Truncated Newton Method

- approximate Newton methods
- truncated Newton methods
- truncated Newton interior-point methods

Newton's method

- minimize convex $f : \mathbf{R}^n \to \mathbf{R}$
- Newton step $\Delta x_{\rm nt}$ found from (SPD) Newton system

$$\nabla^2 f(x) \Delta x_{\rm nt} = -\nabla f(x)$$

  using Cholesky factorization

- backtracking line search on function value $f(x)$ or norm of gradient $\|\nabla f(x)\|$
- stopping criterion based on Newton decrement $\lambda^2/2 = -\nabla f(x)^T \Delta x_{\rm nt}$ or norm of gradient $\|\nabla f(x)\|$

Approximate or inexact Newton methods

- use as search direction an *approximate solution* Δx of Newton system
- idea: no need to compute $\Delta x_{\rm nt}$ exactly; only need a good enough search direction
- number of iterations may increase, but if effort per iteration is smaller than for Newton, we win
- examples:
  - solve $\hat{H}\Delta x = -\nabla f(x)$, where $\hat{H}$ is diagonal or band of $\nabla^2 f(x)$
  - factor $\nabla^2 f(x)$ every k iterations and use most recent factorization

Truncated Newton methods

- approximately solve Newton system using CG or PCG, terminating (sometimes way) early
- also called *Newton-iterative methods*; related to limited memory Newton (or BFGS)
- total effort is measured by cumulative sum of CG steps done
- for good performance, need to tune CG stopping criterion, to use just enough steps to get a good enough search direction
- less reliable than Newton's method, but (with good tuning, good preconditioner, fast $z \rightarrow \nabla^2 f(x) z$ method, and some luck) can handle very large problems

Truncated Newton method

- backtracking line search on $\|\nabla f(x)\|$
- typical CG termination rule: stop after $N_{\max}$ steps or

$$\eta = \frac{\|\nabla^2 f(x)\Delta x + \nabla f(x)\|}{\|\nabla f(x)\|} \leq \epsilon_{\rm pcg}$$

- with simple rules, $N_{\max}$, $\epsilon_{\rm pcg}$ are constant
- more sophisticated rules adapt $N_{\max}$ or $\epsilon_{\rm pcg}$ as algorithm proceeds (based on, *e.g.*, value of $\|\nabla f(x)\|$, or progress in reducing $\|\nabla f(x)\|$)

  $\eta = \min(0.1, \|\nabla f(x)\|^{1/2})$ guarantees (with large $N_{\max}$) superlinear convergence

CG initialization

- we use CG to approximately solve $\nabla^2 f(x)\Delta x + \nabla f(x) = 0$
- if we initialize CG with $\Delta x = 0$
  - after one CG step, Δx points in direction of negative gradient (so, $N_{\mathrm{max}} = 1$ results in gradient method)
  - all CG iterates are descent directions for f
- another choice: initialize with $\Delta x = \Delta x_{\mathrm{prev}}$, the previous search step
  - initial CG iterates need not be descent directions
  - but can give advantage when N_{max} is small

- simple scheme: if $\Delta x_{\rm prev}$ is a descent direction ($\Delta x_{\rm prev}^T \nabla f(x) < 0$) start CG from

$$\Delta x = \frac{-\Delta x_{\rm prev}^T \nabla f(x)}{\Delta x_{\rm prev}^T \nabla^2 f(x) \Delta x_{\rm prev}} \Delta x_{\rm prev}$$

otherwise start CG from $\Delta x = 0$

Example

ℓ_2-regularized logistic regression

$$\text{minimize} \quad f(w) = (1/m)\sum_{i=1}^m \log\left(1+\exp(-b_i x_i^T w)\right) + \sum_{i=1}^n \lambda_i w_i^2$$

- variable is $w \in \mathbf{R}^n$
- problem data are $x_i \in \mathbf{R}^n$, $b_i \in \{-1, 1\}$, $i = 1, \ldots, m$, and regularization parameter $\lambda \in \mathbf{R}_+^n$
- n is number of features; m is number of samples/observations

Hessian and gradient

$$\nabla^2 f(w) = A^T D A + 2\Lambda, \qquad \nabla f(w) = A^T g + 2\Lambda w$$

where

$$A = [b_1 x_1 \cdots b_m x_m]^T, \quad D = \mathbf{diag}(h), \quad \Lambda = \mathbf{diag}(\lambda)$$

$$\begin{aligned} g_i &= -(1/m)/(1 + \exp(Aw)_i) \\ h_i &= (1/m)\exp(Aw)_i/(1 + \exp(Aw)_i)^2 \end{aligned}$$

we never form $\nabla^2 f(w)$; we carry out multiplication $z \to \nabla^2 f(w) z$ as

$$\nabla^2 f(w) z = \left(A^T D A + 2\Lambda\right) z = A^T \left(D(Az)\right) + 2\Lambda z$$

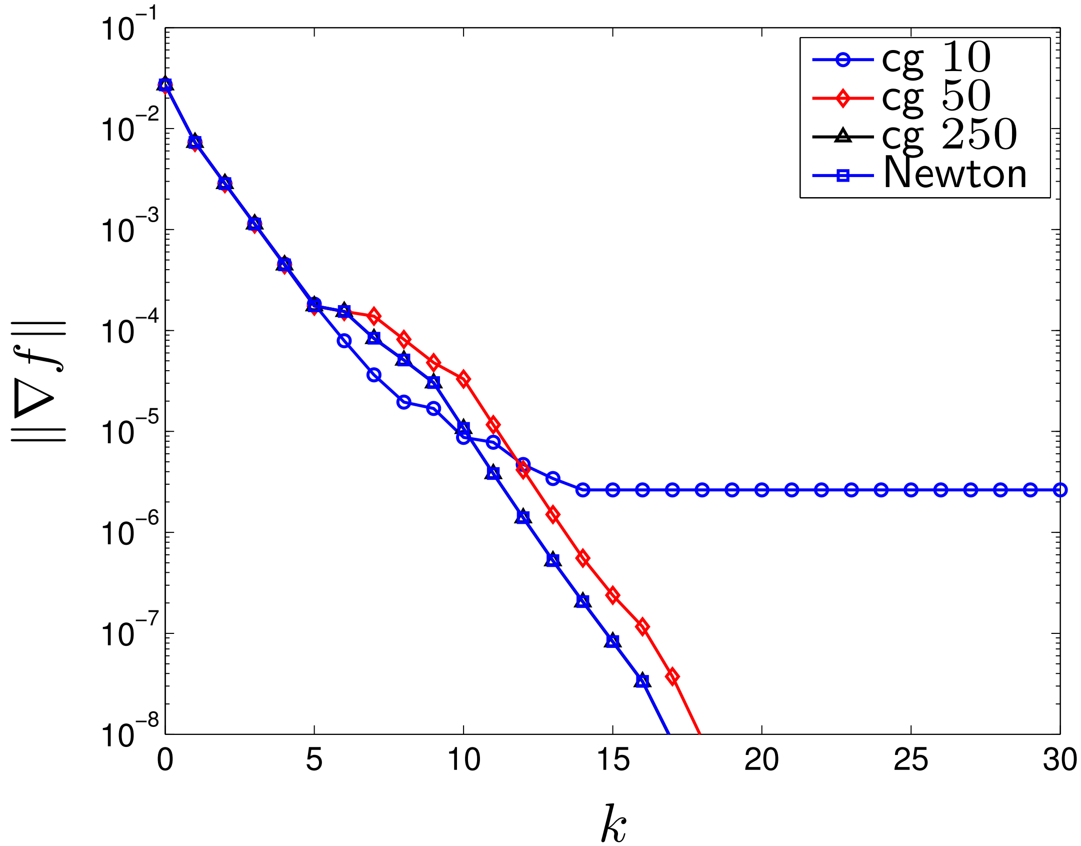
Problem instance

- $n = 10000$ features, $m = 20000$ samples (10000 each with $b_i = \pm 1$)
- x_i have random sparsity pattern, with around 10 nonzero entries
- nonzero entries in x_i drawn from $\mathcal{N}(b_i, 1)$
- $\lambda_i = 10^{-8}$
- around 500000 nonzeros in $\nabla^2 f$, and 30M nonzeros in Cholesky factor

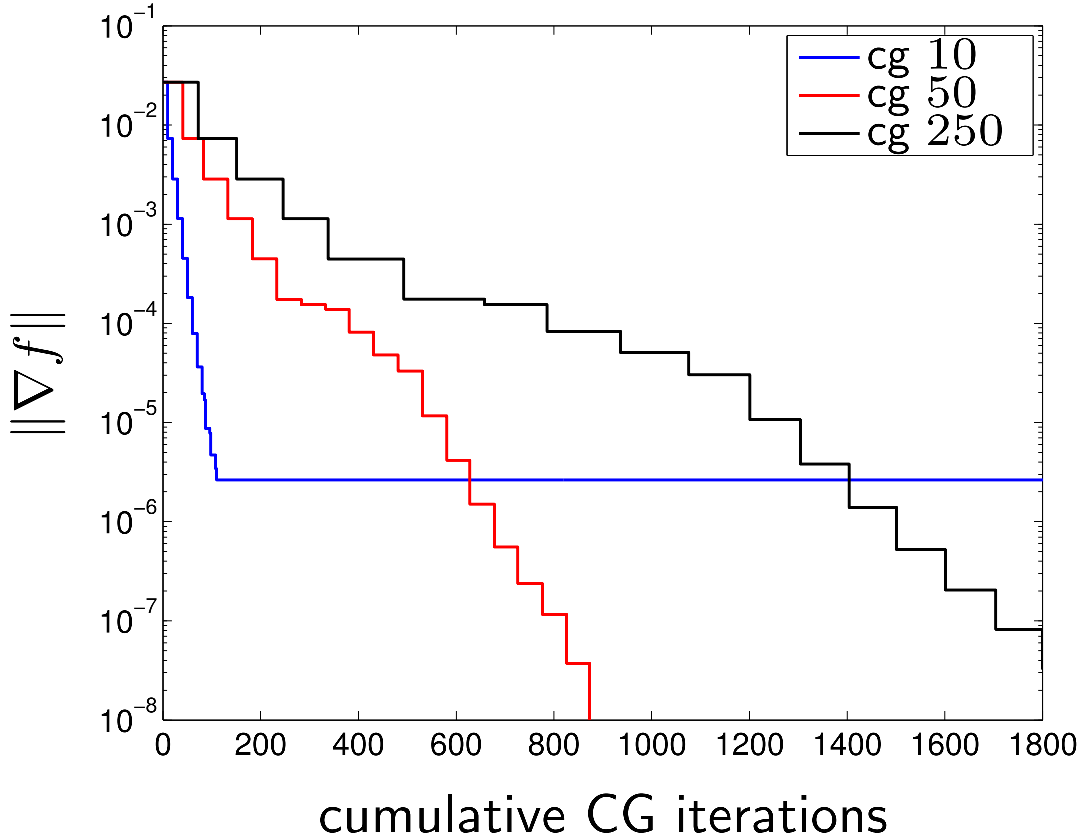
Methods

- Newton (using Cholesky factorization of $\nabla^2 f(w)$)
- truncated Newton with $\epsilon_{\rm cg} = 10^{-4}$, $N_{\rm max} = 10$
- truncated Newton with $\epsilon_{\rm cg} = 10^{-4}$, $N_{\rm max} = 50$
- truncated Newton with $\epsilon_{\rm cg} = 10^{-4}$, $N_{\rm max} = 250$

Convergence versus iterations



Convergence versus cumulative CG steps



- convergence of exact Newton, and truncated Newton methods with $N_{\max} = 50$ and 250 essentially the same, in terms of iterations

- in terms elapsed time (and memory!), truncated Newton methods far better than Newton

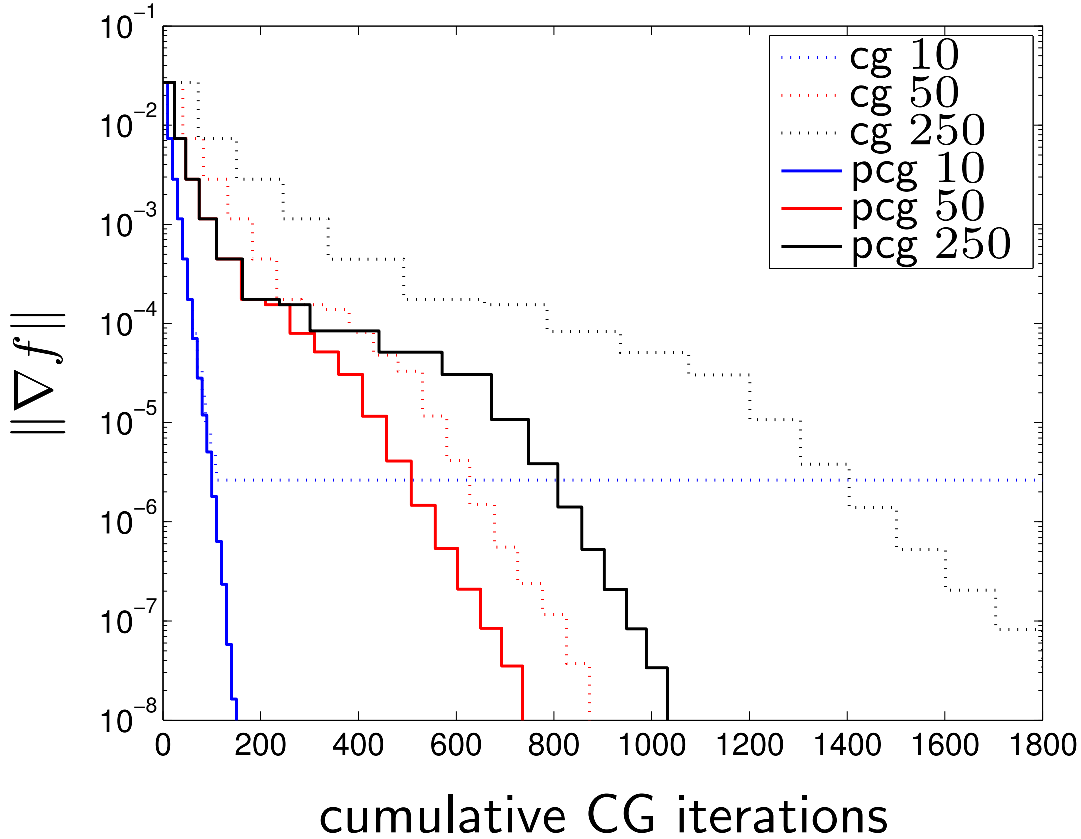
- truncated Newton with $N_{\max} = 10$ seems to jam near $\|\nabla f(w)\| \approx 10^{-6}$

- times (on AMD270 2GHz, 12GB, Linux) in sec:

method	$\|\nabla f(w)\| \leq 10^{-5}$	$\|\nabla f(w)\| \leq 10^{-8}$
Newton	1600	2600
cg 10	4	—
cg 50	17	26
cg 250	35	54

Truncated PCG Newton method

approximate search direction found via diagonally preconditioned PCG



- diagonal preconditioning allows $N_{\max} = 10$ to achieve high accuracy; speeds up other truncated Newton methods

- times:

method	$\|\nabla f(w)\| \leq 10^{-5}$	$\|\nabla f(w)\| \leq 10^{-8}$
Newton	1600	2600
cg 10	4	—
cg 50	17	26
cg 250	35	54
pcg 10	3	5
pcg 50	13	24
pcg 250	23	34

- speedups of $1600:3$, $2600:5$ are not bad (and we really didn't do much tuning . . .)

Extensions

- can extend to (infeasible start) Newton's method with equality constraints
- since we don't use exact Newton step, equality constraints not guaranteed to hold after finite number of steps (but $\|r_p\| \to 0$)
- can use for barrier, primal-dual methods

Truncated Newton interior-point methods

- use truncated Newton method to compute search direction in interior-point method
- tuning PCG parameters for optimal performance on a given problem class is tricky, since linear systems in interior-point methods often become ill-conditioned as algorithm proceeds
- but can work well (with luck, good preconditioner)

Network rate control

rate control problem

$$\begin{array}{ll} \text{minimize} & -U(f) = -\sum_{j=1}^n \log f_j \\ \text{subject to} & Rf \preceq c \end{array}$$

with variable f

- $f \in \mathbf{R}^n_{++}$ is vector of flow rates
- $U(f) = \sum_{j=1}^n \log f_j$ is flow utility
- $R \in \mathbf{R}^{m \times n}$ is route matrix ($R_{ij} \in \{0, 1\}$)
- $c \in \mathbf{R}^m$ is vector of link capacities

Dual rate control problem

dual problem

$$\begin{array}{ll} \text{maximize} & g(\lambda) = n - c^T\lambda + \sum_{i=1}^m \log(r_i^T\lambda) \\ \text{subject to} & \lambda \succeq 0 \end{array}$$

with variable $\lambda \in \mathbf{R}^m$

duality gap

$$\begin{aligned} \eta &= -U(f) - g(\lambda) \\ &= -\sum_{j=1}^n \log f_j - n + c^T\lambda - \sum_{i=1}^m \log(r_i^T\lambda) \end{aligned}$$

Primal-dual search direction (BV §11.7)

primal-dual search direction Δf, $\Delta\lambda$ given by

$$(D_1 + R^T D_2 R)\Delta f = g_1 - (1/t)R^T g_2, \qquad \Delta\lambda = D_2 R\Delta f - \lambda + (1/t)g_2$$

where $s = c - Rf$,

$$D_1 = \mathbf{diag}(1/f_1^2, \ldots, 1/f_n^2), \qquad D_2 = \mathbf{diag}(\lambda_1/s_1, \ldots, \lambda_m/s_m)$$

$$g_1 = (1/f_1, \ldots, 1/f_n), \qquad g_2 = (1/s_1, \ldots, 1/s_m)$$

Truncated Newton primal-dual algorithm

primal-dual residual:

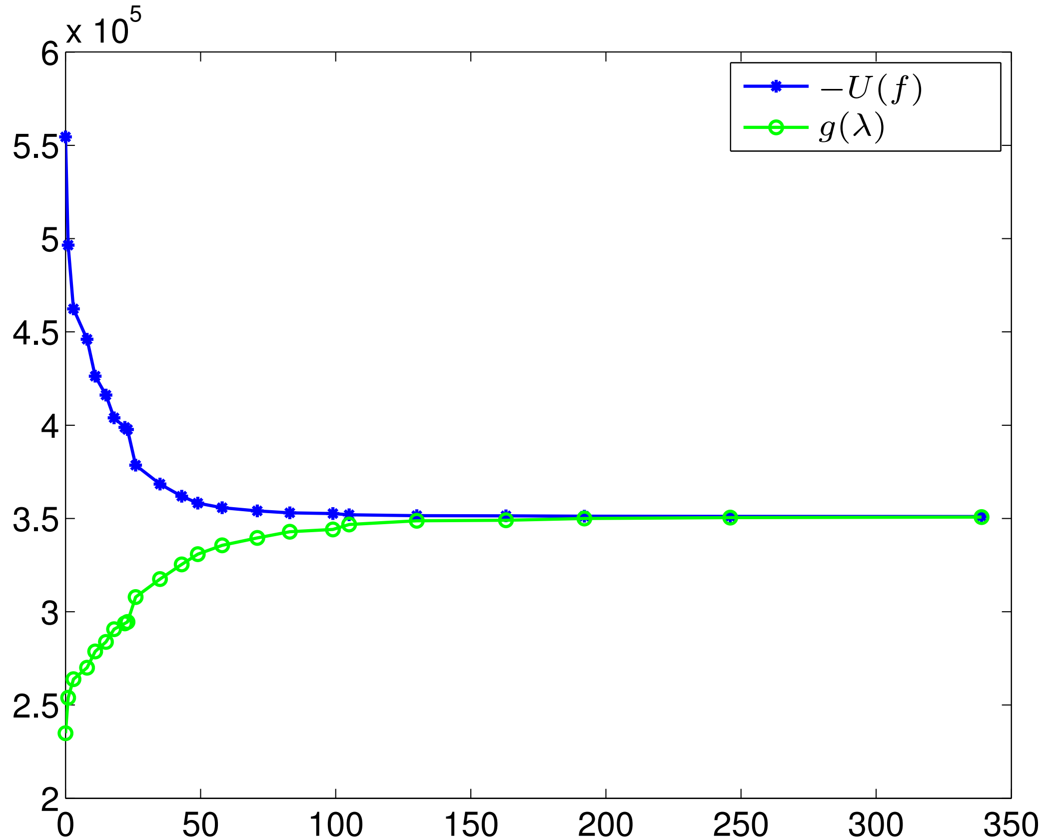
$$r = (r_{\text{dual}}, r_{\text{cent}}) = \left(-g_2 + R^T\lambda,\ \mathbf{diag}(\lambda)s - (1/t)\mathbf{1}\right)$$

given f with $Rf \prec c$; $\lambda \succ 0$
while $\eta/g(\lambda) > \epsilon$
    $t := \mu m/\eta$
    compute Δf using PCG as approximate solution of
        $(D_1 + R^T D_2 R)\Delta f = g_1 - (1/t)R^T g_2$
    $\Delta\lambda := D_2 R\Delta f - \lambda + (1/t)g_2$
    carry out line search on $\|r\|_2$, and update:
        $f := f + \gamma\Delta f$, $\lambda := \lambda + \gamma\Delta\lambda$

- problem instance
  - $m = 200000$ links, $n = 100000$ flows
  - average of 12 links per flow, 6 flows per link
  - capacities random, uniform on $[0.1, 1]$

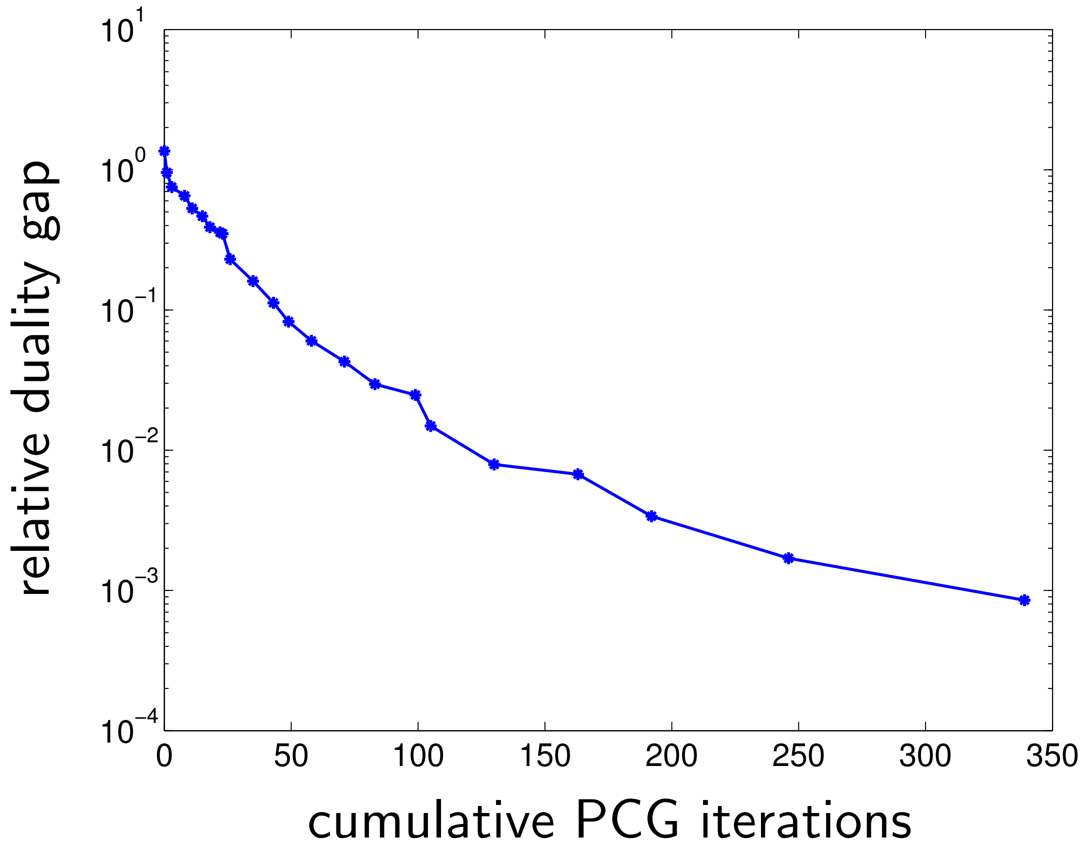
- algorithm parameters
  - truncated Newton with $\epsilon_{\mathrm{cg}} = \min(0.1, \eta/g(\lambda))$, $N_{\max} = 200$ ($N_{\max}$ never reached)
  - diagonal preconditioner
  - warm start
  - $\mu = 2$
  - $\epsilon = 0.001$ ($i.e.$, solve to guaranteed 0.1% suboptimality)

Primal and dual objective evolution

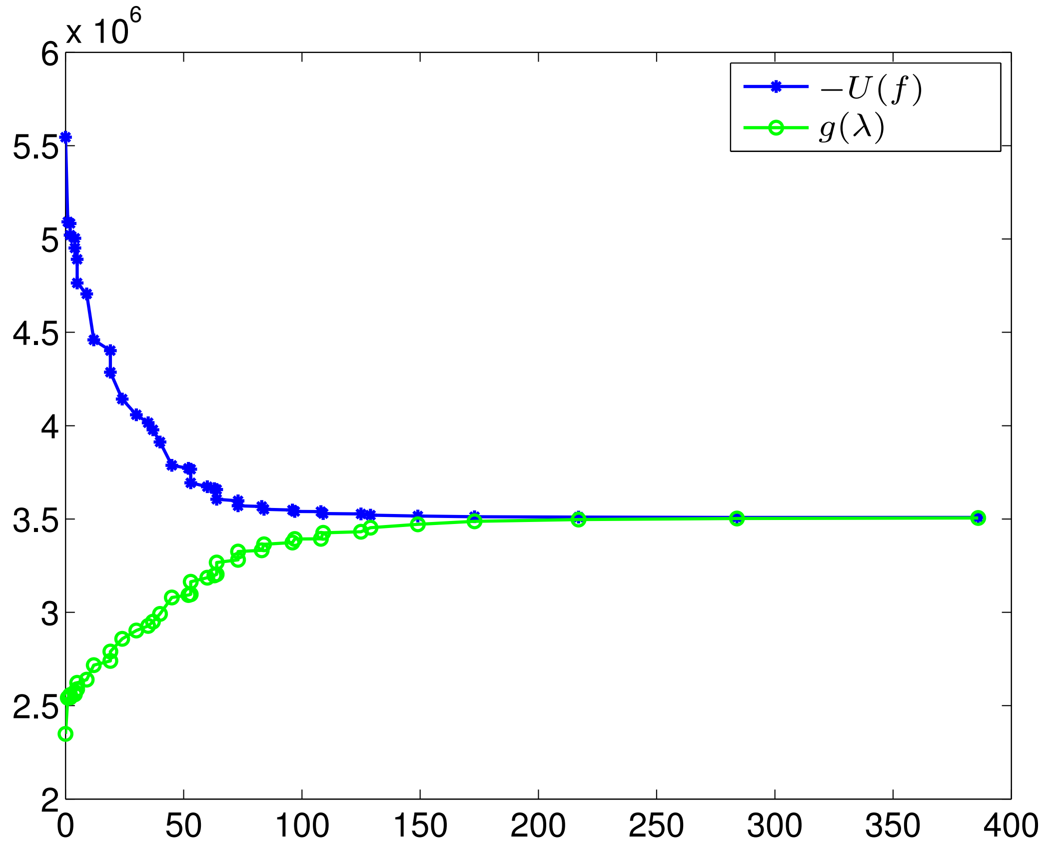


cumulative PCG iterations

Relative duality gap evolution



Primal and dual objective evolution ($n = 10^6$)



cumulative PCG iterations

Relative duality gap evolution ($n = 10^6$)