Computed Tomography: Algorithms, Insight, and Just Enough Theory

Chapter 13: Optimization Methods for Tomography

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Outline

Optimization Problems in Computed Tomography

- Tomographic Reconstruction: Inverse problem Ax = b
  Solve the least-squares problem:

$$x_{LS} = \arg\min_x \frac{1}{2} \|b - Ax\|_2^2$$

- Cimmino's Method:

$$x^{k+1} = \frac{1}{m} \sum_{i=1}^{m} P_i(x^{(k)})$$

- SIRT:

$$x^{k+1} = x^k + D_1 A^T M_1 (b - Ax^{(k)})$$

- Regularization methods:
  - Tikhonov Regularization:

$$\min_{x} \left\{ \frac{1}{2}\|b - Ax\|_2^2 + \alpha \frac{1}{2}\|x\|_2^2 \right\}$$

  - Total Variation Regularization
    - anisotropic TV

$$TV_a(x) = \|(I_N \otimes D_M)x\|_1 + \|(D_N \otimes I_M)x\|_1$$

    - isotropic TV

$$TV_i(x) = \sum_{i=1}^{n} \sqrt{[(I_N \otimes D_M)x]_i^2 + [(D_N \otimes I_M)x]_i^2}$$

Goal:

- Discuss first-order optimization methods related to these problems

Optimization problem

General form:

$$\textit{minimise } g(x)$$
or
$$\textit{minimise } -g(x)$$

$$\text{subject to } C$$

with $g(x)$ as the *objective function* and a *set of constraints C*

- *C* empty -> unconstrained optimization problem
- *C* non-empty -> constrained optimization problem

Outline

Gradient of a multivariate function

Consider:

$$g : D \subseteq \mathbb{R}^n \to \mathbb{R}, \quad \boldsymbol{x} = (x_1, ..., x_n)^\top \mapsto g(x_1, ..., x_n)$$

$$\nabla g(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial g}{\partial x_1} \\ \vdots \\ \frac{\partial g}{\partial x_n} \end{pmatrix}$$

gives us the direction of steepest ascent of g at point $\boldsymbol{x}$

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We conclude:

$$-\nabla g(\boldsymbol{x})$$

gives us

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We conclude:

$$-\nabla g(\boldsymbol{x})$$

gives us the direction of steepest descent of g at point $\boldsymbol{x}$

Minimising a function locally using the gradient

$$\text{minimise } g(x)$$

with $x \in \mathbb{R}^n$ and $g : \mathbb{R}^n \to \mathbb{R}$ continuously differentiable

- $\boldsymbol{x}^*$ global minimizer of $g \iff g(y) \geq g(\boldsymbol{x}^*) \quad \forall y \in \mathbb{R}^n$
- *first-order necessary condition:* $\nabla g(\boldsymbol{x}^*) = 0$ (stationary point)

Find a stationary point relative to an initial guess $\underline{\boldsymbol{x}^{(\mathbf{0})}}$

$$x^{(k+1)} = x^{(k)} - t_k \nabla g(x^{(k)}), \quad k = 0, 1, 2, \ldots$$

with $-\nabla g(x^{(k)})$ as the descent direction and t_k as a sufficiently small step size

Gradient method with a constant step size

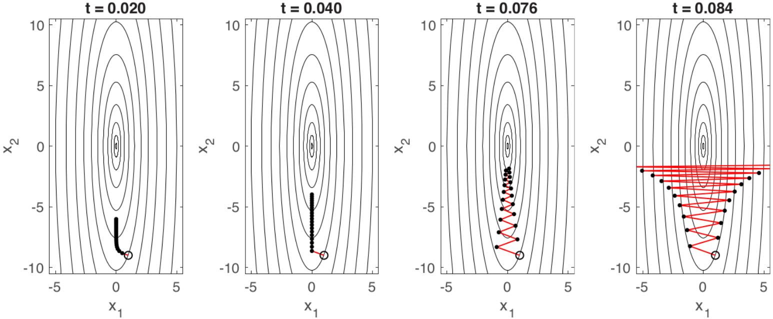

Figure 13.3. *Contour plots of g with the first* 20 *iterations of the gradient method using a constant step size. The initial guess is marked with a circle, and the subsequent iterations are marked with solid black dots connected by a red line that indicates the order of the iterates.*

[4]

Outline

Definition

A function g is ***Lipschitz continuous*** if and only if

$$\exists L \in \mathbb{R}. \quad \forall x, y \in \mathbb{R}^n. \quad \|g(x) - g(y)\| \leq L\|x - y\|$$

How is this helpful?

If the gradient of g is Lipschitz continuous with constant L:

$$g(y) \leq g(x) + \nabla g(x)^\top (y - x) + \frac{L}{2}\|y - x\|_2^2 \quad \forall x, y \in \mathbb{R}^n$$

Example: Least-squares problem

$g(x) = \frac{1}{2}\|b - Ax\|_2^2$

$$\boldsymbol{\nabla g(x) = A^\top (Ax - b)}$$

From this we derive that:

$$\begin{aligned} \boldsymbol{\|\nabla g(y) - \nabla g(x)\|_2} &= \|A^\top (Ay - b) - A^\top (Ax - b)\|_2 \\ &= \|A^\top A(y - x)\|_2 \\ &\boldsymbol{\leq \|A^\top A\|_2 \|y - x\|_2} \end{aligned}$$

We can deduce: ∇g is Lipschitz continuous with constant $L = \|A^\top A\|_2$

Boundedness of the Hessian Matrix

Let g be twice continuously differentiable, the *Hessian matrix of g* corresponds to

$$H(x) = \nabla^2 g(x) = \begin{pmatrix} \frac{\partial^2 g(x)}{\partial x_1^2} & \frac{\partial^2 g(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 g(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 g(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 g(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 g(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 g(x)}{\partial x_n \partial x_1} & \frac{\partial^2 g(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 g(x)}{\partial x_n^2} \end{pmatrix}$$

We can show that if $\|\nabla^2 g(x)\|_2 \leq L$ for all x then the gradient of g is Lipschitz continuous with constant L.

(using the Cauchy-Schwarz inequality and the fundamental theorem of calculus on $\|\nabla g(y) - \nabla g(x)\|_2$)

Converse also true

Power iteration

For $g(x) = \frac{1}{2}\|b - Ax\|_M^2$ with M positive definite

$$H = A^\top M A \quad \text{and} \quad L = \|A^\top M A\|_2$$

However H can be very large and difficult to work with! Since $\|H\|_2 = \lambda_{max}(H)$

- **power iteration** to approximate the largest eigenvalue.
- **algorithm:**

---

parameters: relative tolerance $\epsilon > 0$
$x^{(0)}$ =random vector
$x^{(0)} = x^{(0)}/\|x^{(0)}\|_2$
$\hat{\lambda}^{(0)} = 0$
for $k = 0, 1, 2, \ldots$ **do**
    $w = Hx^{(k)}$
    $\hat{\lambda}^{(k+1)} = \|w\|_2$
    $x^{(k+1)} = w/\hat{\lambda}^{(k+1)}$
    stop if $|\hat{\lambda}^{(k+1)} - \hat{\lambda}^{(k)}| \leq \hat{\lambda}^{(k)}\epsilon$
end for

Majorization

$\psi(y;x)$ is a majorization of g at x if

$$\psi(x;x) = g(x) \quad and \quad \psi(y;x) \geq g(y) \quad \forall y$$

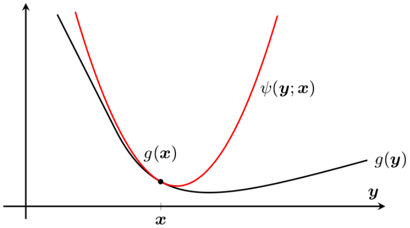

Figure 13.4. *The function $\psi(\boldsymbol{y};\boldsymbol{x})$ is a majorization of g at $\boldsymbol{x}$ since $\psi(\boldsymbol{x};\boldsymbol{x}) = g(\boldsymbol{x})$ and $\psi(\boldsymbol{y};\boldsymbol{x}) \geqslant g(\boldsymbol{x})$ for all $\boldsymbol{y}$.*

[4]

Minimizing the majorization

With an initial guess $x^{(0)}$:

$$x^{(k+1)} = \arg\min_{y} \left\{ \psi(y; x^{(k)}) \right\}, \quad k = 0, 1, 2, \ldots$$

Hence

$$g(x^{(k+1)}) \leq \psi(x^{(k+1)}; x^{(k)}) \leq \psi(x^{(k)}; x^{(k)}) = g(x^{(k)})$$

*Sufficient for descent property:

$$\psi(x^{(k+1)}; x^{(k)}) \leq \psi(x^{(k)}; x^{(k)})$$

Majorization minimization with Lipschitz continuous ∇g

Let $\nabla g(x)$ be Lipschitz continuous with constant L.

$$\begin{aligned}\boldsymbol{x^{(k+1)}} &= \arg\min_y \{g(x^{(k)}) + \nabla g(x^{(k)})^\top (y - x^{(k)}) + \frac{L}{2}\|y - x^{(k)}\|_2^2\} \\ &= \boldsymbol{x^{(k)} - \frac{1}{L}\nabla g(x^{(k)})}\end{aligned}$$

We can show that:

$$g(x^{(k+1)}) \leq g(x^{(k)}) - \frac{1}{2L}\|\nabla g(x^{(k)})\|_2^2$$

We can also show that:

$$\lim_{k\to\infty} \nabla g(x^{(k)}) = 0$$

We converge to a stationary point of g!

Example of a majorization minimization algorithm

General class of SIRT-like algorithms in the form:

$$x^{(k+1)} = x^{(k)} - \lambda_k D A^\top M (A x^{(k)} - b)$$

with $\lambda_k > 0$ as a scalar parameter and D and M positive definite and diagonal

- minimise objective function: $g(x) = \frac{1}{2}\|b - Ax\|_M^2$ via a scaled gradient method
- $\nabla g(x)$ is Lipschitz continuous with constant $L = 1$ under the assumption that $\|M^{1/2} A D^{1/2}\|_2 \leq 1$
  We construct the majorization:

$$g(y) \leq g(x) + \nabla g(x)^\top (y - x) + \frac{1}{2}(y - x)^\top D^{-1}(y - x)$$

- Minimise the right-hand side:

$$y = x - D \nabla g(x)$$

- Substitute $x^{(k)}$ for x and $x^{(k+1)}$ for y, we get the iteration:

$$x^{(k+1)} = x^{(k)} - \lambda_k D \nabla g(x^{(k)})$$

- We get a new upper bound:

$$g(x^{(k+1)}) \leq g(x^{(k)}) - \frac{2\lambda_k - \lambda_k^2}{2} \|\nabla g(x^{(k)})\|_D^2$$

(descent method for $\lambda_k \in (0, 2)$)

- The above analysis can be done for diagonal matrices:

$$D_{jj} = \left(\sum_{i=1}^{m} |A_{ij}|^{\alpha} \right)^{-1}, \qquad M_{ii} = \left(\sum_{j=1}^{n} |A_{ij}|^{2-\alpha} \right)^{-1}$$

$\alpha \in [0, 2]$ and $|A_{ij}|^0 = 1$ when $A_{ij} = 0$
$\rightarrow$ Cimmino method for $\alpha = 0$, SIRT method for $\alpha = 1$

Outline

Convexity

$g : \mathbb{R}^n \to \mathbb{R}$ is convex if and only if

$$\boldsymbol{g(\gamma x + (1-\gamma)y) \leq \gamma g(x) + (1-\gamma)g(y), \quad \gamma \in [0,1] \quad \forall x, y \in \mathbb{R}^n} \tag{1}$$

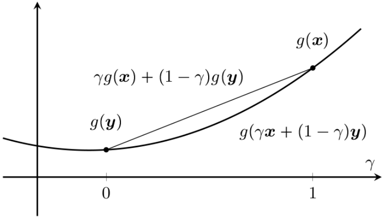

Figure 13.5. *A function g is convex if every line segment that joins two points on its graph (parametrized by $\gamma \in [0,1]$) does not lie below the graph at any point.*

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Any stationary point of a convex function is a minimizer.

If g is continuously differentiable, then (1) is equivalent to

$$g(y) \geq g(x) + \nabla g(x)^\top (y - x), \quad \forall x, y \in \mathbb{R}^n$$

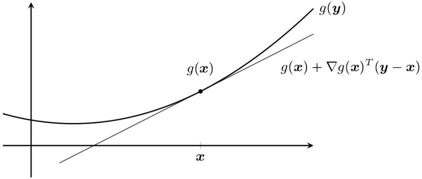

Figure 13.6. *The linearization of a continuously differentiable convex function yields a global linear lower bound.*

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A stationary point is also a global minimizer.

Convergence of the gradient method

$g^* = \inf_x g(x)$ finite and attained at x^* with g being a differentiable convex function with Lipschitz continuous gradient.
Considering the gradient method with $t = \frac{\gamma}{L}$, $\gamma \in (0,2)$:

$$g(x^{(k)}) - g^* \leq \frac{2L\|x^{(0)} - x^*\|_2^2}{4 + \gamma(2-\gamma)k}$$

- objective suboptimality in $O(\frac{1}{k}) \longrightarrow g(x^{(k)})$ converges to g^* sublinearly
- sublinear convergence slower than linear convergence
- best upper bound for $\gamma = 1$, $t_k = \frac{1}{L}$
- $x^{(k)}$ with $g(x^{(k)}) - g(x^*) \leq \epsilon$ attained in at most $O(\frac{1}{\epsilon})$ iterations

Strong convexity

Function g is strongly convex with parameter $\mu > 0$ if

$$\tilde{g}(x) = g(x) - \frac{\mu}{2}\|x\|_2^2 \quad \text{is convex or}$$

$$g(\gamma x + (1-\gamma)y) \leq \gamma g(x) + (1-\gamma)g(y) - \frac{\gamma(1-\gamma)\mu}{2}\|x-y\|_2^2, \quad \forall \gamma \in [0,1], \forall x, y$$

If g is also continuously differentiable we can construct a convex quadratic global underestimator of g at any x:

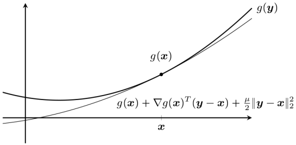

Figure 13.7. *A strongly convex function has a global convex* quadratic *lower bound at all points* $\boldsymbol{x}$.

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Usefulness of strong convexity

- a stationary point x^* of g is a unique minimizer
- bounds that will be useful later:
  - upper bound on the objective suboptimality at x:

$$g(x) - g(x^*) \leq \frac{1}{2\mu}\|\nabla g(x)\|_2^2$$

  - upper bound on the distance from any x to the unique minimizer:

$$\|x^* - x\|_2 \leq \frac{2}{\mu}\|\nabla g(x)\|_2$$

- gradient method with the function being strongly convex with Lipschitz continuous gradient converges linearly to x^* (for $t_k = \frac{\gamma}{(L+\mu)}$ and $\gamma \in (0, 2]$)

$$\|x^{(k)} - x^*\|_2 \leq \left(1 - \frac{2\gamma\mu L}{(L+\mu)^2}\right)^{\frac{k}{2}} \|x^{(0)} - x^*\|_2$$

Convergence results

Using strong convexity we can deduce the following convergence results:

- Landweber's method

$$\|x^{(k)} - \overline{x}\|_2 \leq \left(1 - \frac{2}{1 + \mathsf{cond}(A)^2}\right)^k \|x^{(0)} - \overline{x}\|_2$$

- Cimmino's method

$$\|x^{(k)} - \overline{x}\|_2 \leq \left(1 - \frac{2}{1 + \mathsf{cond}(A^\top M A)}\right)^k \|x^{(0)} - \overline{x}\|_2$$

- Tikhonov regularization

$$\|x^{(k)} - x_{Tik}\|_2 \leq \left(1 - \frac{2}{2 + \|A\|_2^2/\alpha)}\right)^k \|x^{(0)} - x_{Tik}\|_2$$

Visualisation: Tikhonov regularization using the gradient method

Example 13.6:

$$\text{minimise} \frac{1}{2} \left\| \begin{pmatrix} A \\ \sqrt{\alpha} I \end{pmatrix} x - \begin{pmatrix} b \\ 0 \end{pmatrix} \right\|_2^2 \tag{2}$$

Reminder: For g convex, $t_k = \frac{\gamma}{L}$ and $\gamma \in (0, 2]$:

$$g(x^{(k)}) - g^* \leq \frac{2L\|x^{(0)} - x^*\|_2^2}{4 + \gamma(2-\gamma)k} \tag{3}$$

For g strongly convex, $t_k = \frac{\gamma}{(L+\mu)}$ and $\gamma \in (0, 2]$:

$$g(x^{(k)}) - g(x^*) \leq \frac{L}{2} \left(\frac{\frac{L}{\mu} - 1}{\frac{L}{\mu} + 1} \right)^{2k} \|x^{(0)} - x^*\|_2^2 \tag{4}$$

Asymptotic behaviour

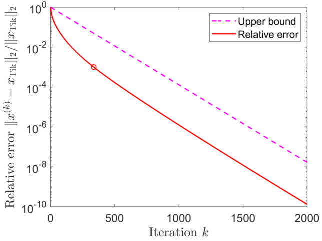

Figure 13.8. *Using the gradient method to solve the Tikhonov problem in Example 13.6. We show the relative error $\|\boldsymbol{x}^{(k)} - \boldsymbol{x}_{\mathrm{Tik}}\|_2/\|\boldsymbol{x}_{\mathrm{Tik}}\|_2$ versus the number of iterations k, together with the upper bound according to (13.37). A relative error of 10^{-3} is achieved after 336 iterations, as indicated by the circle.*

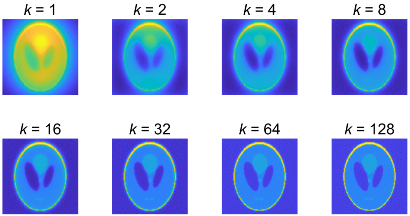

Figure 13.9. *Selected iterations from application of the gradient method to the Tikhonov problem in Example 13.6.*

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For a strongly convex function (4) is asymptotically a better bound.

Nonasymptotic behaviour

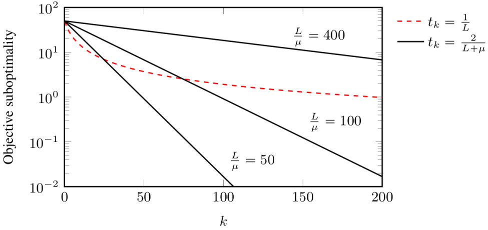

Figure 13.10. *Plot of the worst-case upper bounds* (13.22) *and* (13.28) *when* $L = 100$ *and* $\|\boldsymbol{x}^{(0)} - \boldsymbol{x}^\star\|_2 = 1$. *The latter bound depends on the ratio* L/μ.

[4]

Nonasymptotically, bound (4) is not necessarily better since it depends on $\frac{L}{\mu}$.

Outline

Exact line search

Reminder: Gradient method

$$x^{(k+1)} = x^{(k)} - t_k \nabla g(x^{(k)})$$

Goal: Find t_k such that the descent property holds $(g(x^{(k+1)}) < g(x^{(k)}))$

Possible solution: We define a step size that reduces our function optimally in the current iteration's search direction ("greedy algorithm")

$$t_k = \arg\min_{t>0} \{g(x^{(k)} - t \nabla g(x^{(k)}))\}$$

Problem: can be very inefficient (usage only in special scenarios)

Backtracking Line Search

- inexact line search method
- basis: **Armijo condition** for the gradient method with $\alpha \in]0, \frac{1}{2}[$

$$\boldsymbol{g(x^{(k)} - t\nabla g(x^{(k)})) \leq g(x^{(k)}) - \alpha t \|\nabla g(x^{(k)})\|_2^2}$$

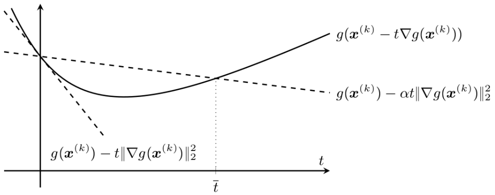

Figure 13.12. *Illustration of the Armijo condition* (13.38).

[4]

the reduction should be proportional to the step length and directional derivative

- **algorithm:**

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parameters: $\alpha \in]0, \frac{1}{2}[$, $\beta \in (0, 1)$ and $t = t_0 > 0$
while $g(x^{(k)} - t\nabla g(x^{(k)})) > g(x^{(k)}) - \alpha t \|\nabla g(x^{(k)})\|_2^2$ **do**
  $t \longleftarrow t\beta$
end while

- **parameter α:** trade-off between the allowed step length and the required decrease, often smaller values chosen to allow bigger step sizes

- **parameter β:** trade-off between number of iterations of the algorithm and step length

BB Step Sizes

- adaptive step sizes without line search and no guaranteed descent
- **two rules:** Let Δy and Δs be

$$\boldsymbol{\Delta y} = \nabla g(x^{(k)}) - \nabla g(x^{(k-1)}) \text{ and } \boldsymbol{\Delta s} = x^{(k)} - x^{(k-1)}$$

  - BB1 step size

$$\boldsymbol{t_k^{BB1}} = \alpha_k^{-1}, \quad \alpha_k = \arg\min_{\alpha}\{\|\Delta y - \alpha\Delta s\|_2^2\} = \frac{\Delta s^\top \Delta y}{\|\Delta s\|_2^2}$$

  - BB2 step size

$$\boldsymbol{t_k^{BB2}} = \arg\min_{\beta}\{\|\beta\Delta y - \Delta s\|_2^2\} = \frac{\Delta s^\top \Delta y}{\|\Delta y\|_2^2}$$

- The first step size must be evaluated using a different method!
- Convergence is guaranteed under certain conditions (e.g. strongly convex and quadratic functions)

Associate plot with step size method

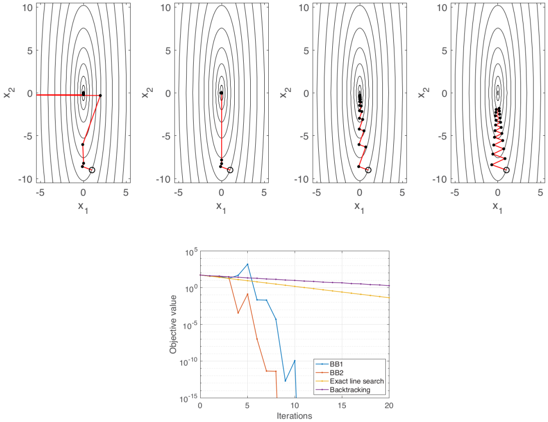

Figure 13.13. *Illustration of the gradient method applied to a quadratic function of two variables with the different step size rules. Each plot shows the initial point* $\boldsymbol{x}^{(0)}$ *(marked with a circle) and the first* 20 *iterations.*

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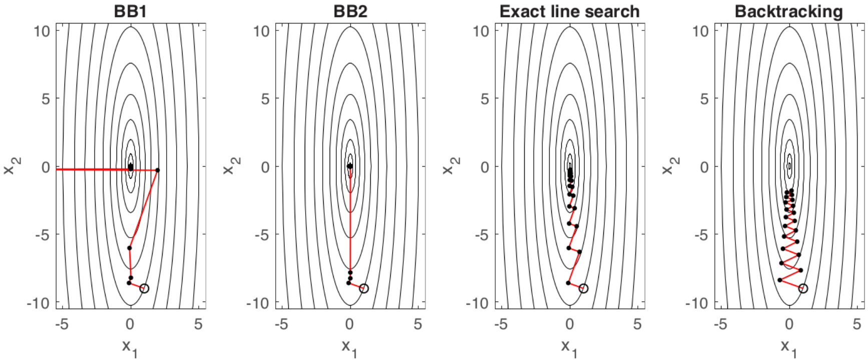
Associate plot with step size method



Stopping Criteria

As seen the gradient method converges to a stationary point under some conditions.

But do we always have to keep iterating until we reach a stationary point?

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No! Oftentimes it is sufficient to iterate until we reach a certain predefined termination condition.

Do you have any ideas for a simple stopping criterion?

Stopping Criteria

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But do we always have to keep iterating until we reach a stationary point?

No! Oftentimes it is sufficient to iterate until we reach a certain predefined termination condition.

Do you have any ideas for a simple stopping criterion?

For example:

$$\|\nabla g(x^{(k)})\|_2 \leq \epsilon$$

for a case-specific tolerance $\epsilon > 0$

Other options

$$\|x^{(k+1)} - x^{(k)}\|_2 \leq \epsilon \|x^{(k)}\|_2$$

which can be interpreted as the relative parameter change.

- Satisfied when $x^{(k+1)} \approx x^{(k)}$

Problem: scale invariance
Modification of variable: $x = Cy$ with $C \in \mathbb{R}^{n \times n}$ a nonsingular matrix

$$\tilde{g}(y) = g(Cy)$$

Then

$$\|\nabla g(x^{(k)})\|_2 \leq \epsilon$$

turns into

$$\|\nabla \tilde{g}(y^{(k)})\|_2 = \|C^\top \nabla g(x^{(k)})\|_2 \leq \epsilon$$

More options

- $g(x^{(k)}) - g(x^{(k+1)}) \leq \epsilon$
- limit the number of iterations

To be used with care!

Special case: strongly convex functions

Reminder:

$$g(x) - g(x^*) \leq \frac{1}{2\mu}\|\nabla g(x)\|_2^2 \qquad \|x^* - x\|_2 \leq \frac{2}{\mu}\|\nabla g(x)\|_2$$

- $\|\nabla g(x^{(k)})\|_2 \leq \sqrt{2\mu\epsilon_{obj}} \quad \Longrightarrow \quad g(x^{(k)}) - g(x^*) \leq \epsilon_{obj}$
- $\|\nabla g(x^{(k)})\|_2 \leq \frac{\mu\epsilon_{dist}}{2} \quad \Longrightarrow \quad \|x^{(k)} - x^*\|_2 \leq \epsilon_{dist}$

Outline

Constrained optimization problem

$$\text{minimise } \{g(x) + h(x)\}$$

with $g : \mathbb{R}^n \to \mathbb{R}$ convex and differentiable and $h : \mathbb{R}^n \to \mathbb{R} \cup \{-\infty, \infty\}$ closed convex

Let us look at the constrained optimization problem

$$\begin{gathered}\text{minimise } g(x) \\ \text{subject to } x \in C\end{gathered}$$

with $C \subseteq \mathbb{R}^n$ closed and convex

that we get for $h(x) = I_C(x)$

$$I_C(x) = \begin{cases} 0, & x \in C \\ \infty, & x \notin C \end{cases}$$

Proximal gradient methods

Proximal operator

$$prox_{th}(x) = \arg\min_y \left\{ th(y) + \frac{1}{2}\|y - x\|_2^2 \right\}$$

If g Lipschitz continuous with constant L

$$\psi(y; x) = g(x) + \nabla g(x)^\top (y - x) + \frac{L}{2}\|y - x\|_2^2 + h(y)$$

via majorization minimization:

$$\begin{aligned} x^{(k+1)} &= \arg\min_y \{\psi(y; x^{(k)})\} \\ &= \arg\min_y \{h(y) + \frac{L}{2}\|y - (x^{(k)} - (1/L)\nabla g(x^{(k)}))\|_2^2\} \\ &= prox_{th}(x^{(k)} - t\nabla g(x^{(k)})) \qquad \text{with } t = 1/L \end{aligned}$$

$x^{(0)} =$ initial vector

$t = 1/L$, where L is a Lipschitz constant associated with ∇g

for k=0,1,2,... **do**

$x^{(k+1)} = prox_{th}(x^{(k)} - t\nabla g(x^{(k)}))$

end for

algorithm:

$x^{(0)} =$ initial vector

$t = 1/L$, where L is a Lipschitz constant associated with ∇g

for k=0,1,2,... **do**

$$x^{(k+1)} = prox_{th}(x^{(k)} - t\nabla g(x^{(k)}))$$

end for

What would the running-time cost of this algorithm depend on?

algorithm:

$x^{(0)} =$ initial vector

$t = 1/L$, where L is a Lipschitz constant associated with ∇g

for k=0,1,2,... **do**

$$x^{(k+1)} = prox_{th}(x^{(k)} - t\nabla g(x^{(k)}))$$

end for

What would the running-time cost of this algorithm depend on?

The cost of the evaluation of the proximal operator

algorithm:

$x^{(0)} =$ initial vector
$t = 1/L$, where L is a Lipschitz constant associated with ∇g
for k=0,1,2,... **do**
$\quad x^{(k+1)} = prox_{th}(x^{(k)} - t\nabla g(x^{(k)}))$
end for

What would the running-time cost of this algorithm depend on?

The cost of the evaluation of the proximal operator

- in general same worst-case suboptimality bound as the gradient method **however**

  if g is strongly convex, the PG method with $t = 1/L$ converges linearly

Accelerated proximal gradient method (FISTA)

$x^{(0)} =$ initial vector
$y = x^{(0)}$
$t_0 = 1$
for k=0,1,2,... **do**
$\quad x^{(k+1)} = prox_{(1/L)h}(y - (1/L)\nabla g(y))$
$\quad t_{k+1} = \frac{1+\sqrt{1+4t_k^2}}{2}$
$\quad y = x^{(k+1)} + \frac{t_k - 1}{t_{k+1}}(x^{(k+1)} - x^{(k)})$
end for

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end for

- worst-case suboptimality $f(x^{(k)}) - f(x^*) = O(\frac{1}{k^2})$ (sublinear)
- not a descent method

Visualization

Problem:

$$\text{minimize } \{\tfrac{1}{2}\|b - Ax\|_2^2 + \tfrac{\gamma}{2}\|x\|_2^2\}$$
$$\text{subject to } x_i \geq 0, \quad i = 1, \ldots, n$$

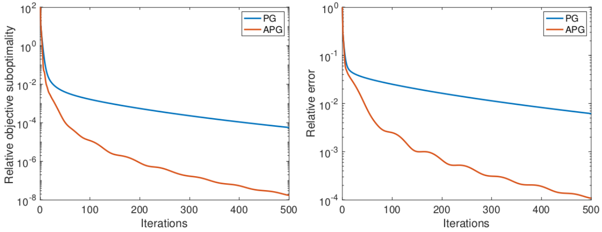

Figure 13.16. *Relative objective suboptimality* $(f(\boldsymbol{x}^{(k)}) - f(\boldsymbol{x}^\star))/|f(\boldsymbol{x}^\star)|$ *(left) and relative error* $\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^\star\|_2/\|\boldsymbol{x}^\star\|_2$ *(right) for the PG and APG methods.*

[4]

Outline

Regularized least-squares problems

$$\text{minimise } \{\tfrac{1}{2}\|b - Ax\|_2^2 + \alpha J(x)\}$$

$$\text{subject to } x \in C$$

$x \in \mathbb{R}^n$, $\alpha > 0$ as the regularization parameter, C as a closed, convex set and a closed, convex regularization function $J(x)$

- bicriterion optimization function:
  - minimise the residual norm
  - minimise $J(x)$

Here our solution depends on α!

The trade-off curve

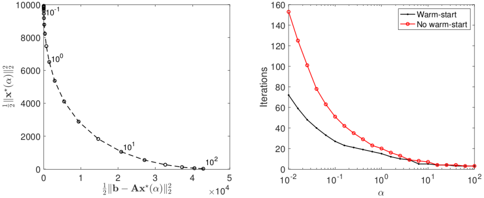

Figure 13.17. *Trade-off curve (left) and the number of iterations using a warm-start approach (right).*

[4]

- we solve the problem for different regularization parameters
- $x^*(\alpha)$ is a solution to the problem with parameter α

The trade-off curve

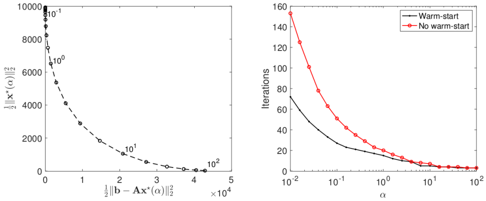

Figure 13.17. *Trade-off curve (left) and the number of iterations using a warm-start approach (right).*

[4]

- we solve the problem for different regularization parameters
- $x^*(\alpha)$ is a solution to the problem with parameter α
- warm start: if α close to α' often $x^*(\alpha)$ is close to $x^*(\alpha')$ too!
  How could we use this to speed things up?

The trade-off curve

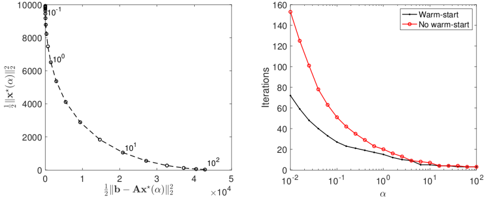

Figure 13.17. *Trade-off curve (left) and the number of iterations using a warm-start approach (right).*

[4]

- we solve the problem for different regularization parameters
- $x^*(\alpha)$ is a solution to the problem with parameter α
- warm start: if α close to α' often $x^*(\alpha)$ is close to $x^*(\alpha')$ too!
  How could we use this to speed things up?
  - use $x^*(\alpha)$ as the initial guess for solving $x^*(\alpha')$

TV regularisation

Goal: consider gradient method for nonsmooth functions

We will look at anisotropic TV of an $M \times N$ image with $x \in \mathbb{R}^{MN}$ as our representation of the image:

$$TV_a(x) = \|Dx\|_1, \qquad D = \begin{pmatrix} I_N \otimes D_M \\ D_N \otimes I_M \end{pmatrix}$$

We want to apply the gradient method to our regularization problem.

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The function is convex but not differentiable

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We want to apply the gradient method to our regularization problem.
What could be the problem?

The function is convex but not differentiable

Solution:
smoothing technique $\rightarrow$ approximate 1-norm by a continuously differentiable function

$$\|y\|_1 = \sum_{i=1}^{n} |y_i| \approx \sum_{i=1}^{n} \phi_\delta(y_i)$$

Possible approximating functions:

1. Lifting:

$$\phi_\delta(\tau) = \sqrt{\tau^2 + \delta^2} = \left\| \begin{pmatrix} \tau \\ \delta \end{pmatrix} \right\|_2$$

   with $\delta > 0$

2. Huber penalty function scaled by $\frac{1}{\delta}$:

$$\phi_\delta(\tau) = \sup_{|v| \le 1} \left\{ \tau v - \frac{\delta}{2} v^2 \right\} = \begin{cases} \frac{\tau^2}{2\delta}, & |\tau| \le \delta \\ |\tau| - \frac{\delta}{2}, & |\tau| > \delta \end{cases}$$

   - derivative is not differentiable!

3. Based on $|\tau| = \max(-\tau, \tau)$

$$\phi_\delta(\tau) = \delta \log(e^{\tau/\delta} + e^{-\tau/\delta})$$

with $\delta > 0$ controlling the quality of the approximation
Problem: the function can cause numerical overflow
Solution: equivalent approximation

$$\phi_\delta(\tau) = |\tau| + \delta \log(1 + e^{-2|\tau|/\delta})$$

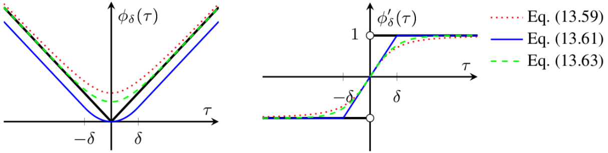


Figure 13.18. *Smooth approximations to the absolute value function.*

[4]

Comparison

(Very similar approaches can be done for the 2-norm of the isotropic TV.)

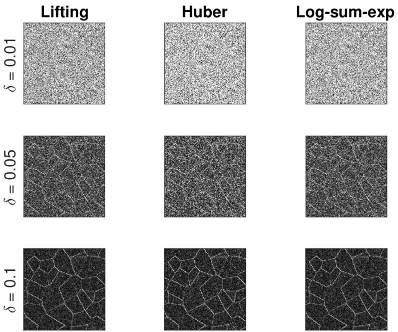


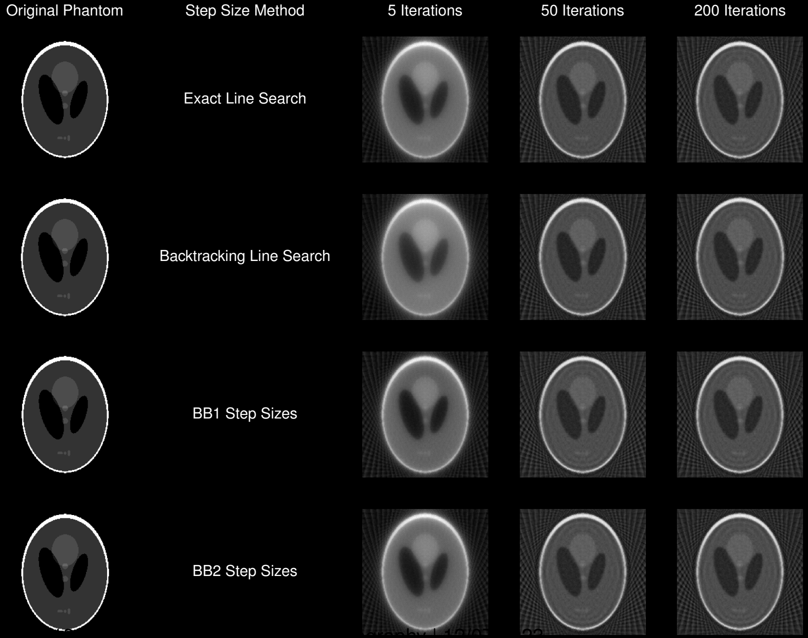
Figure 13.19. *Pixelwise magnitude of* $\nabla \mathrm{TV}_{\mathrm{i}}(\boldsymbol{x})$ *for different values of the smoothing parameter* δ *and where* $\boldsymbol{x}$ *represents the "grains" phantom from AIR Tools* II *with additive noise.*

[4]

Implementation

Gradient method with variable step size

```matlab
function [] = gradientmethod(step_size_method, maxiterations)
%function that uses the gradient method to approximate the least-squares solution of 1/2||Ax-b||²_2
%:param step_size_method: choice of step sizes methods between 'exact line search', 'backtracking line
%search', 'BB1 step sizes' and 'BB2 step sizes'
%:param maxiterations: maximum number of iterations

%set default step size method
if isempty(step_size_method)
   step_size_method = 'exact line search';
end

%test example created using AIR Tools II,
%generation of a 2-D parallel-beam tomography problem
N = 200; theta = 0:5:179; p = 2*N;
[A, b, x] = paralleltomo(N,theta,p);

%define starting point
x_0 = zeros(N*N, 1);

%define tolerance
epsilon = 1e-3;

%define provisory step size
t = 0.05;

%define current number of iterations
iteration = 0;

%define starting vector
currentX = x_0;
x_minus1 = zeros(N*N, 1);

%define objective function
f = @(x) (1/2) * (norm(A*x-b)^2);

grad_f = grad(currentX, A, b);

while and(norm(grad_f)>=epsilon, iteration<maxiterations)
    %define the correct step size depending on parameter 'step_size_method'
    switch step_size_method
        case 'exact line search'
            t = norm(grad(currentX, A, b))^2/norm(A*grad(currentX, A , b))^2;
        case 'backtracking line search'
            t = backtracking(currentX, f, A, b);
        case 'BB1 step sizes'
            if(iteration == 0)
               t = backtracking(currentX, f, A, b);
            else
               t = bb(currentX, x_minus1, A, b, 1);
            end
        case 'BB2 step sizes'
            if(iteration == 0)
               t = backtracking(currentX,f, A ,b);
            else
               t = bb(currentX, x_minus1, A, b, 2);
            end
        otherwise
    end

    %calculate new x
    newX = currentX- t*grad_f;

    if ~isfinite(newX)
        error('x is inf or NaN')
    end

    %update values
    iteration = iteration + 1;
    x_minus1 = currentX;
    currentX = newX;
    grad_f = grad(currentX, A, b);
end

%plot original phantom and result
x = reshape(x,N,N);
subplot(2, 2, 1);
imshow(x, []);
title('Original Phantom');

x_grad = reshape(currentX, [N, N]);
subplot(2, 2, 2);
imshow(x_grad, []);
title(sprintf('Approximated phantom in %d iterations', iteration));

%calculates gradient at x
function g = grad(x, A, b)
g = A'*(A*x-b);

%backtracking line search with alpha = 1e-2 and beta = 0.5
function t_k = backtracking(x, func, A, b)
t_k = 1;
alpha = 1e-2;
beta = 0.5;
while func(x-t_k*grad(x, A, b)) > func(x)-alpha * t_k * norm(grad(x, A ,b))^2
    t_k = t_k * beta;
end

%BB step sizes
%calculates the BB1 or BB2 step size depending on parameter 'version'
function t_k = bb(x, x_minus1, A, b, version)
delta_y = grad(x, A, b) - grad(x_minus1, A , b);
delta_s = x - x_minus1;
if(version == 1)
    alpha_k = (delta_s' * delta_y) / norm(delta_s)^2;
    t_k = 1 / alpha_k;
else
    t_k = (delta_s' * delta_y) / norm(delta_y)^2;
end
```


Original Phantom
Step Size Method
5 Iterations
50 Iterations
200 Iterations
Exact Line Search
Backtracking Line Search
BB1 Step Sizes
BB2 Step Sizes

References

[1] Prof. Dr. Hans-Joachim Bungartz. *Lecture notes in Modeling and Simulation*.

[2] *EPFL lecture notes: Chapter 4 Unconstrained optimization*. Apr. 2022.

[3] “Line Search Methods”. In: *Numerical Optimization*. New York, NY: Springer New York, 2006, pp. 30–65. ISBN: 978-0-387-40065-5. DOI: 10.1007/978-0-387-40065-5_3. URL: https://doi.org/10.1007/978-0-387-40065-5_3.

[4] Jakob Sauer Jørgensen William R. B. Lionheart Per Christian Hansen. “Chapter 13: Optimization Methods for Tomography”. In: *Computed Tomography: Algorithms, Insight, and Just Enough Theory*, pp. 275–315.