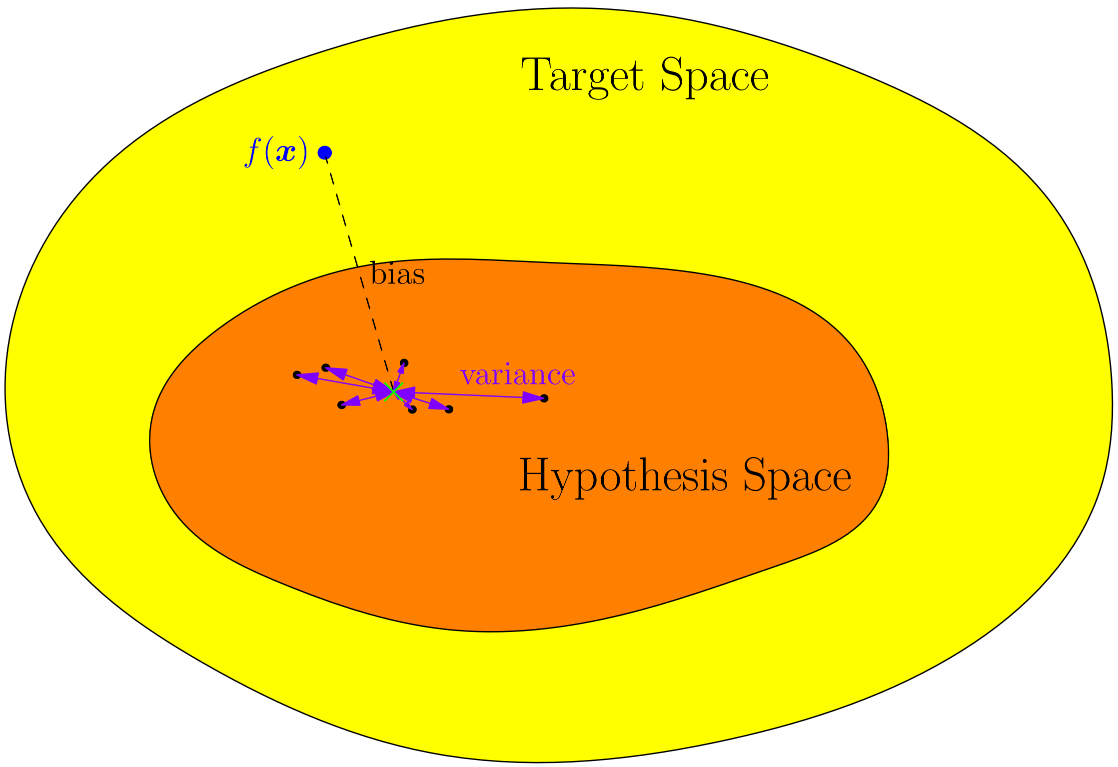
Advanced Machine Learning

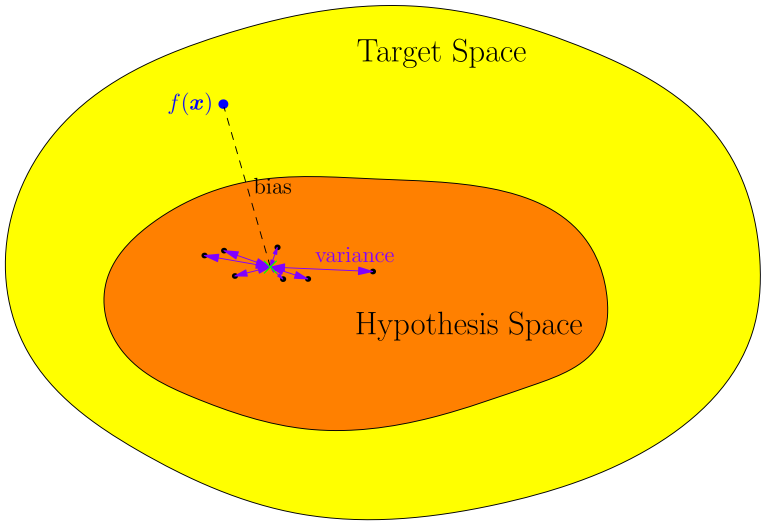
When Machine Learning Works



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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What Makes Machine Learning Hard?

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

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

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

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

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

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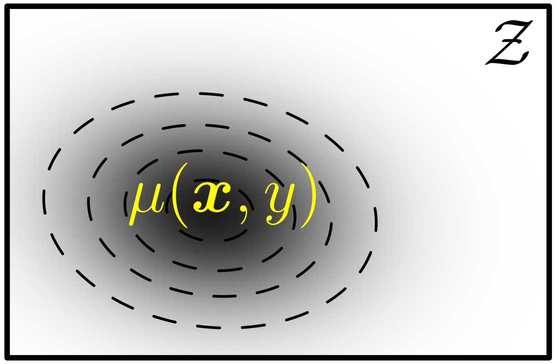

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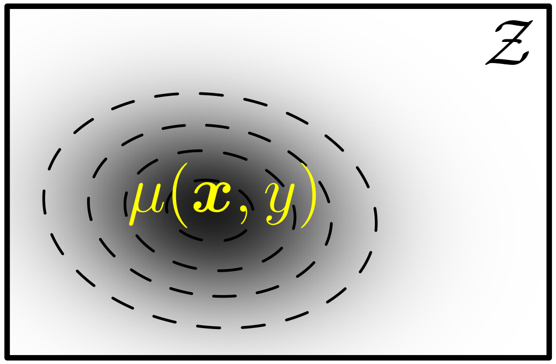

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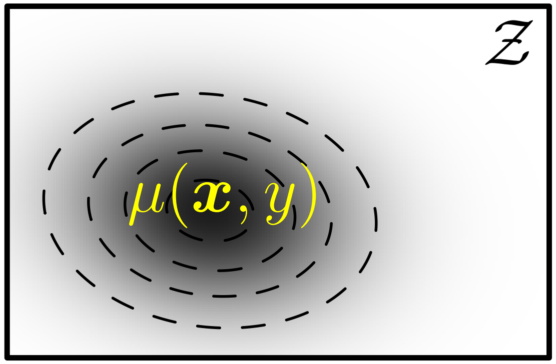

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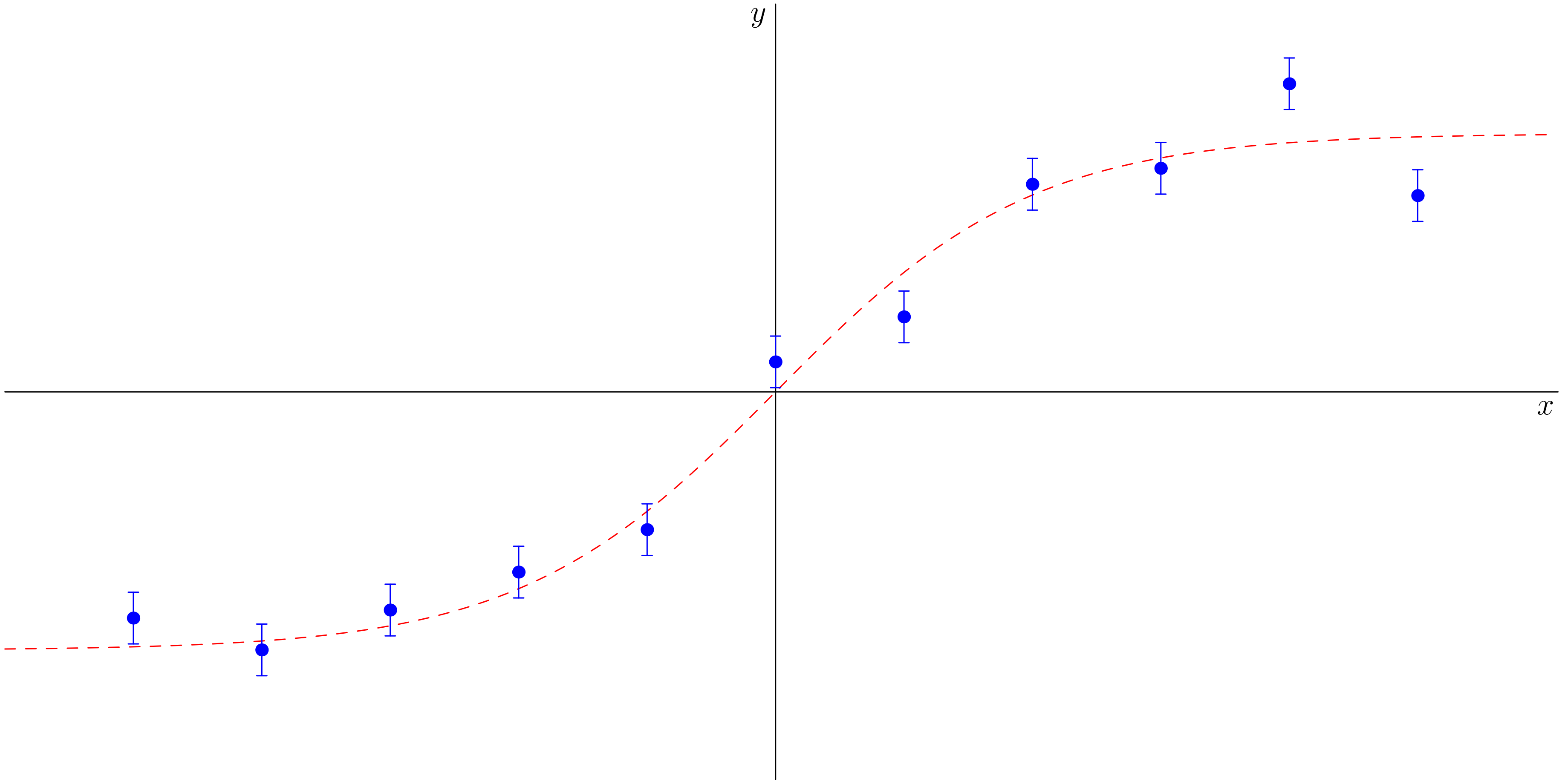

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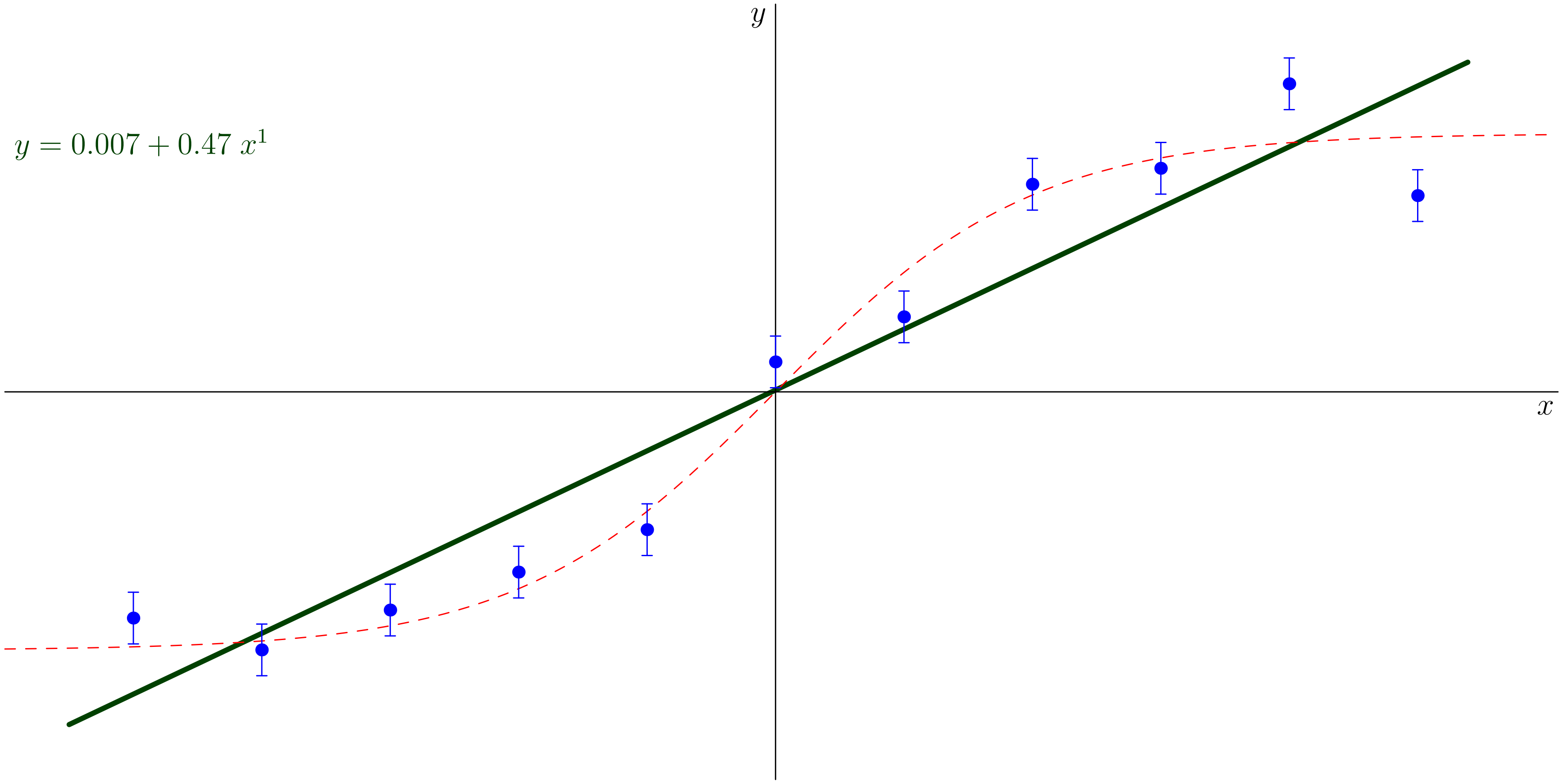

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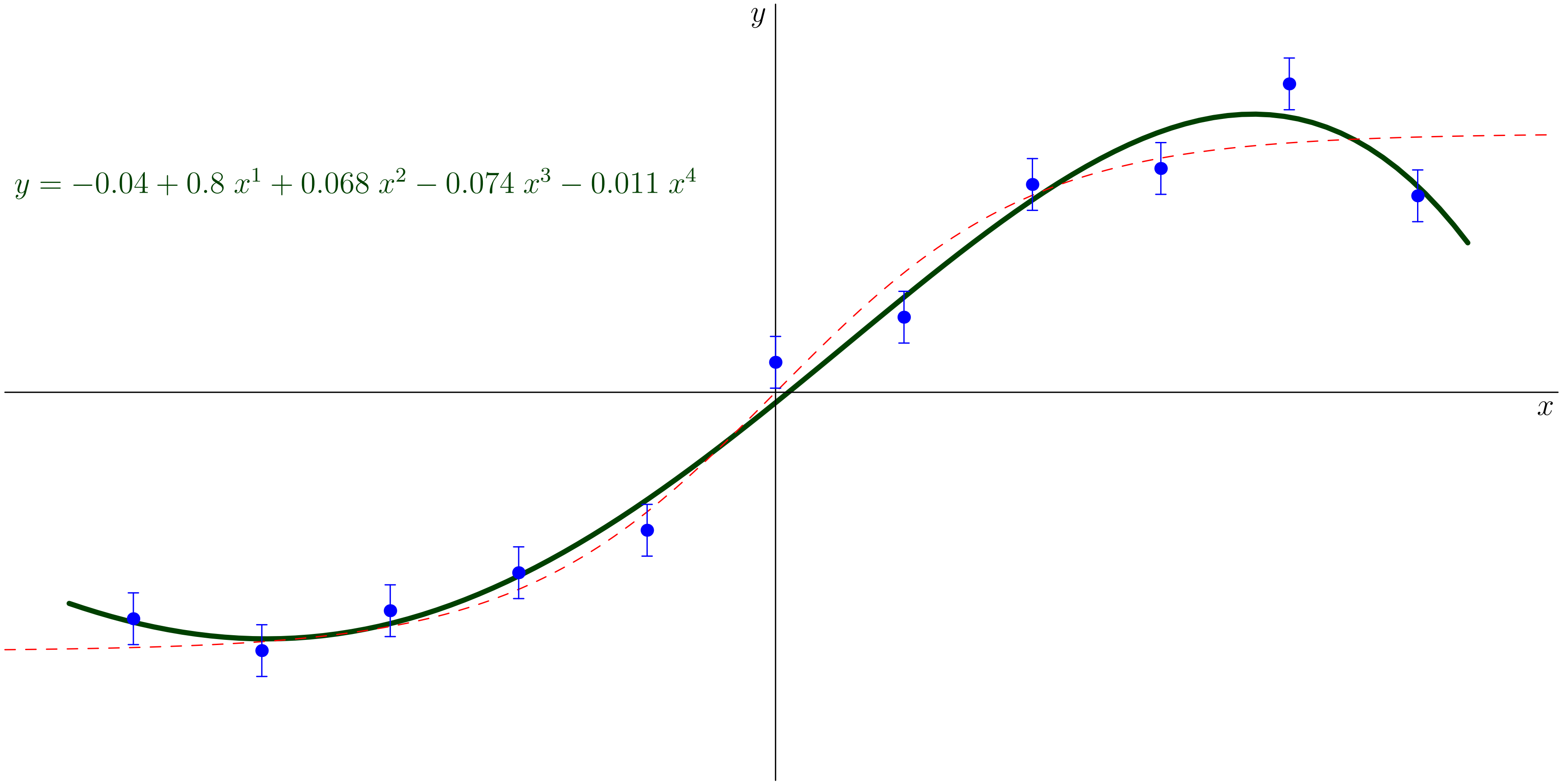

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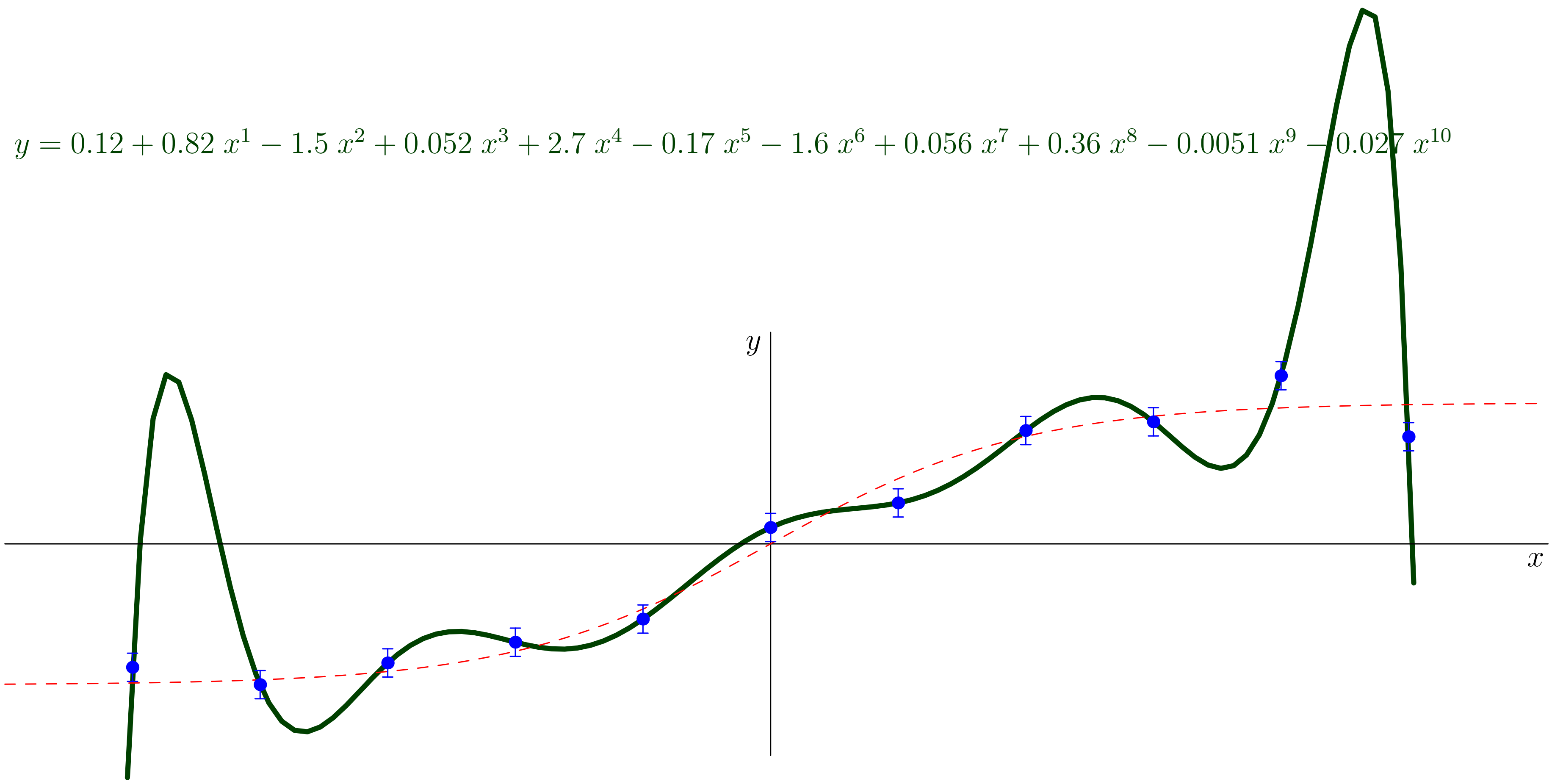
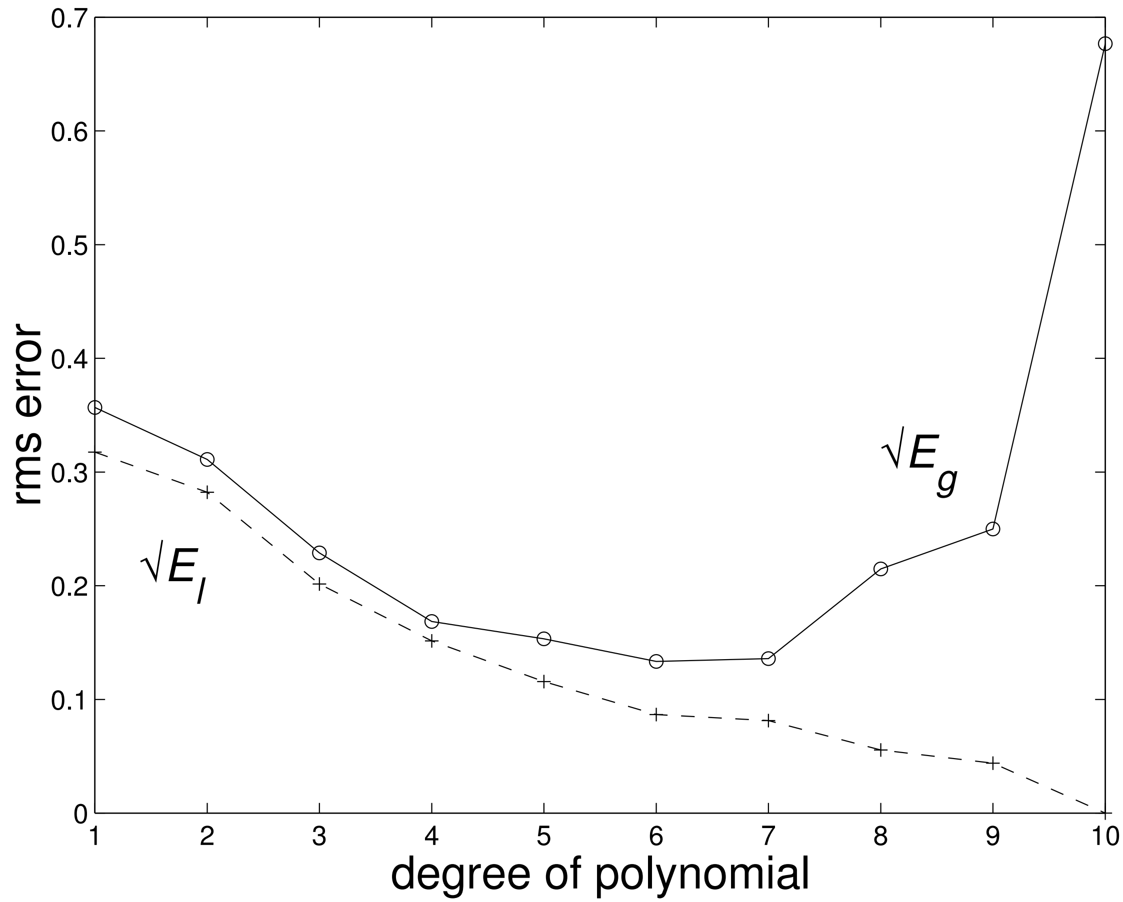


Measuring Generalisation Error for Regression

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



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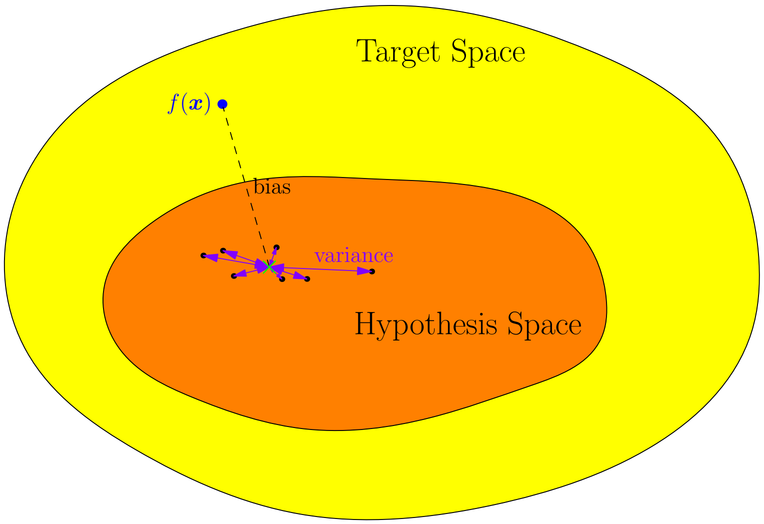

Expected Generalisation Performance

- 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 $\mu(\boldsymbol{x}, y)$
- For each data set, $\mathcal{D}$, we would learn a different approximator $\hat{f}(\boldsymbol{x}|\boldsymbol{\theta}_{\mathcal{D}})$
- 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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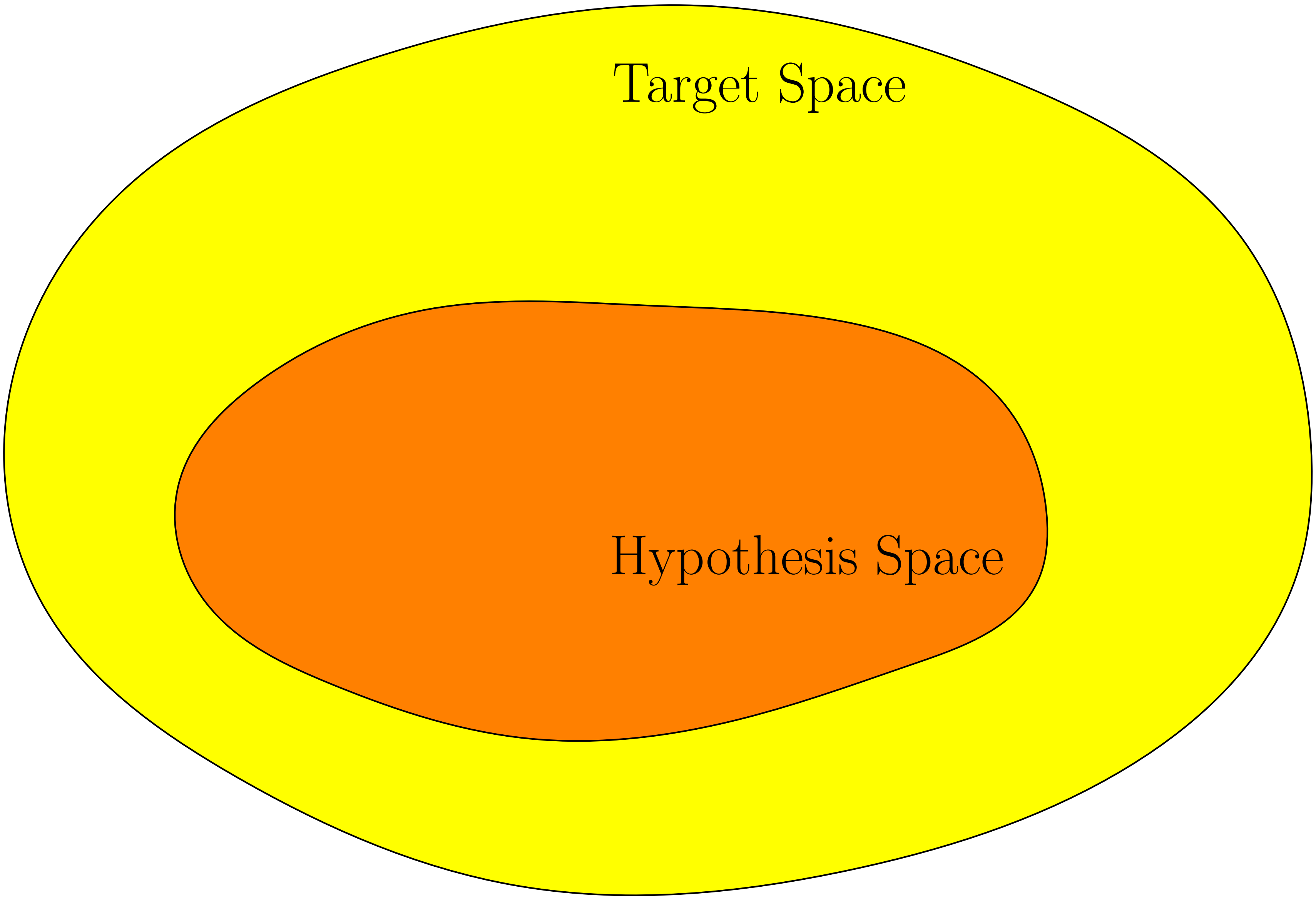

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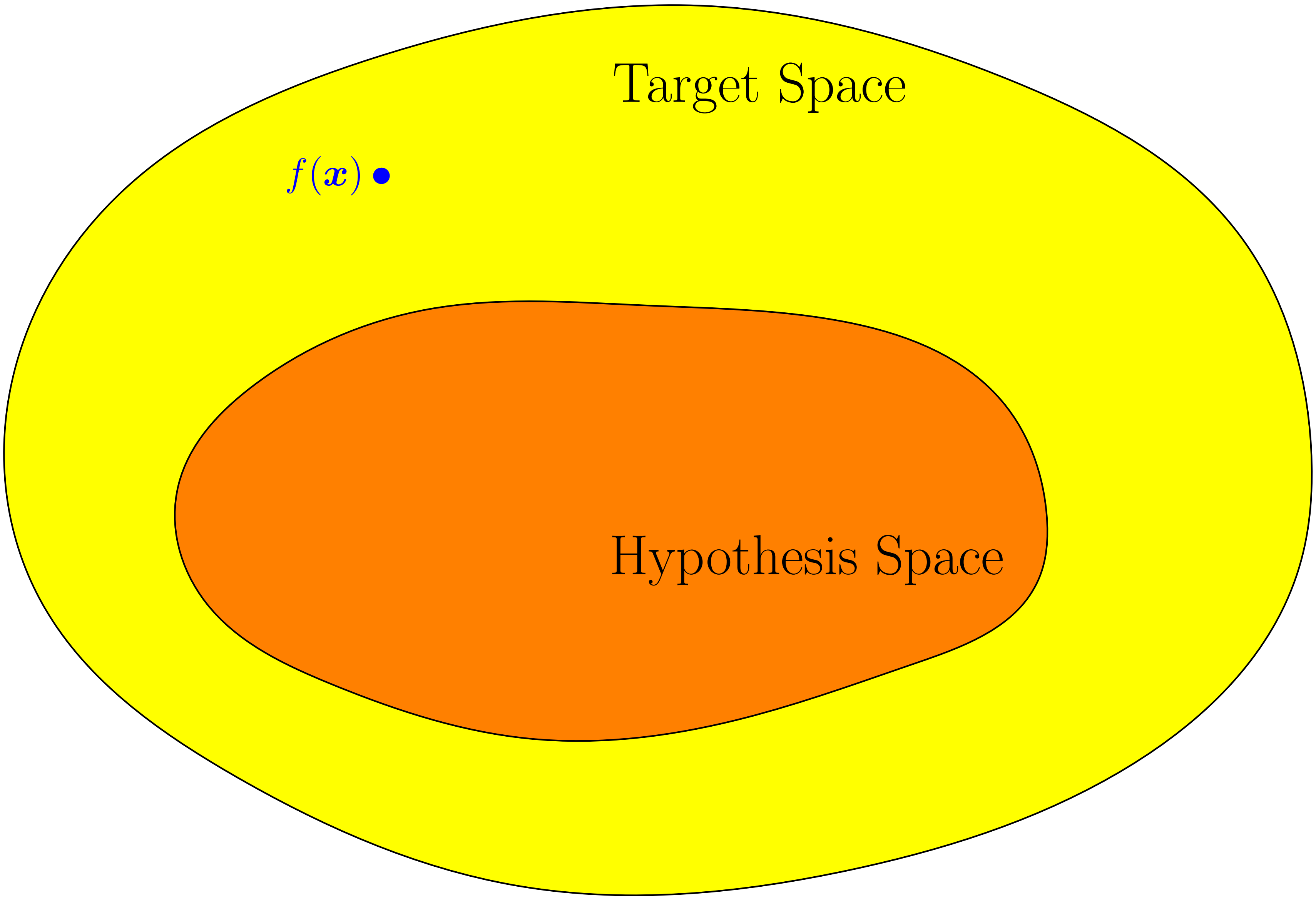

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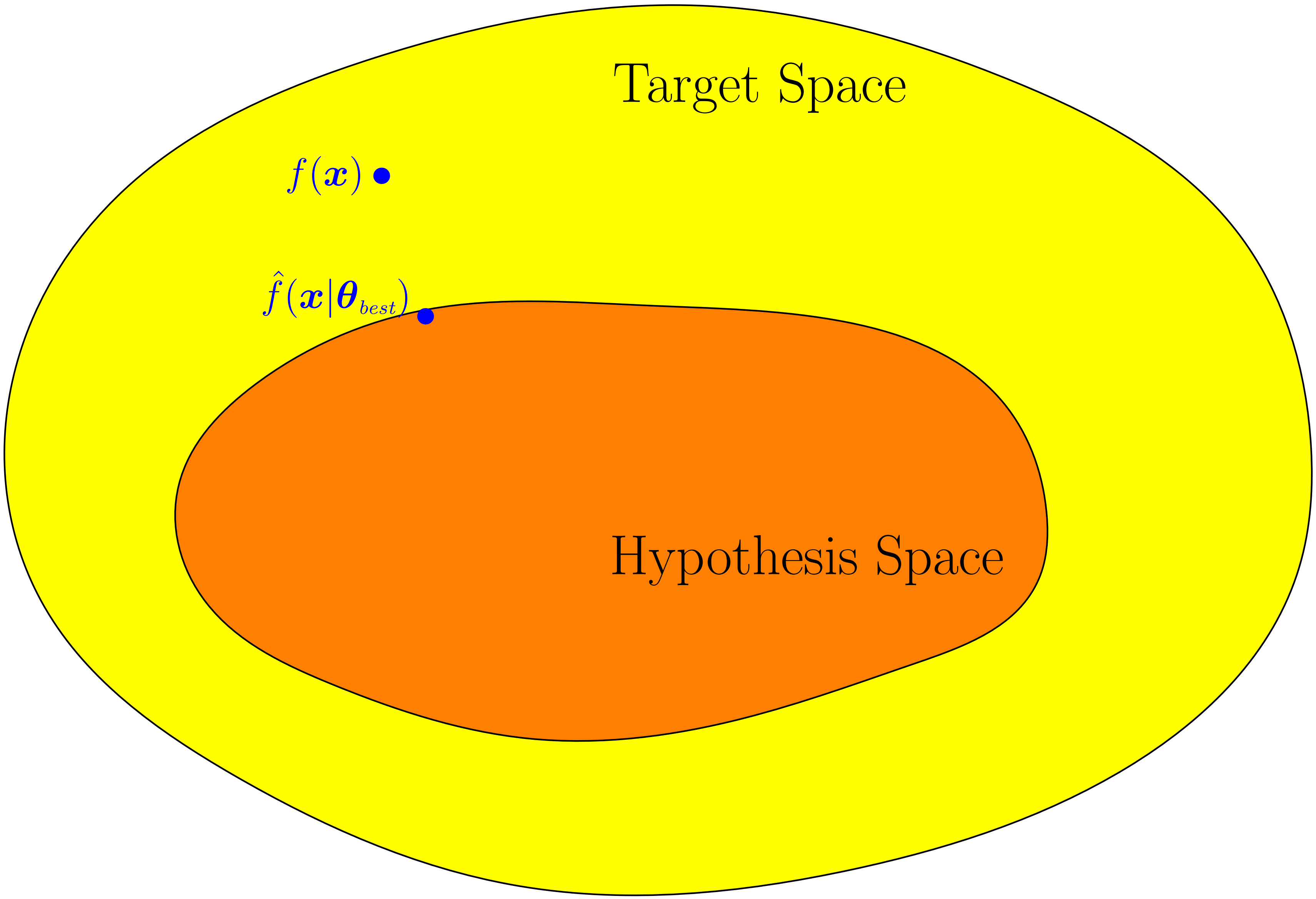

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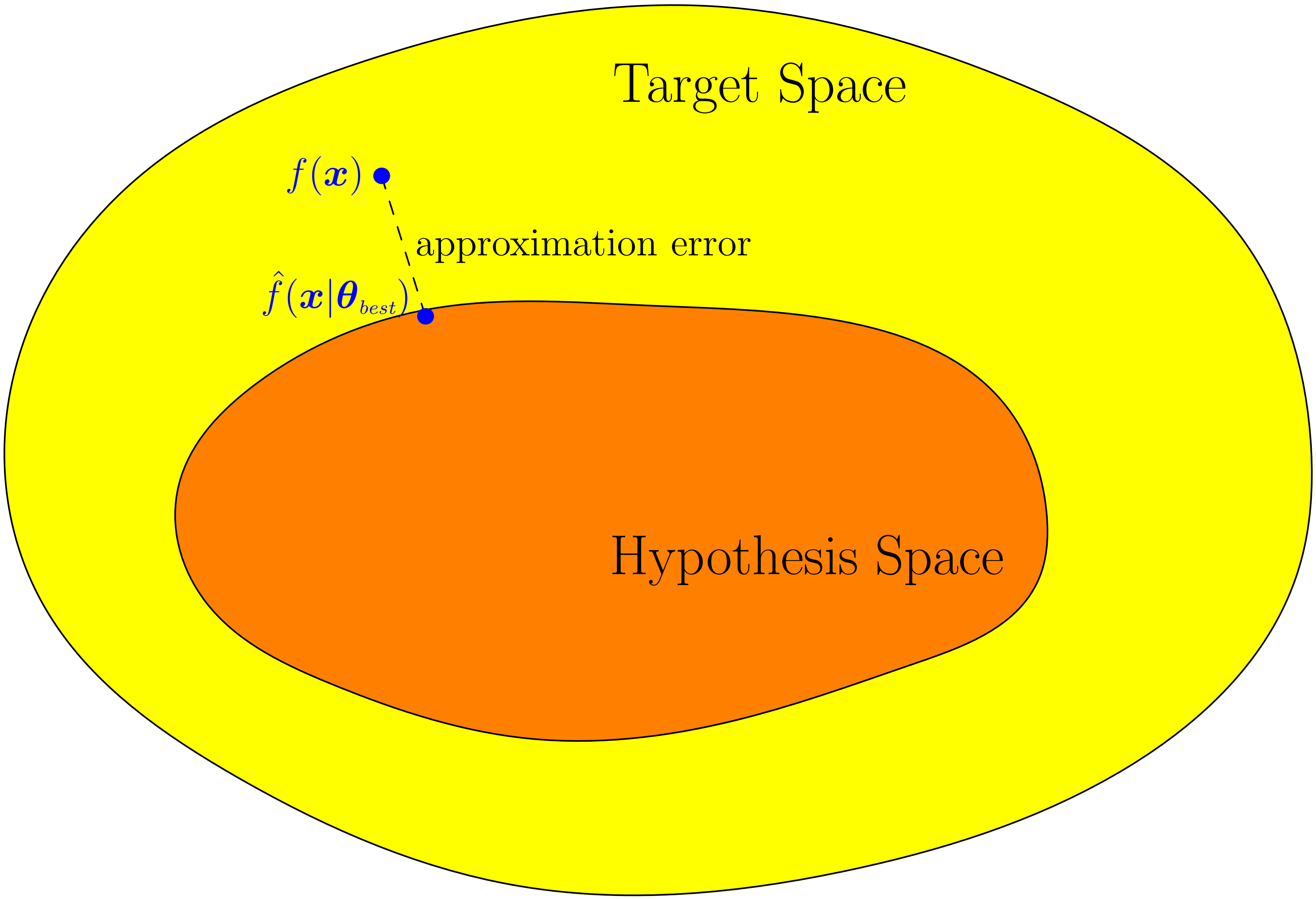

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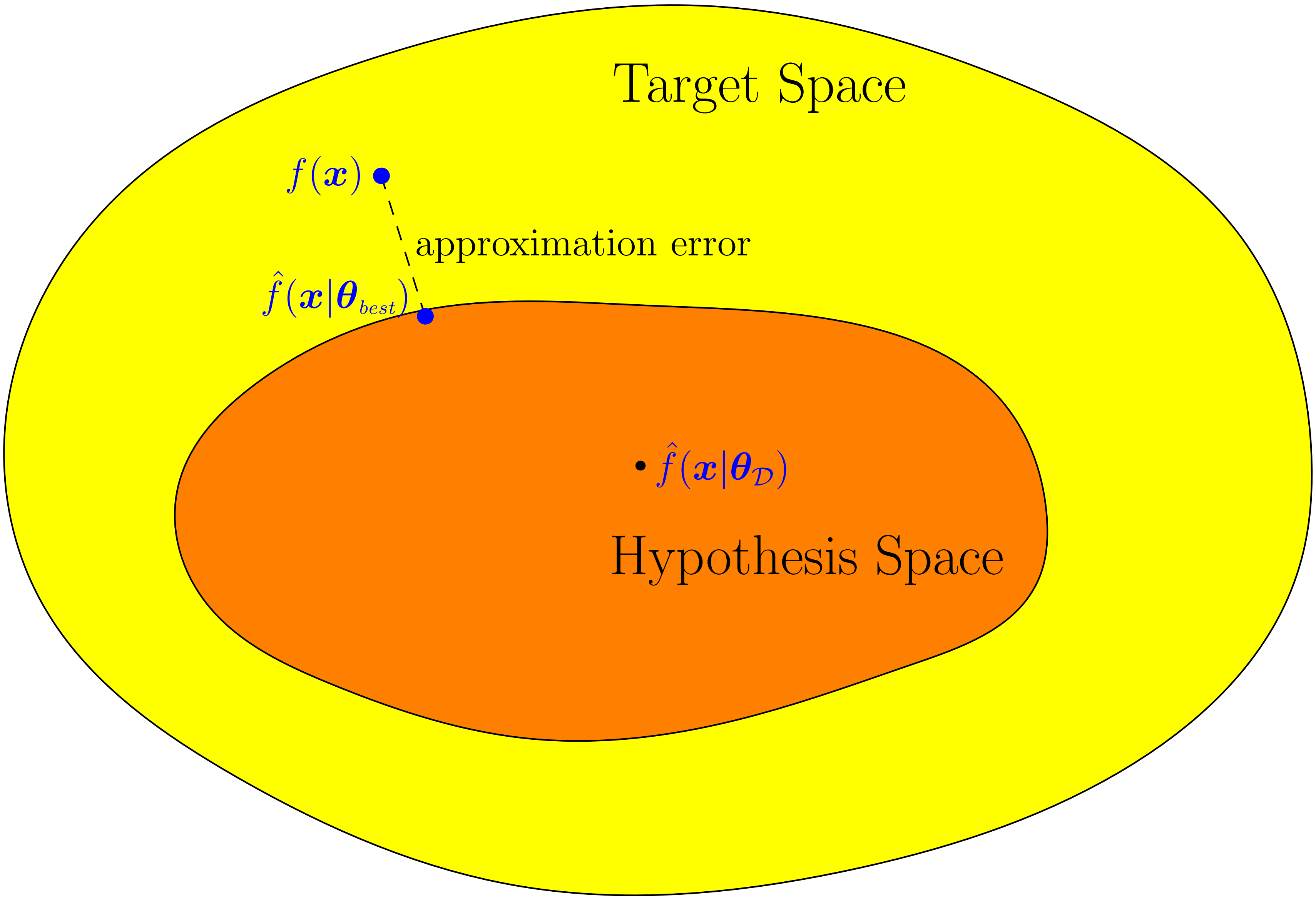

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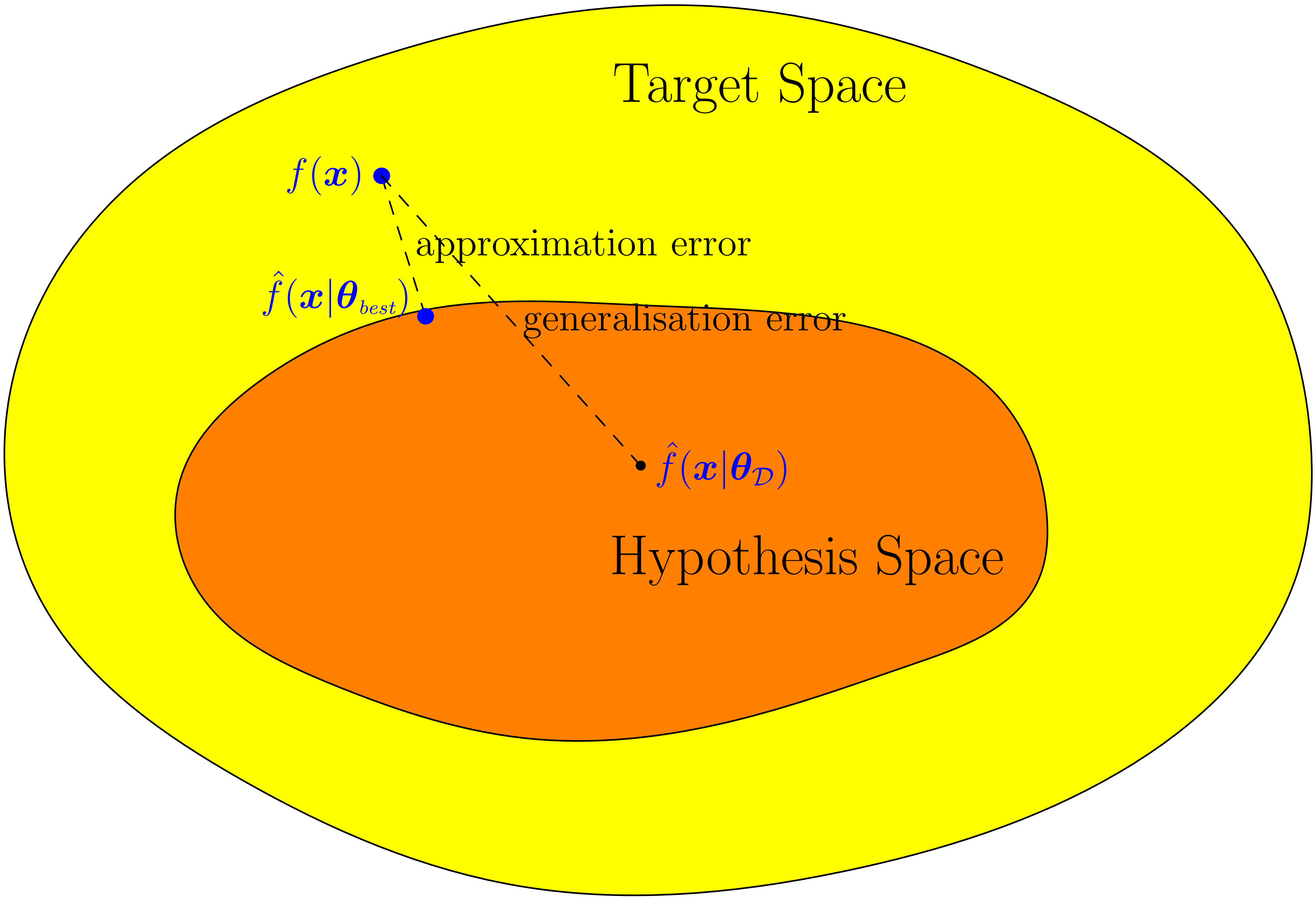

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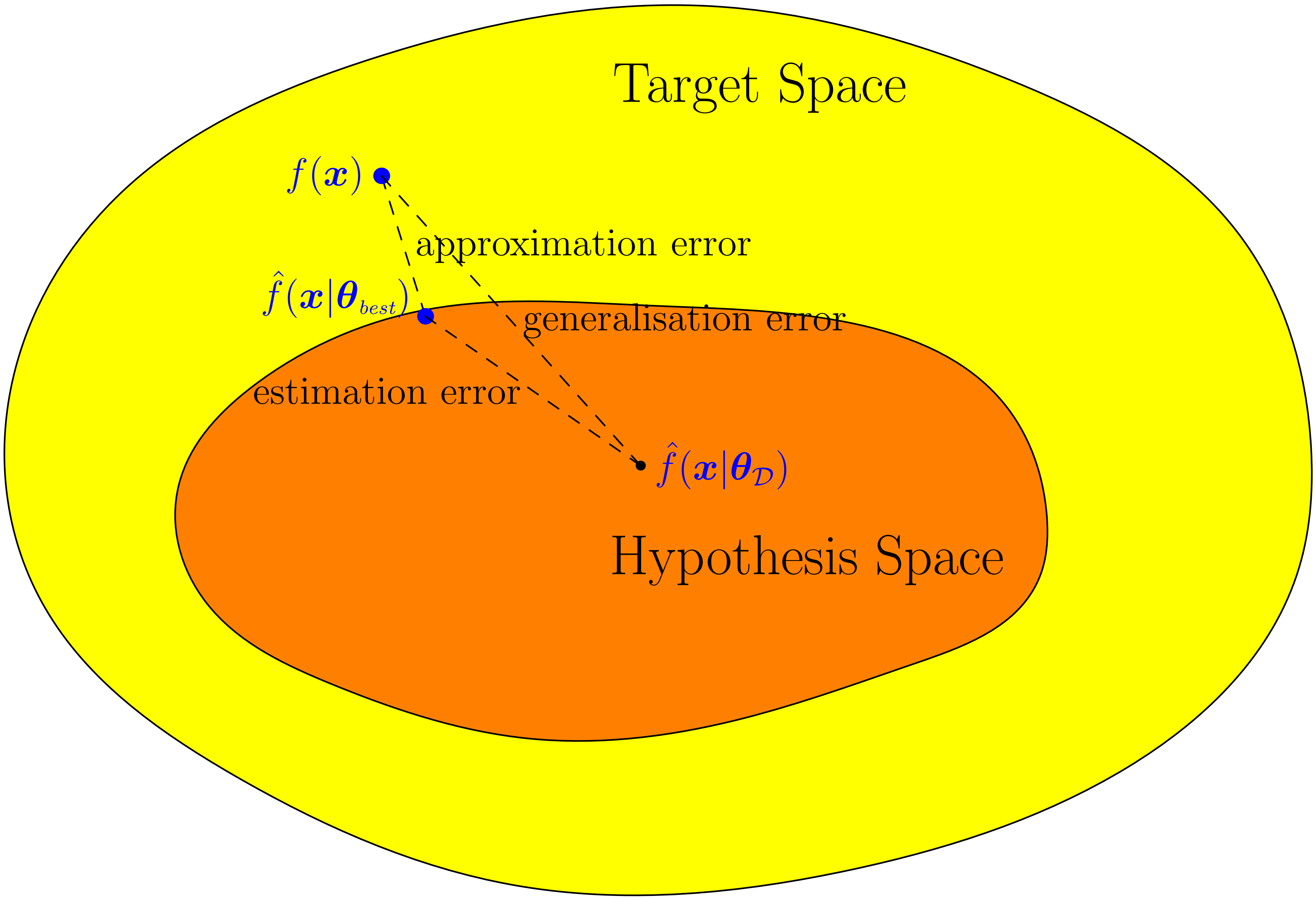

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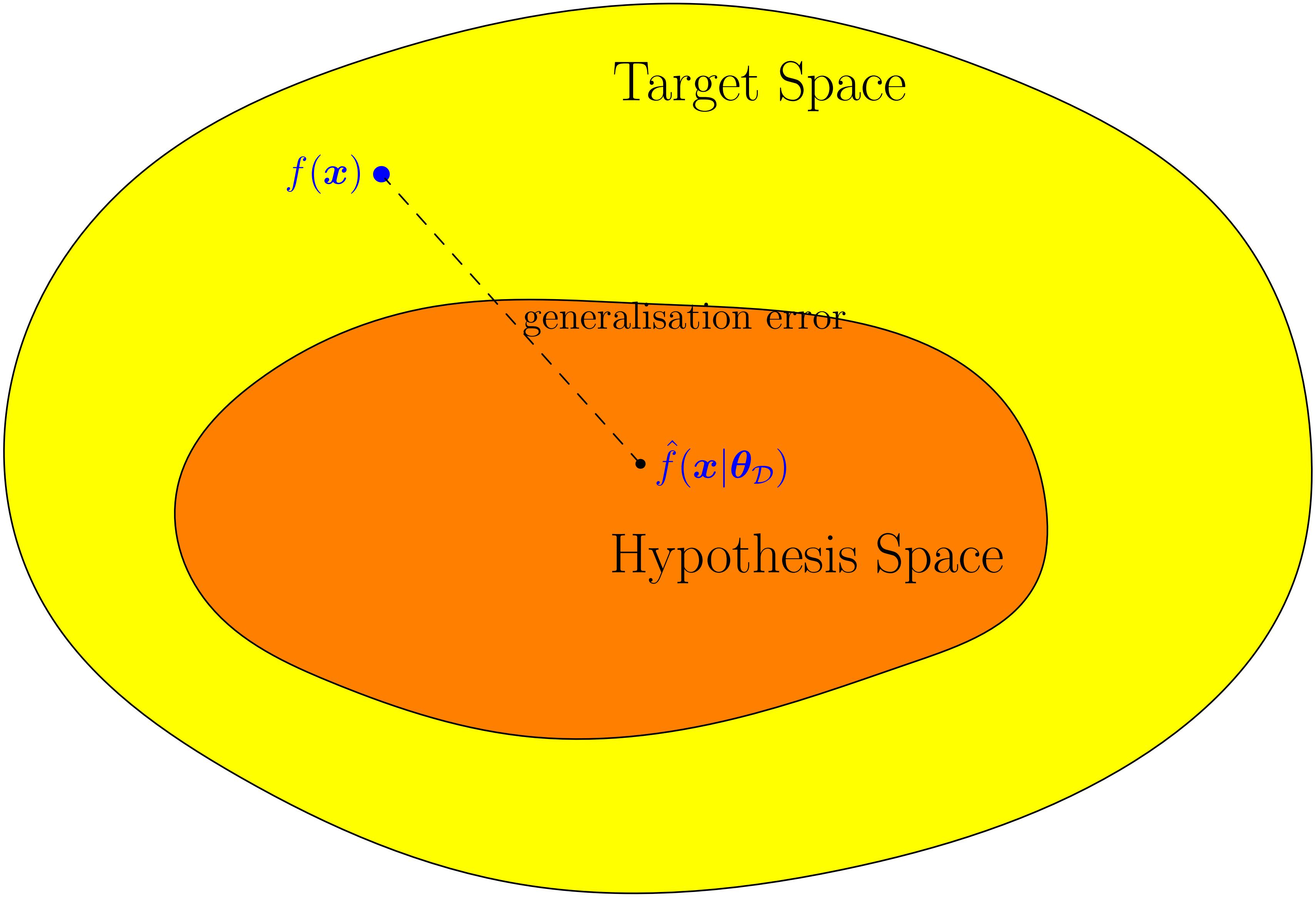

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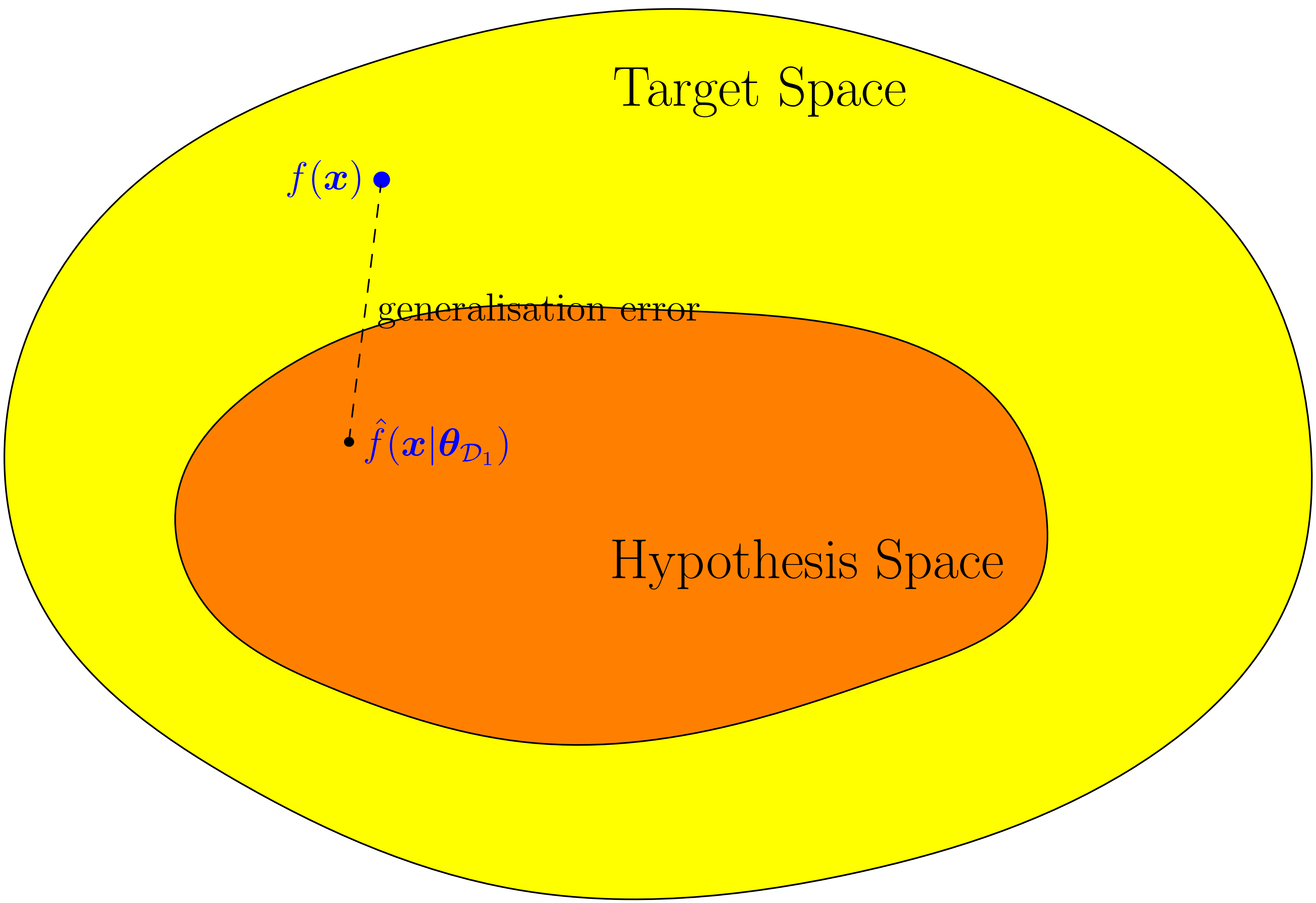

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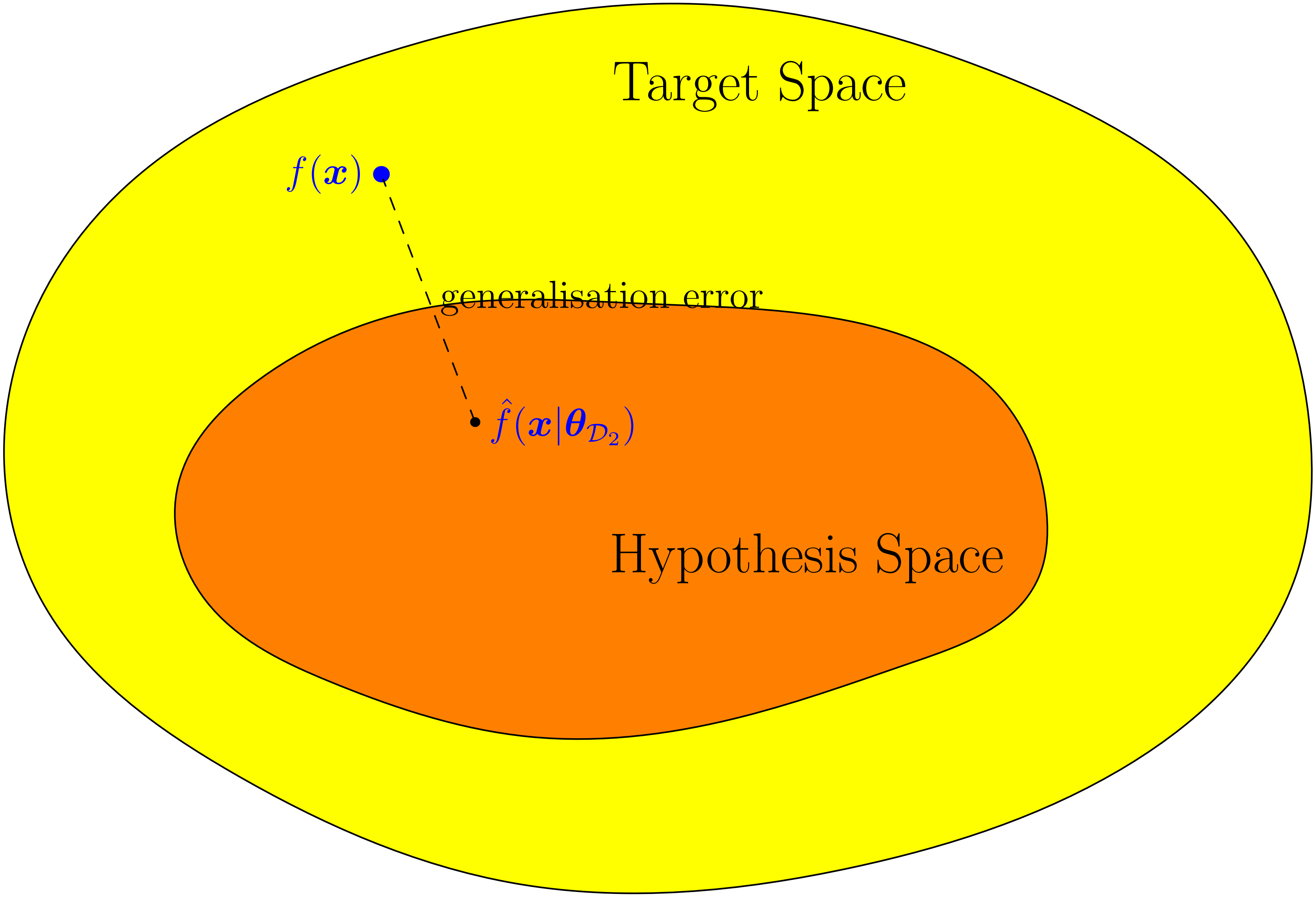

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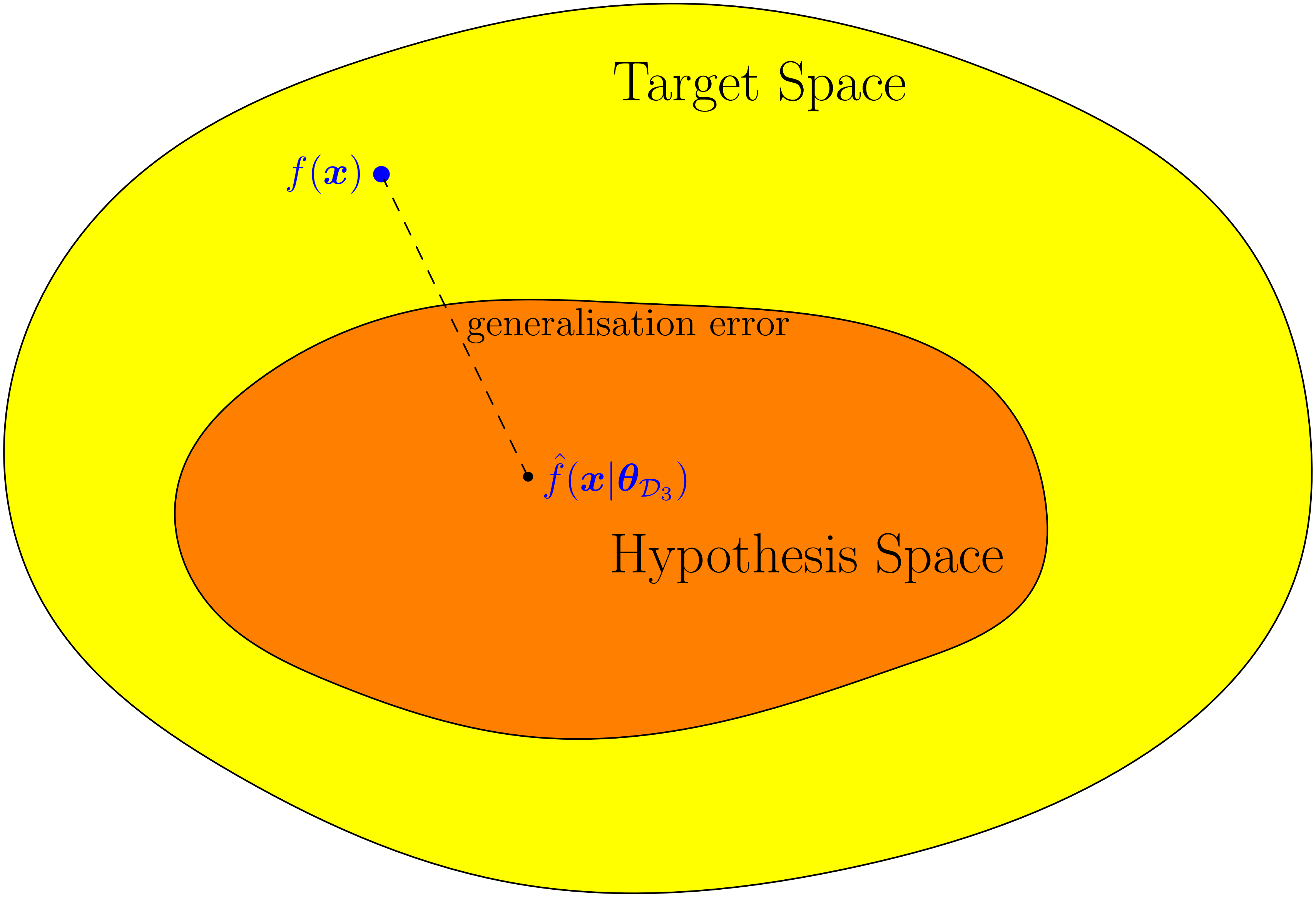

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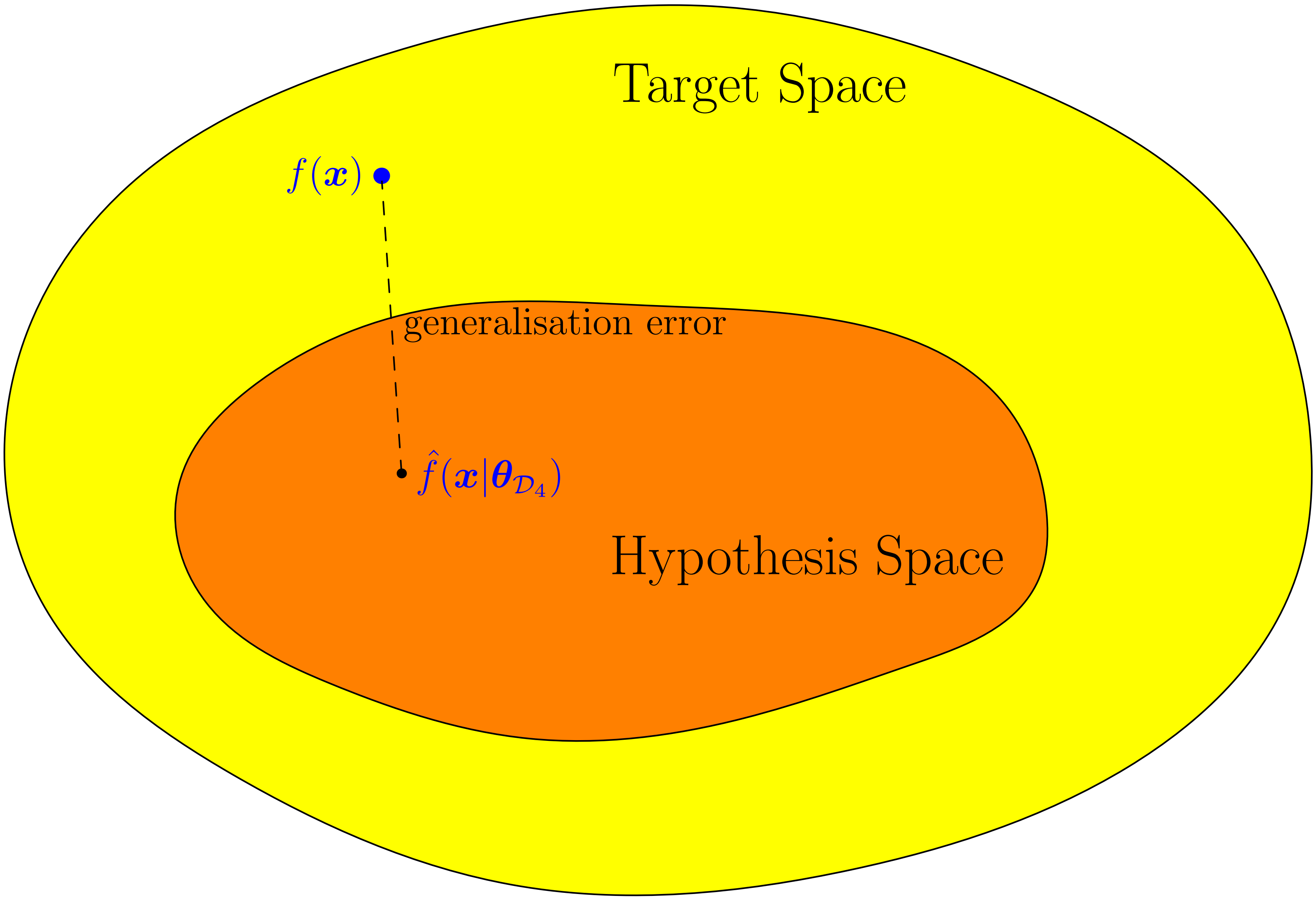

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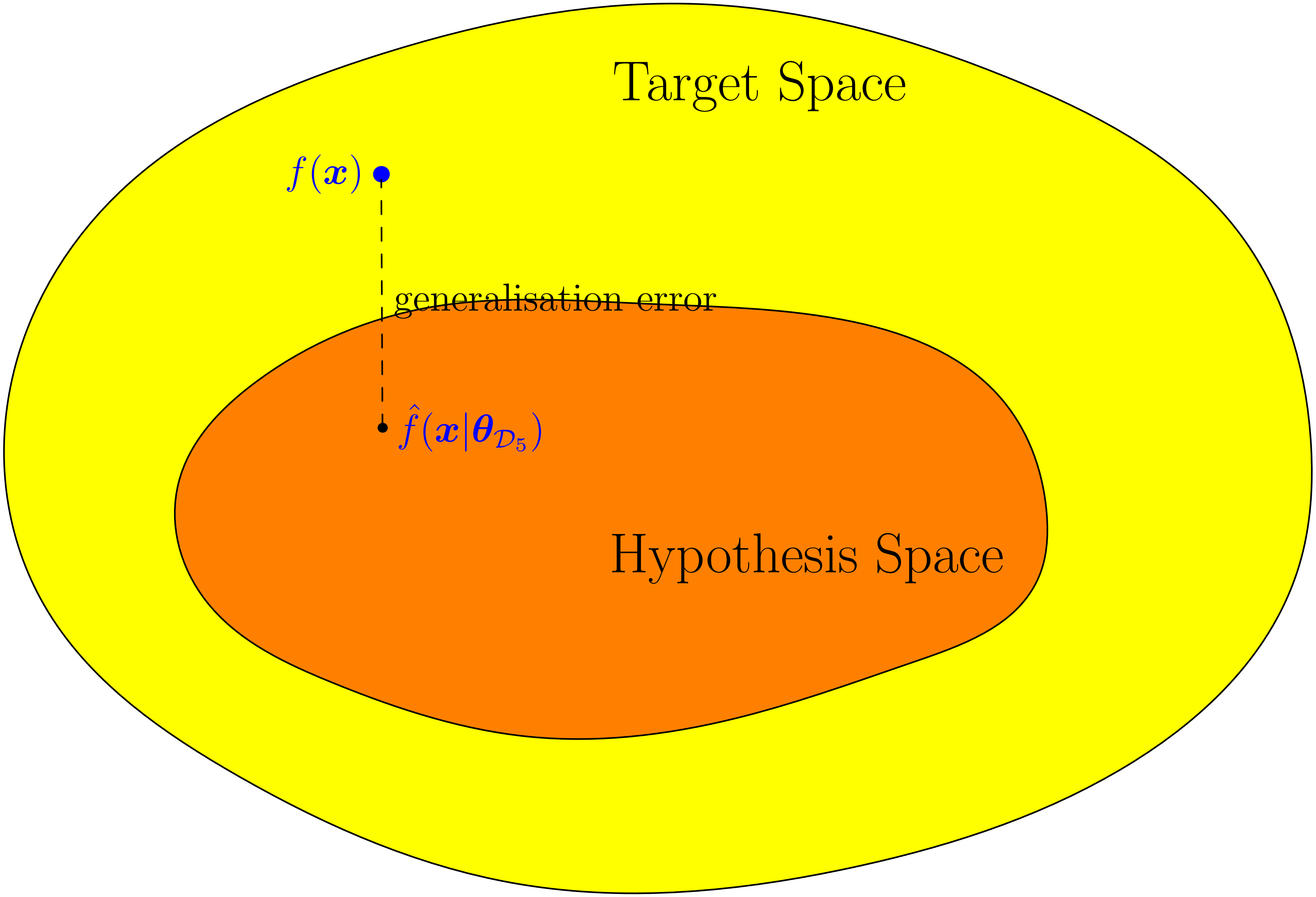

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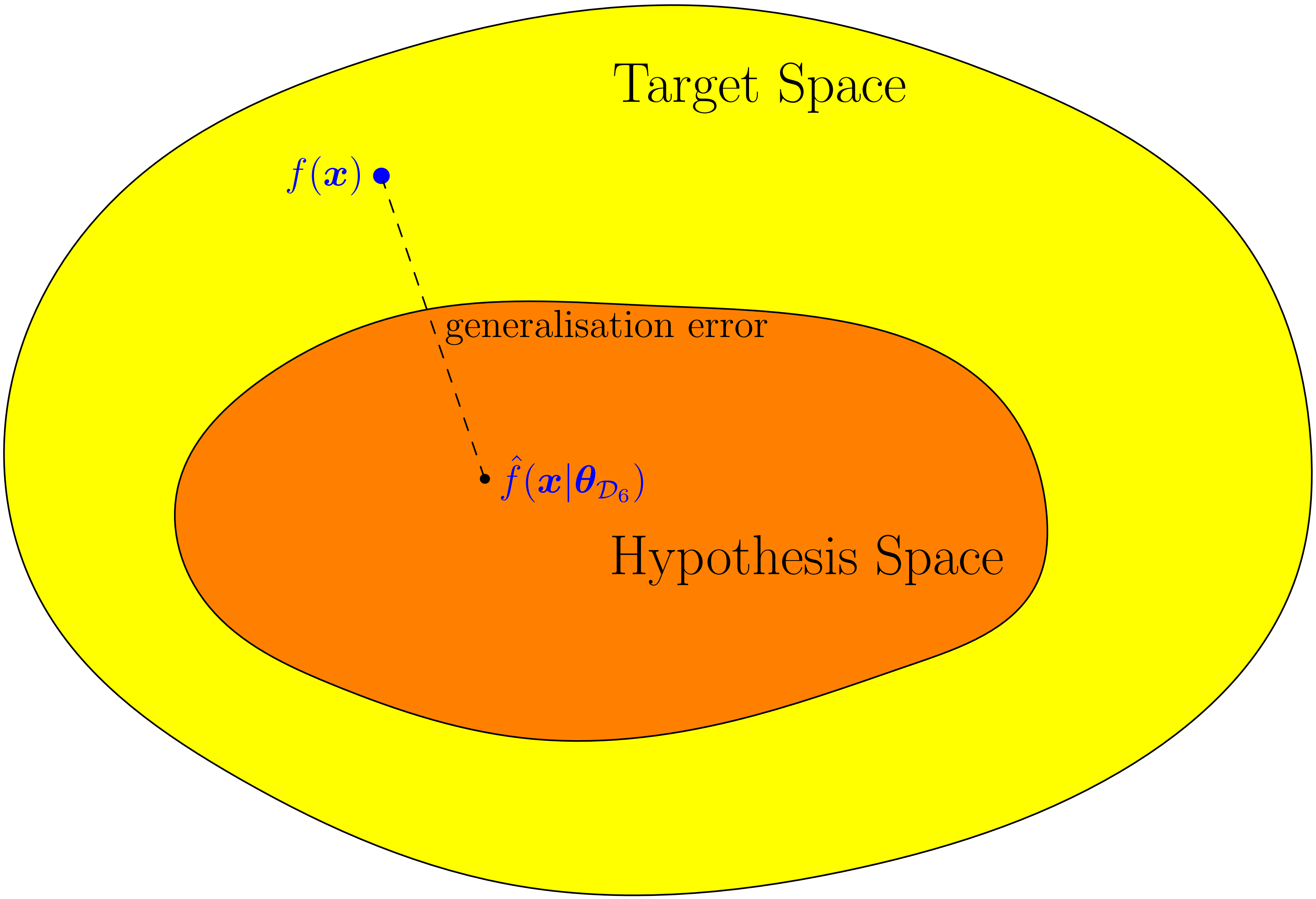

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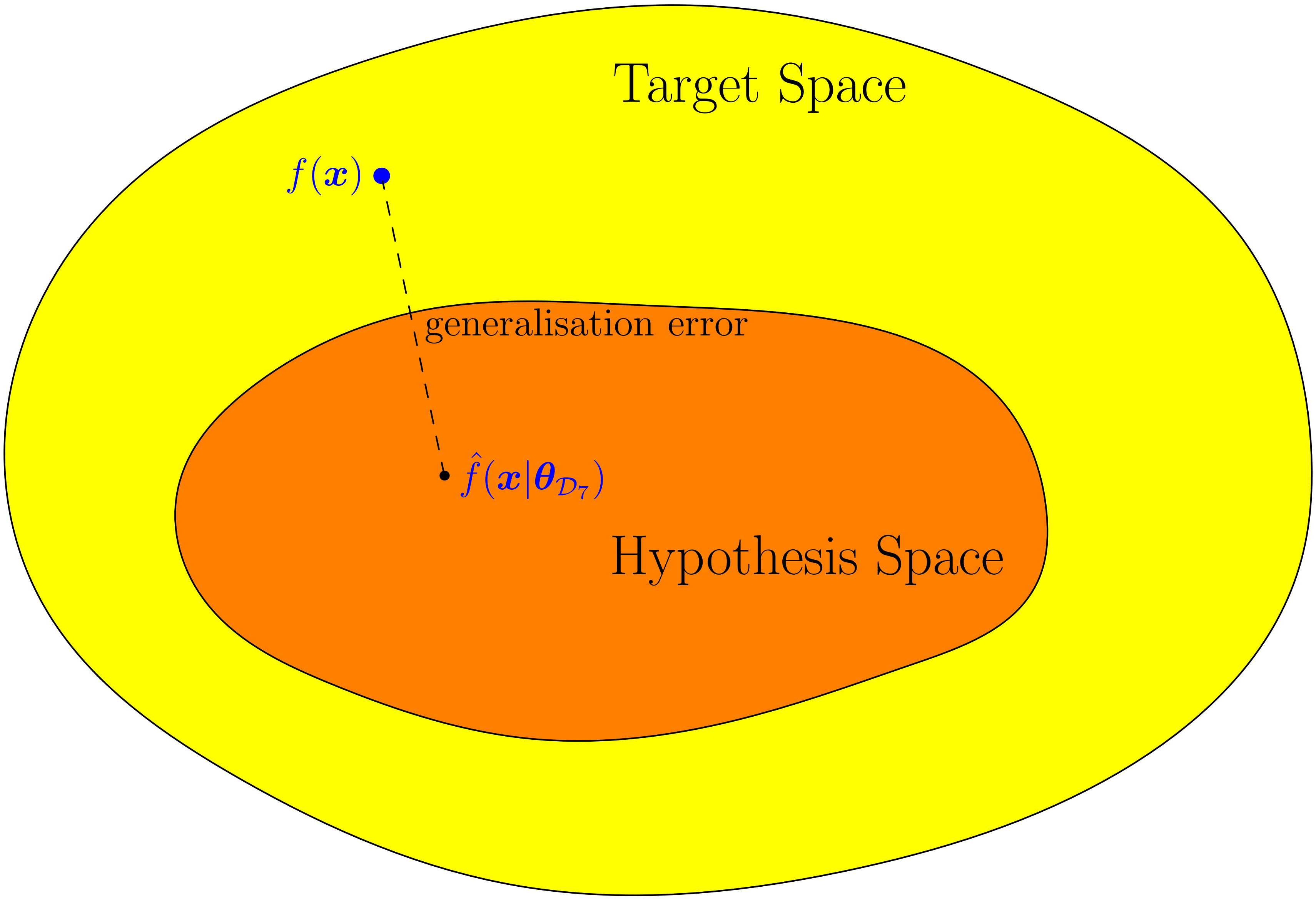

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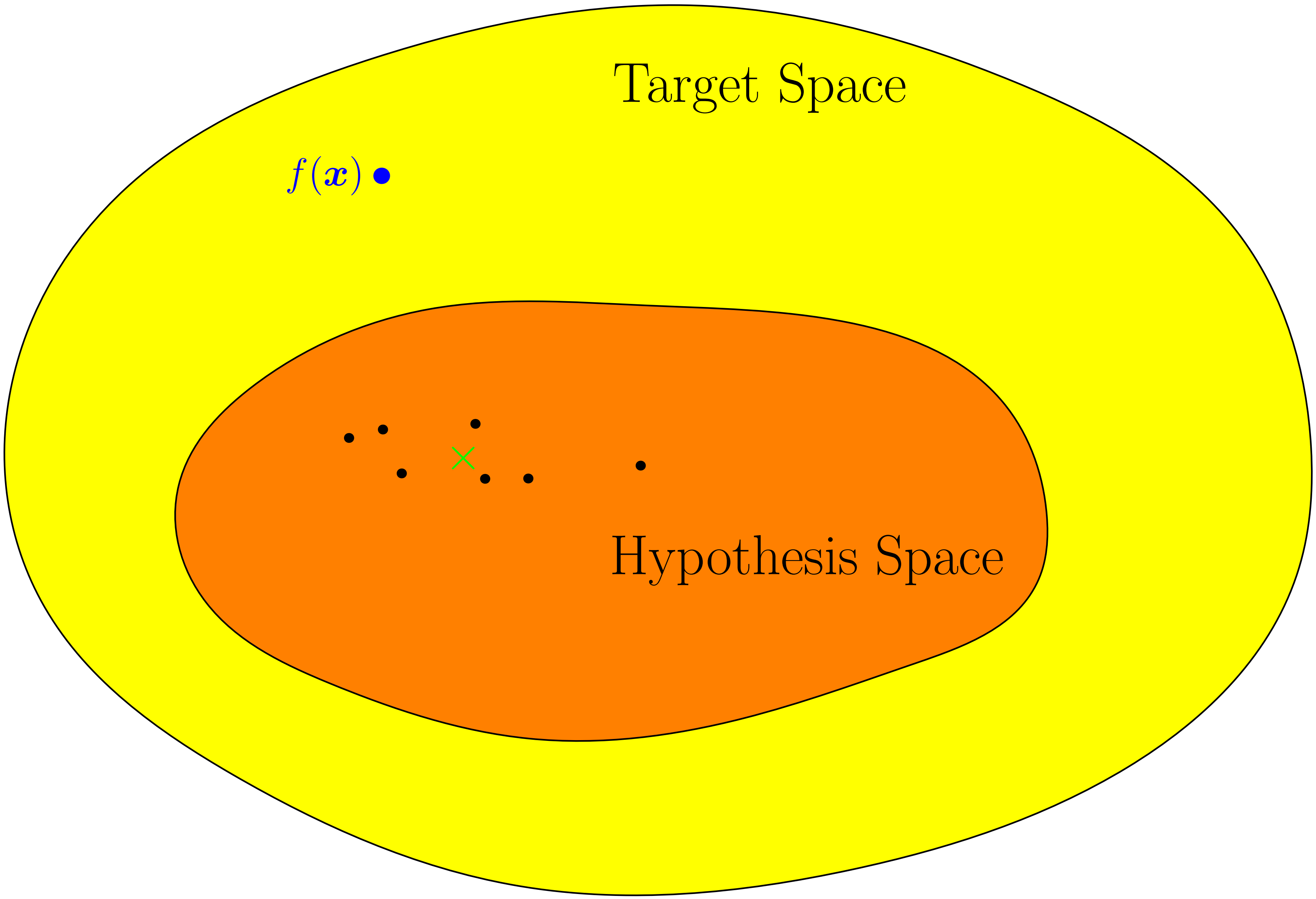

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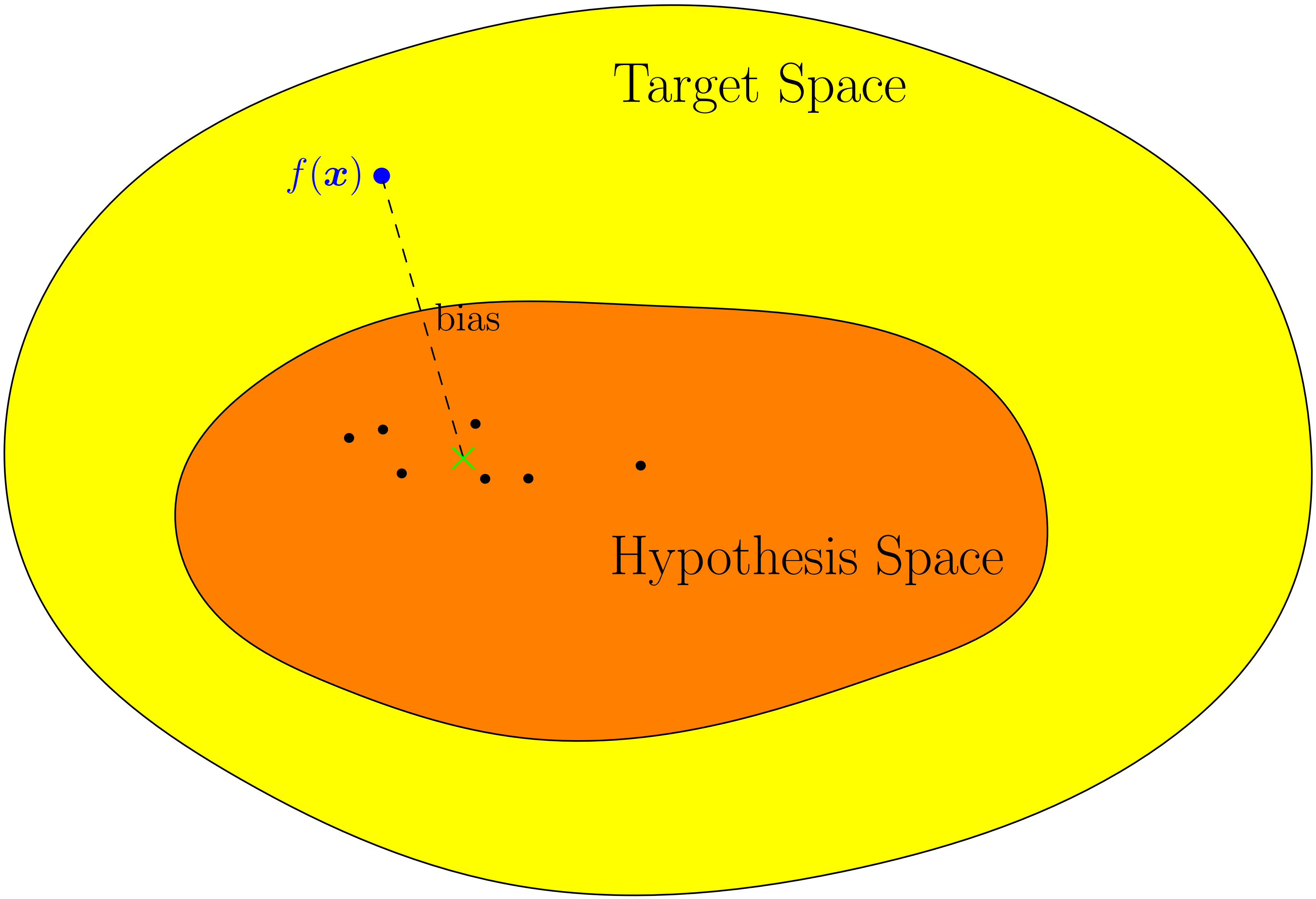

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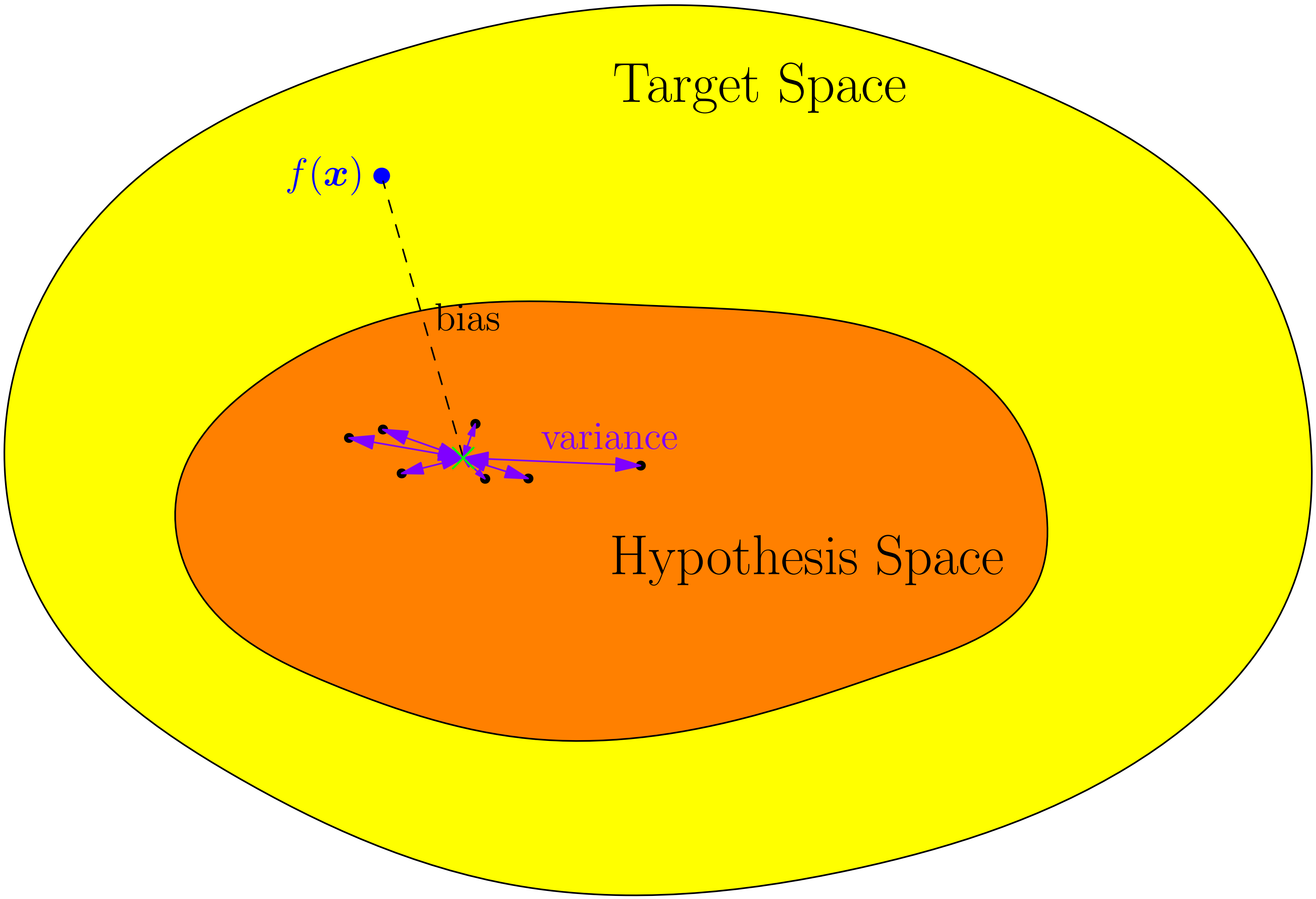

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$$\hat{f}_m(\boldsymbol{x}) = \mathbb{E}_{\mathcal{D}}\left[\hat{f}\left(\boldsymbol{x}|\boldsymbol{\theta}_{\mathcal{D}}\right)\right]$$

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

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

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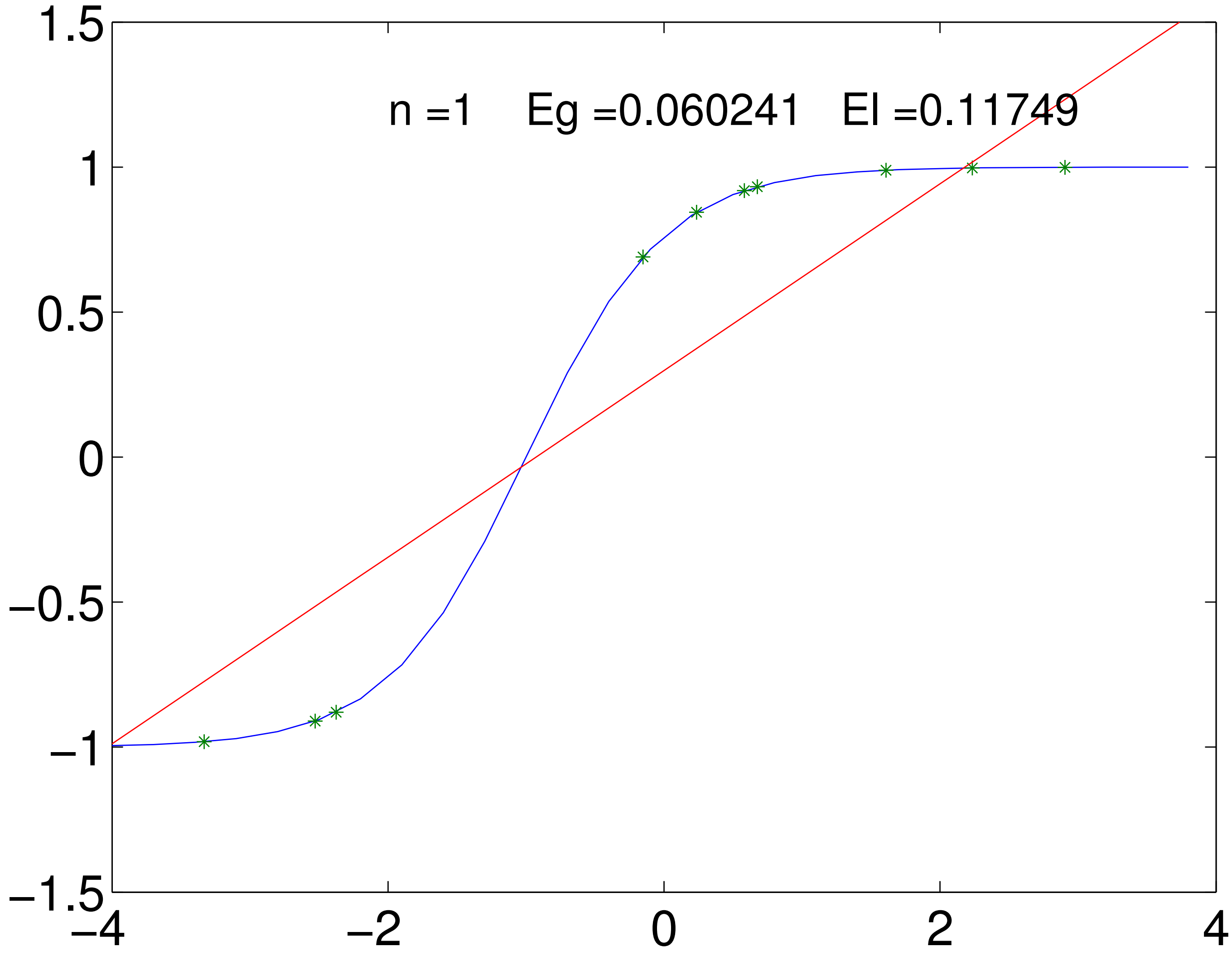

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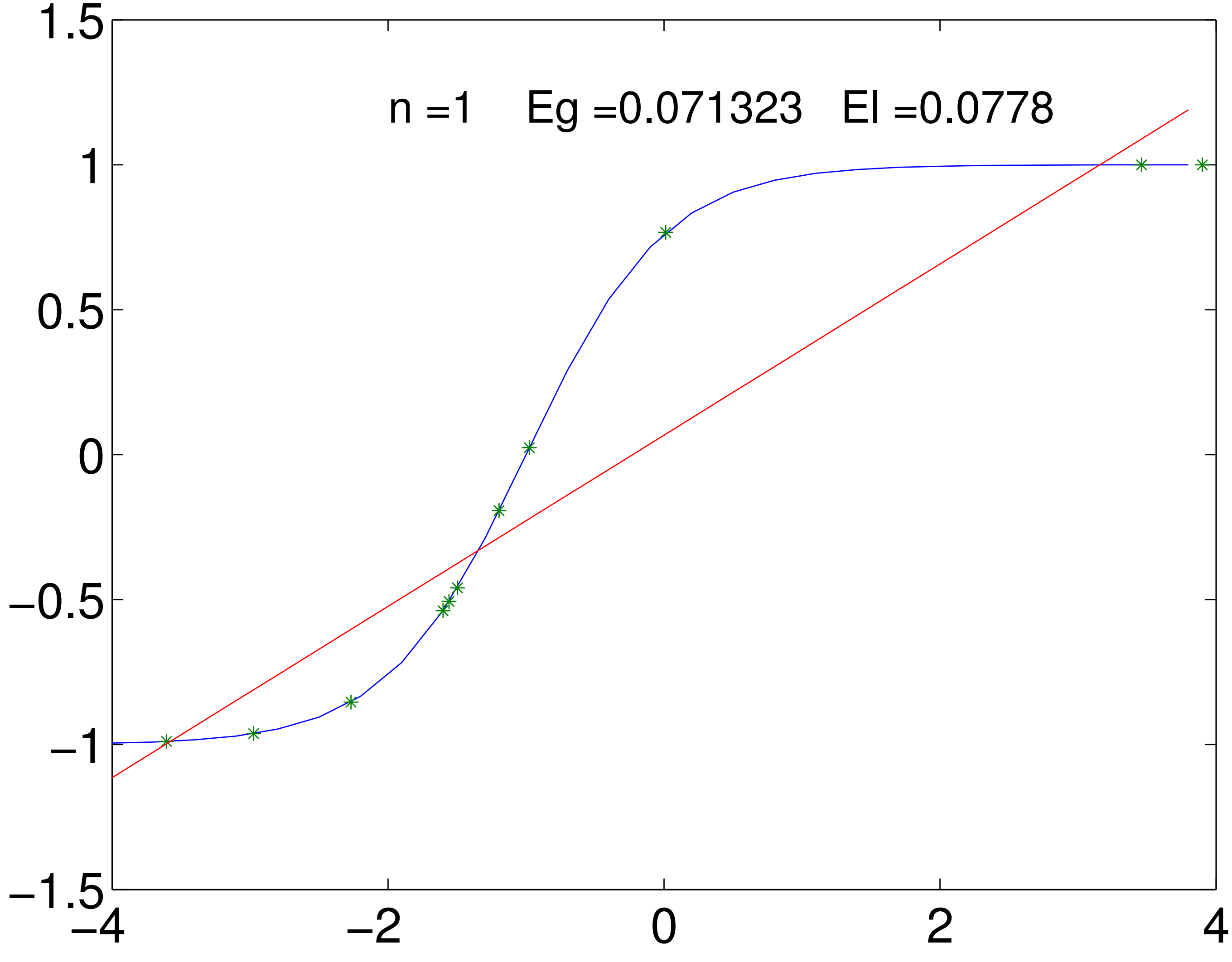

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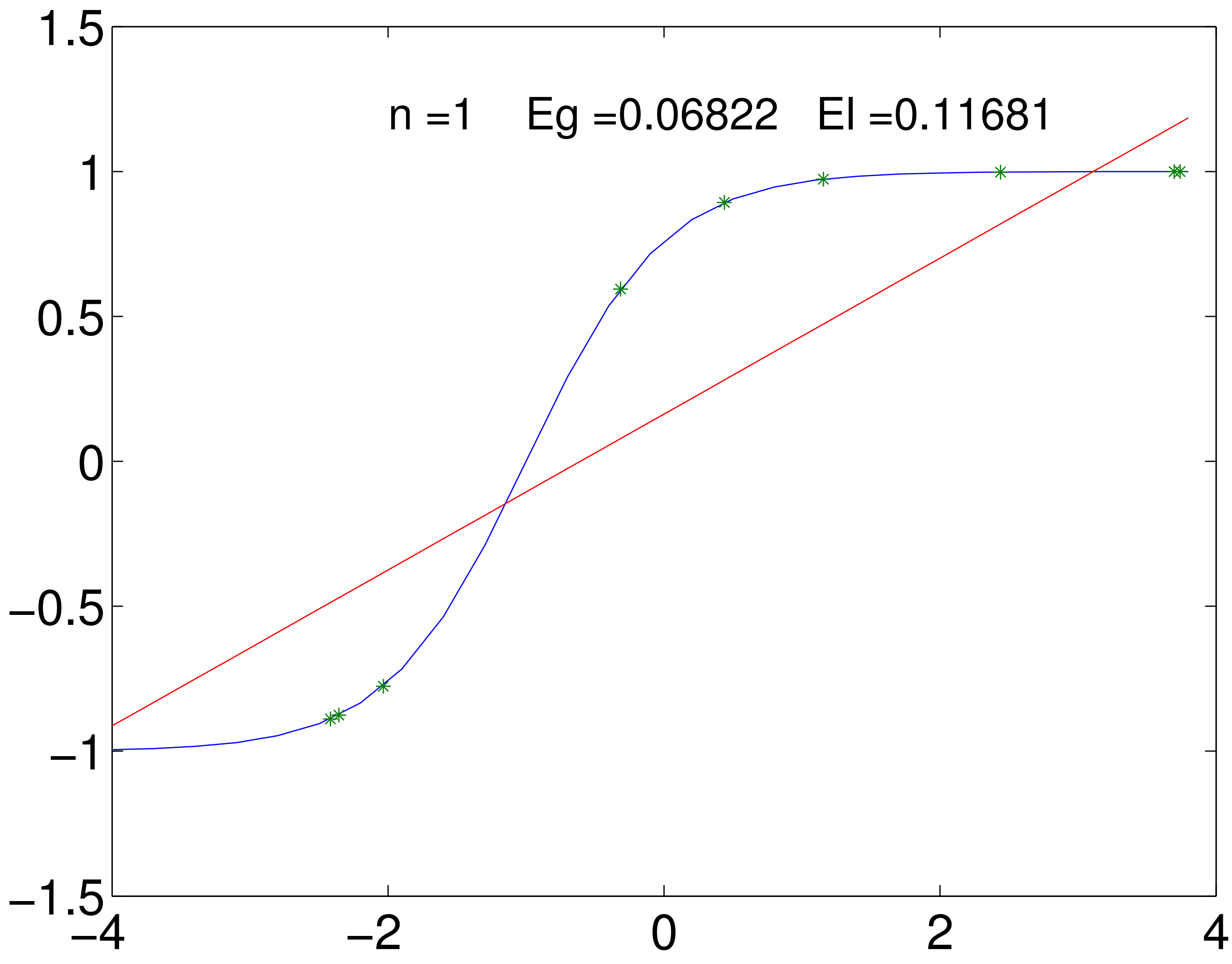

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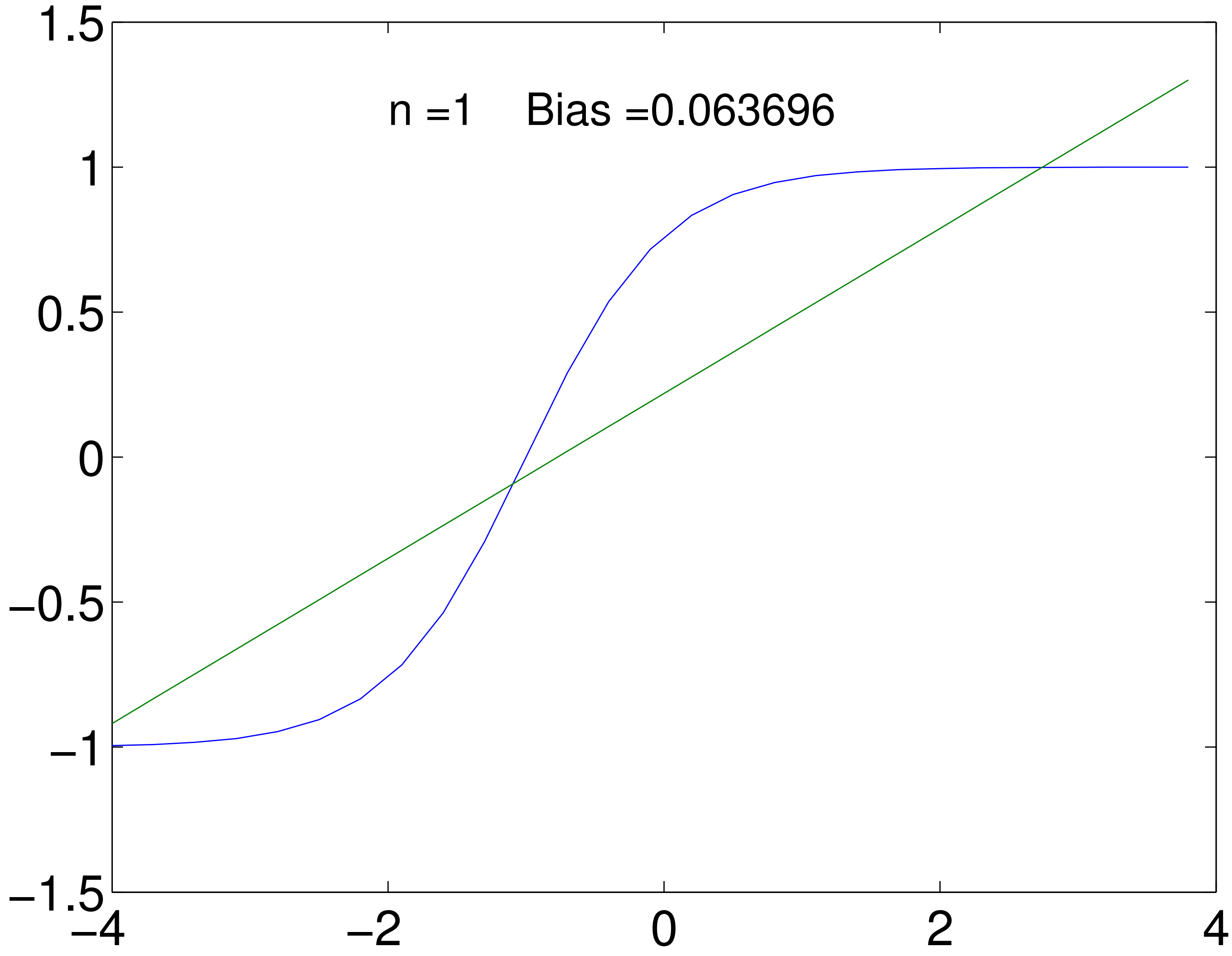

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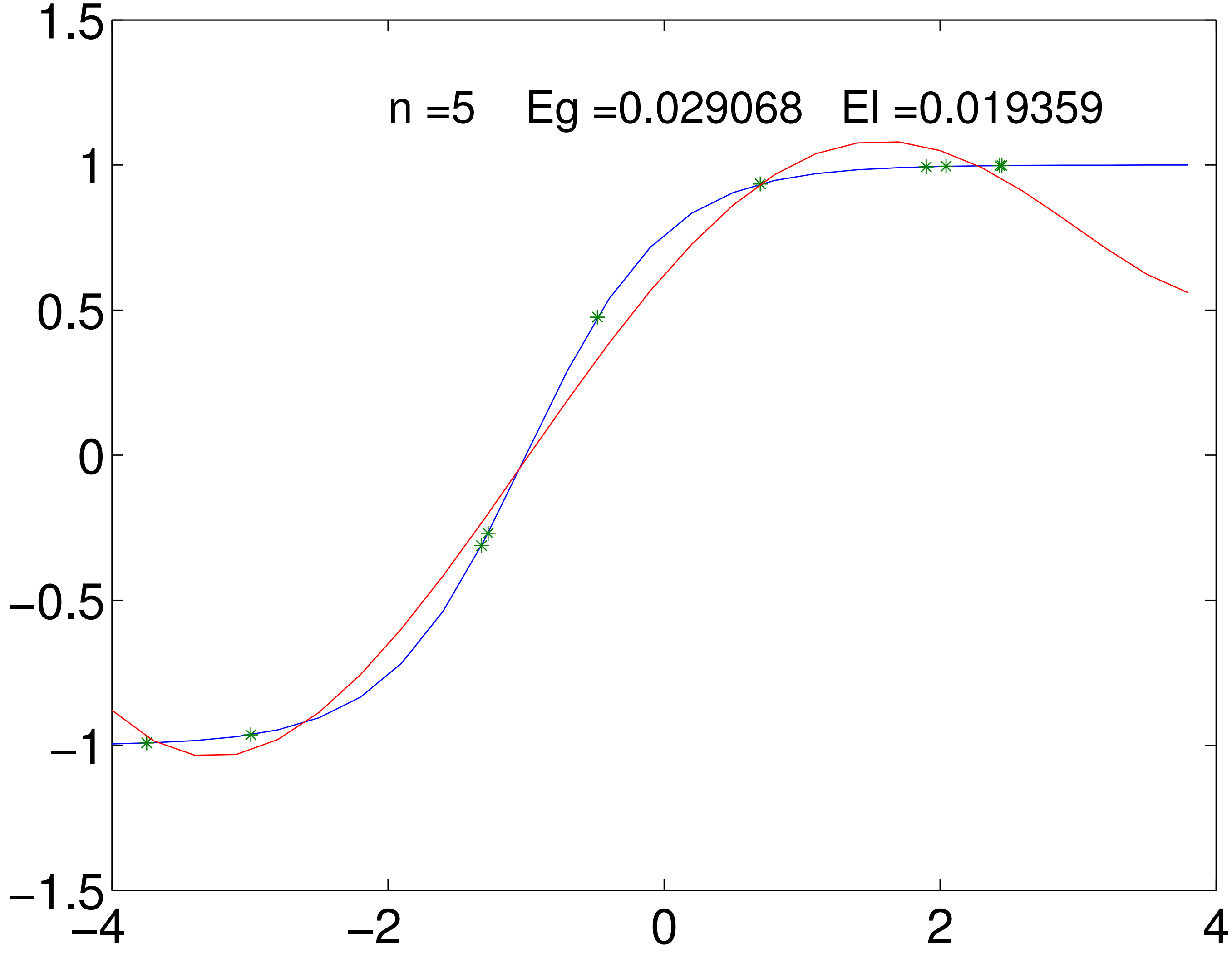

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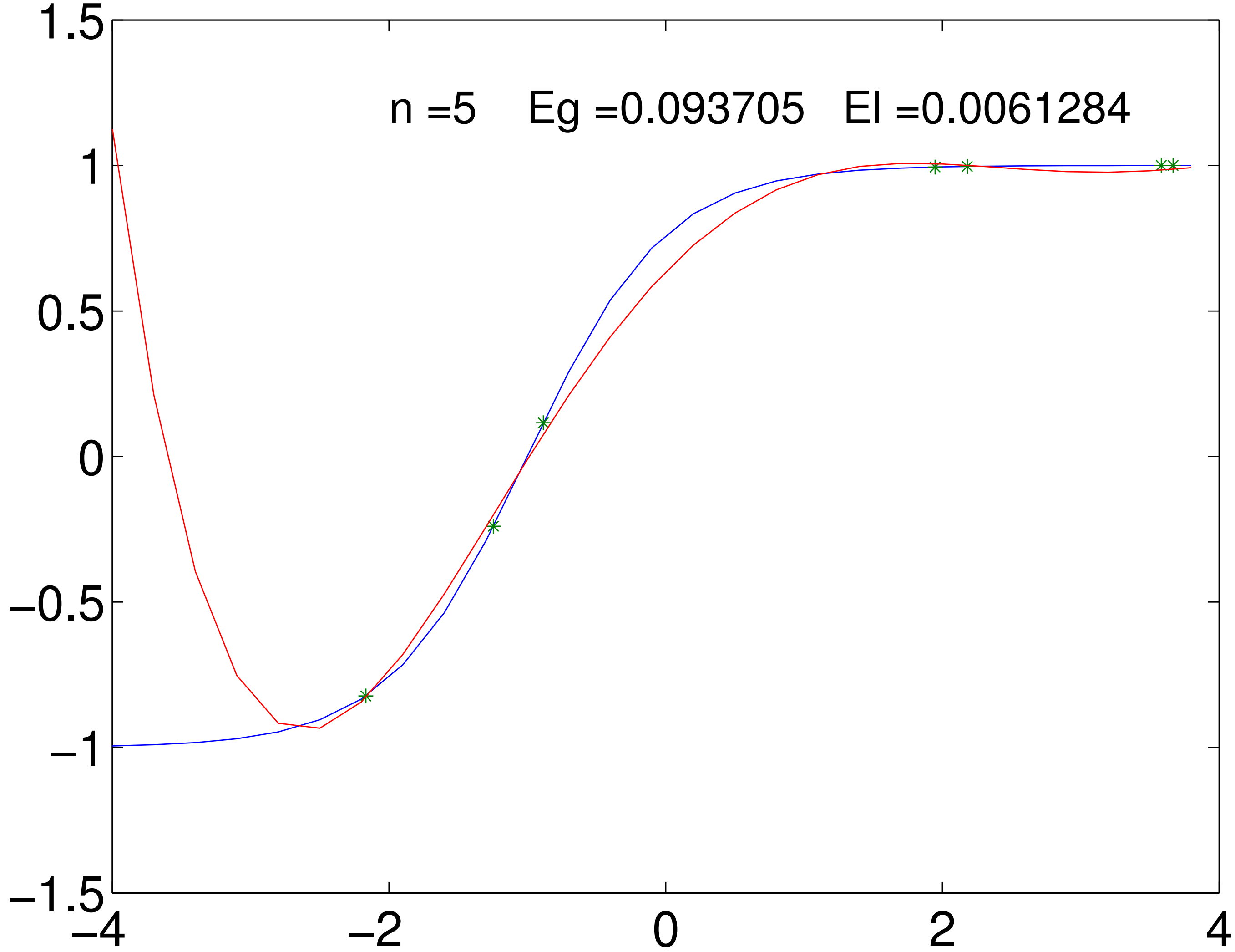

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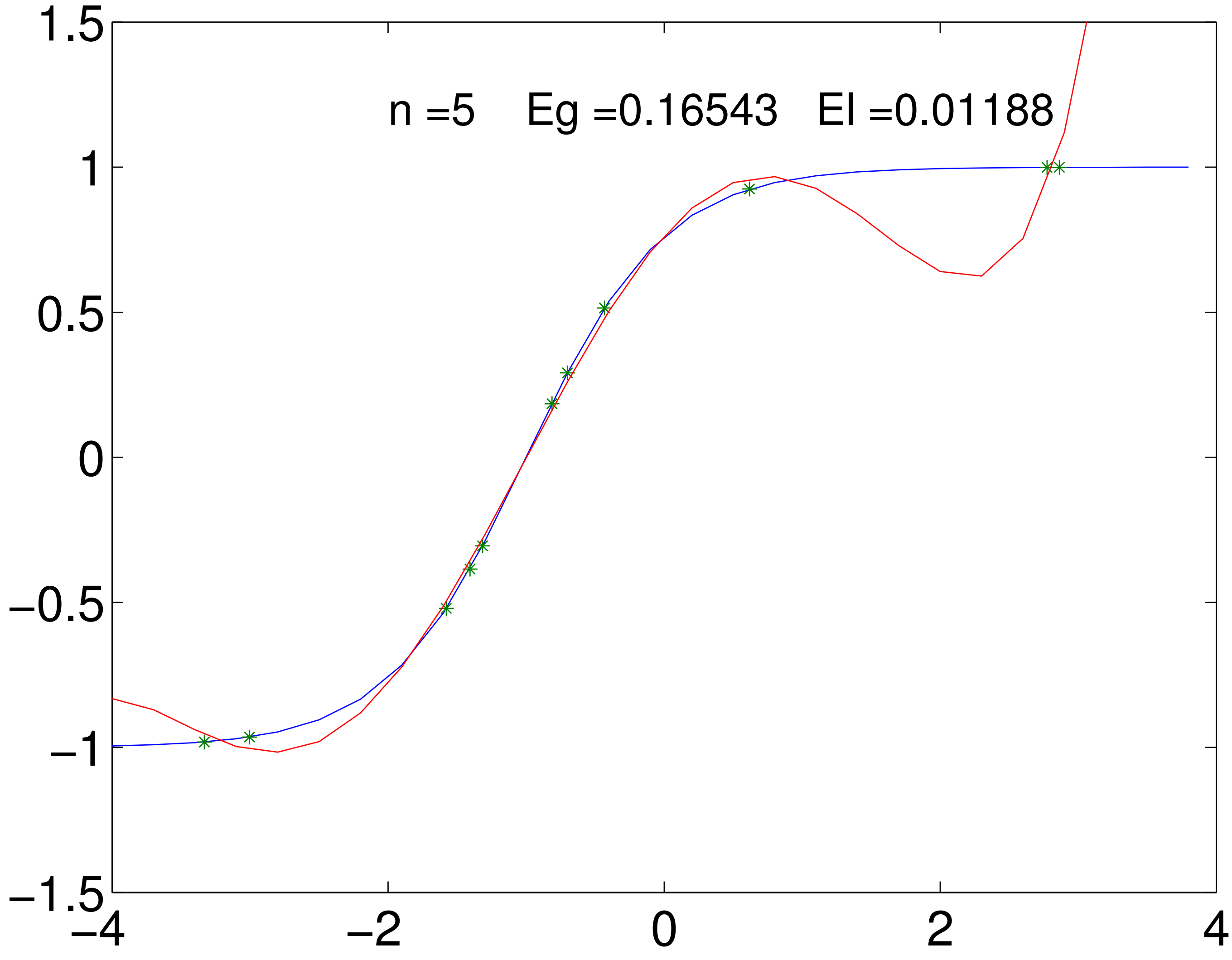

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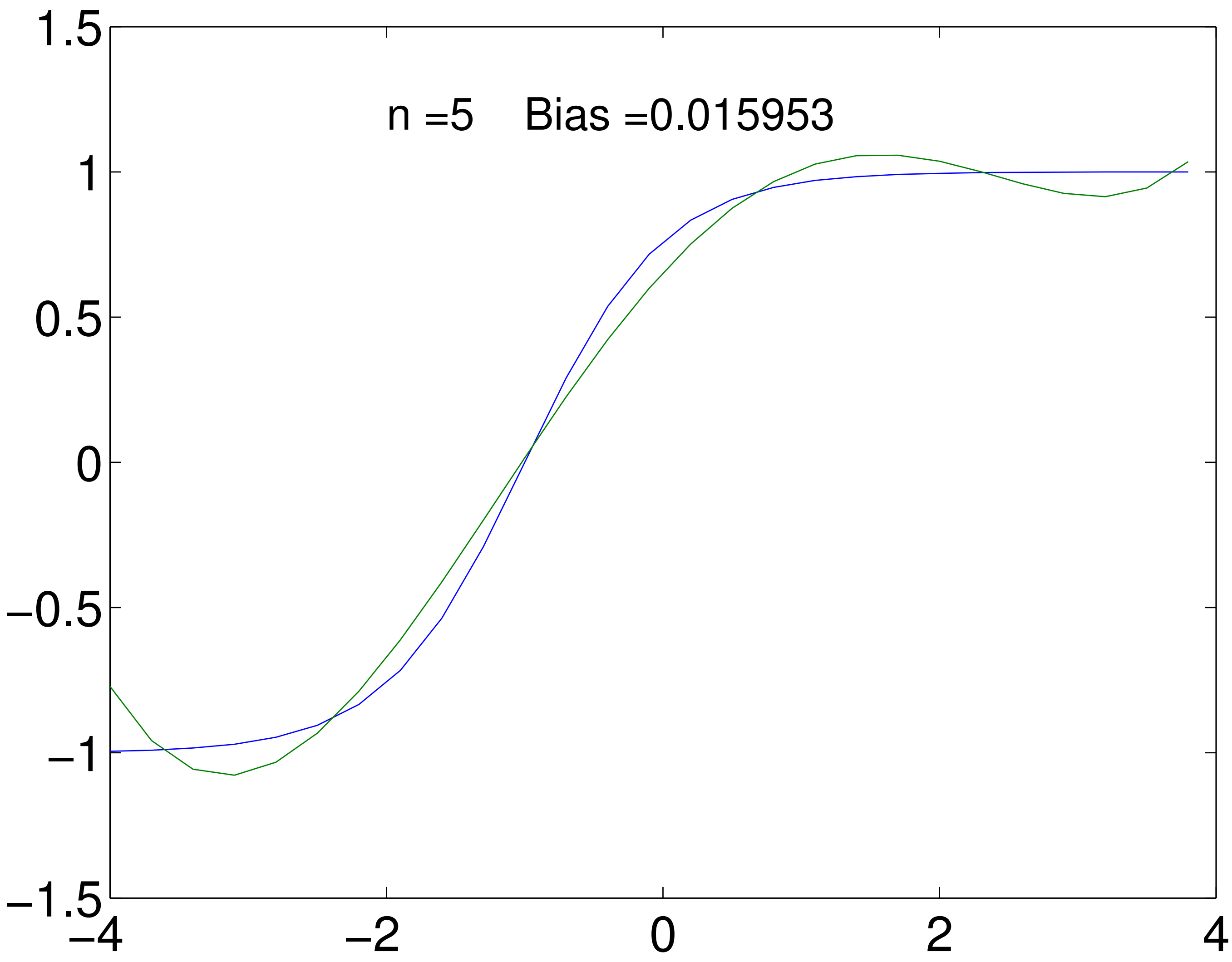

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Bias and Variance

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

Cross Term

- The cross term vanishes

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

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

Bias and Variance

- We can write the expected generalisation loss as

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

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

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Bias-Variance Dilemma

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

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

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

- The variance is usually large if we have a complex machine

- Striking the right balance is often the key to getting good results

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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
- Good machines are powerful enough to capture complex data sets, but they can control their own capacity (ability to (over-)fit the data)

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