# Sparse methods for machine learning

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# Sparse methods for machine learning Outline

- Sparse linear estimation with the  $\ell_1\text{-norm}$ 
  - Lasso
  - Important theoretical results
- Structured sparse methods on vectors
  - Groups of features / Multiple kernel learning
- Sparse methods on matrices
  - Multi-task learning
  - Matrix factorization (low-rank, sparse PCA, dictionary learning)

## Supervised learning and regularization

- Data:  $x_i \in \mathcal{X}$ ,  $y_i \in \mathcal{Y}$ ,  $i = 1, \dots, n$
- Minimize with respect to function  $f : \mathcal{X} \to \mathcal{Y}$ :



- Two theoretical/algorithmic issues:
  - 1. Loss
  - 2. Function space / norm

## Regularizations

- Main goal: avoid overfitting
- Two main lines of work:
  - 1. Euclidean and Hilbertian norms (i.e.,  $\ell_2$ -norms)
    - Possibility of non linear predictors
    - Non parametric supervised learning and kernel methods
    - Well developped theory and algorithms (see, e.g., Wahba, 1990;
       Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004)

## Regularizations

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    - Well developped theory and algorithms (see, e.g., Wahba, 1990;
       Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004)
  - 2. Sparsity-inducing norms
    - Usually restricted to linear predictors on vectors  $f(x) = w^\top x$
    - Main example:  $\ell_1$ -norm  $||w||_1 = \sum_{i=1}^p |w_i|$
    - Perform model selection as well as regularization
    - Theory and algorithms "in the making"

## $\ell_2$ -norm vs. $\ell_1$ -norm

- $\ell_1$ -norms lead to interpretable models
- $\ell_2$ -norms can be run implicitly with very large feature spaces (e.g., kernel trick)
- Algorithms:
  - Smooth convex optimization vs. nonsmooth convex optimization
- Theory:
  - better predictive performance?

## $\ell_2$ vs. $\ell_1$ - Gaussian hare vs. Laplacian tortoise



- First-order methods (Fu, 1998; Beck and Teboulle, 2009)
- Homotopy methods (Markowitz, 1956; Efron et al., 2004)

## Why $\ell_1$ -norm constraints leads to sparsity?

- Example: minimize quadratic function Q(w) subject to ||w||₁ ≤ T.
   coupled soft thresholding
- Geometric interpretation
  - NB : penalizing is "equivalent" to constraining



## $\ell_1$ -norm regularization (linear setting)

- Data: covariates  $x_i \in \mathbb{R}^p$ , responses  $y_i \in \mathcal{Y}$ ,  $i = 1, \dots, n$
- Minimize with respect to loadings/weights  $w \in \mathbb{R}^p$ :

$$J(w) = \sum_{i=1}^{n} \ell(y_i, w^{\top} x_i) + \lambda \|w\|_1$$
  
Error on data + Regularization

- Including a constant term *b*? Penalizing or constraining?
- square loss ⇒ basis pursuit in signal processing (Chen et al., 2001), Lasso in statistics/machine learning (Tibshirani, 1996)

#### Lasso - Two main recent theoretical results

 Support recovery condition (Zhao and Yu, 2006; Wainwright, 2009; Zou, 2006; Yuan and Lin, 2007): the Lasso is sign-consistent if and only if

$$\|\mathbf{Q}_{\mathbf{J}^{c}\mathbf{J}}\mathbf{Q}_{\mathbf{J}\mathbf{J}}^{-1}\operatorname{sign}(\mathbf{w}_{\mathbf{J}})\|_{\infty} \leq 1,$$

where  $\mathbf{Q} = \lim_{n \to +\infty} \frac{1}{n} \sum_{i=1}^{n} x_i x_i^{\top} \in \mathbb{R}^{p \times p}$  and  $\mathbf{J} = \operatorname{Supp}(\mathbf{w})$ 

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- The Lasso is usually not model-consistent
  - Selects more variables than necessary (see, e.g., Lv and Fan, 2009)
    Fixing the Lasso: adaptive Lasso (Zou, 2006), relaxed Lasso (Meinshausen, 2008), thresholding (Lounici, 2008), Bolasso (Bach, 2008a), stability selection (Meinshausen and Bühlmann, 2008)

#### Adaptive Lasso and concave penalization

- Adaptive Lasso (Zou, 2006; Huang et al., 2008)
  - Weighted  $\ell_1$ -norm:  $\min_{w \in \mathbb{R}^p} L(w) + \lambda \sum_{j=1}^p \frac{|w_j|}{|\hat{w}_j|^{\alpha}}$
  - $\hat{w}$  estimator obtained from  $\ell_2$  or  $\ell_1$  regularization
- Reformulation in terms of concave penalization

$$\min_{w \in \mathbb{R}^p} L(w) + \sum_{j=1}^p g(|w_j|)$$



- Example:  $g(|w_j|) = |w_j|^{1/2}$  or  $\log |w_j|$ . Closer to the  $\ell_0$  penalty
- Concave-convex procedure: replace  $g(|w_j|)$  by affine upper bound
- Better sparsity-inducing properties (Fan and Li, 2001; Zou and Li, 2008; Zhang, 2008b)

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 Exponentially many irrelevant variables (Zhao and Yu, 2006; Wainwright, 2009; Bickel et al., 2009; Lounici, 2008; Meinshausen and Yu, 2008): under appropriate assumptions, consistency is possible as long as

$$\log p = O(n)$$

# Alternative sparse methods Greedy methods

- Forward selection
- Forward-backward selection
- Non-convex method
  - Harder to analyze
  - Simpler to implement
  - Problems of stability
- Positive theoretical results (Zhang, 2009, 2008a)
  - Similar sufficient conditions than for the Lasso
- **Bayesian methods** : see Seeger (2008)

# Comparing Lasso and other strategies for linear regression

- Compared methods to reach the least-square solution
  - Ridge regression:  $\min_{w \in \mathbb{R}^{p}} \frac{1}{2} \|y Xw\|_{2}^{2} + \frac{\lambda}{2} \|w\|_{2}^{2}$ - Lasso:  $\min_{w \in \mathbb{R}^{p}} \frac{1}{2} \|y - Xw\|_{2}^{2} + \lambda \|w\|_{1}$
  - Forward greedy:
    - \* Initialization with empty set
    - \* Sequentially add the variable that best reduces the square loss
- Each method builds a path of solutions from 0 to ordinary least-squares solution

#### **Simulation results**

- $\bullet$  i.i.d. Gaussian design matrix,  $k=4\text{, }n=64\text{, }p\in[2,256]\text{, }\mathsf{SNR}=1$
- Note stability to non-sparsity and variability



## **Extensions** - **Going beyond the Lasso**

- $\ell_1$ -norm for linear feature selection in high dimensions
  - Lasso usually not applicable directly

## **Extensions** - Going beyond the Lasso

- $\ell_1$ -norm for **linear** feature selection in **high dimensions** 
  - Lasso usually not applicable directly
- Sparse methods are not limited to the square loss
  - logistic loss: algorithms (Beck and Teboulle, 2009) and theory (Van De Geer, 2008; Bach, 2009)
- Sparse methods are not limited to supervised learning
  - Learning the structure of Gaussian graphical models (Meinshausen and Bühlmann, 2006; Banerjee et al., 2008)
  - Sparsity on matrices (last part of this session)
- Sparse methods are not limited to linear variable selection
  - Multiple kernel learning (next part of this session)

# Sparse methods for machine learning Outline

- Sparse linear estimation with the  $\ell_1\text{-norm}$ 
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  - Matrix factorization (low-rank, sparse PCA, dictionary learning)

# Penalization with grouped variables (Yuan and Lin, 2006)

- Assume that  $\{1, \ldots, p\}$  is **partitioned** into m groups  $G_1, \ldots, G_m$
- Penalization by  $\sum_{i=1}^{m} \|w_{G_i}\|_2$ , often called  $\ell_1$ - $\ell_2$  norm
- Induces group sparsity
  - Some groups entirely set to zero
  - no zeros within groups
- In this tutorial:
  - Groups may have infinite size  $\Rightarrow$  MKL
  - Groups may overlap  $\Rightarrow$  structured sparsity

#### Linear vs. non-linear methods

- All methods in this tutorial are **linear in the parameters**
- By replacing x by features  $\Phi(x)$ , they can be made **non linear in** the data
- Implicit vs. explicit features
  - $\ell_1$ -norm: explicit features
  - $\ell_2$ -norm: representer theorem allows to consider implicit features if their dot products can be computed easily (kernel methods)

#### Kernel methods: regularization by $\ell_2$ -norm

• Data:  $x_i \in \mathcal{X}, y_i \in \mathcal{Y}, i = 1, ..., n$ , with features  $\Phi(x) \in \mathcal{F} = \mathbb{R}^p$ 

– Predictor  $f(x) = w^{\top} \Phi(x)$  linear in the features

• Optimization problem:  $\lim_{w \in \mathbb{R}^p} \sum_{\ell \in \mathbb{R}^p} \ell(w)$ 

$$\min_{w \in \mathbb{R}^p} \sum_{i=1}^n \ell(y_i, w^\top \Phi(x_i)) + \frac{\lambda}{2} \|w\|_2^2$$

#### Kernel methods: regularization by $\ell_2$ -norm

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• Optimization problem: 
$$\lim_{w \in \mathbb{R}^p} \sum_{i=1}^n \ell(y_i, w^\top \Phi(x_i)) + \frac{\lambda}{2} \|w\|_2^2$$

• Representer theorem (Kimeldorf and Wahba, 1971): solution must be of the form  $w = \sum_{i=1}^{n} \alpha_i \Phi(x_i)$ 

- Equivalent to solving: 
$$\lim_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \ell(y_i, (K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha$$

- Kernel matrix  $K_{ij} = k(x_i, x_j) = \Phi(x_i)^{\top} \Phi(x_j)$ 

# Multiple kernel learning (MKL) (Lanckriet et al., 2004b; Bach et al., 2004a)

- Sparsity with non-linearities
  - replace  $f(x) = \sum_{j=1}^{p} w_j^{\top} x_j$  with  $x \in \mathbb{R}^p$  and  $w_j \in \mathbb{R}$
  - by  $f(x) = \sum_{j=1}^{p} w_j^{\top} \Phi_j(x)$  with  $x \in \mathcal{X}$ ,  $\Phi_j(x) \in \mathcal{F}_j$  an  $w_j \in \mathcal{F}_j$
- Replace the  $\ell_1$ -norm  $\sum_{j=1}^p |w_j|$  by "block"  $\ell_1$ -norm  $\sum_{j=1}^p ||w_j||_2$
- Multiple feature maps / kernels on  $x \in \mathcal{X}$ :
  - p "feature maps"  $\Phi_j : \mathcal{X} \mapsto \mathcal{F}_j, j = 1, \dots, p$ .
  - Predictor:  $f(x) = w_1^{\top} \Phi_1(x) + \dots + w_p^{\top} \Phi_p(x)$
  - Generalized additive models (Hastie and Tibshirani, 1990)

#### **Regularization for multiple features**

- Regularization by  $\sum_{j=1}^{p} \|w_j\|_2^2$  is equivalent to using  $K = \sum_{j=1}^{p} K_j$ 
  - Summing kernels is equivalent to concatenating feature spaces

#### **Regularization for multiple features**

- Regularization by  $\sum_{j=1}^{p} \|w_j\|_2^2$  is equivalent to using  $K = \sum_{j=1}^{p} K_j$
- Regularization by  $\sum_{j=1}^{p} \|w_j\|_2$  imposes sparsity at the group level
- Main questions when regularizing by block  $\ell_1$ -norm:
  - 1. Algorithms (Bach et al., 2004a; Rakotomamonjy et al., 2008)
  - 2. Analysis of sparsity inducing properties (Bach, 2008b)
  - 3. Equivalent to learning a sparse combination  $\sum_{j=1}^{p} \eta_j K_j$

## **Applications of multiple kernel learning**

- Selection of hyperparameters for kernel methods
- Fusion from heterogeneous data sources (Lanckriet et al., 2004a)
- Two regularizations on the same function space:
  - Uniform combination  $\Leftrightarrow \ell_2$ -norm
  - Sparse combination  $\Leftrightarrow \ell_1$ -norm
  - MKL always leads to more interpretable models
  - MKL does not always lead to better predictive performance
     \* In particular, with few well-designed kernels
    - \* Be careful with normalization of kernels (Bach et al., 2004b)

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- **Sparse methods**: new possibilities and new features

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## Learning on matrices - Image denoising

- Simultaneously denoise all patches of a given image
- Example from Mairal, Bach, Ponce, Sapiro, and Zisserman (2009b)



## **Learning on matrices - Collaborative filtering**

- Given  $n_{\mathcal{X}}$  "movies"  $\mathbf{x} \in \mathcal{X}$  and  $n_{\mathcal{Y}}$  "customers"  $\mathbf{y} \in \mathcal{Y}$ ,
- predict the "rating"  $z(\mathbf{x},\mathbf{y})\in\mathcal{Z}$  of customer  $\mathbf{y}$  for movie  $\mathbf{x}$
- Training data: large  $n_X \times n_Y$  incomplete matrix  $\mathbf{Z}$  that describes the known ratings of some customers for some movies
- **Goal**: complete the matrix.



## Learning on matrices - Multi-task learning

- k linear prediction tasks on same covariates  $\mathbf{x} \in \mathbb{R}^p$ 
  - k weight vectors  $\mathbf{w}_j \in \mathbb{R}^p$
  - Joint matrix of predictors  $\mathbf{W} = (\mathbf{w}_1, \dots, \mathbf{w}_k) \in \mathbb{R}^{p imes k}$
- Classical application
  - Multi-category classification (one task per class) (Amit et al., 2007)
- Share parameters between tasks
- Joint variable selection (Obozinski et al., 2009)
  - Select variables which are predictive for all tasks
- Joint feature selection (Pontil et al., 2007)
  - Construct linear features common to all tasks

#### **Matrix factorization - Dimension reduction**

- Given data matrix  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n) \in \mathbb{R}^{p imes n}$ 
  - Principal component analysis:  $| \mathbf{x}_i \approx \mathbf{D} \boldsymbol{\alpha}_i \Rightarrow \mathbf{X} = \mathbf{D} \mathbf{A} |$



# Two types of sparsity for matrices $\mathbf{M} \in \mathbb{R}^{n \times p}$ I - Directly on the elements of $\mathbf{M}$

• Many zero elements:  $\mathbf{M}_{ij} = 0$ 



• Many zero rows (or columns):  $(\mathbf{M}_{i1}, \ldots, \mathbf{M}_{ip}) = 0$ 



Two types of sparsity for matrices  $M \in \mathbb{R}^{n \times p}$ II - Through a factorization of  $M = \mathbf{U}\mathbf{V}^{\top}$ 

- Matrix  $\mathbf{M} = \mathbf{U}\mathbf{V}^{ op}$ ,  $\mathbf{U} \in \mathbb{R}^{n imes k}$  and  $\mathbf{V} \in \mathbb{R}^{p imes k}$
- Low rank: *m* small

$$\mathbf{M} = \mathbf{U}^{\mathrm{T}}$$

 $\bullet$  Sparse decomposition: U sparse

$$\mathbf{M} = \mathbf{U} \mathbf{U} \mathbf{V}^{\mathrm{T}}$$

## Structured sparse matrix factorizations

• Matrix  $\mathbf{M} = \mathbf{U}\mathbf{V}^{ op}$ ,  $\mathbf{U} \in \mathbb{R}^{n imes k}$  and  $\mathbf{V} \in \mathbb{R}^{p imes k}$ 

#### $\bullet$ Structure on ${\bf U}$ and/or ${\bf V}$

- Low-rank:  ${\bf U}$  and  ${\bf V}$  have few columns
- Dictionary learning / sparse PCA:  ${\bf U}$  has many zeros
- Clustering (k-means):  $\mathbf{U} \in \{0,1\}^{n \times m}$ ,  $\mathbf{U1} = \mathbf{1}$
- Pointwise positivity: non negative matrix factorization (NMF)
- Specific patterns of zeros (Jenatton et al., 2010)
- Low-rank + sparse (Candès et al., 2009)
- etc.
- Many applications
- Many open questions (Algorithms, identifiability, etc.)

# Low-rank matrix factorizations Trace norm

- Given a matrix  $\mathbf{M} \in \mathbb{R}^{n \times p}$ 
  - Rank of M is the minimum size m of all factorizations of M into  $\mathbf{M} = \mathbf{U}\mathbf{V}^{\top}$ ,  $\mathbf{U} \in \mathbb{R}^{n \times m}$  and  $\mathbf{V} \in \mathbb{R}^{p \times m}$
  - Singular value decomposition:  $\mathbf{M} = \mathbf{U} \operatorname{Diag}(\mathbf{s}) \mathbf{V}^{\top}$  where  $\mathbf{U}$  and  $\mathbf{V}$  have orthonormal columns and  $\mathbf{s} \in \mathbb{R}^m_+$  are singular values
- $\bullet$  Rank of  ${\bf M}$  equal to the number of non-zero singular values

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- $\bullet$  Rank of  ${\bf M}$  equal to the number of non-zero singular values
- **Trace-norm (a.k.a. nuclear norm)** = sum of singular values
- Convex function, leads to a semi-definite program (Fazel et al., 2001)
- First used for collaborative filtering (Srebro et al., 2005)

#### Sparse principal component analysis

- Given data  $\mathbf{X} = (\mathbf{x}_1^{\top}, \dots, \mathbf{x}_n^{\top}) \in \mathbb{R}^{p \times n}$ , two views of PCA:
  - Analysis view: find the projection  $\mathbf{d} \in \mathbb{R}^p$  of maximum variance (with deflation to obtain more components)
  - Synthesis view: find the basis  $d_1, \ldots, d_k$  such that all  $x_i$  have low reconstruction error when decomposed on this basis
- For regular PCA, the two views are equivalent



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#### • Sparse extensions

- Interpretability
- High-dimensional inference
- Two views are differents
  - \* For analysis view, see d'Aspremont, Bach, and El Ghaoui (2008)

# Sparse principal component analysis Synthesis view

• Find  $\mathbf{d}_1, \dots, \mathbf{d}_k \in \mathbb{R}^p$  sparse so that

$$\sum_{i=1}^{n} \min_{\boldsymbol{\alpha}_{i} \in \mathbb{R}^{m}} \left\| \mathbf{x}_{i} - \sum_{j=1}^{k} (\boldsymbol{\alpha}_{i})_{j} \mathbf{d}_{j} \right\|_{2}^{2} = \sum_{i=1}^{n} \min_{\boldsymbol{\alpha}_{i} \in \mathbb{R}^{m}} \left\| \mathbf{x}_{i} - \mathbf{D} \boldsymbol{\alpha}_{i} \right\|_{2}^{2} \text{ is small}$$

- Look for  $\mathbf{A} = (\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_n) \in \mathbb{R}^{k \times n}$  and  $\mathbf{D} = (\mathbf{d}_1, \dots, \mathbf{d}_k) \in \mathbb{R}^{p \times k}$ such that  $\mathbf{D}$  is sparse and  $\|\mathbf{X} - \mathbf{DA}\|_F^2$  is small

# Sparse principal component analysis Synthesis view

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- Sparse formulation (Witten et al., 2009; Bach et al., 2008)
  - Penalize/constrain  $\mathbf{d}_j$  by the  $\ell_1$ -norm for sparsity
  - Penalize/constrain  $lpha_i$  by the  $\ell_2$ -norm to avoid trivial solutions

$$\min_{\mathbf{D},\mathbf{A}} \sum_{i=1}^{n} \|\mathbf{x}_{i} - \mathbf{D}\boldsymbol{\alpha}_{i}\|_{2}^{2} + \lambda \sum_{j=1}^{k} \|\mathbf{d}_{j}\|_{1} \text{ s.t. } \forall i, \|\boldsymbol{\alpha}_{i}\|_{2} \leq 1$$

#### **Sparse PCA vs. dictionary learning**

• Sparse PCA:  $\mathbf{x}_i \approx \mathbf{D} \boldsymbol{lpha}_i$ ,  $\mathbf{D}$  sparse



#### **Sparse PCA vs. dictionary learning**

• Sparse PCA:  $\mathbf{x}_i pprox \mathbf{D} \boldsymbol{lpha}_i$ ,  $\mathbf{D}$  sparse



• Dictionary learning:  $\mathbf{x}_i pprox \mathbf{D} \boldsymbol{lpha}_i$ ,  $\boldsymbol{lpha}_i$  sparse



## Structured matrix factorizations (Bach et al., 2008)

$$\min_{\mathbf{D},\mathbf{A}} \sum_{i=1}^{n} \|\mathbf{x}_{i} - \mathbf{D}\boldsymbol{\alpha}_{i}\|_{2}^{2} + \lambda \sum_{j=1}^{k} \|\mathbf{d}_{j}\|_{\star} \text{ s.t. } \forall i, \|\boldsymbol{\alpha}_{i}\|_{\bullet} \leqslant 1$$
$$\min_{\mathbf{D},\mathbf{A}} \sum_{i=1}^{n} \|\mathbf{x}_{i} - \mathbf{D}\boldsymbol{\alpha}_{i}\|_{2}^{2} + \lambda \sum_{i=1}^{n} \|\boldsymbol{\alpha}_{i}\|_{\bullet} \text{ s.t. } \forall j, \|\mathbf{d}_{j}\|_{\star} \leqslant 1$$

- Optimization by alternating minimization (non-convex)
- $\alpha_i$  decomposition coefficients (or "code"),  $d_j$  dictionary elements
- Two related/equivalent problems:
  - Sparse PCA = sparse dictionary ( $\ell_1$ -norm on  $\mathbf{d}_j$ )
  - Dictionary learning = sparse decompositions ( $\ell_1$ -norm on  $\alpha_i$ ) (Olshausen and Field, 1997; Elad and Aharon, 2006; Lee et al., 2007)

#### **Probabilistic topic models and matrix factorization**



- Latent Dirichlet allocation (Blei et al., 2003)
  - For a document, sample  $\theta \in \mathbb{R}^k$  from a Dirichlet $(\alpha)$
  - For the n-th word of the same document,
    - \* sample a topic  $z_n$  from a multinomial with parameter  $\theta$
    - \* sample a word  $w_n$  from a multinomial with parameter  $\beta(z_n,:)$

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- Interpretation as multinomial PCA (Buntine and Perttu, 2003)
  - Marginalizing over topic  $z_n$ , given  $\theta$ , each word  $w_n$  is selected from a multinomial with parameter  $\sum_{z=1}^k \theta_k \beta(z, z) = \beta^\top \theta$
  - Row of  $\beta = {\rm dictionary}$  elements,  $\theta$  code for a document

## **Probabilistic topic models and matrix factorization**

- Two different views on the same problem
  - Interesting parallels to be made
  - Common problems to be solved
- Structure on dictionary/decomposition coefficients with adapted priors (Blei et al., 2004; Jenatton et al., 2010)
- Identifiability and interpretation/evaluation of results
- Discriminative tasks (Blei and McAuliffe, 2008; Lacoste-Julien et al., 2008; Mairal et al., 2009a)
- Optimization and local minima
  - Online learning (Mairal et al., 2009c)

Sparse methods for machine learning Why use sparse methods?

- Sparsity as a proxy to interpretability
  - Structured sparsity
- Sparsity for high-dimensional inference
  - Influence on feature design
- Sparse methods are not limited to least-squares regression
- Faster training/testing
- Better predictive performance?
  - Problems are sparse if you look at them the right way

## **Conclusion - Interesting questions/issues**

#### • Exponentially many features

- Can we algorithmically achieve  $\log p = O(n)$ ?
- Use structure among features (Bach, 2008c)
- Norm design
  - What type of behavior may be obtained with sparsity-inducing norms?

#### • Overfitting convexity

- Do we actually need convexity for matrix factorization problems?
- Convexity used in inner loops
- Joint convexity requires reformulation (Bach et al., 2008)

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