

Exercise A: Least square problems

A1

Proof. Minimising $\|Ax - b\|_2$ with respect to x means finding x such that the derivative of $\|Ax - b\|_2$ with respect to x is equal to zero. Equivalently, we can minimise the square of the norm which can be developed as follows:

$$\begin{aligned}\|Ax - b\|_2^2 &= \|Ax\|_2^2 - 2\langle Ax, b \rangle + \|b\|_2^2 \\ &= x^\top A^\top Ax - 2x^\top A^\top b + b^\top b.\end{aligned}$$

The derivative of this expression with respect to x is

$$\begin{aligned}\frac{\partial \|Ax - b\|_2^2}{\partial x} &= \frac{\partial (x^\top A^\top Ax - 2x^\top A^\top b + b^\top b)}{\partial x} \\ &= \frac{\partial (x^\top A^\top Ax)}{\partial x} - \frac{\partial (2x^\top A^\top b)}{\partial x} + \frac{\partial (b^\top b)}{\partial x} \\ &= 2A^\top Ax - 2A^\top b + 0.\end{aligned}$$

We set this derivative to zero to obtain the following:

$$\begin{aligned}\frac{\partial \|Ax - b\|_2^2}{\partial x} &= 0 \\ \iff 2A^\top Ax - 2A^\top b &= 0 \\ \iff 2A^\top Ax &= 2A^\top b \\ \iff A^\top Ax &= A^\top b.\end{aligned}$$

To prove that when A has full column rank, i.e. $\text{rank}(A) = n$, the solution is unique, we first show that $\text{Ker}(A^\top A) = \text{Ker}(A)$:

$$\forall x \in \text{Ker}(A) : Ax = 0 \iff A^\top Ax = 0 \iff x \in \text{Ker}(A^\top A) \implies \text{Ker}(A) \subseteq \text{Ker}(A^\top A).$$

$$\begin{aligned}\forall x \in \text{Ker}(A^\top A) : A^\top Ax = 0 &\iff x^\top A^\top Ax = 0 \iff \|Ax\|_2 = 0 \iff Ax = 0 \iff x \in \text{Ker}(A) \\ &\implies \text{Ker}(A^\top A) \subseteq \text{Ker}(A).\end{aligned}$$

Combining these results, we have $\text{Ker}(A^\top A) = \text{Ker}(A)$.

According to the rank-nullity theorem,

$$\text{rank}(A) = n - \dim(\text{Ker}(A)).$$

However, $\text{rank}(A) = n$, and thus

$$\begin{aligned}n &= n - \dim(\text{Ker}(A)) \\ \iff \dim(\text{Ker}(A)) &= 0 = \dim(\text{Ker}(A^\top A)) \\ \implies \text{Ker}(A^\top A) &= \{0\}.\end{aligned}$$

As $\text{Ker}(A^\top A) = \{0\}$ and $A^\top A$ is square, we deduce that $A^\top A$ is invertible. It then follows from Theorem 2.1 of the lecture notes that the solution of the system is unique. \square

A2

Suppose the QR decomposition of A is given by $Q \begin{pmatrix} R \\ 0 \end{pmatrix}$, where $Q \in \mathbb{R}^{m \times m}$ is unitary and $R \in \mathbb{R}^{n \times n}$ is upper triangular. We will express the solution of

$$A^\top Ax = A^\top b \tag{1}$$

in terms of the QR decomposition of A .

Let $R_f = \begin{pmatrix} R \\ 0 \end{pmatrix}$. We can rewrite (1) as

$$\begin{aligned} (QR_f)^\top QR_f x &= (QR_f)^\top b \\ R_f^\top Q^\top QR_f x &= R_f^\top Q^\top b. \end{aligned}$$

As Q is unitary and hence $Q^\top Q = I$, we have

$$\begin{pmatrix} R^\top & 0 \end{pmatrix} \begin{pmatrix} R \\ 0 \end{pmatrix} x = \begin{pmatrix} R^\top & 0 \end{pmatrix} Q^\top b.$$

If we call \hat{Q} the matrix consisting of the first n columns of Q , (1) becomes

$$R^\top R x = R^\top \hat{Q}^\top b.$$

From Theorem 2.8 of the lecture notes, we know that every matrix $A \in \mathbb{C}^{m \times n}$ of full column rank admits a factorization $A = Q_1 R_1$ where $Q_1 \in \mathbb{C}^{m \times n}$ is an isometry and $R_1 \in \mathbb{C}^{n \times n}$ is an upper triangular matrix with positive diagonal. The matrix Q_1 corresponds to \hat{Q} and R_1 simply to R . Hence, we deduce that R is invertible. This allows us to premultiply both sides of the equation by the inverse of R^\top :

$$\begin{aligned} R^{-\top} R^\top R x &= R^{-\top} R^\top \hat{Q}^\top b \\ R x &= \hat{Q}^\top b. \end{aligned}$$

The solution of (1) is therefore $x = R^{-1} \hat{Q}^\top b$ and the computation of the solution is reduced to the resolution of a single triangular system of linear equations (which can be solved efficiently using backward substitution).

Exercise B: Low-rank approximation

B1

For every matrix $A \in \mathbb{R}^{m \times n}$, there exist unitary transformations $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ such that

$$A = U \Sigma V^*, \quad \text{where} \quad \Sigma = \left[\begin{array}{ccc|ccc} \sigma_1 & & & & & 0 \\ & \ddots & & & & \\ 0 & & \sigma_r & & & 0_{r \times (n-r)} \\ \hline & & & 0_{(m-r) \times r} & & 0_{(m-r) \times (n-r)} \end{array} \right],$$

with real positive singular values $\sigma_1 \geq \dots \geq \sigma_r > 0$. These singular values are unique. Indeed, they can be derived from the eigenvalues of the Hermitian matrix $A^* A$ (as explained on p. 39 of the course notes) which are uniquely defined.

Next, we show that the rank of a matrix is equal to its number of nonzero singular values.

Proof. We first prove that if A is a $k \times \ell$ matrix and B is a full-rank $\ell \times \ell$ matrix then $\text{rank}(AB) = \text{rank}(A)$. Let S_1 be the space generated by the columns of A and S_2 the space generated by the columns of AB . If $x \in S_1$ then there exists $y \in \mathbb{R}^{\ell \times 1}$ such that $x = Ay$. Considering $\hat{y} = B^{-1}y$, we note that $x = ABB^{-1}y = (AB)\hat{y}$ and so $x \in S_2$. If $x \in S_2$ then there exists $y \in \mathbb{R}^{\ell \times 1}$ such that $x = (AB)y$. We note that $x = A(By)$ and so $x \in S_1$. This shows that the spaces generated by the columns of A and AB coincide and hence $\text{rank}(A) = \text{rank}(AB)$.

Similarly we prove that if A is a $k \times \ell$ matrix and B is a full-rank $k \times k$ matrix then $\text{rank}(BA) = \text{rank}(A)$. Let S_1 be the space generated by the rows of A and S_2 the space generated by the rows of BA . If $x \in S_1$ then there exists $y \in \mathbb{R}^{1 \times k}$ such that $x = yA$. Considering $\hat{y} = yB^{-1}$ we note that $x = yB^{-1}BA = \hat{y}(BA)$ and so $x \in S_2$. If $x \in S_2$ then there exists $y \in \mathbb{R}^{1 \times k}$ such that $x = y(BA)$. We note $x = (yB)A$ and so $x \in S_1$. This shows that the spaces generated by the rows of A and AB coincide and hence $\text{rank}(A) = \text{rank}(BA)$.

We know that the rank of a diagonal matrix is equal to the number of its nonzero entries. We also note that in the decomposition $A = U \Sigma V^*$, U and V^* have full rank. Therefore, $\text{rank}(A) = \text{rank}(\Sigma) = r$ where r is the number of nonzero singular values. \square

B2

Let $x \in \mathbb{R}^{m \times n}$ be such that $|X_{ij}| \leq \varepsilon$ for all $i \in \{1, \dots, m\}$ and $j \in \{1, \dots, n\}$. Let $\|X\|_2$ be the 2-norm of X and let $\|X\|_F$ be its Frobenius norm. We show that $\|X\|_2 \leq \|X\|_F \leq \sqrt{mn}\varepsilon$.

Proof. First, we show the first inequality. We know from the lecture notes that

$$\begin{aligned}\|X\|_2 &= \sigma_{\max}, \\ \|X\|_F &= \left[\sum_i \sigma_i^2 \right]^{1/2},\end{aligned}$$

where σ_i are the singular values of X . From this, it is immediately clear that $\|X\|_2 \leq \|X\|_F$.

Next, we use an equivalent form of the Frobenius norm to show the second inequality:

$$\|X\|_F = \left[\sum_{i,j} |X_{ij}|^2 \right]^{1/2}.$$

Knowing that $|X_{ij}| \leq \varepsilon$, it is immediate that $\|X\|_F \leq \left[\sum_{i,j} \varepsilon^2 \right]^{1/2} = [mn\varepsilon^2]^{1/2} = \sqrt{mn}\varepsilon$. This concludes the proof. \square

We also give an example where these bounds are tight. Indeed, consider the matrix $X = \varepsilon \in \mathbb{R}^{1 \times 1}$. Clearly, we have $|X_{ij}| \leq \varepsilon$ for all i, j (only one value is possible for each). We know that the only singular value of this matrix is ε , and hence

$$\|X\|_2 = \|X\|_F = \sqrt{1 \cdot 1}\varepsilon = \varepsilon.$$

B3

We start by observing that if $B = A + X$, then by Theorem 3.28 in the lecture notes, we can write

$$\begin{aligned}\sigma_{\min(m,n)-j+1}(B) &= \min_{\mathcal{S}_j} \max_{x \in \mathcal{S}_j \setminus \{0\}} \frac{\|Bx\|_2}{\|x\|_2} \\ &= \min_{\mathcal{S}_j} \max_{x \in \mathcal{S}_j \setminus \{0\}} \frac{\|(A+X)x\|_2}{\|x\|_2} \\ &\leq \min_{\mathcal{S}_j} \max_{x \in \mathcal{S}_j \setminus \{0\}} \left(\frac{\|Ax\|_2}{\|x\|_2} + \frac{\|Xx\|_2}{\|x\|_2} \right) \\ &\leq \sigma_{\min(m,n)-j+1}(A) + \sigma_{\min(m,n)-j+1}(X).\end{aligned}$$

However, we know that A has rank r , and hence by the result of B1, we find that if $\min(m,n) - j + 1 > r$, the singular value of A in the expression is zero, and hence that

$$\begin{aligned}\sigma_{\min(m,n)-j+1}(B) &\leq \sigma_{\min(m,n)-j+1}(X) \\ &\leq \sqrt{mn}\varepsilon,\end{aligned}$$

where the last inequality is a consequence of B2.

A criterion that can then be used to estimate the rank r of A is then to take the smallest r such that $\sigma_{r+1}(B) \leq \sqrt{mn}\varepsilon$. This is very similar to the description given on p. 60 of the lecture notes, concerning the numerical rank of the matrix A .

Exercise C: Realization theory

In this last exercise, we are interested in finding an AR model corresponding to the data obtained during the coronavirus pandemic. Indeed, we want to find the parameters α_i of

$$y(t) = \alpha_0 + \sum_{i=1}^p \alpha_i y(t-i)$$

Let us rewrite the problem as a system of linear equations:

$$\begin{pmatrix} 1 & y(p-1) & y(p-2) & \dots & y(0) \\ 1 & y(p) & y(p-1) & \dots & y(1) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & y(N-1) & y(N-2) & \dots & y(N-p) \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_p \end{pmatrix} = \begin{pmatrix} y(p) \\ \vdots \\ y(N) \end{pmatrix} \quad (2)$$

Note that we consider $\hat{y}(0) = y(0), \dots, \hat{y}(p-1) = y(p-1)$ as initial conditions.

We want to solve the system (2) to obtain an estimate of the optimal parameters α_i . We call A the matrix and we observe that it usually has more lines than columns. Therefore, it is of interest to solve the system using the least squares method. To do so, we can use what we obtained in question A2 to solve the problem with a QR decomposition and backward substitution. Indeed, we must simply solve the triangular system :

$$Rx = \hat{Q}^\top b,$$

where \hat{Q} and R are derived from the QR decomposition of A .

We consider two cases: the lockdown mode and the social distancing mode. Moreover, for each case, we divide the data set into a training set (70 % of the data) and a validation set (30 % of the data).

Considering one mode, (2) has to be solved using the data of the training set. Next, an estimate y that we call \hat{y} can be reconstructed using the AR model equation. The first p components of \hat{y} are given by the initial conditions and then the next components are constructed based on the previously computed estimates:

$$\hat{y}(t) = \alpha_0 + \sum_{i=1}^p \alpha_i \hat{y}(t-i)$$

The error between the true y and the estimate \hat{y} can be computed on both the training and validation set. This allows one to judge the quality of the model.

Next, we show the results we obtained while varying the parameter p .

Lockdown mode First, we study the lockdown mode. As one can see in Figure 1, when the parameter p increases, the training error has a tendency to decrease. Indeed, the AR model that we obtain is able to better represent our training set data as the size of the history grows.

Then, in Figure 2, we observe that the validation error decreases (approximatively) until $p = 19$, and from then on, the error rises again. Through this, we can understand that around $p = 20$, the model starts “overfitting” our training set, and so it gives a good approximation for the training set but performs poorly on the validation set.

Social distancing mode In the social distancing mode, we can make the same observations (in Figures 3 and 4) as in the previous mode: the error in the training set decreases when p increases except at some peaks. For the validation set, we once again observe overfitting when p is higher than 19.

Discussion

In both modes, we have confirmed our intuition that the error in the training set should decrease. However, it is not monotonic and we still observe some peaks. One way to try to explain this is that when we solve the least squares problem, we minimize the error between the real values $y(t)$ and $\hat{y}(t) = f(y(t-1), \dots, y(t-p))$: $e_1 = \|y - \hat{y}\|_2$. However, when we compute the error on the training set, we consider $\tilde{y}(t) = f(\tilde{y}(t-1), \dots, \tilde{y}(t-p))$: $e_2 = \|\tilde{y} - \hat{y}\|_2$, and so we propagate the errors along the time t . Clearly, this last error e_2 is bigger than the first one e_1 . So our intuition that the error should decrease monotonically only applies to the error e_1 (which we have indeed observed) and not to e_2 .

Then, about the validation set errors, we can conclude that overfitting a training set doesn't yield good results for future predictions.

Note that in the analysis above, we only considered values of p such that the linear system of equations has more rows than columns. In the case that we have more columns than rows, our system is underdetermined and so solving the system yields an infinity of solutions that are exact (if there are no linear combinations in the rows of course) which means that our training error is zero in theory (in practice, we have errors of order 10^{-4} , for the confinement mode, and 10^{-9} for the social distancing mode, due to numerical imprecisions). For the validation error, we still overfit, so the error is very big for both modes.

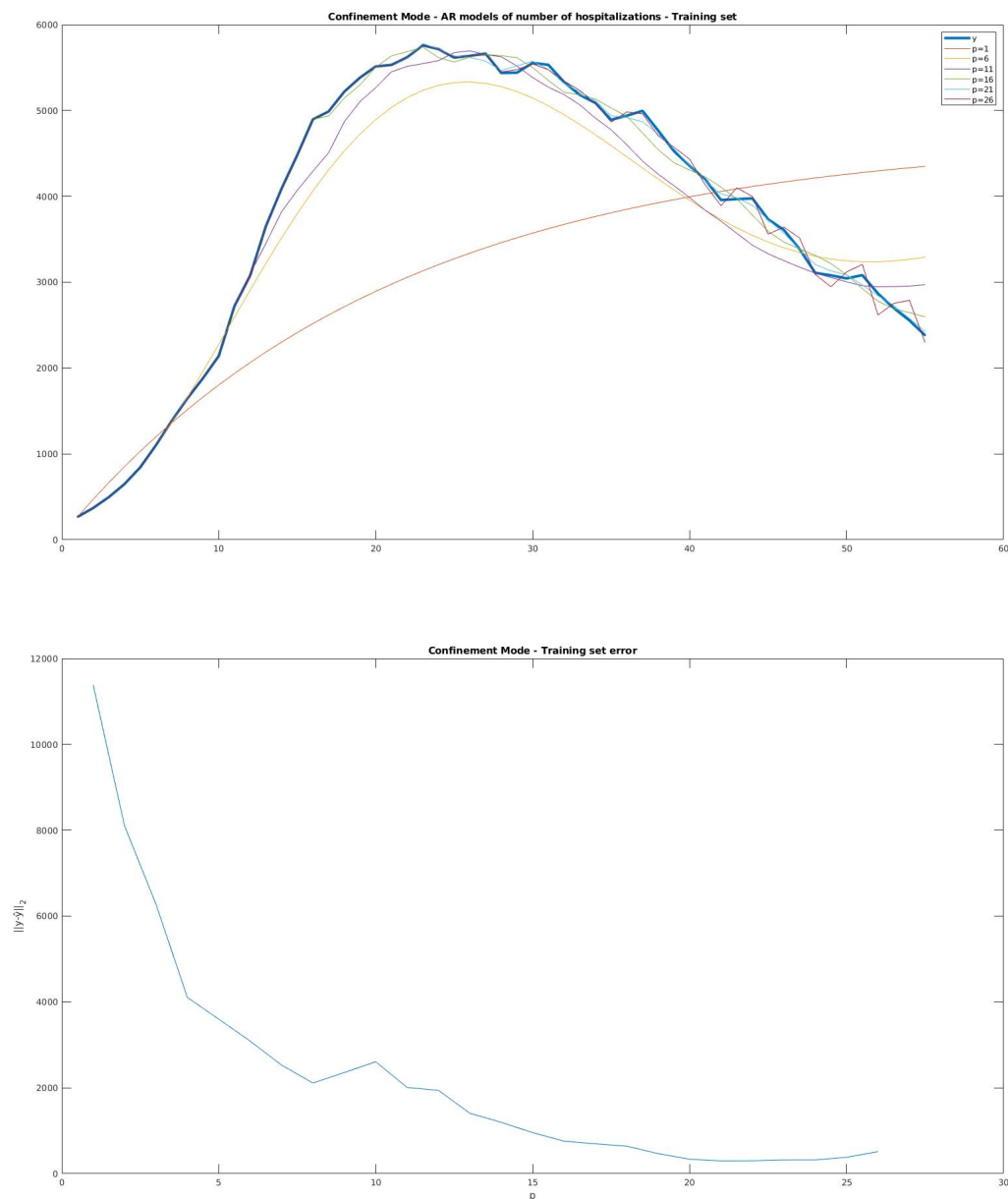


Figure 1: Lockdown mode: training set predictions and error using the AR model, for different values of p .

Bonus question

If we approximate the model in real time with data that we receive at fixed intervals, we will have to solve a new “full-size” least squares problem everytime we want to include new data to improve the system. This can be expensive especially if the system is big.

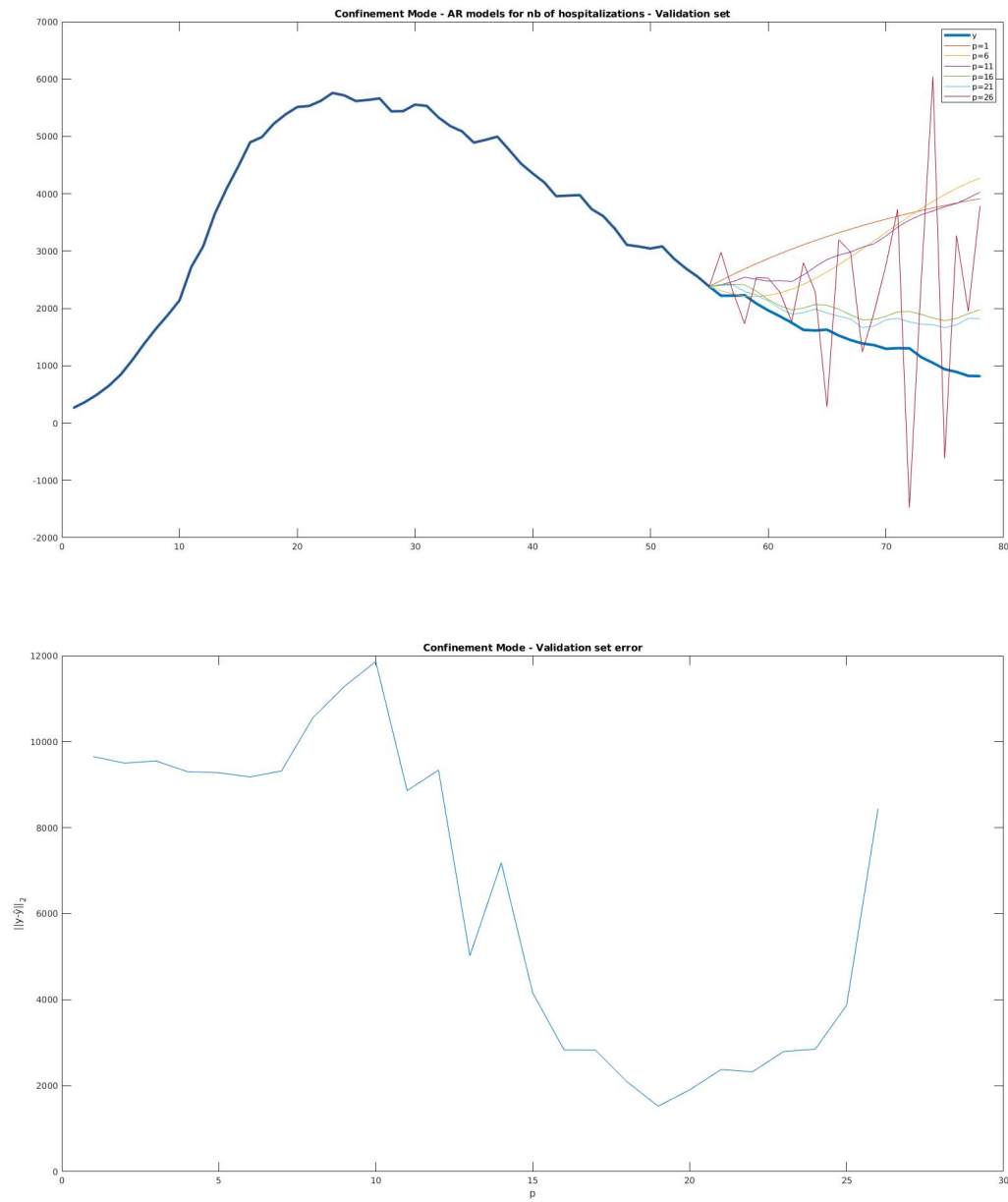


Figure 2: Lockdown mode: validation set predictions and error using the AR model, for different values of p .

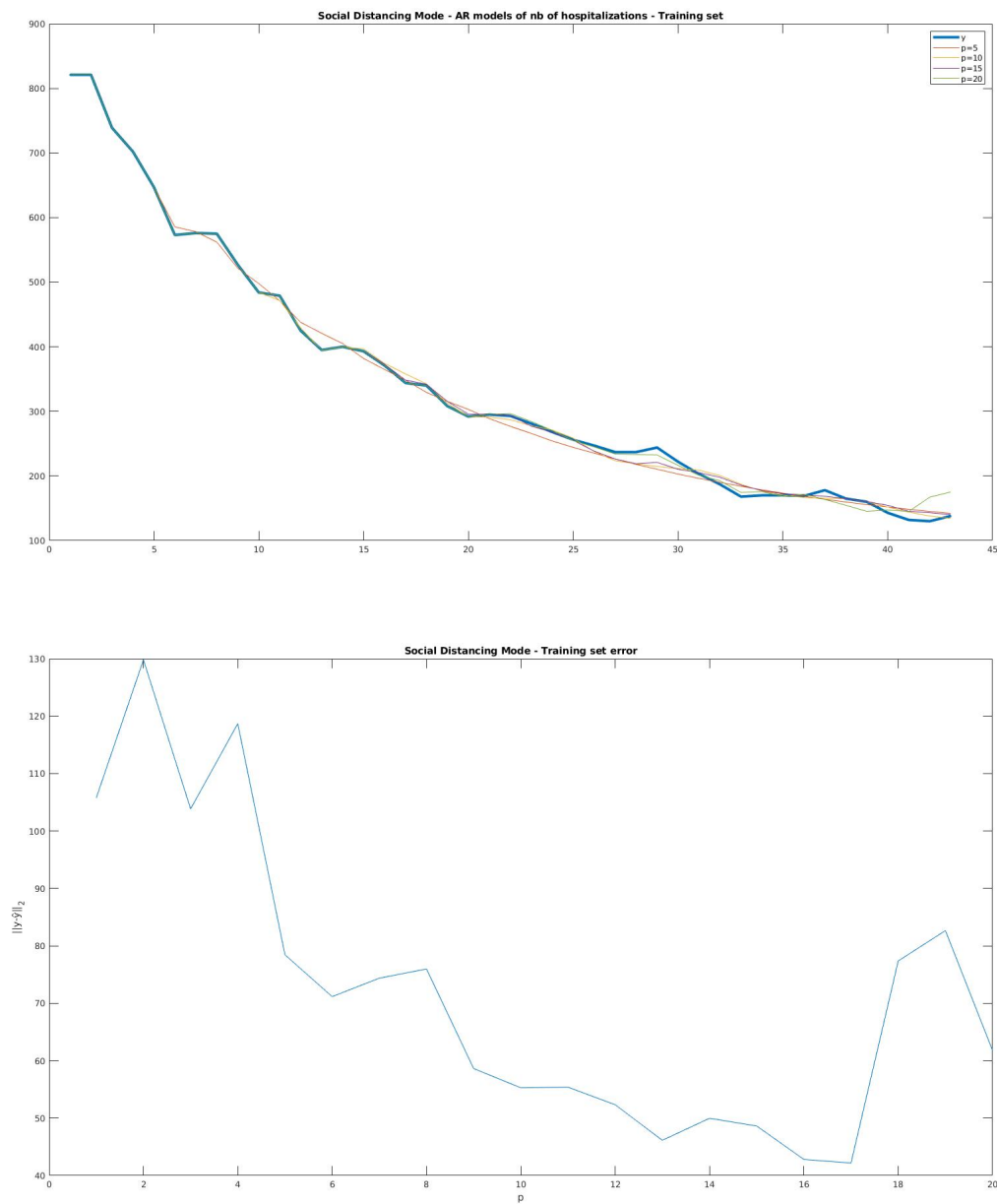


Figure 3: Social distancing mode: training set predictions and error using the AR model, for different values of p .

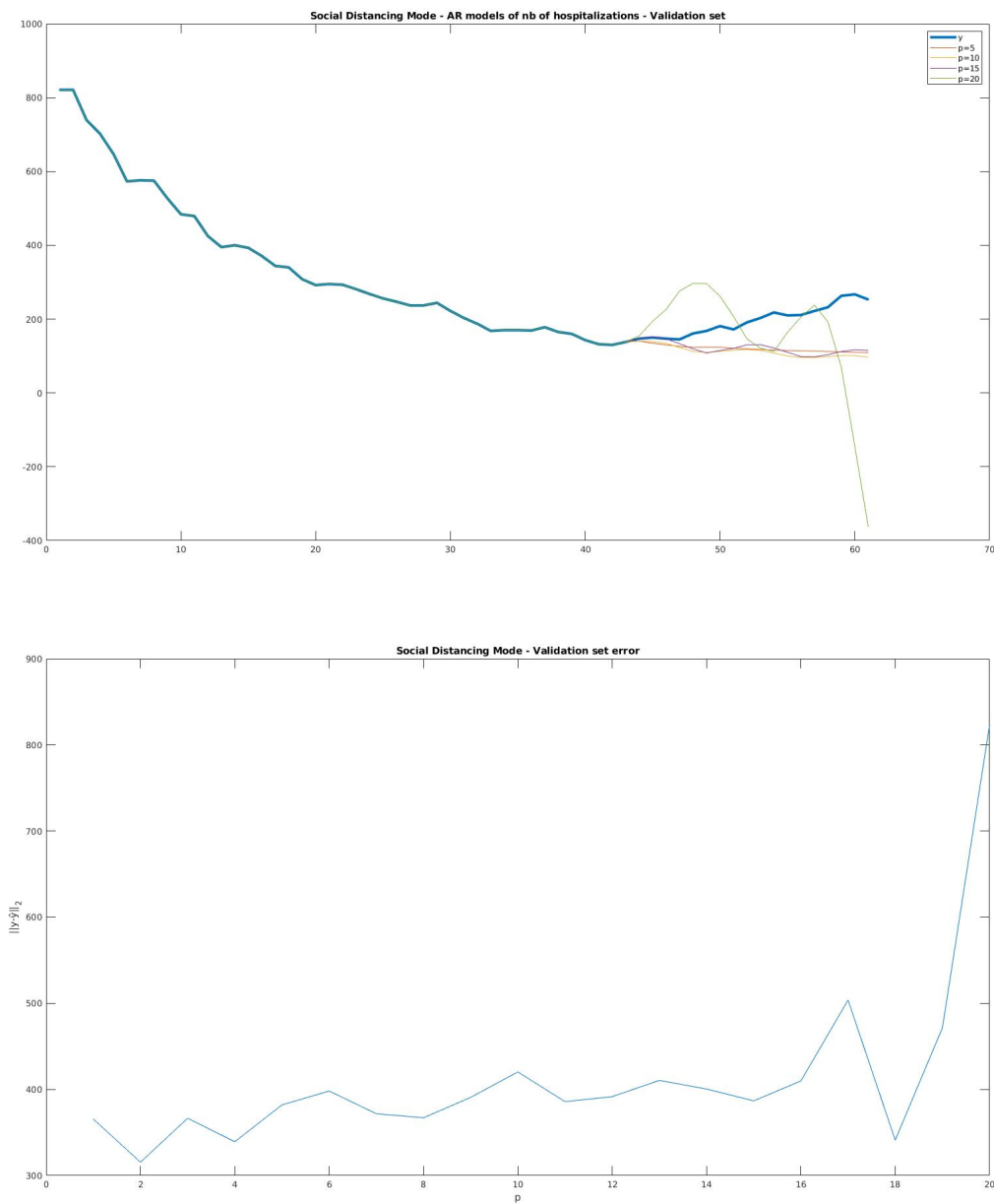


Figure 4: Lockdown mode: validation set predictions and error using the AR model, for different values of p .