# Lecture 18: Constrained & Penalized Optimization

*36-350*

*27 October 2014*

## Agenda

- Optimization under constraints
- Lagrange multipliers
- Penalized optimization
- Statistical uses of penalied optimization

## Maximizing a multinomial likelihood

I roll dice $n$ times; $n_1, \ldots n_6$ count the outcomes

Likelihood and log-likelihood:

$$\begin{aligned} L(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6) &= \frac{n!}{n_1! n_2! n_3! n_4! n_5! n_6!} \prod_{i=1}^{6} \theta_i^{n_i} \\ \ell(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6) &= \log \frac{n!}{n_1! n_2! n_3! n_4! n_5! n_6!} + \sum_{i=1}^{6} n_i \log \theta_i \end{aligned}$$

Optimize by taking the derivative and setting to zero:

$$\begin{aligned} \frac{\partial \ell}{\partial \theta_1} &= \frac{n_1}{\theta_1} = 0 \\ \therefore \theta_1 &= \infty \end{aligned}$$

## Maximizing a multinomial likelihood

We forgot that $\sum_{i=1}^{6} \theta_i = 1$

We could use the constraint to eliminate one of the variables

$$\theta_6 = 1 - \sum_{i=1}^{5} \theta_i$$

Then solve the equations

$$\frac{\partial \ell}{\partial \theta_i} = \frac{n_1}{\theta_i} - \frac{n_6}{1 - \sum_{j=1}^{5} \theta_j} = 0$$

BUT eliminating a variable with the constraint is usually messy

# Lagrange Multipliers

$$g(\theta) = c \;\Leftrightarrow\; g(\theta) - c = 0$$

**Lagrangian**:

$$\mathcal{L}(\theta, \lambda) = f(\theta) - \lambda(g(\theta) - c)$$

$= f$ when the constraint is satisfied

Now do *unconstrained* minimization over $\theta$ and $\lambda$:

$$\begin{aligned} \nabla_\theta \mathcal{L}|_{\theta^*, \lambda^*} &= \nabla f(\theta^*) - \lambda^* \nabla g(\theta^*) = 0 \\ \left.\frac{\partial \mathcal{L}}{\partial \lambda}\right|_{\theta^*, \lambda^*} &= g(\theta^*) - c = 0 \end{aligned}$$

optimizing **Lagrange multiplier** $\lambda$ enforces constraint

More constraints, more multipliers

# Lagrange Multipliers

Try the dice again:

$$\begin{aligned} \mathcal{L} &= \log \frac{n!}{\prod_i n_i!} + \sum_{i=1}^{6} n_i \log(\theta_i) - \lambda \left( \sum_{i=1}^{6} \theta_i - 1 \right) \\ \left.\frac{\partial \mathcal{L}}{\partial \theta_i}\right|_{\theta_i = \theta_i^*} &= \frac{n_i}{\theta_i^*} - \lambda^* = 0 \\ \frac{n_i}{\lambda^*} &= \theta_i^* \\ \sum_{i=1}^{6} \frac{n_i}{\lambda^*} &= \sum_{i=1}^{6} \theta_i^* = 1 \\ \lambda^* &= \sum_{i=1}^{6} n_i \;\Rightarrow \theta_i^* = \frac{n_i}{\sum_{i=1}^{6} n_i} \end{aligned}$$

# Thinking About the Lagrange Multipliers

Constrained minimum value is generally higher than the unconstrained

Changing the constraint level $c$ changes $\theta^*$, $f(\theta^*)$

$$\begin{aligned} \frac{\partial f(\theta^*)}{\partial c} &= \frac{\partial \mathcal{L}(\theta^*, \lambda^*)}{\partial c} \\ &= \left[\nabla f(\theta^*) - \lambda^* \nabla g(\theta^*)\right] \frac{\partial \theta^*}{\partial c} - \left[g(\theta^*) - c\right] \frac{\partial \lambda^*}{\partial c} + \lambda^* = \lambda^* \end{aligned}$$

$\lambda^*$ = Rate of change in optimal value as the constraint is relaxed

$\lambda^*$ = "Shadow price": How much would you pay for minute change in the level of the constraint

## Inequality Constraints

What about an *inequality* constraint?

$$h(\theta) \leq d \;\Leftrightarrow\; h(\theta) - d \leq 0$$

The region where the constraint is satisfied is the **feasible set**

*Roughly* two cases:

1. Unconstrained optimum is inside the feasible set $\Rightarrow$ constraint is **inactive**
2. Optimum is outside feasible set; constraint **is active**, **binds** or **bites**; *constrained* optimum is usually on the boundary

Add a Lagrange multiplier; $\lambda \neq 0 \Leftrightarrow$ constraint binds

## Mathematical Programming

Older than computer programming...

Optimize $f(\theta)$ subject to $g(\theta) = c$ and $h(\theta) \leq d$

"Give us the best deal on $f$, keeping in mind that we've only got $d$ to spend, and the books have to balance"

Linear programming (Kantorovich, 1938)

1. $f$, $h$ both linear in $\theta$
2. $\theta^*$ always at a corner of the feasible set

## Back to the Factory

Revenue: 13k per car, 27k per truck

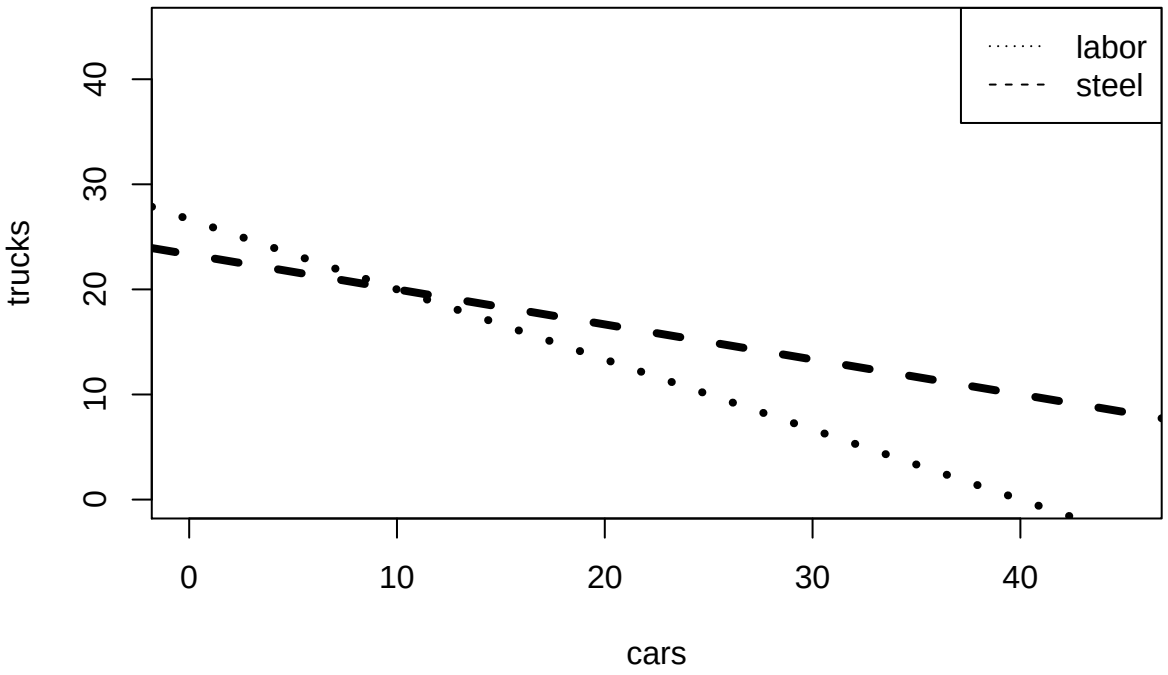
Constraints:

$$\begin{aligned} 40 * \text{cars} + 60 * \text{trucks} &< 1600\text{hours} \\ 1 * \text{cars} + 3 * \text{trucks} &< 70\text{tons} \end{aligned}$$

Find the revenue-maximizing number of cars and trucks to produce

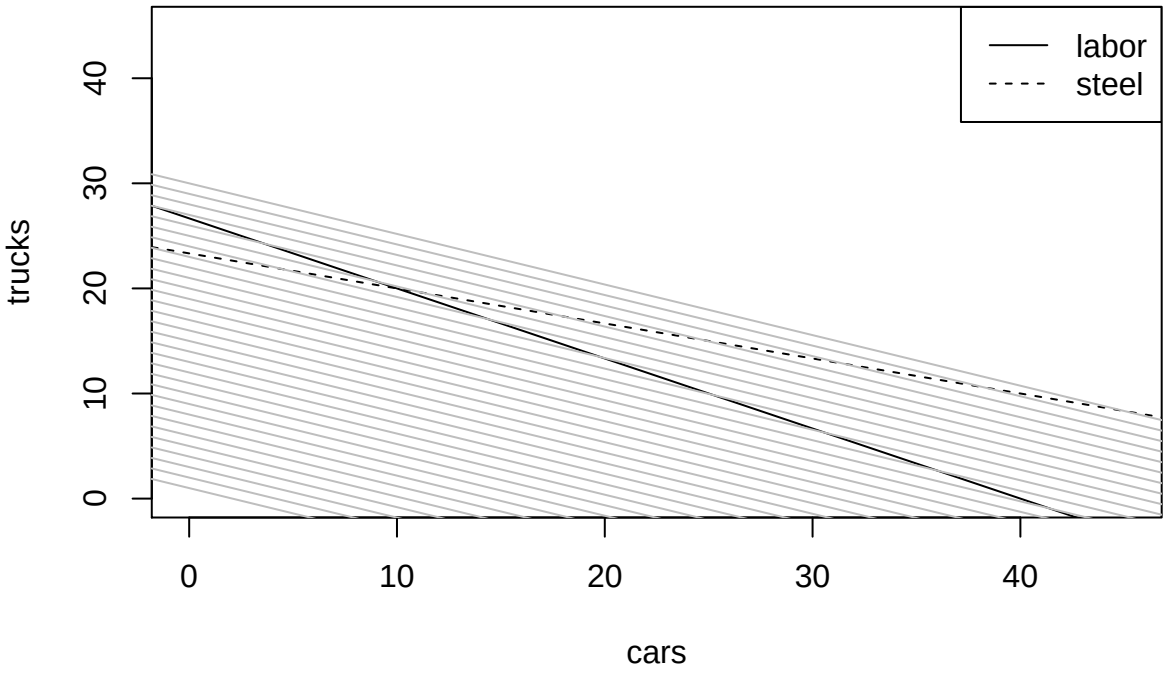
## Back to the Factory

The feasible region:




## Back to the Factory

The feasible region, plus lines of equal profit




## The Equivalent Capitalist Problem

. . . *is* that problem

> the Walrasian model [of economics] is essentially about allocations and only tangentially about markets — as one of us (Bowles) learned when he noticed that the graduate microeconomics course that he taught at Harvard was easily repackaged as 'The Theory of Economic Planning' at the University of Havana in 1969. (S. Bowles and H. Gintis, "Walrasian Economics in Retrospect", *Quarterly Journal of Economics*, 2000)

## The Slightly More Complex Financial Problem

*Given*: expected returns $r_1, \ldots r_p$ among $p$ financial assets, their $p \times p$ matrix of variances and covariances $\Sigma$

*Find*: the portfolio shares $\theta_1, \ldots \theta_n$ which maximizes expected returns

*Such that*: total variance is below some limit, covariances with specific other stocks or portfolios are below some limit
e.g., pension fund should not be too correlated with parent company

Expected returns $f(\theta) = r \cdot \theta$

Constraints: $\sum_{i=1}^{p} \theta_i = 1$, $\theta_i \geq 0$ (unless you can short)
Covariance constraints are linear in $\theta$
Variance constraint is quadratic, over-all variance is $\theta^T \Sigma \theta$

## Barrier Methods

(a.k.a. "interior point", "central path", etc.)

Having constraints switch on and off abruptly is annoying
especially with gradient methods

Fix $\mu > 0$ and try minimizing

$$f(\theta) - \mu \log (d - h(\theta))$$

"pushes away" from the barrier — more and more weakly as $\mu \to 0$

## Barrier Methods

1. Initial $\theta$ in feasible set, initial $\mu$
2. While ((not too tired) and (making adequate progress))
    a. Minimize $f(\theta) - \mu \log (d - h(\theta))$
    b. Reduce $\mu$
3. Return final $\theta$

## R implementation

`constrOptim` implements the barrier method

Try this:

```
factory <- matrix(c(40,1,60,3),nrow=2,
  dimnames=list(c("labor","steel"),c("car","truck")))
available <- c(1600,70); names(available) <- rownames(factory)
prices <- c(car=13,truck=27)
revenue <- function(output) { return(-output %*% prices) }
plan <- constrOptim(theta=c(5,5),f=revenue,grad=NULL,
  ui=-factory,ci=-available,method="Nelder-Mead")
plan$par
```

```
## [1] 10 20
```

`constrOptim` only works with constraints like $\mathbf{u}\theta \geq c$, so minus signs

## Constraints vs. Penalties

$$\text{argmin}_{\theta:h(\theta)\leq d} f(\theta) \Leftrightarrow \text{argmin}_{\theta,\lambda} f(\theta) - \lambda(h(\theta) - d)$$

$d$ doesn't matter for doing the second minimization over $\theta$

We could just as well minimize

$$f(\theta) - \lambda h(\theta)$$

| Constrained optimization | Penalized optimization |
|---|---|
| Constraint level $d$ | Penalty factor $\lambda$ |

"A fine is a price"

## Statistical Applications of Penalization

Mostly you've seen unpenalized estimates (least squares, maximum likelihood)

Lots of modern advanced methods rely on penalties

- For when the direct estimate is too unstable
- For handling high-dimensional cases
- For handling non-parametrics

## Ordinary Least Squares

No penalization; minimize MSE of linear function $\beta \cdot x$:

$$\hat{\beta} = \text{argmin}_{\beta} \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta \cdot x_i)^2 = \text{argmin}_{\beta} MSE(\beta)$$

Closed-form solution if we can invert matrices:

$$\hat{\beta} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y}$$

where $\mathbf{x}$ is the $n \times p$ matrix of $x$ vectors, and $\mathbf{y}$ is the $n \times 1$ matrix of $y$ values.

## Ridge Regression

Now put a penalty on the *magnitude* of the coefficient vector:

$$\tilde{\beta} = \text{argmin}_\beta MSE(\beta) + \mu \sum_{j=1}^{p} \beta_j^2 = \text{argmin}_\beta MSE(\beta) + \mu \|\beta\|_2^2$$

Penalizing $\beta$ this way makes the estimate more *stable*; especially useful for - Lots of noise - Collinear data ($\mathbf{x}$ not of "full rank") - High-dimensional, $p > n$ data (which implies collinearity)

This is called **ridge regression**, or **Tikhonov regularization**

Closed form:

$$\tilde{\beta} = (\mathbf{x}^T\mathbf{x} + \mu I)^{-1}\mathbf{x}^T\mathbf{y}$$

## The Lasso

Put a penalty on the sum of coefficient's absolute values:

$$\beta^\dagger = \text{argmin}_\beta MSE(\beta) + \lambda \sum_{j=1}^{p} |\beta_j| = \text{argmin}_\beta MSE(\beta) + \lambda \|\beta\|_1$$

This is called **the lasso**

- Also stabilizes (like ridge)
- Also handles high-dimensional data (like ridge)
- Enforces **sparsity**: it likes to drive small coefficients exactly to 0

No closed form, but very efficient interior-point algorithms (e.g., `lars` package)

## Spline Smoothing

"Spline smoothing": minimize MSE of a smooth, nonlinear function, plus a penalty on curvature:

$$\hat{f} = \text{argmin}_f \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \int (f''(x))^2 dx$$

This fits smooth regressions without assuming any specific functional form

- Lets you check linear models
- Makes you wonder why you bother with linear models

Many different R implementations, starting with `smooth.spline`

## How Big a Penalty?

Rarely know the constraint level or the penalty factor $\lambda$ from on high

Lots of ways of picking, but often **cross-validation** works well:

- Divide the data into parts
- For each value of $\lambda$, estimate the model on one part of the data
- See how well the models fit the other part of the data
- Use the $\lambda$ which extrapolates best on average

## Summary

- We use Lagrange multipliers to turn constrained optimization problems into unconstrained but penalized ones
  - Optimal multiplier values are the prices we'd pay to weaken the constraints
- The nature of the penalty term reflects the sort of constraint we put on the problem
  - Shrinkage
  - Sparsity
  - Smoothness

## Hypothesis Testing

Test the hypothesis that the data are distributed $\sim P$ against the hypothesis that they are distributed $\sim Q$

$P$ = noise, $Q$ = signal

Want to maximize **power**, probability the test picks up the signal when it's present

Need to limit false alarm rate, probability the test claims "signal" in noise

## Hypothesis Testing

Say "signal" whenever the data falls into some set $S$

Power = $Q(S)$

False alarm rate = $P(S) \leq \alpha$

$$\max_{S:P(S)\leq\alpha} Q(S)$$

With Lagrange multiplier,

$$\max_{S,\lambda} Q(S) - \lambda(P(S) - \alpha)$$

Looks like we have to do ugly calculus over set functions...

## Hypothesis Testing

Pick any point $x$: should we add it to $S$?

Marginal benefit $= dQ/dx = q(x)$

Marginal cost $= \lambda dP/dx = \lambda p(x)$

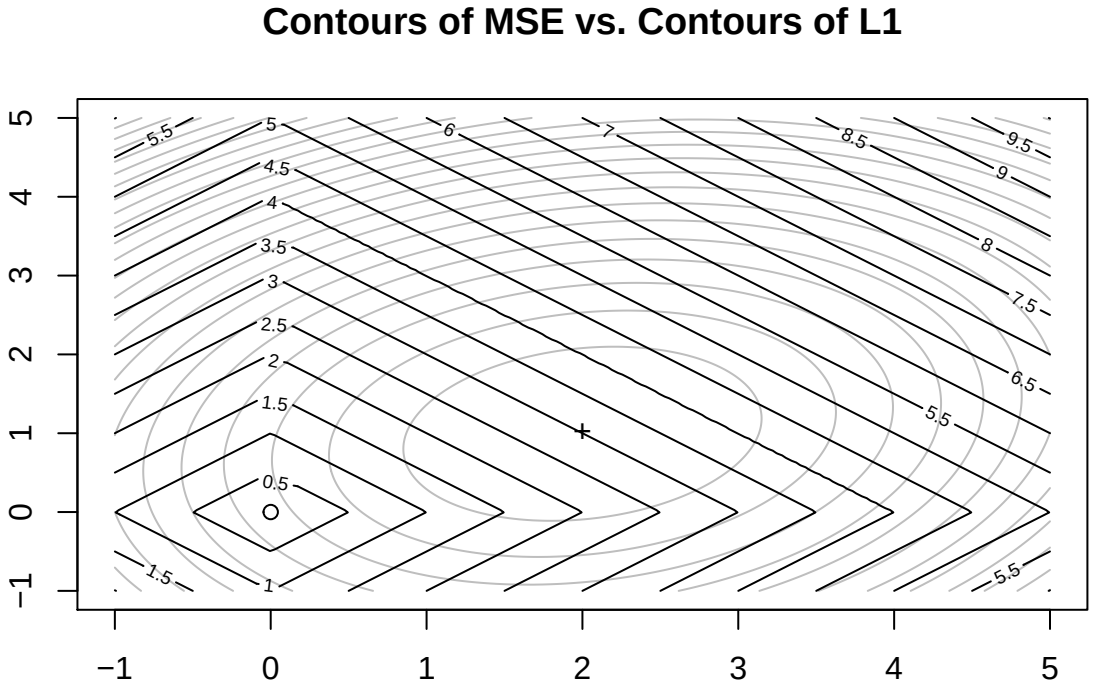
Keep expanding $S$ until marginal benefit = marginal cost so $q(x)/p(x) = \lambda$

$q(x)/p(x) =$ **likelihood ratio**; optimal test is **Neyman-Pearson test**

$\lambda =$ critical likelihood ratio = shadow price of power

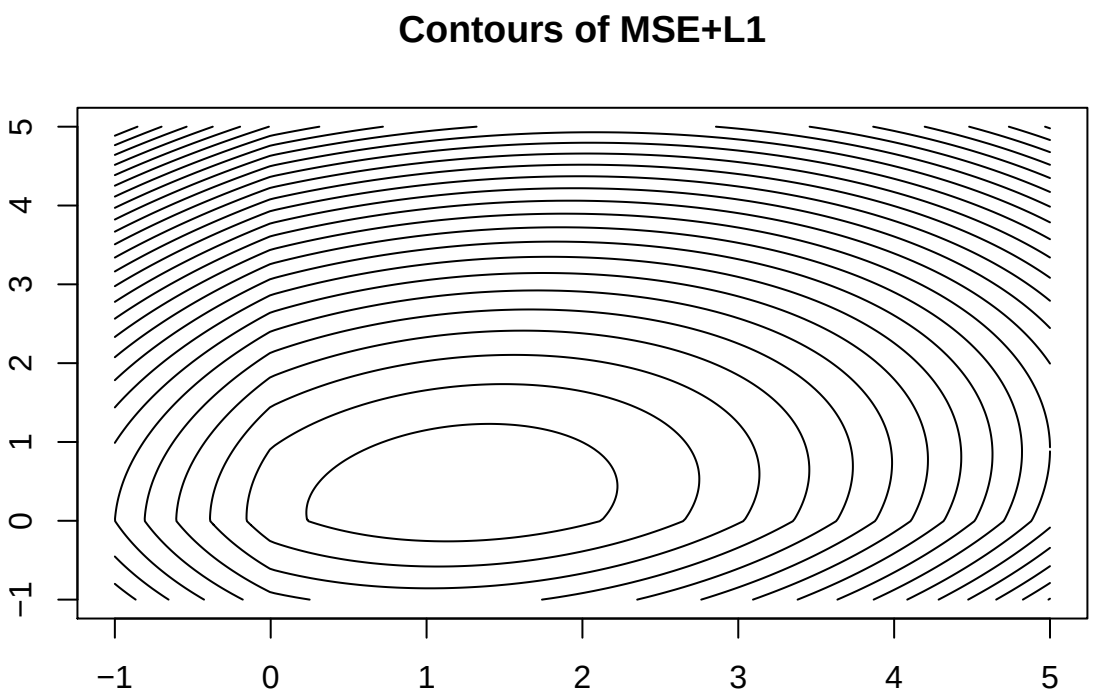
## Lasso Example

```
x <- matrix(rnorm(200),nrow=100)
y <- (x %*% c(2,1))+ rnorm(100,sd=0.05)
mse <- function(b1,b2) {mean((y- x %*% c(b1,b2))^2)}
coef.seq <- seq(from=-1,to=5,length.out=200)
m <- outer(coef.seq,coef.seq,Vectorize(mse))
l1 <- function(b1,b2) {abs(b1)+abs(b2)}
l1.levels <- outer(coef.seq,coef.seq,l1)
ols.coefs <- coefficients(lm(y~0+x))
contour(x=coef.seq,y=coef.seq,z=m,drawlabels=FALSE,nlevels=30,col="grey",
  main="Contours of MSE vs. Contours of L1")
contour(x=coef.seq,y=coef.seq,z=l1.levels,nlevels=20,add=TRUE)
points(x=ols.coefs[1],y=ols.coefs[2],pch="+")
points(0,0)
```



## Lasso Example

```
contour(x=coef.seq,y=coef.seq,z=m+l1.levels,drawlabels=FALSE,nlevels=30,
  main="Contours of MSE+L1")
```




## Augmented Lagrangian Methods

A simple trick for constrained optimization: minimize

$$f(\theta) + r(g(\theta) - c)^2$$

over and over, letting $r \to \infty$

Drawback: really unstable when $r$ is huge

Augmented Lagrangian trick: fix $r$ and a guess at $\lambda$, then minimize

$$f(\theta) + \lambda(g(\theta) - c) + r(g(\theta) - c)^2$$

Now crank up $r$ and update $\lambda$ by an amount that reflects how badly the constraint was violated

Often converges at finite $r$

## Augmented Lagrangian Methods

Same ideas work for inequality constraints

Unlike interior-point methods, initial guess needn't be in feasible set

R impelementation: `alabama` package