First-order Methods

Unconstrained optimization

- Problem

$$\min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x})$$

- First-order optimality condition

$$\nabla f(\mathbf{x}^\star) = 0.$$

Gradient descent method

- Iteration:

$$\boxed{\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \gamma_t \nabla f(\mathbf{x}^{(t)})}$$

for some step size γ_t. This is a special case of the Netwon-type algorithms with $\mathbf{H}_t = \mathbf{I}$ and $\Delta\mathbf{x} = \nabla f(\mathbf{x}^{(t)})$.

- Idea: iterative linear approximation (first-order Taylor series expansion).

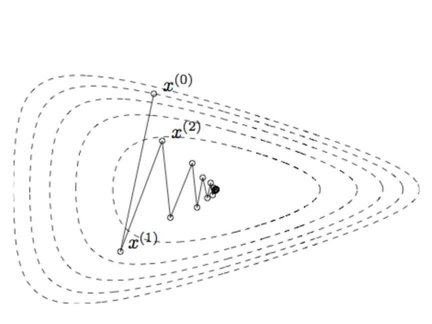
$$f(\mathbf{x}) \approx f(\mathbf{x}^{(t)}) + \nabla f(\mathbf{x}^{(t)})^T(\mathbf{x} - \mathbf{x}^{(t)})$$

and then minimize the linear approximation within a compact set: let $\Delta\mathbf{x} = \mathbf{x}^{(t+1)} - \mathbf{x}^{(t)}$ to choose. Solve

$$\min_{\|\Delta\mathbf{x}\|_2\le 1} \nabla f(\mathbf{x}^{(t)})^T\Delta\mathbf{x}$$

to obtain $\Delta\mathbf{x} = -\nabla f(\mathbf{x}^{(t)})/\|f(\mathbf{x}^{(t)})\|_2 \propto -\nabla f(\mathbf{x}^{(t)})$.

- Step sizes are chosen so that the descent property is maintained (e.g., line search).
  - Step size *must* be chosen at any time, since unlike Netwon's method, first-order approximation is always unbounded below.
- Pros
  - Each iteration is inexpensive.
  - No need to derive, compute, store and invert Hessians; attractive in large scale problems.
- Cons
  - Slow convergence (zigzagging).



  - Do not work for non-smooth problems.

Convergence

- In general, the best we can obtain from gradient descent is linear convergence (cf. quadratic convergence of Newton).
- Example (Boyd & Vandenberghe Section 9.3.2)

$$f(\mathbf{x}) = \frac{1}{2}(x_1^2 + cx_2^2), \quad c > 1$$

  The optimal value is 0.

  It can be shown that if we start from $x^{(0)} = (c, 1)$, then

$$f(\mathbf{x}^{(t)}) = \left(\frac{c-1}{c+1}\right)^t f(\mathbf{x}^{(0)})$$

  and

$$\|\mathbf{x}^{(t)} - \mathbf{x}^\star\|_2 = \left(\frac{c-1}{c+1}\right)^t \|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2$$

- More generally, if

  1. f is convex and differentiable over $\mathbb{R}^d$;
  2. f has L-Lipschitz gradients, i.e., $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \le L\|\mathbf{x} - \mathbf{y}\|_2$;
  3. $p^\star = \inf_{\mathbf{x}\in\mathbb{R}^d} f(x) > -\infty$ and attained at $\mathbf{x}^\star$,

  then

$$f(\mathbf{x}^{(t)}) - p^\star \le \frac{1}{2\gamma t}\|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2 = O(1/t).$$

  for constant step size ($\gamma_t = \gamma \in (0, 1/L]$), a *sublinear* convergence. Similar upper bound with line search.
- If we further assume that f is α-strongly convex, i.e., $f(\mathbf{x}) - \frac{\alpha}{2}\|\mathbf{x}\|_2^2$ is convex for some $\alpha > 0$, then

$$f(\mathbf{x}^{(t)}) - p^\star \le \frac{L}{2}\left(1 - \gamma\frac{2\alpha L}{\alpha + L}\right)^t \|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2$$

  and

$$\|\mathbf{x}^{(t)} - \mathbf{x}^\star\|_2^2 \le \left(1 - \gamma\frac{2\alpha L}{\alpha + L}\right)^t \|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2$$

  for constant step size $\gamma \in (0, 2/(\alpha + L)]$.

Examples

- Least squares: $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2 = \frac{1}{2}\mathbf{x}^T\mathbf{A}^T\mathbf{A}\mathbf{x} - \mathbf{x}^T\mathbf{A}^T\mathbf{y} + \frac{1}{2}\mathbf{y}^T\mathbf{y}$
- Gradient $\nabla f(\mathbf{x}) = \mathbf{A}^T\mathbf{A}\mathbf{x} - \mathbf{A}^T\mathbf{y}$ is $\|\mathbf{A}^T\mathbf{A}\|_2$-Lipschitz. Hence $\gamma \in (0, 1/\sigma_{\max}(\mathbf{A})^2]$ guarantees descent property and convergence.
- If $\mathbf{A}$ is full column rank, then f is also $\sigma_{\min}(\mathbf{A})^2$-strongly convex and the convergence is linear. Otherwise it is sublinear.
- Logistic regression: $f(\beta) = -\sum_{i=1}^n \left[y_i\mathbf{x}_i^T\beta - \log(1 + e^{\mathbf{x}_i^T\beta})\right]$
- Gradient $\nabla f(\beta) = -\mathbf{X}^T(\mathbf{y} - \mathbf{p})$ is $\frac{1}{4}\|\mathbf{X}^T\mathbf{X}\|_2$-Lipschitz.
- Even if $\mathbf{X}$ is full column rank, f may not be strongly convex.
- Adding a ridge penalty $\frac{\rho}{2}\|\mathbf{x}\|_2^2$ makes the problems *always* strongly convex.

Accelerated gradient descent

First-order methods

- Iterative algorithm that generates sequence $\{\mathbf{x}^{(t)}\}$ such that

$$\mathbf{x}^{(t)} \in \mathbf{x}^{(0)} + \text{span}\{\nabla f(\mathbf{x}^{(0)}), \dots, \nabla f(\mathbf{x}^{(t-1)})\}.$$

- Examples:
  - Gradient descent: $\mathbf{x}^{(t)} = \mathbf{x}^{(t-1)} - \gamma_t\nabla f(\mathbf{x}^{(t)})$.
  - Momentum method: $\mathbf{y}^{(t)} = \mathbf{x}^{(t-1)} - \gamma_t\nabla f(\mathbf{x}^{(t)})$, $\mathbf{x}^{(t)} = \mathbf{y}^{(t)} + \alpha_k(\mathbf{y}^{(t)} - \mathbf{y}^{(t-1)})$.
- In general, a first-order method generates

$$\mathbf{x}^{(t)} = \mathbf{x}^{(0)} - \sum_{k=1}^{t-1}\gamma_{t,k}\nabla f(\mathbf{x}^{(k)}) =: M_t(f, \mathbf{x}^{(0)}).$$

- Collection of all first-order method can be considered as the set of all M_N. Let's denote it by $\mathcal{M}_N$.
- Then we want to find a method $M_N \in \mathcal{M}_N$ that minimizes

$$\sup_{f\in\mathcal{F}} f(M_N(f, \mathbf{x}^{(0)})) - p^\star.$$

  for a class of functions $\mathcal{F}$.
- Typically we choose the class of functions as $\mathcal{F}_L$, the set of functions satisfying the 3 assumptions used for convergence analysis of GD:

  1. f is convex and differentiable over $\mathbb{R}^d$;
  2. f has L-Lipschitz gradients, i.e., $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \le L\|\mathbf{x} - \mathbf{y}\|_2$;
  3. $p^\star = \inf_{\mathbf{x}\in\mathbb{R}^d} f(x) > -\infty$ and attained at $\mathbf{x}^\star$.
- We have seen that for gradient descent with a step size $1/L$,

$$\sup_{f\in\mathcal{F}_L} f(M_N(f, \mathbf{x}^{(0)})) - p^\star \le \frac{L}{2N}\|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2 = O(1/N).$$

- Nesterov (1983) showed that for $d \ge 2N + 1$ and every $\mathbf{x}^{(0)}$, there exists $f \in \mathcal{F}_L$ such that **for any** $M_N \in \mathcal{M}_N$,

$$f(\mathbf{x}^{(N)}) - p^\star \ge \frac{3L}{32(N+1)^2}\|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2.$$

  suggesting that the minimax optimal rate of first order methods is at most $O(1/N^2)$.
- This also suggests that the $O(1/N)$ rate of GD can be improved.
- Nesterov's (1983) accelerated gradient method achieves the optimal rate:

$$\begin{aligned}
\mathbf{y}^{(t+1)} &= \mathbf{x}^{(t)} - \frac{1}{L}\nabla f(\mathbf{x}^{(t)}) \\
\gamma_{t+1} &= \frac{1}{2}(1 + \sqrt{1 + 4\gamma_t^2}) \\
\mathbf{x}^{(t+1)} &= \mathbf{y}^{(t+1)} + \frac{\gamma_t - 1}{\gamma_{t+1}}(\mathbf{y}^{(t+1)} - \mathbf{y}^{(t)})
\end{aligned}$$

  with initializtion $\mathbf{y}^{(0)} = \mathbf{x}^{(0)}$ and $\gamma_0 = 1$.
- Theorem (Nesterov, 1983): Nesterov's accelerated gradient method algorithm satisfies

$$f(\mathbf{y}^{(t)}) - p^\star \le \frac{2L}{(t+1)^2}\|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2.$$

  for $f \in \mathcal{F}_L$.
- Kim & Fessler's (2016) algorithm improved this rate by a factor of two:

$$f(\mathbf{x}^{(N)}) - p^\star \le \frac{L}{(N+1)^2}R^2$$

  for $f \in \mathcal{F}_L$ and $\|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2 \le R$.

Steepest descent method

- Recall the idea of GD: iterative linear approximation (first-order Taylor series expansion).

$$f(\mathbf{x}) \approx f(\mathbf{x}^{(t)}) + \nabla f(\mathbf{x}^{(t)})^T(\mathbf{x} - \mathbf{x}^{(t)})$$

  and then minimize the linear approximation within a compact set:

$$\min_{\|\Delta\mathbf{x}\|_2\le 1} \nabla f(\mathbf{x}^{(t)})^T\Delta\mathbf{x}.$$

- The compact set need not be limitted to the ℓ_2 norm ball in order to obtain a descent direction. For any unit norm ball,

$$\min_{\|\Delta\mathbf{x}\|\le 1} \nabla f(\mathbf{x}^{(t)})^T\Delta\mathbf{x} = -\|\nabla f(\mathbf{x}^{(t)})\|_*$$

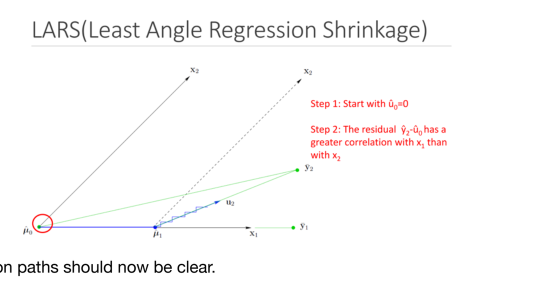
- In particular, if ℓ_1 norm ball is used, then

$$\min_{\|\Delta\mathbf{x}\|_1\le 1} \nabla f(\mathbf{x}^{(t)})^T\Delta\mathbf{x} = -\|\nabla f(\mathbf{x}^{(t)})\|_\infty = -\max_{i=1,\dots,d}|[\nabla f(\mathbf{x}^{(t)})]_i|$$

  and the descent direction is given by the convex hull of the elementary unit vectors corresponding to the coordinates of the maximum absolute derivatives. In other words,

$$\Delta\mathbf{x} = \sum_{i\in J}\alpha_i\,\text{sign}([\nabla f(\mathbf{x}^{(t)})]_i)\mathbf{e}_i, \quad \alpha_i \ge 0, \ \sum_{i\in J}\alpha_i = 1, \quad J = \{j : |[\nabla f(\mathbf{x}^{(t)})]_j| = \|\nabla f(\mathbf{x}^{(t)})\|_\infty\}.$$

- Consider a linear regression setting. Assume each coordinate is standardized. If $\alpha_i = 1/|J|$ for $i \in J$, then the ℓ_1-steepest descent update with a line search strategy of finding the maximal step size with which J does not vary is the least angle regression (LAR). If only one coordinate is chosen and a very small step size ϵ is used, then this update is ϵ-forward stagewise regression.



  Why these algorithms generate sparse solution paths should now be clear.

Proximal gradient methods

Constrained optimization

- Problem

$$\min_{\mathbf{x}\in C\subset\mathbb{R}^d} f(\mathbf{x}) = \min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x}) + \iota_C(\mathbf{x})$$

  where $\iota_C(\mathbf{x})$ is the indicator function of the constrained set C.
- Can be viewed as an unconstrained but nonsmooth problem.
- Recall that GD does not work for non-smooth problems. Need a new first-order method.
- Consider a genearalization

$$\min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x}) + g(\mathbf{x})$$

  where f is smooth but g is nonsmooth.

First-order optimality condition

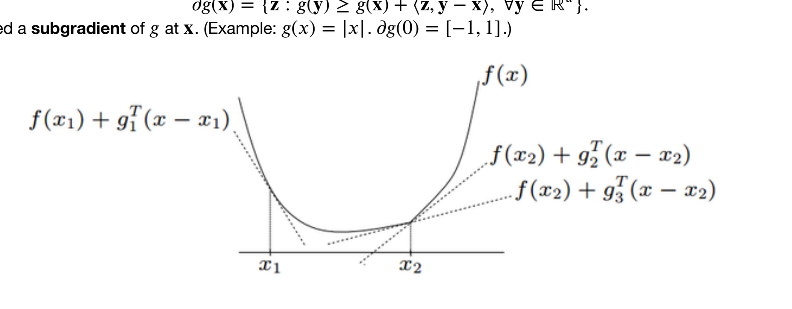
- Assume convexity of f and g. Then $\mathbf{x}^\star$ minimizes $f(\mathbf{x}) + g(\mathbf{x})$ if and only if

$$\nabla f(\mathbf{x}^\star) + \partial g(\mathbf{x}^\star) \ni 0,$$

  where $\partial g(\mathbf{x})$ is the **subdifferential** of g at $\mathbf{x}$:

$$\partial g(\mathbf{x}) = \{\mathbf{z} : g(\mathbf{y}) \ge g(\mathbf{x}) + \langle\mathbf{z}, \mathbf{y} - \mathbf{x}\rangle, \ \forall\mathbf{y} \in \mathbb{R}^d\}.$$

  Vector $\mathbf{z} \in \partial g(\mathbf{x})$ is called a **subgradient** of g at $\mathbf{x}$. (Example: $g(x) = |x|$. $\partial g(0) = [-1, 1]$.)



Proximal gradient

- Proximal gradient solves the nonsmooth first-order opitimality condition in the same spirit as GD.
- Motivation: alternative view of GD

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)}) = \arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{f(\mathbf{x}^{(t)}) + \langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x} - \mathbf{x}^{(t)}\rangle + \frac{1}{2\gamma_t}\|\mathbf{x} - \mathbf{x}^{(t)}\|_2^2\right\}$$

  Thus consider

$$\begin{aligned}
\mathbf{x}^{(t+1)} &= \arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{f(\mathbf{x}^{(t)}) + \langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x} - \mathbf{x}^{(t)}\rangle + \frac{1}{2\gamma_t}\|\mathbf{x} - \mathbf{x}^{(t)}\|_2^2 + g(\mathbf{x})\right\} \\
&= \arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\gamma_t g(\mathbf{x}) + \frac{1}{2}\|\mathbf{x} - [\mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)})]\|_2^2\right\}.
\end{aligned}$$

- The map

$$\mathbf{x} \mapsto \arg\min_{\mathbf{y}\in\mathbb{R}^d}\left\{\phi(\mathbf{y}) + \frac{1}{2}\|\mathbf{y} - \mathbf{x}\|_2^2\right\}$$

  is called the proximal map, proximal operator, or proximity operator of ϕ, denoted by

$$\mathbf{prox}_\phi(\mathbf{x}).$$

- Thus the new update rule is

$$\boxed{\mathbf{x}^{(t+1)} = \mathbf{prox}_{\gamma_t g}\left(\mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)})\right)}$$

  and called the **proximal gradient method**.

Proximal maps

- A key to success of the proximal gradient method is the ease of evaluation of the proximal map $\mathbf{prox}_{\gamma g}(\cdot)$. Often proximal maps have closed-form solutions.
- Examples

  1. If $g(\mathbf{x}) \equiv 0$, then $\mathbf{prox}_{\gamma g}(\mathbf{x}) = \mathbf{x}$. PG reduces to GD.
  2. If $g(\mathbf{x}) = \iota_C(\mathbf{x})$ for a closed convex set C, then $\mathbf{prox}_{\gamma g}(\mathbf{x}) = P_C(\mathbf{x})$, or the orthogonal projection of $\mathbf{x}$ to set C. Proximal gradient reduces to projected gradient.
  3. If $g(\mathbf{x}) = \lambda\|\mathbf{x}\|_1$, then $\mathbf{prox}_{\gamma g}(\mathbf{x}) = S_{\lambda\gamma}(\mathbf{x}) = (\text{sign}(x_i)(|x_i| - \lambda\gamma))_{i=1}^d$, the soft-thresholding operator.
  4. If $g(\mathbf{x}) = \lambda\|\mathbf{x}\|_2$, then

$$\mathbf{prox}_{\gamma g}(\mathbf{x}) = \begin{cases}(1 - \lambda\gamma/\|\mathbf{x}\|_2)\mathbf{x}, & \|\mathbf{x}\|_2 \ge \lambda\gamma \\ \mathbf{0}, & \text{otherwise}\end{cases}$$

  5. If $g(\mathbf{X}) = \lambda\|\mathbf{X}\|_*$ (nuclear norm), then $\mathbf{prox}_{\gamma g}(\mathbf{X}) = \mathbf{U}\text{diag}((\sigma_1 - \lambda\gamma)_+, \dots, (\sigma_r - \lambda\gamma)_+)\mathbf{V}^T$, when the SVD of $\mathbf{X}$ is $\mathbf{X} = \mathbf{U}\text{diag}(\sigma_1, \dots, \sigma_r)\mathbf{V}^T$.
- Lasso

$$\min_\beta \frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda\|\beta\|_1$$

  - $f(\beta) = \frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|_2^2$, $\nabla f(\beta) = \mathbf{X}^T(\mathbf{X}\beta - \mathbf{y})$
  - $g(\beta) = \lambda\|\beta\|_1$.
  - Update rule: $\beta^{(t+1)} = S_{\lambda\gamma_t}\left(\beta^{(t)} - \gamma_t\mathbf{X}^T(\mathbf{X}\beta^{(t)} - \mathbf{y})\right)$. Can be computed in parallel (including matrix-vector multiplications).

Convergence

- It can be shown that if

  1. f is convex and differentiable over $\mathbb{R}^d$;
  2. f has L-Lipschitz gradients, i.e., $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \le L\|\mathbf{x} - \mathbf{y}\|_2$;
  3. g is a closed convex function (i.e., $\mathbf{epi}f$ is closed);
  4. $p^\star = \inf_{\mathbf{x}\in\mathbb{R}^d} f(x) + g(x) > -\infty$ and attained at $\mathbf{x}^\star$.

  then proximal gradient method converges to an optimal solution, at the same rate (in terms of objective values) as GD. For example, with a constant step size $\gamma_t = \gamma = 1/L$,

$$f(\mathbf{x}^{(t)}) + g(\mathbf{x}^{(t)}) - p^\star \le \frac{L}{2t}\|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2.$$

  A similar rate holds with backtracking.
- If f or g is strongly convex, linear convergence.

FISTA: accelerated proximal gradient

- Fast Iterative Shrinkage-Thresholding Algorithm (Beck & Tebolle, 2009)

$$\begin{aligned}
\mathbf{y} &= \mathbf{x}^{(t)} + \frac{t-1}{t+2}(\mathbf{x}^{(t)} - \mathbf{x}^{(t-1)}) \\
\mathbf{x}^{(t+1)} &= \mathbf{prox}_{\gamma_t g}(\mathbf{y} - \gamma_t\nabla g(\mathbf{y}))
\end{aligned}$$

with initialization $\mathbf{x}^{(-1)} = \mathbf{x}^{(0)}$.

- Proximal gradient version of Nesterov's (1983) accelerated gradient algorithm.
- Under the above assumptions and with a constant step size $\gamma_t = \gamma = 1/L$,

$$f(\mathbf{x}^{(N)}) + g(\mathbf{x}^{(N)}) - p^\star \le \frac{L}{2(N+1)^2}\|\mathbf{x}^{(0)} - \mathbf{x}^\star\|_2^2.$$

Mirror descent method

- Again, constrained optimization problem

$$\min_{\mathbf{x}\in C\subset\mathbb{R}^d} f(\mathbf{x}).$$

- Second alternative view of GD

$$\begin{aligned}
\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)}) &= \arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{f(\mathbf{x}^{(t)}) + \langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x} - \mathbf{x}^{(t)}\rangle + \frac{1}{2\gamma_t}\|\mathbf{x} - \mathbf{x}^{(t)}\|_2^2\right\} \\
&= \arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle + \frac{1}{2\gamma_t}\|\mathbf{x} - \mathbf{x}^{(t)}\|_2^2\right\}
\end{aligned}$$

- or projected (proximal) gradient

$$\mathbf{x}^{(t+1)} = P_C\left(\mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)})\right) = P_C\left(\arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle + \frac{1}{2\gamma_t}\|\mathbf{x} - \mathbf{x}^{(t)}\|_2^2\right\}\right)$$

- This relies too much on the (Euclidean) geometry of $\mathbb{R}^d$: $\|\cdot\|_2 = \langle\cdot,\cdot\rangle$.
- If the distance measure $\frac{1}{2}\|\mathbf{x} - \mathbf{y}\|_2^2$ is replaced by something else (say $d(\mathbf{x}, \mathbf{y})$) that better reflects the geometry of C, then update such as

$$\mathbf{x}^{(t+1)} = P_C^d\left(\arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle + \frac{1}{\gamma_t}d(\mathbf{x}, \mathbf{x}^{(t)})\right\}\right)$$

  may converge faster. Here,

$$P_C^d(\mathbf{y}) = \arg\min_{\mathbf{x}\in C} d(\mathbf{x}, \mathbf{y})$$

  to reflect the geometry.

Bregman divergence

- Let $\phi : \mathcal{X} \to \mathbb{R}$ be a continuously differentiable, strictly convex function defined on a vector space $\mathcal{X} \subset \mathbb{R}^d$. The **Bregman divergence** with respect to ϕ is defined by

$$B_\phi(\mathbf{x}\|\mathbf{y}) = \phi(\mathbf{x}) - \phi(\mathbf{y}) - \langle\nabla\phi(\mathbf{y}), \mathbf{x} - \mathbf{y}\rangle$$

- It can be shown that $B_\phi(\mathbf{x}\|\mathbf{y}) \ge 0$ and $B_\phi(\mathbf{x}\|\mathbf{y}) = 0 \iff \mathbf{x} = \mathbf{y}$. But $B_\phi(\mathbf{x}\|\mathbf{y}) \ne B_\phi(\mathbf{y}\|\mathbf{x})$ in general.
- Examples
  - $\phi(\mathbf{x}) = \frac{1}{2}\|\mathbf{x}\|_2^2$, $\mathcal{X} = \mathbb{R}^d$: $B_\phi(\mathbf{x}\|\mathbf{y}) = \frac{1}{2}\|\mathbf{x} - \mathbf{y}\|_2^2$.
  - $\phi(\mathbf{x}) = \sum_{i=1}^d x_i\log x_i - \sum_{i=1}^d x_i$, $\mathcal{X} = \mathbb{R}_{++}^d$ (generalized negative entropy): $B_\phi(\mathbf{x}\|\mathbf{y}) = \sum_{i=1}^d x_i\log\frac{x_i}{y_i} - \sum_{i=1}^d x_i - \sum_{i=1}^d y_i$ (generalized Kullback-Leibler divergence).
  - $\phi(\mathbf{X}) = -\log\det\mathbf{X}$, $\mathcal{X} = \mathbb{S}_{++}^d$: $B_\phi(\mathbf{X}, \mathbf{Y}) = \mathbf{tr}(\mathbf{X}\mathbf{Y}^{-1}) - d - \log\det(\mathbf{X}\mathbf{Y}^{-1})$ (log-det divergence).
- If ϕ is α-strongly convex with respect to norm $\|\cdot\|$, i.e.,

$$\phi(\mathbf{y}) \ge \phi(\mathbf{x}) + \langle\nabla\phi(\mathbf{y}, \mathbf{y} - \mathbf{x}\rangle + \frac{\alpha}{2}\|\mathbf{y} - \mathbf{x}\|^2,$$

  then

$$B_\phi(\mathbf{x}\|\mathbf{y}) \ge \frac{\alpha}{2}\|\mathbf{x} - \mathbf{y}\|^2.$$

  - Negative entropy is 1-strongly convex with respect to $\|\cdot\|_1$.
- Projection onto $C \subset \mathcal{X}$ under the Bregman divergence

$$P_C^\phi(\mathbf{y}) = \arg\min_{\mathbf{x}\in C} B_\phi(\mathbf{x}\|\mathbf{y}) = \arg\min_{\mathbf{x}\in C}\{\phi(\mathbf{x}) - \phi(\mathbf{y}) - \langle\nabla\phi(\mathbf{y}), \mathbf{x} - \mathbf{y}\rangle\} = \arg\min_{\mathbf{x}\in C}\{\phi(\mathbf{x}) - \langle\nabla\phi(\mathbf{y}), \mathbf{x}\rangle\}$$

Mirror descent

- Minimization over a closed convex set $C \subset \mathcal{X}$ by:

$$\begin{aligned}
\mathbf{x}^{(t+1)} &= P_C^\phi\left(\arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle + \frac{1}{2\gamma_t}B_\phi(\mathbf{x}\|\mathbf{x}^{(t)})\right\}\right) \\
&= P_C^\phi\left(\arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\gamma_t\langle\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle + \phi(\mathbf{x}) - \phi(\mathbf{x}^{(t)}) - \langle\nabla\phi(\mathbf{x}^{(t)}), \mathbf{x} - \mathbf{x}^{(t)}\rangle\right\}\right) \\
&= P_C^\phi\left(\arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\phi(\mathbf{x}) - \langle\nabla\phi(\mathbf{x}^{(t)}) - \gamma_t\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle\right\}\right).
\end{aligned}$$

- In the inner (unconstrained) minimization step, the optimiality condition is

$$\nabla\phi(\mathbf{x}) = \nabla\phi(\mathbf{x}^{(t)}) - \gamma_t\nabla f(\mathbf{x}^{(t)})$$

  If ϕ is strongly convex, then this is equivalent to

$$\mathbf{x} = \nabla\phi^*\left(\nabla\phi(\mathbf{x}^{(t)}) - \gamma_t\nabla f(\mathbf{x}^{(t)})\right),$$

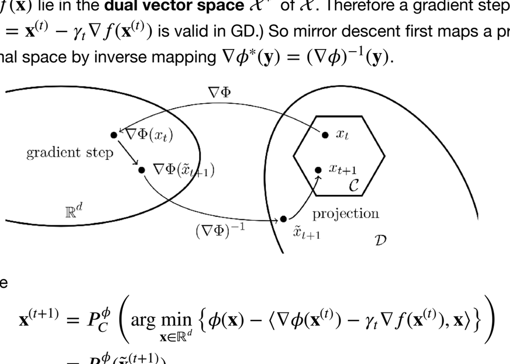
  where $\phi^*(\cdot)$ is the **Fenchel conjugate** function of ϕ:

$$\phi^*(\mathbf{y}) = \sup_{\mathbf{x}\in\mathbb{R}^d}\langle\mathbf{x}, \mathbf{y}\rangle - \phi(\mathbf{x})$$

  (assuming $\phi(\mathbf{x}) = \infty$ if $\mathbf{x} \notin \mathcal{X}$).
  - If $\phi(\cdot)$ is strongly convex, $\phi^*(\cdot)$ is *differentiable*. Hence $\nabla\phi^*(\cdot)$ is well-defined. Furthermore, $\nabla\phi^*(\nabla\phi(\mathbf{x})) = \mathbf{x}$.
- Hence a mirror descent iteration consists of:

$$\begin{aligned}
\mathbf{y}^{(t+1)} &= \nabla\phi(\mathbf{x}^{(t)}) - \gamma_t\nabla f(\mathbf{x}^{(t)}) \quad \text{(gradient step)} \\
\tilde{\mathbf{x}}^{(t+1)} &= \nabla\phi^*(\mathbf{y}^{(t+1)}) \quad \text{(mirroring step)} \\
\mathbf{x}^{(t+1)} &= P_C^\phi(\tilde{\mathbf{x}}^{(t+1)}) \quad \text{(projection step)}
\end{aligned}$$

- Technically speaking, gradients $\nabla\phi(\mathbf{x})$, $\nabla f(\mathbf{x})$ lie in the **dual vector space** $\mathcal{X}^*$ of $\mathcal{X}$. Therefore a gradient step should be taken in the dual space. (If $\mathcal{X} = \mathbb{R}^d$, then $\mathcal{X}^* = \mathcal{X}$. That's why $\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)})$ is valid in GD.) So mirror descent first maps a primal point $\mathbf{x}$ to its dual point $\phi(\mathbf{x})$, takes a gradient step, and maps it back to the primal space by inverse mapping $\nabla\phi^*(\mathbf{y}) = (\nabla\phi)^{-1}(\mathbf{y})$.



- Actual computation can be simplified, since

$$\begin{aligned}
\mathbf{x}^{(t+1)} &= P_C^\phi\left(\arg\min_{\mathbf{x}\in\mathbb{R}^d}\left\{\phi(\mathbf{x}) - \langle\nabla\phi(\mathbf{x}^{(t)}) - \gamma_t\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle\right\}\right) \\
&= P_C^\phi(\tilde{\mathbf{x}}^{(t+1)}) \\
&= \arg\min_{\mathbf{x}\in C}\left\{\phi(\mathbf{x}) - \langle\nabla\phi(\tilde{\mathbf{x}}^{(t+1)}), \mathbf{x}\rangle\right\} \\
&= \arg\min_{\mathbf{x}\in C}\left\{\phi(\mathbf{x}) - \langle\mathbf{y}^{(t+1)}, \mathbf{x}\rangle\right\} \\
&= \arg\min_{\mathbf{x}\in C}\left\{\phi(\mathbf{x}) - \langle\nabla\phi(\mathbf{x}^{(t)}) - \gamma_t\nabla f(\mathbf{x}^{(t)}), \mathbf{x}\rangle\right\}.
\end{aligned}$$

  Compare the first and the last lines.
- Convergence rates are similar to GD, with smaller constants.

Mirror descent example

- Optimization over probability simplex $\Delta^{d-1} = \{\mathbf{x} \in \mathcal{X} = \mathbb{R}_{++}^d : \sum_{i=1}^d x_i = 1\}$.
- Appropriate Bregman divergence: Kullback-Leibler. $\phi(\mathbf{x}) = \sum_{i=1}^d x_i\log x_i - \sum_{i=1}^d x_i$.
  - Fact: $\phi(\cdot)$ is 1-strongly convex with respect to $\|\cdot\|_1$. (Pinsker's inequality)
  - $\nabla\phi(\mathbf{x}) = (\log x_1, \dots, \log x_d)^T = \log\mathbf{x}$.
  - $\nabla\phi^*(\mathbf{y}) = (\nabla\phi)^{-1}(\mathbf{y}) = (e^{y_1}, \dots, e^{y_d})^T = \exp(\mathbf{y})$.
  - Update:

$$\begin{aligned}
\mathbf{y}^{(t+1)} &= \log\mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)}) \\
\tilde{\mathbf{x}}^{(t+1)} &= \exp\big(\log\mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)})\big) \\
\mathbf{x}^{(t+1)} &= \exp\big(\log\mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)})\big)/Z_t \\
&= \mathbf{x}^{(t)}\exp\big(-\gamma_t\nabla f(\mathbf{x}^{(t)})\big)/Z_t, \quad Z_t = \sum_{i=1}^d x_i^{(t)}\exp\big(-\gamma_t\nabla f(\mathbf{x}^{(t)})_i\big) = \mathbf{1}^T\exp\big(\log\mathbf{x}^{(t)} - \gamma_t\nabla f(\mathbf{x}^{(t)})\big),
\end{aligned}$$

  - The last step is because

$$P_{\Delta^{d-1}}^\phi(\mathbf{y}) = \arg\min_{\mathbf{x}\in\Delta^{d-1}} KL(\mathbf{x}\|\mathbf{y}) = \arg\min_{x_i\ge 0,\sum_{i=1}^d x_i=1}\sum_{i=1}^d\left(x_i\log\frac{x_i}{y_i} - x_i + y_i\right) = \arg\min_{x_i\ge 0,\sum_{i=1}^d x_i=1}\sum_{i=1}^d\left(x_i\log\frac{x_i}{y_i}\right).$$

    Lagrangian

$$\mathcal{L}(\mathbf{x}, \mu) = \sum_{i=1}^d\left(x_i\log\frac{x_i}{y_i}\right) + \mu\left(\sum_{i=1}^d x_i - 1\right)$$

    yields

$$\log\frac{x_i}{y_i} + 1 + \mu = 0 \quad \iff \quad x_i = y_i\exp(-\mu - 1) = cy_i, \ c > 0, \quad i = 1, \dots, d.$$

    Summing up yields $c = 1/(\sum_{i=1}^d y_i)$ to have

$$x_i = \frac{y_i}{\sum_{j=1}^d y_j}, \quad i = 1, \dots, d.$$

  - This special case is called the *exponentiated gradient method*.

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