Mathematics of Data: From Theory to Computation

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Lecture 8: Composite convex minimization I

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Outline

Today

- 1. Motivation for non-smooth optimization
- 2. Composite minimization
- 3. Proximal operator and computational complexity
- 4. Proximal gradient method Convex case

Next week

- 1. Proximal gradient method Nonconvex case
- 2. Adaptive constrained optimization
- 3. Stochastic proximal methods (Convex+nonconvex)



Recommended reading material

- A. Beck and M. Tebulle, A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems, SIAM J. Imaging Sciences, 2(1), 183–202, 2009.
- Y. Nesterov, Smooth minimization of non-smooth functions, Math. Program, 103(1), 127–152, 2005.
- Q. Tran-Dinh, A. Kyrillidis and V. Cevher, Composite Self-Concordant Minimization, LIONS-EPFL Tech. Report. http://arxiv.org/abs/1308.2867, 2013.
- N. Parikh and S. Boyd, Proximal Algorithms, Foundations and Trends in Optimization, 1(3):123-231, 2014.



Composite minimization:

Motivation

Data analytics problems in various disciplines can often be simplified to nonsmooth composite minimization problems. To this end, this lecture provides efficient numerical solution methods for such problems.

Intriguingly, composite minimization problems are far from generic nonsmooth problems and we can exploit individual function structures to obtain numerical solutions nearly as efficiently as if they are smooth problems.





Nonsmooth: When smooth models are deficient

Example: Linear Regression

Consider the classical linear regression problem:

$$\mathbf{b} = \mathbf{A} \mathbf{x}^{\natural} + \mathbf{w}$$

with $\mathbf{b} \in \mathbb{R}^n$, $\mathbf{A} \in \mathbb{R}^{n \times p}$ are known, \mathbf{x}^{\natural} is unknown, and \mathbf{w} is noise. Assume for now that $n \ge p$ (more later).

Standard approach: Least squares: $\hat{\mathbf{x}}_{LS} \in \arg\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{Ax}\|_2^2$

• Convex, smooth, and an *explicit solution*: $\hat{\mathbf{x}}_{LS} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b} = \mathbf{A}^{\dagger} \mathbf{b}$

Practical performance of an estimator $\hat{\mathbf{x}}$

Denote the numerical approximation by $\mathbf{x}_{\epsilon}^{\star}.$ The practical performance is determined by

$$\left\| \mathbf{x}_{\epsilon}^{\star} - \mathbf{x}^{\natural} \right\|_{2} \leq \underbrace{\left\| \mathbf{x}_{\epsilon}^{\star} - \hat{\mathbf{x}} \right\|_{2}}_{\text{approximation error}} + \underbrace{\left\| \hat{\mathbf{x}} - \mathbf{x}^{\natural} \right\|_{2}}_{\text{statistical error}}$$

Motivation: *non-smooth* estimators of \mathbf{x}^{\natural} can help *reduce the statistical error*.



Non-smooth unconstrained convex minimization

Alternative approach for Linear Regression: Least absolute value deviation:

$$\hat{\mathbf{x}} \in \arg\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_1.$$

- The advantage: Improved robustness against outliers (high noise values)
- The bad (!) news: A non-differentiable objective function

Problem (Mathematical formulation)

How can we find an optimal solution to the following optimization problem?

$$F^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) \tag{1}$$

where f is proper, closed, convex, but not everywhere differentiable, $f \in \mathcal{F}$.



Subdifferentials: A generalization of the gradient

Definition

Let $f: \mathcal{Q} \to \mathbb{R} \cup \{+\infty\}$ be a convex function. The subdifferential of f at a point $\mathbf{x} \in \mathcal{Q}$ is defined by the set:

$$\partial f(\mathbf{x}) = \{ \mathbf{v} \in \mathbb{R}^p \ : \ f(\mathbf{y}) \ge f(\mathbf{x}) + \langle \mathbf{v}, \ \mathbf{y} - \mathbf{x} \rangle \text{ for all } \mathbf{y} \in \mathcal{Q} \} \,.$$

Each element \mathbf{v} of $\partial f(\mathbf{x})$ is called *subgradient* of f at \mathbf{x} .

Lemma

Let $f : \mathcal{Q} \to \mathbb{R} \cup \{+\infty\}$ be a differentiable convex function. Then, the subdifferential of f at a point $\mathbf{x} \in \mathcal{Q}$ contains only the gradient, i.e., $\partial f(\mathbf{x}) = \{\nabla f(\mathbf{x})\}$.



Figure: (Left) Non-differentiability at point y. (Right) Gradient as a subdifferential with a singleton entry.

(Sub)gradients in convex functions



Figure: Subdifferentials of f(x) = |x| in \mathbb{R} .





Subdifferentials: Two basic results

Lemma (Necessary and sufficient condition)

 $\mathbf{x}^{\star} \in \operatorname{dom}(F)$ is a globally optimal solution to (1) iff $0 \in \partial F(\mathbf{x}^{\star})$.

Sketch of the proof.

• \Rightarrow : For any $\mathbf{x} \in \mathbb{R}^p$, by definition of $\partial F(\mathbf{x}^{\star})$:

$$F(\mathbf{x}) - F(\mathbf{x}^{\star}) \ge 0^T (\mathbf{x} - \mathbf{x}^{\star}) = 0,$$

that is, \mathbf{x}^{\star} is a global solution to (1).

• \Leftarrow : If \mathbf{x}^{\star} is a global of (1) then for every $\mathbf{x} \in \operatorname{dom}(F)$, $F(\mathbf{x}) \ge F(\mathbf{x}^{\star})$ and hence

$$F(\mathbf{x}) - F(\mathbf{x}^{\star}) \ge 0^T (\mathbf{x} - \mathbf{x}^{\star}), \forall \mathbf{x} \in \mathbb{R}^p,$$

which leads to $0 \in \partial F(\mathbf{x}^{\star})$.

Theorem (Moreau-Rockafellar's theorem [8])

Let ∂f and ∂g be the subdifferential of f and g, respectively. If $f, g \in \mathcal{F}(\mathbb{R}^p)$ and $\operatorname{dom}(f) \cap \operatorname{dom}(g) \neq \emptyset$, then:

$$\partial(f+g)=\partial f+\partial g.$$

Non-smooth unconstrained convex minimization

Problem (Non-smooth convex minimization)

$$F^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$$
 (2)

Subgradient method

The subgradient method relies on the fact that even though f is non-smooth, we can still compute its **subgradients**, informing of the local descent directions.

Subgradient method			
1 . Choose $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point.			
2 . For $k = 0, 1, \cdots$, perform:			
$\left\{ egin{array}{cc} \mathbf{x}^{k+1} &= \mathbf{x}^k - lpha_k \mathbf{d}^k, \end{array} ight.$	(3)		
where $\mathbf{d}^k \in \partial f(\mathbf{x}^k)$ and $\alpha_k \in (0,1]$ is a given step size.			



Convergence of the subgradient method

Theorem

Assume that the following conditions are satisfied:

1. $\|\mathbf{g}\|_2 \leq G$ for all $\mathbf{g} \in \partial f(\mathbf{x})$ for any $\mathbf{x} \in \mathbb{R}^p$.

2.
$$\|\mathbf{x}^0 - \mathbf{x}^\star\|_2 \le R$$

Let the stepsize be chosen as

$$\alpha_k = \frac{R}{G\sqrt{k}}$$

then the iterates generated by the subgradient method satisfy

$$\min_{0 \le i \le k} f(\mathbf{x}^i) - f^* \le \frac{RG}{\sqrt{k}}$$

Remarks

- Condition (1) holds, for example, when f is G-Lipschitz.
- The convergence rate of $O(1/\sqrt{k})$ is the slowest we have seen so far!

Today: Achieving guarantees for (many) non-smooth optimization problems that are just as good as those for smooth ones



Stochastic subgradient methods

• An unbiased stochastic subgradient

$$\mathbb{E}[G(\mathbf{x})|\mathbf{x}] \in \partial f(\mathbf{x}).$$

• Algorithms in Lecture 7 can be extended using unbiased subgradients instead of unbiased gradients.

 The classic stochastic subgradient methods (SG)

 1. Choose $\mathbf{x}_1 \in \mathbb{R}^p$ and $(\gamma_k)_{k \in \mathbb{N}} \in]0, +\infty[^{\mathbb{N}}.$

 2. For $k = 1, \ldots$ perform:

 $\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k G(\mathbf{x}_k).$

Theorem (Convergence in expectation [10])

Suppose that:

1. $\mathbb{E}[\|G(\mathbf{x}^k)\|^2] \leq M^2$,

2.
$$\gamma_k = \gamma_0 / \sqrt{k}$$
.

Then,

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \le \left(\frac{D^2}{\gamma_0} + \gamma_0 M^2\right) \frac{2 + \log k}{\sqrt{k}}.$$

• Note: Rate is $\mathcal{O}(\log k/\sqrt{k})$ instead of $\mathcal{O}(1/\sqrt{k})$ for the deterministic algorithm.

Composite convex minimization

Problem (Unconstrained composite convex minimization)

$$F^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ F(\mathbf{x}) := f(\mathbf{x}) + g(\mathbf{x}) \right\}$$
(4)

- ▶ f and g are both proper, closed, and convex.
- ▶ $\operatorname{dom}(F) := \operatorname{dom}(f) \cap \operatorname{dom}(g) \neq \emptyset$ and $-\infty < F^{\star} < +\infty$.
- The solution set $S^* := {\mathbf{x}^* \in \text{dom}(F) : F(\mathbf{x}^*) = F^*}$ is nonempty.

Two remarks

Nonsmoothness: At least one of the two functions f and g is **nonsmooth**

- General nonsmooth convex optimization methods (e.g., classical subgradient methods, level, or bundle methods) lack efficiency and numerical robustness.
 - ▶ Require $\mathcal{O}(\epsilon^{-2})$ iterations to reach a point $\mathbf{x}_{\epsilon}^{\star}$ such that $F(\mathbf{x}_{\epsilon}^{\star}) F^{\star} \leq \epsilon$. Hence, to reach $\mathbf{x}_{0.01}^{\star}$ such that $F(\mathbf{x}_{0.01}^{\star}) F^{\star} \leq 0.01$, we need $\mathcal{O}(10^4)$ iterations.
- Generality: it covers a wider range of problems than smooth unconstrained problems, e.g., when handling regularized *M*-estimation,
 - f is a loss function, a data fidelity, or negative log-likelihood function.
 - \blacktriangleright g is a regularizer, encouraging structure and/or constraints in the solution.

Example 1: Sparse regression in generalized linear models (GLMs)

Problem (Sparse regression in GLM)

Our goal is to estimate $\mathbf{x}^{\natural} \in \mathbb{R}^{p}$ given $\{b_{i}\}_{i=1}^{n}$ and $\{\mathbf{a}_{i}\}_{i=1}^{n}$, knowing that the likelihood function at y_{i} given \mathbf{a}_{i} and \mathbf{x}^{\natural} is given by $\mathcal{L}(b_{i}; \langle \mathbf{a}_{i}, \mathbf{x}^{\natural} \rangle)$, and that \mathbf{x}^{\natural} is sparse.



Optimization formulation

$$\min_{\mathbf{x}\in\mathbb{R}^p} \left\{ \underbrace{-\sum_{i=1}^n \log \mathcal{L}(b_i; \langle \mathbf{a}_i, \mathbf{x} \rangle)}_{f(\mathbf{x})} + \underbrace{\rho_n \|\mathbf{x}\|_1}_{g(\mathbf{x})} \right\}$$

where $\rho_n>0$ is a parameter which controls the strength of sparsity regularization.

Theorem (cf. [5] for details)

Under some technical conditions, there exists $\{\rho_i\}_{i=1}^{\infty}$ such that with high probability,

$$\left\| \mathbf{x}^{\star} - \mathbf{x}^{\natural} \right\|_{2}^{2} = \mathcal{O}\left(\frac{s \log p}{n}\right), \quad \text{supp } \mathbf{x}^{\star} = \text{supp } \mathbf{x}^{\natural}.$$

$$\underset{\textit{Recall ML: }}{\text{Recall ML: }} \left\| \mathbf{x}_{\textit{ML}} - \mathbf{x}^{\natural} \right\|_{2}^{2} = \mathcal{O}\left(p/n \right).$$





Example 2: Image processing

Problem (Imaging denoising/deblurring)

Our goal is to obtain a clean image x given "dirty" observations $\mathbf{b} \in \mathbb{R}^{n \times 1}$ via $\mathbf{b} = \mathcal{A}(\mathbf{x}) + \mathbf{w}$, where \mathcal{A} is a linear operator, which, e.g., captures camera blur as well as image subsampling, and w models perturbations, such as Gaussian or Poisson noise.



where $\rho > 0$ is a regularization parameter and $\|\cdot\|_{TV}$ is the total variation (TV) norm:

$$\|\mathbf{x}\|_{\mathrm{TV}} := \begin{cases} \sum_{i,j} |\mathbf{x}_{i,j+1} - \mathbf{x}_{i,j}| + |\mathbf{x}_{i+1,j} - \mathbf{x}_{i,j}| & \text{anisotropic case}, \\ \sum_{i,j} \sqrt{|\mathbf{x}_{i,j+1} - \mathbf{x}_{i,j}|^2 + |\mathbf{x}_{i+1,j} - \mathbf{x}_{i,j}|^2} & \text{isotropic case} \end{cases}$$





Example 3: Confocal microscopy with camera blur and Poisson observations





Example 4: Sparse inverse covariance estimation

Problem (Graphical model selection)

Given a data set $\mathcal{D} := \{\mathbf{x}_1, \cdots, \mathbf{x}_N\}$, where \mathbf{x}_i is a Gaussian random variable. Let Σ be the covariance matrix corresponding to the graphical model of the Gaussian Markov random field. Our goal is to learn a sparse precision matrix Θ (i.e., the inverse covariance matrix Σ^{-1}) that captures the Markov random field structure.



Optimization formulation

$$\min_{\Theta \succ 0} \left\{ \underbrace{\operatorname{tr}(\Sigma\Theta) - \log \det(\Theta)}_{f(\mathbf{x})} + \underbrace{\lambda \|\operatorname{vec}(\Theta)\|_{1}}_{g(\mathbf{x})} \right\}$$
(5)

where $\Theta \succ 0$ means that Θ is symmetric and positive definite and $\lambda > 0$ is a regularization parameter and vec is the vectorization operator.





Question: How do we design algorithms for finding a solution $\mathbf{x}^\star ?$

Philosophy

We cannot immediately design algorithms just based on the original formulation

$$F^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ F(\mathbf{x}) := f(\mathbf{x}) + g(\mathbf{x}) \right\}.$$
(6)

- \blacktriangleright We need intermediate tools to characterize the solutions \mathbf{x}^{\star} of this problem
- One key tool is called the optimality condition



A short detour: Proximal-point operators

Definition (Proximal operator [9])

Let $g \in \mathcal{F}(\mathbb{R}^p)$ and $\mathbf{x} \in \mathbb{R}^p$. The proximal operator (or prox-operator) of f is defined as:

$$\operatorname{prox}_{g}(\mathbf{x}) \equiv \arg\min_{\mathbf{y}\in\mathbb{R}^{p}} \left\{ g(\mathbf{y}) + \frac{1}{2} \|\mathbf{y} - \mathbf{x}\|_{2}^{2} \right\}.$$
(7)





A short detour: Proximal-point operators

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(7)

Numerical efficiency: Why do we need proximal operator?

For problem (4):

- For many well-known convex functions g, we can compute $prox_g(\mathbf{x})$ analytically or very efficiently.
- ▶ If $f \in \mathcal{F}_L^{1,1}(\mathbb{R}^p)$, and $\operatorname{prox}_g(\mathbf{x})$ is cheap to compute, then solving (4) is as efficient as solving $\min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$ in terms of complexity.
- If $\operatorname{prox}_{f}(\mathbf{x})$ and $\operatorname{prox}_{g}(\mathbf{x})$ are both cheap to compute, then *convex splitting* (4) is also efficient.

Tractable prox-operators

Processing non-smooth terms in (4)

- We handle the nonsmooth term g in (4) using the proximal mapping principle.
- Computing proximal operator $prox_g$ of a general convex function g

$$\operatorname{prox}_{g}(\mathbf{x}) \equiv \arg\min_{\mathbf{y}\in\mathbb{R}^{p}} \left\{ g(\mathbf{y}) + (1/2) \|\mathbf{y} - \mathbf{x}\|_{2}^{2} \right\}.$$

can be computationally demanding.

• If we can efficiently compute prox_F , we can use the **proximal-point algorithm** (PPA) [4, 9] to solve (4). Unfortunately, PPA is hardly used in practice to solve (4) since computing $\operatorname{prox}_{\lambda F}(\cdot)$ can be as almost hard as solving (4).

Definition (Tractable proximity)

Given $g \in \mathcal{F}(\mathbb{R}^p)$. We say that g is proximally tractable if prox_g defined by (7) can be computed efficiently.

- "efficiently" = {closed form solution, low-cost computation, polynomial time}.
- We denote $\mathcal{F}_{prox}(\mathbb{R}^p)$ the class of proximally tractable convex functions.





Tractable prox-operators

Example

For separable functions, the prox-operator can be efficient. For instance, $g(\mathbf{x}) := \|\mathbf{x}\|_1 = \sum_{i=1}^n |\mathbf{x}_i|$, we have

$$\operatorname{prox}_{\lambda g}(\mathbf{x}) = \operatorname{sign}(\mathbf{x}) \otimes \max\{|\mathbf{x}| - \lambda, 0\}.$$

For smooth functions, we can computer the prox-operator via basic algebra. For instance, $g(\mathbf{x}) := (1/2) \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$, one has

$$\mathrm{prox}_{\lambda g}(\mathbf{x}) = \left(\mathbb{I} + \lambda \mathbf{A}^T \mathbf{A}\right)^{-1} \left(\mathbf{x} + \lambda \mathbf{A} \mathbf{b}\right).$$

For the indicator functions of simple sets, e.g., $g(\mathbf{x}) := \delta_{\mathcal{X}}(\mathbf{x})$, the prox-operator is the projection operator

$$\operatorname{prox}_{\lambda g}(\mathbf{x}) := \pi_{\mathcal{X}}(\mathbf{x})$$

the projection of x onto \mathcal{X} . For instance, when $\mathcal{X} = \{ \mathbf{x} : \|\mathbf{x}\|_1 \leq \lambda \}$, the projection can be obtained efficiently.





Computational efficiency - Example

Proximal operator of quadratic function

The proximal operator of a quadratic function $g(\mathbf{x}) := \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$ is defined as

$$\operatorname{prox}_{\lambda g}(\mathbf{x}) := \arg\min_{\mathbf{y}\in\mathbb{R}^p} \left\{ \frac{1}{2} \|\mathbf{A}\mathbf{y} - \mathbf{b}\|_2^2 + \frac{1}{2\lambda} \|\mathbf{y} - \mathbf{x}\|_2^2 \right\}.$$
(8)





Computational efficiency - Example

Proximal operator of quadratic function

The proximal operator of a quadratic function $g(\mathbf{x}) := rac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$ is defined as

$$\operatorname{prox}_{\lambda g}(\mathbf{x}) := \arg\min_{\mathbf{y}\in\mathbb{R}^p} \left\{ \frac{1}{2} \|\mathbf{A}\mathbf{y} - \mathbf{b}\|_2^2 + \frac{1}{2\lambda} \|\mathbf{y} - \mathbf{x}\|_2^2 \right\}.$$
(8)

How to compute $\operatorname{prox}_{\lambda g}(\mathbf{x})$?

The optimality condition implies that the solution of (8) should satisfy the following linear system: $\mathbf{A}^T(\mathbf{A}\mathbf{y} - \mathbf{b}) + \lambda^{-1}(\mathbf{y} - \mathbf{x}) = 0$. As a result, we obtain

$$\operatorname{prox}_{\lambda g}(\mathbf{x}) = \left(\mathbb{I} + \lambda \mathbf{A}^T \mathbf{A}\right)^{-1} \left(\mathbf{x} + \lambda \mathbf{A} \mathbf{b}\right).$$

- When A^TA is efficiently diagonalizable (e.g., U^TA^TAU := Λ, where U is a unitary matrix and Λ is a diagonal matrix) then prox_{λg}(x) can be cheap prox_{λg}(x) = U (I + λΛ)⁻¹ U^T (x + λAb).
 - Matrices A such as TV operator with periodic boundary conditions, index subsampling operators (e.g., as in matrix completion), and circulant matrices (e.g., typical image blur operators) are efficiently diagonalizable with the Fast Fourier transform U.
- ► If $\mathbf{A}\mathbf{A}^T$ is diagonalizable (e.g., a tight frame \mathbf{A}), then we can use the identity $(\mathbb{I} + \lambda \mathbf{A}^T \mathbf{A})^{-1} = \mathbb{I} - \mathbf{A}^T (\lambda^{-1}\mathbb{I} + \mathbf{A}\mathbf{A}^T)^{-1}\mathbf{A}.$

A non-exhaustive list of proximal tractability functions

Name	Function	Proximal operator	Complexity
ℓ_1 -norm	$f(\mathbf{x}) := \ \mathbf{x}\ _1$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = \operatorname{sign}(\mathbf{x}) \otimes [\mathbf{x} - \lambda]_{+}$	$\mathcal{O}(p)$
ℓ_2 -norm	$f(\mathbf{x}) := \ \mathbf{x}\ _2$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = [1 - \lambda / \ \mathbf{x}\ _2]_+ \mathbf{x}$	$\mathcal{O}(p)$
Support function	$f(\mathbf{x}) := \max_{\mathbf{y} \in \mathcal{C}} \mathbf{x}^T \mathbf{y}$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = \mathbf{x} - \lambda \pi_{\mathcal{C}}(\mathbf{x})$	
Box indicator	$f(\mathbf{x}) := \delta_{[\mathbf{a},\mathbf{b}]}(\mathbf{x})$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = \pi_{[\mathbf{a},\mathbf{b}]}(\mathbf{x})$	$\mathcal{O}(p)$
Positive semidefinite	$f(\mathbf{X}) := \delta_{\mathbb{S}^p}(\mathbf{X})$	$\mathrm{prox}_{\lambda f}(\mathbf{X}) = \mathbf{U}[\Sigma]_{+}\mathbf{U}^{T}$, where $\mathbf{X} =$	$\mathcal{O}(p^3)$
cone indicator	+	$U\Sigma U^T$	
Hyperplane indicator	$f(\mathbf{x}) := \delta_{\mathcal{X}}(\mathbf{x}), \ \mathcal{X} :=$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = \pi_{\mathcal{X}}(\mathbf{x}) = \mathbf{x} +$	$\mathcal{O}(p)$
	$\{\mathbf{x} : \mathbf{a}^T \mathbf{x} = b\}$	$\left(\frac{b-\mathbf{a}^T\mathbf{x}}{\ \mathbf{a}\ _2}\right)\mathbf{a}$	
Simplex indicator	$f(\mathbf{x}) = \delta_{\mathcal{X}}(\mathbf{x}), \mathcal{X} :=$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = (\mathbf{x} - \nu 1)$ for some $\nu \in \mathbb{R}$,	$\tilde{O}(p)$
	$\{\mathbf{x} : \mathbf{x} \ge 0, \ 1^T \mathbf{x} = 1\}$	which can be efficiently calculated	
Convex quadratic	$f(\mathbf{x}) := (1/2)\mathbf{x}^T \mathbf{Q}\mathbf{x} +$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = (\lambda \mathbb{I} + \mathbf{Q})^{-1} \mathbf{x}$	$\mathcal{O}(p \log p) \rightarrow$
	$\mathbf{q}^T \mathbf{x}$	-	$\mathcal{O}(p^3)$
Square ℓ_2 -norm	$f(\mathbf{x}) := (1/2) \ \mathbf{x}\ _2^2$	$\operatorname{prox}_{\lambda f}(\mathbf{x}) = (1/(1+\lambda))\mathbf{x}$	$\mathcal{O}(p)$
log-function	$f(\mathbf{x}) := -\log(x)$	$\operatorname{prox}_{\lambda f}(x) = ((x^2 + 4\lambda)^{1/2} + x)/2$	O(1)
$\log \det$ -function	$f(\mathbf{x}) := -\log \det(\mathbf{X})$	$\operatorname{prox}_{\lambda f}(\mathbf{X})$ is the log-function prox ap-	$\mathcal{O}(p^3)$
		plied to the individual eigenvalues of ${f X}$	

Here: $[\mathbf{x}]_+ := \max\{0, \mathbf{x}\}$ and $\delta_{\mathcal{X}}$ is the indicator function of the convex set \mathcal{X} , sign is the sign function, \mathbb{S}^p_+ is the cone of symmetric positive semidefinite matrices.

For more functions, see [1, 7].



A short detour: Basic properties of prox-operator

Property (Basic properties of prox-operator)

- 1. $\operatorname{prox}_g(\mathbf{x})$ is well-defined and single-valued (i.e., the prox-operator (7) has a unique solution since $g(\cdot) + (1/2) \|\cdot -\mathbf{x}\|_2^2$ is strongly convex).
- 2. Optimality condition:

 $\mathbf{x} \in \operatorname{prox}_{g}(\mathbf{x}) + \partial g(\operatorname{prox}_{g}(\mathbf{x})), \ \mathbf{x} \in \mathbb{R}^{p}.$

3. \mathbf{x}^{\star} is a fixed point of $\operatorname{prox}_{q}(\cdot)$:

$$0 \in \partial g(\mathbf{x}^{\star}) \quad \Leftrightarrow \quad \mathbf{x}^{\star} = \operatorname{prox}_{q}(\mathbf{x}^{\star}).$$

4. Nonexpansiveness:

$$\|\operatorname{prox}_{g}(\mathbf{x}) - \operatorname{prox}_{g}(\tilde{\mathbf{x}})\|_{2} \leq \|\mathbf{x} - \tilde{\mathbf{x}}\|_{2}, \quad \forall \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^{p}.$$





- \blacktriangleright $\mathcal{F}_L^{1,1}$ and \mathcal{F}_2 are the class of convex functions with Lipschitz gradient and self-concordant, respectively.
- *F*_{prox} is the class of convex functions with proximity operator (defined in the next slides).
- "smoothable" is defined in the next lectures.



Solution methods

Composite convex minimization

$$F^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} \bigg\{ F(\mathbf{x}) := f(\mathbf{x}) + g(\mathbf{x}) \bigg\}.$$
(1)

Choice of numerical solution methods

• Solve (4) = Find $\mathbf{x}^k \in \mathbb{R}^p$ such that

$$F(\mathbf{x}^k) - F^\star \le \varepsilon$$

for a given tolerance $\varepsilon > 0$.

• Oracles: We can use one of the following configurations (oracles):

- 1. $\partial f(\cdot)$ and $\partial g(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.
- 2. $\nabla f(\cdot)$ and $\operatorname{prox}_{\lambda q}(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.
- 3. $\operatorname{prox}_{\lambda f}$ and $\operatorname{prox}_{\lambda q}(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.
- 4. $\nabla f(\cdot)$, inverse of $\nabla^2 f(\cdot)$ and $\operatorname{prox}_{\lambda q}(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.

Using different oracle leads to different types of algorithms



Proximal-gradient method: A quadratic majorization perspective

Definition (Proximal operator [9]) Let $g \in \mathcal{F}(\mathbb{R}^p)$. The proximal operator (or prox-operator) of g is defined as:

$$\operatorname{prox}_{g}(\mathbf{x}) \equiv \arg\min_{\mathbf{y}\in\mathbb{R}^{p}} \left\{ g(\mathbf{y}) + \frac{1}{2} \|\mathbf{y} - \mathbf{x}\|_{2}^{2} \right\}.$$

Quadratic upper bound for fFor $f \in \mathcal{F}_L^{1,1}(\mathbb{R}^p)$, we have, $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^p$

$$f(\mathbf{x}) \leq f(\mathbf{y}) +
abla f(\mathbf{y})^T (\mathbf{x} - \mathbf{y}) + rac{L}{2} \|\mathbf{x} - \mathbf{y}\|_2^2 \coloneqq Q_L(\mathbf{x}, \mathbf{y})$$

Quadratic *majorizer* for f + g

Of course, $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^p$,

 $f(\mathbf{x}) \leq Q_L(\mathbf{x}, \mathbf{y}) \quad \Rightarrow \quad f(\mathbf{x}) + g(\mathbf{x}) \leq Q_L(\mathbf{x}, \mathbf{y}) + g(\mathbf{x}) \coloneqq P_L(\mathbf{x}, \mathbf{y})$

Proximal-gradient from the majorize-minimize perspective

$$\mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} P_L(\mathbf{x}, \mathbf{x}^k) = \operatorname{prox}_{g/L}(\mathbf{x} - \nabla f(\mathbf{x}^k)/L)$$

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Geometric illustration





Proximal-gradient algorithm

Basic proximal-gradient scheme (ISTA) 1. Choose $\mathbf{x}^0 \in \text{dom}(F)$ arbitrarily as a starting point. 2. For $k = 0, 1, \cdots$, generate a sequence $\{\mathbf{x}^k\}_{k\geq 0}$ as: $\mathbf{x}^{k+1} := \text{prox}_{\alpha g} \left(\mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k)\right)$, where $\alpha := \frac{1}{L}$.





Proximal-gradient algorithm

Basic proximal-gradient scheme (ISTA) 1. Choose $\mathbf{x}^0 \in \text{dom}(F)$ arbitrarily as a starting point. 2. For $k = 0, 1, \cdots$, generate a sequence $\{\mathbf{x}^k\}_{k \ge 0}$ as: $\mathbf{x}^{k+1} := \text{prox}_{\alpha g} \left(\mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k) \right)$, where $\alpha := \frac{1}{T}$.

Theorem (Convergence of ISTA [2])

Let $\{\mathbf{x}^k\}$ be generated by ISTA. Then:

$$F(\mathbf{x}^k) - F^* \le \frac{L_f \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2}{2(k+1)}$$

The worst-case complexity to reach $F(\mathbf{x}^k) - F^* \leq \varepsilon$ of (ISTA) is $\mathcal{O}\left(\frac{L_f R_0^2}{\varepsilon}\right)$, where $R_0 := \max_{\mathbf{x}^* \in S^*} \|\mathbf{x}^0 - \mathbf{x}^*\|_2.$

A line-search procedure can be used to estimate L_k for L based on $(0 < c \le 1)$:

$$f(\mathbf{x}^{k+1}) \le f(\mathbf{x}^k) - \frac{c}{2L_k} \|\nabla f(\mathbf{x}^k)\|^2.$$



Fast proximal-gradient algorithm

Fast proximal-gradient scheme (FISTA) 1. Choose $\mathbf{x}^0 \in \text{dom}(F)$ arbitrarily as a starting point. 2. Set $\mathbf{y}^0 := \mathbf{x}^0$ and $t_0 := 1$. 3. For $k = 0, 1, \dots$, generate two sequences $\{\mathbf{x}^k\}_{k \ge 0}$ and $\{\mathbf{y}^k\}_{k \ge 0}$ as: $\begin{cases}
\mathbf{x}^{k+1} &:= \text{prox}_{\alpha g} \left(\mathbf{y}^k - \alpha \nabla f(\mathbf{y}^k) \right), \\
t_{k+1} &:= (1 + \sqrt{4t_k^2 + 1})/2, \\
\mathbf{y}^{k+1} &:= \mathbf{x}^{k+1} + \frac{t_{k-1}}{t_{k+1}} (\mathbf{x}^{k+1} - \mathbf{x}^k).
\end{cases}$ where $\alpha := L^{-1}$.

From $\mathcal{O}\left(\frac{L_f R_0^2}{\epsilon}\right)$ to $\mathcal{O}\left(R_0 \sqrt{\frac{L_f}{\epsilon}}\right)$ iterations at almost no additional cost!.

Complexity per iteration

- One gradient $\nabla f(\mathbf{y}^k)$ and one prox-operator of g;
- ▶ 8 arithmetic operations for t_{k+1} and γ_{k+1} ;
- ▶ 2 more vector additions, and **one** scalar-vector multiplication.

The cost per iteration is almost the same as in gradient scheme if proximal operator of g is efficient.

Example 1: ℓ_1 -regularized least squares

Problem (ℓ_1 -regularized least squares)

Given $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$, solve:

$$F^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ F(\mathbf{x}) := \frac{1}{2} \| \mathbf{A}\mathbf{x} - \mathbf{b} \|_2^2 + \lambda \| \mathbf{x} \|_1 \right\},\tag{9}$$

where $\lambda > 0$ is a regularization parameter.

Complexity per iterations

- Evaluating $\nabla f(\mathbf{x}^k) = \mathbf{A}^T (\mathbf{A}\mathbf{x}^k \mathbf{b})$ requires one $\mathbf{A}\mathbf{x}$ and one $\mathbf{A}^T \mathbf{y}$.
- One soft-thresholding operator $\operatorname{prox}_{\lambda q}(\mathbf{x}) = \operatorname{sign}(\mathbf{x}) \otimes \max\{|\mathbf{x}| \lambda, 0\}.$
- **Optional**: Evaluating $L = ||\mathbf{A}^T \mathbf{A}||$ (spectral norm) via power iterations (e.g., 20 iterations, each iteration requires one $\mathbf{A}\mathbf{x}$ and one $\mathbf{A}^T\mathbf{y}$).

Synthetic data generation

- $\mathbf{A} := \operatorname{randn}(n, p)$ standard Gaussian $\mathcal{N}(0, \mathbb{I})$.
- x^{*} is a k-sparse vector generated randomly.
- $\mathbf{b} := \mathbf{A}\mathbf{x}^* + \mathcal{N}(0, 10^{-3}).$

Example 1: Theoretical bounds vs practical performance





l₁-regularized least squares formulation has restricted strong convexity. The proximal-gradient method can automatically exploit this structure.



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Adaptive Restart

It is possible the preserve $\mathcal{O}(1/k^2)$ convergence guarantee !

One needs to slightly modify the algorithm as below.

 $\begin{array}{l} \hline \textbf{Generalized fast proximal-gradient scheme} \\ \textbf{1. Choose } \mathbf{x}^0 = \mathbf{x}^{-1} \in \mathrm{dom}\,(F) \text{ arbitrarily as a starting point.} \\ \textbf{2. Set } \theta_0 = \theta_{-1} = 1 \\ \textbf{3. For } k = 0, 1, \dots, \text{ generate two sequences } \{\mathbf{x}^k\}_{k \geq 0} \text{ and } \{\mathbf{y}^k\}_{k \geq 0} \text{ as:} \\ & \left\{ \begin{array}{l} \mathbf{y}^k := \mathbf{x}^k + \theta_k(\theta_{k-1}^{-1} - 1)(\mathbf{x}^k - \mathbf{x}^{k-1}) \\ \mathbf{x}^{k+1} := \mathrm{prox}_{\lambda g}\left(\mathbf{y}^k - \lambda \nabla f(\mathbf{y}^k)\right), \\ & \text{if restart test holds} \\ \theta_{k-1} = \theta_k = 1 \\ & \mathbf{y}^k = \mathbf{x}^k \\ & \mathbf{x}^{k+1} := \mathrm{prox}_{\lambda g}\left(\mathbf{y}^k - \lambda \nabla f(\mathbf{y}^k)\right) \end{array} \right. \end{array}$

where $\lambda := L_f^{-1}$.

θ_k is chosen so that it satisfies

$$\theta_{k+1} = \frac{\sqrt{\theta_k^4 + 4\theta_k^2 - \theta_k^2}}{2} < \frac{2}{k+3}$$

Adaptive Restart: Guarantee

Theorem (**Global complexity** [3]) The sequence $\{\mathbf{x}^k\}_{k>0}$ generated by the modified algorithm satisfies

$$F(\mathbf{x}^{k}) - F^{\star} \leq \frac{2L_{f}}{(k+2)^{2}} \left(R_{0}^{2} + \sum_{k_{i} \leq k} \left(\|\mathbf{x}^{\star} - \mathbf{x}^{k_{i}}\|_{2}^{2} - \|\mathbf{x}^{\star} - \mathbf{z}^{k_{i}}\|_{2}^{2} \right) \right) \quad \forall k \geq 0.$$
(11)

where $R_0 := \min_{\mathbf{x}^{\star} \in S^{\star}} \|\mathbf{x}^0 - \mathbf{x}^{\star}\|$, $\mathbf{z}^k = \mathbf{x}^{k-1} + \theta_{k-1}^{-1}(\mathbf{x}^k - \mathbf{x}^{k-1})$ and $k_i, i = 1...$ are the iterations for which the restart test holds.

Various restarts tests that might coincide with $\|\mathbf{x}^* - \mathbf{x}^{k_i}\|_2^2 \le \|\mathbf{x}^* - \mathbf{z}^{k_i}\|_2^2$

- Exact non-monotonicity test: $F(\mathbf{x}^{k+1}) F(\mathbf{x}^k) > 0$
- ▶ Non-monotonicity test: $\langle (L_F(\mathbf{y}^{k-1} \mathbf{x}^k), \mathbf{x}^{k+1} \frac{1}{2}(\mathbf{x}^k + y^{k-1}) \rangle > 0$ (implies exact non-monotonicity and it is advantageous when function evaluations are expensive)
- Gradient-mapping based test: $\langle (L_f(\mathbf{y}^k \mathbf{x}^{k+1}), \mathbf{x}^{k+1} \mathbf{x}^k \rangle > 0$



Example 2: Sparse logistic regression

Problem (Sparse logistic regression)

Given $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \{-1, +1\}^n$, solve:

$$F^{\star} := \min_{\mathbf{x},\beta} \left\{ F(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^{n} \log \left(1 + \exp \left(-\mathbf{b}_j(\mathbf{a}_j^T \mathbf{x} + \beta) \right) \right) + \rho \|\mathbf{x}\|_1 \right\}$$

Real data

- ▶ Real data: w8a with n = 49'749 data points, p = 300 features
- Available at http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html.

Parameters

- $ightarrow
 ho = 10^{-4}.$
- Number of iterations 5000, tolerance 10^{-7} .
- ▶ Ground truth: Solve problem up to 10⁻⁹ accuracy by TFOCS to get a high accuracy approximation of x^{*} and F^{*}.



Example 2: Sparse logistic regression - numerical results



	ISTA	LS-ISTA	FISTA	FISTA-R	LS-FISTA	LS-FISTA-R
Number of iterations	5000	5000	4046	2423	447	317
CPU time (s)	26.975	61.506	21.859	18.444	10.683	6.228
Solution error $(\times 10^{-7})$	29370	2.774	1.000	0.998	0.961	0.985

Strong convexity case: Algorithms

Proximal-gradient scheme (ISTA_µ) 1. Given $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point. 2. For $k = 0, 1, \cdots$, generate a sequence $\{\mathbf{x}^k\}_{k \ge 0}$ as: $\mathbf{x}^{k+1} := \operatorname{prox}_{\alpha_k g} \left(\mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k) \right),$ where $\alpha_k := 2/(L_f + \mu)$ is the optimal step-size.

Fast proximal-gradient scheme (FISTA_{\mu})1. Given $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point. Set $\mathbf{y}^0 := \mathbf{x}^0$.2. For $k = 0, 1, \cdots$, generate two sequences $\{\mathbf{x}^k\}_{k\geq 0}$ and $\{\mathbf{y}^k\}_{k\geq 0}$ as: $\{\mathbf{x}^{k+1} := \operatorname{prox}_{\alpha_k g} \left(\mathbf{y}^k - \alpha_k \nabla f(\mathbf{y}^k) \right),$ $\mathbf{y}^{k+1} := \mathbf{x}^{k+1} + \left(\frac{\sqrt{c_f}-1}{\sqrt{c_f}+1} \right) (\mathbf{x}^{k+1} - \mathbf{x}^k),$ where $\alpha_k := L_f^{-1}$ is the optimal step-size.





Strong convexity case: Convergence

Assumption

f is strongly convex with parameter $\mu > 0$, i.e., $f \in \mathcal{F}_{L,\mu}^{1,1}(\mathbb{R}^p)$. Condition number: $c_f := \frac{L_f}{\mu} \ge 0$.

Theorem (**ISTA** $_{\mu}$ [6])

$$F(\mathbf{x}^k) - F^\star \le \frac{L_f}{2} \left(\frac{c_f - 1}{c_f + 1} \right)^{2k} \| \mathbf{x}^0 - \mathbf{x}^\star \|_2^2.$$

Convergence rate: Linear with contraction factor: $\omega := \left(\frac{c_f - 1}{c_f + 1}\right)^2 = \left(\frac{L_f - \mu}{L_f + \mu}\right)^2$.

Theorem (**FISTA**_{μ} [6])

$$F(\mathbf{x}^k) - F^\star \le \frac{L_f + \mu}{2} \left(1 - \sqrt{\frac{\mu}{L_f}} \right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2.$$

Convergence rate: Linear with contraction factor: $\omega_f = \frac{\sqrt{L_f} - \sqrt{\mu}}{\sqrt{L_f}} < \omega$.





A practical issue

Stopping criterion

Fact: If $\mathcal{PG}_{\mathcal{L}}(\mathbf{x}^{\star}) = 0$, then \mathbf{x}^{\star} is optimal to (4), where

$$\mathcal{PG}_{\mathcal{L}}(\mathbf{x}) = L\left(\mathbf{x} - \operatorname{prox}_{(1/L)g}\left(\mathbf{x} - (1/L)\nabla f(\mathbf{x})\right)\right).$$

Stopping criterion: (relative solution change)

$$L_k \|\mathbf{x}^{k+1} - \mathbf{x}^k\|_2 \le \varepsilon \max\{L_0 \|\mathbf{x}^1 - \mathbf{x}^0\|_2, 1\},\$$

where ε is a given tolerance.



Summary of the worst-case complexities

Software

TFOCS is a good software package to learn about first order methods. http://cvxr.com/tfocs/

Comparison with gradient scheme $(F(\mathbf{x}^k) - F^* \leq \varepsilon)$

Complexity	Proximal-gradient scheme	Fast proximal-gradient
		scheme
Complexity $[\mu = 0]$	$\mathcal{O}\left(R_0^2(L_f/arepsilon) ight)$	$\mathcal{O}\left(R_0 \sqrt{L_f/arepsilon} ight)$
Per iteration	1-gradient, 1-prox, 1-sv, 1-	1-gradient, 1-prox, 2-sv, 3-
	v+	v+
Complexity $[\mu > 0]$	$\mathcal{O}\left(\kappa\log(\varepsilon^{-1})\right)$	$\mathcal{O}\left(\sqrt{\kappa}\log(\varepsilon^{-1})\right)$
Per iteration	1-gradient, 1-prox, 1-sv, 1-	1-gradient, 1-prox, 1-sv, 2-
	v+	v+

Here: sv = scalar-vector multiplication, v+=vector addition. $R_0 := \max_{\mathbf{x}^{\star} \in S^{\star}} \|\mathbf{x}^0 - \mathbf{x}^{\star}\|$ and $\kappa = L_f/\mu_f$ is the condition number.

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Per iteration	1-gradient, 1-prox, 1- sv , 1-	1-gradient, 1-prox, 2-sv, 3-
	v+	v+
Complexity $[\mu > 0]$	$\mathcal{O}\left(\kappa \log(\varepsilon^{-1})\right)$	$\mathcal{O}\left(\sqrt{\kappa}\log(\varepsilon^{-1})\right)$
Per iteration	1-gradient, 1-prox, 1- sv , 1- $v+$	1-gradient, 1-prox, 1- sv , 2- $v+$

Here: sv = scalar-vector multiplication, v+=vector addition. $R_0 := \max_{\mathbf{x}^{\star} \in S^{\star}} \|\mathbf{x}^0 - \mathbf{x}^{\star}\|$ and $\kappa = L_f/\mu_f$ is the condition number.

Need alternatives when

- f is only self-concordant
- \blacktriangleright computing $\nabla f(\mathbf{x})$ is much costlier than computing prox_g



*Examples

Example (Sparse graphical model selection) $\min_{\Theta \succ 0} \left\{ \underbrace{\operatorname{tr}(\Sigma\Theta) - \log \det(\Theta)}_{f(\mathbf{x})} + \underbrace{\rho \|\operatorname{vec}(\Theta)\|_{1}}_{g(\mathbf{x})} \right\}$

where $\Theta \succ 0$ means that Θ is symmetric and positive definite, and $\rho > 0$ is a regularization parameter and vec is the vectorization operator.

- Computing the gradient is expensive: $\nabla f(\Theta) = \Theta^{-1}$.
- ► $f \in \mathcal{F}_2$ is self-concordant. However, if $\alpha \mathbf{I} \preceq \Theta \preceq \beta \mathbf{I}$, then $f \in \mathcal{F}_{L,\mu}^{2,1}$ with $L = \sqrt{p}/\alpha^2$ and $\mu = (\beta^2 \sqrt{p})^{-1}$.





* Examples (Learned ISTA)



Figure: a) Traditional machine learning approaches b) End-to-end deep learning methods [11]

Example

In sparse coding, given a an overcomplete family basis vectors, we would like to find the optimal sparse code vector $Z^* \in \mathbb{R}^m$ to reconstruct the input vector $X \in \mathbb{R}^n$

$$Z^* = \arg\min_{Z} \frac{1}{2} \|X - W_d Z\|_2^2 + \alpha \|Z\|_1,$$
(12)

where W_d is $n \times m$ dictionary matrix, whose columns are normalized basis vectors.

Too slow for real-time applications



* Examples (Learned ISTA)



ISTA method for sparse coding



Learned ISTA - time unfolded version of the ISTA block diagram

Example

$$\mathcal{L}(W) = \frac{1}{P} \sum_{p=0}^{(P-1)} \underbrace{\frac{1}{2} \|Z^{*p} - f_e(W, X_p)\|^2}_{L(W, X_p)}$$
(13)

where (X_1, \ldots, X_P) are some samples, and Z^{*p} is the optimal code for sample X^p . Parameters of the encoder are chosen as minimizers of $\mathcal{L}(W)$.

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