Augmented Lagrangian Methods

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Consider the linearly constrained problem,

$$\min f(x) \text{ s.t. } Ax = b,$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is smooth. How do we recognize that a point x^* is a solution of this problem? (Such optimality conditions can provide the foundation for algorithms.)

Karush-Kuhn-Tucker (KKT) condition is a "first-order necessary condition." If x^* is a local solution, there exists a vector of Lagrange multipliers $\lambda^* \in \mathbb{R}^m$ such that

$$\nabla f(x^*) = -A^T \lambda^*, \quad Ax^* = b.$$

When f is smooth and convex, these conditions are also sufficient. (In fact, it's enough for f to be convex on the null space of A.)

Minimization with Linear Constraints

Define the Lagrangian function:

$$\mathcal{L}(x,\lambda) := f(x) + \lambda^{T}(Ax - b).$$

Can write the KKT conditions in terms of $\ensuremath{\mathcal{L}}$ as follows:

$$abla \mathcal{L}(x^*,\lambda^*) = egin{bmatrix}
abla_x \mathcal{L}(x^*,\lambda^*) \
abla_\lambda \mathcal{L}(x^*,\lambda^*) \end{bmatrix} = 0.$$

Suppose now that f is convex but not smooth. First-order optimality conditions (necessary and sufficient) are that there exists $\lambda^* \in \mathbb{R}^m$ such that

$$-A^T\lambda^* \in \partial f(x^*), \quad Ax^* = b,$$

where ∂f is the subdifferential. In terms of the Lagrangian, we have

$$0\in\partial_x\mathcal{L}(x^*,\lambda^*),\quad
abla_\lambda\mathcal{L}(x^*,\lambda^*)=0.$$

Augmented Lagrangian Methods

• With *f* proper, lower semi-continuous, and convex, consider:

min f(x) s.t. Ax = b.

• The augmented Lagrangian is (with $\rho > 0$)

$$\mathcal{L}(x,\lambda;\rho) := \underbrace{f(x) + \lambda^{T}(Ax - b)}_{\text{Lagrangian}} + \underbrace{\frac{\rho}{2} \|Ax - b\|_{2}^{2}}_{\text{"augmentation"}}$$

• Basic augmented Lagrangian (a.k.a. method of multipliers) is

$$x_{k} = \arg\min_{x} \mathcal{L}(x, \lambda_{k-1}; \rho)$$
$$\lambda_{k} = \lambda_{k-1} + \rho(Ax_{k} - b);$$

(Hestenes, 1969; Powell, 1969)

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A Favorite Derivation

...more or less rigorous for convex f.

• Write the problem as

$$\min_{x} \max_{\lambda} f(x) + \lambda^{T} (Ax - b).$$

Obviously, the max w.r.t. λ will be $+\infty$, unless Ax = b, so this is equivalent to the original problem.

This equivalence is not very useful, computationally: the max_λ function is highly nonsmooth w.r.t. x. Smooth it by adding a "proximal point" term, penalizing deviations from a prior estimate λ

$$\min_{x} \left\{ \max_{\lambda} f(x) + \lambda^{T} (Ax - b) - \frac{1}{2\rho} \|\lambda - \bar{\lambda}\|^{2} \right\}.$$

• Maximization w.r.t. λ is now trivial (a concave quadratic), yielding

$$\lambda = \bar{\lambda} + \rho(Ax - b).$$

A Favorite Derivation (Cont.)

• Inserting
$$\lambda = \overline{\lambda} + \rho(Ax - b)$$
 leads to

$$\min_{x} f(x) + \overline{\lambda}^{T} (Ax - b) + \frac{\rho}{2} \|Ax - b\|^{2} = \mathcal{L}(x, \overline{\lambda}; \rho).$$

• Hence can view the augmented Lagrangian process as:

- \checkmark min_x $\mathcal{L}(x, \overline{\lambda}; \rho)$ to get new x;
- ✓ Shift the "prior" on λ by updating to the latest max: $\bar{\lambda} + \rho(Ax - b)$.
- ✓ repeat until convergence.
- Add subscripts, and we recover the augmented Lagrangian algorithm of the first slide!
- Can also increase ρ (to sharpen the effect of the prox term), if needed.

Inequality Constraints, Nonlinear Constraints

• The same derivation can be used for inequality constraints:

min f(x) s.t. $Ax \ge b$.

• Apply the same reasoning to the constrained min-max formulation:

$$\min_{x} \max_{\lambda \geq 0} f(x) - \lambda^{T} (Ax - b).$$

• After the prox-term is added, can find the minimizing λ in closed form (as for prox-operators). Leads to update formula:

$$\max\left(ar{\lambda}+
ho(Ax-b),0
ight).$$

 This derivation extends immediately to nonlinear constraints c(x) = 0 or c(x) ≥ 0.

"Explicit" Constraints, Inequality Constraints

- There may be other constraints on x (such as x ∈ Ω) that we prefer to handle explicitly in the subproblem.
- For the formulation $\min_{x} f(x)$, s.t. Ax = b, $x \in \Omega$, the min_x step can enforce $x \in \Omega$ explicitly:

$$\begin{aligned} x_k &= \arg\min_{x\in\Omega} \mathcal{L}(x,\lambda_{k-1};\rho);\\ \lambda_k &= \lambda_{k-1} + \rho(Ax_k - b); \end{aligned}$$

• This gives an alternative way to handle inequality constraints: introduce slacks *s*, and enforce them explicitly. That is, replace

$$\min_{x} f(x) \text{ s.t. } c(x) \ge 0,$$

by

$$\min_{x} f(x) \text{ s.t. } c(x) = s, \ s \ge 0.$$

"Explicit" Constraints, Inequality Constraints (Cont.)

• The augmented Lagrangian is now

$$\mathcal{L}(x,s,\lambda;\rho) := f(x) + \lambda^{\mathsf{T}}(c(x)-s) + \frac{\rho}{2} \|c(x)-s\|_2^2.$$

• Enforce $s \ge 0$ explicitly in the subproblem:

$$egin{aligned} &(x_k,s_k) = rg\min_{x,s}\mathcal{L}(x,s,\lambda_{k-1};
ho), & ext{s.t.} \;\; s \geq 0; \ &\lambda_k = \lambda_{k-1} +
ho(c(x_k) - s_k) \end{aligned}$$

There are good algorithmic options for dealing with bound constraints s ≥ 0 (gradient projection and its enhancements). This is used in the Lancelot code (Conn et al., 1992).

Quick History of Augmented Lagrangian

- Dates from at least 1969: Hestenes, Powell.
- Developments in 1970s, early 1980s by Rockafellar, Bertsekas, and others.
- Lancelot code for nonlinear programming: Conn, Gould, Toint, around 1992 (Conn et al., 1992).
- Lost favor somewhat as an approach for general nonlinear programming during the next 15 years.
- Recent revival in the context of sparse optimization and its many applications, in conjunction with splitting / coordinate descent.

Alternating Direction Method of Multipliers (ADMM)

• Consider now problems with a separable objective of the form

$$\min_{(x,z)} f(x) + h(z) \quad \text{s.t.} \quad Ax + Bz = c,$$

for which the augmented Lagrangian is

$$\mathcal{L}(x,z,\lambda;\rho) := f(x) + h(z) + \lambda^T (Ax + Bz - c) + \frac{\rho}{2} \|Ax - Bz - c\|_2^2.$$

- Standard AL would minimize L(x, z, λ; ρ) w.r.t. (x, z) jointly.
 However, since coupled in the quadratic term, separability is lost.
- In ADMM, minimize over x and z separately and sequentially:

$$\begin{aligned} x_k &= \arg\min_{x} \mathcal{L}(x, z_{k-1}, \lambda_{k-1}; \rho); \\ z_k &= \arg\min_{z} \mathcal{L}(x_k, z, \lambda_{k-1}; \rho); \\ \lambda_k &= \lambda_{k-1} + \rho(Ax_k + Bz_k - c). \end{aligned}$$

Main features of ADMM:

- Does one cycle of block-coordinate descent in (x, z).
- The minimizations over x and z add only a quadratic term to f and h, respectively. Usually does not alter the cost much.
- Can perform the (x, z) minimizations inexactly.
- Can add explicit (separated) constraints: $x \in \Omega_x$, $z \in \Omega_z$.
- Many (many!) recent applications to compressed sensing, image processing, matrix completion, sparse principal components analysis....

ADMM has a rich collection of antecendents, dating even to the 1950s (operator splitting).

For an comprehensive recent survey, including a diverse collection of machine learning applications, see Boyd et al. (2011).

ADMM for Consensus Optimization

Given the unconstrained (but separable) problem

$$\min \sum_{i=1}^m f_i(x),$$

form m copies of the x, with the original x as a "master" variable:

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$$\min_{x,x^1,x^2,...,x^m} \sum_{i=1}^m f_i(x^i) \text{ subject to } x^i - x = 0, \ i = 1, 2, ..., m.$$

Apply ADMM, with $z = (x^1, x^2, \dots, x^m)$. Get

$$\mathcal{L}(x, x^1, x^2, \dots, x^m, \lambda^1, \dots, \lambda^m; \rho) = \sum_{i=1}^m f_i(x^i) + (\lambda^i)^T (x^i - x) + \frac{\rho}{2} \|x^i - x\|_2^2.$$

The minimization w.r.t. $z = (x^1, x^2, \dots, x^m)$ is separable!

$$x_{k}^{i} = \arg\min_{x^{i}} f_{i}(x^{i}) + (\lambda_{k-1}^{i})^{T}(x^{i} - x_{k-1}) + \frac{\rho_{k}}{2} \|x^{i} - x_{k-1}\|_{2}^{2}, \ i = 1, 2, \dots, m.$$

Can be implemented in parallel.

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Consensus, continued

The minimization w.r.t. x can be done explicitly — averaging:

$$x_k = \frac{1}{m} \sum_{i=1}^m \left(x_k^i + \frac{1}{\rho_k} \lambda_{k-1}^i \right).$$

Update to λ^i can also be done in parallel, once the new x_k is known (and communicated):

$$\lambda_k^i = \lambda_{k-1}^i + \rho_k (x_k^i - x_k), \quad i = 1, 2, \dots, m.$$

If the initial λ_0^i have $\sum_{i=1}^m \lambda_0^i =$, can see that $\sum_{i=1}^m \lambda_k^i = 0$ at all iterations k. Can simplify the update for x_k :

$$x_k = \frac{1}{m} \sum_{i=1}^m x_k^i.$$

"Gather-Scatter" implementation.

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ADMM for Awkward Intersections

The feasible set is sometimes an intersection of two or more convex sets that are easy to handle separately (e.g. projections are easily computable), but whose intersection is more difficult to work with.

Example: Optimization over the cone of doubly nonnegative matrices:

$$\min_X f(X) \text{ s.t. } X \succeq 0, X \ge 0.$$

General form:

min
$$f(x)$$
 s.t. $x \in \Omega_i$, $i = 1, 2, \ldots, m$

Again, use a different copy x^i for each set, and constrain them all to be the same:

$$\min_{x,x^1,x^2,...,x^m} f(x) \text{ s.t. } x^i \in \Omega_i, \ x^i - x = 0, \ i = 1, 2, ..., m.$$

ADMM for Awkward Intersections

Separable minimizations over Ω_i , i = 1, 2, ..., m:

$$x_k^i = rg\min_{x_i \in \Omega_i} (\lambda_{k-1}^i)^T (x^i - x_{k-1}) + rac{
ho_k}{2} \|x_k - x^i\|_2^2, \ \ i = 1, 2, \dots, m.$$

Optimize over the master variable (unconstrained, with quadratic added to f):

$$x_{k} = \arg\min_{x} f(x) + \sum_{i=1}^{m} (\lambda_{k-1}^{i})^{T} (x - x_{k-1}^{i}) + \frac{\rho_{k}}{2} \|x - x_{k-1}^{i}\|_{2}^{2},$$

Update multipliers:

$$\lambda_k^i = \lambda_{k-1}^i + \rho_k(x_k - x_k^i), \ i = 1, 2, \dots, m.$$

- Often, a simpler version is enough: $\min_{(x,z)} f(x) + h(z)$ s.t. Ax = z, equivalent to $\min_{x} f(x) + h(Ax)$, often the one of interest.
- In this case, the ADMM can be written as

$$x_{k} = \arg\min_{x} f(x) + \frac{\rho}{2} ||Ax - z_{k-1} - d_{k-1}||_{2}^{2}$$
$$z_{k} = \arg\min_{z} h(z) + \frac{\rho}{2} ||Ax_{k-1} - z - d_{k-1}||_{2}^{2}$$
$$d_{k} = d_{k-1} - (Ax_{k} - z_{k})$$

the so-called "scaled version" (Boyd et al., 2011).

- Updating z_k is a proximity computation: $z_k = \text{prox}_{h/\rho} (A x_{k-1} d_{k-1})$
- Updating x_k may be hard: if f is quadratic, involves matrix inversion; if f is not quadratic, may be as hard as the original problem.

ADMM: Convergence

- Consider the problem $\min_{x} f(x) + h(Ax)$, where f and h are lower semi-continuous, proper, convex functions and A has full column rank.
- The ADMM algorithm presented in the previous slide converges (for any ρ > 0) to a solution x*, if one exists, otherwise it diverges.

This is a cornerstone result by Eckstein and Bertsekas (1992).

- As in IST/FBS/PGA, convergence is still guaranteed with inexactly solved subproblems, as long as the errors are absolutely summable.
- The recent explosion of interest in ADMM is clear in the citation records of the review paper of Boyd et al. (2011) (2800 and counting) and of the paper by Eckstein and Bertsekas (1992):



ADMM for a More General Problem

- Consider the problem $\min_{x \in \mathbb{R}^n} \sum_{i=1}^{J} g_j(H^{(j)}x)$, where $H^{(j)} \in \mathbb{R}^{p_j \times n}$, and $g_1, ..., g_J$ are l.s.c proper convex fuctions.
- Map it into $\min_{x} f(x) + h(Ax)$ as follows (with $p = p_1 + \dots + p_J$): • f(x) = 0• $A = \begin{bmatrix} H^{(1)} \\ \vdots \\ H^{(J)} \end{bmatrix} \in \mathbb{R}^{p \times n},$ • $h : \mathbb{R}^{p_1 + \dots + p_J} \to \overline{\mathbb{R}}, \quad h\left(\begin{bmatrix} z^{(1)} \\ \vdots \\ z^{(J)} \end{bmatrix} \right) = \sum_{j=1}^{J} g_j(z^{(j)})$

• This leads to a convenient version of ADMM.

ADMM for a More General Problem (Cont.)

Resulting instance of

$$\begin{aligned} x_{k} &= \arg\min_{x} \|Az - z_{k} - d_{k}\|_{2}^{2} = \left(\sum_{j=1}^{J} (H^{(j)})^{T} H^{(j)}\right)^{-1} \left(\sum_{j=1}^{J} (H^{(j)})^{T} (z_{k-1}^{(j)} + d_{k-1}^{(j)})\right) \\ z_{k}^{(1)} &= \arg\min_{u} g_{1} + \frac{\rho}{2} \|u - H^{(1)} x_{k-1} + d_{k-1}^{(1)}\|_{2}^{2} = \operatorname{prox}_{g_{1}/\rho} (H^{(1)} x_{k-1} - d_{k-1}^{(1)}) \\ \vdots & \vdots & \vdots \\ z_{k}^{(J)} &= \arg\min_{u} g_{J} + \frac{\rho}{2} \|u - H^{(J)} x_{k-1} + d_{k-1}^{(J)}\|_{2}^{2} = \operatorname{prox}_{g_{J}/\rho} (H^{(J)} x_{k-1} - d_{k-1}^{(J)}) \\ d_{k} &= d_{k-1} - A x_{k} + z_{k} \end{aligned}$$

Key features: matrices are handled separately from the prox operators; the prox operators are decoupled (can be computed in parallel); requires a matrix inversion (can be a curse or a blessing).

(Afonso et al., 2010; Setzer et al., 2010; Combettes and Pesquet, 2011)

Special Case: ℓ_2 - ℓ_1

Standard problem: $\min_x \frac{1}{2} ||Ax - b||_2^2 + ||x||_1$ In this case, the ADMM becomes

$$x_{k} = \arg\min_{x} ||x||_{1} + \frac{\rho}{2} ||Ax - z_{k-1} - d_{k-1}||_{2}^{2}$$
$$z_{k} = \arg\min_{z} h(z) + \frac{\rho}{2} ||Ax_{k-1} - z - d_{k-1}||_{2}^{2}$$
$$d_{k} = d_{k-1} - (Ax_{k} - z_{k})$$

Subproblems are

$$\begin{aligned} x_k &:= (A^T A + \rho_k I)^{-1} (A^T b + \rho_k z_{k-1} - \lambda_k), \\ z_k &:= \min_{z} \tau \|z\|_1 + (\lambda_k)^T (x_k - z) + \frac{\rho_k}{2} \|z - x_k\|_2^2 \\ &= \operatorname{prox}_{\tau/\rho_k} (x_k + \lambda_k/\rho_k) \\ \lambda_{k+1} &:= \lambda_k + \rho_k (x_k - z_k). \end{aligned}$$

Solving for x_k is the most complicated part of the calculation. If the least-squares part is underdetermined (A is $m \times n$ with n > m), can make

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Augmented Lagrangian

Moreover, in some compressed sensing applications, we have $AA^T = I$. In this case, x_k can be recovered at the cost of two matrix-vector multiplications involving A.

Otherwise, can solve for x_k inexactly, using a few steps of an iterative method.

The YALL1 code solves this problem, and other problems with more general regularizers (e.g. groups).

The subproblems are **not** too different from those obtained in prox-linear algorithms (e.g. SpaRSA):

- λ_k is asymptotically similar to the gradient term in prox-linear, that is, λ_k ≈ ∇f(x_k);
- Thus, the minimization over z is quite similar to the prox-linear step.

ADMM for Sparse Inverse Covariance

$$\max_{X \succ 0} \log \det(X) - \langle X, S \rangle - \tau \|X\|_1,$$

Reformulate as

$$\max_{X\succ 0} \log \det(X) - \langle X,S\rangle - \tau \|Z\|_1 \quad \text{s.t.} \ X - Z = 0.$$

Subproblems are:

$$\begin{split} X_k &:= \arg\max_X \log \det(X) - \langle X, S \rangle - \langle U_{k-1}, X - Z_{k-1} \rangle \\ &\quad - \frac{\rho_k}{2} \| X - Z_{k-1} \|_F^2 \\ &:= \arg\max_X \log \det(X) - \langle X, S \rangle - \frac{\rho_k}{2} \| X - Z_{k-1} + U_k / \rho_k \|_F^2 \\ Z_k &:= \operatorname{prox}_{\tau / \rho_k} (X_k + U_k); \\ U_{k+1} &:= U_k + \rho_k (X_k - Z_k). \end{split}$$

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Solving for X

Get optimality condition for the X subproblem by using $\nabla_X \log \det(X) = X^{-1}$, when X is s.p.d. Thus,

$$X^{-1} - S - \rho_k (X - Z_{k-1} + U_k / \rho_k) = 0,$$

which is equivalent to

$$X^{-1} - \rho_k X - (S - \rho_k Z_{k-1} + U_k) = 0.$$

Form eigendecomposition

$$(S - \rho_k Z_{k-1} + U_k) = Q \Lambda Q^T,$$

where Q is $n \times n$ orthogonal and Λ is diagonal with elements λ_i . Seek X with the form $Q \tilde{\Lambda} Q^T$, where $\tilde{\Lambda}$ has diagonals $\tilde{\lambda}_i$. Must have

$$\frac{1}{\tilde{\lambda}_i} - \rho_k \tilde{\lambda}_i - \lambda_i = 0, \quad i = 1, 2, \dots, n.$$

Take positive roots: $\tilde{\lambda}_i = [\lambda_i + \sqrt{\lambda_i^2 + 4\rho_k}]/(2\rho_k)$, i = 1, 2, ..., n.

Further Reading

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