Learning how to act: making good decisions with machine learning

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June 8, 2016

1 Problem Summary

Learning the outcome of an action is central to many real world problems. Does de-worming children in poor countries improve health and educational outcomes [Miguel and Kremer, 2004, Davey et al., 2015]? Would increasing the minimum wage lead to higher unemployment? Will offering this customer a discount improve my revenue? These questions are difficult as they require more than identifying a pattern in data. There are two, very different, approaches to this problem within the machine learning community: reinforcement learning and causal inference.

Reinforcement learning addresses the problem of learning from explicitly taking actions. There is typically some state or environment. An agent chooses an action from those available in the current state. The state then evolves stochastically as a function of the selected action and the agent receives some feedback or reward that is a function of the new state. This setting differs from the standard classification problem in that the agent must learn from feedback on the selected action, rather than being presented with the correct action for a given state. A common modelling assumption is that the state evolves only as a function of the previous state and the action chosen, and given these, is independent of the previous history of states and actions. This is known as a Markov decision process or MDP. A particularly well studied and understood model is the singe state MDP. In this case, there are a set of actions, each associated with a fixed but unknown reward distribution and at each time step our agent selects an action and receives corresponding feedback. This is known as the multi-armed bandit problem.

Causal inference makes use of assumptions to allow the outcome of actions to be predicted from observational data. The key to causal inference is a framework that can model how actions change the state of the world. This framework then allows us to map information collected in one setting to another.

Both approaches can be seen as extensions to the concept of randomised controlled trials. Bandit algorithms deal with the sequential nature of the decision making process, causal inference with the problem that full randomisation is not always feasible, affordable or ethical. The similarities between the problems that these techniques have been developed to address raises the question of if there are problems best addressed by a combination of these approaches and how they can be combined. The goal of my thesis is to explore these questions. In the next sections I review the key literature in causal inference and bandits. I then present a general approach to how causal models might be incorporated into bandit settings and conclude by demonstrating an algorithm that leverages causal assumptions to improve performance in a specific bandit setting.

Part I

Literature review

2 Causal Inference

2.1 Models of causality and intervention

Predicting the outcome of actions without explicitly taking them requires assumptions about how the actions will change the system. A very powerful and general model that underlies much of the recent work in causality is the causal bayesian network. A causal bayesian network, or directed acyclic graph (DAG), is a bayesian network in which a link $V_i \rightarrow V_j$ is defined to mean V_i directly causes V_j. This means that if we intervene and change the value of V_i, we expect V_j to change, but if we intervene to change V_j, V_i will not change. More generally, if G is a causal network for a distribution P defined over variables $V_1 ... V_N$, then the distribution after an intervention where we set $X \subset V$ to x, denoted $do(X = x)$ is obtained by simply dropping the terms for each of the variables in X from the factorization given by the network. This is referred to as the truncated product formula [Pearl, 2000].

If the network contains latent (unobservable) variables we will not be able to calculate all the terms in the truncated product formula. However, it may still be possible to determine the post-interventional distribution of specific variables of interest. A general causal query $P(Y|do(X = x))$ is identifiable if it can be shown to be equivalent to an expression containing only pre-interventional quantities. This means that, asymptotically, we can obtain an unbiased estimate for the distribution after an intervention based on purely observational data.

The do calculus is a set of three rules that allow transformations of interventional terms to non-interventional ones, given a causal graph [Pearl, 2000]. They are derived directly from d-seperation properties of graphical models and the definition of intervention in causal DAGs. These rules are complete. A query is identifiable if and only if it can be transformed to contain only non-interventional terms via the do-calculus [Shpitser and Pearl, 2006, Huang and Valtorta, 2006]. There is an equivalent algorithm that can take any causal graph and query and determine identifiability [Shpitser and Pearl, 2008] (see `http://finnhacks42.github.io/causal_identify` for a javascript demonstration of this algorithm). If a query is not identifiable, it may still be possible to get bounds for causal effects, for example using instrumental variables [Angrist and Pischke, 2009] or by making additional assumptions.

There are two other key frameworks that arise in causal inference. Counterfactuals and structural equation models. Counterfactuals are statements about imagined or alternate realities, are prevalent in everyday language and may play a role in the development of causal reasoning in humans [Weisberg and Gopnik, 2013]. Causal effects are differences in counterfactual variables; what is the difference between what would happen if we did one thing versus what would happen if we did something else [Rubin, 1974, Rubin, 1978, Rosenbaum and Rubin, 1983, Rubin, 2005, Rubin, 2008].

For example, if we wanted to estimate the causal effect of a medical treatment, then we might let Y^1 be a counterfactual random variable representing the (binary) potential outcome if treated. The distribution of Y^1 is the distribution we would see in the outcome Y if everyone was treated. Similarly Y^0 represents the potential outcome for the placebo. The causal effect of the drug is the difference between the probability of recovery, across the population, if everyone was treated, and the probability of recovery given placebo $P(Y^1) - P(Y^0)$. This quantity can be estimated from observational data if we assume $X \perp\!\!\!\perp Y^0$ and $X \perp\!\!\!\perp Y^1$. These assumptions

are referred to as ignoreability assumptions [Rosenbaum and Rubin, 1983]. They state that the treatment each person receives is independent of whether they would recover if treated and if they would recover if not treated. Graphically, this is equivalent to the assumption that there is no variable that is a parent of both the treatment X and the outcome Y.

Structural equation models (SEMs) describe a deterministic world, where underlying mechanisms determine the output of any process for a given input. The mechanism (but not the output) is assumed to be independent of what is fed into it. Linear structural equation models have a long history for causal estimation [Wright, 1921, Haavelmo, 1943]. Mathematically, each variable is a deterministic function of its direct causes and a noise term that captures unmeasured variables. The noise terms are required to be mutually independent. If there is the possibility that an unmeasured variable influences more than one variable of interest in a study, it must be modelled explicitly as a latent (unobserved) variable. Structural equation models can be represented visually as a network. Each variable is a node and arrows are drawn from causes to their effects. If the network for a structural equation model is acyclic then it implies a recursive factorization of the joint distribution over its variables. In other words, it is a causal bayesian network.

Remarkably for models developed relatively independently in fields with very different approaches and problems, the models we have discussed are functionally very similar. To determine if and how an interventional query can be non-parametrically identified, it is equivalent to specify assumptions graphically in terms of bayesian networks or as structural equation models or as conditional independence statements involving counterfactual variables (ignorability assumptions).

It is possible to pose causal queries in terms of counterfactuals that are not interventional and cannot be phrased in terms of the do-notation. The scientific and philosophical validity of such counterfactual queries remains under question [Dawid, 2000, Dawid, 2014], however they are nonetheless widely posed in the form of attribution of causal effects to different pathways and mediation [Pearl, 2014, Imai et al., 2010, VanderWeele and Hernández-Diaz, 2011].

There are differences between the models we have considered when it comes to these non-interventional queries. Counterfactuals are not defined in causal bayesian networks, as they only encode information on the interventional distribution over variables. Counterfactuals can be defined in terms of structural equation models [Pearl, 2000] but there are subtle differences depending on the form of assumptions made. Structural equation models with independent errors allow the identification of quantities in mediation studies, which are not identifiable with the weak ignorability assumptions and cannot be tested experimentally [Richardson and Robins, 2013].

In practice, differences in focus and approach across different fields eclipse the actual differences in the models. The work on causal graphical models [Pearl, 2000, Spirtes et al., 2000] focuses on non-parametric estimation in the population limit and rigorous theoretical foundations. The Neyman-Rubin framework builds on our understanding of randomized experiment and generalizes to quasi-exeperimental and observational settings, with a particular focus on non-random assignment to treatment. This research emphasises estimating average causal effects and provides practical methods for estimation, in particular, propensity scores; a method to control for multiple variables in high dimensional settings with finite data [Rosenbaum and Rubin, 1983]. In economics, inferring causal effects from non-experimental data so as to support policy decisions is central to the field. Economists are often interested in broader measures of the distribution of causal effects than the mean and make extensive use of structural equation models, generally with strong parametric assumptions [Heckman, 2008]. In addition, the parametric structural equation models favoured in economics can be extended to analyse cyclic (otherwise referred to as non-recursive) models.

2.2 Discovering causal structure

In the previous section we discussed when assumptions about the structure of the variables in a specific problem is sufficient to identify a causal effect. This approach relies on having enough prior knowledge or theory about the problem to allow you to, at least partially, specify the causal network. In this section, we consider the much harder problem of causal inference where you need to learn the network. Causal inference might seem impossible without specific assumptions about the structure of the variables involved but, amazingly, some aspects of causal structure can be determined from much more general assumptions.

2.2.1 Discovery based on conditional independence

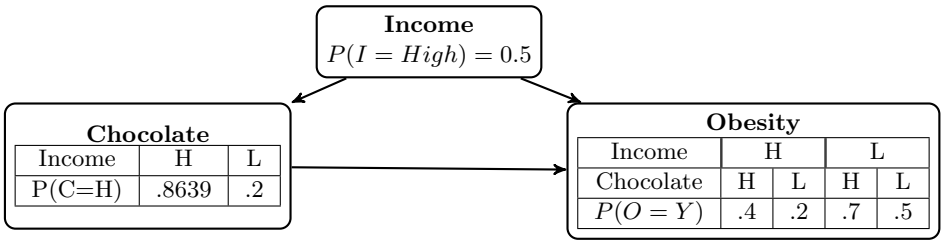
One general approach is to look for clues about the structure of the network in the conditional independence relations in the distribution. Assume there is some acyclic causal network G that generated the distribution $P(\boldsymbol{V})$ from which our data has been sampled. Our goal is to recover the network from this data.

Since G is a bayesian network, if Z d-separates X and Y in G then $(X \perp\!\!\!\perp Y|Z)$ in P . However, we want to work in the other direction, from conditional independence in the distribution to the structure of the network. This requires that we assume the reverse condition: $(X \perp\!\!\!\perp Y|Z)$ in P must imply Z d-separates X and Y in G. This assumption, commonly referred to as ***faithfulness***, says there are no additional independence relations that are satisfied in P but not in all distributions $\boldsymbol{P'}$ that are compatible with G. Stating that P is faithful to G is equivalent to G is a ***perfect map*** for P.

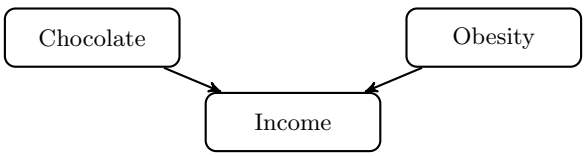
Faithfulness is an assumption. It does not always hold and we cannot verify it from the observational data we wish to use for causal inference. However, most distributions generated by a causal bayesian network will be faithful to that network. For faithfulness to be violated, different causal effects must exactly balance one-another out. For example, consider a simple binary variable model of chocolate consumption, income and obesity, figure 1. If the coefficients in the conditional probability tables are just right then the direct effect of chocolate on obesity will exactly balance the indirect effect through income and obesity will appear independent of chocolate consumption. However, this independence is not stable. It would disappear under a small perturbation to any of the parameters.

Figure 1: Example of a data generated from a causal graph violating the faithfulness assumption

(a) True causal graph generating P



(b) Perfect map for P, $(C \perp\!\!\!\perp O)$



Given the faithfulness assumption, our causal discovery problem reduces to finding the set of bayesian networks that have exactly the dependency structure as we observe in P. A wide range of algorithms have been developed based on this key observation, see table 1. Constraint based methods such as the PC algorithm [Spirtes et al., 2000], FCI algorithm [Spirtes et al., 2000] and RFCI algorithm [Colombo et al., 2012], perform sequential conditional independence tests and eliminate inconsistent graphs. Search and score based methods, such as GES [Chickering, 2002], search over the space of graphs and score them according to how well they fit the independences given a complexity penalising prior. Constraint based methods are faster, particularly for sparse graphs, but can lack robustness as errors in early conditional independence tests can propagate. Search and score based methods are more robust for small samples sizes but difficult to scale to larger graphs. This has led to the development of hybrid approaches, such as the MMHC algorithm [Tsamardinos et al., 2006]. A key component of causal discovery is the ability to do high dimensional non-parametric conditional independence tests. Developments in kernalized conditional independence tests,[Gretton et al., 2008, Zhang et al., 2012] have made this possible.

Table 1: A comparison of key causal discovery algorithms

Alg.	**Method**	**Scales (num.vars)**	**$\sim$ Vars**	**Latent**
PC	Constraint based	Worst case exponential, polynomial for sparse graphs	5000	No
FCI	Constraint based	Worst case exponential, polynomial variant FCI+ for sparse graphs	30	Yes
RFCI	Constraint based	?	500	Yes
GES	Search & Score	Worst case exponential	50	No
MMHC	Hybrid	?	5000	No

If the end goal of causal discovery is to estimate causal effects, then it may not be necessary to learn the entire graph, only the subset of the graph surrounding target variables of interest. Such local causal discovery techniques can be scaled to problems with many more variables [Aliferis and Tsamardinos, 2002]. Once a set of causal graphs has been identified, causal effects of interest can be bounded by combining the results for the all the networks. This procedure is the IDA algorithm [Maathuis et al., 2009] and has been found to outperform standard regularization techniques at finding causal effects in a high-dimensional yeast gene expression data set [Maathuis et al., 2010]. An implementation is available in the R package pcalg [Kalisch et al., 2012]

2.2.2 Discovery with functional models

All of the algorithms we have considered so far return a Markov equivalence class. They cannot distinguish between two models that result in the same set of conditional independence relations. Consider the very simple case where we have only two variables and the only possible causal structures are $X \to Y$ or $Y \to X$. These models have the same dependency structure but in one case $P(Y|do(X)) = P(Y|X)$ and in the other $P(Y|do(X)) = P(Y)$. No algorithm relying purely on conditional independence relations can separate these two cases.

One solution is to utilize structural equation models to specify additional assumptions. For

example, if we assume that noise is additive, such that $X \to Y \implies Y = f(X)+\epsilon$, then this will only be invertible such that $X = g(Y)+\epsilon'$ for specific pairs of functions f and noise distributions ϵ. Thus in general we will be able to identify the causal direction [Hoyer et al., 2009]. This can be extended to post-non-linear additive noise, $Y = h(f(X) + \epsilon)$, [Zhang and Hyvärinen, 2008]. These techniques can also be applied over more than two variables [Peters et al., 2014].

A more general approach is to leverage the assumption that the functions are independent of inputs [Janzing et al., 2012]. This leads to the idea that $P(X)$ and $P(Y|X)$ are independent if $X \to Y$ but not if $Y \to X$. [Janzing and Peters, 2012] propose testing for this by applying both semi-supervised and standard techniques to estimate $P(Y|X)$. Semi-supervised methods, which utilize additional points from $P(X)$ to learn $P(Y|X)$ should only be able to outperform standard methods if $Y \to X$.

Finally, rather than explicitly developing an algorithm based on a specific asymmetry between cause and effect, [Lopez-Paz et al., 2014] propose learning what causality looks like from data. They take as input a dataset where each row of data is itself a dataset in which either $X \to Y$ or $Y \to X$ and a corresponding label. Estimates of the distributions $P(X)$, $P(Y)$ and $P(X, Y)$ for each row are then mapped to features in some kernel space via mean kernel embeddings and finally a standard classification algorithm can be trained to learn the labels. New datasets, where the direction of causality is unknown, are then simply mapped to the kernel space and the causal direction is classified according to the trained classifier. In practice, the classifier is trained mostly on simulated data as it is difficult to find a sufficient set of causal problems with only two variables, where the direction of causality is known.

3 Multi-armed Bandits

In its classic formulation [Robbins, 1952] the (stochastic) K-armed bandit describes a sequential decision making problem, with K possible actions or arms. Each arm i is associated with a fixed but unknown reward distribution ν_i [1]. For each timestep t upto a horizon T the learner selects an action $I_t \in \{1...K\}$ and receives a reward, $g_{I_t,t}$, sampled i.i.d from ν_i. The goal of the learner is to maximize the total reward they receive. This problem introduces the fundamental exploration-exploitation trade-off. The learner must balance playing arms that have yielded good results previously with exploring arms about which they are uncertain.

The performance of bandit algorithms is generally described by the (pseudo) regret, $R(T)$. This is the difference between the expected reward obtained by the algorithm and the expected reward of selecting the best action in every timestep.

$$R(T) = max_{\{i=1...K\}}\mathbb{E}\left[\sum_{t=1}^{T} g_{i,t}\right] - \mathbb{E}\left[\sum_{t=1}^{T} g_{I_t,t}\right] \tag{1}$$

If we let $\mu_i = \mathbb{E}[\nu_i]$ denote the expected reward for each arm i and $\mu^* = max_{\{i=1...K\}}(\mu_i)$ denote the reward for the best arm:

$$R(T) = T\mu^* - \sum_{t=1}^{T} E[\mu_{I_t}] \tag{2}$$

[1] In order to obtain regret bounds, some assumptions are required on the distributions ν_i. It sufficient to assume they are sub-gaussian

An algorithm is learning if it obtains regret that is sublinear in T. The lower bound on the worst case regret for any algorithm (stochastic or adversarial) for the K-armed bandit problem is $\Omega\left(\sqrt{TK}\right)$ [Auer et al., 1995].

A key algorithm for stochastic bandits, with tractable analysis and strong performance guarantees, is the UCB algorithm [Auer et al., 2002]. They key to this algorithm is that it keeps track of an upper confidence bound (hence UCB) on the expected reward for each arm and selects the arm with the highest one. This balances exploration and exploitation as an arm with a high upper confidence bound must have either a high expected reward or large uncertainty on the expected reward. Assume for notational simplicity that $\mu_1 > \mu_2 > ... > \mu_K$, such that $\mu^* = \mu_1$, and let $\Delta_i = \mu_i - \mu^*$ be the sub-optimality for each arm. The (problem dependent) regret for UCB is bounded by:

$$R^{ucb}(T) \in \mathcal{O}\left(\sum_{i=2}^{K} \frac{1}{\Delta_i} \log(T)\right) \tag{3}$$

This bound blows up as differences $\Delta_i \to 0$, however the regret itself does not - since although we may not be able to distinguish arms with very small Δ_i from the optimal arm, we also do not lose much by selecting them. In the worst case, $R^{ucb}(T) = \mathcal{O}\left(\sqrt{TK\log(T)}\right)$ [Bubeck, 2012]. Subtle modifications to the UCB algorithm can eliminate the logarithmic term in this worst case regret bound. This yields $R^{ucb}(T) = \mathcal{O}\left(\sqrt{TK}\right)$ and closes the gap with the worst case lower bound [Audibert and Bubeck, 2009, Lattimore, 2015], whilst retaining a good problem dependent bound of the form achieved by UCB [Lattimore, 2015].

Adversarial bandits are an alternate, widely studied, setting that relaxes the assumption that rewards are generated stochastically. Instead, simultaneously with the learner selecting an action I_t, a potentially malicious adversary selects the reward vector $\boldsymbol{g}_t$. As in the stochastic setting, the learner then receives reward $g_{I_t,t}$. The seminal algorithm for adversarial bandits is Exp-3, which, like UCB, obtains regret $\mathcal{O}\left(\sqrt{TK\log(T)}\right)$ regret [Auer et al., 1995]. Optimal algorithms, with $R(T) = \mathcal{O}\left(\sqrt{TK}\right)$, have also been demonstrated for the adversarial setting [Audibert and Bubeck, 2009].

Another problem that has attracted a lot of recent attention [Bubeck et al., 2009, Audibert and Bubeck, 2010, Gabillon et al., 2012, Karnin et al., 2013] within the multi-armed bandit framework is *pure exploration* or *best arm identification*. In this setting, the horizon T represents a fixed budget for exploration after which the algorithm outputs a single best arm i. The performance of the algorithm is measured by the simple regret; the expected difference between the mean reward of the (truly) optimal arm and the mean reward of the arm selected by the algorithm, $R_s(T) = \mu^* - \mathbb{E}\left[\mu_i\right]$. This problem arises naturally in applications where there is a testing or evaluation phase, during which regret is not incurred, followed by a commercialization or exploitation phase. For example, many strategies might be assessed via simulation prior to one being selected and deployed. The simple regret for a K-armed bandit is lower bounded by $\mathcal{O}\left(\sqrt{K/T}\right)$ [Bubeck et al., 2009].

The classic multi-armed bandit is a powerful tool for sequential decision making. However, the regret grows linearly with the number of (sub-optimal) actions and many real world problems have large or even infinite action spaces. This has led to the development of a wide range of models that assume some structure across the reward distributions for different arms, for example generalized linear bandits [Filippi et al., 2010], dependent bandits [Pandey et al., 2007],

X-armed bandits [Bubeck et al., 2010] and gaussian process bandits [**?**], or that consider more complex feedback, for example the recent work on graph feedback [Mannor and Shamir, 2011, Lelarge and Ens, 2012, Alon and Cesa-Bianchi, 2013, Buccapatnam et al., , Kocák et al., 2014, Alon et al., 2015] and partial monitoring [Piccolboni and Schindelhauer, 2001, Bartók et al., 2014].

Part II

Approach and expected outcomes

The goal of my research is to explore a number of questions around learning to make good decisions.

- Develop a framework to unify concepts causal inference concepts with reinforcement learning, starting with multi-armed bandits.(DONE - see section 4)
- Demonstrate combining concepts from causal inference with multi-armed bandit algorithms can improve on state of the art performance in sequential decision making (DONE - paper submitted for NIPS 2016)
- Causal privacy paper
- something about identifiability

4 Unifying the frameworks

A natural way to connect the causal framework with the bandit setting is to model the problem as a causal directed acyclic graph. Each possible assignment of variables to values is an action (bandit arm). See figure 2 for a simple example. The reward could be a general function of the action selected and the final state of the graph. However for simplicity, we will consider the reward to be the value of a single specified node minus the cost of the selected action. The number of actions or arms grows exponentially with the number of variables in the graph, making it important to use algorithms that take account of the graph structure to reduce the search space.

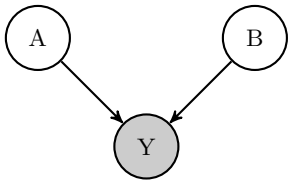
Modelling a problem as a causal graph only makes sense when rewards are generated stochastically - since causal graphs fundamentally model probability distributions over variables. Thus the connection is to stochastic bandit problems (although adversarial bandits algorithms may be applied to stochastic problems).

If we begin by considering the case where the causal graph is known, problems then take on characteristics of different bandit settings depending on the assumptions we make about what subset of actions can be taken, what variables are observable and whether they are observed before or after an action is selected.

If feedback is received only on the reward node then the do-calculus can be applied to eliminate some actions immediately, before any experiments are performed and then a standard bandit algorithm can be run on the remaining actions. See figure 3 as an example.

If we receive feedback on additional nodes, the problem can be more interesting. In addition to being able to eliminate some actions prior to sampling any data as in the previous case, taking one action may give us some information on actions that were not selected. Consider again the model in figure 2. The causal structure implies:

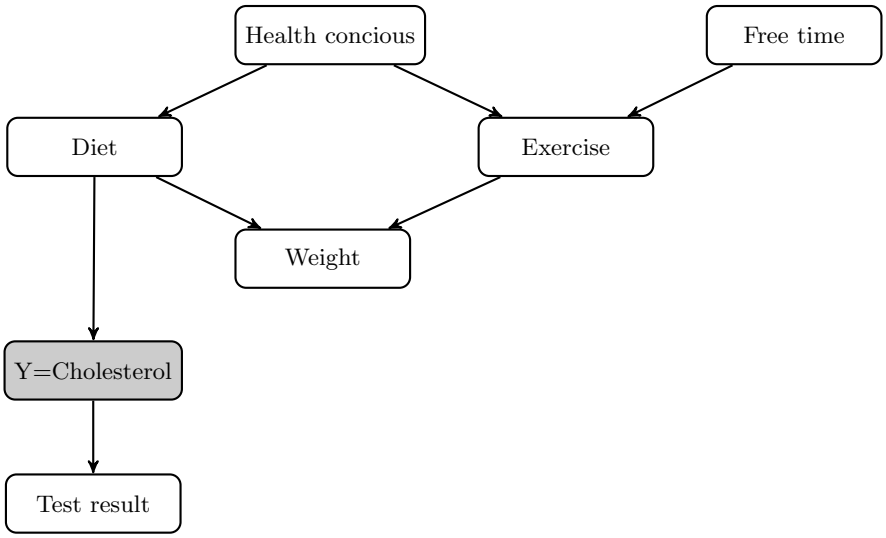
Figure 2: A simple causal graphical model and corresponding complete action space. A and B represent binary variables that can be intervened on and Y represents the reward.



Actions =

do(A=0,B=0)
do(A=0,B=1)
do(A=1,B=0)
do(A=1,B=1)
do(A=0)
do(A=1)
do(B=0)
do(B=1)
do()

Figure 3: Example causal graph (based on [Koller and Friedman, 2009]) where the outcome of interest (reward) is cholesterol level . The do-calculus can be applied to eliminate some actions immediately without the need to do any experiments. For example, no actions involving 'Test Result' need to be considered and interventions on 'Diet' do not need to be considered in conjunction with any other variables.



$$P(Y|do(A=0)) = P(Y|do(), A=0) \tag{4}$$
$$= P(Y|do(B=0), A=0)P(B=0) + P(Y|do(B=1), A=0)P(B=1) \tag{5}$$

Thus we gain information about the reward for the action $do(A=0)$ from selecting the action $do()$ or $do(B=b)$ and then observing $A=0$.

We only get this form of side information for actions that don't specify the value of every variable, ie those in the bottom half of the table in figure 2. Since the reward distribution for actions that set a subset of the variables is the result of marginalizing out other variables, they can only be optimal if they have lower cost. So if the cost of all actions is constant (no matter how many variables must be set), then the problem has the same characteristics as if only the reward node were observable.

If the information on the value of additional nodes is available prior to selecting an action the problem resembles a contextual bandit. For example if we observe $A=0$ then, in deciding between the actions $do(B=0)$ and $do(B=1)$, we would want information on $P(Y|A=0, B=$

0) and $P(Y|A = 0, B = 1)$. Note, side information can still arise if we learn the value of some variables prior to selecting an action and some afterwards.

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