Section 3D. Coefficient Uncertainty Statistics for Data Science

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Coefficients Accuracy

Assume that we observe data generated by an additive linear model of the form

$$\mathbf{x}_i \sim f_X$$
 and $\mathbf{y} = M_X \beta + \varepsilon$, where $\varepsilon_i \sim f_{\varepsilon}$

- We can estimate the linear coefficients as $\widehat{\beta} = (M_X^{\mathsf{T}} M_X)^{-1} M_X^{\mathsf{T}} \mathbf{y}$. Note that, since the datapoints (\mathbf{x}_i, y_i) are random, the coefficients $\widehat{\beta}_i$ are random variables themselves!
- Mean analysis: One can prove that E [β̄_i] ← β_i (or all i (unbiased estimator)
 Covariance analysis: Assuming that we are given a data matrix M_X, the covariance matrix of β̄ satisfies (without proof)

$$\operatorname{\mathsf{Cov}}\left[\widehat{\beta}|M_X\right]
otin \sigma^2 \left(M_X^{\mathsf{T}} M_X\right)^{-1}$$

Coefficients Accuracy: Univariate Case

- lacktriangle For the particular case p=1, the linear regression takes the form $\widehat{Y}
 eq \widehat{eta}_0 + \widehat{eta}_1 X$
- ► The diagonal elements of the covariance matrix are the variances of the estimated coefficients. These variances are:

$$SD\left(\widehat{\beta}_{1}\right)^{2} = Var\left[\widehat{\beta}_{1} | \left\{x_{i}\right\}_{i=1}^{N}\right] \left(=\frac{\sigma^{2}}{\sum_{i=1}^{N}\left(x_{i} - \overline{x}\right)^{2}}\right)$$

$$SD\left(\widehat{\beta}_{0}\right)^{2} = Var\left[\widehat{\beta}_{0} | \left\{x_{i}\right\}_{i=1}^{N}\right] \left(=\sigma^{2} - \frac{1}{N} + \frac{\overline{x}^{2}}{\sum_{i=1}^{n}\left(x_{i} - \overline{x}\right)^{2}}\right)$$

with $\sigma^2 = \text{Var}(\varepsilon)$, $\overline{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$ and $\overline{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$. In this course, we use SD(·) to denote the Standard Deviation of a r.v.

Coefficients Accuracy: Numerical Example

Numerical validation: Let us consider an unrealistic, but illustrative situation

- ▶ Consider 1,000 independent realizations of a training dataset, \mathcal{D}_{Tr}^k for k = 1, 2, ..., 1000. Notice that, in practice, we will only have access to a single realization of a training dataset!
- Each dataset contains N = 100 sample points $\mathcal{D}_{\mathsf{Tr}}^k = \left\{ \left(\mathbf{x}_1^k, y_1^k \right), \dots, \left(\mathbf{x}_{100}^k, y_{100}^k \right) \right\}$.

 For each $\mathcal{D}_{\mathsf{Tr}}^k$, we compute the corresponding estimates $\widehat{\beta}_0^k$ and $\widehat{\beta}_1^k$ for $k = 1, 2, \dots$, 1000

Coefficients Accuracy: Numerical Example

In this example,
$$\beta_1 = \mathbb{E}\left[\widehat{\beta}_1\right] \notin 0.5$$
 and $\operatorname{Var}\left[\widehat{\beta}_1 | \{x_i\}_{i=1}^N\right] \notin 0.05^2$.

Figure: Histogram of the values of $\widehat{\beta}_1^k$. We have used a linear model $Y=1+0.5X+\varepsilon$, where $X\sim\mathcal{N}\left(0,1\right)$ and $\mathrm{Var}\left(\varepsilon\right)=\sigma^2=1$.



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