1. Original Procedure for Choosing λ

To quote from Storey and Taylor 2004, the bootstrap procedure for choosing λ is:

- Step 1: for some range of λ, say $\mathcal{R} = \{0, 0.05, 0.10, \ldots, 0.95\}$, calculate $\hat{\pi}_0(\lambda)$ as in Section 2.
- Step 2: for each $\lambda \in \mathcal{R}$, form B bootstrap versions $\pi_0^{*b}(\lambda)$ of the estimate, $b = 1, ..., B$, by taking bootstrap samples of the p-values.
- Step 3: for each $\lambda \in \mathcal{R}$, estimate its respective MSE as
$$\hat{\text{MSE}}(\lambda) = \frac{1}{B}\sum_{b=1}^{B}[\pi_0^{*b}(\lambda) - \min_{\lambda' \in \mathcal{R}}\{\hat{\pi}_0(\lambda')\}]$$
- Step 4: set $\hat{\lambda} = \text{argmin}_{\lambda \in \mathcal{R}}\{\hat{\text{MSE}}(\lambda)\}$

2. Distribution of Bootstrap Estimator

As defined in Table 1 of Storey 2004, let $W(\lambda) = \sum_{i=1}^{m} I\{p_i > \lambda\}$, the number of p-values greater than λ. This means that (as described in Storey 2004 Eq 4):
$$\hat{\pi}_0(\lambda) = \frac{W(\lambda)}{m(1-\lambda)}$$
Let $q_{1 \ldots m}^{*b}$ be the resampled p-values in bootstrap sample b (as done in Step 2 above), and let $W^{*b}(\lambda)$ be this value calculated for bootstrap sample b.
$$W^{*b}(\lambda) = \sum_{i=1}^{m} I_{q_i > \lambda}$$
Since there are $W(\lambda)$ p-values greater than λ out of a set of m, this means
$$P(q_i^{*b} > \lambda) = \frac{W(\lambda)}{m}$$
and therefore, since the sum of iid Bernoulli variables is binomial:
$$W^{*b}(\lambda) \sim \text{Binom}(m, \frac{W(\lambda)}{m})$$
which means
$$E[W^{*b}(\lambda)] = W(\lambda)$$
$$\text{Var}[W^{*b}(\lambda)] = m\frac{W(\lambda)}{m}(1 - \frac{W(\lambda)}{m}) = W(\lambda)(1 - \frac{W(\lambda)}{m})$$
$$E[\pi_0^{*b}(\lambda)] = \frac{W(\lambda)}{m(1-\lambda)}$$
$$\text{Var}[\pi_0^{*b}(\lambda)] = \frac{1}{m^2(1-\lambda)^2}\text{Var}[W^{*b}(\lambda)] = \frac{W(\lambda)}{m^2(1-\lambda)^2}(1 - \frac{W(\lambda)}{m})$$
This is a closed form solution for the distribution of $\pi_0^{*b}(\lambda)$ in terms of $W(\lambda)$ and m, which means we can remove the need for bootstrap estimation. Specifically,
$$\lim_{b \to \infty} M\hat{S}E(\lambda) = \text{Var}[\pi_0^{*b}(\lambda)] + (E[\pi_0^{*b}(\lambda)] - \min_{\lambda' \in \mathcal{R}}\{\hat{\pi}_0(\lambda')\})^2$$
$$= \frac{W(\lambda)}{m^2(1-\lambda)^2}(1 - \frac{W(\lambda)}{m}) + (\hat{\pi}_0(\lambda) - \min_{\lambda' \in \mathcal{R}}\{\hat{\pi}_0(\lambda')\})^2$$

3. New Procedure

- Step 1: for some range of λ, say $R = \{0, 0.05, 0.10, \ldots, 0.95\}$, calculate $\hat{\pi}_0(\lambda)$ as in Section 2, and $W(\lambda)$ as above.
- Step 2: for each $\lambda \in \mathcal{R}$, estimate its respective MSE as
$$\hat{\text{MSE}}(\lambda) = \frac{W(\lambda)}{m^2(1-\lambda)^2}(1 - \frac{W(\lambda)}{m}) + (\hat{\pi}_0(\lambda) - \min_{\lambda' \in \mathcal{R}}\{\hat{\pi}_0(\lambda')\})^2$$
- Step 3: set $\hat{\lambda} = \text{argmin}_{\lambda \in \mathcal{R}}\{\hat{\text{MSE}}(\lambda)\}$