

Statistical Methods III: Spring 2013

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QP + constrained inference

Outline

- 1 Quadratic programming
- 2 Testing inequality constraints
- 3 Ordered means

OLS

Scalar notation

$$\arg \min_{\beta} \sum (y_i - \mathbf{x}^\top \beta)^2$$

Matrix notation

$$\arg \min_{\beta} (\mathbf{Y} - \mathbf{X}\beta)^\top (\mathbf{Y} - \mathbf{X}\beta)$$

Matrix notation expansion

$$\arg \min_{\beta} \beta^\top \mathbf{X}^\top \mathbf{X} \beta - 2\mathbf{Y}^\top \mathbf{X} \beta + \mathbf{Y}^\top \mathbf{Y}$$

- No constraints on β

Reviewing (and rewriting) OLS

Matrix notation expansion

$$\arg \min_{\beta} \beta^{\top} X^{\top} X \beta - 2 Y^{\top} X \beta + Y^{\top} Y$$

multiply by 1/2, and drop $Y^{\top} Y$ (why allowed?)

$$\arg \min_{\beta} \frac{1}{2} \beta^{\top} X^{\top} X \beta - Y^{\top} X \beta$$

If we write in form of,

$$\arg \min_{\beta} d^{\top} \beta + \frac{1}{2} \beta^{\top} W \beta$$

then

- $W = X^{\top} X$. What is W^{-1} ?
- $d = -Y^{\top} X$

OLS - with restrictions

OLS solution places no restriction on β .
The optimization problem

$$\arg \min_{\beta} \frac{1}{2} \beta^{\top} X^{\top} X \beta - Y^{\top} X \beta$$

restricted inequality constraints on β , for example,

$$\beta \geq 0$$

can be solved with “quadratic programming”

Quadratic programming

Definition (Quadratic programming problem)

Let $\beta \in R^n$, W be symmetric $n \times n$ matrix,

$$\arg \min_{\beta} d^T \beta + \frac{1}{2} \beta^T W \beta$$

subject to

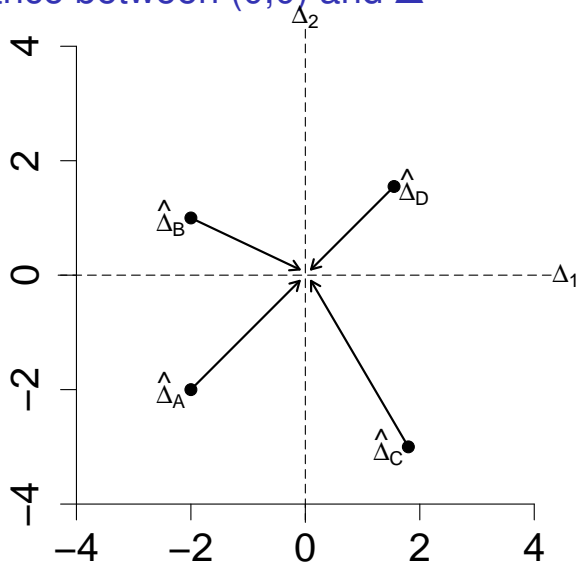
$$R_1^T \beta \geq b_1$$

$$R_2^T \beta = b_2$$

Notes

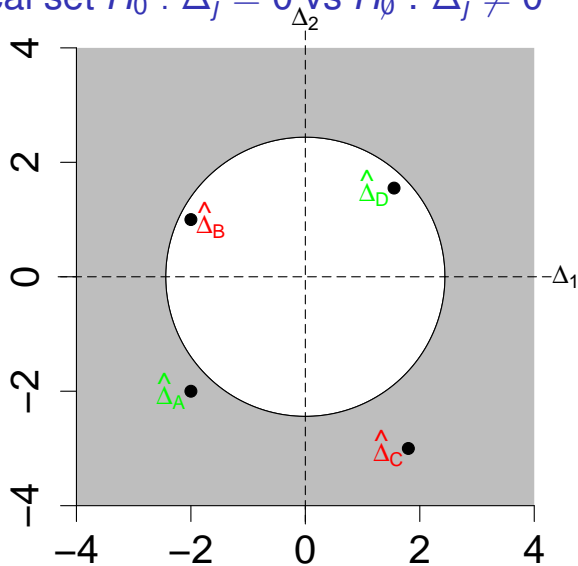
- d , W , R , and b are fixed for a given optimization
- β is unknown

Distance between $(0,0)$ and $\hat{\Delta}$



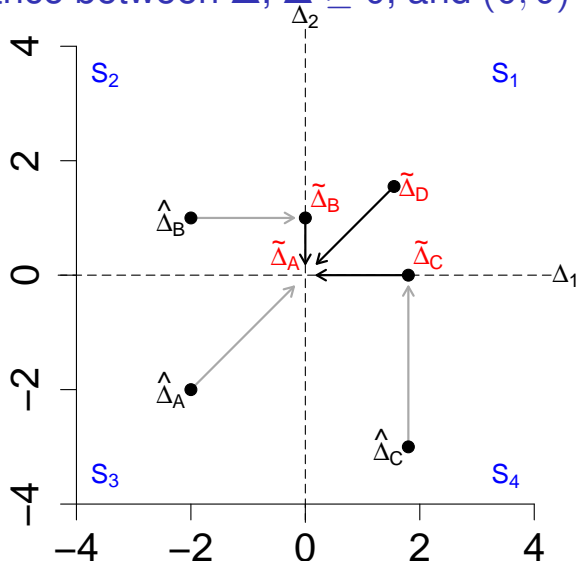
$$\Delta_1^2 + \Delta_2^2 \sim \chi_2^2$$

Critical set $H_0 : \Delta_j = 0$ vs $H_\emptyset : \Delta_j \neq 0$



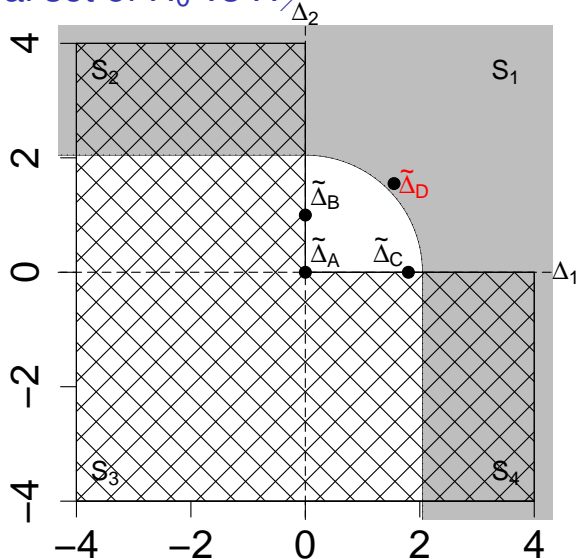
Critical value $\chi_{2,\alpha=.05}^2 = 6$, so $\sqrt{\Delta_1^2 + \Delta_2^2} = \sqrt{6} = \text{radius}$

Distance between $\hat{\Delta}$, $\tilde{\Delta} \geq 0$, and $(0, 0)$



$$\tilde{\Delta}_A \sim 0 \quad \tilde{\Delta}_B, \tilde{\Delta}_C \sim \chi_1^2 \quad \tilde{\Delta}_D \sim \chi_2^2$$

Critical set of H_0 vs H_1



$$P(\bar{\chi}_{+, \alpha}^2 > \bar{c}) = 1/4 P(\chi_2^2 > \bar{c}) + 1/2 P(\chi_1^2 > \bar{c}) + 1/4 = \alpha$$

Constrained estimation: dimensions and distance

Constrained estimates $\tilde{\Delta}$, subject to $\Delta > 0$

$$\tilde{\Delta} = \begin{cases} (\hat{\Delta}_1, \hat{\Delta}_2) & \text{if } \hat{\Delta}_1 \geq 0 \text{ and } \hat{\Delta}_2 \geq 0 \\ (\hat{\Delta}_1, 0) & \text{if } \hat{\Delta}_1 \geq 0 \text{ and } \hat{\Delta}_2 < 0 \\ (0, \hat{\Delta}_2) & \text{if } \hat{\Delta}_1 < 0 \text{ and } \hat{\Delta}_2 \geq 0 \\ (0, 0) & \text{if } \hat{\Delta}_1 < 0 \text{ and } \hat{\Delta}_2 < 0 \end{cases}$$

How many free parameters? 2 (S1), 1 (S2, S4), or 0 (S3).

What is probability of being “far” from H_0 ? By quadrant:

$$P(\tilde{\Delta}_1^2 + \tilde{\Delta}_2^2 < c' \mid \hat{\Delta} \in S_1) = P(\chi_2^2 < c')$$

$$P(\tilde{\Delta}_1^2 + 0 < c' \mid \hat{\Delta} \in S_2) = P(\chi_1^2 < c')$$

$$P(0 + \tilde{\Delta}_2^2 < c' \mid \hat{\Delta} \in S_4) = P(\chi_1^2 < c')$$

$$P(0 + 0 < c' \mid \hat{\Delta} \in S_3) = 1$$

Constrained estimation: dimensions and distance

In this simple example, each of quadrants is equally likely under H_0

$$P(\tilde{\Delta}_1^2 + \tilde{\Delta}_2^2 < c' \mid \hat{\Delta} \in S_1) = P(\chi_2^2 < c')$$

$$P(\tilde{\Delta}_1^2 + 0 < c' \mid \hat{\Delta} \in S_2) = P(\chi_1^2 < c')$$

$$P(0 + \tilde{\Delta}_2^2 < c' \mid \hat{\Delta} \in S_4) = P(\chi_1^2 < c')$$

$$P(0 + 0 < c' \mid \hat{\Delta} \in S_3) = 1$$

So for given α , solve for c'

$$P(\bar{\chi}^2 < c') = 1/4P(\chi_2^2 < c') + 1/2P(\chi_1^2 < c') + 1/4 = 1 - \alpha$$

Distribution of hypothesis tests

- Equality restriction versus unconstrained
 - ▶ Fixed difference in dimensionality of models

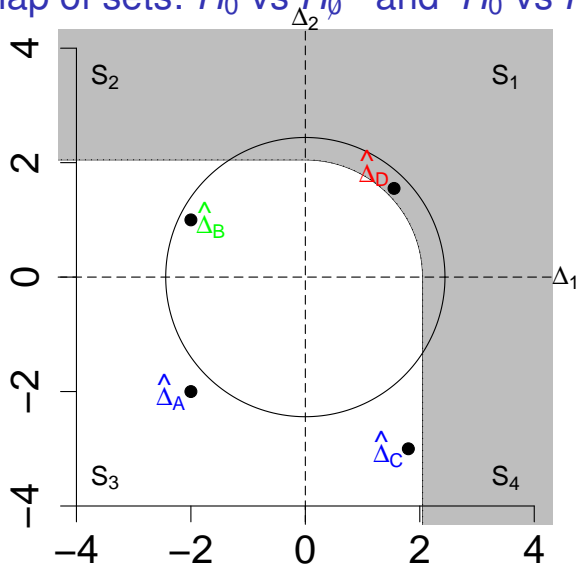
$$Pr(-2[L(\tilde{\theta}) - L(\hat{\theta})] > c) = Pr(\chi_r^2 > c)$$

- But number of free – restricted parms is stochastic if
 - ▶ Equality restrictions versus inequality restriction
 - ▶ Inequality restricted vs unconstrained
 - ▶ Inequality restricted versus additional inequalities

$$\begin{aligned} Pr(-2[L(\tilde{\theta}) - L(\hat{\theta})] > c') &= Pr(\bar{\chi}^2 > c') \\ &= \sum_{k=1}^K w_k Pr(\chi_k^2 > c') \end{aligned}$$

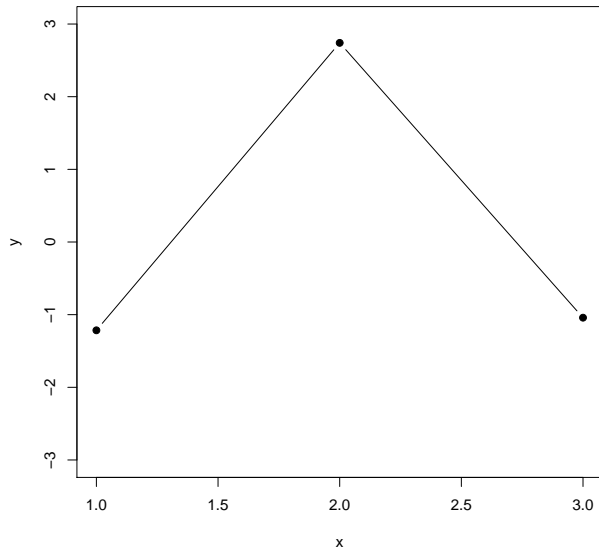
where w_k is the probability of having a difference of k degrees of freedom between models

Overlap of sets: H_0 vs H_\emptyset and H_0 vs H_{\nearrow}



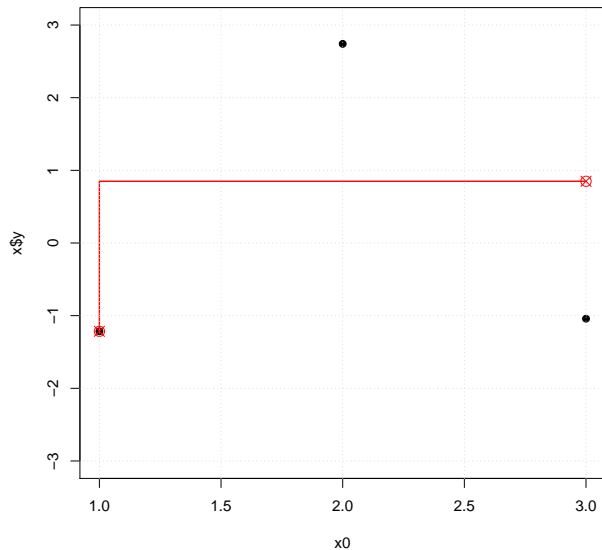
$$\sqrt{\chi_{2,\alpha}^2} = \text{radius}_\emptyset = 2.45 \quad \text{vs} \quad \sqrt{\bar{\chi}_{+,\alpha}^2} = \text{radius}_{\nearrow} = 2.05$$

Sequence of means

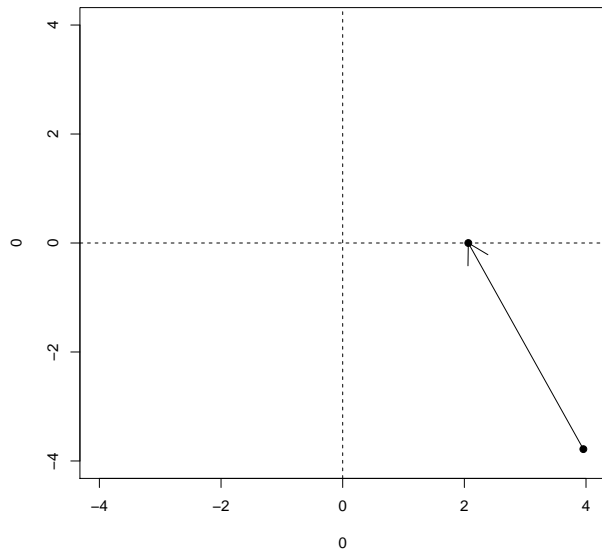


Best fitting mono inc.

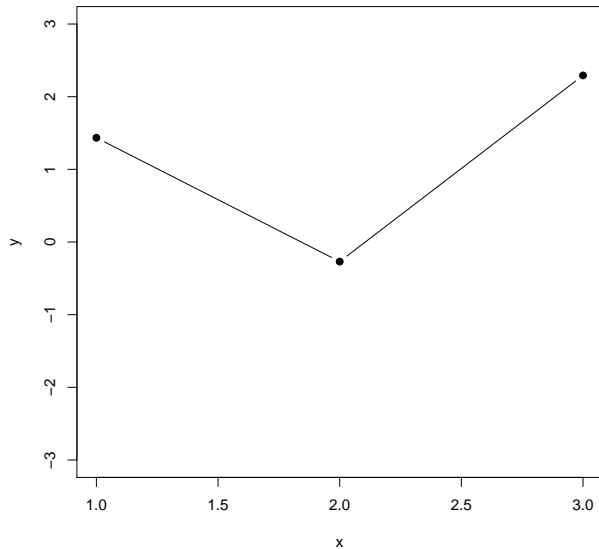
Isotonic regression $\text{isoreg}(x = x, y = y)$



Diff in adjacent mean, unconstrained to constrained

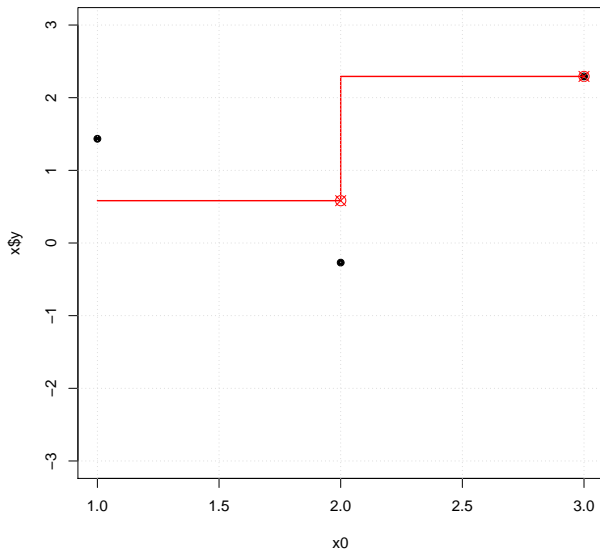


Sequence of means

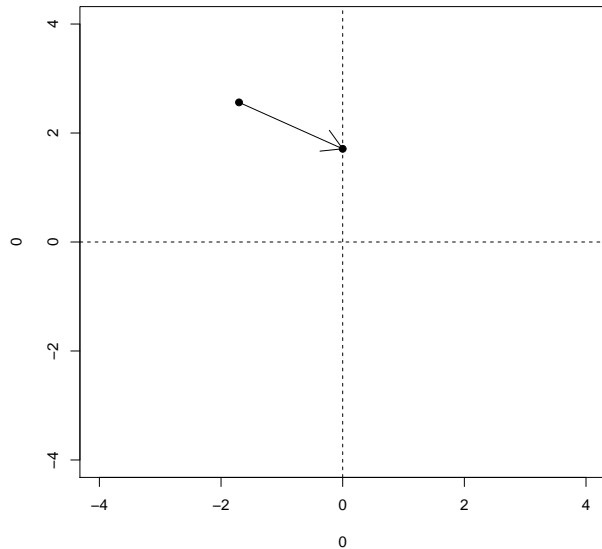


Best fitting mono inc.

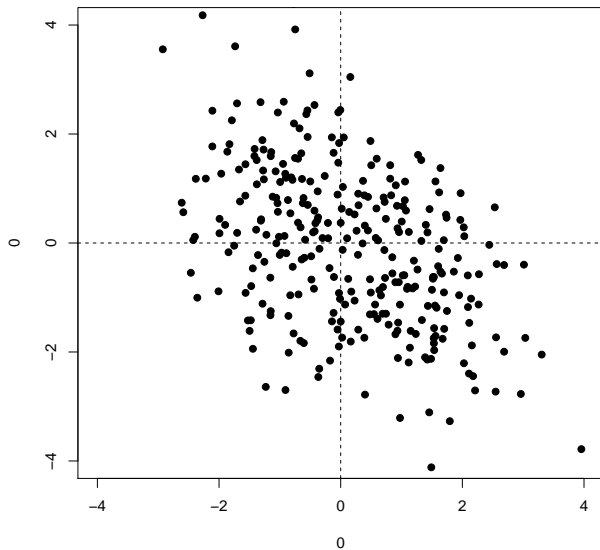
Isotonic regression $\text{isoreg}(x = x, y = y)$



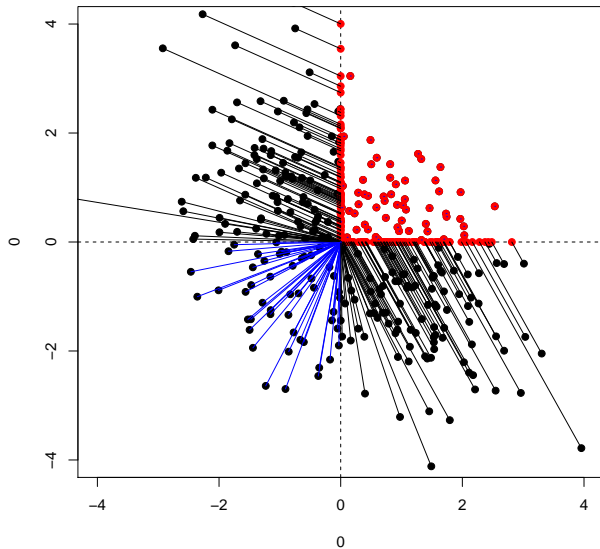
Diff in adjacent mean, unconstrained to constrained



Lots of draws of unconstrained diff means



Constrained v mono inc diff

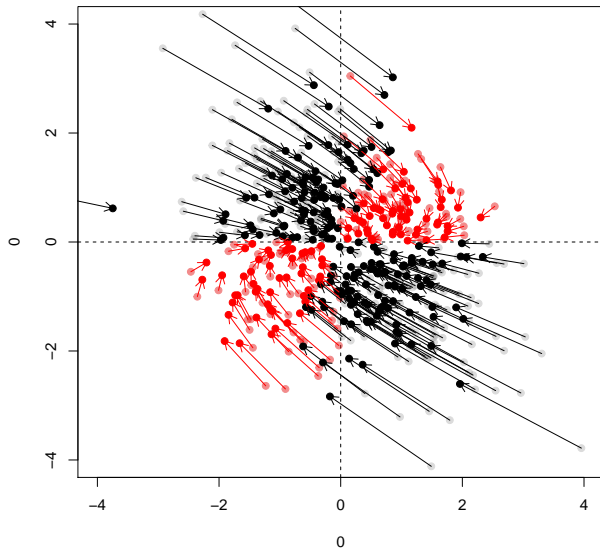


Constrained v mono inc diff

In simulation,

- could you determine w , probability of model dimensionality
- what is the distribution of the fits in constrained?

Transformation via cholesky

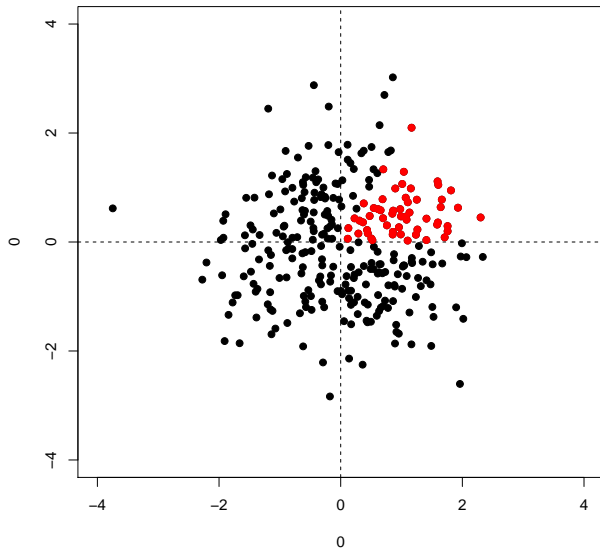


Transformation via cholesky

```
Y <- matrix(rnorm(3*n), ncol=3)
d <- t(apply(Y, 1, diff))
z <- t(apply(Y, 1, function(x) isoreg(x)$yf))
d2 <- t(apply(z, 1, diff))

(V <- cov(d))
Vi <- solve(V)
A <- t(chol(Vi))
Ai <- solve(A)
d3 <- d %*% A
```

... now iid bivariate normal



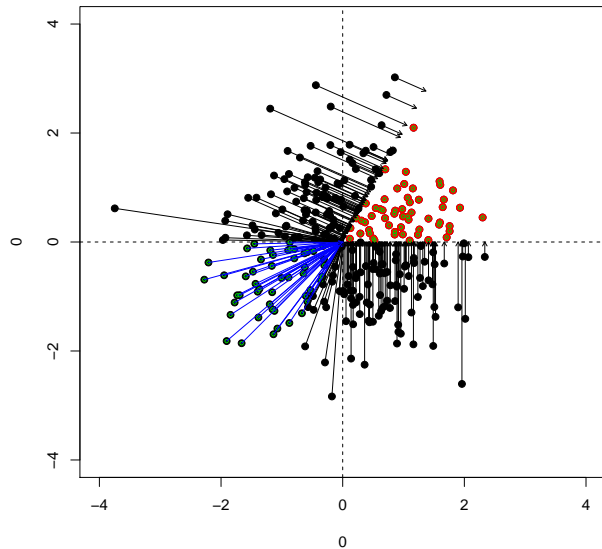
Transformed optimization problem...

```
d <- t(apply(Y,1,diff))
d2<- t(apply(z,1,diff))
(V <- cov(d))
Vi<- solve(V)
A <- t(chol(Vi))
Ai<- solve(A)
d3 <- d %*% A

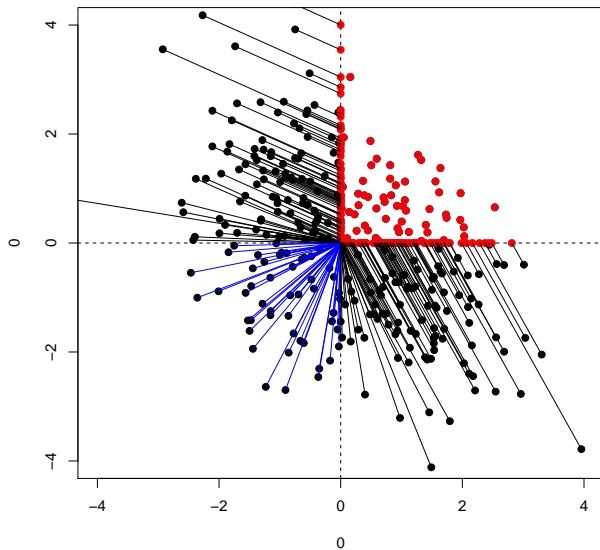
qp2 <- function(X)
  solve.QP( Dmat = Ai%*%Vi%*%t(Ai),
           dvec = X %*% A ,
           Amat = t(R %*% t(Ai)) ,
           bvec = c(0,0))

X <- d[i,]
d4 <- qp2(X)
```

Constrained fit on transformed means



Constrained v mono inc diff



Transformed vs untransformed

In simulation,

- R and V determine cone/constraint
- note: perpendicular: closest fitting point
compare with untransformed
- could you determine w , probability of model dimensionality (any different from untransformed?)
- what is the distribution of the fits in constrained?