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

\[
\minimize_x f(x) := g(x) + h(x)
\]

- \( g \) and \( h \) are convex functions
- \( g \) is continuously differentiable, and its gradient \( \nabla g \) is Lipschitz continuous
- \( h \) is not necessarily everywhere differentiable, but its *proximal mapping* can be evaluated efficiently
Minimizing composite functions: Examples

\( \ell_1 \)-regularized logistic regression:

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

Sparse inverse covariance:

\[
\min_{\Theta} -\log \det(\Theta) + \text{tr}(S\Theta) + \lambda \|\Theta\|_1
\]
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

\[ \min_x g(x) + 1_C(x) \]

Equivalent to solving

\[ \min_{x \in C} g(x) \]
The proximal mapping of a convex function $h$ is

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

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

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

$$\text{prox}_{t\|\cdot\|_1}(x) = \text{sign}(x) \cdot \max\{|x| - t, 0\}.$$
The proximal gradient step

\[ x_{k+1} = \text{prox}_{t_k h} (x_k - t_k \nabla g(x_k)) \]
\[ = \arg \min_y h(y) + \frac{1}{2t_k} \| y - (x_k - t_k \nabla g(x_k)) \|^2 \]
\[ = x_k - t_k G_{t_k f}(x_k) \]

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

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

- \( G_f(x) \) can be thought of as a generalized gradient of \( f(x) \). Simplifies to the gradient descent on \( g(x) \) when \( h = 0 \).
Algorithm 1  The proximal gradient method

Require: starting point \( x_0 \in \text{dom} \, f \)

1: repeat
2: \quad Compute a *proximal gradient step*:
3: \quad \quad \quad G_{t_k} f(x_k) = \frac{1}{t_k} \left( x_k - \text{prox}_{t_k h}(x_k - t_k \nabla g(x_k)) \right).
4: \quad Update: \quad x_{k+1} \leftarrow x_k - t_k G_{t_k} f(x_k).
5: until stopping conditions are satisfied.
Minimizing composite functions

**Proximal Newton-type methods**

Inexact search directions

Computational experiments
Proximal Newton-type methods

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

\[
\Delta x_k := \arg \min_d \nabla g(x_k)^T d + \frac{1}{2} d^T H_k d + h(x_k + d).
\]

Solve the above subproblem and update

\[
x_{k+1} = x_k + t_k \Delta x_k.
\]
Algorithm 2 A generic proximal Newton-type method

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

1: repeat
2: Choose an approximation to the Hessian $H_k$.
3: Solve the subproblem for a search direction:
   \[ \Delta x_k \leftarrow \arg \min_d \nabla g(x_k)^T d + \frac{1}{2} d^T H_k d + h(x_k + d). \]
4: Select $t_k$ with a backtracking line search.
5: Update: $x_{k+1} \leftarrow x_k + t_k \Delta x_k$.
6: 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

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

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: $\ell_1$-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 \( \nabla g \):

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

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: $\|x_k - x^*\|^2 \leq c^{2^k}$ or $\log \log \frac{1}{\epsilon}$ iterations to achieve $\epsilon$ 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 $\left\| \left( H_k - \nabla^2 g(x^*) \right)(x_{k+1} - x_k) \right\|_2 \rightarrow 0$.
- 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 $x^*$, 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

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

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 $\eta_k$ 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 $\eta_k$.
- 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:

\[
\min_{\Theta} -\log\det(\Theta) + \text{tr}(S\Theta) + \lambda \|\Theta\|_1
\]

- \(S\) is a sample covariance, and estimates \(\Sigma\) 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 \(\Sigma^{-1}\)
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:

\[
\min_w \frac{1}{n} \sum_{i=1}^{n} - \log(1 + \exp(-y_i w^T x_i)) + \lambda \|w\|_1
\]
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

\[
\minimize_{\theta} - \sum_{(r,j) \in E} \theta_{rj}(x_r, x_j) + \log Z(\theta) + \sum_{(r,j) \in E} \left( \lambda_1 \|\theta_{rj}\|_2 + \lambda_F \|\theta_{rj}\|_{F}^2 \right).
\]

**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 $g$, $\nabla g$ is expensive to evaluate compared to $h$, $\text{prox}_h$. 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?