Active Subspaces for nonlinear models

- consider the model

$$y = f(\vec{x}; \vec{\theta}), \quad \vec{\theta} \in \mathbb{R}^p$$

- note that we cannot directly apply linear theory.

Approach

- Assume that f is Lipschitz continuous & differentiable s.t. $\|\nabla_\theta f(\vec{\theta})\| \leq L$, where $\nabla_\theta f = \left[\frac{\partial f}{\partial \theta_1}, \ldots, \frac{\partial f}{\partial \theta_p}\right]$,

- We can construct a $p \times p$ matrix given by

$$\underset{\sim}{C} = \int_\Gamma (\nabla_\theta f)(\nabla_\theta f)^T \rho(\vec{\theta})\, d\vec{\theta}, \quad \text{where } \vec{\theta} \in \Gamma \subset \mathbb{R}^p$$

& $\rho(\vec{\theta})$ is a density

- Note that $\underset{\sim}{C}$ is the average gradient-outer product, $\underset{\sim}{C} \in \mathbb{R}^{p \times p}$
- we know that $\underset{\sim}{C}$ is symmetric & nonnegative definite since

$$\vec{v}^T \underset{\sim}{C} \vec{v} = \int_\Gamma \left[\vec{v}^T \nabla_\theta f\right]^2 \rho(\vec{\theta})\, d\vec{\theta} \geq 0$$

- Because $\underset{\sim}{C}$ is symmetric & nonnegative definite, we can use an eigendecomposition

$$\underset{\sim}{C} = \underset{\sim}{W} \underset{\sim}{\Lambda} \underset{\sim}{W}^T, \quad \underset{\sim}{\Lambda} = \operatorname{diag}(\lambda_1, \ldots, \lambda_p)$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p \geq 0$.

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- The eigenvalues of $\underset{\sim}{C}$ correspond to eigenvectors

$$\underset{\sim}{W} = \left[\vec{\omega}_1, \vec{\omega}_2, \dots, \vec{\omega}_p\right], \ \& \ \underset{\sim}{W} \text{ is orthogonal.}$$

- We can express any λ_i as

$$\lambda_i = \vec{\omega}_i^T \underset{\sim}{C} \vec{\omega}_i = \int_{\Gamma} \left(\left(\nabla_{\theta} f \right)^T \vec{\omega}_i \right)^2 \rho(\vec{\theta}) \, d\vec{\theta}$$

i.e., mean square changes in $f(\underset{\sim}{q}; \vec{\theta})$ along $\vec{\omega}_i$ are given by λ_i.

. If $\lambda_i \simeq 0$, f is relatively constant for linear combination of parameters in direction $\vec{\omega}_i$.

- In practice, $\lambda_i \neq 0$, but may be "relatively small."

- We can split our eigendecomposition into

$$\underset{\sim}{\Lambda} = \begin{bmatrix} \underset{\sim}{\Lambda}_1 & \\ & \underset{\sim}{\Lambda}_2 \end{bmatrix}, \quad \underset{\sim}{W} = \begin{bmatrix} \underset{\sim}{W}_1 & \underset{\sim}{W}_2 \end{bmatrix}$$

where $\underset{\sim}{\Lambda}_1$ & $\underset{\sim}{W}_1$ denote the eigenpairs prior to a significant gap in λ_i, that is

$$\Rightarrow \underset{\sim}{\Lambda}_1 \in \mathbb{R}^{m \times m}, \quad \lambda_m \gg \lambda_{m+1}$$

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- Then the rotated coordinate frame (active subspace) for our parameters is given by

$$\vec{z} = \underset{\sim}{W}_1^T \vec{\theta}, \quad \vec{\chi} = \underset{\sim}{W}_2^T \vec{\theta}$$

where $\vec{z} \in \mathbb{R}^m$ is the active variable + $\vec{\chi} \in \mathbb{R}^{p-m}$ is inactive.

☆ Goal: Find $\underset{\sim}{W}_1^T \in \mathbb{R}^{p \times m}$ where $m \ll p$. ☆

Things to consider

i) What is $\rho(\vec{\theta})$ + Γ?

ii) How do we approximate $\underset{\sim}{C}$?

iii) How do we approximate $\nabla_\theta f$?

iv) What does $\lambda_m \gg \lambda_{m+1}$ mean?

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i) Choosing $\rho(\vec{\theta})$ + Γ

- Typically assume $\pm 20\%$ from some $\hat{\vec{\theta}}$

$$\Rightarrow \theta_i \sim U(0.8\, \hat{\theta}_i, 1.2\, \hat{\theta}_i)$$

- or $\vec{\theta} \sim MVN(\vec{\mu}, \underset{\sim}{V})$

ii) Approximating $\underset{\sim}{C}$

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- Quadrature works well when p is small
- Monte Carlo does best for large p

Algorithm

1) Draw $\vec{\theta}^1, \dots, \vec{\theta}^M$

2) Compute

$$\nabla_\theta f^j = \nabla_\theta f(\vec{\theta}^j) \quad (p+1 \text{ evals for Fwd. diff})$$

3) Calculate

$$\hat{\underset{\sim}{C}} = \frac{1}{M} \sum_{j=1}^{M} (\nabla_\theta f^j)(\nabla_\theta f^j)^T$$

4) Compute $\hat{\underset{\sim}{C}} = \hat{\underset{\sim}{W}} \hat{\underset{\sim}{\Lambda}} \hat{\underset{\sim}{W}}^T$

5) Find n s.t. $\lambda_n >> \lambda_{n+1}$ + $\hat{\underset{\sim}{\Lambda}} = \begin{bmatrix} \hat{\underset{\sim}{\Lambda}}_1 & \\ & \hat{\underset{\sim}{\Lambda}}_2 \end{bmatrix}$

6) Define $\vec{z} = \hat{\underset{\sim}{W}}_1^T \vec{\theta}$, $\vec{z} \in \mathbb{R}^n$, + (hopefully) $n << p$.