Stepwise Variable Selection in Nonparametric Additive Models

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Outline

1. Problem and Method
   - Nonparametric Sparse Regression
   - Iterative Variable Selection
   - Estimation, Selection, and Screening
   - Forward Addition
2. Empirical Studies
   - Simulation Settings
   - Empirical Performances

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Sparse Additive Regression Model

- Consider $Y_i = \eta(x_i) + \epsilon_i = \eta_\emptyset + \sum_{j=1}^{p} \eta_j(x_{i\langle j\rangle}) + \epsilon_i$, $i = 1, \ldots, n$, where $x_i = (x_{i\langle 1\rangle}, \ldots, x_{i\langle p\rangle}) \in [0,1]^p$ and $\epsilon_i \sim N(0, \sigma^2)$.
- Task: Only $d < p$ of the η_j's are nonzero, which we try to identify.
- Existing algorithms are largely LASSO-variants, using some L_1-type penalties to weed out inactive variables.
  - COSSO (Lin & Zhang 2006), SpAM (Ravikumar et al 2007), penGAM (Meier et al 2009), etc.
  - When $p \gg n$, variable-screening is needed to pare down the variable list for the algorithms to work (Fan et al 2011).
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Iterative Variable Selection

- Working with a pair of dynamic variable sets $\mathcal{P} \supseteq \mathcal{S}$, one may separate variable selection from estimation.
  1. Estimation: Given a variable pool $\mathcal{P}$, fit $\hat{\eta}(x)$ of form $\eta(x_i) = \eta_\emptyset + \sum_{j\in\mathcal{P}} \eta_j(x_{i\langle j\rangle})$ to the data.
  2. Variable Selection: Pick selection set $\mathcal{S} \subseteq \mathcal{P}$ such that $\tilde{\eta}(x)$ of form $\eta(x_i) = \eta_\emptyset + \sum_{j\in\mathcal{S}} \eta_j(x_{i\langle j\rangle})$ nearly achieves the goodness-of-fit of $\hat{\eta}(x)$.
  3. Screening and Updating: Rank variables in $\mathcal{P}^c$ to obtain $\tilde{\mathcal{P}}$, and augment $\mathcal{S}$ by $\tilde{\mathcal{P}}$ to update $\mathcal{P} = \mathcal{S} \cup \tilde{\mathcal{P}}$.
- The size $\tilde{p}$ of $\tilde{P}$ is capped at a moderate number, say 5; $\tilde{p}$ varies with the amount of agreement between consecutive $\mathcal{S}$'s.
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Cubic Spline Additive Models

- For estimation given $\mathcal{P}$, one may use cubic spline additive models.
- To fit $Y_i = \eta(x_i) + \epsilon_i = \eta_\emptyset + \sum_{j\in\mathcal{P}} \eta_j(x_{i\langle j\rangle}) + \epsilon_i$, one minimizes
$$\frac{1}{n}\sum_{i=1}^n \Big(Y_i - \eta_\emptyset - \sum_j \eta_j(x_{i\langle j\rangle})\Big)^2 + \lambda \sum_j \theta_j^{-1} \int_0^1 \big(\eta_j''(x_{\langle j\rangle})\big)^2 dx_{\langle j\rangle}$$
with $\eta(x) = d_0 + \sum_j d_j\phi(x_{\langle j\rangle}) + \sum_{i=1}^n c_i\big(\sum_j \theta_j R(x_{i\langle j\rangle}, x_{\langle j\rangle})\big)$, where $\phi(x)$ and $R(x,y)$ are known functions (Kimeldorf & Wahba 1971).
- Fixing θ_j, one may select λ using GCV (Craven & Wahba 1979).
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- It is clear that $\eta_j(x_{\langle j \rangle}) = d_j \phi(x_{\langle j \rangle}) + \theta_j \sum_i c_i R(x_{i\langle j \rangle}, x_{\langle j \rangle})$.
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- One may calculate an asymptotically efficient approximation of form $\eta(x) = d_0 + \sum_j d_j\phi(x_{\langle j\rangle}) + \sum_{k=1}^q c_k\big(\sum_j \theta_j R(z_{k\langle j\rangle}, x_{\langle j\rangle})\big)$, for $\{z_k\} \subset \{x_i\}$ a random subset of size $q \asymp n^{2/9}$ (Gu & Kim 2002).
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- For θ_j, use the starting value algorithm of Gu & Wahba (1991).
- $\sum_j \theta_j^{-1}\int_0^1 \big(\eta_j''(x_{\langle j\rangle})\big)^2 dx_{\langle j\rangle} = \sum_j \theta_j\, \mathbf{c}^T Q_j \mathbf{c}$; $\int_0^1 \big(\eta_j''(x_{\langle j\rangle})\big)^2 dx_{\langle j\rangle} = \theta_j^2\, \mathbf{c}^T Q_j \mathbf{c}$.
- First set $\tilde\theta_j^{-1} \propto \mathrm{tr} Q_j$ and fit $\tilde\eta$, then set $\theta_j \propto \tilde\theta_j^2\, \tilde{\mathbf{c}}^T Q_j \tilde{\mathbf{c}}$.

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- $\sum_j \theta_j^{-1}\int_0^1 \big(\eta_j''(x_{\langle j\rangle})\big)^2 dx_{\langle j\rangle} = \sum_j \theta_j\, \mathbf{c}^T Q_j \mathbf{c}$; $\int_0^1 \big(\eta_j''(x_{\langle j\rangle})\big)^2 dx_{\langle j\rangle} = \theta_j^2\, \mathbf{c}^T Q_j \mathbf{c}$.
- First set $\tilde{\theta}_j^{-1} \propto \mathrm{tr} Q_j$ and fit $\tilde{\eta}$, then set $\theta_j \propto \tilde{\theta}_j^2\, \tilde{\mathbf{c}}^T Q_j \tilde{\mathbf{c}}$.

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- The computational cost is comparable to that with $p = 1$.

Square Error Projection

- To select $\mathcal{S} \subseteq \mathcal{P}$, one may use square error projection, which is designed to "test" $H_0 : \eta \in \mathcal{H}_0$ versus $H_a : \eta \in \mathcal{H}_0 \oplus \mathcal{H}_1$.
- Given $\hat{\eta} \in \mathcal{H}_0 \oplus \mathcal{H}_1$, minimize $\mathrm{KL}(\hat{\eta}, \eta)$ over $\eta \in \mathcal{H}_0$ to get $\tilde{\eta}$. Inspect $\mathrm{KL}(\hat{\eta}, \eta_c) = \mathrm{KL}(\hat{\eta}, \tilde{\eta}) + \mathrm{KL}(\tilde{\eta}, \eta_c)$ for some η_c degenerate. (Gu 2004)
- We use $\mathrm{KL}(g, h) = \mathrm{SE}(g, h) = \frac{1}{n} \sum_i \big(g(x_i) - h(x_i)\big)^2$ and $\eta_c = \bar{Y}$.
- Forward Variable Selection: Given $\hat{\eta}$ fitted to variables in $\mathcal{P}$,
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  3. If $\mathrm{SE}(\hat{\eta}_*, \tilde{\eta}_*)$ exceeds a threshold, add $x_{\langle * \rangle}$ to $\mathcal{S}$, go to Step 1. Otherwise stop.
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Outline

Simulation Settings

- Simulations are conducted on some standard test examples in the literature. (Lin & Zhang 2006, Fan et al 2011, etc)

- Two test functions based on univariate g_1, g_2, g_3, g_4, and $\epsilon \sim N(0,1)$:

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Y &= 5g_1(x_{\langle 1\rangle}) + 3g_2(x_{\langle 1\rangle}) + 4g_3(x_{\langle 1\rangle}) + 6g_4(x_{\langle 1\rangle}) + \sqrt{1.74}\,\epsilon; \\
Y &= g_1(x_{\langle 1\rangle}) + g_2(x_{\langle 2\rangle}) + g_3(x_{\langle 3\rangle}) + g_4(x_{\langle 4\rangle}) \\
&\quad + 1.5\{g_1(x_{\langle 5\rangle}) + g_2(x_{\langle 6\rangle}) + g_3(x_{\langle 7\rangle}) + g_4(x_{\langle 8\rangle})\} \\
&\quad + 2\{g_1(x_{\langle 9\rangle}) + g_2(x_{\langle 10\rangle}) + g_3(x_{\langle 11\rangle}) + g_4(x_{\langle 12\rangle}) + \sqrt{.5184}\,\epsilon.
\end{aligned}
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- Three designs: $x_{\langle j\rangle} = (w_j + \alpha u)/(1+\alpha)$, for $w_j, u \sim U(0,1)$ and $\alpha = 0, 1, 3$.
- One hundred replicates each with $n = 400$ and $p = 100, 1000$.

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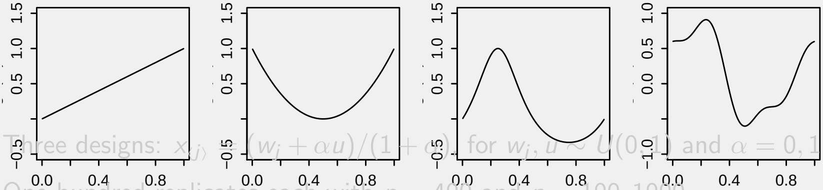

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- Selection results from 100 replicates each, for $p = 1000$ and $p = 100$:

- The numbers look okay for the independent and the mildly correlated designs, but not so good for the highly correlated design.
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	$d = 4$		$d = 12$	
	TP	FP	TP	FP
$\alpha = 0$	4.00, (4,4)	0.03, (0,1)	10.82, (9,12)	0.03, (0,1)
	4.00, (4,4)	0.03, (0,1)	11.58, (9,12)	0.03, (0,1)
$\alpha = 1$	3.99, (3,4)	0.15, (0,2)	9.18, (6,11)	0.18, (0,2)
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$\alpha = 3$	3.23, (2,4)	0.19, (0,2)	5.54, (4,8)	0.11, (0,2)
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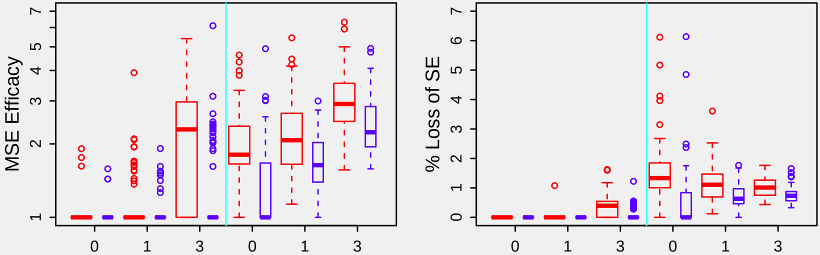

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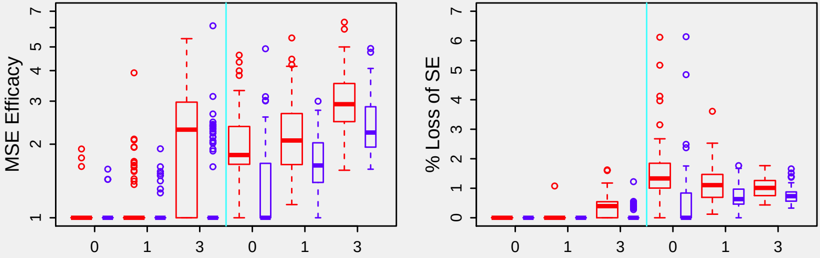

Behind the Scene

```
[1] "p=100"
[1] "initial"
[1] "X12" "X8"  "X71" "X10" "X11" "X74"
[1] "phase 1"
[1] "X12" "X8"  "X11" "X10" "X7"
[1] "phase 2"
[1] "X12" "X8"  "X11" "X10" "X7"  "X3"
[1] "X12" "X8"  "X11" "X10" "X7"  "X3"  "X4"

[1] "p=1000"
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[1] "X968" "X662" "X367" "X242" "X195" "X3"
[1] "phase 1"
[1] "X12"  "X8"   "X11"  "X195" "X4"
[1] "X12" "X8"  "X11" "X10" "X4"  "X6"
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The End

Thank You!