Optimization Methods for Machine Learning

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Outline

- Data Analysis and Machine Learning
    - Context
    - Applications / Examples, including formulation as optimization problems
- Optimization in Data Analysis
    - Relevant Algorithms

Optimization is being revolutionized by its interactions with machine learning and data analysis.

- new algorithms, and new interest in *old* algorithms;
- challenging formulations and new paradigms;
- renewed emphasis on certain topics: convex optimization algorithms, complexity, structured nonsmoothness, ...
- many new (excellent) researchers working on the machine learning / optimization spectrum.

Data Analysis

Related Terms: Machine Learning, Statistical Inference, Data Mining.

- Extract meaning from data: Understand statistical properties, learn important features and fundamental structures in the data.
- Use this knowledge to make predictions about other, similar data.

Highly multidisciplinary area!

- Foundations in Statistics;
- Computer Science: AI, Machine Learning, Databases, Parallel Systems;
- Optimization provides a toolkit of modeling/formulation and algorithmic techniques.

Modeling and domain-specific knowledge is vital: “80% of data analysis is spent on the process of cleaning and preparing the data.” [Dasu and Johnson, 2003].

(Most academic research deals with the other 20%.)

The Age of "Big Data"

New "Data Science Centers" at many institutions, new degree programs (e.g. Masters in Data Science), new funding initiatives.

- Huge amounts of data are collected, routinely and continuously.
  - Consumer and citizen data: phone calls and text, social media apps, email, surveillance cameras, web activity, online shopping,...
  - Scientific data (particle colliders, satellites, biological / genomic, astronomical,...)
- Affects everyone directly!
- Powerful computers and new specialized architectures make it possible to handle larger data sets and analyze them more thoroughly.
- Methodological innovations in some areas. e.g. Deep Learning.
  - Speech recognition in smart phones
  - AlphaGo: Deep Learning for Go.
  - Image recognition

Typical Setup

After cleaning and formatting, obtain a data set of m objects:

- Vectors of features: a_j, $j = 1, 2, \dots, m$.
- Outcome / observation / label y_j for each feature vector.

The outcomes y_j could be:

- a real number: **regression**
- a label indicating that a_j lies in one of M classes (for $M \geq 2$): **classification**
- multiple labels: classify a_j according to multiple criteria.
- no labels (y_j is null):
  - **subspace identification:** Locate low-dimensional subspaces that approximately contain the (high-dimensional) vectors a_j;
  - **clustering**: Partition the a_j into a few clusters.

  (Structure may reveal which features in the a_j are important / distinctive, or enable predictions to be made about new vectors a.)

Fundamental Data Analysis Task

Seek a function ϕ that:

- approximately maps a_j to y_j for each j: $\phi(a_j) \approx y_j$ for $j = 1, 2, \dots, m$
- if there are no labels y_j, or if some labels are missing, seek ϕ that does something useful with the data $\{a_j\}$, e.g. assigns each a_j to an appropriate cluster or subspace.
- satisfies some additional properties — simplicity, structure — that make it "plausible" for the application, robust to perturbations in the data, generalizable to other data samples.

Can usually define ϕ in terms of some parameter vector x — thus identification of ϕ becomes a data-fitting problem: Find the best x.

Objective function in this problem often built up of m terms that capture mismatch between predictions and observations for each (a_j, y_j).

The process of finding ϕ is called learning or training.

What's the use of the mapping ϕ?

- Analysis: ϕ — especially the parameter x that defines it — reveals structure in the data. Examples:
  - Feature selection: reveal the components of vectors a_j that are most important in determining the outputs y_j, and quantifies the importance of these features.
  - Uncovers some hidden structure, e.g.
    - finds some low-dimensional subspaces that contain the a_j;
    - find clusters that contain the a_j;
    - find a decision tree that builds intuition about how outputs y_j depend on inputs a_j.
- Prediction: Given new data vectors a_k, predict outputs $y_k \leftarrow \phi(a_k)$.

Complications

- **noise or errors** in a_j and y_j. Would like ϕ (and x) to be robust to this. We want the solution to generalize to perturbations of the observed data. Often achieve this via regularized formulations.
- **avoid overfitting**: Observed data is viewed as an empirical, sampled representation of some underlying reality. Want to avoid overfitting to the particular sample. (Training should produce a similar result for other samples from the same data set.) Again, generalization / regularization.
- **missing data**: Vectors a_j may be missing elements (but may still contain useful information).
- **missing labels:** Some or all y_j may be missing or null — semi-supervised or unsupervised learning.
- **online learning**: Data (a_j, y_j) is arriving in a stream rather than all known up-front.

Application I: Least Squares

$$\min_x f(x) := \frac{1}{2}\sum_{j=1}^{m}(a_j^T x - y_j)^2 = \frac{1}{2}\|Ax - y\|_2^2.$$

[Gauss, 1799], [Legendre, 1805]; see [Stigler, 1981].

Here the function mapping data to output is linear: $\phi(a_j) = a_j^T x$.

- ℓ_2 regularization reduces sensitivity of the solution x to noise in y.

$$\min_x \frac{1}{2}\|Ax - y\|_2^2 + \lambda\|x\|_2^2.$$

- ℓ_1 regularization yields solutions x with few nonzeros:

$$\min_x \frac{1}{2}\|Ax - y\|_2^2 + \lambda\|x\|_1.$$

  Feature selection: Nonzero locations in x indicate important components of a_j.

- Nonconvex separable regularizers (SCAD, MCP) have nice statistical properties, but lead to nonconvex optimization formulations.

Application II: Matrix Completion

Regression over a structured matrix: Observe a matrix X by probing it with linear operators $\mathcal{A}_j(X)$, giving observations y_j, $j = 1, 2, \dots, m$. Solve a regression problem:

$$\min_X \frac{1}{2m} \sum_{j=1}^{m} (\mathcal{A}_j(X) - y_j)^2 = \frac{1}{2m} \|\mathcal{A}(X) - y\|_2^2.$$

Each $\mathcal{A}_j$ may observe a single element of X, or a linear combination of elements. Can be represented as a matrix A_j, so that $\mathcal{A}_j(X) = \langle A_j, X \rangle$.

Seek the "simplest" X that satisfies the observations. Nuclear-norm (sum-of-singular-values) regularization term induces low rank on X:

$$\min_X \frac{1}{2m} \|\mathcal{A}(X) - y\|_2^2 + \lambda \|X\|_*, \quad \text{for some } \lambda > 0.$$

[Recht et al., 2010]

Explicit Low-Rank Parametrization

Compact, nonconvex formulation is obtained by parametrizing X directly:

$$X = LR^T, \quad \text{where } L \in \mathbb{R}^{m\times r},\ R \in \mathbb{R}^{n\times r},$$

where r is known (or suspected) rank.

$$\min_{L,R} \frac{1}{2m} \sum_{j=1}^{m} (\mathcal{A}_j(LR^T) - y_j)^2.$$

For symmetric X, write $X = ZZ^T$, where $Z \in \mathbb{R}^{n\times r}$, so that

$$\min_{Z} \frac{1}{2m} \sum_{j=1}^{m} (\mathcal{A}_j(ZZ^T) - y_j)^2.$$

(No need for regularizer — rank is hard-wired into the formulation.)

Despite the nonconvexity, near-global minima can be found when $\mathcal{A}_j$ are incoherent. Use appropriate initialization [Candès et al., 2014], [Zheng and Lafferty, 2015] or the observation that all local minima are near-global [Bhojanapalli et al., 2016].

Matrix Completion from Individual Entries

When the observations $\mathcal{A}_j$ are of individual elements, recovery is still possible when the true matrix X is itself low-rank and incoherent (i.e. not too "spiky" and with singular vectors randomly oriented).

Need sufficiently many observations [Candès and Recht, 2009].

Procedures based on trimming + truncated singular value decomposition (for initialization) and projected gradient (for refinement) produce good solutions [Keshavan et al., 2010].

Application III: Nonnegative Matrix Factorization

Given $m \times n$ matrix Y, seek factors L $(m \times r)$ and R $(n \times r)$ that are element-wise positive, such that $LR^T \approx Y$.

$$\min_{L,R} \frac{1}{2}\|LR^T - Y\|_F^2 \text{ subject to } L \geq 0,\ R \geq 0.$$

Applications in computer vision, document clustering, chemometrics, ...

Could combine with matrix completion, when not all elements of Y are known, if it makes sense on the application to have nonnegative factors.

If positivity constraint were not present, could solve this in closed form with an SVD, since Y is observed completely.

Application IV: Sparse Inverse Covariance

Let $Z \in \mathbb{R}^p$ be a (vector) random variable with zero mean. Let $z_1, z_2, \dots, z_N$ be samples of Z. Sample covariance matrix (estimates covariance between components of Z):

$$S := \frac{1}{N-1} \sum_{\ell=1}^{N} z_\ell z_\ell^T.$$

Seek a sparse inverse covariance matrix: $X \approx S^{-1}$.

X reveals dependencies between components of Z: $X_{ij} = 0$ if the i and j components of Z are conditionally independent.

(Nonzeros in X indicate arcs in the dependency graph.)

Obtain X from the regularized formulation:

$$\min_X \langle S, X \rangle - \log\det(X) + \lambda \|X\|_1, \quad \text{where } \|X\|_1 = \textstyle\sum_{i,j} |X_{ij}|.$$

[d'Aspremont et al., 2008, Friedman et al., 2008].

Application V: Sparse Principal Components (PCA)

Seek sparse approximations to the leading eigenvectors of the sample covariance matrix S.

For the leading sparse principal component, solve

$$\max_{v \in \mathbb{R}^n} v^T S v = \langle S, vv^T \rangle \quad \text{s.t. } \|v\|_2 = 1,\ \|v\|_0 \le k,$$

for some given $k \in \{1, 2, \dots, n\}$. Convex relaxation replaces vv^T by an $n \times n$ positive semidefinite proxy M:

$$\max_{M \in S\mathbb{R}^{n \times n}} \langle S, M \rangle \quad \text{s.t. } M \succeq 0,\ \langle I, M \rangle = 1,\ \|M\|_1 \le R,$$

where $| \cdot |_1$ is the sum of absolute values [d'Aspremont et al., 2007].

Adjust the parameter R to obtain desired sparsity.

Sparse PCA (rank r)

For sparse leading rank-r eigenspace, seek $V \in \mathbb{R}^{n \times r}$ with orthonormal columns such that $\langle S, VV^T \rangle$ is maximized, and V has at most k nonzero rows. Convex relaxation:

$$\max_{M \in S\mathbb{R}^{n \times n}} \langle S, M \rangle \quad \text{s.t. } 0 \preceq M \preceq I, \; \langle I, M \rangle \le r, \; \|M\|_1 \le R.$$

Explicit low-rank formulation is

$$\max_{F \in \mathbb{R}^{n \times r}} \langle S, FF^T \rangle \quad \text{s.t. } \|F\|_2 \le 1, \; \|F\|_{2,1} \le \bar{R},$$

where $\|F\|_{2,1} := \sum_{i=1}^{n} \|F_{i\cdot}\|_2$.

[Chen and Wainwright, 2015]

Application VI: Sparse + Low-Rank

Given $Y \in \mathbb{R}^{m \times n}$, seek low-rank M and sparse S such that $M + S \approx Y$.

Applications:

- Robust PCA: Sparse S represents "outlier" observations.
- Foreground-Background separation in video processing.
  - Each column of Y is one frame of video, each row is one pixel evolving in time.
  - Low-rank part M represents background, sparse part S represents foreground.

Convex formulation:

$$\min_{M,S} \|M\|_* + \lambda \|S\|_1 \quad \text{s.t. } Y = M + S.$$

[Candès et al., 2011, Chandrasekaran et al., 2011]

Sparse + Low-Rank: Compact Formulation

Compact formulation: Variables $L \in \mathbb{R}^{n\times r}$, $R \in \mathbb{R}^{m\times r}$, $S \in \mathbb{R}^{m\times n}$ sparse.

$$\min_{L,R,S} \frac{1}{2}\|LR^T + S - Y\|_F^2 + \lambda\|S\|_1 \quad \text{(fully obvserved)}$$

$$\min_{L,R,S} \frac{1}{2}\|P_\Phi(LR^T + S - Y)\|_F^2 + \lambda\|S\|_1 \quad \text{(partially observed)},$$

where Φ represents the locations of the observed entries.
[Chen and Wainwright, 2015, Yi et al., 2016].

(For well-posedness, need to assume that the "true" L, R, S satisfy certain incoherence properties.)

Application VII: Subspace Identification

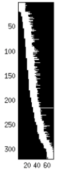
Given vectors $a_j \in R^n$ with missing entries, find a subspace of $\mathbb{R}^n$ such that all "completed" vectors a_j lie approximately in this subspace.

If $\Omega_j \subset \{1, 2, \ldots, n\}$ is the set of observed elements in a_j, seek $X \in \mathbb{R}^{n \times d}$ such that

$$[a_j - X s_j]_{\Omega_j} \approx 0,$$

for some $s_j \in \mathbb{R}^d$ and all $j = 1, 2, \ldots$.
[Balzano et al., 2010, Balzano and Wright, 2014].

Application: Structure from motion. Reconstruct opaque object from planar projections of surface reference points.



Application VIII: Linear Support Vector Machines

Each item of data belongs to one of two classes: $y_j = +1$ and $y_j = -1$.

Seek (x, β) such that

$$\begin{aligned} a_j^T x - \beta &\geq 1 && \text{when } y_j = +1; \\ a_j^T x - \beta &\leq -1 && \text{when } y_j = -1. \end{aligned}$$

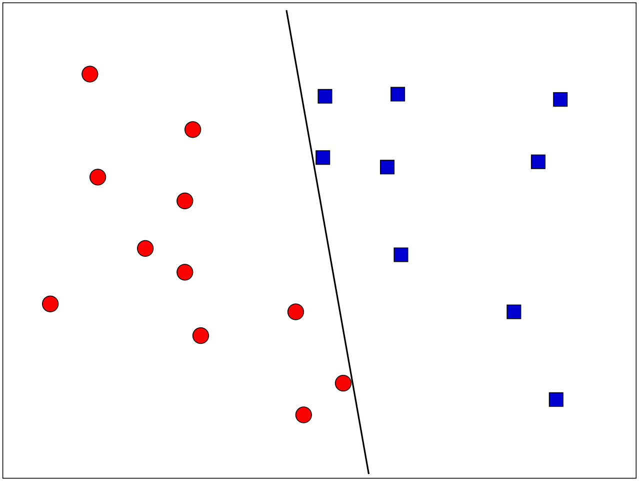
The mapping is $\phi(a_j) = \text{sign}(a_j^T x - \beta)$.

Design an objective so that the jth loss term is zero when $\phi(a_j) = y_j$, positive otherwise. A popular one is hinge loss:

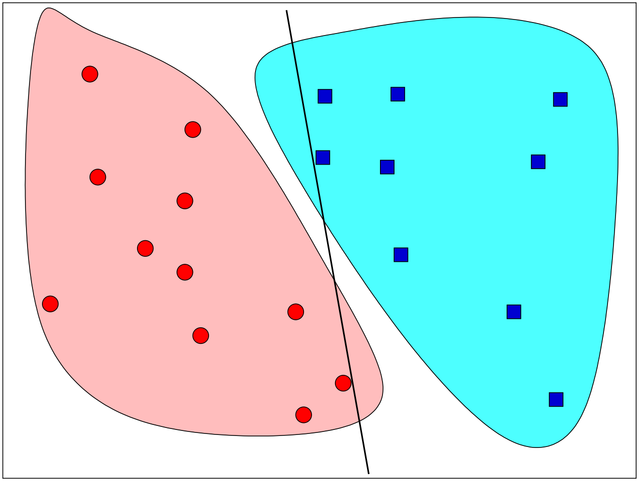
$$H(x) = \frac{1}{m} \sum_{j=1}^{m} \max(1 - y_j(a_j^T x - \beta), 0).$$

Add a regularization term $(\lambda/2)\|x\|_2^2$ for some $\lambda > 0$ to maximize the margin between the classes.

Regularize for Generalizability



Regularize for Generalizability



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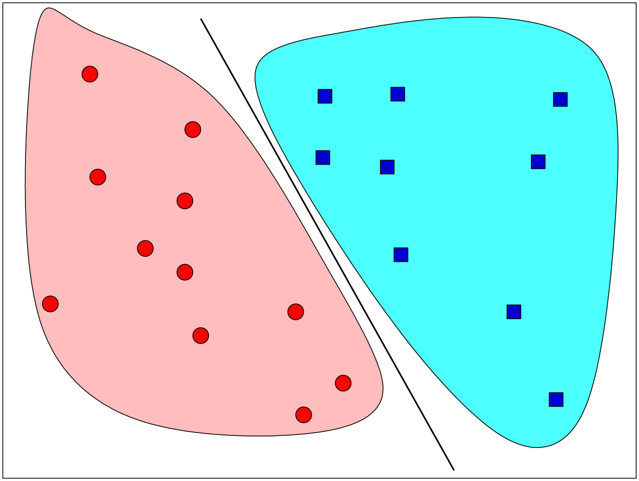

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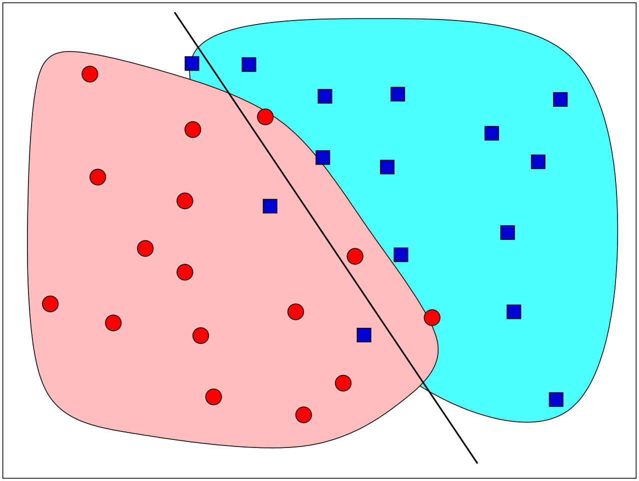
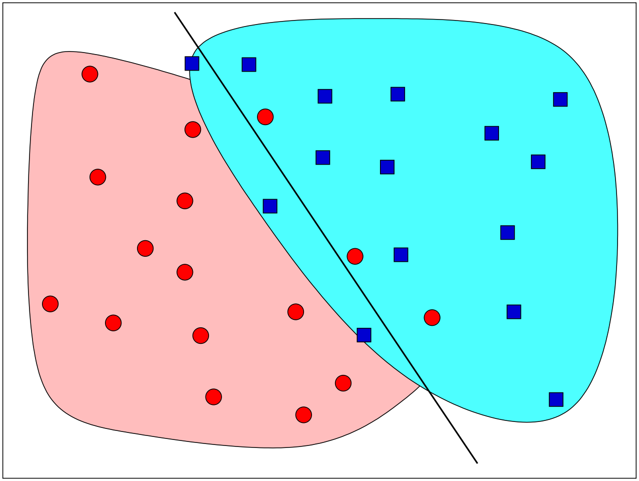


Regularize for Generalizability



Application IX: Nonlinear SVM

Data a_j, $j = 1, 2, \ldots, m$ may not be *separable* neatly into two classes $y_j = +1$ and $y_j = -1$. Apply a nonlinear transformation $a_j \to \psi(a_j)$ ("lifting") to make separation more effective. Seek (x, β) such that

$$\begin{aligned} \psi(a_j)^T x - \beta &\geq 1 && \text{when } y_j = +1; \\ \psi(a_j)^T x - \beta &\leq -1 && \text{when } y_j = -1. \end{aligned}$$

Leads to the formulation:

$$\min_x \frac{1}{m} \sum_{j=1}^{m} \max(1 - y_j(\psi(a_j)^T x - \beta), 0) + \frac{1}{2}\lambda \|x\|_2^2.$$

Can avoid defining ψ explicitly by using instead the dual of this QP.

Nonlinear SVM: Dual

Dual is a quadratic program in m variables, with simple constraints:

$$\min_{\alpha \in \mathbb{R}^m} \frac{1}{2}\alpha^T Q\alpha - e^T\alpha \text{ s.t. } 0 \le \alpha \le (1/\lambda)e, \quad y^T\alpha = 0.$$

where $Q_{k\ell} = y_k y_\ell \psi(a_k)^T \psi(a_\ell)$, $y = (y_1, y_2, \ldots, y_m)^T$, $e = (1, 1, \ldots, 1)^T$.

No need to choose $\psi(\cdot)$ explicitly. Instead choose a kernel K, such that

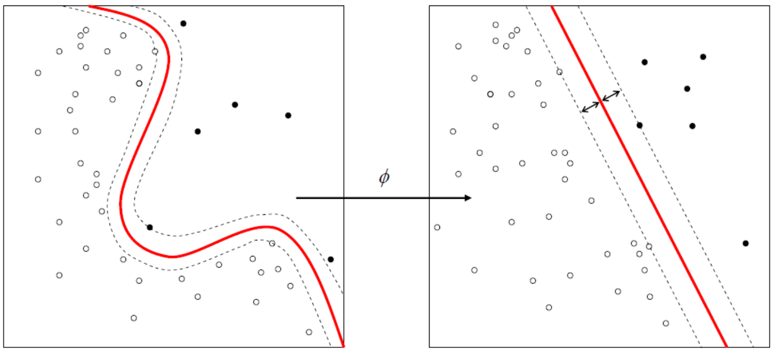
$$K(a_k, a_\ell) \sim \psi(a_k)^T \psi(a_\ell).$$

[Boser et al., 1992, Cortes and Vapnik, 1995]. "Kernel trick."

Gaussian kernels are popular:

$$K(a_k, a_\ell) = \exp(-\|a_k - a_\ell\|^2/(2\sigma)), \quad \text{for some } \sigma > 0.$$

Nonlinear SVM



Application X: Logistic Regression

Binary logistic regression is similar to binary SVM, except that we seek a function p that gives odds of data vector a being in class 1 or class 2, rather than making a simple prediction.

Seek odds function p parametrized by $x \in \mathbb{R}^n$:

$$p(a; x) := (1 + e^{a^T x})^{-1}.$$

Choose x so that $p(a_j; x) \approx 1$ when $y_j = 1$ and $p(a_j; x) \approx 0$ when $y_j = 2$.

Choose x to minimize a negative log likelihood function:

$$\mathcal{L}(x) = -\frac{1}{m}\left[\sum_{y_j=2} \log(1 - p(a_j; x)) + \sum_{y_j=1} \log p(a_j; x)\right]$$

Sparse solutions x are interesting because the indicate which components of a_j are critical to classification. Can solve: $\min_z \mathcal{L}(z) + \lambda\|z\|_1$.

Multiclass Logistic Regression

Have M classes instead of just 2. M can be large e.g. identify phonemes in speech, identify line outages in a power grid.

Labels $y_{j\ell} = 1$ if data point j is in class ℓ; $y_{j\ell} = 0$ otherwise; $\ell = 1, \dots, M$.

Find subvectors $x_{[\ell]}$, $\ell = 1, 2, \dots, M$ such that if a_j is in class k we have

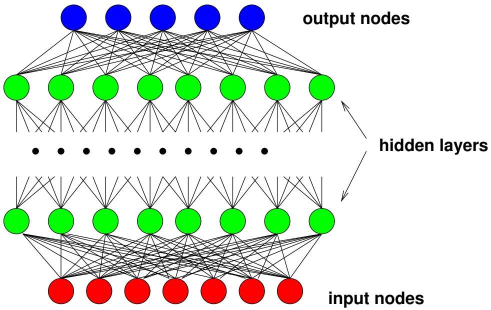
$$a_j^T x_{[k]} \gg a_j^T x_{[\ell]} \quad \text{for all } \ell \neq k.$$

Find $x_{[\ell]}$, $\ell = 1, 2, \dots, M$ by minimizing a negative log-likelihood function:

$$f(x) = -\frac{1}{m} \sum_{j=1}^{m} \left[\sum_{\ell=1}^{M} y_{j\ell}(a_j^T x_{[\ell]}) - \log \left(\sum_{\ell=1}^{M} \exp(a_j^T x_{[\ell]}) \right) \right]$$

Can use group LASSO regularization terms to select important features from the vectors a_j, by imposing a common sparsity pattern on all $x_{[\ell]}$.

Application XI: Deep Learning



Inputs are the vectors a_j, outputs are odds of a_j belonging to each class (as in multiclass logistic regression).

At each layer, inputs are converted to outputs by a linear transformation composed with an element-wise function:

$$a^{\ell+1} = \sigma(W^\ell a^\ell + g^\ell),$$

where a^ℓ is node values at layer ℓ, (W^ℓ, g^ℓ) are *parameters* in the network, σ is the element-wise function.

Deep Learning

The element-wise function σ makes transformations to scalar input:

- Logistic function: $t \to 1/(1+e^{-t})$;
- Hinge: $t \to \max(t, 0)$;
- Bernoulli: random! $t \to 1$ with probability $1/(1+e^{-t})$ and $t \to 0$ otherwise (inspired by neuron behavior).

The example depicted shows a completely connected network — but more typically networks are engineered to the application (speech processing, object recognition, . . .).

- local aggregation of inputs: pooling;
- restricted connectivity + constraints on weights (elements of W^ℓ matrices): convolutions.

Training Deep Learning Networks

The network contains many parameters — (W^ℓ, g^ℓ), $\ell = 1, 2, \dots, L$ in the notation above — that must be selected by training on the data (a_j, y_j), $j = 1, 2, \dots, m$.

Objective has the form:

$$\sum_{j=1}^{m} h(x; a_j, y_j)$$

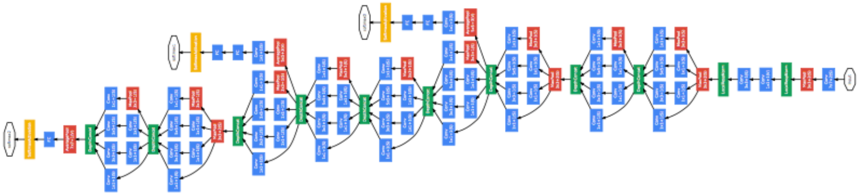
where $x = (W^1, g^1, W^2, g^2, \dots)$ are the parameters in the model and h measures the mismatch between observed output y_j and the outputs produced by the model (as in multiclass logistic regression).

Nonlinear, Nonconvex. It's also random in some cases (but then we can work with expectation).

Composition of many simple functions.

GoogLeNet

Visual object recognition: Google's prize-winning network from 2014 [Szegedy et al., 2015].



How Does a Neural Network Make The Problem Easier?

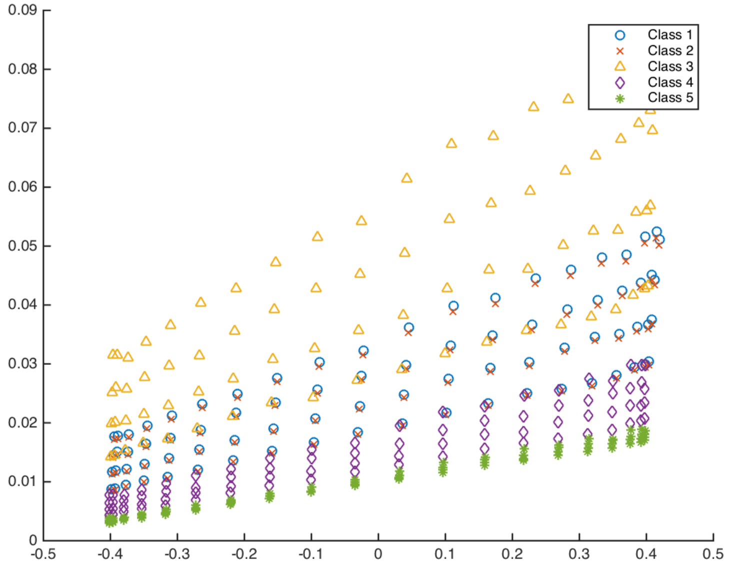
Can think of the neural network as transforming the raw data in a way that makes the ultimate task (regression, classification) easier.

We consider a multiclass classification application in power systems. The *raw data* is PMU measurements at different points in a power grid, under different operating conditions. The goal is to use this data to detect line outages. Each class corresponds to outage of a particular line.

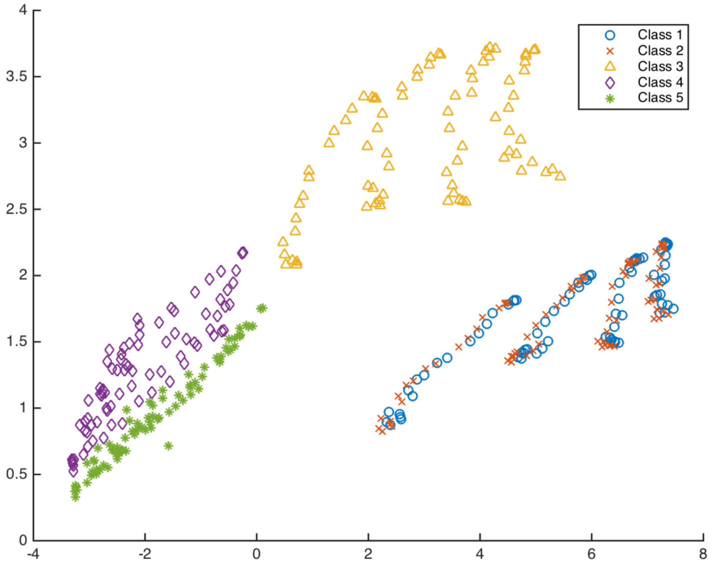
High-dimensional. Can illustrate by doing a singular value decomposition of the data matrix and plotting pairs of principal components on a 2-d graph.

Do this before and after transformation. One hidden layer with 200 nodes.

Raw Data (Before Transformation)



After Transformation by One Layer



A Basic Paradigm

Many optimization formulations in data analysis have this form:

$$\min_x \frac{1}{m} \sum_{j=1}^m h_j(x) + \lambda \Omega(x),$$

where

- h_j depends on parameters x of the mapping ϕ, and data items (a_j, y_j);
- Ω is the regularization term, often nonsmooth, convex, and separable in the components of x (but not always!).
- $\lambda \geq 0$ is the regularization parameter.
- (Ω could also be an indicator for simple set e.g. $x \geq 0$.)

Alternative formulation:

$$\min_x \frac{1}{m} \sum_{j=1}^m h_j(x) \quad \text{s.t. } \Omega(x) \leq \tau.$$

Structure in $h_j(x)$ and Ω strongly influences the choice of algorithms.

Optimization in Data Analysis: Some Background

Optimization formulations of data analysis / machine learning problems were popular, and becoming more so... but not universal:

- Heuristics are popular: k-means clustering, random forests.
- Linear algebra approaches are appropriate in some applications.
- Greedy feature selection.

Algorithmic developments have sometimes happened independently in the machine learning and optimization communities, e.g. stochastic gradient from 1980s-2009.

Occasional contacts in the past:

- Mangasarian solving SVM formulations [Mangasarian, 1965, Wohlberg and Mangasarian, 1990, Bennett and Mangasarian, 1992]
- Backpropagation in neural networks equivalent to gradient descent [Mangasarian and Solodov, 1994]
- Basis pursuit [Chen et al., 1998].

...but now, crossover is much more frequent and systematic.

Optimization in Learning: Context

Naive use of "standard" optimization algorithms is usually not appropriate.

Large data sets make some standard operations expensive: Evaluation of gradients, Hessians, functions, Newton steps, line searches.

The optimization formulation is viewed as a sampled, empirical approximation of some underlying "infinite" reality.

- Don't need or want an exact minimizer of the stated objective — this would be overfitting the empirical data. An approximate solution of the optimization problem suffices.
- Choose the regularization parameter λ so that ϕ gives best performance on some "holdout" set of data: validation, tuning.

Desired solution property is called generalizability.

Low-Dimensional Structure

Generalizability often takes the form of low-dimensional structure, when the function is parametrized appropriately.

- Variable vector x may be sparse (feature selection, compressed sensing).
- Variable matrix X may be low-rank, or low-rank + sparse.
- Data objects a_j lie approximately in a low-dimensional subspace.

Convex formulations with regularization are often tractable and efficient in practice.

Discrete or nonlinear formulations are more natural, but harder to solve and analyze. Recent advances make discrete formulations more appealing (Bertsimas et al.)

ALGORITHMS

Seek optimization algorithms — mostly elementary — that can exploit the structure of the formulations above.

- Full-gradient algorithms.
  - with projection and shrinking to handle Ω
- Accelerated gradient
- Stochastic gradient
  - and hybrids with full-gradient
- Coordinate descent
- Conditional gradient
- Newton's method, and approximate Newton
- Augmented Lagrangian / ADMM

Everything Old is New Again

"Old" approaches from the optimization literature have become popular:

- Nesterov acceleration of gradient methods [Nesterov, 1983].
- Alternating direction method of multipliers (ADMM) [Eckstein and Bertsekas, 1992].
- Parallel coordinate descent and incremental gradient algorithms [Bertsekas and Tsitsiklis, 1989]
- Stochastic gradient [Robbins and Monro, 1951]
- Frank-Wolfe / conditional gradient [Frank and Wolfe, 1956, Dunn, 1979].

Many extensions have been made to these methods and their convergence analysis. Many variants and adaptations proposed.

Gradient Methods

Basic formulation, without regularization:

$$\min_x H(x) := \frac{1}{m} \sum_{j=1}^{m} h_j(x).$$

Steepest descent takes steps in the negative gradient direction:

$$x^{k+1} \leftarrow x^k - \alpha_k \nabla H(x^k).$$

Classical analysis applies for H smooth, convex, and

$$\begin{aligned} \textbf{Lipschitz:} \quad & \|\nabla H(x) - \nabla H(z)\| \le L\|x - z\|, \quad && \text{for some } L > 0, \\ \textbf{Lojasiewicz:} \quad & \|\nabla H(x)\|^2 \ge 2\mu[H(x) - H^*], && \text{for some } \mu \ge 0. \end{aligned}$$

$\mu = 0$: sublinear convergence for $\alpha_k \equiv 1/L$: $H(x^k) - H^* = O(1/k)$.
$\mu > 0$: linear convergence with $\alpha_k \equiv 1/L$:

$$H(x^k) - H^* \le \left(1 - \frac{\mu}{L}\right)^k [H(x^0) - H^*].$$

Shrinking, Projecting for Ω

In the regularized form:

$$\min_x \; H(x) + \lambda\Omega(x),$$

the gradient step in H can be combined with a shrink operation in which the effect of Ω is accounted for exactly:

$$x^{k+1} = \arg\min_z \; \nabla H(x^k)^T(z - x^k) + \frac{1}{2\alpha_k}\|z - x_k\|^2 + \lambda\Omega(z).$$

When Ω is the indicator function for a convex set, x^{k+1} is the projection of $x^k - \alpha_k \nabla H(x^k)$ onto this set: gradient projection.

For many Ω of interest, this problem can be solved quickly (e.g. $O(n)$).

Algorithms and convergence theory for steepest descent on smooth H usually extend to this setting (for convex Ω).

Accelerated Gradient and Momentum

Accelerated gradient methods [Nesterov, 1983] highly influential.

Fundamental idea: **Momentum!** Search direction at iteration k depends on the latest gradient $\nabla H(x^k)$ and also the search direction at iteration $k-1$, which encodes gradient information from earlier iterations.

Heavy-ball & conjugate gradient (incl. nonlinear CG) also use momentum.

Heavy-Ball for $\min_x H(x)$:

$$x^{k+1} = x^k - \alpha \nabla H(x^k) + \beta(x^k - x^{k-1}).$$

Nesterov's optimal method:

$$x^{k+1} = x^k - \alpha_k \nabla H(x^k + \beta_k(x^k - x^{k-1})) + \beta_k(x^k - x^{k-1}).$$

Typically $\alpha_k \approx 1/L$ and $\beta_k \approx 1$.

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Typically $\alpha_k \approx 1/L$ and $\beta_k \approx 1$.

Accelerated Gradient Convergence

Typical convergence:

$$\text{Weakly convex } \mu = 0: \quad H(x^k) - H^* = O(1/k^2);$$

$$\text{Strongly convex } \mu > 0: \quad H(x^k) - H^* \le M \left(1 - \sqrt{\frac{\mu}{L}}\right)^k [H(x^0) - H^*].$$

- Approach can be extended to regularized functions $H(x) + \lambda\Omega(x)$ [Beck and Teboulle, 2009].
- Partial-gradient approaches (stochastic gradient, coordinate descent) can be accelerated in similar ways.
- Some fascinating new interpretations have been proposed recently
  - Algebraic analysis based on lower-bounding quadratics [Drusvyatskiy et al., 2016];
  - Geometric derivation [Bubeck et al., 2015].

Full Gradient: Does It Make Sense?

The methods above, based on full gradients, are useful for some problems in which X is a matrix, in which full gradients are practical to compute.

- Matrix completion, including explicitly parametrized problems with $X = LR^T$ or $X = ZZ^T$; nonnegative matrix factorization.
- Subspace identification;
- Sparse covariance estimation;

They are less appealing when the objective is the sum of m terms, with m large. To calculate

$$\nabla H(x) = \frac{1}{m} \sum_{j=1}^{m} \nabla h_j(x),$$

generally need to make a full pass through the data.

Often not practical for massive data sets. But can be hybridized with stochastic gradient methods (see below).

Stochastic Gradient (SG)

For $H(x) = (1/m)\sum_{j=1}^{m} h_j(x)$, iteration k has the form:

- Choose $j_k \in \{1, 2, \ldots, m\}$ uniformly at random;
- Set $x^{k+1} \leftarrow x^k - \alpha_k \nabla h_{j_k}(x^k)$.

$\nabla h_{j_k}(x^k)$ is a proxy for $\nabla H(x^k)$ but it depends on just one data item a_{j_k} and is much cheaper to evaluate.

Unbiased — $\mathbb{E}_j \nabla h_j(x) = \nabla H(x)$ — but the variance may be very large.

- Average the iterates for more robust convergence:

$$\bar{x}^k = \frac{\sum_{\ell=1}^{k} \gamma_\ell x^\ell}{\sum_{\ell=0}^{k} \gamma_\ell}, \text{where } \gamma_\ell \text{ are positive weights.}$$

- Minibatch: Use a set $J_k \subset \{1, 2, \ldots, m\}$ rather than a single item. (Smaller variance in the gradient estimate.)

See [Nemirovski et al., 2009] and many other works.

Stochastic Gradient (SG)

Convergence results for h_j convex require bounds on the variance of the gradient estimate:

$$\frac{1}{m}\sum_{j=1}^{m}\|\nabla h_j(x)\|_2^2 \le B^2 + L_g\|x-x^*\|^2.$$

Analyze expected convergence, e.g. $\mathbb{E}(f(x^k)-f^*)$ or $\mathbb{E}(f(\bar{x}^k)-f^*)$, where the expectation is over the sequence of indices $j_0, j_1, j_2, \ldots$.

Sample results:

- H strongly convex, $\alpha_k \sim 1/k$: $\mathbb{E}(H(x^k)-H^*) = O(1/k)$;
- H weakly convex, $\alpha_k \sim 1/\sqrt{k}$: $\mathbb{E}(H(\bar{x}^k)-H^*) = O(1/\sqrt{k})$.
- $B=0$, H strongly convex, $\alpha_k = \text{const}$: $\mathbb{E}(\|x^k-x^*\|_2^2) = O(\rho^k)$ for some $\rho \in (0,1)$.

Generalizes beyond finite sums, to $H(x) = \mathbb{E}_\xi f(x;\xi)$, where ξ is random.

Stochastic Gradient Applications

SG fits well the summation form of H (with large m), so has widespread applications:

- SVM (primal formulation).
- Logistic regression: binary and multiclass.
- **Deep Learning.** The Killer App! (Nonconvex) [LeCun et al., 1998]
- Subspace Identification (GROUSE): Project stochastic gradient searches onto subspace [Balzano and Wright, 2014].

Hybrids of Full Gradient and Stochastic Gradient

Stabilize SG by hybridizing with steepest descent (full-gradient). Get *linear convergence* for strongly convex functions, sublinear for weakly convex.

SAG: [LeRoux et al., 2012] Maintain approximations g_j to ∇h_j, use search direction $-(1/m)\sum_{j=1}^m g_j$. At iteration k, choose j_k at random, and update $g_{j_k} = \nabla h_{j_k}(x^k)$.

SAGA: [Defazio et al., 2014] Similar to SAG, but use search direction

$$-\nabla h_{j_k}(x^k) + g_{j_k} - \frac{1}{m}\sum_{j=1}^m g_j.$$

SVRG: [Johnson and Zhang, 2013] Similar again, but periodically do a full gradient evaluation to refresh all g_j.

Too much storage, **BUT** when h_j have the "ERM" form $h_j(a_j^T x)$ (linear least squares, linear SVM), all gradients can be stored in a scalar:

$$\nabla_x h_j(a_j^T x) = a_j h_j'(a_j^T x).$$

Coordinate Descent (CD) Framework

... for smooth unconstrained minimization: $\min_x H(x)$:

```
Set Choose $x^1 \in \mathbb{R}^n$;
for $\ell = 0, 1, 2, \dots$ (epochs) do
    for $j = 1, 2, \dots, n$ (inner iterations) do
        Define $k = \ell n + j$
        Choose index $i = i(\ell, j) \in \{1, 2, \dots, n\}$;
        Choose $\alpha_k > 0$;
        $x^{k+1} \leftarrow x^k - \alpha_k \nabla_i H(x^k) e_i$;
    end for
end for
```

where

- $e_i = (0, \dots, 0, 1, 0, \dots, 0)^T$: the ith coordinate vector;
- $\nabla_i H(x) =$ ith component of the gradient $\nabla H(x)$;
- $\alpha_k > 0$ is the step length.

CD Variants

- CCD (Cyclic CD): $i(\ell, j) = j$.
- RCD (Randomized CD a.k.a. Stochastic CD): $i(\ell, j)$ is chosen uniformly at random from $\{1, 2, \ldots, n\}$.
- RPCD (Randomized Permutations CD):
  - At the start of epoch ℓ, we choose a random permutation of $\{1, 2, \ldots, n\}$, denoted by π_ℓ.
  - Index $i(\ell, j)$ is chosen to be the jth entry in π_ℓ.

Important quantities in analysis:

- $L_{\max}$: componentwise Lipschitz constant for ∇H:

$$|\nabla_i H(x + te_i) - \nabla_i H(x)| \le L_i |t|, \quad L_{\max} = \max_{i=1,2,\ldots,n} L_i.$$

- L: usual Lipschitz constant: $|\nabla H(x + d) - \nabla H(x)| \le L \|d\|$.
- Lojasiewicz constant μ: $\|\nabla H(x)\|^2 \ge 2\mu[H(x) - H^*]$

Randomized CD Convergence

Of the three variants, convergence of the randomized form has by far the most elementary analysis [Nesterov, 2012].

Get convergence rates for quantity $\phi_k := \mathbb{E}(H(x^k) - x^*)$.

$$\begin{aligned} \mu > 0: &\quad \phi_{k+1} \le \left(1 - \frac{\mu}{nL_{\max}}\right)\phi_k, \quad && k = 1, 2, \dots, \\ \mu = 0: &\quad \phi_k \le \frac{2nL_{\max}R_0^2}{k}, && k = 1, 2, \dots, \end{aligned}$$

where R_0 bounds distance from x^0 to solution set.

If the economics of evaluating gradient components are right, this can be a factor $L/L_{\max}$ faster than full-gradient steepest descent!

This ratio is in range $[1, n]$. Maximized by $H(x) = (\mathbf{1}\mathbf{1}^T)x$.

Functions like this are good cases for RCD and RPCD, which are much faster than CCD or steepest descent.

Cyclic and Random-Permutations CD Convergence

Analysis of [Beck and Tetruashvili, 2013] treats CCD as an approximate form of Steepest Descent, bounding improvement in f over one cycle in terms of the gradient at the start of the cycle.

Get linear and sublinear rates that are slower than both RCD and Steepest Descent. This analysis is fairly tight — recent analysis of [Sun and Ye, 2016] confirms slow rates on a worst-case example.

Same analysis applies to Randomized Permutations (RPCD), but practical results for RPCD are much better, and usually at least as good as RCD. Results on quadratic function

$$H(x) = (1/2)x^T Ax$$

demonstrate this behavior (see [Wright, 2015] and my talks in 2015).

We can explain good behavior of RCCD now, on the worst-case example for CCD. [Lee and Wright, 2016]

CD Extensions

- Block CD: Replace single component i by block $I \subset \{1, 2, \dots, n\}$.
- Dual nonlinear SVM [Platt, 1999]. Choose *two* components of α per iteration, to stay feasible w.r.t. constraint $y^T \alpha = 0$.
- Can be accelerated (efficiently) using "Nesterov" techniques: [Nesterov, 2012, Lee and Sidford, 2013].
- Adaptable to the separable regularized case $H(x) + \lambda \Omega(x)$.
- Parallel asynchronous variants, suitable for implementation on shared-memory multicore computers, have been proposed and analyzed. [Bertsekas and Tsitsiklis, 1989, Liu and Wright, 2015, Liu et al., 2015]

Conditional Gradient / "Frank-Wolfe"

$$\min_{x \in \Omega} f(x),$$

where f is a convex function and Ω is a closed, bounded, convex set.

Start at $x_0 \in \Omega$. At iteration k:

$$v_k := \arg\min_{v \in \Omega} v^T \nabla f(x_k);$$
$$x_{k+1} := x_k + \alpha_k (v_k - x_k), \quad \alpha_k = \frac{2}{k+2}.$$

- Potentially useful when it is easy to minimize a linear function over the *original* constraint set Ω;
- Admits an elementary convergence theory: $1/k$ sublinear rate.
- Same convergence rate holds if we use a line search for α_k.

Revived by [Jaggi, 2013].

Newton's Method

$$\min_{x \in \mathbb{R}^n} f(x), \quad \text{with } f \text{ smooth.}$$

Newton's method motivated by the second-order Taylor-series approximation at current iterate x^k:

$$f(x^k + p) = f(x^k) + \nabla f(x^k)^T p + \frac{1}{2} p^T \nabla^2 f(x^k) p + O(\|p\|^3). \tag{1}$$

When $\nabla^2 f(x^k)$ is positive definite, can choose p to minimize the quadratic

$$p^k = \arg\min_p \; f(x^k) + \nabla f(x^k)^T p + \frac{1}{2} p^T \nabla^2 f(x^k) p,$$

which is

$$p^k = -\nabla^2 f(x^k)^{-1} \nabla f(x^k) \quad \text{Newton step!}$$

Thus, basic form of Newton's method is

$$x^{k+1} = x^k - \nabla^2 f(x^k)^{-1} \nabla f(x^k). \tag{2}$$

Practical Newton

If x^* satisfies second-order sufficient conditions:

$$\nabla f(x^*) = 0, \quad \nabla^2 f(x^*) \text{ positive definite,}$$

then Newton's method has local quadratic convergence:

$$\|x^{k+1} - x^*\| \le C\|x^k - x^*\|^2, \quad \text{for all } k \ge \bar{k},$$

when $\|x^{\bar{k}} - x^*\|$ is sufficiently small.

When $\nabla^2 f(x^k)$ is not positive semidefinite, motivation for Newton step (as minimizer of the second-order Taylor series expansion) no longer applies.

Newton can be modified to retain its validity as a descent method, and still retain fast local convergence to second-order sufficient solutions.

If $\nabla^2 f(x^k)$ is indefinite, can modify p^k:

- Add positive values to the diagonal of $\nabla^2 f(x^k)$ while factorizing it during the calculation of p^k;
- Redefine
$$p^k := -[\nabla^2 f(x^k) + \lambda_k I]^{-1} \nabla f(x^k),$$
for some $\lambda_k > 0$, so that the modified Hessian is positive definite and p^k is a descent direction.
- (Equivalent) Redefine p^k as solution of a trust-region subproblem:
$$\min_p \; f(x^k) + \nabla f(x^k)^T p + \frac{1}{2} p^T \nabla^2 f(x^k) p \quad \text{subject to } \|p\|_2 \le \Delta_k.$$
- Cubic regularization: Given Lipschitz constant L for $\nabla^2 f(x)$, solve
$$\min_p \; f(x^k) + \nabla f(x^k)^T p + \frac{1}{2} p^T \nabla^2 f(x^k) p + \frac{L}{6} \|p\|^3.$$

Global Convergence

(Assume that f is bounded below.)

Methods that calculate a descent direction p^k via modified Newton, then do a line search typically have accumulation points that are stationary: $\nabla f(x^*) = 0$.

Special trust-region, line-search, and cubic regularization methods have stronger guarantees e.g. accumulation points satisfy second-order necessary conditions: $\nabla f(x^*) = 0$, $\nabla^2 f(x^*)$ positive semidefinite.

$$\begin{aligned} \|\nabla f(x^k)\| \le \epsilon \quad & \text{within } k = O(\epsilon^{-3/2}) \text{ iterations;} \\ \nabla^2 f(x^k) \ge -\epsilon I \quad & \text{within } k = O(\epsilon^{-3}) \text{ iterations,} \end{aligned}$$

where the constants in $O(\cdot)$ depend on $[f(x^0) - \bar{f}]$ and L.
[Nesterov and Polyak, 2006, Royer and Wright, 2017], others.

Augmented Lagrangian

Consider the linearly constrained problem,

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

where $f : \mathbb{R}^n \to \mathbb{R}$ is convex.

Define the Lagrangian function:

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

x^* is a solution if and only if there exists a vector of Lagrange multipliers $\lambda^* \in \mathbb{R}^m$ such that

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

or equivalently:

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

Augmented Lagrangian

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

$$\mathcal{L}(x, \lambda; \rho) := \underbrace{f(x) + \lambda^T(Ax - b)}_{\text{Lagrangian}} + \underbrace{\frac{\rho}{2}\|Ax - b\|_2^2}_{\text{“augmentation”}}.$$

Basic Augmented Lagrangian (a.k.a. method of multipliers) is

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

[Hestenes, 1969, Powell, 1969]

Some constraints on x (such as $x \in \Omega$) can be handled explicitly:

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

Alternating Direction Method of Multipliers (ADMM)

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

for which the Augmented Lagrangian is

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

Standard AL would minimize $\mathcal{L}(x, z, \lambda; \rho)$ w.r.t. (x, z) jointly. However, since coupled in the quadratic term, separability is lost.

In ADMM, minimize over x and z separately and sequentially:

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

Extremely useful framework for many data analysis / learning settings.
Major references: [Eckstein and Bertsekas, 1992, Boyd et al., 2011]

Not Discussed!

Many interesting topics not mentioned, including

- quasi-Newton methods.
- Linear equations $Ax = b$: Kaczmarz algorithms.
- Image and video processing: denoising and deblurring.
- Graphs: detect structure and cliques, consensus optimization, ...
- Integer and combinatorial formulations.
- Parallel variants: synchronous and asynchronous.
- Online learning.

Conclusions: Optimization in Data Analysis

- HUGE interest across multiple communities.
- Ongoing challenges because of increasing scale and complexity of machine learning / data analysis applications. Also because of the computational platforms.
- Optimization methodology is integrated with the applications.
- The optimization / data analysis / machine learning research communities are becoming integrated too!

FIN

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