CPSC 540: Machine Learning

Proximal-Gradient

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Admin

- Auditting/registration forms:
  - Pick up after class today.
- Assignment 1:
  - 2 late days to hand in tonight.
- Drop deadline is today.
  - Last chance to withdraw.
- Assignment 2:
  - First question up now.
  - Due in 2 weeks.

Last Time: Projected-Gradient

- We discussed minimizing smooth functions with simple convex constraints,

$$\operatorname*{argmin}_{w \in \mathcal{C}} f(w).$$

- With simple constraints, we can use projected-gradient:

$$w^{k+\frac{1}{2}} = w^k - \alpha_k \nabla f(w^k) \qquad \text{(gradient step)}$$

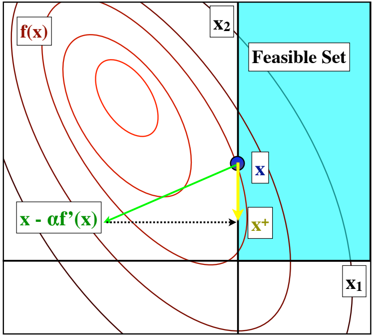
$$w^{k+1} = \operatorname*{argmin}_{v \in \mathcal{C}} \|v - w^{k+\frac{1}{2}}\| \qquad \text{(projection)}$$

- Very similar properties to gradient descent when ∇f is Lipschitz:
  - $O(\log(1/\epsilon))$ iterations required if f is strongly-convex.
  - Setting $\alpha_k < 2/L$ guarantees we decerase objective.
  - We have practical line-search strategies that improve performance.
  - Solutions are "fixed points".
  - We can add momentum or make Newton-like versions.

Last Time: Projected-Gradient

$$w^{k+\frac{1}{2}} = w^k - \alpha_k \nabla f(w^k) \qquad \text{(gradient step based on function } f\text{)}$$

$$w^{k+1} = \underset{v \in \mathcal{C}}{\text{argmin}} \|v - w^{k+\frac{1}{2}}\| \qquad \text{(projection onto feasible set } \mathcal{C}\text{)}$$



Why the Projected Gradient?

- We want to optimize f (smooth but possibly non-convex) over some convex set $\mathcal{C}$,

$$\mathop{\mathrm{argmin}}_{w \in \mathcal{C}} f(w).$$

- Recall that we can view gradient descent as minimizing quadratic approximation

$$w^{k+1} \in \mathop{\mathrm{argmin}}_{v} \left\{ f(w^k) + \nabla f(w^k)(v - w^k) + \frac{1}{2\alpha_k}\|v - w^k\|^2 \right\},$$

  where we've written it with a general step-size α_k instead of $1/L$.
  - Solving the convex quadratic argmin gives $w^{k+1} = w^k - \alpha_k \nabla f(w^k)$.

- We could minimize quadratic approximation to f subject to the constraints,

$$w^{k+1} \in \mathop{\mathrm{argmin}}_{v \in \mathcal{C}} \left\{ f(w^k) + \nabla f(w^k)^T(v - w^k) + \frac{1}{2\alpha_k}\|v - w^k\|^2 \right\},$$

Why the Projected Gradient?

- We write this "minimize quadratic approximation over the set $\mathcal{C}$" iteration as

$$\begin{aligned}
w^{k+1} &\in \operatorname*{argmin}_{y \in \mathcal{C}} \left\{ f(w^k) + \nabla f(w^k)^T(v - w^k) + \frac{1}{2\alpha_k}\|v - w^k\|^2 \right\} \\
&\equiv \operatorname*{argmin}_{v \in \mathcal{C}} \left\{ \alpha_k f(w^k) + \alpha_k \nabla f(w^k)^T(v - w^k) + \frac{1}{2}\|v - w^k\|^2 \right\} \quad \text{(multiply by } \alpha_k\text{)} \\
&\equiv \operatorname*{argmin}_{v \in \mathcal{C}} \left\{ \frac{\alpha_k^2}{2}\|\nabla f(w^k)\|^2 + \alpha_k \nabla f(w^k)^T(v - w^k) + \frac{1}{2}\|v - w^k\|^2 \right\} \quad (\pm \text{ const.}) \\
&\equiv \operatorname*{argmin}_{v \in \mathcal{C}} \left\{ \|(v - w^k) + \alpha_k \nabla f(w^k)\|^2 \right\} \quad \text{(complete the square)} \\
&\equiv \operatorname*{argmin}_{v \in \mathcal{C}} \left\{ \|v - \underbrace{(w^k - \alpha_k \nabla f(w^k))}_{\text{gradient descent}}\| \right\},
\end{aligned}$$

which gives the projected-gradient algorithm: $w^{k+1} = \text{proj}_{\mathcal{C}}[w^k - \alpha_k \nabla f(w^k)]$.

Simple Convex Sets

- Projected-gradient is only efficient if the projection is cheap.
- We say that $\mathcal{C}$ is simple if the projection is cheap.
  - For example, if it costs $O(d)$ then it adds no cost to the algorithm.
- For example, if we want $w \geq 0$ then projection sets negative values to 0.
  - Non-negative constraints are "simple".
- Another example is $w \geq 0$ and $w^T 1 = 1$, the probability simplex.
  - There are $O(d)$ algorithm to compute this projection (similar to "select" algorithm)

Simple Convex Sets

- Other examples of simple convex sets:
  - Having upper and lower bounds on the variables, $LB \leq x \leq UB$.
  - Having a linear equality constraint, $a^T x = b$, or a small number of them.
  - Having a half-space constraint, $a^T x \leq b$, or a small number of them.
  - Having a norm-ball constraint, $\|x\|_p \leq \tau$, for $p = 1, 2, \infty$ (fixed τ).
  - Having a norm-cone constraint, $\|x\|_p \leq \tau$, for $p = 1, 2, \infty$ (variable τ).
- It's easy to minimize smooth functions with these constraints.

Intersection of Simple Convex Sets: Dykstra's Algorithm

- Often our set $\mathcal{C}$ is the intersection of simple convex set,

$$\mathcal{C} \equiv \cup_i \mathcal{C}_i.$$

- For example, we could have a large number linear constraints.
- Dykstra's algorithm can compute the projection in this case.
  - On each iteration, it projects a vector onto one of the sets $\mathcal{C}_i$.
  - Requires $O(\log(1/\epsilon))$ such projections to get within ϵ.

(This is not the shortest path algorithm of "Dijkstra".)

Outline

Solving Problems with Simple Regularizers

- We were discussing how to solve non-smooth L1-regularized objectives like

$$\underset{w \in \mathbb{R}^d}{\text{argmin}} \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_1.$$

- Use our trick to formulate as a quadratic program?
  - $O(d^2)$ or worse.
- Make a smooth approximation to the L1-norm?
  - Destroys sparsity (we'll again just have one subgradient at zero).
- Use a subgradient method?
  - Needs $O(1/\epsilon)$ iterations even in the strongly-convex case.
- Transform to "smooth f with simple constraints" and use projected-gradient?
  - Works well (bonus), but increases problem size and destroys strong-convexity.

- For "simple" regularizers, proximal-gradient methods don't have these drawbacks

Quadratic Approximation View of Gradient Method

- We want to solve a smooth optimization problem:

$$\operatorname*{argmin}_{w\in\mathbb{R}^d} f(w).$$

- Iteration w^k works with a quadratic approximation to f:

$$f(v) \approx f(w^k) + \nabla f(w^k)^T(v-w^k) + \frac{1}{2\alpha_k}\|v-w^k\|^2,$$

$$w^{k+1} \in \operatorname*{argmin}_{v\in\mathbb{R}^d}\left\{f(w^k) + \nabla f(w^k)^T(v-w^k) + \frac{1}{2\alpha_k}\|v-w^k\|^2\right\}.$$

We can equivalently write this as the quadratic optimization:

$$w^{k+1} \in \operatorname*{argmin}_{v\in\mathbb{R}^d}\left\{\frac{1}{2}\|v-(w^k-\alpha_k\nabla f(w^k))\|^2\right\},$$

and the solution is the gradient algorithm:

$$w^{k+1} = w^k - \alpha_k\nabla f(w^k).$$

Quadratic Approximation View of Proximal-Gradient Method

- We want to solve a smooth plus non-smooth optimization problem:

$$\underset{w \in \mathbb{R}^d}{\operatorname{argmin}}\, f(w) + r(w).$$

- Iteration w^k works with a quadratic approximation to f:

$$f(v) + r(v) \approx f(w^k) + \nabla f(w^k)^T (v - w^k) + \frac{1}{2\alpha_k}\|v - w^k\|^2 + r(v),$$

$$w^{k+1} \in \underset{v \in \mathbb{R}^d}{\operatorname{argmin}} \left\{ f(w^k) + \nabla f(w^k)^T (v - w^k) + \frac{1}{2\alpha_k}\|v - w^k\|^2 + r(v) \right\}.$$

We can equivalently write this as the proximal optimization:

$$w^{k+1} \in \underset{v \in \mathbb{R}^d}{\operatorname{argmin}} \left\{ \frac{1}{2}\|v - (w^k - \alpha_k \nabla f(w^k))\|^2 + \alpha_k r(v) \right\},$$

and the solution is the proximal-gradient algorithm:

$$w^{k+1} = \operatorname{prox}_{\alpha_k r}[w^k - \alpha_k \nabla f(w^k)].$$

Proximal-Gradient for L1-Regularization

- The proximal operator for L1-regularization when using step-size α_k,

$$\text{prox}_{\alpha_k\lambda\|\cdot\|_1}[w^{k+\frac{1}{2}}] \in \underset{v\in\mathbb{R}^d}{\text{argmin}}\left\{\frac{1}{2}\|v - w^{k+\frac{1}{2}}\|^2 + \alpha_k\lambda\|v\|_1\right\},$$

  involves solving a simple 1D problem for each variable j:

$$w_j^{k+1} \in \underset{v_j\in\mathbb{R}}{\text{argmin}}\left\{\frac{1}{2}(v_j - w_j^{k+\frac{1}{2}})^2 + \alpha_k\lambda|v_j|\right\}.$$

- The solution is given by applying "soft-threshold" operation:
  1. If $|w_j^{k+\frac{1}{2}}| \leq \alpha_k\lambda$, set $w_j^{k+1} = 0$.
  2. Otherwise, shrink $|w_j^{k+\frac{1}{2}}|$ by $\alpha_k\lambda$.

Proximal-Gradient for L1-Regularization

- An example sof-threshold operator with $\alpha_k \lambda = 1$:

$$\begin{array}{ccc} \text{Input} & \text{Threshold} & \text{Soft-Threshold} \\ \begin{bmatrix} 0.6715 \\ -1.2075 \\ 0.7172 \\ 1.6302 \\ 0.4889 \end{bmatrix} & \begin{bmatrix} 0 \\ -1.2075 \\ 0 \\ 1.6302 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ -0.2075 \\ 0 \\ 0.6302 \\ 0 \end{bmatrix} \end{array}$$

- Symbolically, the soft-threshold operation computes

$$w_j^{k+1} = \underbrace{\text{sign}(w^{k+\frac{1}{2}})}_{-1 \text{ or } +1} \max\left\{0, |w_j^{k+\frac{1}{2}}| - \alpha_k \lambda\right\}.$$

- Has the nice property that iterations w^k are sparse.
  - Compared to subgradient method which wouldn't give exact zeroes.

Proximal-Gradient Method

- So proximal-gradient step takes the form:

$$w^{k+\frac{1}{2}} = w^k - \alpha_k \nabla f(w^k)$$
$$w^{k+1} = \operatorname*{argmin}_{v \in \mathbb{R}^d} \left\{ \frac{1}{2}\|v - w^{k+\frac{1}{2}}\|^2 + \alpha_k r(v) \right\}.$$

- Second part is called the proximal operator with respect to a convex $\alpha_k r$.
  - We say that r is simple if you can efficiently compute proximal operator.

- Very similar properties to projected-gradient when ∇f is Lipschitz-continuous:
  - Guaranteed improvement for $\alpha < 2/L$, practical backtracking methods work better.
  - Solution is a fixed point, $w^* = \text{prox}_r[w^* - \nabla f(w^*)]$.
  - If f is strongly-convex then

$$F(w^k) - F^* \leq \left(1 - \frac{\mu}{L}\right)^k \left[F(w^0) - F^*\right],$$

where $F(w) = f(w) + r(w)$.

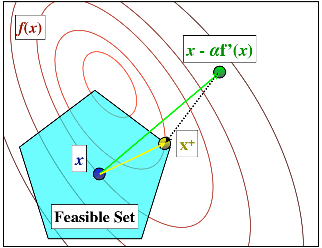
Projected-Gradient is Special case of Proximal-Gradient

- Projected-gradient methods are a special case:

$$r(w) = \begin{cases} 0 & \text{if } w \in \mathcal{C} \\ \infty & \text{if } w \notin \mathcal{C} \end{cases}, \quad (\text{indicator function for convex set } \mathcal{C})$$

gives

$$w^{k+1} \in \underbrace{\operatorname*{argmin}_{v \in \mathbb{R}^d} \frac{1}{2}\|v - w^{k+\frac{1}{2}}\|^2 + r(v)}_{\text{proximal operator}} \equiv \operatorname*{argmin}_{v \in \mathcal{C}} \frac{1}{2}\|v - w^{k+\frac{1}{2}}\|^2 \equiv \underbrace{\operatorname*{argmin}_{v \in \mathcal{C}} \|v - w^{k+\frac{1}{2}}\|}_{\text{projection}}.$$



Proximal-Gradient Linear Convergence Rate

- Simplest linear convergence proofs are based on the proximal-PL inequality,

$$\frac{1}{2}\mathcal{D}_r(w, L) \geq \mu(F(w) - F^*),$$

where compared to PL inequality we've replaced $\|\nabla f(w)\|^2$ with

$$\mathcal{D}_r(w, \alpha) = -2\alpha \min_v \left[\nabla g(w)^T(v - w) + \frac{\alpha}{2}\|v - w\|^2 + r(v) - r(w)\right],$$

and recall that $F(w) = f(w) + r(w)$ (bonus).

- This non-intuitive property holds for many important problems:
  - L1-regularized least squares.
  - Any time f is strong-convex (i.e., add an L2-regularizer as part of f).
  - Any $f = g(Ax)$ for strongly-convex g and r being indicator for polyhedral set.
- But it can be painful to show that functions satisfy this property.

Outline

Motivation for Group Sparsity

- Recall that multi-class logistic regression uses
$$\hat{y}^i = \operatorname*{argmax}_c \{w_c^T x^i\},$$
where we have a parameter vector w_c for each class c.
- We typically use softmax loss and write our parameters as a matrix,
$$W = \begin{bmatrix} | & | & | & & | \\ w_1 & w_2 & w_3 & \cdots & w_k \\ | & | & | & & | \end{bmatrix}$$
- Suppose we want to use L1-regularization for feature selection,
$$\operatorname*{argmin}_{W \in \mathbb{R}^{d \times k}} \underbrace{f(W)}_{\text{softmax loss}} + \underbrace{\lambda \sum_{c=1}^{k} \|w_c\|_1}_{\text{L1-regularization}}.$$
- Unfortunately, setting elements of W to zero may not select features.

Motivation for Group Sparsity

- Suppose L1-regularizationgives a sparse W with a non-zero in each row:

$$W = \begin{bmatrix} -0.83 & 0 & 0 & 0 \\ 0 & 0 & 0.62 & 0 \\ 0 & 0 & 0 & -0.06 \\ 0 & 0.72 & 0 & 0 \end{bmatrix}.$$

- Even though it's very sparse, it uses all features.
  - Remember that classifier multiplies feature j by each value in row j.
  - Feature 1 is used in w_1.
  - Feature 2 is used in w_3.
  - Feature 3 is used in w_4.
  - Feature 4 is used in w_2.
- In order to remove a feature, we need its entire row to be zero.

Motivation for Group Sparsity

- What we want is group sparsity:

$$W = \begin{bmatrix} -0.77 & 0.04 & -0.03 & -0.09 \\ 0 & 0 & 0 & 0 \\ 0.04 & -0.08 & 0.01 & -0.06 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

- Each row is a group, and we want groups (rows) of variables that have all zeroes.
  - If row j is zero, then x_j is not used by the model.
- Pattern arises in other settings where each row gives parameters for one feature:
  - Multiple regression, multi-label classification, and multi-task classification.

Motivation for Group Sparsiy

- Categorical features are another setting where group sparsity is needed.
- Consider categorical features encoded as binary indicator features ("1 of k"):

City	Age
Vancouver	22
Burnaby	35
Vancouver	28

Vancouver	Burnaby	Surrey	Age ≤ 20	20 < Age ≤ 30	Age > 30
1	0	0	0	1	0
0	1	0	0	0	1
1	0	0	0	1	0

- A linear model would use

$$\hat{y}^i = w_1 x_{\text{van}} + w_2 x_{\text{bur}} + w_3 x_{\text{sur}} + w_4 x_{\leq 20} + w_5 x_{21-30} + w_6 x_{>30}.$$

- If we want feature selection of original categorical variables, we have 2 groups:
  - $\{w_1, w_2, w_3\}$ correspond to "City" and $\{w_4, w_5, w_6\}$ correspond to "Age".

Group L1-Regularization

- Consider a problem with a set of disjoint groups $\mathcal{G}$.
  - For example, $\mathcal{G} = \{\{1,2\},\{3,4\}\}$.

- Minimizing a function f with group L1-regularization:

$$\underset{w \in \mathbb{R}^d}{\text{argmin}}\, f(w) + \lambda \sum_{g \in \mathcal{G}} \|w_g\|_p,$$

  where g refers to individual group indices and $\|\cdot\|_p$ is some norm.

- For certain norms, it encourages sparsity in terms of groups g.
  - Variables x_1 and x_2 will either be both zero or both non-zero.
  - Variables x_3 and x_4 will either be both zero or both non-zero.

Group L1-Regularization

- Why is it called group L1-regularization?

- Consider $G = \{\{1,2\},\{3,4\}\}$ and using L2-norm,

$$\sum_{g\in G}\|w_g\|_2 = \sqrt{w_1^2 + w_2^2} + \sqrt{w_3^2 + w_4^2}.$$

- If vector v contains the group norms, it's the L1-norm of v:

$$\text{If } v \triangleq \begin{bmatrix}\|w_{12}\|_2 \\ \|w_{34}\|_2\end{bmatrix} \text{ then } \sum_{g\in G}\|w_g\|_2 = \|w_{12}\|_2+\|w_{34}\|_2 = v_1+v_2 = |v_1|+|v_2| = \|v\|_1.$$

- So groups L1-regularization encourages sparsity in the group norms.
  - When the norm of the group is 0, all group elements are 0.

Group L1-Regularization: Choice of Norm

- The group L1-regularizer is sometimes written as a "mixed" norm,

$$\|w\|_{1,p} \triangleq \sum_{g \in \mathcal{G}} \|w_g\|_p.$$

- The most common choice for the norm is the L2-norm:
  - If $\mathcal{G} = \{\{1,2\},\{3,4\}\}$ we obtain

$$\|w\|_{1,2} = \sqrt{w_1^2 + w_2^2} + \sqrt{w_3^2 + w_4^2}.$$

- Another common choice is the L∞-norm,

$$\|w\|_{1,\infty} = \max\{|w_1|,|w_2|\} + \max\{|w_3|,|w_4|\}.$$

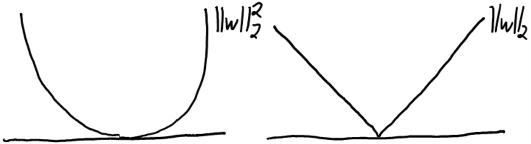
- But note that the L1-norm does not give group sparsity,

$$\|w\|_{1,1} = |w_1| + |w_2| + |w_3| + |w_4| = \|w\|_1,$$

as it's equivalent to non-group L1-regularization.

Sparsity from the L2-Norm?

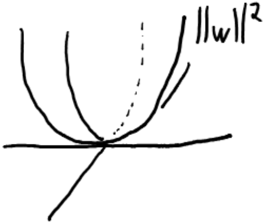
- Didn't we say sparsity comes from the L1-norm and not the L2-norm?
  - Yes, but we were using the squared L2-norm.
- Squared vs. non-squared L2-norm in 1D:

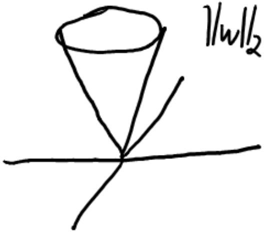


- Non-squared L2-norm is absolute value.
  - Non-squared L2-regularizer will set $w = 0$ for some finite λ.
- Squaring the L2-norm gives a smooth function but destroys sparsity.

Sparsity from the L2-Norm?

- Squared vs. non-squared L2-norm in 2D:





- The squared L2-norm is smooth and has no sparsity.
- Non-squared L2-norm is non-smooth at the zero vector.
  - It doesn't encourage us to set any $w_j = 0$ as long as one $w_{j'} \neq 0$.
  - But if λ is large enough it encourages all w_j to be set to 0.

Sub-differential of Group L1-Regularization

- For our group L1-regularization objective with the 2-norm,

$$F(w) = f(w) + \lambda \sum_{g \in \mathcal{G}} \|w_g\|_2,$$

  the indices g in the sub-differential are given by

$$\partial_g F(w) \equiv \nabla_g f(w) + \lambda \partial \|w_g\|_2.$$

- In order to have $0 \in \partial F(w)$, we thus need for each group that

$$0 \in \nabla_g f(w) + \lambda \partial \|w_g\|_2,$$

  and subtracting $\nabla_g f(w)$ from both sides gives

$$-\nabla_g f(w) \in \lambda \partial \|w_g\|_2.$$

Sub-differential of Group L1-Regularization

- So at minimizer w^* we must have for all groups that

$$-\nabla_g f(w^*) \in \lambda \partial \|w_g^*\|_2.$$

- The sub-differential of the scaled L2-norm is given by

$$\partial \|w\|_2 = \begin{cases} \left\{ \frac{w}{\|w\|_2} \right\} & w \neq 0 \\ \{v \mid \|v\|_2 \leq 1\} & w = 0. \end{cases}$$

- So at a solution w^* we have for each group that

$$\begin{cases} -\nabla_g f(w^*) = \lambda \frac{w_g^*}{\|w_g^*\|_2} & w_g \neq 0, \\ \|\nabla_g f(w^*)\| \leq \lambda & w_g^* = 0. \end{cases}$$

- For sufficiently-large λ we'll set the group to zero.
  - With squared group norms we would need $\nabla_g f(w^*) = 0$ with $w_g^* = 0$ (unlikely).

Summary

- Simple convex sets are those that allow efficient projection.
- Simple regularizers are those that allow efficient proximal operator.
- Proximal-gradient: linear rates for sum of smooth and simple non-smooth.
- Group L1-regularization encourages sparsity in variable groups.

- Next time: going beyond L1-regularization to "structured sparsity".

Should we use projected-gradient for non-smooth problems?

- Some non-smooth problems can be turned into smooth problems with simple constraints.

- But transforming might make problem harder:
  - For L1-regularization least squares,

$$\underset{w \in \mathbb{R}^d}{\text{argmin}} \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_1,$$

  we can re-write as a smooth problem with bound constraints,

$$\underset{w_+ \geq 0,\, w_- \geq 0}{\text{argmin}} \|X(w_+ - w_-) - y\|^2 + \lambda\sum_{j=1}^{d}(w_+ + w_-).$$

  - Doubles the number of variables.
  - Transformed problem is not strongly convex even if the original was.

Projected-Newton Method

- We discussed how the naive projected-Newton method,

$$x^{t+\frac{1}{2}} = x^t - \alpha_t [H_t]^{-1} \nabla f(x^t) \qquad \text{(Newton-like step)}$$

$$x^{t+1} = \mathop{\text{argmin}}_{y \in \mathcal{C}} \|y - x^{t+\frac{1}{2}}\| \qquad \text{(projection)}$$

  will not work.

- The correct projected-Newton method uses

$$x^{t+\frac{1}{2}} = x^t - \alpha_t [H_t]^{-1} \nabla f(x^t) \qquad \text{(Newton-like step)}$$

$$x^{t+1} = \mathop{\text{argmin}}_{y \in \mathcal{C}} \|y - x^{t+\frac{1}{2}}\|_{H_t} \qquad \text{(projection under Hessian metric)}$$

Projected-Newton Method

- Projected-gradient minimizes quadratic approximation,

$$x^{t+1} = \operatorname*{argmin}_{y \in C} \left\{ f(x^t) + \nabla f(x^t)(y - x^t) + \frac{1}{2\alpha_t}\|y - x^t\|^2 \right\}.$$

- Newton's method can be viewed as quadratic approximation (wth $H_t \approx \nabla^2 f(x^t)$):

$$x^{t+1} = \operatorname*{argmin}_{y \in \mathbb{R}^d} \left\{ f(x^t) + \nabla f(x^t)(y - x^t) + \frac{1}{2\alpha_t}(y - x^t)H_t(y - x^t) \right\}.$$

- Projected Newton minimizes constrained quadratic approximation:

$$x^{t+1} = \operatorname*{argmin}_{y \in C} \left\{ f(x^t) + \nabla f(x^t)(y - x^t) + \frac{1}{2\alpha_t}(y - x^t)H_t(y - x^t) \right\}.$$

- Equivalently, we project Newton step under different Hessian-defined norm,

$$x^{t+1} = \operatorname*{argmin}_{y \in C} \|y - (x^t - \alpha_t H_t^{-1}\nabla f(x^t))\|_{H_t},$$

where general "quadratic norm" is $\|z\|_A = \sqrt{z^T A z}$ for $A \succ 0$.

Discussion of Projected-Newton

- Projected-Newton iteration is given by

$$x^{t+1} = \operatorname*{argmin}_{y \in C} \left\{ f(x^t) + \nabla f(x^t)(y - x^t) + \frac{1}{2\alpha_t}(y - x^t)H_t(y - x^t) \right\}.$$

- But this is expensive even when $\mathcal{C}$ is simple.
- There are a variety of practical alternatives:
  - If H_t is diagonal then this is typically simple to solve.
  - Two-metric projection methods are special algorithms for upper/lower bounds.
    - Fix problem of naive method in this case by making H_t partially diagonal.
  - Inexact projected-Newton: solve the above approximately.
    - Useful when f is very expensive but H_t and $\mathcal{C}$ are simple.
    - "Costly functions with simple constraints".

Properties of Proximal-Gradient

- Two convenient properties of proximal-gradient:
  - Proximal operators are non-expansive,

$$\|\text{prox}_r(x) - \text{prox}_r(y)\| \leq \|x - y\|,$$

    it only moves points closer together.

    (including x^k and x^*)
  - For convex f, only fixed points are global optima,

$$x^* = \text{prox}_r(x^* - \alpha \nabla f(x^*)),$$

    for any $\alpha > 0$.

    (can test $\|x^t - \text{prox}_r(x^t - \nabla f(x^t))\|$ for convergence)
- Proximal gradient/Newton has two line-searches (generalized projected variants):
  - Fix α_t and search along direction to x^{t+1} (1 proximal operator, non-sparse iterates).
  - Vary α_t values (multiple proximal operators per iteration, gives sparse iterations).

Implicit subgradient viewpoint of proximal-gradient

- The proximal-gradient iteration is

$$w^{k+1} \in \operatorname*{argmin}_{v \in \mathbb{R}^d} \frac{1}{2}\|v - (w^k - \alpha_k \nabla f(w^k))\|^2 + \alpha_k r(v).$$

- By non-smooth optimality conditions that 0 is in subdifferential, we have that

$$0 \in (w^{k+1} - (w^k - \alpha_k \nabla f(w^k)) + \alpha_k \partial r(w^{k+1}),$$

  which we can re-write as

$$w^{k+1} = w^k - \alpha_k(\nabla f(w^k) + \partial r(w^{k+1})).$$

- So proximal-gradient is like doing a subgradient step, with
  1. Gradient of the smooth term at w^k.
  2. A particular subgradient of the non-smooth term at w^{k+1}.
     - "Implicit" subgradient.

Proximal-Gradient Convergence under Proximal-PL

- By Lipschitz continuity of g we have

$$
\begin{aligned}
F(x_{k+1}) &= g(x_{k+1}) + r(x_k) + r(x_{k+1}) - r(x_k) \\
&\leq F(x_k) + \langle \nabla g(x_k), x_{k+1} - x_k \rangle + \frac{L}{2}||x_{k+1} - x_k||^2 + r(x_{k+1}) - r(x_k) \\
&\leq F(x_k) - \frac{1}{2L}\mathcal{D}_r(x_k, L) \\
&\leq F(x_k) - \frac{\mu}{L}[F(x_k) - F^*],
\end{aligned}
$$

and then we can take our usual steps.

Faster Rate for Proximal-Gradient

- It's possible to show a slightly faster rate for proximal-gradient using $\alpha_t = 2/(\mu + L)$.
- See `http://www.cs.ubc.ca/~schmidtm/Documents/2014_Notes_ProximalGradient.pdf`

Proximal-Newton

- We can define proximal-Newton methods using

$$x^{t+\frac{1}{2}} = x^t - \alpha_t [H_t]^{-1} \nabla f(x^t) \qquad \text{(gradient step)}$$

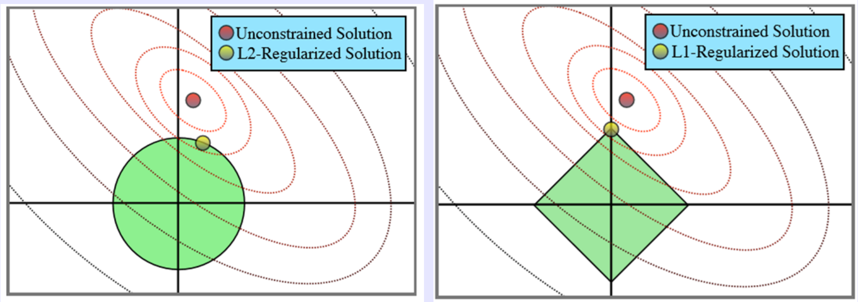
$$x^{t+1} = \operatorname*{argmin}_{y \in \mathbb{R}^d} \left\{ \frac{1}{2} \|y - x^{t+\frac{1}{2}}\|_{H_t}^2 + \alpha_t r(y) \right\} \qquad \text{(proximal step)}$$

- This is expensive even for simple r like L1-regularization.
- But there are analogous tricks to projected-Newton methods:
  - Diagonal or Barzilai-Borwein Hessian approximation.
  - "Orthant-wise" methods are analogues of two-metric projection.
  - Inexact methods use approximate proximal operator.

L1-Regularization vs. L2-Regularization

- Last time we looked at sparsity using our constraint trick,

$$\operatorname*{argmin}_{w \in \mathbb{R}^d} f(w) + \lambda \|w\|_p \quad \Leftrightarrow \quad \operatorname*{argmin}_{w \in \mathbb{R}^d, \tau \in \mathbb{R}} f(w) + \lambda\tau \text{ with } \tau \geq \|w\|_p.$$

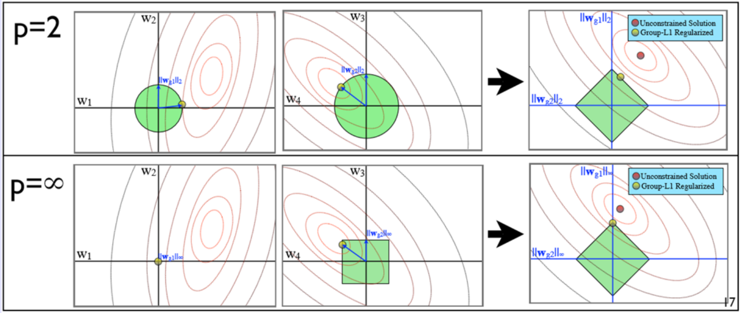


- Note that we're also minimizing the radius τ.
  - If τ shrinks to zero, all w are set to zero.
  - But if τ is squared there is virtually no penalty for having τ non-zero.

Group L1-Regularization

- Minimizing a function f with group L1-regularization,

$$\underset{w\in\mathbb{R}^d}{\text{argmin}}\, f(w) + \lambda\|w\|_{1,p} \quad \Leftrightarrow \quad \underset{w\in\mathbb{R}^d,\tau\in\mathbb{R}^{|\mathcal{G}|}}{\text{argmin}}\, f(w) + \lambda\sum_{g=1}^{|\mathcal{G}|}\tau_g \text{ with } \tau_g \geq \|w\|_p.$$



- We're minimizing $f(w)$ plus the radiuses τ_g for each group g.
  - If τ_g shrinks to zero, all w_g are set to zero.

Group L1-Regularization

- We can convert the non-smooth group L1-regularization problem,

$$\mathop{\text{argmin}}_{x \in \mathbb{R}^d} g(x) + \lambda \sum_{g \in G} \|x_g\|_2,$$

into a smooth problem with simple constraints:

$$\mathop{\text{argmin}}_{x \in \mathbb{R}^d} \underbrace{g(x) + \lambda \sum_{g \in G} r_g}_{f}, \quad \text{subject to } r_g \geq \|x_g\|_2 \text{ for all } g.$$

- Here the constraitnts are separable:
  - We can project onto each norm-cone separately.
- Since norm-cones are simple we can solve this with projected-gradient.
  - But we have more variables in the transformed problem and lose strong-convexity.

Proximal-Gradient for L0-Regularization

- There are some resutls on proximal-gradient for non-convex r.
- Most common case is L0-regularization,

$$f(w) + \lambda \|w\|_0,$$

  where $\|w\|_0$ is the number of non-zeroes.
  - Includes AIC and BIC from 340.
- The proximal operator for $\alpha_k \lambda \|w\|_0$ is simple:
  - Set $w_j = 0$ wihenever $|w_j| \leq \alpha_k \lambda$ ("hard" thresholding).
- Analysis is complicated a bit because discontinuity of prox as function of α_k.