Optimization for Machine Learning

Lecture 13: EM, CCCP, and friends

6.881: MIT

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06 Apr, 2021

Motivation

(example task)

Nonnegative matrix factorization

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- SVD yields dense B and C
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$$\boxed{\textbf{NMF} \text{ imposes } B \geq 0, C \geq 0}$$

Algorithms

$$\boxed{A \approx BC \quad \text{s.t. } B, C \geq 0}$$

Least-squares NMF

$$\min \quad \tfrac{1}{2}\|A - BC\|_{\mathrm{F}}^2 \quad \text{s.t. } B, C \geq 0.$$

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We'll look at simple (local) methods

Background on NMF Algorithms

- Hack: Compute TSVD; "zero-out" negative entries
- Alternating minimization (AM)
- Majorize-Minimize based (MM)
- Global optimization (not covered)
- "Online" algorithms (not covered)

AltMin / AltDesc

$$\min \quad F(B, C)$$

Alternating Descent

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4. $k \leftarrow k+1$, and repeat until stopping criteria met.

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$$\text{(Observe:)} \quad F(B^{k+1}, C^{k+1}) \leq F(B^k, C^{k+1}) \leq F(B^k, C^k)$$

AltMin for NMF: naive version

Alternating Least Squares (ALS)

$$C = \underset{C}{\operatorname{argmin}} \quad \|A - B^k C\|_F^2;$$

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$$\|A - B^{k+1}C^{k+1}\|_F^2 \leq \|A - B^k C^{k+1}\|_F^2 \leq \|A - B^k C^k\|_F^2$$

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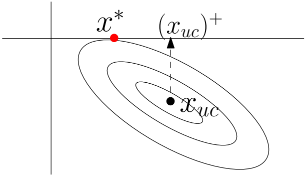
descent **can fail to hold!**



NMF AltMin: correct way

Use alternating **nonnegative least-squares**

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Advantages: Guaranteed descent. Theory of two-block BCD guarantees convergence to a *stationary point*.

Disadvantages: more complex; slower than ALS

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Explore. Faster methods; e.g., an SGD-style method for NMF?

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Ref. Mairal, Bach, Ponce, Sapiro. *Online Learning for Matrix Factorization and Sparse Coding*. JMLR 11(2):19–60, 2010.

Just Descend

(EM, CCCP, MM methods!)

Revisiting NMF

Consider $F(B, C) = \frac{1}{2}\|A - BC\|_F^2$: convex separately in B and C

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Since $F(C)$ *separable* (over cols of C), we just illustrate

$$\min_{c \geq 0} \quad f(c) = \tfrac{1}{2}\|a - Bc\|_2^2$$

Remark. This is the well-known NNLS problem.

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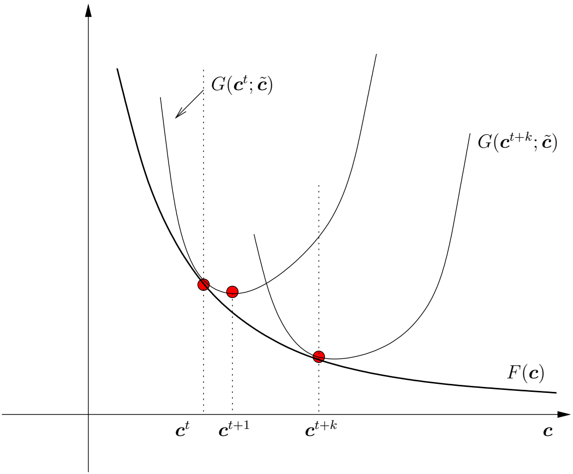
$$\boxed{\text{Doing descent (not necc minimization) over } f!}$$

The Majorize-Minimize (MM) idea



(**Majorize:** get upper bound; Minorize: minimize this bound)

Descent technique

$$\min_{c\geq 0} \quad f(c) = \tfrac{1}{2}\|a - Bc\|_2^2$$

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$$\begin{aligned} g(c,c) &= f(c), && \text{for all} \quad c,\\ g(c,\tilde{c}) &\geq f(c), && \text{for all} \quad c,\tilde{c}. \end{aligned}$$

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Constructing g for $f(c) = \|a - Bc\|^2$

We exploit that $h(x) = \frac{1}{2}x^2$ is a *convex function*

$$\boxed{h\left(\sum_i \lambda_i x_i\right) \leq \sum_i \lambda_i h(x_i), \text{ where } \lambda_i \geq 0, \sum_i \lambda_i = 1}$$

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&=: g(c, \tilde{c}), \quad \text{where} \quad \lambda_{ij} \quad \text{are convex coeffts}
\end{aligned}$$

Constructing $g(c, \tilde{c})$

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Exercise: Verify that $g(c,c) = f(c)$;

Exercise: Let $f(c) = \sum_i a_i \log(a_i/(Bc)_i) - a_i + (Bc)_i$. Derive an auxiliary function $g(c,\tilde{c})$ for this $f(c)$.

Reapting the benefits of g

Key step

$$
\begin{aligned}
g(c, \tilde{c}) &= \tfrac{1}{2}\|a\|_2^2 - \sum\nolimits_i a_i b_i^T c + \tfrac{1}{2}\sum\nolimits_{ij} \lambda_{ij}\left(b_{ij}c_j/\lambda_{ij}\right)^2 \\
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Exercise: Solve $\partial g(c,c^t)/\partial c_p = 0$ to obtain ***closed form***

$$c_p = c_p^t \frac{[B^T a]_p}{[B^T B c^t]_p}$$

Reapting the benefits of g

Key step

$$\begin{aligned} g(c,\tilde{c}) &= \tfrac{1}{2}\|a\|_2^2 - \sum\nolimits_i a_i b_i^T c + \tfrac{1}{2}\sum\nolimits_{ij} \lambda_{ij}\left(b_{ij}c_j/\lambda_{ij}\right)^2 \\ c^{t+1} &= \operatorname*{argmin}_{c\geq 0} g(c, c^t) \end{aligned}$$

Exercise: Solve $\partial g(c,c^t)/\partial c_p = 0$ to obtain ***closed form***

$$c_p = c_p^t \frac{[B^T a]_p}{[B^T B c^t]_p}$$

This yields the famous "multiplicative update" algorithm of Lee/Seung (1999) – the paper that popularized NMF.

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Exercise: View few other optim methods via MM lens

Explore: Various other ways of doing MM!

Some key MM methods

- Expectation Maximization (EM) algorithm exploits convexity of $-\log x$
- Convex-Concave Procedure (CCCP)
- Variational Methods
- **Explore:** More broadly, ***d.c. programming***

Example: Variational Methods

Examples

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\begin{aligned}
-\log x &= \min_{\lambda} \lambda x - \log \lambda - 1 \\
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An Introduction to Variational Methods for Graphical Models

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See also: *Francis Bach's blog, Posts Jul 1 & Aug 5, 2019.*

Blei, Kucukelbir, McAuliffe. *Variational Inference: A Review for Statisticians*

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Exercise: Derive a "stochastic" version of EM.

Convex-Concave Procedure

$$\boxed{\min_x F(x) := f(x) - h(x), \text{ where } f, h \text{ are both convex.}}$$

Difference of convex (DC) functions widely studied in d.c. programming. They have many nice properties, including: set of dc functions is a vector space; dc functions are locally Lipschitz on the interior of their domain, etc.

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Observe: $F(x) = G(x, x)$ and $F(x) \leq G(x, y)$. CCCP algo is

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CCCP often quite useful: always try as a baseline!

Example 1 – Sinkhorn's method

Theorem. (Sinkhorn, 1964). Let A be a strictly positive matrix. There exists a unique doubly stochastic matrix $M = EAD$, where E and D are strictly positive diagonal matrices. Moreover, the iterative procedure of alternatingly normalizing the rows and columns of A to sum to 1 converges to M.

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Theorem. (Yuille, Rangarajan, 2002). Sinkhorn's algorithms is CCCP with cost function: $\phi(r) = -\sum_i \log r_i + \sum_i \log\left(\sum_j r_j A_{ij}\right)$ where $\{r_i\}$ are the diagonal elements of E and the diagonal elements of D are given by $\left(\sum_j r_j A_{ij}\right)^{-1}$.

Exercise: Verify the above claim.

Explore CCCP applied to the so-called *operator scaling problem*

Example 2 – Learning DPP Kernels

$$\max_{L \succ 0} \ \phi(L) := \frac{1}{n} \sum\nolimits_{i=1}^{n} \log\det(U_i^* L U_i) - \log\det(I + L)$$

MLE for learning DPP kernel L; U_i: compression matrices

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Remarkably, this generates monotonic $\uparrow$ sequence $\{\phi(L_k)\}_{k \geq 1}$.

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Conjecture. For every "step-size" $\alpha \in (0, \gamma)$, the iteration $L_{k+1} = L_k + \alpha L_k \Delta_k L_k$ generates monotonic $\phi(L_k)$ values.

DC Programming

$$f(x) - g(x)$$

DC programming

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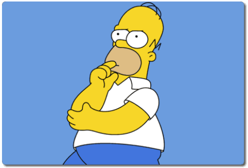
Explore: DC programming theory, algos, applications.

Amusement

$$I(p) := \sqrt{p} \int_0^\infty \left|\frac{\sin x}{x}\right|^p dx$$



$\boxed{\text{Is } I(p) = f(p) - h(p) \text{ for convex } f, h \text{ for } p \geq 1?}$