Optimization: Uphill simplex method

Nelder & Mead (1965) Computer Journal 7:308-313
Numerical Recipes in C, §10.4

Why mention this algorithm?

- It's cute.
- Nelder (as in McCullagh and Nelder) is a very interesting statistician.
- The method is completely different from the others we've discussed (as are its convergence properties).

Other points:

- Only requires function evaluations
- Not very fast
- Requires *a lot* of function evalutations
- Best when you need to get something going quickly and when function evaluations are cheap

Basic description:

- Seek to maximize a function $l(\theta)$ where θ is a p-vector.
- Start with $p+1$ points defining a simplex in p-space.
- Roll/stretch/contract the simplex through p-space to find the maximum of $l(\theta)$

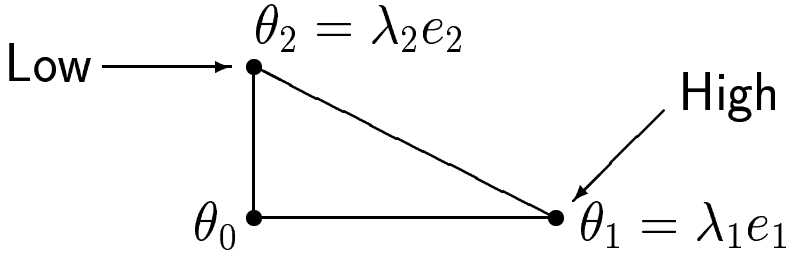
Uphill simplex method (continued)

Start:

$\theta_0 =$ starting point

$\theta_i = \theta_o + \lambda_i e_i$

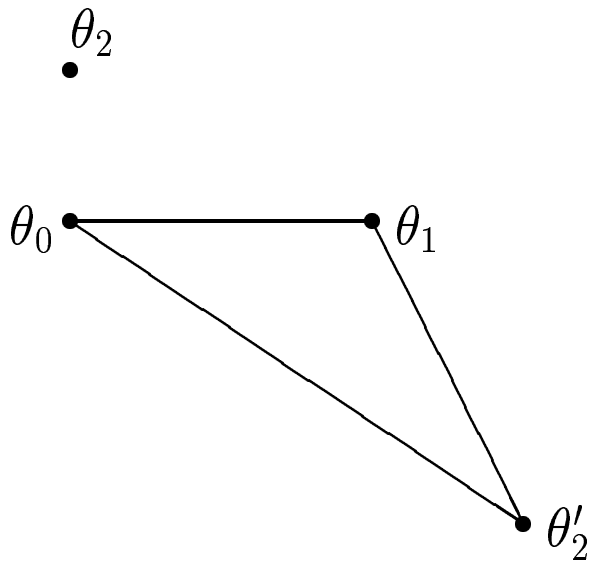
where e_i is the unit vector in the ith direction and λ_i is the *scale* of θ_{0i}.



Move A: (reflect and expand)

Suppose $i^\star = \arg\min_i l(\theta_i)$.

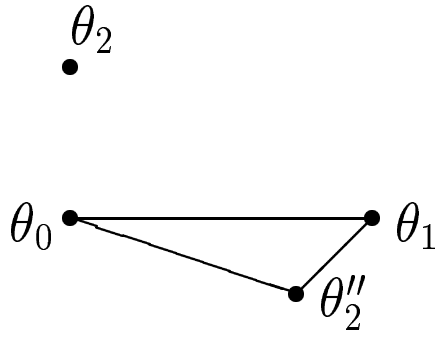
Replace $\theta_{i^\star}$ by reflecting it across the opposite face and expanding by a factor of 2, to give $\theta'_{i^\star}$.



Uphill simplex method (continued)

Move B: (reflect and contract)
If $l(\theta'_{i^\star}) < l(\theta_{i^\star})$:

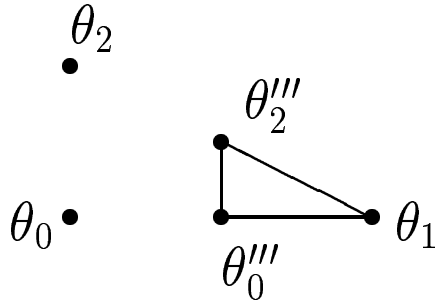
Try reflecting $\theta_{i^\star}$ across the opposite face but contracting by a factor of 2, to give $\theta''_{i^\star}$.



Move C: (multiple contraction)
If also $l(\theta''_{i^\star}) < l(\theta_{i^\star})$:

Find $i^{\star\star} = \arg\max_i l(\theta_i)$

Contract all points except $\theta_{i^{\star\star}}$ towards $\theta_{i^{\star\star}}$ by a factor of 2.



Stopping criterion:

Stop when $|l(\theta_{i^{\star\star}}) - l(\theta_{i^\star})| < \{|l(\theta_{i^{\star\star}})| + |l(\theta_{i^\star})|\}/(2\epsilon)$ or maybe $\max\{||\theta_i - \theta_{i^{\star\star}}||\} < \epsilon$

L_p regression

We wish find $\hat{\beta}$ minimizing $S_p(\beta) = \sum_i |y_i - x_i'\beta|^p$
for $0 < p < 2$.
Special case: when $p = 1$ we have *least absolute deviations* regression

IRLS method:

Note that $S_p(\beta) = \sum_i w_i(\beta)(y_i - x_i'\beta)^2$
where $w_i(\beta) = |y_i - x_i'\beta|^{p-2}$

This suggests using IRLS:

1. Find a starting point $\hat{\beta}^{(0)}$ (eg, by least squares)
2. Form the weights $w_i(\hat{\beta}^{(s)}) = |y_i - x_i'\hat{\beta}^{(s)}|^{p-2}$
3. Get new estimates $\hat{\beta}^{(s+1)}$ by using least squares with weights $w_i(\hat{\beta}^{(s)}$.

Problem: 0 residuals

Solution: Take $w_i(\beta) = \max\{\epsilon, |y_i - x_i'\beta|\}^{p-2}$
for some small ϵ (eg, 10^{-8}).

This isn't a very stable or fast solution (though it does work, pretty much). A better solution for the case $p = 1$ will be shown later.

L_p regression: code

```
lp <-
function(x,y,p=1,tol=1e-6,eps=1e-12,maxit=1000)
{
  beta.old <- lm(y~x)$coef

  for(i in 1:maxit) {
    r <- abs(y-cbind(1,x)%*%beta.old)
    r[r < eps] <- eps
    w <- as.numeric(r^(p-2))

    beta <- lm(y~x,weights=w)$coef

    if(all(abs(beta-beta.old) <
       tol*(abs(beta.old)+tol*100))) break;

    beta.old <- beta
  }
  cat("Number of iterations:", i, "\n")
  beta
}
```

```
> print(a <- lm(y~x)$coef,dig=2)
    9.26  0.30 -0.46  0.24  0.45

> unix.time(b <- lp(x,y))
Number of iterations: 41
[1] 4.33 0.52 4.91 0.00 0.00

> print(b,dig=2)
    9.45  0.11 -0.44  0.29  0.51
```

Constrained optimization

Maximize $l(\theta)$ for $\theta \in \Theta \subset R^p$

Easiest approach:

Hope/pray that $\hat{\theta} = \arg\max_{\theta \in R^p} l(\theta)$ satisfies $\hat{\theta} \in \Theta$.

Usual situation:

Maximize $l(\theta)$ subject to

Equality constraints: $c_1(\theta) = 0, \ldots, c_E(\theta) = 0$

Inequality constraints: $c_{E+1}(\theta) \geq 0, \ldots, c_{E+I}(\theta) \geq 0$

Linear programming:

l and the c_j are linear in θ.

Quadratic programming:

l is quadratic; the c_j are linear.

Nasty enough:

l is more complex than quadratic; the c_j are linear.

LAD regression

A linear programming formulation for the case $p = 1$:

Minimize $\sum e_i^+ + \sum e_i^-$
Subject to the constraints

$$y = X\beta + e^+ - e^-$$
$$e^+ \geq 0$$
$$e^- \geq 0$$

Here we have $2n + p$ unknowns (namely β, e^+ and e^-). Since $y_i = x_i\beta + (e_i^+ - e_i^-)$, at the solution either $e_i^+ = 0$ or $e_i^- = 0$ or both.

Efficient implementations make use of the relationships among the $2n + p$ variables.

If you're interested, see SC Narula (1982) Optimization techniques in linear regression. In Zanakis and Rustagi (eds), *Optimization in statistics*, Elsevier, New York, pp 11-29.

LS w/ linear equality constraints

[Seber (1977) Linear regression analysis. Wiley. §3.9.]

Minimize $(y - X\beta)'(y - X\beta)$ with constraint $A\beta = c$
where X is $n \times p$ with rank p
and A is $q \times p$ with rank $q < p$.

Solution using Lagrange multipliers:

Consider $r = (y - X\beta)'(y - X\beta) + (\beta' A' - c')\lambda$

Note that $\partial(\beta' a)/\partial\beta = a$ and
$\partial(\beta' W\beta)/\partial\beta = 2W\beta$ (if W is symmetric).

Thus $\partial r/\partial\beta = 2X'y + 2X'X\beta + A'\lambda$.

We seek $\hat{\beta}_H$ and $\hat{\lambda}_H$ satisfying $A\hat{\beta}_H = c$
and $2X'y + 2X'X\hat{\beta}_H + A'\hat{\lambda}_H = 0$.

$$\begin{aligned} \hat{\beta}_H &= (X'X)^{-1}X'y - (X'X)^{-1}A'\hat{\lambda}_H/2 \\ &= \hat{\beta} - (X'X)^{-1}A'\hat{\lambda}_H/2 \\ c &= A\hat{\beta} - A(X'X)^{-1}A'\hat{\lambda}_H/2 \\ \Longrightarrow\ \hat{\lambda}_H/2 &= \{A(X'X)^{-1}A'\}^{-1}(A\hat{\beta} - c) \end{aligned}$$

$$\Longrightarrow\ \hat{\beta}_H = \hat{\beta} + (X'X)^{-1}A'\{A(X'X)^{-1}A'\}^{-1}(c - A\hat{\beta})$$

LS w/ lin eq constraints (continued)

Three other points:

1. An interesting geometric derivation of $\hat{\beta}_H$, using projections and nullspaces, appears in Seber (1977) §3.9, and is worth looking at.

2. Since $\hat{\beta}_H = G\hat{\beta} + k$, we have $\text{var}(\hat{\beta}_H) = G\,\text{var}(\hat{\beta})\,G'$
   Using $G = I - (X'X)^{-1}A'\{A(X'X)^{-1}A'\}^{-1}A$,
   we appear to obtain $\text{var}(\hat{\beta}_H) = \sigma^2 G(X'X)^{-1}$

3. I can't remember my third point.

Example

Consider the model $y = \beta_0 + \sum_{j=1}^{4} \beta_i x_i + \epsilon$
Suppose we have the constraints $2\beta_1 = \beta_4$ and $3\beta_2 - 5\beta_3$.
Then $c = 0$ and

$$A = \begin{pmatrix} 0 & 2 & 0 & 0 & -1 \\ 0 & 0 & 3 & 5 & 0 \end{pmatrix}$$

With the data I played with above in LAD regression,

$\hat{\beta} \approx (9.26, 0.30, -0.46, 0.24, 0.45)$ and
$\hat{\beta}_H = G\hat{\beta} \approx (9.30, 0.23, -0.45, 0.25, 0.47)$.

$\hat{SE}(\hat{\beta}) \approx (0.59, 0.14, 0.12, 0.14, 0.11)$
$\hat{SE}(\hat{\beta}_H) \approx (0.51, 0.03, 0.12, 0.07, 0.07)$

LS with linear inequality constraints

This is an example of *quadratic programming*.

Note:

A consistent set of linear inequality constraints of full rank can be reduced by reparameterization to a set of nonnegativity constraints. [Thisted, 1988]

Problem:

minimize $(y - X\beta)'(y - X\beta)$
with constraints $\beta_j \geq 0$ for $j \in J$

Algorithm:

Let $\hat{\beta}$ be the unconstr'd sol'n, $C = J \setminus \{j : \hat{\beta}_j \geq 0\}$ (the "active" constraints), and $M = \{1, \ldots, p\} \setminus J$.

The constr'd sol'n to the problem is equiv't to the unconstr'd sol'n dropping the columns of X with $j \in C$.

Thus to solve the constrained problem, we need to find the maximal set M for which the unconstrained estimates $\hat{\beta}_j$ all satisfy the constraints.

At the worst, we may need to fit $2^{|J|}$ models. But a stepwise selection procedure can get the job done.

Example

Consider the model $y = \beta_0 + \sum_{j=1}^{4} x_j + \epsilon$
where we constrain $\beta_j \geq 0$ for $j > 0$.

```
> lm(y ~ x)$coef
     int       X1       X2       X3       X4
-0.0822 -0.0388  0.1221  0.0016  0.1226

> lm(y ~ x[,-1])$coef
     int       X2       X3       X4
-0.0867  0.1071 -0.0107  0.1271

> lm(y ~ x[,-3])$coef
     int       X1       X2       X4
-0.0823 -0.0384  0.1228  0.1225

> lm(y ~ x[,-c(1,3)])$coef
     int       X2       X4
-0.0861  0.1009  0.1289
```

The last model, with $\hat{\beta}_1 = \hat{\beta}_3 = 0$, is the one we choose.

Another example: Isotonic regression

Consider pairs (x_i, y_i) with $x_1 \leq x_2 \leq \ldots \leq x_n$.

Suppose $y_i|x_i \sim \mathsf{N}(\mu_i, \sigma^2)$ with $\mu_1 \leq \mu_2 \leq \ldots \leq \mu_n$.

$\rightarrow$ Find $\hat{\mu}_i$ minimizing $\sum(y_i - \mu_i)^2$ with this constraint.

If $y_1 \leq y_2 \leq \ldots \leq y_n$, then things are easy: $\hat{\mu}_i = y_i$!

Otherwise:

1. Let $\beta_1 = \mu_1$ and $\beta_i = \mu_i - \mu_{i-1}$ for $i > 1$.
   Let $X_{ij} = 1$ if $i \geq j$ or 0 otherwise.
   Then $y = X\beta + \epsilon$, $\epsilon \sim \mathsf{N}(0, \sigma^2)$, $\beta_i \geq 0$ for $i > 1$.
   Use the previously described method!
2. "Pool adjacent violators"
   See Barlow, Bartholomew, Bremner and Brunk (1972) Statistical inference under order restrictions; the theory and application of isotonic regression. Wiley.

Example

Suppose $k_{ij} \sim$ indep Poisson(λ_i)
for $i = 1, \ldots, G$ and $j = 1, \ldots, n_i$.

$l(\lambda|k) = -\sum_i n_i \lambda_i + \sum_i \log \lambda_i \sum_j k_{ij}$

$\partial l / \partial \lambda_i = -n_i + \sum_j k_{ij} / \lambda_i$

MLE: $\hat{\lambda}_i = \sum_j k_{ij} / n_i$

Constraint: $\lambda_1 \leq \lambda_i$ for all i.

If $\hat{\lambda}_1 \leq \hat{\lambda}_i$ for all $i \rightarrow$ done!

Otherwise, suppose $\hat{\lambda}_i < \hat{\lambda}_1$ for $i \in I$.

Then $\hat{\lambda}'_1 = \sum_{i \in I \cup \{1\}} \sum_j k_{ij} / \sum_{i \in I \cup \{1\}} n_i$

and $\hat{\lambda}'_i = \hat{\lambda}'_1$ for $i \in I$

Nonquad programming w/ lin eq constr

We seek to maximize $l(\theta)$ with the constraint $A\theta = b$ where A is $q \times p$ with rank $q < p$.

Let Z be a $p \times (p-q)$ orthonormal matrix satisfying $AZ = 0$ (and $Z'Z = I$).

Basic algorithm:

1. **Start**: Pick $\hat{\theta}^{(0)}$ satisfying $A\hat{\theta}^{(0)} = b$.
2. **Steps**: Take $\hat{\theta}^{(s+1)} = \hat{\theta}^{(s)} + \alpha_s \delta_s$ where $\delta_s = Zy$ for some $(p-q)$-vector y.

Let $g^{(s)}$ and $G^{(s)}$ be the gradient and Hessian of l, respectively, evaluated at $\hat{\theta}^{(s)}$.

Steepest ascent: $\delta_s = ZZ'g^{(s)}$

Newton-Raphson: $\delta_s = -Z\{Z'G^{(s)}Z\}^{-1}Z'\hat{g}^{(s)}$

Ref: Gill et al (1981) Practical optimization. Academic press. (ch 5)

Nonquad programming w/ lin ineq constr

We seek to maximize $l(\theta)$ with the constraint $A\theta \geq b$ where A is $q \times p$ of rank $q < p$.

The following is what is called an *active set algorithm*.

1. Find a starting point $\hat{\theta}^{(0)}$ satisfying $A\theta \geq b$. (For example, find the unconstrained maximum and project into onto the feasible set $\{\theta : A\theta \geq b\}$.
2. Define the set of *active constraints* by $C_s = \{i : a_i'\hat{\theta^{(s)}} = b_i\}$ where a_i' is the ith row of A.

   Let A_s and b_s denote the A and b with the inactive constraints dropped.
3. Consider dropping a constraint from the active set.
4. Compute a feasible direction, $\delta_s = Z_s y$ where $A_s Z_s = 0$ and $Z_s' Z_s = I$, as if we were maximizing $l(\theta)$ with just the active constraints $A_s\theta = b_s$.
5. Calculate $\bar{\alpha}_s$, the maximum value of α such that $A(\hat{\theta}^{(s)} + \alpha\delta_s) \geq b$

   Find $0 < \alpha_s \leq \bar{\alpha}_s$ so that $l(\hat{\theta}^{(s)} + \alpha_s\delta_s) > l(\hat{\theta}^{(s)})$.
6. Take $\hat{\theta}^{(s+1)} = \hat{\theta}^{(s)} + \alpha_s\delta_s$.
7. If $\alpha_s = \bar{\alpha}_s$, add the corresponding inactive constraint to the active set.