Statistical Computing (36-350)

Lecture 19: Optimization III: Constrained and Stochastic Optimization

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30 October 2013

Agenda

- Constraints and penalties
- Stochastic optimization methods

READING (big picture): Francis Spufford, *Red Plenty*
OPTIONAL READING (big picture): Herbert Simon, *The Sciences of the Artificial*
OPTIONAL READING (close up): Bottou and Bosquet, “The Tradeoffs of Large Scale Learning”

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:

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

or $n_1 = 0$

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:

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

$= f$ when the constraint is satisfied

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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

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 $\theta^*, f(\theta^*)$

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

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λ^* = Rate of change in optimal value as the constraint is relaxed
λ^* = "Shadow price": How much would you pay for minute change in the level of the constraint

Inequality Constraints

What about an *inequality* constraint?

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

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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)

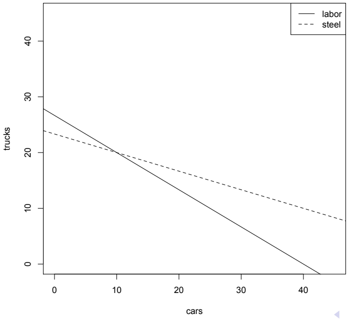
- f, h both linear in θ
- θ^* always at a corner of the feasible set

Back to the Factory

Constraints:

$$\begin{aligned} 40(\text{cars}) + 60(\text{trucks}) &\leq 1600 \\ 1(\text{cars}) + 3(\text{trucks}) &\leq 70 \end{aligned}$$

Revenue: \$13k/car, \$27k/truck
The feasible region:



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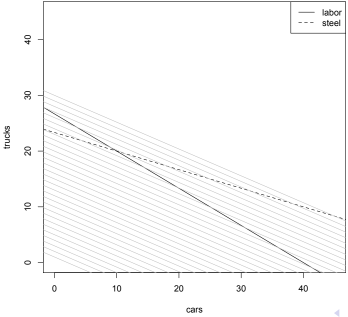

Barrier Methods

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

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

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

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Constrained optimization	$\Leftrightarrow$	Penalized optimization
Constraint level d	$\Leftrightarrow$	Penalty factor λ

Statistical Applications of Penalization

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Usually decide on penalty factor/constraint level by trying to predict out of sample

R implementation

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In penalty form, just chose λ and modify your objective function
`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
```

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

Problems with Big Data

Typical statistical objective function, mean-squared error:

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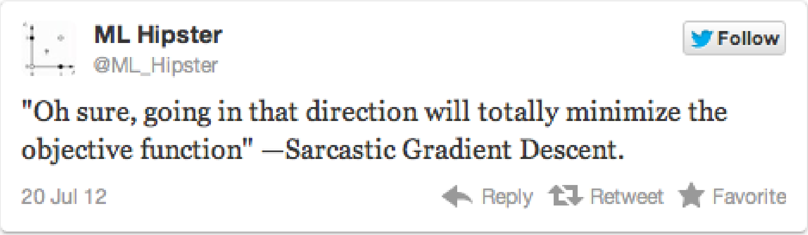
Not bad when $n = 100$ or even $n = 10^4$, but if $n = 10^9$ or $n = 10^{12}$ we don't even know which way to move


ML Hipster
@ML_Hipster
Follow
"Oh sure, going in that direction will totally minimize the objective function" —Sarcastic Gradient Descent.
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Reply
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Sampling, the Alternative to Sarcastic Gradient Descent

Pick *one* data point I at random (uniform on $1:n$)
Loss there, $(y_I - m(x_I, \theta))^2$, is random, but

$$\mathbb{E}\left[(y_I - m(x_I, \theta))^2\right] = f(\theta)$$

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Generally, if $f(\theta) = n^{-1} \sum_{i=1}^{n} f_i(\theta)$ and f_i are well-behaved,

$$\begin{aligned} \mathbb{E}\left[f_I(\theta)\right] &= f(\theta) \\ \mathbb{E}\left[\nabla f_I(\theta)\right] &= \nabla f(\theta) \\ \mathbb{E}\left[\nabla^2 f_I(\theta)\right] &= \mathbf{H}(\theta) \end{aligned}$$

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\mathbb{E}\left[\nabla f_I(\theta)\right] &= \nabla f(\theta) \\
\mathbb{E}\left[\nabla^2 f_I(\theta)\right] &= \mathbf{H}(\theta)
\end{aligned}$$

$\therefore$ Don't optimize with all the data, optimize with random samples

Stochastic Gradient Descent

Draw lots of one-point samples, let their noise cancel out:

1. Start with initial guess θ, learning rate η
2. While ((not too tired) and (making adequate progress))
    1. At t^{th} iteration, pick random I uniformly
    2. Set $\theta \leftarrow \theta - t^{-1}\eta\nabla f_I(\theta)$
3. Return final θ

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(Variants: put points in some random order, only check progress after going over each point once, adjust $1/t$ rate, average a couple of random data points, etc.)

```
stoch.grad.descent <- function(f,theta,df,max.iter=1e6,rate=1e-6) {
  stopifnot(require(numDeriv))
  for (t in 1:max.iter) {
    g <- stoch.grad(f,theta,df)
    theta <- theta - (rate/t)*g
  }
  return(x)
}

stoch.grad <- function(f,theta,df) {
  i <- sample(1:nrow(df),size=1)
  noisy.f <- function(theta) { return(f(theta, data=df[i,])) }
  stoch.grad <- grad(noisy.f,theta)
  return(stoch.grad)
}
```

Stochastic Newton's Method

a.k.a. 2nd order stochastic gradient descent

1. Start with initial guess θ
2. While ((not too tired) and (making adequate progress))
    1. At t^{th} iteration, pick uniformly-random I
    2. $\theta \leftarrow \theta - t^{-1}\mathbf{H}_I^{-1}(\theta)\nabla f_I(\theta)$
3. Return final θ

+ all the Newton-ish tricks to avoid having to recompute the Hessian

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Often low computational cost to get within *statistical* error of the optimum

Simulated Annealing

Use Metropolis to sample from a density $\propto e^{-f(\theta)/T}$
Samples will tend to be near small values of f
Keep lowering T as we go along ("cooling", "annealing")

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2. While ((not too tired) and (making adequate progress))
    1. Proposal: $Z \leftarrow r(\cdot|\theta)$ (e.g., Gaussian noise)
    2. Draw $U \sim \mathrm{Unif}(0, 1)$
    3. Acceptance: If $U < e^{-\frac{f(Z)-f(\theta)}{T}}$ then $\theta \leftarrow Z$
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No derivatives, works for discrete problems, few guarantees

Summary

- Constraints are usually part of optimization
    - Constrained optimum generally at the boundary of feasible set
    - Lagrange multipliers turn constrained problems into unconstrained ones
    - Multipliers are prices: trade-off between tightening constraint and worsening optimal value
- Stochastic optimization methods use probability in the search
    - Stochastic gradient descent samples the data; gives up precision for speed
    - Simulated annealing randomly moves against the objective function; escapes local minima