An  $I_1$ -Augmented Lagrangian algorithm and why, at least sometimes, it is a very good idea

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# Four Fundamental Transparent(?) Unproved Statements:

All computational mathematics is essentially linear.

- First derivatives characterise optima.
- The derivative of a quadratic is linear
- So we need only talk about quadratic problems to understand optimization.



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## The paradigm unconstrained problem:

#### Optimize a quadratic.

For example

 $\min_x f(x) = a + b^\top x + \frac{1}{2}x^\top H x$ 

Motivated by the statements

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# Characterisation of Optimality: Unconstrained Case.





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Note: the (first-order) characterisation for a min or max is the same.



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 $\min_{x|g_i(x) \le 0} g_0(x)$  optimal if  $\nabla g_0(x) = \sum_i \lambda_i \nabla g_i(x), \lambda_i \le 0$ 

Equivalent to a stationary point of the Lagrangian  $L(x, \lambda) = g_0(x) - \sum_i \lambda_i g_i(x)$ 



Characterisation of Optimality: Constrained Case.

We note that the characterisation

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Although it suggests the Lagrangian is only locally meaningful!



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We are not very good at designing algorithms to find saddle points

# Background

The intuitive idea of penalty functions:

 $\min_{x\in\mathbb{R}^n} f(x)$ 

subject to  $c_j(x) = 0, j \in \{1, \ldots, m\}.$ 

The idea[ Courant, 1943], was to replace it with

 $\min_{x \in \mathbb{R}^n} p(x, \mu) = f(x) + \mu \sum_{j \in \{1, ..., m\}} c_j^2(x)$ 

and then

$$\lim_{\mu\to\infty} x(\mu) = x^*$$



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# The above motivated the idea of combining the Lagrangian with the penalty function

The augmented Lagrangian [Hestenes and Powell, 1969], is defined by  $\min_{x \in \mathbb{R}^n} \mathcal{L}(x, \lambda, \mu) =$  $f(x) + \sum_{i \in \{1,...,m\}} \lambda_i c_i(x) + \mu \sum_{j \in \{1,...,m\}} c_j^2(x)$ 

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 $\nabla \mathcal{L}(x,\lambda,\mu) =$  $\nabla f(x) + \sum_{i \in \{1,\dots,m\}} \lambda_i \nabla c_i(x) + 2.0 \ \mu \sum_{j \in \{1,\dots,m\}} c_j(x) \ \nabla c_j(x)$ 

which looking at the terms in  $\nabla c_j(x)$  suggests the update formula,

 $\lambda_j^+ = \lambda_j + 2.0 \ \mu c_j(x)$ 

If not sufficiently feasible  $\mu$  alone is increased, otherwise the  $\lambda {\rm s}$  alone are updated

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The idea: [Zangwill, 1967], replace the constrained problem with  $\min_{x \in \mathbb{R}^n} \quad p(x, \mu) = f(x) + \mu \sum_{j \in \{1, \dots, m\}} |c_j(x)|$ 

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 $\mu < \mu^*$  implies that  $x(\mu) = x^*$ 

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#### If I have quadratic constraints

the quadratic penalty function is a quartic.

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the exact penalty function is piecewise quadratic.

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# Projection onto a Hyperplane

Assume that the columns of A,  $a_i$ ,  $j \in \{1, ..., m\}$  are a **basis** of normals for the hyperplane in question

Define the projection operator P by

$$P = I - A(A^{\top}A)^{-1}A^{\top}$$

Note that, assuming that  $A^{\top}N = 0$ ,

PA = 0 and PN = N,

where the columns of N are the generators for the hyperplane.

So Px projects x on to the hyperplane.



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# Making an Exact Penalty Function Practical

#### Basic idea was my Ph.D thesis [1971]

- Consider  $\min_{x \in \mathbb{R}^n} f(x)$  subject to  $c_j(x) \le 0, j \in I$ .
- The penalty function  $p(x, \mu) = f(x) + \mu \sum_{j \in I} \max\{c_j(x), 0\}$  is only non-differentiable in the neighbourhood of active constraints

Define  $A_{\epsilon} = \{j \in I : |c_j^k(\mathbf{x})| \le \epsilon\}$  and  $V_{\epsilon} = \{j \in I : c_j^k(\mathbf{x}) > \epsilon\}$ 

So the idea is to define  $r(x,\mu) = f(x) + \mu \sum_{j \in I \setminus A_{\epsilon}} \max\{c_j(x), 0\}$ 

or equivalently  $r(x,\mu) = f(x) + \mu \sum_{j \in V_{\epsilon}} c_j(x)$ ,



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# A Practical First-Order Method

Base the search direction on  $r(x, \mu)$  by projecting orthogonal to the space spanned by  $\nabla c_i(x), i \in A_{\epsilon}$ 

In other words, we have completely accurate information about the change in p if we take our fundamental subproblem as  $\min_{d \in \mathbb{R}^n} r(x + d, \mu)$  subject to  $c_j(x + d) = c_j(x), j \in A_{\epsilon}$ .

So, up to first-order define  $d = -P\nabla r(x, \mu)$  orthogonal to the space spanned by  $\nabla c_j(x)$ ,  $j \in A_{\epsilon}$ .

Important Observation 1: If  $-P\nabla r(x,\mu)$  is small then  $\nabla r(x,\mu) \approx \sum_{j \in A_{\epsilon}} \lambda_j \nabla c_j(x)$  and we can obtain a good estimate for the  $\lambda$ 's. (which connects up with the "local" issue)

This tells us if and how we can obtain descent by releasing a single activity **and gives us optimality conditions**.



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In other words, we have completely accurate information about the change in p if we take our fundamental subproblem as  $\min_{d \in \mathbb{R}^n} r(x + d, \mu)$  subject to  $c_j(x + d) = c_j(x), j \in A_{\epsilon}$ .

So, up to first-order define  $d = -P\nabla r(x,\mu)$  orthogonal to the space spanned by  $\nabla c_j(x)$ ,  $j \in A_{\epsilon}$ .

Important Observation 1: If  $-P\nabla r(x,\mu)$  is small then  $\nabla r(x,\mu) \approx \sum_{j \in A_{\epsilon}} \lambda_j \nabla c_j(x)$  and we can obtain a good estimate for the  $\lambda$ 's. (which connects up with the "local" issue)

This tells us if and how we can obtain descent by releasing a single activity **and gives us optimality conditions**.



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Now, the subproblem we really wish to solve is

$$\min_{\boldsymbol{d}\in\mathbb{R}^n} \qquad \nabla_{\boldsymbol{x}} \boldsymbol{r}(\tilde{\boldsymbol{x}},\boldsymbol{\mu})^\top \boldsymbol{d} + \frac{1}{2} \boldsymbol{d}^\top \nabla_{\boldsymbol{x}\boldsymbol{x}} \boldsymbol{r}(\tilde{\boldsymbol{x}},\boldsymbol{\mu}) \boldsymbol{d}$$

subject to  $\nabla c_j(\tilde{x})^\top d + \frac{1}{2}d^\top \nabla^2 c_j(\tilde{x})d = 0, \quad j \in A_\epsilon.$ 

In other words, we have completely accurate information about the change in p up to second order

We can improve the activity values via

$$J_{A_{\epsilon}}(\tilde{x})^{\top}v = -\phi_{A_{\epsilon}}(\tilde{x}+d)$$



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### A Practical Second-Order Method: Observations

We know how to solve

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subject to 
$$\nabla c_i(\tilde{x})^\top d = 0, \quad j \in A_{\epsilon}.$$

Claim: If  $-P\nabla r(x,\mu)$  is large then we can ignore the constraint curvature

We already observed that if  $-P\nabla r(x,\mu)$  is small then we can obtain a good estimate for the  $\lambda$ 's in.

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abla c_j( ilde{x})^{ op}d+rac{1}{2}d^{ op}
abla^2 c_j( ilde{x})d = 0, \quad j\in A_\epsilon. \end{aligned}$$

We need  $abla_{\mathsf{x}} r(\tilde{x}, \mu) + 
abla_{\mathsf{xx}} r(\tilde{x}, \mu) d = \sum_{j \in \mathcal{A}_{\epsilon}} \lambda_j \left\{ \nabla c_j(\tilde{x}) + \nabla_{\mathsf{xx}} c_j(\tilde{x}, \mu) d \right\}$ 

Or using our good lambda estimate,  $\hat{\lambda}$  $\nabla_{\mathbf{x}} r(\tilde{\mathbf{x}}, \mu) + \nabla_{\mathbf{xx}} r(\tilde{\mathbf{x}}, \mu) d \approx \sum_{j \in A_{\mathbf{x}}} \left\{ \lambda_j \nabla c_j(\tilde{\mathbf{x}}) + \hat{\lambda}_j \nabla_{\mathbf{xx}} c_j^k(\tilde{\mathbf{x}}, \mu) d \right\}$ .

Compare with KKT for

min d∈ℝ″  $\nabla_{\mathbf{x}} r(\tilde{\mathbf{x}}, \mu)^{\top} d + \frac{1}{2} d^{\top} \left( \nabla_{\mathbf{x}\mathbf{x}} r(\tilde{\mathbf{x}}, \mu) - \hat{\lambda} \nabla_{\mathbf{x}\mathbf{x}} c_j^k(\tilde{\mathbf{x}}, \mu) \right) d\mathbf{x}$ 

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#### We need $\nabla_x r(\tilde{x}, \mu) + \nabla_{xx} r(\tilde{x}, \mu) d = \sum_{j \in A_{\epsilon}} \lambda_j \{ \nabla c_j(\tilde{x}) + \nabla_{xx} c_j(\tilde{x}, \mu) d \}$

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 $\min_{d\in\mathbb{R}^n}$ 

subject to  $\nabla c_j(\tilde{x})^\top d = 0, \quad j \in A_\epsilon.$ 



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#### Remark

The usual  $(l_2)$ -Augmented Lagrangian is a combination of the (inexact) quadratic penalty with the Lagrangian which is motivated as a means to prevent the necessity of requiring the penalty parameter for the quadratic penalty to tend to infinity

Thus it seems eccentric to augment an exact penalty function

But one can obtain a better estimate of the multipliers

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It is just a small step to define an  $I_1$ -analogue to the augmented Lagrangian

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 $f(x) - \sum_{i} \lambda_{i} c_{i}(x) + \mu \sum_{j \in \{1,...,m\}} \max\{c_{j}(x), 0\}$ 

and again only one of  $\mu$  and the  $\lambda$ s needs to be updated

Furthermore, the "gradient" of the augmented Lagrange compared with the Lagrangian gives the  $\lambda$  update.



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Now, the subproblem we wish to solve for a second-order method is

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Model Problem Observation

As already stated, the model based upon a quadratic objective function and quadratic constraints should be the paradigm optimization problem

If solved via the quadratic penalty function or (*I*<sub>2</sub>-)augmented Lagrangian it is more complex than quadratic (i.e. quartic)

If solved via an  $l_1$ -penalty function or an  $l_1$ -augmented Lagrangian it is piecewise quadratic



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# An *I*<sub>1</sub> augmented Lagrangian for equality constraints

For simplicity assume all general constraints are equality constraints and now

- The  $l_1$ -exact penalty is  $f(x) + \mu \sum_{i=1}^{m_e} |c_j(x)|$ ,
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where  $\sigma_j$  is the sign of  $c_j(x)$ .

The optimality conditions are that, for all  $j\in A_\epsilon$ 

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For bounds we need an additional (trivial) projection,  $\mathcal{P}_{\mathcal{B}}$ In other words we deal with them directly. If we have just x > 0For any  $x^{(k)}$ , we have two possibilities for each component:  $\begin{array}{lll} \textit{Dominated} & (i) & 0 \le x_i^{(k)} \le \left( \nabla_x \ L_D^k(x^k, \lambda^{(k)}, \mu^{(k)}, \hat{\lambda}^{(k)}) \right)_i, \text{ or} \\ \textit{Floating} & (ii) & \left( \nabla_x \ L_D^k(x^k, \lambda^{(k)}, \mu^{(k)}, \hat{\lambda}^{(k)}) \right)_i < x_i^{(k)}, & \text{when} \end{array}$ where



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### The Algorithm

where  $\hat{\lambda}^{(k)}$  is a (least squares) estimate for

$$\nabla_{x} D^{k}(x^{(k)}, \lambda^{(k)}, \mu^{(k)}) = \sum_{j \in A_{\epsilon}} \hat{\lambda}_{j}^{(k)} \nabla_{x} c_{j}^{k}(x^{(k)}).$$

$$\begin{split} & \text{If } \|c(x^{(k)}\| \leq \eta^{(k)} \text{ execute Step 3. Otherwise execute Step 4.} \\ & \text{Step 3:Test for convergence and update Lagrange multiplier estimates.} \\ & \text{If } \|L_D^k(x^k, \lambda^{(k)}, \mu^{(k)}, \hat{\lambda}^{(k)})\| \leq \omega_* \text{ and } \|c(x^{(k)}\| \leq \eta_* \text{ stop. Otherwise, set} \\ & \lambda^{(k+1)} = \bar{\lambda}(x^{(k)}, \lambda^{(k)}, \mu^{(k)}), \quad \mu^{(k+1)} = \mu^{(k)}, \\ & \alpha^{(k+1)} = \min(\mu^{(k+1)}, \gamma_l), \\ & \omega^{(k+1)} = \omega^{(k)}(\alpha^{(k+1)})^{\beta_{\omega}}, \\ & \eta^{(k+1)} = \eta^{(k)}(\alpha^{(k+1)})^{\beta_{\eta}}. \end{split}$$

increment k by one and go to Step 2.

Step 4:Increase the penalty parameter. Set

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### What can we prove? Essentially the same as LANCELOT

 $x^*$  is any limit of the sequence  $\{x^{(k)}\}$  generated by our Algorithm:

Assume: The functions and constraints are twice continuously differentiable, the iterates  $x^{(k)}$  lie in a closed, bounded domain and the Jacobian matrix of active constraints,  $\hat{A}(x^*)$ , has full column rank at any limit point,  $x^*$ , of the sequences  $x^{(k)}$ , Let K be the indices of an infinite subsequence of  $x^{(k)}$  with limit  $x^*$ .

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(i) There are positive constants  $a_1, a_2$  and an integer  $k_0$  such that  $\|\bar{\lambda}(x^{(k)}, \lambda^{(k)}, \mu^{(k)}) - \lambda^*\| \le a_1 \omega^{(k)} + a_2 \|x^{(k)} - x^*\|,$ 

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Assume: The functions and constraints are twice continuously differentiable, the iterates  $x^{(k)}$  lie in a closed, bounded domain and the Jacobian matrix of active constraints,  $\hat{A}(x^*)$ , has full column rank at any limit point,  $x^*$ , of the sequences  $x^{(k)}$ , Let K be the indices of an infinite subsequence of  $x^{(k)}$  with limit  $x^*$ .

#### Then

(i) There are positive constants  $a_1, a_2$  and an integer  $k_0$  such that  $\|\bar{\lambda}(x^{(k)}, \lambda^{(k)}, \mu^{(k)}) - \lambda^*\| \le a_1 \omega^{(k)} + a_2 \|x^{(k)} - x^*\|,$ 

and

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$$\begin{array}{ll} \min\limits_{x\in\mathcal{B}} & f(x)\\ \text{subject to} & c_j(x)=0, \ j\in E=\{1,\cdots,m_e\}, \end{array} \tag{1}$$

where  $\mathcal{B} = \{x \in \mathbb{R}^n \mid x \ge 0\}$ ,  $\lambda^*$  is the corresponding vector of Lagrange multipliers, and the sequences  $\{\bar{\lambda}(x^{(k)}, \lambda^{(k)}, \mu^{(k)})\}$  and  $\{\lambda(x^{(k)})\}$  converges to  $\lambda^*$  for  $k \in K$ ,

(iii) The gradient  $\nabla_x L_D^k(x^k, \lambda^{(k)}, \mu^{(k)}, \hat{\lambda}^{(k)})$  converges so that

 $g_L(x^k, \lambda^{(k+1)}) = \nabla f^k(x^k) + \left\{ \sum_{j=1}^m \lambda_j - \sum_{j \in A_\epsilon} \hat{\lambda}_j^{(k)} \right\} \nabla_x c_j^k(x^k) = 0,$ and  $g_L(x^*, \lambda^*) = 0$ , for  $k \in K$ , where  $g_L$  is the gradient with respect to x of the Lagrangian corresponding to (1).



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Suppose further that the iterates  $\{x^{(k)}\}$  converges to a single limit point  $x^*$ , then there is a constant  $\mu > 0$  such that  $\mu^{(k)} \le \mu$  for all k.

Suppose strict complementary slackness holds. Then for k sufficiently large, the set of floating variables are precisely those which lie away from their bounds at  $x^*$ .

The iterates  $x^k$  and the Lagrange multiplier estimates are at least R-linearly convergent

For all exterior penalty function methods, it is possible to converge to a non-feasible stationary point; usually easily rectified.



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Numerical results with MADS implemented as Nomad: Thanks to Nadir Amaioua

MADS is a well-known derivative-free direct search optimization method.

The search step of MADS uses a model trust region approach.

It naturally uses quadratic models for the objective and the constraints when doing the search step.



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# Numerical results with MADS implemented as Nomad

These results are on 20 constrained problems, with the largest having 20 variables and 15 constraints, and 4 simulation problems, with the largest having 10 variables and 10 constraints.

The comparisons are made with the QPQC subproblems solved by:

- MADS,
- the exact penalty function,
- the usual augmented Lagrangian,
- the *l*<sub>1</sub>-augmented Lagrangian, and
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The latter is a well-known smooth penalty function approach that uses the log barrier with a linesearch



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### MADS on constrained problems in brief:



Fraction of problems you were less than  $\alpha$  as bad as the best



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Fraction of problems you were less than  $\alpha$  as bad as the best



### The Aircraft Range simulation problem: 50 instances

10 variables and 10 constraints Simulation in days





### The Simplified Wing simulation problem: 50 instances

7 variables and 3 constraints Simulation in days





### 200 instances of the 4 simulation-based applications







#### MADS on constrained problems in brief (data profiles)



Fraction of problems that can be solved with  $\alpha$  function evaluations



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#### Lockwood simulation problem: 50 instances:data profile





#### Lockwood simulation problem: 50 instances:data profile



Fraction of problems solved with  $\alpha$  function evaluations

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The Welded simulation problem:

Just in case you think we always win: 4 variables and 6 constraints





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### What next?

Is it better to handle inequalities directly?

#### Consider adaptive strategies for updating the penalty parameter.



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