Lecture 4
Bias-Variance Tradeoff
&
Intro to Probabilistic Inference

How to quantify expected *out-of-sample* error?

$$y = f(\boldsymbol{x}) + \epsilon \quad \text{with} \quad \epsilon \in \mathcal{N}(0, \sigma_\epsilon^2)$$

$$\ell(\boldsymbol{y}, h(\boldsymbol{X}; \boldsymbol{\theta})) = \sum_i \left(y_i - h\left(\boldsymbol{x}_i; \boldsymbol{\theta}\right)\right)^2$$

Given a fixed training set D, the empirically optimal hypothesis is parametrised by

$$\hat{\boldsymbol{\theta}}_D = \arg\min_{\boldsymbol{\theta}} \ell(\boldsymbol{y}, h(\boldsymbol{X}; \boldsymbol{\theta}))$$

On average, how well does our empirically optimal hypothesis $h_S^* \equiv h\left(\boldsymbol{x}, \hat{\boldsymbol{\theta}}_D\right)$ *make prediction*?

In other words, we want to quantify how well our empirically optimal hypothesis from finite samples predict the value of the unknown god-given function f.

We'll perform a bias-variance decomposition to do quantify this.

Let's calculate the out-of-sample error, averaged over multiple data samples D and noise realisation ϵ

$$\mathbb{E}_{D,\epsilon}\left[\ell\left(\boldsymbol{y}, h\left(\boldsymbol{X};\hat{\boldsymbol{\theta}}_D\right)\right)\right] = \mathbb{E}_{D,\epsilon}\left[\sum_i \left(y_i - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right]$$

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$$= \mathbb{E}_{D,\epsilon}\left[\sum_i \left(y_i - f\left(\boldsymbol{x}_i\right) + f\left(\boldsymbol{x}_i\right) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right]$$

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$$= \sum_i \mathbb{E}_{\epsilon}\left[\left(y_i - f\left(\boldsymbol{x}_i\right)\right)^2\right] + \mathbb{E}_{D,\epsilon}\left[\left(f\left(\boldsymbol{x}_i\right) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right]$$

$$+2\mathbb{E}_{\epsilon}\left[y_i - f\left(\boldsymbol{x}_i\right)\right]\mathbb{E}_{D}\left[f\left(\boldsymbol{x}_i\right) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]$$

Let's calculate the out-of-sample error, averaged over multiple data samples D and noise realisation ϵ

$$
\begin{aligned}
\mathbb{E}_{D,\epsilon}\left[\ell\left(\boldsymbol{y}, h\left(\boldsymbol{X};\hat{\boldsymbol{\theta}}_D\right)\right)\right] &= \mathbb{E}_{D,\epsilon}\left[\sum_i \left(y_i - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right] \\
&= \mathbb{E}_{D,\epsilon}\left[\sum_i \left(y_i - f\left(\boldsymbol{x}_i\right) + f\left(\boldsymbol{x}_i\right) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right] \\
&= \sum_i \mathbb{E}_{\epsilon}\left[\left(y_i - f\left(\boldsymbol{x}_i\right)\right)^2\right] + \mathbb{E}_{D,\epsilon}\left[\left(f\left(\boldsymbol{x}_i\right) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right] \\
&\quad + 2\mathbb{E}_{\epsilon}\left[y_i - f\left(\boldsymbol{x}_i\right)\right]\mathbb{E}_{D}\left[f\left(\boldsymbol{x}_i\right) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right] \\
&= \sum_i \sigma_\epsilon^2 + \sum_i \mathbb{E}_{D}\left[\left(f\left(\boldsymbol{x}_i\right) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right]
\end{aligned}
$$

measurement error (noise) *finite-size sampling error (noise independent)*

Let's look at the last term

finite-size sampling error

$$\sum_i \mathbb{E}_D\left[\left(f(\boldsymbol{x}_i) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right] = \sum_i \mathbb{E}_D\left[\left\{f(\boldsymbol{x}_i) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]} + \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]} - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right\}^2\right]$$

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$$
\begin{aligned}
\sum_i \mathbb{E}_D\left[\left(f(\boldsymbol{x}_i) - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right)^2\right] &= \sum_i \mathbb{E}_D\left[\left\{f(\boldsymbol{x}_i) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]} + \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]} - h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right\}^2\right] \\
&= \sum_i \mathbb{E}_D\left[\left\{f(\boldsymbol{x}_i) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}^2\right] + \mathbb{E}_D\left[\left\{h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}^2\right] \\
&\quad + 2\mathbb{E}_D\left[\left\{f(\boldsymbol{x}_i) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}\left\{h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}\right]
\end{aligned}
$$

Let's look at the last term

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$$= \sum_i \mathbb{E}_D\left[\left\{f(\boldsymbol{x}_i) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}^2\right] + \mathbb{E}_D\left[\left\{h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}^2\right]$$

$$+2\mathbb{E}_D\left[\left\{f(\boldsymbol{x}_i) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}\left\{h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}\right]$$

$$= \sum_i \left(f(\boldsymbol{x}_i) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right)^2 + \sum_i \mathbb{E}_D\left[\left\{h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}^2\right]$$

Bias^2 Variance

How to quantify expected *out-of-sample* error? Putting them altogether

$$\mathbb{E}_{D,\epsilon}\left[\ell\left(\boldsymbol{y}, h\left(\boldsymbol{X};\hat{\boldsymbol{\theta}}_D\right)\right)\right] = \sum_i \left(f\left(\boldsymbol{x}_i\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right)^2$$

Bias²

$+$

$$+\sum_i \mathbb{E}_D\left[\left\{h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i;\hat{\boldsymbol{\theta}}_D\right)\right]}\right\}^2\right]$$

Variance

$+$

$$+\sum_i \sigma_\epsilon^2$$

Measurement error
(Noise)

How to quantify expected *out-of-sample* error? Putting them altogether

$$\mathbb{E}_{D,\epsilon}\left[\ell\left(\boldsymbol{y}, h\left(\boldsymbol{X}; \hat{\boldsymbol{\theta}}_D\right)\right)\right] = \sum_i \left(f\left(\boldsymbol{x}_i\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i; \hat{\boldsymbol{\theta}}_D\right)\right]}\right)^2$$

Bias^2

+

$$+ \sum_i \mathbb{E}_D\left[\left\{h\left(\boldsymbol{x}_i; \hat{\boldsymbol{\theta}}_D\right) - \underline{\mathbb{E}_D\left[h\left(\boldsymbol{x}_i; \hat{\boldsymbol{\theta}}_D\right)\right]}\right\}^2\right]$$

Variance

sample size dependent!

+

$$+ \sum_i \sigma_\epsilon^2$$

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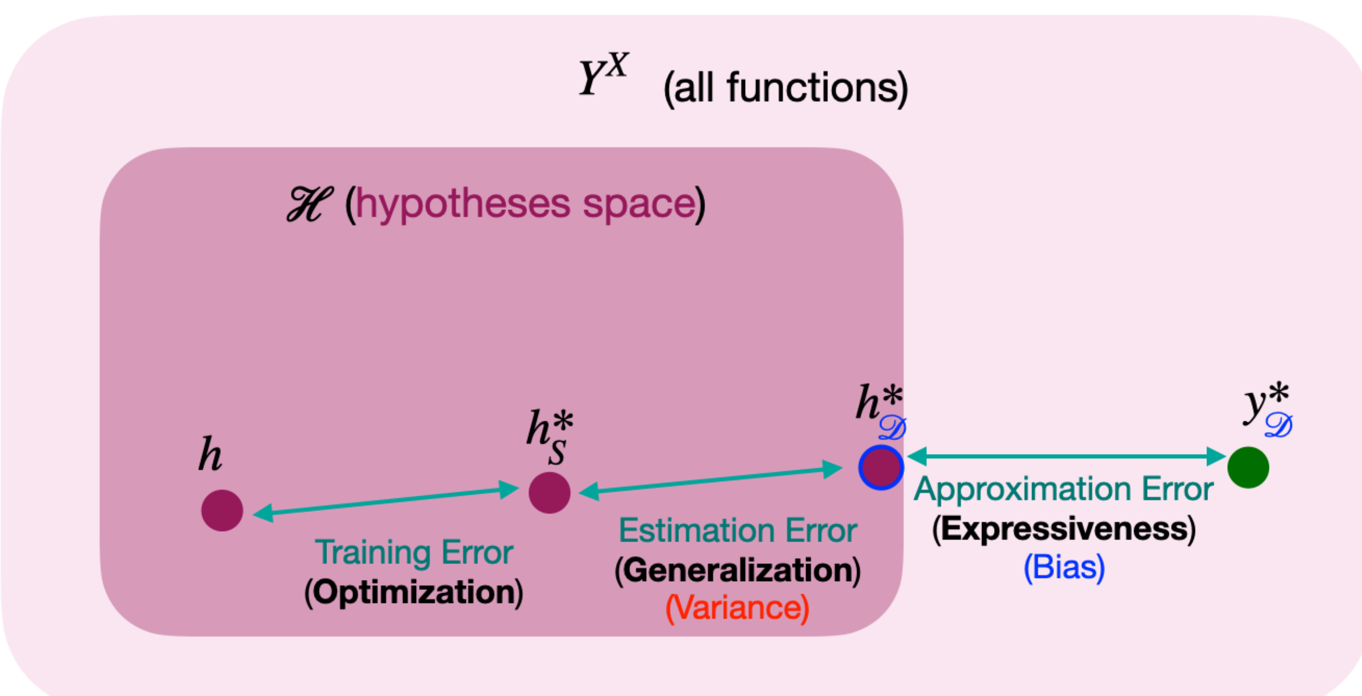

This picture is valid if the consistency condition holds

$$\underline{\mathbb{E}_D\left[h\left(\boldsymbol{x};\hat{\boldsymbol{\theta}}_D\right)\right]} \approx \lim_{m\to\infty} h_S^* = h_{\mathscr{D}}^*.$$

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$$\mathbb{E}_{D,\epsilon}\left[\ell\left(y, h\left(X;\hat{\theta}_D\right)\right)\right] = \sum_i \left(f\left(x_i\right) - \underline{\mathbb{E}_D\left[h\left(x_i;\hat{\theta}_D\right)\right]}\right)^2$$

Bias²

$$+\sum_i \mathbb{E}_D\left[\left\{h\left(x_i;\hat{\theta}_D\right) - \underline{\mathbb{E}_D\left[h\left(x_i;\hat{\theta}_D\right)\right]}\right\}^2\right]$$

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sample size dependent!

$$+\sum_i \sigma_\epsilon^2$$

+

Measurement error
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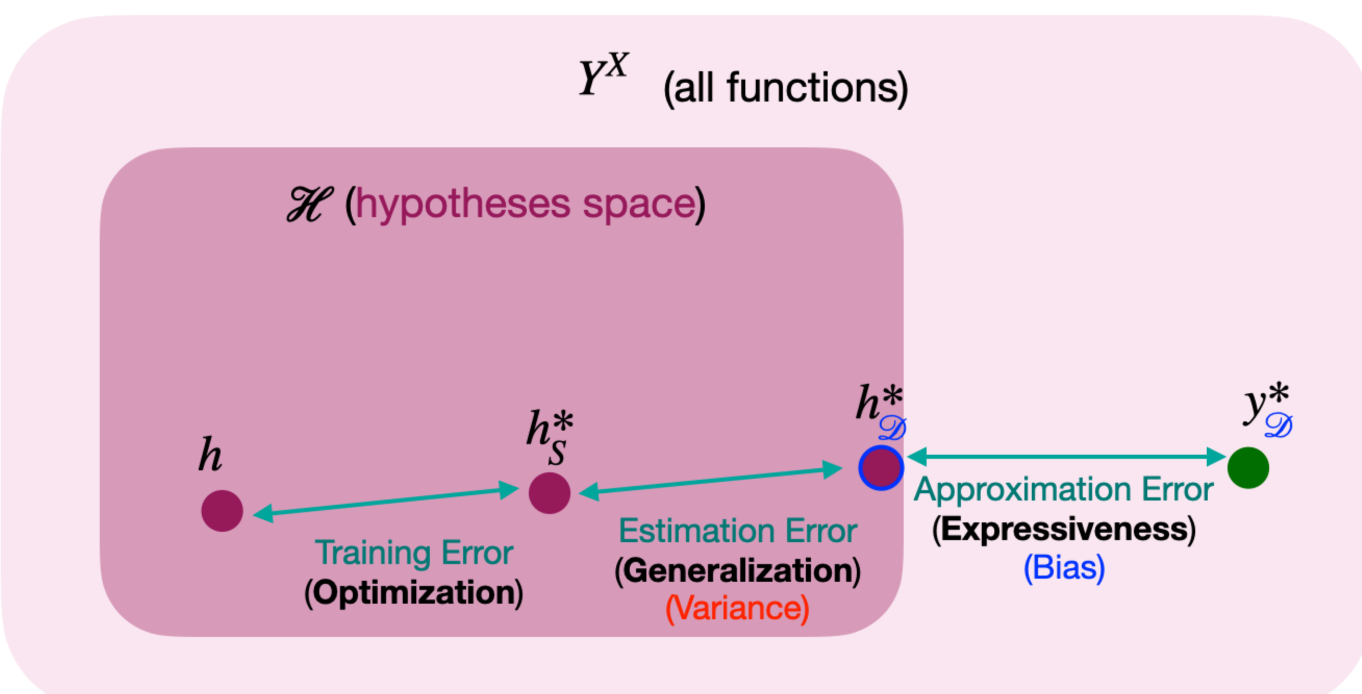

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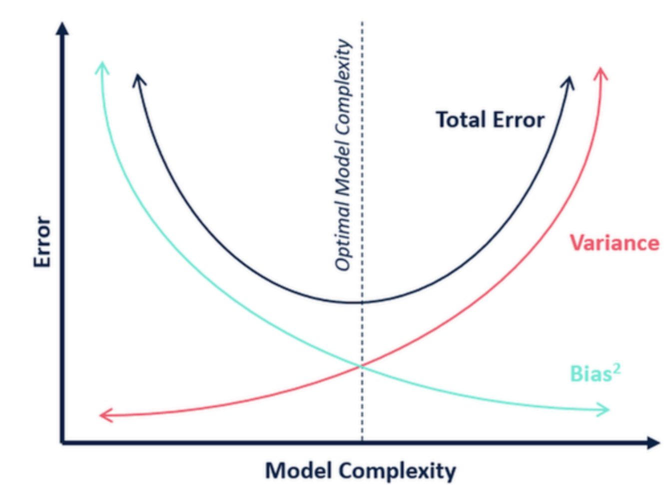
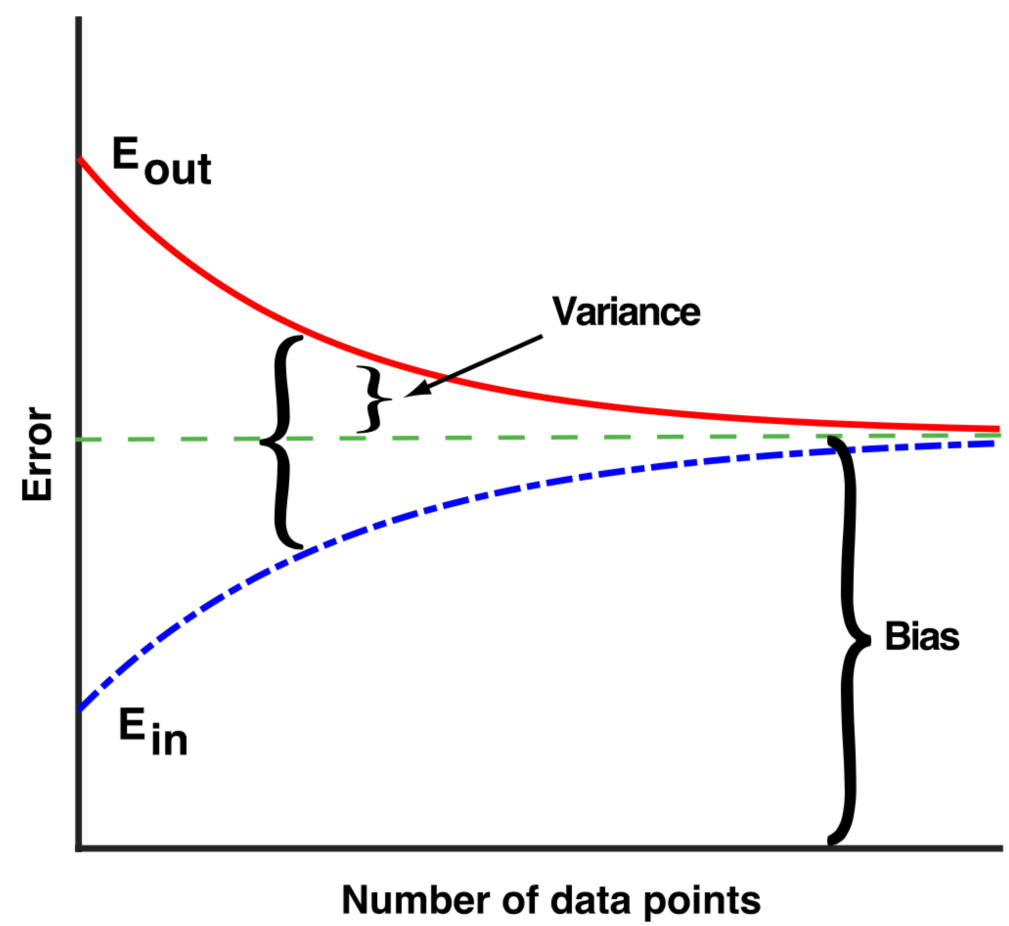


Note: this graph is not quite right…



Measurement error is troublesome!

It makes out-of-sample non-zero even our hypothesis class the same as the god-given signal!

Can we design an alternative approach to learn both signal and noise?

Yes! Bayesian and Probabilistic Inference

Back to a noisy god-given rule

$$y = f(\boldsymbol{x}) + \epsilon \quad \text{with} \quad \epsilon \in \mathcal{N}(0, \sigma_\epsilon^2)$$

We can write this rule for generating the continuous label as

$$P(y \mid \boldsymbol{x}, \boldsymbol{\theta}) = \mathcal{N}\left(f(\boldsymbol{x}), \sigma_\epsilon^2\right)$$

This is a *generative model* (probabilistic model that generates data label, given input).

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What's the framework to evaluate the hypothesis function?

Frequentist's Interpretation of Probability

$P(A)$ = *long-run relative frequency* with which A occurs in identical repeats of an experiment.
"A" restricted to propositions about *random variables*.

Law of large number relates frequency of events in repeated experiments to theoretical probability.

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Bayesian Interpretation of Probability

$P(A \mid B)$ = a real number measure of *the plausibility of a proposition/hypothesis A*, given (conditional on) *the truth* of the information represented by proposition B.
"A" can be *any logical proposition*, <u>not restricted to</u> propositions about random variables.

Both views follow the same mathematical rules of probability theory…

One useful rule (Bayes' Rule)

$$\boxed{P(A \mid B) = \frac{P(A, B)}{P(B)} = \frac{P(B \mid A)P(A)}{P(B)}}$$

Bayes' rule for evaluating plausibility of a scientific hypothesis, given data.

$$\boxed{P\left(H_i \mid D, I\right) = \frac{P\left(H_i \mid I\right) P\left(D \mid H_i, I\right)}{P(D \mid I)}}$$

H_i = proposition asserting the truth of a hypothesis of interest

I = proposition representing our prior information

D = proposition representing data

$P\left(D \mid H_i, I\right)$ = probability of obtaining data D; if H_i and I are true (Likelihood function)

$P\left(H_i \mid I\right)$ = Prior probability of hypothesis

$P\left(H_i \mid D, I\right)$ = Posterior probability of hypothesis

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Bayes' rule allows you to evaluate the probability that the hypothesis is true once new data arrives! (How your belief changes depending on the incoming data)