A guided tour in targeted learning territory

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1 Introduction

This is a very first draft of our article. The current *tentative* title is "A guided tour in targeted learning territory".

Explain our objectives and how we will meet them.

Use sectioning a lot to ease cross-referencing.

```
set.seed(54321) ## because reproducibility matters...
suppressMessages(library(R.utils)) ## make sure it is installed
suppressMessages(library(ggplot2)) ## make sure it is installed
expit <- plogis
logit <- qlogis
```

2 A simulation study

blabla

2.1 Reproducible experiment as a law. We are interested in a reproducible experiment. The generic summary of how one realization of the experiment unfolds, our observation, is called O. We view O as a random variable drawn from what we call the law P_0 of the experiment. The law P_0 is viewed as an element of what we call the model. Denoted by $\mathcal{M}$, the model is the collection of *all* laws from which O can be drawn and that meet some constraints. The constraints translate the knowledge we have about the experiment. The more we know about the experiment, the smaller is $\mathcal{M}$. In all our examples, model $\mathcal{M}$ will put very few restrictions on the candidate laws.

Consider the following chunk of code:

```
drawFromExperiment <- function(n, full = FALSE) {
  ## preliminary
  n <- Arguments$getInteger(n, c(1, Inf))
  full <- Arguments$getLogical(full)
  ## ## 'gbar' and 'Qbar' factors
  gbar <- function(W) {
```

```r
    expit(-0.3 + 2 * W - 1.5 * W^2)
  }
  Qbar <- function(AW) {
    A <- AW[, 1]
    W <- AW[, 2]
    A * cos(2 * pi * W) + (1 - A) * sin(2 * pi * W^2)
  }
  ## sampling
  ## ## context
  W <- runif(n)
  ## ## counterfactual rewards
  zeroW <- cbind(A = 0, W)
  oneW <- cbind(A = 1, W)
  Yzero <- rnorm(n, mean = Qbar(zeroW), sd = 1)
  Yone <- rnorm(n, mean = Qbar(oneW), sd = 1)
  ## ## action undertaken
  A <- rbinom(n, size = 1, prob = gbar(W))
  ## ## actual reward
  Y <- A * Yone + (1 - A) * Yzero
  ## ## observation
  if (full) {
    obs <- cbind(W = W, Yzero = Yzero, Yone = Yone, A = A, Y = Y)
  } else {
    obs <- cbind(W = W, A = A, Y = Y)
  }
  attr(obs, "gbar") <- gbar
  attr(obs, "Qbar") <- Qbar
  attr(obs, "QW") <- dunif
  ##
  return(obs)
}
```

We can interpret `drawFromExperiment` as a law P_0 since we can use the function to sample observations from a common law. It is even a little more than that, because we can tweak the experiment, by setting its `full` argument to `TRUE`, in order to get what appear as intermediary (counterfactual) variables in the regular experiment. The next chunk of code runs the (regular) experiment five times independently:

```r
(five.obs <- drawFromExperiment(5))
```

```
##              W A          Y
## [1,] 0.4290078 1 -0.4410530
## [2,] 0.4984304 0  0.1905250
## [3,] 0.1766923 0 -0.1325567
## [4,] 0.2743935 1 -1.6415356
## [5,] 0.2165102 0  0.6829717
## attr(,"gbar")
## function (W)
## {
##     expit(-0.3 + 2 * W - 1.5 * W^2)
## }
## <bytecode: 0x4f0d808>
## <environment: 0x225df18>
## attr(,"Qbar")
## function (AW)
```

```
## {
##     A <- AW[, 1]
##     W <- AW[, 2]
##     A * cos(2 * pi * W) + (1 - A) * sin(2 * pi * W^2)
## }
## <bytecode: 0x52d4690>
## <environment: 0x225df18>
## attr(,"QW")
## function (x, min = 0, max = 1, log = FALSE)
## .Call(C_dunif, x, min, max, log)
## <bytecode: 0x5273870>
## <environment: namespace:stats>
```

The `attributes` of the object `obs` are visible because, in this section, we act as oracles, *i.e.*, we know completely the nature of the experiment. From a probabilistic point of view, the attributes `gbar`, `Qbar` and `QW` are infinite-dimensional features of P_0. There is more to P_0 than $\bar{g}_0$ (`gbar`), $\bar{Q}_0$ (`Qbar`), formally defined by

$$\bar{g}_0(W) \equiv P_0(A = 1|W), \quad \bar{Q}_0(A, W) \equiv E_{P_0}(Y|A, W), \tag{1}$$

and the marginal distribution $Q_{0,W}$ of W under P_0 (`QW`), for instance the conditional distribution (not expectation) of Y given (A, W), but $\bar{g}_0$, $\bar{Q}_0$ and $Q_{0,W}$ will play a prominent role in our story.

2.2 The parameter of interest, first pass. It happens that we especially care for a finite-dimensional feature of P_0 that we denote by ψ_0. Its definition involves the aforementioned infinite-dimensional features:

$$\begin{aligned} \psi_0 &\equiv E_{P_0}\left(\bar{Q}_0(1, W) - \bar{Q}_0(0, W)\right) \\ &= \int \left(\bar{Q}_0(1, w) - \bar{Q}_0(0, w)\right) dQ_{0,W}(w). \end{aligned} \tag{2}$$

Acting as oracles, we can compute explicitely the numerical value of ψ_0.

Our interest in ψ_0 is of causal nature. Taking a closer look at `drawFromExperiment` reveals indeed that the random making of an observation O drawn from P_0 can be summarized by the following causal graph and nonparametric system of structural equations:

```
## plot the causal diagram
```

and, for some deterministic functions f_w, f_a, f_y and independent sources of randomness U_w, U_a, U_y,

1. sample the context where the rest of the experiment will take place, $W = f_w(U_w)$;
2. sample the two counterfactual rewards of the two actions that can be undertaken, $Y_0 = f_y(0, W, U_y)$ and $Y_1 = f_y(1, W, U_y)$;
3. sample which action is carried out in the given context, $A = f_a(W, U_a)$;
4. define the corresponding reward, $Y = AY_1 + (1 - A)Y_0$;
5. summarize the course of the experiment with the observation $O = (W, A, Y)$, thus concealing Y_0 and Y_1.

The above description of the experiment `drawFormExperiment` is useful to ram home what it means to run the "full" experiment by setting argument `full` to `TRUE` in a call to `drawFormExperiment`. Doing so triggers a modification of the nature of the experiment, enforcing that the counterfactual rewards Y_0 and Y_1 be part of the summary of the experiment eventually. In light of the above enumeration, $\mathbb{O} \equiv (W, Y_0, Y_1, A, Y)$ is output, as opposed to its summary measure O. This defines another experiment and its law, that we denote $\mathbb{P}_0$.

It is well known (do we give the proof or refer to other articles?) that

$$\psi_0 = E_{\mathbb{P}_0}\left(Y_1 - Y_0\right).$$

Thus, ψ_0 compares (additively) the averages of the two counterfactual rewards. In other words, ψ_0 quantifies the difference in average of the reward one would get in a world where one would always enforce action $a = 1$ with the reward one would get in a world where one would always enforce action $a = 0$. This said, it is worth emphasizing that ψ_0 is a well defined parameter beyond its causal interpretation.

To conclude this subsection, we draw advantage from the possibility to sample full observations from `drawFromExperiment` by setting its argument `full` to `TRUE` in order to numerically approximate ψ_0. By the law of large numbers, the following chunk of code approximates ψ_0:

```
B <- 1e6
full.obs <- drawFromExperiment(B, full = TRUE)
(psi.hat <- mean(full.obs[, "Yone"] - full.obs[, "Yzero"]))
```

```
## [1] -0.170182
```

In fact, the central limit theorem and Slutsky's lemma allow us to build a confidence interval with asymptotic level 95% for ψ_0:

```
sd.hat <- sd(full.obs[, "Yone"] - full.obs[, "Yzero"])
alpha <- 0.05
(psi.CI <- psi.hat + c(-1, 1) * qnorm(1 - alpha / 2) * sd.hat / sqrt(B))
```

```
## [1] -0.1738905 -0.1664735
```

2.3 The parameter of interest, second pass. Suppose we know beforehand that O drawn from P_0 takes its values in $\mathcal{O} \equiv [0,1] \times \{0,1\} \times [0,1]$ and that $P_0(A = 1|W)$ is bounded away from zero and one $Q_{0,W}$-almost surely (this is the case indeed). Then we can define model $\mathcal{M}$ as the set of all laws P on $\mathcal{O}$ such that $\bar{g}(W) \equiv P(A = 1|W)$ is bounded away from zero and one Q_W-almost surely, where Q_W is the marginal distribution of W under P.

Let us also define generically $\bar{Q}$ as

$$\bar{Q}(A, W) \equiv E_P(Y|A, W).$$

Central to our approach is viewing ψ_0 as the value at P_0 of the statistical mapping Ψ from $\mathcal{M}$ to $[0,1]$ characterized by

$$\begin{aligned}\Psi(P) &\equiv E_P\left(\bar{Q}(1, W) - \bar{Q}(0, W)\right) \\ &= \int \left(\bar{Q}(1, w) - \bar{Q}(0, w)\right) dQ_W(w),\end{aligned}$$

a clear extension of (2). For instance, although the law $\Pi_0 \in \mathcal{M}$ encoded by default (*i.e.*, with `h=0`) in `drawFromAnotherExperiment` defined below differs starkly from P_0,

```
drawFromAnotherExperiment <- function(n, h = 0) {
  ## preliminary
  n <- Arguments$getInteger(n, c(1, Inf))
  h <- Arguments$getNumeric(h)
  ## ## 'gbar' and 'Qbar' factors
  gbar <- function(W) {
```

```
    sin((1 + W) * pi / 6)
  }
  Qbar <- function(AW, hh = h) {
    A <- AW[, 1]
    W <- AW[, 2]
    expit( logit( A *  W + (1 - A) * W^2 ) +
           hh * 10 * sqrt(W) * A )
  }
  ## sampling
  ## ## context
  W <- rbeta(n, shape1 = 2, shape2 = 2)
  ## ## action undertaken
  A <- rbinom(n, size = 1, prob = gbar(W))
  ## ## reward
  QAW <- Qbar(cbind(A, W))
  Y <- rbeta(n, shape1 = 1, shape2 = (1 - QAW) / QAW)
  ## ## observation
  obs <- cbind(W = W, A = A, Y = Y)
  attr(obs, "gbar") <- gbar
  attr(obs, "Qbar") <- Qbar
  attr(obs, "QW") <- dunif
  ##
  return(obs)
}
```

parameter $\Psi(\Pi_0)$ is well defined, and approximated by `psi.Pi.zero` in the following chunk of code:

```
obs.from.another.experiment <- drawFromAnotherExperiment(1)
integrand <- function(w) {
  Qbar <- attr(obs.from.another.experiment, "Qbar")
  QW <- attr(obs.from.another.experiment, "QW")
  ( Qbar(cbind(1, w)) - Qbar(cbind(0, w)) ) * QW(w)
}
(psi.Pi.zero <- integrate(integrand, lower = 0, upper = 1)$val)
```

```
## [1] 0.1666667
```

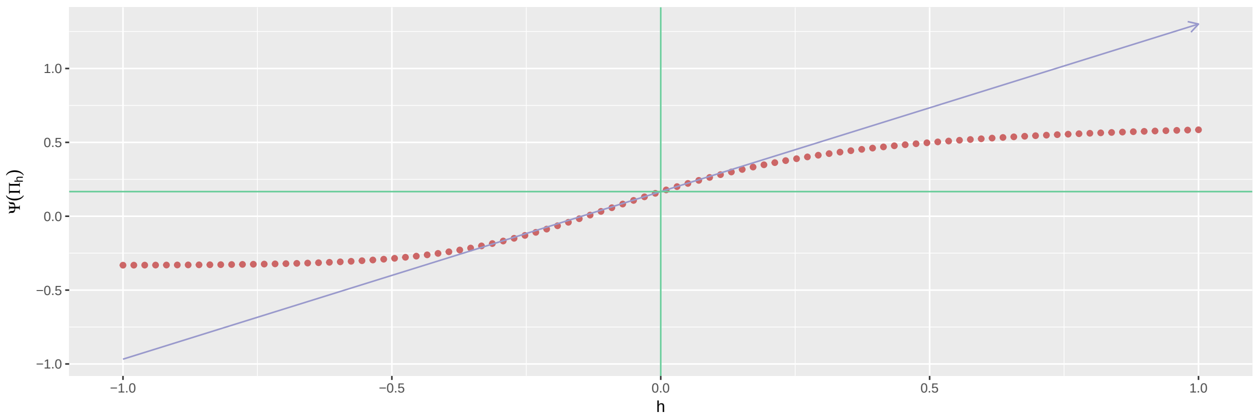
(easy algebra reveals that $\Psi(\Pi_0) = 1/6$ indeed).

Luckily, the statistical mapping Ψ is well behaved, or smooth. Here, this colloquial expression refers to the fact that, for each $P \in \mathcal{M}$, if $P_h \to_h P$ in $\mathcal{M}$ from a direction s when the real parameter $h \to 0$, then not only $\Psi(P_h) \to_h \Psi(P)$ (continuity), but also $h^{-1}[\Psi(P_h) - \Psi(P)] \to_h c$, where the real number c depends on P and s (differentiability).

For instance, let $\Pi_h \in \mathcal{M}$ be the law encoded in `drawFromAnotherExperiment` with `h` ranging over $[-1, 1]$. We will argue shortly that $\Pi_h \to_h \Pi_0$ in $\mathcal{M}$ from a direction s when $h \to 0$. The following chunk of code evaluates and represents $\Psi(\Pi_h)$ for h ranging in a discrete approximation of $[-1, 1]$:

```
approx <- seq(-1, 1, length.out = 1e2)
psi.Pi.h <- sapply(approx, function(t) {
  obs.from.another.experiment <- drawFromAnotherExperiment(1, h = t)
  integrand <- function(w) {
    Qbar <- attr(obs.from.another.experiment, "Qbar")
    QW <- attr(obs.from.another.experiment, "QW")
    ( Qbar(cbind(1, w)) - Qbar(cbind(0, w)) ) * QW(w)
  }
```

```r
  integrate(integrand, lower = 0, upper = 1)$val
})
slope <- (psi.Pi.h - psi.Pi.zero) / approx
slope <- slope[min(which(approx > 0))]
ggplot() +
  geom_point(data = data.frame(x = approx, y = psi.Pi.h), aes(x, y),
             color = "#CC6666") +
  geom_segment(aes(x = -1, y = psi.Pi.zero - slope, xend = 1, yend = psi.Pi.zero + slope),
               arrow = arrow(length = unit(0.03, "npc")),
               color = "#9999CC") +
  geom_vline(xintercept = 0, color = "#66CC99") +
  geom_hline(yintercept = psi.Pi.zero, color = "#66CC99") +
  labs(x = "h", y = expression(Psi(Pi[h])))
```



The dotted curve represents the function $h \mapsto \Psi(\Pi_h)$. The blue line represents the tangent to the previous curve at $h = 0$, which is indeed differentiable around $h = 0$. It is derived by simple geometric arguments. In the next subsection, we formalize what it means to be smooth for the statistical mapping Ψ. Once the presentation is complete, we will be able to derive a closed-form expression for the slope of the blue curve from the chunk of code where `drawFromAnotherExperiment` is defined.

2.4 The parameter of interest, third pass.