Selective sampling after solving a convex problem

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Abstract: We consider the problem of selective inference after solving a (randomized) convex statistical learning program in the form of a penalized or constrained loss function. Our first main result is a change-of-measure formula that describes many conditional sampling problems of interest in selective inference. Our approach is model-agnostic in the sense that users may provide their own statistical model for inference, we simply provide the modification of each distribution in the model after the selection.

Our second main result describes the geometric structure in the Jacobian appearing in the change of measure, drawing connections to curvature measures appearing in Weyl-Steiner volume-of-tubes formulae. This Jacobian is necessary for problems in which the convex penalty is not polyhedral, with the prototypical example being group LASSO or the nuclear norm. We derive explicit formulae for the Jacobian of the group LASSO.

To illustrate the generality of our method, we consider many examples throughout, varying both the penalty or constraint in the statistical learning problem as well as the loss function, also considering selective inference after solving multiple statistical learning programs. Penalties considered include LASSO, forward stepwise, stagewise algorithms, marginal screening and generalized LASSO. Loss functions considered include squared-error, logistic, and log-det for covariance matrix estimation.

Having described the appropriate distribution we wish to sample from through our first two results, we outline a framework for sampling using a projected Langevin sampler in the (commonly occurring) case that the distribution is log-concave.

1. Introduction

Based on the explosion of freely available and high quality statistical software, practicing data scientists or statisticians can rely on untold numbers of statistical learning methods that explore their data. Having found an interesting pattern through such methods, in order to report their findings in the scientific literature, the data scientist is confronted in defending the significance of their findings. Naively assessing significance using methods that ignore their exploration is recognized as flawed. A common, though not often used, solution is to use data splitting to evaluate the significance. There has been significant recent research on developing methods of inference that have the same type of guarantees as data splitting but offer more power. These methods are generally referred to as methods for selective inference (Benjamini, 2010; Berk et al., 2013; Barber and Candes, 2014; Fithian et al., 2014; Lee et al., 2016; Tian et al., 2015; Tian and Taylor, 2015). Loosely speaking, selective inference recognizes the in-
herent selection biases in reporting the most “significant” results from various statistical models and attempts to adjust for the bias in a rigorous framework.

At a high level, selective inference involves two stages: first, query the data by applying some function. Often this function might be the solution of some convex optimization problem. Second, posit a model based on the outcome of the query and perform inference for the parameters or statistical functionals in such models. In order to perform valid inference in this second stage, a common approach espoused above is to condition on the result of the query. An alternative approach is to address the problem via reduction to a problem of simultaneous inference Berk et al. (2013). Under the conditional approach, when the query involves solving a convex problem, we are interested in distributions of the form

\[ S|\hat{\beta}(S) \in A \]  

where \( S \sim F \) represents our data, \( \hat{\beta} \) denotes the solution to a convex optimization problem and \( A \) is some event of interest, set by the data analyst.

In this paper, we address computational problems in the conditional approach to selective inference. In adopting this conditional approach, it quickly becomes apparent distributions of the form (1) can be rather complex. In this work, we propose a unified sampling approach that is feasible for a wide variety of problems. Combined with the randomization idea in Tian and Taylor (2015), this significantly improve both the applicability of selective inference in practice, and the power of the selective tests.

1.1. A canonical example

As a concrete example, we consider solving the LASSO Tibshirani (1996a) at some fixed \( \lambda \), as considered in Lee et al. (2016). Suppose we observe data \((X, y)\), with \( X \in \mathbb{R}^{n \times p} \) and \( y \in \mathbb{R}^n \). The query by the data analyst returns \( \text{sign}(\hat{\beta}(X, y; \lambda)) \) (with \( \text{sign}(0) = 0 \)) where

\[ \hat{\beta}(X, y; \lambda) = \arg\min_{\beta} \frac{1}{2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1. \]  

(2)

The sign vector can be expressed in terms of \( \hat{E} \), the support of \( \hat{\beta} \) and \( \hat{z}_E \) the signs of the non-zero coefficients of \( \hat{\beta} \). In principle, after observing \((\hat{E}, \hat{z}_E) = (\hat{E}_{\text{obs}}, \hat{z}_{E,\text{obs}})\), there is no restriction on the choice of models. For simplicity, we posit a parametric normal model that is based on \( E \) (dropping the ‘obs’ notation) and fixed \( X \),

\[ \mathcal{M}_E = \{N(X_E b_E, \sigma^2_E I) : b_E \in \mathbb{R}^E \} \]  

(3)

with \( \sigma^2_E \) known. Target of inference is naturally \( b_{j|E} \), the parameters of this model. Selective inference essentially takes any distribution \( F \in \mathcal{M}_E \) and consider its corresponding selective distribution by conditioning on \( \{(\hat{E}, \hat{z}_E) = (\hat{E}_{\text{obs}}, \hat{z}_{E,\text{obs}})\} \). In this case, our selective distribution is exactly of the form
of (1), with $A$ being the quadrant specified by the nonzero coefficients $E$ and their signs $z_E$.

Despite the simple form of $A$, the constraint induced a much more intricate set in the space of $y$. In this special case, Lee et al. (2016) has worked out the constraint set on $y$ and selective tests can be computed explicitly. However, this is not generally true, especially in the context of randomized selection procedures proposed by Tian and Taylor (2015); Fithian et al. (2014). In many cases, the form of selective distributions are not explicitly computable and we have to use sampling methods to approximate the conditional distribution. Given a large enough sample from such distribution, we can construct the selective tests. In the following paragraph, we first introduce the randomized Lasso procedure which is a special case of randomized selection procedures proposed in Tian and Taylor (2015). Then we would illustrate what is the appropriate conditional distribution to sample and given a large sample from this distribution, how we carry out the tests for $b_{j|E}$.

First, we propose to incorporate randomness into (2). In particular, we consider solving

$$
\hat{\beta}(X, y, \omega; \lambda) = \arg\min_{\beta} \frac{1}{2} \|y - X\beta\|^2 + \lambda \|\beta\|_1 - \omega^T \beta + \frac{\epsilon}{2} \|\beta\|^2
$$

(4)

where $\omega \sim G$ is a random vector independent of $(X, y)$, whose distribution is chosen by the data analyst, hence known. We will assume that $G$ is supported on all of $\mathbb{R}^p$ with density $g$. The ridge term with small parameter $\epsilon$ ensures the problem above has a solution. This resembles the ridge term in the elastic net proposed by Zou and Hastie (2005).

This type of randomized convex program has been considered in Tian and Taylor (2015). It is espoused as it significantly increase the power in the inference stage without much loss in the quality of the selected model. In particular, increasing the scale of the randomization inevitably deteriorates the model selection quality, similar to using a smaller training set to choose a model in the context of data splitting. However, even a small amount of randomization has empirically shown a fairly noticeable increase in power. Another benefit of randomization include a form of robustness to rare selection events in the selective CLT of Tian and Taylor (2015).

After solving (4), we use its solution $\hat{\beta}(X, y, \omega; \lambda)$ for model selection. Similar to unrandomized version, the appropriate law after model selection is

$$
y | \hat{\beta}(X, y, \omega; \lambda) \in A, \quad y \sim F,
$$

where $F$ is a member of the parametric normal model specified by (3).

Various selective tests can be constructed based on this law including the goodness-of-fit tests and the $p$-values and confidence intervals for $b_{j|E}$. We discuss how to construct tests for $b_{j|E}$ here as they are a special case of testing a single parameter in a multi-parameter exponential family. The general approach is laid out in Fithian et al. (2014).
Selective inference recognizes the fact that interest in \( b_{ij|E} \) is due to the query returning \( E \) as the nonzero variables of the solution to (4). In order to provide valid inference, we therefore consider only the part of sample space that will yield the same model, i.e. conditioning on \( \{(\hat{E}, \hat{z}_E) = (E_{\text{obs}}, z_{E,\text{obs}})\} \). Conditioning each model in \( \mathcal{M}_E \) yields a new parametric model, the selective model

\[
\mathcal{M}^*(E_{\text{obs}}, z_{E,\text{obs}}) = \left\{ F^* : \frac{dF^*}{dF}(\cdot) \propto 1\{ (\hat{E}, \hat{z}_E) = (E_{\text{obs}}, z_{E,\text{obs}}), F \in \mathcal{M}_E \} (\cdot) \right\},
\]

(5)

where \( (E_{\text{obs}}, z_{E,\text{obs}}) \) are the observed variables and signs.

Note that this approach is not tied to the parametric model in (3). In particular, when the parametric normal model is not appropriate, one might replace \( \mathcal{M} \) with some other statistical model (i.e. some other collection of distributions) and carry out statistical inference in this new selective model. This approach was laid out in detail in Fithian et al. (2014), with some asymptotic justification for nonparametric models developed in Tian and Taylor (2015). In fact, in the Lee et al. (2016) the (pre-conditioning) statistical model proposed was not \( \mathcal{M}_E \), rather it was the saturated model

\[
\mathcal{M} = \{ N(\mu, \sigma^2 I) : \mu \in \mathbb{R}^n \}.
\]

(6)

A fairly simple calculation shows that the hypothesis tests and confidence intervals are exactly the same whether we had started with (6) or (3). However this is not the case for examples like forward stepwise, discussed below and in Fithian et al. (2015); Tibshirani et al. (2014).

Let us now consider how we might go about inference in (5). For instance, suppose we are simply interested in a goodness-of-fit test and we will consider the model \( \mathcal{M} = \{ F_0 \} \) so that \( \mathcal{M}^* \) consists of \( F_0^* \) restricted to the event that fixes the active set and signs of the LASSO to be \( (E_{\text{obs}}, z_{E,\text{obs}}) \). Call this distribution \( F_0^* \). A natural way to test \( H_0 : F = F_0 \) would be follow Fisher’s approach by choosing some test statistic \( T = T(X,y) \) and compare our observed value \( T_{\text{obs}} \) to the distribution of \( T \) under \( F_0^* \). In order to do this, it is sufficient to describe the law \( \hat{\beta}_{\lambda,s}(F_0) \), i.e. the push forward of \( F_0 \) and condition this law on the event that fixes the active set and signs to be \( (E_{\text{obs}}, z_{E,\text{obs}}) \). Unfortunately, this is no easy task. Of course, a natural alternative is to use Monte Carlo. A large enough sample from \( F_0^* \) is sufficient to carry out this goodness-of-fit test. A version of this goodness-of-fit test is considered in Section 4.7 below.

The issue of what Monte Carlo method to use remains. Our main contribution in this work is an explicit description of how to sample from distributions such as \( F_0^* \). To be precise, we describe how to sample from conditional distributions where the conditioning depends on the solution to a convex problem. A naive way to sample from this distribution would be to take a Monte Carlo sampler to draw from \( F_0 \), retaining only those points where the active set and signs of the LASSO agree with \( (E_{\text{obs}}, z_{E,\text{obs}}) \). This requires solving (2) at each sample point, and is clearly infeasible. We might say that this is a direct way to condition the push-forward distribution \( \hat{\beta}_{\lambda,s}(F_0) \) on the selection event.
Our approach here relies on what is essentially the pull-back of the conditional distribution itself. In concrete terms, we construct an explicit inverse map to problems like (2) on the selection event. Then, instead of sampling (1), we realize the law $F_0^*$ by sampling $\tilde{\beta}_\lambda$ together with some auxiliary variables on the conditioning event. After acquiring these samples, we can use the inverse map to reconstruct $y$ that is essentially distributed according to the law $F_0^*$. The construction for (2) is described in Section 2.2.

We will see that the pull-back construction is particularly simple for the randomized lasso (4). The randomization was inspired by the differential privacy literature Dwork et al. (2015), though we will see below that it is already very similar to data splitting. Besides making the pull-back simple to compute, we advocate the use of randomization in the query stage in that conditional inference in the second stage is often more powerful if the selection stage is carried out with randomization than without Fithian et al. (2014); Tian and Taylor (2015). Increasing the scale of the randomization inevitably deteriorates the model selection quality, similar to using a smaller training set to choose a model in the context of data splitting. However, even a small amount of randomization has empirically shown a fairly noticeable increase in power. Another benefits of randomization include a form of robustness to rare selection events in the selective CLT of (Tian and Taylor, 2015).

Inference for linear functionals is slightly more complicated than the simple goodness-of-fit test. To conclude this section, let us describe the form of the pull-back construction when we have solved (4) and observed the active set and signs $(E, z_E)$ (dropping the ‘obs’ notation). In principle, there is no restriction on the choice of models. For simplicity, we posit a parametric normal model that is based on a subset of variables $\bar{E}$:

$$ M_{E} = \{ N(X_{\bar{E}}\beta_{\bar{E}}, \sigma_{\bar{E}}^2 I) : \beta_{\bar{E}} \in \mathbb{R}^{\bar{E}} \} $$

with $\sigma_{\bar{E}}^2$ known. Often, the data analyst may opt to take $\bar{E} = E_{obs}$, though this is not strictly necessary. Based on $(E, z_E)$ she might consult the relevant literature (or data independent of $y$) and choose to include or delete some variables from the set $E$. When the variance is unknown, one can either plug in a consistent estimate of $\sigma_{\bar{E}}^2$ (c.f. Lemma 14 of Tian and Taylor (2015)) or include the parameter $\sigma_{\bar{E}}^2$ in the model and solve instead the square-root Lasso Belloni et al. (2014). If a parametric model is not appropriate then one might use a normal approximation for the pair $X^T y$, and rewrite the selection event in terms of this statistic as opposed to just $y$. Such an approach is considered in Tian and Taylor (2015), appealing to the selective CLT.

Having fixed model $M_{\bar{E}}$, and knowing the density $g$ for the randomization $\omega$, suppose the data analyst now wants to test $H_0: \beta_{j|\bar{E}}$ under the assumption $F \in M_{\bar{E}}$. Let $P_{E \setminus j}$ denote orthogonal projection onto col$(X_{E \setminus j})$. In the normal $z$-test for $\beta_{j|\bar{E}}$, we essentially consider the distribution of

$$ r_j = y - \mu_{E \setminus j}, \quad \mu_{E \setminus j} = P_{E \setminus j} y. $$

$r_j$ can be recognized as the residual from the model with variables $E \setminus j$. Select-
tive tests for $\beta_{j | \bar{E}}$ is essentially considering the law of $r_j$ under the conditional distributions. An application of our main result Theorem 1 implies that this law (with the appropriate augmentation variables) has density proportional to

$$(r_j, \hat{\beta}_{E}, \hat{z}_{-E}) \mapsto \exp \left( -\frac{1}{2\sigma_E^2} \| \mu_{E \setminus j} + r_j \|_2^2 \right) \cdot g \left( X^T X_{E} \hat{\beta}_{E} + \lambda \cdot \left( \hat{z}_{E} \right) + \epsilon \cdot \left( \beta_{E} \right) \right)$$

supported on

$$\text{col}(P_{E \setminus j})^\perp \times \{ (\hat{\beta}_E, \hat{z}_{-E}) : \text{sign}(\hat{\beta}_E) = \hat{z}_E, \| \hat{z}_{-E} \|_\infty \leq 1 \}.$$  

The augmentation variables $(\hat{\beta}_E, \hat{z}_{-E})$ are variables involved in the optimization problem (4). Their support ensures we stay on the selection event of interest. In fact, their support is recognizable as a subset of

$$\left\{ (\hat{\beta}, \hat{z}) : \hat{z} \in \partial(\| \cdot \|_1)(\hat{\beta}) \right\},$$

with $\partial$ denoting the subdifferential with respect to $\hat{\beta}$. In particular, this is the subset for which the non-zero coefficients of $\hat{\beta}$ are $E$ with signs $\hat{z}_E$.

In this simple case, the construction of the inverse map is remarkably simple. If we write out the KKT condition for the optimization problem (4), we have

$$X^T X \hat{\beta} - X^T y + \lambda \cdot \hat{z} - \omega + \epsilon \hat{\beta} = 0$$

which can be rewritten as

$$\omega = X^T X \hat{\beta} - X^T y + \lambda \hat{z} + \epsilon \hat{\beta}.$$  

where $(\hat{\beta}, \hat{z})$ are the optimization variables and the subgradient of (4). In this sense, we have inverted the KKT conditions on the selection event of interest, explicitly parameterizing the pairs $(y, \omega)$ that yield active set and signs $(E, z_E)$.

We call this density the pull-back as this is recognizable precisely as the differential geometric pull-back of a differential form on the interior of the selection event, a subset of the manifold $\mathbb{R}^n \times \mathbb{R}^p$. As $g$ is assumed to have a density, the boundary of the selection event is ignorable. To those readers who do not recognize the term pull-back, Theorem 1 essentially just applies a standard change of variables to realize a conditional law for $(y, \omega)$ via a law for $(r_j, \beta_{E}, \hat{z}_{-E})$. Note that the unselective law of $r_j$ is that of $y$ projected onto the residual space form model $\bar{E} \setminus j$.

The reader may ask what we have gained through this exercise. By constructing an inverse map for $(y, \omega)$ on the selection event, we do not have to check whether the pair $(y, \omega) = (y, X^T X \hat{\beta} - X^T y + \lambda \cdot \hat{z} + \epsilon \cdot \hat{\beta})$ satisfy the KKT conditions for the pair $(E, z_E)$. That is, we have removed the difficulty of conditioning from the problem. We are still left with a sampling problem, though we have an explicit density as well as a fairly simple support. Further, the density (7) is log-concave in $(r_j, \beta_{E}, \hat{z}_{-E})$ with a simple support hence methods such as
projected Langevin Bubeck et al. (2015) may be run efficiently as the projection operator is cheap to compute. Section 7 discusses several other examples.

Finally, and most importantly, the reader who may also be the data scientist may ask what to do with samples from this density in order to carry out a test of \( H_0 : \beta_{j|\bar{E}}(F) = 0 \). Let \( \hat{\beta}_{j|\bar{E}} : \mathbb{R}^n \to \mathbb{R} \) denote the map that computes OLS coefficient \( j \) in the model with variables \( \bar{E} \). Then, given a sufficiently large sample \((r_{j,b}, \beta_{E,b}, z_{-E,b})_{b=1}^B\) from density (7), the data analyst will compare the empirical distribution of

\[
\left( \hat{\beta}_{j|\bar{E}}(\mu_{E\setminus j} + r_{j,b}) \right)_{b=1}^B = \left( \hat{\beta}_{j|\bar{E}}(r_{j,b}) \right)_{b=1}^B
\]

to the observed value \( \hat{\beta}_{j|\bar{E}}(y) \). Selective confidence intervals can be constructed by tilting the empirical distribution, though if the true parameter is far from 0, then a reference distribution other than (7) is perhaps more appropriate. One might try replacing \( r_{j,\perp} \) in the density above with \( r_{j,\perp} - \hat{\beta}_{j|\bar{E}} \) where \( \hat{\beta}_{j|\bar{E}} \) is an approximate selective MLE or pseudo MLE Panigrahi et al. (2016). We do not pursue this further here, leaving this for future work. A data analyst concerned about slow mixing in a given MCMC scheme to draw from (7) may take some reversible MCMC algorithm and carry out the exact tests described in Besag and Clifford (1989).

1.2. General approach

Having described what might be the canonical example, the LASSO with a parametric Gaussian model for inference, we now lay out our general approach.

We consider a randomized version of the optimization problem in (1) formulated as

\[
\hat{\beta}(S, \omega) = \arg\min_{\beta \in \mathbb{R}^p} \ell(\beta; S) + \mathcal{P}(\beta) - \omega^T \beta + \frac{\epsilon}{2} \| \beta \|^2
\]

where \( \ell \) is some smooth loss involving the data, \( \mathcal{P} \) is some structure inducing convex function, \( \epsilon > 0 \) is some small parameter that is sometimes necessary in order to assure the program has a solution and \( \omega \sim G \) is a randomization chosen by the data analyst. Our main goal is to sample

\[
(S, \omega) | \hat{\beta}(S, \omega) \in A
\]

Our reasons for considering the problem (8) rather than an unrandomized problem are described in the LASSO example above and also hold for the optimization and sampling problems.

Namely, we expect an increase in power in the second stage following even a small randomization. Further, as in the LASSO example above, this randomization often allows us to cast the sampling problem as sampling from a distribution on a space that is much simpler than if we had not randomized. That is, the law induced by the pull-back measure in a randomized program is often supported on a simpler region, as opposed to the push-forward measure.
of the non-randomized program. For inference in the non-randomized case, one might take the approach of sending the scale of randomization to 0, though we do not pursue this here.

Another feature of the sampling problem related to (8) is that the sampler somewhat decouples the statistical model from the optimization variables. In this sense, our main result provides ways to sample in a model-agnostic fashion: data analysts can supply their own model $M$, resulting in selective model $M^\ast$. Of course, for inference in $M^\ast$, the analyst may have to use other techniques to reduce their problem to sampling from a particular distribution in $M^\ast$. In the example above, standard exponential family techniques were used to eliminate nuisance parameters $\beta_{E\setminus j} E(F)$ and the problem was reduced to sampling from only one distribution, constructed by conditioning a distribution in $M^\ast$ on the sufficient statistic corresponding to the nuisance parameters.

By decoupling, we do not mean statistical independence in any sense. We mean that each distribution in the corresponding selective model is supported on $\Omega \times C$ where $\Omega$ is the original probability space for our data $S$ and $C$ is a set of optimization variables related to the structure inducing function $P$. Formally, we should note that in the pull-back variables, the selective model describes the distribution of tuples $(s, \beta, z)$ rather than the original probability space $\Omega \times \mathbb{R}^p$. Hence, our sampler produces tuples $(s, \beta, z)$ rather than pairs $(s, \omega)$ though $\omega$ can always be reconstructed via the map $\omega = \nabla \ell(\beta; S) + z + \epsilon \cdot \beta$.

The two most common examples of interest in statistical learning are

$$P(\beta) = h_K(\beta) = \sup_{\nu \in K} \nu^T \beta$$

for some convex $K \ni 0$, i.e. a seminorm. In this case, $C$ is typically a subset of the normal bundle of $K$ (c.f. Adler and Taylor (2007); Schneider (1993))

$$\{ (\beta, z) : \beta \in N_z K \}$$

where $N_z K$ is the normal cone of $K$ at $z$, polar to the support cone of $K$ at $z$. The other common example is a constraint on a seminorm, i.e.

$$P(\beta) = I_K(\beta) = \begin{cases} 0 & \beta \in K \\ \infty & \beta \notin K \end{cases}$$

(10)

where $K = \{ b : \| b \| \leq 1 \}$ for some seminorm $\| \cdot \|$. In this case $C$ is again typically a subset of $N(K)$ of the form

$$\{ (\beta, z) : z \in N_{\beta} K \}.$$  (11)

Such sets arise naturally from the KKT conditions of (8):

$$\omega = \nabla \ell(\beta; S) + z + \epsilon \cdot \beta.$$  

Queries related to active sets of variables in the case of the LASSO or group LASSO or the rank of matrices in the case of the nuclear norm correspond
to smooth subsets of the corresponding normal bundles. When the structure 
inducing penalty is polyhedral in nature, the sets \( C \) are typically polyhedral. 
For norms with curved unit balls this is no longer the case, and curvature comes 
in to play. We treat the group LASSO as a canonical example of this in Section 
5.

1.3. Related work

Most of the theoretical work on high-dimensional data focuses on consistency, 
either the consistency of solutions Negahban et al. (2010); Van de Geer (2008) 
or the consistency of the models Wainwright (2009); Zhao and Yu (2006).

In the post selection literature, Berk et al. (2013) proposed the PoSI ap-
proach, which reduce the problem to a simultaneous inference problem. Because 
of the simultaneity, it prevents data snooping from any selection procedure, but 
also results in more conservative inference. In addition, the PoSI method has 
extremely high computational cost, and is only applicable when the dimension 
\( p < 30 \) or for very sparse models. The authors Meinshausen et al. (2012) pro-
posed a method for computing p-values that controls false discovery rate (FDR) 
among all variables. The knockoff filter of Barber and Candes (2014) provides 
similar control of FDR for all variables in the full model. What distinguishes 
the conditional approach from these simultaneous approaches is that the hypothe-
ses tested, or parameters for which intervals are formed, in selective inference 
are chosen as a function of the data. Hence, the methods of inference are not 
always directly comparable.

1.4. Outline of paper

We propose the main Theorem 1 of this paper in Section 3, putting forth the 
sampling density conditional on a selection event. The highlight of this theo-
rem is the reparametrization map that allows to reconstruct the randomization 
as a function of optimization variables and data and allows us to compute the 
required conditional density explicitly, up to a normalizing constant. This is fol-
lowed by a variety of examples of convex optimization programs. The support 
of the selective density in the first set of examples- LASSO and variants in Sec-
tion B, graphical models in Section 4.8, forward stepwise in Section 4.4 can be 
described by polyhedral geometry. We follow this up with a section describing 
more complex problems where the Jacobian involves a curvature component, the 
group lasso illustrated as the prototypical example. We extend the selective sam-
pler to the case in which the data analyst considers multiple views, or queries, 
of the data in Section 6. A selective version of Fisher’s exact test in which the 
data analyst chooses the sufficient statistics based on the data is described in 
Section 4.7. Finally, we advocate the projected Langevin sampling technique 
Bubeck et al. (2015) in Section 7 to sample from a log-concave selective den-
sity as described in earlier examples. Each update in such an implementation 
involves a projection onto a set of constraints induced by the selection event.
The computational cost of each step is often minimal due to a much simpler constraint region using our reparametrization.

2. Inverting the optimization map

In this section, we consider the general problem of constructing an explicit inverse to the solution of a convex problem. In this section, we focus on convex problems without additional randomization, deferring randomization to Section 3.

Consider a statistical learning problem of the form

$$\min_{\beta \in \mathbb{R}^p} \ell(\beta; S) + \mathcal{P}(\beta), \quad S \sim F,$$

where $F$ is some distribution in some model $M$ and $\mathcal{P}$ is some structure inducing convex function, typically of the form (10) or (11). Cone constraints are also easily handled.

The subgradient equation for such a problem at a solution $\hat{\beta}(S)$ reads

$$0 \in \hat{\alpha}(S) + \hat{z}(S)$$

with

$$(S, \hat{\beta}(S), \hat{\alpha}(S), \hat{z}(S)) \in \mathcal{S}^F(\ell, \mathcal{P}),$$

where

$$\mathcal{S}^F(\ell, \mathcal{P}) \overset{\text{def}}{=} \{(s, \beta, \alpha, z) :$$

$$s \in \text{supp}(F),$$

$$\ell(\beta; s) < \infty,$$

$$\alpha \in \partial \ell(\beta; s),$$

$$\mathcal{P}(\beta) < \infty,$$

$$z \in \partial \mathcal{P}(\beta)\}.$$  

Above, and throughout, $\partial$ and $\nabla$ will denote subdifferentials and derivatives with respect to $\beta$ unless otherwise noted.

The set $\mathcal{S}^F(\ell, \mathcal{P})$ can be described by the “base space” $\text{supp}(F)$ and “fibers”

$$\{(\beta, \alpha, z) : \ell(\beta; s) < \infty, \alpha \in \partial \ell(\beta; s), \mathcal{P}(\beta) < \infty, z \in \partial \mathcal{P}(\beta)\}.$$  

We call the map

$$s \mapsto (s, \hat{\beta}(s), \hat{\alpha}(s), \hat{z}(s)) \in \mathcal{S}^F(\ell, \mathcal{P})$$

the *optimization map*. In practice, given data $S$, a computer solves the problem, i.e. produces a point in $\hat{\theta}(S) \subset \mathcal{S}^F(\ell, \mathcal{P})$. Specifically, a solver produces a point in the range of the optimization map:

$$\mathcal{S}^F(\ell, \mathcal{P}) = \{(s, \beta, \alpha, z) \in \mathcal{S}^F(\ell, \mathcal{P}) : \alpha + z = 0\}.$$  

Formally speaking, the program (12) may have no solutions. On this set $\hat{\theta}(s) = \emptyset$. In all of our examples except the dual problem considered in Section B.4, we will assume enough so that our convex programs have unique solutions, when they have any.

The selection events Lee et al. (2016); Fithian et al. (2014) we are most interested in are typically of the form

$$S^F_B(\ell, \mathcal{P}) = \{(s, \beta, \alpha, z) \in S^F_0(\ell, \mathcal{P}) : (\beta, \alpha, z) \in B(s)\}$$

for some nice set-valued function $B(s)$ which could be specified by the zero-set of a function $h^B$:

$$(\beta, \alpha, z) \in B(s) \iff h^B(s, \beta, \alpha, z) = 0.$$  

In all examples below except basis pursuit in Section B.2, $B(s) = \mathcal{B}$ does not depend on $s$. This set also has the form of a bundle with base space $\text{supp}(F)$ and fibers

$$\{(\beta, \alpha, z) \in B(s) : \alpha + z = 0\}.$$  

We call $S^F_B(\ell, \mathcal{P})$ parametrizable if there exists a measurable parametrization $\psi$ defined on some domain $D$ with range $S^F_B(\ell, \mathcal{P})$. The map $\psi$ is typically constructed to be an inverse of the optimization map $\hat{\theta}$ on $S^F_B(\ell, \mathcal{P})$.

Given a parameterization, we will typically construct a change of measure using $\phi = \pi_B \circ \psi$ to simplify sampling from $\{s : \pi_B^{-1}(s) \neq \emptyset\}$ by sampling from $S^F_B(\ell, \mathcal{P})$ itself, where $\pi_B$ is the projection onto the base of $S^F_B(\ell, \mathcal{P})$. Our construction is similar to what Zhou (2014) called estimator augmentation. By construction, then, $\pi_B(s, \beta, \alpha, z)$ is such that $\hat{\theta} \circ \pi_B = \text{id}|_{S^F_B(\ell, \mathcal{P})}$ with $\text{id}$ the identity map.

Transforming the probability space and constructing new data vectors that solve (12) as functions of optimization problems is key to our approach of sampling. The explicit parametrization changes with each problem. Typically, in selective inference examples, we condition on some function of $\hat{\beta}$, perhaps its support $E$ and possibly the signs $z_E$ of the non-zero coefficients. More generally, might condition on something besides $(E, z_E)$ which we might denote by $q$. The selection event, i.e. the quantity we condition on determines the set of constraints $B_q$. We shall denote the parametrization map in our problems as $\psi_q$, so often we will write $\psi_{(E,z_E)}$. The map $\psi_q$ always produces a point $(s, \beta, \alpha, z) \in S^F_B(\ell, \mathcal{P})$, while the domain of this parametrization can vary with the problem at hand, that is

$$\psi_q : D_q \rightarrow S^F_B(\ell, \mathcal{P}),$$

for a problem specific domain $D_q$.  

2.1. Inverting the MLE

We now begin to describe our approach to inverting the optimization map. Our first example is classical: the density of the MLE of the natural parameters of an exponential family. The formula is not new, going back at least to Fisher (Barndorff-Nielsen, 1983; Efron and Hinkley, 1978). Nevertheless, it serves to illustrate the general approach we take for the general cases later.

Our loss function is

$$\ell(\beta; S) = \Lambda(\beta) - \beta^T S$$

where

$$e^{\Lambda(\beta)} = \mathbb{E}_{F_0}[e^{\beta^T S}]$$

is the moment generating function in the exponential family with reference measure $F_0$ and sufficient statistic $S$ with $F_\beta$ the law of $S$ above and in what follows. We also assume that $F_0$ has a density $f_0$ with respect to Lebesgue measure.

As we are computing the MLE, our penalty function is $\mathcal{P}(\beta) \equiv 0$. The convex program we solve is

$$\text{minimize}_{\beta \in \mathbb{R}^p} \Lambda(\beta) - \beta^T S.$$  \hspace{1cm} (19)

The KKT conditions or subgradient equation here is just the usual score equation

$$\nabla \Lambda(\hat{\beta}(S)) = S$$

where

$$\nabla \Lambda(\beta) = \int_{\mathbb{R}^p} s f_\beta(ds).$$

Our parameterization of $S_0^F(\ell, \mathcal{P} = 0)$ is

$$\psi(\beta) = (\nabla \Lambda(\beta), \beta, 0, 0)$$

which can be interpreted as reconstructing $S$ given $\beta$.

Standard multivariate calculus then tells us that the density of $\hat{\beta}(S)$ under the distribution $F_{\beta_0}$ is

$$e^{\nabla \Lambda(\beta)^T \beta_0 - \Lambda(\beta_0)} \det(\nabla^2 \Lambda(\beta)) f_0(\nabla \Lambda(\beta)).$$  \hspace{1cm} (20)

where $\nabla^2 \Lambda(\beta)$ is the observed information (Efron and Hinkley, 1978).

If $\beta_0$ is the true parameter, then, at the cost of changing the reference measure by a factor of $\exp(s^T \hat{\beta}(s) - \Lambda(\hat{\beta}(s))) \det(\nabla^2 \Lambda(\beta))^{1/2}$ yielding a new Lebesgue density $h_0$, we can rewrite this as

$$e^{\Lambda(\beta) - \Lambda(\beta_0) + \nabla \Lambda(\beta)^T (\beta_0 - \beta)} \det(\nabla^2 \Lambda(\beta))^{1/2} h_0(\nabla \Lambda(\beta)).$$  \hspace{1cm} (21)

As pointed out in (Barndorff-Nielsen, 1983) ignoring the term $h_0(\nabla \Lambda(\beta))$ (which is the constant 1 in the Gaussian case) yields the usual saddle-point approximation to the density of the MLE, up to the constant of integration. The exponential above can be rewritten as

$$-\frac{1}{2}(\beta - \beta_0)^T \nabla^2 \Lambda(\beta)(\beta - \beta_0) + R(\beta; \beta_0).$$
Note that even ignoring the remainder, this is quadratic in $\beta_0$ the parameter, and not $\beta$ the variable of integration in the density.

In principle, nothing above really relies on the exponential family structure for the model, though it does rely somewhat on the fact that the loss we use came from an exponential family. It relies on this in that we use the form of the loss to reconstruct data $S$ from optimization variables $\beta$. This is similar to what we see in the LASSO example below.

Nevertheless, the same argument above shows that if we solve the program (19) then, so long as $S \sim F$ has a Lebesgue density the density of $\hat{\beta}(S)$ is
\[
 f(\nabla \Lambda(\beta)) \cdot |\det(\nabla^2 \Lambda(\beta))|.
\]
(22)

In this sense, the above display provides an exact recipe to compute the density of the MLE under model misspecification. This is somewhat similar to the general approach taken in Hillier and Armstrong (1999), though we are considering this only in a very restricted setting.

### 2.2. Pull-Back of the LASSO with fixed design matrix

As a second example of a pull-back, we look at the canonical example in the class of regularized convex optimization problems: the LASSO (Tibshirani 1996b). The LASSO program is defined for each $(X, y, \lambda) \in \mathbb{R}^{n \times p} \times \mathbb{R}^n \times (0, \infty)$ as
\[
 \min_{\beta \in \mathbb{R}^p} \frac{1}{2} \| y - X\beta \|_2^2 + \lambda \| \beta \|_1.
\]
(23)

In this example, $X$ is considered fixed and $F = \mathcal{L}(P_Cy|X)$ where $P_C$ is projection onto col$(X)$. The law $F$ is supported on col$(X)$ because the optimization map depends only on $P_Cy$. In our general notation, we can take
\[
 S = P_Cy,
\]
\[
 \ell(\beta; y) = \frac{1}{2} \| y - X\beta \|_2^2,
\]
\[
 \mathcal{P}(\beta) = \lambda \| \beta \|_1.
\]
(24)

The familiar subgradient equations of the LASSO are
\[
 -\dot{\alpha}(y) = X^T(y - X\hat{\beta}(y)) = \check{\varepsilon}(y), \quad \check{\varepsilon}(y) \in \partial(\lambda \| \cdot \|_1)(\hat{\beta}(y)).
\]
(25)

Note also that (25) contains the implicit constraint $\check{\varepsilon}(y) \in \text{row}(X)$ where row$(X)$ is the rowspace of $X$. This can be seen from the structure of
\[
 S^F_0(\ell, \mathcal{P}) = \left\{ (y, \beta, \alpha, z) \in S^F(\ell, \mathcal{P}) : X^T(X\beta - y) + z = 0 \right\}
\]
as each point in \( \mathcal{S}^E_0(\ell, \mathcal{P}) \) has \( z \in \text{row}(X) \).

In Lee et al. (2016), the authors assume general position so the map \( \hat{\theta} \) is single valued Tibshirani (2013). The authors then considered the active set and signs of the LASSO solution, conditioning on their value \((E, z_E)\) and the design \(X\). This is the event

\[
\left\{ y : (y, \hat{\beta}(y), \hat{\alpha}(y), \hat{z}(y)) \in \mathcal{S}^E_0(\ell, \mathcal{P}), \text{diag}(z_E)\hat{\beta}_E(y) > 0, \hat{\beta}_{-E}(y) = 0 \right\}.
\] (26)

Note that this event is equivalent to

\[
\hat{\theta}(y) \in \{(y, \beta, \alpha, z) : \text{diag}(z_E)\beta_E > 0, \beta_{-E} = 0\}.
\]

This is our canonical example of a parameterizable set where

\[
\mathcal{B} = \mathcal{B}(E, z_E) = \{(\beta, \alpha, z) : \text{diag}(z_E)\beta_E > 0, \beta_{-E} = 0, z_E = \lambda \text{ sign}(\beta_E), \|z_{-E}\|_{\infty} \leq \lambda\}.
\]

The above constraints on \( \beta \) induce further restrictions on the range of the solver

\[
\mathcal{S}^E_{B(E,z_E)}(\ell, \mathcal{P}) = \{(s, \beta, \alpha, z) \in \mathcal{S}^E_0(\ell, \mathcal{P}) : \beta \in \mathcal{B}(E, z_E)\}
\]

\[
= \{(s, \beta, \alpha, z) : \text{diag}(z_E)\beta_E > 0, \beta_{-E} = 0, \alpha = -X^T(s - X\beta) = -z, z_E = \lambda \text{ sign}(\beta_E), \|z_{-E}\|_{\infty} < \lambda\}.
\]

The authors in Lee et al. (2016) then carry out selective inference for linear functionals \( \eta^T \mu \) in the saturated model

\[
\mathcal{M} = \{N(\mu, \sigma^2) : \mu \in \mathbb{R}^n\}
\] (27)

with \( \sigma^2 > 0 \) considered known. In this context, selective inference corresponds to taking each \( F \in \mathcal{M} \) and conditioning it on the event (26) which can be rewritten as

\[
\pi_S \left( \mathcal{S}^E_{B(E,z_E)}(\ell, \mathcal{P}) \right)
\]

where \( \pi_S \) denotes projection onto the data coordinate. The resulting selective model

\[
\mathcal{M}^* = \left\{ F^* : \frac{dF^*}{dF}(y) \propto \begin{cases} 1 & y \in \pi_S \left( \mathcal{S}^E_{B(E,z_E)}(\ell, \mathcal{P}) \right) \\ 0 & \text{otherwise.} \end{cases} \right\}
\]

is an exponential family and sampling is generally not necessary in the saturated model as valid inference typically requires conditioning on sufficient statistic related to nuisance parameters as described in Lee et al. (2016); Fithian et al. (2014).

Nevertheless, if sampling were necessary, a naive accept reject sampling scheme for inference in this setting draws vectors \( y \) on \( \mathbb{R}^n \) according to \( N(\mu, \sigma^2) \) solves the LASSO with the triple \((y, X, \lambda)\) and checks whether the result lies in (26). Due to the nature of the LASSO, this check can be reduced to verifying whether \( y \) satisfies a set of affine inequalities Lee et al. (2016).
2.2.1. Parametrization and pull-back of the LASSO

What if we did not have to check these affine inequalities in our sampling scheme? This is the essence of what we propose in this work. We will ultimately see that our approach is essentially equivalent to that of Lee et al. (2016) but the probability space of our sampler is different. The approach we take is similar to (Zhou, 2014). We will see later that, after randomization, the parameter space is generically simpler than if we had not randomized.

Our first example of a parameterization is

$$
\psi_{(E,z)}(\beta,z) = (X\beta + (X^T)^+z, \beta, z, z)
$$

with domain

$$
D_{(E,z)} = \{ (\beta, z) : \text{diag}(z_E)\beta_E > 0, \beta_{-E} = 0,
\text{ } z \in \text{row}(X), z_E = \lambda \text{ sign}(\beta_E), \|z_{-E}\|_\infty \leq \lambda \}
$$

and corresponding data reconstruction map $\phi_{(E,z)} : D_{(E,z)} \rightarrow \text{col}(X)$ defined by

$$
\phi_{(E,z)}(\beta,z) = X\beta + (X^T)^+z.
$$

We see that $\psi_{(E,z)}$ is indeed a parameterization of $S^F_0(\ell, P)$. Hence, on the range of $\phi_{(E,z)}$, we do not actually have to check the affine inequalities of (Lee et al., 2016) as they are satisfied by construction.

The set $D_{(E,z)}$ is a subset of a $2p$-dimensional set but is in fact of dimension $\text{rank}(X)$ whenever $|E| < \text{rank}(X)$. Hence, it has Lebesgue measure 0 in $\mathbb{R}^{2p}$ but it is a subset of an affine space so that it inherits a Hausdorff measure $\mathcal{H}_{\text{rank}(X)}$.

In a formal sense, the map $\phi_{(E,z)}$ is the inverse of the optimization map.

Lemma 1. On the set of $y$ where that the solution to (23) is unique ($X$ being considered fixed), the following equality holds

$$
\hat{\theta}_{-y,0} \circ \phi_{(E,z)}(\beta,z) = (\beta,z) \quad \text{for } (\beta,z) \in D_{(E,z)},
$$

where $\hat{\theta}_{-y,0}(y) = (\hat{\beta}(y), \hat{z}(y))$. Hence, $\hat{\theta}_{-y,0} \circ \phi_{(E,z)}$ is equivalent to the identity map on $D_{(E,z)}$.

More generally, the set (26) is equal to $\phi_{(E,z)}(D_{(E,z)})$.

Proof. Direct verification of (25). □

Now choose an element in $\mathcal{M}$, i.e. fix some $\mu \in \mathbb{R}^n$ and consider the $N(\mu, \sigma^2 I)$ density. We define its pull-back to be the law $F^*_{\mu}$ supported on $D_{(E,z)}$ with $\mathcal{H}_{\text{rank}(X)}$ density

$$
f^*_{\mu}(\beta,z) \propto \exp \left( -\frac{1}{2\sigma^2} \| \phi_{(E,z)}(\beta,z) - \mu \|^2_2 \right) \cdot |J\phi_{(E,z)}(\beta,z)|,
$$

where $J\phi_{(E,z)}$ is the Jacobian of the projection of the parameterization, which depends only on $X$ in this case (and can be treated as a constant). We use the
name pull-back as this density is precisely the pull-back of the measure with Lebesgue density $f_\mu$ under the reconstruction map $\phi_{(E,z_E)}$.

As each density has a pull-back, the model itself has a pull-back $\mathcal{M}^*$ comprising the pull-back of each density. The model also inherits the exponential family structure of $\mathcal{M}$. Taking $f_0^*$ to be the reference measure, we can choose the natural parameter to be $\mu/\sigma^2$ and sufficient statistic to be $\phi_{(E,z_E)}((\beta,z))$.

Finally, note that nothing about our construction so far has anything to do with the parametric model $(27)$. In fact, as long as $F$ has a Lebesgue density the pull-back is well-defined.

**Lemma 2.** Suppose $F = \mathcal{L}(P_C y | X)$ has density $f$ on $C = \text{col}(X)$ and the solution to $(23)$ is $F$-a.s. unique. Then, the following equality holds

$$
\mathcal{L}_{y \sim F}(P_C y \mid (y,\hat{\beta}(y),\hat{\alpha}(y),\hat{z}(y)) \in \mathcal{S}_F^F(\ell,P), \text{diag}(z_E)\hat{\beta}_E(y) > 0, \hat{\beta}_{-E}(y) = 0, X) = \mathcal{L}_{(\beta,z) \sim F^*}(\phi_{(E,z_E)}(\beta,z)) X),
$$

where $F^*$ is supported on $\text{relint}(D_{(E,z_E)})$ and has $\mathcal{H}_{\text{rank}(X)}$ density

$$f^*(\beta,z) \propto f(\phi_{(E,z_E)}(\beta,z)) \cdot |J\phi_{(E,z_E)}(\beta,z)|.$$

**Proof.** Follows from Lemma 1 and standard multivariate calculus combined with the fact that the existence of the density $f$ implies that

$$F(\phi_{(E,z_E)}(D_{(E,z_E)} \setminus \text{relint}(D_{(E,z_E)})) = 0.
$$

**Remark 1.** One of the consequences of the above is that one can draw response vectors $y$ that have the same active set and signs from a density with relatively simple support when row $X) = \mathbb{R}^p$. Hence, sampling IID from some density on this support allows one to use importance sampling with the above explicit density as numerator in the importance weight.

When row $X) \subseteq \mathbb{R}^p$, the support is still somewhat complex. For instance, the subgradients $z$ must be in the intersection of a face of the $\ell_\infty$ ball which may be a difficult set to describe. We will see that after randomization, this complexity often disappears.

**Remark 2.** In theory, one might want to drop the uniqueness assumption above. If uniqueness of the solution does not hold then the parameterization is not injective and the event we condition on should be replaced with the event $\theta(y) \cap \mathcal{S}_F^F(\ell,P) \neq \emptyset$.

In this case, it may still be possible to derive a formula for the law of $P_C y$ by invoking the co-area formula Federer (1959); Diaconis et al. (2013). We do not pursue this generalization here.

In order to carry out selective inference for a linear functional $\eta^T \mu$, the authors of Lee et al. (2016) conditioned on $P_C^\perp y$. This is also possible in the pull-back model. Fix a linear subspace $L \subset \text{col}(X)$ considered to be the model...
subspace so that
\[ M_L = \{ N(\mu, \sigma^2 I) : \mu \in L \} \].

For each linear function of interest \( \eta \in L \), one generally must condition on \((P_L - P_\eta)y\) to eliminate the nuisance parameter \((P_L - P_\eta)\mu\). If \( w \) is the observed value of \((P_L - P_\eta)y\), a straightforward modification of the argument above shows that the appropriate distribution is supported on the \( \text{rank}(X) - \text{dim}(L) + 1 \) dimensional set
\[
D_{(E,z_E)}(w) = \{ (\beta, z) \in D_{(E,z_E)} : (P_L - P_\eta)\phi(E,z_E)(\beta, z) = w \}
\]
with \( H_{\text{rank}(X) - \text{dim}(L) + 1} \) density proportional to \( f^* \). In this case, even if \( \text{row}(X) = \mathbb{R}^p \), the support is somewhat complex.

3. Inverting the optimization map of a randomized convex program

In this section, we describe how to invert the KKT conditions for our family of randomized convex programs. As mentioned in the introduction, randomization comes with advantages like enhanced statistical power in the inference stage, as well as a simplification of the support of the relevant reference distribution. In what follows, all of our convex programs have random variables appearing linearly in the subgradient, so that these random variables can be reconstructed from optimization variables. The random variable is one introduced by a data analyst through additional randomization as described in (Dwork et al., 2015; Tian and Taylor, 2015).

Let \( G \) be a distribution on \( \mathbb{R}^p \) and \( \epsilon \geq 0 \) a small parameter. Given a canonical problem specified by \( (F, \ell, P) \) we define its randomized version as
\[
\min_{\beta \in \mathbb{R}^p} \ell(\beta; S) + P(\beta) - \omega^T \beta + \frac{\epsilon}{2} \| \beta \|^2_2, \quad (S, \omega) \sim F \times G. \tag{33}
\]

A natural question to ask at this point is: why randomize the program in the above way? One of the inspirations for selective inference after randomization, the topic considered in (Tian and Taylor, 2015) are techniques used in differential privacy (Dwork et al., 2015). The other was the empirical finding in (Fithian et al., 2014) that holding out some data before carrying out selective inference as in Lee et al. (2016) also showed an improvement in selective power.

This increase in selective power can be attributed to the fact that choosing a model with a randomized response has more leftover information as defined in Fithian et al. (2014) after model selection than choosing a model with the original response.

The choice to add \( \frac{\epsilon}{2} \| \beta \|^2_2 - \omega^T \beta \) to the objective is not the only reasonable choice. The main property we want of the perturbation \( \Delta(\beta, \omega) \) is that \( \omega = \phi(\beta, v) \) where \( (\beta, v) \in \partial \Delta(\beta, \omega) \). That is, given the value of \( \beta \) and the subgradient \( v \) we can reconstruct \( \omega \).
Remark 3. Addition of the term $\frac{\epsilon}{2} \|eta\|_2^2$ to the objective ensures that the set of $(s, \omega)$ such that (33) has a solution contains the set

\[ \{(s, \omega) : \hat{\theta}(s) \neq \emptyset, \omega \in \text{supp}(G)\}. \]

To see this, note that solving (33) is equivalent to computing

\[ \hat{\beta}(s, \omega) = \text{prox}_{\frac{1}{2}(\ell(\cdot; s) + \mathcal{P}(\beta))}(\omega/\epsilon). \]

Whenever $\hat{\theta}(s) \neq \emptyset$, the objective $\ell(\cdot; s) + \mathcal{P}(\beta)$ is a closed proper convex function, hence its proximal mapping is well-defined and $\hat{\beta}(s, \omega)$ is well-defined.

If $\ell$ is strongly convex a.s.-$F$ and $\mathcal{P}$ is closed and proper then we can take $\epsilon = 0$.

3.1. Data splitting as randomization

The suggested randomization above may strike some readers as lacking motivation. A randomization mechanism probably familiar to most readers is data splitting (Cox, 1975), i.e. randomly partitioning the dataset into two pieces of size $(n_1, n - n_1)$. We will see that solving a convex program after data splitting is essentially an example of (33).

For a specific example, suppose we fit the graphical LASSO Friedman et al. (2008) based on a data matrix $X \in \mathbb{R}^{n \times p}$ but we first randomly split the data. That is, we form

\[ S_1(g) = \frac{1}{n_1}X_1(g)^T \left( I_{n_1} - \frac{1}{n_1}1_{n_1}1_{n_1}^T \right) X_1(g), \]

with $g$ denoting the random partition of the data into two groups and $X_1(g)$ denoting the data in the first group.

Next, we solve the program

\[ \minimize_{\Theta : \Theta^T = \Theta, \Theta > 0} - \log \det(\Theta) + \text{Tr}(S_1(g)\Theta) + \lambda \mathcal{P}(\Theta) \]

with the usual caveat that the penalty does not charge diagonal elements of $\Theta$.

This program is equivalent to solving the problem

\[ \minimize_{\Theta : \Theta^T = \Theta, \Theta > 0} - \log \det(\Theta) + \text{Tr}(S\Theta) + \text{Tr}((S_1(g) - S)\Theta) + \lambda \mathcal{P}(\Theta), \]

where

\[ S = \frac{1}{n}X^T \left( I - \frac{1}{n}1_n1_n^T \right) X. \]

This is very close to (33) with $\omega = \omega(g) = S - S_1(g)$ which is orthogonal to, but not necessarily independent of the full covariance $S$. As described in Fithian et al. (2014), data splitting can be interpreted as simply conditioning on the value $(S_1(g), g)$ as the only variation in $\mathcal{L}(S|S_1(g), g)$ is $S_2(g)$, the second stage data.
3.2. The selective sampler

In this section, we describe our main tool for inference after solving a convex program randomized in the above fashion. We call this tool the selective sampler.

A solver for the program (33) produces a point in

\[ \mathcal{S}^F(G, \epsilon, \ell, P) = \{ (s, \omega, \beta, \alpha, z) : \]
\[ s \in \text{supp}(F), \]
\[ \omega \in \text{supp}(G), \]
\[ \ell(\beta; s) < \infty, \]
\[ \alpha \in \partial\ell(\beta; s), \]
\[ P(\beta) < \infty, \]
\[ z \in \partial P(\beta) \}. \] (34)

More precisely, it produces a point in

\[ \mathcal{S}^F_0(G, \epsilon, \ell, P) = \{ (s, \omega, \beta, \alpha, z) \in \mathcal{S}^F(G, \epsilon, \ell, P) : \epsilon \cdot \beta + \alpha + z - \omega = 0 \}. \] (35)

Our statistical learning task is typically to infer something about \( F \) in some model \( \mathcal{M} \). As we are free to choose \( G \) however we want, a natural choice is to choose \( G \) to have a Lebesgue density supported on all of \( \mathbb{R}^p \). In this case, inspection of the KKT conditions or subgradient equation of (33) read

\[ \omega = \hat{\alpha}(s, \omega) + \hat{\epsilon}(s, \omega) + \epsilon \cdot \hat{\beta}(s, \omega). \] (36)

The subgradient equation determines a canonical map

\[ \psi : \mathcal{S}^F(\ell, P) \to \mathcal{S}^F_0(G, \epsilon, \ell, P) \] (37)

defined naturally as

\[ \psi(s, \beta, \alpha, z) = (s, \alpha + z + \epsilon \cdot \beta, \beta, \alpha, z). \] (38)

As in the non-randomized case, we are typically interested in some selection events of the form

\[ \mathcal{S}^F_0(G, \epsilon, \ell) = \{ (s, \omega, \beta, \alpha, z) \in \mathcal{S}^F_0(G, \epsilon, \ell, P) : (\beta, \alpha, z) \in \mathcal{B}(\beta) \}. \]

The corresponding randomization reconstruction map is then

\[ \phi(\beta, \alpha, z) = \alpha + z + \epsilon \cdot \beta, \]

defined on a domain

\[ \{ (\beta, \alpha, z) \in \mathcal{B}(\beta) : \alpha + z + \epsilon \cdot \beta \in \text{supp}(G) \}. \]
for a suitable $\mathcal{B}(S)$, defined by the selection event. It turns out that many selection events of interest are such that the restriction of $\psi$ to these events have a simple structure which allows for straightforward description of the selective model. The canonical example of conditioning on the set of active variables and signs of the LASSO as in (Lee et al., 2016) was described in Section 1.1.

**Theorem 1** (Selective sampler). Suppose that $\omega$ is independent of $S$ with distribution $G$ such that $\text{supp}(G) \subset \mathbb{R}^p$ has non-empty interior with Lebesgue density $g$ on $\text{supp}(G)$.

Then, the map

$$
\psi(s,\beta,\alpha,z) = (s, \epsilon \cdot \beta + \alpha + z, \beta, \alpha, z)
$$

restricted to

$$
D_G = \{(s, \beta, \alpha, z) \in \mathcal{S}^F(\ell, \mathcal{P}) : \epsilon \cdot \beta + \alpha + z \in \text{supp}(G)\}
$$

is onto $\bar{\mathcal{S}}^F(\mathcal{G}, \ell, \mathcal{P})$. Further, the law

$$
\mathcal{L}_{\mathcal{F} \times \mathcal{G}}((S, \omega) | (S, \omega, \hat{\beta}(S, \omega), \hat{\alpha}(S, \omega), \hat{\varphi}(S, \omega)) \in \bar{\mathcal{S}}^F(\mathcal{G}, \ell, \mathcal{P})) = \mathcal{L}((S, \epsilon \beta + \alpha + z) | (s, \beta, \alpha, z) \in D_G, (\beta, \alpha, z) \in \mathcal{B}(S))
$$

(39)

for suitable $\mathcal{B}(S)$ and $(S, \beta, \alpha, z)$ has density proportional to

$$
f(s) \cdot g(\epsilon \cdot \beta + \alpha + z) \cdot |J\psi(s, \beta, \alpha, z)| \cdot 1_{D_G}(s, \beta, \alpha, z) \cdot 1_{\mathcal{B}(s)}(\beta, \alpha, z)
$$

(40)

with the Jacobian denoting the derivative of the map $\psi$ with respect to $(\beta, \alpha, z)$ on the fiber over $s$.

**Proof.** The fact that $\psi$ restricted to $D_G$ is onto follows from its construction. Let $\mathcal{F}(s) = \{(\beta, \alpha, z) : \alpha \in \partial \ell(\beta; s), z \in \partial \mathcal{P}(\beta)\}$ denote the fiber over $s$ and assume that $\mathcal{B}(s) = \mathcal{B}$ does not vary with $s$. In this case, in any local coordinates on $\mathcal{F}(s)$ standard multivariate calculus yields the density (40) as the derivative of the map

$$(s, \beta, \alpha, z) \mapsto (s, \alpha + z + \epsilon \cdot \beta)$$

takes the form

$$
\begin{pmatrix}
I_{n \times n} & 0_{n \times p} \\
D_s \phi & D_{(\beta,\alpha,z)} \phi
\end{pmatrix}
$$

with determinant $|\text{det}(D_{(\beta,\alpha,z)} \phi)|$. The result then follows by integrating over $\text{supp}(\mathcal{F})$ with density $f(s)$. If $S$ does not have a density then (39) can be derived via the Kac-Rice formula Taylor et al. (2013); Adler and Taylor (2007).

If $\mathcal{B}$ depends on $s$ then the Kac-Rice formula may often be used to derive the above density given the $\mathcal{B}$ can be described as the zero set of some smooth function $h^\mathcal{B}$. As most of our examples are such that $\mathcal{B}$ does not depend on $s$ we omit the details. □
Remark 4. The correct interpretation of (39) has as conditioning event

$$\bar{\theta}-(s,\omega)(s,\omega) \cap B(s) \neq \emptyset$$

where $\bar{\theta}$ is the map

$$\bar{\theta}(s,\omega) = (s,\omega, \hat{\beta}(s,\omega), \hat{\alpha}(s,\omega), \hat{z}(s,\omega)).$$

Remark 5. When $\text{supp}(G) = \mathbb{R}^p$ then $D_G = S^F(\ell, \mathcal{P})$.

Remark 6. Above, we have constructed $\omega$ as a function of $(s, \beta, \alpha, z)$. This is similar to the LASSO case in Section 2.2 in that we construct new random variables out of optimization variables. Often, it is also possible to construct $s$ from $(\omega, \beta, \alpha, z)$ though there is no canonical embedding unless we provide more structure to the map $\ell$. If $\ell$ is an exponential family negative log-likelihood so that

$$\ell(\beta; s) = \Lambda(\beta) - s^T \beta$$

then this is certainly possible. However, in order to have a change of measure result as in Theorem 1, the law of $S$ should have a density on $\mathbb{R}^n$.

Remark 7. Often, we will want to condition on some functions of $S$. Theorem 1 formally holds unchanged for any distribution supported on a lower dimensional subset of $S$. One simply replaces the law $F$ with the appropriate law supported on a lower dimensional set. This device was used in Section 1.1. A further example of this is considered in Appendix A below.

Remark 8. The theorem assumes $\omega$ is independent of the data $S$. It is straightforward to see that a similar result holds if we replace throughout the density $g$ above with $K(\omega; s)$ a kernel for the conditional density of $\omega|s$.

4. Polyhedral examples

We now begin describing several instances of the selective sampler. In this section, the penalties or constraints are polyhedral. In this case, the reconstruction maps are typically affine in the optimization variables but may be non-trivial in the data. Some of these examples were also considered in Tian et al. (2016). We repeat them here, in more explicit detail, as concrete examples of the selective sampler.

4.1. LASSO with Gaussian errors and fixed design matrix

As is often the case, the LASSO serves as a canonical example. We denote the parametrization, based on the active set and signs as $\psi(E, z_E)$ on domain $D_{\psi(E, z_E)}$ and the reconstruction map for randomization $\omega$ as $\phi(E, z_E)$ throughout. In all the below examples, we are implicitly thinking of cases when $\text{supp}(G) = \mathbb{R}^p$ and $G$ has a Lebesgue density, the canonical example being $N(0, \sigma^2_\omega I_p)$.
This example was addressed in Section 1.1, though we present it here in the
general notation developed so far. The embedding in Theorem 1 plays the role
of $\psi(E,z_E)$ in the parametric LASSO example. The randomized LASSO program
Tian and Taylor (2015) with randomization $G$ is defined for each $(y,X,\lambda,\omega) \in \mathbb{R}^n \times \mathbb{R}^{n \times p} \times (0,\infty) \times \mathbb{R}^p$ as

$$\minimize_{\beta \in \mathbb{R}^p} \frac{1}{2} \|y - X\beta\|_2^2 + \frac{\epsilon}{2} \|\beta\|_2^2 - \omega^T\beta + \lambda \|eta\|_1, \quad y | X \sim F, \omega \sim G$$

with $\omega$ independent of $(X,y)$.

When $G = \delta_0$, we recover the parametric LASSO with $\epsilon = 0$ and the parametric Elastic Net if $\epsilon > 0$ Zou and Hastie (2005). Supposing then that $\supp(G) = \mathbb{R}^p$, and the canonical selection event given by

$$B(E,z_E) = \{ \beta : \text{diag}(z_E)\beta_E > 0, \beta_{-E} = 0 \}. \quad (41)$$

A parametrization of

$$\{(s,\omega,\beta,\alpha,z) \in S^P_0(G,\epsilon,\ell,P) : \beta \in B(E,z_E)\}$$

is given by

$$\psi(E,z_E)(y,\beta_E,u_{-E}) = \left( y, \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - X^T(y - X\beta_E) + \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix}, \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - X^T(y - X\beta_E), \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix} \right)$$

with the domain

$$D(E,z_E) = \{ (y,\beta_E,u_{-E}) : \text{diag}(z_E)\beta_E > 0, \|u_{-E}\|_\infty \leq 1 \}. \quad (42)$$

The reconstruction map for $\omega$ is given by

$$\phi(E,z_E)(y,\beta_E,u_{-E}) = \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - X^T(y - X\beta_E) + \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix}, \quad (43)$$

again with the same support as the parametrization map. For the canonical event $B(E,z_E)$, we therefore need to sample from a density proportional to

$$f_\mu(y) \cdot g \left( \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - X^T(y - X\beta_E) + \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix} \right) \cdot |\det(X_E^TX_E + \epsilon I)| \quad (44)$$

supported on $D(E,z_E)$, where $f_\mu$ is the $N(\mu,\sigma^2 I_n)$ density. As above, the same expression holds if our model for $y|X$ is not from the normal family.

A common variant of the LASSO implemented in Friedman et al. (2010) is

$$\minimize_{\beta \in \mathbb{R}^p} \frac{\|y - X\beta\|_2^2}{2\|X^Ty\|_\infty} + \lambda \|eta\|_1. \quad (45)$$
A randomized version of this is easily handled, changing the density to be proportional to

\[ f_\mu(y) \cdot g \left( \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - \frac{X^T(y - X_E \beta_E)}{||X^Ty||_\infty} + \lambda \begin{pmatrix} z_E \\ u_E \end{pmatrix} \right) \cdot \left| \det \left( \frac{X_E^T X_E + \epsilon I}{||X^Ty||_\infty} \right) \right| \]

and supported on the same set as in (42). Another variant Sabourin et al. (2014) replaces \( ||X^Ty||_\infty \) with a resampling based quantity median(\( X^Ty \)) resulting in a similar change in the sampling density.

**Remark 9.** Conditioning on Nuisance Statistics: As detailed in Fithian et al. (2014), we condition not just on the selection event \( B_{(E,z_E)} \), but also on the sufficient statistics corresponding to nuisance parameters to obtain optimal UMPU selective tests/ intervals. In such a case, the support for \( y \) in the selective sampling density is restricted to a set, denoted as \( D_{obs} \). This has been sketched for interested readers in A in the appendix.

### 4.2. The selective sampler is model agnostic: LASSO without parametric assumptions

Up this point, we have assumed so far that \( X \) is fixed and the law of \( y | X \) was from the parametric model \( \{ N(\mu, \sigma^2 I) : \mu \in \mathbb{R}^n \} \).

We now remove this assumption, assuming that the law \( F \) is now just a law for the pair \( (X,y) \in \mathbb{R}^{n \times p} \times \mathbb{R}^n \). A common assumption is the pairs model: \( (x_i, y_i) \overset{\text{iid}}{\sim} \tilde{F} \) for some distribution \( \tilde{F} \) on \( \mathbb{R}^p \times \mathbb{R}^n \), where \( x_i^T \) are the rows of \( X \).

While we keep this model in mind, it is not necessary in order to define the appropriate sampler. This section serves as an example of the sense in which our main result Theorem 1 is agnostic to the underlying statistical model.

In the notation established so far

\[ S = (X, y) \in \mathbb{R}^n \times \mathbb{R}^{n \times p}, \]

\[ \ell(\beta; (X, y)) = \frac{1}{2} ||y - X \beta||_2^2, \]

\[ P(\beta) = \lambda ||\beta||_1. \]

Therefore, we must sample from a density proportional to

\[ f(X, y) \cdot g \left( \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - X^T(y - X_E \beta_E) + \lambda \begin{pmatrix} z_E \\ u_E \end{pmatrix} \right) \cdot \left| \det(X_E^T X_E + \epsilon I) \right| \]

supported on

\[ \{(X, y, \beta_E, u_E) : \text{diag}(z_E) \beta_E > 0, ||u_E||_\infty \leq 1 \}. \quad (46) \]

In order to use this result for particular applications of inference, one may have to reduce the problem to sampling from a particular reference distribution perhaps by conditioning on appropriate sufficient statistics, as described in Appendix A.
4.3. Selective CLT: \( \ell_1 \)-penalized logistic regression

In this section, we describe an application of the selective CLT of Tian and Taylor (2015), applied to the case of logistic regression with random design matrix \( X \in \mathbb{R}^{n \times p} \) with rows \( x_i^T, i = 1, \ldots, n \). Suppose

\[
x_i \overset{iid}{\sim} F_X, \quad x_i \in \mathbb{R}^p, \quad y_i | x_i \sim \text{Bernoulli}(\pi(x_i^T b)),
\]

where \( \pi(x) = \exp(x)/(1 + \exp(x)) \) and \( b \in \mathbb{R}^p \) is unknown, \( p \) fixed, \( S = (X, y) \). With logistic loss,

\[
\ell(\beta; (X, y)) = -\frac{1}{\sqrt{n}} \left[ \sum_{i=1}^{n} y_i \log \pi(x_i^T \beta) + (1 - y_i) \log(1 - \pi(x_i^T \beta)) \right],
\]

we solve randomized \( \ell_1 \)-penalized logistic regression introduced in Tian and Taylor (2015),

\[
\min_{\beta \in \mathbb{R}^p} \ell(\beta; (X, y)) - \omega^T \beta + \frac{\epsilon}{2} \| \beta \|_2^2 + \lambda \| \beta \|_1.
\]

(47)

On the usual selection event of observing active set and signs \((E, z_E)\), the randomization reconstruction map is

\[
\phi_{(E, z_E)}(y, \beta_E, u_{-E}) = \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - \frac{1}{\sqrt{n}} X_T(y - \pi(x_E \beta_E)) + \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix}.
\]

And, the sampling density becomes proportional to

\[
f(X, y) \cdot g \left( \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - \frac{1}{\sqrt{n}} X_T(y - \pi(x_E \beta_E)) + \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix} \right) \cdot \left| \det \left( \frac{1}{\sqrt{n}} X_E^T W(X_E \beta_E) X_E + \epsilon I \right) \right|,
\]

(48)

where \( W(X) = \text{diag}(\pi(X)(1 - \pi(X))) \) is the Hessian matrix of the loss and the density above is supported on the same set as in (46). Sampling \((X, y)\) jointly is not feasible when \( F_X \) is unknown. Denoting \( \bar{\beta}_E = \arg\min_{\beta \in \mathbb{R}^{|E|}} -\frac{1}{\sqrt{n}} \sum_{i=1}^{n} y_i \log \pi(x_{E,i}^T \beta) + (1 - y_i) \log(1 - \pi(x_{E,i}^T \beta)) \),

(49)

the MLE for the unpenalized logistic regression with only the variables in \( E \), a Taylor series expansion of \( \nabla \ell(\beta; (X, y)) \) gives\(^2\)

\[
\nabla \ell(\beta; (X, y)) \approx \sqrt{n} \begin{pmatrix} Q(\beta_E - t_E) \\ -t_{-E} + C(\beta_E - t_E) \end{pmatrix}.
\]

\(^1\)With slight abuse of notation, we allow \( \pi : \mathbb{R}^n \to \mathbb{R}^n, x \mapsto \pi(x) \) to be the function applied on each coordinate of \( x \in \mathbb{R}^n \).

\(^2\)Alternatively, we might take \( \bar{\beta}_E \) to be the one-step estimator in the selected model starting from \( \beta_E \) Taylor and Tibshirani (2016).
Here, $t$ is the observed value of the random vector
\[
T = \left( \frac{1}{n} X^T E (\bar{\beta}_E) \right); 
\]
(50)
\[
Q = \frac{1}{n} X^T E W (X E \bar{\beta}_E) X_E \quad \text{and} \quad C = \frac{1}{n} X^T E W (X E \bar{\beta}_E) X_E. 
\]
With $p$ is fixed, pre-selected, $T$ properly scaled is asymptotically normal
\[
\sqrt{n} \left( T - \left( \frac{b_E}{\gamma_{-E}} \right) \right) \xrightarrow{D} N(0, \Sigma), 
\]
(51)
where $\Sigma$ is estimable from the data. When the selected parametric model is correct ($E \supseteq \text{supp } b$) we note that $\gamma_{-E} = 0$ and $\Sigma$ is in fact block-diagonal (Taylor and Tibshirani, 2016). When the selected parametric model is not correct, one can estimate this covariance nonparametrically, using bootstrap (see Section 7). Since asymptotically $T$ is from an exponential family with parameters $b_E$, we could base inference on $b_E$ by sampling from the distribution of $T$ instead of $(X, y)$.

In this case, the parametrization map becomes
\[
\psi_{(E, z_E)}(t, \beta_E, u_{-E}) = \left( t, \epsilon \left( \frac{\beta_E}{0} \right), \sqrt{n} \left( \frac{Q(\beta_E - t_E)}{-t_{-E} + C(\beta_E - t_E)} \right), \lambda \left( \frac{z_E}{u_{-E}} \right) \right), 
\]
(52)
with the domain $\mathbb{R}^p \times \mathbb{R}^{\vert E \vert} \times [-1, 1]^{p-\vert E \vert}$. Hence, the density we sample from is proportional to
\[
f(t) \cdot g \left( \epsilon \left( \frac{\beta_E}{0} \right), \sqrt{n} \left( \frac{Q(\beta_E - t_E)}{-t_{-E} + C(\beta_E - t_E)} \right), \lambda \left( \frac{z_E}{u_{-E}} \right) \right), 
\]
(53)
restricted on the domain of $\psi_{(E, z_E)}$, where $f$ here is the density of $\mathcal{N} \left( \begin{pmatrix} b_E \\ 0 \end{pmatrix}, \Sigma \right)$.

We note that, in order to construct a valid test about some linear functional of $b_E$ we can always condition on the observed $u_{-E}$ and $/ or \beta_E$ if we desire. The upside to such conditioning is that the sampling problem becomes easier, with the downside usually being a loss in selective power.

### 4.4. First step of forward stepwise

The Kac-Rice tests, described in Taylor et al. (2013) are based on the solution of
\[
\max_{\eta \in \mathcal{K}} \eta^T X^T y, \quad \text{where } y \sim F, 
\]
(54)
$X \in \mathbb{R}^{n \times p}$ is a fixed design, $K$ a convex set that can be stratified into smooth disjoint manifolds and the process $\eta^T X^T y$ is Morse for almost every $y \in \mathbb{R}^n$. The simplest example of such tests is one step of forward stepwise model selection, in which case $K$ is the $\ell_1$ ball of radius 1. In this case $X$ will be usually centered and scaled so that $X^T y$ corresponds to the marginal $Z$ statistics for $p$ different simple linear regressions.

Inference in this broad class of problems, for the global null, is based on the test statistic $\eta^* X^T y$, where

$$\eta^* = \arg\max_{\eta \in K} \eta^T X^T y,$$

with $K$ being the polar set of convex set $C$. Since, the null distribution of the above test statistic is intractable, we could instead provide inference based on the conditional law

$$\mathcal{L}\left(\eta^* X^T y \bigg| \eta^* = \arg\max_{\eta \in K} \eta^T X^T y\right).$$

With this brief description of inference based on Kac-Rice tests, we focus back on the randomized versions of the Kac-Rice objective in (54). The randomized objective is given by

$$\max_{\eta \in \mathbb{R}^p} \eta^T (X^T y + \omega) - I_K(\eta), \quad \text{where } y \times \omega \sim F \times G,$$

with $\omega \in \mathbb{R}^p$ and penalty manifests as the characteristic function of convex set $K$, that is

$$I_K(\eta) = \begin{cases} 0 & \text{if } \eta \in K, \\ \infty & \text{otherwise}. \end{cases}$$

Here we set $\epsilon = 0$, as the above optimization problem does always have a solution. Having $\epsilon > 0$ would allow for several variables to be selected.

As mentioned above, perhaps the simplest example of the randomized optimization problem in (56) is forward stepwise problem with a single step. Specifically, that is consider

$$\max_{\eta \in K} \eta^T (X^T y + \omega),$$

for

$$K = \{\eta \in \mathbb{R}^p : \|\eta\|_1 \leq 1\}.$$ 

The above optimization problem yields the optimal direction

$$\eta^*_j = \begin{cases} s^* & \text{if } j = j^* \\ 0 & \text{otherwise}, \end{cases}$$

for

$$j = 1, \ldots, p,$$

where

$$j^* = \arg\max_{1 \leq j \leq p} |X^T_j y + w_j|.$$
coordinate with the maximum absolute value, and
\[ s^* = \text{sign}(X^T_{j^*} y + w_{j^*}), \]
the corresponding sign. Thus, we condition on the first active direction (both \( s^* \) and \( j^* \)), which gives rise to selection event
\[ \hat{E}_{(s^*, j^*)} = \{(y, \omega) \in \mathbb{R}^n \times \mathbb{R}^p : \text{sign}(X^T_{j^*} y + \omega_{j^*}) = s^*, \]
\[ s^* (X^T_{j^*} y + \omega_{j^*}) \geq \max_{1 \leq j \leq p} |X^T_j y + \omega_j| \} \].

The subgradient equation yields the reconstruction map
\[ \phi_{(j^*, s^*)}(y, z) = z - X^T y, \]
where \( z \in \partial I_K(\eta^*) \), the set of sub-gradients to \( K \) at \( \eta^* \), given by the normal cone
\[ \partial I_K(\eta^*) = \{c(u_1, \ldots, u_{j^*} - 1, s^*, u_{j^*} + 1, \ldots, u_p) : u_i \in \mathbb{R}, |u_i| \leq 1, c > 0 \}. \]

We can reparametrize the set
\[ \left\{ (y, \omega, \beta, \alpha, z) \in \bar{S}_F^p (G, \epsilon = 0, \ell, P) : (y, \omega) \in \hat{E}_{(s^*, j^*)} \right\} \]
using
\[ \psi_{(s^*, j^*)}(y, z) = (y, z - X^T y, \eta^*, X^T y, z), \]
\( (\eta^*_j = s^* \mathbb{I}_{\{j = j^*\}}, j = 1, \ldots, p) \), with the domain \( \mathbb{R}^n \times \partial I_K(\eta^*) \).

With the above reparametrization, we sample \((y, z)\) from a density proportional to
\[ f(y) \cdot g(z - X^T y), \quad (57) \]
supported on \( \mathbb{R}^n \times \partial I_K(\eta^*) \).

**Remark 10.** The set of sub-gradients at \( \eta^* \) for \( s^* > 0 \) can be identified as the epigraph of the \( \ell_\infty \) norm (modulo a permutation of the maximum coordinate \( j^* \)) and for \( s^* < 0 \), \( \partial I_K(\eta^*) \) is the polar cone of the epigraph of \( \ell_1 \) norm.

**Remark 11.** Of course, it is usually of interest to take more than one step of forward stepwise. Inference after several steps of forward stepwise is considered in Tibshirani et al. (2014); Fithian et al. (2015). We consider several steps of forward stepwise in Section 6.

**Remark 12.** The data analyst may have some set of variables \( \bar{E} \) that she insists on controlling for. In this case, instead of just assuming \( X \) is centered, we might assume that \( P_{\bar{E}} X = X \) and its columns normalized, where \( P_{\bar{E}} \) denotes projection onto the column space of \( X_{\bar{E}} \). In this way, centering \( X \) corresponds to the common practice controlling for an intercept in the model.
Remark 13. Forward stepwise is also used in generalized linear models such as logistic regression. In this case, the quantity $X_T P_{E'} y$ that appears in the least squares setting can be replaced either by the Wald Z-statistics or the score Z-statistics. For example, for logistic regression, the score Z-statistics take the form

$$Z_j = \frac{X_T^j (y - \pi(X_{E'} \hat{\beta}_{E'}))}{(X_T^j W(X_{E'} \hat{\beta}_{E'}))^{1/2}}, \quad 1 \leq j \leq p$$

(58)

where $\hat{\beta}_{E'}$ is the unpenalized MLE for the model with variables $E'$ and

$$W(X_{E'} \hat{\beta}_{E'}) = \text{diag}(\pi(X_{E'} \hat{\beta}_{E'})(1 - \pi(X_{E'} \hat{\beta}_{E'})))$$

is a consistent estimate of the variance of $y$ under the model with variables $E'$. While this is the typical parametric estimate of variance forward stepwise would use, one might prefer using a jackknife or bootstrap estimate of this variance if one is unsure whether the model with variables $E'$ is correctly specified, as would be the case early on in building a model via forward stepwise. Using Wald type Z statistics would require fitting $p$ different logistic regression models which has some computational burden.

Having computed the $Z_j$'s one might then consider a randomized version of the problem

$$\max \sum_{i=1}^{p} |\eta_i|$$

$$\text{subject to } \|\eta\|_1 \leq c$$

and proceed as above with $S$ being the vector $Z$.

4.5. Marginal screening

Marginal screening computes marginal Z statistics

$$Z_j = \frac{X_T^j y}{\sigma \|X_j\|_2}$$

or T statistics

$$T_j = \frac{X_T^j y}{\sigma_j \|X_j\|_2}$$

for each of $p$ centered variables $X_j$ and thresholds their absolute value at some threshold, perhaps $z_{1-\alpha/2}$ where $\alpha$ is some nominal $p$-value threshold. This can be expressed in optimization form as

$$\min_{\|\eta\|_{\infty} \leq c} \frac{1}{2} \|\eta - T\|_2^2.$$

Selective inference in the nonrandomized setting for this problem was considered in (Lee and Taylor, 2014).

A natural randomized version would be

$$\min_{\|\eta\|_{\infty} \leq c} \frac{1}{2} \|\eta - T\|_2^2 - \omega^T \eta.$$
Conditioning on the set achieving the threshold \( c \) and their signs to be \((E, z_E)\), we see that this event is
\[
\{(T, \eta, z) : \eta_E = c \cdot z_E, \text{diag}(z_E)z_E \geq 0, \|\eta - E\|_{\infty} < c, z_{-E} = 0\} \tag{59}
\]
and the randomization reconstruction map becomes
\[
\phi_{(E, z_E)}(T, \eta_{-E}, z_E) = \left(\frac{c \cdot z_E}{\eta_E} - T + \left(\frac{z_E}{0}\right)\right).
\]
We thus sample \((y, X, \eta_{-E}, z_E)\) (or \((T, \eta_{-E}, z_E)\) if \(X\) is random) from a selective density proportional to
\[
f(T) \cdot g\left(\left(\frac{c \cdot z_E}{\eta_E} - T + \left(\frac{z_E}{0}\right)\right)\right) \tag{60}
\]
and supported on the event in (59), where \(f\) is the unselective law of \(T\). For logistic regression, one can replace the \(T\) statistics above with the score statistics as described in Remark 13.

### 4.6. Full model screening

Another possible way to screen variables is to threshold the coefficients from the output of an unpenalized, randomized selection program given by
\[
\min_{\beta \in \mathbb{R}^p} \frac{1}{2} \|y - X\beta\|^2_2 + \frac{\epsilon}{2} \|\beta\|^2_2 - \omega^T \beta, \quad ((X,y), \omega) \sim F \times G, \tag{61}
\]
Based on the solution \(\hat{\beta}((X,y), \omega)\), we define the threshold model \((E, z_E)\) as
\[
E = \{i : |\hat{\beta}_i((X,y), \omega)| \geq a\sigma\}
\]
and signs \(z_E = \text{sign}(\hat{\beta}_E((X,y), \omega))\), where \(a\) is a constant (e.g. \(1 - \alpha\) quantile of the standard normal or the \(t\)-distribution for some nominal level \(\alpha\)) and \(\sigma\) is the scaling. The canonical event of interest is
\[
B_{(E,z_E)} = \{\beta \in \mathbb{R}^p : |\beta_i| \geq a\sigma \forall i \in E, \|\beta_{-E}\|_{\infty} < a\sigma, \text{diag}(z_E)\beta_E > 0\}. \]
A parametrization of
\[
\{(X,\omega, \beta, \alpha, z) \in \tilde{S}^R_0(G, \epsilon, \ell, \mathcal{P}) : \beta \in B_{(E,z_E)}\}
\]
is given by
\[
\psi_{(E,z_E)}((X,y), \beta) = ((X,y), \epsilon\beta - X^T(y - X\beta), \beta, -X^T(y - X\beta), 0)
\]
with the domain
\[
D_{(E,z_E)} = \{((X,y), \beta) : \text{diag}(z_E)\beta_E > 0, |\beta_i| \geq a\sigma \forall i \in E, \|\beta_{-E}\|_{\infty} < a\sigma\}. \]
For the canonical event $B_{(E,z,E)}$, we therefore need to sample $((X,y),\beta)$ from a density proportional to

$$f(X,y) \cdot g\left(\epsilon\beta - X^T(y - X\beta)\right) \cdot \left| \det(X^TX + \epsilon I) \right|$$  \hspace{1cm} (62)$$

supported on $D_{(E,z,E)}$, where $f$ and $g$ are the densities of $F$ and $G$, respectively. If $X$ is random, the sampling of the data simplifies as in Section 4.3. The scaling $\sigma$ can be estimated as the variance of noise from the selected model with response $y$ and matrix of predictors $X_E$. As long as the estimate of $\sigma$ is consistent, we can treat it as a constant in the selection event, hence have the selection event as the polyhedral region.

### 4.7. Selective sampler based on a penalized MLE: Fisher’s exact selective test

In Section 2.1, we considered the pull-back of the unpenalized MLE for an exponential family. Allowing for penalization in the problem (19) as well as randomization yields programs of the form

$$\min_{\beta \in \mathbb{R}^p} \Lambda(\beta) - S^T\beta + \frac{\epsilon}{2}\|\beta\|_2^2 - \omega^T\beta + \mathcal{P}(\beta), \quad (S,\omega) \sim F \times G.$$  

We describe a version of Fisher’s exact test based on observing some function of the solution to the above program. As we saw in the LASSO, the penalty $\mathcal{P}$ is often chosen such that the solution set

$$\{(\beta,z) : z \in \partial\mathcal{P}(\beta)\}$$

possesses a nice stratification into a discrete collection of bundles $C$, the canonical example being the $\ell_1$ norm, or perhaps non-negative constraints. In particular, if $\mathcal{P}$ is the support function of some convex set $K$, then (4.7) is seen to be the normal bundle of $K$ which itself often has a nice stratification.

Fixing $C$ to be one of these strata, the subgradient equations of the optimization problem yields a reconstruction map

$$\phi_C(s,\beta,z) = \nabla\Lambda(\beta) - s + z + \epsilon \beta$$

where $(\beta,z) \in C$ and $s \in \text{supp}(F)$. In this case, the parametrization map of

$$\{ (s,\omega,\beta,\alpha,z) \in \tilde{S}_0(G,\epsilon,\ell,\mathcal{P}) : (\beta,z) \in C \}$$

becomes

$$\psi_C(s,\beta,z) = (s,\nabla\Lambda(\beta) - s + \epsilon\beta + z,\beta,\nabla\Lambda(\beta) - s, z)$$

and the sampling density proportional to

$$f(s) \cdot g(\nabla\Lambda(\beta) - s + \epsilon\beta + z) \cdot |J\phi_C(s,\beta,z)|$$

and restricted to $(s,\beta,z) \in M \times C$.  

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We now describe a stylized instance of such a problem used in the context of goodness-of-fit tests. Much of the effort in selective inference has been focused on finding tools for inference about specific parameters in a model, i.e. inference about statistical functionals $\theta : \mathcal{M} \to \mathbb{R}$. Two examples in the literature that employ such goodness-of-fit tests are Choi et al. (2014); Fithian et al. (2015).

In this case, we assume the data analyst will use the data to decide what sufficient statistics to use in constructing the goodness-of-fit test. Suppose our data $S$ is a Poisson process $N$ with points in $X$ and intensity measure modeled with density $d\lambda(\beta)d\mu(x) = \exp\left(\sum_{j=1}^{p} \beta_j h_j(x)\right)$ with respect to some reference probability measure $\mu$ on $X$.

If $X = [0, 1]$ and $h_j = 1_{[l_j, u_j]}$ were a collection of indicator functions, this would correspond to a change-point model. We might then use something like the fused LASSO in which we can take the intervals to be the step functions $[l_j, u_j] = [(j-1)/p, 1]$ or perhaps a multiscale approach as in Frick et al. (2014); Chan and Walther (2011); Rivera and Walther (2013) and use the penalty

$$P(\beta) = \sum_{j=1}^{p} \lambda_j |\beta_j|$$

a weighted $\ell_1$ penalty$^3$. Usually, the background rate is included in such a model by fixing $h_1$ to be the constant function 1. An unpenalized fit for this variable corresponds to its corresponding $\lambda$ being 0.

Depending on our choice of penalty, we might then solve the following randomized program

$$\min_{\beta \in \mathbb{R}^p} \Lambda(\beta) - \sum_{j=1}^{p} \left( \beta_j \int_X h_j(x) N(dx) \right) + P(\beta) + \frac{\epsilon}{2} \|\beta\|_2^2 - \omega^T \beta$$

where

$$\Lambda(\beta) = \log \left[ \int_X \left[ \exp\left(\sum_{j=1}^{p} \beta_j h_j(x)\right) - 1 \right] \mu(dx) \right].$$

Having solved the above problem, the data analyst now observes that $(\hat{\beta}(N, \omega), \hat{z}(N, \omega))$ are in some subbundle $C$ of the set of variable-subgradient pairs. When $P$ is a weighted $\ell_1$ penalty, the conditioning event

$$\{(N, \omega) : \hat{E}(N, \omega) = E, \hat{z}_{\hat{E}(N, \omega)} = z_E\}$$

where

$$\hat{E}(N, \omega) = \left\{ j : \hat{\beta}_j(N, \omega) \neq 0, \lambda_j > 0 \right\}$$

$^3$The multiscale approach described in Frick et al. (2014); Chan and Walther (2011); Rivera and Walther (2013) is formally a testing approach. The penalized version above was proposed in Tian et al. (2015) based on the dual of the test statistic in the multiscale literature.
are the selected penalized coordinates. The corresponding subbundle is the set
\[ C = \{ (\beta_E, \beta_U, z_{-E}) : \text{diag}(z_E)\beta_E \geq 0, \|z_{-E}\|_\infty \leq 1, \beta_U \in \mathbb{R}^U \} \]
where \( U = \{ j : \lambda_j = 0 \} \) is the set of unpenalized coordinates. With some abuse of notation, we write \( z = (z_E, z_U, z_{-E}) = (z_E, 0, z_{-E}) \) as the full subgradient where \( z_E \) are held fixed on \( C \) and \( z_U = 0 \) as these coordinates are unpenalized.

The data analyst now decides to test the null hypothesis
\[ H_{0,j|E} : \beta_j|E = 0, \quad j \neq 1 \]
in the model
\[ \log \lambda(\beta) = \sum_{j \in E} \beta_j \int_X h_j(x) \mu(dx). \]
Following the exponential family setup in Fithian et al. (2014), we might condition on the nuisance sufficient statistics
\[ \int_X h_i(x) N(dx), \quad i \in E \setminus j. \]
Assuming we have included a background rate in the model, this fixes the total number of points in the Poisson process to be \( N(X) \) the observed number of points.

If we had not used the data to select the intervals, conditioning on these sufficient statistics and resampling points is exactly Fisher’s exact test modulo the choice of test statistic. That is, the appropriate reference measure can be constructed by sampling from a Binomial process \( \tilde{N} \) with \( n = N(X) \) points and distribution \( \mu \) conditioned to satisfy
\[ \int_X h_i(x) \tilde{N}(dx) = \int_X h_i(x) N(dx), \quad i \in E \setminus j. \]
where the right hand side are the values observed in the data. When \( X \) is a discrete space, this is a generalization of Fisher’s exact test. Sampling for such problems has a fairly rich literature (c.f. (Diaconis and Sturmfels, 1998)). When \( X \) is Euclidean or a manifold, the conditioning event above corresponds to a subset of the configurations of \( N(X) \) points on \( X \) and is generally a nontrivial task. See (Diaconis et al., 2013) for further discussion and examples.

Having used the data to choose which sufficient statistics to use, we must use an appropriate selective distribution. Beyond just sampling \( \tilde{N} \) from the conditional density, we must sample \( (\beta_E, \beta_U, z_{-E}) \). Conditional on \( \tilde{N} \) we see that the appropriate density of the joint law with respect to the product of the law of \( \tilde{N} \) and \( p \)-dimensional Hausdorff measure on \( C \) is proportional to
\[ (\tilde{N}, \beta_E, \beta_U, z) \mapsto g \left( \nabla \Lambda(\beta) - \int_X h(x) d\tilde{N}(x) + \epsilon \cdot \beta + \text{diag}(\lambda) z \right) \]
with
\[ \nabla \Lambda(\beta) = \frac{\int_X h(x) \exp \left( \sum_{i \in E \cup U} \beta_i h_i(x) \right) \mu(dx)}{\int_X \exp \left( \sum_{i \in E \cup U} \beta_i h_i(x) \right) \mu(dx)} \]

For computational reasons, to evaluate the integrals over $\mathcal{X}$ above, it may be simpler to use a discretization of $\mathcal{X}$ as in Lindsey’s method Efron and Tibshirani (1996).

Finally, while we have considered using a weighted LASSO to choose the sufficient statistics, one might use a penalty with some curvature as well, requiring the modifications discussed in Section 5.

### 4.8. Graphical models

Gaussian graphical models are a popular way to study network structures. In particular, it has often been used on many types of genome data, e.g. gene expression, metabolite concentrations, etc. Specifically, consider the $p$-dimensional normally distributed random variable

$$X = (x_1, \ldots, x_p) \sim N(\mu, \Sigma).$$

It is of interest to study the conditional independence structure of the variables $\{1, 2, \ldots, p\}$. The conditional independence structure is conveniently represented by an undirectional graph $(\gamma, \mathcal{E})$, where the nodes are $\gamma = \{1, 2, \ldots, p\}$, and there is an edge $(i, j) \in \mathcal{E}$ if and only if $x_i \perp x_j$ conditional on all the other variables $\gamma \setminus \{i, j\}$. Moreover, assuming the covariance matrix $\Sigma$ is not singular, we denote the inverse covariance matrix $\Theta = \Sigma^{-1}$, then

$$x_i \perp x_j | X_\gamma \setminus \{i, j\} \iff \Theta_{ij} = 0.$$

In many applications of Gaussian graphical models, we assume the sparse edge structure, where we can hope to uncover the network structure even in the high-dimensional setting. We discuss applying the selective sampler to the graphical LASSO Friedman et al. (2008). Another graphical model selection, neighborhood selection, is discussed in Appendix C.

The randomized graphical LASSO with randomization $\omega \sim G$ is the convex program

$$\min_{\Theta : \Theta^T = \Theta, \Theta > 0} -\log \det(\Theta) + \text{Tr}((S - \omega)\Theta) + \lambda \mathcal{P}(\Theta), \quad (S, \omega) \sim F \times G, \quad (63)$$

where

$$\mathcal{P}(\Theta) = \sum_{(i, j) : i \neq j} |\Theta|_{ij}$$

and

$$S \in M_k = \{A : A^T = A, A \geq 0, \text{rank}(A) = k\}, \quad k \leq p.$$ 

Usually,

$$S = \frac{1}{n} X^T \left( I - \frac{1}{n} 11^T \right) X, \quad X \in \mathbb{R}^{n \times p}$$

for some data matrix so that $k$ is generically min$(n - 1, p)$. Note that $\Theta, S, \omega$ are $p \times p$ matrices.
The subgradient equations read as
\[
\omega = \tilde{\Theta}^{-1}(S, \omega) + S + \hat{z}(S, \omega),
\]
where \( \hat{z}(S, \omega) \in \partial \mathcal{P}(\tilde{\Theta}(S, \omega)) \). For \( E \subset \{ (i, j) : i \neq j \} \), the natural selection event of interest is
\[
S = \left\{ (S, \omega) : \exists \Theta = \tilde{\Theta}(S, \omega) \text{ s.t. } \text{sign}(\Theta_E) = z_E, \Theta_{(E \cap \{(i, j) : 1 \leq i \leq p\})} = 0 \right\},
\]
Owing to symmetry in \( \Theta \), on \( S \) we have
\[
\hat{z}_{ij}(S, \omega) = \frac{\partial \mathcal{P}(\tilde{\Theta}(S, \omega))}{\partial \Theta_{ij}} = \begin{cases} 
2\lambda s_{ij} & (i, j) \in E \\
0 & i = j \\
2\lambda u_{ij} & (i, j) \notin E \text{ and } i \neq j,
\end{cases}
\]
where
\[
u_{ij} = u_{ji} \text{ satisfies } \| u \|_\infty \leq 1 \text{ for } (i, j) \notin E, i \neq j,
\]
and
\[
s_{ij} = \text{sign}(\Theta_{ij}).
\]
Due to symmetry, we can parametrize \( \omega \) by the active elements in \( \Theta \) along with its diagonal elements (dimension \(|E|/2 + p\)) and the inactive elements of the penalty subgradient (dimension \((p^2 - |E|)/2\)), corresponding to the inactive elements, both restricted to the upper triangular part of \( \Theta \). To fix notations, denote
\[
E^* = \{(i, j) \in E : i \leq j \} \cup \{(i, j) : i = j \},
\]
the set of active coordinates in the upper triangular part of \( \Theta \) along with its diagonal elements.

This leads us to the following parameterization of \( \{(S, \omega, \Theta, \alpha, z) \in \tilde{S}_0(G, \epsilon = 0, \ell, \mathcal{P}) : (S, \omega) \in S\}
\]
\[
\psi_{(E, z_E)}(S, \Theta_{E^*}, u_{-E^*}) = (S, \Theta^{-1}(E^*) + S + z(u_{-E^*}), \Theta(E^*), \\
\Theta^{-1}(E^*) + S, z(u_{-E^*})),
\]
where \( \Theta(E^*) \) is the matrix with \( E^* \) entries from \( \Theta_{E^*} \) and zeroes elsewhere, \( z_{ij}(u) = 2\lambda (s_{ij} I_{(i, j) \in E} + u_{ij} I_{(i, j) \notin E, i \neq j}) \) and the domain of \( \psi_{(E, z_E)} \) is restricted to \( \| u_{-E^*} \|_\infty \leq 1 \).

The randomization reconstruction map can be written as
\[
\phi_{(E, z_E)}(S, \Theta_{E^*}, u_{-E^*}) = \Theta^{-1}(E^*) + S + z(u_{-E^*}).
\]
With this parametrization, we can sample from the density proportional to
\[
f(S) \cdot g(\Theta^{-1}(E^*) + S + z(u_{-E^*})) \cdot |J\psi(S, \Theta_{E^*}, u_{-E^*})|.
\]
and restricted to \( \| u_{-E^*} \|_\infty \leq 1 \). The computation of above Jacobian involves (see the Appendix of Taylor and Tibshirani (2016))
\[
\left( \frac{\partial \phi_{(E, z_E)}}{\partial \Theta_{ij}} \right)_{kl} = 2(\sigma_{il} \sigma_{jk} + \sigma_{ik} \sigma_{jl}) \text{ for } (i, j) \in E^*,
\]
\[
\left( \frac{\partial \phi(E,z_E)}{\partial u_{ij}} \right)_{kl} = 2\lambda \delta_{ik} \delta_{lj} \text{ for } (i, j) \notin E^*, i \leq j.
\]

where \( \sigma_{ij} \) are the elements of \( \Sigma \) and \( \delta_{ij} \) is Kronecker delta function.

The above computations give the \((k, l)\) coordinate of the \((i, j)\)th upper triangular matrix and as again, we simply restrict attention to \(\{(k, l) : k \leq l\}\), the upper triangular half of randomization map.

More polyhedral examples, as well as the generalized LASSO are presented in Appendix B.

5. Curvature

Up to now, our examples have been polyhedral in nature. In most examples above, the selection event was some part of the normal bundle of such a polyhedral convex set. Not all problems can be described by such polyhedral sets. In this section we give some examples with non-trivial curvature. As above, many of the interesting selection events are still parts of the normal bundle.

5.1. Projection onto a convex set

The problem of projection onto a closed convex set \( K \) is canonical example of a convex program. Hence, it seems to be a natural place to start to introduce curvature into our discussion. (Indeed two variants of the LASSO above can be expressed in terms of projection onto a convex set.) Let

\[
\ell(\beta; s) = \frac{1}{2} \| \beta - s \|_2^2
\]

\[
\mathcal{P}(\beta) = \begin{cases} 
0 & \beta \in K \\
\infty & \text{otherwise.}
\end{cases}
\]

In this case, with \( \epsilon = 0 \) the randomized program takes the form

\[
\text{minimize } \frac{1}{2} \| \beta - s \|_2^2 - \omega^T \beta.
\]

with solution

\[
\hat{\beta}(s, \omega) = \mathcal{P}_K(s + \omega),
\]

where \( \mathcal{P}_K \) is the Euclidean metric projection onto the set \( K \) (i.e. the projection with metric induced by the \( \ell_2 \) norm).

The subgradients to our penalty are

\[
\partial \mathcal{P}(\beta) = N_\beta(K),
\]

the normal cone of \( K \) at \( \beta \).

In this case, the subgradient equations take the form

\[
s + \omega = \beta + z, \quad \beta \in K, z \in N_\beta(K).
\]
The normal cone $N_\beta(K)$ can be parameterized by its unit vectors

$$S(N_\beta(K)) = \{ u \in N_\beta(K) : \| u \|_2 = 1 \}$$

and their length $r \in [0, \infty)$.

We can therefore draw from the joint distribution of $(s, \omega)$ with a density proportional to

$$f(s) \cdot g(\beta + r \cdot u - s) \cdot |J_\psi(\beta, r, u)|,$$

where

$$\psi(s, \beta, r, z) = (s, \beta + r \cdot u - s, \beta - s, r \cdot u) \quad \beta \in K, u \in S(N_\beta(K)), r \geq 0.$$

Integrating out $s$ yields the density

$$(f * g)(\beta + r \cdot u) \cdot |J_\psi(\beta, r, u)|,$$

where $f * g$ is the density of the convolution $F * G$.

The Jacobian here is recognizable as that in the Weyl-Steiner volume of tubes formula Weyl (1939); Hotelling (1939); Johnstone and Siegmund (1989); Takemura and Kuriki (2002); Sun (1993); Adler and Taylor (2007)

$$J_\psi(\beta, r, u) = \det (I + r \cdot C_{-u}) = \det (I + C_{-r \cdot u}),$$

where $C_\eta$ is the curvature matrix of $\partial K$ at $\beta$ in the direction $\eta$ normal to $\partial K$.

Suppose now $K$ is compact and that $F * G$ is the uniform distribution on $K \oplus \delta B_2$. This can be achieved by taking $F = \delta_0$, say and $G$ the uniform distribution itself. In this case, $\text{supp}(G) = K \oplus \delta B_2$ and we arrive at Weyl-Steiner’s tube formula

$$1 = \frac{1}{H_p(K \oplus \delta B_2)} \int_{\{ \beta : \beta + r \cdot u \in K \oplus \delta B_2 \}} J_\psi(\beta, r, u) \ d\beta \ dr \ du$$

$$= \int_0^\delta \left[ \int_{\partial K} J_\psi(\beta, r, u) \ d\beta \ du \right] \ dr.$$

The formula above must be interpreted as a sum over pieces or strata of $K$ of different dimensions so that $d\beta$ properly refers to Hausdorff measure of differing dimensions and the matrix in (65) is also of differing dimensions. We refer the readers to Takemura and Kuriki (2002); Adler and Taylor (2007) for further details and points of entry into the volume-of-tubes literature. When $K$ is a smooth body, i.e. its boundary is a differentiable $(p - 1)$-dimensional hypersurface then there is only stratum and the tube formula reads

$$H_p(K \oplus \delta B_2) = \int_0^\delta \int_{\partial K} J_\psi(\beta, r, \eta_\beta) \ d\beta \ dr,$$

where $\eta_\beta$ is the outward pointing unit normal vector field.

---

4: This parameterization is slightly different than our usual one, in that it constructs $s + \omega$ instead of $\omega$, but the difference is not important.
When \( F \ast G \) is not the uniform distribution on \( K \oplus \delta B_2 \) we might instead try to compute
\[
(F \ast G)(K \oplus \delta B_2) = \int_{(\beta,r,u):\beta+r \cdot u \in K \oplus \delta B_2} (f \ast g)(\beta + r \cdot u) \cdot J_\psi(\beta, r, u) \, d\beta \, dr \, du
\]
\[
= \int_{\delta} \left[ \int_{\delta} (f \ast g)(\beta + r \cdot u) \cdot J_\psi(\beta, r, u) \, d\beta \, du \right] \, dr.
\]
This problem is considered in some generality when \( f \ast g \) is a smooth density in Chapter 10 of Adler and Taylor (2007). When \( F \ast G = N(0, I_p) \), their probability, expanded in a power series in \( \delta \) plays an important role in the Gaussian Kinematic Formula Taylor (2006); Taylor and Adler (2009).

Unlike in the Weyl-Steiner formula, while the first steps are similar and are what Weyl said was something any student of calculus could do Weyl (1939), the above probability are not Riemannian invariants of \( K \) but depend on how the law \( F \ast G \) relates to \( K \).

While the connections to curvature measures and volume-of-tubes formulae are enlightening, we feel concrete examples are also very important. In this section, we consider the group LASSO as a canonical example of a statistical learning problem with curvature.

### 5.2. Forward stepwise with groups of variables: Kac-Rice with groups

This example is a generalization of the first-step of forward stepwise when we allow groups of variables to enter, and is a second example of the Kac-Rice test described above. Non-randomized approaches to this problem are considered in Loftus and Taylor (2014); Yang et al. (2016).

The randomized version of the Kac-Rice objective with a group LASSO penalty determined by a partition \( \{1, 2, \ldots, p\} = \bigcup_{g \in G} g \) can be written as
\[
\text{maximize } \eta^T (X^T y + \omega) - I_K(\eta), \ y \times \omega \in F \times H \tag{66}
\]
where
\[
K = \{ \eta \in \mathbb{R}^p : \sum_{g \in G} \lambda_g \| \eta_g \|_2 \leq 1 \}
\]
and \( I_K \) is the usual characteristic function of set \( K \). In this section we have denoted the law of \( \omega \) by \( H \) with density \( h \) to distinguish the density from the group index \( g \). In this case, the optimal \( \eta = \eta^* \) is given by
\[
\eta_g^* = \begin{cases} \frac{X_g^T y + \omega_g}{\lambda_g \| X_g^T y + \omega_g \|_2} & \text{if } g = g^* \\ 0 & \text{otherwise} \end{cases}
\]
where
\[
g^* = \arg\max_{g \in G} \frac{1}{\lambda_g} \| X_g^T y + \omega_g \|_2.
\]
Conditioning on the selection event
\[ \tilde{E}_g^* = \left\{ (y, \omega) : g^* = \arg\max_{g \in G} \| X^T g y + \omega_g \|_2 / \lambda_g \right\}, \]
the subgradient equation leads to the reconstruction map
\[
\omega = \phi_{g^*}(y, c, z_{g^*}, (z_g)_{g \neq g^*}) = -X^T y + c \left( z_{g^*} \right),
\]
subject to constraints
\[
c > 0, \| z_{g^*} \|_2 = \lambda_{g^*}, \| z_g \|_2 \leq \lambda_g \text{ for } g \neq g^*.
\]
Thus we sample \((y, c, z_{g^*}, (z_g)_{g \neq g^*})\) from a density proportional to
\[ f(y) \cdot h(cz - X^T y) \cdot c^{|g^*|-1} \]
and supported on
\[ \text{supp}(F) \times \mathbb{R}_+ \times \lambda_{g^*} S(\mathbb{R}^{|g^*|}) \times \prod_{g \in G, g \neq g^*} \lambda_g B_2(\mathbb{R}^{|g|}), \]
where \(\lambda_{g^*} S(\mathbb{R}^{|g^*|})\) is a sphere with radius \(\lambda_{g^*}\) in \(\mathbb{R}^{|g^*|}\) and \(\lambda_g B_2(\mathbb{R}^{|g|})\) is an \(\ell_2\) ball in \(\mathbb{R}^{|g|}\). The Jacobian here, is the determinant of the derivative of the map
\[
(z_{g^*}, c) \mapsto -X^T y + cz_{g^*},
\]
which equals \(\det \left( c V_{g^*} \cdot z_{g^*} \right) = \lambda_{g^*} c^{|g^*|-1}\), where \(V_{g^*} \in \mathbb{R}^{|g^*|} \times \mathbb{R}^{|g^*|} \) be an orthonormal basis completion of \(z_{g^*}\).

5.3. Group LASSO

As mentioned above, the LASSO (23) can be expressed in terms of metric projection, as can many problems when \(\ell\) is squared-error loss and \(P\) is either a (semi-)norm in or a constraint on a seminorm. When the seminorm is polyhedral the Jacobian in our parameterization typically depends only on the design matrix \(X\). If the unit ball of the seminorm is not polyhedral, the Jacobian of the parameterization involves a curvature term which depends on the design matrix \(X\).

We consider the group LASSO Ming and Lin (2005). The group LASSO norm, defined by a partition
\[ \bigcup_{g \in G} g = \{1, \ldots, p\} \]
and weights \((\lambda_g)_{g \in G}\) is defined as
\[ P(\beta) = P_{G, (\lambda_g)_{g \in G}}(\beta) = \sum_{g \in G} \lambda_g \| \beta_g \|_2, \quad (67) \]
where $\beta_g = \beta[g]$ are the coefficients in the $g$-th group.

The group LASSO problem is defined by

$$
\minimize_{\beta \in \mathbb{R}^p} \frac{1}{2} \| y - X\beta \|_2^2 + \sum_{g \in G} \lambda_g \| \beta_g \|_2. 
$$

(68)

Losses other than squared-error can of course be used with this penalty – it is the penalty that is the group LASSO. The square-root group LASSO Bunea et al. (2013) replaces the squared-error loss above with the $\ell_2$ loss $\| y - X\beta \|_2$.

The randomized version of the group LASSO is

$$
\minimize_{\beta \in \mathbb{R}^p} \frac{1}{2} \| y - X\beta \|_2^2 - \omega^T \beta + \frac{\epsilon}{2} \| \beta \|_2^2 + \sum_{g \in G} \lambda_g \| \beta_g \|_2 
$$

(69)

where $\omega \sim H$ with density $h$.

Having solved (69) with solution $\hat{\beta}(X, y, \omega)$, we define the set of active groups as

$$
\hat{E}(X, y, \omega) = \{ g : \hat{\beta}_g(X, y, \omega) \neq 0 \}.
$$

The canonical event of interest here is

$$
\{(X, y, \omega) : \hat{E}(X, y, \omega) = E \}.
$$

(70)

On this event, the subgradient equation gives the randomization reconstruction map

$$
\omega = \phi_E(y, (\beta_g)_{g \in E}, (z_h)_{h \in -E})
= (X^T X + \epsilon I) \left( \begin{array}{c} (\beta_g)_{g \in E} \\ 0 \end{array} \right) - X^T y + \left( \begin{array}{c} (\lambda_g \beta_g/\| \beta_g \|_2)_{g \in E} \\ (z_h)_{h \in -E} \end{array} \right),
$$

(71)

with the restriction on the inactive subgradients as

$$
\| z_h \|_2 \leq \lambda_h, \ h \in -E.
$$

We may choose to parameterize

$$
\{(y, \omega, \beta, \alpha, z) \in S^E_0(G, \epsilon, \ell, \mathcal{P}) : \beta_h = 0 \ \forall h \in -E \}
$$

in terms of $(y, (\beta_g)_{g \in E}, (z_h)_{h \in -E})$ as

$$
\psi_E(y, (\beta_g)_{g \in E}, (z_h)_{h \in -E})
= \left( y, (X^T X + \epsilon I) \left( \begin{array}{c} (\beta_g)_{g \in E} \\ 0 \end{array} \right) - X^T y + \left( \begin{array}{c} (\lambda_g \beta_g/\| \beta_g \|_2)_{g \in E} \\ (z_h)_{h \in -E} \end{array} \right), \left( \begin{array}{c} (\beta_g)_{g \in E} \\ 0 \end{array} \right),
\right.
- X^T \left( y - X^T \left( \begin{array}{c} (\beta_g)_{g \in E} \\ 0 \end{array} \right) \right) + \left( \begin{array}{c} (\lambda_g \beta_g/\| \beta_g \|_2)_{g \in E} \\ (z_h)_{h \in -E} \end{array} \right))
$$

with the restriction on the inactive subgradient

$$
(z_h)_{h \in -E} \in \prod_{h \in -E} \lambda_h B_2(\mathbb{R}^{|h|}),
$$

(72)
where $B_2(\mathbb{R}^{|h|})$ is the $\ell_2$ ball in $\mathbb{R}^{|h|}$. The density to sample from thus is proportional to
\begin{equation}
 f(y) \cdot g(\phi_E(y, (\beta_g)_{g \in E}, (z_h)_{h \in -E})) \cdot |D((\beta_g)_{g \in E}, (z_h)_{h \in -E})\phi_E|,
\end{equation}
restricted to (72). Denoting $M = \cup_{g \in E} g$, the set of active predictors, and their cardinality as $|M| = \sum_{g \in E} |g|$, where $|g|$ is size of each group, the non-trivial Jacobian term is precisely given by
\begin{equation}
 D((\beta_g)_{g \in E}, (z_h)_{h \in -E})\phi_E
 = \det \left( \begin{bmatrix}
 X_M^T X_M + \epsilon I + D_1 & 0_{|M| \times (p-|M|)} \\
 X_{-M}^T X_M & I_{p-|M|}
 \end{bmatrix} \right)
 = \det(X_M^T X_M + \epsilon I + D_1),
\end{equation}
where $D_1$ is a block diagonal matrices of the form
\begin{equation}
 D_1 = \text{diag} \left( \frac{\lambda_g}{\|\beta_g\|_2} \left( I - \frac{\beta_g \beta_g^T}{\|\beta_g\|_2^2} \right) \right)_{g \in E} \in \mathbb{R}^{|M| \times |M|}.
\end{equation}

Remark 14. For groups that are singletons ($|g| = 1$ for all $g \in G$), the matrix $D_1$ is zero as $\beta_g/\|\beta_g\|_2 \in \{1, -1\}$.

5.4. Conditioning on active directions in group LASSO

If we choose to condition additionally on the active directions
\begin{equation}
 \left\{ u_g = \frac{\beta_g}{\|\beta_g\|_2}, \ g \in E \right\},
\end{equation}
writing
\begin{equation}
 \beta_g = \gamma_g \cdot u_g, \ \gamma_g > 0, \quad g \in E; \\
 \|z_h\|_2 \leq \lambda_h, \quad h \in -E,
\end{equation}
we may express the reconstruction in (71) in terms of $(y, (\gamma_g)_{g \in E}, (z_h)_{h \in -E})$ as
\begin{equation}
 \phi_{(E,(u_g))}(y, (\gamma_g)_{g \in E}, (z_h)_{h \in -E})
 = (X^T X + \epsilon I) \begin{pmatrix} R \gamma_g u_g \end{pmatrix}_{g \in E} - X^T y + \begin{pmatrix} (\lambda_y u_g)_{g \in E} \\
 (z_h)_{h \in -E} \end{pmatrix}
\end{equation}
restricted to
\begin{equation}
 (y, (\gamma_g)_{g \in E}, (z_h)_{h \in -E}) \in \mathbb{R}^n \times (0, \infty)^{|E|} \times \prod_{h \in -E} \lambda_h B_2(\mathbb{R}^{|h|}).
\end{equation}

In this case the density we sample from is proportional to
\begin{equation}
 f(y) \cdot g(\phi_{(E,(u_g))}(y, (\gamma_g)_{g \in E}, (z_h)_{h \in -E})) \cdot |D((\gamma_g)_{g \in E}, (z_h)_{h \in -E})\phi_{(E,(u_g))}|,
\end{equation}
restricted to (72).
restricted to support above. The Jacobian of the map in this case can be computed as polynomial in \((\gamma_g)_{g \in E}\) by taking a geometric approach outlined below. Hence, conditioning further on the active directions allows us to sample from a log-concave density.

To see an explicit computation of the Jacobian, let \(V_g \in \mathbb{R}^{|g| \times (|g|-1)}\), \(g \in E\), denote a matrix whose columns are orthonormal and orthogonal to \(u_g\) and set

\[
V = \text{diag}((V_g)_{g \in E}) \in \mathbb{R}^{|E| \times (|E|-1)}, \quad U = \text{diag}((u_g)_{g \in E}) \in \mathbb{R}^{|E| \times |E|}.
\]

Finally set

\[
\Gamma = \text{diag}((\gamma_gI_{|g|})_{g \in E}) \in \mathbb{R}^{|M| \times |M|}.
\]

The Jacobian is the derivative of the map

\[(U, \gamma) \mapsto \nabla \tilde{\ell}(\Gamma U) + \Lambda U,
\]

where

\[
\nabla \tilde{\ell}(\Gamma U) = (X_M^T X_M + \epsilon I_{|M|}) \Gamma U,
\]

and

\[
\Lambda = \text{diag}((\lambda_gI_g)_{g \in E}) \in \mathbb{R}^{|M| \times |M|}.
\]

Differentiating first with respect to \(V\) (i.e. tangent to \(U\)) and then \(\gamma\), the derivative can be written as

\[
((\nabla^2 \tilde{\ell}(\Gamma U) + \Lambda)V \nabla^2 \ell(\Gamma U)U) = (\nabla^2 \tilde{\ell}(\Gamma U)\Gamma + \Lambda V V^T) (V \Gamma^{-1} U).
\]

Since \(\tilde{\ell}\) is quadratic, \(Q = \nabla^2 \ell(\Gamma U) = X_M^T X_M + \epsilon I_{|M|}\) does not involve \(\Gamma U\), the determinant of the above expression is equivalent to

\[
\det \left( \begin{pmatrix} V^T & U^T \end{pmatrix} Q^{-1} \begin{pmatrix} (Q \Gamma + \Lambda) & V \end{pmatrix} \right).
\]

Letting

\[
\Gamma^- = \text{diag}((\gamma_gI_{|g|-1})_{g \in E}), \quad \bar{\Gamma} = \begin{pmatrix} \Gamma^- & 0 \\ 0 & I_{|E|} \end{pmatrix},
\]

the Jacobian reduces to computing

\[
\det \left( \begin{pmatrix} \Gamma^- & 0 \\ 0 & \Gamma^{-1} \end{pmatrix} \begin{pmatrix} V^T Q^{-1} \Lambda V & 0 \\ Z^T Q^{-1} \Lambda V & 0 \end{pmatrix} \right) = \det (\Gamma^- + V^T Q^{-1} \Lambda V).
\]

Conditioning on \(U\) is now straightforward as \(V\) will then be fixed in the above density.

---

5 Since we condition on the active directions, \(U\) and \(V\) are fixed matrices hence \((V \ U)^T Q^{-1}\) is fixed as well.
5.5. General geometric approach

More generally, one can take a geometric approach to obtain the Jacobian, even when we do not condition on the active directions.

For the group LASSO, in computing the Jacobian it is convenient to assume that $\ell$ is somewhat arbitrary but twice-differentiable and to introduce a new Riemannian metric on the fiber of optimization variables $((\gamma_g)_{g \in E}, (z_g)_{g \in E})$ over the data point $s$. The convenience is that the structure of the Jacobian is similar for many problems in which the penalty is a seminorm appearing in Lagrange form. We expect a similar formula to hold when the penalty is a seminorm appearing in bound form. In the interest of space, we do not pursue this here.

The Riemannian metric we use is the pull-back of the following metric on $\mathbb{R}^p$:

$$
(V_\beta, Z_\beta)_{(s, \beta)} = V_\beta^T \left( \nabla^2 \ell(\beta; s) + \epsilon I \right)^{-1} Z_\beta.
$$  \hfill (77)

With $\epsilon = 0$ and $\ell$ the log-likelihood of an exponential family, in local coordinates the above metric is inverse of the observed information metric \textit{Efron and Hinkley} (1978) evaluated at the point estimate $\beta$. It is perturbed by $\epsilon$ times the Euclidean metric above as we have modified our convex program in randomizing it.

For the group LASSO, we then now differentiate the parameterization in coordinates $\gamma_E, (z_g)_{g \in G}$. The main reason for introducing this metric is that the image tangent vectors in the face

$$
\mathcal{F} = \left( \prod_{g \in E} \lambda_g \cdot S(\mathbb{R}^{|g|}) \right) \times \left( \prod_{h \in -E} \lambda_h B_2(\mathbb{R}^{|h|}) \right)
$$

remain orthogonal to the normal vectors $\sum_{g \in E} \gamma_g z_g$. The next theorem derives the Jacobian when curvature component is present in the geometry.

\textbf{Theorem 2} (Jacobian meta-theorem). Consider the randomized version of the problem

$$
\min_{\beta \in \mathbb{R}^p} \ell(\beta; S) + \|\beta\|
$$

for some $F$-a.s. twice-differentiable convex $\ell$ and some seminorm

$$
\|\beta\| = \sup_{z \in K} \beta^T z.
$$

Let

- $\mathcal{F}$ be a smooth face of $K$;
- $(\eta_i)_{i \in I}$ be an orthonormal (in the Euclidean metric) frame field normal to $\mathcal{F}$;
- $(V_j)_{j \in A}$ be an orthonormal (in the Euclidean metric) frame field tangent to $\mathcal{F}$,
and let $\psi$ denote the parameterization
\[
\psi(s, z, \gamma) = \nabla \ell(\beta(z, \gamma); s) + \epsilon \cdot \beta(z, \gamma) + z
\]
restricted to $N(F)$ with $\beta(z, \gamma) = \sum_{i \in I} \gamma_i \eta_i$. Then,
\[
\langle \eta_i, \frac{\partial}{\partial \gamma_i} \psi \rangle_{(s, \beta)} = \delta_{il}
\]
and
\[
\langle V_j, \frac{\partial}{\partial \gamma_i} \psi \rangle_{(s, \beta)} = 0
\]
(78)
where $S_\eta$ is the shape operator of $F$ as it sits in $\mathbb{R}^p$. Finally,
\[
J\psi(s, z, \gamma) = \det(\nabla^2 \ell(\beta; s) + \epsilon \cdot I) \cdot \det(G(s, z, \gamma) + C_{-\beta}(z, \gamma))
\]
\[
= \det(I + G(s, z, \gamma)^{-1} C_{-\beta}(z, \gamma)) / \det(H(s, z, \gamma)),
\]
(79)
where $G(s, z, \gamma)_{jk} = \langle V_j, V_k, z \rangle_{(s, \beta)}$
\[
H(s, z, \gamma)_{il} = \langle P_{(s, \beta)}^\perp \eta_i, z, P_{(s, \beta)}^\perp \eta_l, z \rangle_{(s, \beta)},
\]
where $P_{(s, \beta)}^\perp$ is projection orthogonal to the tangent space of $F$ in the metric (77) and $C_{-\beta}(z, \gamma)$ is the Euclidean curvature matrix of $F$ in the basis $V_i, 1 \leq i \leq \dim(F)$.

Proof. The reconstruction map reads
\[
\omega = \nabla \ell \left( \sum_i \gamma_i \eta_i; s \right) + \epsilon \left( \sum_i \gamma_i \eta_i \right) + z
\]
with the constraint $\sum_i \gamma_i \eta_i$ is normal to $K$ at $z \in F$. We now compute
\[
\frac{\partial}{\partial \gamma_i} \psi(s, z, \gamma) = \left( \nabla^2 \ell \left( \sum_i \gamma_i \eta_i; s \right) + \epsilon \cdot I \right) \eta_i
\]
\[
V_j \psi(s, z, \gamma) = \left( \nabla^2 \ell \left( \sum_i \gamma_i \eta_i; s \right) + \epsilon \cdot I \right) V_j \left( \sum_i \gamma_i \eta_i \right) + V_j.
\]
This is enough to establish (78). Now, the determinant we want to compute is the determinant of the matrix
\[
\begin{pmatrix}
V \psi & \frac{\partial}{\partial \gamma_i} \psi
\end{pmatrix}
\]
where $V \psi$ is the matrix whose columns are $V_j \psi$, and $\frac{\partial}{\partial \gamma_i} \psi$ is the matrix whose columns are $\frac{\partial}{\partial \gamma_i} \psi$. 
Factoring out $\nabla^2 \ell (\sum_i \gamma_i \eta_i; s) + \epsilon I$ and then multiplying by the orthogonal matrix 
\[
\begin{pmatrix}
V^T \\
\gamma^T
\end{pmatrix}
\]
shows that the determinant we want to compute is $\det(\nabla^2 \ell (\beta; s) + \epsilon I)$ times the determinant of the matrix
\[
\begin{pmatrix}
S_{-\beta}(V_j, V_k) + \langle V_j, V_k \rangle_{(s,\beta)} & 0 \\
\vdots & I
\end{pmatrix}.
\]
Relation (79) now follows, with the second display simply a familiar formula for the determinant expressed in block form
\[
\det(\nabla^2 \ell (\beta; s) + \epsilon \cdot I)^{-1} = \det(G(s, z, \gamma)) \cdot \det(H(s, z, \gamma)).
\]
When the loss is quadratic, or we use a quadratic approximation for the loss, we see that if we condition on $z$, then the term $\det(H(s, z, \gamma))$ is constant and only the first term must be computed. \hfill \square

**Remark 15.** We note that while $\mathcal{F}$ may not be convex, when $\ell$ is quadratic (or a quadratic approximation is used for inference) and we condition on $z$ the distribution for inference is log-concave in $\gamma$. More generally, if $f$ is log-concave in $s$ as well, then the relevant distribution of $(s, \gamma)|z$ is jointly log-concave in $(s, \gamma)$.

This general theorem can be applied to compute the Jacobian of the group LASSO with a parametrization in terms of the active and inactive directions and the magnitudes of active coefficients. We refer the readers to Appendix D for a rederivation of this Jacobian using the above geometric perspective.

**6. Multiple views of the data**

Often, an analyst might try fitting several models to a data set. These models might have different numbers of parameters, and different objective functions. Examples include fitting a regularization path \cite{Friedman2010} or stability selection \cite{Meinshausen2010}.

Nevertheless, if each model is an instance of (33), then there is a straightforward procedure to construct a selective sampler.

Given a collection $(G, \epsilon, \ell, P)_{i \in I}$, the appropriate density is proportional to
\[
f(s) \cdot \left( \prod_{i \in I} g_i(\epsilon_i \beta_i + \alpha_i + z_i) \cdot J \psi_i(s, \beta_i, \alpha_i, z_i) \right)
\]
supported on some subset of
\[
\bigcup_{s \in \text{supp}(F)} \left( \prod_{i \in I} \{ (\beta_i, \alpha_i, z_i) : \beta_i \in \mathbb{R}^{p_i}, \alpha_i \in \partial \ell_i(\beta_i; s), z_i \in \partial P_i(\beta_i) \} \right).
\]
This set has the form of a bundle with base space \( \text{supp}(F) \) and fibers as described above. Typically, each \( \psi_i \) will be restricted to some canonical event \( B_i \). For example, in something similar to stability selection, each \( B_i \) might identify the set of variables and signs chosen by the \( i \)-th randomized LASSO program.

We see that given \( s \), the variables in the fiber are independent. Hence, these can be sampled in parallel. For instance, on different machines initiated with the same random seed, we can sample \( s \) IID from density \( f \), then run Gibbs or other samplers to sample \((\beta_i, \alpha_i, z_i)\).

### 6.1. Multiple steps of forward stepwise

As an example, we consider taking \( K \) steps of forward stepwise. The Kac-Rice test can be extended to \( K \) steps of forward stepwise, where the selection event is characterized by a sequence of indices with the corresponding signs that constitute the active set at step \( K \). To make it more explicit, say we consider a sequence of active variables \((j_1, \ldots, j_K)\) with corresponding signs \((s_1, s_2, \ldots, s_K)\), in the order in which the randomized variables enter the model. The \( k \)-th optimization in the set of \( K \) optimizations can be written as

\[
\max_{\eta \in \mathbb{R}^{p-k+1}} \eta^T (X^T_{-A_{k-1}} P_{A_{k-1}} y + \omega_k) - I_{K_k}(\eta), \quad \text{where } y \times \omega_k \sim F \times G_k, \tag{81}
\]

\( A_k = \{j_1, j_2, \ldots, j_k\} \) is the active set including the \( k \)-th step, \( X_{-A_k} \) are the columns of \( X \) except for the ones corresponding to the current active set \( A_k \), the characteristic function

\[
I_{K_k}(\eta) = \begin{cases} 0 & \text{if } \eta \in K_k \\ \infty & \text{otherwise} \end{cases}
\]

and

\[
K_k = \{\eta \in \mathbb{R}^{p-k+1} : \|\eta\|_1 \leq 1\}.
\]

Here, \( \{\omega_k\}_{k=1}^{K} \) is a sequence of independent randomization variables with \( \omega_k \) coming from a given distribution \( G_k \) in \( \mathbb{R}^{p-k+1} \) and corresponding density \( g_k \).

The projection \( P_{A_k} \) is onto \( X_{A_k} \) and \( P_{A_k}^\perp \) is the residual after this projection. The selection event after \( K \) steps can be written as

\[
\hat{E}_{\{(s_k, j_k)\}_{k=1}^{K}} = \left\{ (y, \{\omega_k\}_{k=1}^{K}) \in \mathbb{R}^n \times \prod_{k=1}^{K} \mathbb{R}^{p-k+1} : \text{sign}(X_{j_k}^T P_{A_{k-1}}^\perp y + \omega_{k,j_k}) = s_k, \right. \\
\left. s_k(X_{j_k}^T P_{A_{k-1}}^\perp y + \omega_{k,j_k}) \geq \max_{j \in A_{k-1}} |X_j^T P_{A_{k-1}}^\perp y + \omega_{k,j}|, k = 1, \ldots, K \right\}.
\]

The randomization reconstruction map for the \( k \)-th step, from the subgradient equation is given by

\[
\phi_k(y, z_k) = -X^T_{-A_{k-1}} P_{A_{k-1}}^\perp y + z_k.
\]
where, sub-differential $z_k \in \mathbb{R}^{p-k+1}$ from the $k$-th step is restricted to

$$z_k \in \partial I_{K_k}(\eta^*_k),$$

and $\eta^*_k \in \mathbb{R}^{n-k+1}$ is the optimal solution for the $k$-th optimization, as stated in (81). More explicitly, the normal cone is given by

$$\partial I_{K_k}(\eta^*_k) = \{ c \cdot u : u \in \mathbb{R}^{p-k+1}, u_j = s_k, |u_j| \leq 1 \forall j \in A_{k-1}, c > 0 \}. \quad (82)$$

The sampler density is thus proportional to

$$f(y) \cdot \prod_{k=1}^K g_k (z_k - X^T - A_{k-1} P_{A_{k-1}} y), \quad (83)$$

supported on

$$(y, z_1, \ldots, z_k) \in \mathbb{R}^n \times \prod_{k=1}^K \partial I_{K_k}(\eta^*_k).$$

For logistic regression, one can replace the $T$ statistics above with the score statistics as described in Remark 13.

Further examples of algorithms that choose a variable based on multiple views of the data are presented in Appendix E.

7. Selective sampling via projected Langevin

In the examples above, we sample from a joint density of data $S \in \mathbb{R}^n$ and optimization variables $T \in \mathbb{R}^p$, from a probability space on $(S, T)$, achieved via a reparametrization. The selective sampler now samples from a pull back measure on a transformed probability space under a reconstruction map for randomization $\omega$. This idea implemented on randomized convex programs typically allow us to sample from a joint density that is supported on a relatively simpler region.

On a canonical selection event $B(E, z_E)$, defined by the active variables $E$ and their signs/directions $z_E$, the joint sampling density is

$$h(s, t) \propto f(s) \cdot g(\phi(E, z_E)(s, t)) \cdot |D_t \phi(E, z_E)(s, t)| \cdot 1_{D(E, z_E)}(s, t), \quad (84)$$

supported on constraint set $D(E, z_E) \subset \mathbb{R}^n \times \mathbb{R}^p$, under reconstruction map $\phi(E, z_E)$.

When we consider

$$f(s) \propto \exp(-\tilde{f}(s)) \quad \text{and} \quad g(\omega) \propto \exp(-\tilde{g}(\omega)),$$

the negative of logarithm of the sampling density is proportional to

$$\tilde{h}(s, \phi(E, z_E)(s, t)) = -\tilde{f}(s)) + \tilde{g}(\phi(E, z_E)(s, t)) - \log |D_t \phi(E, z_E)(s, t)| \quad (85)$$
supported on set $D_{(E,z_E)}$.

We sample from the target density $\tilde{h}$ using updates from a projected Langevin random walk.

**Projected Langevin Updates**

**Iterative update $[k+1]$**: The $(k+1)$ update based on previous update $(s^{(k)}, t^{(k)})$ is given by

$$
\begin{aligned}
(s^{(k+1)}, t^{(k+1)}) &= \mathcal{P} \left( s^{(k)}, t^{(k)} - \eta \left( \nabla_s \tilde{h}(s^{(k)}, \phi(E,z_E)(s^{(k)}, t^{(k)})) \right) + \sqrt{2\eta} \left( \xi_1^{(k)}, \xi_2^{(k)} \right) \right)
\end{aligned}
$$

for step-size $\eta, \xi_1^{(k)} \times \xi_2^{(k)} \sim \mathcal{N}(0, I_n) \times \mathcal{N}(0, I_p)$ and $\mathcal{P}$ is projection onto set $D_{(E,z_E)}$.

Computing the $(k+1)$ update based on previous update $(s^{(k)}, t^{(k)})$ thus involves two steps:

1: Computing gradient of the negative of log density w.r.t. $(s, t)$, that is

$$
\begin{aligned}
&\nabla_s \tilde{h}(s^{(k)}, \phi(E,z_E)(s^{(k)}, t^{(k)})) \\
&\nabla_t \tilde{h}(s^{(k)}, \phi(E,z_E)(s^{(k)}, t^{(k)}))
\end{aligned}
$$

2: Compute projection of update from a noisy version of gradient descent of the log density

$$
\begin{aligned}
&s^{(k)} - \eta \left( \nabla_s \tilde{h}(s^{(k)}, \phi(E,z_E)(s^{(k)}, t^{(k)})) \right) + \sqrt{2\eta} \left( \xi_1^{(k)}, \xi_2^{(k)} \right) \\
&\text{onto constraint set } D_{(E,z_E)}.
\end{aligned}
$$

When $\tilde{h}(s, \phi(E,z_E)(s, t))$ is a convex function on restriction $D_{(E,z_E)}$ and satisfies smoothness properties

$$
\left| \nabla \tilde{h}(s_1, \omega_1) - \nabla \tilde{h}(s_2, \omega_2) \right| \leq \beta \left| (s_1, \omega_1) - (s_2, \omega_2) \right|
$$

$$
\left| \nabla \tilde{h}(s_1, \omega_1) \right| \leq C,
$$

for all $(s_1, \omega_1), (s_2, \omega_2) \in D_{(E,z_E)}$, and the support $D_{(E,z_E)}$ is convex with non-empty interior and contained in a finite Euclidean ball, the projected Langevin sampler indeed converges to the target density in (84) as proved in Bubeck et al. (2015).

**Remark 16.** For most examples, data $S$ is sampled from a Gaussian density, in which case, $\nabla \tilde{f}$ is unbounded. One should be able to remove this condition by considering a restriction of $\tilde{f}$ to a bounded set of probability close to 1 under Gaussian density $f$.

**Remark 17.** The choices for randomizations typically include a Gaussian, Laplacian or Logistic distribution. Under a Logistic density, $\tilde{g}$ is seen to satisfy the smoothness conditions. Qualitatively, our samples do not change much with any of these choices of randomization.

---

6Tian and Taylor (2015) use heavy-tailed distributions such as Laplace or logistic as choices for randomization.
Remark 18. Typically, the support set $D_{(E,z_E)}$ is convex, but not bounded. We could again remove the boundedness condition on $D_{(E,z_E)}$, by considering a compact subset of probability close to 1 under sampling density $h$.

7.1. Examples

We revisit few examples like the LASSO with fixed and random design, the Kac-Rice with forward stepwise, the $\ell_1$-penalized Logistic to implement the projected Langevin sampler. We offer inference on the parameters in the selected model $E$ conditional on the canonical selection event $B_{(E,z_E)}$ and their signs/ directions, obtained upon solving the corresponding randomized programs. We base our tests on the randomized pivot, developed in Tian and Taylor (2015) for selective inference in a randomized setting.\footnote{To construct the pivots from Tian and Taylor (2015) we can either integrate over the null statistic or condition on it. In the case of LASSO or $\ell_1$-penalized logistic with random design, the null statistic is $T_{E,E}$ defined in (50). In the case of LASSO with fixed $X$, the null statistic is $X_{E}^Tb$. Here we report the results where we integrate over the null statistic (conditioning on the null is easier computationally since it reduces the size of the sampling space).}

Example 7.1. LASSO with fixed design (Section 4.1): The response $y$ is modeled as $\mathcal{N}(Xb,\sigma^2)$ with $|\text{supp}(b)| = s$ and $\sigma^2 = 1$. We test the null hypothesis $H_0 : b_{E,j} = 0$, $b_{E,j}$ denoting the $j$-th coefficient in the selected model $E$, conditioning on the selection event $B_{(E,z_E)}$ and sufficient statistics $P_{E \setminus j}y$, corresponding to nuisance parameters as discussed in A. Thus, the sampling density is proportional to (44) on the support

$$\{ (y, \beta_E, u_{-E}) : P_{E \setminus j}y = Y_{obs}, \text{diag}(z_E)\beta_E > 0, \|u_{-E}\|_\infty \leq 1 \}$$

The updates from projected Langevin sampler can be written as

$$\begin{pmatrix} \hat{y}^{(k+1)} \\ \beta_E^{(k+1)} \\ u_{-E}^{(k+1)} \end{pmatrix} = \begin{pmatrix} y^{(k)} - \eta \hat{y}^{(k)} / \sigma^2 - \eta \nabla y \hat{g}(\phi_{(E,z_E)}(y^{(k)}, \beta_E^{(k)}, u_{-E}^{(k)})) + \sqrt{2}\eta \xi_1^{(k)} \\ \mathcal{P}_1 \left( \beta_E^{(k)} - \eta \nabla \beta_E \hat{g}(\phi_{(E,z_E)}(y^{(k)}, \beta_E^{(k)}, u_{-E}^{(k)})) + \sqrt{2}\eta \xi_2^{(k)} \right) \\ \mathcal{P}_2 \left( u_{-E}^{(k)} - \eta \nabla u_{-E} \hat{g}(\phi_{(E,z_E)}(y^{(k)}, \beta_E^{(k)}, u_{-E}^{(k)})) + \sqrt{2}\eta \xi_3^{(k)} \right) \end{pmatrix},$$

where $(\xi_1^{(k)}, \xi_2^{(k)}, \xi_3^{(k)}) \sim \mathcal{N}(0, I_s) \times \mathcal{N}(0, I_{|E|}) \times \mathcal{N}(0, I_{p-|E|})$ and independent of everything else and $\mathcal{P}_1$ is projection onto the orthant $\mathbb{R}_{z_E}^{|E|}$ and $\mathcal{P}_2$ is the projection onto the cube $[-1,1]^{p-|E|}$. The conditioning on nuisance statistic is implemented by fixing $P_{E \setminus j}y$ with the update being

$$y^{(k+1)} = Y_{obs} + \mathcal{P}_{E \setminus j}^\perp \hat{g}^{(k+1)},$$

where $\mathcal{P}_{E \setminus j}$ is the projection onto the column space of $X_{E \setminus j}$.

Example 7.2. $\ell_1$-penalized logistic & LASSO with random design matrix (Section 4.3): In $\ell_1$-penalized logistic the response $y$ is modeled as i.i.d. Bernoulli$(\pi(x_i^Tb))$, with $|\text{supp}(b)| = s$, with the same null hypothesis as above. In the case of LASSO
with random design, the response is modeled as \( y \sim \mathcal{N}(Xb, \sigma^2I_n) \) with \( \sigma^2 = 1 \). If we denote as \( \hat{\beta}_E \) the unpenalized MLE using only selected covariates \( X_E \) in the respective problems, then we can describe the inference for both problems at once. We sample from the selective density in (53), supported on

\[
\{(t, \beta_E, u_{-E}) : \mathcal{P}_{E \setminus j} t = T_{obs}, \text{diag}(z_E)\beta_E > 0, \|u_{-E}\|\infty \leq 1\},
\]

conditioning again on selection event \( B_{(E,z_E)} \) and nuisance statistics. Here, \( \mathcal{P}_{E \setminus j} \) is the projection onto the column space of \( \begin{pmatrix} \hat{\Sigma}_{E,E} & 0 \\ 0 & 0 \end{pmatrix} \) and the nuisance statistic equals

\[
\mathcal{P}_{E \setminus j} T = \hat{\Sigma}_{E,E}\hat{\beta}_E
\]

where \( \Sigma_{E,E} \) is the covariance of \( \hat{\beta}_E \) (we use a bootstrap estimate of this covariance in the shown results) and \( \hat{\Sigma}_{E,E} = \Sigma_{E,E} - \Sigma_{E,E,E,E,E,E,j} / \Sigma_{E,j,E,E,E,j} \). The updates in the projected Langevin sampler are

\[
\left( \hat{t}^{(k+1)}, \hat{\beta}_E^{(k+1)}, u_{-E}^{(k+1)} \right) = \left( \hat{t}^{(k)} - \eta \hat{\Sigma}^{-1} (t^{(k)} - \eta \hat{\Sigma} g(\hat{\phi}_E, z_E)(t^{(k)}, \beta_E^{(k)}, u_{-E}^{(k)})) + \sqrt{2\eta} \xi_1^{(k)} ), \right.
\]

\[
\left. \quad \mathcal{P}_1 \left( \beta_E^{(k)} - \eta \sqrt{\beta_E g(\hat{\phi}_E, z_E)(t^{(k)}, \beta_E^{(k)}, u_{-E}^{(k)})) + \sqrt{2\eta} \xi_1^{(k)} \right) \right)
\]

\[
\left( u_{-E}^{(k)} - \eta \sqrt{u_{-E} g(\hat{\phi}_E, z_E)(t^{(k)}, \beta_E^{(k)}, u_{-E}^{(k)})) + \sqrt{2\eta} \xi_2^{(k)} \right)
\]

where \( (\xi_1^{(k)}, \xi_2^{(k)}, \xi_3^{(k)}) \sim \mathcal{N}(0, I_p) \times \mathcal{N}(0, I_{|E|}) \times \mathcal{N}(0, I_{p-|E|}) \) and independent of everything else and \( \mathcal{P}_1 \) is projection onto the orthant \( \mathbb{R}_E^{p} \) and \( \mathcal{P}_2 \) is the projection onto the cube \([-1,1]^p\). The conditioning as usual is implemented by keeping \( \mathcal{P}_{E \setminus j} \) fixed and updating

\[
t^{(k+1)} = T_{obs} + \mathcal{P}_{E \setminus j} \hat{t}^{(k+1)}.
\]

**Example 7.3.** Forward stepwise for Kac-Rice (Section 6.1): We perform \( K \) steps of randomized forward stepwise as in (81) with the response generated as \( y \sim \mathcal{N}(Xb, \sigma^2I_n) \) and \( |\text{supp}(b)| = s \). The null hypothesis is \( H_0 : b_{jk} = 0 \), where \( j_k \) is the predictor chosen by the algorithm in the \( k \)th step, \( k = 1, \ldots, K \). We sample from the density (53) with \( s = K - 1 \) supported on

\[
\{(y, z_1, \ldots, z_K) : \mathcal{P}_{A_{K-1}} y = Y_{obs}, z_k \in \partial I_{X_k}(y_{jk}), k = 1, \ldots, K\}
\]

where we condition on the sufficient statistic for the nuisance parameters in the selected model consisting of predictors \( X_{A_K} \). The updates from projected Langevin sampler when one computes the Kac-Rice objective conditional on the selection event determined by forward stepwise with \( K \) steps are

\[
\left( \bar{y}, z_1, \ldots, z_K \right)^{(i+1)} = \left( \frac{y^{(i)} - \eta \bar{y}^{(i)} / \sigma^2 - \eta \nabla_{\bar{y}} \left( \sum_{k=1}^{K} \bar{g}_k(y^{(i)}, z_k^{(i)}) \right)}{\mathcal{P}_1 \left( z_1^{(i)} - \eta \nabla_{z_1} \bar{g}_1(y^{(i)}, z_1^{(i)}) + \sqrt{2\eta} \xi_1^{(i)} \right)} \right.
\]

\[
\left. \quad \mathcal{P}_K \left( z_K^{(i)} - \eta \nabla_{z_K} \bar{g}_K(y^{(i)}, z_K^{(i)}) + \sqrt{2\eta} \xi_K^{(i)} \right) \right),
\]
where $P_k$ is the projection onto $\partial I_{K_k}(\eta^*_k)$, given in (82), for all $k = 1, \ldots, K$.\footnote{This projection is easily done using Remark 10.} The conditioning step is then done as above by updating $y$ while keeping $P_{A_{K-1}} y$ fixed.

**Example 7.4.** Group LASSO with fixed $X$ (Section 5.4): The response $y$ is modeled as $\mathcal{N}(X \beta, \sigma^2)$ with $|\text{supp}(\beta)| = s$ and $\sigma^2 = 1$. We test the null hypothesis $H_0 : b_{E,g} = 0, b_{E,g}$ denoting the coefficient corresponding to group $g$, $g \in E$, conditioning on the selection event $B_{E,(u_g)_{g \in E}}$.\footnote{This includes conditioning on the active directions as well to get a log-concave density (Section 5.4).} Additionally, we condition on the sufficient statistics for the nuisance parameters, $\mathcal{P}_{E \setminus y}$. The sampling density is proportional to (75) on the support

$$\left\{ (y, (\gamma_g)_{g \in E}, (z_h)_{h \in E}) \in \mathbb{R}^n \times (0, \infty)^{|E|} \times \prod_{h \in E} \lambda_h B_{2}(\mathbb{R}^{|h|}) : \mathcal{P}_{E \setminus y} = Y_{\text{obs}} \right\}.$$ 

The updates for

$$\left( \begin{array}{c}
\tilde{y}^{(k+1)} \\
(\gamma_g)^{(k+1)}_{g \in E} \\
(z_h)^{(k+1)}_{h \in E-E}
\end{array} \right)$$

from projected Langevin sampler can be written as

$$\mathcal{P}_1 \left( (\gamma_g)^{(k)}_{g \in E} - \eta \nabla \tilde{y}^{(k)} + \sqrt{2\eta} \xi_1^{(k)} \\
\mathcal{P}_2 \left( (z_h)^{(k+1)}_{h \in E-E} - \eta \nabla(y, (\gamma_g)^{(k)}_{g \in E}, (z_h)^{(k)}_{h \in E-E}) + \sqrt{2\eta} \xi_2^{(k)} \right) \right),$$

where

$$\phi^{(k)} = \phi_{(E,(u_g)_{g \in E})}(\tilde{y}^{(k)}, (\gamma_g)^{(k)}_{g \in E}, (z_h)^{(k)}_{h \in E-E}),$$

$$(\xi_1^{(k)}, \xi_2^{(k)}, \xi_3^{(k)}) \sim \mathcal{N}(0, I_n) \times \mathcal{N}(0, I_{|E|}) \times \mathcal{N}(0, I_{|E|-|M|}),$$

independent of everything else, $\mathcal{P}_1$ is projection onto the orthant $(0, \infty)^{|E|}$ and $\mathcal{P}_2$ is the projection onto the product of balls $\prod_{h \in E-E} \lambda_h B_{2}(\mathbb{R}^{|h|})$. Here, term $(\text{Tr}(G_g^{(k)}))_{g \in E}$ comes from differentiating the logarithm of the Jacobian (76) with respect to $(\gamma_g)_{g \in E}$ at iteration $k$:

$$D_g^{(k)} = \left((\Gamma^{-1})^{(k)} + V^T Q^{-1} AV\right)^{-1} G_g,$$

where

$$G_g = \frac{\partial V^T Q^{-1} AV}{\partial \lambda_g}$$

and $(\Gamma^{-1})^{(k)} = \text{diag} \left((\gamma_g^{(k)} I_{|g|-1})_{g \in E}\right)$.

Note that $G_g$ is a fixed matrix, thus at every iteration we just need to invert $(\Gamma^{-1})^{(k)} + V^T Q^{-1} AV$ in order to compute $D_g^{(k)}$. The conditioning on $\mathcal{P}_{E \setminus y}$ is done as in the above examples.
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Appendix A: Nuisance parameters & conditional distributions

In forming selective hypothesis tests or intervals when the model $M$ is an exponential family, it was noted in Fithian et al. (2014) that the classical approach of conditioning on appropriate sufficient statistics can be used to eliminate nuisance parameters. In this section we describe selective samplers that can be used to sample from such conditional distributions.

Specifically, suppose we use the randomized Lasso (41) with $X$ considered fixed and $E$ is a subset of features that we will use to form the selected model $M_{\bar{E}} = \{ N(X_\bar{E}\beta_\bar{E},\sigma^2_\bar{E}) : \beta_\bar{E} \in \mathbb{R}^{|\bar{E}|}, \sigma^2_\bar{E} > 0 \}$. (86)

Often, for a given $(E,s_E)$ observed after fitting the randomized Lasso, we will choose $\bar{E} = E$ but this is not strictly necessary. As $\sigma^2_E$ is part of the indexing set for $M_{\bar{E}}$, we are assuming $\sigma^2_E$ is unknown.

Suppose we want a selective test of $H_{0,j|\bar{E}}: \beta_{j|\bar{E}} = 0$ in the model $M_{\bar{E}}$. Standard exponential family calculations detailed in Fithian et al. (2014) tell us that we can construct such a test in the presence of the nuisance parameters $(\beta_{E\setminus\bar{E}},\sigma^2_\bar{E})$ by conditioning on the appropriate sigma-algebra:

$$\sigma \left( X_{E\setminus\bar{E}}^T y, \|y\|_2^2 \right) = \sigma \left( P_{E\setminus\bar{E}} y, \|(I - P_{E\setminus\bar{E}}) y\|_2^2 \right).$$

For any fixed values of the sufficient statistics, say $(W_{obs},SSE_{obs})$ (with $P_{E\setminus\bar{E}} W_{obs} = W_{obs}$) the conditional distribution for any $F \in M_{\bar{E}}$ is supported on the set

$$D_{obs} = \{ y : y = W_{obs} + r, P_{E\setminus\bar{E}} r = 0, \|r\|_2 = SSE_{obs} \}.$$

Under $H_{0,j|\bar{E}}$ it is uniformly distributed over the above set.

We must therefore sample from the set

$$\{ (y,\beta_E,u_{-E}) : y \in D_{obs}, \text{diag}(s_E)\beta_E > 0, \|u\|_{-E} \leq 1 \}$$

with a density proportional to

$$f(y) \cdot g \left( \beta_E^0 - X^T (y - X_E\beta_E) + \lambda \left( \begin{array}{c} s_E \\ u_{-E} \end{array} \right) \right).$$

Appendix B: LASSO and variants

In this section, we describe two common variants of the LASSO.
B.1. LASSO in bound form

The LASSO program in bound form is defined as

\[
\begin{align*}
\minimize_{\beta \in \mathbb{R}^p : \|\beta\|_1 \leq \delta} & \quad \frac{1}{2} \left\|y - X\beta\right\|_2^2 \\
\end{align*}
\]

(87)

with its corresponding randomized version

\[
\begin{align*}
\minimize_{\beta \in \mathbb{R}^p : \|\beta\|_1 \leq \delta} & \quad \frac{1}{2} \left\|y - X\beta\right\|_2^2 + \frac{\epsilon}{2} \|\beta\|_2^2 - \omega^T \beta.
\end{align*}
\]

(88)

In the notation established so far

\[
S = \frac{1}{2} \left\|y - X\beta\right\|_2^2
\]

\[
\ell(\beta; y) = \frac{1}{2} \left\|y - X\beta\right\|_2^2
\]

\[
P(\beta) = \begin{cases} 
0 & \|\beta\|_1 \leq \delta \\
\infty & \text{otherwise.}
\end{cases}
\]

Typically, we will be interested in doing inference when the constraint above is tight. In this case, for the canonical event \(B_{(E,z_E)}\), the set \(S_0^F(G, \epsilon, \ell, P)\) can be parametrized by

\[
\left\{(y, \beta_E, u_E, c) : y \in \mathbb{R}^n, \beta_E \in \mathbb{R}^{|E|}, \|\beta_E\|_1 = \delta, \text{diag}(z_E)\beta_E > 0, u_E \in \mathbb{R}^{p-|E|}, \|u_E\|_\infty \leq 1, c \in \mathbb{R}, c > 0 \right\}.
\]

Another possible reparametrization, can be stated as

\[
\left\{(y, \beta_{E\setminus1}, u_E, c) : y \in \mathbb{R}^n, \beta_{E\setminus1} \in \mathbb{R}^{|E|-1}, s_{E,1}\beta_{E,1} = \delta - s_{E\setminus1}^T \beta_{E\setminus1}, \text{diag}(s_{E\setminus1})\beta_{E\setminus1} > 0, u_E \in \mathbb{R}^{p-|E|}, \|u_E\|_\infty \leq 1, c \in \mathbb{R}, c > 0 \right\},
\]

where \(\beta_{E\setminus1} = (\beta_{E,2}, \ldots, \beta_{E,|E|})\) and similarly \(s_{E\setminus1}\). The above parameterization can be expressed as

\[
\psi_{(E,z_E)}(y, \beta_{E\setminus1}, u_E, c) = \begin{pmatrix} y, c \begin{pmatrix} \beta_{E,1} \\ 0 \end{pmatrix} - X^T(y - X_E\beta_E) + c \begin{pmatrix} z_E \\ u_E \end{pmatrix}, \\
\begin{pmatrix} \beta_{E,1} \\ 0 \end{pmatrix}, -X^T(X - X_E\beta_E), c \begin{pmatrix} z_E \\ u_E \end{pmatrix} \end{pmatrix},
\]
where $\beta_E$ is expressed in terms of $\beta_{E\setminus 1}$ as above and the corresponding randomization reconstruction map is

$$
\phi_{(E,z_E)}(y,\beta_{E\setminus 1},u_{-E},c) = \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - X^T(y - Z_E\beta_E) + c \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix},
$$

where

$$
\beta_E = \begin{pmatrix} \delta - s_{E\setminus 1}^T\beta_{E\setminus 1}s_{E\setminus 1} \\ \beta_{E\setminus 1} \\ 0 \end{pmatrix}.
$$

The sampling density is proportional to

$$
f(y) \cdot g \left( \phi_{(E,z_E)}(y,\beta_{E\setminus 1},u_{-E},c) \right) \cdot \left| \det(D(\beta_{E\setminus 1},u_{-E},c,\phi_{(E,z_E)})) \right|;
$$

where the last determinant equals

$$
-\epsilon^{|E|} \det \left( -\epsilon s_{E\setminus 1}^T s_{E\setminus 1} + X_1^T(-s_{E\setminus 1} X_1 s_{E\setminus 1} + X_{E\setminus 1}) s_{E\setminus 1} \right).
$$

### B.2. Basis pursuit

The basis pursuit problem Chen et al. (1998) is defined as

$$
\begin{aligned}
\text{minimize} & \quad \beta \in \mathbb{R}^p : \|y - X\beta\|_2 \leq \delta, \\
\end{aligned}
$$

(89)

In the notation established so far

$$
S = y, \\
\ell(\beta; y) = \begin{cases} 0 & \|y - X\beta\|_2 \leq \delta \\ \infty & \text{otherwise} \end{cases}, \\
\mathcal{P}(\beta) = \|\beta\|_1.
$$

The set on which the problem (89) has a solution is

$$
\left\{ y : \hat{\theta}(y) \neq \emptyset \right\} = \left\{ y : \|(I - P_C)y\|_2 \leq \delta \right\},
$$

where $P_C$ denotes projection onto col($X$).

Its randomized version is

$$
\begin{aligned}
\text{minimize} & \quad \beta \in \mathbb{R}^p : \|y - X\beta\|_2 \leq \delta, \\
& \quad \frac{\epsilon}{2}\|\beta\|_2^2 - \omega^T \beta + \|\beta\|_1,
\end{aligned}
$$

(90)

This problem, with non-random choices of $\omega$ is considered in Becker et al. (2010). We see that

$$
\left\{ (y, \omega) : \hat{\theta}(y, \omega) \neq \emptyset \right\} = \left\{ (y, \omega) : \hat{\theta}(y) \neq \emptyset \right\}.
$$
Generically, when a solution exists, the constraint will be tight, hence our events of interest will typically condition on $\|y - X\beta\|_2 = \delta$. We see then

$$\bar{S}_0^F(G, \epsilon, \ell, P) = \{(y, \omega, \alpha, z) : y \in \text{supp}(F), \|y - X\beta\|_2 = \delta, \omega \in \text{supp}(G),$$

$$\omega = c\beta + \alpha + z, \alpha = cX^T(X\beta - y), c > 0, z \in \partial P(\beta)\}.$$ 

For the canonical event $B_{(E,z_E)}$, the set $\bar{S}_B^F(G, \epsilon, \ell, P)$ can be parameterized by

$$\left\{(y, \beta_E, u_E, c) : \|(I - P_C)y\|_2 \leq \delta, \beta_E \in \mathbb{R}^{|E|}, \text{diag}(z_E)\beta_E > 0, \|y - X_E\beta_E\|_2 = \delta, u_E \in \mathbb{R}^{p - |E|}, \|u_E\|_{\infty} \leq 1, c \in \mathbb{R}, c > 0\right\}. \quad (91)$$

This set has the form of a bundle over a subset of $\mathbb{R}^n$, with fibers that are the product a $|E| - 1$ dimensional ellipse, a $p - |E|$ dimensional cube and a half-line.

The parameterization is

$$\psi_{(E,z_E)}(y, \beta_E, u_E, c) = \left(\begin{array}{cc} y, \epsilon & \beta_E \\ 0, 0 \end{array}\right) - cX^T(y - X_E\beta_E) + \left(\begin{array}{c} z_E \\ u_E \end{array}\right).$$

Denoting $\phi_{(E,z_E)}(\beta_E, u_E, c) = \epsilon \left(\begin{array}{cc} \beta_E \\ 0 \end{array}\right) - cX^T(y - X_E\beta_E) + \left(\begin{array}{c} z_E \\ u_E \end{array}\right)$, the sampling density is proportional to

$$f(y) \cdot g(\phi_{(E,z_E)}(\beta_E, u_E, c)) \cdot |\text{det}(D(\phi_{(E,z_E)}(\beta_E, u_E, c)))|$$

and restricted to (91), where $\text{det}(D(\phi_{(E,z_E)}(\beta_E, u_E, c)))$ is the Jacobian of the parameterization in the coordinates described above, i.e. coordinates on the product of an $|E| - 1$ dimensional ellipse, an $p - |E|$ dimensional cube and a half-line.

**B.3. Square-root LASSO**

Using the LASSO with an unknown noise level is somewhat of a chicken-and-egg problem, as knowing which value of $\lambda$ to choose is somewhat difficult. Suppose that instead we use the square-root LASSO. The square-root LASSO program Belloni et al. (2014); Sun and Zhang (2011) is defined as

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|_2 + \lambda\|\beta\|_1. \quad (92)$$
Selective inference for this program was considered in (Tian et al., 2015). This program has the advantage that it is possible to choose a reasonable value of $\lambda$ without knowing anything about the noise level. Its randomized version is

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|_2 + \frac{\epsilon}{2}\|\beta\|_2^2 - \omega^T \beta + \lambda \|\beta\|_1. \quad (93)$$

We can take the law of $\omega$ to be independent of any particular noise level, though we probably should choose $\epsilon = O(n^{-1/2})$ if thinking of something like the pairs model.

In the notation established so far

$$S = y, \quad \ell(\beta; y) = \|y - X\beta\|_2, \quad P(\beta) = \lambda \|\beta\|_1.$$

We are most interested in inference when $y - X\hat{\beta}(y, \omega) \neq 0$ on which $\ell$ is differentiable and for the canonical event $B_{(E,z_E)} = \{\beta : \text{diag}(z_E)\beta_E > 0, \beta_{-E} = 0\}$ we can parametrize $\{(y, \omega, \beta, \alpha, z) \in \bar{S}_0(G, \epsilon, \ell, P) : y \in D_{\text{obs}}, \beta \in B_{(E,z_E)}\}$ as

$$\psi_{(E,z_E)}(y, \beta_E, u_{-E}) = \left( y, \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix}, \frac{X^T(y - X_E\beta_E)}{\|y - X_E\beta_E\|_2} \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix}, \frac{X^T(y - X_E\beta_E)}{\|y - X_E\beta_E\|_2}, \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix} \right),$$

with the domain $D_{\text{obs}} \times \mathbb{R}^{[E]} \times [-1, 1]^{p-[E]}$. We therefore must sample from a density proportional to

$$f(y) \cdot g \left( \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix}, \frac{X^T(y - X_E\beta_E)}{\|y - X_E\beta_E\|_2} \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix} \right) \left| \det \left( \frac{X^T R(y, \beta_E) X_E}{\|y - X_E\beta_E\|_2} + \epsilon I \right) \right|$$

and restricted to the domain of $\psi_{(E,z_E)}$, where

$$R(y, \beta_E) = I_n - \frac{(y - X_E\beta_E)(y - X_E\beta_E)^T}{\|y - X_E\beta_E\|_2^2}.$$ 

B.4. More complex penalties: generalized LASSO and other quadratic programs

Clearly, not every statistical learning problem of interest can be expressed in terms of the LASSO or forward stepwise. For example, the generalized LASSO (Tibshirani and Taylor, 2011) considers a penalty of the form

$$P(\beta) = \lambda \|D\beta\|_1.$$ 

Selective inference for the entire solution path of the generalized LASSO, analogous to the solution path of Least Angle Regression and LASSO in Tibshirani et al.
Tian Harris et al./Selective sampling (2014) has been considered in Hyun et al. (2016). We consider a fixed value of \( \lambda \) combined with randomization. For some \( D \), the programs can be re-expressed as LASSO problems but not all \( D \) (c.f. Tibshirani and Taylor (2011)). More generally, we might be confronted with solving a problem of the form

\[
\minimize_{\beta} \ell(\beta; S) + \bar{\mathcal{P}}(D\beta - \gamma).
\]  

(94)

That is, we consider our usual problem with

\[
\mathcal{P}(\beta) = \bar{\mathcal{P}}(D\beta - \gamma).
\]

For example, a linearly constrained quadratic program might take the form

\[
\minimize_{\beta} \frac{1}{2} \beta^T Q\beta - S^T \beta
\]

subject to \( D\beta \leq \gamma \) with \( S \sim F \). In this case, \( \bar{\mathcal{P}} \) is the non-positive cone constraint.

Sometimes, the Fenchel conjugate \( \mathcal{P}^* \) is simple in the sense that its naturally associated selection events are easy to parametrize. In this case, we can proceed as before and simply consider randomized programs of the form

\[
\minimize_{\beta} \frac{1}{2} \beta^T Q\beta - (S + \omega)^T \beta + \bar{\mathcal{P}}(D\beta - \gamma) + \frac{\epsilon}{2} \|\beta\|_2^2.
\]  

(96)

However, when \( \mathcal{P}^* \) is complex, then our usual approach may be computationally expensive. In this section, we describe an alternative randomization scheme that may yield simpler sampling algorithms as described in Section 7.

For concreteness, we consider the quadratic program (96). Similar calculations hold for the generalized LASSO by simply replacing one convex conjugate with another. The issue of parameterization of selection events arises quickly upon inspection of the subgradient equation for the randomized program (96).

It will often be of interest to condition on the set of tight constraints

\[ \hat{E}(S, \omega) = \{ j : D_T^E \hat{\beta}(S, \omega) = \gamma_j \}. \]

On this event, the subgradient equation reads

\[ \omega = Q\beta - S + D_T^E z_E \]

where \( z_E \geq 0 \) and \( D_E\beta = \gamma_E \). We see the sub-gradient \( D_T^E z_E \) lies in the cone generated by the rows of \( D_E \). If we were to parametrize this selection event, we might write it as

\[ \omega = Q\beta - S + \bar{z}_E \]

where \( \bar{z}_E \in \text{cone}(D_E) \). For arbitrary \( D \) and \( E \), this cone may be rather complex. Each step of the projected Langevin implementation described in Section 7 requires projection onto this set. Projection onto this set can be achieved via a
non-negative least squares problem, which would in principal need to be re-run for every step of the sampler.

We shall instead solve the corresponding randomized dual program. Introducing variable \( v = D\beta - \gamma \), the dual of (95) which solves

\[
\max_{u} \left\{ \min_{\beta, v : v \leq 0} \frac{1}{2} \beta^T Q\beta - S^T \beta + \frac{\epsilon}{2} \|\beta\|_2^2 + u^T (D\beta - \gamma - v) \right\},
\]

subject to \( u \geq 0 \) is equivalent to solving

\[
\min_{u} \frac{1}{2} (D^T u - S)^T (Q + \epsilon I)^{-1} (D^T u - S) + u^T (\gamma - \omega)
\]

subject to \( u \geq 0 \) (for the generalized LASSO, the non-negative cone constraint is replaced with the constraint \( \|u\|_\infty \leq \lambda \)). The set of tight constraints can be thought of as corresponding to non-zero \( u \)'s in this dual problem \( E \).

When the dual problem is strongly convex this is a one-to-one correspondence, though if it is not strongly convex there may be more than one dual solution Tibshirani and Taylor (2012).

The randomized dual problem solves the program

\[
\min_{u} \frac{1}{2} (D^T u - S)^T (Q + \epsilon I)^{-1} (D^T u - S) + u^T (\gamma - \omega)
\]

subject to \( u \geq 0 \), which is dual to

\[
\min_{\beta} \frac{1}{2} \beta^T Q\beta - S^T \beta + \frac{\epsilon}{2} \|\beta\|_2^2 + I_K(\beta)
\]

with

\[
K = \{ \beta : D\beta - \gamma + \omega \leq 0 \}
\]

and \( I_K \) denoting its characteristic function. However, for the above randomized QP that we propose to solve, the law of \( \omega \) has to supported on the set

\[
\{ \omega : \cap_j \{ \beta : D_j^T \beta \leq \gamma_j - \omega_j \} \neq \emptyset \}.
\]

to ensure feasibility of the primal problem, though the dual problem always has a solution.

Remark 19. Generally, this is not a problem in examples like the generalized LASSO, where \( P \) is finite everywhere. Further, in the applications of selective inference we have in mind, a data analyst is typically solving statistical learning programs to suggest parameters of interest. For example, Heirnet Bien et al. (2013) is a statistical learning method that seeks hierarchical interactions that can be expressed as a linearly constrained quadratic program. In this case, a randomization which makes the primal problem infeasible is not catastrophic.

Denoting

\[
Q_\epsilon = (Q + \epsilon I)^{-1},
\]
one solution to the above problem that ensures feasibility of the primal problem is to instead consider

$$\begin{align*}
\text{minimize} & \quad \frac{1}{2} (D^T u - S)^T Q_e (D^T u - S) + u^T (\gamma - \omega) + \frac{\epsilon'}{2} \| u \|_2^2 \\
\text{subject to} & \quad u \geq 0 \quad \text{for} \quad \epsilon' > 0.
\end{align*}$$

(98)

This always yields a feasible primal

$$\begin{align*}
\text{minimize} & \quad \frac{1}{2} z^T (DQ_e D^T + \epsilon' I)^{-1} z - (DQ_e D^T + \epsilon' I)^{-1} (DQ_e S - \gamma + \omega),
\end{align*}$$

as $DQ_e D^T + \epsilon' I$ is a positive definite matrix with added positive $\epsilon'$. The reconstruction map in this case is given by

$$\omega = \phi_E(S, u, z - E) = DQ_e (D_E^T u_E - S) + \epsilon' \begin{pmatrix} u_E \\ 0 \end{pmatrix} + \gamma + \begin{pmatrix} 0 \\ z - E \end{pmatrix},$$

(99)

which allows us to sample $(S, u_E, z - E)$ from a sampling density proportional to

$$f(S) : g(\phi_E(S, u_E, z - E))$$

and supported on $	ext{supp}(F) \times \mathbb{R}_+^{[E]} \times \mathbb{R}_{-E}^{[E]}$, where $\mathbb{R}_+ = \{x \in \mathbb{R} : x \geq 0\}$ and $\mathbb{R}_- = \{x \in \mathbb{R} : x \leq 0\}$.

Another possibility is to consider the dual of the randomized objective (96) given by

$$\begin{align*}
\text{minimize} & \quad \frac{1}{2} (D^T u - S - \omega)^T Q_e (D^T u - S - \omega) + u^T \gamma,
\end{align*}$$

which lead to reconstruction map

$$DQ_e \omega = DQ_e D_E^T u_E - DQ_e S + \gamma + \begin{pmatrix} 0 \\ z - E \end{pmatrix},$$

where we have conditioned on the value of the set

$$\hat{E}(S, \omega) = \{j : \hat{u}_j(S, \omega) > 0\}$$

of being $E$. As noted above, the set $\hat{E}(S, \omega)$ may not be unique even when $E(S, \omega)$ is (c.f. Tibshirani and Taylor (2012)). In this sense, we are conditioning on a particular value of the boundary set, the boundary set determined by the solver we use to solve this dual problem.

Denoting the density of $DQ_e \omega$ as $\tilde{g}$, the sampling density of $(S, u_E, z - E)$ is now proportional to

$$f(S) : \tilde{g} \left( DQ_e D_E^T u_E - DQ_e S + \gamma + \begin{pmatrix} 0 \\ z - E \end{pmatrix} \right)$$

and restricted to

$$z - E \leq 0, \quad u_E \geq 0 \quad \text{and} \quad z - E + \gamma - E \in \text{col}(D_{-E}).$$
To avoid enforcing the implicit constraint of $P_{D_{z,E}}^\perp(z_E + \gamma - E)$ being 0 at each step of the sampler, we can sample from an approximate density for $(S,u,E,z_E - E(\gamma - E))$ with a smoothed version, an example being

$$f(S)\cdot \hat{g}
\left(DQ\cdot D_E^T u_E - DQ\cdot S + \gamma + \left(0\right)_{z-E}\right)\cdot \exp\left(-\frac{1}{2\epsilon^2}\left\|P_{D_{z,E}}^\perp(z_E + \gamma - E)\right\|^2_2\right)$$

supported on $\text{supp}(F) \times \mathbb{R}^{[E]} \times \mathbb{R}^{p-[E]}$, a much simpler constraint set.

**Appendix C: Neighborhood selection**

We now consider neighborhood selection (a selective sampler for which appears in Tian et al. (2016)). Meinshausen and Bühlmann (2006) proposed neighborhood selection with the LASSO to achieve this goal. The algorithm can be formulated as the following optimization problem, for any node $i$

$$\hat{\beta}_{i,\lambda} = \arg\min_{\beta \in \mathbb{R}^p, \beta_i = 0} \|x_i - X\beta\|^2_2 + \lambda \|\beta\|_1,$$

(100)

where with slight abuse of notation, $X \in \mathbb{R}^{n \times p}$ is the data matrix observed from $n$ i.i.d observations, and $x_i$ is the $i$-th column of $X$. Choice of $\lambda$ is discussed in Chapter 3 of Meinshausen and Bühlmann (2006). Denote $\hat{B} = (\hat{\beta}_1, \hat{\beta}_2, ..., \hat{\beta}_p)$, we propose the randomized version of (100),

$$\hat{B} = \arg\min_{B \in \mathbb{R}^p \times p, B_{ii} = 0 \forall i \in \{1, ..., p\}} \|X - XB\|^2_F + \lambda \|B\|_1 + \frac{\epsilon}{2} \|B\|^2_F - \Omega B,$$

(101)

where $\Omega = (\omega_1, ..., \omega_p)$ i.i.d $G$. This is the matrix form of (33), and the KKT conditions are decomposable across the nodes.

Suppose for node $i$, $E^i$ is the active set for (100), $s^i$ is the corresponding signs, $\lambda \cdot u^i$ is the subgradient corresponding to the inactive variables except the $i$-th and $X_{-,i}$ is the columns of $X$ except the $i$-th column. For every node $i$, the $i$-th coordinate of $\beta^i$ is held to be zero, and (100) is in fact a regression of dimension $p - 1$, thus

$$\alpha^i = -X^T_{-,i}(x_i - X_E \beta^i_{E^-}),$$

(102)

and the reparametrization map,

$$\psi_{(E,D)}(X, B^-, u) = (X, \alpha + z + \epsilon B^-, B^-, \alpha, z),$$

where

$$\alpha = (\alpha_1, \alpha_2, ..., \alpha_p), \alpha_i \text{ from (102)},$$

$$z = (z_1, z_2, ..., z_p), \quad z^i = \lambda \left(s^i\right),$$

$$B^- \in \mathbb{R}^{(p-1)\times p} \text{ is } p \times p \text{ matrix without the diagonal elements}.$$
Since $\omega^i$, $1 \leq i \leq p$, are independent, and the Jacobian
\[
J \psi_{(E, z_t)}(X, B^-, u) = \prod_{i \in \Gamma} \det(X_{Ei}^T X_{Ei} + \epsilon I),
\]
conditioning on $(E^i, s^i)$, the distribution for selective inference has the following density,
\[
f(X) \cdot \prod_{i \in \Gamma} g \left( \epsilon \begin{pmatrix} \beta^i_e \\ 0 \end{pmatrix} + \lambda \begin{pmatrix} s^i \\ u^i \end{pmatrix} - X_{-i}^T (x_i - X_{Ei} \beta^i_e) \right) \cdot \prod_{i \in \Gamma} \left| \det(X_{Ei}^T X_{Ei} + \epsilon I) \right|. \tag{103}
\]

After seeing the active set $E = (E^1, \ldots, E^p)$, it is natural to choose the selected model (i.e. the edge set $E$) to be $E$. However, since the active set $E$ is not necessarily symmetric, we choose the edge set $E$ to be $E^\vee$, where
\[
E^\vee = \{(i, j) \mid E_{ij} = 1 \text{ or } E_{ji} = 1\}.
\]
Under this model, the distribution of $X$ is an exponential family. More specifically, conditioning on the set of edges $E^\vee$,
\[
f(X) \propto \exp \left( -\frac{1}{2} \text{Tr}(\Theta X^T X) \right)
= \exp \left( -\sum_{(i, j) \in E^\vee} \Theta_{ij} x_i^T x_j - \frac{1}{2} \sum_{i \in \Gamma} \Theta_{ii} ||x_i||^2 \right).
\]
Note that this is an exponential family with sufficient statistics
\[
\{x_i^T x_j, (i, j) \in E^\vee, ||x_i||^2, i \in \Gamma\}.
\]
Therefore, the law for selective inference (103) is also an exponential family with the same sufficient statistics. To construct the UMPU tests as in Fithian et al. (2014) for the null hypothesis $H_{0, ij} : \Theta_{ij} = 0$, we condition on the sufficient statistics corresponding to the nuisance parameter and sample from the law (103).

**Appendix D: Recomputing Jacobian for group lasso**

We apply the Jacobian meta theorem 2 to the group Lasso to re-derive the Jacobian in the selective sampler density from a geometric perspective. For the tangential frame $V_{i, z}$ we can split this over groups as
\[
(\Pi^T_g (V_{g, j, z_g}))_{1 \leq j \leq |g|-1})_{g \in E} = (V_{g, z_g})_{g \in E}
\]
where $\Pi_g : \mathbb{R}^p \rightarrow \mathbb{R}^g$ is projection onto the $g$ coordinates represented by the matrix $\Pi_g \in \mathbb{R}^{g \times p}$. The the vectors $V_{g, j, z_g}$ are chosen to be are orthonormal.
within $T_g(\lambda_g S(\mathbb{R}^q))$ additionally satisfying $V^T_{g,j} z_g = 0$. For the normal frame we can take $\eta_g = z_g / \lambda_g$ and

$$\beta = \sum_{g \in G} \gamma_g z_g / \lambda_g.$$  

In the standard basis of $T_\beta \mathbb{R}^p$, the metric (77) has matrix

$$X^T X + \epsilon I.$$  

The curvature matrix $C_{-\beta}$ is 0 except on the tangent spaces coming from active groups, on which it is block diagonal with blocks

$$\frac{\gamma_g}{\lambda_g} I_{|g|-1}, g \in E.$$  

Hence the matrix of interest is

$$G(z, \gamma)^{-1} C_{-\beta}(z, \gamma) = \begin{pmatrix} G_E(z, \gamma)^{-1} C_{E,-\beta}(z, \gamma) & 0 \\ 0 & 0 \end{pmatrix}$$

where the blocks of $G_E$ are

$$G_{E, gh}(z, \gamma) = V^T_{g, z_g} \Pi_g (X^T X + \epsilon I)^{-1} \Pi^T_h V_{h, z_h}, \quad g, h \in E.$$  

The eigenvalues of the matrix which show up in the determinant are the same as the reciprocal of the eigenvalues of the matrix with blocks

$$\tilde{G}_{E, gh}(z, \gamma) = \frac{\lambda_g^{1/2}}{\gamma_g} V^T_{g, z_g} (X^T X + \epsilon I)^{-1} V_{h, z_h} \frac{\lambda_h}{\gamma_h}, \quad g, h \in E. \quad (104)$$

Finally, the matrix $H(z, \gamma)$ can be ignored if we consider $X$ to be fixed.

**Appendix E: Multiple views of the data**

In this section, we consider three more algorithms that choose variables by querying the data several times.

**E.1. Top K screening**

A simple way of variable selection called top K screening selects the K most correlated features $X_j$ with response vector $y$. For a given K, the unrandomized version of such a screening selects most correlated variables ($j_1, j_2, \ldots, j_K$) with corresponding signs ($s_1, s_2, \ldots, s_K$), such that

$$s_1 X^T_{j_1} y \geq s_2 X^T_{j_2} y \geq \cdots \geq s_K X^T_{j_K} y \geq \max_{j \notin \{j_1, \ldots, j_K\}} |X^T_j y|.$$  

Selective inference in the nonrandomized setting for this problem was considered in (Lee and Taylor, 2014).
Here, we consider a randomized version of the optimization above yielding the $k$-th most correlated variable for $1 \leq k \leq K$, with added independent randomization variable $\omega_k \sim G_k \in \mathbb{R}^{p-k+1}$ and corresponding density $g_k$ is given by

$$
\max_{\eta \in \mathbb{R}^{p-k+1}} \eta^T (X^T_{-A_k-1} y + \omega_k) - I_{K_k}(\eta), \quad \text{where } y \sim F. \tag{105}
$$

Here, $A_k = \{j_1, j_2, \ldots, j_k\}$ is the active set including the $k$-th step, $X_{-A_k}$ are the columns of $X$ except for the ones corresponding to the current active set $A_k$, $\omega_k$ is a sequence of randomizations and $I_{K_k}(\eta)$ is the characteristic function of

$$
K_k = \{\eta \in \mathbb{R}^{p-k+1} : \|\eta\|_1 \leq 1\},
$$

that is,

$$
I_{K_k}(\eta) = \begin{cases} 
0 & \text{if } \eta \in K_k \\
\infty & \text{otherwise.}
\end{cases}
$$

Denote the optimal solution of (105) as

$$
\eta^*_{k,j} = \begin{cases} 
s_k & \text{if } j = j_k \\
0 & \text{otherwise,}
\end{cases} \quad \text{(106)}
$$

where $j \in \{1, \ldots, p\} \setminus A_{k-1} = A_{k-1}^c$ and $j_k = \arg\max_{j \in A_{k-1}^c} |X^T_j y + \omega_{k,j}|$. The subgradient equation in $k$-th step leads to a reconstruction map for the randomization given by

$$
\omega_k = \phi_k(y, z_k) = -X^T_{-A_{k-1}} y + z_k,
$$

constraining sub-differential $z_k \in \mathbb{R}^{p-k+1}$ to

$$
z_k \in \partial I_{K_k}(\eta^*_k) = \{c \cdot u : u \in \mathbb{R}^{p-k+1}, u_{j_k} = s_k, |u_j| \leq 1 \ \forall j \in A_{k-1}^c, c > 0\}.
$$

Conditioning on the selection event of choosing the $K$ most correlated variables with their corresponding signs

$$
E_{\{s_k, j_k\}}^K = \left\{ (y, \{\omega_k\}_{k=1}^K) \in \mathbb{R}^n \times \prod_{k=1}^K \mathbb{R}^{p-k+1} : \text{sign}(X^T_{j_k} y + \omega_k) = s_k, \right. \\
\left. s_k(X^T_{j_k} y + \omega_k) \geq \max_{j \in A_{k-1}^c} |X^T_j y + \omega_k|, k = 1, \ldots, K \right\},
$$

we sample $(y, z_1, \ldots, z_k)$ from the selective sampling density proportional to

$$
f(y) \cdot \prod_{k=1}^K g_k \left(z_k - X^T_{-A_{k-1}} y\right), \quad \text{(107)}
$$

$\eta^*_k \in \mathbb{R}^{p-k+1}$ is indexed by this set and all $p-k+1$-dimensional vectors in this and the following section will be indexed by $A_{k-1}^c$. 

---

10 $\eta^*_k \in \mathbb{R}^{p-k+1}$ is indexed by this set and all $p-k+1$-dimensional vectors in this and the following section will be indexed by $A_{k-1}^c$. 

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supported on
\[ \mathbb{R}^n \times \prod_{k=1}^{K} \partial I_{K_k} (\eta_k^*) . \]

For logistic regression, one can replace the \( T \) statistics above with the score statistics as described in Remark 13.

### E.2. Stagewise algorithms

Instead of fully projecting out the current variables at each step as in forward stepwise, one can use an incremental approach as in a stagewise algorithm Tibshirani (2015). The first step of a randomized version of such an algorithm might consist of solving the problem

\[
\max_{\eta: \|\eta\|_1 \leq 1} \eta^T (X^T (y - X \alpha) + \omega_1)
\]

with \( \alpha_0 = \eta_0^* = 0 \). We update
\[ \alpha_1 = \alpha_0 + \delta \cdot \eta_0^* \]
for some learning rate \( \delta > 0 \). Subsequent problems are given by

\[
\max_{\eta: \|\eta\|_1 \leq 1} \eta^T (X^T (y - X \alpha) + \omega_k)
\]

with solution \( \eta_k^* \) and
\[ \alpha_k = \delta \cdot \sum_{j=0}^{k-1} \eta_j^* . \]

After \( K \) steps, the sampler density is thus proportional to

\[
f(y) \cdot \prod_{k=1}^{K} g_k (z_k - X^T (y - X \alpha_{k-1})) ,
\]

\[ (y, z_1, \ldots, z_k) \in \mathbb{R}^n \times \prod_{k=1}^{K} \partial I_{K_k} (\eta_k^*) . \]

with \( \mathcal{K} = \{ \eta \in \mathbb{R}^p : \|\eta\|_1 \leq 1 \} \).

### E.3. Screening via thresholding randomized Post-LASSO

An alternative way to screen is through the following two-stage procedure where we use randomized LASSO as in (41) in the first stage to select the model \((E, z_E)\). In the second stage, we solve an unpenalized, randomized program as in (61) with the selected predictors \( X_E \)

\[
\min_{\gamma \in \mathbb{R}^{|E|}} \frac{1}{2} \|y - X_E \gamma\|^2 + \frac{c_1}{2} \|\gamma\|^2 - \omega^T \gamma , \quad ((X, y), \omega) \sim F \times G_1 ,
\]

\[(y, z_1, \ldots, z_k) \in \mathbb{R}^n \times \prod_{k=1}^{K} \partial I_{K_k} (\eta_k^*) . \]

with \( \mathcal{K} = \{ \eta \in \mathbb{R}^p : \|\eta\|_1 \leq 1 \} \).
where $G_1$ is a known distribution on $\mathbb{R}^{|E|}$ and $\omega_1$ is independent from the randomization variable $\omega$ used in the first stage. We perform a second stage of selection based on the output of the above convex program to threshold the resulting coefficients of $\hat{\gamma}((X, y), \omega_1)$ resulting in a further selected model

$$E = \{ i : |\hat{\gamma}_i((X, y), \omega_1)| > a\sigma \}$$

with their signs $\tilde{z}_E = \text{sign}(\hat{\gamma}_E((X, y), \omega_1))$, where $a$ is a constant and $\sigma$ is again the scaling which can be estimated by the noise variance of the selected model as in Section 4.6. The canonical event of interest from the two-step procedure becomes

$$B_{(E, z_E, \tilde{E}, \tilde{z}_E)} = \{ (\beta_E, u_{-E}, \gamma) : \text{diag}(z_E)\beta_E > 0, \|u_{-E}\|_\infty \leq 1, \text{diag}(\tilde{z}_E)\gamma_E > 0, |\gamma_i| \geq a\sigma \forall i \in \tilde{E}, \|\gamma_{-\tilde{E}}\|_\infty < a\sigma \}.$$ 

Now the sampling density on $((X, y), \beta_E, u_{-E}, \gamma)$ becomes proportional to

$$f(X, y) \cdot g \left( \epsilon \begin{pmatrix} \beta_E \\ 0 \end{pmatrix} - X^T (y - X_E\beta_E) + \lambda \begin{pmatrix} z_E \\ u_{-E} \end{pmatrix} \right) \cdot g_1 \left( \epsilon_1 \gamma - X^T (y - X\gamma) \right)$$

where the optimization variables $(\beta_E, u_{-E}, \gamma)$ are restricted to $B_{(E, z_E, \tilde{E}, \tilde{z}_E)}$. 