LINKÖPING UNIVERSITY

Advanced Computational Statistics – Spring 2025
Assignment for Lecture 4

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Perform the solutions individually and send your report **until April 28** by email to me. Try to keep this deadline. However, if you have problems with it, there will be a final deadline on September 30 for all assignments. Please send me one **pdf-file** with your report and additionally, please send me your code in one separate **plain-text file**. **Both Problems 4.1 and 4.2 are mandatory.**

Problem 4.1

We want to determine the D-optimal design for cubic regression where the independent variable x is allowed to have values between 0 and 10. Four different $x_i \in [0, 10], i = 1, 2, 3, 4$, can be chosen by the experimenter and the proportion of observations done at each x_i is $w_i \geq 0$ with $\sum_{i=1}^{4} w_i = 1$. The D-optimal design maximises

$$\det\left(\sum_{i=1}^{4} w_i \mathbf{f}(x_i)\mathbf{f}(x_i)^\top\right), \text{ with } \mathbf{f}(x) = (1, x, x^2, x^3)^\top,$$

under the restrictions mentioned above.

a. Determine a matrix $\mathbf{U}$ and a vector $\mathbf{c}$ such that the constraints can be written in the form $\mathbf{U}\mathbf{y} - \mathbf{c} \geq 0$, where $\mathbf{y}$ is the vector of parameters to be optimised over.

b. Determine the D-optimal design using a constrained optimisation function in your programming language, e.g., `constrOptim` in `R`. Does the result make sense?

c. Let $\tilde{g}(\mathbf{y}) = \mu \cdot b(\mathbf{y}) + g(\mathbf{y})$, where $\mu \cdot b(\mathbf{y})$ are log barriers at all constraints and g is the function to be maximised. Program a function for $\tilde{g}$. The value μ could be a parameter in the function such that you easily can modify it.

d. Choose some reasonable values for μ and compute the optimal value of g using unconstrained optimisation. For this, you can use an available optimiser in your programming language, e.g., `optim` in `R`. Report results for a sequence of decreasing μ, where you use the solution $\mathbf{y}^*$ as starting value for the next μ. Do you obtain similar results as in b. when using small μ?

Problem 4.2

We consider again as in Problem 3.1 the experiment investigating how the growth of garden cress depends on a (potentially) toxic fertilizer. The data is on the homepage in the file `cressdata.txt` (columns: observation number, fertilizer concentration, yield).

We want to estimate now a third-degree polynomial (cubic), again using least squares with L_1-regularisation. In contrast to the penalized objective function in Problem 3.1, we use now the constrained objective function

$$\text{Minimise } g(\boldsymbol{\beta}) = \|\mathbf{X}\boldsymbol{\beta} - \mathbf{y}\|_2^2 \text{ subject to } \|\tilde{\boldsymbol{\beta}}\|_1 \leq t, \tag{1}$$

where $\mathbf{X}$ is the design matrix with columns 1, fertilizer, fertilizer^2, fertilizer^3, $\tilde{\boldsymbol{\beta}} = (\beta_1, \beta_2, \beta_3)^\top$ is the parameter vector without intercept, $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2, \beta_3)^\top$ is the complete parameter vector and $\mathbf{y}$ is the yield-data. The constant $t \geq 0$ is now the regularisation constant. t and λ (in Problem 3.1) are related such that a t in the constrained problem corresponds to a λ in the penalised problem which gives the same solution.

Note that now, $t = \infty$ corresponds to the least squares estimation, where the solution for $\boldsymbol{\beta}$ of the optimisation problem is $(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$.

a. Write the constraint $\|\tilde{\boldsymbol{\beta}}\|_1 \leq t$ in terms of eight linear constraints $\mathbf{u}_i^\top\boldsymbol{\beta} + c_i \geq 0$ (or as $\mathbf{U}\boldsymbol{\beta} - \mathbf{c} \geq \mathbf{0}$ with a matrix $\mathbf{U}$ with 8 rows).

b. Compute the Lasso-estimate using a constrained optimization function which can handle linear inequality constraints like `constrOptim` in `R` for $t = 1000, 100, 40, 10$. Describe which optimization algorithm is used in your function. Check $\|\tilde{\boldsymbol{\beta}}\|_1$ for the solutions: Is the inequality constraint active or not?

c. Implement the projected gradient algorithm and solve the constrained optimization problem for $t = 1000, 100, 40, 10$. Compare with the result in part b.