`CMregr` – A Matlab software package for finding CM-Estimates for Regression

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1 Introduction

This paper describes how to use the Matlab software package `CMregr`, and also gives some limited information on the CM-estimation problem itself. For detailed information on the algorithms used in `CMregr` as well as extensive testings, please refer to (Arslan, Edlund & Ekblom 2002) and (Edlund & Ekblom 2002).

New methods for robust estimation regression have been developed during the last decades. Two important examples are M-estimates (Huber 1981) and S-estimates (Rousseeuw & Yohai 1984). A more recent suggestion is Constrained M-estimates – or CM-estimates for short – where the good local properties of the M-estimates and good global robustness properties of the S-estimates are combined (Mendes & Tyler 1995). CM-estimates maintain an asymptotic breakdown point of 50% without sacrificing high asymptotic efficiency.

Until recently, there was no satisfying method for fast computation of CM-estimates, with high precision. The Matlab code `CMregr` presented here is an implementation of a new algorithm for CM-estimates for regression presented in (Arslan et al. 2002) and (Edlund & Ekblom 2002), that addresses these issues.

We can formulate CM-estimation for regression in the following way. Consider the linear model $y = X\beta + e$, where $y = (y_1, y_2, ..., y_n)^T$ is the response vector, X is an $(n \times p)$ design matrix, β a p-dimensional vector of unknowns and $e = (e_1, e_2, ..., e_n)^T$ the error vector. Alternatively we may write

$$y_i = x_i^T \beta + e_i, \qquad i = 1, 2, ..., n$$

where x_i is the i:th row in X. Define the residuals as $r_i = y_i - x_i^T \beta, \quad i = 1, 2, ..., n$. The CM-estimation problem is to find the global minimum of

$$L(\beta, \sigma) = c\,\frac{1}{n}\sum_{i=1}^{n} \rho(r_i/\sigma) + \log\sigma \tag{1}$$

over $\beta \in \mathbb{R}^p$ and $\sigma \in \mathbb{R}_+$ subject to the constraint

$$\frac{1}{n}\sum_{i=1}^{n}\rho(r_i/\sigma) \leq \varepsilon\,\rho(\infty) \tag{2}$$

Here $\rho(t)$ is a bounded function, symmetric around zero and nondecreasing for $t \geq 0$, and c and ε are tuning parameters that need to be chosen carefully, as described in Section 2.

If strict inequality holds in the constraint above we get the redescending M-estimating equations for β and σ. Equality in the constraint instead gives the S-estimate, where σ is minimized with respect to (2). The reason is that for equality constraint we have $L(\beta, \sigma) = \text{constant} + \log(\sigma)$, which is minimized by minimizing σ. Thus the S- and CM-estimates are closely related. However, the CM-estimates have some nice properties not shared by the S-estimates as exemplified in Section 2.

Two ρ-functions are considered in this paper: Tukey biweight

$$\rho(t) = \begin{cases} \frac{t^2}{2} - \frac{t^4}{2} + \frac{t^6}{6}, & \text{for } |t| \leq 1 \\ \frac{1}{6}, & \text{for } |t| > 1 \end{cases}$$

and Welsh

$$\rho(t) = \frac{1}{2}(1 - e^{-t^2}) \ .$$

In `CMregr` these two functions are referred to as `tukey` and `welsh` respectively. As shown in Section 5, it is easy to add customized ρ-functions to `CMregr`, to calculate other CM-estimates.

2 Estimation parameters and how to choose them

The parameters c and ε in (1) and (2) are used for tuning the CM-estimates.

The parameter ε controls the asymptotic breakdown point: The asymptotic breakdown point is given by $\min(\varepsilon, 1-\varepsilon)$. By choosing $\varepsilon = 0.5$, the highest possible asymptotic breakdown point is achieved. No other choice is sensible when CM-estimates are considered.

This means that the only parameter that really matters for CM-estimates is c. If c is small, the S-estimate for $\varepsilon = 0.5$ is found rather than an CM-estimate. For normally distributed residuals, it is in general required that $c > 15$ (Tukey) and $c > 5.3$ (Welsh) to get a CM-estimate rather than an S-estimate.

The properties of the estimate varies with c. Mendes & Tyler (1995) made a theoretical investigation of the *asymptotic relative efficiency*, and the *residual gross error sensitivity*: γ_r^*. When those results are applied to Tukey biweight and Welsh, it is revealed that the sensitivity γ_r^* has a minimum for some c, and that the efficiency is an increasing function of c. This implies that it is pointless to choose c smaller than the minimizer of γ_r^*, but it may

be worthwhile to choose a greater value. For Tukey, γ_r^* is minimized by $c = 19.62$, and for Welsh the minimizer is $c = 7.348$. Other possible choices are given in Table 1.

Table 1: Asymptotic relative efficiency and residual gross error sensitivity (γ_r^*) for varying choices of c in Tukey biweight and Welsh CM-estimates.

Tukey biweight			*Welsh*		
c	eff	γ_r^*	c	eff	γ_r^*
19.62	0.847	1.64	7.348	0.838	1.58
22.57	0.900	1.66	8.930	0.900	1.61
28.97	0.950	1.77	12.07	0.950	1.73
41.68	0.980	2.01	18.39	0.980	2.02
56.02	0.990	2.28	25.54	0.990	2.31

The table for Tukey biweight in (Mendes & Tyler 1995) looks different since they use a slightly modified ρ-function in their analysis. The values in Table 1 hold for `tukey` and `welsh` in `CMregr`.

It is possible to use `CMregr` for finding S-estimates by setting $c = 0$. Then the properties of the estimate are controlled by changing the asymptotic breakdown point ε. As a comparison, Table 2 shows the values of ε corresponding to Table 1, with the addition of $\varepsilon = 0.5$. A table for Tukey biweight with some more reasonable choices of ε can be found in (Rousseeuw & Yohai 1984).

Table 2: Asymptotic relative efficiency for varying choices of asymptotic breakdown point ε in Tukey biweight and Welsh S-estimates.

Tukey biweight		*Welsh*	
ε	eff	ε	eff
0.5000	0.287	0.5000	0.289
0.2001	0.847	0.1835	0.838
0.1638	0.900	0.1400	0.900
0.1194	0.950	0.0963	0.950
0.0786	0.980	0.0596	0.980
0.0570	0.990	0.0417	0.990

Figure 1 illustrates the difference in efficiency between some estimates with breakdown point 0.5, and least squares. High efficiency means that the regression line is close to the least squares solution if there are no outliers.

In Figure 2 we see the price one has to pay in S-estimates to get the same asymptotic relative efficiency as in CM-estimates. In the right graph of Figure 2, the S-estimate "breaks down" when one more outlier is added compared to the left graph. This is because of the very low breakdown point required for S-estimates to get high efficiency.

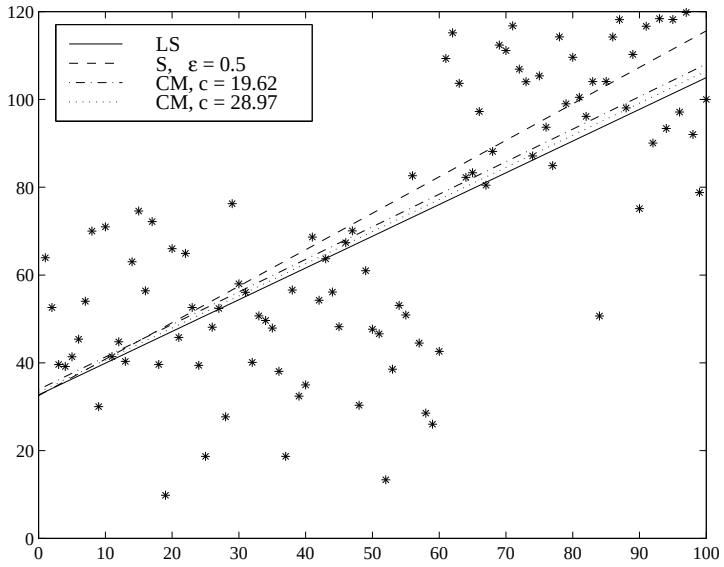


Figure 1: Regression lines for least squares (LS), S-estimate with $\varepsilon = 0.5$ and CM-estimates with $c = 19.62$ and $c = 28.97$ using Tukey biweight.

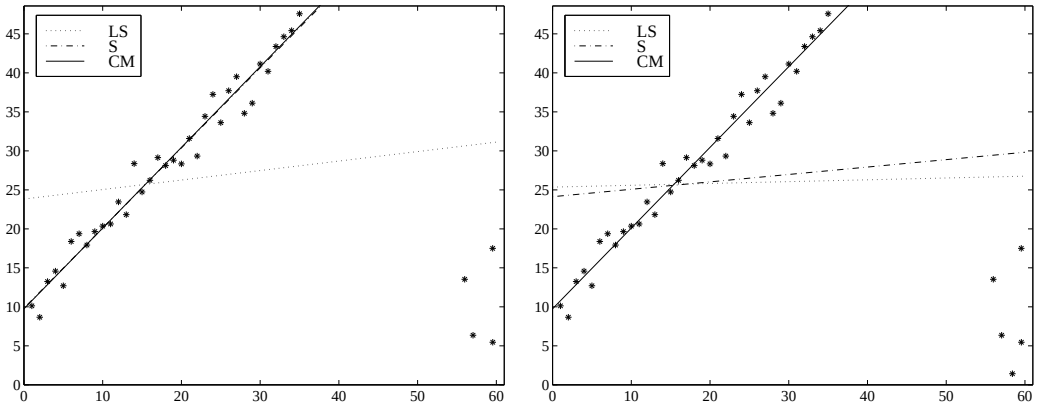


Figure 2: Regression lines for least squares (LS), S-estimate with $\varepsilon = 0.1194$ and CM-estimate with $c = 28.97$ using Tukey biweight. Both parameters correspond to an asymptotic efficiency of 0.95.

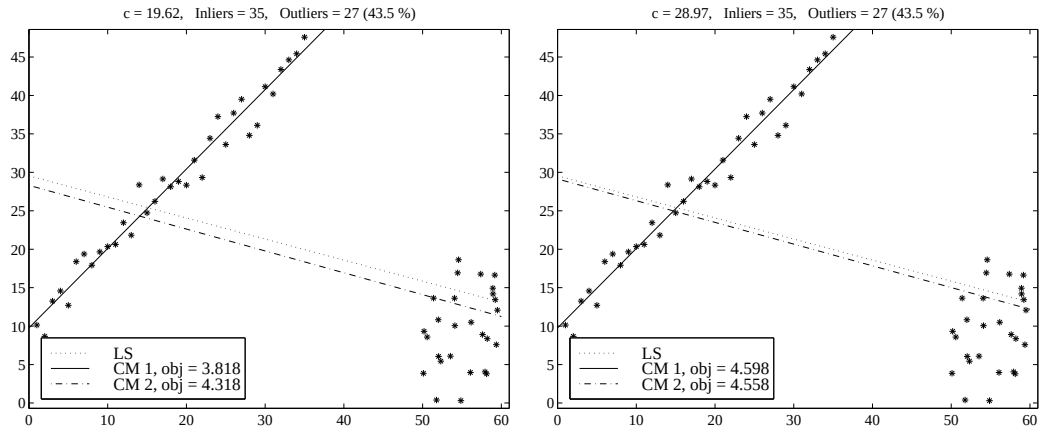


Figure 3: Regression lines for least squares (LS), and for the two local minima of the CM-estimate with $c = 19.62$ in the left graph, and with $c = 28.97$ in the right graph, using Tukey biweight. The values of the corresponding objective functions (1) are in the label box.

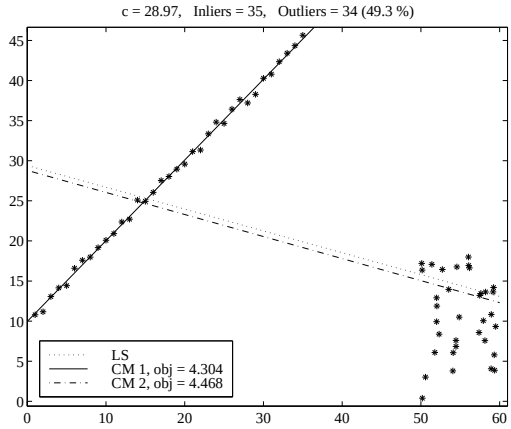


Figure 4: Regression lines for least squares (LS), and for the two local minima of the CM-estimate with $c = 28.97$, using Tukey biweight. The values of the corresponding objective functions (1) are in the label box.

The optimization problem of finding the CM-estimates shares the property, that there may be a few local minima, with the S-estimates. Figure 3 shows the two local minima for CM with two choices for the parameter c. The data-sets are the same in the two graphs with 43.5% outliers in the data. The right graph has the greater c corresponding to a higher efficiency, but then the objective function (1) reports the "wrong" solution as the best one.

The CM-estimate has an asymptotic 50% breakdown point, but that is not achieved in this case. This is what can be expected when the "good data" is too scattered. Figure 4 shows that for better behaved "good data", the 50% breakdown point is achieved, even for greater values of c. It is however obvious that the observed breakdown point may drop a bit. And the drop is generally greater for CM-estimates with higher efficiency.

3 The algorithm

The CM-estimates cannot be expressed explicitly. Computing these estimates numerically is a challenging problem, since we like to minimize an objective function where many local minima may exist.

If σ is held fixed in (1), we have a linear model M-estimation problem. The algorithms in (Arslan et al. 2002) and (Edlund & Ekblom 2002) make use of the fact that very good algorithms exist for this problem (Edlund 1997). So the solution is found by solving a series of linear model M-estimation problems.

The updating of σ is done as a separate step, that requires much less calculations, since we have a one-dimensional problem at hand. Details on this issue is found in (Edlund & Ekblom 2002).

To find the global minimum, good starting points for the local iteration above is generated by considering many subsamples with p observations (Arslan et al. 2002).

4 Invoking the software

There are two commands in `CMregr` for calculating CM-estimates: `globalCMregr` and `localCMregr`. The first of these tries to find the "global minimum" using the technique described above, while `localCMregr` needs a user-supplied starting point.

globalCMregr

$[\beta, \sigma, \texttt{stat}] = \texttt{globalCMregr}(\rho\text{-fun}, c, \varepsilon, X, y)$

or

$[\beta, \sigma, \texttt{stat}] = \texttt{globalCMregr}(\rho\text{-fun}, c, \varepsilon, X, y, \texttt{iters})$

Input parameters

ρ-fun – the chosen ρ-function as a Matlab string e.g. `'tukey'` or `'welsh'`.
c – the tuning parameter, from Table 1.
ε – asymptotic breakdown point. Always use 0.5 for CM-estimates.
X – the design matrix.
y – the response vector.
`iters` – the number of subsamples to investigate for a good starting point. If this is omitted, the routine makes a guess of the number of subsamples to use.

Output parameters

β & σ – the calculated solution.

`stat` – some additional data on the solution.
`stat.border` is 1 if the solution fulfills (2) with equality, and 0 if (2) is fulfilled with strict inequality.
`stat.obj` is the value of the objective function (1) at the solution.
`stat.constr` is the difference between the left and right hand sides of (2).

Example

Let us define a design matrix and a response vector:

```
>>X = [1 0;1 1;1 3;1 4;1 8]
X =
     1     0
     1     1
     1     3
     1     4
     1     8
>>y = [1 2 3 4 0.5]';
```

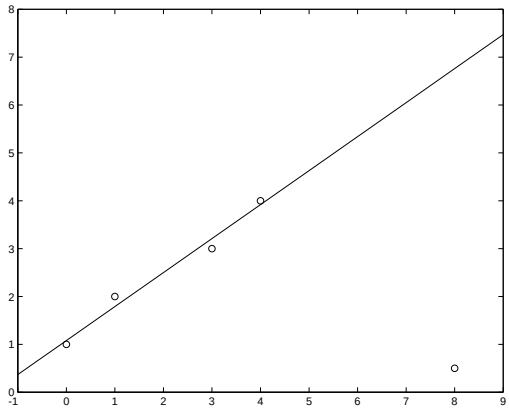
The Tukey biweight CM-estimate with $c = 19.62$ (see Table 1) is then found by

```
>>[b,s,stat] = globalCMregr('tukey',19.62,0.5,X,y)
b =
   1.07973997179869
   0.71013001410066
s =
   0.54750922628337
stat =
    border: 0
       obj: 0.63014080945719
    constr: -0.02051392582918
```

Since `stat.border` = 0, the solution is in the interior of the feasible region, i.e. (2) is not fulfilled with equality. If the number of outliers would increase, the solution would eventually reach the border. In a sense one could say that, if outliers are plentiful, the S-estimate kicks in and saves the day.

Plotting the regression line yields:

```
>>t = -1:9;
>>plot(X(:,2),y,'o',t,b(1)+b(2)*t)
```



localCMregr

$[\beta, \sigma, \texttt{stat}] = \texttt{localCMregr}(\rho\text{-fun}, c, \varepsilon, X, y, \beta_{\text{start}})$

Input parameters

ρ-fun – the chosen ρ-function as a Matlab string e.g. `'tukey'` or `'welsh'`.
c – the tuning parameter, from Table 1.
ε – asymptotic breakdown point. Always use 0.5 for CM-estimates.
X – the design matrix.
y – the response vector.
β_{start} – the initial guess of the solution β. The algorithm searches from this point and finds a local minimum.

Output parameters

β & σ – the calculated solution.
`stat` – some additional data on the solution.
`stat.border` is 1 if the solution fulfills (2) with equality, and 0 if (2) is fulfilled with strict inequality.
`stat.obj` is the value of the objective function (1) at the solution.
`stat.constr` is the difference between the left and right hand sides of (2).

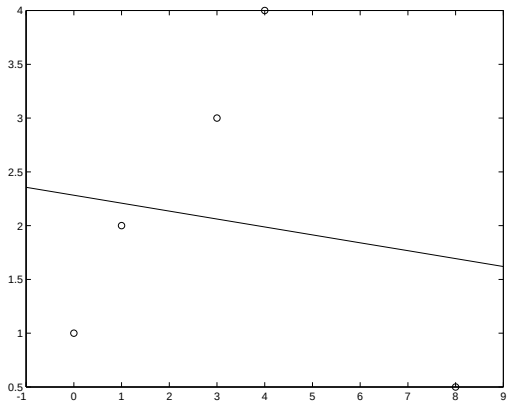
Example

Using the same design matrix and response vector as in the previous example, we want to calculate the Welsh estimate with $c = 12.07$ (see Table 1) and starting from the least squares solution:

```
>>[b,s,stat] = localCMregr('welsh',12.07,0.5,X,y,X\y)
b =
   2.28257700557494
  -0.07363502459208
s =
   4.06413162024954
```

```
stat =
    border: 0
       obj: 1.94453719549732
    constr: -0.20506734889203
```

Also in this example the solution is in the interior of the feasible region (`stat.border` = 0). Plotting the solution yields:



The badly chosen starting point results in a solution that is a local minimum, and not the global minimum we were interested in.

5 Adding customized ρ-functions

The ρ-functions that are supplied with `CMregr` are implemented as Matlab-functions. This means that it is quite easy to add new ones manually. The Matlab-function that implements the ρ-function must obey the following rules:

1. If the Matlab-function is called with one vector as input, it should return a vector with the ρ-function applied to each element in the input vector. *Example:*

   ```
   >>welsh([-1 0 1 2])
   ans =
       0.3161         0    0.3161    0.4908
   ```

2. If the vector is followed by the parameter 0 (zero), the same vector as above should be returned. *Example:*

   ```
   >>welsh([-1 0 1 2],0)
   ans =
       0.3161         0    0.3161    0.4908
   ```

3. If the vector is followed by the parameter 1, the Matlab-function should return a vector with the derivative ρ' applied to each element in the input vector. *Example:*

   ```
   >>welsh([-1 0 1 2],1)
   ans =
      -0.3679         0    0.3679    0.0366
   ```

4. If the vector is followed by the parameter 2, the Matlab-function should return a vector with the second derivative ρ'' applied to each element in the input vector. *Example:*

```
>>welsh([-1 0 1 2],2)
ans =
   -0.3679    1.0000   -0.3679   -0.1282
```

The routines in `CMregr` make use of all these four cases. This puts some restrictions on what ρ-functions can be used. The ρ-function has to be twice differentiable!

The code for the `welsh` function of `CMregr` serves as an example of how to implement such a function, and may serve as a template for customized ρ-functions in `CMregr`:

```
function v = welsh(r,diff)

if nargin==1
    diff = 0;
elseif nargin~=2
    error('Wrong number of input arguments')
end

switch diff
case 0
    v = 0.5*(1–exp(–r.^2));
case 1
    v = r.*exp(–r.^2);
case 2
    r2 = r.^2;
    v = (1–2*r2).*exp(–r2);
otherwise
    error('Illegal order of differentiation')
end
```

References

Arslan, O., Edlund, O. & Ekblom, H. (2002), 'Algorithms to compute CM- and S-estimates for regression', *Metrika* **55**, 37–51.

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Mendes, B. & Tyler, D. E. (1995), Constrained M-estimates for regression, *in* 'Robust Statistics; Data Analysis and Computer Intensive Methods', Vol. 109 of *Lecture Notes in Statistics*, Springer, New York, pp. 299–320.

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