

# Collaborative filtering in Hilbert spaces with spectral regularization

Jacob Abernethy<sup>1</sup>   Francis Bach<sup>2</sup>  
Theodoros Evgeniou<sup>3</sup>   Jean-Philippe Vert<sup>4</sup>

<sup>1</sup>UC Berkeley

<sup>2</sup>INRIA / Ecole normale superieure de Paris

<sup>3</sup>INSEAD

<sup>4</sup>Mines ParisTech / Institut Curie / INSERM

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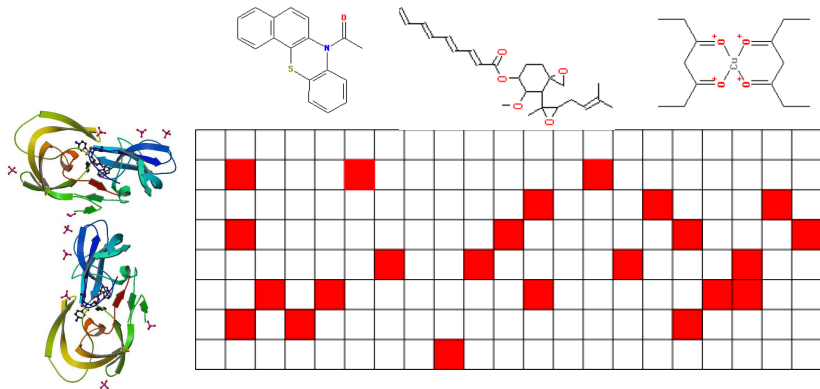
# The NETFLIX challenge

← 18,000 movies →

480,000 users

x	1	1	x	...	x
x	x	x	5	...	x
x	x	3	x	...	x
x	4	3	x	...	2
...	x	x	x	...	x
x	5	x	1	...	x
x	x	3	3	...	x
x	1	x	x	...	2

# *In silico* chemogenomics



## The problem

- $\mathcal{X}$  and  $\mathcal{Y}$  two sets ("customers" and "movies").
- **Training data:**  $(\mathbf{x}_i, \mathbf{y}_i, t_i)_{i=1, \dots, n} \in (\mathcal{X}, \mathcal{Y}, \mathbb{R})^n$  some ratings  $t_i$  by customer  $\mathbf{x}_i$  for movie  $\mathbf{y}_i$
- $n_{\mathcal{X}} \leq n$  (resp.  $n_{\mathcal{Y}} \leq n$ ) the number of **different** customers (resp. movies) in the training data.
- **Goal:** learn the "rating function"  $f : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$ .

## Existing strategies

- 1 Collaborative filtering
- 2 Regression over pairs

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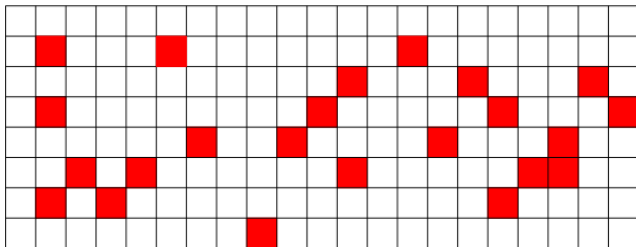
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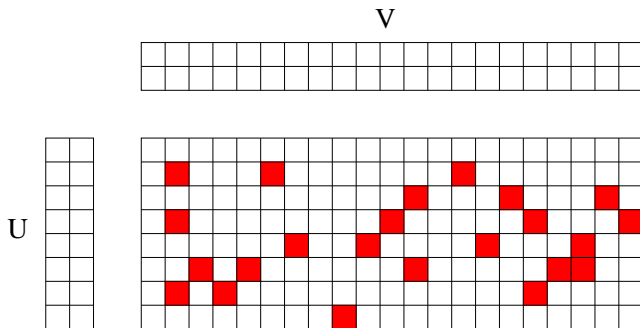
# Strategy 1: Collaborative Filtering (CF)

- Ignore any information about movies and customers
- $\mathcal{X} = \{\mathbf{x}^1, \dots, \mathbf{x}^{n_x}\}$  and  $\mathcal{Y} = \{\mathbf{y}^1, \dots, \mathbf{y}^{n_y}\}$  are finite
- Training data: large  $n_x \times n_y$  incomplete matrix  $F$  that describes the known ratings of some customers for some movies
- Goal: complete the matrix.



# CF by low-rank matrix approximation

- A common strategy for CF
- $F$  has rank less than  $k \Leftrightarrow F = UV^T$   $U \in \mathbb{R}^{n_x \times k}$ ,  $V \in \mathbb{R}^{n_y \times k}$
- 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  $F$  into the (**convex**) **trace norm** of  $F$ : if  $\sigma_i(F)$  are the singular values of  $F$ ,

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

- $i$ -th observation  $t_i$  corresponding to  $\mathbf{x}_i = \mathbf{x}^{u(i)}$  and  $\mathbf{y}_i = \mathbf{y}^{v(i)}$ :

$$\min_{F \in \mathbb{R}^{n_x \times n_y}} \sum_{i=1}^n \ell(t_i, F_{u(i), v(i)}) + \lambda \|F\|_*,$$

where  $\ell(z, z')$  is a convex loss function.

- This is an SDP if  $\ell$  is SDP-representable



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## Strategy 2: Regression over pairs

- $\mathcal{X}$  and  $\mathcal{Y}$  represent the attributes of each customer/movie
- This is a classical regression problem over  $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$
- For example, take  $\mathbf{z} = \mathbf{x} \otimes \mathbf{y}$  and find

$$f(\mathbf{x}, \mathbf{y}) = \mathbf{w}^\top \mathbf{z} = \mathbf{w}^\top (\mathbf{x} \otimes \mathbf{y})$$

by solving

$$\min_{\mathbf{w} \in \mathcal{X} \otimes \mathcal{Y}} \sum_{i=1}^n \ell(t_i, \mathbf{w}^\top (\mathbf{x}_i \otimes \mathbf{y}_i)) + \lambda \|\mathbf{w}\|^2.$$

- **Kernel methods** (SVM...) are efficient methods to solve problems of the form

$$\min_{\mathbf{w} \in \mathcal{Z}} \sum_{i=1}^n \ell(t_i, \mathbf{w}^\top \mathbf{z}_i) + \lambda \|\mathbf{w}\|^2.$$

- They require the definition of the kernel:

$$\begin{aligned} K_Z(\mathbf{z}, \mathbf{z}') &= \mathbf{z}^\top \mathbf{z}' \\ &= (\mathbf{x} \otimes \mathbf{y})^\top (\mathbf{x} \otimes \mathbf{y}') \\ &= (\mathbf{x}^\top \mathbf{x}') \times (\mathbf{y}^\top \mathbf{y}') \\ &= K_X(\mathbf{x}, \mathbf{x}') K_Y(\mathbf{y}, \mathbf{y}'). \end{aligned} \tag{1}$$

# Comparison of both strategies

## Collaborative filtering

$$\min_{F \in \mathbb{R}^{n_x \times n_y}} \sum_{i=1}^n \ell(t_i, F_{u(i), v(i)}) + \lambda \|F\|_* .$$

- Use various spectral penalties of the matrix (rank, trace norm)
- No use of attribute, no prediction outside the training set

## Regression over pairs

$$\min_{\mathbf{w} \in \mathcal{X} \otimes \mathcal{Y}} \sum_{i=1}^n \ell(t_i, \mathbf{w}^\top (\mathbf{x}_i \otimes \mathbf{y}_i)) + \lambda \|\mathbf{w}\|^2 .$$

- Flexible use of attributes with kernels
- No special treatment of repetitions in the training set

## Goal

- Make a link between collaborative filtering and regression over pairs
- Develop methods that combine the advantages of both strategies

## Contributions

- A **general framework** for CF **with or without attributes**, using **kernels** to describe attributes (“kernel-CF”)
- A **family of algorithms** in this setting

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# From CF to regression over pairs

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

$$\phi_X(\mathbf{x}^i) = \mathbf{e}_i, \quad \phi_Y(\mathbf{y}^j) = \mathbf{f}_j.$$

- The rating  $F_{i,j}$  of  $\mathbf{x}^i$  for  $\mathbf{y}^j$  is given by

$$F_{i,j} = \mathbf{e}_i^\top F \mathbf{y}_j = \text{Tr} \left( F^\top (\phi_X(\mathbf{x}^i) \otimes \phi_Y(\mathbf{y}^j)) \right).$$

- We can thus rewrite CF as

$$\min_{F \in \mathbb{R}^{n_x \times n_y}} \sum_{i=1}^n \ell(t_i, \text{Tr} \left( F^\top (\phi_X(\mathbf{x}_i) \otimes \phi_Y(\mathbf{y}_i)) \right)) + \lambda \|F\|_*.$$

# The idea

$$\min_{\mathbf{w} \in \mathcal{X} \otimes \mathcal{Y}} \sum_{i=1}^n \ell(t_i, \mathbf{w}^\top (\mathbf{x}_i \otimes \mathbf{y}_i)) + \lambda \|\mathbf{w}\|^2.$$

$$\min_{F \in \mathbb{R}^{n_X \times n_Y}} \sum_{i=1}^n \ell(t_i, \text{Tr} \left( F^\top (\phi_X(\mathbf{x}_i) \otimes \phi_Y(\mathbf{y}_i)) \right)) + \lambda \|F\|_*.$$

- Put the attribute informations in  $\phi_X(\mathbf{x})$  and  $\phi_Y(\mathbf{y})$ , like in regression
- Investigate penalties beyond the  $\ell_2$  norm, like in CF
- For this we need to work with "infinite-dimensional matrices", i.e., compact operators

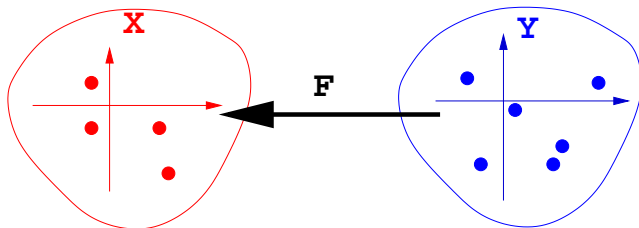


# Setting

- Movies: points in a Hilbert space  $\mathcal{X}$
- Customers: points in a Hilbert space  $\mathcal{Y}$
- We model the preference of customer  $\mathbf{y}$  for a movie  $\mathbf{x}$  by a bilinear form:

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

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



## Classical results

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

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

- Any compact operator  $F : \mathcal{Y} \rightarrow \mathcal{X}$  admits a spectral decomposition:

$$F = \sum_{i=1}^{\infty} \sigma_i \mathbf{u}_i \otimes \mathbf{v}_i.$$

where the  $\sigma_i \geq 0$  are the **singular values** and  $(\mathbf{u}_i)_{i \in \mathbb{N}}$  and  $(\mathbf{v}_i)_{i \in \mathbb{N}}$  are orthonormal families in  $\mathcal{X}$  and  $\mathcal{Y}$ .

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

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

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## Hilbert-Schmidt operators

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

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

- They form a **Hilbert space** with inner product:

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

- It is isomorphic to the reproducing kernel Hilbert space used in regression over pairs

## Definition

A function  $\Omega : \mathcal{B}_0(\mathcal{Y}, \mathcal{X}) \mapsto \mathbb{R} \cup \{+\infty\}$  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:

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

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## Setting

- **Training set:**  $(\mathbf{x}_i, \mathbf{y}_i, t_i)_{i=1, \dots, N}$  a set of (movie, customer, preference).
- **Loss function**  $l(t, t')$  : cost of predicting preference  $t$  instead of  $t'$ .
- **Empirical risk** of an operator  $F$ :

$$R_N(F) = \frac{1}{N} \sum_{i=1}^N l(\langle \mathbf{x}_i, F \mathbf{y}_i \rangle_{\mathcal{X}}, t_i) .$$

## Learning an operator

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

# Learning operator with spectral regularization

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# Particular cases

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

## CF

- $K_X(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x}, \mathbf{x}')$  ,  $K_Y(\mathbf{y}, \mathbf{y}') = \delta(\mathbf{y}, \mathbf{y}')$
- $\Omega(F) = \|F\|_*$  or  $\text{rank}(F)$

## Pairwise regression

- $K_X(\mathbf{x}, \mathbf{x}')$  and  $K_Y(\mathbf{y}, \mathbf{y}')$  defined by attributes
- $\Omega(F) = \|F\|_{Fro}^2$

## Many variants, e.g., multitask learning

- $K_X(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x}, \mathbf{x}')$  and  $K_Y(\mathbf{y}, \mathbf{y}')$  defined by attributes
- $\Omega(F) = \|F\|_*$

## 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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## Theorem

If  $\hat{F}$  is a solution the problem:

$$\min_{F \in \mathcal{B}_2(\mathcal{Y}, \mathcal{X})} \left\{ R_N(F) + \lambda \sum_{i=1}^{\infty} \sigma_i(F)^2 \right\},$$

then it is necessarily in the linear span of  $\{\mathbf{x}_i \otimes \mathbf{y}_i : i = 1, \dots, N\}$ , i.e., it can be written as:

$$\hat{F} = \sum_{i=1}^N \alpha_i \mathbf{x}_i \otimes \mathbf{y}_i,$$

for some  $\alpha \in \mathbb{R}^N$ .

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

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

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

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

- 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.  $\square$

# A generalized representer theorem

## Theorem

For **any spectral penalty function**  $\Omega : \mathcal{B}_0(\mathcal{Y}, \mathcal{X}) \mapsto \mathbb{R}$ , let the optimization problem:

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

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**  $\alpha \in \mathbb{R}^{m_x \times m_y}$  **such that:**

$$F = \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} \alpha_{ij} \mathbf{u}_i \otimes \mathbf{v}_j ,$$

where  $(\mathbf{u}_1, \dots, \mathbf{u}_{m_x})$  and  $(\mathbf{v}_1, \dots, \mathbf{v}_{m_y})$  form orthonormal bases of  $\mathcal{X}_N$  and  $\mathcal{Y}_N$ , respectively.

- 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  $G \in \mathcal{X}_N \otimes \mathcal{Y}_N$ .  $\square$

## Theorem (cont.)

The coefficients  $\alpha$  that define the solution by

$$F = \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} \alpha_{ij} \mathbf{u}_i \otimes \mathbf{v}_j,$$

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

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

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  $K = XX^\top$  and  $G = YY^\top$  for the two Gram matrices  $K$  and  $G$  of  $\mathcal{X}_N$  and  $\mathcal{Y}_N$ .

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

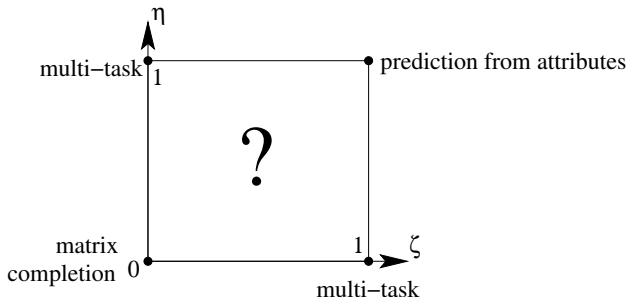


# A family of kernels

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

$$\begin{cases} K = \eta K_{Attribute}^x + (1 - \eta) K_{Dirac}^x, \\ G = \zeta K_{Attribute}^y + (1 - \zeta) K_{Dirac}^y, \end{cases}$$

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



## Experiment

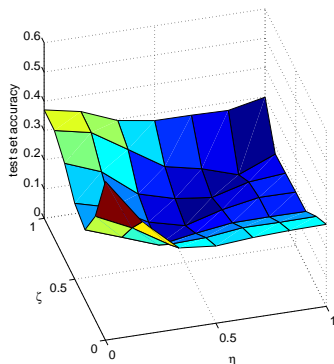
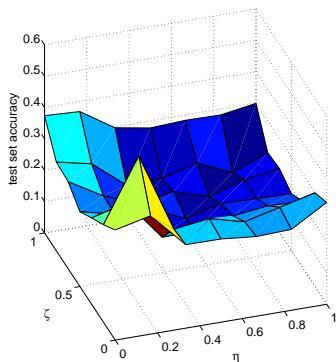
- Generate data  $(\mathbf{x}, \mathbf{y}, z) \in \mathbb{R}^{f_X} \times \mathbb{R}^{f_Y} \times \mathbb{R}$  according to

$$z = \mathbf{x}^\top \mathbf{B} \mathbf{y} + \varepsilon$$

- 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)

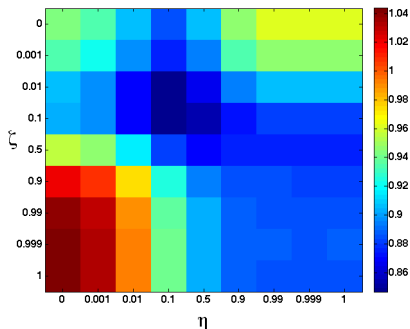
# Simulated data: results

- 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  $\{1, \dots, 5\}$
- 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

J. Abernethy, F. Bach, T. Evgeniou and J.-P. Vert, “A new approach to collaborative filtering: operator estimation with spectral regularization”, *Journal of Machine Learning Research*, 10:803-826, 2009.