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Uncertainty estimation

Outline

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Introduction

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- A **single prediction** is a piece of information, but a limited one.
- The algorithm takes a "decision", but how certain is the algorithm about it?
- In order to answer that, we need to discuss the **sources of uncertainty**
- **<u>Statistical uncertainty</u>**: Inherent to the process and its environment. Irreducible in practice.
- **<u>Epistemic uncertainty</u>**: Coming from the fact that a model explains data, which itself explains the process. So two related deviations occur.
- Most of the applications come from Statistics and are exclusive for regression problems, because the error can be directly quantified.
- Nevertheless, in classification problems we can also estimate uncertainties

Introduction

- Uncertainty yes, but where? And how?

- **Model parameters**, e.g. *a* and *b* in simple linear regression $\hat{Y} = f(X) = a + bX$. Confidence intervals on the parameters.

- **Model general behavior**, i.e. the global error. Confidence intervals on the model error.

- **Model single prediction**. Prediction intervals on single predictions.

- In general, the calculations of the intervals is not simple in general. We will focus on statistical regression models, concretely on simple linear regression.

Confidence intervals for model parameters

- The most common way is by means of **bootstrapping**. The steps would be
- Create k datasets by sampling with replacement
- Train the model for all of them
- Store all k parameter collections obtained
- Use percentiles to cut the tails (usually 2.5% on each side)
- The remaining 95% of values determine the intervals (one per parameter)

Confidence intervals for standard error

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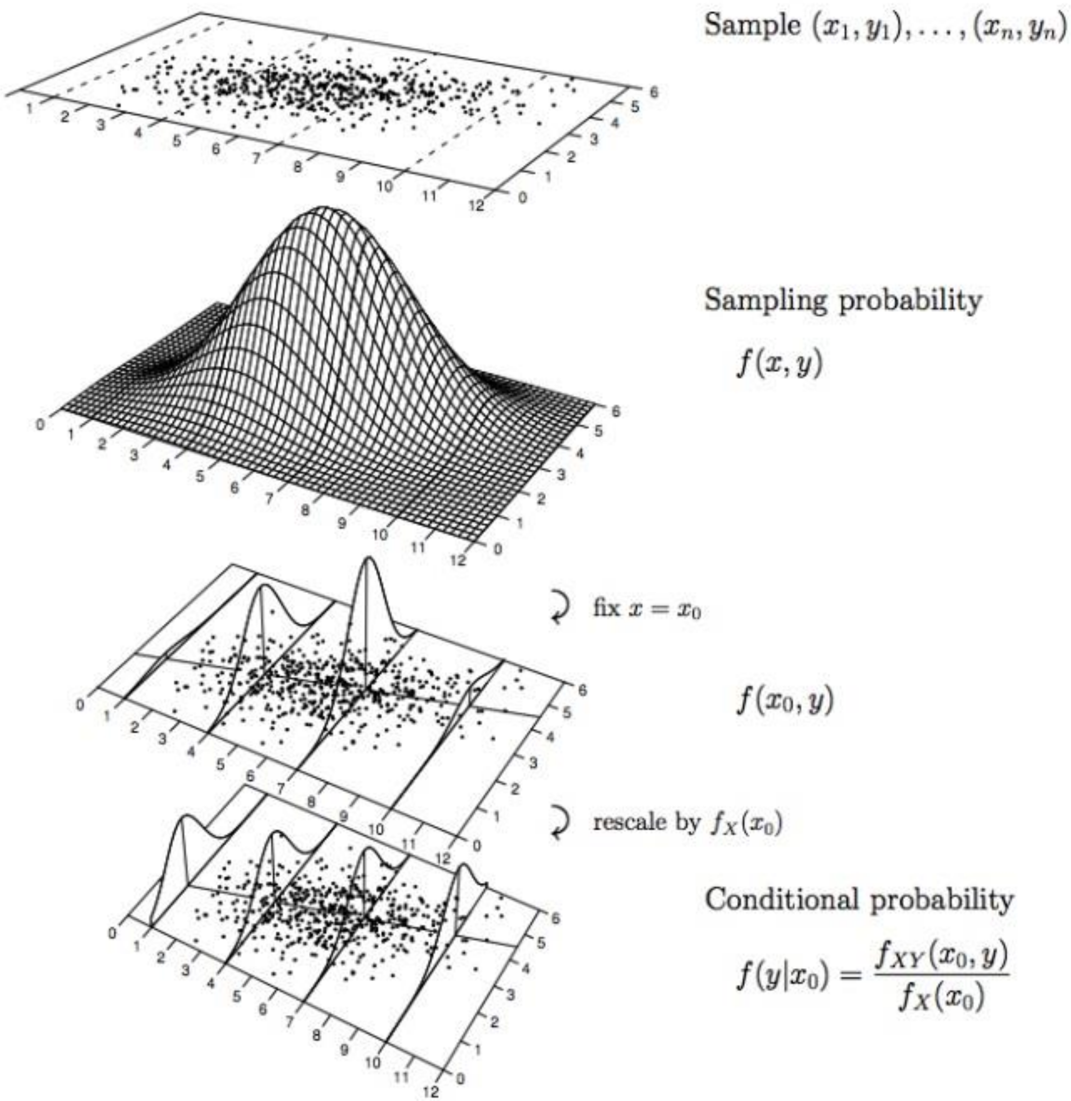


Prediction variance

$$\mathrm{Var}\left(\hat{\alpha} + \hat{\beta} x_d\right) = \mathrm{Var}(\hat{\alpha}) + \left(\mathrm{Var}\,\hat{\beta}\right) x_d^2 + 2 x_d \,\mathrm{Cov}\left(\hat{\alpha}, \hat{\beta}\right)$$

$$\mathrm{Var}\left(\hat{\alpha} + \hat{\beta} x_d\right) = \sigma^2 \left(\frac{1}{m} + \frac{(x_d - \bar{x})^2}{\sum (x_i - \bar{x})^2}\right)$$

Prediction standard deviation

$$s_{\mu_{y|x}} = \sqrt{Var(\hat{\alpha} + \hat{\beta} x_d)}$$

Confidence interval for standard error

$$\boxed{\mu_{y|x} \pm t_{1-\alpha/2, n-2} s_{\mu_{y|x}}}$$

Prediction intervals

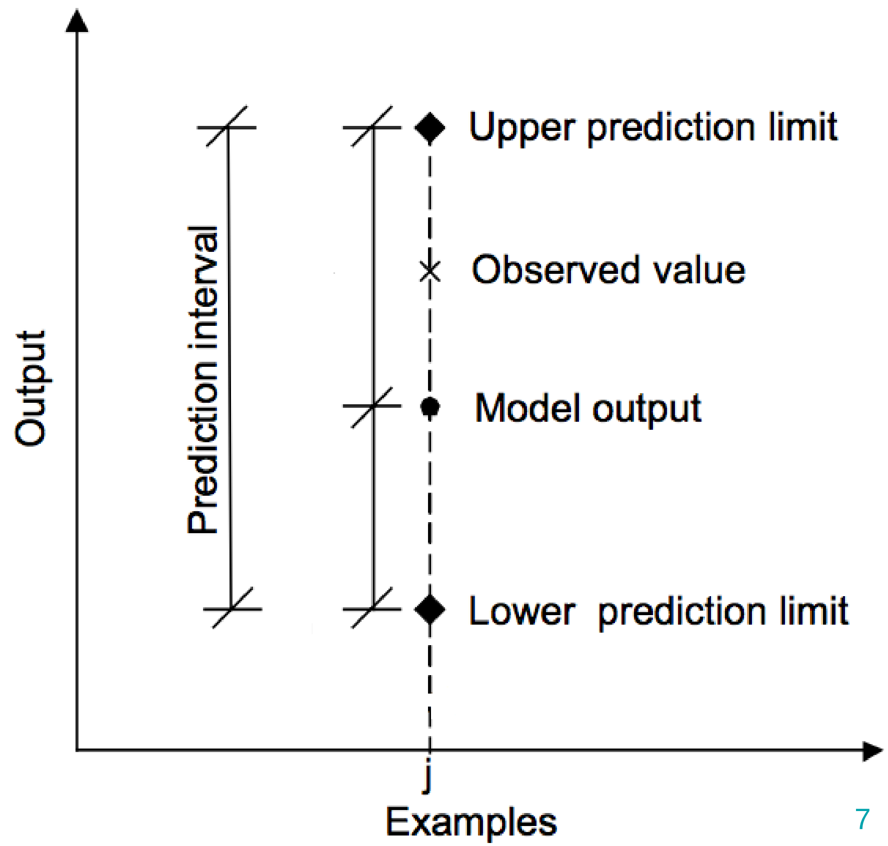
- They quantify the **uncertainty in every single prediction**

- The main difference with the confidence intervals for standard error is that they consider also the dispersion on the target, i.e. they consider that the standard deviation of prediction is

$$s_{y|x} = \sqrt{Var(y_d) + Var(\hat{\alpha} + \hat{\beta}x_d)}$$

- Because of that difference, prediction intervals are wider than confidence intervals wrt similar zones of the prediction space.

- When we plot them, they look like vertical error bars, that form an error band when plotted together.



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Muchas gracias

Thank you

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