Semismooth Newton Augmented Lagrangian Method for Solving Lasso Problems

with Implementation in R

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Final Year Project Presentation

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Outline

What is Lasso Regression

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- This *Lagrangian* form is equivalent to a constrained minimisation problem

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- The optimal case would be *best-subset selection*, when all possible combinations of regressors are tried to produce the one with the lowest sum of squares for a given number of non-zero parameters.
- This is computationally costly, since it is $O(m!)$, but Lasso gives a very good approximation to it.
- Both ridge and Lasso are *convex* problems, and can be solved with the correct numerical, computational methods

Original Paper

- *A highly efficient semismooth Newton augmented Lagrangian method for solving Lasso problems*, Li, Xudong, Sun, Defeng and Toh, Kim-Chuan, *SIAM Journal on Optimization*, Vol. 28(1), pp 433-458, **2018**, *SIAM*

Convex Composite

Primal Problem

$$(\mathbf{P}) \quad \min \left\{ \frac{1}{2}\|Ax - b\|^2 + \lambda\|x\|_1 \right\}$$

where $A : \mathcal{X} \to \mathcal{Y}$, $h : \mathcal{Y} \to \mathbb{R}$, $p : \mathcal{X} \to (-\infty, +\infty]$ and $c \in \mathcal{X}$ is a vector.
$h(\xi) = \frac{1}{2}\|\xi - b\|^2$ and $p(x) = \lambda\|x\|_1$

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Dual Problem

$$(\mathbf{D}) \quad \max \left\{ -\frac{1}{2}\|\xi\|^2 + \langle b, \xi \rangle \mid A^T\xi + u - c = 0, \|u\|_\infty \leq \lambda \right\}$$

where $h^*(\xi) = -\frac{1}{2}\|\xi\|^2 + \langle b, \xi \rangle$ and $p^*(x) = \mathbb{I}_{\|x\|_\infty}$
p^* and h^*: the Fenchel conjugate functions of p and h

Assumptions on the loss function

Assumption 1.

1. $h^*(\cdot)$ is essentially smooth where h^* is differentiable on $\text{int}(\text{dom } h^*) \neq \emptyset$ and $\lim_{k\to\infty}\|h^*(\xi^k)\| = +\infty$ whenever $\{\xi^k\}$ is a sequence in $\text{int}(\text{dom } h^*)$ converging to a boundary point ξ of $\text{int}(\text{dom } h^*)$.
2. $p^*(\cdot)$ is either an indicator function $\delta_p(\cdot)$ or a support function δ_p^* for some nonempty polyhedral convex set $P \subseteq \mathcal{X}$.

Assumption 2.

$h : \mathcal{Y} \to \mathbb{R}$ is a convex differentiable function whose gradient is $\frac{1}{\alpha_h}$ *Lipschitz continuous* i.e.

$$\|\nabla h(\xi') - \nabla h(\xi)\| \leq \frac{1}{\alpha_h}\|\xi' - \xi\|, \quad \forall \xi', \xi \in \mathcal{Y}$$

($h^*(\cdot)$ is strongly convex with modulus α_k)

Assumptions on the loss function

Assumption 3.

h is essentially locally strongly convex, i.e. for any compact and convex set $K \subset dom\ \partial h$, there exists $\beta_K > 0$ s.t.

$$(1-\lambda)h(\xi') + \lambda h(\xi) \le h((1-\lambda)\xi' + \lambda\xi) + \frac{1}{2}\beta_K \lambda(1-\lambda)\|\xi' - \xi\|^2, \quad \forall \xi', \xi \in K$$

($\nabla h^*(\cdot)$ is locally *Lipschitz continuous* and directionally differentiable on int(dom h^*))

Assumption 4.

The Karush Kuhn Tucker (**KKT**) system is nonempty and its solution is denoted as $\bar{\xi}, \bar{u}$ and $\bar{x}$.

An augmented Lagrangian method for (D)

- The Lagrangian function of (**D**) is,

$$\ell(\xi, u; x) = h^*(\xi) + p^*(u) - \langle x, A^*\xi + u - c\rangle, \quad \forall (\xi, u; x) \in \mathcal{Y} \times \mathcal{X} \times \mathcal{X}$$

- Given $\sigma > 0$, the augmented Lagrangian function of (**D**) is,

$$\mathcal{L}_\sigma(\bar{\xi}, \bar{u}; \bar{x}) := \ell(\xi, u; x) + \frac{\sigma}{2}\|A^*\xi + u - c\|^2, \ \forall (\xi, u; x) \in \mathcal{Y} \times \mathcal{X} \times \mathcal{X}$$

- $\mathrm{Prox}_{\sigma\lambda\|\cdot\|_1}(x) = \arg\min_u\{\frac{1}{2}\|u - x\|^2 + \sigma\lambda\|u\|_1\}$ and $\mathrm{Prox}_{\sigma p}(x) = \mathrm{sgn}(x) \circ \max\{|x| - \sigma\lambda, 0\}$.

Algorithm 1

Algorithm Inexact Augmented Lagrangian Method

Let $\sigma_0 > 0$ be a given penalty parameter.
Choose $(\xi^0, u^0, x^0) \in \mathrm{int}(\mathrm{dom}\, h^*) \times \mathrm{dom}\, p^* \times \mathcal{X}$.

for $i = 0, 1, \ldots, \infty$ **do**

(1) **Compute**

$$(\xi^{k+1}, u^{k+1}) \approx \arg\min\{\Psi_k(\xi, u) := \mathcal{L}_{\sigma_k}(\xi, u; x^k)\} \tag{1}$$

(2) **Compute**

$$x^{k+1} = x^k - \sigma_k(A^*\xi^{k+1} + u^{k+1} - c) \ \& \ \textbf{update} \quad \sigma_{k+1} \uparrow \sigma_\infty \leq \infty$$

Global and Local Convergence

From [Rockafellar, 1976a[1] and 1976b[2]],

Convergence Criterion for inner subproblem (1)

$$(A) \quad \Psi_k(\xi^{k+1}, u^{k+1}) - \inf \Psi_k \leq \frac{\varepsilon_k^2}{2\sigma_k}, \sum_{k=0}^{\infty} \varepsilon_k < \infty$$

$$(B1) \quad \Psi_k(\xi^{k+1}, u^{k+1}) - \inf \Psi_k \leq \left(\frac{\delta_k^2}{2\sigma_k}\right) \|x^{k+1} - x^k\|^2, \ \delta_k \geq 0, \ \sum_{k=0}^{\infty} \delta_k < \infty$$

$$(B2) \quad \mathrm{dist}(0, \partial \Psi_k(\xi^{k+1}, u^{k+1})) \leq \left(\frac{\delta_k'}{\sigma_k}\right) \|x^{k+1} - x^k\|, \ 0 \leq \delta_k' \to 0$$

where, $\mathrm{dist}(x, \mathcal{C}) := \inf_{x' \in \mathcal{C}} \|x - x'\|$ for any $x \in \mathcal{X}$ and any $\mathcal{C} \subset \mathcal{X}$

[1] Rockafellar, R.T., 1976. Monotone operators and the proximal point algorithm. SIAM journal on control and optimization, 14(5), pp.877-898.

[2] Rockafellar, R.T., 1976. Augmented Lagrangians and applications of the proximal point algorithm in convex programming. Mathematics of operations research, 1(2), pp.97-116.

Semismooth Newton method for inner problems

Definition (Semismoothness) [Miffin, 1977][3]

Suppose that $M : \mathcal{X} \rightrightarrows \mathcal{L}(\mathcal{X}, \mathcal{Y})$ & $F : \mathcal{X} \to \mathcal{Y}$, is a locally *Lipschitz continuous* function. F is said to be semismooth at $x \in \mathcal{X}$ if F is directionally differentiable at x and for any $G \in \partial F(x + \Delta x) = M(x + \Delta x)$ & $\Delta x \to 0$.

$$F(x + \Delta x) - F(x) - G(\Delta x) = o(\|\Delta x\|)$$

F is said to be strongly semismooth at $x \in \mathcal{X}$ if,

$$F(x + \Delta x) - F(x) - G(\Delta x) = O(\|\Delta x\|^2)$$

Then F is said to be semismooth (strongly semismooth) function on $\mathcal{X}$ if it is semismooth (strongly semismooth) everywhere in $\mathcal{X}$

[3] Mifflin, Robert. "Semismooth and semiconvex functions in constrained optimization". In: SIAM Journal on Control and Optimization 15.6 (1977),pp. 959–972

Semismooth Newton method for inner problems

- While fixing $\sigma > 0$, we newly denote for $\xi \in \text{int}(\text{dom}\, h^*)$,

$$\begin{aligned}\psi(\xi) &:= \inf_u \Psi(\xi, u) = \inf \mathcal{L}_\sigma(\xi, u; x) \\ &= h^*(\xi) + p^*(\text{Prox}_{p^*/\sigma})(\bar{x}/\sigma - A^*\xi + c) \\ &+ \frac{1}{2\sigma}\|\text{Prox}_{\sigma p}(\bar{x} - \sigma(A^*\xi - c))\|^2 - \frac{1}{2\sigma}\|\bar{x}\|^2\end{aligned}$$

- We compute the 1^{st} and 2^{nd} derivatives

$$\begin{aligned}\nabla\psi(\xi) &= \nabla h^*(\xi) - A\,\text{Prox}_{\sigma p}(\bar{x} - \sigma(A^*\xi - c)),\ \forall\xi \in \text{int}(\text{dom}\, h^*) \\ \hat{\partial}^2\psi(\xi) &= \nabla^2 h^*(\xi) + \sigma A\,\text{Prox}_{\sigma p}(\bar{x} - \sigma(A^*\xi - c))A^*\end{aligned}$$

- where $\partial^2 h^*(\xi)$ is the Clarke subdifferential of $\nabla h^*(\cdot)$ at ξ and $\partial\,\text{Prox}_{\sigma p}(\bar{x} - \sigma(A^*\xi - c))$ is the Clarke subdifferential of the *Lipschitz continuous* mapping and Jacobian of $\text{Prox}_{\sigma p}(\cdot)$ at $\bar{x} - \sigma(A^*\xi - c)$.

Semismooth Newton method for inner problems

- Then solve the semismooth equation,

$$\nabla \psi(\xi) = 0, \quad \xi \in \mathrm{int}(\mathrm{dom}\, h^*)$$

- Then we define the generalised Hessian of ψ at ξ,

$$V := H + \sigma A P A^*$$

with $H \in \partial^2 h^*(\xi)$ and $P \in \partial\,\mathrm{Prox}_{\sigma p}(\bar{x} - \sigma(A^*\xi - c))$ where for the case of our paper, $h(\xi) = \frac{1}{2}\|\xi\|^2 + b^T\xi$, $\nabla h^*(\xi) = \xi + b$, $\nabla^2 h^*(\xi) = \mathbb{I}_m$. $h^*(\cdot)$ is twice differentiable and $\mathrm{Prox}_{\lambda\|\cdot\|}$ is a piecewise linear function which are strongly semismooth.

Algorithm 2

Algorithm Semismooth Newton Method

Given the hyperparameter, $\mu \in (0, \frac{1}{2}), \tilde{\eta} \in (0,1), \tau \in (0,1]$ & $\delta \in (0,1)$.
Choose $\xi^0 \in \text{int}(\text{dom}\, h^*)$ and **for** $j = 0, 1, \ldots, \infty$ **do**
(1) **Choose** $H_j \in \partial^2(\nabla h^*)(\xi^j)$ & $P_j \in \partial\, \text{Prox}_{\sigma p}(\tilde{x} - \sigma(A^*\xi^j - c))$. **Let** $V_j := H_j + \sigma A P_j A^*$. **Solve** the following Linear System exactly or by the conjugate gradient algorithm to find d^j

$$V_j d + \nabla\psi(\xi^j) = 0, \text{where } d = \Delta\xi$$
$$\text{s.t. } \|V_j d^j + \nabla\psi(\xi^j)\| \leq \min(\tilde{\eta}, \|\nabla\psi(\xi^j)\|)^{1+\tau}$$

(2) **Set** $\alpha = \delta^{m_j}$ where m_j is the first nonnegative integer m for which,

$$\xi^j + \delta^m d^j \in \text{int}(\text{dom}\, h^*) \text{ and } \psi(\xi^j + \delta^m d^j) \leq \psi(\xi^j) + \mu\delta^m\langle\nabla\psi(\xi^j), d^j\rangle$$

(3) **Set** $\xi^{j+1} = \xi^j + \alpha_j d^j$

Convergence of semismooth Newton method

Let the sequence $\{\xi^j\}$ be generated by **Algorithm 2**,

Theorem

Assume that $\nabla h^*(\cdot)$ and $\text{Prox}_{\sigma p}(\cdot)$ are strongly semismooth on $\int(\text{dom}\, h^*)$ and $\mathcal{X}$ then ξ^j converges to the unique optimal solution $\bar{\xi} \in \text{int}(\text{dom}\, h^*)$ and $\bar{u} = \bar{x} - \sigma(A^T\bar{\xi} - c)$ at least superlinearly, i.e.,

$$\|\xi^{j+1} - \bar{\xi}\| = O(\|\xi^j - \bar{\xi}\|^{1+\tau}), \text{ for any } j \geq 0, V_j \in \partial^2\psi(\xi^j)$$

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Then, the implementable stopping criterion from the stopping criteria (A), (B1) and (B2)

$$(A') \quad \|\psi_k(\xi^{k+1})\| \leq \frac{\varepsilon_k}{\sqrt{\sigma_k/\alpha_h}}$$

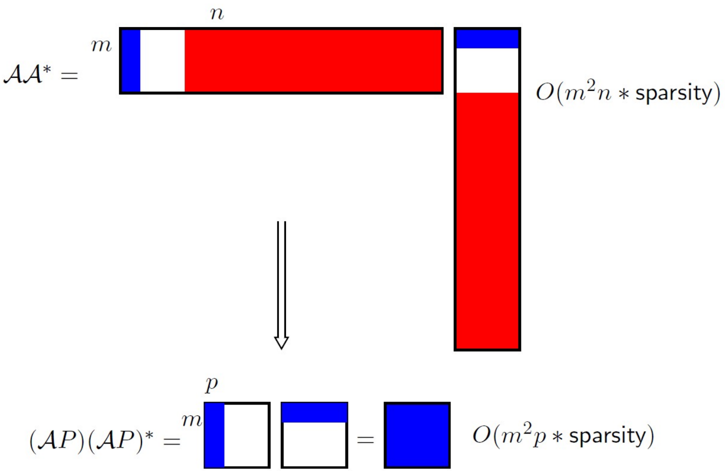
$$(B1') \quad \|\nabla\psi_k(\xi^{k+1})\| \leq \sqrt{\alpha_h\sigma_k}\delta_k\|A^*\xi^{k+1} + u^{k+1} - c\|$$

$$(B2') \quad \|\nabla\psi_k(\xi^{k+1})\| \leq \delta'\|A^*\xi^{k+1} + u^{k+1} - c\|, \ 0 \leq \delta'_k \to 0$$

where $\sum_{k=0}^{\infty}\varepsilon_k < \infty$ and $\sum_{k=0}^{\infty}\delta_k < \infty$ and $\|\nabla\psi_k(\xi^{k+1})\|$ is sufficiently small.

Semismooth Newton method

We can exploit the second order sparsity,



Semismooth Newton method

- We solve the linear system,

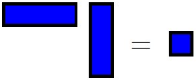
$$(\mathbb{I}_m + \sigma \mathcal{A} P \mathcal{A}^T)d = -\nabla \psi(\xi)$$

- We let $\mathcal{J} := \{j \mid |x_j| > \sigma\lambda, \ j = 1, ..., n\}$ and $|\mathcal{J}| = r$, the cardinality of $\mathcal{J}$. Then we have

$$\mathcal{A} P \mathcal{A}^T = (\mathcal{A}P)(\mathcal{A}P)^T = \mathcal{A}_{\mathcal{J}} \mathcal{A}_{\mathcal{J}}^T$$

- For the case when $p << m$, instead of factorising an $m \times m$ matrix, we can invert a much smaller, $p \times p$, matrix by using the Sherman-Morrison-Wood formula,

$$(\mathbb{I}_m + \sigma \mathcal{A} P \mathcal{A}^T)^{-1} = (\mathbb{I}_m + \sigma \mathcal{A}_{\mathcal{J}} \mathcal{A}_{\mathcal{J}}^T)^{-1} = \mathbb{I}_m - \mathcal{A}_{\mathcal{J}}(\sigma^{-1}\mathbb{I}_r + \mathcal{A}_{\mathcal{J}}^T \mathcal{A}_{\mathcal{J}})^{-1} \mathcal{A}_{\mathcal{J}}^T$$

$(\mathcal{A}P)^*(\mathcal{A}P) =$  $O(p^2 m * \text{sparsity})$

Semismooth Newton method

The relative KKT residual:

$$\eta = \frac{\|\bar{x} - \mathrm{Prox}_{\lambda\|\cdot\|}(\bar{x} - A^*(A\bar{x} - b))\|}{1 + \|\bar{x}\| + \|A\bar{x} - b\|} < \varepsilon$$

Number of nonzeros: $\mathrm{nnz} := \min\left\{ k \mid \sum_{t=1}^{k} |\hat{x}_t| \geq 0.999\|x\|_1 \right\}$

Datasets

Data	Dimension(m; n)	$\lambda_{max}(AA^*)$
pyrim5	74; 201376	1.22e+06
triazines4	186; 635376	2.07e+07
abalone7	4177; 6435	5.21e+05
bodyfat7	252; 116280	5.29e+04
housing7	506; 77520	3.28e+05
mpg7	392; 3432	1.28e+04
space_ga9	3107; 5005	4.01e+03

Table: UCI and Statlib Testing Instances

- Methylation data - 450k CpG methylation sites for 656 patients, and their ages

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3. Then, we made drafts in R of the original MATLAB code with reference to the pseudocode in [Li et al, 2018]
4. Changed norms, matrix-vector algebra functions, preconditioning functions, workflow and parameterisation as necessary.

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- To begin, this was only performed on *abalone7* data at one particular value of λ

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3. Towards the end of the algorithm, very slight differences (on the order of 10^{-5}, and relatively small also) were observed
4. We attributed to different handling of floating point extrema.
5. However, this did lead in general to the R code taking a few more iterations than MATLAB.

Implementation details

- Nevertheless, after de-scaling and transforming the output vectors, we obtained the exact same results as the MATLAB code in terms of objective values, minimum and maximum parameter estimates and number of non-zeros calculated according to:
- nnz $:= \min \left\{ k \mid \sum_{t=1}^{k} |\hat{x}_t| \geq 0.999 \|x\|_1 \right\}$

Overall results

Data	λ_c	Time (s)	Objective Value
		Matlab — R-SSNAL — *glmnet*	Matlab — R-SSNAL — *glmnet*
pyrim5	10^{-3}	2.16 — 9.92 — 0.40	0.07511 — 0.07511 — 0.0795
(74;201376)	10^{-4}	2.63 — 27.82 — 0.26	0.0109 — 0.0108 — 0.0260
triazines4	10^{-3}	13.79 — 170.92 — 3.3	0.5452 — 0.5452 — 0.5548
(186;635376)	10^{-4}	27.90 — 1580.88 — 5.48	0.1156 — 0.1156 — 0.1524
abalone7	10^{-3}	1.95 — 6.84 — 1.04	11407 — 11407 — 12158
(4177;6435)	10^{-4}	3.47 — 18.14 — 2.48	9289 — 9289 — 9716
bodyfat7	10^{-3}	1.64 — 5.00 — 0.30	0.2925 — 0.2925 — 1.334
(252;116280)	10^{-4}	2.27 — 7.52 — 0.98	0.03031 — 0.03031 — 0.2372
housing7	10^{-3}	2.92 — 13.88 — 0.60	2775 — 2775 — 2819
(506;77520)	10^{-4}	2.27 — 7.52 — 0.98	920.3 — 920.3 — 987.1
mpg7	10^{-3}	0.32 — 1.02 — 0.04	1669 — 1669 — 2076
(392;3432)	10^{-4}	0.37 — 2.90 — 0.16	890 — 890 — 985.57
space_ga9	10^{-3}	0.81 — 2.34 — 0.10	31.9 — 31.9 — 62.08
(3107;5005)	10^{-4}	2.27 — 7.52 — 0.98	19.88 — 19.88 — 31.63

Table: Performance comparisons of SSNAL in Matlab and R and *glmnet*

Overall results

Data	λ_c	min	max	NNZ
		Matlab — R-SSNAL — *glmnet*	Matlab — R-SSNAL — *glmnet*	Matlab — R-SSNAL — *glmnet*
pyrim5	10^{-3}	-0.0422 — -0.0422 — -0.1732	0.165 — 0.166 — 0.1067	70 — 70 — 166
(74;201376)	10^{-4}	-0.0897 — -0.0896 — -0.63454	0.172 — 0.172 — 0.064	77 — 78 — 1643
triazines4	10^{-3}	-0.163 — -0.163 — -0.163	0.161 — 0.161 — 0.182	565 — 572 — 292
(186;635376)	10^{-4}	-0.458 — -0.458 — -0.4525	0.300 — 0.296 — 0.2465	261 — 261 — 1573
abalone7	10^{-3}	-8.13 — -8.13 — -13.49	11.7 — 11.7 — 11.7	24 — 24 — 21
(4177;6435)	10^{-4}	-13.3 — -13.3 — -12.97	16.1 — 16.1 — 7.96	59 — 59 — 129
bodyfat7	10^{-3}	-0.0465 — -0.0465 — -0.8133	1.05 — 1.05 — 1.202	2 — 2 — 17
(252;116280)	10^{-4}	-0.0526 — -0.0526 — -1.06	1.05 — 1.045 — 1.314	3 — 3 — 49
housing7	10^{-3}	-7.37 — -7.37 — -8.02	3.25 — 3.25 — 4.114	158 — 158 — 163
(506;77520)	10^{-4}	-13.1 — -13.1 — -19.7	11.3 — 11.27 — 8.39	281 — 281 — 484
mpg7	10^{-3}	-5.08 — -5.08 — -23.68	17 — 16.98 — 14.99	47 — 47 — 46
(392;3432)	10^{-4}	-11.8 — -11.8 — -18.93	15.3 — 15.3 — 16.38	128 — 128 — 172
space_ga9	10^{-3}	-1.14 — -1.14 — -3.68	0.978 — 0.978 — 3.77	14 — 14 — 19
(3107;5005)	10^{-4}	-3.56 — -3.56 — -4.59	2.64 — 2.64 — 4.71	38 — 38 — 58

Table: Performance comparisons of **SSNAL** in **Matlab** and **R** and *glmnet*

Implementation details

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7. Altogether, around 1,800 lines of code.

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Cross-validation: UCI and Statlib

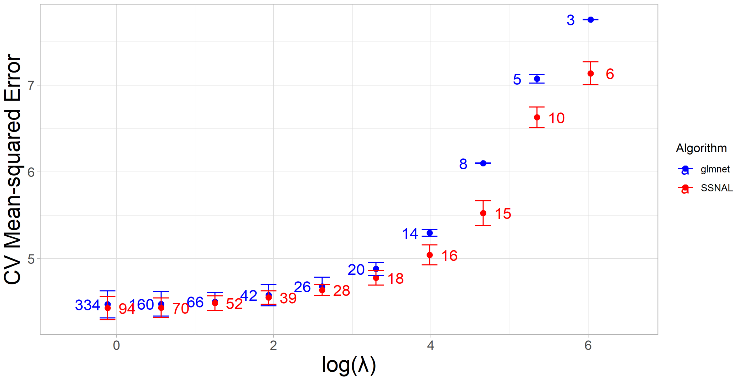
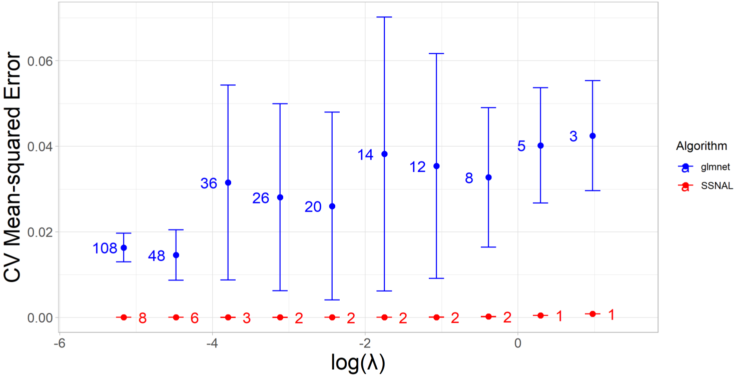


Figure: abalone

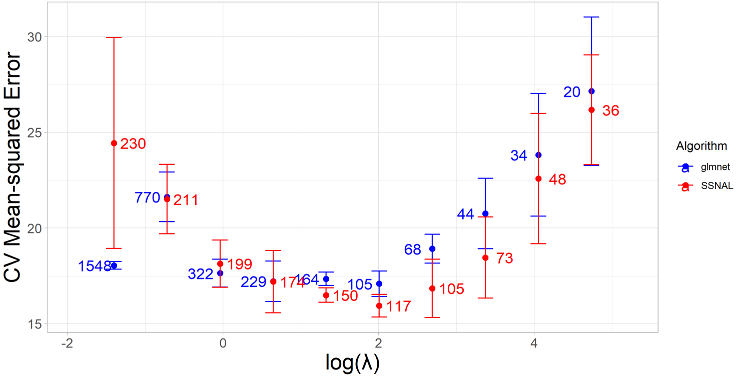
Cross-validation: UCI and Statlib

Figure: bodyfat



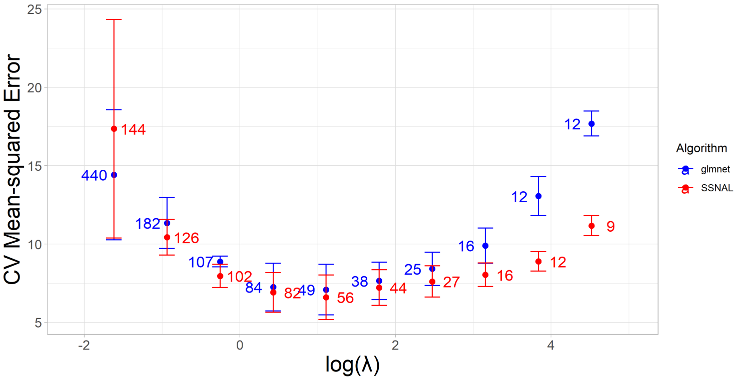
Cross-validation: UCI and Statlib

Figure: housing



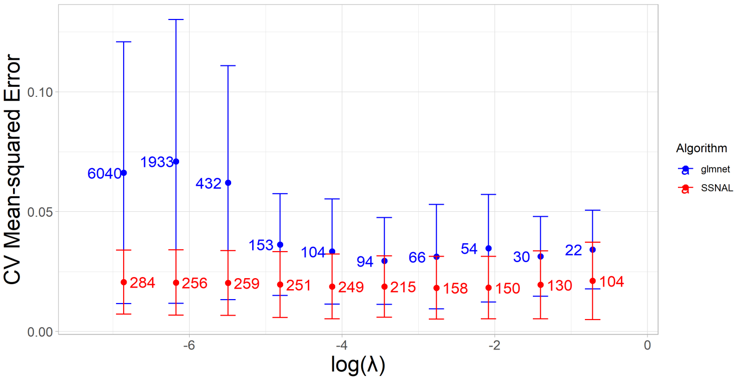
Cross-validation: UCI and Statlib

Figure: mpg



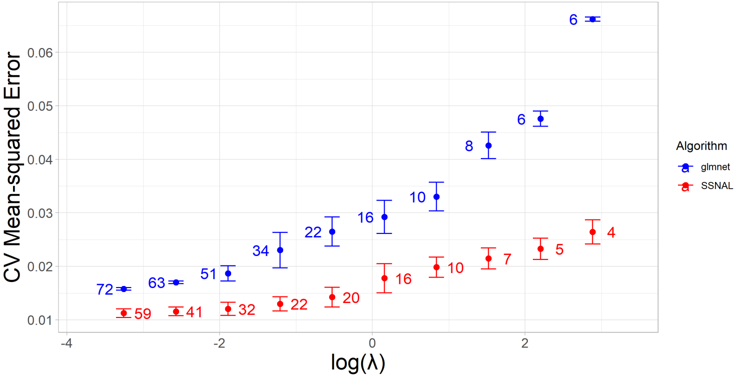
Cross-validation: UCI and Statlib

Figure: pyrim



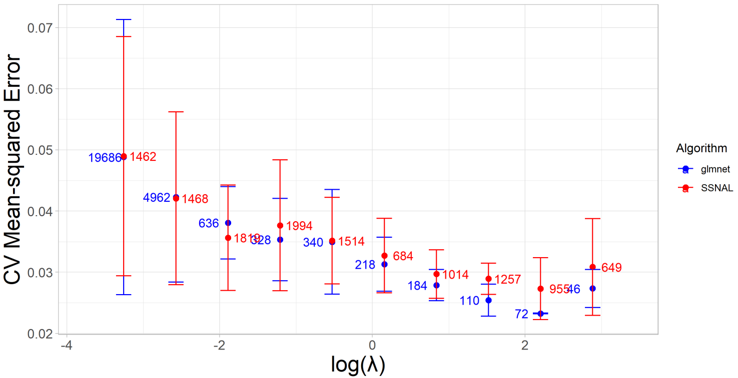
Cross-validation: UCI and Statlib

Figure: space_ga



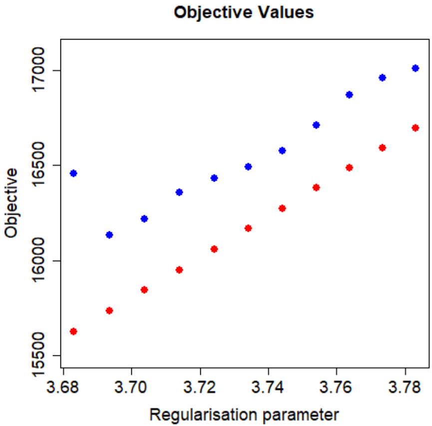
Cross-validation: UCI and Statlib

Figure: triazines



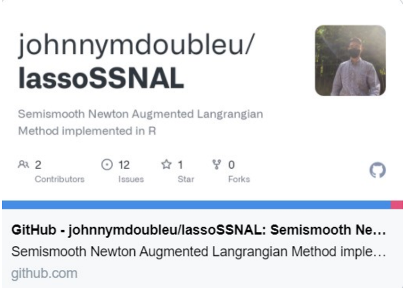
Objective values: methylation data

Figure: Methylation data



Code

▸ Github Repository



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4. Future Work: on developing a more generalised SSNAL method to apply on Elastic Net, fused Lasso and many more.

Thank you for your attention!