Trust Regions in Large-Scale Optimization and Regularization

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Danny C. Sorensen, Rice, USA

Thanks
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Outline

- Trust Regions in Optimization
- Trust Regions in Regularization
- The Trust-Region Subproblem (TRS)
- Methods for the large-scale TRS
- Comparisons
- Applications
- Concluding Remarks

Trust Regions in Optimization

Unconstrained Optimization

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Two strategies to move from x_k to $x_{k+1} = x_k + d$:
Line Search and Trust Region.

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Consider the following quadratic model of f at x_k

$$q_k(d) = f(x_k) + \nabla f(x_k)^T d + \tfrac{1}{2} d^T H d,$$

where H is a symmetric matrix.

Line Search Methods:

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- Search along d_k for a suitable step length α.
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Trust-Region Methods:

- Find a minimizer of q_k in $\{d \in \mathbb{R}^n s.t. \|d\| \leq \Delta_k, \Delta_k > 0\}$.
- $\{d \in \mathbb{R}^n s.t. \|d\| \leq \Delta_k\}$ is the trust region:
  a region where we trust the model q_k to be a good representation of f.
- Δ_k is the trust-region radius.
- d_k is the step.
- Do not require positive definite H.

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- Trust-Region Methods are slightly more robust.
- The Levenberg-Marquardt Method (1944, 1963) for nonlinear least squares problems is considered as the first trust-region method (Moré 1978).

Given x_0 and Δ_0
begin
    $k := 1$; $\Delta := \Delta_0$;
    repeat
        set d_k as a solution to

$$\min q_k(d) \text{ s.t. } \|d\| \leq \Delta;$$

        $\varrho := \frac{f(x_k)-f(x_{k+1})}{q_k(0)-q_k(d_k)}$;   % gain factor
        if $\varrho > 0.75$ $\Delta := 2 * \Delta$; **end**
        if $\varrho < 0.25$ $\Delta := \Delta/3$; **end**
        if $\varrho > 0$
            $x_k := x_{k-1} + d_k$;
        end
        $k := k + 1$;
    until *convergence*
end

Trust-Region Methods

Main calculation per iteration: Trust-Region Subproblem (TRS)

$$\begin{array}{ll} \min & \frac{1}{2} d^T H d + g^T d \\ s.t. & \|d\| \leq \Delta \end{array}$$

where:

- $g = \nabla f(x_k)$.
- H is a symmetric matrix, usually an approximation to $\nabla^2 f(x_k)$.
- $\Delta > 0$.

Trust Regions in Regularization

Regularization: Linear

Tikhonov Regularization:

$$\min_{x \in \mathbb{R}^n} \quad \frac{1}{2}\|Ax - b\|_2^2 + \lambda \|x\|_2^2$$

- $A \in \mathbb{R}^{m \times n}$, $m \geq n$ large, from ill-posed problems.
- $b \in \mathbb{R}^m$, containing noise, and $A^T b \neq 0$.
- $\lambda > 0$ is the Tikhonov regularization parameter.

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$$\begin{array}{ll} \min & \frac{1}{2}\|Ax - b\|_2^2 \qquad (\text{TRS}) \\ s.t. & \|x\|_2 \leq \Delta \end{array}$$

where $\Delta > 0$, plays the role of the regularization parameter.

Regularization: Nonlinear, Constrained

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where f, g are nonlinear functions, $S \subset \mathbb{R}^n$, and λ is a regularization parameter.

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Example 2: $\min \; \frac{1}{2}\|Ax - b\|_2$ s.t. $\|x\|_2 \le \Delta$, $x \ge 0$.
Could be solved with a trust-region-based method
(R & Steihaug 2002).

TRS in Optimization and Regularization

Optimization	**Regularization**
Several TRS	Linear: One TRS Nonlinear, Constrained: Several TRS
(potential) Hard Case not common	(potential) Hard Case (Near HC) likely

The Trust-Region Subproblem

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$$\begin{array}{ll} \min & \frac{1}{2}x^T H x + g^T x \\ s.t. & \|x\| \leq \Delta \end{array}$$

- $H \in \mathbb{R}^{n \times n}$, $H = H^T$, n large.
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- $\| \cdot \|$ is the Euclidean norm.

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- In optimization: $H \approx \nabla^2 f(x_k)$, $g = \nabla f(x_k)$.
- In (linear) regularization: $H = A^T A$, $g = -A^T b$.

Characterization of solutions. Gay 1981, Sorensen 1982.

x_* with $\|x_*\| \le \Delta$ is a solution of TRS with Lagrange multiplier λ_*, if and only if

(i) $(H - \lambda_* I)x_* = -g$.
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Remark: $\|x\| - \Delta = 0$ is the secular equation.

Solutions to TRS

Notation:

- $\delta_1 \leq \delta_2 \leq \ldots \leq \delta_n$ are the eigenvalues of H.
- $\mathcal{S}_1$ is the eigenspace associated with δ_1, the smallest eigenvalue of H.

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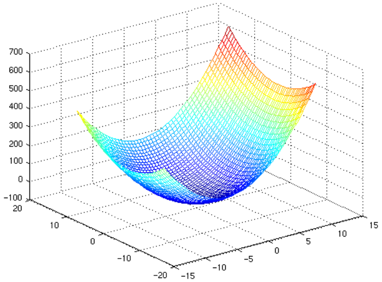

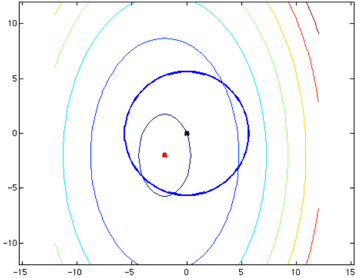

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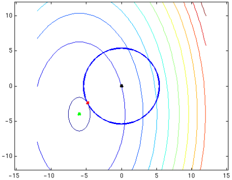

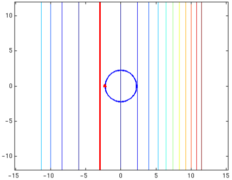

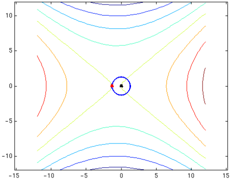

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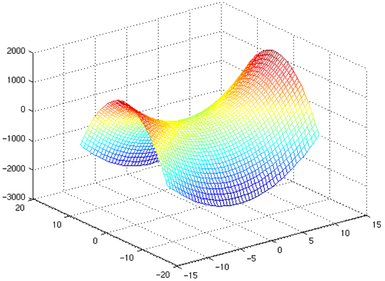

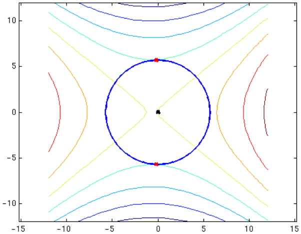

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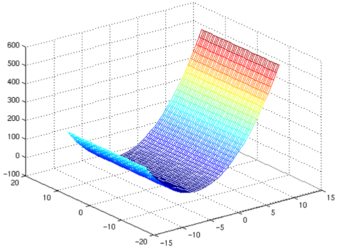

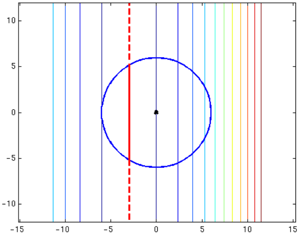

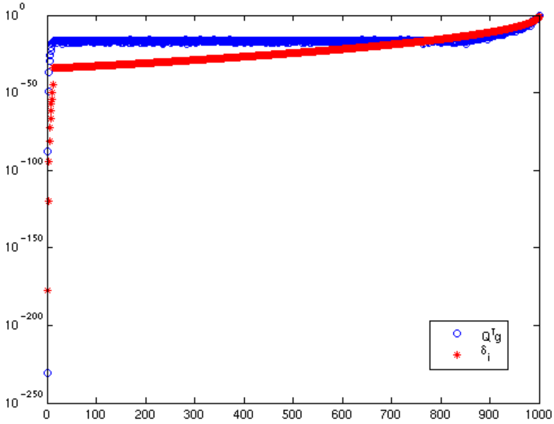

Problem **heat** from P.C. Hansen's Regularization Tools.
$m = n = 1000$; $\circ$ $Q^T g$; $*$ δ_i.

Methods for Large-Scale TRS

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- SSM: Hager 2001.
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Nearly-Exact:

- Moré and Sorensen 1983:
  Newton's method on $\dfrac{1}{\|x_\lambda\|^2} - \dfrac{1}{\Delta^2} = 0$.
- Golub and von Matt 1991.
  Moments, quadrature, Lanczos bidiagonalization to compute lower and upper bounds for $\|x_\lambda\|^2$, $\Delta < \|H^\dagger g\|$.
- Sorensen 1997.
- SDP: Rendl and Wolkowicz 1997, Fortin and Wolkowicz 2004.
- LSTRS: R, Santos and Sorensen 2000, 2008.
  Rational interpolation + parameterized eigenvalue problems.

Secular Functions and Equations

Let $\quad H = Q \; diag(\delta_1, \delta_2, \ldots, \delta_n) \; Q^T \;$ and $\; \gamma = Q^T g.$

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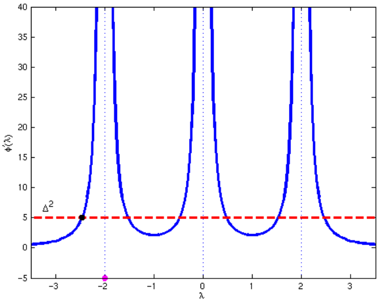
Then $\quad \phi'(\lambda) = x^T x$.

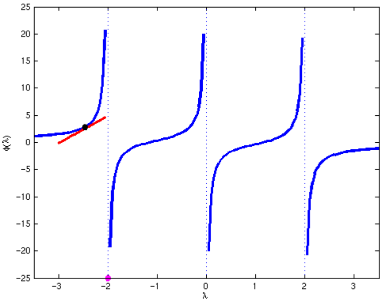
Secular Equation: $\phi'(\lambda) = \Delta^2$.

Secular Equations - standard case

$\phi'(\lambda)$



$\phi(\lambda)$



Secular Equations - hard case

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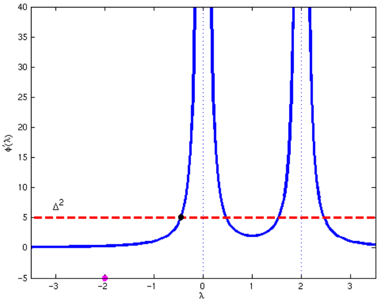
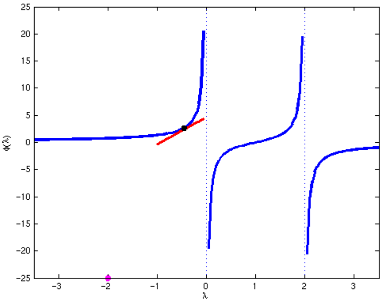
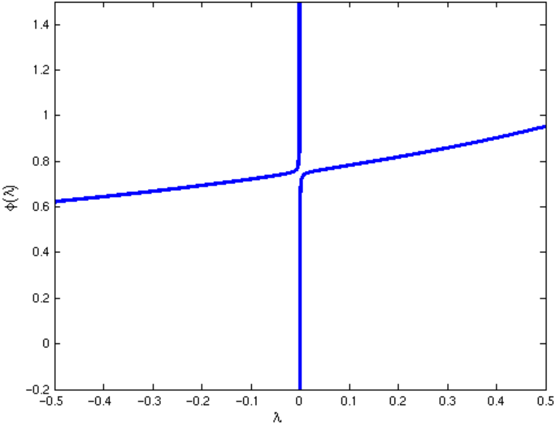


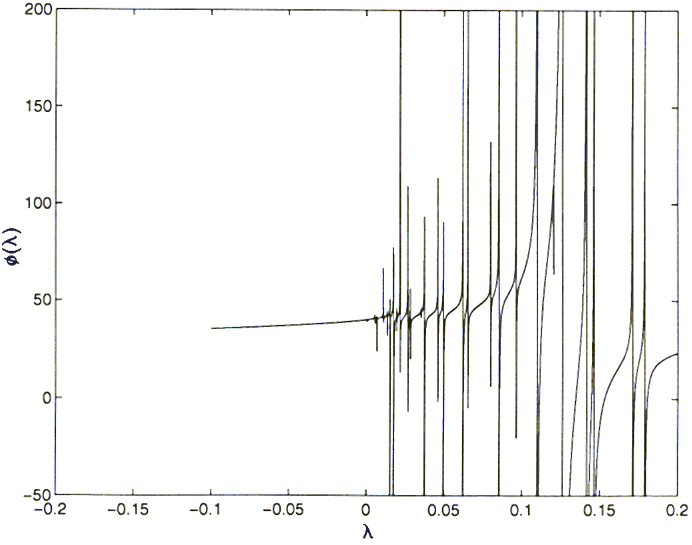
$\phi(\lambda)$



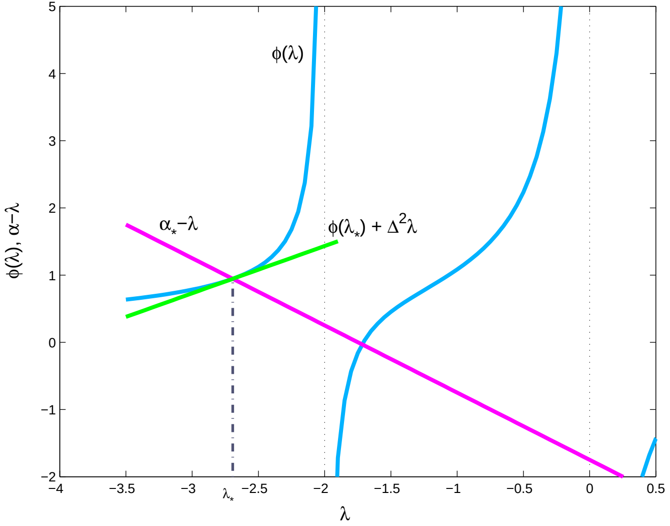
Potential (near) hard case: $g \approx\perp \mathcal{S}_1$



Ill-posed problems: $g \approx\perp \mathcal{S}_i, i = 1, 2, \ldots, k$



LSTRS - standard case



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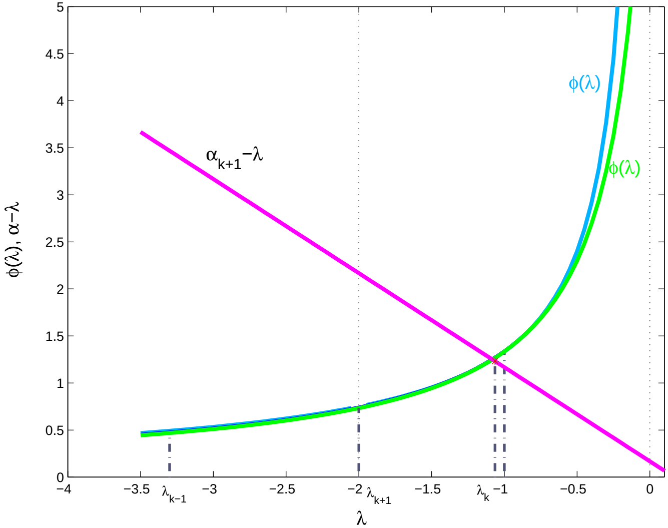

Comparisons

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  Hager 2001.
- SDP - Semidefinite Programming approach.
  Rendl and Wolkowicz 1997, Fortin and Wolkowicz 2004.
- GLTR - Generalized Lanczos Trust Region method.
  Gould, Lucidi, Roma, and Toint 1999.
- LSTRS.
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  Rendl and Wolkowicz 1997, Fortin and Wolkowicz 2004.
- GLTR - Generalized Lanczos Trust Region method.
  Gould, Lucidi, Roma, and Toint 1999.
- LSTRS.
  R, Santos and Sorensen 2000, 2008.
- All: matrix-free.
- LSTRS, SDP, SSM: limited-memory.

Average results for 2-D Laplacian, $n = 1024$. Easy Case.

METHOD	MVP	STORAGE	$\frac{\|(H - \lambda I)x+g\|}{\|g\|}$
LSTRS	127.1	10	2.32×10^{-6}
SSM	67.3	10	9.53×10^{-7}
SSM_d	67.3	10	9.53×10^{-7}
SDP	595	10	3.17×10^{-5}
GLTR	81.6	41.3	8.56×10^{-6}

Average results for 2-D Laplacian, $n = 1024$. Hard Case.

METHOD	MVP	STORAGE	$\frac{\\|(H - \lambda I)x+g\\|}{\\|g\\|}$
LSTRS	252.6	10	6.91×10^{-6}
SSM	377.9	10	1.42×10^{-6}
SSM_d	377.9	10	1.42×10^{-6}
SDP	2023.8	10	5.76×10^{-2}
GLTR	151.8	76.4	8.37×10^{-6}

Inverse Heat Equation, $n = 1000$. Mildly Ill-Posed.

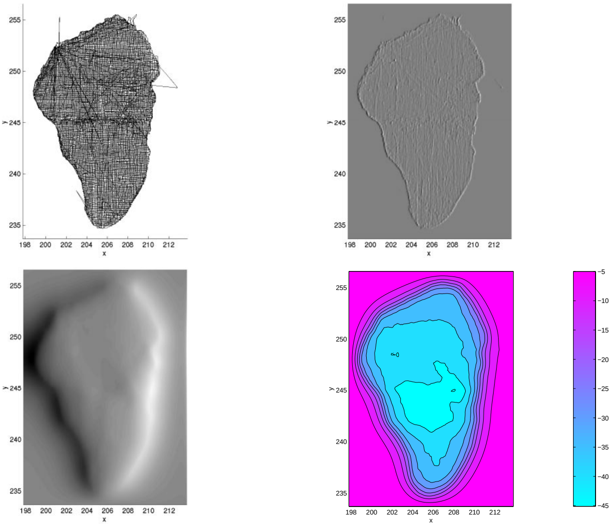
METHOD	MVP	STORAGE	$\frac{\|(H - \lambda I)x+g\|}{\|g\|}$	$\frac{\|x-x_{IP}\|}{\|x_{IP}\|}$
LSTRS	265	8	9.12×10^{-6}	6.13×10^{-4}
SSM	700	8	2.99×10^{-9}	2.41×10^{-4}
SSM_d	649	8	2.74×10^{-9}	4.57×10^{-4}
SDP	5700	8	2.73×10^{-7}	3.63×10^{-4}

Inverse Heat Equation, $n = 1000$. Severely Ill-Posed.

METHOD	MVP	STORAGE	$\frac{\|(H - \lambda I)x+g\|}{\|g\|}$	$\frac{\|x-x_{IP}\|}{\|x_{IP}\|}$
LSTRS	552	8	7.05×10^{-6}	5.49×10^{-2}
SSM	512	8	1.81×10^{-7}	3.75×10^{-2}
SSM$_d$	215	8	2.04×10^{-7}	2.25×10^{-2}
SDP	4600	8	2.27×10^{-4}	2.08×10^{-1}

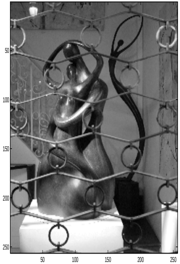
Applications (LSTRS)

Inverse Interpolation: Bathymetry of the Sea of Galilee

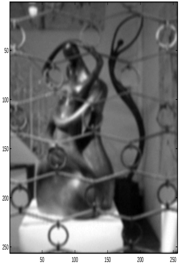


Dimension: 40401. Vectors: 5. MVP: 206.

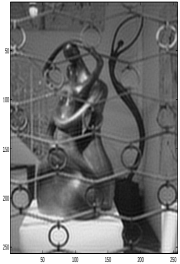
Image Restoration



True image



Blurred and noisy image



LSTRS restoration

Dimension:	**65536**
Vectors:	**7**
MVP:	**201**

Using function **blur** from P.C. Hansen's Regularization Tools.

Other applications

- Large-scale non-negative regularization (R & Steihaug 2002).
- Confidence intervals for solutions of large-scale discrete ill-posed problems (Eldén, Hansen & R 2005).

Other applications

- Large-scale non-negative regularization (R & Steihaug 2002).
- Confidence intervals for solutions of large-scale discrete ill-posed problems (Eldén, Hansen & R 2005).
- Large-scale computer vision.
  Kahl and collaborators, Lund University, Sweden.
- 3D electrical impedance tomography.
  Soleimani and collaborators, University of Bath, U.K.

Concluding Remarks

- Trust regions yield efficient methods for solving general nonlinear optimization problems, and for both linear and nonlinear regularization problems.
- TRS is the main calculation in trust-region methods.
- The special features of the TRS in regularization problems influence the design of methods.
- There exist efficient methods for solving large-scale TRS arising in general optimization problems and in regularization.

REFERENCES

Trust-Region Methods:

- A.R. Conn, N.I.M. Gould, and Ph.L. Toint. *Trust-Region Methods*, SIAM, Philadelphia, 2000.
- J. Nocedal and S.J. Wright. *Numerical Optimization*. Springer, New York, 2nd. ed., 2006.

Trust Regions and Regularization, LSTRS:

Thesis, Papers and Software can be downloaded from:

`http://www.imm.dtu.dk/~mr`