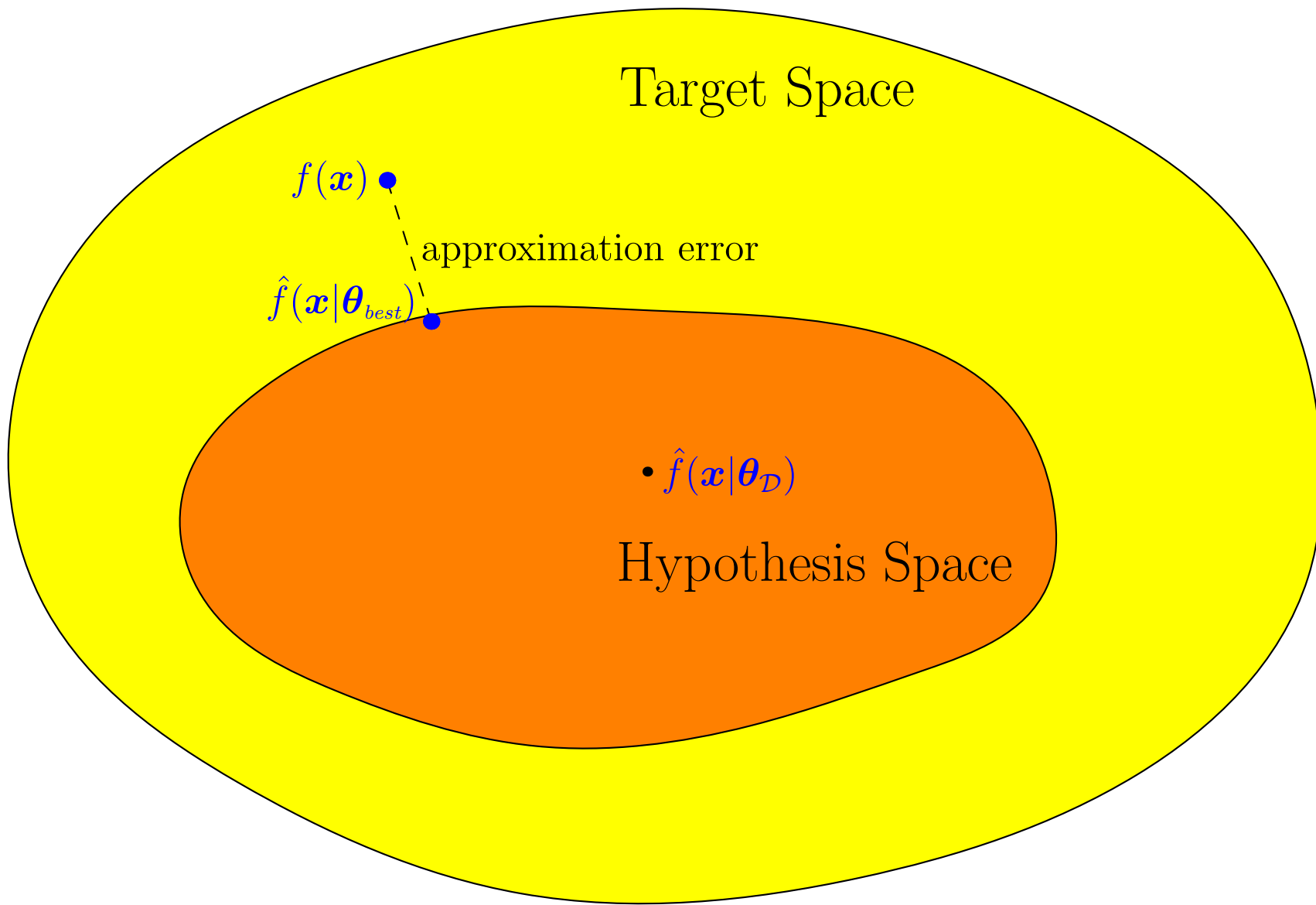
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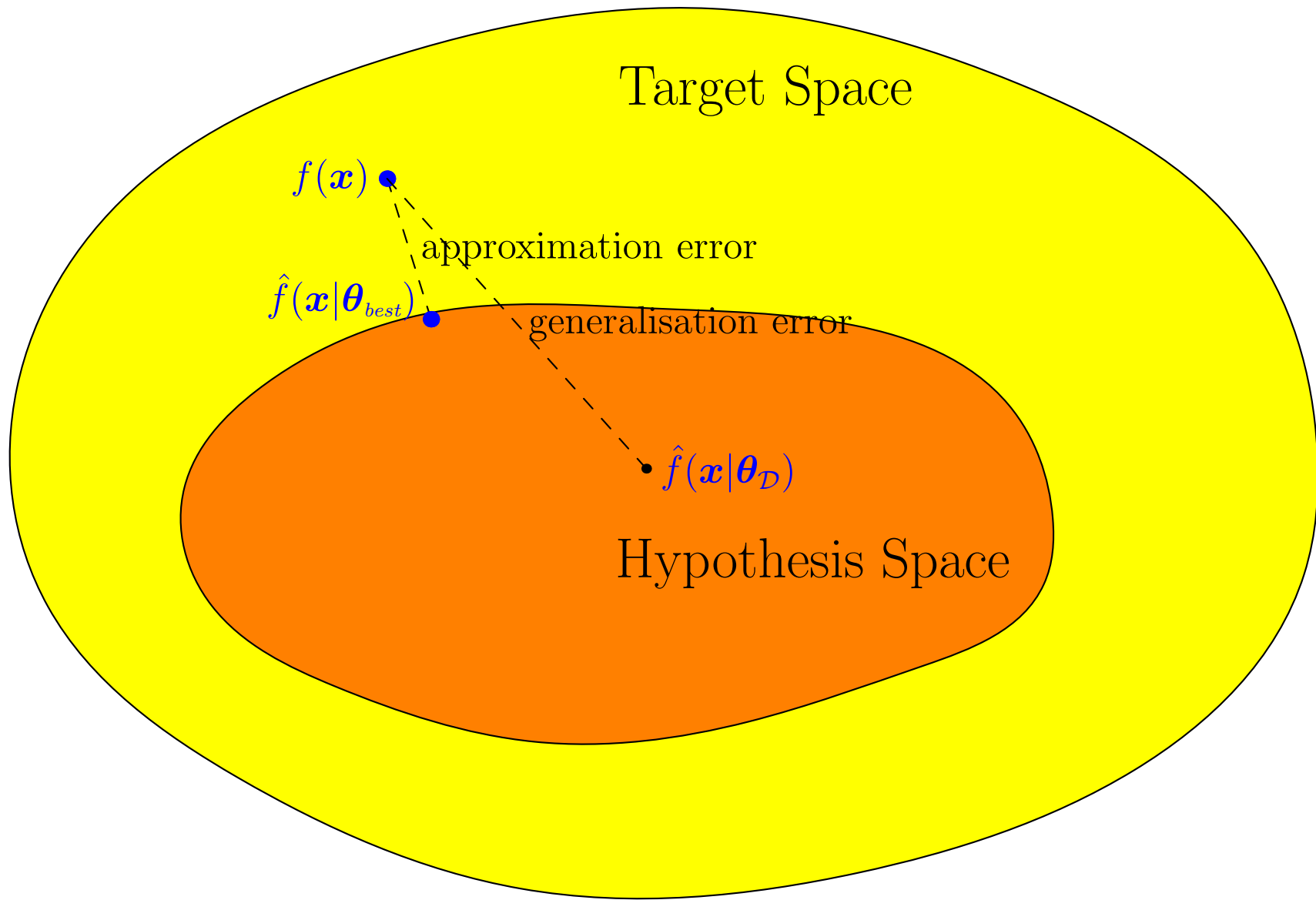
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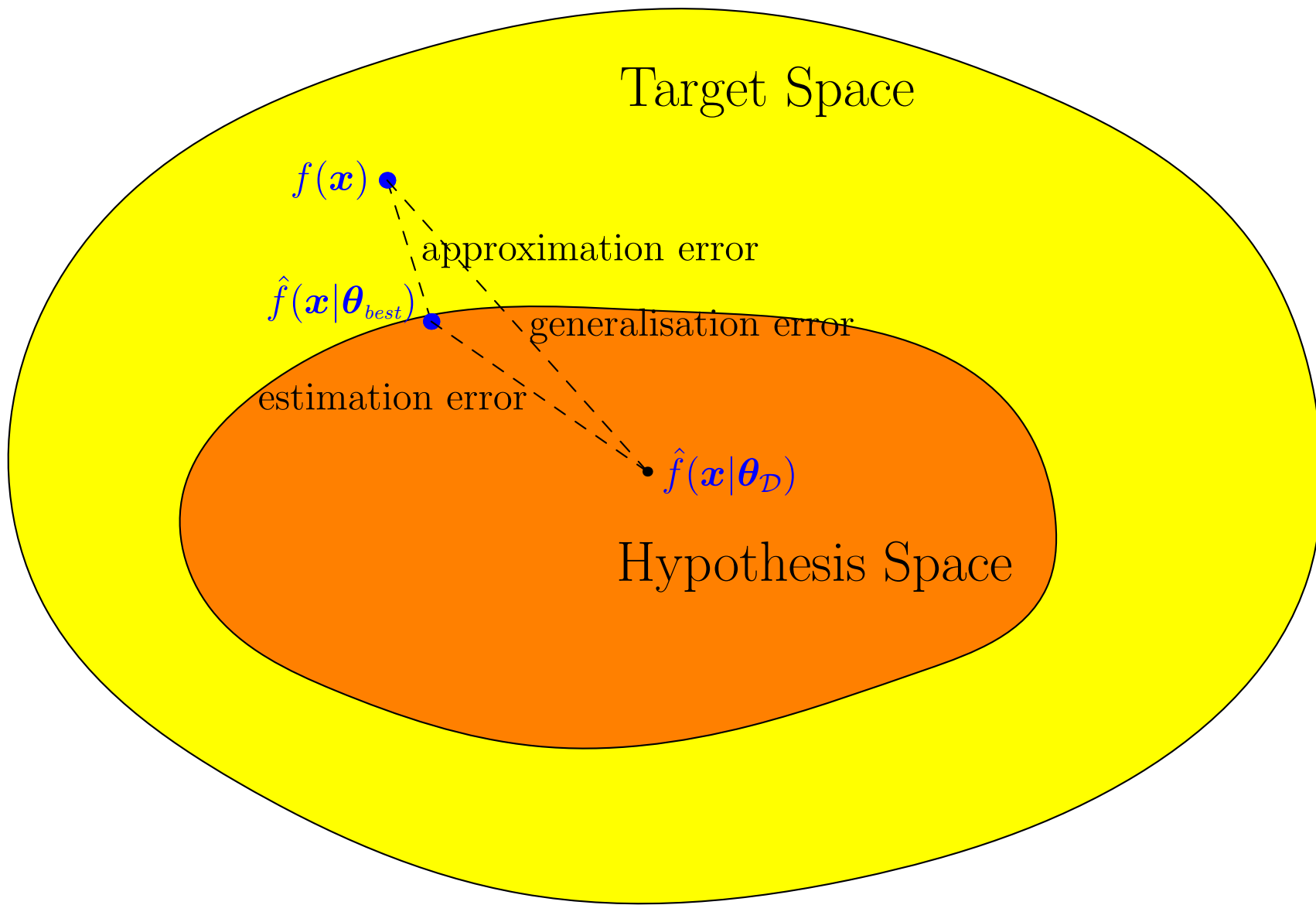
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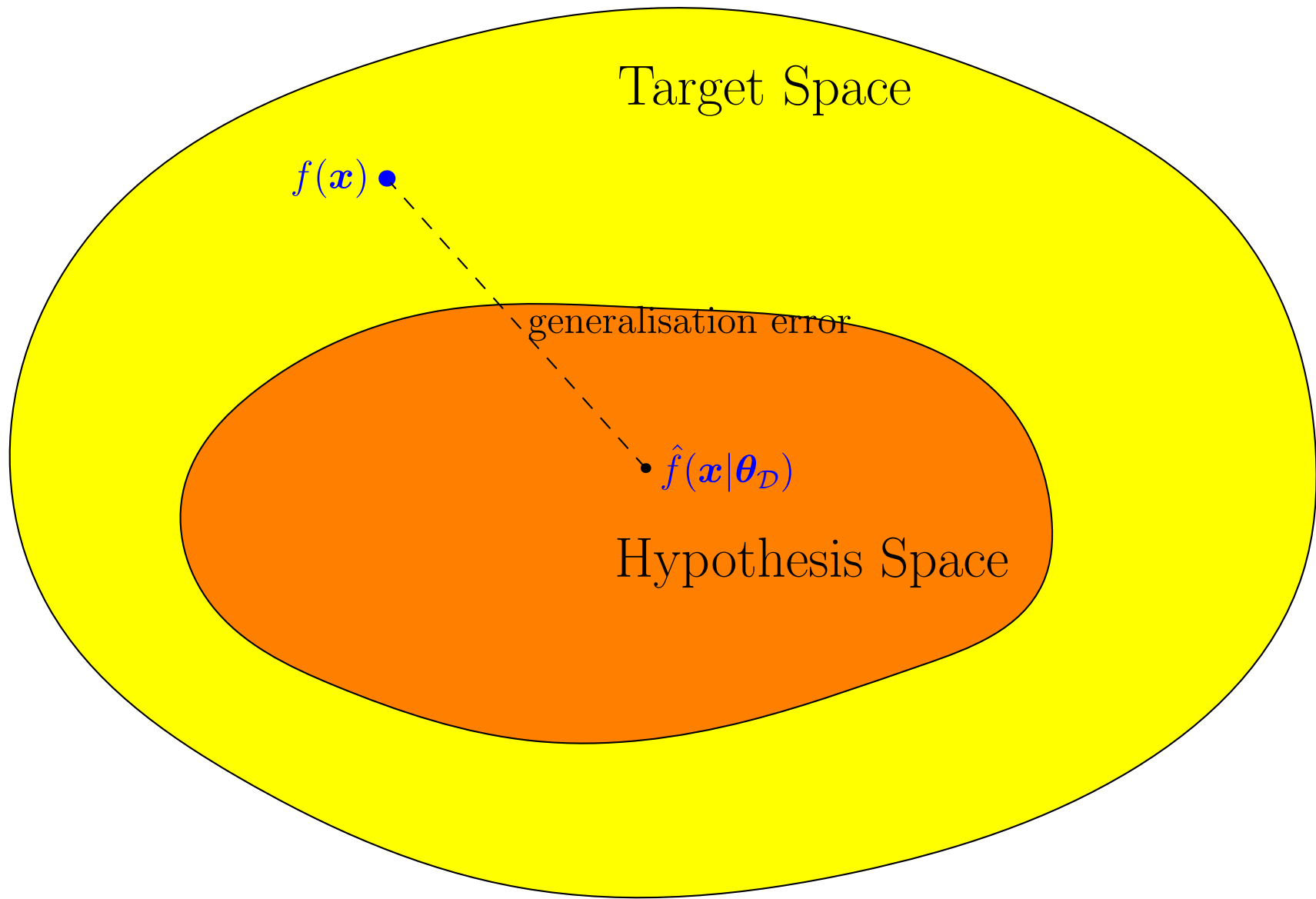
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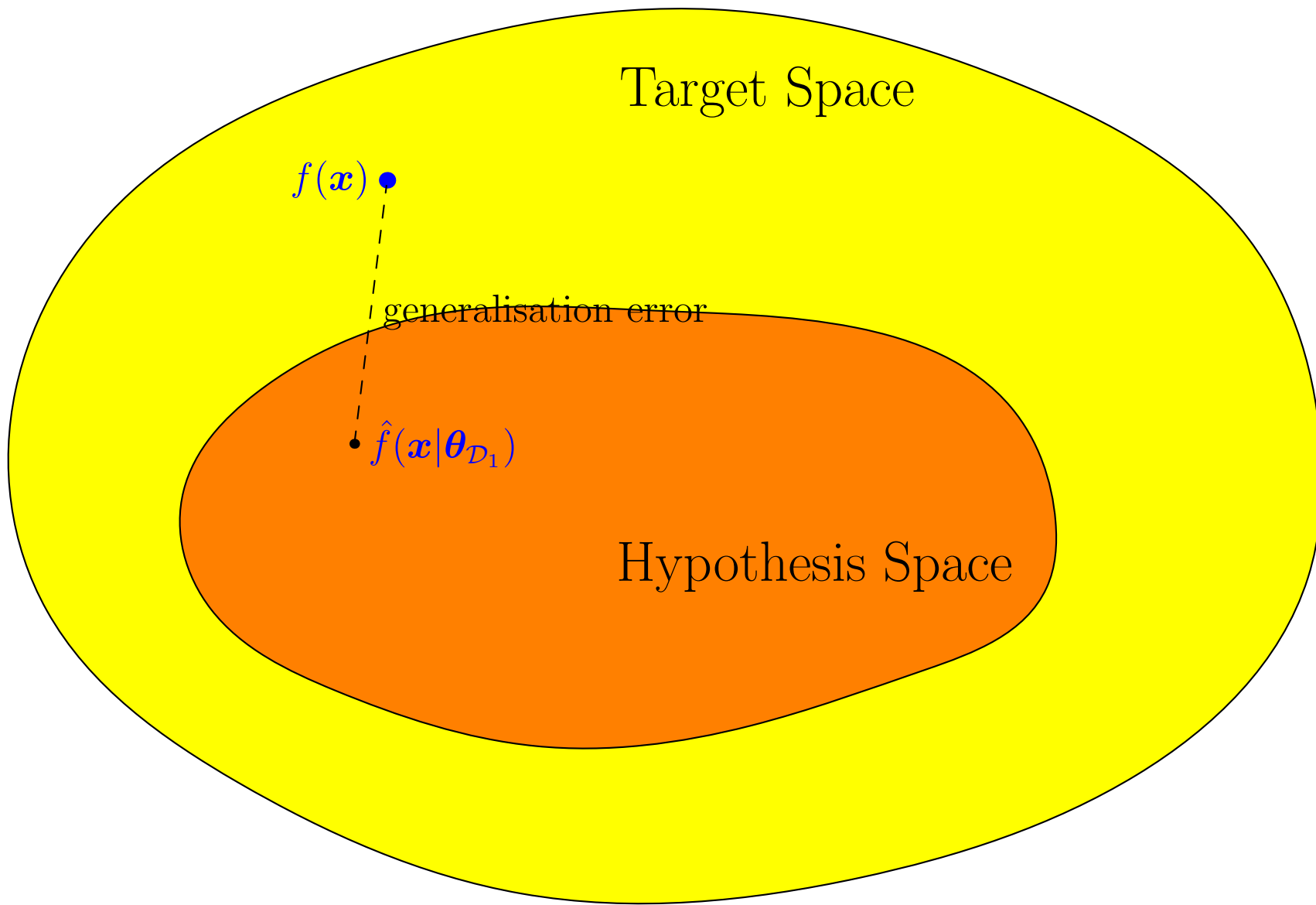
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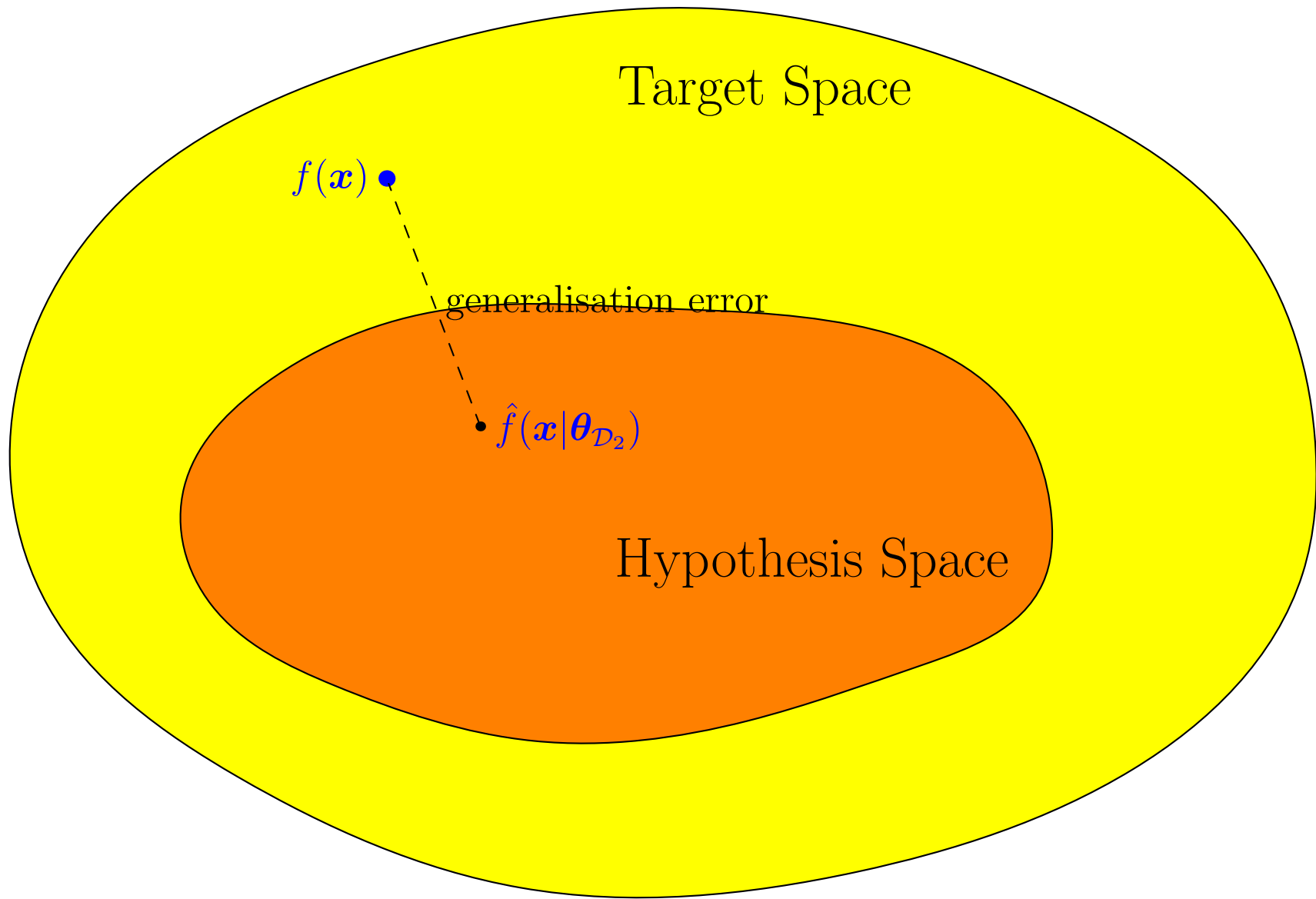
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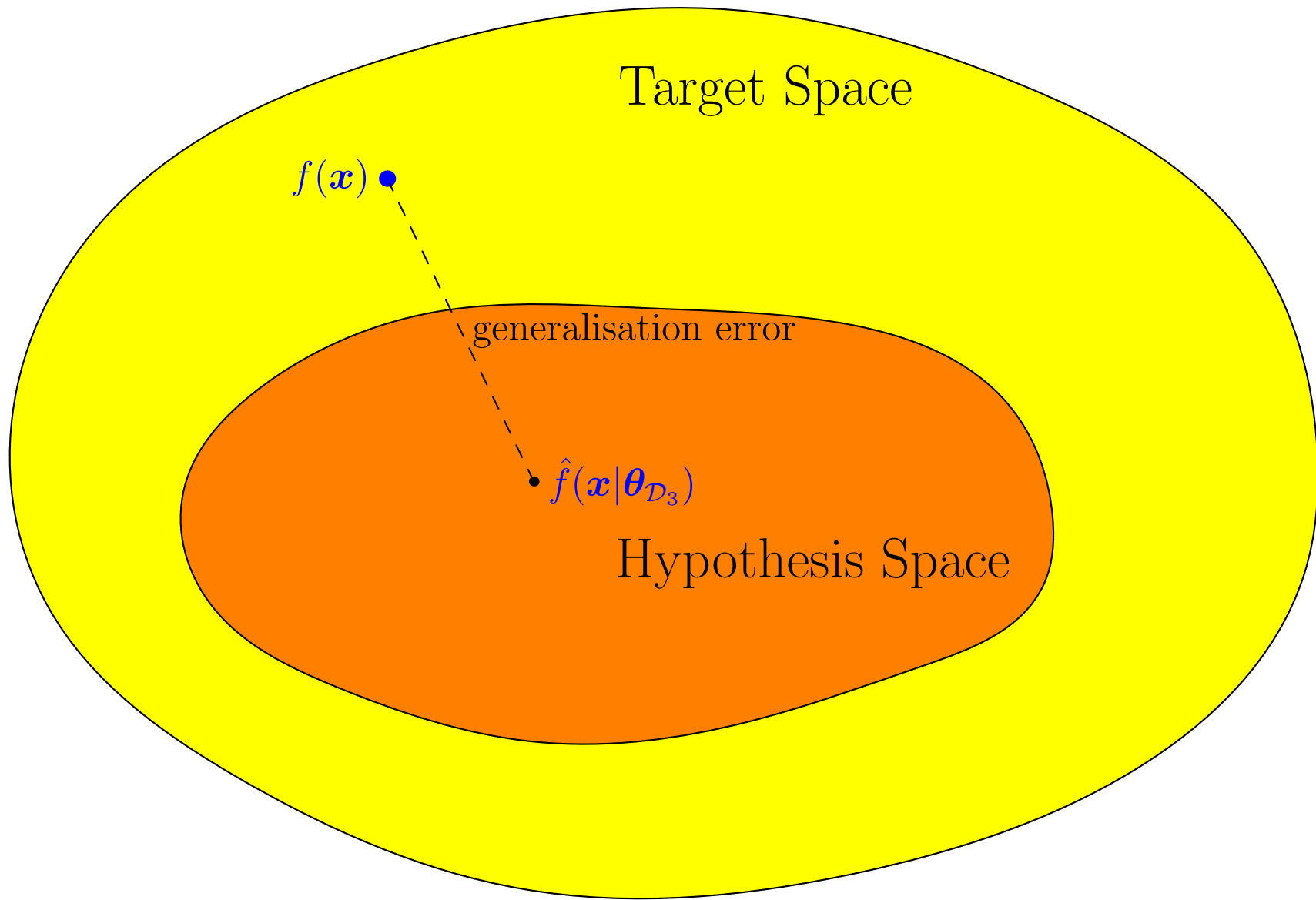
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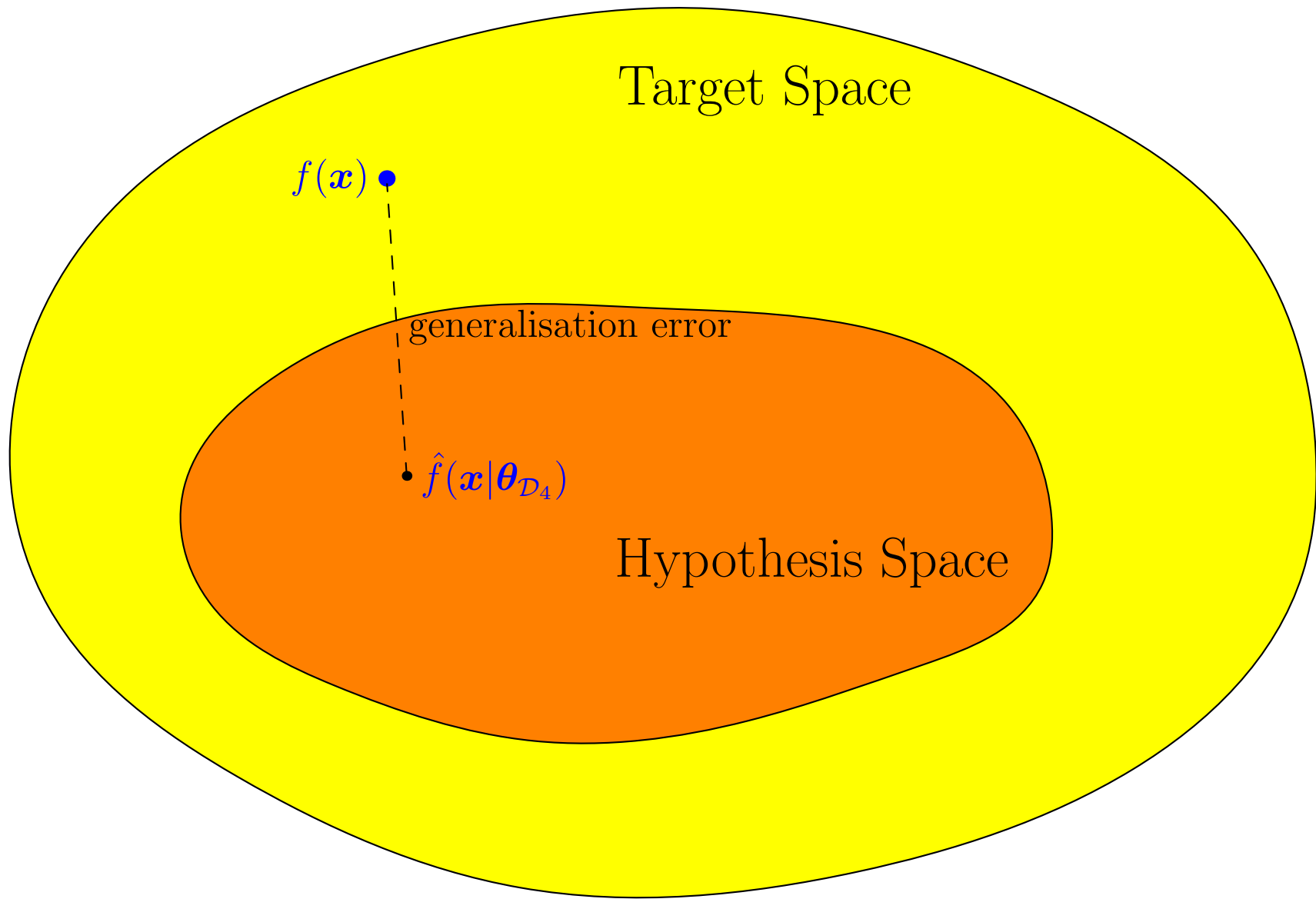
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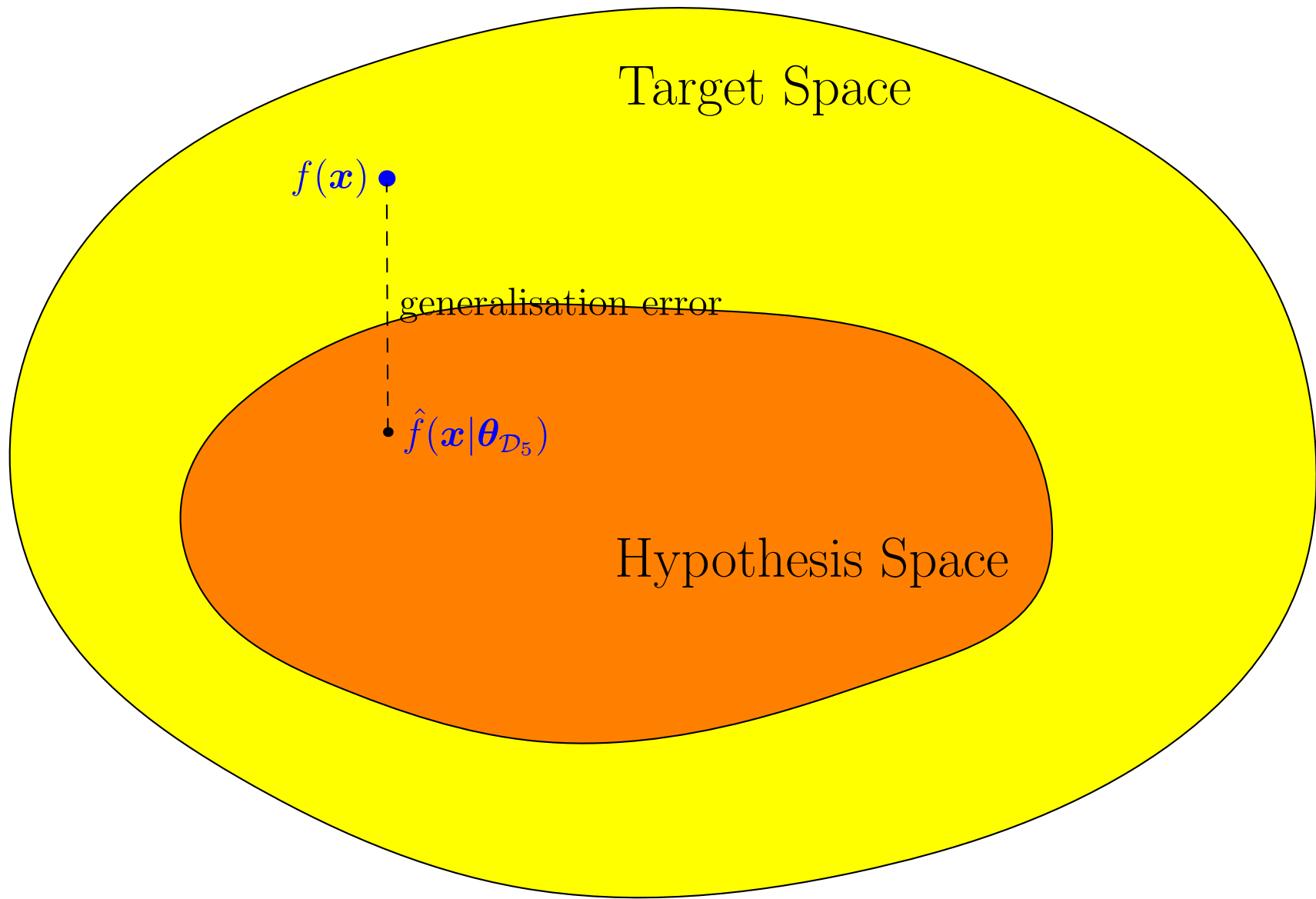
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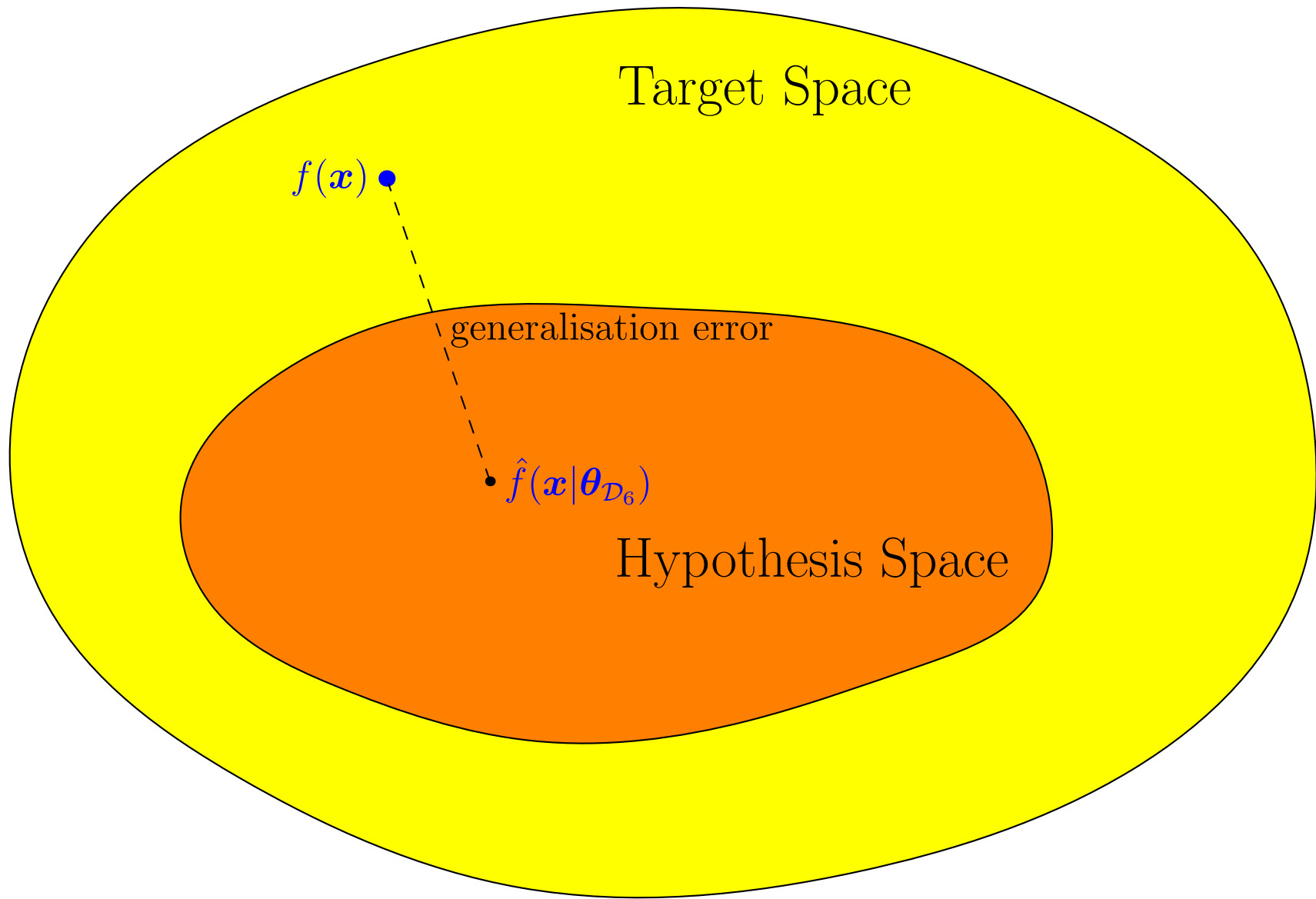
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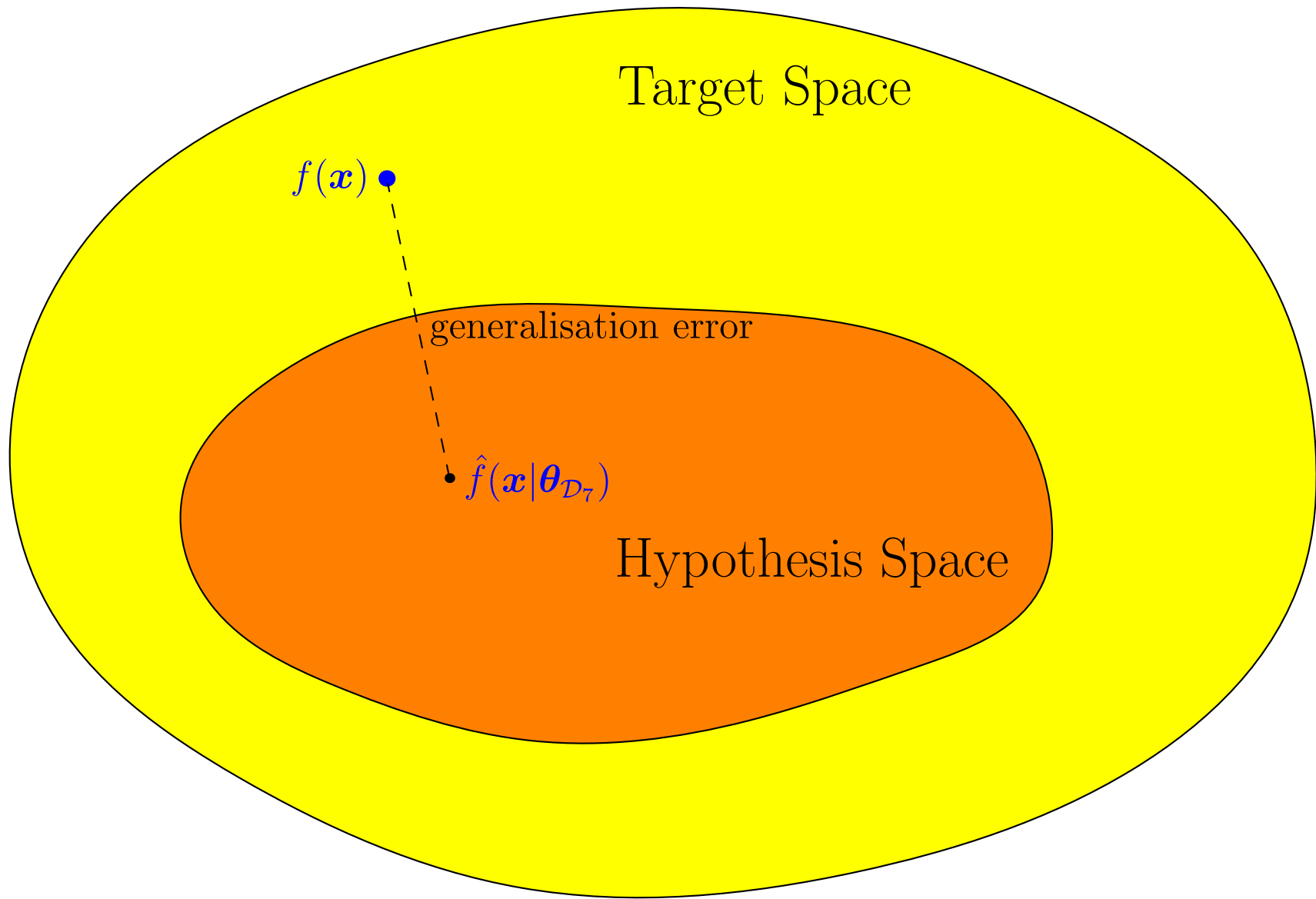
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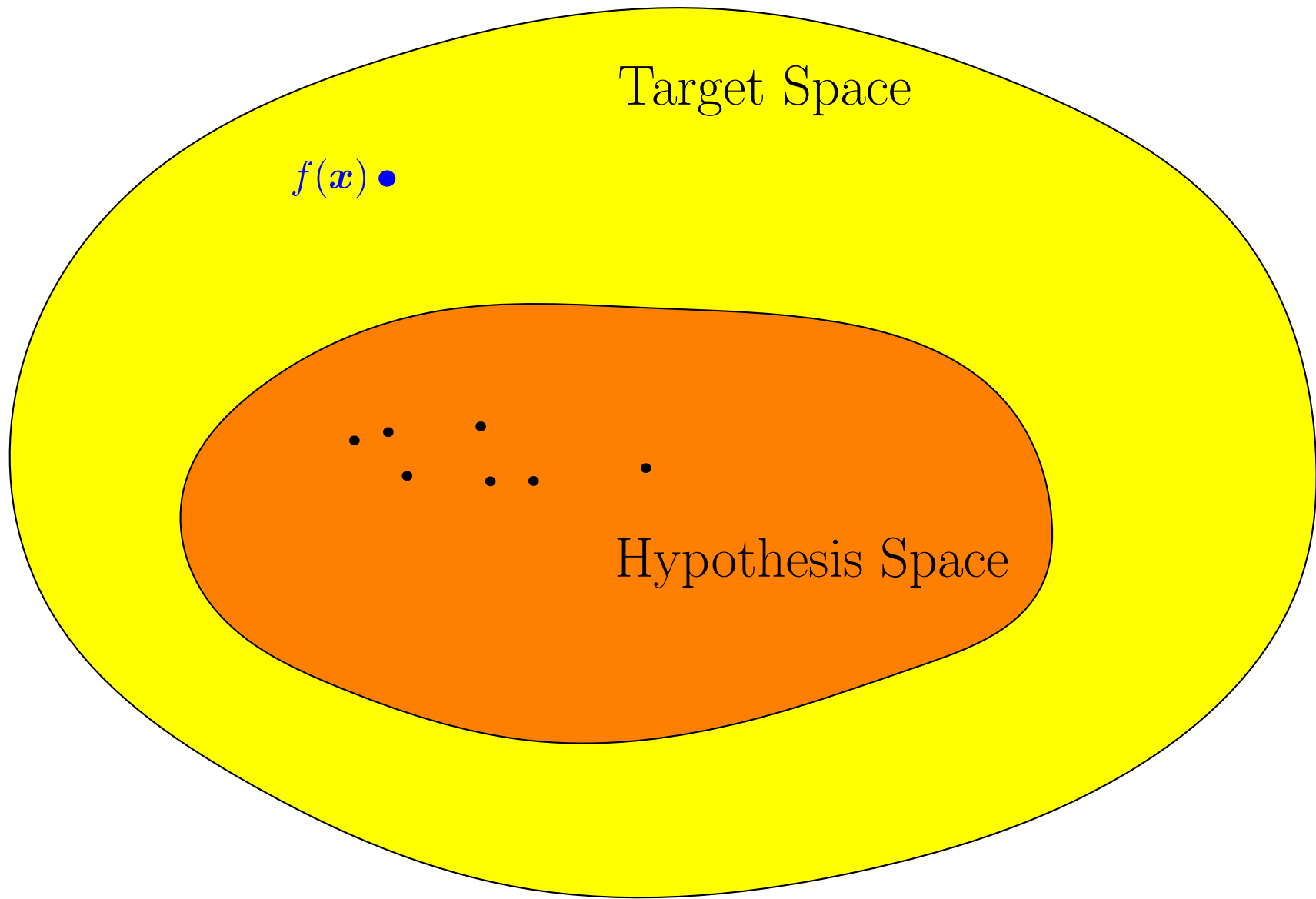
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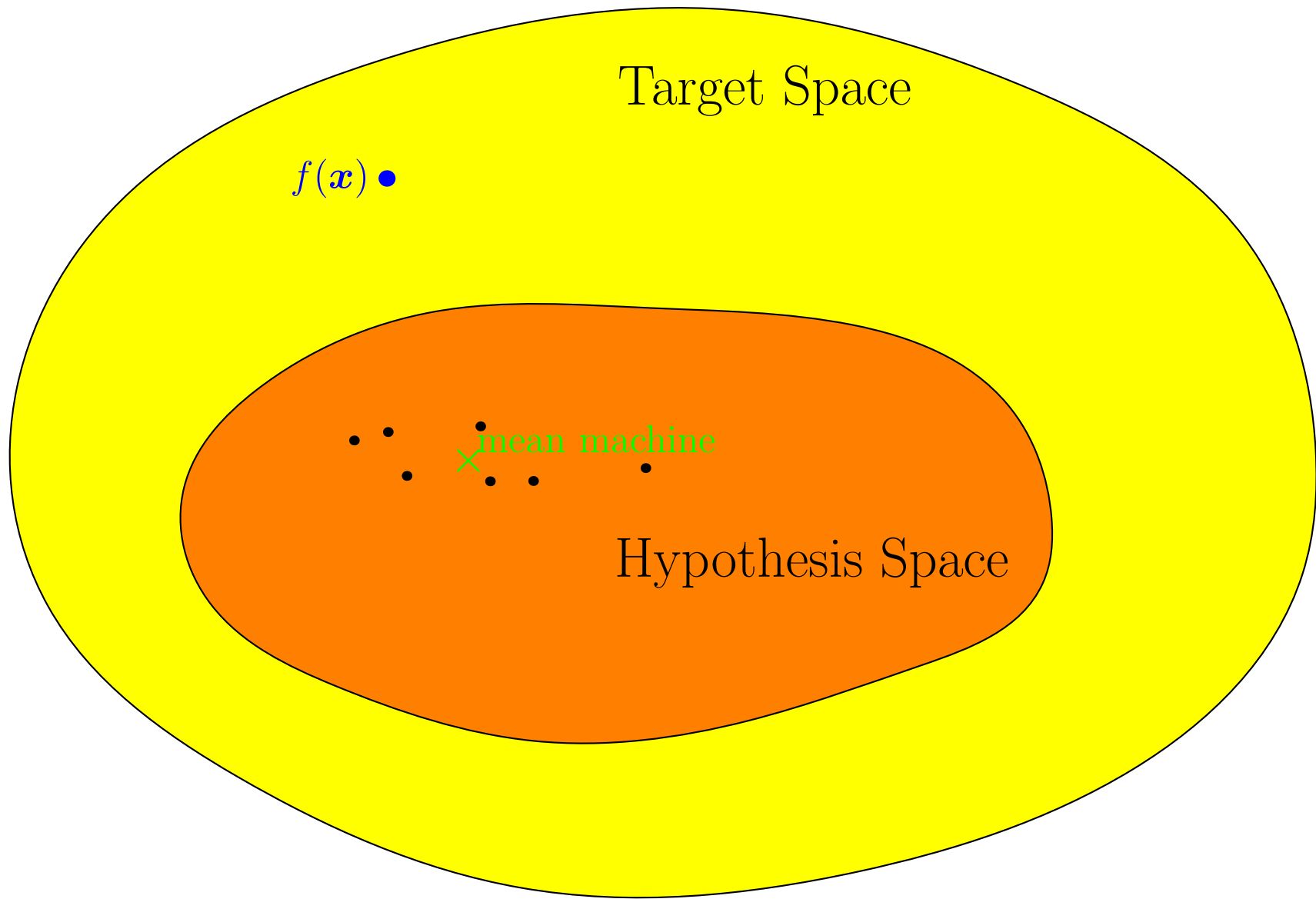
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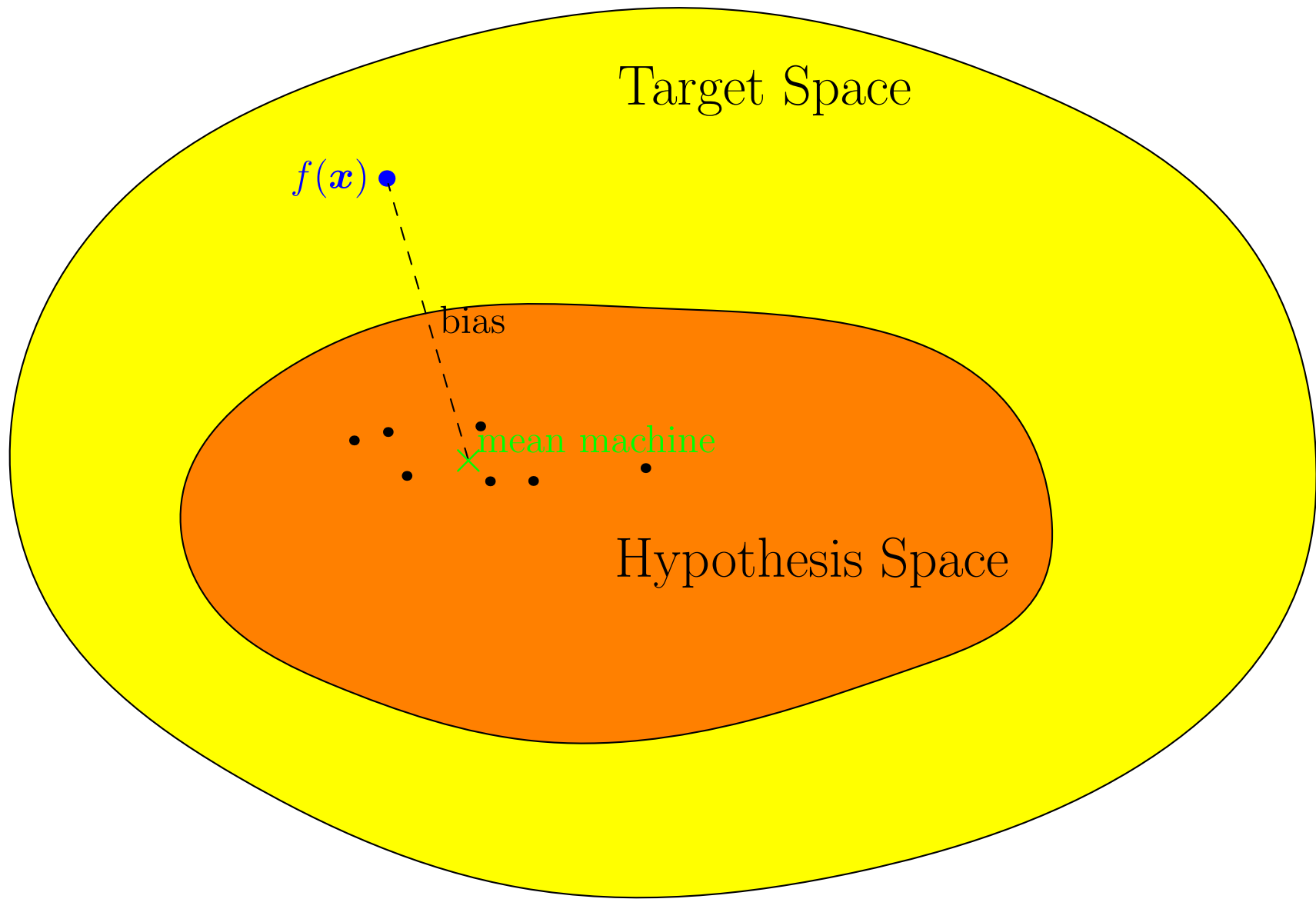
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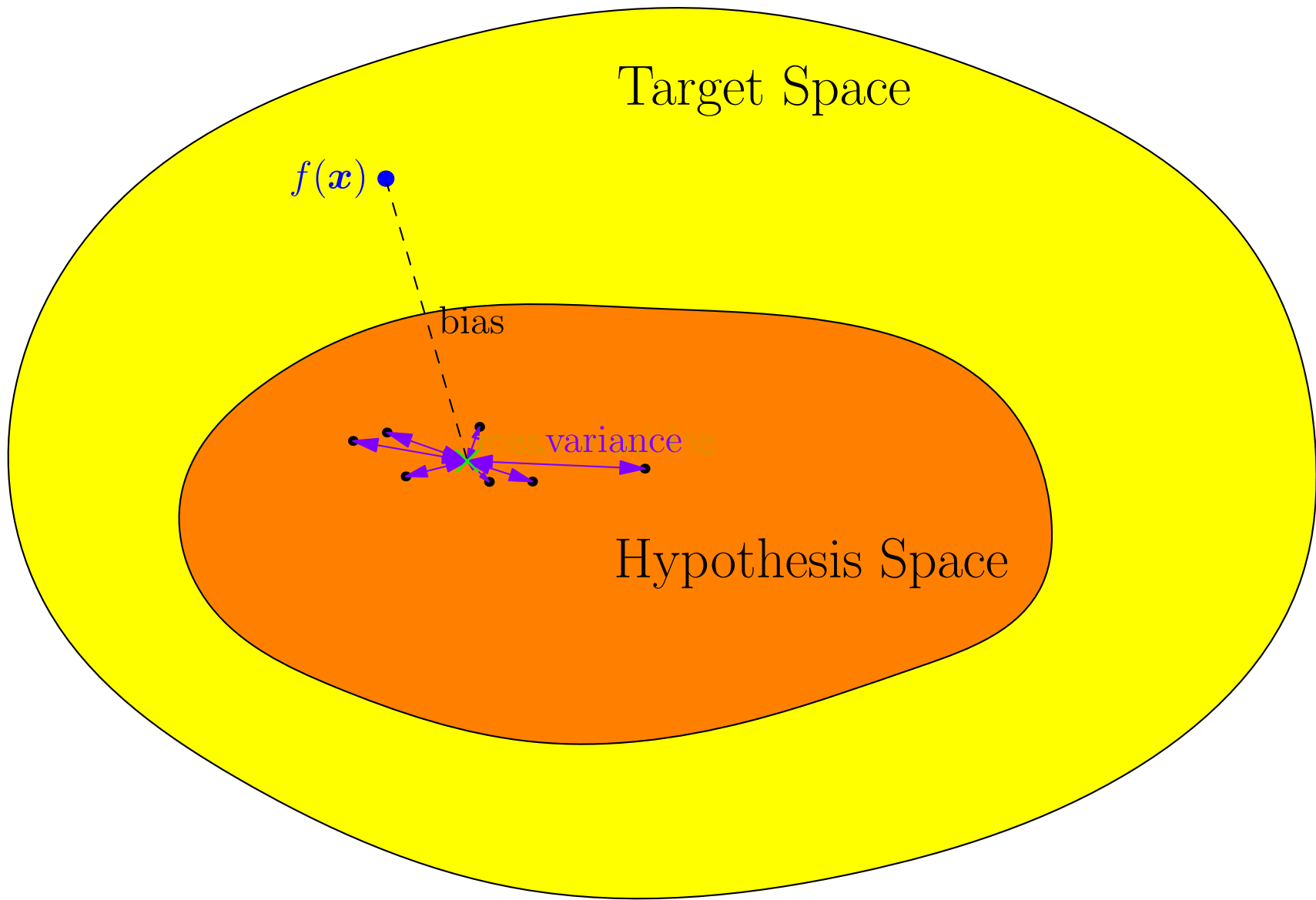
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Mean Machine

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

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

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

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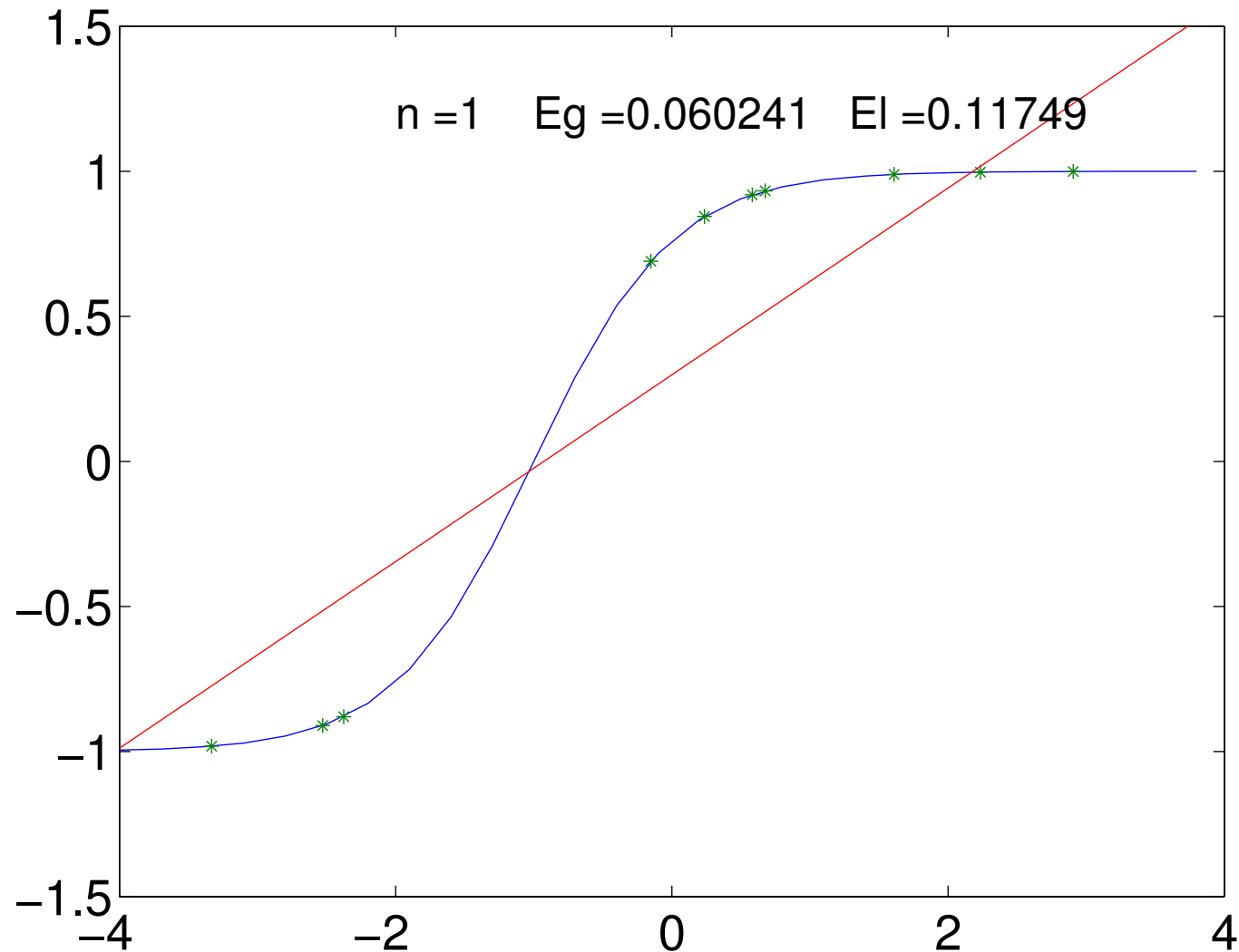
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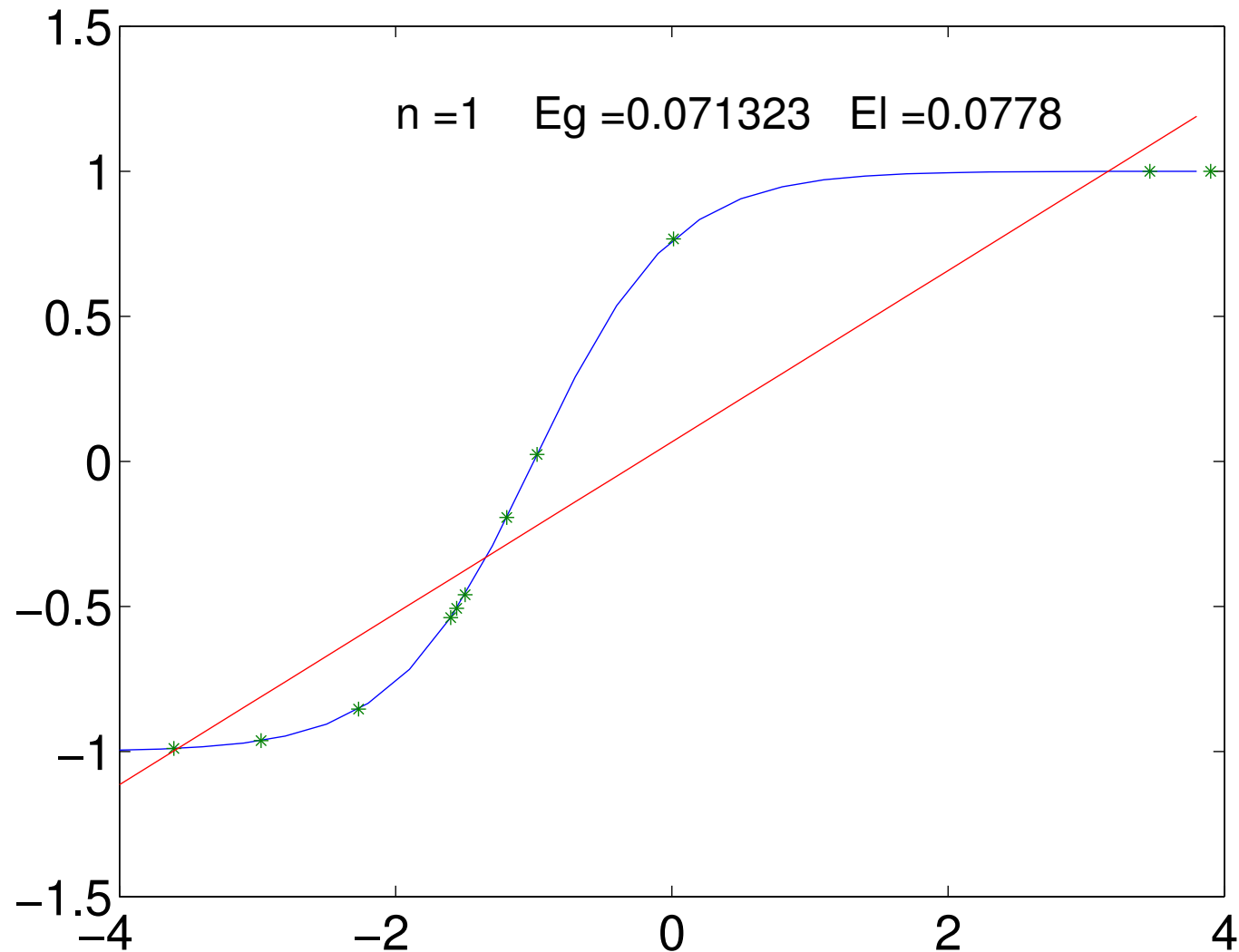
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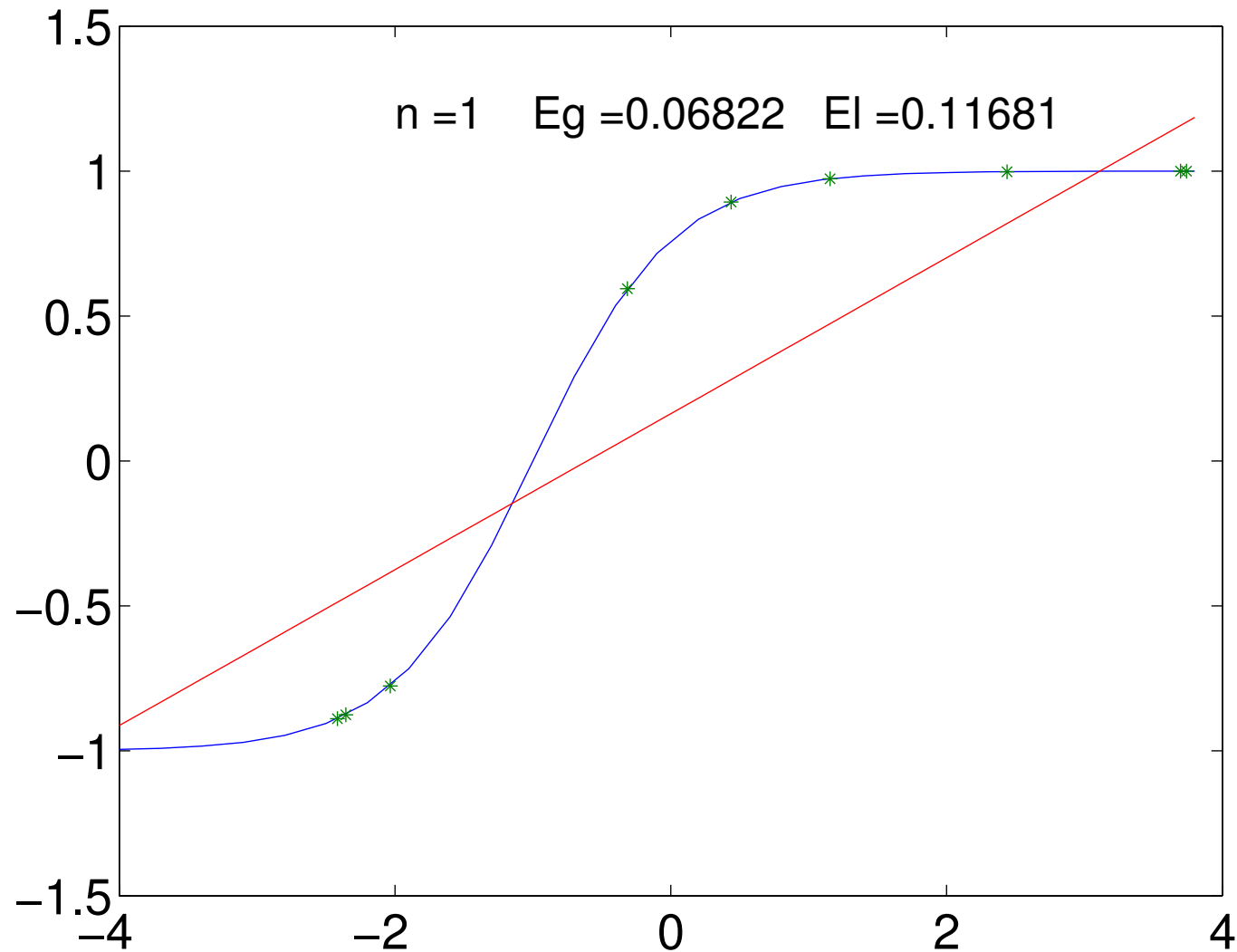
Regression Example $n = 1$



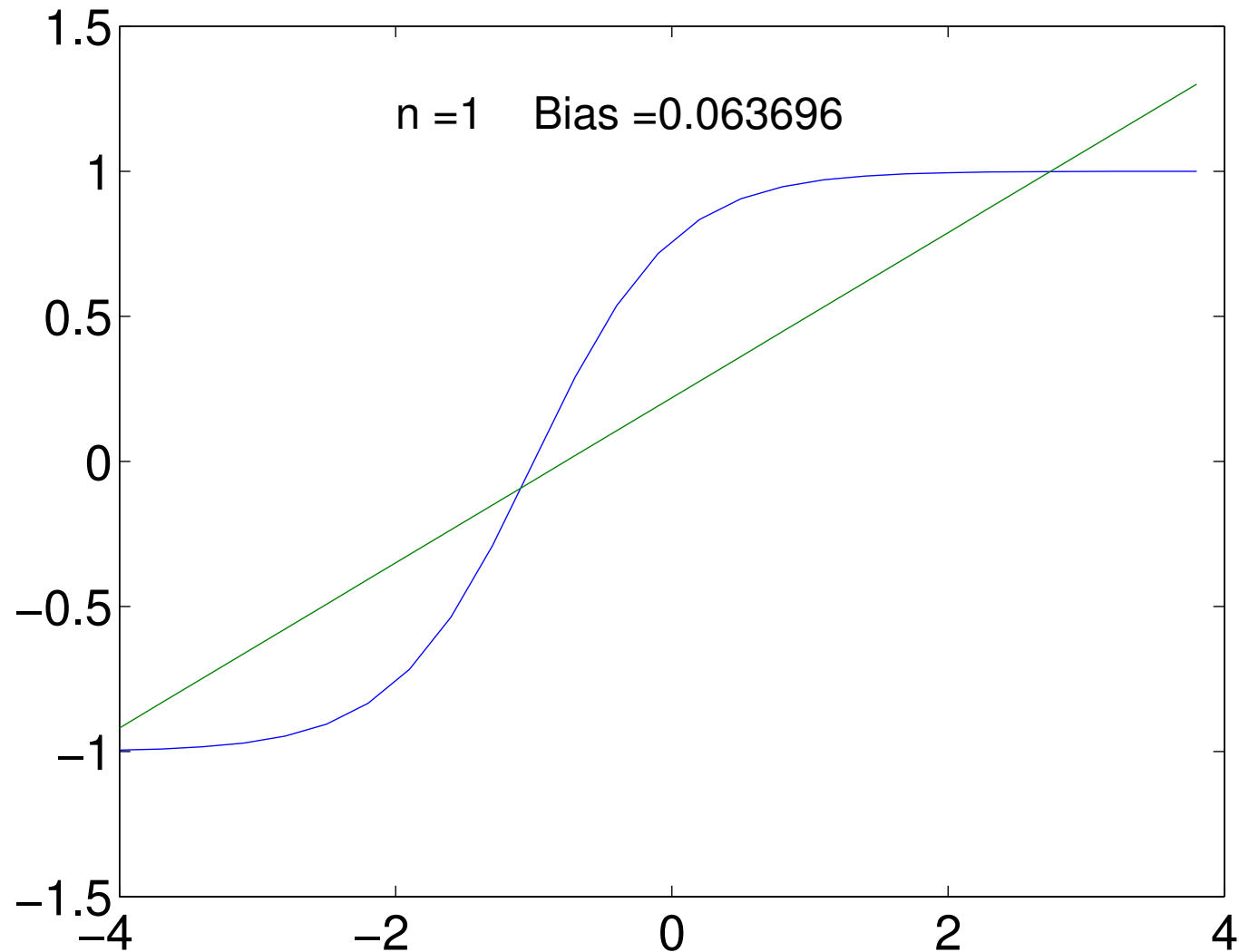
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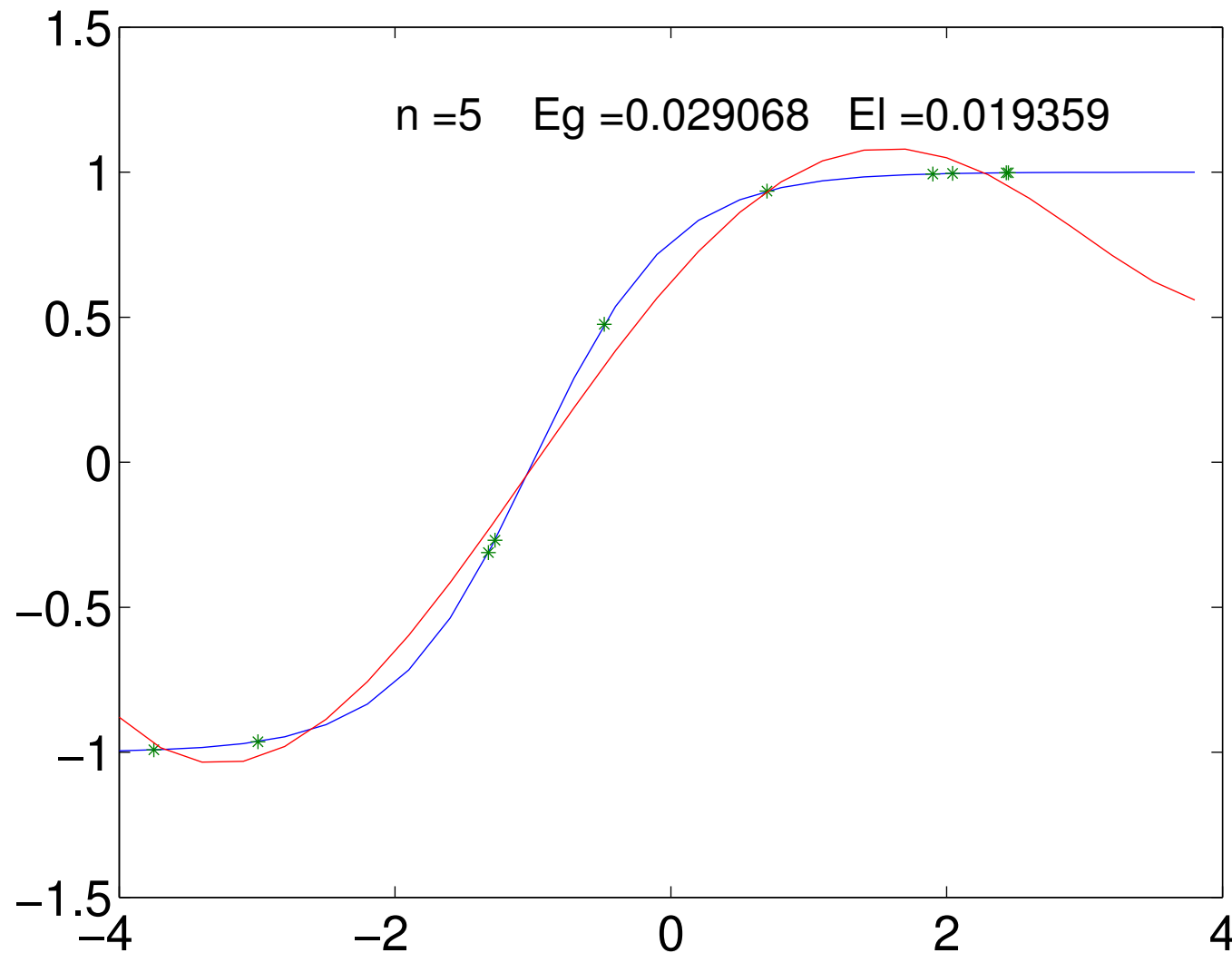
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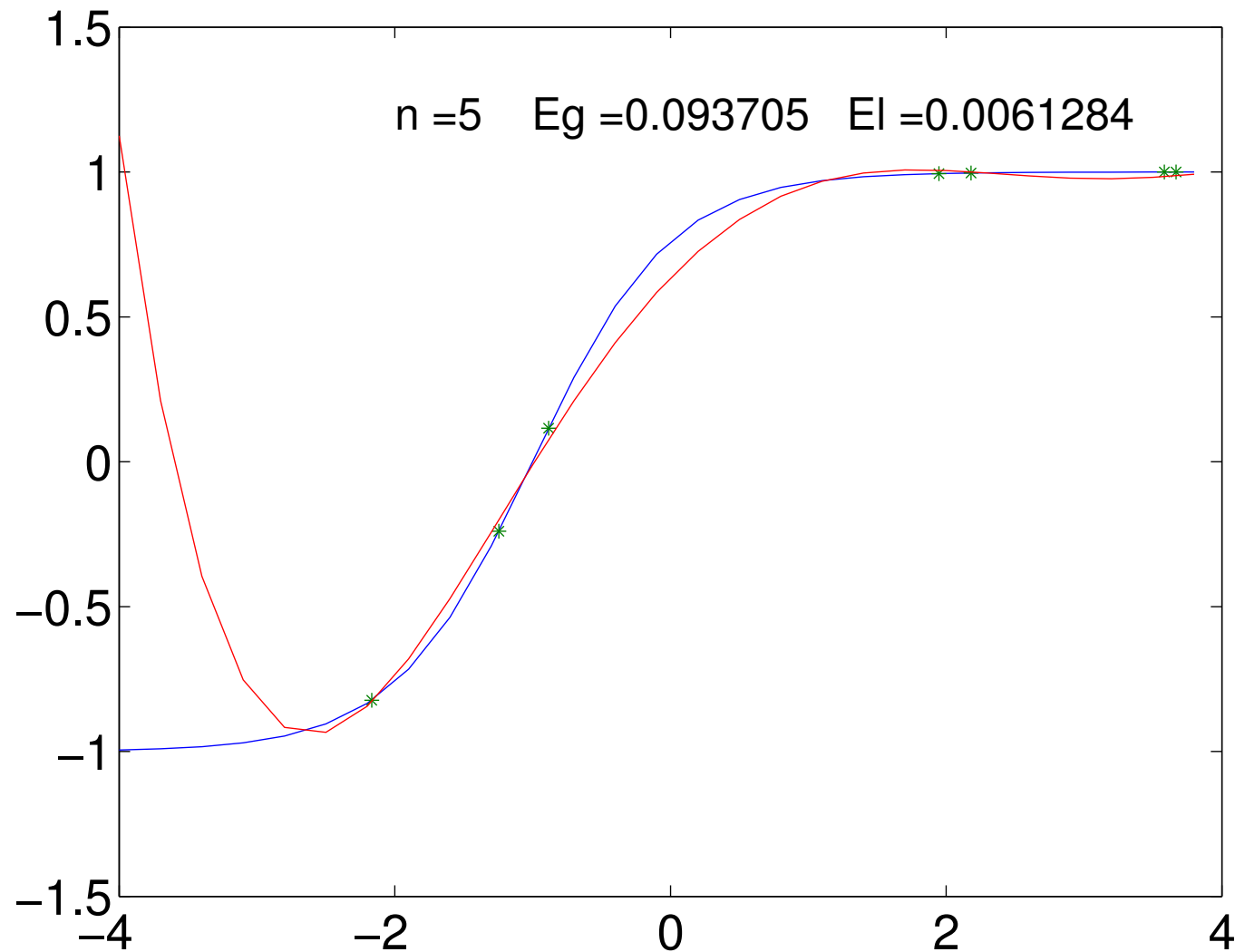
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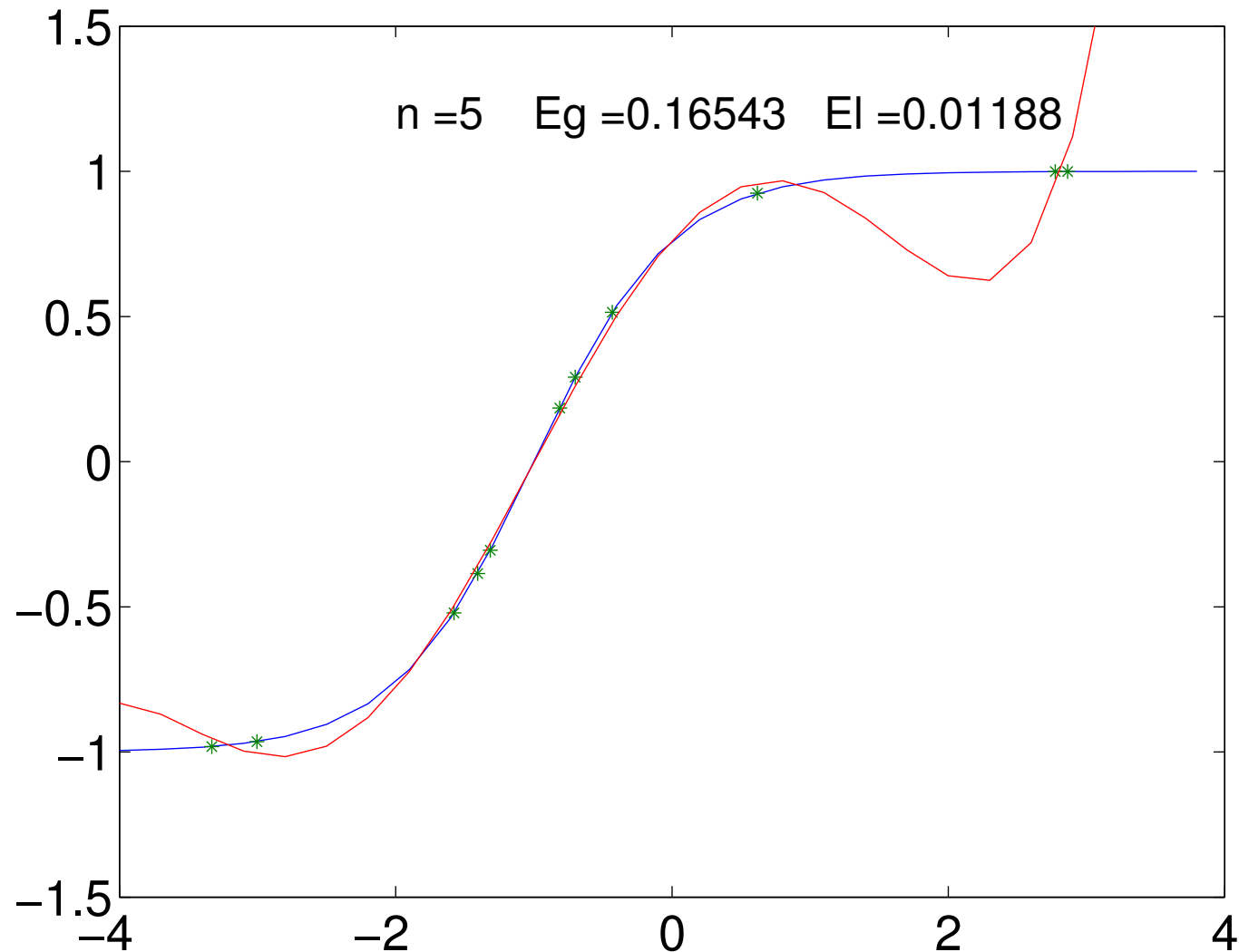
Regression Example $n = 5$



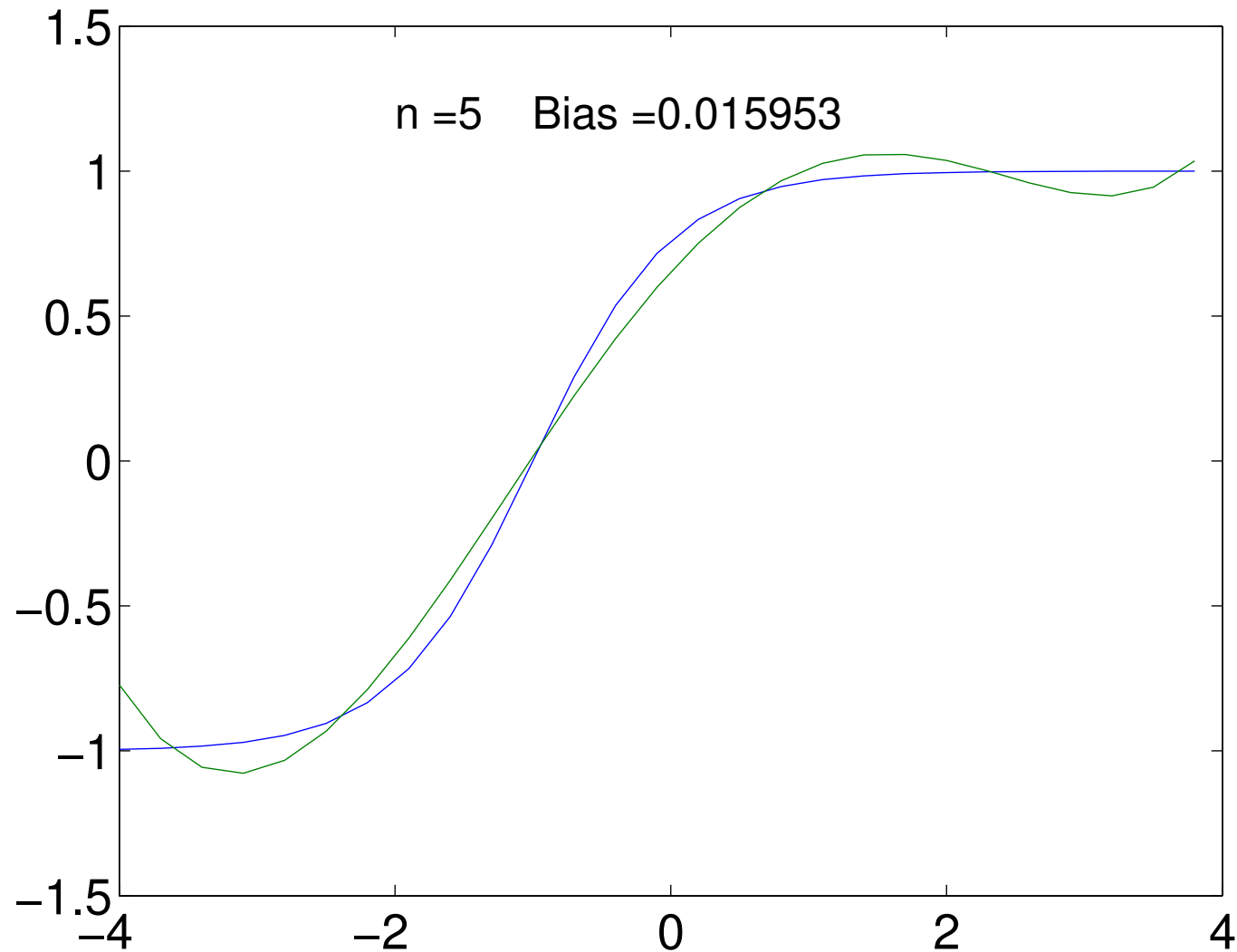
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Bias and Variance

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

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

Cross Term

- The cross term vanishes

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

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- Thus

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Bias and Variance

- We can write the expected generalisation loss as

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

- 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 machines 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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Lessons

- This course is about understanding machine learning techniques that work well
- Which one to use will depend on the data set
- One of the most useful intuitions about what works is the bias-variance framework
- The bias is high for simple machines that can't capture the data
- The variance is high for complex machines that are sensitive to the training set
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