Missing data, IPW, Imputation, Covariate shift

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Contents

Missing data setup

MCAR setup

- We want to estimate $\mathbb{E}Y$ for $Y \sim p(y)$.
- **Full data**: $Y_1, \ldots, Y_n$ i.i.d. $p(y)$.
- Response indicators: $R, R_1, \ldots, R_n \in \{0, 1\}$ are i.i.d.
  - with $\mathbb{P}(R = 1) = \pi$.
- What we actually observe:

$$(R_1, R_1 Y_1), \ldots, (R_n, R_n Y_n).$$

- **Complete cases** are observations with $R_i = 1$.
- **Incomplete cases** are observations with $R_i = 0$.
- **MCAR assumption**: $R_i \perp\!\!\!\perp Y_i$ for each i

MAR setup

- Assume we have **covariate** X_i about each individual i.
- Also assume that X_i is **never missing**.
- Full data: $(X_1, Y_1), \ldots, (X_n, Y_n)$ i.i.d $p(x, y)$.
- What we actually observe:

$$(X_1, R_1, R_1 Y_1), \ldots, (X_n, R_n, R_n Y_n).$$

- **MAR assumption**: $R_i \perp\!\!\!\perp Y_i \mid X_i$ for each i
    - i.e.$p(r, y \mid x) = p(r \mid x) p(y \mid x)$

The propensity score

- Key piece in the MAR setting is the model for missingness:

$$\mathbb{P}(R=1 \mid X=x, Y=y) = \mathbb{P}(R=1 \mid X=x) = \pi(x).$$

- $\pi(x)$ is called the **propensity score**.
- If the propensity score is 0, we have a blind spot in our input space
  - can't do anything about it (at least with our estimators)

Assumption

Unless otherwise noted, we will always assume that propensity scores are strictly positive: $\pi(x) > 0$.

Inverse propensity score estimators

Observed responses represent multiple unobserved responses

- Suppose $\mathcal{X} = \{0, 1\}$ corresponding to two types of people.
- When $X_i = 1$, response probability $\pi(1) = \mathbb{P}(R_i = 1 \mid X_i = 1) = 0.2$
- When $X_i = 0$, response probability $\pi(0) = \mathbb{P}(R_i = 1 \mid X_i = 0) = 0.1$
- If we observe Y_i for an individual with $X_i = 1$,
  - That individual represents roughly 5 people from the full data.
- If we observe Y_i for an individual with $X_i = 0$,
  - That individual represents roughly 10 people from the full data.

Inverse propensity weighted (IPW) Mean

- When[1] $\pi(x) > 0 \ \forall x \in \mathcal{X}$,
  we can define the **IPW mean estimator** for $\mathbb{E}Y$:

$$
\begin{aligned}
\hat{\mu}_{\text{ipw}} &= \frac{1}{n} \sum_{i:R_i=1} \frac{Y_i}{\pi(X_i)} \\
&= \frac{1}{n} \sum_{i=1}^{n} \frac{R_i Y_i}{\pi(X_i)}
\end{aligned}
$$

- $\hat{\mu}_{\text{ipw}}$ is **unbiased** for $\mathbb{E}Y$ (i.e. $\mathbb{E}\hat{\mu}_{\text{ipw}} = \mathbb{E}Y$.)
- $\hat{\mu}_{\text{ipw}}$ is **consistent** for $\mathbb{E}Y$ (i.e. $\hat{\mu}_{\text{ipw}} \xrightarrow{P} \mathbb{E}Y$ as $n \to \infty$)

[1] We assume here and everywhere below that $\pi(x) > 0 \ \forall x \in \mathcal{X}$.

The complete case mean estimator

- The **complete case mean estimator** is defined as

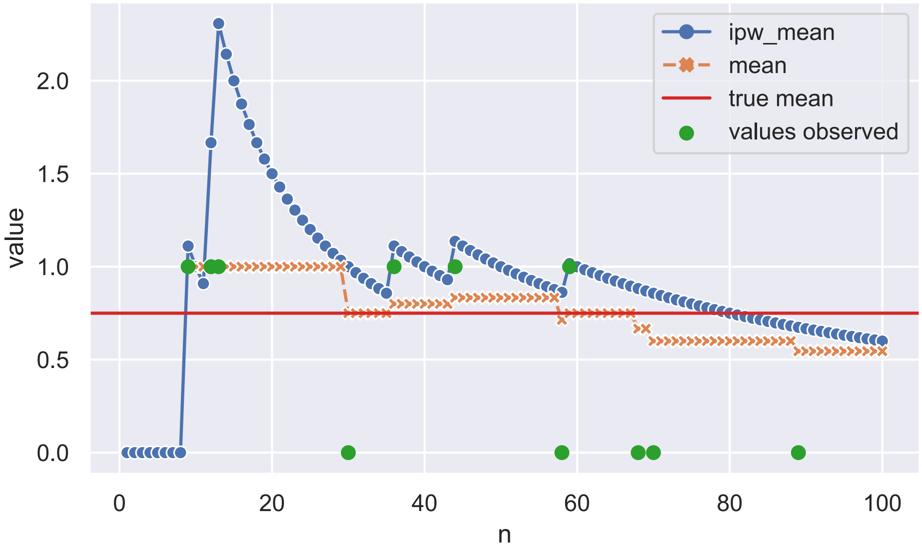
$$\hat{\mu}_{\text{cc}} = \frac{\sum_{i=1}^{n} R_i Y_i}{\sum_{i=1}^{n} R_i}.$$

- i.e. just take the average of the observed Y_i's

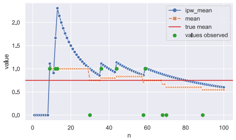
MCAR example

- For $i = 1, \ldots, n$
    - Let R_i be independent of (X_i, Y_i).
    - $\pi(x) = \mathbb{P}(R_i = 1 \mid X_i = x) \equiv 0.1$.
    - Let $Y_i \in \{0, 1\}$ with $\mathbb{P}(Y_i = 1) = 0.75$

IPW vs complete case mean for MCAR



IPW vs complete case mean for MCAR



- We've added in the orange line here, which represent the mean of the complete cases.
- Note that the orange line is constant between observations, and jumps whenever we get a new observation.

IPW vs complete case mean, 5000x

- We repeat the experiment[2] above 5000 times ($n = 100$ samples in each) and get the following.
- Recall that the true mean is $\mu = 0.75$.

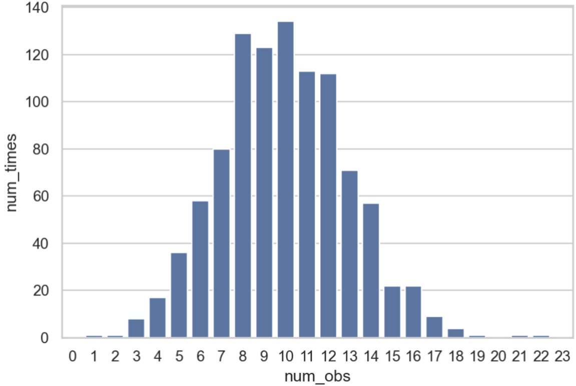
estimator	mean	SD	SE	bias	RMSE
mean	0.751654	0.143943	0.002036	0.001654	0.143953
ipw_mean	0.752540	0.262224	0.003708	0.002540	0.262237

[2] In the very rare event that the sample in a particular repetition has 0 complete cases, we take $\hat{\mu}_{cc} = 0$.

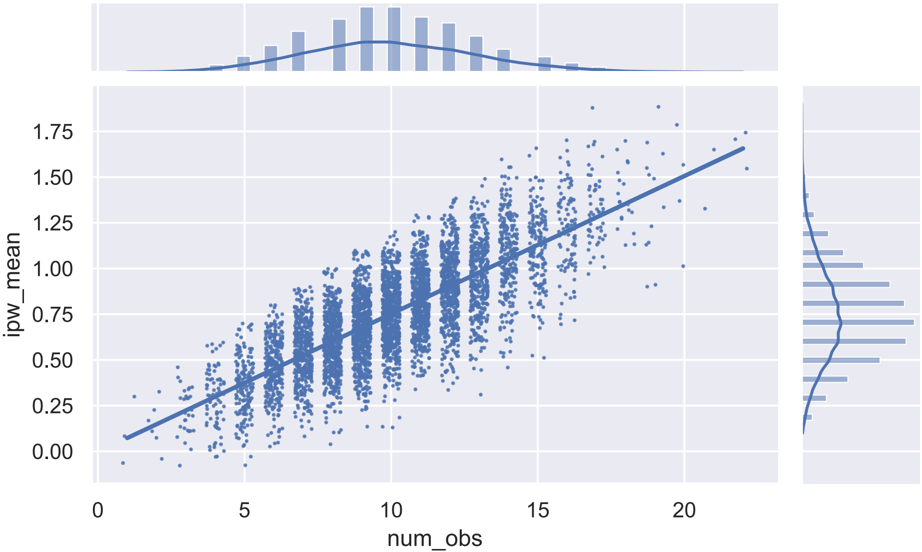
Variance of IPW

Probability review: how many responses will we get?

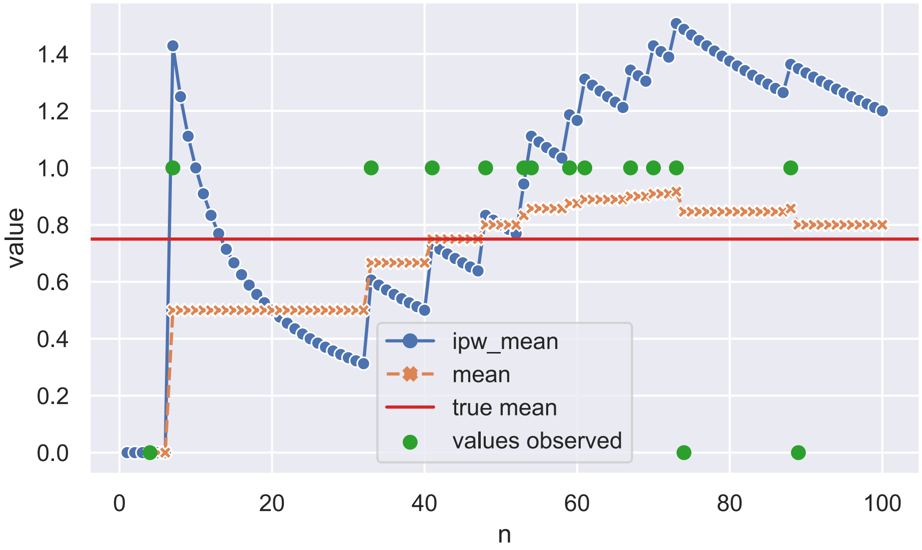
- $R, R_1, \ldots, R_n \in \{0,1\}$ are i.i.d. with $\mathbb{P}(R=1) = 0.1$.
- Number of observations: $N = \sum_{i=1}^{n} R_i$.
- Expected number of responses is $\mathbb{E}N = 0.1n$ and $N \sim \text{Binom}(n, p = 0.1)$.
- Histogram of N from 1000 simulations of our setup with $n = 100$:



IPW mean vs number of observations



IPW mean for "too many" observations



IPW: Can we improve this estimator for MCAR?

- IPW for constant observation probability π:

$$\hat{\mu}_{\text{ipw}} = \frac{1}{n}\sum_{i=1}^{n}\frac{R_i Y_i}{\pi}$$

- Idea: Rather than dividing by n,
  - divide by actual number of observations $N = \sum_{i=1}^{n} R_i$.
- This exactly gives us back

$$\hat{\mu}_{\text{cc}} = \frac{\sum_{i=1}^{n} R_i Y_i}{\sum_{i=1}^{n} R_i}.$$

- Have we gone in a useless circle?
- Not at all! Let's try to apply this "correction" to the more general MAR case...

Self-normalized IPW for MAR

Weights

- We can write

$$\hat{\mu}_{\text{ipw}} = \frac{1}{n}\sum_{i=1}^{n}\frac{R_iY_i}{\pi(X_i)} = \frac{1}{n}\sum_{i=1}^{n}W_iR_iY_i,$$

where

$$W_i := \frac{1}{\pi(X_i)} = \frac{1}{p(R_i = 1 \mid X_i)}.$$

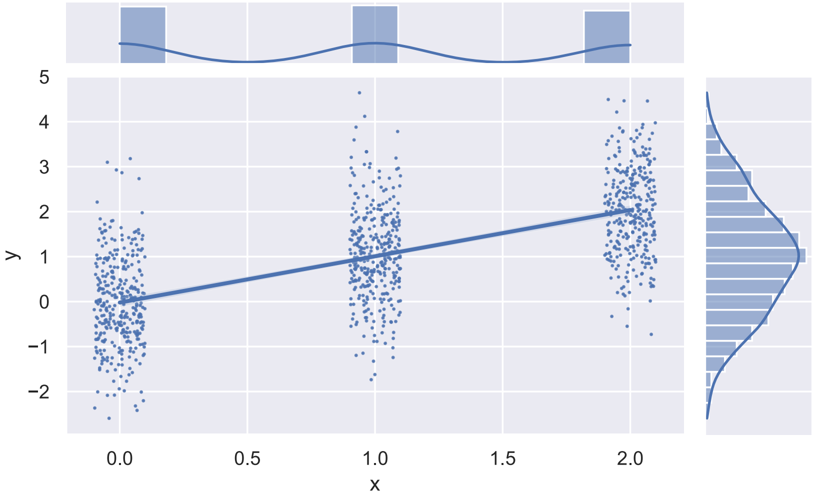
- We'll refer to W_i as the **weight** for observation Y_i.
- It's like each observed response Y_i (with $R_i = 1$) represents W_i responses in the full data.
- Upweighting by W_i makes up for the zeros when $R_i = 0$.

IPW in MAR: very large or small number of observations?

- If each observed response Y_i represents W_i responses in the full data,
  - then our observed data represents $\sum_{i=1}^{n} W_i R_i$ people.
- The IPW estimate normalizes by n: $\hat{\mu}_{\text{ipw}} = \frac{1}{n}\sum_{i=1}^{n} W_i R_i Y_i$.
- But what if $\sum_{i=1}^{n} W_i R_i$ is much smaller or larger than n?
- Then it seems like we're normalizing by the wrong thing...

MAR: “SeaVan1” distribution illustrated

A sample of size 1000 from the full data distribution is shown below:



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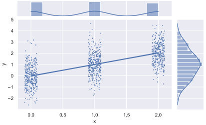
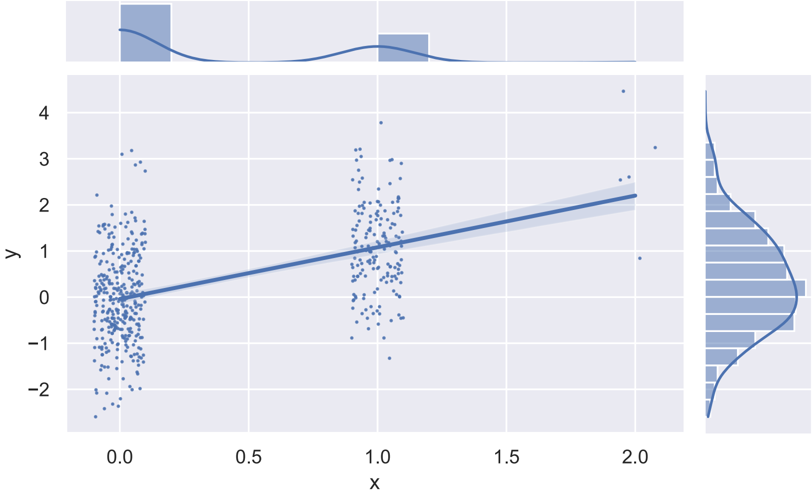


We’ve added jitter to the x values so that it’s easier to see the distribution.

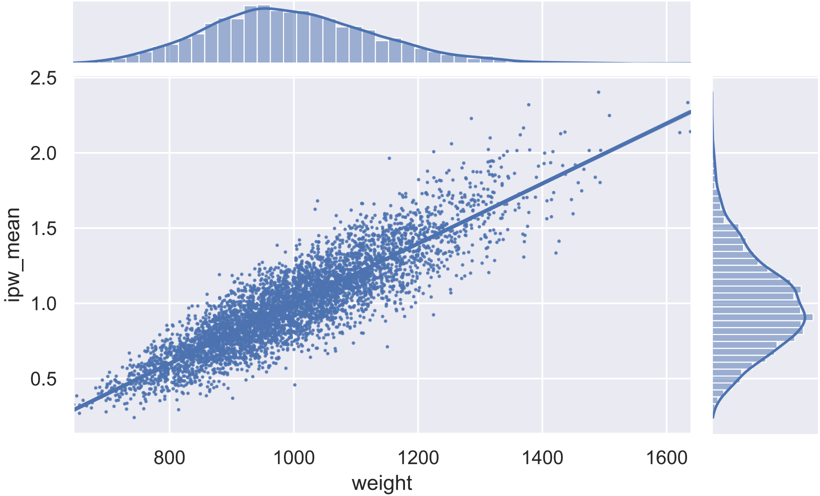
MAR: "SeaVan1" distribution illustrated

(X_i, Y_i) for which $R_i = 1$, i.e. the complete cases.



IPW vs total weight of observations

- The points below have correlation 0.885.



The self-normalized IPW estimator

- If we normalize by $\sum_{i=1}^n W_i R_i$ instead of n, we get

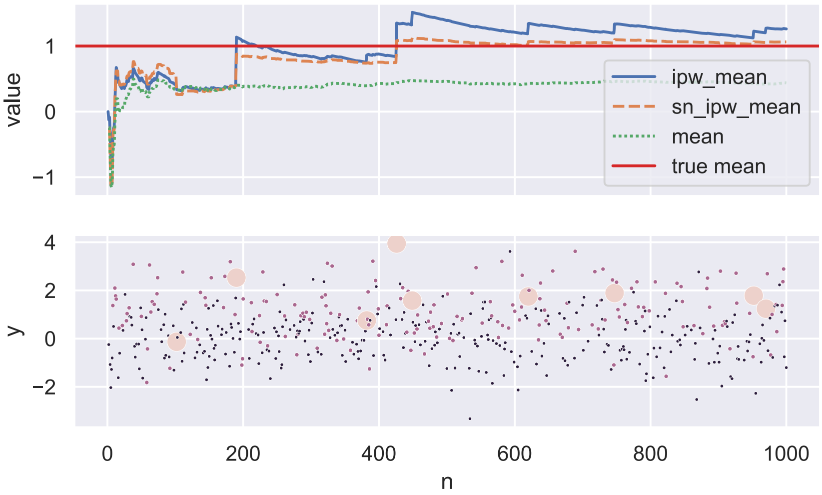
Definition (Self-normalized IPW mean)

For a dataset $(W_1, R_1, Y_1), \ldots, (W_n, R_n, Y_n)$ as described above,

$$\hat{\mu}_{\text{sn\_ipw}} = \frac{\sum_{i=1}^n W_i R_i Y_i}{\sum_{i=1}^n W_i R_i}$$

- In the MCAR case with $\pi(x) \equiv p$, $\hat{\mu}_{\text{sn\_ipw}} = \hat{\mu}_{\text{cc}}$ and seems preferable to $\hat{\mu}_{\text{ipw}}$.

Self-normalized IPW estimator on SeaVan1



IPW vs self-normalized IPW: 5000x

- We repeat the experiment above 5000 times (1000 samples each) and get the following.
- Recall that the true mean is $\mu = 1.0$.

estimator	mean	SD	SE	bias	RMSE
mean ($\hat{\mu}_{cc}$)	0.357244	0.050305	0.000711	-0.643534	0.645497
ipw_mean ($\hat{\mu}_{ipw}$)	0.995142	0.308634	0.004365	-0.005635	0.308686
sn_ipw_mean ($\hat{\mu}_{sn\_ipw}$)	0.978119	0.197319	0.002791	-0.022659	0.198615

Regression imputation

Regression imputation: basic idea

X	R	Y
x_1	1	y_1
x_2	0	?
x_3	0	?
x_4	1	y_4
$\vdots$	$\vdots$	$\vdots$
x_n	1	y_n

$\Longrightarrow$

X	R	Y
x_1	1	y_1
x_2	0	$\hat{f}(x_2)$
x_3	0	$\hat{f}(x_3)$
x_4	1	y_4
$\vdots$	$\vdots$	$\vdots$
x_n	1	y_n

- Fit $\hat{f}(x)$ on complete cases $(R=1)$ to approximate $\mathbb{E}[Y \mid X=x]$.
- **Regression imputation estimator:** Estimate $\mathbb{E}Y$ with

$$\frac{1}{n}\left(y_1+\hat{f}(x_2)+\hat{f}(x_3)+y_4+\cdots+y_n\right).$$

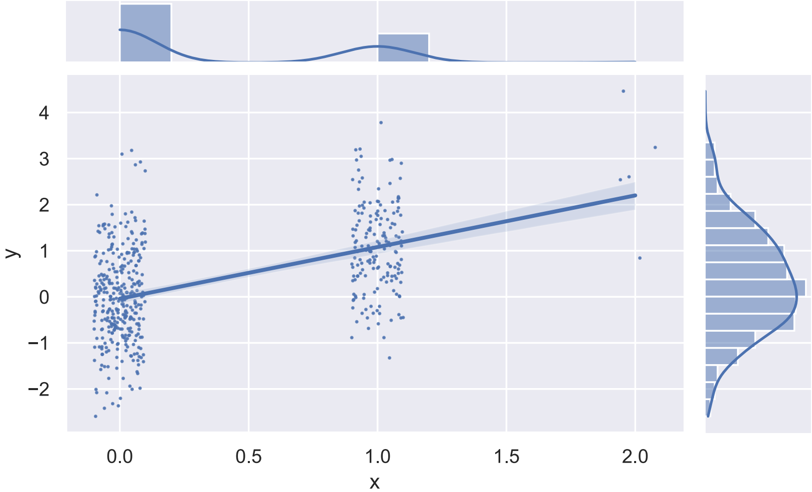
Well-specified and misspecified models

- In statistics, a **model** is a set of distributions
  - (or conditional distributions).
- A model is **well specified** if it contains the data-generating distribution.
  - Also referred to as **correctly specified.**
- If a model is not well specified, we say it's **misspecified** or **incorrectly specified**.
- We'll see that regression imputation has the following performance characteristics:

	MCAR	MAR
well specified	Good	Good
misspecified	OK/Good	Bad

MAR: SeaVan1 distribution illustrated

(X_i, Y_i) for which $R_i = 1$, i.e. the complete cases.



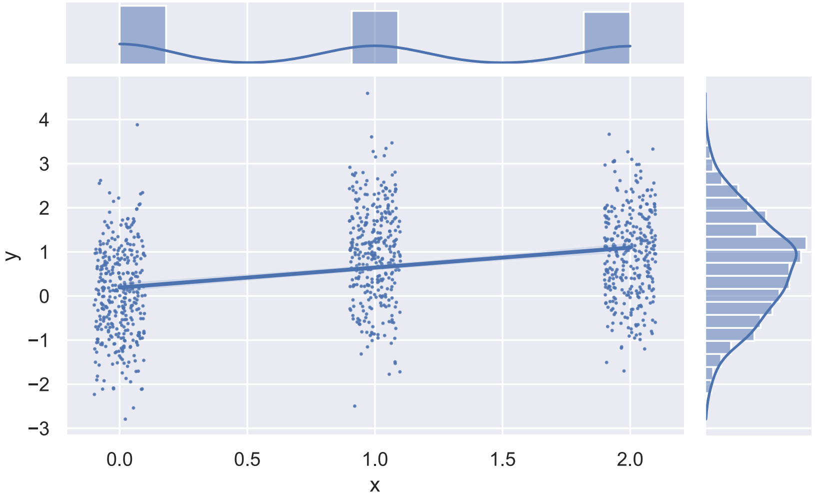
Performance on SeaVan1

- Fit $\hat{f}(x) = a + bx$ to the complete cases.
- Impute missing Y_i's with $\hat{f}(X_i)$...

estimator	mean	SD	SE	bias	RMSE
mean ($\hat{\mu}_{\text{cc}}$)	0.3572	0.0503	0.0007	-0.6435	0.6455
ipw_mean ($\hat{\mu}_{\text{ipw}}$)	0.9951	0.3086	0.0044	-0.0056	0.3087
sn_ipw_mean ($\hat{\mu}_{\text{sn\_ipw}}$)	0.9781	0.1973	0.0028	-0.0227	0.1986
impute_linear ($\hat{\mu}_{\hat{f}}$)	0.9989	0.0777	0.0011	-0.0018	**0.0777**

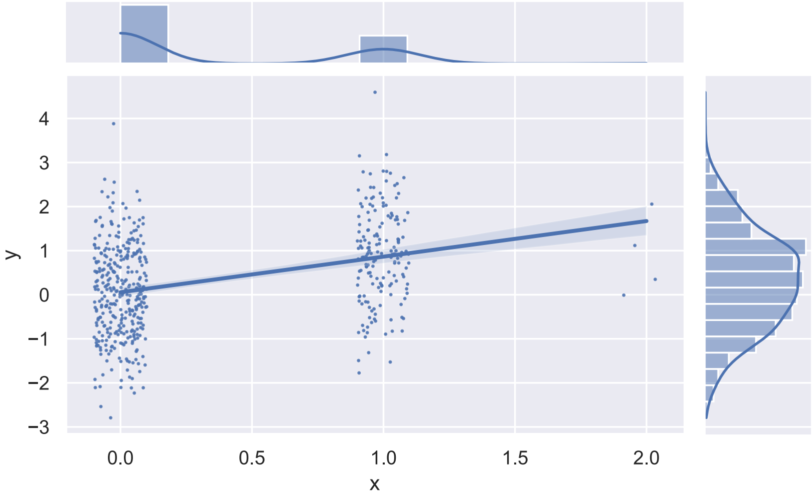
MAR: "SeaVan2" distribution illustrated

- Full data for sample of size $n = 1000$; $\mathbb{E}[Y \mid X = x] = \mathbb{1}[x \geqslant 1]$.



MAR: "SeaVan2" distribution illustrated

- Complete cases in sample of size $n = 1000$



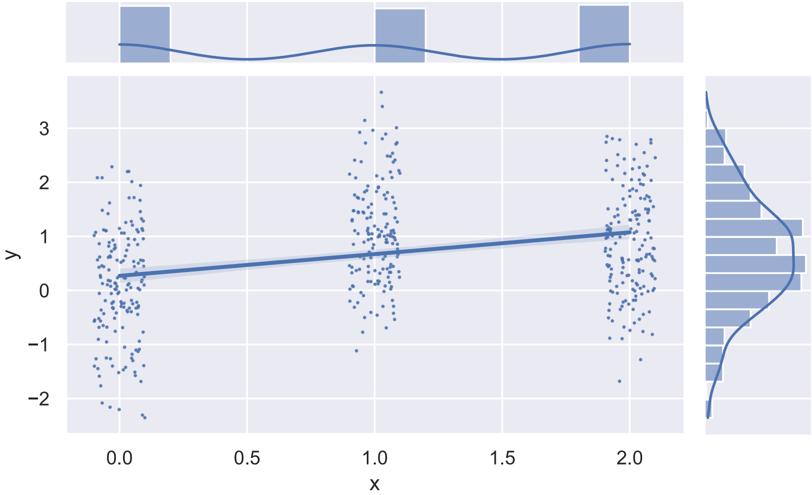
Performance on SeaVan2

- Fit $\hat{f}(x) = a + bx$ to the complete cases.

estimator	mean	SD	SE	bias	RMSE
mean ($\hat{\mu}_{\text{cc}}$)	0.3453	0.0497	0.0007	-0.3221	0.3259
ipw_mean ($\hat{\mu}_{\text{ipw}}$)	0.6634	0.1977	0.0028	-0.0040	0.1978
sn_ipw_mean ($\hat{\mu}_{\text{sn\_ipw}}$)	0.6580	0.1462	0.0021	-0.0094	0.1465
impute_linear ($\hat{\mu}_{\hat{f}}$)	0.9382	0.0793	0.0011	0.2708	**0.2821**

SeaVan2_MCAR illustrated

- Complete cases in sample size $n = 1000$



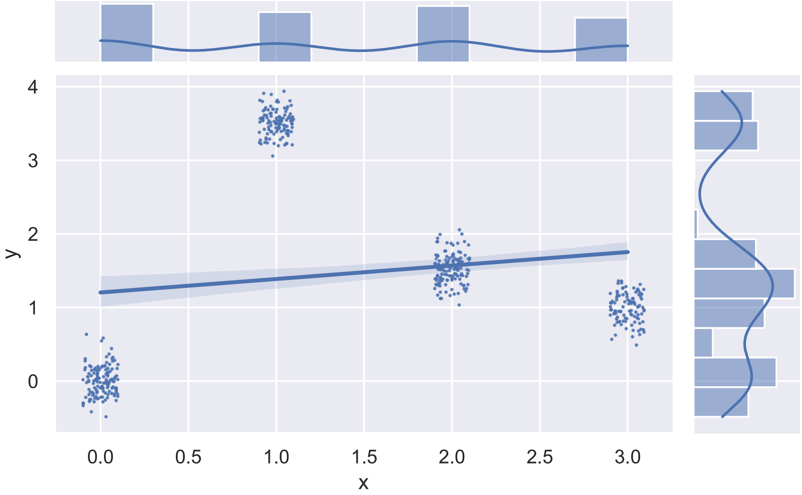
Performance on SeaVan2_MCAR

- Fit $\hat{f}(x) = a + bx$ to the complete cases.
- True mean: 0.667

estimator	mean	SD	SE	bias	RMSE
mean ($\hat{\mu}_{\text{cc}}$)	0.66724	0.05059	0.00226	0.00116	0.05061
ipw_mean ($\hat{\mu}_{\text{ipw}}$)	0.66712	0.05552	0.00248	0.00104	0.05553
sn_ipw_mean ($\hat{\mu}_{\text{sn\_ipw}}$)	0.66724	0.05059	0.00226	0.00116	0.05061
impute_linear ($\hat{\mu}_{\hat{f}}$)	0.66763	0.04953	0.00222	0.00155	**0.04955**

MCAR_normal_nonlinear

Complete cases for $\mathbb{P}(R = 1 \mid X) \equiv 0.5$ and $n = 1000$:



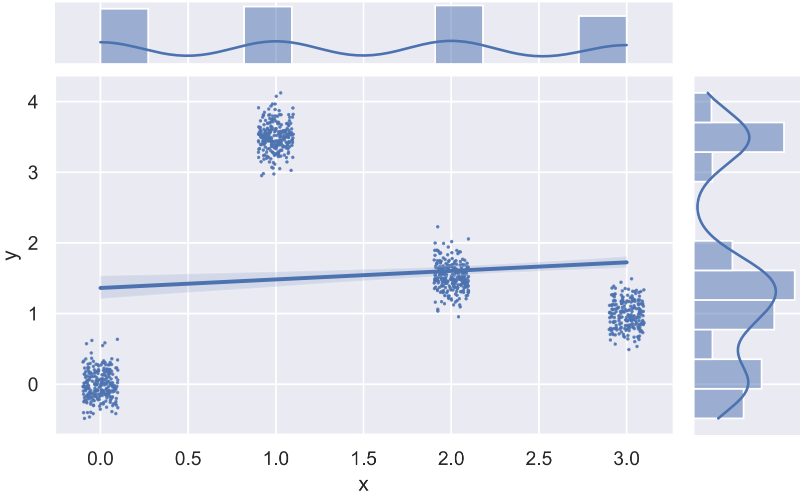
Performance on MCAR_normal_nonlinear

- True mean: 1.50

estimator	mean	SD	SE	bias	RMSE
mean	1.5021	0.0593	0.0019	0.0009	0.0593
ipw_mean	1.5014	0.0759	0.0024	0.0002	0.0759
sn_ipw_mean	1.5021	0.0593	0.0019	0.0009	0.0593
impute_linear	1.5030	0.0592	0.0019	0.0018	**0.0592**

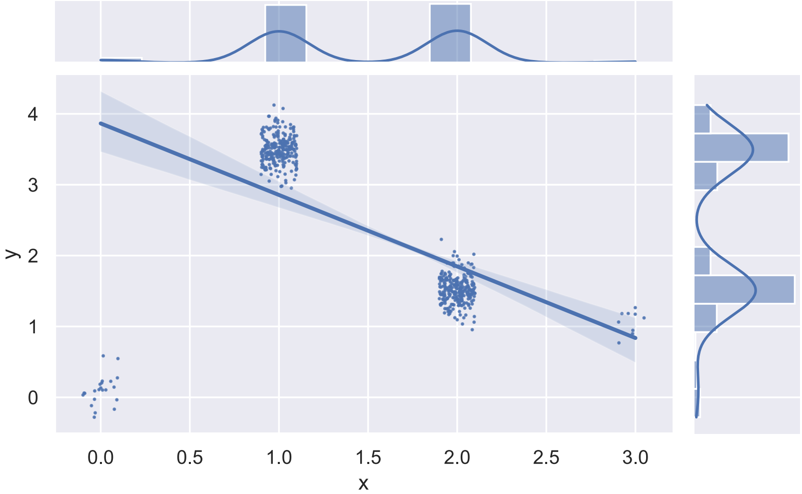
MAR_normal_nonlinear

Full data for $n = 1000$:



MAR_normal_nonlinear

Complete cases for $n = 1000$:



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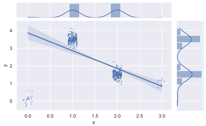

Note that the linear fit is completely off from the fit to the full data (preceding slide) because of the sample bias.

Performance on MAR_normal_nonlinear

- True mean: 1.50

estimator	mean	SD	SE	bias	RMSE
mean	2.4075	0.0476	0.0015	0.9063	0.9075
ipw_mean	1.4985	0.0851	0.0027	-0.0027	0.0852
sn_ipw_mean	1.5070	0.1224	0.0039	0.0057	0.1225
impute_linear	2.4060	0.0583	0.0018	0.9048	**0.9066**

What's going on?

- The best linear fit to the complete cases is
  - COMPLETELY DIFFERENT from the best linear fit to full data.
- Essential issue: model is fit to the **complete cases**,
  - but applied on **incomplete cases.**
- Complete cases and incomplete cases have different distributions!

Covariate shift

Supervised learning framework

- $\mathcal{X}$: input space
- $\mathcal{Y}$: outcome space
- $\mathcal{A}$: action space
- **Prediction function** $f : \mathcal{X} \to \mathcal{A}$ (takes input $x \in \mathcal{X}$ and produces action $a \in \mathcal{A}$)
- **Loss function** $\ell : \mathcal{A} \times \mathcal{Y} \to \mathbb{R}$ (evaluates action a in the context of outcome y).

Risk minimization

- Let $(X,Y) \sim p(x,y)$.
- The **risk** of a prediction function $f: \mathcal{X} \to \mathcal{A}$ is $R(f) = \mathbb{E}\ell(f(X),Y)$.
    - the expected loss of f on a new example $(X,Y) \sim p(x,y)$
- Ideally we'd find the **Bayes prediction function** $f^* \in \arg\min_f R(f)$.

Empirical risk minimization

- Training data: $\mathcal{D}_n = ((X_1, Y_1), \ldots, (X_n, Y_n))$
  - drawn i.i.d. from $p(x, y)$.
- Let $\mathcal{F}$ be a **hypothesis space** of functions mapping $\mathcal{X} \to \mathcal{A}$
- A function $\hat{f}$ is an **empirical risk minimizer** over $\mathcal{F}$ if

$$\hat{f} \in \underset{f \in \mathcal{F}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell(f(X_i), Y_i).$$

- Uses sample $\mathcal{D}_n$ from $p(x, y)$ to estimate expectation w.r.t. $p(x, y)$.
- Most machine learning methods can be written in this form.
- What if we only have a sample from another distribution $q(x, y)$?

Covariate shift

- Goal: Find f minimizing risk $R(f) = \mathbb{E}\ell(f(X), Y)$ where

$$(X, Y) \sim p(x, y) = p(x)p(y \mid x).$$

- Standard: $\mathcal{D}_n = ((X_1, Y_1), \ldots, (X_n, Y_n))$ is i.i.d. from

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- **Covariate shift**: $\mathcal{D}_n = ((X_1, Y_1), \ldots, (X_n, Y_n))$ is i.i.d. from

$$q(x, y) = q(x)p(y \mid x).$$

- The covariate distribution has changed, but
  - the conditional distribution $p(y \mid x)$ is the same in both cases.

Covariate shift: the issue

- Under covariate shift,

$$\mathbb{E}_{(X_i,Y_i)\sim q(x,y)}\left[\frac{1}{n}\sum_{i=1}^{n}\ell(f(X_i),Y_i)\right] \neq \mathbb{E}_{(X,Y)\sim p(x,y)}\ell(f(X),Y).$$

- i.e the empirical risk is a **biased** estimator for risk.
- Naive empirical risk minimization is optimizing the wrong thing.
- Can we get an unbiased estimate of risk with $\mathcal{D}_n \sim q(x,y)$?
- **Importance sampling** is one approach to this problem.

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Empirical risk minimization

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Importance sampling for covariate shift

- $\mathcal{D}_n = ((X_1, Y_1), \ldots, (X_n, Y_n))$ is i.i.d. from

$$q(x, y) = q(x)p(y \mid x).$$

- Then the **importance-sampled empirical risk** is

$$\begin{aligned}
\hat{R}_{\text{IS}}(f) &= \frac{1}{n}\sum_{i=1}^{n} \frac{p(x)p(y \mid x)}{q(x)p(y \mid x)} \ell(f(X_i), Y_i) \\
&= \frac{1}{n}\sum_{i=1}^{n} \frac{p(x)}{q(x)} \ell(f(X_i), Y_i).
\end{aligned}$$

- Note that $\mathbb{E}_{\mathcal{D}_n \sim q(x,y)} \hat{R}_{\text{IS}}(f) = \mathbb{E}_{(X,Y) \sim p(x,y)} \ell(f(X), Y)$.
- So the **importance-sampled empirical risk** is unbiased.

Potential variance issues

- Since the summands are independent, we have

$$\begin{aligned}\text{Var}\left(\hat{R}_{\text{IS}}(f)\right) &= \text{Var}\left(\frac{1}{n}\sum_{i=1}^{n} f(X_i)\frac{p(X_i)}{q(X_i)}\right) \\ &= \frac{1}{n}\text{Var}\left(f(X)\frac{p(X)}{q(X)}\right)\end{aligned}$$

- If $q(x)$ is much smaller than $p(x)$,
  - the importance weight can get very large,
  - variance can blow up.

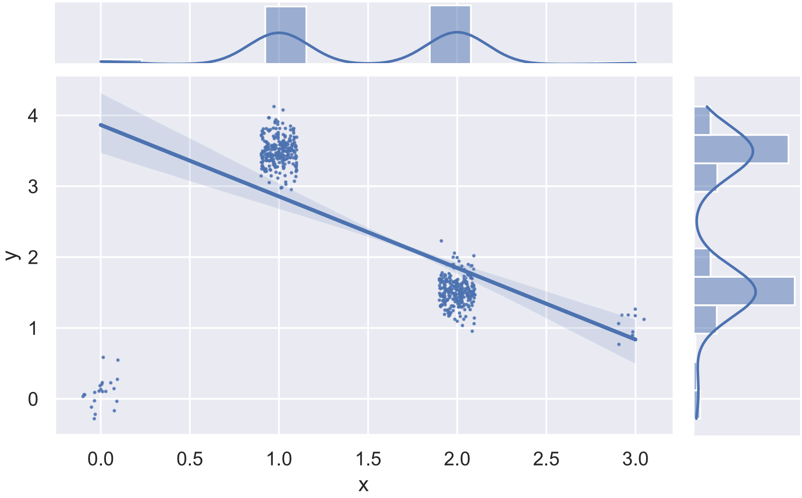
Importance-sampled regression imputation

Importance sampling

- Our linear model is fit to data from the complete case distribution
  - we need it to be fit to the incomplete case distribution
  - or the full data distribution (also common)
- Two new estimators:
  - **impute_IPW_linear:** examples weighted by $\frac{1}{\pi(X_i)}$ so unbiased for full data
  - **impute_IS_linear:** examples weighted by $\frac{1-\pi(X_i)}{\pi(X_i)}$ so unbiased for incomplete data

Recap: MAR_normal_nonlinear

Complete cases for $n = 1000$:



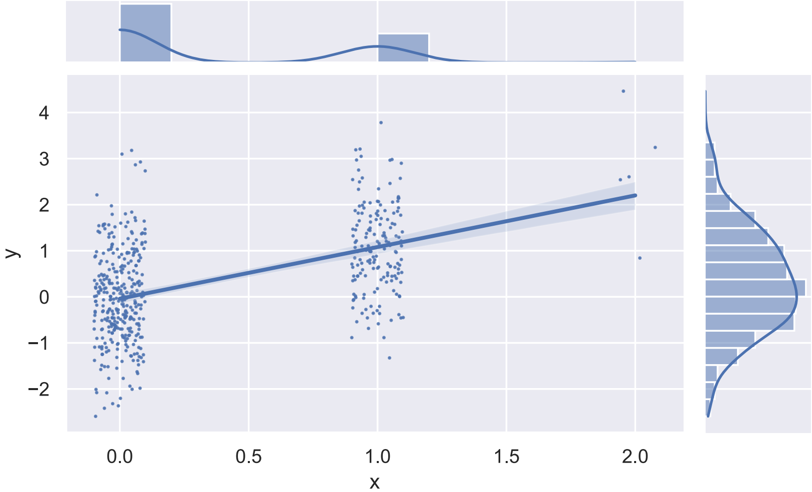
Performance on MAR_normal_nonlinear

- True mean: 1.50

estimator	mean	SD	SE	bias	RMSE
mean	2.4075	0.0476	0.0015	0.9063	0.9075
ipw_mean	1.4985	0.0851	0.0027	-0.0027	0.0852
sn_ipw_mean	1.5070	0.1224	0.0039	0.0057	0.1225
impute_linear	2.4060	0.0583	0.0018	0.9048	**0.9066**
impute_ipw_linear	1.9895	0.0777	0.0025	0.4883	**0.4944**
impute_is_linear	1.5005	0.0466	0.0015	-0.0007	**0.0466**

Recap: SeaVan1 distribution illustrated

(X_i, Y_i) for which $R_i = 1$, i.e. the complete cases.



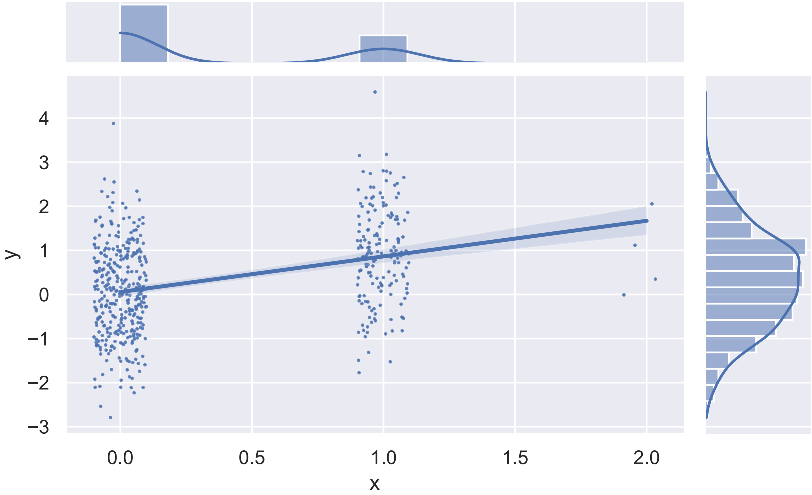
Performance on SeaVan1

- Fit $\hat{f}(x) = a + bx$ to the complete cases.

estimator	mean	SD	SE	bias	RMSE
mean	0.3564	0.0515	0.0016	-0.6431	0.6452
ipw_mean	1.0127	0.2968	0.0094	0.0132	0.2971
sn_ipw_mean	0.9906	0.1890	0.0060	-0.0089	0.1892
impute_linear	1.0022	0.0781	0.0025	0.0027	**0.0782**
impute_ipw_linear	1.0039	0.1439	0.0046	0.0044	**0.1440**
impute_is_linear	1.0047	0.1529	0.0048	0.0052	**0.1530**

MAR: "SeaVan2" distribution illustrated

- Complete cases in sample of size $n = 1000$



Performance on SeaVan2

- Fit $\hat{f}(x) = a + bx$ to the complete cases.

estimator	mean	SD	SE	bias	RMSE
mean	0.3425	0.0493	0.0007	-0.3244	0.3282
ipw_mean	0.6655	0.1939	0.0027	-0.0014	0.1939
sn_ipw_mean	0.6594	0.1446	0.0020	-0.0075	0.1448
impute_linear	0.9364	0.0792	0.0011	0.2695	**0.2809**
impute_ipw_linear	0.6750	0.1503	0.0021	0.0081	**0.1505**
impute_is_linear	0.6677	0.1561	0.0022	0.0008	**0.1561**

Caveat on results

- The importance-sampled regression imputation estimators seem promising.
- The estimators rely on knowing the importance weights $p(x)/q(x)$.
- Performance may be significantly worse when we use estimates $\hat{p}(x)/\hat{q}(x)$.
- This is something we can explore in homeworks and projects.

References

References I