Collaborative filtering in Hilbert spaces with spectral regularization

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Collaborative Filtering (CF)

The problem

- Given a set of $n_x$ “movies” $x \in X$ and a set of $n_y$ “customers” $y \in Y$,
- predict the “rating” $z(x, y) \in Z$ of customer $y$ for movie $x$
- Training data: large $n_x \times n_y$ incomplete matrix $Z$ that describes the known ratings of some customers for some movies
- Goal: complete the matrix.
Another CF example

Drug design

- Given a family of *proteins* of therapeutic interest (e.g., GPCR’s)
- Given all known *small molecules* that bind to these proteins
- Can we predict unknown *interactions*?
A common strategy for CF

$Z$ has rank less than $k \iff Z = UV^\top$, $U \in \mathbb{R}^{n_x \times k}$, $V \in \mathbb{R}^{n_y \times k}$

Examples: PLSA (Hoffmann, 2001), MMMF (Srebro et al, 2004)

Numerical and statistical efficiency
Fitting low-rank models (Srebro et al, 2004)

- Relax the (non-convex) rank of $Z$ into the (convex) trace norm of $Z$: if $\sigma_i(Z)$ are the singular values of $Z$,

$$\text{rank} Z = \sum_i 1_{\sigma_i(Z) > 0} \quad \|Z\|_* = \sum_i \sigma_i(Z).$$

- $n$ observations $z_u$ corresponding to $x_{i(u)}$ and $y_{j(u)}$, $u = 1, \ldots, n$:

$$\min_{Z \in \mathbb{R}^{n \times n \times n \times n}} \sum_{u=1}^n \ell(z_u, Z_{i(u),j(u)}) + \lambda \|Z\|_*,$$

where $\ell(z, z')$ is a convex loss function.
- This is an SDP if $\ell$ is SDP-representable.
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CF with attributes

The problem

- Often we have **additional attributes**:
  - gender, age of customers; type, actors of movies..
  - 3D structures of proteins and ligands for protein-ligand interaction prediction

- **How to include attributes in CF?**

- **Expected gains**: increase performance, allow predictions on new movie and/or customers.

Our contributions

- A general framework for CF with or without attributes, using kernels to describe attributes (“kernel-CF”)

- A family of algorithms for CF in this setting
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The idea

Basic facts

- $n_X$ movies and $n_Y$ customers
- The known rating $z(x_i, y_j)$ of customer $y_j$ for movie $x_i$ is stored in the $(i,j)$-th entry of a matrix $M$ (of size $n_X \times n_Y$).
- $M$ represents a linear application / bilinear form:

$$M : \mathbb{R}^{n_Y} \rightarrow \mathbb{R}^{n_X}$$

defined by:

$$e_i^\top M f_j = M_{i,j}$$

- Rank / trace norm are spectral properties of the linear application
The idea

Reformulations

- **Represent** the $i$-th movie $\mathbf{x}_i \in \mathcal{X}$ (resp. $j$-th customer $\mathbf{y}_j \in \mathcal{Y}$) by the $i$-th basis vector $e_i \in \mathbb{R}^{n_x}$ (resp. $f_j \in \mathbb{R}^{n_y}$):

\[
\phi_X(\mathbf{x}_i) = e_i, \quad \phi_Y(\mathbf{y}_j) = f_j.
\]

- **Approximate** the rating function by a bilinear form:

\[
\forall (\mathbf{x}_i, \mathbf{y}_j) \in \mathcal{X} \times \mathcal{Y}, \quad G_M(\mathbf{x}_i, \mathbf{y}_j) = \phi_X(\mathbf{x}_i)^\top M \phi_Y(\mathbf{y}_j),
\]

by constraining a **spectral property** of $M : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_x}$.

An idea

If we have additional attributes about movies / customer, why not include them in $\phi_X(\mathbf{x})$ and $\phi_Y(\mathbf{y})$?
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An idea

If we have additional attributes about movies / customer, why not include them in $\phi_X(x)$ and $\phi_Y(y)$?
Movies: points in a Hilbert space $\mathcal{X}$
Customers: points in a Hilbert space $\mathcal{Y}$

We model the preference of customer $y$ for a movie $x$ by a bilinear form:

$$f(x, y) = \langle x, Fy \rangle_{\mathcal{X}},$$

where $F \in \mathcal{B}_0(\mathcal{Y}, \mathcal{X})$ is a compact linear operator (i.e., a “matrix”).
Spectra of compact operators

Classical results

- For \((x, y)\) in \(\mathcal{X} \times \mathcal{Y}\) the tensor product \(x \otimes y\) is the operator

\[
\forall h \in \mathcal{Y}, \quad (x \otimes y) h = \langle y, h \rangle_\mathcal{Y} x.
\]

- Any compact operator \(F : \mathcal{Y} \to \mathcal{X}\) admits a spectral decomposition:

\[
F = \sum_{i=1}^{\infty} \sigma_i u_i \otimes v_i.
\]

where the \(\sigma_i \geq 0\) are the singular values and \((u_i)_{i \in \mathbb{N}}\) and \((v_i)_{i \in \mathbb{N}}\) are orthonormal families in \(\mathcal{X}\) and \(\mathcal{Y}\).

- The spectrum of \(F\) is the set of singular values sorted in decreasing order: \(\sigma_1(F) \geq \sigma_2(F) \geq \ldots \geq 0\).

- This is the natural generalization of singular values for matrices.
For \((x, y)\) in \(X \times Y\), the tensor product \(x \otimes y\) is the operator

\[\forall h \in Y, \quad (x \otimes y)h = \langle y, h \rangle_Y x.\]

Any compact operator \(F : Y \rightarrow X\) admits a spectral decomposition:

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Useful classes for operators

Operators of finite rank

- The rank of an operator is the number of strictly positive singular values.
- Hence operators of rank smaller or equal to $k$ are characterized by:

$$\sigma_{k+1}(F) = 0.$$ 

Trace-class operators

The trace-class operators are the compact operators $F$ that satisfy:

$$\| F \|_* := \sum_{i=1}^{\infty} \sigma_i(F) < \infty.$$ 

$\| F \|_*$ is a norm over the trace-class operators, called the trace norm.
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Hilbert-Schmidt operators

The Hilbert-Schmidt operators are compact operators $F$ that satisfy:

$$\| F \|_{\text{Fro}}^2 := \sum_{i=1}^{\infty} \sigma_i(F)^2 < \infty.$$  

They form a Hilbert space with inner product:

$$\langle x \otimes y, x' \otimes y' \rangle_{X \otimes Y} = \langle x, x' \rangle_{X} \langle y, y' \rangle_{Y}.$$
Definition

A function $\Omega : B_0 (\mathcal{Y}, \mathcal{X}) \mapsto \mathbb{R} \cup \{+\infty\}$ is called a spectral penalty function if it can be written as:

$$\Omega(F) = \sum_{i=1}^{\infty} s_i(\sigma_i(F)),$$

where for any $i \geq 1$, $s_i : \mathbb{R}^+ \mapsto \mathbb{R}^+ \cup \{+\infty\}$ is a non-decreasing penalty function satisfying $s_i(0) = 0$. 
Examples

- **Rank constraint**: take $s_{k+1}(0) = 0$ and $s_{k+1}(u) = +\infty$ for $u > 0$, and $s_i = 0$ for $i \geq k$. Then

  $$\Omega(F) = \begin{cases} 
  0 & \text{if } \text{rank}(F) \leq k, \\
  +\infty & \text{if } \text{rank}(F) > k.
  \end{cases}$$

- **Trace norm**: take $s_i(u) = u$ for all $i$, then:

  $$\Omega(F) = \| F \|_*.$$

- **Hilbert-Schmidt norm**: take $s_i(u) = u^2$ for all $i$, then

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Spectral penalty function

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Learning operator with spectral regularization

Setting

- Training set: \((x_i, y_i, t_i)_{i=1,...,N}\) a set of (movie, customer, preference).
- Loss function \(l(t, t')\): cost of predicting preference \(t\) instead of \(t'\).
- Empirical risk of an operator \(F\):

\[
R_N(F) = \frac{1}{N} \sum_{i=1}^{N} l(\langle x_i, Fy_i \rangle, t_i).
\]

Learning an operator

\[
\min_{F \in \mathcal{B}_0(Y, X), \Omega(F) < \infty} \left\{ R_N(F) + \lambda \Omega(F) \right\}.
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Questions

Theory

Is it a "good" algorithm in theory?

- To be investigated...
- See Srebro et al. (2004), Bach (2007) for preliminary results with the trace norm

Practice

Can we implement it? Does it work on real data?

- Optimization problem in the space of compact operators... but we show later that it boils down to a finite-dimensional optimization problem
- Promising results on real data
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A classical representer theorem

**Theorem**

If \( \hat{F} \) is a solution to the problem:

\[
\min_{F \in B_2(\mathcal{Y}, \mathcal{X})} \left\{ R_N(F) + \lambda \sum_{i=1}^{\infty} \sigma_i(F)^2 \right\},
\]

then it is necessarily in the linear span of \( \{ x_i \otimes y_i : i = 1, \ldots, N \} \), i.e., it can be written as:

\[
\hat{F} = \sum_{i=1}^{N} \alpha_i x_i \otimes y_i,
\]

for some \( \alpha \in \mathbb{R}^N \).
Proof sketch

- $\mathcal{B}_2 (\mathcal{Y}, \mathcal{X})$ is isomorphic to the RKHS of the tensor product kernel:

$$k \otimes ( (x, y), (x', y') ) = \langle x, x' \rangle_\mathcal{X} \langle y, y' \rangle_\mathcal{Y},$$

by $f(x, y) = \langle x, Fy \rangle_\mathcal{X}$. In particular,

$$\| f \|_{\mathcal{H} \otimes}^2 = \| F \|_2^2 = \Omega(F).$$

- The problem is therefore a classical kernel method:

$$\min_{f \in \mathcal{H} \otimes} \left\{ R_N(f) + \lambda \| f \|_{\otimes}^2 \right\},$$

so the classical representer theorem can be used. □
For any spectral penalty function $\Omega : \mathcal{B}_0(\mathcal{Y}, \mathcal{X}) \mapsto \mathbb{R}$, let the optimization problem:

$$\min_{F \in \mathcal{B}_0(\mathcal{Y}, \mathcal{X}), \Omega(F) < \infty} \left\{ R_N(F) + \lambda \Omega(F) \right\}.$$ 

If the set of solutions is not empty, then there is a solution $F$ in $\mathcal{X}_N \otimes \mathcal{Y}_N$, i.e., there exists $\alpha \in \mathbb{R}^{m_{\mathcal{X}} \times m_{\mathcal{Y}}}$ such that:

$$F = \sum_{i=1}^{m_{\mathcal{X}}} \sum_{j=1}^{m_{\mathcal{Y}}} \alpha_{ij} u_i \otimes v_j,$$

where $(u_1, \ldots, u_{m_{\mathcal{X}}})$ and $(v_1, \ldots, v_{m_{\mathcal{Y}}})$ form orthonormal bases of $\mathcal{X}_N$ and $\mathcal{Y}_N$, respectively.
Proof sketch

For any operator \( F \in \mathcal{B}_0(\mathcal{Y}, \mathcal{X}) \), let

\[
G = \Pi_{\mathcal{X}_N} F \Pi_{\mathcal{Y}_N},
\]

where \( \Pi_U \) is the orthogonal projection onto \( U \).

Lemma: we can show that for all \( i \geq 0 \):

\[
\sigma_i(G) \leq \sigma_i(F).
\]

Therefore \( \Omega(G) \leq \Omega(F) \).

On the other hand \( R_N(G) = R_N(F) \).

Consequently for any solution \( F \) we have another solution \( G \in \mathcal{X}_N \otimes \mathcal{Y}_N \). □
The coefficients $\alpha$ that define the solution by

$$F = \sum_{i=1}^{m_X} \sum_{j=1}^{m_Y} \alpha_{ij} u_i \otimes v_j,$$

can be found by solving the following finite-dimensional optimization problem:

$$\min_{\alpha \in \mathbb{R}^{m_X \times m_Y}, \Omega(\alpha) < \infty} R_N \left( \text{diag} \left( X\alpha Y^T \right) \right) + \lambda \Omega(\alpha),$$

where $\Omega(\alpha)$ refers to the spectral penalty function applied to the matrix $\alpha$ seen as an operator from $\mathbb{R}^{m_Y}$ to $\mathbb{R}^{m_X}$, and $X$ and $Y$ denote any matrices that satisfy $K = XX^T$ and $G = YY^T$ for the two Gram matrices $K$ and $G$ of $\mathcal{X}_N$ and $\mathcal{Y}_N$. 
Summary

We obtain various algorithms by choosing:

1. A loss function (depends on the application)
2. A spectral regularization (that is amenable to optimization)
3. Two Gram matrices (aka kernel matrices)

Both kernels and spectral regularization can be used to constrain the solution.
A family of kernels

Taken $K_\otimes = K \times G$ with

\[
\begin{align*}
K &= \eta K_{\text{Attribute}}^x + (1 - \eta) K_{\text{Dirac}}^x, \\
G &= \zeta K_{\text{Attribute}}^y + (1 - \zeta) K_{\text{Dirac}}^y,
\end{align*}
\]

for $0 \leq \eta \leq 1$ and $0 \leq \zeta \leq 1$
Simulated data

Experiment

- Generate data \((x, y, z) \in \mathbb{R}^{f_X} \times \mathbb{R}^{f_Y} \times \mathbb{R}\) according to

\[
z = x^\top By + \varepsilon
\]

- Observe only \(n_X < f_X\) and \(n_Y < f_Y\) features
  - Low-rank assumption will find the missing features
  - Observed attributes will help the low-rank formulation to concentrate mostly on the unknown features

- Comparison of
  - Low-rank constraint without tracenorm (note that it requires regularization)
  - Trace-norm formulation (regularization is implicit)
Simulated data: results

- Compare MSE
- Left: rank constraint (best: 0.1540), right: trace norm (best: 0.1522)
Movies

- MovieLens 100k database, ratings with attributes
- Experiments with 943 movies and 1,642 customers, 100,000 rankings in \{1, \ldots, 5\}
- Train on a subset of the ratings, test on the rest
- error measured with MSE (best constant prediction: 1.26)
Conclusion

What we saw

- A general framework for CF with or without attributes
- A generalized representation theorem valid for any spectral penalty function
- A family of new methods;

Future work

- The bottleneck is often practical optimization. Online version possible.
- Automatic choice of the kernel

Reference