Detection of Cooperative Interactions in Logistic Regression Models

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- Parameter estimation:

$$(\tilde{\beta}_1, \tilde{\beta}_2, \ldots, \tilde{\beta}_d) = \arg\min_{\beta_1, \beta_2, \ldots, \beta_d} \frac{1}{n} \sum_{t=1}^{n} \left| y^{(t)} - (\beta_1 x_1^{(t)} + \ldots + \beta_d x_d^{(t)}) \right|^2$$

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- Test sample: $(x_1^{\text{test}}, x_2^{\text{test}}, \ldots, x_d^{\text{test}})$
- Prediction:

$$y^{\text{test}} = \tilde{\beta}_1 x_1^{\text{test}} + \cdots + \tilde{\beta}_d x_d^{\text{test}}$$

Logistic Regression Models

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Individual Effects and Pairwise Interactions

Logistic regression model with individual effects and pairwise interactions

$$\Pr(Y = +1|\mathbf{X}) = \sigma(\beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_d X_d$$

Individual Effects and Pairwise Interactions

Logistic regression model with individual effects and pairwise interactions

$$\Pr(Y = +1|\mathbf{X}) = \sigma(\beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_d X_d \\ + \beta_{1,2} X_1 X_2 + \beta_{1,3} X_1 X_3 + \cdots + \beta_{d-1,d} X_{d-1} X_d)$$

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- $\beta_i \neq 0$: X_i has an individual effect.
- $\beta_i = 0$: X_i has no individual effect.
- $\beta_{i,j} \neq 0$: X_i and X_j has a pairwise interaction.
- $\beta_{i,j} = 0$: X_i and X_j has no pairwise interaction.

System Model

- $X_1, X_2, \ldots, X_d$ are independent variables with $\Pr\{X_i = +1\} = \Pr\{X_i = -1\} = 1/2$, for $i = 1, 2, \ldots, d$.
- Y is a binary outcome variable

$$
\begin{aligned}
\Pr\{Y = +1 | X_1, X_2, \ldots, X_d\} &= \sigma\Big(\sum_{i=1}^{d} \beta_i X_i + \sum_{1 \le i < j \le d} \beta_{i,j} X_i X_j\Big) \\
\Pr\{Y = -1 | X_1, X_2, \ldots, X_d\} &= 1 - \Pr\{Y = +1 | X_1, X_2, \ldots, X_d\} \\
&= \sigma\Big(-\sum_{i=1}^{d} \beta_i X_i - \sum_{1 \le i < j \le d} \beta_{i,j} X_i X_j\Big)
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\end{aligned}$$

Target:

Detect all individual effects and pairwise interactions in logistic regression models from a limited number of samples.

Motivation 1: Detection of the Graph Underlying an Ising Model [Bresler (2015)]

- Ising models on a graph $G = (V, E)$ with $|V| = d$:

$$p(X_1, X_2, \ldots, X_d) = \exp\left\{\sum_{i \in V} \beta_i X_i + \sum_{\{i,j\} \in E} \beta_{i,j} X_i X_j - \Phi(\beta)\right\}$$

- parameter vector: $\beta = \{\beta_i\}_{i \in V} \cup \{\beta_{i,j}\}_{\{i,j\} \in E}$
- normalizing constant: $\Phi(\beta)$
- the maximum degree of nodes is p (constant)
- $|\beta_i| \leq h$ and $\lambda \leq |\beta_{i,j}| \leq \mu$.

Motivation 1: Detection of the Graph Underlying an Ising Model [Bresler (2015)] (Continued)

Theorem (Bresler 2015)

Let $\delta = \frac{1}{2}e^{-2(\mu p + h)}$, $\tau^* = \frac{\lambda^2 \delta^{4p+1}}{16 p \mu}$, $\epsilon^* = \frac{\tau^*}{2}$, $\ell^* = \frac{8}{(\tau^*)^2}$. *Suppose we observe* n *samples with*

$$n \geq \frac{144(\ell^* + 3)}{(\epsilon^*)^2 \delta^{2\ell^*}} \log \frac{d}{\zeta}.$$

Then with probability at least $1 - \zeta$, *there exists an algorithm to detect the structure of* G *running in polynomial time* $O(\ell^* dn)$.

Motivation 2: Chow-Liu Tree [Chow & Liu (1968)]

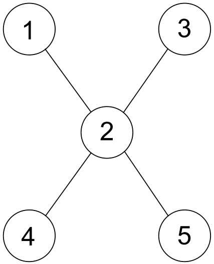
Chow-Liu representation:

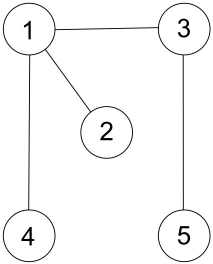
$$
\begin{aligned}
& p(X_1, X_2, X_3, X_4, X_5) \\
= \; & p(X_1) \cdot p(X_2|X_1) \cdot p(X_3|X_1, X_2) \cdot p(X_4|X_1, X_2, X_3) \cdot p(X_5|X_1, X_2, X_3, X_4) \\
\approx \; & p(X_1) \cdot p(X_2|X_1) \cdot p(X_3|X_2) \qquad \cdot p(X_4|X_2) \qquad \cdot p(X_5|X_2) \\
& \text{(first-order product approximation)} \\
= \; & p'(X_1, X_2, X_3, X_4, X_5)
\end{aligned}
$$

Target: Find p' to minimize the Kullback-Leibler distance $D(p||p')$ between p and p'.

Motivation 2: Chow-Liu Tree [Chow & Liu (1968)] (Continued)

Dependency Relationship





$$p(X_1, X_2, X_3, X_4, X_5) \approx p(X_1)p(X_2|X_1)p(X_3|X_2)p(X_4|X_2)p(X_5|X_2)$$

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Motivation 2: Chow-Liu Tree [Chow & Liu (1968)] (Continued)

Chow-Liu Algorithm:

- Construct a weighted complete graph $G = (V, E)$ with $V = \{v_1, v_2, \ldots, v_d\}$.
- The weight $w(v_i, v_j)$ of edge (v_i, v_j) is assigned to be $I(X_i; X_j)$.
- Find a maximum spanning tree T of G (by Kruskal's algorithm or Prim's algorithm).
- Set an arbitrarily node v to be the root of T, then rank the other nodes by their depths.

Our Work

- Model all individual effects and pairwise interaction by a so-called interaction graph.

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Our Work

- Model all individual effects and pairwise interaction by a so-called interaction graph.
- Establish an algorithm with a similar style as Chow-Liu algorithm to detect the structure of the interaction graph from a limited number of samples.
- No assumption of the maximum degree of nodes.
- Sample complexity and running time are both polynomial functions of the number of features.

Model with only Pairwise Interactions

- **Assumption:**
  No individual effects ($\beta_i = 0$ for $1 \leq i \leq d$).

- **For example:**
  - 5 variables X_1, X_2, X_3, X_4, X_5
  - $\beta_{1,2}, \beta_{2,3}, \beta_{2,4}, \beta_{2,5} \neq 0$ and other $\beta_{i,j} = 0$

$$\begin{aligned}
\Pr\{Y = +1 | X_1, X_2, X_3, X_4, X_5\} &= \sigma(\beta_{1,2}X_1X_2 + \beta_{2,3}X_2X_3 \\
&\quad + \beta_{2,4}X_2X_4 + \beta_{2,5}X_2X_5) \\
\Pr\{Y = -1 | X_1, X_2, X_3, X_4, X_5\} &= 1 - \Pr\{Y = +1 | X_1, X_2, X_3, X_4, X_5\}
\end{aligned}$$

Interaction Graph

Interaction graph: Let $G = (V, E)$ be the interaction graph with $V = \{v_1, v_2, \dots, v_d\}$, and the edge $(v_i, v_j) \in E$ if and only if the coefficient $\beta_{i,j}$ corresponding to X_i and X_j is nonzero.

For example:

$$\begin{aligned}
&\Pr\{Y = +1 | X_1, X_2, X_3, X_4, X_5\} \\
&\quad = \sigma(\beta_{1,2}X_1X_2 + \beta_{2,3}X_2X_3 \\
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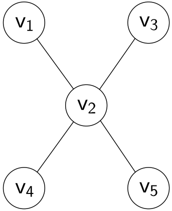

$\beta_{1,2}, \beta_{2,3}, \beta_{2,4}, \beta_{2,5} \neq 0$

Assumption, Difficulty & Target

- **Assumption:**

  The interaction graph $G = (V, E)$ is acyclic.

  - When the model contains at most two interactions, G is always acyclic.
  - When the number of interactions is far less than the number of features, G is acyclic with a high probability.
  - The model contains at most $d - 1$ interactions.

- **Difficulty:**

  We don't know which edges this graph has.

- **Target:**

  Detect the structure of the interaction graph from a limited number of samples.

Construction of a Weighted Complete Graph

Construction:

Construct a weighted complete graph $G' = (V', E')$ by

- $V' = (v'_1, v'_2, \dots, v'_d)$
- The weight of any edge $(v'_i, v'_j) \in E'$ is

$$w_{\{i,j\}} = \big| \Pr\{Y = +1 | X_i = +1, X_j = +1\} - \Pr\{Y = -1 | X_i = +1, X_j = +1\} \big|.$$

Structure Detection of the Interaction Graph (Case 1)

- Case 1: The third-order joint probability $p(X_i, X_j, Y)$ is known.
- $w_{\{i,j\}}$ can be calculated from the third-order joint distribution of X_i, X_j, Y

$$
\begin{aligned}
& w_{\{i,j\}} \\
= & |\Pr\{Y = +1|X_i = +1, X_j = +1\} - \Pr\{Y = -1|X_i = +1, X_j = +1\}| \\
= & |8 \Pr\{X_i = +1, X_j = +1, Y = +1\} - 1|
\end{aligned}
$$

Theorem on Detection (Case 1)

Theorem

Let $T = (V', E_T)$ be a maximum spanning tree of G'. Then

$$(v_i, v_j) \in E \text{ if and only if } (v_i', v_j') \in E_T \text{ and } w_{\{i,j\}} > 0.$$

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edges in the interaction graph

$\Updownarrow$

non-zero weighted edges in the maximum spanning tree

Detection Algorithm (Case 1)

Algorithm (Detecting the interaction graph)

- *Construct a weighted graph* $G' = (V', E')$ *with* $V' = \{v'_1, v'_2, \ldots, v'_d\}$.
- *The weight* $w_{\{i,j\}}$ *of edge* (v'_i, v'_j) *is assigned to be* $|\Pr\{Y = +1 | X_i = +1, X_j = +1\} - \Pr\{Y = -1 | X_i = +1, X_j = +1\}|$.
- *Find a maximum spanning tree* $T' = (V', E_T)$ *of* G' *(by Kruskal's algorithm or Prim's algorithm).*
- *Then the set of the edges in* G *is* $\{(v_i, v_j) : (v'_i, v'_j) \in E_T \text{ and } w_{\{i,j\}} > 0\}$.

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- *Then the set of the edges in* G *is* $\{(v_i, v_j) : (v'_i, v'_j) \in E_T \text{ and } w_{\{i,j\}} > 0\}$.

The algorithm is executed in polynomial time $O(d^2)$.

Structure Detection of the Interaction Graph (Case 2)

- Case 2:
  - The third-order joint probability $p(X_i, X_j, Y)$ is unknown.
  - Any non-zero parameter $\beta_{i,j}$ satisfies that

$$\lambda \leq |\beta_{i,j}| \leq \mu.$$

- Weight Assignment: With n samples $(Y^{(t)}, X_1^{(t)}, X_2^{(t)}, \ldots, X_d^{(t)})$ for $1 \leq t \leq n$, we estimate

$$w_{\{i,j\}} = |8\,\mathrm{Pr}\{X_i = +1, X_j = +1, Y = +1\} - 1|$$

by

$$\hat{w}_{\{i,j\}} = \left| \frac{8}{n} \sum_{t=1}^{n} \mathbf{1}_{(X_i^{(t)}, X_j^{(t)}, Y^{(t)}) = (+1,+1,+1)} - 1 \right|.$$

Theorem on Detection (Case 2)

Let

$$\gamma = \sqrt{\frac{2}{\pi d}} \left[\sigma(\lambda + 3\mu) - \sigma(-\lambda + 3\mu)\right].$$

Theorem

Assume for $1 \leq i < j \leq d$,

$$|\hat{w}_{\{i,j\}} - w_{\{i,j\}}| < \gamma/2.$$

Let $T = (V', E_T)$ *be a maximum spanning tree of* G'. *Then*

$$(v_i, v_j) \in E \text{ if and only if } (v_i', v_j') \in E_T \text{ and } \hat{w}_{\{i,j\}} > \gamma/2.$$

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edges in the interaction graph

$\Updownarrow$

large weighted edges in the maximum spanning tree

Detection Algorithm (Case 2)

Algorithm (Detecting the interaction graph)

- *Construct a weighted graph* $G' = (V', E')$ *with* $V' = \{v'_1, v'_2, \ldots, v'_d\}$.
- *The weight* $w_{\{i,j\}}$ *of edge* (v'_i, v'_j) *is assigned to be*

$$\left| \frac{8}{n} \sum_{t=1}^{n} \mathbf{1}_{(X_i[t], X_j[t], Y[t]) = (+1,+1,+1)} - 1 \right|.$$

- *Find a maximum spanning tree* $T' = (V', E_T)$ *of* G' *(by Kruskal's algorithm or Prim's algorithm).*
- *Then the set of the edges in* G *is* $\{(v_i, v_j) : (v'_i, v'_j) \in E_T \text{ and } w_{\{i,j\}} > \gamma/2\}$.

The algorithm is executed in polynomial time $O(nd^2)$.

Sample Complexity (Case 2)

Theorem

Fix $0 < \epsilon < 1$ and let n be a positive integer such that

$$n \geq \frac{128}{\gamma^2} \log \frac{d^2}{\epsilon} = \frac{64\pi d}{[\sigma(\lambda + 3\mu) - \sigma(-\lambda + 3\mu)]^2} \log \frac{d^2}{\epsilon}. \quad (1)$$

Then with probability at least $1 - \epsilon$, the algorithm can successfully detect the graph G from n i.i.d. samples of $(X_1, X_2, \ldots, X_d, Y)$.

The order of sample complexity: $\Theta\left(d \log \frac{d}{\epsilon}\right)$
Running time: $O(d^3 \log \frac{d}{\epsilon})$

Models with both Individual Effects and Pairwise Interactions

- **For example:**
  - 4 variables X_1, X_2, X_3, X_4
  - $\beta_2, \beta_{1,2}, \beta_{2,3}, \beta_{2,4} \neq 0$ and other $\beta_i, \beta_{i,j} = 0$

$$\begin{aligned}\Pr\{Y = +1 | X_1, X_2, X_3, X_4\} &= \sigma(\beta_2 X_2 + \beta_{1,2} X_1 X_2 \\ &\quad + \beta_{2,3} X_2 X_3 + \beta_{2,4} X_2 X_4) \\ \Pr\{Y = -1 | X_1, X_2, X_3, X_4\} &= 1 - \Pr\{Y = +1 | X_1, X_2, X_3, X_4\}\end{aligned}$$

Extended Interaction Graph

For extended interaction graph $G = (V, E)$,

- $V = \{v_0(\text{virtual vertex}), v_1, v_2, \ldots, v_d\}$
- $(v_0, v_i) \in E$ if and only if X_i has an individual effect
- $(v_i, v_j) \in E$ if and only if X_i and X_j have a cooperative interaction

With the help of the virtual vertex v_0, G can capture all individual effects and pairwise interactions.

For example:

$$\begin{aligned}
&\Pr\{Y = +1 | X_1, X_2, X_3, X_4\} \\
&\quad = \sigma(\beta_2 X_2 + \beta_{1,2} X_1 X_2 \\
&\qquad + \beta_{2,3} X_2 X_3 + \beta_{2,4} X_2 X_4)
\end{aligned}$$

$$\begin{aligned}
&\Pr\{Y = -1 | X_1, X_2, X_3, X_4\} \\
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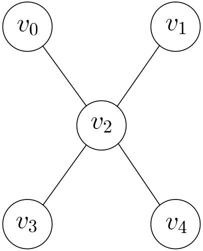


$\beta_2, \beta_{1,2}, \beta_{2,3}, \beta_{2,4} \neq 0$

Auxiliary Model

- **Assumption:**

  The extended interaction graph $G = (V, E)$ is acyclic.

- **Auxiliary model:** $\Pr\{\tilde{X}_i = +1\} = \Pr\{\tilde{X}_i = -1\} = 1/2$ for $0 \leq i \leq d$.

  ($\tilde{X}_0$: the virtual feature corresponding to the virtual node v_0)

$$\Pr\{\tilde{Y} = +1 | \tilde{X}_0, \tilde{X}_1, \tilde{X}_2, \ldots, \tilde{X}_d\} = \sigma\Big(\sum_{i=1}^{d} \beta_i \tilde{X}_0 \tilde{X}_i + \sum_{1 \leq i < j \leq d} \beta_{i,j} \tilde{X}_i \tilde{X}_j\Big)$$

$$\begin{aligned}\Pr\{\tilde{Y} = -1 | \tilde{X}_0, \tilde{X}_1, \tilde{X}_2, \ldots, \tilde{X}_d\} &= 1 - \Pr\{\tilde{Y} = +1 | \tilde{X}_0, \tilde{X}_1, \tilde{X}_2, \ldots, \tilde{X}_d\} \\ &= \sigma\Big(-\sum_{i=1}^{d} \beta_i \tilde{X}_0 \tilde{X}_i - \sum_{1 \leq i < j \leq d} \beta_{i,j} \tilde{X}_i \tilde{X}_j\Big)\end{aligned}$$

Relationship between Original Model and its Auxiliary Model

- **Original model:**

$$
\begin{aligned}
w_{\{0,i\}} &:= |\Pr(Y = +1|X_i = +1) - \Pr(Y = -1|X_i = +1)| \\
w_{\{i,j\}} &:= |\Pr\left(Y = +1|X_i = +1, X_j = +1\right) \\
&\quad + \Pr\left(Y = +1|X_i = -1, X_j = -1\right) - 1|
\end{aligned}
$$

- **Auxiliary model:**

$$
\tilde{w}_{\{i,j\}} := \left|\Pr(\tilde{\mathrm{Y}} = +1|\tilde{\mathrm{X}}_i = +1, \tilde{\mathrm{X}}_j = +1) - \Pr(\tilde{\mathrm{Y}} = -1|\tilde{\mathrm{X}}_i = +1, \tilde{\mathrm{X}}_j = +1)\right|
$$

Theorem

For $0 \le i < j \le d$,

$$
w_{i,j} = \tilde{w}_{i,j}
$$

Idea of Converting

- Original model and auxiliary model share the same interaction graph.
- Auxiliary model contains only pairwise interactions.
- Assign the empirical weight of the original model into each edge of the auxiliary model.

Detection Algorithm of Extended Interaction Graphs

Algorithm

- *Construct a weighted complete graph* $G' = (V', E')$ *with* $V' = \{v'_0, v'_1, v'_2, \ldots, v'_d\}$.
- *For* $1 \leq i \leq d$, *the weight* $w_{\{0,i\}}$ *of edge* (v'_0, v'_i) *is assigned to be*

$$\left| \frac{4}{n} \sum_{t=1}^{n} \mathbf{1}((\mathrm{x}_i[t], \mathrm{y}[t]) = (+1, +1)) - 1 \right| ;$$

for $1 \leq i < j \leq d$, *the weight* $w_{\{i,j\}}$ *of edge* (v'_i, v'_j) *is assigned to be*

$$\left| \frac{4}{n} \sum_{t=1}^{n} \mathbf{1}((\mathrm{x}_i[t], \mathrm{x}_j[t], \mathrm{y}[t]) = (+1, +1, +1)) + \frac{4}{n} \sum_{t=1}^{n} \mathbf{1}((\mathrm{x}_i[t], \mathrm{x}_j[t], \mathrm{y}[t]) = (-1, -1, +1)) - 1 \right| .$$

Detection Algorithm of Extended Interaction Graphs (Continued)

Algorithm

- *Find a maximum spanning tree* $T' = (V', E_T)$ *of* G' *(by Kruskal's algorithm or Prim's algorithm).*
- *Then the set of the edges in* G *is* $\{(v_i, v_j) : (v'_i, v'_j) \in E_T \text{ and } w_{\{i,j\}} > \gamma'/2\}$, *with*

$$\gamma' = \sqrt{\frac{2}{\pi(d+1)}} \left[\sigma(\lambda + 3\mu) - \sigma(-\lambda + 3\mu)\right].$$

The algorithm is also executed in polynomial time.

Non-Uniform Case

- **Assumption:**
  - $X_1, X_2, \ldots, X_d$ are independent variables with $\Pr\{X_i = +1\} = p_i$, $\Pr\{X_i = -1\} = q_i$ with $p_i + q_i = 1$, for $i = 1, 2, \ldots, d$ (non-uniform features)
  - The interaction graph $G = (V, E)$ is simply a path of length at most 4.
- **Target:**

  Reconstruct the graph from the samples of $(Y, X_1, X_2, \ldots, X_d)$.
- **Construction:**

  Construct a weighted complete graph $G' = (V', E')$ by
  - $V' = (v'_1, v'_2, \ldots, v'_d)$
  - The weight of any edge $(v'_i, v'_j) \in E'$ is assigned to be

$$w_{\{i,j\}} = \Big| Q^{i,j}_{+1,+1,+1} + Q^{i,j}_{-1,-1,+1} + Q^{i,j}_{-1,+1,-1} + Q^{i,j}_{+1,-1,-1} - Q^{i,j}_{+1,+1,-1} - Q^{i,j}_{-1,-1,-1} - Q^{i,j}_{-1,+1,+1} - Q^{i,j}_{+1,-1,+1} \Big|.$$

$(Q^{i,j}_{i_1,i_2,i_3} := \Pr\{Y = i_3 | X_i = i_1, X_j = i_2\})$

Theorem on Detection (Non-uniform Case)

Theorem

Let $T = (V', E_T)$ *be a maximum spanning tree of* G'. *Then*

$$(v_i, v_j) \in E \text{ if and only if } (v_i', v_j') \in E_T \text{ and } w_{\{i,j\}} > 0.$$

Hardness of Detection (Non-uniform Case)

Theorem

Assume that the interaction graph is simply a path of length 5. If the weight of edge (v_i', v_j') in G' is assigned to be

$$w_{\{i,j\}} = \left| \sum_{i_1, i_2, i_3 \in \{+1,-1\}} \alpha_{i_1,i_2,i_3} Q^{i,j}_{i_1,i_2,i_3} \right|,$$

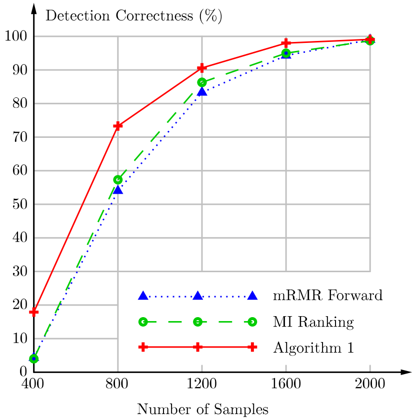
for any constants $\{\alpha_{i_1,i_2,i_3} : i_1, i_2, i_3 \in \{+1,-1\}\}$, then there exists a counterexample where we cannot correctly detect the structure of the interaction graph by finding a maximum spanning tree of G'.

The theorem for the uniform cases cannot be extended into the generic non-uniform cases.

Simulation Experiments

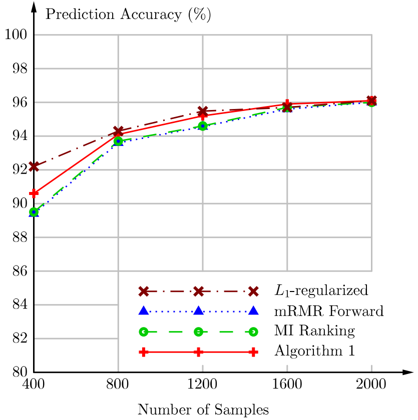
- 1000 logistic regression models
- 15 features, 5 individual effects, 10 pairwise interactions
- 400, 800, 1,200, 1,600, 2,000 samples
- Detection of the interaction graphs

Results of Simulation Experiments - Part 1



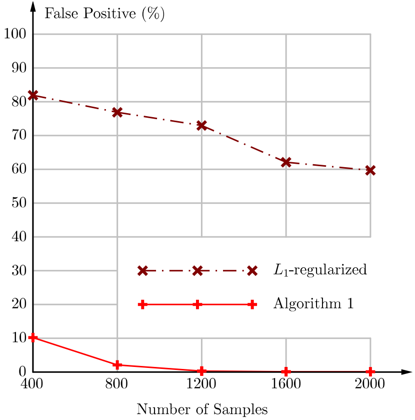
Comparison of detection correctness among mRMR forward selection [Peng, Long & Ding (2005)], feature ranking based on mutual information estimation [Paninski (2003)], and our algorithm.

Results of Simulation Experiments - Part 2



Comparison of prediction correctness among mRMR forward selection [Peng, Long & Ding (2005)], feature ranking based on mutual information estimation [Paninski (2003)], and L_1-penalized logistic regression [Park & Hastie (2007)], and our algorithm.

Results of Simulation Experiments - Part 3



Comparison of false positive rates for detection between L_1-penalized logistic regression [Park & Hastie (2007)] and our Algorithm.

Summary

- Logistic regression models:

$$\Pr\{Y = +1 | X_1, X_2, \ldots, X_d\} = \sigma\Big(\sum_{1 \le i \le d} \beta_i X_i + \sum_{1 \le i < j \le d} \beta_{i,j} X_i X_j\Big)$$

$$\Pr\{Y = -1 | X_1, X_2, \ldots, X_d\} = 1 - \Pr\{Y = +1 | X_1, X_2, \ldots, X_d\}$$

- Interaction graph $G = (V, E)$:

$$(v_i, v_j) \in E \iff \beta_{i,j} \neq 0.$$

- Detection of the interaction graph:
  - Construct a weighted complete graph.
  - Find its maximum spanning tree.
  - Pick the edges with large weights.
- Extended to the models with both individual effects and pairwise interactions

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Thank you!