Proximal Newton-type methods for minimizing composite functions

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Minimizing composite functions

Proximal Newton-type methods

Inexact search directions

Computational experiments

Minimizing composite functions

$$\underset{x}{\text{minimize}}\ f(x) := g(x) + h(x)$$

- g and h are convex functions
- g is continuously differentiable, and its gradient ∇g is Lipschitz continuous
- h is not necessarily everywhere differentiable, but its *proximal mapping* can be evaluated efficiently

Minimizing composite functions: Examples

ℓ_1-regularized logistic regression:

$$\min_{w \in \mathbf{R}^p} \; \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-y_i w^T x_i)) + \lambda \|w\|_1.$$

Sparse inverse covariance:

$$\min_{\Theta} \; -\text{logdet}(\Theta) + \mathbf{tr}(S\Theta) + \lambda \|\Theta\|_1$$

Minimizing composite functions: Examples

Graphical Model Structure Learning

$$\min_{\theta} \; - \sum_{(r,j)\in E} \theta_{rj}(x_r, x_j) + \log Z(\theta) + \lambda \sum_{(r,j)\in E} \|\theta_{rj}\|_F.$$

Multiclass Classification:

$$\min_{W} \sum_{i=1}^{n} - \log \left(\frac{e^{w_{y_i}^T x_i}}{\sum_k e^{w_k^T x_i}} \right) + \|W\|_*$$

Minimizing composite functions: Examples

Arbitrary convex program

$$\min_x \ g(x) + \mathbf{1}_C(x)$$

Equivalent to solving

$$\min_{x \in C} \ g(x)$$

The proximal mapping

The proximal mapping of a convex function h is

$$\operatorname{prox}_h(x) = \arg\min_y \; h(y) + \frac{1}{2}\|y - x\|_2^2 .$$

- $\operatorname{prox}_h(x)$ exists and is unique for all $x \in \operatorname{dom} h$
- proximal mappings generalize projections onto convex sets

Example: soft-thresholding: Let $h(x) = \|x\|_1$. Then

$$\operatorname{prox}_{t\|\cdot\|_1}(x) = \operatorname{sign}(x) \cdot \max\{|x| - t, 0\}.$$

The proximal gradient step

$$
\begin{aligned}
x_{k+1} &= \text{prox}_{t_k h}\left(x_k - t_k \nabla g(x_k)\right) \\
&= \arg\min_y h(y) + \frac{1}{2t_k}\left\|y - (x_k - t_k \nabla g(x_k))\right\|^2 \\
&= x_k - t_k G_{t_k f}(x_k)
\end{aligned}
$$

- $G_{t_k f}(x_k)$ minimizes a simple quadratic model of f:

$$
-t_k G_{t_k f}(x_k) = \arg\min_d \; \nabla g(x_k)^T d + \underbrace{\frac{1}{2t_k}\|d\|_2^2}_{\text{simple quadratic}} + h(x_k + d).
$$

- $G_f(x)$ can be thought of as a generalized gradient of $f(x)$. Simplifies to the gradient descent on $g(x)$ when $h = 0$.

The proximal gradient method

Algorithm 1 The proximal gradient method

Require: starting point $x_0 \in \operatorname{dom} f$

1: **repeat**

2: Compute a *proximal gradient step*:
$$G_{t_k f}(x_k) = \frac{1}{t_k}\left(x_k - \operatorname{prox}_{t_k h}(x_k - t_k \nabla g(x_k))\right).$$

3: Update: $x_{k+1} \leftarrow x_k - t_k G_{t_k f}(x_k)$.

4: **until** stopping conditions are satisfied.

Proximal Newton-type methods

Main idea: use a local quadratic model (in lieu of a simple quadratic model) to account for the curvature of g:

$$\Delta x_k := \arg\min_d \nabla g(x_k)^T d + \underbrace{\frac{1}{2} d^T H_k d}_{\text{local quadratic}} + h(x_k + d).$$

Solve the above subproblem and update

$$x_{k+1} = x_k + t_k \Delta x_k.$$

A generic proximal Newton-type method

Algorithm 2 A generic proximal Newton-type method

Require: starting point $x_0 \in \operatorname{dom} f$

repeat

    Choose an approximation to the Hessian H_k.

    Solve the subproblem for a search direction:

    $$\Delta x_k \leftarrow \arg\min_d \nabla g(x_k)^T d + \frac{1}{2} d^T H_k d + h(x_k + d).$$

    Select t_k with a backtracking line search.

    Update: $x_{k+1} \leftarrow x_k + t_k \Delta x_k$.

until stopping conditions are satisfied.

Why are these proximal?

Definition (Scaled proximal mappings)

Let h be a convex function and H, a positive definite matrix. Then the scaled proximal mapping of h at x is defined to be

$$\text{prox}_h^H(x) = \arg\min_y \; h(y) + \frac{1}{2}\|y - x\|_H^2.$$

The proximal Newton update is

$$x_{k+1} = \text{prox}_h^{H_k}\left(x_k - H_k^{-1}\nabla g(x_k)\right)$$

and analogous to the proximal gradient update

$$x_{k+1} = \text{prox}_{h/L}\left(x_k - \frac{1}{L}\nabla g(x_k)\right)$$

$\Delta x = 0$ if and only if x minimizes $f = g + h$.

A classical idea

Traces back to:

- Projected Newton-type methods
- Generalized proximal point methods

Popular methods tailored to specific problems:

- `glmnet`: lasso and elastic-net regularized generalized linear models
- LIBLINEAR: ℓ_1-regularized logistic regression
- QUIC: sparse inverse covariance estimation

Choosing an approximation to the Hessian

1. **Proximal Newton method:** use Hessian $\nabla^2 g(x_k)$
2. **Proximal quasi-Newton methods:** build an approximation to $\nabla^2 g(x_k)$ using changes in ∇g:

$$H_{k+1}(x_{k+1} - x_k) = \nabla g(x_k) - \nabla g(x_{k+1})$$

3. If problem is large, use limited memory versions of quasi-Newton updates (e.g. L-BFGS)
4. Diagonal+rank 1 approximation to the Hessian.

Bottom line: Most strategies for choosing Hessian approximations Newton-type methods also work for proximal Newton-type methods

Theoretical results

Take home message:

The convergence of proximal Newton methods parallel those of the regular Newton Method.

Global convergence:

- smallest eigenvalue of H_k's bounded away from zero

Quadratic convergence (prox-Newton method):

- Quadratic convergence: $\|x_k - x^\star\|^2 \le c^{2^k}$ or $\log\log\frac{1}{\epsilon}$ iterations to achieve ϵ accuracy.
- Assumptions: g is strongly convex, and $\nabla^2 g$ is Lipschitz continuous

Superlinear convergence (prox-quasi-Newton methods):

- BFGS, SR1, and many other hessian approximations. Dennis-More condition $\frac{\left\|\left(H_k - \nabla^2 g(x^\star)\right)(x_{k+1} - x_k)\right\|_2}{\|x_{k+1} - x_k\|_2} \to 0.$
- Superlinear convergence means it is faster than any linear rate. E.g. c^{k^2} converges superlinearly to 0.

Questions so far?

Any Questions?

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Computational experiments

Solving the subproblem

$$\Delta x_k = \arg\min_d \; \nabla g(x_k)^T d + \frac{1}{2} d^T H_k d + h(x_k + d)$$
$$= \arg\min_d \; \hat{g}_k(x_k + d) + h(x_k + d)$$

Usually, we must use an iterative method to solve this subproblem.

- Use proximal gradient or coordinate descent on the subproblem.
- A gradient/coordinate descent iteration on the subproblem is much cheaper than a gradient iteration on the original function f, since it does not require a pass over the data. By solving the subproblem, we are more efficiently using a gradient evaluation than gradient descent.
- H_k is commonly a L-BFGS approximation, so computing a gradient takes $O(Lp)$. A gradient of the original function takes $O(np)$. The subproblem is independent of n.

Inexact Newton-type methods

Main idea: no need to solve the subproblem exactly only need a good enough search direction.

- We solve the subproblem approximately with an iterative method, terminating (sometimes very) early
- number of iterations may increase, but computational expense per iteration is smaller
- many practical implementations use inexact search directions

What makes a stopping condition good?

We should solve the subproblem more precisely when:

1. x_k is close to $x^\star$, since Newton's method converges quadratically in this regime.
2. $\hat{g}_k + h$ is a good approximation to f in the vicinity of x_k (meaning H_k has captured the curvature in g), since minimizing the subproblem also minimizes f.

Early stopping conditions

For regular Newton's method the most common stopping condition is

$$\|\nabla \hat{g}_k(x_k + \Delta x_k)\| \leq \eta_k \|\nabla g(x_k)\| .$$

Analogously,

$$\underbrace{\left\|G_{(\hat{g}_k+h)/M}(x_k + \Delta x_k)\right\|}_{\text{optimality of subproblem solution}} \leq \eta_k \underbrace{\left\|G_{f/M}(x_k)\right\|}_{\text{optimality of } x_k}$$

Choose η_k based on how well $G_{\hat{g}_k+h}$ approximates G_f:

$$\eta_k \sim \frac{\left\|G_{(\hat{g}_{k-1}+h)/M}(x_k) - G_{f/M}(x_k)\right\|}{\left\|G_{f/M}(x_{k-1})\right\|}$$

Reflects the Intuition: solve the subproblem more precisely when

- $G_{f/M}$ is small, so x_k is close to optimum.
- $G_{\hat{g}+h} - G_f \approx 0$, means that H_k is accurately capturing the curvature of g.

Convergence of the inexact prox-Newton method

- Inexact proximal Newton method converges superlinearly for the previous choice of stopping criterion and η_k.
- In practice, the stopping criterion works extremely well. It uses approximately the same number of iterations as solving the subproblem exactly, but spends much less time on each subproblem.

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Computational experiments

Sparse inverse covariance (Graphical Lasso)

Sparse inverse covariance:

$$\min_{\Theta} -\text{logdet}(\Theta) + \mathbf{tr}(S\Theta) + \lambda\|\Theta\|_1$$

- S is a sample covariance, and estimates Σ the population covariance.

$$S = \sum_{i=1}^{p}(x_i - \mu)(x_i - \mu)^T$$

- S is not of full rank since $n < p$, so S^{-1} doesn't exist.
- Graphical lasso is a good estimator of Σ^{-1}

Sparse inverse covariance estimation

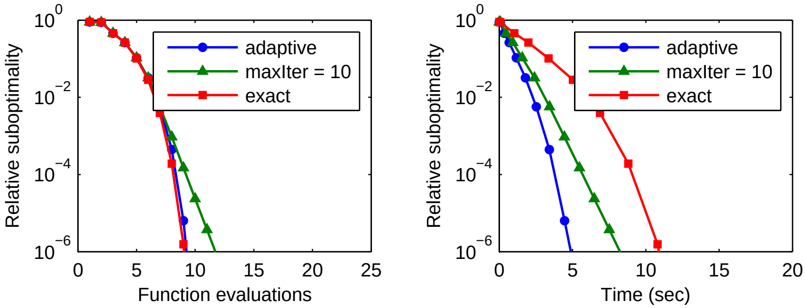
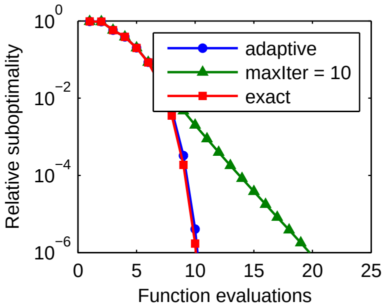


Figure: Proximal BFGS method with three subproblem stopping conditions (Estrogen dataset $p = 682$)

Sparse inverse covariance estimation



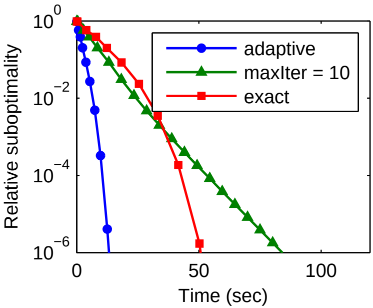


Figure: Leukemia dataset $p = 1255$

Another example

Sparse logistic regression

- training data: $x^{(1)}, \ldots, x^{(n)}$ with labels $y^{(1)}, \ldots, y^{(n)} \in \{0, 1\}$
- We fit a sparse logistic model to this data:

$$\underset{w}{\text{minimize}} \ \frac{1}{n} \sum_{i=1}^{n} -\log(1 + \exp(-y_i w^T x_i)) + \lambda \|w\|_1$$

Sparse logistic regression

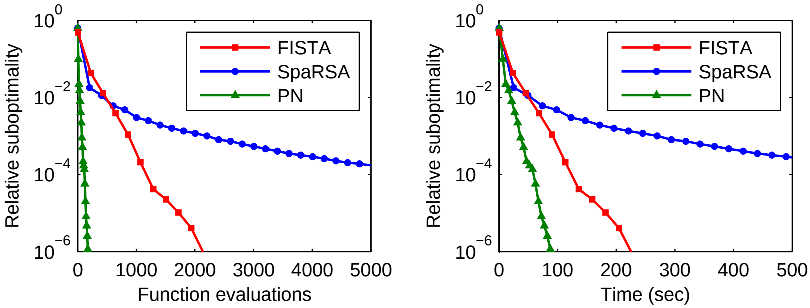
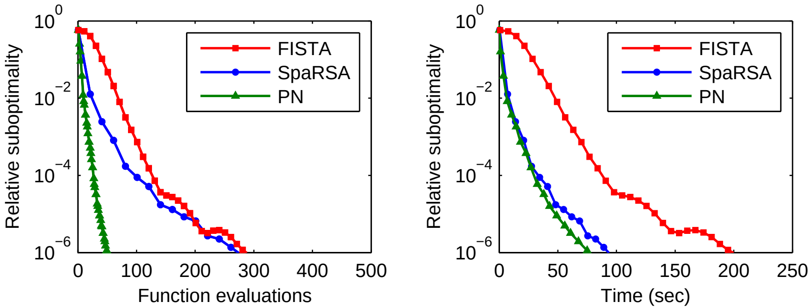


Figure: Proximal L-BFGS method vs. FISTA and SpaRSA (`gisette` dataset, $n = 5000$, $p = 6000$ and dense)

Sparse logistic regression

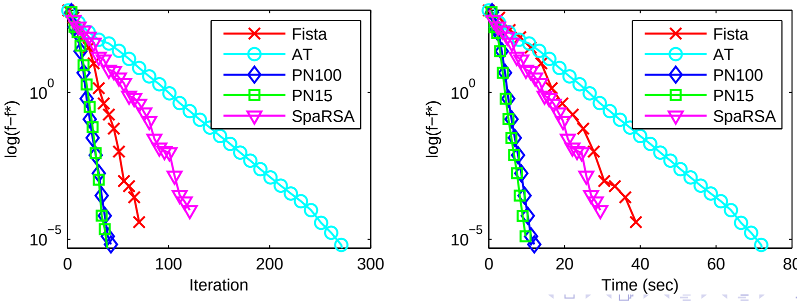
Figure: `rcv1` dataset, $n = 47,000$, $p = 542,000$ and 40 million nonzeros



Markov random field structure learning

$$\underset{\theta}{\text{minimize}} \; -\sum_{(r,j)\in E} \theta_{rj}(x_r, x_j) + \log Z(\theta) + \sum_{(r,j)\in E} \left(\lambda_1 \|\theta_{rj}\|_2 + \lambda_F \|\theta_{rj}\|_F^2\right).$$

Figure: Markov random field structure learning



Summary

Proximal Newton-type methods

- converge rapidly near the optimal solution, and can produce a solution of high accuracy
- are insensitive to the choice of coordinate system and to the condition number of the level sets of the objective
- are suited to problems where g, ∇g is expensive to evaluate compared to h, prox_h. This is the case when $g(x)$ is a loss function and computing the gradient requires a pass over the data.
- "more efficiently uses" a gradient evaluation of $g(x)$.

Thank you for your attention. Any questions?