Optimization II

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Agenda

- Optimization with `optim()` and `nls()`
- Optimization under constraints
- Lagrange multipliers
- Penalized optimization
- Statistical uses of penalized optimization

Optimization in R: optim()

`optim(par, fn, gr, method, control, hessian)`

- `fn`: function to be minimized; mandatory
- `par`: initial parameter guess; mandatory
- `gr`: gradient function; only needed for some methods
- `method`: defaults to a gradient-free method ("Nedler-Mead"), could be BFGS (Newton-ish)
- `control`: optional list of control settings
  - (maximum iterations, scaling, tolerance for convergence, etc.)
- `hessian`: should the final Hessian be returned? default FALSE

Return contains the location (`$par`) and the value (`$val`) of the optimum, diagnostics, possibly `$hessian`

Optimization in R: optim()

```
gmp <- read.table("gmp.dat")
gmp$pop <- gmp$gmp/gmp$pcgmp
library(numDeriv)
```

```
## Warning: package 'numDeriv' was built under R version 4.0.2
```

```
mse <- function(theta) {
  mean((gmp$pcgmp - theta[1]*gmp$pop^theta[2])^2)
  }
grad.mse <- function(theta) { grad(func=mse,x=theta) }
theta0=c(5000,0.15)
fit1 <- optim(theta0,mse,grad.mse,method="BFGS",hessian=TRUE)
```

Optimization in R: optim()

- fit1: Newton-ish BFGS method

```
fit1[1:3]
```

```
## $par
## [1] 6493.2563739    0.1276921
##
## $value
## [1] 61853983
##
## $counts
## function gradient
##       63       11
```

Optimization in R: optim()

- fit1: Newton-ish BFGS method

```
fit1[4:6]
```

```
## $convergence
## [1] 0
##
## $message
## NULL
##
## $hessian
##               [,1]          [,2]
## [1,]      52.5021       4422071
## [2,] 4422071.3594 375729087979
```

Optimization in R: nls()

- `optim` is a general-purpose optimizer
- `nlm` is another general-purpose optimizer; nonlinear least squares
- Try them both if one doesn't work

Optimization in R: nls()

```
nls(formula, data, start, control, [[many other options]])
```

- `formula`: Mathematical expression with response variable, predictor variable(s), and unknown parameter(s)
- `data`: Data frame with variable names matching `formula`
- `start`: Guess at parameters (optional)
- `control`: Like with `optim` (optional)
- Returns an `nls` object, with fitted values, prediction methods, etc. The default optimization is a version of Newton's method.

Optimization in R: nls()

- fit2: Fitting the Same Model with nls()

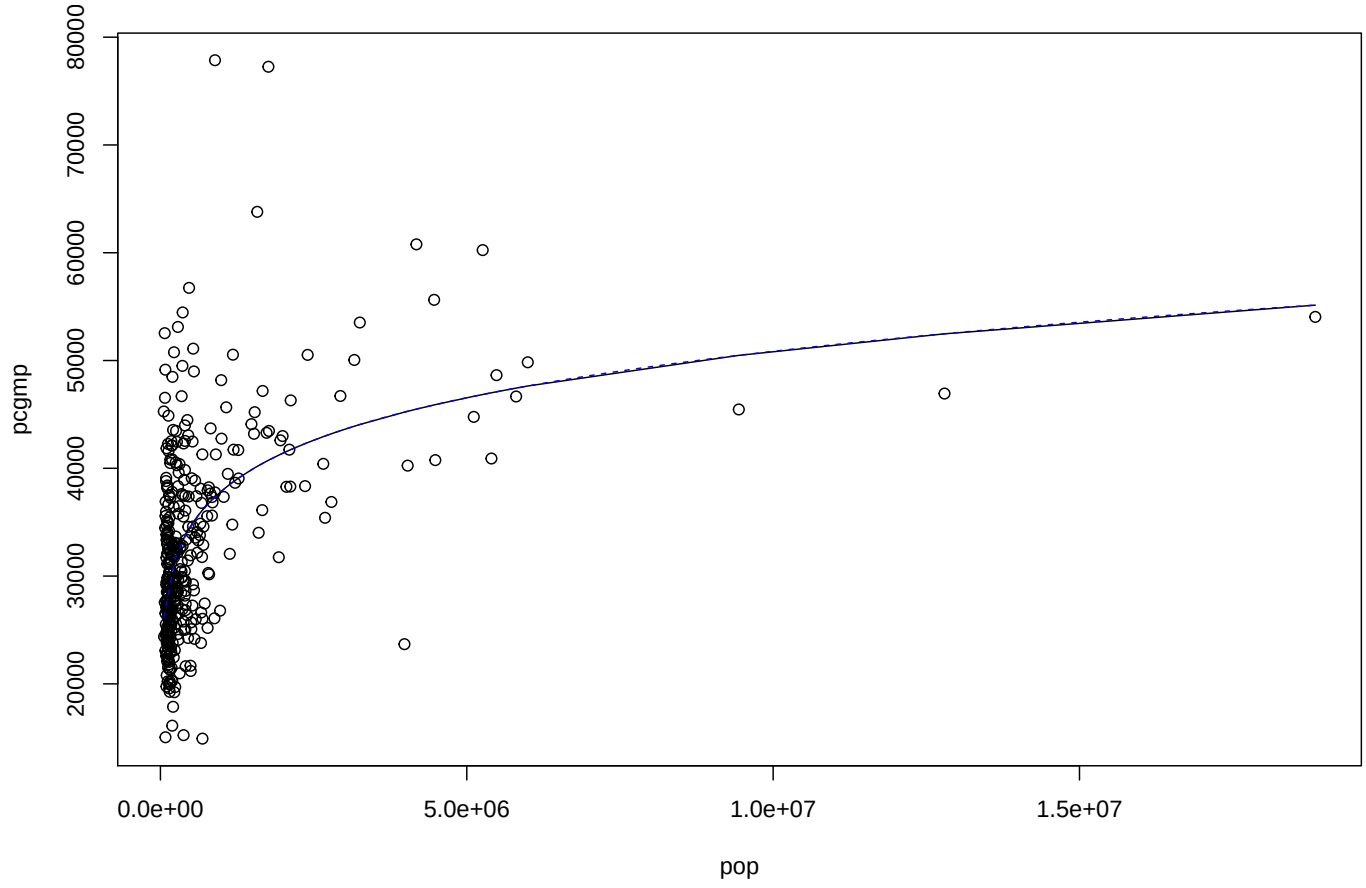
```
fit2 <- nls(pcgmp~y0*pop^a,data=gmp,start=list(y0=5000,a=0.1))
summary(fit2)
```

```
##
## Formula: pcgmp ~ y0 * pop^a
##
## Parameters:
##     Estimate Std. Error t value Pr(>|t|)
## y0 6.494e+03  8.565e+02   7.582 2.87e-13 ***
## a  1.277e-01  1.012e-02  12.612  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7886 on 364 degrees of freedom
##
## Number of iterations to convergence: 5
## Achieved convergence tolerance: 1.819e-07
```

Optimization in R: nls()

- fit2: Fitting the Same Model with nls()

```
plot(pcgmp~pop,data=gmp)
pop.order <- order(gmp$pop)
lines(gmp$pop[pop.order],fitted(fit2)[pop.order])
curve(fit1$par[1]*x^fit1$par[2],add=TRUE,lty="dashed",col="blue")
```



Example: Multinomial

- Roll dice n times; $n_1, \ldots n_6$ count the outcomes
- Likelihood and log-likelihood

$$L(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6) = \frac{n!}{n_1! n_2! n_3! n_4! n_5! n_6!} \prod_{i=1}^{6} \theta_i^{n_i}$$

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

- Optimize by taking the derivative and setting to zero

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

Example: Multinomial

- 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 θ and λ

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

- Optimizing **Lagrange multiplier** λ enforces constraint
- More constraints, more multipliers

Lagrange multipliers

- Try the dice again

$$\mathcal{L} = \log \frac{n!}{\prod_i n_i!} + \sum_{i=1}^{6} n_i \log(\theta_i) - \lambda \left(\sum_{i=1}^{6} \theta_i - 1 \right)$$

$$\left. \frac{\partial \mathcal{L}}{\partial \theta_i} \right|_{\theta_i = \theta_i^*} = \frac{n_i}{\theta_i^*} - \lambda^* = 0$$

$$\frac{n_i}{\lambda^*} = \theta_i^*$$

$$\sum_{i=1}^{6} \frac{n_i}{\lambda^*} = \sum_{i=1}^{6} \theta_i^* = 1$$

$$\lambda^* = \sum_{i=1}^{6} n_i \;\; \Rightarrow \theta_i^* = \frac{n_i}{\sum_{i=1}^{6} n_i}$$

Lagrange multipliers

- Constrained minimum value is generally higher than the unconstrained
- Changing the constraint level c changes θ^*, $f(\theta^*)$

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

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

Example: Factory

- Revenue: 13k per car, 27k per truck
- Constraints

$$40 * \text{cars} + 60 * \text{trucks} < 1600 \text{hours}$$

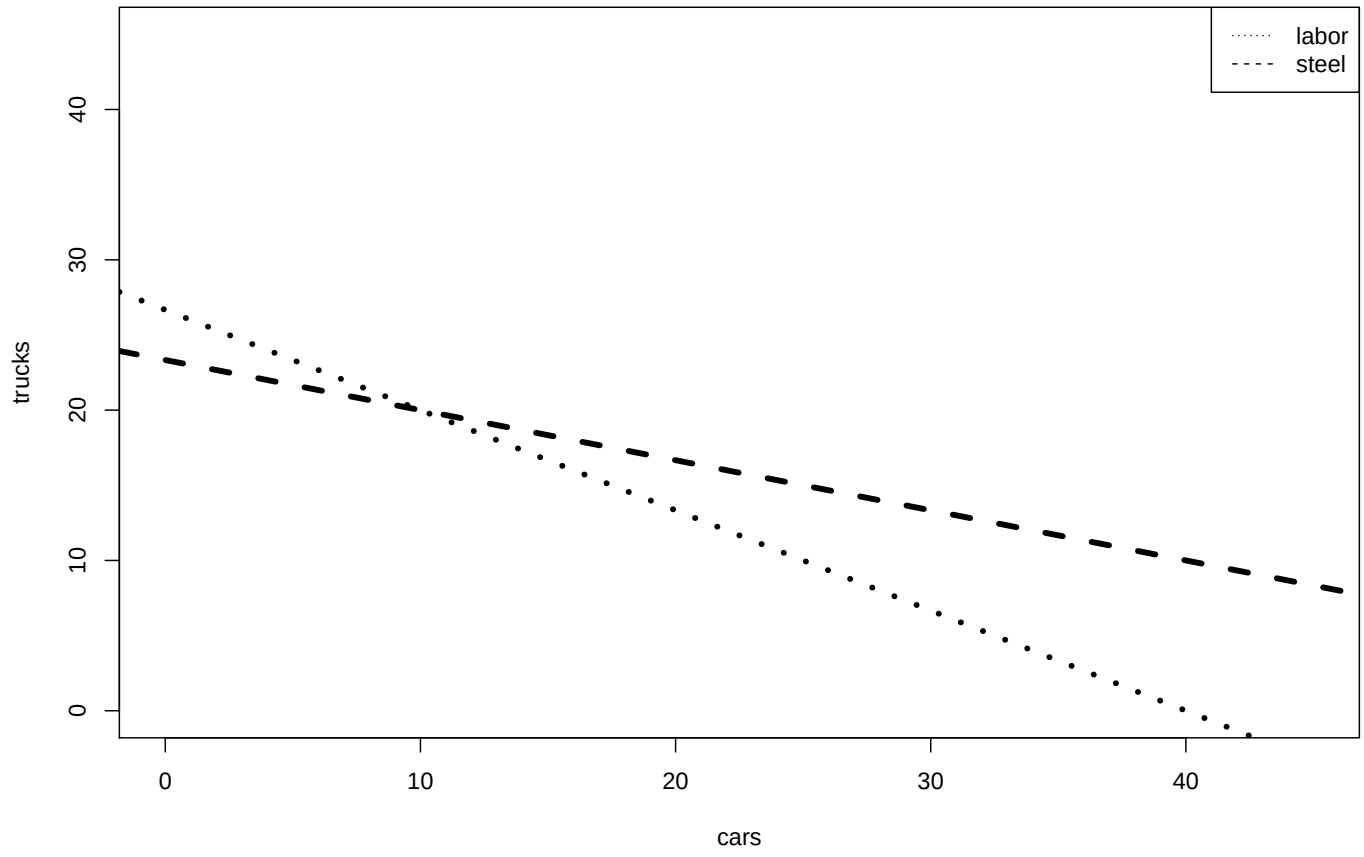
$$1 * \text{cars} + 3 * \text{trucks} < 70 \text{tons}$$

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

Example: Factory

- The feasible region

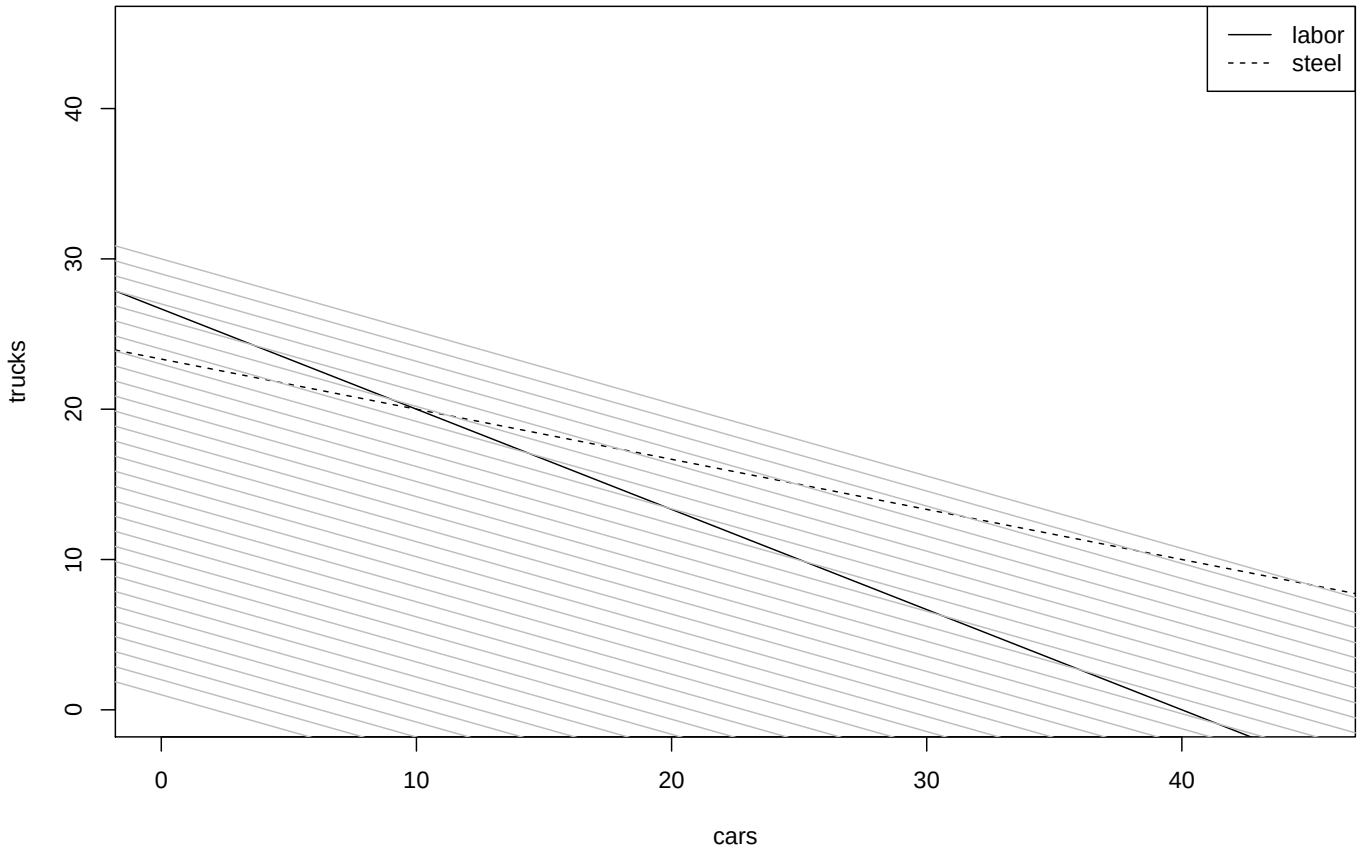
```
plot(0,type="n",xlim=c(0,45),ylim=c(0,45),xlab="cars",ylab="trucks")
abline(70/3,-1/3,lty="dashed",lwd=4)
abline(80/3,-2/3,lty="dotted",lwd=4)
legend("topright",legend=c("labor","steel"),lty=c("dotted","dashed"))
```



Example: Factory

- The feasible region, plus lines of equal profit

```
plot(0,type="n",xlim=c(0,45),ylim=c(0,45),xlab="cars",ylab="trucks")
abline(70/3,-1/3,lty="dashed")
abline(80/3,-2/3)
legend("topright",legend=c("labor","steel"),lty=c("solid","dashed"))
for (i in 1:30) {abline(i,-13/27,col="grey",lwd=1)}
```



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 Σ
- *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
  - For example, 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 θ
  - Variance constraint is quadratic, over-all variance is $\theta^T \Sigma \theta$

Barrier Methods

- Also known as "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 θ in feasible set, initial μ
2. While *not too tired* and *making adequate progress*
   a. Minimize $f(\theta) - \mu \log(d - h(\theta))$
   b. Reduce μ
3. Return final θ

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]  9.999896 20.000035
```

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

Constraints vs. Penalties

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

- d doesn't matter for doing the second minimization over θ
- We could just as well minimize

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

Constrained optimization	Penalized optimization
Constraint level d	Penalty factor λ

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 $\beta \cdot x$

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

- 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

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

- Penalizing β 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 solution

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

The Lasso

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

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

- 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

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

- 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 λ from on high
- Lots of ways of picking, but often **cross-validation** works well
  - Divide the data into parts
  - For each value of λ, estimate the model on one part of the data
  - See how well the models fit the other part of the data
  - Use the λ which extrapolates best on average

Summary

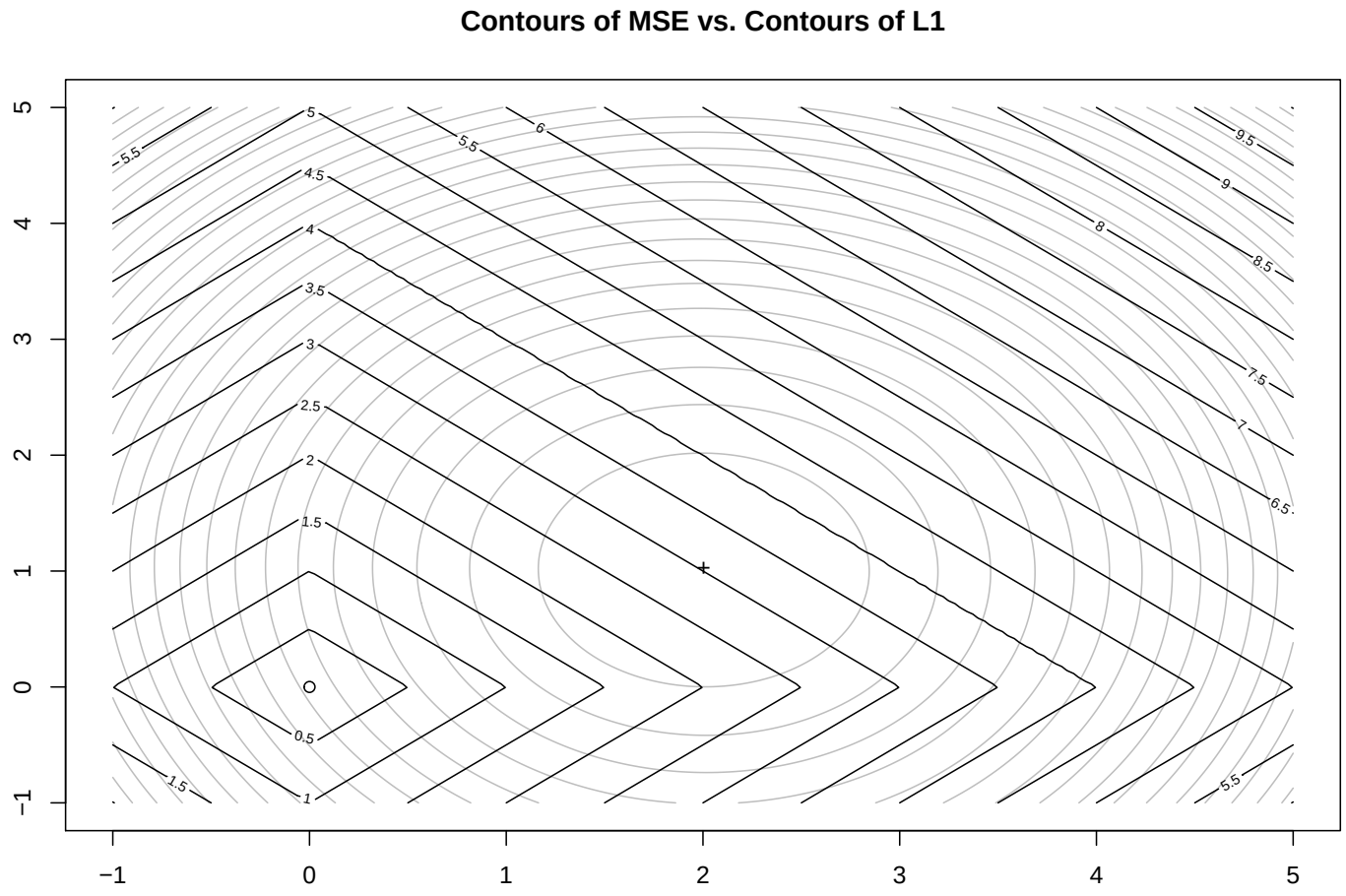
- Start with pre-built code like `optim` or `nls`, implement your own as needed
- Use Lagrange multipliers to turn constrained optimization problems into unconstrained but penalized ones
  - Optimal multiplier values are the prices we'd pay to weaken the constraints
- The nature of the penalty term reflects the sort of constraint we put on the problem
  - Shrinkage
  - Sparsity
  - Smoothness

Example: Lasso

```
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))
```

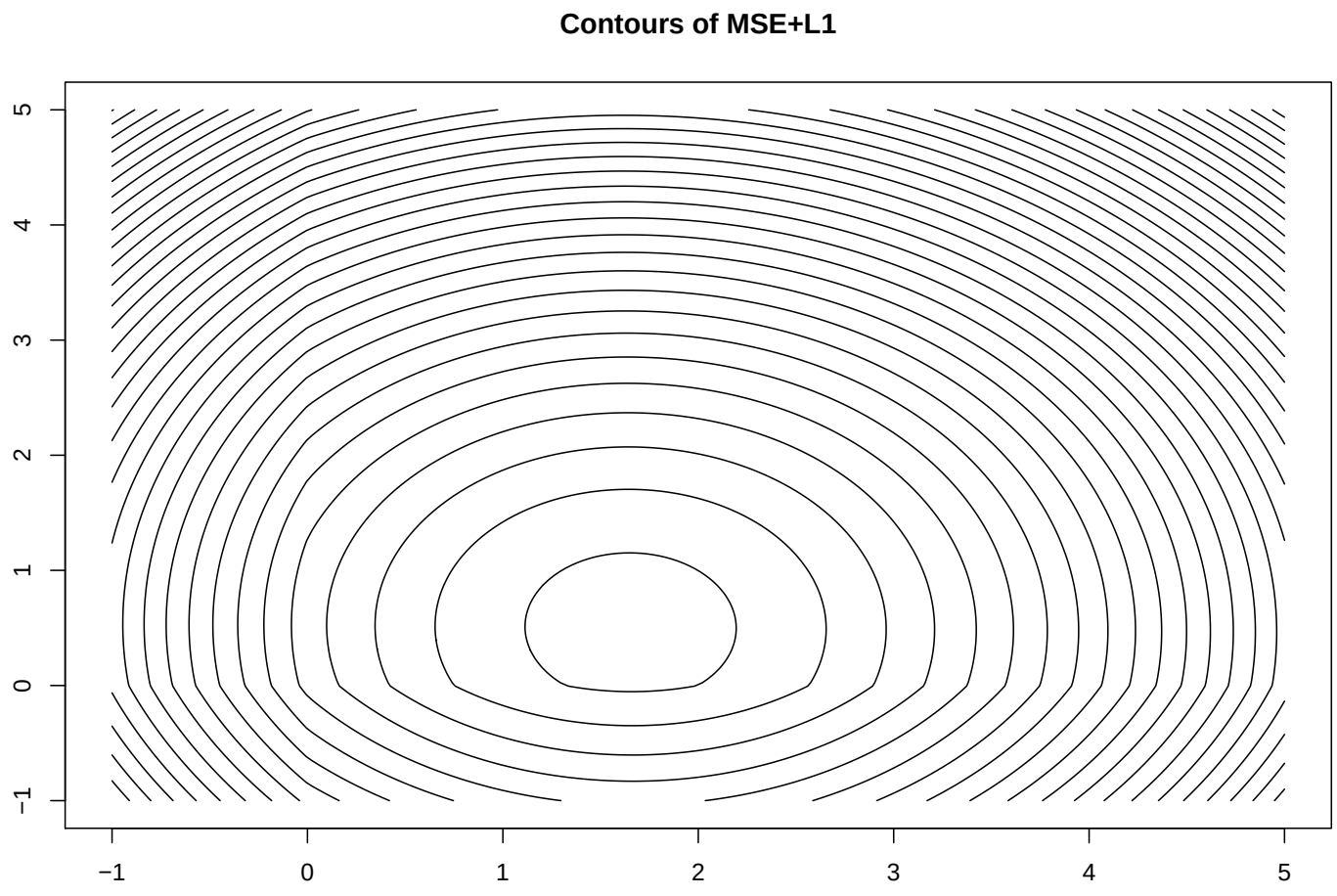
Example: Lasso

```
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)
```



Example: Lasso

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



Bonus: Writing Our Own gradient()

- Suppose we didn't know about the `numDeriv` package..
- Use the simplest possible method: change `x` by some amount, find the difference in `f`, take the slope

  `method="simple"` option in `numDeriv::grad`
  - Start with pseudo-code

```
gradient <- function(f,x,deriv.steps) {
  # not real code
  evaluate the function at x and at x+deriv.steps
  take slopes to get partial derivatives
  return the vector of partial derivatives
}
```

Bonus Example: gradient()

- A naive implementation would use a `for` loop

```
gradient <- function(f,x,deriv.steps,...) {
  p <- length(x)
  stopifnot(length(deriv.steps)==p)
  f.old <- f(x,...)
  gradient <- vector(length=p)
  for (coordinate in 1:p) {
   x.new <- x
   x.new[coordinate] <- x.new[coordinate]+deriv.steps[coordinate]
   f.new <- f(x.new,...)
   gradient[coordinate] <- (f.new - f.old)/deriv.steps[coordinate]
  }
  return(gradient)
}
```

- Works, but it's so repetitive!

Bonus Example: gradient()

- Better: use matrix manipulation and `apply`

```
gradient <- function(f,x,deriv.steps,...) {
  p <- length(x)
  stopifnot(length(deriv.steps)==p)
  x.new <- matrix(rep(x,times=p),nrow=p) + diag(deriv.steps,nrow=p)
  f.new <- apply(x.new,2,f,...)
  gradient <- (f.new - f(x,...))/deriv.steps
  return(gradient)
}
```

- Clearer and half as long
- Presumes that `f` takes a vector and returns a single number
- Any extra arguments to `gradient` will get passed to `f`
- Check: Does this work when `f` is a function of a single number?

Bonus Example: gradient()

- Acts badly if `f` is only defined on a limited domain and we ask for the gradient somewhere near a boundary
- Forces the user to choose `deriv.steps`
- Uses the same `deriv.steps` everywhere, imagine $f(x) = x^2 \sin x$
- . . . and so on through much of a first course in numerical analysis