Uncertainty Propagation (Chapter 13)

- Once we have $\vec{\theta} \in \mathbb{R}^p$ + information about $\vec{\theta}$ (e.g., estimate from OLS, maybe upper + lower bounds, or $\pi(\vec{\theta} \mid \vec{y})$).
  - How do we quantify the uncertainty in $f(\vec{x}; \vec{\theta})$?
  - E.g., if $f(\vec{x}; \vec{\theta}) = \vec{y} \in \mathbb{R}^{N_y}$.

E.g.) Once we have $\vec{\theta}$, what is

$$E\left[f(\vec{x}; \vec{\theta})\right] = \int_{\mathbb{R}^p} f(\vec{x}; \vec{\theta})\, \rho(\vec{\theta})\, d\vec{\theta}, \quad \rho(\vec{\theta}) \text{ is a density}$$

$$Var\left[f(\vec{x}; \vec{\theta})\right] = \int_{\mathbb{R}^p} \left[f(\vec{x}; \vec{\theta}) - E\left[f(\vec{x}; \vec{\theta})\right]\right]^2 \rho(\vec{\theta})\, d\vec{\theta}$$

Linear Models in Frequentist Perspective

- Consider

$$\vec{y} = \underset{\sim}{X}\vec{\theta} + \vec{\varepsilon}, \quad \varepsilon_i \sim N(0, \sigma_\varepsilon^2), \quad \underset{\sim}{X} \in \mathbb{R}^{N_x \times p}$$

- Given $\vec{\theta}$ s.t. $E[\vec{\theta}] = \vec{\theta}^*$

$$\Rightarrow \quad E[\vec{y}] = E[\underset{\sim}{X}\vec{\theta} + \vec{\varepsilon}] = \underset{\sim}{X}\, E[\vec{\theta}] + \vec{0}$$

$$= \underset{\sim}{X}\, \vec{\theta}^*$$

$$\Rightarrow \quad Cov[\underset{\sim}{X}\vec{\theta}] = \underset{\sim}{X}\, Cov(\vec{\theta})\, \underset{\sim}{X}^T = \underset{\sim}{X}\, \underset{\sim}{V}_\theta\, \underset{\sim}{X}^T, \quad \underset{\sim}{V}_\theta = Cov(\vec{\theta})$$

$$\Rightarrow \mathrm{Cov}[\underset{\sim}{X}\vec{\theta}] = \underset{\sim}{X}\,\mathrm{Cov}(\theta \ldots$$

$$\Rightarrow \mathrm{Cov}[\vec{y}] = \mathrm{Cov}[\underset{\sim}{X}\vec{\theta} + \vec{\varepsilon}] = \mathrm{Cov}[\underset{\sim}{X}\vec{\theta}] + \mathrm{Cov}[\vec{\varepsilon}]$$

$$\Rightarrow \mathrm{Cov}[\vec{y}] = \underset{\sim}{X}\,\underset{\sim}{V}_\theta\,\underset{\sim}{X}^T + \underset{\sim}{V}_{obs}, \quad \text{if } \varepsilon_i \overset{iid}{\sim} N(0, \sigma_\varepsilon^2)$$

$$\Rightarrow \underset{\sim}{V}_{obs} = \sigma_\varepsilon^2\,\underset{\sim}{I}_{N_x}$$

- If each θ_i is independent

$$\Rightarrow \underset{\sim}{V}_\theta = \mathrm{diag}[\mathrm{var}(\theta_1), \mathrm{var}(\theta_2), \ldots, \mathrm{Var}(\theta_p)]$$

$$\Rightarrow \begin{aligned} \underset{\sim}{X}\vec{\theta} &\sim N(\underset{\sim}{X}\vec{\theta}^*, \underset{\sim}{X}\,\underset{\sim}{V}_\theta\,\underset{\sim}{X}^T) \\ \vec{y} &\sim N(\underset{\sim}{X}\vec{\theta}^*, \underset{\sim}{X}\,\underset{\sim}{V}_\theta\,\underset{\sim}{X}^T + \underset{\sim}{V}_{obs}) \end{aligned}$$

- Hence, a confidence interval on $\vec{y}$ with significance α, is

$$CI \equiv \left[\vec{y} \pm t_{N_y - P}^{1-\alpha/2}\sqrt{\sigma_\varepsilon^2\,(\underset{\sim}{X}^T\underset{\sim}{X})^{-1}}\right], \quad \text{Since } \mathrm{Cov}(\hat{\theta}) = \sigma_\varepsilon^2\,(\underset{\sim}{X}^T\underset{\sim}{X})^{-1}$$

- The prediction interval is

$$PI \equiv \left[\vec{y} \pm t_{N_y - P}^{1-\alpha/2}\sqrt{\sigma_\varepsilon^2 + \sigma_\varepsilon^2\,(\underset{\sim}{X}^T\underset{\sim}{X})^{-1}}\right]$$

Nonlinear Models under Frequentist Assumption

- Assume that $f(\underset{\sim}{q};\vec{\theta})$ can be accurately represented by a first order Taylor expansion.

$$\Rightarrow f(\underset{\sim}{q};\vec{\theta}) \approx f(\underset{\sim}{q};\vec{\theta}^*) + \sum_{j=1}^{p} \left.\frac{\partial f}{\partial \theta_j}\right|_{\vec{\theta}^*} \cdot \Delta\theta_j, \quad \Delta\theta_j = \theta_j - \theta_j^*$$

P

$$\Rightarrow f(y;\theta) \approx \text{[illegible]} \quad {}_{j=1}$$

$$= \bar{F} + \sum_{j=1}^{p} \vec{S}_j \Delta\theta_j$$

$$\Rightarrow E\left[f(y;\vec{\theta})\right] \approx E\left[\bar{F} + \sum_{j=1}^{p} \vec{S}_j \Delta\theta_j\right] = E\left[\bar{F}\right] + E\left[\sum_{j=1}^{p} \vec{S}_j \Delta\theta_j\right]$$

$$= \int_{\mathbb{R}^p} \bar{F} \cdot \rho(\vec{\theta})\, d\vec{\theta} + \int_{\mathbb{R}^p} \sum_{i=1}^{p} \vec{S}_j \cdot (\theta_j - \theta_j^*)\, \rho(\vec{\theta})\, d\vec{\theta}$$

$$= \bar{F} + \sum_{j=1}^{p} \vec{S}_j \int_{\mathbb{R}^p} (\theta_j - \theta_j^*)\, \rho(\vec{\theta})\, d\theta$$

- Let's assume that $\rho(\vec{\theta})$ is symmetric (e.g., Uniform, Gaussian)

$$\Rightarrow \int_{\mathbb{R}^p} (\theta_j - \theta_j^*)\, \rho(\vec{\theta})\, d\vec{\theta} = 0$$

$$\Rightarrow E\left[f(y;\vec{\theta})\right] = \bar{F} + 0$$

- Now for Variance

$$\mathrm{Var}\left[f(y;\vec{\theta})\right] = E\left[\left(\bar{F} + \sum_{j=1}^{p} \vec{S}_j \Delta\theta_j - \bar{F}\right)^2\right]$$

$$= E\left[\left(\sum_{j=1} \vec{S}_j \cdot \Delta\theta_j\right)^2\right]$$

$$= E\left[\sum_{j=1}^{p} \vec{S}_j^2 \Delta\theta_j^2 + \sum_{j=1}^{p} \sum_{\substack{q=1 \\ q \neq j}}^{p} \vec{S}_j \vec{S}_q \Delta\theta_j \Delta\theta_q\right]$$

$$= E\left[\sum_{j=1}^{p} \vec{S}_j^2 \Delta\theta_j^2\right] + E\left[\sum_{j=1}^{p} \sum_{\substack{q=1 \\ q \neq j}}^{p} \vec{S}_j \vec{S}_q \Delta\theta_j \Delta\theta_q\right]$$

$$= \sum_{j=1}^{p} \vec{S}_j^2 \underbrace{\int_{\mathbb{R}^p} (\theta_j - \theta_j^*)^2 \rho(\vec{\theta})\, d\vec{\theta}}_{\mathrm{Var}(\vec{\theta})} + \sum_{j=1}^{p} \sum_{\substack{q=1 \\ q \neq j}}^{p} \vec{S}_j \vec{S}_q \int_{\mathbb{R}^p} (\theta_j - \theta_j^*)(\theta_q - \theta_q^*)\, \rho(\vec{\theta})\, d\vec{\theta}$$

$$\sum_{j=1} S_j \ \mathbb{R}^p \underbrace{\qquad\qquad}_{Var(\vec{\theta})} \qquad \sum_{j=1} \ \sum_{q\neq j}$$

$$= \sum_{j=1}^{p} \vec{S}_j^{\,2} \, Var(\theta_j) + \sum_{j=1}^{p} \sum_{\substack{q=1 \\ q\neq p}}^{p} \vec{S}_j \vec{S}_q \, cov(\theta_j, \theta_q)$$

$$\boxed{= \underset{\sim}{S} \, \underset{\sim}{V}_\theta \, \underset{\sim}{S}^T}$$

$$\Rightarrow Var[f(y;\vec{\theta})] \approx \underset{\sim}{S} \, \underset{\sim}{V}_\theta \, \underset{\sim}{S}^T$$

$$\Rightarrow f \overset{apx}{\sim} N(f, \underset{\sim}{S} \, \underset{\sim}{V}_\theta \, \underset{\sim}{S}^T), \quad \text{where } \underset{\sim}{S} = \left[\frac{\partial f}{\partial \theta_j}\right]_{j=1,\dots,p}$$

$$\Rightarrow PI = \left[\bar{Y}_{\vec{\theta}^*} \pm t^{1-\alpha/2}_{N_y-p} \sqrt{\sigma_\varepsilon^2 + \sigma_\varepsilon^2 \, \underset{\sim}{S}^* (\underset{\sim}{S}^T \underset{\sim}{S})^{-1} \underset{\sim}{S}^{*T}}\right]$$

where $\underset{\sim}{S}^* = \left.\frac{\partial f}{\partial \theta_j}\right|_{\vec{\theta}^*, \vec{y}}$