The Merits of Keeping it Smooth: Implementing a Smooth Exact Penalty Function for Nonlinear Optimization

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Constrained Optimization

Equality-constrained nonlinear program:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad f(x) \quad \text{subject to} \quad c(x) = 0,$$

with n variables, $m \leq n$ constraints, and $f, c \in C_3$.

Focus on equality constraints only for now, discuss inequality/bound constraints later.

Such problems are ubiquitous in the computational sciences for applications including:

- Structural Design
- Systems biology
- Machine learning
- Optimal control
- Robotics planning
- ...

Example: PDE-Constrained Optimal Control

Inverse Poisson Problem:

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

where $\Omega = [0,1]^2$, $\bar{u}$ is observed data, and f is given source.

- u is the *state* (e.g., temperature)
- z is the *control* (e.g., heat conduction coefficient)

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- u is the *state* (e.g., temperature)
- z is the *control* (e.g., heat conduction coefficient)

Problem structure:

- Want computed state to match observations
- Want control variable to be "reasonable" (regularization)
- State must be physically meaningful given control

Solving Constrained Optimization Problems

Necessary conditions for optimal primal-dual solution (x^*, y^*):

$$\begin{aligned} c(x^*) &= 0, \\ g(x^*) &= A(x^*)y^*. \end{aligned}$$

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

$$\nabla L(x^*, y^*) = 0.$$

Constrained solvers built around root-finding of above equations.

Notation:

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

Solving Constrained Optimization Problems

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

Common difficulties with constrained methods:

- Finding a feasible point is just as difficult as solving problem
- Complicated heuristics to trade off optimality vs. feasibility
- Require feasibility restoration phases
- Most solvers built using explicit matrix-factorizations

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Alternative approach:

- Move constraint violation into the objective
- Solve unconstrained problem
- Additionally: want to avoid matrix-factorizations

Penalty methods for Nonlinear Programming

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**

$$\min_{x} f(x) - y_k^T c(x) + \frac{\sigma_k}{2}\|c(x)\|_2^2$$

  - Need to solve sequence of problems.

Penalty methods

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- **Augmented Lagrangian method**

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

  - 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:

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

Notation:

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

Variations

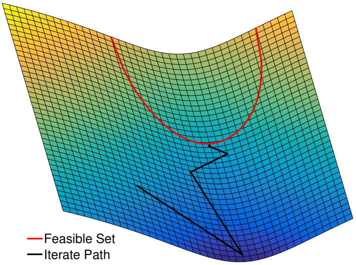
Smooth Primal (Fletcher, 1970)

$$\phi_{0,\rho}(x) := f(x) - y(x)^T c(x) + \tfrac{1}{2}\rho\|c(x)\|_2^2$$

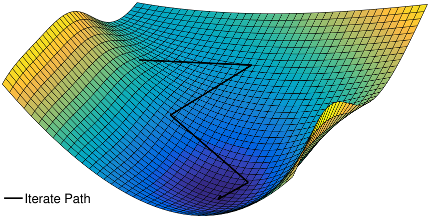
Smooth Primal-Dual (Di Pillo and Grippo, 1989; Zavala and Anitescu, 2014)

$$\psi_{\alpha,\beta}(x,y) := L(x,y) + \tfrac{1}{2}\alpha\|c(x)\|_2^2 + \tfrac{1}{2}\beta\|\nabla L(x,y)\|_2^2$$

An Illustration



(a) 'hs007' with feasible set.



(b) ϕ_σ for problem 'hs007'.

Derivatives

More notation (sorry!):

$$g_\sigma(x) = \nabla_x L(x, y_\sigma), \qquad H_\sigma(x) = \nabla_{xx} L(x, y_\sigma)$$

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Gradient of penalty function:

$$\nabla \phi_\sigma(x) = g_\sigma - Y_\sigma c$$

Hessian of penalty function:

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

First-Order Optimality Conditions

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

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

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

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

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

Second-Order Optimality Conditions

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

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

Second-Order Optimality Conditions

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

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Hessian of Penalty function:

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

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

Second-Order 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 $\nabla^2\phi_\sigma(x_*) \succeq 0 \iff \sigma \geq \sigma_* = \frac{1}{2}\lambda_{\max}(P_A H_\sigma P_A)$

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

Solving NLP with ϕ_σ

$\phi_\sigma(x)$ 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)
- Can use $\phi_{\sigma,\rho} = \phi_\sigma(x) + \frac{1}{2}\rho\|c(x)\|_2^2$ to resolve this

Benefits of this approach

- Conceptually simple minimization (no optimality/feasibility trade-off heuristics)
- No feasibility restoration*
- No Maratos effect (slow convergence for nonsmooth penalties)
- Solve single unconstrained problem if σ known in advance

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- Conceptually simple minimization (no optimality/feasibility trade-off heuristics)
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- Solve single unconstrained problem if σ known in advance
- Naturally accommodates *matrix-free* optimization (only matrix-vector products; no factorizations)
- Naturally accommodates inexact optimization

The technical part

In order to minimize ϕ_σ, need procedures for:

- function evaluation, $\phi_\sigma(x)$,
- gradient evaluation, $\nabla\phi_\sigma(x)$, and
- approximate Hessian-vector products: compute for any $v \in \mathbb{R}^n$

$$u = B(x)v, \qquad B(x) \approx \nabla^2\phi_\sigma(x)$$

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Therefore need procedures for computing:

- y_σ
- products with Y_σ and Y_σ^T

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

$$S(x,v)u = \begin{bmatrix} v^TH_1u \\ \vdots \\ v^TH_mu \end{bmatrix}, \qquad S(x,v)^Tu = \sum_{i=1}^m u_iH_iv$$

(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

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

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:

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

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

Two augmented system solves per product.

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Two augmented system solves per product.

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

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A few notes and observations:

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

Solving the Augmented System

- Direct Solvers
  - Factorize augmented system once per iteration
  - Sparse LDL
  - Semi-normal equations (Q-less QR) + iterative refinement
- Iterative methods
  - Results in *matrix-free* implementation
  - Inexact function/gradient evaluation controlled via iterative solver tolerance
  - Efficient with good preconditioners

Solving the Augmented System: LSLQ/LNLQ

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

- Equivalent to SYMMLQ on normal equations
- Given $\sigma_{est} \leq \sigma_{\min}(A)$, 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 $\sigma_{\min}\left(\mathcal{P}^{-1} A^T A\right) \geq 1$

Inexact Evaluation

Certain trust-region methods (Conn, Gould and Toint 2000; Heinkenschloss and Ridzal, 2014) converge provided that

$$\begin{aligned} \|\phi_\sigma - \widetilde{\phi_\sigma}\| &\le M\eta_1, \\ \|\nabla\phi_\sigma - \widetilde{\nabla\phi_\sigma}\| &\le M\eta_2, \end{aligned}$$

where η_i is a prescribed accuracy, and $M > 0$ is a fixed constant (need not be known).

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where η_i is a prescribed accuracy, and $M > 0$ is a fixed constant (need not be known).

Can bound terms according to residual or error of augmented system.

Error expressions tedious—in practice, use ad-hoc fixed error bound.

Handling Linear Constraints

Suppose some constraints are linear:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad f(x) \quad \text{subject to} \quad c(x) = 0, \qquad B^T x = d,$$

Handling Linear Constraints

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Change penalty function minimization to:

$$\begin{aligned} \min_{x} \quad & \phi_\sigma(x) := f(x) - c(x)^T y_\sigma(x) \\ \text{s.t.} \quad & B^T x = d \end{aligned}$$

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Benefits:

- Threshold value σ_* decreases
- Penalty function better conditioned

Regularization

If $A = \nabla c$ is rank-deficient, then ϕ_σ can be undefined.

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Regularize least-squares problem:

$$\begin{aligned}
\phi_\sigma(x;\delta) &= f(x) - c(x)^T y_\sigma(x;\delta) \\
y_\sigma(x;\delta) &= \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
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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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---

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

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

Inequality Constraints

Consider problem

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Modify Fletcher's penalty function to

$$\begin{aligned} \min_x \quad & \phi_\sigma(x) := f(x) - c(x)^T y_\sigma(x) \\ \text{s.t.} \quad & x \geq 0 \\ & y_\sigma(x) := \arg\min_y \frac{1}{2}\|g - Ay\|_{X}^2 + \sigma c(x)^T y \end{aligned}$$

Inequality Constraints

- Minimize smooth function over bound constraints
- Smoothness holds for $x > 0$ (use interior method)
- Exactness still holds
- Need to now solve augmented system:

$$\begin{bmatrix} I & X^{\frac{1}{2}}A \\ A^T X^{\frac{1}{2}} & 0 \end{bmatrix} \begin{bmatrix} w \\ v \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

Numerical Experiments: Inverse Poisson Problem

Solve inverse-poisson problem from earlier.

Discretize using finite elements, $n = 2050$, $m = 961$, $\alpha = 10^{-4}$.

Use Matlab implementation of Newton-CG trust-region solver (TRON). Solve linear system with error accuracy η:

η	Iter.	$\#Hv$	$\#Av$	$\#A^Tv$
10^{-2}	29	874	1794	2608
10^{-4}	27	830	1950	2728
10^{-6}	27	866	2317	3129
10^{-8}	27	866	2673	3485
10^{-10}	27	866	3145	3957

Thanks to Drew Kouri (Sandia) for implementing the model!

Numerical Experiments: Linear Constraints

Problem	n	m_{lin}	m_{nln}	σ^*_{impl}	σ^*_{expl}	σ	Impl.	Expl.
Chain100	202	102	1	0.0047	0	10^{-3} 0.005	$*$ 8	13 10
Chain200	402	202	1	0.0024	0	10^{-3} 0.003	$*$ 7	11 10
Chain400	802	402	1	0.0012	0	10^{-3} 0.002	$*$ 7	10 10
Channel100	800	400	400	0	0	10^{-3} 1	– –	5 5
Channel200	1600	800	800	0	0	10^{-3} 1	– –	5 5
Channel400	1600	800	800	0	0	10^{-3} 1	– –	5 5

Numerical Experiments: Regularization (mss1)

- $n = 90$, $m = 73$, $\sigma = 10^3$
- Fails at step 1 when $\delta_0 = 0$
- Start with $\delta_0 = 10^{-2}$

iter	merit	objective	opt Error	du Feas	nln Feas	||y||	penalty	delta
0	3.525544e+05	-4.050000e+03	5.964e+03	4.979e+02	8.900e+01	1.818e+06	1.0e+03	1.0e-02
1	3.388800e+05	-1.806637e+03	8.528e+03	3.277e+02	3.915e+01	1.815e+06		
2	3.369551e+05	-1.802047e+03	8.540e+03	3.263e+02	3.905e+01	1.810e+06		
3	3.350170e+05	-1.797264e+03	8.533e+03	3.271e+02	3.896e+01	1.804e+06		
4	3.330739e+05	-1.792274e+03	8.507e+03	3.279e+02	3.886e+01	1.799e+06		
5	3.311332e+05	-1.787067e+03	8.465e+03	3.287e+02	3.877e+01	1.794e+06		
...								
45	-1.600001e+01	-1.600155e+01	8.443e-04	4.761e-02	1.656e-06	1.741e+02		
46	-1.600001e+01	-1.600154e+01	6.603e-05	4.748e-02	1.656e-06	1.741e+02		1.0e-04
47	-1.600000e+01	-1.599998e+01	6.924e-03	3.513e-03	3.921e-07	1.753e+02		
48	-1.600000e+01	-1.600000e+01	1.898e-04	1.905e-04	9.392e-10	1.753e+02		
49	-1.600000e+01	-1.600000e+01	1.762e-05	1.762e-05	2.893e-10	1.753e+02		
50	-1.600000e+01	-1.600000e+01	1.813e-06	5.356e-06	1.674e-10	1.753e+02		
51	-1.600000e+01	-1.600000e+01	5.934e-08	5.361e-06	1.660e-10	1.753e+02		
52	-1.600000e+01	-1.600000e+01	4.840e-09	5.554e-06	1.663e-10	1.753e+02		1.0e-07
53	-1.600000e+01	-1.600000e+01	7.565e-08	3.905e-08	4.923e-12	1.753e+02		

EXIT: Optimal solution found

Conclusions and Future Work

Simpler* approach to nonlinear programming!

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Many practical matters to be resolved:

- Robust tolerance rules for inexact solves
- Good heuristics for updating penalty parameter
- Stability of inequality constrained problems near boundary
- Test on more PDE-constrained optimization problems!