Optimisation et apprentissage.

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Complexity.

In the course. . .

- Randomness helps. Getting a solution with a small probability of failure is often much easier than solving the problem exactly.
- Random instances of some optimization problems are easier to solve.

Today...

- Focus on **convexity** and its impact on complexity.
- Convex approximations, duality.
- Applications in learning.

In optimization.

Twenty years ago. . .

- Solve realistic large-scale problems using naive algorithms.
- Solve small, naive problems using serious algorithms.

Twenty years later. . .

- Solve realistic problems in e.g. statistics, signal processing, using efficient algorithms with explicit complexity bounds.
- Statisticians have started to care about complexity.
- Optimizers have started to care about statistics.

Introduction

Convexity.



Key message from complexity theory: as the problem dimension gets large

- all convex problems are easy,
- most nonconvex problems are hard.

Convex problem.

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & a_i^T x = b_i, \quad i = 1, \dots, p \end{array}$$

 f_0 , f_1 , ..., f_m are convex functions, the equality constraints are all affine.

• Strong assumption, yet **surprisingly expressive**.

Good convex approximations of nonconvex problems.

Introduction

First-order condition. Differentiable f with convex domain is convex iff

$$f(y) \ge f(x) + \nabla f(x)^T (y - x)$$
 for all $x, y \in \operatorname{dom} f$



First-order approximation of f is global underestimator

Ellipsoid method

Ellipsoid method. Developed in 70s by Shor, Nemirovski and Yudin.

- Function $f : \mathbb{R}^n \to \mathbb{R}$ convex (and for now, differentiable)
- **problem:** minimize *f*
- oracle model: for any x we can evaluate f and $\nabla f(x)$ (at some cost)



By evaluating ∇f we rule out a halfspace in our search for x^{\star} .

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Ellipsoid method

Suppose we have evaluated $\nabla f(x_1), \ldots, \nabla f(x_k)$,



on the basis of $\nabla f(x_1), \ldots, \nabla f(x_k)$, we have **localized** x^* to a polyhedron.

Question: what is a 'good' point x_{k+1} at which to evaluate ∇f ?

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Ellipsoid algorithm

Idea: localize x^* in an **ellipsoid** instead of a polyhedron.



Compared to cutting-plane method:

- Iocalization set doesn't grow more complicated
- easy to compute query point
- but, we add unnecessary points in step 4

Challenges in cutting-plane methods:

- can be difficult to compute appropriate next query point
- Iocalization polyhedron grows in complexity as algorithm progresses

Ellipsoid method:

- Simple formula for $\mathcal{E}^{(k+1)}$ given $\mathcal{E}^{(k)}$
- $\operatorname{vol}(\mathcal{E}^{(k+1)}) < e^{-\frac{1}{2n}} \operatorname{vol}(\mathcal{E}^{(k)})$

Ellipsoid Method: example





Duality

A linear program (LP) is written

$$\begin{array}{ll} \text{minimize} & c^T x\\ \text{subject to} & Ax = b\\ & x \geq 0 \end{array}$$

where $x \ge 0$ means that the coefficients of the vector x are nonnegative.

- Starts with Dantzig's simplex algorithm in the late 40s.
- First proofs of polynomial complexity by Nemirovskii and Yudin [1979] and Khachiyan [1979] using the ellipsoid method.
- First efficient algorithm with polynomial complexity derived by Karmarkar [1984], using interior point methods.

Duality

Duality. The two linear programs

 $\begin{array}{ll} \text{minimize} & c^T x\\ \text{subject to} & Ax = b\\ & x \geq 0 \end{array}$

 $\begin{array}{ll} \text{maximize} & y^T b\\ \text{subject to} & c - A^T y \geq 0 \end{array}$

have the same optimal values.

Similar results hold for most **convex** problems.

- Usually both primal and dual have a natural interpretation.
- Many algorithms solve both problems simultaneously.

Support Vector Machines

Simplest version. . .

- Input: A set of points (in 2D here) and labels (black & white).
- **Output**: A linear classifier separating the two groups.



Text Classification

Example: word frequencies.

- In blue: good news
- In red: bad news.



Improving these results. . .

- Are we restricted to **linear** classifiers?
- What happens when the two classes are not perfectly **separable**?

Linear Classification

The linear separation problem.

Inputs:

- Data points $x_j \in \mathbb{R}^n$, $j = 1, \ldots, m$.
- Binary Labels $y_j \in \{-1, 1\}, j = 1, ..., m.$

Problem:

find $w \in \mathbb{R}^n$ such that $\langle w, x_j \rangle \ge 1$ for all j such that $y_j = 1$ $\langle w, x_j \rangle \le -1$ for all j such that $y_j = -1$

Output:

• The classifier vector w.

Linear Classification

Nonlinear classification.

The problem:

find wsuch that $\langle w, x_j \rangle \ge 1$ for all j such that $y_j = 1$ $\langle w, x_j \rangle \le -1$ for all j such that $y_j = -1$

is linear in the variable w. Solving it amounts to solving a linear program.
Suppose we want to add quadratic terms in x:

find
$$w$$

such that $\langle w, (x_j, x_j^2) \rangle \ge 1$ for all j such that $y_j = 1$
 $\langle w, (x_j, x_j^2) \rangle \le -1$ for all j such that $y_j = -1$

this is still a (larger) linear program in the variable w.

Nonlinear classification is as easy as linear classification.

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Classification

This trick means that we are not limited to linear classifiers:



Separation by ellipsoid

Separation by 4th degree polynomial

Both are **equivalent** to linear classification. . . just increase the dimension.

Classification: margin

Suppose the two sets are not separable. We solve instead

$$\begin{array}{ll} \text{minimize} & \mathbf{1}^T u + \mathbf{1}^T v \\ \text{subject to} & \langle w, x_j \rangle \geq 1 - u_j & \text{for all } j \text{ such that } y_j = 1 \\ & \langle w, x_j \rangle < -(1 - v_j) & \text{for all } j \text{ such that } y_j = -1 \\ & u \succeq 0, \quad v \succeq 0 \end{array}$$

Can be interpreted as a heuristic for minimizing the number of misclassified points.



Robust linear discrimination

Suppose instead that the two data sets are well **separated**.

(Euclidean) distance between hyperplanes

$$\mathcal{H}_1 = \{z \mid a^T z + b = 1\}$$
$$\mathcal{H}_2 = \{z \mid a^T z + b = -1\}$$

is $\operatorname{dist}(\mathcal{H}_1, \mathcal{H}_2) = 2/\|a\|_2$



to separate two sets of points by maximum margin,

minimize
$$(1/2) ||a||_2$$

subject to $a^T x_i + b \ge 1$, $i = 1, \dots, N$ (1)
 $a^T y_i + b \le -1$, $i = 1, \dots, M$

(after squaring objective) a QP in a, b

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In practice. . .

- The data has very high dimension.
- The classifier is highly nonlinear.
- Overfitting is a problem: in high dimensional spaces it is always possible to find a classifier, but the classifier itself can become somewhat meaningless.
 - Maximizing the margin helps.
 - Determine the tradeoff between error and margin by **cross-validation**.

Support Vector Machines: Duality

Given m data points $x_i \in \mathbb{R}^n$ with labels $y_i \in \{-1, 1\}$.

The maximum margin classification problem can be written

minimize
$$\frac{1}{2} ||w||_2^2 + C \mathbf{1}^T z$$

subject to $y_i(w^T x_i) \ge 1 - z_i, \quad i = 1, \dots, m$
 $z \ge 0$

in the variables $w, z \in \mathbb{R}^n$, with parameter C > 0.

• The Lagrangian is written

$$L(w, z, \alpha) = \frac{1}{2} \|w\|_2^2 + C \mathbf{1}^T z + \sum_{i=1}^m \alpha_i (1 - z_i - y_i w^T x_i)$$

with dual variable $\alpha \in \mathbb{R}^m_+$.

Support Vector Machines: Duality

The Lagrangian can be rewritten

$$L(w, z, \alpha) = \frac{1}{2} \left(\left\| w - \sum_{i=1}^{m} \alpha_i y_i x_i \right\|_2^2 - \left\| \sum_{i=1}^{m} \alpha_i y_i x_i \right\|_2^2 \right) + (C\mathbf{1} - \alpha)^T z + \mathbf{1}^T \alpha$$

with dual variable $\alpha \in \mathbb{R}^n_+$.

 \blacksquare Minimizing in (w,z) we form the dual problem

maximize
$$-\frac{1}{2} \left\| \sum_{i=1}^{m} \alpha_i y_i x_i \right\|_2^2 + \mathbf{1}^T \alpha$$

subject to $0 \le \alpha \le C$

• At the optimum, we must have

$$w = \sum_{i=1}^{m} \alpha_i y_i x_i$$
 and $\alpha_i = C$ if $z_i > 0$

(this is the representer theorem).

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Support Vector Machines: the kernel trick

If we write X the data matrix with columns x_i , the dual can be rewritten

$$\begin{array}{ll} \text{maximize} & -\frac{1}{2}\alpha^T \operatorname{diag}(y) X^T X \operatorname{diag}(y) \alpha + \mathbf{1}^T \alpha \\ \text{subject to} & 0 \leq \alpha \leq C \end{array} \\ \end{array}$$

This means that the data only appears in the dual through the gram matrix

$$K = X^T X$$

which is called the **kernel** matrix.

- In particular, the original dimension n does not appear in the dual.
- SVM complexity only grows with the number of samples, typically $O(m^{1.5})$.
- For linear classifiers: the magnitude of w_i gives a hint on the importance of variable i (for text: important words).

Support Vector Machines: the kernel trick

Kernels.

- All matrices written $K = X^T X$ can be kernel matrices.
- Easy to construct from highly diverse data types.

Examples. . .

Kernels for voice recognition



Kernels for gene sequence alignment

AAB24882 AAB24881	TYHMCQFHCRYVNNHSGEKLYECNERSKAFSCPSHLQCHKRRQIGEKTHEHNQCGKAFPT 60 YECNQCGKAFAQHSSLKCHYRTHIGEKPYECNQCGKAFSK 40
	**** *** * * * * * * * * * * * * * * * *
AAB24882	PSHLQYHERTHTGEKPYECHQCGQAFKKCSLLQRHKRTHTGEKPYE-CNQCGKAFAQ- 116
AAB24881	HSHLQCHKRTHTGEKPYECNQCGKAFSQHGLLQRHKRTHTGEKPYMNVINMVKPLHNS 98
	**** * ********** *** *** *** *********

Support Vector Machines: the kernel trick

Kernels for images



Kernels for text classification

Ryanair Q3 profit up 30%, stronger than expected. (From Reuters.) DUBLIN, Feb 5 (Reuters) - Ryanair (RYA.I: Quote, Profile, Research) posted a 30 pct jump in third-quarter net profit on Monday, confounding analyst expectations for a fall, and ramped up its full-year profit goal while predicting big fuel-cost savings for the following year (...).

profit	loss	up	down	jump	fall	below	expectations	ramped up
3	0	2	0	1	1	0	1	1

Consider the following underdetermined linear system



where $A \in \mathbb{R}^{m \times n}$, with $n \gg m$.

Can we find the **sparsest** solution?

- Signal processing: We make a few measurements of a high dimensional signal, which admits a sparse representation in a well chosen basis (e.g. Fourier, wavelet). Can we reconstruct the signal exactly?
- Coding: Suppose we transmit a message which is corrupted by a few errors. How many errors does it take to start losing the signal?
- **Statistics:** Variable selection in regression (LASSO, etc).

Why **sparsity**?

- Sparsity is a proxy for **power laws**. Most results stated here on sparse vectors apply to vectors with a power law decay in coefficient magnitude.
- Power laws appear everywhere. . .
 - Zipf law: word frequencies in natural language follow a power law.
 - Ranking: pagerank coefficients follow a power law.
 - Signal processing: 1/f signals
 - Social networks: node degrees follow a power law.
 - Earthquakes: Gutenberg-Richter power laws
 - River systems, cities, net worth, etc.



Frequency vs. word in Wikipedia (from Wikipedia).

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Frequency vs. magnitude for earthquakes worldwide. [Christensen et al., 2002]



Pages vs. Pagerank on web sample. [Pandurangan et al., 2006]

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Cumulative degree distribution in networks. [Newman, 2003]

• Getting the sparsest solution means solving:

minimize Card(x)subject to Ax = b

which is a (hard) **combinatorial** problem in $x \in \mathbb{R}^n$.

• A classic heuristic is to solve instead:

minimize $||x||_1$ subject to Ax = b

which is equivalent to an (easy) linear program.

Example: we fix A, we draw many **sparse** signals e and plot the probability of perfectly recovering e by solving

minimize $||x||_1$ subject to Ax = Ae

in $x \in \mathbb{R}^n$, with n = 50 and m = 30.



- For some matrices A, when the solution e is sparse enough, the solution of the **linear program** problem is also the **sparsest** solution to Ax = Ae. [Donoho and Tanner, 2005, Candès and Tao, 2005]
- Let k = Card(e), this happens even when $\mathbf{k} = O(\mathbf{m})$ asymptotically, which is provably optimal.



Semidefinite Programming

A linear program (LP) is written

minimize
$$c^T x$$

subject to $Ax = b$
 $x \ge 0$

where $x \ge 0$ means that the coefficients of the vector x are nonnegative.

A semidefinite program (SDP) is written

minimize
$$\operatorname{Tr}(CX)$$

subject to $\operatorname{Tr}(A_iX) = b_i, \quad i = 1, \dots, m$
 $X \succeq 0$

where $X \succeq 0$ means that the matrix variable $X \in \mathbf{S}_n$ is **positive semidefinite**.

- Nesterov and Nemirovskii [1994] showed that the interior point algorithms used for linear programs could be extended to semidefinite programs.
- Key result: self-concordance analysis of Newton's method (affine invariant smoothness bounds on the Hessian).

Modeling

- Linear programming started as a toy problem in the 40s, many applications followed.
- Semidefinite programming has much stronger expressive power, many new applications being investigated today (cf. this talk).
- Similar conic duality theory.
- Algorithms
 - Robust solvers for solving large-scale linear programs are available today (e.g. MOSEK, CPLEX, GLPK).
 - Not (yet) true for semidefinite programs. Very active work now on first-order methods, motivated by applications in statistical learning (matrix completion, NETFLIX, structured MLE, . . .).

Mixing rates for Markov chains & maximum variance unfolding

- Let G = (V, E) be an **undirected graph** with n vertices and m edges.
- We define a **Markov chain** on this graph, and let $w_{ij} \ge 0$ be the transition rate for edge $(i, j) \in V$.



• Let $\pi(t)$ be the state distribution at time t, its evolution is governed by the heat equation

$$d\pi(t) = -L\pi(t)dt$$

with

$$L_{ij} = \begin{cases} -w_{ij} & \text{if } i \neq j, \ (i,j) \in V \\ 0 & \text{if } (i,j) \notin V \\ \sum_{(i,k) \in V} w_{ik} & \text{if } i = j \end{cases}$$

the graph Laplacian matrix, which means

$$\pi(t) = e^{-Lt}\pi(0).$$

[Sun, Boyd, Xiao, and Diaconis, 2006]

Maximizing the mixing rate of the Markov chain means solving

maximize
$$t$$

subject to $L(w) \succeq t(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T)$
 $\sum_{(i,j)\in V} d_{ij}^2 w_{ij} \le 1$
 $w \ge 0$

in the variable $w \in \mathbb{R}^m$, with (normalization) parameters $d_{ij}^2 \ge 0$.

Since L(w) is an affine function of the variable $w \in \mathbb{R}^m$, this is a semidefinite program in $w \in \mathbb{R}^m$.

[Weinberger and Saul, 2006, Sun et al., 2006]

The **dual** means solving

maximize
$$\operatorname{Tr}(X(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T))$$

subject to $X_{ii} - 2X_{ij} + X_{jj} \leq d_{ij}^2$, $(i, j) \in V$
 $X \succeq 0$,

in the variable $X \in \mathbf{S}_n$.

This is a maximum variance unfolding problem.





From [Sun et al., 2006]: we are given pairwise 3D distances for k-nearest neighbors in the point set on the right. We plot the maximum variance point set satisfying these pairwise distance bounds on the right.

The NETFLIX challenge

- Video On Demand and DVD by mail service in the United States, Canada, Latin America, the Caribbean, United Kingdom, Ireland, Sweden, Denmark, Norway, Finland.
- About 25 million users and 60,000 films.
- Unlimited streaming, DVD mailing, cheaper than CANAL+ :)
- Online movie recommendation engine.

Collaborative prediction

• Users assign **ratings** to a certain number of movies:



Objective: make recommendations for other movies. . .

NETFLIX

Just for Kids Taste Profile

· DVDs

alexandre d'Aspr... Your Account Help Movies, TV shows, actors, directors, genres

Top 10 for alexandre

Instant

Queue



Popular on Netflix



Infer user preferences and movie features from user ratings.

A linear prediction model

$$\operatorname{rating}_{ij} = u_i^T v_j$$

where u_i represents user characteristics and v_j movie features.

This makes collaborative prediction a **matrix factorization** problem, We look for a linear model by factorizing $M \in \mathbb{R}^{n \times m}$ as:

$$M = U^T V$$

where $U \in \mathbb{R}^{n \times k}$ represents user characteristics and $V \in \mathbb{R}^{k \times m}$ movie features.

• Overcomplete representation. . . We want k to be as small as possible, i.e. we seek a low rank approximation of M.

We would like to solve

minimize
$$\operatorname{\mathbf{Rank}}(X) + c \sum_{(i,j) \in S} \max(0, 1 - X_{ij}M_{ij})$$

non-convex and numerically hard. . .

Relaxation result in Fazel et al. [2001]: replace $\mathbf{Rank}(X)$ by its convex envelope on the spectahedron to solve:

minimize
$$||X||_* + c \sum_{(i,j) \in S} \max(0, 1 - X_{ij}M_{ij})$$

where $||X||_*$ is the **nuclear norm**, *i.e.* sum of the singular values of X.

• This is a convex **semidefinite program** in X.

NETFLIX challenge.

- NETFLIX offered \$1 million to the team who could improve the quality of its ratings by 10%, and \$50.000 to the first team to improve them by 1%.
- It took two weeks to beat the 1% mark, and three years to reach 10%.
- Very large number of scientists, students, postdocs, etc. working on this.
- The story could end here. But all this work had surprising outcomes...

Phase Recovery

Molecular imaging



(from [Candes et al., 2011b])

CCD sensors only record the magnitude of diffracted rays, and loose the phase

Fraunhofer diffraction: phase is required to invert the 2D Fourier transform

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Focus on the phase retrieval problem, i.e.

find
$$x$$

such that $|\langle a_i, x \rangle|^2 = b_i^2$, $i = 1, \dots, n$

in the variable $x \in \mathbf{C}^p$.

[Shor, 1987, Lovász and Schrijver, 1991] write

$$|\langle a_i, x \rangle|^2 = b_i^2 \quad \Longleftrightarrow \quad \mathbf{Tr}(a_i a_i^* x x^*) = b_i^2$$

 [Chai et al., 2011] and [Candes et al., 2011a] formulate phase recovery as a matrix completion problem

Minimize
$$\operatorname{\mathbf{Rank}}(X)$$

such that $\operatorname{\mathbf{Tr}}(a_i a_i^* X) = b_i^2, \quad i = 1, \dots, n$
 $X \succeq 0$

[Recht et al., 2007, Candes and Recht, 2008, Candes and Tao, 2010] show that under certain conditions on A and x_0 , it suffices to solve

Minimize $\operatorname{Tr}(X)$ such that $\operatorname{Tr}(a_i a_i^* X) = b_i^2$, $i = 1, \dots, n$ $X \succeq 0$

which is a (convex) semidefinite program in $X \in \mathbf{H}_p$.

- Solving the convex semidefinite program yields a solution to the combinatorial, hard reconstruction problem.
- Apply results from **collaborative filtering** (NETFLIX) to **molecular imaging**.

Merci!

*

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