DUAL CYCLIC COORDINATE DESCENT ALGORITHMS FOR INEQUALITY CONSTRAINED LEAST SQUARES

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1. Problem

The problem we solve in this note is

(1)
$$\min_{\beta} \left\{ \frac{1}{2} (y - X\beta)' W (y - X\beta) \mid AX\beta \ge c \right\}.$$

We assume that W is positive definite and diagonal, and that X has full column rank. It is convenient to make a change of variables first. Suppose X = QR, with Q'WQ = I and R upper triangular. Define $y = R\beta$, $z = Q'W\gamma$, and D = AQ. Then

$$(\gamma - X\beta)'W(\gamma - X\beta) = \gamma'W\gamma - z'z + (\gamma - z)'(\gamma - z),$$

and Problem (1) can be solved by solving

(2)
$$\min_{\gamma} \left\{ \frac{1}{2} (z - \gamma)'(z - \gamma) \mid D\gamma \ge c \right\},$$

If \hat{y} is the solution of (2), then $\hat{\beta} = R^{-1}\hat{y}$ solves (1), and $X\hat{\beta} = Q\hat{y}$.

Problem (2) is the *primal problem*. It can also be written as

(3)
$$\min_{\substack{y \in \lambda > 0}} \max_{\lambda > 0} \frac{1}{2} (z - y)'(z - y) - \lambda'(Dy - c).$$

The *dual problem* is obtained by interchanging the min and the max in (3). Some simple computation gives

$$\max_{\lambda \geq 0} \min_{\gamma} \frac{1}{2} (z - \gamma)'(z - \gamma) - \lambda'(D\gamma - c) = -\min_{\lambda \geq 0} \frac{1}{2} \lambda' DD'\lambda + \lambda' r,$$

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where r = Dz - c. By the Fenchel Duality Theorem [Rockafellar, 1970] if $\hat{\lambda} \ge 0$ is a solution of the dual problem, then $\hat{y} = z + D'\hat{\lambda}$ is a solution of the primal problem (2) and thus of the primal problem (1)

2. ALGORITHM

We give an iterative algorithm of the coordinate descent type [Hildreth, 1957; D'Esopo, 1959; Tseng, 1993]. It solves the dual problem, i.e. minimizes

$$\sigma(\lambda) = \frac{1}{2}\lambda' DD'\lambda + \lambda' r$$

over non-negative λ . It is convenient to define a vector δ with the diagonal elements of DD' and a vector $\tau = D'\lambda$. For row i of D we write d_i .

The algorithm starts with $\lambda = 0$ and then cycles through the coordinates in order. Each coordinate step replaces λ by $\lambda + \theta e_i$, where e_i is one of the unit vectors (with all elements zero, except element i which is one). Now

$$\sigma(\lambda + \theta e_i) = \sigma(\lambda) + \frac{1}{2}\theta^2 \delta_i + \theta(d_i'\tau + r_i),$$

which is minimized by choosing

$$\hat{\theta} = \max(-\lambda_i, -\frac{d_i'\tau + r_i}{\delta_i}).$$

Update

$$\hat{\lambda} = \lambda + \hat{\theta}e_i,$$

 $\hat{\tau} = \tau + \hat{\theta}d_i,$

 $\hat{\gamma} = z + \hat{\tau}.$

Then go the next coordinate, unless we have completed a cycle, in which case we start with the first coordinate again. And so on, until convergence.

Observe that this is a dual algorithm, which means that only at convergence will we actually have $AQy \ge c$. All the intermediate solutions will be infeasible. If feasibility is critical we may have to iterate to rather high precision.

3. APPLICATIONS

In the Appendix we give an \mathbb{R} function for the algorithm in this note. By default the monRegCCA() function does an unwieghted monotone regression, i.e. it chooses X=W=I and c=0, while A takes successive differences. By choosing $c\neq 0$ we can do bounded monotone regression. By choosing only certain rows of the difference matrix we can fit partial orders.

Using the same finite difference matrix A but choosing monomials for X means fitting a monotone polynomial. In the same way choosing a B-spline basis for X, for instance by using the bs() function from the splines package, will fit a monotone spline.

REFERENCES

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APPENDIX A. CODE

```
monRegCCA < -function(y, x = \frac{diag(length(y))}{diag(length(y))})
          , c = rep(0, nrow(a)), w = rep(1, length(y)), eps = 1e - 15, itmax = 100,
          verbose=FALSE,itout=TRUE) {
    m \leftarrow -nrow(a); n \leftarrow -ncol(x)
     \underline{qr} \leftarrow \underline{qr} (\underline{sqrt}(w) \underline{*}x); \underline{q} \leftarrow \underline{qr}.\underline{Q}(\underline{qr}) \underline{/sqrt}(w); \underline{r} \leftarrow \underline{qr}.\underline{R}(\underline{qr})
     z \leftarrow colSums(y*w*q); d \leftarrow a%*q; lbd \leftarrow rep(0,m); gam \leftarrow z
 5 ss < (sum(w*y^2) - sum(z^2))/2; tau < -rep(0,n); r < -drop(d%*%z) - c
     del < rowSums(d^2); itel < 1; sold < -0
     repeat {
          snew<-sold
                for (i in 1:m) {
                            di \leftarrow d[i,]; deli \leftarrow del[i]; lbdi \leftarrow lbd[i]
10
                            ri \leftarrow r[i]; taudi \leftarrow sum(tau \cdot di)
                            topt<-max(-lbdi,-(taudi+ri)/deli)
                            lbd[i]<-lbdi+topt; tau<-tau+topt*di; gam<-z+tau
                            snew < -snew + (deli * topt ^ 2) / 2 + topt * (taudi + ri)
                            if (verbose)
15
                                        cat("Cycle:", formatC(itel, digits=3,
                                             width=3),
                                                    "Coordinate: _ " , <a href="formate">formatC</a>(i , digits)
                                                         =3, width=3),
                                                   "Loss: _ ", formatC (ss-snew, digits
                                                         =6, width=10, format="f"),
                                                    "\n")
20
                            }
                if (itout)
                            cat("Cycle:_", formatC(itel, digits=3, width=3),
                                        "<u>************</u>",
                                        "Previous Loss: , ", formatC (ss-sold,
                                             digits = 6, width = 10, format = "f"),
                                        "Current_Loss:_ ", <a href="formate">formate</a> (ss-snew, digits
25
                                             =6, width=10, format="f"),
                                        "\n")
                if (((sold-snew) < eps) || (itel == itmax)) break()</pre>
                sold<-snew; itel<-itel+1</pre>
```

```
}
30 <u>return(list(yhat=q%*%gam,s=ss-snew,k=itel))</u>
}
```

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