

**MLCC 2019**  
**Variable Selection and Sparsity**

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# Outline

Variable Selection

Subset Selection

Greedy Methods: (Orthogonal) Matching Pursuit

Convex Relaxation: LASSO & Elastic Net

## Prediction and Interpretability

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We look at this question from the perspective of **variable selection**

# Linear Models

Consider a linear model

$$f_w(x) = w^T x = \sum_{i=1}^v w^i x^i$$

Here

- ▶ the components  $x^j$  of an input can be seen as **measurements** (pixel values, dictionary words count, gene expressions, ...)

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# Notation

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- ▶  $Y_n \in \mathbb{R}^n$  the output vector

# High-dimensional Statistics

Estimating a linear model corresponds to solving a linear system

$$X_n w = Y_n.$$

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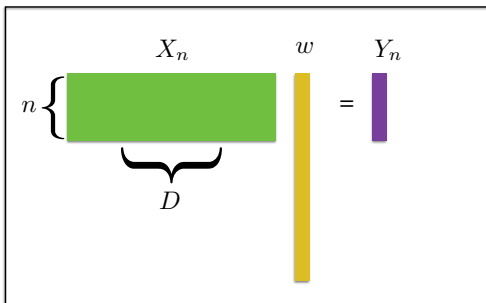
- ▶ Classically  $n \gg D$  **low dimension/overdetermined system**
- ▶ Lately  $n \ll D$  **high dimensional/underdetermined system**

Buzzwords: compressed sensing, high-dimensional statistics . . .

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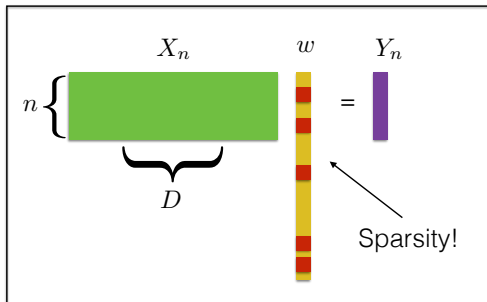
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If we consider the square loss, it can be shown that a **regularization** approach is given by

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^n (y_i - f_w(x_i))^2 + \lambda \|w\|_0$$

## The Brute Force Approach is Hard

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^n (y_i - f_w(x_i))^2 + \lambda \|w\|_0$$

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The computational complexity is combinatorial. In the following we consider two possible approximate approaches:

- ▶ greedy methods
- ▶ convex relaxation

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3. update the index set to include the index of such variable
4. update/compute coefficient vector
5. update residual.

The simplest such procedure is called forward stage-wise regression in statistics and matching pursuit (MP) in signal processing

## Initialization

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The MP algorithm starts by initializing the residual  $r \in \mathbb{R}^n$ , the coefficient vector  $w \in \mathbb{R}^D$ , and the index set  $I \subseteq \{1, \dots, D\}$

$$r_0 = Y_n, \quad w_0 = 0, \quad I_0 = \emptyset$$

## Selection

The variable most correlated with the residual is given by

$$k = \arg \max_{j=1, \dots, D} a_j, \quad a_j = \frac{(r_{i-1}^T X^j)^2}{\|X^j\|^2},$$

where we note that

$$v^j = \frac{r_{i-1}^T X^j}{\|X^j\|^2} = \arg \min_{v \in \mathbb{R}} \|r_{i-1} - X^j v\|^2, \quad \|r_{i-1} - X^j v^j\|^2 = \|r_{i-1}\|^2 - a_j$$



## Selection (cont.)

Such a selection rule has two interpretations:

- ▶ We select the variable with larger **projection** on the output, or equivalently
- ▶ we select the variable such that the corresponding column best explains the the output vector in a **least squares sense**

## Active Set, Solution and residual Update

Then, index set is updated as  $I_i = I_{i-1} \cup \{k\}$ , and the coefficients vector is given by

$$w_i = w_{i-1} + w_k, \quad w_k k = v_k e_k$$

where  $e_k$  is the element of the canonical basis in  $\mathbb{R}^D$  with  $k$ -th component different from zero

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Finally, the residual is updated

$$r_i = r_{i-1} - X w^k$$

## Orthogonal Matching Pursuit

A variant of the above procedure, called Orthogonal Matching Pursuit, is also often considered, where the coefficient computation is replaced by

$$w_i = \arg \min_{w \in \mathbb{R}^D} \|Y_n - X_n M_{I_i} w\|^2,$$

where the  $D$  by  $D$  matrix  $M_I$  is such that  $(M_I w)^j = w^j$  if  $j \in I$  and  $(M_I w)^j = 0$  otherwise. Moreover, the residual update is replaced by

$$r_i = Y_n - X_n w_i$$

## Theoretical Guarantees

If

- ▶ the solution is sparse, and
- ▶ the data matrix has columns "not too correlated"

OMP can be shown to recover with high probability the right vector of coefficients

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## $\ell_1$ Norm and Regularization

Another popular approach to find sparse solutions is based on a **convex relaxation**

Namely, the  $\ell_0$  norm is replaced by the  $\ell_1$  norm,

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Namely, the  $\ell_0$  norm is replaced by the  $\ell_1$  norm,

$$\|w\|_1 = \sum_{j=1}^D |w^j|$$

In the case of least squares, one can consider

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^n (y_i - f_w(x_i))^2 + \lambda \|w\|_1$$



## Convex Relaxation

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^n (y_i - f_w(x_i))^2 + \lambda \|w\|_1.$$

- ▶ The above problem is called LASSO in statistics and Basis Pursuit in signal processing
- ▶ The objective function defining the corresponding minimization problem is convex but not differentiable
- ▶ Tools from non-smooth convex optimization are needed to find a solution

## Iterative Soft Thresholding

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$$w_0 = 0, \quad w_i = S_{\lambda\gamma}\left(w_{i-1} - \frac{2\gamma}{n}X_n^T(Y_n - X_n w_{i-1})\right), \quad i = 1, \dots, T_{\max}$$

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At each iteration a non linear soft thresholding operator is applied to a gradient step

## Iterative Soft Thresholding (cont.)

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- ▶ the iteration should be run until a convergence criterion is met, e.g.  $\|w_i - w_{i-1}\| \leq \epsilon$ , for some precision  $\epsilon$ , or a maximum number of iteration  $T_{\max}$  is reached
- ▶ To ensure convergence we should choose the step-size

$$\gamma = \frac{n}{2\|X_n^T X_n\|}$$

## Splitting Methods

In ISTA the contribution of error and regularization are **split**:

- ▶ the argument of the soft thresholding operator corresponds to a step of gradient descent

$$\frac{2}{n} X_n^T (Y_n - X_n w_{i-1})$$

- ▶ The soft thresholding operator depends only on the regularization and acts component wise on a vector  $w$ , so that

$$S_\alpha(u) = ||u| - \alpha|_+ \frac{u}{|u|}.$$

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This can be contrasted to Tikhonov regularization where this is hardly the case



## Lasso meets Tikhonov: Elastic Net

Indeed, it is possible to see that:

- ▶ while Tikhonov allows to compute a stable solution, in general its solution is not sparse
- ▶ On the other hand the solution of LASSO, might not be stable

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- ▶ On the other hand the solution of LASSO, might not be stable

The elastic net algorithm, defined as

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^n (y_i - f_w(x_i))^2 + \lambda(\alpha \|w\|_1 + (1 - \alpha) \|w\|_2^2), \quad \alpha \in [0, 1] \quad (2)$$

can be seen as hybrid algorithm which interpolates between Tikhonov and LASSO

## ISTA for Elastic Net

The ISTA procedure can be adapted to solve the elastic net problem, where the gradient descent step incorporates also the derivative of the  $\ell^2$  penalty term. The resulting algorithm is

$$\begin{aligned}w_0 &= 0, \\ \text{for } & i = 1, \dots, T_{\max} \\ w_i &= S_{\lambda\alpha\gamma}((1 - \lambda\gamma(1 - \alpha))w_{i-1} - \frac{2\gamma}{n}X_n^T(Y_n - X_n w_{i-1})),\end{aligned}$$

To ensure convergence we should choose the step-size

$$\gamma = \frac{n}{2(\|X_n^T X_n\| + \lambda(1 - \alpha))}$$

# Wrapping Up

Sparsity and interpretable models

- ▶ greedy methods
- ▶ convex relaxation

## Next Class

*unsupervised learning*: dimensionality reduction!