ElasticNet avec gestion des interactions et débiaisage

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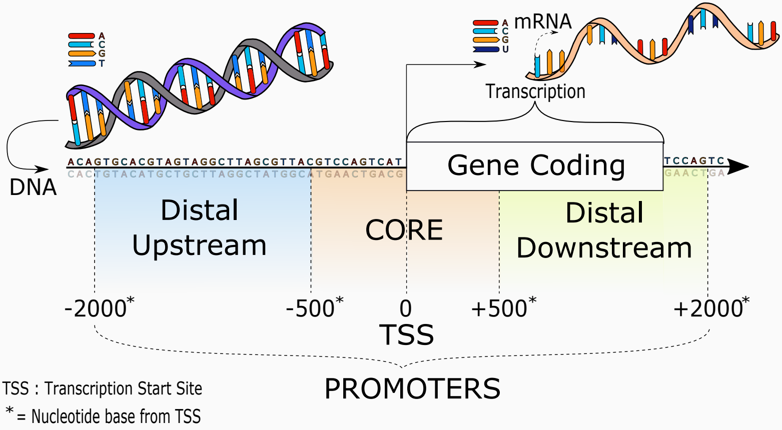
Motivation



- linear model[1] to explain mRNA count (y) from DNA sequence resume (X)

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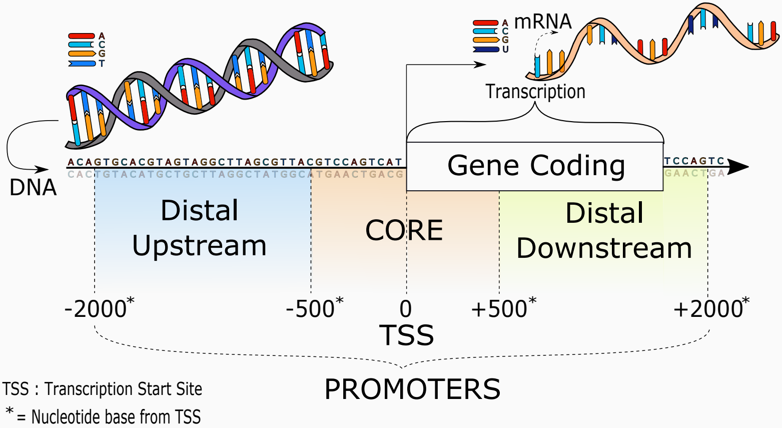

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- X : frequency of 1-letter and 2-letter words (AA, AC, AG, ...)

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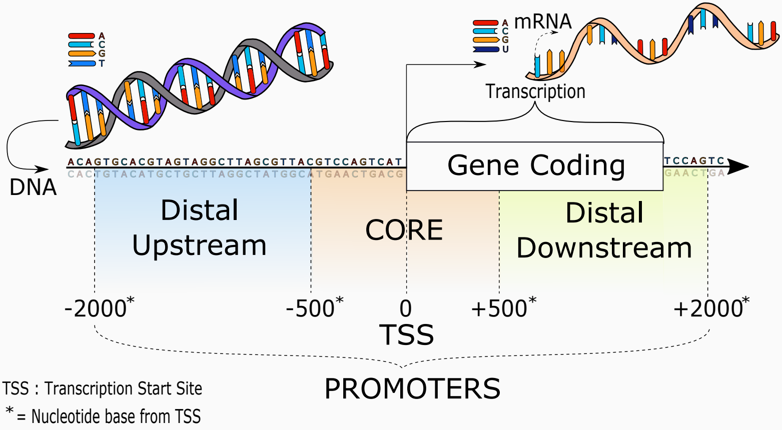

- linear model[1] to explain mRNA count (y) from DNA sequence resume (X)
- X : frequency of 1-letter and 2-letter words (AA, AC, AG, . . .)
- Add (2nd order) interactions between variables to improve the model

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Model: sparse linear regression model with interactions :

$$y = X\beta + Z\Theta + \text{ error}$$

where :

- $y \in \mathbb{R}^n$ (response vector): mRNA log transformed counts ;
- $X \in \mathbb{R}^{n \times p}$ design matrix of main variables :

$$X = [x_1, x_2, \ldots, x_p]$$

- $Z \in \mathbb{R}^{n \times q}$ design matrix of interaction variables, $q = \frac{p(p+1)}{2}$:

$$Z = [x_1 \odot x_1, \ldots, x_1 \odot x_p, x_2 \odot x_2, \ldots, x_{p-1} \odot x_p, x_p \odot x_p]$$

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$$\text{Here : } \begin{cases} n \approx 20\ 000 : \text{genes number} \\ p \approx 500 : \text{number of main features} \\ q \approx 140\ 000 : \text{number of quadratic features} \end{cases}$$

ElasticNet with interactions

The usual ElasticNet[2] (shortly Enet) estimator is defined as :

$$\hat{\beta} \in \arg\min_{\beta \in \mathbb{R}^p} \frac{\|y - X\beta\|^2}{2n} + \underbrace{\alpha_{1,1}\|\beta\|_1}_{\ell_1 \text{ regularization}} + \underbrace{\alpha_{2,1}\frac{\|\beta\|^2}{2}}_{\ell_2 \text{ regularization}}$$

1. ℓ_1 regularization to enforce sparsity[3]
2. adding ℓ_2 regularization to detect correlated features

[2] H. Zou and T. J. Hastie (2005). "Regularization and variable selection via the elastic net". In: *J. R. Stat. Soc. Ser. B Stat. Methodol.* 67.2, pp. 301–320.

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Q: How to solve it ? A: Coordinate Descent[4] algorithm

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Algorithm 1: Coordinate Descent for ElasticNet with interactions (1 epoch)

input : $X \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$, $\alpha = (\alpha_{1,1}, \ldots, \alpha_{2,2})^\top$, $\bar{x}$, $\bar{z}$, $\mathrm{std}(x)$, $\mathrm{std}(z)$ ...

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for $j_1 = 1, \ldots, p$ **do**

$\quad x = \frac{x_{j_1} - \bar{x}_{j_1}}{\mathrm{std}(x_{j_1})}$

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    $jj \mathrel{+}= 1$

output : $\widehat{\beta}^{k+1}$, $\widehat{\Theta}^{k+1}$

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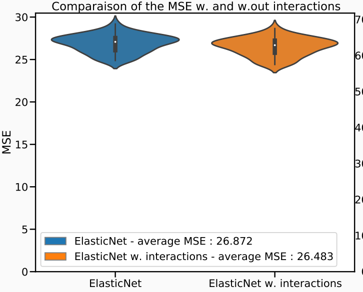
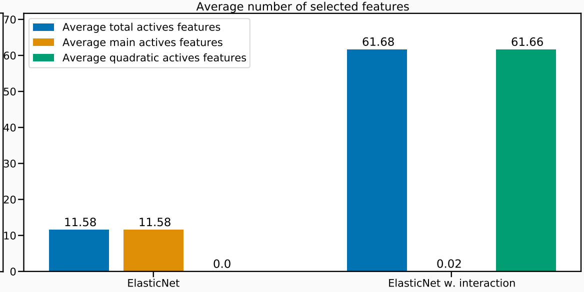
First real data result[5] : only CORE promoter part



(a) MSE error



(b) Distribution of actives features

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[5] Data and parameters : $n = 19393$, $p = 20$, $q = 210$, 50 repetitions of 5-folds CV, `l1_ratio` $\in \{1, 0.99, 0.95, 0.9\}$, duality gap fix to 10^{-4}, $\alpha_{\min} = \dfrac{\alpha_{\max}}{1000}$ and X, Z standardize

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   - Handle quadratic interactions, whatever the datasets
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2. Cons
   - ElasticNet shrinks large coefficients toward 0 (bias).

Debiasing the ElasticNet

A simple remedy : Naive LS ElasticNet

[6] C.-A. Deledalle et al. (2017). "CLEAR: Covariant LEAst-square Re-fitting with applications to image restoration". In: *SIAM J. Imaging Sci.* 10.1, pp. 243–284.

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$$\hat{\beta}_{\alpha}^{\text{LSEnet}}, \hat{\Theta}_{\alpha}^{\text{LSEnet}} := \mathop{\arg\min}_{\substack{\beta \in \mathbb{R}^p, \Theta \in \mathbb{R}^q \\ \mathrm{supp}(\beta) = \mathrm{supp}(\beta^{\text{Enet}}_{\alpha_{1,2}, \alpha_{2,2}}) \\ \mathrm{supp}(\Theta) = \mathrm{supp}(\Theta^{\text{Enet}}_{\alpha_{1,1}, \alpha_{2,1}})}} \frac{1}{2n} \|y - X\beta - Z\Theta\|_2^2$$

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Naive LS ElasticNet issues (w. interactions) :

❶ Require LeastSquares solver with interactions for large datasets ;

❷ Require to cross validate the whole pipeline ;

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We want to debiased on the fly without building Z : CLEAR[6] .

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CLEAR estimator is associated to an differentiable estimator $\mathbb{R}^n \ni y \to \widehat{\beta}(y) \in \mathbb{R}^p$ is, for all $y \in \mathbb{R}^n$, given by :

$$\mathcal{R}_{\widehat{\beta}}(y) := \widehat{\beta}(y) + \rho J \cdot (y - X\widehat{\beta}(y)) \text{ with } \rho := \begin{cases} \frac{\langle XJ\delta | \delta \rangle}{\|XJ\delta\|^2} & , \text{ if } XJ\delta \neq 0, \\ 1 & , \text{ otherwise,} \end{cases}$$

where $\delta = y - X\widehat{\beta}(y)$, $J = J_{\widehat{\beta}}(y) \in \mathbb{R}^{p \times n}$ is the **Jacobian** of $\widehat{\beta}(y)$.

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$$(J_{\widehat{\Theta}^{k+1}} r^{k+1})_{jj} = \frac{z_{jj}^\top \left((z_{jj} e_{jj}^\top - Z) J_{\widehat{\Theta}^k} + (\mathrm{Id}_n - X J_{\widehat{\beta}^k}) \right) r^k}{\|z_{jj}\|^2 + n\alpha_{2,2}} \mathbb{1}_{\left\{ \left| z_{jj}^\top \left(r^k + \widehat{\Theta}_{jj}^k z_{jj} \right) \right| \geqslant n\alpha_{1,2} \right\}}$$

Pro : updating scheme well fitted for coordinate descent.

Simulation Study : $y = X\beta^\star + Z\Theta^\star + \varepsilon$ w. $n = 100$, $p = 50$, $q = 1275$

- study different interaction hierarchical[7] cases : strong, weak and random.
- $X \sim \mathcal{N}(0_p, \Sigma_{p\times p})$, $\Sigma_{p\times p}$ produce correlation Toeplitz on X :

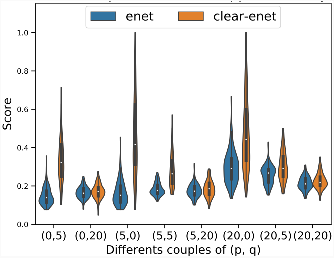
$$\Sigma_{p\times p} = \begin{pmatrix} 1 & 0.9 & 0.9^2 & \dots & 0.9^{p-2} & 0.9^{p-1} \\ 0.9 & 1 & 0.9 & \dots & 0.9^{p-3} & 0.9^{p-2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0.9^{p-1} & 0.9^{p-2} & 0.9^{p-3} & \dots & 0.9 & 1 \end{pmatrix}$$

- $\beta^\star$ and $\Theta^\star$: coefficients randomly chosen and equals ± 1 ;
- $\varepsilon \sim \mathcal{N}(0_n, \sigma^2 \, \mathrm{Id}_n)$ according to SNR[8] ≈ 16

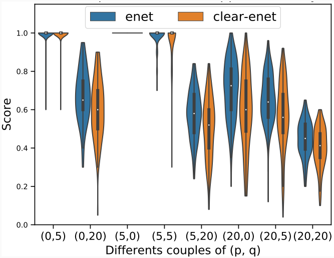
[7] J. Bien, J. Taylor, and R. Tibshirani (2013). "A lasso for hierarchical interactions". In: *Ann. Statist.* 41.3, pp. 1111–1141.

[8] P. Bühlmann and J. Mandozzi (2014). "High-dimensional variable screening and biais in subsequent inference, with an empirical comparison". In: *Computational Statistics* 29.3, pp. 407–430.

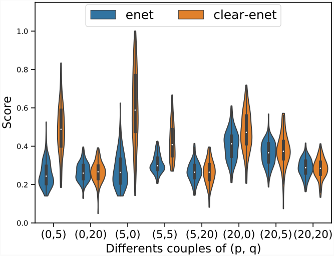
Simulated result in random cases : 100 repetitions of 5-folds CV.[9]



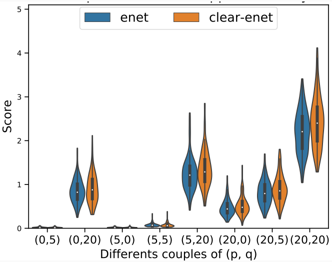
(a) Precision



(b) Recall



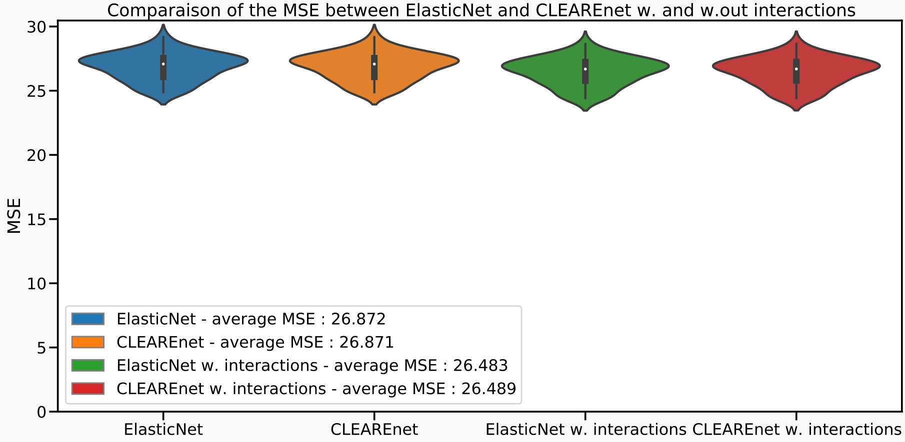
(c) F1 score



(d) MSE

[9] **Parameters :** `l1_ratio` $\in \{1, 0.99, 0.95, 0.9\}$, **duality gap fix to** 10^{-4}, $\alpha_{\min} = \dfrac{\alpha_{\max}}{100}$ **and** X, Z **standardize**

First real data result[10] : only CORE promoter part



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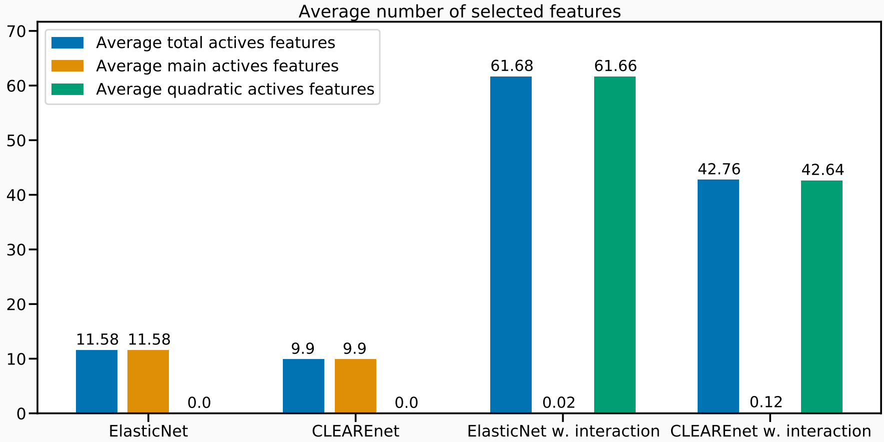

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Perspectives :

1. Speed-up the method, e. g. with working set strategies[12] ;
2. Scaling up experiment : both on simulated and real data ;
3. Clever hyperparameters tuning[13] (in $\mathbb{R}^2$ or $\mathbb{R}^4$).

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1. Speed-up the method, e. g. with working set strategies[12] ;
2. Scaling up experiment : both on simulated and real data ;
3. Clever hyperparameters tuning[13] (in $\mathbb{R}^2$ or $\mathbb{R}^4$).

Thanks for your attention.

[12] M. Massias, A. Gramfort, and J. Salmon (2018). "Celer: a Fast Solver for the Lasso with Dual Extrapolation". In: *ICML*.

[13] Q. Bertrand et al. (2020). "Implicit differentiation of Lasso-type models for hyperparameter optimization". In: *ICML*.

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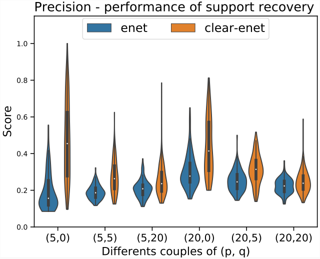
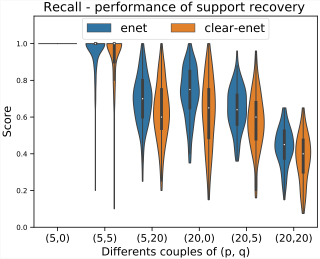
Appendix

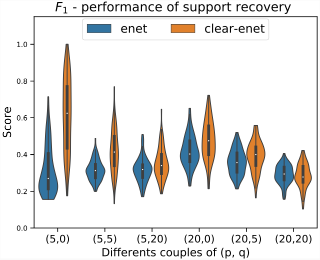
Strong cases : Result after 100 repetition of 5-folds CV.[14]



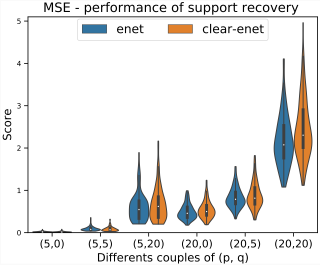
(a) Precision



(b) Recall



(c) F1 score



(d) MSE

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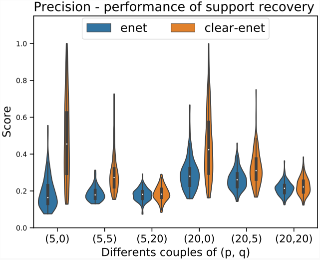
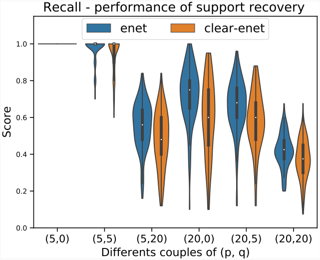
[14] **Others parameters** : `l1_ratio` $\in \{1, 0.99, 0.95, 0.9\}$, **duality gap fix to** 10^{-4}, $\alpha_{\min} = \dfrac{\alpha_{\max}}{100}$ **and** X, Z **standardized.**

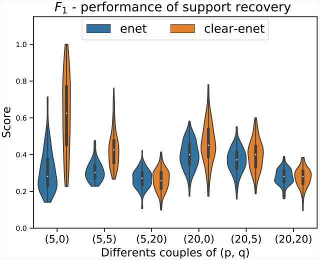
Weak cases : Result after 100 repetition of 5-folds CV.[15]



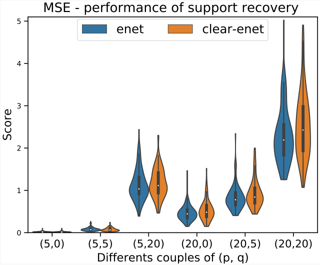
(a) Precision



(b) Recall



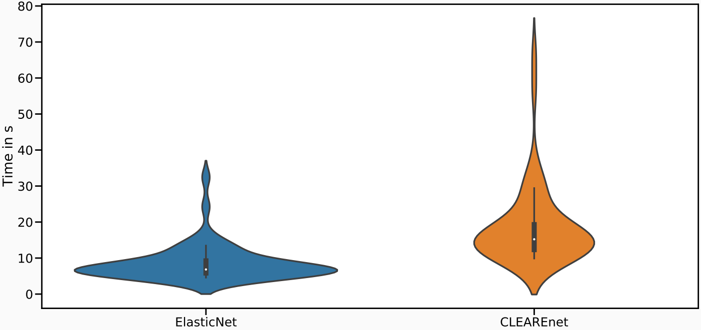
(c) F1 score



(d) MSE

[15] **Others parameters** : `l1_ratio` $\in \{1, 0.99, 0.95, 0.9\}$, **duality gap fix to** 10^{-4}, $\alpha_{\min} = \dfrac{\alpha_{\max}}{100}$ **and** X, Z **standardized.**

Time comparaison : ElasticNet and CLEAREnet



Correlation Matrix :