Is it a computing algorithm or a statistical procedure:
Can you tell or should you care?

Xiao-Li Meng

Harvard University

Lee, Li and Meng (2019) ***Likelihood-free EM: Self Consistency as a Dual Principle for Incomplete or Irregular-Pattern Data***.

Machine Learning v.s. Statistics

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- Stereotypical complaint about statisticians: Excessive worries over modeling and inferential principles, to a degree of being willing to produce nothing
- Stereotypical complaint about machine learners: Strong tendency to let ease of implementation or good performance trump principled justification, to a point of being willing to deliver anything

Principled Corner Cutting (PC^2)

- ***Principle Oriented*** v.s. ***Performance Oriented***

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- ***Principle Oriented*** v.s. ***Performance Oriented***
- We need BOTH in order to reach a sensible compromise between statistical efficiency and computational efficiency
- We need to train more ***Principled Corner Cutters***: Who can formulate the solution from the soundest principles available but are at ease of cutting corners guided by these principles, to achieve as much statistical efficiency as feasible while maintaining computational efficiency under time and resource constraints.

But can you tell which is which?

- Mr. Littlestat was given a **black box** which computes the Least Squares Estimate (LSE) of β for the linear regression

$$y_i = \beta x_i + \epsilon_i, \quad i = 1, \ldots, n, \quad \epsilon_i \; i.i.d. \sim F[0,1].$$

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- And it only works when $n = 2^4 = 16$, outputting

$$\hat{\beta}_{16}(y_1, \ldots, y_{16}) = \frac{\sum_{i=1}^{16} y_i x_i}{\sum_{i=1}^{16} x_i^2}.$$

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- But Mr. Littlestat only has $n = 13$. Can he still use the same program?

Is it possible?

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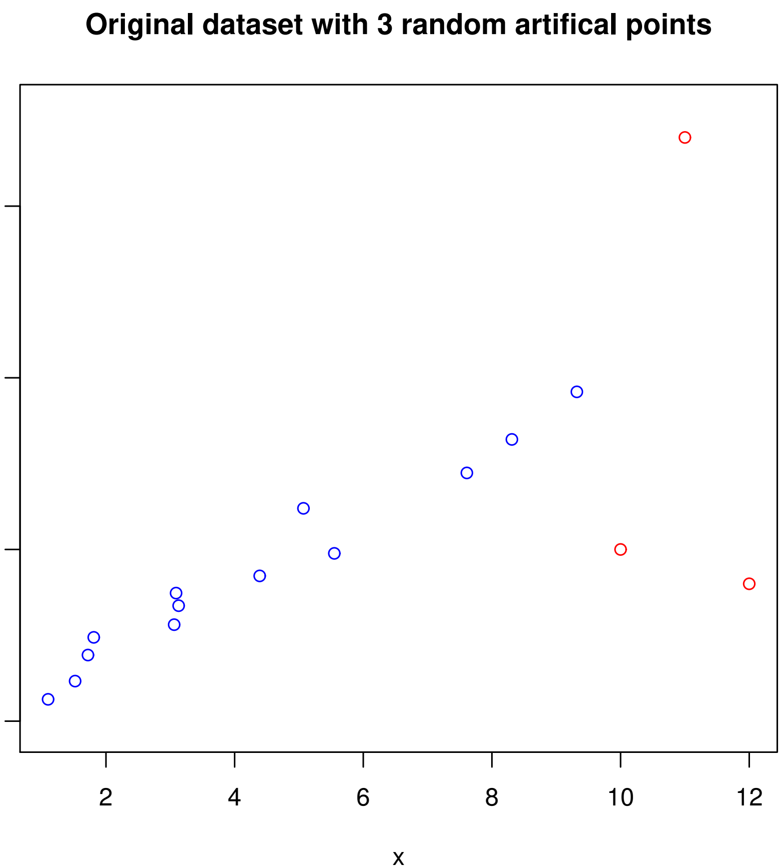
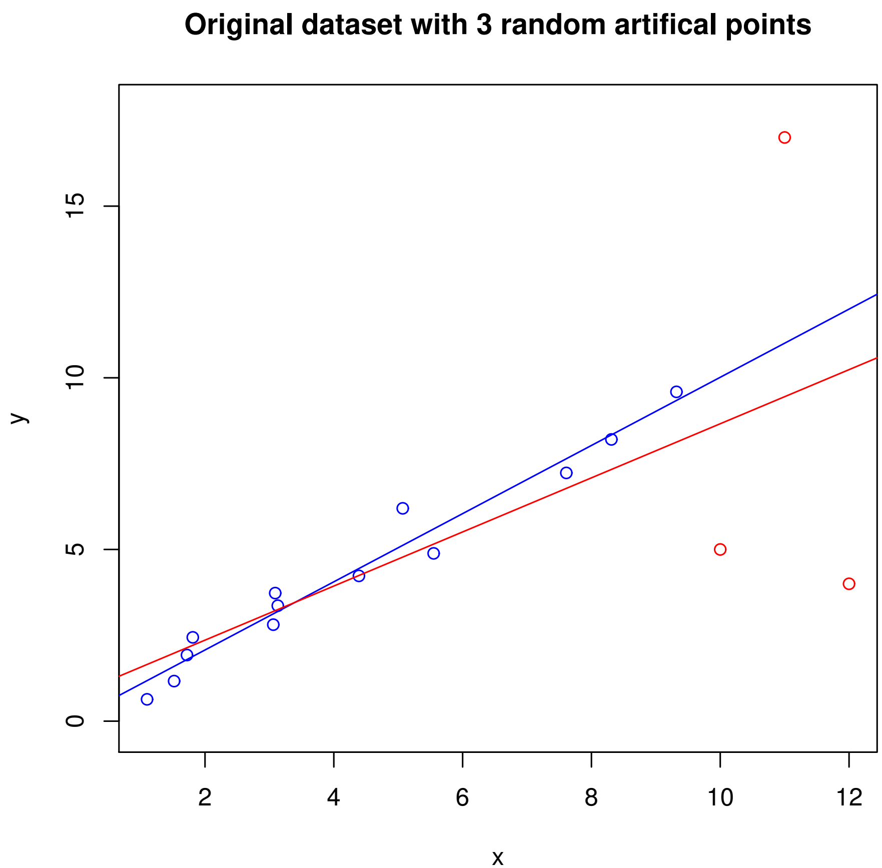
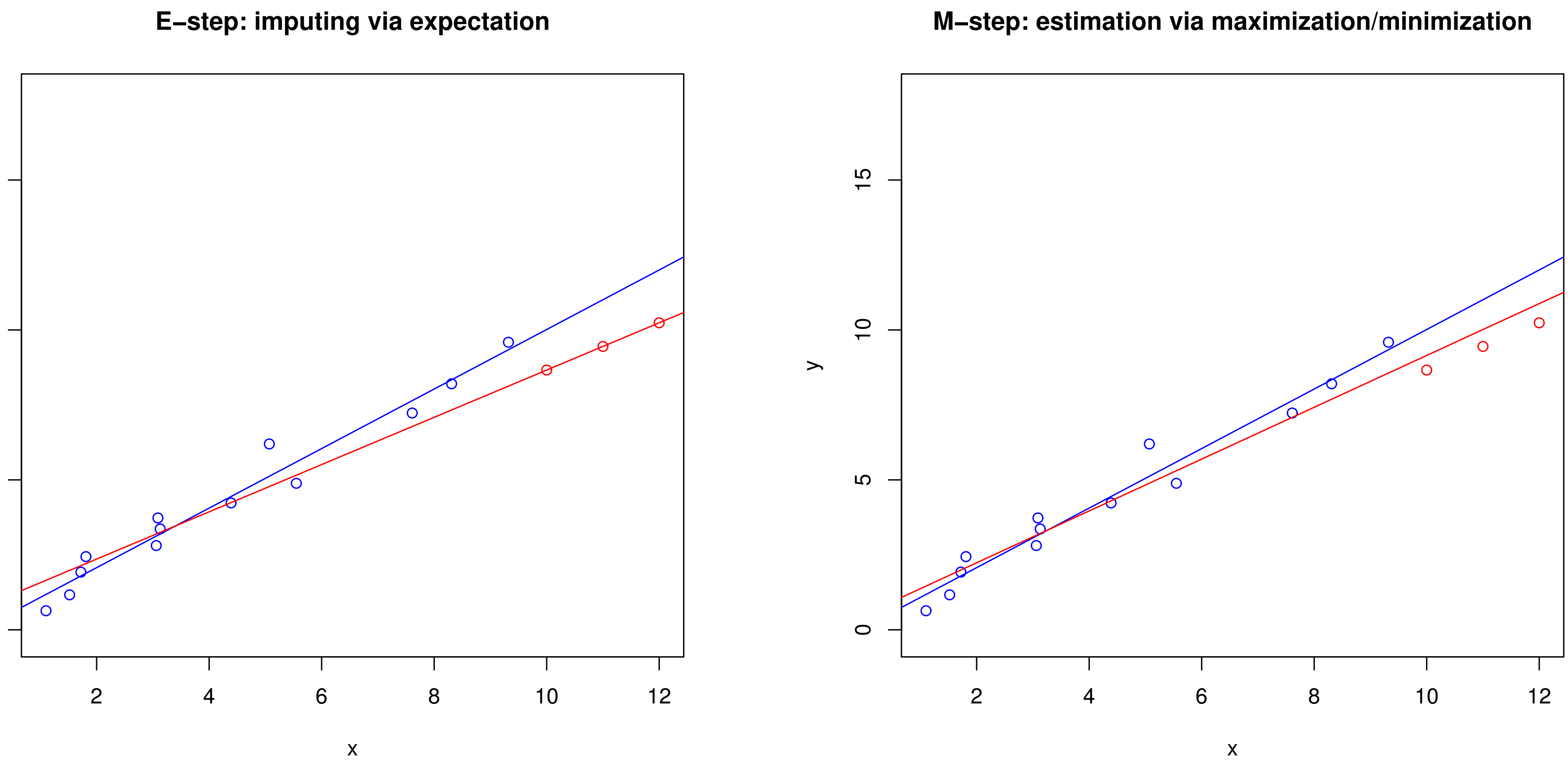
- The answer has to be **YES** because ...
- The ***Principle of Selection Bias***!

A Numerical Illustration



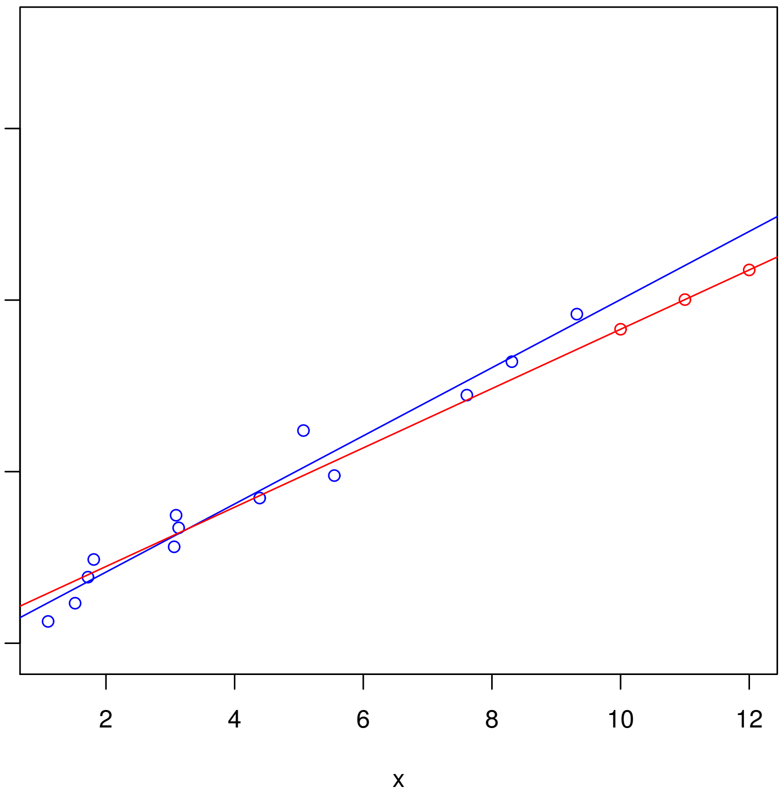


Iteration 1

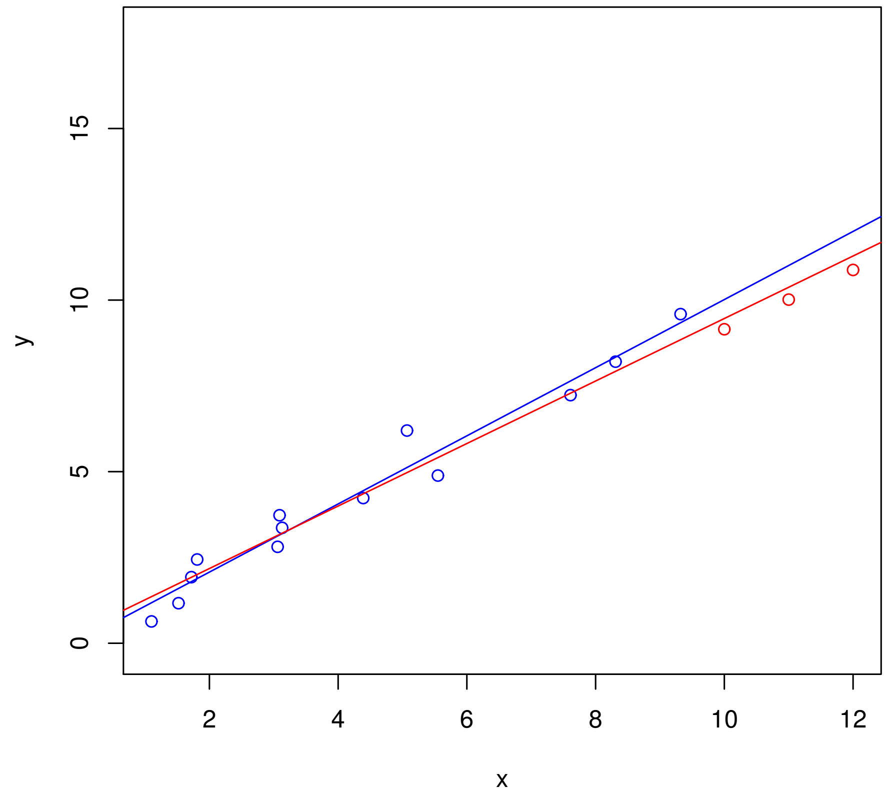

E−step: imputing via expectation
M−step: estimation via maximization/minimization
x
y
2
4
6
8
10
12
0
5
10
15

Iteration 2

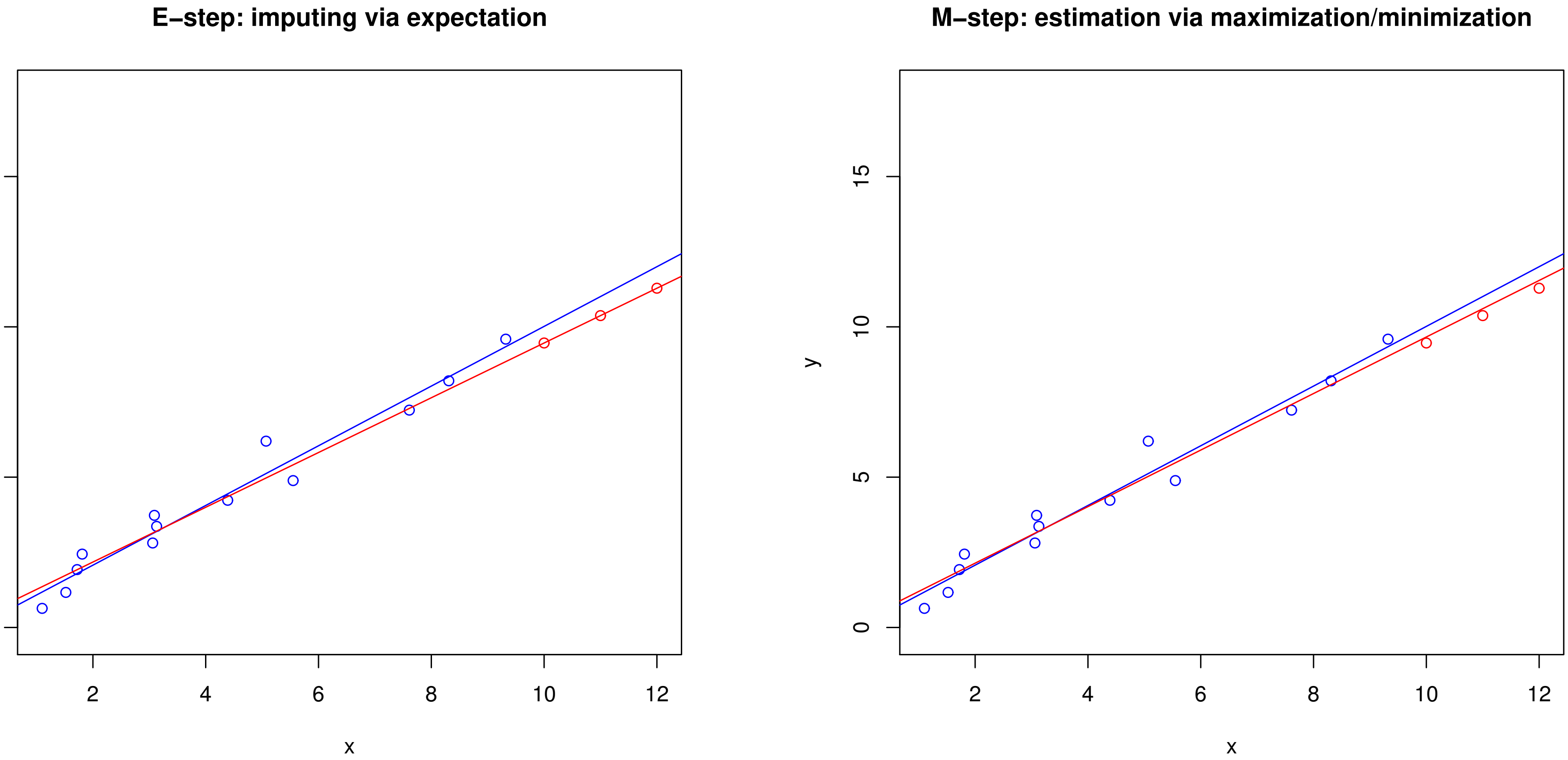
E–step: imputing via expectation



M–step: estimation via maximization/minimization



Iteration 3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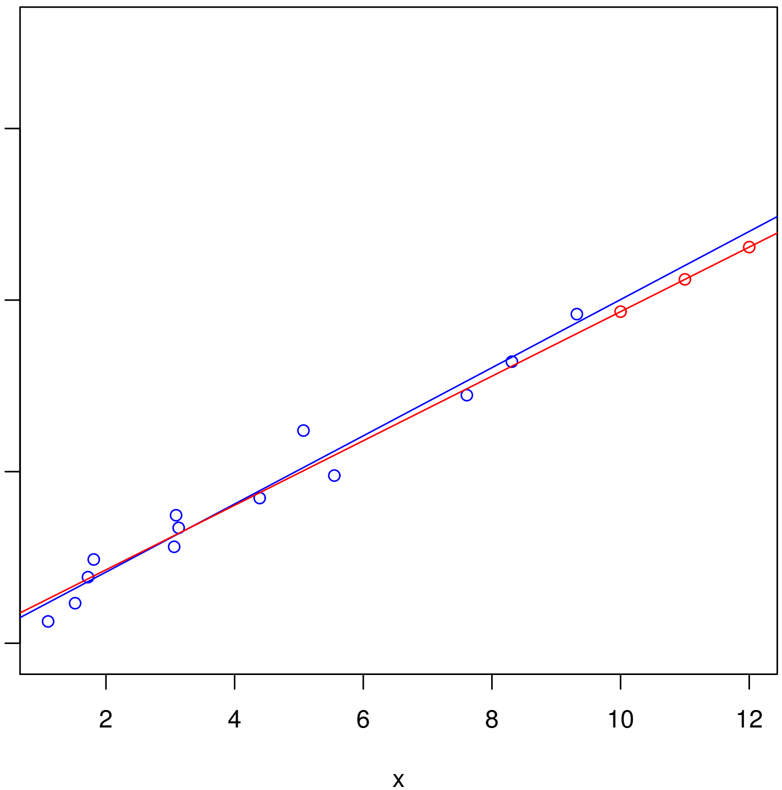
Iteration 4

E−step: imputing via expectation



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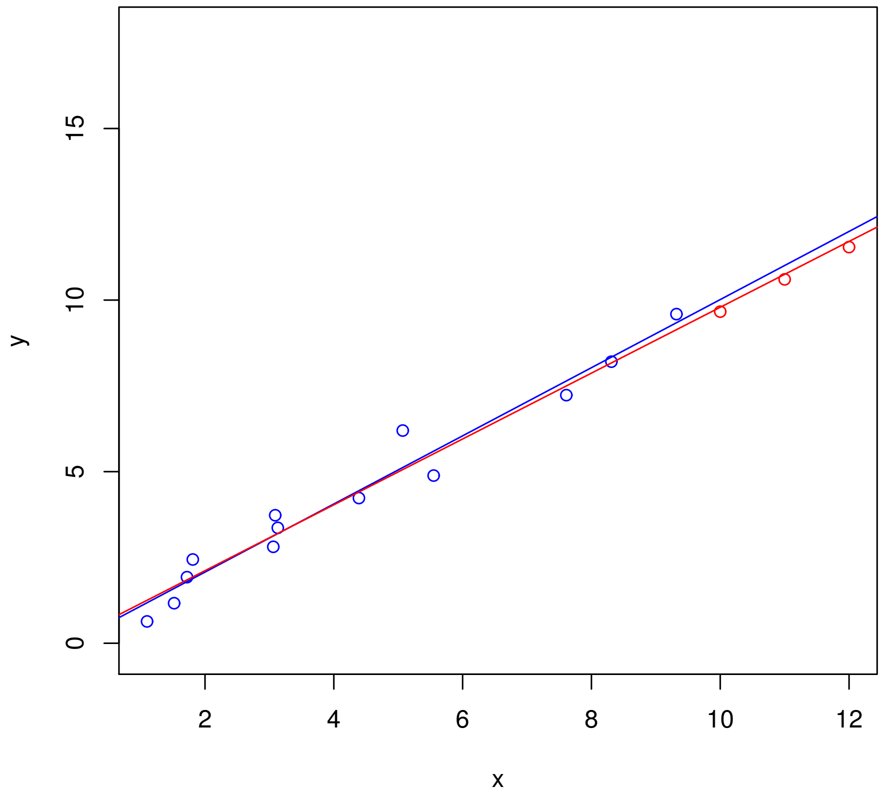
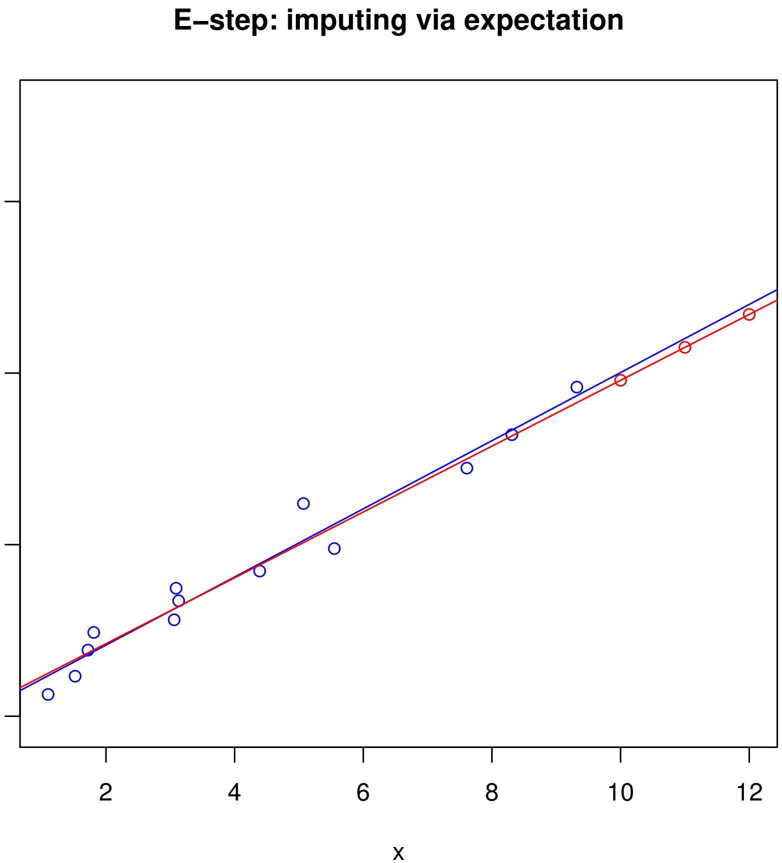


Iteration 5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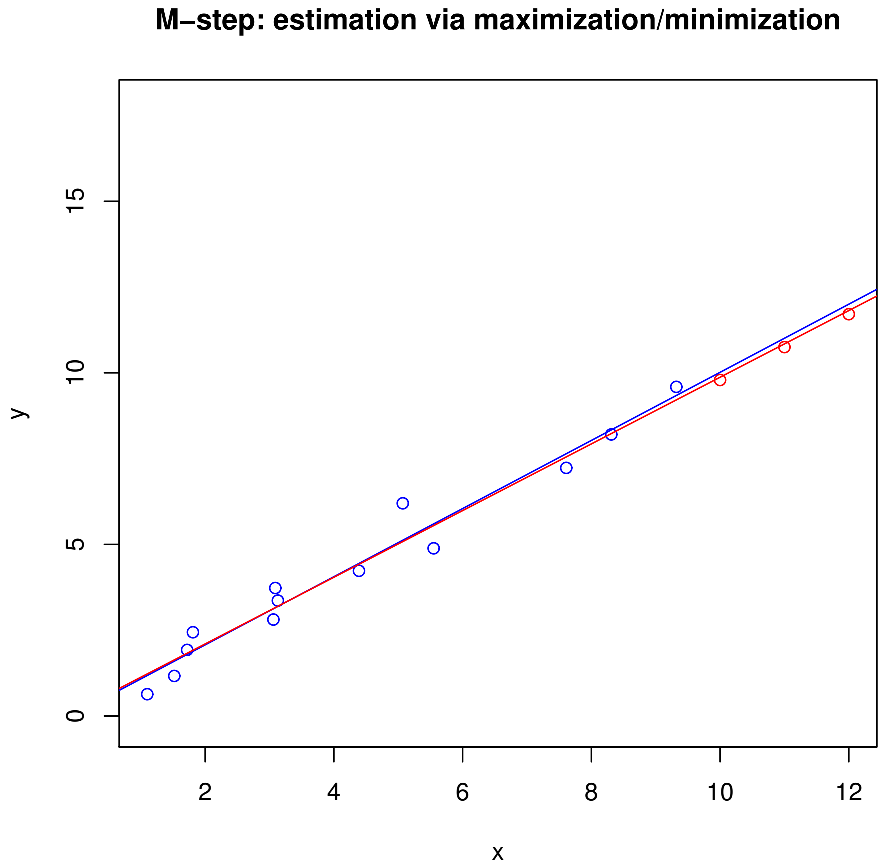
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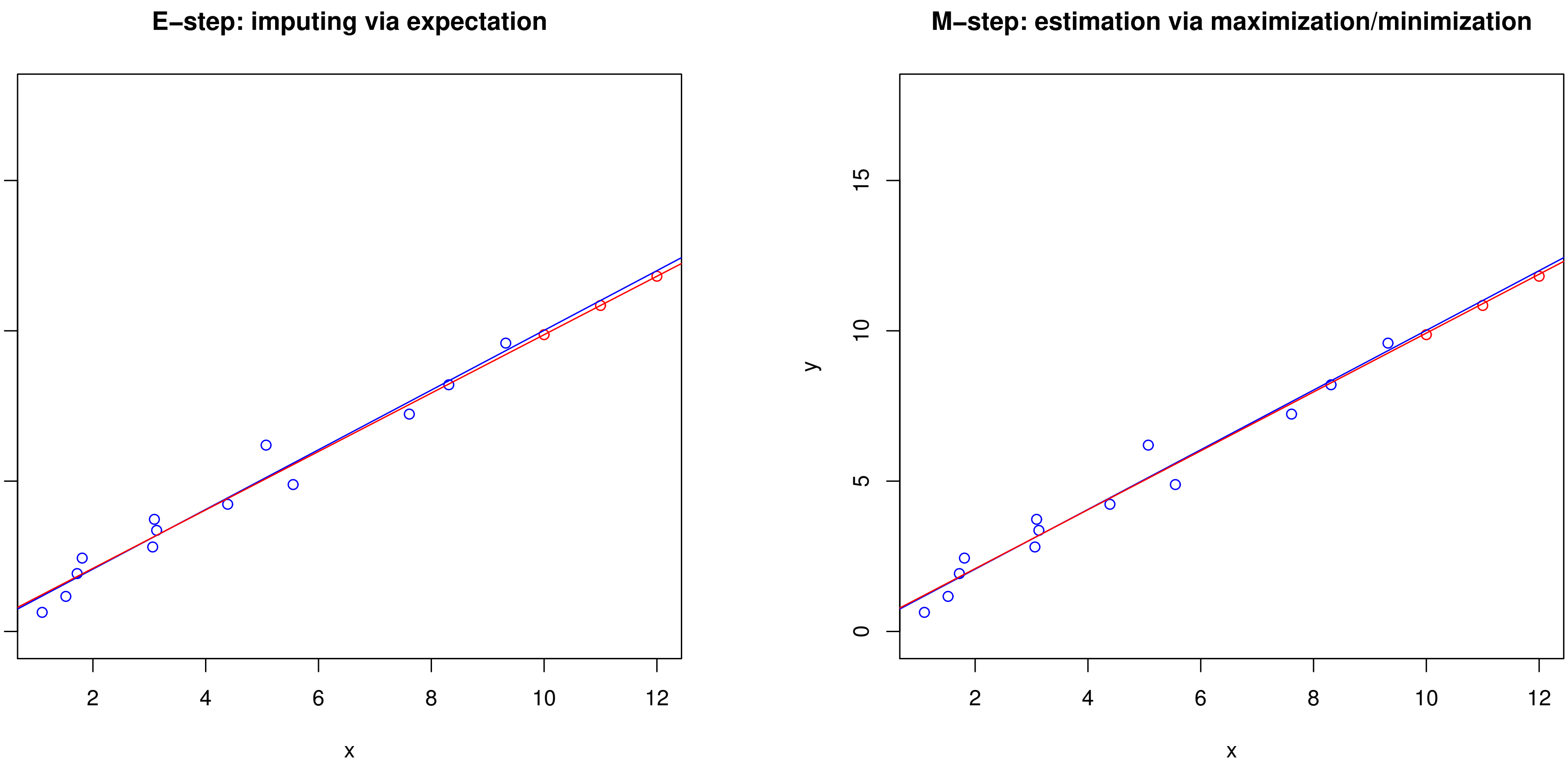
Iteration 6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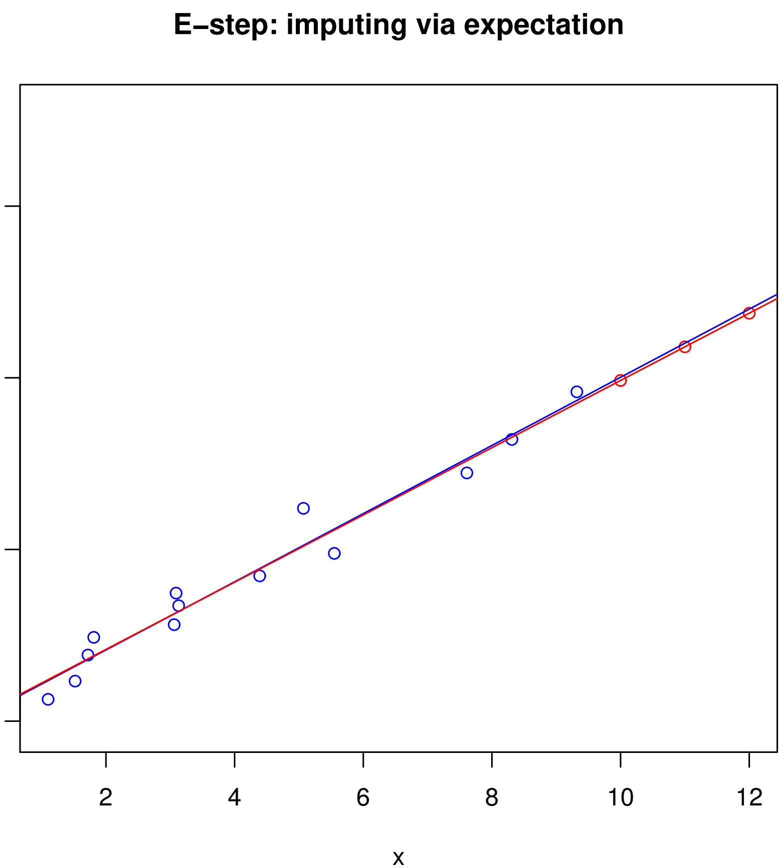

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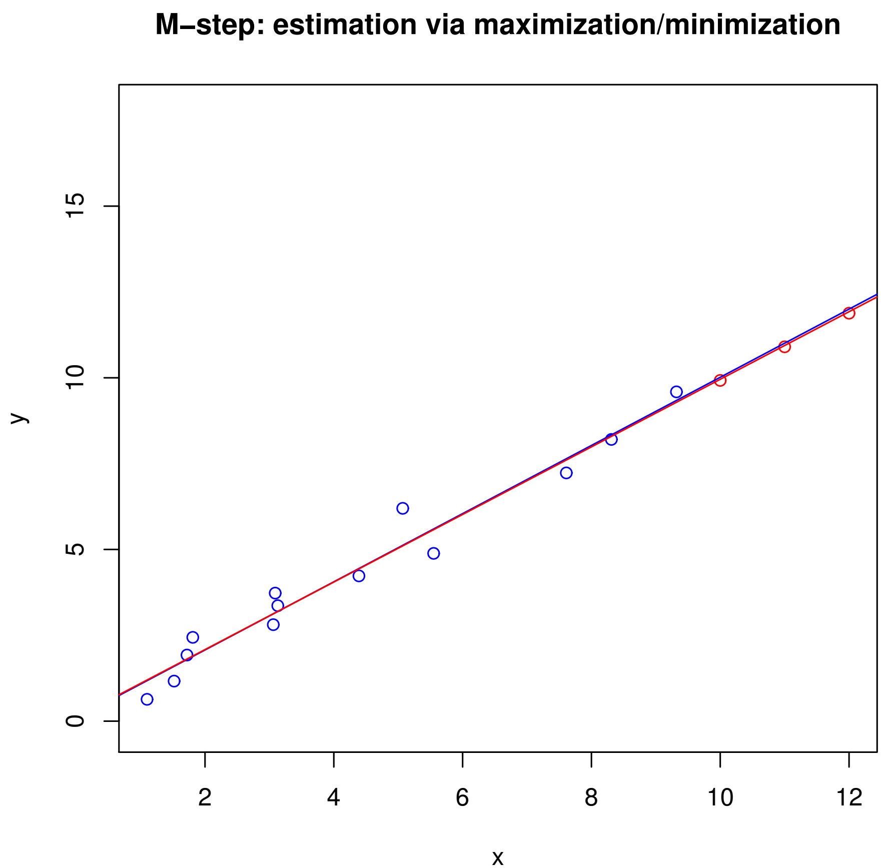

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- Is this a computing algorithm or a statistical procedure?
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- Well, do you want to know how general it is?

If you do, then ...

- From a statistical estimation perspective: What’s the statistical principle behind it? Is it consistent? Is it (asymptotically) efficient in some sense? What assumptions on missing-data mechanism are needed to justify its validity?

If you do, then ...

- From a statistical estimation perspective: What's the statistical principle behind it? Is it consistent? Is it (asymptotically) efficient in some sense? What assumptions on missing-data mechanism are needed to justify its validity?
- From an algorithmic implementation perspective: How many iterations usually does it take? Does the number of iterations depend on where I put the initial points? Does the method scalable to high dimensional data sets? Can it be implemented generically?

The Self-Consistency Principle

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- But we only observed data $\boldsymbol{y}_{\mathrm{obs}}$.
- Intuitively, the “best" estimate of f given the procedure $\hat{\boldsymbol{f}}_{\mathrm{com}}$ and the imputation model $p(\boldsymbol{y}_{\mathrm{com}}|\boldsymbol{y}_{\mathrm{obs}}, f)$, $\hat{\boldsymbol{f}}_{\mathrm{obs}}$, should satisfy the fixed-point equation

$$E\left[\hat{\boldsymbol{f}}_{\mathrm{com}}(\cdot)\middle|\boldsymbol{y}_{\mathrm{obs}}; \boldsymbol{f}=\hat{\boldsymbol{f}}_{\mathrm{obs}}\right]=\hat{\boldsymbol{f}}_{\mathrm{obs}}(\cdot)$$

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  where $\hat{\boldsymbol{F}}_{\rm com}$ is the complete-data empirical CDF.
- Considerable progresses by Turnbull (1974, 1976), Tasi and Crowley (1985), Tasi (1986), Chan and Yang (1987), Ren and Mykland (1996), Van der Laan (1997, 1998, etc. under more general censoring.

Least Squares Estimator is Self-consistent

- Seek $\hat{\beta}_{13}$:

$$E\left[\hat{\beta}_{16}(y_1,\ldots,y_{16})\middle| y_1,\ldots,y_{13};\beta=\hat{\beta}_{13}\right]=\hat{\beta}_{13},$$

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- Starting with $\beta_{13}^{(0)}$, (1) impute the missing y_i by $y_i^{(t)} = \beta_{13}^{(t)} x_i$ and (2) compute

$$\beta_{13}^{(t+1)} = \hat{\beta}_{16}(y_1, \ldots, y_{13}, y_{14}^{(t)}, y_{15}^{(t)}, y_{16}^{(t)}).$$

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- The limit $\hat{\beta}_{13}$ satisfies

$$\hat{\beta}_{13}=\frac{\sum_{i=1}^{13}y_ix_i+\hat{\beta}_{13}\sum_{i=14}^{16}x_i^2}{\sum_{i=1}^{16}x_i^2}\Longrightarrow\hat{\beta}_{13}=\frac{\sum_{i=1}^{13}y_ix_i}{\sum_{i=1}^{13}x_i^2}$$

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- score $S(\theta|\boldsymbol{y}_{\rm com})$ & expected Fisher information $I(\theta)$

$$\hat{\theta}_{\rm com} - \theta = \frac{S(\theta|\boldsymbol{y}_{\rm com})}{I(\theta)} + o_p(n_{\rm com}^{-1/2}).$$

$$E[\hat{\theta}_{\rm com}|\boldsymbol{y}_{\rm obs};\theta] - \theta = \frac{E[S(\theta|\boldsymbol{y}_{\rm com})|\boldsymbol{y}_{\rm obs};\theta]}{I(\theta)} + o_p(n_{\rm obs}^{-1/2})$$

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- Because of the Fisher's identity (fundamental for EM)

$$E[S(\theta|\boldsymbol{y}_{\text{com}})|\boldsymbol{y}_{\text{obs}};\theta] = S(\theta|\boldsymbol{y}_{\text{obs}})$$

& $S(\hat{\theta}_{\text{obs}}|\boldsymbol{y}_{\text{obs}}) = 0$, observed-data MLE $\hat{\theta}_{\text{obs}}$ must satisfy

$$E[\hat{\theta}_{\text{com}}|\boldsymbol{y}_{\text{obs}}, \theta = \hat{\theta}_{\text{obs}}] = \hat{\theta}_{\text{obs}} + o_p(n_{\text{obs}}^{-1/2}).$$

A Multiple Imputation Self-Consistent (MISC) Algorithm

Starting from $\hat{\boldsymbol{f}}^{(0)}$, for $t = 1, \ldots,$ iterating three steps:

1. Multiple Imputation: for $\ell = 1, \ldots, m$, draw independently $\boldsymbol{y}_{\text{mis}}^{\ell} \sim P(\boldsymbol{y}_{\text{mis}} \big| \boldsymbol{y}_{\text{obs}}; \boldsymbol{f} = \hat{\boldsymbol{f}}^{(t-1)})$
2. Applying the complete-data procedure to $\boldsymbol{y}^{\ell} = \{\boldsymbol{y}_{\text{obs}}, \boldsymbol{y}_{\text{mis}}^{\ell}\}$ to compute $\hat{\boldsymbol{f}}_{\ell}$, $\ell = 1, \ldots, m$
3. Combining Estimates:

   Under L^2 : $\quad \hat{\boldsymbol{f}}^{(t)} = \frac{1}{m} \sum_{\ell=1}^{m} \hat{\boldsymbol{f}}_{\ell}.$

   Under L^1 : $\quad \hat{\boldsymbol{f}}^{(t)} = \text{Median}\{\hat{\boldsymbol{f}}_{\ell},\ \ell = 1, \ldots, m\}$

   (nuisance part of f can be handled differently.)

MISC: No corner cutting, but ...

- Advantages:
  1. A generic algorithm: can be applied with any complete-data *procedure*;
  2. Any error norm: simply modify the combining rule accordingly.
  3. Additional programming is often easy.
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- Disadvantage: computationally very expensive, especially when the Monte Carlo size m is large.

So What Are The Theoretical Guarantees?

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$$||\hat{f}_{\text{com}} - f||_p = \left[E\left(\int |\hat{f}_{\text{com}}(t) - f(t)|^p dt\right)\right]^{1/p}$$

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$$M(f; \boldsymbol{y}_{\text{obs}}) = \text{argmin}_g E\left[\int |\hat{f}_{\text{com}}(t) - g(t)|^p dt \middle| \boldsymbol{y}_{\text{obs}}; f \right]$$

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- For $p = 2$, $M(f; \boldsymbol{y}_{\rm obs})(t) = E[\hat{f}_{\rm com}(t) | \boldsymbol{y}_{\rm obs}; f]$
- $M(\hat{f}) \equiv M(f = \hat{f}; \boldsymbol{y}_{\rm obs})$ a map from $\mathcal{F}_{\rm obs}$—a sub-space of L^p that contains the true f_0—into itself.

The Power of Contraction Mapping

- Define $|f|_p = \left[\int |f(t)|^p dt\right]^{1/p}$. If $M(f)$ contracts on $\mathcal{F}_{\text{obs}}$ wrt $|f|_p$, then there exists a unique solution to $M(\hat{f}_{\text{obs}}) = \hat{f}_{\text{obs}}$.

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- Suppose there exists a $0 \le \delta < 1$ such that $\forall \hat{f}_1, \hat{f}_2 \in \mathcal{F}_{\rm obs}$, $||M(\hat{f}_1) - M(\hat{f}_2)||_p \le \delta||\hat{f}_1 - \hat{f}_2||_p$. Then for any $f \in \mathcal{F}_{\rm obs}$,

$$||\hat{f}_{\rm obs} - f||_p \le 2\frac{||\hat{f}_{\rm com} - f||_p}{1-\delta}$$

Proof: $||\hat{f}_{\rm obs} - f||_p \le ||M(\hat{f}_{\rm obs}) - M(f)||_p + ||M(f) - f||_p$

$$||\hat{f}_{\rm obs} - f||_p \le \delta||\hat{f}_{\rm obs} - f||_p + ||M(f) - f||_p$$

$$||M(f) - f||_p \le ||M(f) - \hat{f}_{\rm com}||_p + ||\hat{f}_{\rm com} - f||_p \le 2||\hat{f}_{\rm com} - f||_p$$

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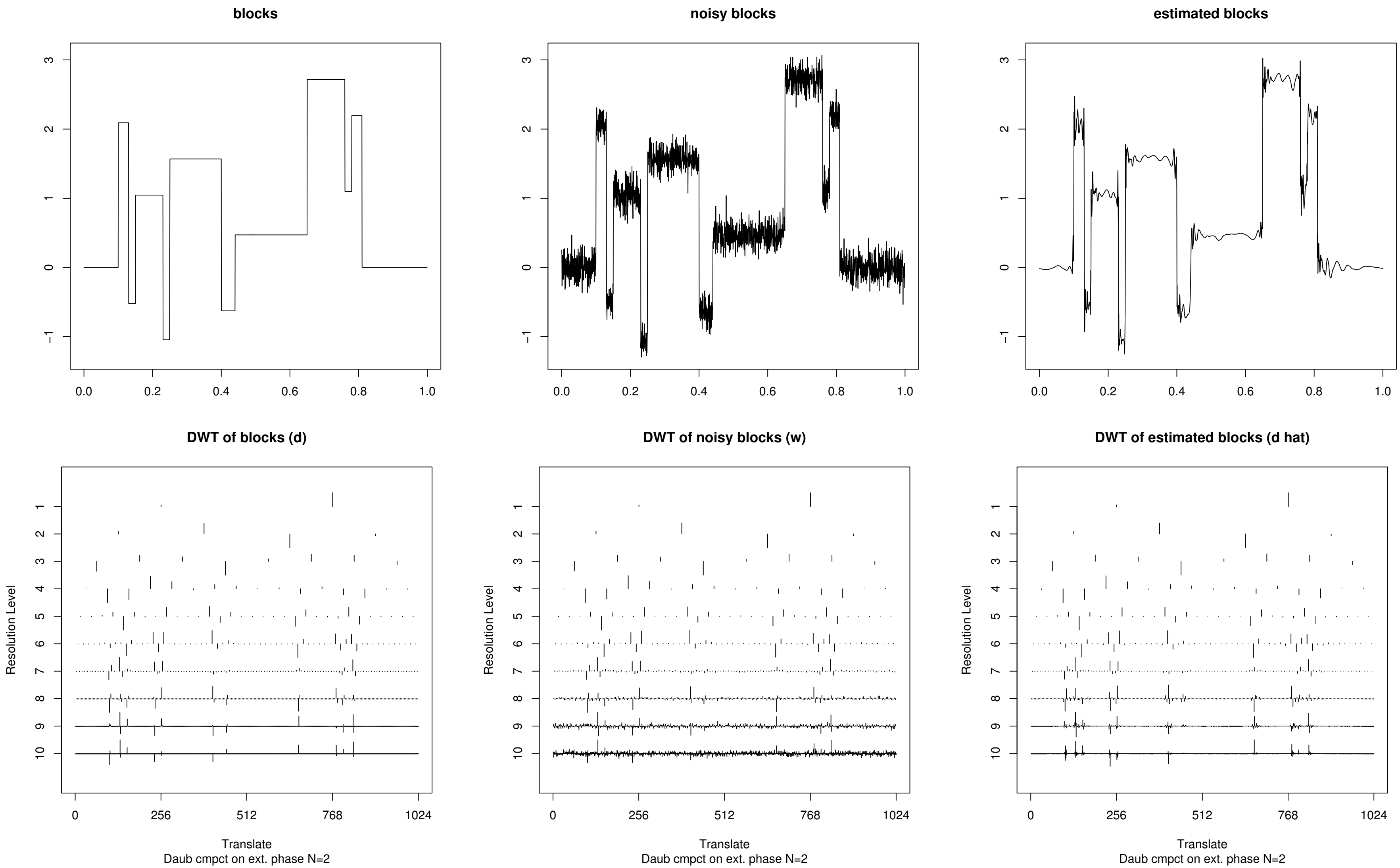
- $M(f)$ is *not* a contraction map for hard thresholding.

Wavelet Denoising (e.g., Donoho and Johnstone, 1994)



Incomplete Designs

- We observe $\boldsymbol{y}_{\text{obs}} = \{x_i, y_i\}_{i=1}^n$:

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- **Key idea:** View $\boldsymbol{y}_{\text{obs}}$ as incomplete data from $\boldsymbol{y}_{\text{com}} = \{x_i = \frac{i}{N}, y_i\}_{i=0}^{N-1}$ with y_i missing when $x_i \notin \boldsymbol{X}_{\text{obs}}$.

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- Applications:
  1. Actual missing y's with a regular design.
  2. Deleting outliers from a regular design data set.
  3. Cross-validation for a regular design problem.

Incomplete/Missing Data in 2D

- instrument malfunction, damaged photos, etc.

airplane

murder in progress

A Simple (SIM) Approximated Algorithm

- Starting with $\hat{\boldsymbol{f}}^{(0)}$ and $\hat{\sigma}^{(0)}$, for $t = 1, \ldots,$ iterating:
  1. Impute the missing y_i by $y_i^{(t)} = \hat{f}_i^{(t-1)}$ and create $\boldsymbol{y}^{(t)} = \{y_i : y_i \text{ is observed}\} \cup \{y_i^{(t)} : y_i \text{ is missing}\}$
  2. Obtain $\boldsymbol{w}^{(t)} = \boldsymbol{W}\boldsymbol{y}^{(t)}$ & “finest scale" estimate $\tilde{\sigma}^{(t)}$
  3. Use the variance inflation formula to compute

$$\hat{\sigma}^{(t)} = \sqrt{[\tilde{\sigma}^{(t)}]^2 + C_m[\hat{\sigma}^{(t-1)}]^2},$$

     where $C_m = 1 - \frac{n}{N}$ is fraction of missing data
  4. Threshold $\boldsymbol{w}^{(t)}$ with $g(\hat{\sigma}^{(t)})$ (e.g. $g(\sigma) = \sigma\sqrt{2\log N}$) to obtain $\hat{\boldsymbol{w}}^{(t)}$, and then $\hat{\boldsymbol{f}}^{(t)} = \boldsymbol{W}^T\hat{\boldsymbol{w}}^{(t)}$

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- Extreme corner cutting, but we understand when it can help and when it will do great harm.

A Refined (REF) Algorithm: Much More Principled Corner Cutting

- Similar to SIM, but much better approximation to the E-step $\hat{w}_l^{(t)} \equiv E\left[1_{|w_l| \geq g(\tilde{\sigma})} w_l \middle| \boldsymbol{y}_{\text{obs}}, \boldsymbol{f} = \hat{\boldsymbol{f}}^{(t-1)}\right]$ pretending $c = g(\tilde{\sigma})$ is fixed. Under normality:

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\hat{w}_l^{(t)} &= \alpha(w_l^{(t)}, \eta_l) + \beta(w_l^{(t)}, \eta_l) \times w_l^{(t)} \\
\text{with } \alpha(w, \eta) &= \sqrt{\eta}\sigma \left[\phi\left(\frac{c - w}{\sqrt{\eta}\sigma}\right) - \phi\left(\frac{c + w}{\sqrt{\eta}\sigma}\right)\right], \\
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Contracting Properties for Soft-Thresholding

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- Conjecture: $\exists\, \rho < 1$ independent of n,

$$||M(\hat{w}^{(t)}) - M(w)||_{2,n} \leq \sqrt{\rho}||\hat{w}^{(t)} - w||_{2,n}$$

Simulation Experiments

- compared 6 procedures:
  - a: MISC, L_1 norm, EBayes of Johnstone & Silverman (2005) for $\hat{f}_{\mathrm{com}}$
  - b: MISC, L_2 norm, EBayes of Johnstone & Silverman (2005) for $\hat{f}_{\mathrm{com}}$
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  - e: REF with hard thresholding
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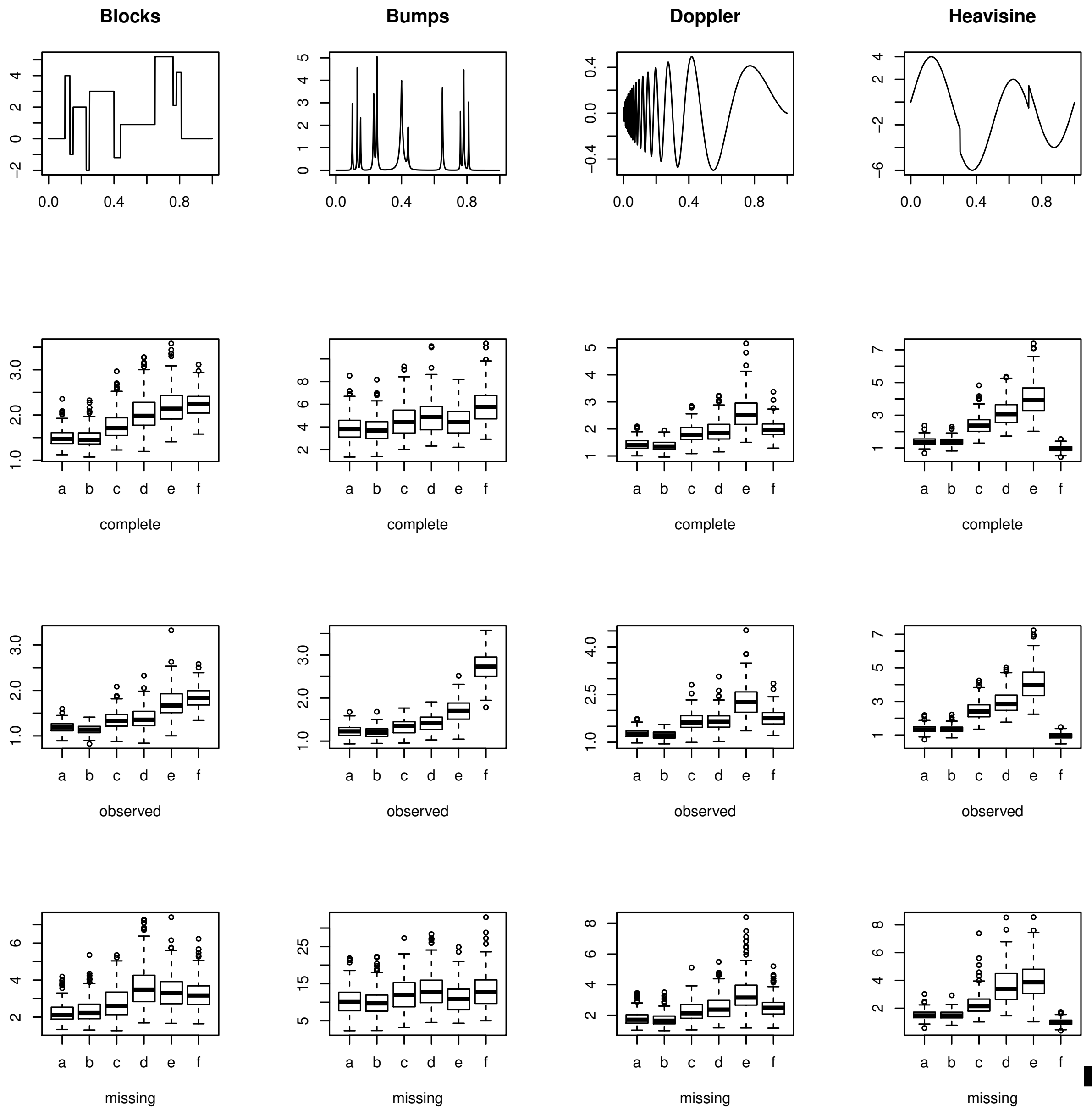
Boxplots of MSE: snr=3, 30% missing (results similar for MAE)



Let's see how it works - Airplane

degraded

reconstructed

Murder in Progress

degraded

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- conducted experiments to compare PPV and NPV:

$$\text{PPV} = \frac{\text{number of selected significant variables}}{\text{number of true significant variables}}$$

$$\text{NPV} = \frac{\text{number of removed non-significant variables}}{\text{number of true non-significant variables}}$$

Experimental Results

method		LCLM	HCLM	LCHM	HCHM	mean	weighted mean
1	PPV	85.4	67.3	85.4	67.3	76.4	87.9
	NPV	93.5	92.2	93.5	92.2	92.8	
2	PPV	80.6	56.5	72.7	46.6	64.1	86.4
	NPV	95.9	94.9	97.2	95.9	96.0	
3	PPV	88.1	70.1	83.7	64.4	76.6	84.2
	NPV	88.6	87.1	88.7	85.3	87.4	
4	PPV	79.8	55.9	71.5	45.1	63.1	86.1
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- Tested 4 methods:
  1. complete data available (for benchmark comparison)
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- BUT, there are a lot more to be done ...

A Telescopic, Microscopic, and Kaleidoscopic View of Data Science

HDSR

HARVARD DATA SCIENCE REVIEW