

Experimental Design and Linear Estimators

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Linear Model

- $a, b, c = -1$ or 1
- y : A function of a, b, c with Gaussian noise

A linear model :

$$y = \mu + \beta_a a + \beta_b b + \beta_c c + \varepsilon$$

↑ ↑ ↑ ↑ ↑
 unknown noise

Problem Estimate some of the unknown parameters from the experiments ↴

There are $2^3 = 8$ types of experiments.

	①	②	③	④	⑤	⑥	⑦	⑧
(μ)	1	1	1	1	1	1	1	1
a	-1	1	-1	1	-1	1	-1	1
b	-1	-1	1	1	-1	-1	1	1
c	-1	-1	-1	-1	1	1	1	1
outputs	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

Each column corresponds to an experiment.

Linear Estimator

A linear model :
($a, b, c = -1$ or 1)

$$y = \underbrace{\mu}_{\text{unknown}} + \underbrace{\beta_a}_{\text{unknown}} a + \underbrace{\beta_b}_{\text{unknown}} b + \underbrace{\beta_c}_{\text{unknown}} c + \underbrace{\varepsilon}_{\text{noise}}$$

	①	②	③	④	⑤	⑥	⑦	⑧
(μ)	1	1	1	1	1	1	1	1
a	-1	-1	-1	-1	1	1	1	1
b	-1	-1	1	1	-1	-1	1	1
c	-1	1	-1	1	-1	1	-1	1
outputs	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

An example of linear (unbiased) estimator of β_a

ε : ignored

$$\hat{\beta}_a = \frac{1}{2} \{-y_1 + y_5\} = \frac{1}{2} \{-(\mu - \beta_a - \beta_b - \beta_c) + (\mu + \beta_a - \beta_b - \beta_c)\} = \beta_a$$

The linear estimator of β_a :

$$\hat{\beta}_a = \sum_{g=1}^8 x_{ag} Y_g$$

($x_{a1}, \dots, x_{a8} \in \mathbf{R}$)

Design of Experiments

One of the purpose of design of experiments is to construct the optimal experimental design.

	①	②	③	④	⑤	⑥	⑦	⑧
(μ)	1	1	1	1	1	1	1	1
a	-1	-1	-1	-1	1	1	1	1
b	-1	-1	1	1	-1	-1	1	1
c	-1	1	-1	1	-1	1	-1	1
outputs	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

Problem Choose fewer experiments among ①, ..., ⑧ with the minimum loss of information to estimate some of the unknown parameters.

Model selection, sparse modeling, ...

Group Lasso

A linear model : $y = \mu + \beta_a a + \beta_b b + \beta_c c + \varepsilon$

Problem



- Obtain the **good linear unbiased estimators**.
- Choose **fewer** experiments.

Assume that we want to estimate β_a and β_b .



$$\begin{aligned} &\underset{x_a, x_b \in \mathbb{R}^8}{\text{minimize}} \quad \underbrace{\left\{ \|x_a\|^2 + \|x_b\|^2 \right\}}_{\substack{\text{Variances} \\ (\Rightarrow \text{good estimators})}} + \underbrace{\sum_{g=1}^8 \lambda_g \left| \sqrt{x_{ag}^2 + x_{bg}^2} \right|}_{\substack{\text{Sparseness} \\ (\Rightarrow \text{fewer experiments})}} \\ &\text{subject to} \quad \underbrace{\begin{pmatrix} Mx_a \\ Mx_b \end{pmatrix} = \begin{pmatrix} e_a \\ e_b \end{pmatrix}}_{\substack{\text{Unbiasedness} \\ (\Rightarrow \text{linear unbiased estimators})}} \end{aligned}$$

Numerical Examples

(<https://github.com/tanaken-basis/explasso>)

$$y = \mu + \beta_a a + \beta_b b + \beta_c c + \varepsilon$$

Example 1) Assume that we want to estimate β_a, β_b

⇒ $(\lambda_1, \dots, \lambda_8) = (10, 100, 20, 200, 40, 400, 80, 800)$

⇒ Solve the problem of **Group lasso**

⇒ The optimal solution :

	①	③	⑤
(μ)	1	1	1
a	-1	-1	1
b	-1	1	-1
c	-1	-1	-1

Example 2) Assume that we want to estimate $\beta_a, \beta_b, \beta_c$

⇒ $(\lambda_1, \dots, \lambda_8) = (100, 0, 0, 100, 0, 100, 100, 0)$

⇒ **Group lasso** ⇒ **L4**

	⑧	⑤	③	②
(μ)	1	1	1	1
a	1	1	-1	-1
b	1	-1	1	-1
c	1	-1	-1	1

Patterns of the solution

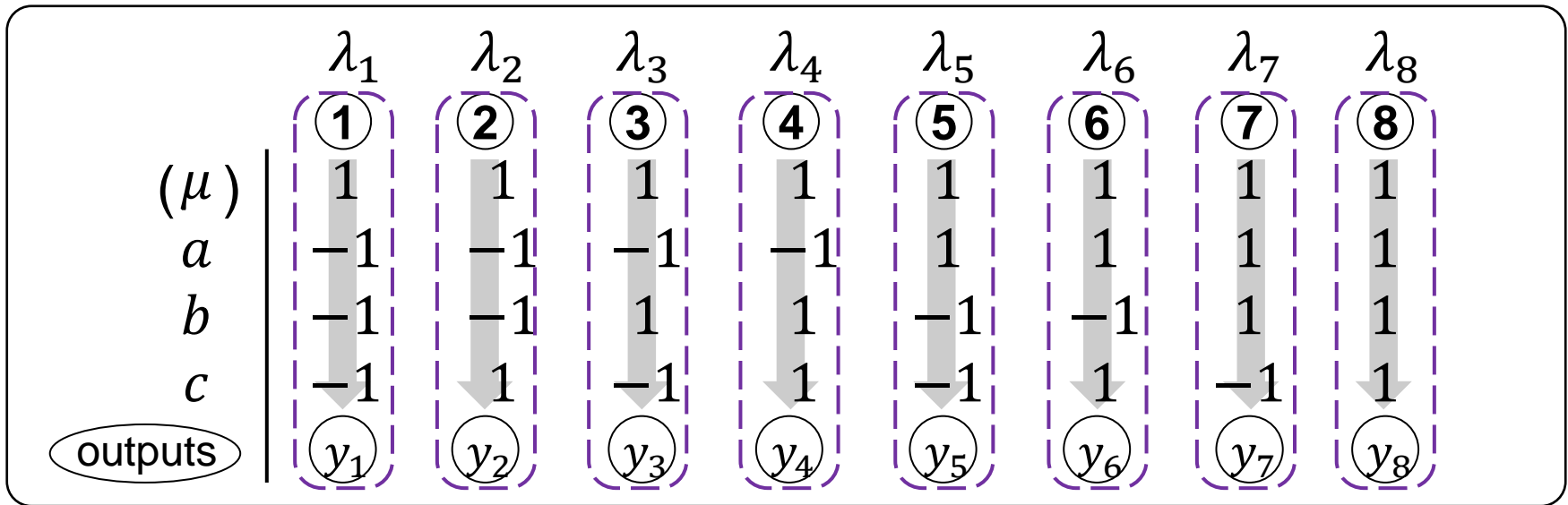
The selection of the experiments strongly depends on the tuning parameters!

$$\begin{aligned} & \underset{\mathbf{x}_a, \mathbf{x}_b \in \mathbb{R}^8}{\text{minimize}} \left\{ \|\mathbf{x}_a\|^2 + \|\mathbf{x}_b\|^2 \right\} + \sum_{g=1}^8 \lambda_g \left| \sqrt{x_{ag}^2 + x_{bg}^2} \right| \\ & \text{subject to } \begin{pmatrix} \mathbf{M} \mathbf{x}_a \\ \mathbf{M} \mathbf{x}_b \end{pmatrix} = \begin{pmatrix} \mathbf{e}_a \\ \mathbf{e}_b \end{pmatrix} \end{aligned}$$

λ_g : unwantedness of the g -th experiment

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
(μ)	①	②	③	④	⑤	⑥	⑦	⑧
a	1	1	1	1	1	1	1	1
b	-1	-1	-1	-1	1	1	1	1
c	-1	1	-1	1	-1	-1	-1	1
outputs	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

Patterns of the solution



Example 3) Assume that we want to estimate β_a, β_b

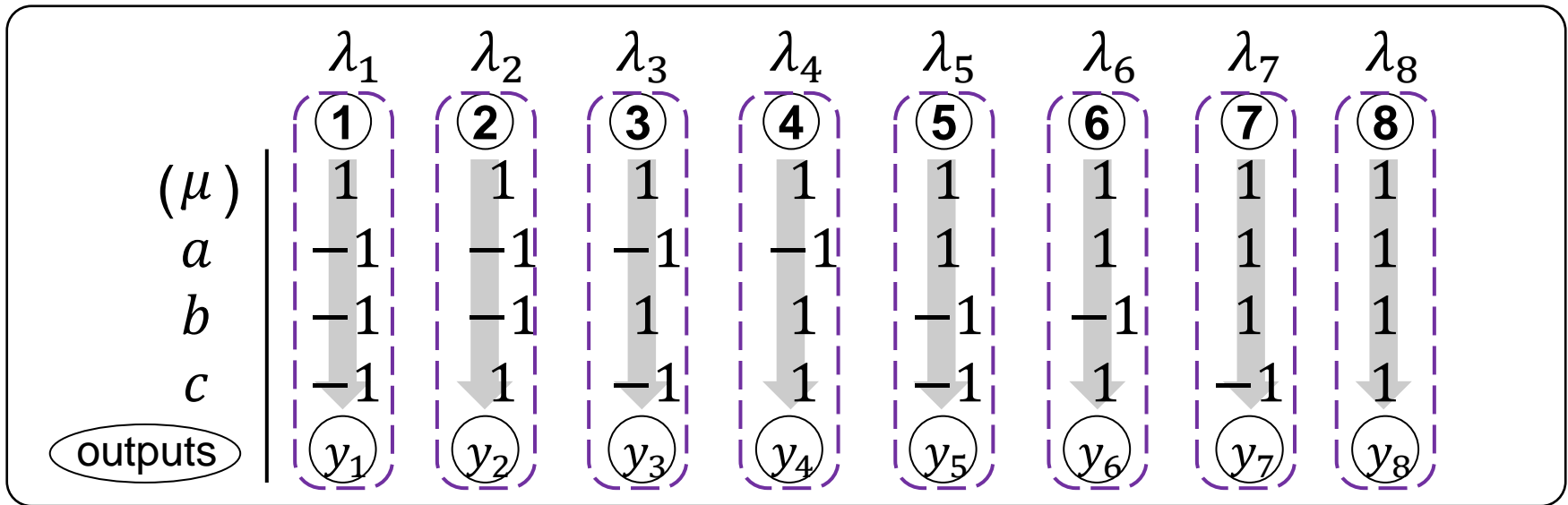
$\Rightarrow \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = \lambda_7 = \lambda_8$ (highly symmetric)

\Rightarrow **Group lasso** \Rightarrow

	①	②	③	④	⑤	⑥	⑦	⑧
(μ)	1	1	1	1	1	1	1	1
a	-1	-1	-1	-1	1	1	1	1
b	-1	-1	1	1	-1	-1	1	1
c	-1	1	-1	1	-1	1	-1	1

Sparse solutions (asymmetric solutions) are never obtained from ...

Patterns of the solution



Example 4) Assume that we want to estimate β_a, β_b

$$\Rightarrow \lambda_1, \lambda_3, \lambda_5 < \lambda_2, \lambda_4, \lambda_6, \lambda_7, \lambda_8$$

\Rightarrow **Group lasso** \Rightarrow

	①	③	⑤
(μ)	1	1	1
a	-1	-1	1
b	-1	1	-1
c	-1	-1	-1

or

	①	③	⑤	⑦
(μ)	1	1	1	1
a	-1	-1	1	1
b	-1	1	-1	-1
c	-1	-1	-1	1

or...

Patterns of the solution

Example 5) Assume that we want to estimate β_a, β_b

$$\Rightarrow \lambda_1, \lambda_2, \lambda_5 < \lambda_4 < \lambda_3, \lambda_6, \lambda_7, \lambda_8$$

\Rightarrow **Group lasso** \Rightarrow

	①	②	④	⑤	
(μ)	1	1	1	1	
a	-1	-1	-1	1	or...
b	-1	-1	1	-1	
c	-1	1	1	-1	

Example 6) Assume that we want to estimate β_a, β_b

$$\Rightarrow \lambda_1, \lambda_2, \lambda_4 < \lambda_5 < \lambda_3, \lambda_6, \lambda_7, \lambda_8$$

\Rightarrow **Group lasso** \Rightarrow

	①	②	④	⑤	
(μ)	1	1	1	1	
a	-1	-1	-1	1	or...
b	-1	-1	1	-1	
c	-1	1	1	-1	

The different orderings of $\lambda_1, \dots, \lambda_8$ can give the same structure of the solution.

Question What makes the patterns of the solutions? \Rightarrow **Gröbner basis**

Linear Unbiased Estimator

A linear model :
($a, b, c = -1$ or 1)

$$y = \underbrace{\mu}_{\text{unknown}} + \underbrace{\beta_a}_{\text{unknown}} a + \underbrace{\beta_b}_{\text{unknown}} b + \underbrace{\beta_c}_{\text{unknown}} c + \underbrace{\varepsilon}_{\text{noise}}$$

	①	②	③	④	⑤	⑥	⑦	⑧
(μ)	1	1	1	1	1	1	1	1
a	-1	-1	-1	-1	1	1	1	1
b	-1	-1	1	1	-1	-1	1	1
c	-1	1	-1	1	-1	1	-1	1
outputs	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

An example of linear (unbiased) estimator of β_a

ε : ignored

$$\begin{aligned} \hat{\beta}_a &= \frac{1}{2} \{-y_1 + y_5\} = \frac{1}{2} \{-(\mu - \beta_a - \beta_b - \beta_c) + (\mu + \beta_a - \beta_b - \beta_c)\} = \beta_a \\ &= (\mu \quad \beta_a \quad \beta_b \quad \beta_c) \left\{ -\frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ -1 \\ -1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} \right\} = (\mu \quad \beta_a \quad \beta_b \quad \beta_c) \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \beta_a \end{aligned}$$

Linear Unbiased Estimator

A linear model :
 $(a, b, c = -1 \text{ or } 1)$

$$y = \underbrace{\mu}_{\text{unknown}} + \underbrace{\beta_a}_{\text{unknown}} a + \underbrace{\beta_b}_{\text{unknown}} b + \underbrace{\beta_c}_{\text{unknown}} c + \underbrace{\varepsilon}_{\text{noise}}$$

	①	②	③	④	⑤	⑥	⑦	⑧
(μ)	1	1	1	1	1	1	1	1
a	-1	-1	-1	-1	1	1	1	1
b	-1	-1	1	1	-1	-1	1	1
c	-1	1	-1	1	-1	1	-1	1
outputs	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

T : a subset of the columns ①,...,⑧

A linear combination of T
 is a linear unbiased estimator of β_a



$$(\text{A linear combination of } T) = \begin{pmatrix} 0 \\ k \\ 0 \\ 0 \end{pmatrix}$$

$(k \neq 0)$

Linear Unbiased Estimator

$$\begin{array}{c} (\mu) \\ a \\ b \\ c \end{array} \left| \begin{array}{cccccccc} \textcircled{1} & \textcircled{2} & \textcircled{3} & \textcircled{4} & \textcircled{5} & \textcircled{6} & \textcircled{7} & \textcircled{8} \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} \right| = M$$

$$\begin{array}{c} (\mu) \\ a \\ b \\ c \end{array} \left| \begin{array}{cccccccc} \textcircled{1} & \textcircled{2} & \textcircled{3} & \textcircled{4} & \textcircled{5} & \textcircled{6} & \textcircled{7} & \textcircled{8} \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} \right| = M_{-a}$$

Lemma

T : a subset of the columns $\textcircled{1}, \dots, \textcircled{8}$

$$\begin{array}{l} \text{(A linear combination of } T \text{)} \\ (k \neq 0) \end{array} = \begin{pmatrix} 0 \\ k \\ 0 \\ 0 \end{pmatrix}$$



$$T \in \ker M_{-a} / \ker M$$

Gröbner basis

$$\begin{array}{c} (\mu) \\ a \\ b \\ c \end{array} \left| \begin{array}{cccccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} \right| = M$$

$$\begin{array}{c} (\mu) \\ a \\ b \\ c \end{array} \left| \begin{array}{cccccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} \right| = M_{-a}$$

$$\left\{ \begin{array}{l} \ker M : \text{toric ideal} = \langle x_1x_4 - x_2x_3, x_1x_6 - x_2x_5, x_1x_8 - x_2x_7, \dots \rangle \\ \ker M_a : \text{toric ideal} = \langle x_1 - x_5, x_2 - x_6, x_3 - x_7, x_4 - x_8, x_1x_4 - x_2x_3 \rangle \\ \ker M / \ker M_a : \langle x_1 - x_5, x_2 - x_6, x_3 - x_7, x_4 - x_8 \rangle \end{array} \right.$$

Gröbner bases

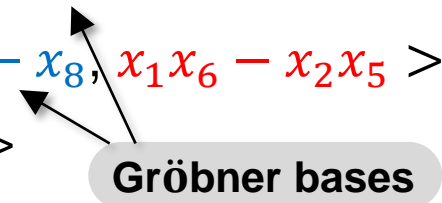
\Rightarrow Any linear unbiased estimator of β_a is a linear combination of $y_1 - y_5, y_2 - y_6, y_3 - y_7, y_4 - y_8$.

Gröbner basis

$$\begin{array}{c} (\mu) \\ a \\ b \\ c \end{array} \left| \begin{array}{cccccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} \right| = M$$

$$\begin{array}{c} (\mu) \\ a \\ \del{b} \\ c \end{array} \left| \begin{array}{cccccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ \del{-1} & \del{-1} & \del{1} & \del{1} & \del{-1} & \del{-1} & \del{1} & \del{1} \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} \right| = M_{-b}$$

$$\left\{ \begin{array}{l} \ker M : \text{ toric ideal} = \langle x_1x_4 - x_2x_3, x_1x_6 - x_2x_5, x_1x_8 - x_2x_7, \dots \rangle \\ \ker M_b : \text{ toric ideal} = \langle x_1 - x_3, x_2 - x_4, x_5 - x_7, x_6 - x_8, x_1x_6 - x_2x_5 \rangle \\ \ker M / \ker M_b : \langle x_1 - x_3, x_2 - x_4, x_5 - x_7, x_6 - x_8 \rangle \end{array} \right.$$


Gröbner bases

\Rightarrow Any linear unbiased estimator of β_b is a linear combination of $y_1 - y_3, y_2 - y_4, y_5 - y_7, y_6 - y_8$.

Linear Unbiased Estimator

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
(μ)	1	1	1	1	1	1	1	1
a	-1	-1	-1	-1	1	1	1	1
b	-1	-1	1	1	-1	-1	1	1
c	-1	1	-1	1	-1	1	-1	1
outputs	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

Assume that we want to estimate β_a, β_b

- Any linear unbiased estimator of β_a is a linear combination of $y_1 - y_5, y_2 - y_6, y_3 - y_7, y_4 - y_8$.
- Any linear unbiased estimator of β_b is a linear combination of $y_1 - y_3, y_2 - y_4, y_5 - y_7, y_6 - y_8$.

$$\lambda_1, \lambda_2, \lambda_5 < \lambda_4 < \lambda_3, \lambda_6, \lambda_7, \lambda_8$$

$$\lambda_1, \lambda_2, \lambda_4 < \lambda_5 < \lambda_3, \lambda_6, \lambda_7, \lambda_8$$

In the both cases, $y_1 - y_5$ and $y_2 - y_4$ are chosen.

Future Work / Conclusion

Lemma (in page 13)

T : a subset of the columns of design matrix.

$$\text{A linear combination of } T = \begin{pmatrix} 0 \\ k \\ 0 \\ 0 \end{pmatrix} \quad (k \neq 0) \quad \longleftrightarrow \quad T \in \ker M_{-a} / \ker M$$

- Any linear unbiased estimator is a linear combination of linear combinations of columns given as Gröbner basis.

Any least square estimator is a linear combination of linear combinations of columns given as Gröbner basis.

Simple linear regression: $\hat{\beta} = \sum_{j < k} \tau_{jk} \left(\frac{y_j - y_k}{x_j - x_k} \right)$, $\tau_{jk} \propto (x_j - x_k)^2$

($x_j - x_k \neq 0$)

Given by Gröbner basis

- If we allow *errors* in the computation of $\ker M$ or $\ker M_{-a}$, the lemma \Uparrow may also be useful for high-dimensional ($n < p$) data.

Future Work / Conclusion

$$y = \mu + \beta_a a + \beta_b b + \beta_c c + \varepsilon$$

$$\begin{array}{c} (\mu) \\ a \\ b \\ c \end{array} \left| \begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{array} \right. = M$$

$\underbrace{\quad}_{y_1} \quad \underbrace{\quad}_{y_2} \quad \underbrace{\quad}_{y_3}$

$\swarrow \text{tolerance}(\text{error})$
 $\ker M \left(\frac{1}{3} \right) = \emptyset$

$$\begin{array}{c} (\mu) \\ b \\ c \end{array} \left| \begin{array}{ccc} 1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{array} \right. = M_{-a}$$

$\underbrace{\quad}_{y_1} \quad \underbrace{\quad}_{y_2} \quad \underbrace{\quad}_{y_3}$

$$\ker M_{-a} \left(\frac{1}{3} \right) = \left\{ \frac{1}{3} (y_1 + y_2 - y_3) \right\}$$

$\longrightarrow \frac{1}{3} (y_1 + y_2 - y_3) \in \ker M_{-a} \left(\frac{1}{3} \right) / \ker M \left(\frac{1}{3} \right)$

\nwarrow Nearly unbiased estimator with tolerance of 1/3

Future Work / Conclusion

Lemma (in page 13)

T : a subset of the columns of design matrix.

$$\text{A linear combination of } T = \begin{pmatrix} 0 \\ k \\ 0 \\ 0 \end{pmatrix} \quad (k \neq 0) \quad \longleftrightarrow \quad T \in \ker M_{-a} / \ker M$$

$$\ker M \subset \ker M_{-a} \subset \ker M_{-ab} \subset \ker M_{-abc} \subset \dots$$

$$\text{coker } M \supset \text{coker } M_{-a} \supset \text{coker } M_{-ab} \supset \text{coker } M_{-abc} \supset \dots$$

$$\ker M(\delta_1) \subset \ker M(\delta_2) \subset \ker M(\delta_3) \subset \ker M(\delta_4) \subset \dots$$

$(\delta_i: \text{tolerance}(\text{error}), \quad 0 < \delta_1 < \delta_2 < \delta_3 < \dots)$

- A connection with homology (matroid) ?
- A connection with persistent homology ?

Future Work / Conclusion

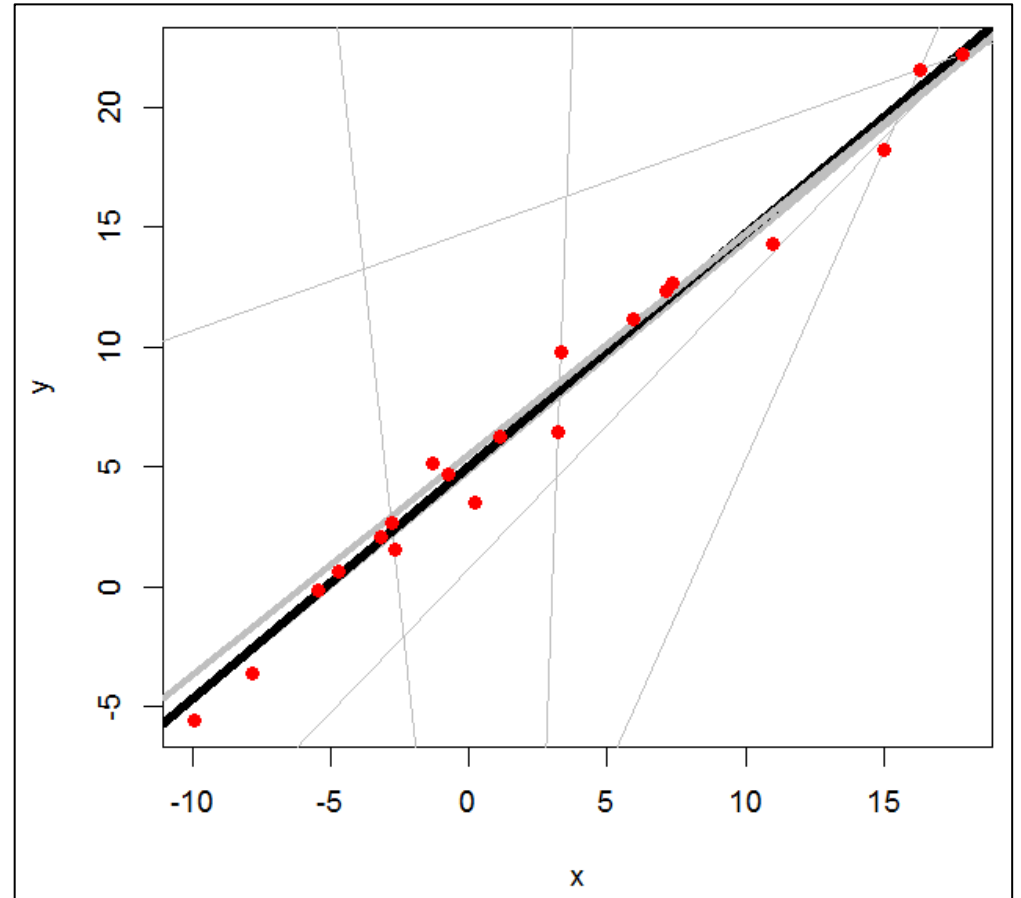
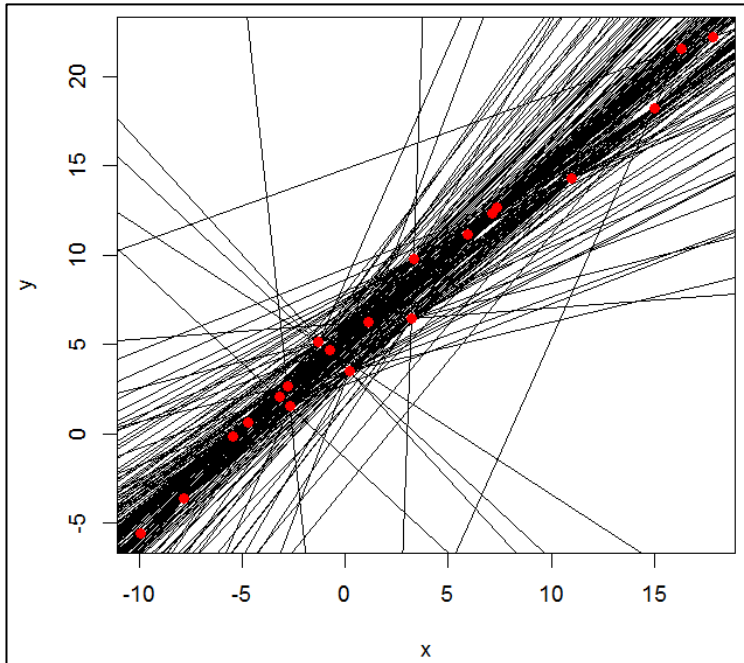
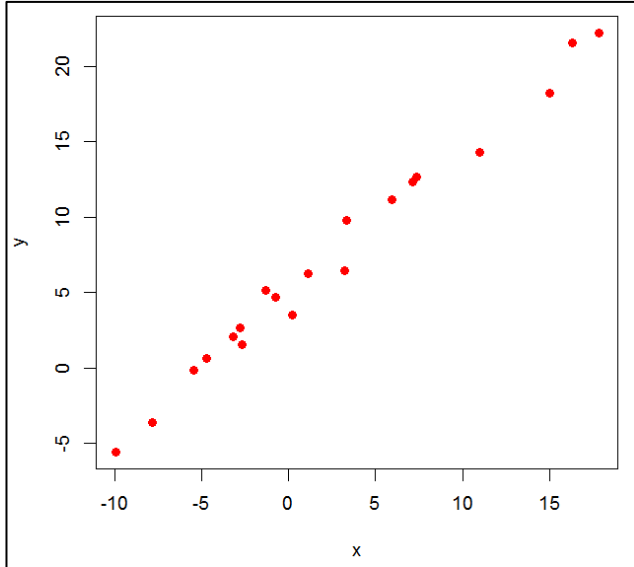
$$\ker M \subset \ker M_{-a} \subset \ker M_{-ab} \subset \ker M_{-abc} \subset \dots$$

$$\begin{array}{c|cccccccc} (\mu) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ a & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ b & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ c & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} = M_{+a}$$

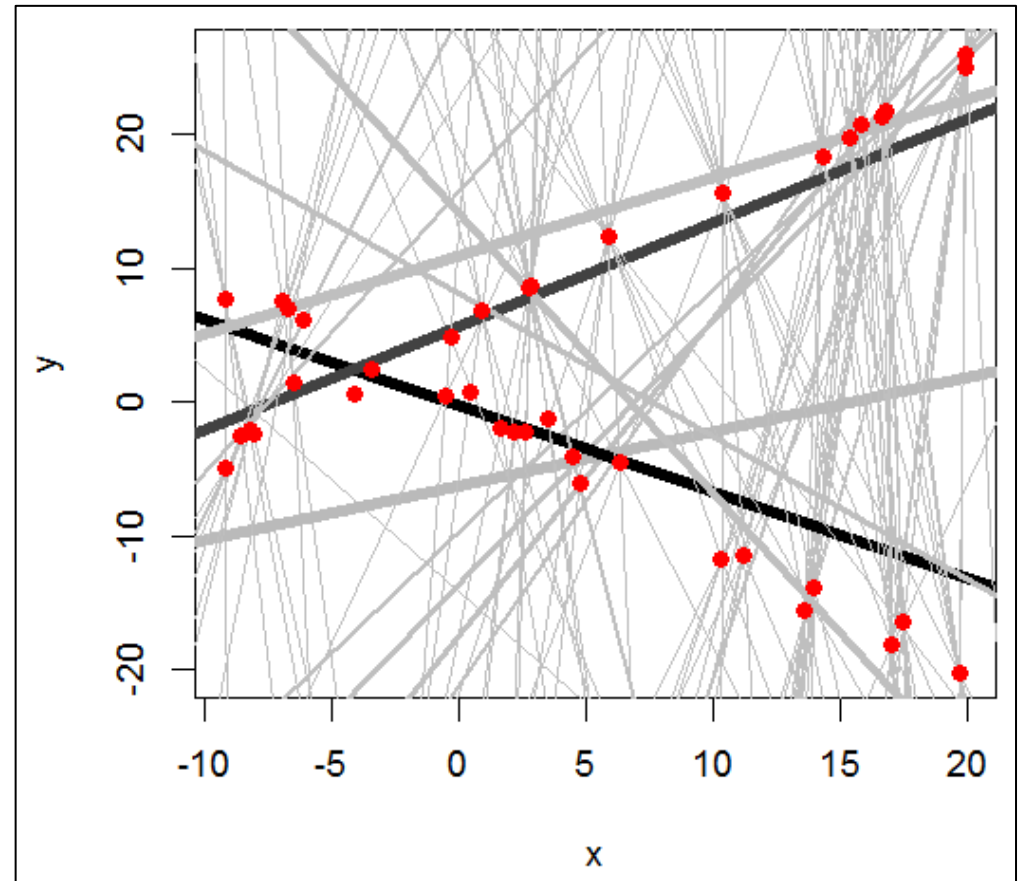
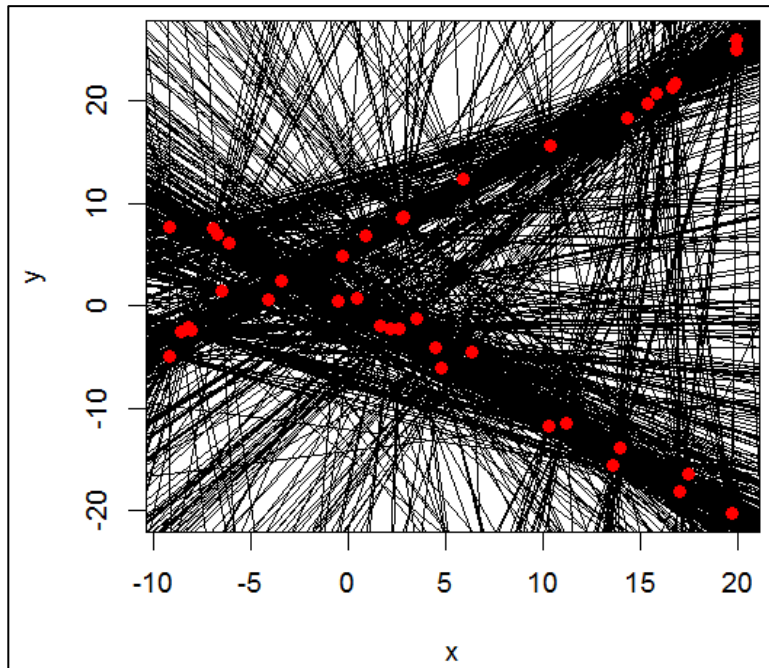
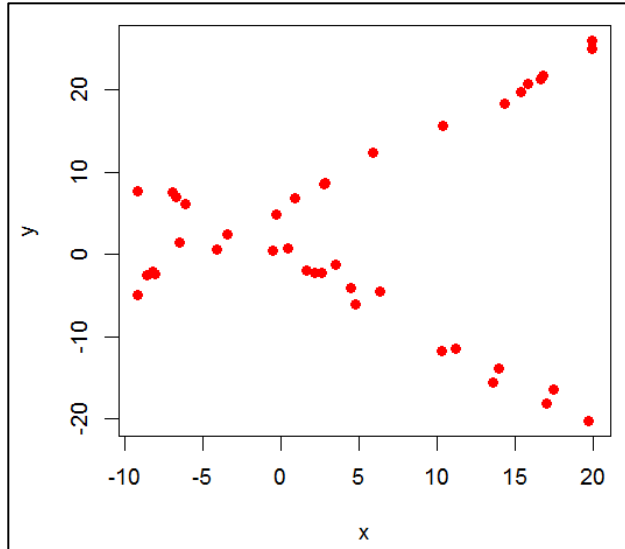
$$\begin{array}{c|cccccccc} & x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ (\mu) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ a & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ b & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ c & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{array} = M_{-ab}$$

$$\ker M_{-b} / \ker M = (\ker M_{-ab} / \ker M_a) \cap \ker M_{+a}$$

Linear regressions

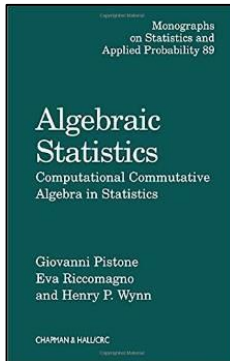


Linear regressions



References

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- Groebner do-jo
(gu re bu na-a, do-o jo-o)

