PFS Per-Exposure Targeting Optimization

Problem Description

The problem description is thanks to my advisor, <u>Peter Melchior</u>. The other sections I have written up.

We assume that we have $i=1,\ldots,N$ galaxies, each of which with a predefined utility u_i . The utilities can be parameterized as $u_i=\hat{u}_i~\sigma((T_i-\hat{T}_i)/\delta T)$ with a maximum utility \hat{u} , which is modulated by a sigmoid function, to create the utility gains only after a desired integration time \hat{T} has been reaching. For future reference, \hat{u} and \hat{T} may be grouped into classes of targets, not individual ones.

The observations are given by L exposures of equal length T_e in time on an instrument with K=2400 fibers. We want to find per-exposure assignments t_{ikl} to

$$egin{aligned} ext{maximize} & \sum_{i=1}^N u_i = \sum_i \hat{u}_i \ \sigma((\sum_{k,l} t_{ikl} - \hat{T}_i)/\delta T) \ ext{subject to} \ orall l: \sum_{k,i} t_{ikl} = K \ & orall k, l: \sum_i t_{ikl} \leq 1 \ & orall i: \sum_k t_{ikl} \leq 1 \ & orall i, k: t_{ikl} \in \{0,1\} \end{aligned}$$

This is combinatorially really hard and practically impossible when only next-exposure decision can be made. In this case, we have some $l \in [1, L]$, and we want to find the best assignments for the next exposure $l = 1, \ldots, L$ such that the solutions approximates the global assignment/scheduling solution. We therefore introduce "intermediate" utilities u_{il} and then determine the targeting assignments s_{il} for the exposure l such that they

$$egin{aligned} ext{maximize} \sum_{i=1}^N u_{il} &= \sum_i \hat{u}_i \, s_{il} \ ext{subject to} \ \sum_i^i s_{il} &= K \ orall i : s_{il} \in \{0,1\} \end{aligned}$$

But that doesn't have any aspect of long-term planning, so this approach goes after the highutility targets whenever it can (not a terrible policy, but not very equitable). Let's see if we can find some more useful structure in lieu of the s_{il} . The idea is to make this problem probabilistic and continuous and

$$egin{aligned} ext{maximize} \sum_{i=1}^N u_{il} &= \sum_i \hat{u}_i \Pr(\sum_{k,l'} t_{ikl'} = \hat{T}_i \mid heta_{il}) \ ext{subject to} & \sum_i heta_{il} = K \ orall i : 0 \leq heta_{il} \leq 1 \end{aligned}$$

where $\Pr(\sum_{k,l'} t_{ikl'} = \hat{T}_i \mid \theta_{il}) = \operatorname{Binom}(L - l, (\hat{T}_i - T_i')/T_e, \theta_{il})$ is the probability of getting the desired total integration by the end of the program. This term provides memory because it includes integration from earlier exposures $T_i' = T_e \sum_{l'=1}^l t_{ikl'}$ and future outlook because it counts the number of choices available to get the remaining exposures.

By optimizing the targeting probabilities θ_{il} we thus strike a balance between high-utility and feasible targets. Since we need to make targeting choices, we would rank-order the targets i by their contribution to eq. (9), and pick the top K.

What remains is the choice of the θ_{il} . If all targets are equally easy to get, the initial probabilities are $\forall i: \theta_{i1} = K/N$. This would pick all possible high-utility targets first, no optimization needed. We should test this as a baseline, but it is likely not close to optimal because it sacrifices all lower-utility targets even if there are so many to have that they have more aggregate utility.

One can think of several ways of determining "better" θ_{ij} :

- Brute-force optimization possible given N is $\mathcal{O}(10^4)$, but likely to get stuck in local minima.
- Introduce classes such that $\theta_{il} \propto N_c K/N$ for $i \in C_c$, which aims to get N_c total objects in class C_c after all exposures are done.
- Minimizing the variance of estimator, which prefers $\theta_{il} \in \{0,1\}$.
- Reinforcement learning: Simulate the policy to find q table as function of \hat{u}_i, l, T_i' and potentially other terms for class-based utilities.

Separability Approach

The primary impetus behind this optimizer is to parallelize the problem to find better θ . In particular, instead of looking at

$$\begin{split} & \text{minimize} & & -\sum_{i=1}^N \hat{u}_i \binom{L-l+1}{R_i} \theta_i^{R_i} (1-\theta_i)^{L-l+1-R_i} \\ & \text{subject to} & & 0 \leq \theta_i \leq 1 \\ & & & \sum_{i=1}^N \theta_i = K \end{split}$$

which for the Subaru PFS is an N=10,000-dimensional nonconvex (but smooth) optimization across K=2400 fibers, instead we first formulate the Lagrangian

$$L(heta_i,\lambda) = -\sum_{i=1}^N \hat{u}_i inom{L-l+1}{R_i} heta_i^{R_i} (1- heta_i)^{L-l+1-R_i} + \lambda \left(\sum_{i=1}^N heta_i - K
ight)$$

Then we solve the problem

$$egin{array}{ll} ext{minimize} & -C_i heta_i^{R_i}(1- heta_i)^{S-R_i}+\lambda heta_i \ ext{subject to} & 0_i\leq heta\leq 1 \end{array}$$

which is smooth over compact domain and thus we simply need to solve a low-degree polynomial (since L is the number of exposures and thus the degree is not too large) by checking vertices and local extrema. Doing so allows us to construct a set of functions $\theta_i(\lambda)$ giving the optimal θ_i . Then to enforce $\sum_{i=1}^N \theta_i = K$, all we must do is solve

$$\Theta(\lambda) = \sum_{i=1}^N heta_i(\lambda) = K$$

which can be done by bisection.

Analytical Form of Polynomial

To solve a problem of form

minimize
$$f(\theta) = -C\theta^R(1-\theta)^{S-R} + \lambda\theta$$

subject to $0 \le \theta \le 1$

we must analytically express the gradient as a polynomial: for $S \geq 2$ and $1 \leq R \leq S-1$,

$$\begin{aligned} 0 &= \frac{df}{d\theta} = C\left[-R\theta^{R-1}(1-\theta)^{S-R} + (S-R)\theta^R(1-\theta)^{S-R-1}\right] + \lambda \\ &= C\theta^{R-1}(1-\theta)^{S-R-1}\left[-R(1-\theta) + (S-R)\theta\right] + \lambda \\ &= C\theta^{R-1}(1-\theta)^{S-R-1}(S\theta - R) + \lambda \end{aligned}$$

Expanding binomial coefficients,

$$\begin{split} 0 &= C\theta^{R-1}(S\theta - R) \left[\sum_{k=0}^{S-R-1} (-1)^k \binom{S-R-1}{k} \theta^k \right] + \lambda \\ &= C\theta^{R-1} \left[S \sum_{k=0}^{S-R-1} (-1)^k \binom{S-R-1}{k} \theta^{k+1} - R \sum_{k=0}^{S-R-1} (-1)^k \binom{S-R-1}{k} \theta^k \right] + \lambda \\ &= C\theta^{R-1} \left[\sum_{k=1}^{S-R} (-1)^{k-1} \binom{S-R-1}{k-1} \theta^k - R \sum_{k=0}^{S-R-1} (-1)^k \binom{S-R-1}{k} \theta^k \right] + \lambda \\ &= C\theta^{R-1} \left[S(-1)^{S-R-1} \theta^{S-R} + \sum_{k=1}^{S-R-1} (-1)^{k-1} \left(S \binom{S-R-1}{k-1} \right) + R \binom{S-R-1}{k} \right) \theta^k - R \right] + \lambda \end{split}$$

from which the optimal value θ^* may be numerically solved (for any given λ).

Meanwhile if S=1 (recall $S\neq 0$ since it is the number of remaining exposures), then the objective for $X\sim \mathrm{Binom}(S,\theta)$ is just

$$egin{cases} -\hat{u}(1- heta)+\lambda & R=0 \ -\hat{u} heta+\lambda & R=1 \ \lambda & ext{otherwise} \end{cases}$$

Of course since the minimization occurs over [0,1] (and looking forward to the sum constraint on θ) this is solved by

$$\theta^* = \begin{cases} 1 & R = 1 \\ 0 & \text{otherwise} \end{cases}$$

Finally consider S>1, but R=0 or R=S. If R=0, then again $\theta^*=0$. If R=S, then

$$\begin{array}{ll} \text{minimize} & -C\theta^S + \lambda\theta \\ \text{subject to} & 0 < \theta < 1 \end{array}$$

reduces to testing $\theta \in \{0, 1, \sqrt[s-1]{\lambda/CS}\}$ from first-order conditions.

Generalizing to Multiple Classes

The original algorithm makes the simplifying assumption that there are simply N individual objects, each with distinct utilities. However, the more realistic scenario is: there are N individual objects partitioned into C classes. Each class $c \subseteq \mathcal{P}([N])$ (where \mathcal{P} denotes power set) has associated utility u_c and a required number of targets X_c . Our original problem P1 is

$$egin{aligned} ext{maximize} & \sum_{i=1}^N u_{il} = \sum_i \hat{u}_i \Pr(\sum_{k,l'} t_{ikl'} = \hat{T}_i \mid heta_{il}) \ ext{subject to} & \sum_i heta_{il} = K \ & orall i : 0 < heta_{il} < 1 \end{aligned}$$

But in order to satisfy class constraints, we cannot simply look at per-exposure optimization anymore. Rather, #todo

Comparison to Other Optimizers

Comparative Advantages

vs. General Nonconvex Methods. Because of the high-dimensional nature of the problem, methods such as differential evolution (and other genetic algorithms), simulated annealing, etc. are too costly in terms of runtime by several orders of magnitude. On the contrary, the

parallelized nature of this problem makes it extremely computationally efficient, as it reduces to solving a large number of one-dimensional polynomial optimizations.

vs. Greedy Optimizers. A greedy optimizer such as

```
if 0 < R[i] <= L - l // time needed to copmlete target i
    score[i] = u_max[i] / R[i]
else
    score[i] = 0
sort reversed [0...N] off key=score
return first K elements</pre>
```

fails to plan ahead successfully, leading to many "wasted" opportunities, i.e. the optimizer runs out of viable targets and is forced to allocate to "already finished" targets.

Robustness. One of the most desirable characteristics of this optimizer is that it has the capability to make next-exposure decisions, while still planning ahead for long-term optimality. This property makes it robust to external disruptions, such as weather or equipment interference, which prevents may prevent Subaru PFS from actually making all of the suggested observations recommended by the optimizer.

An additional desirable trait is the emphasis on high-utility, long-timeframe targets first, which is a policy this program empirically follows. This adds additional robustness to disruption as it gives the PFS more chances to observe vulnerable high-value targets.

Potential Drawbacks

Because of the bracketing involved in finding an optimal Lagrange multiplier at each exposure, in some rare occasions the optimizer will be forced to evaluate $\sqrt[s-1]{\lambda/CS}$ for $\lambda < 0$. The result is a complex value whose imaginary part the optimizer is forced to discard. Since this arises if and only if R = S > 1 (R is the number of necessary exposures for a galaxy, S is the remaining exposures left in the program) it is limited in scope and empirically does not affect the optimizer's success, even when it does occur. However, a more robust treatment could potentially help in some limiting cases where this phenomenon could make a difference.