A Smooth Exact Penalty Function for Nonlinear Optimization

Ron Estrin
ICME, Stanford University

Sandia National Lab
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Joint Work with Michael Friedlander, Dominique Orban, and Michael Saunders

Penalty methods for Nonlinear Programming

Equality constrained nonlinear program

$$\begin{array}{ll} \min\limits_{x} & f(x) \\ \text{s.t.} & c(x) = 0, \end{array}$$

with n variables, $m \leq n$ constraints and $f, c \in C^2$.

Plethora of methods available, but still an active area of research!

Methods for NLP often complicated:

- involve complicated heuristics to trade off optimality vs. feasibility
- feasibility restoration phases required

Penalty methods

Add some measure of constraint violation in objective

- **Quadratic penalty**

$$\min_x f(x) + \frac{\sigma_k}{2}\|c(x)\|_2^2$$

  - Perturbs the solution.
  - Need to solve sequence of problems with $\sigma_k \to \infty$.

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- ℓ_1 **penalty**

$$\min_x f(x) + \sigma \|c(x)\|_1$$

  - Non-smooth.

Penalty methods

Add some measure of constraint violation in objective

- **Augmented Lagrangian method**

$$\min_x f(x) + \lambda_k^T c(x) + \frac{\sigma_k}{2}\|c(x)\|_2^2$$

  - Need to solve sequence of problems.

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$$\min_x f(x) + \lambda_k^T c(x) + \frac{\sigma_k}{2}\|c(x)\|_2^2$$

  - Need to solve sequence of problems.

- Would like exact penalty function which is smooth...

Fletcher's Penalty Function

Primal only Lagrangian:

$$L(x, y) = f(x) - y^T c(x)$$

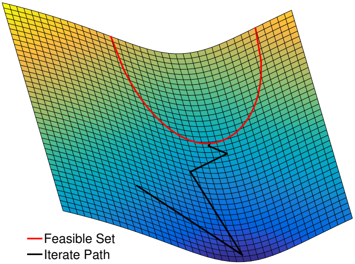
Fletcher's penalty function:

$$\begin{aligned}\phi_\sigma(x) &= f(x) - c(x)^T y_\sigma(x)\\ y_\sigma(x) &= \arg\min_y \frac{1}{2}\|g - Ay\|_2^2 + \sigma c(x)^T y\end{aligned}$$

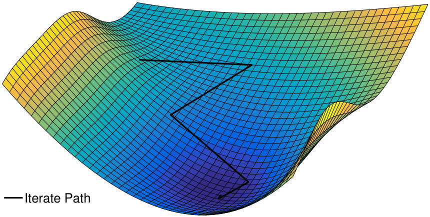
Notation:

$$g = \nabla f(x), \qquad A = \begin{bmatrix} \nabla c(x) \end{bmatrix}, \qquad Y_\sigma = \begin{bmatrix} \nabla y_\sigma(x) \end{bmatrix}.$$

An Illustration



(a) ‘hs007’ with feasible set.



(b) ϕ_σ for problem ‘hs007’.

Derivatives

Gradient of penalty function:

$$\begin{aligned}\nabla\phi_\sigma(x) &= g - Ay_\sigma - Y_\sigma c \\ &= g_\sigma - Y_\sigma c\end{aligned}$$

Hessian of penalty function:

$$\begin{aligned}\nabla^2\phi_\sigma(x) &= H - \sum_{i=1}^{m}(y_\sigma)_i H_i - AY_\sigma^T - Y_\sigma A^T - \nabla[Y_\sigma(\cdot)c] \\ &= H_\sigma - AY_\sigma^T - Y_\sigma A^T - \nabla[Y_\sigma(\cdot)c]\end{aligned}$$

Optimality Conditions

(x_*, y_*) is first-order KKT point:

$$c(x_*) = 0, \qquad g(x_*) - A(x_*)y_* = 0.$$

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Gradient of penalty function:

$$\nabla\phi_\sigma(x) = g - Ay_\sigma - Y_\sigma c.$$

Then $y_* = y_\sigma(x_*)$ and $\nabla\phi_\sigma(x_*) = 0$

$\implies$ **1st order KKT points** are **stationary points** of ϕ_σ.

Optimality Conditions

(x_*, y_*) is second-order KKT point:

$$d^T \nabla^2_{xx} L(x_*, y_*) d \geq 0, \qquad \text{for } d \text{ such that } A(x_*)^T d = 0$$

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Hessian of Penalty function:

$$\begin{aligned} \nabla^2 \phi_\sigma(x_*) &= H_\sigma - AY_\sigma^T - Y_\sigma A^T - \nabla[Y_\sigma(x)c] \\ &= H_\sigma - H_\sigma P_A - P_A H_\sigma + 2\sigma P_A \\ &= \bar{P}_A H_\sigma \bar{P}_A - P_A H_\sigma P_A + 2\sigma P_A \end{aligned}$$

Projectors: $\qquad P_A = A(A^T A)^{-1} A^T, \qquad \bar{P}_A = I - P_A.$

Optimality Conditions

Hessian of Penalty function:

$$\nabla^2 \phi_\sigma(x_*) = \bar{P}_A H_\sigma \bar{P}_A - P_A H_\sigma P_A + 2\sigma P_A$$

Then $\nabla^2 \phi_\sigma(x_*) \succeq 0$ if $\sigma \geq \sigma_* = \frac{1}{2}\|P_A H_\sigma P_A\|_2$

$\implies$ **2nd order KKT points** are **minimizers** of ϕ_σ for $\sigma \geq \sigma_*$.

$\phi_\sigma(x)$ is a smooth, exact penalty function.

If σ is chosen large enough, it is enough to minimize $\phi_\sigma(x)$ once to obtain KKT point to original NLP.

- (Weakly-exact: spurious minima rare but still possible)

How to evaluate function/gradient/products with (approx.) Hessian?

Function Evaluation

Multiplier estimate:

$$y_\sigma(x) = \arg\min_y \frac{1}{2}\|g - Ay\|_2^2 + \sigma c(x)^T y$$

which is solved by

$$A^T A y_\sigma = A^T g - \sigma c$$

or equivalently,

$$\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} g_\sigma \\ y_\sigma \end{bmatrix} = \begin{bmatrix} g \\ \sigma c \end{bmatrix}$$

Products with Y_σ

First, Jacobian of y_σ:

$$Y_\sigma = (H_\sigma - \sigma I)A(A^TA)^{-1} + S(x, g_\sigma)^T(A^TA)^{-1}$$

where

$$S(x, v)u = \begin{bmatrix} v^T H_1 u \\ \vdots \\ v^T H_m u \end{bmatrix}, \qquad S(x, v)^T u = \sum_{i=1}^{m} u_i H_i v$$

(Notice that $S(x_*, g_\sigma) = 0$ since $g_\sigma = 0$ at solution).

Products with Y_σ

$$
\begin{aligned}
Y_\sigma u &= (H_\sigma - \sigma I) A (A^T A)^{-1} u + S(x, g_\sigma)^T (A^T A)^{-1} u \\
&= (H_\sigma - \sigma I)(-w) + \sum_{i=1}^{m} v_i H_i g_\sigma
\end{aligned}
$$

where

$$
\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} w \\ v \end{bmatrix} = \begin{bmatrix} 0 \\ -u \end{bmatrix}.
$$

Products with Y_σ^T

$$
\begin{aligned}
Y_\sigma^T u &= (A^T A)^{-1} A^T (H_\sigma - \sigma I) u + (A^T A)^{-1} S(x, g_\sigma) u \\
&= v
\end{aligned}
$$

where

$$
\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} w \\ v \end{bmatrix} = \begin{bmatrix} (H_\sigma - \sigma I) u \\ -S(x, g_\sigma) u \end{bmatrix}.
$$

Gradient Computation

Gradient:

$$\nabla \phi_\sigma = g_\sigma - Y_\sigma c$$

Need to solve one additional augmented system.

Hessian products

Hessian product:

$$
\begin{aligned}
\nabla^2 \phi_\sigma(x_*) v &= H_\sigma v - A Y_\sigma^T v - Y_\sigma A^T v - \nabla[Y_\sigma(x) c] v \\
&\approx H_\sigma v - A Y_\sigma^T v - Y_\sigma A^T v \qquad \text{(remove third derivatives)} \\
&\approx H_\sigma v - P_A H_\sigma v - H_\sigma P_A v + 2\sigma P_A v
\end{aligned}
$$

Can further approximate by removing terms which are zero at solution.

Two augmented system solves per product.

Hessian products

Hessian product:

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Fletcher showed that even with these approximations, **quadratic convergence** can still be retained.

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The end! Questions?
...Not quite

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A few notes and observations:

- Solving augmented system (direct vs. iterative)
- Singular Jacobians (regularization)
- Trust-region $>$ linesearch (indefinite Hessians)
- Adjusting penalty parameter, initial points, unboundedness...

Solving the Augmented System

- Sparse LDL
- Semi-normal equations (Q-less QR) + iterative refinement
- Iterative methods
  - Efficient with good preconditioners (I've heard these near-optimal preconditioners for PDE's are popular...)
  - Inexact function/gradient evaluation controlled via iterative solver tolerance

Solving the Augmented System: LSLQ/LNLQ

Iterative methods for least-squares (LSLQ) or least-norm problems (LNLQ).

- Equivalent to SYMMLQ on normal equations.
- Given $\sigma_{est} \geq \sigma_{\min}(A)$, can monitor $\|w_* - w_k\|$ and $\|v_* - v\|$.
- For near-optimal preconditioners, where $A^T = \begin{bmatrix} A_u^T & A_z^T \end{bmatrix}$ and $\mathcal{P} = A_u^T A_u$, then $\sigma_{\min}\left(\mathcal{P}^{-1} A^T A\right) \geq 1$.

Regularization

If A is singular, the ϕ_σ can be undefined.
Regularize least-squares problem:

$$\begin{aligned}
\phi_{\sigma\delta}(x) &= f(x) - c(x)^T y_{\sigma\delta}(x) \\
y_{\sigma\delta}(x) &= \arg\min_y \frac{1}{2} \left\| \begin{bmatrix} g \\ 0 \end{bmatrix} - \begin{bmatrix} A \\ \delta I \end{bmatrix} y \right\|_2^2 + \sigma c(x)^T y
\end{aligned}$$

Only change: augmented system becomes

$$\begin{bmatrix} I & A \\ A^T & -\delta^2 I \end{bmatrix} \begin{bmatrix} w \\ v \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}.$$

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Assume that LICQ holds at x_*.

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---

for k=1,2,... **do**
  $\delta_k \leftarrow \max\left\{\delta_{k-1}^2, \|\nabla \phi_{\sigma\delta_{k-1}}(x_k)\|\right\}$
  Get x_{k+1} from one step on $\phi_{\sigma\delta_k}(x_k)$
end for

If quadratically convergent method used, entire method above remains quadratically convergent.

Inequality Constraints

Consider problem

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & c(x) = 0, \\ & x \geq 0. \end{aligned}$$

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- Smoothness holds for $x > 0$ (use interior method)
- Exactness still holds

Inverse Poisson Problem (Thanks Drew!)

$$\begin{aligned} \min_{u,z} \quad & \frac{1}{2}\int_\Omega (u(x) - \bar{u}(x))^2 dx + \frac{\alpha}{2}\int_\Omega z(x)^2 dx \\ \text{s.t} \quad & -\nabla\cdot(z\nabla u) = f, \qquad \text{in } \Omega \\ & u = 0, \qquad \text{on } \partial\Omega \end{aligned}$$

Discretize using finite elements (interlab), run with Matlab implementation of penalty method with:

- $n = 2050$, $m = 961$
- $\alpha = 10^{-4}$, $\sigma = 10^{-2}$
- TRON (Newton-CG) applied on $\phi_\sigma(u, z)$
- LNLQ for augmented system solves, rel. error tol $= 10^{-3}$

Inverse Poisson Problem

iter	merit	objective	opt Error	du Feas	nln Feas	CGits	stat
0	2.997845e+00	1.837255e+00	7.985e-03	7.123e-03	2.000e+00		
1	2.964378e+00	1.820891e+00	7.976e-03	7.087e-03	1.975e+00	1	
2	2.834288e+00	1.755744e+00	7.934e-03	6.938e-03	1.878e+00	1	
3	2.372450e+00	1.498781e+00	7.645e-03	6.225e-03	1.492e+00	1	
4	1.111925e+00	6.183138e-01	6.570e-03	7.431e-03	1.025e+00	1	
5	1.381301e-01	3.408713e-02	3.827e-03	2.515e-03	4.348e-01	2	
6	4.033638e-01	1.108718e-01	4.538e-03	3.096e-03	1.180e+00	2	rej
7	6.599361e-02	1.687954e-02	2.433e-03	2.230e-03	2.004e-01	2	
8	3.608916e-03	9.273160e-04	7.735e-04	4.657e-04	7.073e-02	2	
9	2.334628e-04	2.316148e-04	3.226e-05	1.783e-05	6.444e-03	1	
10	2.306002e-04	2.305667e-04	1.013e-06	8.145e-07	2.053e-04	1	
11	2.081017e-04	1.997098e-04	3.682e-05	2.142e-05	3.505e-03	6	
12	2.052722e-04	2.054533e-04	1.543e-06	8.706e-07	3.129e-04	1	
13	1.905605e-04	1.874832e-04	2.050e-05	1.217e-05	8.842e-04	10	
14	1.898997e-04	1.899435e-04	5.290e-07	3.753e-07	7.993e-05	1	
15	1.854960e-04	1.842241e-04	1.369e-05	8.012e-06	6.028e-04	16	
16	1.853261e-04	1.853453e-04	6.334e-07	3.400e-07	4.926e-05	1	
17	1.848716e-04	1.847335e-04	2.251e-06	1.229e-06	1.597e-04	24	
18	1.848673e-04	1.848701e-04	1.755e-07	9.599e-08	1.207e-05	1	
19	1.848203e-04	1.848129e-04	1.052e-07	5.783e-08	6.837e-06	32	
20	1.848202e-04	1.848205e-04	6.376e-09	3.621e-09	4.582e-07	1	

Inverse Poisson Problem

	Iterations	# Hv	# Jprod	# Adj. Jprod
$\epsilon = 10^{-2}$	22	878	3448	3672
$\epsilon = 10^{-4}$	21	896	4251	4459
$\epsilon = 10^{-6}$	20	744	4651	4928
$\epsilon = 10^{-8}$	20	746	5611	5887
$\epsilon = 10^{-10}$	20	746	6595	6871

ROL_example_PDE-OPT_navier-stokes_example_01

Fletcher solver : Trust_Region

iter	merit	fval	gpnorm	gLnorm	cnorm	snorm	flag	iterCG
0	3.1e-01	3.1e-01	4.1e-02	4.1e-02	4.6e-12			
1	3.1e-01	3.0e-01	4.1e-02	8.9e+00	2.5e-04	6.8e-01	2	48
2	3.1e-01	3.0e-01	4.1e-02	4.1e-02	4.6e-12	1.7e-01	0	2
3	3.1e-01	3.1e-01	9.2e-02	6.1e-02	1.4e-06	4.3e-02	0	1
4	3.0e-01	3.0e-01	5.3e-01	2.8e-01	8.6e-04	1.0e-01	0	4
5	3.0e-01	3.0e-01	4.4e-01	2.2e-01	5.1e-05	1.0e-01	0	7
6	3.0e-01	3.0e-01	9.8e-01	4.9e-01	1.2e-05	1.6e-01	0	42
7	3.0e-01	3.0e-01	1.1e-01	5.8e-02	4.1e-06	6.0e-02	0	31
8	3.0e-01	2.9e-01	4.2e-01	2.1e-01	5.1e-06	1.1e-01	0	39
9	2.9e-01	2.9e-01	8.2e-03	4.2e-03	7.3e-07	1.7e-02	0	25
10	2.9e-01	2.9e-01	6.6e-03	3.3e-03	8.2e-08	1.4e-02	0	27
11	2.9e-01	2.9e-01	5.3e-05	4.9e-05	5.2e-08	1.0e-04	0	7
12	2.9e-01	2.9e-01	1.7e-06	8.9e-07	1.9e-10	2.4e-04	0	44

Conclusions and Future Work

Simpler approach to nonlinear programming!

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- Current implementation Matlab, ROL implementation coming along

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Many practical matters to be resolved:

- Practical tolerance rules for inexact solves
- Good heuristics for updating penalty parameter
- Stability of inequality constrained problems near boundary
- Continue implementation in Matlab and ROL
- Test on more PDE-constrained optimization problems!