

## Lecture 26: March 13

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## 26.1 Stein's Unbiased Risk Estimate (SURE)

Say we have data  $Y \in \mathbb{R}^n$ , and  $Y \sim \mathcal{N}(\mu, I_{n \times n})$  (i.e. covariance known). Say we have  $k$  estimators  $\hat{\theta}_1, \dots, \hat{\theta}_k$  for  $\mu$ , and we wish to choose the “best” one.

One way to do this is to choose the estimator which minimizes squared error risk, i.e.  $R(\mu, \hat{\theta}) = \mathbb{E}_\mu [\|\hat{\theta}(Y) - \mu\|^2]$ .

We can't compute these quantities directly since  $\mu$  is unknown. Stein's Unbiased Risk Estimate (SURE) gives us a way to estimate  $R(\mu, \hat{\theta})$ .

**Definition 26.1** We define **SURE** to be

$$\begin{aligned}\hat{R}(\mu, \hat{\theta}) &= -n + \|Y - \hat{\theta}(Y)\|^2 + 2 \sum_{i=1}^n \frac{\partial \hat{\theta}_i}{\partial Y_i}(Y) \\ &= -n + \|Y - \hat{\theta}(Y)\|^2 + 2 \operatorname{div} \hat{\theta}.\end{aligned}$$

**Proposition 26.2** Under the true distribution, the expected value of SURE is equal to the squared error risk, i.e.

$$\mathbb{E}_\mu[\text{SURE}] = \mathbb{E}_\mu[\hat{R}(\mu, \hat{\theta})] = R(\mu, \hat{\theta}).$$

The proof uses Stein's Lemma:

**Lemma 26.3** Suppose  $Z \sim \mathcal{N}(\mu, 1)$ . Then for smooth  $g$  (such that  $g(z)$  does not grow too quickly as  $|z| \rightarrow \infty$ ),

$$\mathbb{E}_\mu[g(Z)(Z - \mu)] = \mathbb{E}_\mu[g'(Z)].$$

**Proof:** By integration by parts:

$$\begin{aligned}\mathbb{E}_\mu[g(Z)(Z - \mu)] &= \int_{-\infty}^{\infty} g(z)(z - \mu)e^{-(z-\mu)^2/2} dz \\ &= \left[ -g(z)e^{-(z-\mu)^2/2} \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} e^{-(z-\mu)^2/2} g'(z) dz \\ &= \mathbb{E}_\mu[g'(Z)].\end{aligned}$$

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**Proof:** [Proof of Proposition 26.2]

**Case 1:**  $Y \in \mathbb{R}$ .

Note that

$$\mathbb{E}_\mu[\text{SURE}] = \mathbb{E}_\mu \left[ -1 + (Y - \hat{\theta}(Y))^2 + 2 \frac{\partial \hat{\theta}}{\partial Y} \right] = -1 + \mathbb{E}_\mu \left[ (Y - \hat{\theta}(Y))^2 \right] + 2 \mathbb{E}_\mu \left[ \frac{\partial \hat{\theta}}{\partial Y} \right].$$

Let  $g(Y) = \hat{\theta}(Y) - Y$ . Then

$$\begin{aligned} (\hat{\theta}(Y) - \mu)^2 &= (Y - \mu + g(Y))^2 \\ &= (Y - \mu)^2 + 2g(Y)(Y - \mu) + [g(Y)]^2, \\ \mathbb{E}_\mu \left[ (\hat{\theta}(Y) - \mu)^2 \right] &= 1 + 2\mathbb{E}_\mu[g(Y)(Y - \mu)] + \mathbb{E}_\mu[g(Y)^2] \\ &= 1 + 2\mathbb{E}_\mu[g'(Y)] + \mathbb{E}_\mu \left[ (\hat{\theta}(Y) - Y)^2 \right] \\ &= 1 + 2 \left[ -1 + \mathbb{E}_\mu \frac{\partial \hat{\theta}}{\partial Y} \right] + \mathbb{E}_\mu \left[ (\hat{\theta}(Y) - Y)^2 \right] \\ &= \mathbb{E}_\mu[\text{SURE}]. \end{aligned}$$

**Case 2:**  $Y \in \mathbb{R}^n$ .

Let  $g$  be as before. Note that

$$\begin{aligned} \|\hat{\theta}(Y) - \mu\|^2 &= \|Y - \mu + g(Y)\|^2 \\ &= \|Y - \mu\|^2 + 2g(Y)^T(Y - \mu) + \|g(Y)\|^2, \\ \mathbb{E}_\mu \left[ \|\hat{\theta}(Y) - \mu\|^2 \right] &= \mathbb{E} \|Y - \mu\|^2 + 2 \sum_{i=1}^n \mathbb{E}_\mu[g_i(Y)(Y - \mu)] + \mathbb{E}_\mu \|g(Y)\|^2 \\ &= n + 2 \sum_{i=1}^n \mathbb{E}_\mu[g_i(Y)(Y - \mu)] + \mathbb{E}_\mu \left[ \|\hat{\theta}(Y) - Y\|^2 \right], \end{aligned}$$

since  $\|Y - \mu\|^2 \sim \chi_n^2$ . For each  $i$ ,

$$\begin{aligned} \mathbb{E}_\mu[g_i(Y)(Y - \mu)] &= \mathbb{E}_\mu [\mathbb{E}_\mu [g_i(Y)(Y - \mu) \mid Y_{-i}]] \\ &= \mathbb{E}_\mu \left[ \frac{\partial g_i(Y)}{\partial Y_i} \right] \\ &= \mathbb{E}_\mu \left[ -1 + \frac{\partial \hat{\theta}_i(Y)}{\partial Y_i} \right]. \end{aligned}$$

Hence,

$$\begin{aligned} \mathbb{E}_\mu \left[ \|\hat{\theta}(Y) - \mu\|^2 \right] &= n + 2 \sum_{i=1}^n \mathbb{E}_\mu \left[ -1 + \frac{\partial \hat{\theta}_i(Y)}{\partial Y_i} \right] + \mathbb{E}_\mu \left[ \|\hat{\theta}(Y) - Y\|^2 \right] \\ &= -n + 2\mathbb{E}_\mu[\text{div } \hat{\theta}] + \mathbb{E}_\mu \left[ \|\hat{\theta}(Y) - Y\|^2 \right] \\ &= \mathbb{E}_\mu[\text{SURE}]. \end{aligned}$$

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**Definition 26.4** In this context, we define the degrees of freedom of  $\hat{\theta}$  to be

$$df(\hat{\theta}) := \text{div } \hat{\theta}.$$