Stochastic Matching Pursuit for Bayesian Variable Selection and Analysis of Supersaturated Design

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## Variable Selection

$\square$ Model: $Y=\beta_{1} X_{1}+\cdots+\beta_{p} X_{p}+\varepsilon$

- Y: the $n$-dimensional response vector
- $\mathbf{X}_{i}$ : the $n$-dimensional regressor vector
- $\varepsilon$ : white noise
$\square$ Find the "promising" model:

$$
Y=\beta_{1}^{*} X_{1}^{*}+\cdots+\beta_{q}^{*} X_{q}^{*}+\varepsilon
$$

$\square n>p($ Large $n$ Small $p)$
$\square p>n($ Small $n$ Large $p)$

## Variable Selection Methods

$\checkmark$ How to find the "promising" variables, $X_{1}^{*}, \ldots, X_{q}^{*}$ ?

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- Stochastic Search Variable Selection


## Bayesian Variable Selection

$\square$ Stochastic Search Variable Selection (SSVS)

- George and McCulloch (1993, 1997)
- Chipman (1996) and Chipman et al. (1997)
- Smith and Kohn (1996)
$\square$ Applications:
- Supersaturated design: Beattie et al. (2002)
- Signal processing: Wolfe et al. (2004), and Févotte and Godsill (2006)
- Gene selection: Lee et al. (2003)
- ...


## Statistical Model

$\checkmark$ Model:

$$
Y=\mathbf{X} \beta+\epsilon
$$

- $Y$ is an $n \times 1$ response vector.
- $\mathbf{X}=\left[X_{1}, \ldots, X_{p}\right]$ is an $n \times p$ model matrix, and $X_{i}$ is the $i$-th predictor variable or regressor.
- $\beta=\left(\beta_{1}, \ldots, \beta_{p}\right)^{\prime}$ is a $p \times 1$ vector of the unknown coefficients.
- $\epsilon=\left(\epsilon_{1}, \ldots, \epsilon_{n}\right)^{\prime}$ is an $n \times 1$ noise vector that follows $M N\left(\mathbf{0}, \sigma^{2} I_{n}\right)$
$\square$ A $p \times 1$ vector of latent variables, $\gamma=\left(\gamma_{1}, \ldots, \gamma_{p}\right)^{\prime}$ :

$$
\gamma_{i}= \begin{cases}1, & X_{i} \text { is selected } \\ 0, & \text { otherwise }\end{cases}
$$

## Stochastic Search Variable Selection

$\square$ George and McCulloch (1993)
$\checkmark$ Prior assumptions:

- $\left(\beta_{i}, \gamma_{i}\right), i=1,2, \ldots, p$ are assumed to be independent.
- $\gamma: P\left(\gamma_{i}=0\right)=p_{i}$, and $P\left(\gamma_{i}=1\right)=1-p_{i}$.
- $\beta$ :

$$
\left[\beta_{i} \mid \gamma_{i}=0\right] \sim N\left(0, \nu_{0 i}\right), \text { and }\left[\beta_{i} \mid \gamma_{i}=1\right] \sim N\left(0, \nu_{1 i}\right) .
$$

Usually set $\nu_{1 i}=c_{i} \nu_{0 i}$ and $c_{i} \gg 1$, i.e. $\nu_{1 i} \gg \nu_{0 i}$.

- $\sigma: \sigma^{2} \sim I G(\nu / 2, \nu \lambda / 2)$.


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$\square$ The best subset of variables is selected according to the Monte Carlo samples of $\gamma$.
$\square$ The most costly step:

$$
[\beta \mid \gamma, Y, \sigma] \sim N\left(\sigma^{-2} A_{\gamma} \mathbf{X}^{\prime} Y, A_{\gamma}\right)
$$

- $A_{\gamma}=\left(\sigma^{-2} \mathbf{X}^{\prime} \mathbf{X}+D_{\gamma}^{-1} R^{-1} D_{\gamma}^{-1}\right)^{-1}$.
- $R$ is the prior correlation matrix.
- $D_{\gamma}^{-2}=\operatorname{diag}\left[\left(a_{1} \nu_{01}\right)^{-1}, \ldots,\left(a_{p} \nu_{0 p}\right)^{-1}\right]$ with $a_{i}=1$ if $\gamma_{i}=0$, and $a_{i}=c_{i}$ if $\gamma_{i}=1$.


## Stochastic Search Variable Selection

$\square$ Speed up the stochastic search variable selection process:

- Cholesky decomposition for $A_{\gamma}$.
- Sample $\gamma$ componentwise, i.e. $\left[\gamma_{i} \mid \gamma_{-i}, Y\right]$.
- When $\nu_{0 i}=0$, Geweke (1996) suggested to jointly draw $\left(\gamma_{i}, \beta_{i}\right)$.
- Choose conjugate prior for $\beta$. Sample $[\gamma \mid Y]$ directly. (Smith and Kohn, 1996, and George and McCulloch, 1997)


## Componentwise Gibbs Sampler

$\square$ The prior of $\beta: \beta_{i} \mid \gamma_{i} \sim\left(1-\gamma_{i}\right) \delta_{0}+\gamma_{i} N\left(0, \tau_{i}^{2}\right)$.

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$\square$ Assume $\tau_{i}=\tau$.
$\square$ The key step:

$$
\begin{aligned}
& \quad z_{i}=\frac{P\left(Y \mid \gamma_{i}=1,\left\{\beta_{k}, \forall k \neq i\right\}\right)}{P\left(Y \mid \gamma_{i}=0,\left\{\beta_{k}, \forall k \neq i\right\}\right)}=\sqrt{\frac{\sigma_{i \star}^{2}}{\tau^{2}}} \exp \left\{\frac{r_{i}^{2}}{2 \sigma_{i \star}^{2}}\right\}, \\
& \text { where } \sigma_{i \star}^{2}=\frac{\sigma^{2} \tau^{2}}{X_{i}^{\prime} X_{i} \tau^{2}+\sigma^{2}}, r_{i}=\frac{R_{i}^{\prime} X_{i} \tau^{2}}{\sigma^{2}+X_{i}^{\prime} X_{i} \tau^{2}}, \text { and } \\
& R_{i}=Y-\Sigma_{k \neq i} \beta_{k} X_{k} .
\end{aligned}
$$

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where $\sigma_{i \star}^{2}=\frac{\sigma^{2} \tau^{2}}{X_{i}^{\prime} X_{i} \tau^{2}+\sigma^{2}}, r_{i}=\frac{R_{i}^{\prime} X_{i} \tau^{2}}{\sigma^{2}+X_{i}^{\prime} X_{i} \tau^{2}}$, and $R_{i}=Y-\Sigma_{k \neq i} \beta_{k} X_{k}$.
$\square$ Set $p_{i}=\rho$. Then

$$
P\left(\gamma_{i}=1 \mid\left\{\beta_{k}, \forall k \neq i\right\}, Y\right)=\frac{(1-\rho) z_{i}}{\rho+(1-\rho) z_{i}}
$$

## The componentwise Gibbs sampler for variable selection

(I) Randomly select a variable $X_{i}$.
(II) Compute

$$
z_{i}=\frac{p\left(Y \mid \gamma_{i}=1,\left\{\beta_{k}, \forall k \neq i\right\}\right)}{p\left(Y \mid \gamma_{i}=0,\left\{\beta_{k}, \forall k \neq i\right\}\right)}=\sqrt{\sigma_{i \star}^{2} / \tau^{2}} \exp \left\{\frac{r_{i}^{2}}{2 \sigma_{i \star}^{2}}\right\} .
$$

Then evaluate the posterior probability
$P\left(\gamma_{i}=1 \mid\left\{\beta_{k}, \forall k \neq i\right\}, Y\right)=\frac{(1-\rho) z_{i}}{\rho+(1-\rho) z_{i}}$.
(III) Sample $\gamma_{i}$ from the above posterior probability. If $\gamma_{i}=0$, then set $\beta_{i}=0$, otherwise, sample $\beta_{i} \sim N\left(r_{i}, \sigma_{i \star}^{2}\right)$. Go back to (I).
(IV) After a number of iterations of the above steps, compute the current residual vector, Res $=Y-\sum_{i} \beta_{i} X_{i}$. Then sample $\sigma^{2} \sim I G\left(\frac{n+\nu}{2}, \frac{R_{e s} s^{\prime} R e s+\nu \lambda}{2}\right)$. Go back to (I).

## Componentwise Gibbs Sampler

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- The variables are highly correlated.
- The residual variance is small.


## Matching Pursuit

$\checkmark$ Matching Pursuit (Mallat and Zhang, 1993): Suppose $\left\|X_{i}\right\|^{2}=1$. At each iteration,

- Select $X_{j}$ such that

$$
j=\arg \max \left|\left\langle R, X_{i}\right\rangle\right| .
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- Updated $\beta_{i} \leftarrow \beta_{i}+\left\langle R, X_{i}\right\rangle$, and $R \leftarrow R-\left\langle R, X_{i}\right\rangle X_{i}$.


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$\square$ Forward selection


## Metropolized Matching Pursuit

$\square$ Metropolis scheme with a pair of reversible moves: addition and deletion moves based on

$$
z_{i}=P\left(Y \mid \gamma_{i}=1,\left\{\beta_{k}, \forall k \neq i\right\}\right) / P\left(Y \mid \gamma_{i}=0,\left\{\beta_{k}, \forall k \neq i\right\}\right)
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$\square$ The larger $z_{i}$ is, the more promising the variable $X_{i}$ is.

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$\checkmark$ Proposal for the next status:

- Add or delete a variable.
- Addition proposal: Sample a inactive variable with probability proportional to $z_{i}$.
- Deletion proposal: Randomly select one active variable.
$\checkmark$ Acceptance probability for addition move:

$$
\begin{align*}
& p_{\text {accept-add }} \\
= & \min \left[1, \frac{P\left(\gamma_{i}=1 \mid\left\{\beta_{k}, \forall k \neq i\right\}, Y\right)}{P\left(\gamma_{i}=0 \mid\left\{\beta_{k}, \forall k \neq i\right\}, Y\right)} \frac{p_{\text {delete }}}{p_{\text {add }}} \frac{1 /(A+1)}{z_{i} / \sum_{j: \gamma_{j}=0} z_{j}}\right] \\
= & \min \left[1, \frac{(1-\rho)}{\rho} \frac{p_{\text {delete }}}{p_{\text {add }}} \frac{\sum_{j: \gamma_{j}=0} z_{j}}{(A+1)}\right] . \tag{1}
\end{align*}
$$

$\square$ Acceptance probability of the deletion move:

$$
\begin{align*}
& p_{\text {accept-delete }} \\
= & \min \left[1, \frac{P\left(\gamma_{i}=0 \mid\left\{\beta_{k}, \forall k \neq i\right\}, Y\right)}{P\left(\gamma_{i}=1 \mid\left\{\beta_{k}, \forall k \neq i\right\}, Y\right)} \frac{p_{\text {add }}}{p_{\text {delete }}} \frac{z_{i} /\left(\sum_{j: \gamma_{j}=0} z_{j}+z_{i}\right)}{1 / A}\right] \\
= & \min \left[1, \frac{\rho}{(1-\rho)} \frac{p_{\text {add }}}{p_{\text {delete }}} \frac{A}{\sum_{j: \gamma_{j}=0} z_{j}+z_{i}}\right] . \tag{2}
\end{align*}
$$

## Stochastic matching pursuit for variable selection

(I) Let $A$ be the number of active variables. With probability $p_{\text {add }}$, go to (II). With probability $p_{\text {delete }}=1-p_{\text {add }}$ go to (IV).
(II) With probability $p_{\text {accept-add }}$ calculated according to Eq. (1), go to (III), and with probability $1-p_{\text {accept-add }}$ go back to (I).
(III) Among all the inactive variables $i$ with $\gamma_{i}=0$, sample a variable $i$ with probability proportional to $z_{i}$, then let $\gamma_{i}=1$ and sample $\beta_{i}$ as described in (III) of Algorithm 1. Go back to (I).

## Stochastic matching pursuit for variable selection

(IV) If $A>0$, then randomly select an active variable $i$ with $\gamma_{i}=1$.
(V) With probability $p_{\text {accept-delete }}$ calculated according to Eq. (2), accept the proposal of deleting the variable $i$, i.e., set $\gamma_{i}=0$, and $\beta_{i}=0$. With probability
$1-p_{\text {accept-delete }}$, reject the proposal of deleting variable $i$, and sample $\beta_{i}$ as described in (III) of Algorithm 1. Go back to (I).
(VI) After a number of iterations of the above steps, compute the current residual vector, Res $=Y-\sum_{i} \beta_{i} X_{i}$, and then update $\sigma^{2} \sim \operatorname{IG}\left(\frac{n+\nu}{2}, \frac{\text { Res }^{\prime} \operatorname{Res}+\nu \lambda}{2}\right)$. Go back to (I).
$\square$ Combine the strengths of the matching pursuit and the componentwise Gibbs sampler.

1. Pursue proposing variables.
2. Don't need to compute the inverse of the large matrix.

## Implementation Details

$\square$ After a burn-in period, use $\left\{\gamma^{(i)}, i>T\right\}$ to estimate $P\left(\gamma_{j}=1 \mid Y\right)$.
$\square$ Selection criteria:

- The highest posterior probability: $\max P\left(\gamma_{1}, \ldots, \gamma_{p} \mid Y\right)$.
- The median probability criterion in Barbieri and Berger (2004): $X_{i}$ is included in the model if

$$
P\left(\gamma_{i}=1 \mid Y\right) \geq 1 / 2
$$

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- $z_{i}$ is a decreasing function of $\tau$. Then $P\left(\gamma_{i}=1 \mid\left\{\beta_{k}, k \neq i\right\}, Y\right)$ is smaller for larger $\tau$.


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- Cross-Validation approach for selecting $\tau$ : Use $K$-fold CV (or Monte Carlo CV) to choose "proper" value of $\tau$. Thus

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\widehat{\tau}=\arg \min _{\tau} \sum_{k=1}^{K} \sum_{j}\left(y_{k j}-\widehat{y}_{-k j}(\tau)\right)^{2}
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$$

$\square \rho$ can also be selected by this CV approach.

## Large $n$ Small $p$

Example 3.1: $(n, p)=(60,5)$
$\square$ These five variables, $X_{1}, \ldots, X_{5} \stackrel{\text { iid }}{\sim} N_{60}\left(\mathbf{0}, I_{60}\right)$.
$\square$ The response variable is generated by

$$
Y=X_{4}+1.2 X_{5}+\epsilon
$$

where $\epsilon \sim N_{60}\left(\mathbf{0}, I_{60}\right)$.
$\square \operatorname{Set}(\rho, \tau)=(0.5,10)$ for SMP and set $\left(\nu_{0}, c\right)=(0.01,2500)$ for SSVS.
$\square$ Totally there are 1000 replications. Draw 3000 samples from posterior samples.

## Large $n$ Small $p$

Table 1: Variable selection results in Example 3.1

| method |  | Number of selected variables |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | 0 | 1 | 2 | 3 | 4 | 5 |  |
| SMP | $f_{1}$ | 0 | 0 | 997 | 3 | 0 | 0 |
|  | $f_{2}$ | 0 | 0 | 997 | 3 | 0 | 0 |
| SSVS | $f_{1}$ | 0 | 0 | 997 | 3 | 0 | 0 |
|  | $f_{2}$ | 0 | 0 | 997 | 3 | 0 | 0 |

## Large $n$ small $p$

Example 3.2: $(n, p)=(60,10)$
$\square 10$ variables, $X_{1}, \ldots, X_{10} \stackrel{\text { iid }}{\sim} N_{60}\left(\mathbf{0}, I_{60}\right)$.
$\square$ The true model is

$$
Y=2 X_{1}+3 X_{2}+4 X_{5}+5 X_{6}+6 X_{9}+7 X_{10}+\epsilon
$$

where $\epsilon \sim N_{60}\left(0,2.5^{2} I_{60}\right)$.
$\square \operatorname{Set}(\rho, \tau)=(0.5,15)$ for SMP and set $\left(\nu_{0}, c\right)=(0.01,2500)$ for SSVS.
$\square$ Totally there are 1000 replications. In each replication, draw 3000 samples.

## Large $n$ small $p$

Table 2: Variable selection results in Example 3.2

| method |  | Number of selected variables |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  |  | $\leq 3$ | 4 | 5 | 6 | 7 | $\geq 8$ |
| SMP | $f_{1}$ | 0 | 0 | 2 | 961 | 37 | 0 |
|  | $f_{2}$ | 0 | 0 | 0 | 961 | 37 | 0 |
| SSVS | $f_{1}$ | 0 | 0 | 1 | 934 | 64 | 1 |
|  | $f_{2}$ | 0 | 0 | 0 | 934 | 64 | 1 |

## Computational Cost

Table 3: CPU times (in seconds) of 10,000 iterations

|  | SMP | SSVS |
| :---: | :---: | :---: |
| CPU time in Example $3.1(p=5)$ | 14.6 s | 9.3 s |
| CPU time in Example $3.2(p=10)$ | 39.5 s | 20.8 s |
| CPU time with $p=100$ | 2016.6 s | 7266.4 s |

## Small $n$ Large $p$

$\square$ The gene selection problem in microarray experiments: the number of candidate genes, $p>$ the number of available sample size, $n$. (Yi et al., 2003, and Lee et al., 2003)
$\square$ Overcomplete signal representation: the number of basis functions, $p>$ the size of the signal, $n$. (Wolf et al., 2004)
$\square$ Sparse assumption.

## Simulations for Small $n$ Large $p$ Problem

$\square$ Shao and Chow (2007) studied the small $n$ large $p$ problem in microarray experiments.
$\square$ The ridge regression estimator for $\beta$ is $\widehat{\beta}=\left(\mathbf{X}^{\prime} \mathbf{X}+h_{n} I_{p}\right)^{-1} \mathbf{X}^{\prime} Y=R_{D} \mathbf{X}^{\prime} Y$,

- $I_{p}$ is the $p \times p$ identity matrix.
- $h_{n}$ is the ridge parameter.
- $R_{D}=\left(\mathbf{X}^{\prime} \mathbf{X}+h_{n} I_{p}\right)^{-1}$.
$\square$ Screen out $X_{i}$ if $\left|\widehat{\beta}_{i}\right| \leq a_{n}$, and $a_{n} \rightarrow 0$ as $n \rightarrow \infty$.
$\square$ Their procedure is asymptotically consistent and their idea is similar to that of the Lasso method (Tibshirani, 1996).


## Simulation

$\square(n, p)=(50,200)$ and $(100,400)$.
$\square$ There are 5 true active variables, and

$$
\beta=(3,-3.5,4,-2.8,3.2,0, \ldots, 0)^{\prime}
$$

$\square$ The regressor $X_{i}$ is generated by

$$
X_{i}=G_{i}+\lambda G
$$

where $G_{i}$ and $G \sim N_{n}\left(0, I_{n}\right)$, and $\lambda=0$ or 1.
$\square \epsilon \sim N_{n}\left(0, I_{n}\right)$.

## Simulation

$\square$ Three methods are used here, Shao and Chow (2007), SMP and Lasso + CV.
$\square$ The screening method of Shao and Chow (2007): Set $h_{n}=n^{2 / 3}$ and $a_{n}=n^{-1 / 6}$.
$\square$ SMP:

- $\tau$ is selected by 5 -fold CV from $\{80,120,160,220\}$ for $(n, p)=(50,200)$ and from $\{100,150,200,250\}$ for $(n, p)=(100,400)$.
- Draw 2000 posterior samples by taking every $p$ th sample.


## Simulation

$\square$ Lasso + CV: There is a Matlab implementation of the homotopy/LARS-LASSO algorithm for tracing the regularization path of the L1-penalized squared error loss (Rocha, 2006), and this tool-box is available at http://www.stat.berkeley.edu/twiki/Research/YuGroup/Software
$\square$ Stopping criterion:

$$
\left\|\mathbf{X}^{\prime}\left(Y-\mathbf{X}^{\prime} \widehat{\beta}\right)\right\|_{\infty}<b
$$

$\square$ lasso_cv: Fit the parameters of a linear model by using the lasso and $k$-folds cross validation
$\square b \in\left\{2 \times 10^{-1}, 10^{-1}, 10^{-2}, \ldots, 10^{-5}, 10^{-8}\right\}$.
$\square 10$-folds CV is used here.
$\square$ Identify $\left\{i \| \beta_{i} \mid>0\right\}$.

Frequencies based on 100 replications with $(n, p)=(50,200)$


Frequencies based on 100 replications with $(n, p)=(100,400)$


## An illustration in Image Representation

$\square$ Gabor regression model (Wolf et al., 2004) is

$$
f=\sum_{i} c_{i} g_{i}+\varepsilon
$$

where $g_{i}$ 's are the Gabor basis functions.
$\square$ The Gabor basis function can be defined as

$$
\begin{aligned}
g(u, v) & =\exp \left[-\frac{1}{2}\left(\sigma_{u} u^{2}+\sigma_{v} v^{2}\right)\right] \cos \left[\frac{2 \pi u}{\lambda}+\varphi\right] \\
u & =u_{0}+x_{1} \cos \theta-x_{2} \sin \theta \\
v & =v_{0}+x_{1} \sin \theta-x_{2} \cos \theta
\end{aligned}
$$

## Gabor Regression Function


$\square$ Give a grid

$$
\mathcal{X}=\left\{\left(x_{1}, x_{2}\right) \mid x_{1} \in\{22,24, \ldots, 40\} \text { and } x_{2} \in\{7,9, \ldots, 25\}\right\}
$$

$\square$ Totally we have 200 Gabor basis functions on $\mathcal{X}$ by setting $\varphi=0, \sigma_{u}=1$ and $\theta \in\{0,3 / 8 \pi\}$.
$\square$ The response is generated by

$$
Y=7 X_{17}-7 X_{71}+7 X_{161}-7 X_{177}+\varepsilon
$$

$\checkmark$ SMP:

- $\tau$ is chosen from $\mathcal{A}=\{50,100, \ldots, 300\}$ by Monte Carlo cross validation with 100 replications.
- Draw 3000 samples by taking every $p$ th sample.

| Selected Bases |  |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $X_{17}$ | $X_{71}$ | $X_{73}$ | $X_{161}$ | $X_{177}$ | SNR1 | SNR2 |
| 0.9957 | 0.5243 | 0.6317 | 0.6933 | 1.0000 | 0.373 | 0.080 |

## Conjugate Prior for $\beta$

$\checkmark$ Smith and Kohn (1996): The prior of $\beta$ given $\gamma$ is $N\left(\mathbf{0}, c \sigma^{2}\left(\mathbf{X}_{\gamma}^{\prime} \mathbf{X}_{\gamma}\right)^{-1}\right)$.
$\square$ Obtain $[\gamma \mid Y]$ by integrating $\beta$ and $\sigma^{2}$ out.

$$
P(\gamma \mid Y) \propto(1+c)^{-q_{\gamma} / 2} S(\gamma)^{-n / 2} \prod_{i=1}^{p} p_{i}^{\gamma_{i}}\left(1-p_{i}\right)^{1-\gamma_{i}}
$$

where $q_{\gamma}$ is the number of selected variables and

$$
S(\gamma)=Y^{\prime} Y-\frac{c}{1+c} Y^{\prime} \mathbf{X}_{\gamma}\left(\mathbf{X}_{\gamma}^{\prime} \mathbf{X}_{\gamma}\right)^{-1} \mathbf{X}_{\gamma}^{\prime} Y
$$

$\square$ Use Gibbs sampler to generate $\gamma_{i} \mid Y, \gamma_{-i}$.
$\square$ Need to prespecify the prior parameter $c$. When the norm of $X_{i}$ is equal to $1, c \in[10,1000]$.
$\square$ Simulations for the algorithm of Smith and Kohn (1996):

- Fix $p_{i}=\rho=1 / 2$.
- Set $n=50$ and $p=20,50,100,300$.
- The variables, $X_{1}, \ldots, X_{p} \stackrel{\text { iid }}{\sim} N_{n}\left(\mathbf{0}, I_{n}\right)$.
- The response variable is generated by

$$
Y=3 X_{1}+3 X_{2}+\cdots+3 X_{10}+\epsilon
$$

where $\epsilon \sim N_{n}\left(\mathbf{0}, I_{n}\right)$.

- The median probability criterion
- Selection results:

| $c$ | $p=20$ | $p=50$ | $p=100$ | $p=300$ |
| :---: | :---: | :---: | :---: | :---: |
| 10 | $\sqrt{ }$ | $\sqrt{ }$ | $\times$ |  |
| 100 | $\sqrt{ }$ | $\sqrt{ }$ | $\sqrt{ }$ | $\times$ |
| 1000 |  |  | $\sqrt{ }$ | $\times$ |

- SMP with $\tau=250$ works.


## Summarization

$\square$ Stochastic matching pursuit + median probability criterion works for both the cases of large $n$ small $p$ and small $n$ large $p$.
$\square$ Tune the parameters, $\rho$ and $\tau$, via CV approach.
$\square$ "Full" Bayesian procedure
$\square$ CPU times: Componentwise Gibbs sampler $<$ SMP $<$ SSVS
$\square$ Window (or block) version
$\square$ Selection criterion
$\square$ Theoretical Properties
$\checkmark$ Other applications

## Analysis of Supersaturated Design

$\checkmark$ Supersaturate design:

- Investigates $p$ factors in only $n(<p+1)$ experimental runs.
- Particularly useful in factor screening.
$\square$ Analysis methods:
- Lin (1993): Stepwise regression approach.
- Chipman (1996) and Chipman et al. (1997): Propose different priors for SSVS.
- Beattie et al. (2002): A two-stage method via SSVS.
- Phoa et al. (2009): Dantzing selection method.


## Analysis Approach

$\square$ Use componentwise Gibbs sampler:

- The sample correlations between the factors are not so high.
- The variance would not be too small.
$\square$ Follow the pre-process in Phoa et al. (2009), standardize $Y$ and $X_{i}$ 's are unit norm.
$\square$ Use leave-two-out cross-validation approach to choose the proper parameters, $\rho$ and $\tau$.
$\square$ Selection criterion: the median probability criterion and the highest posterior probability criterion.


## Example 1. Cast Fatigue Experiment

| Run | A | B | C | D | E | F | G |
| ---: | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | + | + | - | + | + | + | - |
| 2 | + | - | + | + | + | - | - |
| 3 | - | + | + | + | - | - | - |
| 4 | + | + | + | - | - | - | + |
| 5 | + | + | - | - | - | + | - |
| 6 | + | - | - | - | + | - | + |
| 7 | - | - | - | + | - | + | + |
| 8 | - | - | + | - | + | + | - |
| 9 | - | + | - | + | + | - | + |
| 10 | + | - | + | + | - | + | + |
| 11 | - | + | + | - | + | + | + |
| 12 | - | - | - | - | - | - | - |

## Example 1. Cast Fatigue Experiment

$\square$ Consider main effect model. i.e. $n=12$ and $p=7$.
$\square$ Fix $\rho=1 / 2$.
$\square$ Iterate $10000 \times p$ times and get 1000 samples from last $5000 \times p$ iterations.
$\square \tau$ is select from $\mathcal{A}=\{1,2,3,4,5\}$. $\widehat{\tau}=2$.
$\square$ The marginal posterior probabilities

| Variable | A | B | C | D | E | F | G |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Prob. | 0.350 | 0.353 | 0.341 | 0.553 | 0.292 | 0.899 | 0.279 |

$\square \mathrm{Wu}$ and Hamada (2000) and Phoa et al. (2009): [F (D)]

## Example 1. Cast Fatigue Experiment

$\square$ Consider main effects + two-factor interactions. i.e. $n=12$ and $p=28$.
$\square \tau$ is select from $\mathcal{A}=\{40,80,120,160,200\} . \widehat{\tau}=120$.
$\square$ The marginal posterior probabilities

| Variable | F | FG | AE | AC | BD | BC | AB |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Prob. | 0.763 | 0.759 | 0.129 | 0.015 | 0.014 | 0.014 | 0.014 |

$\square$ The highest posterior probability criterion: [F FG].
$\square$ Same as Phoa et al. (2009) by mAIC.

## Example 2. Blood Glucose Experiment

$\square$ Sample size, $n=18$.
$\square p=15: 1$ two-level factors, $A, 7$ three-level factors, $B, \ldots, H$ and 7 quadratic contrasts of these seven three-level factors, $B^{2}, \ldots, H^{2}$.
$\square \tau$ is select from $\mathcal{A}=\{3,4,5,6,7,8\} . \widehat{\tau}=4$.
$\square$ The marginal posterior probabilities

| Variable | $F^{2}$ | $E^{2}$ | $C$ | $B$ | $G$ | $F$ | $A$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Prob. | 0.596 | 0.538 | 0.384 | 0.383 | 0.378 | 0.364 | 0.322 |

$\square$ Same as Wu and Hamada (2000) and Phoa et al. (2009)

## Example 2. Blood Glucose Experiment

$\square$ Include two-factor interaction terms, $p=113$.
$\square \tau$ is select from $\mathcal{A}=\{40,80,120,160,200\} . \widehat{\tau}=80$.
$\square$ The marginal posterior probabilities

| Variable | $B H^{2}$ | $B^{2} H^{2}$ | $E G$ | $A H^{2}$ | $D E$ | $B C$ | $D E^{2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Prob. | 0.821 | 0.748 | 0.578 | 0.496 | 0.154 | 0.147 | 0.145 |

$\square$ The highest posterior probability criterion:

| Model | Post. Prob. | $R^{2}$ |
| :---: | :---: | :---: |
| $A H^{2} B H^{2} E G B^{2} H^{2}$ | 0.116 | 0.9568 |
| $B H^{2} B^{2} H^{2}$ | 0.027 | 0.7696 |
| $B H^{2} E G B^{2} H^{2}$ | 0.018 | 0.8737 |
| $A H^{2} B H^{2} E G B^{2} H^{2} E^{2} G^{2}$ | 0.017 | 0.9766 |

## Example 3. An Example in Lin (1993)

$\square$ A supersaturated design with $n=14$ and $p=23$.
$\square$ Fix $\rho=1 / 2$.
$\square$ Iterate 10000 times and get 1000 samples from last 5000 iterations.
$\square \tau$ is select from $\mathcal{A}=\{20,40,60,80,100\} . \widehat{\tau}=20$.
$\square$ The marginal posterior probabilities

| Variable | 14 | 12 | 19 | 4 | 10 | 11 | 15 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Prob. | 0.967 | 0.574 | 0.561 | 0.444 | 0.099 | 0.069 | 0.063 |

## Example 3. An Example in Lin (1993)

$\square$ The highest posterior probability criterion:

| Model | Post. Prob. | $R^{2}$ |
| :---: | :---: | :---: |
| 4121419 | 0.206 | 0.9548 |
| 14 | 0.133 | 0.6317 |
| 121419 | 0.034 | 0.8706 |
| 1214 | 0.031 | 0.7401 |
| 1419 | 0.023 | 0.7225 |

$\square \mathrm{Li}$ and Lin (2003): [4 1214 19]
$\square$ Phoa et al. (2009): [14]

## Future Works

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$\square$ Other examples
$\square$ One-stage method or two-stage method?
$\square$ The idea of Chipman (1996) and Chipman et al. (1997)

## Example 3. An Example in Lin (1993)

$\square$ Main effects + Two-factor interaction effects
$\square$ Totally 252 variables $(23+229)$
$\square$ Fix $\rho=1 / 2$.
$\square$ Iterate 10000 times and get 1000 samples from last 5000 iterations.
$\square \tau$ is select from $\mathcal{A}=\{150,170,190,210,230\} . \widehat{\tau}=170$.
$\square$ The marginal posterior probabilities

| Var. | 14 | $7 \times 15$ | $13 \times 20$ | $6 \times 10$ | $3 \times 5$ | $7 \times 19$ | $9 \times 22$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Prob. | 0.367 | 0.133 | 0.116 | 0.059 | 0.057 | 0.056 | 0.053 |

## Example 3. An Example in Lin (1993)

$\square$ Select the variables whose marginal probabilities $>0.04$.
$\square$ Totally 21 variables.
$\square$ Fix $\rho=1 / 2$.
$\square$ Iterate 10000 times and get 1000 samples from last 5000 iterations.
$\square \tau$ is select from $\mathcal{A}=\{5,10,15,20,25\} . \widehat{\tau}=5$.
$\square$ The marginal posterior probabilities

| Var. | $5 \times 20$ | 23 | 14 | $6 \times 10$ | 11 | $9 \times 21$ | $7 \times 15$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Prob. | 0.593 | 0.551 | 0.548 | 0.542 | 0.47 | 0.45 | 0.314 |

