Report for Comp Exam

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1 Problem Setup

Let $\mathcal{T}$ be the set of proposed interventions we wish to consider, X the set of participants, and Y the set of possible outcomes. For each proposed intervention $t \in \mathcal{T}$, let $Y(t) \in Y$ be the potential outcome for x when x is assigned to the intervention t. In randomized control trial (RCT) and observed study, only one outcome is observed for a given participant x; even if the participant is given an intervention and later the other, the participant is not in the same state.

In the binary intervention set, there are two possible interventions $\mathcal{T} = \{0, 1\}$, where intervention 1 is often referred as the "treated" and intervention 0 is the "control." Given a sample of subjects and a treatment, each subject has a pair of potential outcomes: $Y_i(0)$ and $Y_i(1)$, the outcomes under the control and the treatment, respectively. Let t be an indicator variable denoting the treatment received ($t = 0$ for the control and $t = 1$ for the treatment). Only one outcome, $Y_i(Y_i = t \cdot Y_i(1) + (1 - t) \cdot Y_i(0))$, is observed for the subject i.

The individual treatment effect (ITE) can be defined to be $Y_i(1) - Y_i(0)$. The average treatment effect (ATE) is defined to be $E[Y_i(1) - Y_i(0)]$. The ATE is the average treatment effect, at the population level, of moving an entire population from the control to the treatment. A related measure of treatment effect is the average treatment effect for the treated (ATT) [Imbens, 2004]. The ATT is defined as $E[Y(1) - Y(0) \mid t = 1]$. The ATT is the average effect of treatment on those subjects who ultimately received the treatment. In an RCT these tow measures of treatment effects coincide because, due to randomization, the treated population will not, on average, differ systematically from overall population.

1.1 Randomized Controlled Trials

In RCTs, treatment is assigned by randomization. As a consequence of randomization, an unbiased estimate of the ATE can be directly computed from the data. An unbiased estimate of the ATE is $E[Y_i(1) - Y_i(0)] = E[Y(1)] - E[Y(0)]$. This definition allows one to define the ATE in terms of a difference in means (continuous outcomes) or a difference in proportions (binary outcomes).

1.2 Observational Studies

An observational study has the same intent as a randomized experiment: to estimate a causal effect. However, an observational study differs from a RCT in one design issue: the use of randomization to allocate units to treatment and control groups.

In observational studies, the treated subjects often differ systematically from untreated subjects. In general, $E[Y(1) \mid t = 1] \neq E[Y(1)]$ holds. Thus, an unbiased estimate of the average treatment effect cannot be obtained by directly comparing outcomes between the two treatment groups.

1.3 Strong Ignorability

The treatment assignment is defined to be strongly ignorable [Rosenbaum and Rubin, 1983] if the following two conditions hold: 1). $(Y(1), Y(0)) \perp\!\!\!\perp t \mid X$ and 2). $0 < \Pr(t = 1 \mid X) < 1$. The first condition says that treatment assignment is independent of the potential outcomes conditional on the observed baseline covariates. The second condition says that every subject has a nonzero probability to receive either treatment. The aforementioned first condition is also referred to as the "no unmeasured confounders" assumption that all variables that affect treatment assignment and outcome have been measured.

2 Random Causal Forest

[Wager and Athey, 2015] proposed random causal forest (RCF) to infer treatment effect. From the conceptual point of view, trees and forests can be viewed as nearest neighbor methods with an adaptive neighborhood metric. Given observed independent samples (X_i, Y_i, W_i), a causal tree is first built by recursively splitting the feature space until all samples are partitioned into a set of leaves L, each of which contains a few training samples. Then, for a data point x, the predicted outcome $\hat{\mu}(x)$ is evaluated by identifying the leaf $L(x)$ containing x and calculating

$$\hat{\mu} = \frac{1}{|\{i : X_i \in L(x)\}|} \sum_{\{i:X_i \in L(x)\}} Y_i$$

Given a test point x, the closest points to x are those fall in the same leaf as it. The authors believe that the leaf is small enough that the responses Y_i are roughly identically distributed. Then the treatment effect $\hat{\tau}$ for any $x \in L(x)$ is estimated as following:

$$\begin{aligned}\hat{\tau}(x) = & \frac{1}{|\{i : W_i = 1, X_i \in L(x)\}|} \sum_{\{i:W_i=1, X_i \in L(x)\}} Y_i \\ & - \frac{1}{|\{i : W_i = 0, X_i \in L(x)\}|} \sum_{\{i:W_i=0, X_i \in L(x)\}} Y_i \end{aligned} \quad (1)$$

RCF assumes that there is overlapping in the data, i.e., for some $\epsilon > 0$ and all $x \in [0,1]^d$,

$$\epsilon < \mathbb{P}[W = 1 \mid X = x] < 1 - \epsilon$$

This condition effectively guarantees that, for large enough n, there will be enough treatment and control units near any test point x for local methods to work.

2.1 Honest Trees and Forests

A tree is honest if, for each training example i, it only uses the response Y_i to estimate the within-leaf treatment effect τ using Equation 1 or to decide where to place the splits, but not both. [Wager and Athey, 2015] proposed two causal forest algorithms that satisfy this condition.

The first algorithm, which is called double-sample tree, achieves honesty by dividing its training sub-sample into two halves $\mathcal{I}$ and $\mathcal{J}$. Then, it uses the $\mathcal{J}$-sample to place the splits, while holding out the $\mathcal{I}$-sample to do within-leaf estimation. The details of the algorithm is shown in Algorithm 2.

Algorithm 1: Double-sample Causal Trees

Input: n training examples of (X_i, Y_i, W_i), where X_i are features, Y_i is the response, and W_i is the treatment assignment.
A minimum leaf size k.

1 Draw a random subsample of size s from $\{1, \ldots, n\}$ without replacement, and then divide it into two disjoint sets of size $|\mathcal{I}| = \lfloor s/2 \rfloor$ and $|\mathcal{J}| = \lceil s/2 \rceil$

2 Grow a tree via recursive partitioning. The splits are chosen using any data from the $\mathcal{J}$ sample and X- or W-observations from the $\mathcal{I}$ sample, but without using Y-observations from $\mathcal{I}$-sample.

3 Estimate leaf-wise response using only the $\mathcal{I}$-sample observations.

The algorithm estimates $\hat{\tau}(x)$ using Equation 1 on the $\mathcal{I}$ sample. The splitting criteria is to maximize the variance of $\hat{\tau}(X_i)$ for $i \in \mathcal{J}$. Each leaf of the tree must contain k or more $\mathcal{I}$-sample observations of each treatment class.

Another way to build honest trees is to ignore the outcome Y_i when placing splits, and instead first train a classification tree for the treatment assignments W_i. Such propensity trees can be particularly useful in observational studies, where we want to minimize bias due to variation in $e(x)$. Seeking estimators that match training examples based on estimated propensity is a longstanding idea from Propensity Score Matching (PSM).

Algorithm 2: Propensity Trees

Input: n training examples of (X_i, Y_i, W_i), where X_i are features, Y_i is the response, and W_i is the treatment assignment.
A minimum leaf size k.

1 Draw a random subsample $\mathcal{I} \in 1, \ldots, n$ of size $|\mathcal{I}| = s$ (no replacement).
2 Train a classification tree using sample $\mathcal{I}$ where the outcome is the treatment assignment, i.e., on the (X_i, W_i) pairs with $i \in \mathcal{I}$. Each leaf of the tree must have k or more observations of each treatment class.
3 Estimate $\tau(x)$ using Equation 1 on the leaf containing x.

3 Counterfactual Inference

[Johansson et al., 2016] proposed Balancing Neural Networks (BNN) which can be applied to solve the counterfactual inference problem. They used a form of regularizer to enforce the similarity between the distributions of representations learned for populations with different interventions, for example, the representations for students who received text hints versus those who received video hints.This reduces the variance from fitting a model on one distribution and applying it to another. Because of random assignment to the interventions in RCTs, the distributions of the populations within different interventions are highly likely to be identical. However, in the observational study, we may end up with the situation where only male students receive video hints and female students receive text hints. Without enforcing the similarity between the distributions of representations for male and female students, it is not safe to make a prediction of the outcome if male students receive text hints. In machine learning, ”domain adaptation” refers to the dissimilarity of the distributions between the training data and the test data.

In the ”treated” and the ”control” setting, we refer to the observed and unobserved outcomes as the factual outcome $y^F(x)$, and the counterfactual outcome $y^{CF}(x)$ respectively. In other words, when the participant x is assigned to the ”control” $(t = 0)$, $y^F(x)$ is equal to $Y_1(x)$, and $y^{CF}(x)$ is equal to $Y_0(x)$. The other way around, $y^F(x)$ is equal to $Y_0(x)$, and $y^{CF}(x)$ is equal to $Y_1(x)$.

Given n samples $\left\{(x_i, t_i, y_i^F)\right\}_{i=1}^n$, where $y_i^F = t_i \cdot Y_1(x_i) + (1 - t_i)Y_0(x_i)$, a common approach for estimating the ITE is to learn a function $f : X \times T \to Y$ such that $f(x_i, t_i) \approx y_i^F$. The estimated ITE is then:

$$I\hat{T}E(x_i) = \begin{cases} y_i^F - f(x_i, 1 - t_i), & t_i = 1. \\ f(x_i, 1 - t_i) - y_i^F, & t_i = 0. \end{cases}$$

We assume n samples $\left\{(x_i, t_i, y_i^F)\right\}_{i=1}^n$ form an empirical distribution $\hat{p}^F = \{(x_i, t_i)\}_{i=1}^n$. We call this empirical distribution $\hat{p}^F \sim p^F$ the empirical factual distribution. In order to calculate ITE, we need to infer the counterfactual outcome which is dependent on the empirical distribution $\hat{p}^{CF} = \{(x_i, 1 - t_i)\}_{i=1}^n$. We call the empirical distribution $\hat{p}^{CF} \sim p^{CF}$. The p^F and p^{CF} may not be equal because the distributions of the control and the treated populations may be different. The inequality of two distributions may cause the counterfactual inference over a different distribution than the one observed from the experiment. In machine learning terms, this scenario is usually referred to as domain adaptation, where the distribution of features in test data are different than the distribution of features in training data.

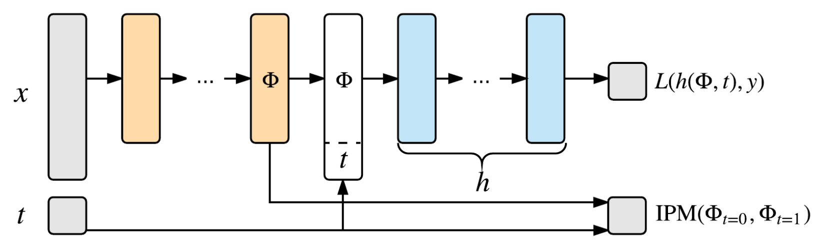

Figure 1: CFR for ITE estimation. L is a loss function, IPM is an integral probability metric

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To learn a representation of deep features Φ, the RCN uses fully connected layers with ReLu activation function, where $Relu(z) = max(0, z)$. We need to generalize from factual distribution to counterfactual distribution in the feature representation Φ to obtain accurate estimation of counterfactual outcome. The common successful approaches for domain adaptation encourage similarity between the latent feature representations w.r.t the different distributions. This similarity is often enforced by minimizing a certain distance between the domain-specific hidden features. The distance between two distributions is usually referred to as the discrepancy distance, introduced by [**?**], which is a hypothesis class dependent distance measure tailored for domain adaptation.

In this paper we use an Integral Probability Metric (IPM) measure of distance between two distributions $p_0 = p(x|t = 0)$, and $p_1 = p(x|t = 1)$, also known as the control and treated distributions. The IPM for p_0 and p_1 is defined as

$$\text{IPM}_{\mathcal{F}}(p_0, p_1) := \sup_{f \in \mathcal{F}} \left| \int_S f dp_0 - \int_S f dp_1 \right|,$$

where $\mathcal{F}$ is a class of real-valued bounded measurable functions on S.

The choice of functions is the crucial distinction between IPMs [**?**]. Two specific IPMs are used in our experiments: the Maximum Mean Discrepancy (MMD), and the Wasserstein distance. $\text{IPM}_{\mathcal{F}}$ is called MMD, when $\mathcal{F} = \{f : \|f\|_{\mathcal{H}} \leq 1\}$, where $\mathcal{H}$ represents a reproducing kernel Hilbert space (RKHS) with k as its reproducing kernel. In other words, the family of norm-1 reproducing kernel Hilbert space (RKHS) functions lead to the MMD. The family of 1-Lipschitz functions $\mathcal{F} = \{f : \|f\|_L \leq 1\}$, where $\|f\|_L$ is the Lipschitz seminorm of a bounded continuous real-valued function f, make IPM the Wasserstein distance. Both the Wasserstein and MMD metrics have consistent estimators which can be efficiently computed in the finite sample case [**?**]. The important property of IPM is that

$$p_0 = p_1 \text{ iff } \mathrm{IPM}_{\mathcal{F}}(p_0, p_1) = 0.$$

The representation with reduction of the discrepancy between the control and the treated populations helps the model to focus on balancing features across two populations when inferring the counterfactual outcomes. For instance, if in an experiment, almost no male student ever received intervention A, inferring how male students would react to intervention A is highly prone to error and a more conservative use of the gender feature might be warranted.

4 Individualized Treatment Rules

In experiments, we observe a triplet $(\mathbf{x}, t, y)$ from each participant, where $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T \in \mathcal{X}$ denotes the participant's covariates, $t \in \mathcal{T} = -1, 1$ denotes the treatment assignment, and $y \in Y$ is the observed outcome, also called the "reward" in the literature on reinforcement learning. Note that $t = -1$ means the control in the context of ITR. Let $p(t|x)$ be the probability of assigning the participant with covariates $\mathbf{x}$ to the intervention t.

An individual treatment rule (ITR) $d : X \to \mathcal{T}$ is a deterministic decision rule from subject x into the intervention space $\mathcal{T}$. The value of d satisfies

$$V(d) = E\left[\frac{y}{p(t|x)} \mathbb{I}_{t=d(\mathbf{x})}\right],$$

where $\mathbb{I}(\cdot)$ is an indicator function. An optimal ITR, d^*, is a rule that has the maximal value such that,

$$d^* \in \arg\max_d V(d).$$

Finding d^* is equivalent to minimizing the following equation:

$$d^* \in \arg\min_d E\left[\frac{y}{p(t|x)} \mathbb{I}_{t \neq d(\mathbf{x})}\right] \tag{2}$$

Assume that the observed data $\{(\mathbf{x}_i, t_i, y_i),\ i = 1, \ldots, n\}$ are collected independently. For any decision function $f(\mathbf{x})$, let $d_f(\mathbf{x}) = sign(f(\mathbf{x}))$ be the associated rule, where $sign(u) = 1$ for $u > 0$ and -1 otherwise. The particular choice of the value of $sign(0)$ is not important. With the observed data, the weighted classification error in Equation 2 can be approximated by the empirical risk

$$\frac{1}{n} \sum_{i=1}^{n} \frac{y_i}{p(t_i|x_i)} \mathbb{I}_{t_i \neq d_f(\mathbf{x_i})}. \tag{3}$$

[Qian and Murphy, 2011] proposed a two-step procedure that first estimates a conditional mean for the outcome and then determines the treatment rule by comparing the conditional means across various treatment.

In contrast, outcome weighted learning (OWL) is proposed by [Zhao et al., 2012] using the hinge loss function and the regularization technique. In other words, instead of minimizing Equation 3, OWL aims to minimize

$$\frac{1}{n}\sum_{i=1}^{n}\frac{y_i}{p(t_i|x_i)}(1-t_i f(\mathbf{x}_i))_+ + \lambda\left\|f\right\|^2 \ , \tag{4}$$

where $(u)_+ = \max(u,0)$ is the positive part of u, $\|f\|$ is some norm for f, and λ is a tuning parameter controlling the trade-off between empirical risk and complexity of the decision function f.

[Zhou et al.,] pointed out that decision rule in Equation 8 is affected by a simple shift of the outcome Y and proposed Residual weighted learning (RWL) to relieve this issue. The idea behind RWL is to introduce a function g to reduce the variance of $\frac{y-g(\mathbf{x})}{p(t|\mathbf{x})}\mathbb{I}_{t\neq d(\mathbf{x})}$ and a reasonable candidate of g is

$$g^*(\mathbf{x}) = \frac{\mathbb{E}(y|\mathbf{x},t=1)+\mathbb{E}(y|\mathbf{x},t=-1)}{2} = \mathbb{E}\left(\frac{y}{2p(t,\mathbf{x})}|\mathbf{x}\right). \tag{5}$$

RWL thus is to minimize the following empirical risk:

$$\frac{1}{n}\sum_{i=1}^{n}\frac{y_i-\hat{g}^*(\mathbf{x}_i)}{p(t_i|\mathbf{x_i})}\mathbb{I}_{t_i\neq d_f(\mathbf{x_i})} \tag{6}$$

where $\hat{g}^*$ is an estimate of g^*. For simplicity, let $\hat{r}_i = y_i - \hat{g}^*(\mathbf{x}_i)$. As in OWL, [Zhou et al.,] consider a surrogate loss function T to replace the 0-1 loss in Equation 6. The non-convex loss T has the following form:

$$T(u) = \begin{cases} 0 & \text{if } u \geq 1, \\ (1-u)^2 & \text{if } 0 \leq u < 1, \\ 2-(1+u)^2 & \text{if } -1 \leq u < 0, \\ 2 & \text{if } u < -1 \end{cases} \tag{7}$$

It is called the smoothed ramp loss in [Zhou et al.,]. By incorporating the regularization, RWL is eventually aimed to minimize the following empirical risk:

$$\frac{1}{n}\sum_{i=1}^{n}\frac{\hat{r}_i}{p(t_i|x_i)}T(t_i f(\mathbf{x}_i))_+ + \lambda\left\|f\right\|^2 \ , \tag{8}$$

where $\|f\|$ is the norm for f, and λ is a tuning parameter.

5 Bayesian Optimization

Bayesian optimization is a sequential model-based approach for global optimization of an unknown objective function f. The problem can be mathematically expressed as:

$$\mathbf{x}^* = \arg\max_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x}) \tag{9}$$

where $\mathcal{X}$ is the design space of interest. Since the objective function is unknown, the Bayesian strategy is to treat it as a random function and place a prior over it. The prior captures our beliefs about the behaviour of the function. After gathering the function evaluations, which are treated as data, the prior is updated to form the posterior distribution over the objective function. Equipped with the posterior distribution, an acquisition function $\alpha : \mathcal{X} \to \mathbb{R}$ is induced to determines what the next query point should be. The acquisition function leverages the uncertainty in the posterior to trade off between the exploration and the exploitation. Examples of acquisition functions includes probability of improvement, expected improvement, Bayesian expected losses, upper confidence bounds (UCB), Thompson sampling and mixtures of these. They all trade-off exploration and exploitation so as to minimize the number of function queries. As such, Bayesian optimization is well suited for functions that are very expensive to evaluate.

In this setting, Bayesian optimization is considered as a sequential search algorithm which, at round n, selects a query point $\mathbf{x}_{n+1}$ at which to evaluate f and observe y_{n+1}. After N queries, the algorithm produces the best estimate $\bar{\mathbf{x}}_N$. Under the context of multi-armed bandit problems, function f is the reward function.

In summary, Bayesian optimization is the combination of two main components: a surrogate probabilistic model which captures our beliefs about the behavior of the unknown objective function and observed information, and an acquisition function which performs the selection of the optimal sequence of queries based on the previous model.

The Gaussian process (GP) is the most popular model due to its accuracy, robustness and flexibility, because Bayesian optimization is mainly usesd in blck-box scenarios. The range of applicaility of a Gaussian process is defined by its kernel function, which sets the family of functions that is able to represent through the reproducing kernel Hilbert space (RKHS). In BO, attributes of the GP such as mean and variance are used to sample successive points. It is suitable for situations where cost function is costly to evaluate and MCMC techniques would not work.

In many applications, the designs available to the experimenter have components that can be varied independently. For example, in designing an advertisement, one has choices such arkwork, font style, and size. If there are five choices for each, the total number of possible configurations is 125.

In general, this number grows combinatorially in the number of components. This presents challenges for approaches such as the independent Thompson sampling, since the Thompson sampling models the arms as independent, which will lead to strategies that must try every option at least once. This rapidly becomes infeasible in the large spaces of real-world problems.

Algorithm 3: Bayesian optimization with Gaussian process

Input: n observations $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ from objective function f

for $t = n+1, n+2, \ldots$ **do**

select new $\mathbf{x}_t$ by maximizing acquisition function α

$$\mathbf{x}_t = \arg\max_{\mathbf{x}} \alpha(\mathbf{x}; \mathcal{D})$$

query objective function to observe $y_t = f(\mathbf{x}_t)$

augment data $\mathcal{D} = \{\mathcal{D}, (\mathbf{x}_t, y_t)\}$

update statistical model

end

5.1 Thompson Sampling

Thompson sampling for Beta-Bernoulli bandit perhaps is the simplest non-trivial multi-armed bandit strategy in Bayesian optimization. Bernoulli bandit problem is the bandit problem when the rewards are either 0 or 1, and for arm i the probability of success (reward=1) is μ_i. The Thompson sampling maintains Bayesian priors on the Bernoulli means μ_i's. Beta distribution turns out to be a very convenient choice of priors for Bernoulli rewards. The pdf of Beta(α, β) with parameters $\alpha > 0, \beta > 0$ is given by

$$f(x; \alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1}. \tag{10}$$

The mean of Beta(α, β) is $\alpha/(\alpha+\beta)$; and higher the α, β, tighter is the concentration of Beta(α, β) around the mean. If the prior for each arm is a Beta(α, β) distribution, then after observing a Bernoulli trial, the posterior distribution is simply Beta$(\alpha+1, \beta)$ or Beta$(\alpha, \beta+1)$, depending on whether the trial resulted in a success or failure, respectively. Thompson sampling then samples from these posterior distributions across all arms and chooses the arm with largest sample value. This procedure is summarized in Algorithm 4.

5.2 Sequential method

The sequential approach is independent of the choice of prior and of the likelihood function and depends only on the assumption of i.i.d data. Sequential methods make use of observations one at a time, or in small batches, and then discard them before the next observations are used. They can be used, for example, in real-time learning scenarios where a steady stream of data is arriving, and predictions must be made before all of the data is seen. Because they do not require the whole data set to be stored or loaded into memory, sequential methods are also useful for large data sets.

Algorithm 4: Thompson sampling for Beta-Bernoulli bandit

Input: α, β: hyperparameters of the beta prior
Initialize $n_{a,0} = n_{a,1} = i = 0$ for all K arms a
repeat
  for $a = 1, \ldots, K$ **do**
    $w_a \sim \text{Beta}(\alpha + n_{a,1}, \beta + n_{a,0})$
  end
  $a_i = \arg\max_a w_a$
  Observe y_i by pulling arm a_i
  if $y_i = 0$ **then**
    $n_{a_i,0} = n_{a_i,0} + 1$
  else
    $n_{a_i,1} = n_{a_i,1} + 1$
  end
  $i = i + 1$
until *stopping criterion reached*;

6 Propensity Score Matching

A propensity score [Rosenbaum and Rubin, 1983] is the probability of a unit (e.g., student, classroom, school) being assigned to a particular treatment given a set of observed covariates. Propensity scores are used to reduce selection bias by equating groups based on these covariates.

Suppose that we have a binary treatment $T = \{0, 1\}$, an outcome Y, and background variables X. The propensity score is defined as the conditional probability of treatment given background variables:

$$p(x) := \Pr(T = 1 \mid X = x)$$

Let $Y(0)$ and $Y(1)$ denote the potential outcomes under the control and the treatment, respectively.

The actual propensity score in observational experiments is unknown and it can be estimated using statistical or machine learning models from the experiment data. The most commonly used model is a logistic regression model, in which treatment assignment T is regressed on background variables X.

Propensity score matching (PSM) entails forming matched sets of treated and untreated subjects who share a similar value of the propensity score. PSM allows one to estimate the average treatment effect for the treated (ATT). The ATT is the average effect of treatment on those subjects who ultimately receive the treatment. The most common implementation of PSM is one-to-one or pair matching, in which pairs of treated and untreated subjects are formed, such that matched subjects have similar values of the propensity score. Once a matched sample has been formed, the treatment effect can be estimated by directly comparing outcomes between treated and untreated subjects in the matched sample. If the outcome is continuous, the effect of treatment can be estimated as the difference between the mean outcome for treated subjects and the mean outcome for untreated subjects in the matched sample. If the outcome is binary, the effect of treatment can be estimated as the difference between the proportion of subjects experiencing the event in each of the two groups (treated vs. untreated) in the matched sample.

The possibility of bias arises because the apparent difference in outcome between these two groups of units may depend on characteristics that affected whether or not a unit received a given treatment instead of due to the effect of the treatment per se. In randomized experiments, the randomization enables unbiased estimation of treatment effects; for each covariate, randomization implies that treatment-groups will be balanced on average, by the law of large numbers. Unfortunately, for observational studies, the assignment of treatments to research subjects is typically not random. Matching attempts to mimic randomization by creating a sample of units that received the treatment that is comparable on all observed covariates to a sample of units that did not receive the treatment.

The analysis of a propensity score matched sample can mimic that of an RCT: one can directly compare outcomes between the treated and control subjects within the propensity score matched sample.

7 Gaussian Processes in Bandit Settings

Bayesian algorithms do not attempt to identify 'best-fit' models of the data (or similarly, make 'best guess' predictions for new test inputs). Instead, they compute a posterior distribution over models (or similarly, compute posterior predictive distributions for new test input). These distributions provide a useful way to quantify our uncertainty in model estimates, and to exploit our knowledge of this uncertainty in order to make more robust predictions on new test points.

The Gaussian process is the extension of multivariate Gaussian to infinite-sized collections of real-valued variables. In particular, this extension will allow us to think of Gaussian processes as distributions not just over random vectors but in fact distributions over random functions.

The Gaussian process $\mathrm{GP}(\mu_0, k)$ is a non-parametric model that is fully characterized by its prior mean function $\mu_0 : \mathcal{X} \to \mathbb{R}$ and its positive-definite kernel, or covariance function, $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.

Let $\mathcal{D}_n = \{(\mathbf{x}_i, y_i)\}$ denote a set of n observations and $\mathbf{x}$ denote the arbitrary test point. The random variable $f(\mathbf{x})$ is also a GP distribution conditioned on observations $\mathcal{D}_n$ with following mean $\mu_n(\mathbf{x})$ and variance $\sigma_n^2(\mathbf{x})$:

$$\mu_n(\mathbf{x}) = \mu_0(\mathbf{x}) + \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}(\mathbf{y} - \mathbf{m}) \tag{11}$$

$$\sigma_n^2(\mathbf{x}) = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{k}(\mathbf{x}) \tag{12}$$

where $m_i := \mu_0(\mathbf{x}_i)$, $K_{i,j} := k(\mathbf{x_i}, \mathbf{x_j})$, and $\mathbf{k}(\mathbf{x})$ is a vector of covariance terms between $\mathbf{x}$ and $\mathbf{x}_{1:n}$.

The posterior mean and variance evaluated at any point $\mathbf{x}$ represent the model's prediction and uncertainty in the objective function at the point $\mathbf{x}$. In order to apply GP under the setting of multi-armed bandit, we need a acquisition function to select the next query point given the posterior model. The acquisition function should be carefully design to trade off exploration of the search area and exploitation of current promising areas.

7.1 GP-UCB

To decrease uncertainty globally, one strategy could be to pick the point which maximums the variance $\mathbf{x}_{n+1} = \underset{\mathbf{x}\in D}{\arg\max}\ \sigma_n(\mathbf{x})$. However, this strategy is not well suited for multi-armed bandit problem since it can be wasteful. Another idea is to select the point which maximizes the expected reward given the posterior model $\mathbf{x}_{n+1} = \underset{\mathbf{x}\in D}{\arg\max}\ \mu_n(\mathbf{x})$. However, this idea is too greedy and tends to end up with a local optima. To balance exploration and exploitation, a combined strategy is to choose

$$\mathbf{x}_{n+1} = \underset{\mathbf{x}\in D}{\arg\max}\, \mu_n(\mathbf{x}) + \beta_n \sigma_n(\mathbf{x}), \tag{13}$$

where β_n are constants. There are theoretically motivated guidelines for setting and scheduling the hyperparameter β_n to achieve optimal regret.

Since Equation 7.1 is an upper confidence bound of the marginal posterior $P(f(\mathbf{x})|\mathbf{y}_n)$, a natural interpretation of this strategy is that it selects the point $\mathbf{x}$ such that $f(\mathbf{x})$ is a reasonable upper bound on $f(\mathbf{x})$. This algorithm is called Gaussian process upper confidence bound (GP-UCB), introduced by [Srinivas et al., 2010]. The GP-UCB selection rule is motivated by the UCB algorithm for the classical multi-armed bandit problem.

7.2 Contextual GP-UCB

Motivated by GP-UCB algorithm mentioned above, [Krause and Ong, 2011] extended the generalization of this algorithm by incorporating contextual information

$$\mathbf{x}_{n+1} = \underset{\mathbf{x}\in D}{\arg\max}\, \mu_n(\mathbf{x}, \mathbf{z}_n) + \beta_n \sigma_n(\mathbf{x}, \mathbf{z}_n), \tag{14}$$

where $z_n \in Z$ is the contextual information from a set Z of contexts, $\mu_n(\cdot)$ and $\sigma_n^2(\cdot)$ are the posterior mean and variance of the GP conditioned on observations $\mathcal{D}_n = \{(\mathbf{x}_i, \mathbf{z}_i, y_i)\}$. The authors called the selection rule the contextual Gaussian process UCB algorithm (GCP-UCB).

To derive the kernel k on the product space $Z \times X$ of contexts and actions, a natural approach to start with kernel functions $k_Z : Z \times Z \to \mathbb{R}$ and $k_X : X \times X \to \mathbb{R}$ on the space of contexts and actions. [Krause and Ong, 2011] proposed two possibilities of constructing composite kernel k from context kernel k_Z and action kernel k_X. One is to calculate a product kernel $k = k_Z \otimes k_X$, by setting

$$(k_Z \otimes k_X)((\mathbf{z}, \mathbf{x}), (\mathbf{z}', \mathbf{x}')) = k_Z(\mathbf{z}, \mathbf{z}')k_X(\mathbf{x}, \mathbf{x}'). \tag{15}$$

An alternative is to calculate the additive kernel $k = k_Z \oplus k_X$, by setting

$$(k_Z \oplus k_X)((\mathbf{z}, \mathbf{x}), (\mathbf{z}', \mathbf{x}')) = k_Z(\mathbf{z}, \mathbf{z}') + k_X(\mathbf{x}, \mathbf{x}'). \tag{16}$$

7.3 Probability distributions over functions with finite domains

Let $\mathcal{X} = \{x_1, x_2, \ldots, x_m\}$ be any finite set of elements. Consider the set $\mathcal{H}$ of all possible functions mapping from $\mathcal{X}$ to $\mathbf{R}$. For instance, one example of a function $f_0(\cdot) \in \mathcal{H}$ is given by

$$f_0(x_1) = 5,\ f_0(x_2) = 2.3, \cdots,\ f_0(x_{m-1}) = -\pi,\ f_0(x_m) = 8.$$

Since the domain of any $f(\cdot) \in \mathcal{H}$ has only m elements, we can always represent $f(\cdot)$ compactly as an m-dimensional vector, $\vec{f} = [f(x_1)\ \ f(x_2)\ \ \ldots\ \ f(x_m)]^T$. In order to specify a probability distribution over functions $f(\cdot) \in \mathcal{H}$, we must associate some "probability density" with each function in $\mathcal{H}$. One natural way to do this is to exploit the one-to-one correspondence between $f(\cdot) \in \mathcal{H}$ and their vector representation, $\vec{f}$. In particular, if we specify that $\vec{f} \sim \mathcal{N}(\vec{\mu}, \sigma^2 I)$, then this in turn implies a probability distribution over functions $f(\cdot)$, whose probability density function is given by

$$p(h) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{1}{2\sigma^2}(f(x_i) - \mu_i)^2)$$

In the example above, we show that probability distributions over functions with finite domains can be represented using a finite-dimensional multivariate Gaussian distribution over function outputs $f(x_1), \ldots, f(x_m)$ at a finite number of input points $x1, \ldots, x_m$

7.4 Probability distributions over functions with infinite domains

A stochastic process is a collection of random variables, $\{f(x) : x \in \mathcal{X}\}$, indexed by elements from some set $\mathcal{X}$, known as the index set. A Gaussian process is a stochastic process such that any finite sub-collection of random variables has a multivariate Gaussian distribution.

In particular, a collection of random variables $\{f(x) : x \in \mathcal{X}\}$ is said to be drawn from a Gaussian process with mean function $m(\cdot)$ and covariance function $k(\cdot, \cdot)$ if for any finite set of elements $x_1, \ldots, x_m \in \mathcal{X}$, the associated finite set of random variables $f(x_1), \ldots, f(x_m)$ have distribution,

$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_m) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_m) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_m) \\ \vdots & \ddots & \vdots \\ k(x_m, x_1) & \cdots & k(x_m, x_m) \end{bmatrix}\right).$$

We denote this using the notation,

$$f(\cdot) \sim \mathcal{GP}(m(\cdot), k(\cdot, \cdot)).$$

In general, any real-valued function $m(\cdot)$ is acceptable, but for $k(\cdot, \cdot)$, it must be the case that for any set of elements $x_1, \ldots, x_m \in \mathcal{X}$, the resulting matrix

$$K = \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_m) \\ \vdots & \ddots & \vdots \\ k(x_m, x_1) & \cdots & k(x_m, x_m) \end{bmatrix}$$

is a valid covariance matrix corresponding to some multivariate Gaussian distribution. A standard result in probability theory states that this is true provided that K is positive semi-definite.

8 Reproducing kernel Hilbert space

In functional analysis, a reproducing kernel Hilbert space (RKHS) is a Hilbert space of functions in which point evaluation is a continuous linear functional. The representer theorem states that every function in an RKHS that minimizes an empirical risk function can be written as a linear combination of the kernel function evaluated at the training points.

9 Information Theory

The entropy of the random variable X, where $p(X = x_i) = p_i$, is defined as:

$$\mathrm{H}[p] = -\sum_i p(x_i) \log p(x_i) \tag{17}$$

Distributions $p(x_i)$ that are sharply peaked around a few values will have a relatively low entropy, whereas those that spread more evenly across many values will have higher entropy. Because $0 \le p_i \ge 1$, the entropy is non-negative, and it will equal its minimum value of 0 when one of the $p_i = 1$ and all other $p_{j \neq i} = 0$. The maximum entropy configuration can be found by maximizing H using a Lagrange multiplier to enforce the constraint on the probabilities.

Now consider the joint distribution between two sets of variables $\mathbf{x}$ and $\mathbf{y}$ given by $p(\mathbf{x}, \mathbf{y})$. If the sets of variables are independent, then their join distribution will factorize into the product of their marginals $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x})p(\mathbf{y})$. If the variables are not independent, we can gain some idea of whether they are 'close' to being independent by considering the Kullback-Leibler divergence between the joint distribution and the product of the marginals, given by

$$\begin{aligned} \mathrm{I}[\mathrm{x}, \mathrm{y}] &= \mathrm{KL}(p(\mathrm{x}, \mathrm{y}) \parallel p(\mathrm{x})p(\mathrm{y})) \\ &= -\iint p(\mathrm{x}, \mathrm{y}) \log \left(\frac{p(\mathrm{x})p(\mathrm{y})}{p(\mathrm{x}, \mathrm{y})} \right) \mathrm{d}x \, \mathrm{d}y \end{aligned} \tag{18}$$

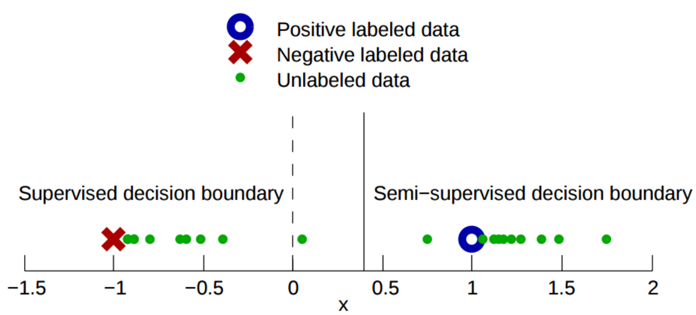
which is called the *mutual information* between the variable x and y. Using the sum and product rules of probability, we see that the mutual information is related to the conditional entropy through

$$\mathrm{I}[\mathrm{x}, \mathrm{y}] = \mathrm{H}[\mathrm{x}] - \mathrm{H}[\mathrm{x}|\mathrm{y}] = \mathrm{H}[\mathrm{y}] - \mathrm{H}[\mathrm{y}|\mathrm{x}] \tag{19}$$

From a Bayesian perspective, we can view $p(x)$ as the prior distribution for x and $p(\mathrm{x}|\mathrm{y})$ as the posterior distribution after we have observed new data y. The mutual information therefore represents the reduction in uncertainty about x as a consequence of the new observation y.

10 Semi-Supervised Learning

In the context of semi-supervised learning, the training data consists of l labeled instances $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$ and u unlabeled instances $\{(\mathbf{x}_j)\}_{j=l+1}^{l+u}$, often with $u \ll l$. The goal of semi-supervised learning is to learn a model with better performance from the training data than from labeled data alone. It is known that the labeled data can be hard and expensive to obtain since labels may require human experts, and the unlabeled data is often cheap in large quantity.



Co-training [Blum and Mitchell, 1998] is a semi-supervised learning technique that requires two views of the data. It assumes that each example is described using two different feature sets that provide different, complementary information about the instance. Co-training first learns a separate classifier for each view using any labeled examples. The most confident predictions of each classifier on the unlabeled data are then used to iteratively construct additional labeled training data. The details of co-training algorithm is described in Algorithm 5.

There are three important assumptions which guarantee the performance of co-training algorithm: 1). feature split $x = [x^{(1)}; x^{(2)}]$ exists; 2). $x^{(1)}$ or $x^{(2)}$ alone is sufficient to train a good classifier; 3). $x^{(1)}$ and $x^{(2)}$ are conditionally independent given the class.

Algorithm 5: Co-training Algorithm for Semi-Supervised Learning

Input: labeled data $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$, unlabeled data $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$
each instance has two views $\mathbf{x}_i = \left[\mathbf{x}_i^{(1)}, \mathbf{x}_i^{(2)}\right]$
and a learning speed k
Let $L_1 = L_2 = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_l, y_l)\}$.
repeat
    Train view-1 $f^{(1)}$ from L_1, view-2 $f^{(2)}$ from L_2
    Classify unlabeled data with $f^{(1)}$ and $f^{(2)}$ separately.
    Add $f^{(1)}$'s top k most-confident predictions $(\mathbf{x}, f^{(1)}(\mathbf{x}))$ to L_2
    Add $f^{(2)}$'s top k most-confident predictions $(\mathbf{x}, f^{(2)}(\mathbf{x}))$ to L_1
    Remove these from the unlabeled data.
until *unlabeled data is used up*;

11 Reliable Crowdsourcing

In order to characterize the learning artifacts for certain features, e.g., media format, pedagogical approach, difficulty to understand, etc, we could crowdsource from students by ask them to rate the learning artifacts along these features. During this process, we might gather noisy rating from students due to the fact that students may have a wide ranging level of rating expertise which are unknown, and in some cases may be adversarial. To learn the ground truth of these learning artifacts, we need to aggregate their opinions to recover the true, unknown label of each learning artifacts.

11.1 Dawid-Skene Model

[Dawid and Skene, 1979] were among the first to consider such a problem setup. They assume each workers are conditionally independent given the true labels and each worker is associated with a probabilistic confusion matrix that generates her labels. Each entry of the matrix indicates the probability that items in one class are labeled as another. Given the observed responses, the true labels for each items and the confusion matrices for each worker can be jointly estimated by a maximum likelihood method. The optimization can be implemented by the expectation-maximization (EM) algorithm.

11.2 GLAD

[Whitehill et al., 2009] proposed a richer graphic model which includes item difficulty and the expertise of the worker. The difficulty of item is modeled by the parameter $1/\beta_j \in [0, \infty)$ where β_j is constrained to be positive. Here $1/\beta_j = \infty$ means the image is very ambiguous and hence the most proficient worker has a random chance of labeling it correctly. $1/\beta_j = 0$ means the item is so easy that even the most obtuse worker will always label it correctly.

The expertise of each worker i is modeled using the parameter $\alpha_i \in (-\infty, +\infty)$. Here $\alpha = +\infty$ means the worker always labels items correctly; $-\infty$ means the worker always labels items incorrectly.

The labels given by worker i to item j are denoted as L_{ij} and are generated as follows:

$$p(L_{ij} = Z_j | \alpha_i, \beta_j) = \frac{1}{1 + e^{-\alpha_i \beta_j}} \tag{20}$$

As the difficulty $1/\beta_j$ of an item increases, the probability of the label being correct moves toward 0.5. Similarly, as the worker's expertise decreases (lower α_i), the chance of correctly labeling drops to 0.5.

11.3 Deep Learning Approach

[Shaham et al., 2016] has proven that the Dawid and Skene model is equivalent to a Restricted Boltzmann Machine (RBM) with a single hidden node under the assumption that all workers are conditionally independent. Thus the posterior probabilities of the true labels can be estimated via a trained RBM.

A RBM is an undirected bipartite graphical model, consisting of a visible layer X and a hidden layer H. The visible layer consists of d binary random variables and the hidden layer m binary random variables. These two layers are fully connected to each other. A RBM is parametrized by $\lambda = (W, a, b)$, where W is the weight matrix of the connections between the visible and hidden units, and a, b are the bias vectors of the visible and hidden layers, respectively.

A RBM implies the conditional probabilities

$$\begin{aligned} p_\lambda(X_i = 1 | H) &= \sigma(a_i + W_{i\cdot} H) \\ p_\lambda(H_j = 1 | X) &= \sigma(b_j + X^T W_{\cdot j}), \end{aligned}$$

where $\sigma(z)$ is the sigmoid function, $W_{i\cdot}$ is the i-th row of W and $W_{\cdot j}$ is its j-th column.

To relax the assumption on the conditional independence of the variables $X_1, \ldots, X_d$, a RBM-based Deep Neural Net (DNN) is proposed to estimate the posterior probabilities $p_\theta(Y|X)$. The mechanism to stack multiple RBMs is that the hidden layer of each RBM is the input for the successive RBM. The RBMs are trained one at a time from bottom to top. Specifically, given training data $x^{(1)}, \ldots, x^{(n)} \in \{0, 1\}^d$, the bottom RBM is trained first, and then obtain the hidden representation of the first layer by sampling $h^{(i)}$ from the conditional RBM distribution $p_\lambda(H|X = x^{(i)})$. The vector $h^{(1)}, \ldots, h^{(n)}$ are then used as a training set for the second RBM and so on.

11.4 Minimax Entropy

[Zhou et al., 2012] proposed a minimax entropy principle to estimate the ground truth given the observed labels by workers. The model is illustrated in Figure 2.

	item 1	item 2	...	item n
worker 1	z_{11}	z_{12}	...	z_{1n}
worker 2	z_{21}	z_{22}	...	z_{2n}
...	...	...	...	...
worker m	z_{m1}	z_{m2}	...	z_{mn}

	item 1	item 2	...	item n
worker 1	π_{11}	π_{12}	...	π_{1n}
worker 2	π_{21}	π_{22}	...	π_{2n}
...	...	...	...	...
worker m	π_{m1}	π_{m2}	...	π_{mn}

Figure 2: Left: observed labels. Right: underlying distributions. Highlights on both tables indicate that rows and columns of the distributions are constrained by sums over observations.

Each row corresponds to a works indexed by i (from 1 to m). Each column corresponds to an item to be labeled, indexed by j (from 1 to n). Each item has an unobserved label represented as a vector y_{jl}, which is 1 when item j is in class l (from 1 to c), and 0 otherwise. Observed data is a tensor of labels z_{ijk}, which is 1 when the item i is labeled as class j by the worker i, and 0 otherwise. We assume that z_{ij} are drawn from π_{ij}. π_{ij} can be represented as a tensor π_{ijk}, which is the probability that worker i labels item j as class k. The proposed model will estimate y_{jl} from the observed z_{ij}.

The maximum entropy model for π_{ij} given y_{jl} is as following:

$$\begin{aligned}
&\max_{\pi} - \sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{c} \pi_{ijk} \ln \pi_{ijk} \\
&\text{s.t.} \sum_{i=1}^{m} \pi_{ijk} = \sum_{i=1}^{m} z_{ijk}, \forall j,k, \quad \sum_{j=1}^{n} y_{jl}\pi_{ijk} = \sum_{j=1}^{n} y_{jl} z_{ijk} \forall i,k,l, \\
&\sum_{k=1}^{c} \pi_{ijk} = 1, \forall i,j, \pi_{ijk} \geq 0, \forall i,j,k.
\end{aligned} \tag{21}$$

To infer y_{jl}, they proposed to choose y_{jl} to minimize the entropy in Equation 21.

$$\begin{aligned}
&\min_{y} \max_{\pi} - \sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{c} \pi_{ijk} \ln \pi_{ijk} \\
&\text{s.t.} \sum_{i=1}^{m} \pi_{ijk} = \sum_{i=1}^{m} z_{ijk}, \forall j,k, \quad \sum_{j=1}^{n} y_{jl}\pi_{ijk} = \sum_{j=1}^{n} y_{jl} z_{ijk} \forall i,k,l, \\
&\sum_{k=1}^{c} \pi_{ijk} = 1, \forall i,j, \pi_{ijk} \geq 0, \forall i,j,k, \sum_{l=1}^{c} y_{jl} = 1, \forall j, y_{jl} \geq 0, \forall j,l.
\end{aligned} \tag{22}$$

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