Numerical Optimization

IN A Few Useful Things to Know about Machine Learning, Pedro Domingos put up a relation: LEARNING = REPRESENTATION + EVALUATION + OPTIMIZATION.

- Representation as the core of the note is the general (mathematical) model that computer can handle.
- Evaluation is **criteria**. An evaluation function (also called objective function, cost function or scoring function) is needed to distinguish good classifiers from bad ones.
- Optimization is aimed to find the parameters that optimizes the evaluation function, i.e.

$$\begin{split} \arg\min_{\theta} f(\theta) &= \{\theta^* | f(\theta^*) = \min f(\theta) \} \, \text{or} \\ \arg\max_{\theta} f(\theta) &= \{\theta^* | f(\theta^*) = \max f(\theta) \}. \end{split}$$

The objective function to be minimized is also called cost function.

Evaluation is always attached with optimization; the evaluation which cannot be optimized is not a good evaluation in machine learning.

- https://www.wikiwand.com/en/Mathematical_optimization
- https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf
- http://www.cs.cmu.edu/~pradeepr/convexopt/
- · An interactive tutorial to numerical optimization
- Patrick Louis' RECENT CONFERENCE TALKS on optimization
- http://awibisono.github.io/2016/06/06/world-of-optimization.html
- http://awibisono.github.io/2016/06/13/gradient-flow-gradient-descent.html
- http://awibisono.github.io/2016/06/20/accelerated-gradient-descent.html

Gradient Descent and More

Each iteration of a line search method computes a search direction p^k and then decides how far to move along that direction. The iteration is given by

$$x^{k+1} = x^k + \alpha_k p^k \tag{Line search}$$

where the positive scalar α_k is called the step length. The success of a line search method depends on effective choices of both the direction p^k and the step length α_k .

Note: we use the notation x^k and α_k to represent the kth iteration of the vector variables x and k th step length, respectively. Most line search algorithms require p^k to be a descent direction — one for which

 $\langle p^k, \nabla f_k \rangle < 0$ — because this property guarantees that the function f can be reduced along this direction, where ∇f_k is the gradient of objective function f at the kth iteration point x_k i.e. $\nabla f_k = \nabla f(x^k)$.

Gradient descent and its variants are to find the local solution of the unconstrained optimization problem:

$$\min f(x)$$

where $x \in \mathbb{R}^n$.

It is not difficult to observe that

$$f(x)pprox f(x^k)+(x-x^k)^T
abla f(x^k)+rac{s_k}{2}\|x-x^k\|_2^2$$

by Taylor expansion of f near the point x^k for some constant s_k .

Let $x^{k+1} = \arg\min_x f(x^k) + (x-x^k)^T \nabla f(x^k) + \frac{s_k}{2} \|x-x^k\|_2^2$, we will obtain $x^{k+1} = x^k - \frac{1}{s_k} \nabla_x f(x^k)$. However, the constant s_k is difficult to estimate.

And the general gradient descent methods are given by

$$x^{k+1} = x^k - lpha_k
abla_x f(x^k)$$

where x^k is the kth iterative result, $\alpha_k \in \{\alpha | f(x^{k+1}) < f(x^k)\}$ and particularly $\alpha_k = \arg\min_{\alpha} f(x^k - \alpha \nabla_x f(x^k))$ so that $f(x^{k+1}) = \min_{\alpha} f(x^k - \alpha \nabla_x f(x^k))$.

- http://59.80.44.100/www.seas.ucla.edu/~vandenbe/236C/lectures/gradient.pdf
- http://wiki.fast.ai/index.php/Gradient_Descent

There are many ways to choose some proper step or learning rate sequence $\{\alpha_k\}$.

The proof of convergence or complexity is often based on the convex case where the objective function is convex, i.e.,

$$f(tx + (1-t)y) \le tf(x) + (1-t)f(y), \quad t \in [0,1].$$

And this optimization is called convex optimization.

Some variants of gradient descent methods are not line search method.

For example, the heavy ball methods or momentum methods:

$$x^{k+1} = x^k - lpha_k
abla_x f(x^k) +
ho_k (x^k - x^{k-1})$$

where the momentum coefficient $\rho_k \in [0,1]$ generally and the step length α_k cannot be determined by line search.

Nesterov accelerated gradient method at the kth step is given by:

$$x^k = y^k - lpha_{k+1}
abla_x f(y^k)$$
 Descent $y^{k+1} = x^k +
ho_k (x^k - x^{k-1})$ Momentum

where the momentum coefficient $ho_k \in [0,1]$ generally.

They are called as inertial gradient methods or accelerated gradient methods. And there are some different forms.

Inventor of Nesterov accelerated Gradient

<img src=https://upload.wikimedia.org/wikipedia/commons/thumb/9/9e/Nesterov_yurii.jpg/440px-Nesterov_yurii.jpg
width = 60% />

- https://blogs.princeton.edu/imabandit/2013/04/01/acceleratedgradientdescent/
- https://blogs.princeton.edu/imabandit/2014/03/06/nesterovs-accelerated-gradient-descent-for-smooth-and-strongly-convex-optimization/
- https://blogs.princeton.edu/imabandit/2015/06/30/revisiting-nesterovs-acceleration/
- https://blogs.princeton.edu/imabandit/2018/11/21/a-short-proof-for-nesterovs-momentum/
- https://blogs.princeton.edu/imabandit/2019/01/09/nemirovskis-acceleration/
- https://zhuanlan.zhihu.com/p/41263068
- https://zhuanlan.zhihu.com/p/35692553
- https://zhuanlan.zhihu.com/p/35323828
- On Gradient-Based Optimization: Accelerated, Asynchronous, Distributed and Stochastic
- https://jlmelville.github.io/mize/nesterov.html
- https://distill.pub/2017/momentum/
- http://www.optimization-online.org/DB_FILE/2018/11/6938.pdf
- https://www.mat.univie.ac.at/~neum/glopt/mss/MasAi02.pdf
- https://www.cs.cmu.edu/~ggordon/10725-F12/slides/09-acceleration.pdf
- https://saugatbhattarai.com.np/what-is-gradient-descent-in-machine-learning/
- https://www.fromthegenesis.com/gradient-descent-part-2/
- http://www.deepideas.net/deep-learning-from-scratch-iv-gradient-descent-and-backpropagation/
- https://ee227c.github.io/notes/ee227c-lecture08.pdf

Variable Metric Methods

Newton's Method

NEWTON'S METHOD and QUASI-NEWTON METHODS are classified to variable metric methods.

It is also to find the solution of unconstrained optimization problems, i.e.

where $x \in \mathbb{R}^n$. Specially, the objective function f(x) is convex so that the local minima is global minima.

If x^* is the extrema of the cost function f(x), it is necessary that $\nabla f(x^*) = 0$.

So if we can find all the solution of the equation system $\nabla f(x)=0$, it helps us to find the solution to the optimization problem $\arg\min_{x\in\mathbb{R}^n}f(x)$.

Newton's method is one of the fixed-point methods to solve nonlinear equation system.

It is given by

$$egin{align} x^{k+1} &= rg \min_x f(x^k) + (x-x^k)^T
abla_x f(x^k) + rac{1}{2lpha_{k+1}} (x-x^k)^T H(x^k) (x-x^k) \ &= x^k - lpha_{k+1} H^{-1}(x^k)
abla_x f(x^k) \ \end{split}$$

where $H^{-1}(x^k)$ is inverse of the Hessian matrix of the function f(x) at the point x^k .

It is called Newton-Raphson algorithm in statistics.

Especially when the log-likelihood function $\ell(\theta)$ is well-behaved,

a natural candidate for finding the MLE is the Newton-Raphson algorithm with quadratic convergence rate.

The Fisher Scoring Algorithm

In maximum likelihood estimation, the objective function is the log-likelihood function, i.e.

$$\ell(heta) = \sum_{i=1}^n \log P(x_i| heta)$$

where $P(x_i|\theta)$ is the probability of realization $X_i=x_i$ with the unknown parameter θ . However, when the sample random variable $\{X_i\}_{i=1}^n$ are not observed or realized, it is best to replace negative Hessian matrix (i.e. $-\frac{\partial^2 \ell(\theta)}{\partial \theta \partial \theta^T}$)

of the likelihood function with the observed information matrix:

$$J(heta) = \mathbb{E}(-rac{\partial^2 \ell(heta)}{\partial heta \partial heta^T}) = -\int rac{\partial^2 \ell(heta)}{\partial heta \partial heta^T} f(x_1, \cdots, x_n | heta) \mathrm{d}x_1 \cdots \mathrm{d}x_n$$

where $f(x_1, \dots, x_n | \theta)$ is the joint probability density function of X_1, \dots, X_n with unknown parameter θ .

And the Fisher scoring algorithm is given by

$$heta^{k+1} = heta^k + lpha_k J^{-1}(heta^k)
abla_{ heta} \ell(heta^k)$$

where $J^{-1}(\theta^k)$ is the inverse of observed information matrix at the point θ^k .

See http://www.stats.ox.ac.uk/~steffen/teaching/bs2HT9/scoring.pdf or https://wiseodd.github.io/techblog/2018/03/11/fisher-information/.

Fisher scoring algorithm is regarded as an example of **Natural Gradient Descent** in information geometry as shown in https://wiseodd.github.io/techblog/2018/03/14/natural-gradient/and https://www.zhihu.com/question/266846405.

Quasi-Newton Methods

Quasi-Newton methods, like steepest descent, require only the gradient of the objective function to be supplied at each iterate.

By measuring the changes in gradients, they construct a model of the objective function that is good enough to produce super-linear convergence.

The improvement over steepest descent is dramatic, especially on difficult problems. Moreover, since second derivatives are not required, quasi-Newton methods are sometimes more efficient than Newton's method.[^1]

In optimization, quasi-Newton methods (a special case of **variable-metric methods**) are algorithms for finding local maxima and minima of functions. Quasi-Newton methods are based on Newton's method to find the stationary point of a function, where the gradient is 0.

In quasi-Newton methods the Hessian matrix does not need to be computed. The Hessian is updated by analyzing successive gradient vectors instead. Quasi-Newton methods are a generalization of the secant method to find the root of the first derivative for multidimensional problems.

In multiple dimensions the secant equation is under-determined, and quasi-Newton methods differ in how they constrain the solution, typically by adding a simple low-rank update to the current estimate of the Hessian.

One of the chief advantages of quasi-Newton methods over Newton's method is that the Hessian matrix (or, in the case of quasi-Newton methods, its approximation) \mathbf{B} does not need to be inverted. The Hessian approximation \mathbf{B} is chosen to satisfy

$$\nabla f(x^{k+1}) = \nabla f(x^k) + B(x^{k+1} - x^k),$$

which is called the **secant equation** (the Taylor series of the gradient itself).

In more than one dimension B is underdetermined. In one dimension, solving for B and applying the Newton's step with the updated value is equivalent to the secant method.

The various quasi-Newton methods differ in their choice of the solution to the **secant equation** (in one dimension, all the variants are equivalent).

The unknown x_k is updated applying the Newton's step calculated using the current approximate Hessian matrix B_k :

- 1. $\Delta x_k = -\alpha_k B_k^{-1} \nabla f(x_k)$, with α chosen to satisfy the Wolfe conditions;
- 2. $x_{k+1} = x_k + \Delta x_k$;
- 3. The gradient computed at the new point $\nabla f(x_{k+1})$, and $y_k = \nabla f(x_{k+1}) \nabla f(x_k)$ is used to update the approximate Hessian B_{k+1} , or directly its inverse $H_{k+1} = B_{k+1}^{-1}$ using the Sherman–Morrison formula.

A key property of the BFGS and DFP updates is that if B_k is positive-definite, and α_k is chosen to satisfy the Wolfe conditions, then B_{k+1} is also positive-definite.

For example,

Method	$B_{k+1}=$	$H_{k+1} = B_{k+1}^{-1} = % \left(\frac{1}{k} - \frac{1}{k} \right) \left(\frac{1}{k} - \frac{1}{k} - \frac{1}{k} \right) \left(\frac{1}{k} - \frac{1}{k} - \frac{1}{k} \right) \left(\frac{1}{k} - \frac{1}{k} - \frac{1}{k} - \frac{1}{k} \right) \left(\frac{1}{k} - $
DFP	$(I - rac{y_k \Delta x_k^{\mathrm{T}}}{y_k^{\mathrm{T}} \Delta x_k}) B_k (I - rac{\Delta x_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} \Delta x_k}) + rac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}}} \Delta x_k$	$H_k + rac{\Delta x_k \Delta x_k^T}{\Delta x_k^T y_k} - rac{H_k y_k y_k^T H_k}{y_k^T H_k y_k}$
BFGS	$B_k + rac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} \Delta x_k} - rac{B_k \Delta x_k (B_k \Delta x_k)^T}{\Delta x_k B_k \Delta x_k}$	$(I-rac{\Delta x_k^{\mathrm{T}}y_k}{y_k^{\mathrm{T}}\Delta x_k})H_k(I-rac{y_k\Delta x_k^{\mathrm{T}}}{y_k^{\mathrm{T}}\Delta x_k})+rac{\Delta x_k\Delta x_k^{\mathrm{T}}}{y_k^{\mathrm{T}}\Delta x_k}$
SR1	$B_k + rac{(y_k - B_k \Delta x_k)(y_k - B_k \Delta x_k)^{\mathrm{T}}}{(y_k - B_k \Delta x_k)^{\mathrm{T}} \Delta x_k}$	$H_k + rac{(\Delta x_k - H_k y_k)(\Delta x_k - H_k y_k)^{\mathrm{T}}}{(\Delta x_k - H_k y_k)^{\mathrm{T}} y_k}$

- Quasi-Newton methods in Wikipedia page
- http://59.80.44.98/www.seas.ucla.edu/~vandenbe/236C/lectures/qnewton.pdf
- http://fa.bianp.net/teaching/2018/eecs227at/quasi_newton.html

The Barzilai-Borwein method

Consider the gradient iteration form

$$x^{k+1} = x^k - lpha_k
abla f(x^k)$$

which can be written as

$$x^{k+1} = x^k - D_k
abla f(x^k)$$

where $D_k = \alpha_k I$.

In order to make the matrix D_k have quasi-Newton property, we compute $lpha_k$ such that

$$\min \|s_{k-1} - D_k y_{k-1}\|$$

which yields

$$\alpha_k = \frac{\langle s_{k-1}, y_{k-1} \rangle}{\langle y_{k-1}, y_{k-1} \rangle} \tag{1}$$

where $s_{k-1} = x_k - x_{k-1}, y_{k-1} = \nabla f(x^k) - \nabla f(x^{k-1}).$

By symmetry, we may minimize $\|D_k^{-1}s_{k-1}-y_{k-1}\|$ with respect to $lpha_k$ and get

$$\alpha_k = \frac{\langle s_{k-1}, s_{k-1} \rangle}{\langle s_{k-1}, y_{k-1} \rangle}.$$
 (2)

In short, the iteration formula of Barzilai-Borwein method is given by

$$x^{k+1} = x^k - \alpha_k
abla f(x^k)$$

where α_k is determined by (1) or (2).

It is easy to see that in this method no matrix computations and no line searches (except k=0) are required.

- https://mp.weixin.qq.com/s/G9HH29b2-VBnk_Sqze8pDg
- http://www.math.ucla.edu/~wotaoyin/math273a/slides/
- http://bicmr.pku.edu.cn/~wenzw/courses/WenyuSun_YaxiangYuan_BB.pdf
- https://www.math.lsu.edu/~hozhang/papers/cbb.pdf
- Wikipedia page on Newton Method
- Newton-Raphson Visualization (1D)
- Newton-Raphson Visualization (2D)
- Using Gradient Descent for Optimization and Learning

Natural Gradient Descent

Natural gradient descent is to solve the optimization problem $\min_{\theta} L(\theta)$ by

$$heta^{(t+1)} = heta^{(t+1)} - lpha_{(t)} F^{-1}(heta^{(t)})
abla_{ heta} L(heta^{(t)})$$

where $F^{-1}(\theta^{(t)})$ is the inverse of Remiann metric at the point $\theta^{(t)}$. And Fisher scoring algorithm is a typical application of Natural Gradient Descent to statistics. Natural gradient descent for manifolds corresponding to exponential families can be implemented as a first-order method through mirror descent (https://www.stat.wisc.edu/~raskutti/publication/MirrorDescent.pdf).

Originator of Information Geometry: Shunichi Amari

- Natural gradient descent and mirror descent
- Online Natural Gradient as a Kalman Filter
- https://www.zhihu.com/question/266846405
- 2016 PKU Mini-Course: Information Geometry
- Information Geometry and Natural Gradients
- Tutorial on Information Geometry and Algebraic Statistics
- True Asymptotic Natural Gradient Optimization
- Shun-ichi Amari's CV in RIKEN

- Energetic Natural Gradient Descent
- · Natural gradients and K-FAC
- http://www.divergence-methods.org/
- http://www.deeplearningpatterns.com/doku.php?id=natural_gradient_descent
- NATURAL GRADIENTS AND STOCHASTIC VARIATIONAL INFERENCE
- 谈谈优化算法 郑思座的文章 知乎
- Accelerating Natural Gradient with Higher-Order Invariance

Trust Region Methods

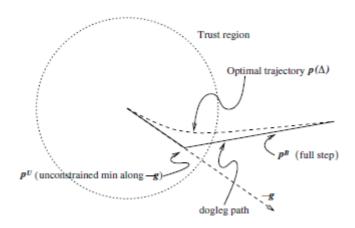
Trust-region methods define a region around

the current iterate within which they trust the model to be an adequate representation of the objective function, and then choose the step to be the approximate minimizer of the model in this region.

If a step is not acceptable, they reduce the size of the region and find a new minimizer. In general, the direction of the step changes whenever the size of the trust region is altered.

$$\min_{p\in\mathbb{R}^n} m_k(p) = f_k + g_k^T p + rac{1}{2} p^T B_k p, \,\, s.\, t. \, \|p\| \leq \Delta_k,$$

where $f_k=f(x^k), g_k=\nabla f(x^k); B_k$ is some symmetric matrix as an approximation to the Hessian $\nabla^2 f(x^k+tp); \Delta_k>0$ is the trust-region radius. In most of our discussions, we define $\|\cdot\|$ to be the Euclidean norm. Thus, the trust-region approach requires us to solve a sequence of subproblems in which the objective function and constraint are both quadratic. Generally, we set $B_k=\nabla^2 f(x^k)$.



- https://optimization.mccormick.northwestern.edu/index.php/Trust-region_methods
- Concise Complexity Analyses for Trust-Region Methods
- https://www.nmr-relax.com/manual/Trust_region_methods.html

Expectation Maximization Algorithm

Expectation-Maximization algorithm, popularly known as the **EM algorithm** has become a standard piece in the statistician's repertoire.

It is used in incomplete-data problems or latent-variable problems such as Gaussian mixture model in maximum likelihood estimation.

The basic principle behind the **EM** is that instead of performing a complicated optimization, one augments the observed data with latent data to perform a series of simple optimizations.

It is really popular for Bayesian statistician.

Let $\ell(\theta|Y_{obs}) \triangleq \log L(\theta|Y_{obs})$ denote the log-likelihood function of observed datum Y_{obs} . We augment the observed data Y_{obs} with latent variables Z so that both the complete-data log-likelihood $\ell(\theta|Y_{obs},Z)$ and the conditional predictive distribution $f(z|Y_{obs},\theta)$ are available. Each iteration of the **EM** algorithm consists of an expectation step (E-step) and a maximization step (M-step) Specifically, let $\theta^{(t)}$ be the current best guess at the MLE $\hat{\theta}$. The E-step is to compute the **Q** function defined by

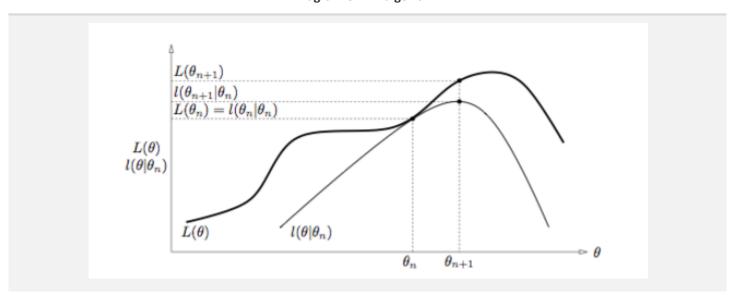
$$egin{aligned} Q(heta| heta^{(t)}) &= \mathbb{E}(\ell(heta|Y_{obs},Z)|Y_{obs}, heta^{(t)}) \ &= \int_{Z} \ell(heta|Y_{obs},Z) imes f(z|Y_{obs}, heta^{(t)}) \mathrm{d}z, \end{aligned}$$

and the M-step is to maximize ${\bf Q}$ with respect to θ to obtain

$$heta^{(t+1)} = rg \max_{ heta} Q(heta| heta^{(t)}).$$

- https://www.wikiwand.com/en/Expectation-maximization_algorithm
- http://cs229.stanford.edu/notes/cs229-notes8.pdf
- EM算法存在的意义是什么? 史博的回答 知乎

Diagram of EM algorithm



Each iteration of the **generalized EM** algorithm consists of an expectation step (E-step) and a maximization step (M-step) Specifically, let $\theta^{(t)}$ be the current best guess at the MLE $\hat{\theta}$. The E-step is to compute the **Q** function defined by

$$egin{aligned} Q(heta| heta^{(t)}) &= \mathbb{E}[\ell(heta|Y_{obs},Z)|Y_{obs}, heta^{(t)}] \ &= \int_{Z} \ell(heta|Y_{obs},Z) imes f(z|Y_{obs}, heta^{(t)}) \mathrm{d}z, \end{aligned}$$

and the another step is to find θ that satisfies $Q(\theta^{t+1}|\theta^t) > Q(\theta^t|\theta^t)$, i.e.

$$heta^{(t+1)} \in \{\hat{ heta}|Q(\hat{ heta}| heta^{(t)} \geq Q(heta| heta^{(t)})\}.$$

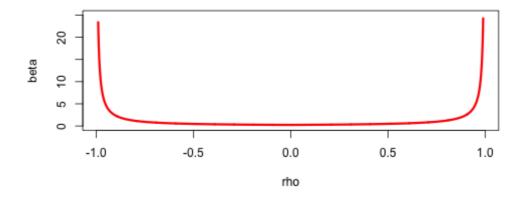
It is not to maximize the conditional expectation.

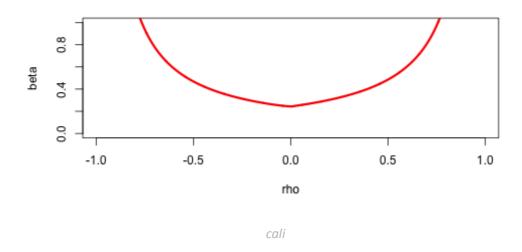
See more on the book The EM Algorithm and Extensions, 2nd Edition by Geoffrey McLachlan, Thriyambakam Krishna.

![projection EM](https://pic4.zhimg.com/80/v2-468b515b4d26ebc4765f82bf3ed1c3bf_hd.jpg =360x328)

- The MM Algorithm by Kenneth Lange
- Majorization Methods
- Tangential Majorization
- Quadratic Majorization
- Sharp Majorization
- Using Higher Derivatives

Quadratic Lower Bound





• http://www.cs.cmu.edu/afs/cs/user/dwoodruf/www/w10b.pdf

Projected Gradient Method and More

We will focus on **projected gradient descent** and its some non-Euclidean generalization in order to solve some simply constrained optimization problems.

If not specified, all these methods are aimed to solve convex optimization problem with explicit constraints, i.e.

$$rg\min_{x\in\mathbb{S}}f(x)$$

where f is convex and differentiable, $\mathbb{S} \subset \mathbb{R}^n$ is convex.

The optimal condition for this constrained optimization problem is that the feasible direction is not the descent or profitable direction: if $x^* \in \mathbb{S}$ is the solution to the problem, we can assert that variational inequality holds:

$$\forall x \in \mathbb{S}, \langle \nabla f(x^{\star}), x - x^{\star} \rangle \geq 0.$$

And it is the optimal condition of constrained optimization problem.

Projected Gradient Descent

Projected gradient descent has two steps:

$$z^{k+1}=x^k-lpha_k
abla_x f(x^k)$$
 Descent $x^{k+1}=Proj_{\mathbb{S}}(z^{k+1})=rg\min_{x\in\mathbb{S}}\|x-z^{k+1}\|^2$ Projection

or in the compact form

$$egin{aligned} x^{k+1} &= rg\min_{x \in \mathbb{S}} \|x - (x^k - lpha_k
abla_x f(x^k))\|^2 \ &= rg\min_x \{\|x - (x^k - lpha_k
abla_x f(x^k))\|^2 + \delta_{\mathbb{S}}(x)\} \end{aligned}$$

where $\delta_{\mathbb{S}}$ is the indictor function of the set \mathbb{S}

$$h(x) = \delta_{\mathbb{S}}(x) = \left\{egin{array}{ll} 0, & ext{if} & x \in \mathbb{S}; \ \infty, & ext{otherwise.} \end{array}
ight.$$

Each projection is an optimization so that the iterative points satisfy the optimal conditions, which also restricts the projection method into the case where the projection is available or simple to compute.

And it is natural to search better Descent step or Projection step.

The following links are recommended if you want more theoretical proof:

- http://maths.nju.edu.cn/~hebma/slides/03C.pdf
- http://maths.nju.edu.cn/~hebma/slides/00.pdf

For the non-differentiable but convex function such as the absolute value function f(x) = |x|, we therefore consider subgradients in place of the gradient, where sub-gradient ϕ at the point \hat{x} is defined as the elements in the domain of convex function f (denoted as D_f), satisfying

$$\langle \phi, x - \hat{x} \rangle \leq f(x) - f(\hat{x}), \forall x \in D_f.$$

Mirror descent

Mirror descent can be regarded as the non-Euclidean generalization via replacing the ℓ_2 norm or Euclidean distance in projected gradient descent by Bregman divergence.

Bregman divergence is induced by convex smooth function h:

$$B_h(x,y) = h(x) - h(y) - \langle \nabla h(y), x - y \rangle$$

where $\langle \cdot, \cdot \rangle$ is inner product and it also denoted as D_h .

The function h is usually required to be strongly convex. And if the convex function h is not differentiable, one element of the sub-gradient $\partial h(y)$ may replace the gradient $\nabla h(y)$.

It is convex in
$$x$$
 and $\frac{\partial B_h(x,y)}{\partial x} = \nabla h(x) - \nabla h(y).$

Especially, when h is quadratic function, the Bregman divergence induced by h is

$$B_h(x,y) = x^2 - y^2 - \langle 2y, x - y \rangle = x^2 + y^2 - 2xy = (x - y)^2$$

i.e. the square of Euclidean distance.

A wonderful introduction to **Bregman divergence** is **Meet the Bregman Divergences** by Mark Reid at http://mark.reid.name/blog/meet-the-bregman-divergences.html.

The Bregman projection onto a convex set $C \subset \mathbb{R}^n$ given by

$$y' = rg \min_{x \in C} B(x,y)$$

is unique.

A generalized Pythagorean theorem holds: for convex $C\subset\mathbb{R}^n$ and for all $x\in C$ and $y\in\mathbb{R}^n$ we have

$$B(x, y) > B(x, y') + B(y', y)$$

where y' is the Bregman projection of y, and equality holds when the convex set C defining the projection y' is affine.

It is given in the projection form:

$$z^{k+1} = x^k - lpha_k
abla_x f(x^k) \qquad ext{Gradient descent} \; ; \ x^{k+1} = rg\min_{x \in \mathbb{S}} B(x, z^{k+1}) \qquad ext{Bregman projection}.$$

In another compact form, mirror gradient can be described in the proximal form:

$$x^{k+1} = \arg\min_{x \in \mathbb{S}} \{ f(x^k) + \left\langle g^k, x - x^k \right\rangle + \frac{1}{\alpha_k} B(x, x^k) \}$$
 (1)

with $q^k = \nabla f(x^k)$.

Note that the next iteration point x^{k+1} only depends the current iteration point x^k no more previous iteration points.

By the optimal conditions of equation (1), the original "mirror" form of mirror gradient method is described as

$$abla h(x^{k+1}) =
abla h(x^k) - lpha_k
abla f(x^k), x \in \mathbb{S}$$

where the convex function h induces the Bregman divergence.

One special method is called entropic mirror descent(Multiplicative Weights Update, Exponential Gradient Descent) when the Bregman divergence induced by e^x and the constraint set $\mathbb{S} \subset \mathbb{R}^n$ is simplex, i.e. $\sum_{i=1}^n x_i = 1, \forall x_i \geq 0.$

Entropic descent method at step k is given as follows:

$$x_i^{k+1} = rac{x_i^k \exp(-lpha
abla f(x^k)_i)}{\sum_{i=1}^n x_i^k \exp(-lpha
abla f(x^k)_i)}, i=1,2,\ldots,n.$$

See more on the following link list.

- Bregman Divergence and Mirror Descent, Xinhua Zhang(张歆华)
- CS 294 / Stat 260, Fall 2014: Learning in Sequential Decision Problems
- ELE522: Large-Scale Optimization for Data Science , Yuxin Chen, Princeton University, Fall 2019
- Mirror Descent and the Multiplicative Weight Update Method, CS 435, 201, Nisheeth Vishnoi
- http://www.divergence-methods.org/
- https://zhuanlan.zhihu.com/p/34299990
- https://blogs.princeton.edu/imabandit/2013/04/16/orf523-mirror-descent-part-iii/
- https://blogs.princeton.edu/imabandit/2013/04/18/orf523-mirror-descent-part-iiii/
- https://tlienart.github.io/pub/csml/cvxopt/mda.html
- https://web.stanford.edu/class/cs229t/2017/Lectures/mirror-descent.pdf
- https://www.cs.ubc.ca/labs/lci/mlrg/slides/mirrorMultiLevel.pdf

Proximal Gradient Method

The proximal mapping (or prox-operator) of a convex function ${f h}$ is defined as

$$prox_h(x) = rg \min_u \{h(u) + rac{1}{2} \|x - u\|_2^2 \}$$

Unconstrained problem with cost function split in two components:

$$minimize f(x) = g(x) + h(x)$$

- *g* is convex, differentiable;
- h is closed, convex, possibly non-differentiable while $prox_h(x)$ is inexpensive.

Proximal gradient algorithm

$$x^k = prox_{t_kh}\{x^{k-1} - t_k
abla g(x^{k-1})\}$$

 $t_k > 0$ is step size, constant or determined by line search.

$$x^+ = prox_{th}(x - t \nabla g(x))$$

from the definition of proximal mapping:

$$x^{+} = \arg\min_{u} (h(u) + \frac{1}{2} \|u - (x - t\nabla g(x))\|_{2}^{2})$$

$$= \arg\min_{u} (h(u) + g(x) + \nabla g(x)^{T} (u - x) + \frac{1}{2t} \|u - x\|_{2}^{2})$$

$$= \arg\min_{u} (h(u) + \nabla g(x)^{T} (u - x) + \frac{1}{2t} \|u - x\|_{2}^{2})$$

 x^+ minimizes h(u) plus a simple quadratic local model of g(u) around x.

And projected gradient method is a special case of proximal gradient methods with

$$h(x) = \delta_C(x) = \left\{ egin{array}{ll} 0, & ext{if} & x \in C; \ \infty, & ext{otherwise}. \end{array}
ight.$$

And it is natural to consider a more general algorithm by replacing the squared Euclidean distance in definition of proximal mapping with a Bregman distance:

$$rg\min_{u}\{h(u)+rac{1}{2}\|x-u\|_{2}^{2}\}
ightarrowrg\min_{u}\{h(u)+B(x,u)\}.$$

so that the primary proximal gradient methods are modified to the Bregman version, which is called as Bregman proximal gradient method.

- http://www.seas.ucla.edu/~vandenbe/236C/lectures/proxgrad.pdf
- https://people.eecs.berkeley.edu/~elghaoui/Teaching/EE227A/lecture18.pdf
- https://arxiv.org/abs/1808.03045
- A unified framework for Bregman proximal methods: subgradient, gradient, and accelerated gradient schemes
- A collection of proximity operators implemented in Matlab and Python.
- Proximal Algorithms, N. Parikh and S. Boyd
- For more (non exhaustive) informations regarding the proximity operator and the associated proximal algorithms

Proximal and Projected Newton Methods

A fundamental difference between gradient descent and Newton's method was that the latter also iteratively minimized quadratic approximations, but these used the local Hessian of the function in question.

Proximal Newton method can be also applied to such optimization problem:

$$y^k = prox_{H_{k-1}}(x^{k-1} - H_{k-1}^{-1}
abla g(x^{k-1})) \ x^k = x^{k-1} + t_k(y^k - x^{k-1}).$$

• http://www.stat.cmu.edu/~ryantibs/convexopt-S15/lectures/24-prox-newton.pdf

Note: the projection from a point x^0 into a subset $C \subset \mathbb{R}^n$ is defined in proximal operator as

$$x^+ = rg \min_x \{ \delta_C(x) + rac{1}{2} \|x - x^0\|_2^2 \}$$

while it can also written in the following form:

$$x^{+} = \arg\min_{x} \{ rac{1}{1_{C}(x)} \cdot \|x - x^{0}\|_{2}^{2} \}$$

where

$$1_C(x) = \left\{ egin{array}{ll} 1, & ext{if} & x \in C, \ 0, & ext{otherwise.} \end{array}
ight.$$

How we can generalize this form into the proximal form? And what is the difference with the original addition proximal operator?

If \boldsymbol{x}^0 is in the set C , the projection can be rewritten in proximal operator:

$$x^+ = rg \min_x \{ \exp[\delta_C(x)] \cdot rac{1}{2} \|x - x^0\|_2^2 \}.$$

How we can generalize the function δ_C to more general convex function? What are the advantages of this generalization? As likelihood and log-likelihood, we can transfer the product of some functions to sum by taking logarithm.

$$egin{aligned} x^+ &= rg \min_x \{ \exp[\delta_C(x)] \cdot rac{1}{2} \|x - x^0\|_2^2 \} \ &= rg \min_x \log \{ \exp[\delta_C(x)] \cdot rac{1}{2} \|x - x^0\|_2^2 \} \ &= rg \min_x \{ \delta_C(x) + \log(\|x - x^0\|_2^2) \}. \end{aligned}$$

Lagrange Multipliers and Duality

It is to solve the constrained optimization problem

$$rg \min_x f(x), \quad s.\, t. \quad g(x) = b.$$

The barrier or penalty function methods are to add some terms to $f(x) + \Omega(g(x) - b)$ converting constrained problems into unconstrained problems by introducing an artificial penalty for violating the constraint.

For example,

$$P(x,\lambda) = f(x) + \lambda \|g(x) - b\|_2^2$$

where the penalty function $\Omega(x)=\left\|x\right\|_{2}^{2}$, $\lambda\in\mathbb{R}^{+}$.

We can regard it as a surrogate loss technique.

Although the penalty function is convex and differentiable, it is more difficult than directly optimizing f(x) when the constrain is complicated.

What is the simplest additional term when the constraint is linear? In following context we will talk the optimization problem with linear constraints:

$$\arg\min_{x} f(x)$$

Lagrange Multipliers and Generalized Lagrange Function

The penalty function methods do not take the optimal conditions into consideration although it works. If x^* is in the solution set of the optimization problem above, it is obvious that $Ax^*=b$ and $L(x^*,\lambda)=f(x^*)$ where

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

In another direction, we want to prove that x^* is the optima of the optimization problem if

$$L(x^\star,\lambda^\star) = \min_x [\max_\lambda L(x,\lambda)].$$

By the definition,

$$L(x^\star,\lambda^\star)\geq L(x^\star,\lambda)=f(x^\star)+\lambda^T(Ax^\star-b)$$
, which implies that $\lambda^T(Ax^\star-b)=0$ i.e., $Ax^\star=b$. And $L(x^\star,\lambda^\star)=f(x^\star)\leq L(x,\lambda^\star) \forall x$ if $Ax=b$

thus x^{\star} is the solution to the primary problem.

It is dual problem is in the following form:

$$\max_{\lambda} [\min_{x} L(x, \lambda)].$$

Note that

$$\min_x L(x,\lambda) \leq L(x,\lambda) \leq \max_\lambda L(x,\lambda)$$

implies

$$\max_{\lambda} [\min_{x} L(x,\lambda)] \leq \max_{\lambda} L(x,\lambda) \leq \min_{x} [\max_{\lambda} L(x,\lambda)].$$

And note that necessary condition of extrema is that the gradients are equal to 0s:

$$rac{\partial L(x,\lambda)}{\partial x} = rac{\partial f(x)}{\partial x} + A\lambda = 0$$
 $rac{\partial L(x,\lambda)}{\partial \lambda} = Ax - b = 0$

Dual Ascent takes advantages of this properties:

1.
$$x^{k+1}=rg\min_x L(x,\lambda);$$
2. $\lambda^{k+1}=\lambda^k+lpha_k(Ax^{k+1}-b).$

Entropy minimization algorithms:

$$x^{k+1} \in rg \min_x \{f(x) + rac{1}{c_k} \sum_{i=1}^n x^i (\ln(rac{x_i}{x_i^k}) - 1)\}.$$

A special case for the convex problem

$$egin{aligned} ext{minimize} & f(x), \ s.\ t.\ g_1(x) \leq 0, g_2(x) \leq 0, \cdots, g_r(x) \leq 0, x \in X \end{aligned}$$

is the exponential augmented Lagrangean method.

It Consists of unconstrained minimizations:

$$x^k \in rg\min_{x \in X} \{f(x) + rac{1}{c_k} \sum_{j=1}^r \mu_j^k \exp(c_k g_j(x))$$

followed by the multiplier iterations

$$\mu_j^{k+1} = \mu_j^k \exp(c_k g_j(x^k)).$$

If the constraints are more complex, KKT theorem may be necessary.

- Duality
- https://cs.stanford.edu/people/davidknowles/lagrangian duality.pdf
- https://people.eecs.berkeley.edu/~elghaoui/Teaching/EE227A/lecture7.pdf
- https://www.svm-tutorial.com/2016/09/duality-lagrange-multipliers/
- https://www.cs.jhu.edu/~svitlana/papers/non refereed/optimization 1.pdf
- http://web.mit.edu/dimitrib/www/lagr mult.html
- https://zhuanlan.zhihu.com/p/50823110

exponential augmented Lagrangian method

- An exponential augmented Lagrangian method with second order convergence
- On the convergence of the exponential multiplier method for convex programming

Splitting Methods

Alternating direction method of multipliers is called **ADMM** shortly. It is aimed to solve the following convex optimization problem:

$$\min F(x,y) \{ = f(x) + g(y) \}$$
 (cost function)

$$Ax + By = b$$
 (constraint)

where f(x) and g(y) is convex; A and B are matrices.

Define the augmented Lagrangian:

$$L_{eta}(x,y) = f(x) + g(y) - \lambda^T(Ax + By - b) + rac{eta}{2} \|Ax + By - b\|_2^2.$$

Augmented Lagrange Method at step k is described as following:

1.
$$(x^{k+1}, y^{k+1}) = \arg\min_{x \in \mathbf{X}} L_{\beta}(x, y, \lambda^{k});$$

2. $\lambda^{k+1} = \lambda^{k} - \beta(Ax^{k+1} + By^{k+1} - b).$

ADMM at step t is described as following:

1.
$$x^{k+1} = \arg\min_{x \in \mathbf{X}} L_{\beta}(x, y^{k}, \lambda^{k});$$

2. $y^{k+1} = \arg\min_{y \in \mathbf{Y}} L_{\beta}(x^{k+1}, y, \lambda^{k});$
3. $\lambda^{k+1} = \lambda^{k} - \beta(Ax^{k+1} + By^{k+1} - b).$

The convergence proof of ADMM in convex optimization can be reduced to verifying the stability of a dynamical system or based on the optimal condition variational inequality like On the O(1/t) convergence rate of alternating direction method.

Linearized ADMM

Note that the \boldsymbol{x} subproblem in ADMM

$$\arg \min_{x} L_{\beta}(x, y^{k}, \lambda^{k})
= \arg \min_{x} \{f(x) + g(y^{k}) + \lambda^{k} (Ax + By^{k} - b) + \frac{\beta}{2} \|Ax + By^{k} - b\|_{2}^{2} \}
= \arg \min_{x} f(x) + \frac{\beta}{2} \|Ax + By^{k} - b - \frac{1}{\beta} \lambda\|_{2}^{2}$$
(1)

However, the

solution of the subproblem (1) does not have the closed form solution because of the general structure of the matrix A. In this case, we linearize the quadratic term of

$$rac{eta}{2}\|Ax+By^k-b-rac{1}{eta}\lambda^k\|_2^2$$

at x^k and add a proximal term $\frac{r}{2}\|x-x^k\|_2^2$ to the objective function.

In another word, we solve the following x subproblem if ignoring the constant term of the objective function:

$$\min_x f(x) + eta(Ax)^T(Ax^k + By^k - b - rac{1}{\lambda^k}) + rac{r}{2} \left\|x - x^k
ight\|_2^2.$$

1.
$$x^{k+1} = \arg\min_{x \in \mathbf{X}} f(x) + \beta (Ax)^T (Ax^k + By^k - b - \frac{1}{\lambda^k}) + \frac{r}{2} \|x - x^k\|_{2^k}^2$$

2.
$$y^{k+1} = \arg\min_{y \in Y} L_{\beta}(x^{k+1}, y, \lambda^{k})$$

3.
$$\lambda^{k+1} = \lambda^k - \beta (Ax^{k+1} + By^{k+1} - b)$$
.

For given eta>0 , choose r such that the matrix $rI_1-eta A^TA$ is definitely positive, i.e.,

$$rI_1 - \beta A^T A > 0.$$

We can also linearize the y subproblem:

1.
$$x^{k+1} = \operatorname{arg\,min}_{x \in \mathbf{X}} L_{\beta}(x, y^k, \lambda^k)$$

2.
$$y^{k+1} = \arg\min_{y \in \mathbf{Y}} g(y) + \beta (By)^T (Ax^{k+1} + By^k - b - \frac{1}{\beta}\lambda^k) + \frac{r}{2} \|y - y^k\|^2$$

3.
$$\lambda^{k+1} = \lambda^k - \beta (Ax^{k+1} + By^{k+1} - b).$$

For given $\beta > 0$, choose r such that

the matrix $rI_2-eta B^TB$ is definitely positive, i.e.,

$$rI_2 - \beta B^TB \geq 0.$$

1.
$$x^{k+1} = \arg\min_{x \in \mathbf{X}} L_{\beta}(x, y^{k}, \lambda^{k}),$$

2. $\lambda^{k+\frac{1}{2}} = \lambda^{k} - \mu \beta (Ax^{k+1} + By^{k} - b),$
3. $y^{k+1} = \arg\min_{y \in \mathbf{Y}} L_{\beta}(x^{k+1}, y, \lambda^{k+\frac{1}{2}}),$
4. $\lambda^{k+1} = \lambda^{k+\frac{1}{2}} - \mu \beta (Ax^{k+1} + By^{k+1} - b).$

http://www.optimization-online.org/DB FILE/2015/05/4925.pdf

Thanks to Professor He Bingsheng who taught me those. [^9]



He Bingsheng

One of the particular ADMM is also called Split Bregman methods. And Bregman ADMM replace the quadratic penalty function with Bregman divergence:

$$L^\phi_eta(x,y) = f(x) + g(y) - \lambda^T(Ax + By - b) + rac{eta}{2}B_\phi(b - Ax, By).$$

where B_ϕ is the Bregman divergence induced by the convex function ϕ .

BADMM

$$\begin{split} & \text{1. } x^{k+1} = \arg\min_{x \in \mathbf{X}} L^{\phi}_{\beta}(x, y^{\pmb{k}}, \lambda^{\pmb{k}}); \\ & \text{2. } y^{k+1} = \arg\min_{y \in \mathbf{Y}} L^{\phi}_{\beta}(x^{\pmb{k+1}}, y, \lambda^{\pmb{k}}); \\ & \text{3. } \lambda^{k+1} = \lambda^k - \beta(Ax^{\pmb{k+1}} + By^{\pmb{k+1}} - b). \end{split}$$

- https://arxiv.org/abs/1306.3203
- https://www.swmath.org/software/20288

Relaxed, Inertial and Fast ADMM

http://bipop.inrialpes.fr/people/malick/Docs/15-titan-iutzeler.pdf

- http://www.iutzeler.org/pres/osl2017.pdf
- https://www.mia.uni-saarland.de/Publications/goldstein-cam12-35.pdf
- The Classical Augmented Lagrangian Method and Nonexpansiveness

Multi-Block ADMM

Firstly we consider the following optimization problem

$$egin{aligned} \min f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n) \ s.\,t. \quad A_1x_1 + A_2x_2 + \cdots + A_nx_n = b, \ x_i \in X_i \in \mathbb{R}^{d_i}, i = 1, 2, \cdots, n. \end{aligned}$$

We defined its augmented Lagrangian multipliers as

$$L^n_eta(x_1, x_2, \cdots, x_n \mid \lambda) = \sum_{i=1}^n f_i(x_i) - \lambda^T (\sum_{i=1}^n A_i x_i - b) + rac{eta}{2} \| \sum_{i=1}^n A_i x_i - b \|^2.$$

Particularly, we firstly consider the case when n = 3:

$$egin{aligned} L^3_eta(x,y,z\mid \lambda) &= f_1(x) + f_2(y) + f_3(z) - \lambda^T (A_1 x + A_2 y + A_3 z - b) \ &+ rac{eta}{2} \|A_1 x + A_2 y + A_3 z - b\|_2^2. \end{aligned}$$

It is natural and computationally beneficial to extend the original ADMM directly to solve the general n-block problem. A counter-example shows that this method diverges.

And Professor Bingsheng He, who taught me this section in his class, and his coauthors proposed some schemes for this problem based on his unified frame work for convex optimization and monotonic variational inequality.

Parallel splitting augmented Lagrangian method (abbreviated to PSALM) is described as follows:

1.
$$x^{k+1} = rg \min_x \{L^3_{eta}(x, y^k, z^k, \lambda^k) \mid x \in \mathbb{X}\};$$

2.
$$y^{k+1} = \arg\min_{x} \{L^3_{\beta}(x^{k+1}, y, z^k, \lambda^k) \mid y \in \mathbb{Y}\};$$

3.
$$z^{k+1} = rg \min_x \{L^3_{\beta}(x^{k+1}, y^k, z, \lambda^k) \mid z \in \mathbb{Z}\};$$

4.
$$\lambda^{k+1} = \lambda^k - \beta(A_1x^{k+1} + A_2y^{k+1} + A_3z^{k+1} - b).$$

We can add one more correction step

$$v^{k+1} := v^k - \alpha(v^k - v^{k+1}), \alpha \in (0, 2 - \sqrt{2})$$

where
$$v^{k+1} = (y^{k+1}, z^{k+1}, \lambda^{k+1}).$$

Another approach is to add an regularized terms:

$$\begin{split} &1.\ x^{k+1} = \arg\min_x \{L_{\beta}^3(x,y^k,z^k,\lambda^k) \mid x \in \mathbb{X}\}, \\ &2.\ y^{k+1} = \arg\min_x \{L_{\beta}^3(x^{k+1},y,z^k,\lambda^k) + \frac{\tau}{2}\beta \|A_2(y-y^k)\|^2 \mid y \in \mathbb{Y}\}, \\ &3.\ z^{k+1} = \arg\min_x \{L_{\beta}^3(x^{k+1},y^k,z,\lambda^k) + \frac{\tau}{2}\beta \|A_3(z-z^k)\|^2 \mid z \in \mathbb{Z}\}, \\ &4.\ \lambda^{k+1} = \lambda^k - \beta(A_1x^{k+1} + A_2y^{k+1} + A_3z^{k+1} - b), \end{split}$$

where $\tau > 1$.

- http://scis.scichina.com/en/2018/122101.pdf
- http://maths.nju.edu.cn/~hebma/slides/17C.pdf
- http://maths.nju.edu.cn/~hebma/slides/18C.pdf
- https://link.springer.com/article/10.1007/s10107-014-0826-5

Davis-Yin three operator splitting

If f_1 is strongly convex, then apply Davis-Yin (to dual problem) gives:

$$\begin{split} &1.\ x^{k+1} = \arg\min_x \{L^3(x,y^k,z^k,\lambda^k) \mid x \in \mathbb{X}\}; \\ &2.\ y^{k+1} = \arg\min_x \{L^3_\beta(x^{k+1},y,z^k,\lambda^k) \mid y \in \mathbb{Y}\}; \\ &3.\ z^{k+1} = \arg\min_x \{L^3_\beta(x^{k+1},y^{k+1},z,\lambda^k) \mid z \in \mathbb{Z}\}; \\ &4.\ \lambda^{k+1} = \lambda^k - \beta(A_1x^{k+1} + A_2y^{k+1} + A_3z^{k+1} - b). \end{split}$$

where the notation $L^3(x,y,z,\lambda)$ is deefined by

$$L^3(x,y,z,\lambda) = f_1(x) + f_2(y) + f_3(z) - \lambda^T (A_1 x + A_2 y + A_3 z - b)$$

is the Lagrangian rather than augmented Lagrangian.

- Three-Operator Splitting
- A Three-Operator Splitting Scheme and its Optimization Applications
- Three-Operator Splitting and its Optimization Applications
- A Three-Operator Splitting Scheme and its Optimization Applications
- A Three-Operator Splitting Scheme and its Applications

Randomly Permuted ADMM given initial values at round k is described as follows:

- 1. Primal update
 - Pick a permutation σ of $1, \ldots, n$ uniformly at random;

 $\circ \hspace{0.2cm}$ For $i=1,2,\cdots,n$, compute $x_{\sigma(i)}^{k+1}$ by

$$x_{\sigma(i)}^{k+1} = rg\min_{x_{\sigma(i)}} L(x_{\sigma(1)}^{k+1}, \cdots, x_{\sigma(i-1)}^{k+1}, x_{\sigma(i)}, x_{\sigma(i+1)}^{k+1}, \cdots \mid \lambda^k).$$

2. Dual update. Update the dual variable by

$$\lambda^{k+1} = \lambda^k - \mu(\sum_{i=1}^n A_i x_i - b).$$

- Randomly Permuted ADMM
- http://opt-ml.org/oldopt/papers/OPT2015_paper_47.pdf
- https://arxiv.org/abs/1503.06387
- Multi-Block ADMM and its Convergence Random Permutation Helps-A talk by Ye
- http://maths.nju.edu.cn/~hebma/
- http://stanford.edu/~boyd/admm.html
- · A General Analysis of the Convergence of ADMM
- 用ADMM实现统计学习问题的分布式计算
- https://www.wikiwand.com/en/Augmented_Lagrangian_method
- 凸优化:ADMM(Alternating Direction Method of Multipliers)交替方向乘子算法
- Splitting methods and ADMM, Thibaut Lienart
- Split Bregman
- Accelerated Bregman operator splitting with backtracking
- Splitting Algorithms, Modern Operator Theory, and Applications (17w5030)
- 17w5030 Workshop on Splitting Algorithms, Modern Operator Theory, and Applications

Primal-dual fixed point algorithm and Primary Dual Hybrid Gradient

- A primal-dual fixed point algorithm for multi-block convex minimization
- A primal–dual fixed point algorithm for convex separable minimization
- A Unified Primal-Dual Algorithm Framework Based on Bregman Iteration
- Proximal ADMM
- PDHG

The methods such as ADMM, proximal gradient methods do not optimize the cost function directly. For example, we want to minimize the following cost function

$$f(x,y) = g(x) + h(y)$$

with or without constraints.

Specially, if the cost function is additionally separable, $f(x)=f_1(x_1)+f_2(x_2)+\cdots+f_n(x_n)$, we would like to minimize the sub-function or component function $f_i(x_i), i=1,2,\cdots,n$ rather than the cost function itself

$$\min_x \sum_i f_i(x_i) \leq \sum_i \min_{x_i} f_i(x_i).$$

And ADMM or proximal gradient methods are to split the cost function to 2 blocks, of which one is differentiable and smooth while the other may not be differentiable. In another word, we can use them to solve some non-smooth optimization problem.

However, what if there is no constraints application to the optimization problem?

Coordinate descent is aimed to minimize the following cost function

$$f(x) = g(x) + \sum_i^n h_i(x_i)$$

where g(x) is convex, differentiable and each $h_i(x)$ is convex.

We can use coordinate descent to find a minimizer: start with some initial guess x^0 , and repeat for $k=1,2,3,\ldots$

$$1. \ x_1^k \in rg \min_{x_1} f(x_1, x_2^{k-1}, x_3^{k-1}, \dots, x_n^{k-1});$$

2.
$$x_2^k \in \arg\min_{x_1} f(x_1^k, x_2, x_3^{k-1}, \dots, x_n^{k-1});$$

3.
$$x_3^k \in \arg\min_{x_1} f(x_1^k, x_2^k, x_3, \dots, x_n^{k-1});$$

5.
$$x_n^k \in \operatorname{arg\,min}_{x_1} f(x_1^k, x_2^k, x_3^k, \dots, x_n)$$
.

It can extended to block coordinate descent($\overline{ ext{BCD}}$) if the variables x_1, x_2, \ldots, x_n are separable in some blocks.

- http://bicmr.pku.edu.cn/conference/opt-2014/index.html
- https://calculus.subwiki.org/wiki/Additively_separable_function
- https://www.cs.cmu.edu/~ggordon/10725-F12/slides/25-coord-desc.pdf
- http://bicmr.pku.edu.cn/~wenzw/opt2015/multiconvex_BCD.pdf

Surrogate Optimization

It is a unified principle that we optimize an objective function via sequentially optimizing surrogate functions such as **EM, ADMM**.

It is obvious that the choice of optimization methods relies on the objective function. Surrogate loss transform the original problem $\min_x f(x)$ into successive trackable subproblems:

$$x^{k+1} = rg \min_x Q_k(x).$$

A good surrogate function should:

- Approximate the objective function.
- · Easy to optimize.

This always leads to the convexification technique where the surrogate function is convex. For example, we can rewrite gradient descent in the following form

$$x^{k+1} = rg \min_x \{f(x^k) + \left\langle
abla f(x^k), x - x^k
ight
angle + rac{1}{2lpha_k} \|x - x^k\|_2^2 \}.$$

In Newton's method, we approximate the objective with a quadratic surrogate of the form:

$$Q_k(x) = f(x^k) + \left\langle
abla f(x^k), x - x^k
ight
angle + rac{1}{2lpha_k} (x - x^k)^T H_k(x - x^k).$$

Note that the Hessian matrix H_k is supposed to be positive definite. The quasi-Newton methods will approximate the Hessian matrix with some inverse symmetric matrix. And they can rewrite in the principle of surrogate function, where the surrogate function is convex in the form of linear function + squared functions in some sense.

Note that momentum methods can be rewrite in the surrogate function form:

$$\begin{split} x^{k+1} &= x^k - \alpha_k \nabla_x f(x^k) + \rho_k (x^k - x^{k-1}) \\ &= \arg \min_x \{ f(x^k) + \left\langle \nabla f(x^k), x - x^k \right\rangle + \frac{1}{2\alpha_k} \|x - x^k - \rho_k (x^k - x^{k-1})\|_2^2 \}. \end{split}$$

PS: How we can extend it to Nesterov gradient methods or stochastic gradient methods? Discover acceleration

It is natural to replace the squared function with some non-negative function such as mirror gradient methods

$$x^{k+1} = rg \min_x \{f(x^k) + \left\langle
abla f(x^k), x - x^k
ight
angle + rac{1}{lpha_k} B(x, x^k) \}.$$

More generally, auxiliary function $g_k(x)$ may replace the Bregman divergence $B(x,x^k)$, where the auxiliary functions $g_k(x)$ have the properties $g_k(x) \ge 0$ and $g_k(x^{k-1}) = 0$.

- http://fa.bianp.net/teaching/2018/eecs227at/
- http://fa.bianp.net/teaching/2018/eecs227at/newton.html
- http://faculty.uml.edu/cbyrne/NBHSeminar2015.pdf

The parameters α_k is chosen so that the surrogate function is convex by observing that the condition number of Hessian matrix is determined by the factor $\frac{1}{\alpha_k}$. And gradient are used in these methods to construct the surrogate function. There are still two problems in unconstrained optimization:

- 1. If the cost function is not smooth or differential such as absolute value function, the gradient is not available so that it is a problem to construct a convex surrogate function without gradient;
- 2. In another hand, there is no unified principle to construct a convex surrogate function if we know more information of higher order derivatives.

Moreau envelope (or Moreau-Yosida regularization) of a convex function f with parameter $\mu>0$ is defined as

$$M_{\mu f}(x) = \inf_z \{f(z) + rac{1}{2\mu} \|z - x\|_2^2\}.$$

Minimizing f and M_f are equivalent. $prox_{\mu f}(x) \mbox{ is unique point that achieves the infimum that defines } M_{\mu f} \mbox{ , i.e.}$

$$M_{\mu f}(x) = f(prox_{\mu f}(x)) + rac{1}{2} \left\| prox_{\mu f}(x) - x
ight\|_2^2 \}.$$

Moreau envelope M_f is continuously differentiable with gradients

$$abla M_{\mu f} = rac{1}{\mu} (prox_{\mu f}(x) - x).$$

This means

$$prox_{uf}(x) = x - \mu \nabla M_{uf}$$

i.e., $prox_{\mu f}(x)$ is gradient step for minimizing $M_{\mu f}$.

Fenchel Conjugate of a function h is is the function h^* defined by

$$h^\star(x) = \sup_z \{\langle z, x
angle - h(z) \}.$$

- Smoothing for nonsmooth optimization, ELE522: Large-Scale Optimization for Data Science
- Smoothing, EE236C (Spring 2013-14)
- Smoothing and First Order Methods: A Unified Framework

Charles Byrne gives a unified treatment of some iterative optimization algorithms such as auxiliary function methods.

Young Recent

Young	Recent
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src=http://faculty.uml.edu/cbyrne/CharlieByrneBookImage.jpg	=https://i1.rgstatic.net/ii/profile.image/551299453919233-
width = 150% />	1508451440729_Q128/Charles_Byrne.jpg width = 200% />

He is a featured author of CRC press and professor in UML

Auxiliary-Function Methods minimize the function

$$G_k(x) = f(x) + g_k(x)$$

over $x\in\mathbb{S}$ for $k=1,2,\cdots$ if $f(x):\mathbb{S}\mapsto\mathbb{R}$ and $g_k(x)$ is auxiliary function.

We do not linearize the cost function as the previous methods.

Auxiliary-Function Methods(AF methods) include

- Barrier- and Penalty-Function Algorithms such as sequential unconstrained minimization (SUM) methods, interior-point methods exterior-point methods;
- Proximal Minimization Algorithms such as majorization minimization.

And an AF method is said to be in the SUMMA class if the SUMMA Inequality holds:

$$G_k(x) - G_k(x^k) \geq g_{k+1}(x), orall x \in \mathbb{S}.$$

Proximal minimization algorithms using Bregman distances, called here PMAB, minimize the function

$$G_k(x) = f(x) + B(x, x^{k-1}), \forall x \in \mathbb{S}.$$

The forward-backward splitting (FBS) methods is to minimize the function

$$f_1(x) + f_2(x)$$

where both functions

are convex and $f_2(x)$ is differentiable with its gradient L-Lipschitz continuous in the Euclidean norm. The iterative step of the FBS algorithm is

$$x^k = prox_{\gamma f_1}(x^{k-1} - \gamma
abla f_2(x^{k-1})).$$

It is equivalent to minimize

$$G_k(x) = f(x) + rac{1}{2\gamma} \|x - x^{k-1}\|_2^2 - B(x, x^{k-1}),$$

where $B(x,x^{k-1})=f_1(x)-f_1(x^{k-1})-\left\langle
abla f_1(x^{k-1}),x-x^{k-1}
ight
angle ,\, 0<\gamma\leq rac{1}{L}.$

Alternating Minimization (AM) can be regarded as coordinate optimization methods with 2 blocks:

•
$$p^{n+1} = \operatorname{arg\,min}_{p \in P} f(p, q^n)$$
,

•
$$q^{n+1} = \arg\min_{p \in Q} f(p^{n+1}, q)$$

where $f(p,q), p \in P, q \in Q$ is the objective function. It is proved that the sequence $f(p^n,q^n)$ converge to the minimizer if the Five-Point Property hold:

$$f(p,q) + f(p,q^{n-1}) \ge f(p,q^n) + f(p^n,q^{n-1}).$$

For each p in the set P, define q(p) in Q as a member of Q for which $f(p;q(p)) \leq f(p;q)$, for all $q \in P$. Let $\hat{f}(p) = f(p;q(p))$. At the nth step of AM we minimize

$$G_n(p) = f(p;q(p)) + [f(p;q^{n-1}) - f(p;q(p))]$$

to get p^n , where $g_n(p)=f(p;q^{n-1})-f(p;q(p))$ is the auxiliary function. So we can write that $G_n(p)=f(p;q(p))+g_n(p)$.

See Iterative Convex Optimization Algorithms; Part Two: Without the Baillon—Haddad Theorem or Alternating Minimization, Proximal Minimization and Optimization Transfer Are Equivalent for more information on AF methods.

Expectation-Maximization can be classified to AF method.

- $Q(\theta|\theta^{(t)}) = \mathbb{E}(\ell(\theta|Y_{obs},Z)|Y_{obs},\theta^{(t)});$
- $\theta^{(t+1)} = \arg\min_{\theta} Q(\theta|\theta^{(t)}).$

The $Q(\theta|\theta^{(t)})$ function is log-likelihood function of complete data (Y_{os}, Z) given $(Y_{obs}, \theta^{(t)})$.

- Iterative Convex Optimization Algorithms; Part Two: Without the Baillon–Haddad Theorem
- Alternating Minimization, Proximal Minimization and Optimization Transfer Are Equivalent
- A unified treatment of some iterative algorithms in signal processing and image reconstruction
- Convergence Rate of Expectation-Maximization

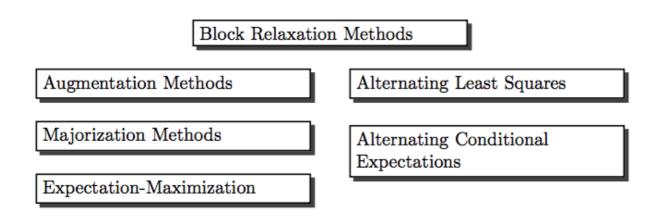
Optimization using surrogate models applied to Gaussian Process models (Kriging).

- Optimization using surrogate models
- Surrogate loss function
- Divergences, surrogate loss functions and experimental design
- Surrogate Regret Bounds for Proper Losses
- Bregman Divergences and Surrogates for Learning
- Meet the Bregman Divergences
- Some Theoretical Properties of an Augmented Lagrangian Merit Function
- https://people.eecs.berkeley.edu/~wainwrig/stat241b/lec11.pdf

http://fa.bianp.net/blog/2014/surrogate-loss-functions-in-machine-learning/

Relaxation and Convexification

The methods discussed in the book Block Relaxation Methods in Statistics are special cases of what we shall call block-relaxation methods, although other names such as decomposition or nonlinear Gauss-Seidel or ping-pong or seesaw methods have also been used.



block relaxation methods

In a block relaxation method we minimize a real-valued function of several variables by partitioning the variables into blocks. We choose initial values for all blocks, and then minimize over one of the blocks, while keeping all other blocks fixed at their current values. We then replace the values of the active block by the minimizer, and proceed by choosing another block to become active. An iteration of the algorithm steps through all blocks in turn, each time keeping the non-active blocks fixed at current values, and each time replacing the active blocks by solving the minimization subproblems. If there are more than two blocks there are different ways to cycle through the blocks. If we use the same sequence of active blocks in each iteration then the block method is called cyclic.

In the special case in which blocks consist of only one coordinate we speak of the coordinate relaxation method or the coordinate descent (or CD) method. If we are maximizing then it is coordinate ascent (or CA). The cyclic versions are CCD and CCA.

Augmentation Methods

Augmentation and Decomposition Methods

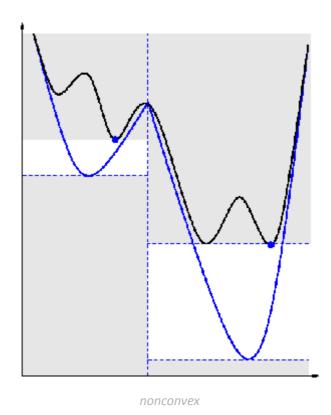
Alternating Conditional Expectations

The alternating descent conditional gradient method

Convex relaxations are one of the most powerful techniques for designing polynomial time approximation algorithms for NP-hard optimization problems such as

Chromatic Number, MAX-CUT, Minimum Vertex Cover etc. Approximation algorithms for these problems are developed by formulating the problem at hand as an integer program.

- https://pratikac.github.io/
- Block Relaxation Methods in Statistics by Jan de Leeuw
- Deep Relaxation: partial differential equations for optimizing deep neural networks
- Deep Relaxation tutorials
- CS 369S: Hierarchies of Integer Programming Relaxations
- Convex Relaxations and Integrality Gaps
- LP/SDP Hierarchies Reading Group
- Proofs, beliefs, and algorithms through the lens of sum-of-squares
- Iterative Convex Optimization Algorithms; Part Two: Without the Baillon-Haddad Theorem
- Relaxation and Decomposition Methods for Mixed Integer Nonlinear Programming



In order for primal-dual methods to be applicable to a constrained minimization problem, it is necessary that restrictive convexity conditions are satisfied.

A nonconvex problem can be convexified and transformed into one which can be solved with the aid of primal-dual methods.

- Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming: Theory, Algorithms, Software, and Applications
- Convexification and Global Optimization of Nonlinear Programs
- Convexification Procedure and Decomposition Methods for Nonconvex Optimization Problem
- Conic Optimization Theory: Convexification Techniques and Numerical Algorithms
- Convexification of polynomial optimization problems by means of monomial patterns
- On convexification/optimization of functionals including an ℓ^2 -misfit term
- Lossless Convexification of Nonconvex Control Bound and Pointing Constraints of the Soft Landing Optimal Control Problem
- A General Class of Convexification Transformation for the Noninferior Frontier of a Multiobjective Program

- Implementation of a Convexification Technique for Signomial Functions
- Sequential quadratic programming
- A method to convexify functions via curve evolution

Fixed Point Iteration Methods

The fixed point algorithm is initially to find approximate solutions of the equation

$$f(x) = 0 (1)$$

where $f: \mathbb{R} \to \mathbb{R}, x \in \mathbb{R}^n$.

In this method, we first rewrite the question(1) in the following form

$$x = g(x) \tag{2}$$

in such a way that any solution of the equation (2), which is a fixed point of the function g, is a solution of equation (1). For example, we can set g(x)=f(x)+x, g(x)=x-f(x). Then consider the following algorithm.

1. Give the initial point x^0 ;

2. Compute the recursive procedure $x^{n+1} = g(x^n), n = 1, 2, ...$

So that finally we obtain an sequence $\{x^0, x^1, \cdots, x^n, \cdots\}$. There are many methods to test whether this sequence is convergent or not as learn in calculus.

In high dimensional space, it is a little different. Fixed point iteration as well as the fixed point itself arises in many cases such as [https://arxiv.org/pdf/1511.06393.pdf].

The contracting mapping $F:\mathbb{R}^d o \mathbb{R}^d$ is defined as

$$||F(x) - F(y)|| \le \alpha ||x - y||, \forall x, y \in \mathbb{R}, \alpha \in [0, 1).$$

Thus
$$\lim_{\|x-y\| o 0} rac{\|F(x)-F(y)\|}{\|x-y\|} \leq lpha \in [0,1).$$

Now we rewrite the necessary condition of unconstrainted optimization problems $\nabla f(x) = 0$ to the fixed point equation:

$$abla f(x) = 0 \Rightarrow x - \alpha \nabla f(x) = x$$

$$abla f(x) = 0 \Rightarrow g(x) - \alpha \nabla f(x) = g(x) \Rightarrow x - g^{-1}(\alpha \nabla f(x)) = x$$

$$abla f(x) = 0 \Rightarrow H(x)x - \alpha \nabla f(x) = H(x)x \Rightarrow x - \alpha H(x)^{-1} \nabla f(x) = x$$

$$abla f(x) = 0 \Rightarrow M(x) \nabla f(x) = 0 \Rightarrow x - \alpha M(x) \nabla f(x) = x$$

where H(x) is the lambda-matrix.

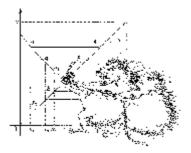
These correspond to gradient descent, mirror gradient methods, Newton's methods and quasi-Newton's methods, respectively.

And the projected (sub)gradient methods are in the fixed-point iterative form:

$$x = Proj_{\mathbb{S}}(x - \alpha \nabla f(x))$$

as well as the mirror gradient and proximal gradient methods different from the projection operator.

Expectation maximization is also an accelerated fixed point iteration as well as Markov chain.



http://www.drkhamsi.com/fpt/books.html

The following figures in the table is form Formulations to overcome the divergence of iterative method of fixed-point in nonlinear equations solution

Fixed Point Iterations

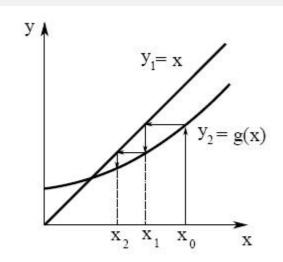


Figure 1. Convergence for 0 < g'(x) < 1 (monotone behavior).

Source: own work.

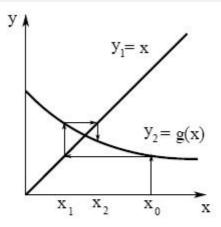


Figure 2. Convergence for -1 < g'(x) < 0 (oscillatory behavior).

Source: own work.

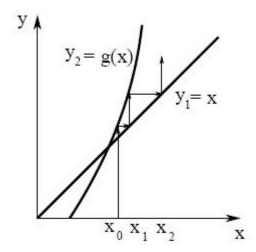


Figure 3. Divergence for g'(x) > 1 (monotone behavior).

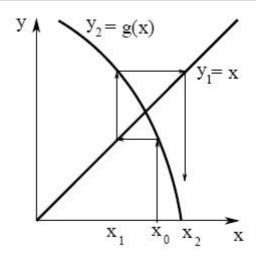


Figure 4. Divergence for g'(x) < -1 (oscillatory behavior).

Source: own work.

- https://www.wikiwand.com/en/Fixed-point_theorem
- Fixed-Point Iteration

Source: own work.

- Lecture 8 : Fixed Point Iteration Method, Newton's Method
- FixedPoint: A suite of acceleration algorithms with Application
- Books on Fixed Point Theory

ISTA and FASTA

The ℓ_1 regularization is to solve the ill-conditioned equations such as

$$\min_{x} \|Ax - b\|_{2}^{2} + \lambda \|x\|_{1}.$$

It is less sensitive to outliers and obtain much more sparse solutions (as opposed to ℓ_2 regularization). Its application includes and is not restricted in *LASSO*, compressed sensing and sparse approximation of signals.

It is clear that the absolute value function is not smooth or differentiable everywhere even the objective function $\|Ax - b\|_2^2 + \lambda \|x\|_1$ is convex.

It is not best to solve this problem by gradient-based methods.

Iterative Shrinkage-Threshold Algorithms(ISTA) for ℓ_1 regularization is

$$x^{k+1} = \mathbf{T}_{\lambda t}(x^k - tA^T(Ax - b))$$

where t>0 is a step size and \mathbf{T}_{lpha} is the shrinkage operator defined by

$$\mathbf{T}_{lpha}(x)_i = (x_i - lpha)_+ sgn(x_i)$$

where x_i is the i th component of $x \in \mathbb{R}^n$.

FISTA with constant stepsize

• $x^k = p_L(y^k)$ computed as ISTA;

$$ullet \ t_{k+1} = rac{1+\sqrt{1+4t_k^2}}{2};$$

•
$$y^{k+1} = x^k + \frac{t_{k-1}}{t_{k+1}}(x^k - x^{k-1}).$$

- A Fast Iterative Shrinkage Algorithm for Convex Regularized Linear Inverse Problems
- https://pylops.readthedocs.io/en/latest/gallery/plot_ista.html
- ORF523: ISTA and FISTA

This will lead to the operator splitting methods analysed by Wotao Yin and others. Wotao Yin wrote a summary on First-order methods and operator splitting for optimization:

First-order methods are described and analyzed with gradients or subgradients, while second-order methods use second-order derivatives or their approximations.

During the 70s–90s the majority of the optimization community focused on second-order methods since they are more efficient for those problems that have the sizes of interest at that time. Beginning around fifteen years ago, however, the demand to solve ever larger problems started growing very quickly. Many large problems are further complicated by non-differentiable functions and constraints. Because simple first-order and classic second-order methods are ineffective or infeasible for these problems, operator splitting methods regained their popularity.

Operators are used to develop algorithms and analyze them for a wide spectrum of problems including optimization problems, variational inequalities, and differential equations. Operator splitting is a set of ideas that generate algorithms through decomposing a problem that is too difficult as a whole into two or more smaller and simpler subproblems. During the decomposition, complicated structures like non-differentiable functions, constraint sets, and distributed problem structures end up in different subproblems and thus can be handled elegantly. We believe ideas from operator splitting provide the most effective means to handle such complicated structures for computational problem sizes of modern interest.

• ORIE 6326: Convex Optimization Operator Splitting

- Monotone Operator Splitting Methods
- A Course on First-Order, Operator Splitting, and Coordinate Update Methods for Optimization
- Operator Splitting Methods for Convex Optimization Analysis and Implementation
- Some Operator Splitting Methods for Convex Optimization

Krasnosel'skii-Mann(KM, or averaged) iterations update \boldsymbol{x}^k in iteration k to

$$x^{k+1} = (1 - \alpha_k)x^k + \alpha_k T(x^k), \alpha_k \in (0, 1)$$

for the fixed point problem (2). Specially, $T(x^k)=x^k-\alpha_k\nabla f(x^k)$ for the convex optimization problems. If the operator T is non-expensive, then the sequence $\{x^k\mid k=0,1,2,\ldots\}$ is convergent by Krasnosel'skii-Mann Theorem .

In 1953, Mann defined an iterative method:

$$x^{k+1}=M(x^k,lpha_k,T)=(1-lpha_k)x^k+lpha_kT(x^k), \ lpha_k\in[0,1) ext{ satisfying } \sum_{k=1}^\inftylpha_k=\infty.$$

The sequence $\{x^k\}$ defined by

$$x^{k+1} = (1 - \alpha_k)x^k + \alpha_k T^k(x^k), 0 < a \le \alpha_k \le b < 1$$

(additionally $\sum_{k=1}^\infty \alpha_k = \infty$)is called a modied Mann iteration . Take $\{\alpha_k,\beta_k\}$ two sequences in [0,1] satisfying

$$\sum_{k=1}^{\infty} lpha_k eta_k = \infty, \lim_{k\infty} eta_k = 0, 0 \leq lpha_k \leq eta_k \leq 1.$$

Then the sequence $\{x^k\}$ defined by

$$x^{k+1} = (1 - \alpha_k)x^k + \alpha_k T^k(y^k),$$

 $y^k = (1 - \beta_k)x^k + \beta_k T(x^k).$

is called the Ishikawa iteration .

Hojjat Afshari and Hassen Aydi proposes another Mann type iteration:

$$x^{k+1} = lpha_k x^k + eta_k T(x^k) + \gamma_k T^2(x^k)$$

where $\alpha_k+\beta_k+\gamma_k=1, \alpha_k, \beta_k, \gamma_k\in [0,1)$ for all $k\geq 1$, $\sum_k^\infty (1-\alpha_k)=\infty$, $\sum_{k=1}^\infty \gamma_k<\infty$.

If the Mann type iteration $\{x^k\}$ converges strongly to a point p, then p is affixed point of T.

Krasnoselskii-Mann method for non-self mappings

- http://www.krasnoselskii.iitp.ru/papereng.pdf
- Strong convergence of the modified Mann iterative method for strict pseudo-contractions
- Some results on a modified Mann iterative scheme in a reflexive Banach space
- Some results about Krasnosel'skii-Mann iteration process
- Convergence theorems for inertial KM-type algorithms

There is an acceleration framework of fixed point iterations for the problem (2) called Anderson Acceleration or regularized nonlinear acceleration:

1.
$$F_k = (h_{k-m_k}, \dots, h_k)$$
 where $h_i = g(x_i) - x_i$;

2. Determine
$$\alpha^k=(\alpha_0^k,\ldots,\alpha_{m_k}^k)^T$$
 that solves $\min_{\alpha^k}\|F_k\alpha^k\|_2^2$ s.t. $\sum_{i=0}^{m_k}\alpha_i^k=1$;

3. Set
$$x_{k+1} = \sum_{i=0}^{m_k} \alpha_i^k g(x_{k-m_k+i})$$
.

It is maybe interesting to introduce some Bregman divergence $D_f(\cdot,\cdot)$ instead of the squared ℓ_2 norm when choosing α^k so that

$$lpha^k = rg \min_{lpha^k} \{D_f(F_k lpha^k) \mid \sum_{i=0}^{m_k} lpha_i^k = 1\}.$$

It is proved that the Anderson acceleration converges if the fixed point mapping is cotractive.

- Anderson acceleration for fixed point iterations
- Anderson Acceleration
- MS142 Anderson Acceleration and Applications
- Anderson Acceleration of the Alternating Projections Method for Computing the Nearest Correlation Matrix
- Convergence Analysis For Anderson Acceleration
- Using Anderson Acceleration to Accelerate the Convergence of Neutron Transport Calculations with Anisotropic Scattering
- Comments on "Anderson Acceleration, Mixing and Extrapolation"

The Baillon-Haddad Theorem provides an important link between convex optimization and fixed-point iteration, which proves that if the gradient of a convex and continuously differentiable function is nonexpansive, then it is actually firmly nonexpansive.

- The Baillon-Haddad Theorem Revisited
- Recent Advances in Convex Optimization and Fixed Point Algorithms by Jean-Christophe Pesquet
- A Generic online acceleration scheme for Optimization algorithms via Relaxation and Inertia
- RELAXATION AND INERTIA IN FIXED-POINT ITERATIONS WITH APPLICATION
- Monotonicity, Acceleration, Inertia, and the Proximal Gradient algorithm
- Globally Convergent Type-I Anderson Acceleration for Non-Smooth Fixed-Point Iterations
- On the Convergence Rate of the Halpern-Iteration
- Iterative Convex Optimization Algorithms; Part One: Using the Baillon-Haddad Theorem

However, it is best to think from the necessary condition of optima in non-convex optimization in my opinion. Another question is to generalize the fixed point iteration to stochastic gradient methods.

Dynamical Systems

We will focus on the optimization methods in the form of fixed point iteration and dynamical systems. It is to minimize the following function

$$f(x), x \in \mathbb{R}^p, \quad \nabla f(x) = g(x), \quad \nabla^2 f(x) = H(x).$$

Iteration ODE

Like Newton interpolation, more points can compute higher order derivatives.

The dynamics of accelerated gradient methods are expected to correspond to higher order differential equations.

Some acceleration methods are iterations of the corresponding algorithms of Asymptotic Vanishing Damping called by Hedy Attouch:

$$\ddot{x}(t) + \frac{\alpha}{t}\dot{x}(t) + \nabla\Phi(x(t)) = 0.$$
 (AVD)

where $\Phi(x(t))$ is dependent on the objective function; $\alpha > 0$ is constant in \mathbb{R} .

The fast minimization properties of the trajectories of the second-order evolution equation is also studied by Hedy's group in 2016:

$$\ddot{x}(t) + \frac{\alpha}{t}\dot{x}(t) + \nabla^2\Phi(x(t))\dot{x}(t) + \nabla\Phi(x(t)) = 0 \tag{HDD}$$

When it comes to numerical solution to differential equations, it is to find the solution of the equations x(t) so that the equations hold; in optimization, the optima is our goal so that the focus is limit order

$$\lim_{t o t_0} x(t) = x^\star$$

if possible where x^* optimizes the cost/objective function f(x) specially $t_0 = \infty$.

<img src="https://i1.rgstatic.net/ii/profile.image/291292945895424-1446461058178_Q128/Hedy_Attouch.jpg" width = "50%"
/>

- https://perso.math.univ-toulouse.fr/spot/resumes/
- Fast convex optimization via inertial dynamics with Hessian driven damping
- A proximal-Newton method for monotone inclusions in Hilbert spaces with complexity $O(1/k^2)$
- https://www.researchgate.net/profile/Hedy_Attouch

- https://www.ljll.math.upmc.fr/~plc/sestri/
- Hedy Attouch at https://biography.omicsonline.org
- Rate of convergence of the Nesterov accelerated gradient method in the subcritical case $lpha \leq 3$
- A Dynamical Approach to an Inertial Forward-Backward Algorithm for Convex Minimization
- An Inertial Proximal Method for Maximal Monotone Operators via Discretization of a Nonlinear Oscillator with Damping
- THE HEAVY BALL WITH FRICTION METHOD, I. THE CONTINUOUS DYNAMICAL SYSTEM: GLOBAL EXPLORATION OF THE LOCAL MINIMA OF A REAL-VALUED FUNCTION BY ASYMPTOTIC ANALYSIS OF A DISSIPATIVE DYNAMICAL SYSTEM
- Viscosity Solutions of Minimization Problems
- Rate of convergence of the Nesterov accelerated gradient method in the subcritical case $lpha \leq 3$
- A dynamic approach to a proximal-Newton method for monotone inclusions in Hilbert spaces, with complexity $O(\frac{1}{n^2})$
- FAST CONVERGENCE OF INERTIAL DYNAMICS AND ALGORITHMS WITH ASYMPTOTIC VANISHING DAMPING

It is difficult to generalize these methods to stochastic cases.

There is a wonderful summary DYNAMICAL, SYMPLECTIC AND STOCHASTIC PERSPECTIVES ON GRADIENT-BASED OPTIMIZATION given by Micheal I Jordan at ICM 2018.

Some new connections between dynamical systems and optimization is found.

- Variational and Dynamical Perspectives On Learning and Optimization
- Continuous and Discrete Dynamics For Online Learning and Convex Optimization
- DYNAMICAL, SYMPLECTIC AND STOCHASTIC PERSPECTIVES ON GRADIENT-BASED OPTIMIZATION
- On Symplectic Optimization
- A variational perspective on accelerated methods in optimization
- A Dynamical Systems Perspective on Nesterov Acceleration
- Generalized Momentum-Based Methods: A Hamiltonian Perspective
- https://people.eecs.berkeley.edu/~jordan/optimization.html

Weijie J. Su (joint with Bin Shi, Simon Du, and Michael Jordan) introduced a set of high-resolution differential equations to model, analyze, interpret, and design accelerated optimization methods.

$$\ddot{x}(t) + 2\sqrt{\mu}\dot{x}(t) + \sqrt{s}\nabla^2 f(x)\dot{x}(t) + (1 + \sqrt{\mu}s)\nabla f(x) = 0$$
 (Su)

- A Differential Equation for Modeling Nesterov's Accelerated Gradient Method: Theory and Insights
- Acceleration via Symplectic Discretization of High-Resolution Differential Equations

- · Understanding the Acceleration Phenomenon via High-Resolution Differential Equations
- Global Convergence of Langevin Dynamics Based Algorithms for Nonconvex Optimization
- Sampling as optimization in the space of measures: The Langevin dynamics as a composite optimization problem
- Optimization and Dynamical Systems
- Direct Runge-Kutta Discretization Achieves Acceleration
- The Physical systems Behind Optimization Algorithms
- ESAIM: Control, Optimization and Calculus of Variations (ESAIM: COCV)
- MCT'03 Louisiana Conference on Mathematical Control Theory
- International Workshop "Variational Analysis and Applications", ERICE, August 28 September 5, 2018
- Games, Dynamics and Optimization, 2019
- System dynamics & optimization
- Introduction to Dynamical Systems by John K. Hunter, Department of Mathematics, University of California at Davis
- Special Focus on Bridging Continuous and Discrete Optimization

https://eta.impa.br/dl/028.pdf

Stochastic Approximation

Clearing the Jungle of Stochastic Optimization

The Tradeoffs of Large-scale Learning

Deterministic

» Objective function

$$\min_{x_0, \dots, x_T} \sum_{t=0}^T c_t x_t$$

» Decision variables:

$$(x_0,...,x_T)$$

» Constraints:

• at time t

$$\left. \begin{array}{l}
 A_t x_t = R_t \\
 x_t \ge 0
 \end{array} \right\} \mathcal{X}_t$$

· Transition function

$$R_{t+1} = b_{t+1} + B_t x_t$$

Stochastic

» Objective function

$$\min_{\pi} E^{\pi} \left\{ \sum_{t=0}^{T} \gamma^{t} C\left(S_{t}, X_{t}^{\pi}\left(S_{t}\right)\right) | S_{0} \right\}$$

» Policy

$$X^{\pi}: S \mapsto \mathcal{X}$$

» Constraints at time t

$$x_t = X_t^{\pi}(S_t) \in \mathcal{X}_t$$

» Transition function

$$S_{t+1} = S^{M}\left(S_{t}, x_{t}, W_{t+1}\right)$$

» Exogenous information

$$(W_1, W_2, ..., W_T)$$

Stochastic approximation methods are a family of iterative methods typically used for *root-finding* problems or for *optimization* problems. The recursive update rules of stochastic approximation methods can be used, among other things, for solving linear systems when the collected data is corrupted by noise, or for approximating extreme values of functions which cannot be computed directly, but only estimated via noisy observations.

- Kiefer-Wolfowitz Algorithm
- Stochastic Process and Application

Robbins–Monro algorithm introduced in 1951 by Herbert Robbins and Sutton Monro, presented a methodology for solving a root finding problem, where the function is represented as an expected value. Assume that we have a function $M(\theta)$, and a constant α , such that the equation $M(\theta)=\alpha$ has a unique root at θ^* . It is assumed that while we cannot directly observe the function $M(\theta)$, we can instead obtain measurements of the random variable $N(\theta)$ where $\mathrm{E}[N(\theta)]=M(\theta)$. The structure of the algorithm is to then generate iterates of the form:

$$\theta_{n+1} = \theta_n - a_n(N(\theta_n) - \alpha)$$

Here, a_1, a_2, \ldots is a sequence of positive step sizes. Robbins and Monro proved , Theorem 2 that θ_n converges in L^2 (and hence also in probability) to θ , and Blum later proved the convergence is actually with probability one, provided that:

 $N(\theta)$ is uniformly bounded,

 $M(\theta)$ is nondecreasing,

 $M'(\theta^*)$ exists and is positive, and

The sequence a_n satisfies the following requirements:

$$\sum_{n=0}^{\infty} a_n = \infty \quad ext{ and } \quad \sum_{n=0}^{\infty} a_n^2 < \infty$$

A particular sequence of steps which satisfy these conditions, and was suggested by Robbins–Monro, have the form:

 $a_n=a/n$, for a>0. Other series are possible but in order to average out the noise in $N(\theta)$, the above condition must be met.

Stochastic Gradient Descent

Stochastic gradient descent is classified to stochastic optimization which is considered as the generalization of gradient descent.

Stochastic gradient descent takes advantages of stochastic or estimated gradient to replace the true gradient in gradient descent.

It is **stochastic gradient** but may not be **descent**.

The name **stochastic gradient methods** may be more appropriate to call the methods with stochastic gradient.

It can date back to **stochastic approximation** in statistics.

It is aimed to solve the problem with finite sum optimization problem, i.e.

$$rg \min_{ heta} rac{1}{n} \sum_{i=1}^n f(heta|x_i)$$

where $n < \infty$ and $\{f(\theta|x_i)\}_{i=1}^n$ are in the same function family and $\{x_i\}_{i=1}^n \subset \mathbb{R}^d$ are constants while $\theta \in \mathbb{R}^p$ is the variable vector.

The difficulty is p, that the dimension of θ , is tremendous. In other words, the model is **overparameterized**. And the number n is far larger than p generally, i.e. $n \gg p \gg d$.

What is worse, the functions $\{f(\theta|x_i)\}_{i=1}^n$ are not convex in most case.

The stochastic gradient method is defined as

$$heta^{k+1} = heta^k - lpha_k rac{1}{m} \sum_{i=1}^m
abla f(heta^k | x_j')$$

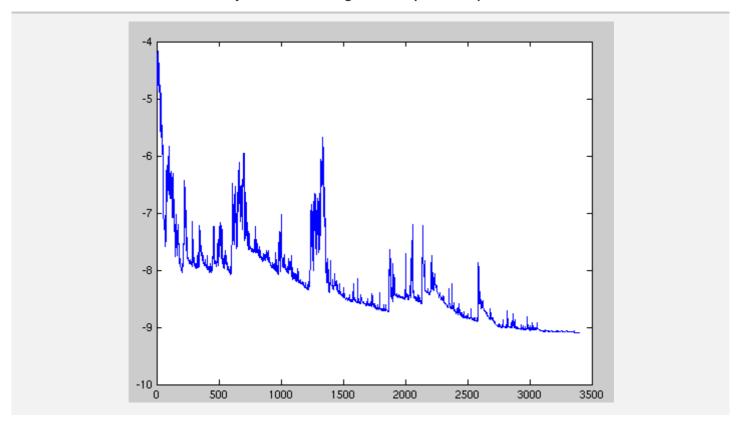
where x_j' is draw from $\{x_i\}_{i=1}^n$ and $m \ll n$ is on random.

It is the fact $m \ll n$ that makes it possible to compute the gradient of finite sum objective function and its side effect is that the objective function is not always descent.

There is fluctuations in the total objective function as gradient steps with respect to mini-batches are taken.

The fluctuations in the objective function as gradient steps with respect to mini-batches are taken

The fluctuations in the objective function as gradient steps with respect to mini-batches are taken



An heuristic proposal for avoiding the choice and for modifying the learning rate while the learning task runs is the **bold driver (BD) method**[^14].

The learning rate increases *exponentially* if successive steps reduce the objective function f, and decreases rapidly if an "accident" is encountered (if objective function f increases), until a suitable value is found.

After starting with a small learning rate, its modifications are described by the following equation:

$$lpha_{k+1} = \left\{ egin{aligned}
holpha_k, & f(heta^{k+1}) < f(heta^k); \ \eta^nlpha_k, & f(heta^{k+1}) > f(heta^k) ext{using } lpha_k, \end{aligned}
ight.$$

where ρ is close to 1 such as $\rho=1.1$ in order to avoid frequent "accidents" because the objective function computation is wasted in these cases, η is chosen to provide a rapid reduction ($\eta=0.5$), and n is the minimum integer such that the reduced rate η^n succeeds in diminishing the objective function.[^13]

The fact that the sample size is far larger than the dimension of parameter, $n \gg p$, that makes it expensive to compute total objective function $f(\theta) = \sum_{i=1}^{n} f(\theta|x_i)$.

Thus it is not clever to determine the learning rate α_k by line search.

And most stochastic gradient methods are to find proper step length α_k to make it converge at least in convex optimization. The variants of gradient descent such as momentum methods or mirror gradient methods have their stochastic counterparts.

- It is simplest to set the step length a constant, such as $lpha_k = 3 imes 10^{-3} \, orall k$.
- There are decay schemes, i.e. the step length α_k diminishes such as $\alpha_k = \frac{\alpha}{k}$, where α is constant.
- And another strategy is to tune the step length adaptively such as AdaGrad, ADAM.

PS: the step length α_k is called **learning rate** in machine learning. Additionally, stochastic gradient descent is also named as increment gradient methods in some case.

We can see some examples to see the advantages of incremental method such as the estimation of mean.

Given x_1, x_2, \ldots, x_n the mean is estimated as $\bar{x} = \frac{\sum_{i=1}^n x_i}{n}$. If now we observed more data y_1, y_2, \ldots, y_m from the population, the mean could be estimated by $\frac{n\bar{x}}{m+n} + \frac{\sum_{j=1}^m y_j}{m+n} = \frac{n\bar{x} + \sum_{j=1}^m y_j}{m+n}$. It is not necessary to summarize x_1, \ldots, x_n .

Another example, it is Newton interpolation formula in numerical analysis. The task is to fit the function via polynomials given some point in th function $(x_i, f(x_i)), i = 1, 2, ..., n$.

The Newton form of the interpolating polynomial is given by

\$\$

$$P_n(x) = a_0 + a_1 (x-x_1) + a_2 (x-x_1)(x-x_2) + \cdot cdots$$

a_n(x-x_1)(x-x_2)(x-x_3)\cdots (x-x_n).\$\$

This form is incremental and if another points $(x_{n+1}, f(x_{n+1}))$ is observed we will fit the function f more precisely just by adding another term $a_{n+1}(x-x_1)(x-x_2)\cdots(x-x_n)(x-x_{n+1})$ where the coefficients a_0, a_1, \cdots, a_n are determined by $f(x_1), f(x_2), \cdots, f(x_n)$.

See the following links for more information on stochastic gradient descent.

- https://www.wikiwand.com/en/Stochastic_gradient_descent
- http://ruder.io/optimizing-gradient-descent/
- https://zhuanlan.zhihu.com/p/22252270
- http://fa.bianp.net/teaching/2018/eecs227at/stochastic_gradient.html
- A Brief (and Comprehensive) Guide to Stochastic Gradient Descent Algorithms
- A look at SGD from a physicist's perspective Part 1
- A look at SGD from a physicists's perspective Part 2, Bayesian Deep Learning
- A look at SGD from a physicists's perspective Part 3, Langevin Dynamics and Applications

The Differences of Gradient Descent and Stochastic Gradient Descent

- Convergence Analysis of Gradient Descent Stochastic Algorithms
- Stochastic Approximations, Diffusion Limit and Small Random Perturbations of Dynamical Systems



Leon Bottou

- http://blavatnikawards.org/honorees/profile/leon-bottou/
- https://leon.bottou.org/projects/sgd
- https://leon.bottou.org/research/stochastic
- https://leon.bottou.org/papers/bottou-bousquet-2008

ADAM and More

- Adam: A Method for Stochastic Optimization
- On the convergence of Adam and Beyond
- http://ruder.io/deep-learning-optimization-2017/

The Differences of Stochastic Gradient Descent and its Variants

PS: Zeyuan Allen-Zhu and others published much work on acceleration of stochastic gradient descent.

- https://arxiv.org/pdf/1811.03962.pdf
- http://www.arxiv-sanity.com/search?q=Zeyuan+Allen-Zhu
- VR-SGD
- Laplacian Smoothing Gradient Descent
- Entropy SGD

Distributed Optimization Methods

Beginning around ten years ago, the single-threaded CPU performance stopped improving significantly, due to physical limitations; it is the numbers of cores in each machine that continue to arise. Today we can buy 8-core phones, 64-core workstations, and 2.5k-core GPUs at affordable prices. On the other hand, most of our algorithms are still single-threaded, and because so, their running time is about the same as it was to ten years ago and will stay so in the future, say, ten or twenty years. To develop faster algorithms, especially for those large-scale problems that arise in signal processing, medical imaging, and machine learning, it is inevitable to consider parallel computing.

Large scale supervised machine learning methods, which are based on gradient to improve their performance, need online near-real-time feedback from massive users. Math 285J: A First Course on Large-Scale Optimization Methods http://bicmr.pku.edu.cn/~wenzw/bigdata2019.html Data Science meet optimization Distributed optimization for control and learning ME 555: Distributed Optimization https://www.euro-online.org/websites/dso/ https://labs.criteo.com/2014/09/poh-part-3-distributed-optimization/ Convex and Distributed Optimization (749g) Accelerated Parallel Alternating Method of Multipliers (ADMM) for Distributed Optimization 8th IEEE Workshop Parallel / Distributed Computing and Optimization (PDCO 2018) **Distributed Optimization and Control** ADOPT: Asynchronous Distributed Constraint Optimization with Quality Guarantees On Distributed Optimization in Networked Systems Distributed Optimization and Control using Operator Splitting Methods Foundations of Distributed and Large Scale Computing Optimization Distributed Optimization of Large-Scale Complex Networks Walkman: A Communication-Efficient Random-Walk Algorithm for Decentralized Optimization **Proportional-Integral Distributed Optimization** NOVEL GRADIENT-TYPE OPTIMIZATION ALGORITHMS FOR EXTREMELY LARGE-SCALE NONSMOOTH CONVEX OPTIMIZATION Projects: Structure Exploitation in Large-Scale Non-Convex Optimisation http://ecee.colorado.edu/marden/files/dist-opt-journal.pdf http://shivaram.org/publications/hemingway-mlsys-2016.pdf http://principlesofoptimaldesign.org/ http://is4.tecnico.ulisboa.pt/~is4.daemon/tasks/distributed-optimization/

Machine learning especially deep learning requires more powerful distributed and decentralized optimization

Parallelizing Stochastic Gradient Descent

• Hogwild: A Lock-Free Approach to Parallelizing Stochastic Gradient Descent

- Asynchronous Decentralized Parallel Stochastic Gradient Descent
- https://arxiv.org/abs/1905.05920v1
- https://ray.readthedocs.io/en/latest/distributed_sgd.html
- https://www.podc.org/data/podc2018/podc2018-tutorial-alistarh.pdf

Stochastic ADMM

methods.

Linearly constrained stochastic convex optimization is given by

$$egin{aligned} \min_{x,y} \mathbb{E}_{artheta}[F(x,artheta)] + h(y), \ s.\,t.\,\,Ax + By = b, x \in \mathbb{X}, y \in \mathbb{Y}. \end{aligned}$$

where typically the expectation $\mathbb{E}_{\vartheta}[F(x,\vartheta)]$ is some loss function and h is regularizer to prevent from over-fitting. The first problem is that the distribution of ϑ is unknown as well as the expectation $\mathbb{E}_{\vartheta}[F(x,\vartheta)]$ in the objective function.

Modified Augmented Lagrangian

Linearize f(x) at x_k and add a proximal term :

$$egin{aligned} L^k_eta(x,y,\lambda) := f(x_k) + \langle x_k, g_k
angle + h(y) - \langle \lambda, Ax + By - b
angle + rac{eta}{2} \|Ax + By - b\|_2^2 \ &+ rac{1}{2\eta_k} \|x - x_k\|^2 \end{aligned}$$

where g_k is a stochastic (sub)gradient of f.

1.
$$x^{k+1} = \operatorname{arg\,min}_{x \in \mathbf{X}} L^k_{\beta}(x, y^k, \lambda^k);$$

2.
$$y^{k+1} = \arg\min_{y \in Y} L_{\beta}^{k}(x^{k+1}, y, \lambda^{k});$$

3.
$$\lambda^{k+1} = \lambda^k - \beta (Ax^{k+1} + By^{k+1} - b).$$

- Stochastic ADMM
- Accelerated Variance Reduced Stochastic ADMM
- Towards optimal stochastic ADMM or the talk in ICML
- V-Cycle or Double Sweep ADMM
- https://arxiv.org/abs/1903.01786

Distributed ADMM

Let us assume that the function F has the following decomposition where each x_i has its own dimension.

$$egin{aligned} \min_x F(x) &\{= \sum_{i=1}^n f_i(x_i)\}, \ s.\, t. \quad x \in \mathrm{C} \end{aligned}$$

We can reformulate the problem to get

$$\min_{x} F(x) + g(y),$$
s. t. $x = y$

where g(z) is the indictor function of set C.

We can dene an augmented Lagrangian

$$egin{aligned} L_{eta}(x,y,\lambda) &= F(x) + g(y) - \lambda^T(x-y) + rac{eta}{2} \|x-y\|_2^2 \ &= \sum_{i=1}^n [f_i(x_i) - \lambda_i(x_i-y_i) + rac{eta}{2} (x_i-y_i)^2] + g(y) \ &= \sum_{i=1}^n L_{(eta,i)}(x_i,y,\lambda_i). \end{aligned}$$

We can split the optimization over x_i :

1.
$$x_i^{k+1} = \arg\min_{x_i} L_{(\beta,i)}(x_i, y^k, \lambda_i^k)$$
 $i = 1, 2, \dots, n;$
2. $y^{k+1} = \arg\min_{x_i} L_{(\beta,i)}(x_i^{k+1}, y, \lambda_i^k);$
3. $\lambda^{k+1} = \lambda^k + \lambda(x^{k+1} - y^{k+1}).$

Then optimization over x_i is done in parallel. Subsequently, the results are communicated back to a master node which performs the y update (usually just a projection as in the example above) and returns back the result to other worker nodes. The update over λ_i is again done independently.

- http://users.isr.ist.utl.pt/~jmota/DADMM/
- http://repository.ust.hk/ir/Record/1783.1-66353
- https://ieeexplore.ieee.org/document/7039496
- DISTRIBUTED ASYNCHRONOUS OPTIMIZATION WITH THE ALTERNATING DIRECTION METHOD OF MULTIPLIERS
- Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers by S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein
- Asynchronous Distributed ADMM for Consensus Optimization
- Notes on Distributed ADMM

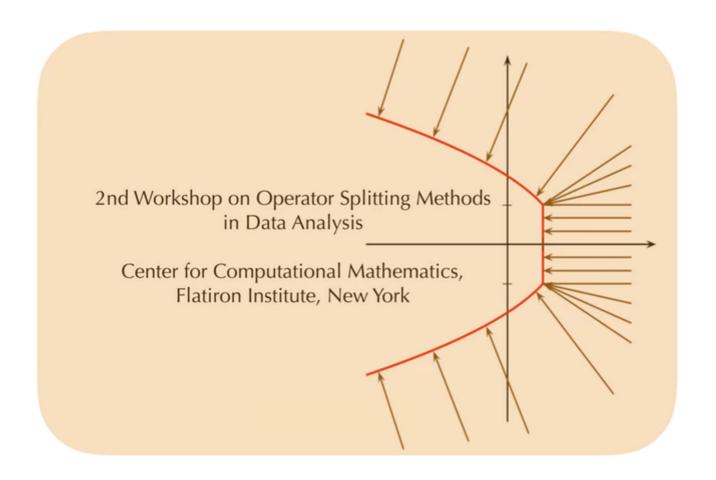
Monotone Operator Splitting Methods for Optimization

Operator splitting is to decompose one omplicated operator(procedure) into some simple operators (procedures). For example, ADMM splits the maxmin operator of the augmented Lagrangian into 3 operators:

$$rg \min_{x,y} \max_{\lambda} L_{eta}(x,y\mid \lambda)$$

to

$$rg \min_x L_eta(x,y\mid \lambda) \circ \ rg \min_y L_eta(x,y\mid \lambda) \circ rg \max_\lambda L_eta(x,y\mid \lambda).$$



conference

They are really some block relaxation techniques.

- https://web.stanford.edu/class/ee364b/lectures/monotone_split_slides.pdf
- Operator Splitting by Professor Udell @ORIE 6326: Convex Optimization
- A note on the equivalence of operator splitting methods
- Splitting methods for monotone operators with applications to parallel optimization
- Operator Splitting Methods for Fast MPC
- https://staffportal.curtin.edu.au/staff/profile/view/Jie.Sun/
- Operator Splitting Methods in Data Analysis

Gradient Free Optimization Methods

As shown in Principle of Optimal Design , nongradient methods are classified into 3 classes:

We organize the discussion of nongradient methods in three parts, direct search methods, heuristic methods, and black-box methods. Direct search methods rely on ranking the objective function values rather than using the objective values themselves. Heuristic methods use some random process to generate new candidate solutions, and so the iteration paths and even the solutions obtained can change each time we perform a search. Black-box methods deal with problems that have no known model function structure that we can exploit. For example, functions generated by simulations have no discernible mathematical properties (like convexity), and so we refer to them as black-box functions. In this sense, all nongradient methods can be used for black-box problems. The two black-box methods described in this chapter were created to address design problems with expensive simulations, and so their main goal is to find an optimum quickly with few function evaluations.

Derivative-free optimization (DFO) algorithms differ in the way they use the sampled function values to determine the new iterate. One class of methods constructs a linear or quadratic model of the objective function and defines the next iterate by seeking to minimize this model inside a trust region. We pay particular attention to these model-based

approaches because they are related to the unconstrained minimization methods described in earlier chapters. Other widely used DFO methods include the simplex-reflection method

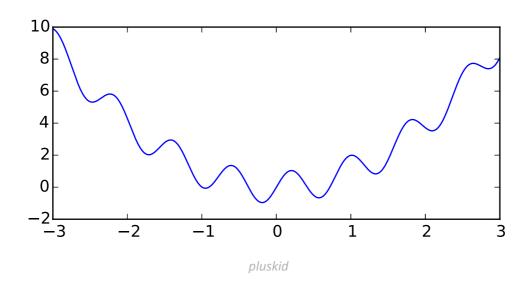
of Nelder and Mead, pattern-search methods, conjugate-direction methods, and simulated annealing.

Heuristic methods will be introduced in computational intelligence as well as Bayesian Optimization .

Let us start with the example and suppose that we want to

$$\arg\min_{x} f(x) = x^2 + 4\sin(2x). \tag{1}$$

The objective function f(x), a non-convex function, has many local minimizer or extrema. The function (1) is upper bounded by x^2+4 and lower bounded by x^2-4 .



Another insightful example is to minimize the following cost function:

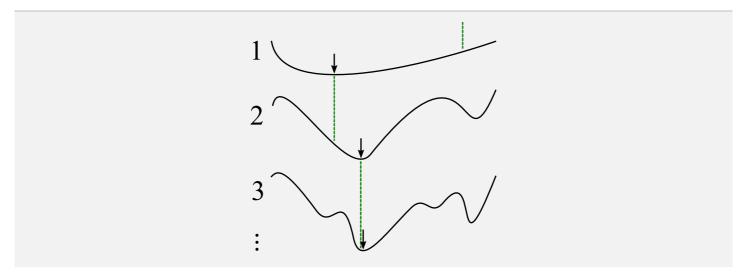
$$x^2 + 4\sin(2x) - 1001 \mathbb{I}_{\sqrt{2}}(x) \tag{2}$$

where the last part $\mathbb{I}_{\sqrt{2}}(x)$ is equal to 1 when $x=\sqrt{2}$ and 0 otherwise, a Dirac function. It is almost equal to the first function (1) except at the point $x=\sqrt{2}$. The minimal value of the above function is $2+4\sin(2\sqrt{2})-1001$ when $x=\sqrt{2}$. And these two functions are two different kinds of non-convex functions.

Another related method is <code>graduated</code> optimization, which is a global optimization technique that attempts to solve a difficult optimization problem by initially solving a greatly simplified problem, and progressively transforming that problem (while optimizing) until it is equivalent to the difficult optimization problem. Further, when certain conditions exist, it can be shown to find an optimal solution to the final problem in the sequence. These conditions are:

- The first optimization problem in the sequence can be solved given the initial starting point.
- The locally convex region around the global optimum of each problem in the sequence includes the point that corresponds to the global optimum of the previous problem in the sequence.

Graduated Optimization



- https://www.wikiwand.com/en/Numerical_continuation
- Multi-Resolution Methods and Graduated Non-Convexity

Kiefer-Wolfowitz Algorithm

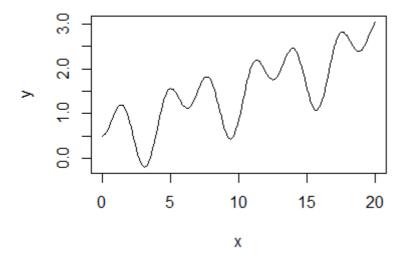
In stochastic gradient descent, the estimated gradient is a partial sum of the population gradient so that it is necessary to compute the gradient of sample function.

Kiefer-Wolfowitz Algorithm is the gradient-free version of stochastic gradient descent.

It is a recursive scheme to approximate the minimum or maximum of the form

$$x^{k+1} = x^k - a_n \Delta(x^k)$$

During the n-th stage, observations y'' and y' are taken at the design levels $x''=x^k+c_k$ and $x'=x^k-c_k$, respectively. And $\Delta(x^k)=\frac{y''-y'}{2c_n}$, a_n and c_n are positive constants so that $c_n\to 0, \sum_{i=0}^\infty (a_n/c_n)^2<\infty, \sum a_n=\infty$.



function with noise

- http://pawel.sawicz.eu/tag/kiefer-wolfowitz/
- A compansion to Kiefer-Wolfowit algorithm
- Archive for Kiefer-Wolfowitz algorithm
- Strong Convergence of a Stochastic Approximation Algorithm
- Almost Sure Approximations to the Robbins-Monro and Kiefer-Wolfowitz Processes with Dependent Noise
- A Kiefer-Wolfowitz Algorithm with Randomized Differences
- Stochastic Approximation by Tze Leung Lai

Multi-Level Optimization is to optimize a related cheap function \hat{f} when the objective function f is very expensive to evaluate.

Multi-level optimization methods repeat three steps:

1. Cheap minimization of modified \hat{f} :

$$y^k = rg\min_{x \in \mathbb{R}^p} + \langle v_k, x
angle \ .$$

2. Use y^k to give descent direction,

$$x^{k+1} = x^k - a_k(x^k - y^k).$$

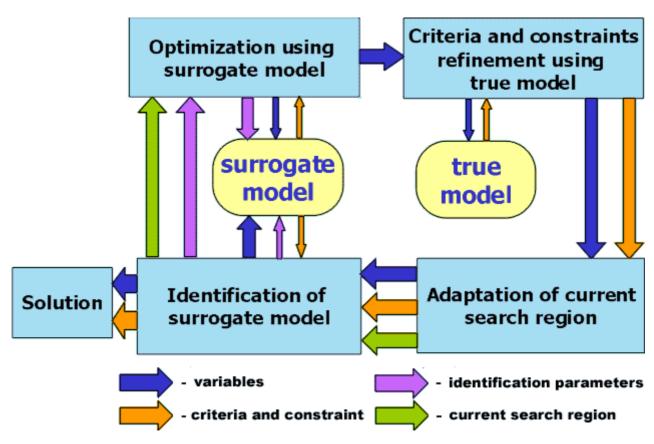
3. Set v_k to satisfy first-order coherence

$$v_{k+1} = rac{L_f}{L_F} F'(x^{k+1}) - f'(x^{k+1}).$$

Panos Parpas Panos Parpas

EMERITUS PROFESSORBERCRUSTEM

- Multilevel Optimization Methods: Convergence and Problem Structure
- A Multilevel Proximal Algorithm for Large Scale Composite Convex Optimization
- Multiresolution Algorithms for Faster Optimization in Machine Learning



The basic scheme of multilevel optimization

The simplified scheme of work for the multilevel optimization procedure can be represented as follows.

- 1. Solving the optimization problem using a surrogate model. For this purpose, the method of indirect optimization based on the self-organization (IOSO) is used. This method allows finding the single solution for single-objective optimization or the Pareto-optimal set of solutions for multi-objective problems.
- 2. For the obtained solution the indicators of efficiency are updated using the high-fidelity analysis tools.
- 3. The adjustment of a current search region is performed.

- 4. The adjustment of the surrogate model is performed. Depending upon the particular features of the applied mathematical simulation, the adjustment procedure can performed using several approaches. One such approach involves constructing non-linear corrective dependencies. This includes evaluation of the results obtained with different fidelity analysis tools. The other possible approach is application of nonlinear estimation of surrogate model internal parameters.
- 5. Replacement of the surrogate model by the adjusted one and the return to step (1).
- Multilevel Optimization: Convergence Theory, Algorithms and Application to Derivative-Free Optimization
- multilevel optimization iosotech
- OptCom: A Multi-Level Optimization Framework for the Metabolic Modeling and Analysis of Microbial Communities

Matrix Multiplicative Weight can be considered as an ensemble method of optimization methods.

The name "multiplicative weights" comes from how we implement the last step: if the weight of the chosen object at step t is w_t before the event, and G represents how well the object did in the event, then we'll update the weight according to the rule:

$$w_{t+1} = w_t(1+G).$$

Multiplicative Weights algorithm

Initialization: Fix an $\eta \leq \frac{1}{2}$. With each decision i, associate the weight $w_i^{(1)} := 1$. **For** t = 1, 2, ..., T:

- 1. Choose decision *i* with probability proportional to its weight $w_i^{(t)}$. I. e., use the distribution over decisions $\mathbf{p}^{(t)} = \{w_1^{(t)}/\Phi^{(t)}, \dots, w_n^{(t)}/\Phi^{(t)}\}$ where $\Phi^{(t)} = \sum_i w_i^{(t)}$.
- Observe the costs of the decisions m^(t).
- 3. Penalize the costly decisions by updating their weights as follows: for every decision i, set

$$w_i^{(t+1)} = w_i^{(t)} (1 - \eta m_i^{(t)})$$
ⁱ知乎 @yrnhuang

Matrix Multiplicative Weight

Jeremy wrote a blog on this topic:

In general we have some set X of objects and some set Y of "event outcomes" which can be completely independent. If these sets are finite, we can write down a table M whose rows are objects, whose columns are outcomes, and whose i,j entry M(i,j) is the reward produced by object x_i when the outcome is y_j . We will also write this as M(x,y) for object x and outcome y. The only assumption we'll make on the rewards is that the values M(x,y) are bounded by some small constant B (by small I mean B should not require exponentially many bits to write down as compared to the size of X). In symbols, $M(x,y) \in [0,B]$. There are minor modifications you can make to the

algorithm if you want negative rewards, but for simplicity we will leave that out. Note the table M just exists for analysis, and the algorithm does not know its values. Moreover, while the values in M are static, the choice of outcome y for a given round may be nondeterministic.

The **MWUA** algorithm randomly chooses an object $x \in X$ in every round, observing the outcome $y \in Y$, and collecting the reward M(x,y) (or losing it as a penalty). The guarantee of the MWUA theorem is that the expected sum of rewards/penalties of MWUA is not much worse than if one had picked the best object (in hindsight) every single round.

Theorem (from Arora et al): The cumulative reward of the MWUA algorithm is, up to constant multiplicative factors, at least the cumulative reward of the best object minus $\log(n)$, where n is the number of objects.

- Matrix Multiplicative Weight (1)
- Matrix Multiplicative Weight (2)
- Matrix Multiplicative Weight (3)
- The Multiplicative Weights Update framework
- The Multiplicative Weights Update Method: a Meta Algorithm and Applications
- Nonnegative matrix factorization with Lee and Seung's multiplicative update rule
- A Combinatorial, Primal-Dual approach to Semidefinite Programs
- Milosh Drezgich, Shankar Sastry. "Matrix Multiplicative Weights and Non-Zero Sum Games".
- The Matrix Multiplicative Weights Algorithm for Domain Adaptation by David Alvarez Melis
- The Reasonable Effectiveness of the Multiplicative Weights Update Algorithm
- Zeroth-Order Method for Distributed Optimization With Approximate Projections
- Derivative-Free Optimization (DFO)
- Derivative Free Optimization / Optimisation sans Gradient
- Delaunay-based derivative-free optimization via global surrogates, part I: linear constraints
- Delaunay-based derivative-free optimization via global surrogates, part II: convex constraints
- https://projects.coin-or.org/Dfo
- https://nlopt.readthedocs.io/en/latest/NLopt_Algorithms/
- http://adl.stanford.edu/aa222/Lecture_Notes_files/chapter6_gradfree.pdf
- https://code.fb.com/ai-research/nevergrad/
- https://github.com/facebookresearch/nevergrad
- https://www.kthohr.com/optimlib.html
- https://www.infoq.com/presentations/black-box-optimization

And there are more topics on optimization such as this site.

And more courses on optimization:

- http://bicmr.pku.edu.cn/~wenzw/opt-2018-fall.html
- http://math.sjtu.edu.cn/faculty/xqzhang/html/teaching.html
- http://mat.uab.cat/~alseda/MasterOpt/
- http://www.math.ucla.edu/~wotaoyin/summer2016/
- http://www.math.ucla.edu/~wotaoyin/math273c/
- http://www.math.ucla.edu/~lvese/273.1.10f/
- http://www.seas.ucla.edu/~vandenbe/ee236b/ee236b.html
- https://people.eecs.berkeley.edu/~elghaoui/Teaching/EECS127/index.html
- https://lavaei.ieor.berkeley.edu/Course_IEOR262B_Spring_2019.html
- https://web.stanford.edu/~boyd/teaching.html
- http://web.stanford.edu/class/ee364b/lectures.html
- http://www.stat.cmu.edu/~ryantibs/convexopt/
- https://nisheethvishnoi.wordpress.com/convex-optimization/
- Optimization by Vector Space Methods
- Algorithms for Convex Optimization

http://niaohe.ise.illinois.edu/IE598_2016/index.html
http://www.optimization-online.org/
http://convexoptimization.com/
More Optimization Online Links
TUTORIALS AND BOOKS at http://plato.asu.edu/sub/tutorials.html.
Provable Nonconvex Methods/Algorithms
https://optimization.mccormick.northwestern.edu/index.php/Main_Page
Non-convex Optimization for Machine Learning
GLOBAL OPTIMALITY CONDITIONS FOR DEEP NEURAL NETWORKS
http://www.vision.jhu.edu/assets/HaeffeleCVPR17.pdf
https://www.springer.com/us/book/9783319314822
https://core.ac.uk/display/83849901
https://core.ac.uk/display/73408878
https://zhuanlan.zhihu.com/p/51514687
http://math.cmu.edu/~hschaeff/research.html
https://people.eecs.berkeley.edu/~elghaoui/Teaching/EECS127/index.html
https://blogs.princeton.edu/imabandit/

http://www.probabilistic-numerics.org/research/index.html	