CSIC

Simulating lateral flow and its contribution to spatial variations of (rainfed) winter wheat yields

Research state, preliminary results and following steps

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Promoters and supervisors: **José A. Gómez & Elías Fereres**

Conceptual background

Point-based model

(1st routine)

Mechanistic modelling of surface run-off and optimization of hydraulic parameters

+

30 year-sequence

Upscaling method

(LIF prediction)

MLR / ANN

(data-driven method)

training and testing sets

+

30 year-sequence

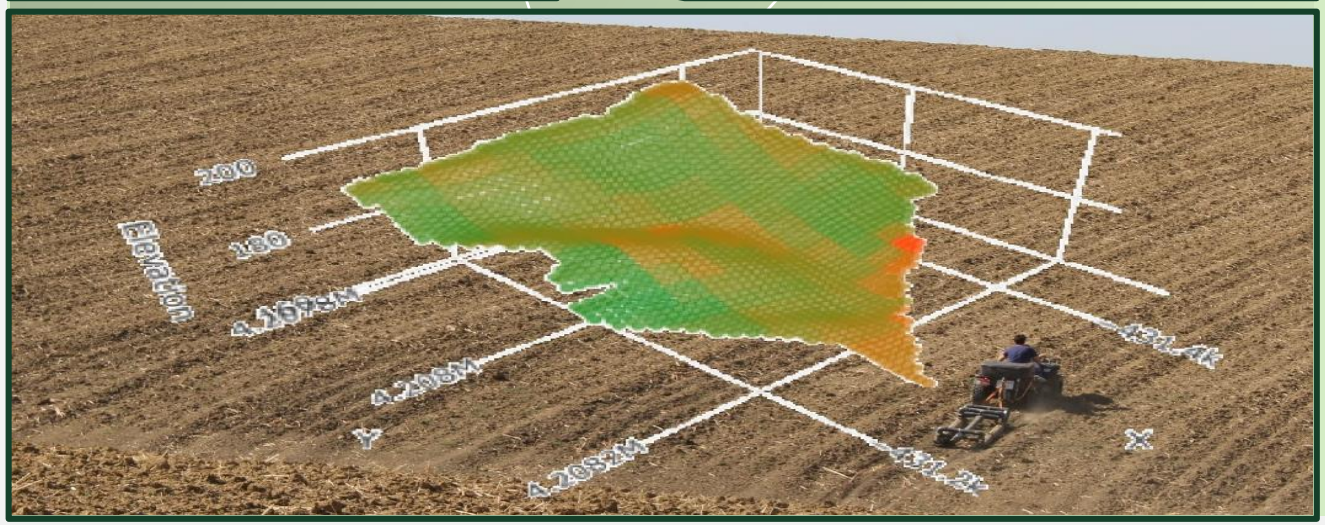
Crop modelling routine

(2nd routine)

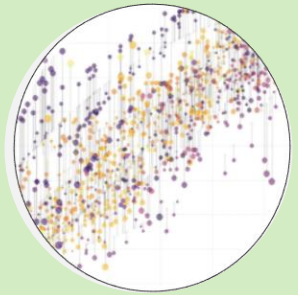
Yield simulations under the 1st vs. 2nd scenario

(with/without LIF)

Probability distribution functions of yield response to LIF

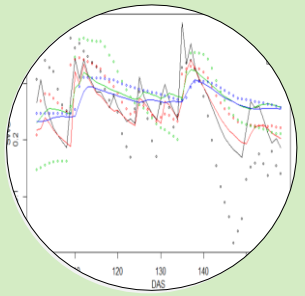


Preliminary results



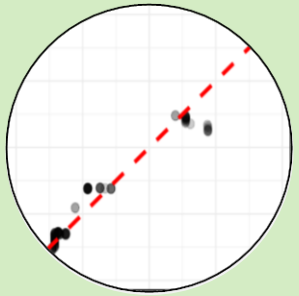
Meta-analysis

Assimilation of NDVI-CC models into HYDRUS-1D



Field datasets

Soil parameterization, root growth rates, phenological development, crop growth and crop management



Upscaling methods

Multiple Linear Reg. models

Artificial Neural Networks

"novel data assimilation algorithms"

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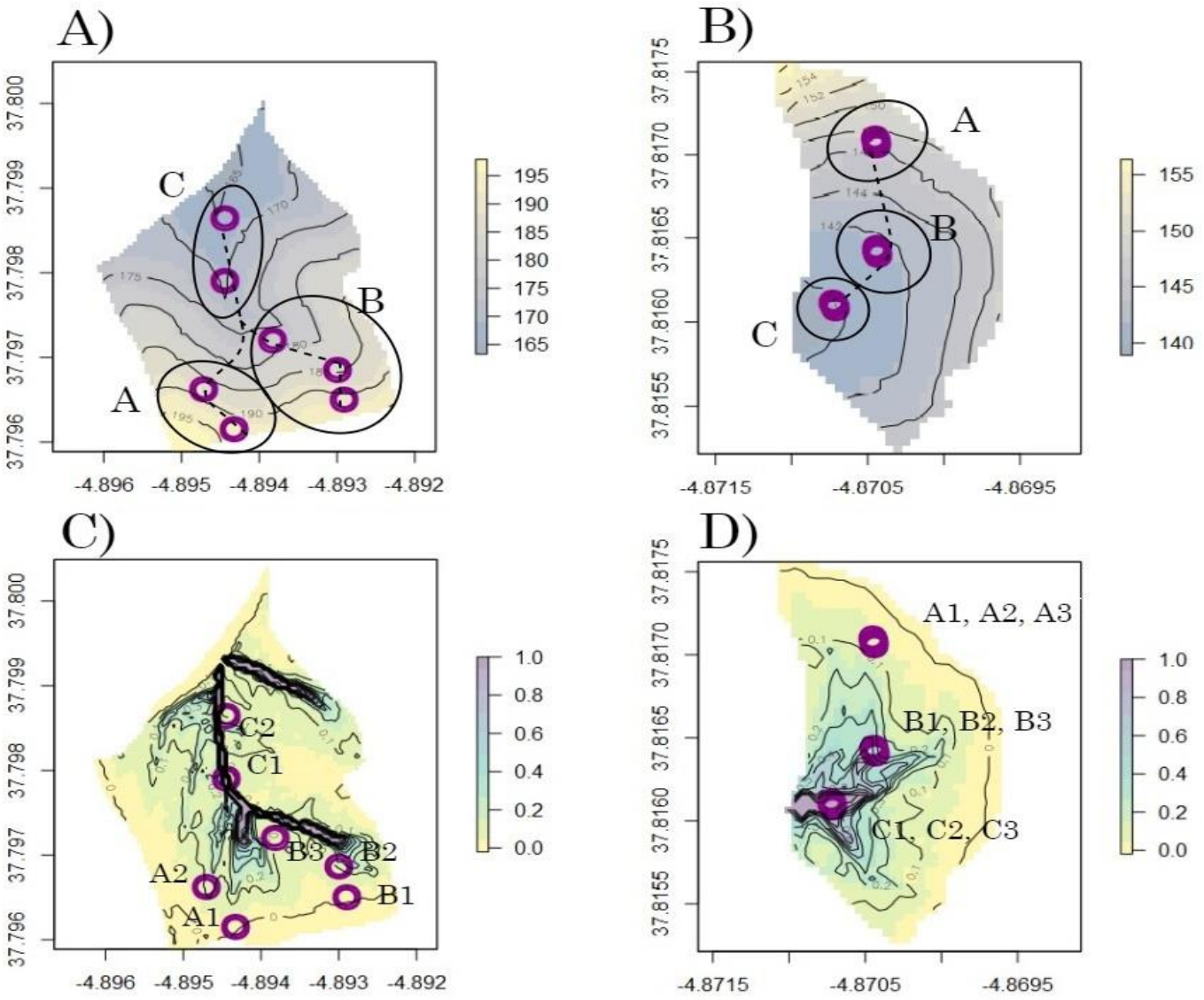
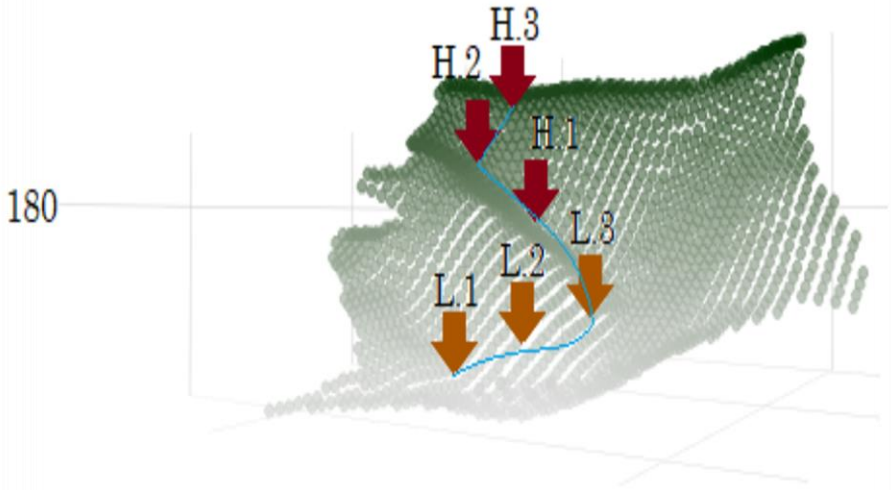
Experimental sites





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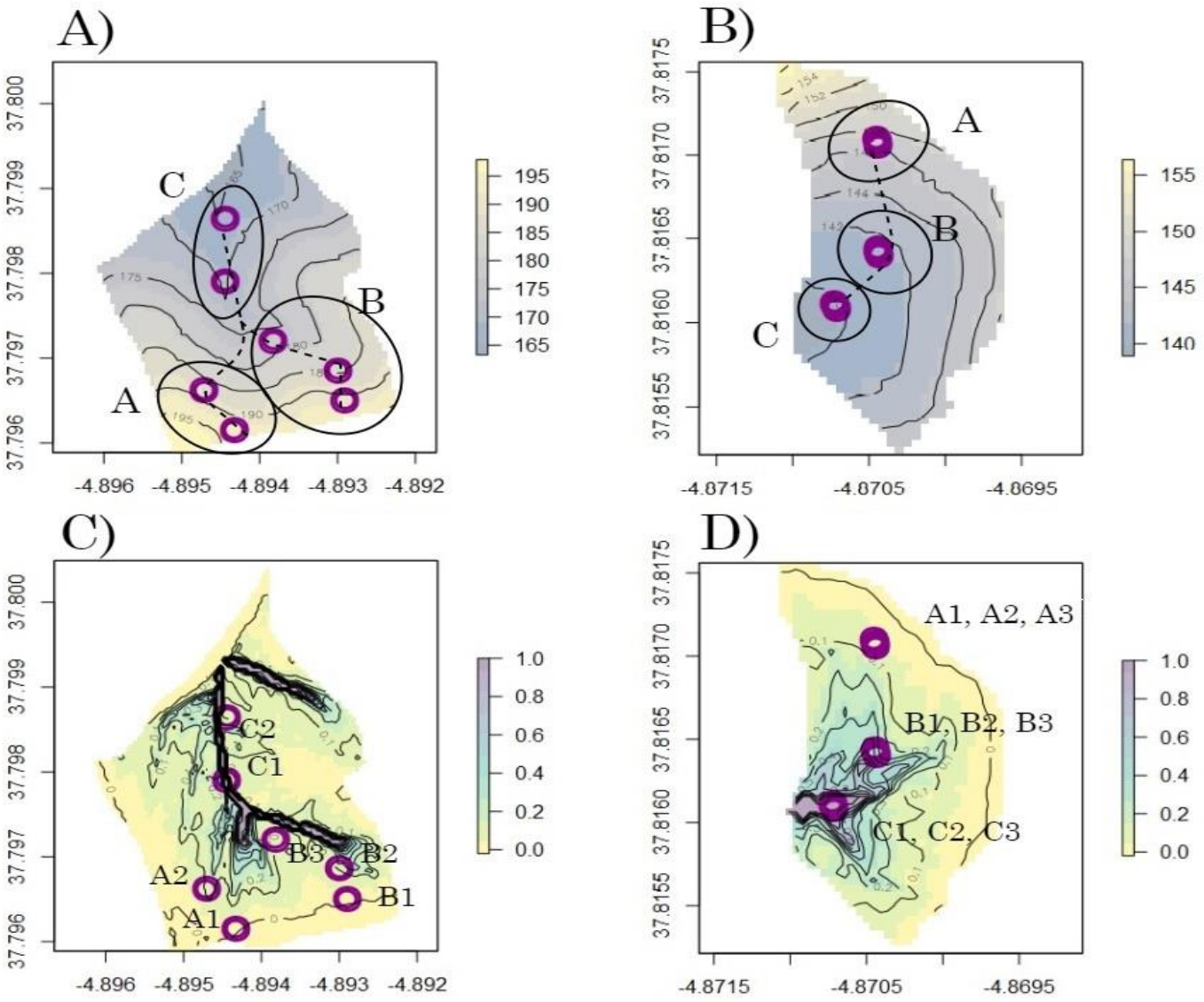
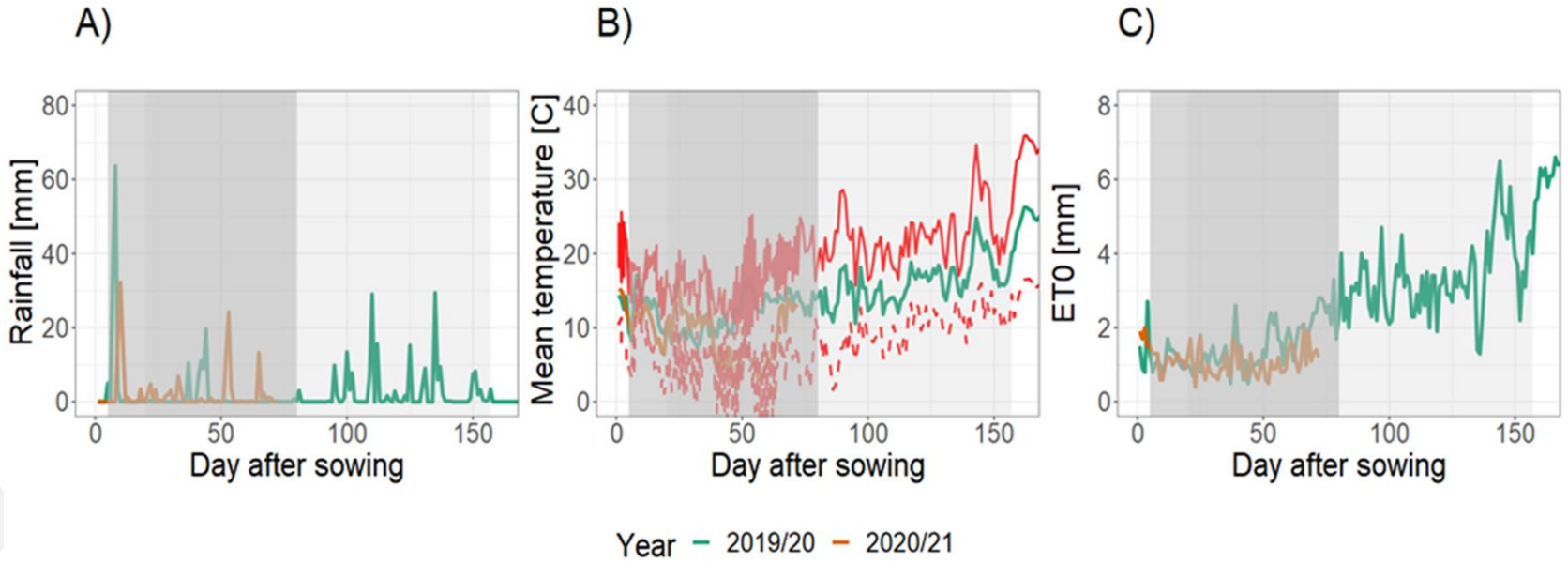
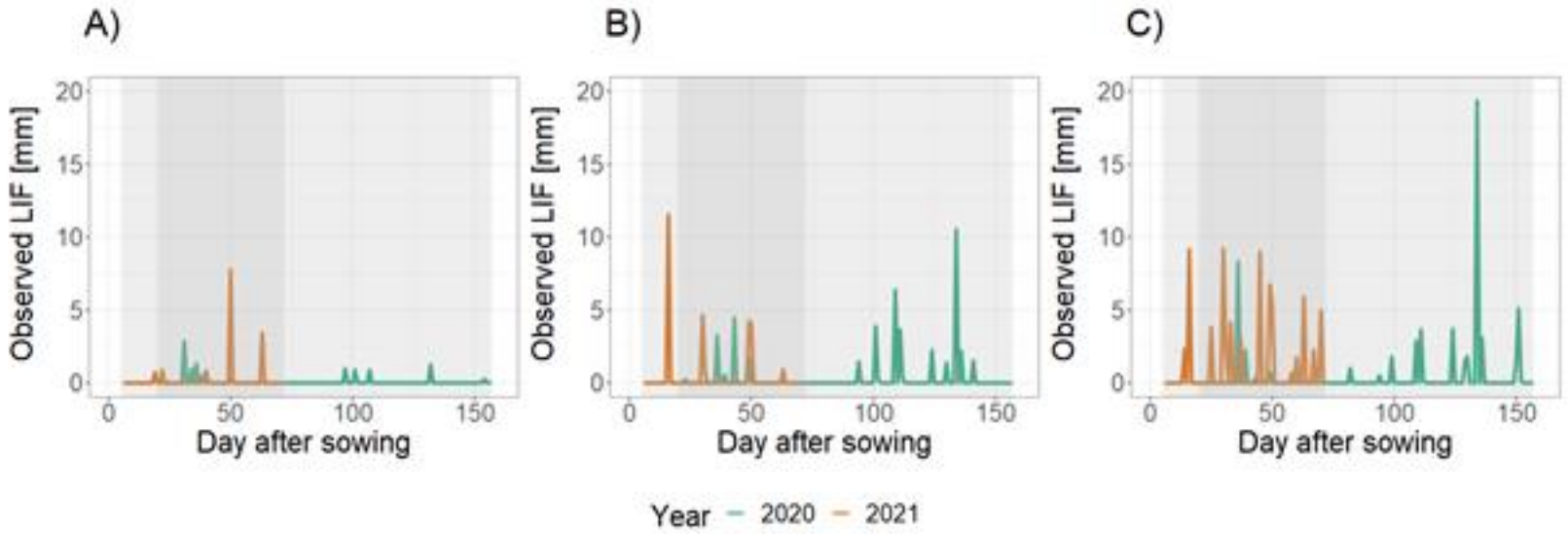


Parameter	Zone	Catchment-1 A	Catchment-1 B	Catchment-1 C	Catchment-2 A	Catchment-2 B	Catchment-2 C
	Sampling points [N]	2	3	2	3	3	3
	[Units]						
Elevation	m (amsl.)	187 (2.4)	184 (5.1)	168 (2.3)	147 (0.5)	141 (0.3)	139 (0.3)
ECa	dS/m	0.31 (0.08)	0.28 (0.09)	0.48 (0.06)	-	-	-
%Clay	%	45 (3.4)	42 (3.3)	50 (3.4)	44 (2.8)		
%Sand	%	18 (2.6)	22 (2.9)	15 (2.8)	22 (3.2)		
Bulk density	g/cm3	1.78 (0.06)	1.81 (0.04)	1.74 (0.05)	1.66 (0.05)		
FAI	[0;1]	0.09 (0.021)	0.12 (0.082)	0.72 (0.218)	0.07 (0.005)	0.42 (0.002)	0.98 (0.011)

Rainfall and meteorological data

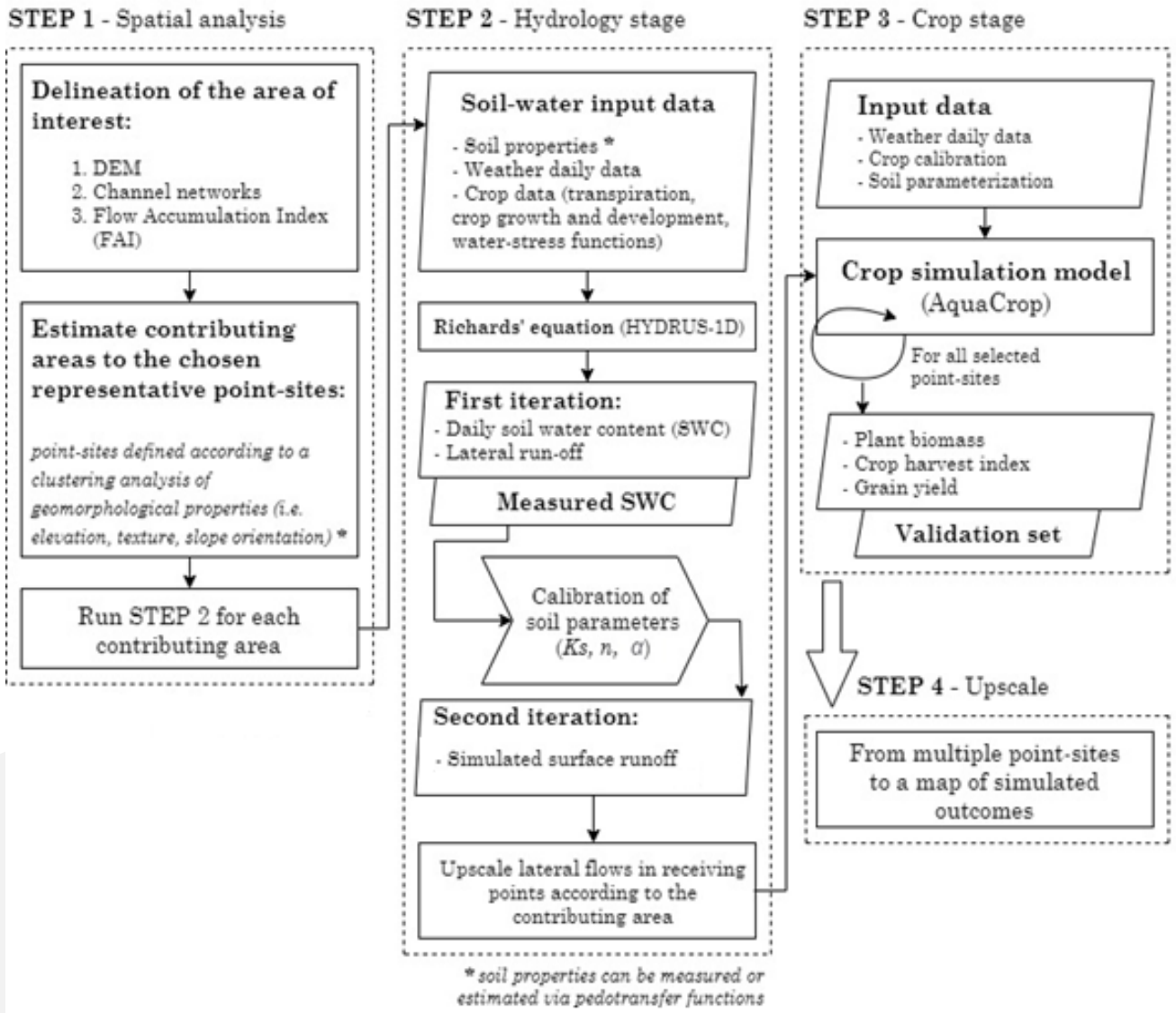


Lateral inflows
(inferred from field observations)

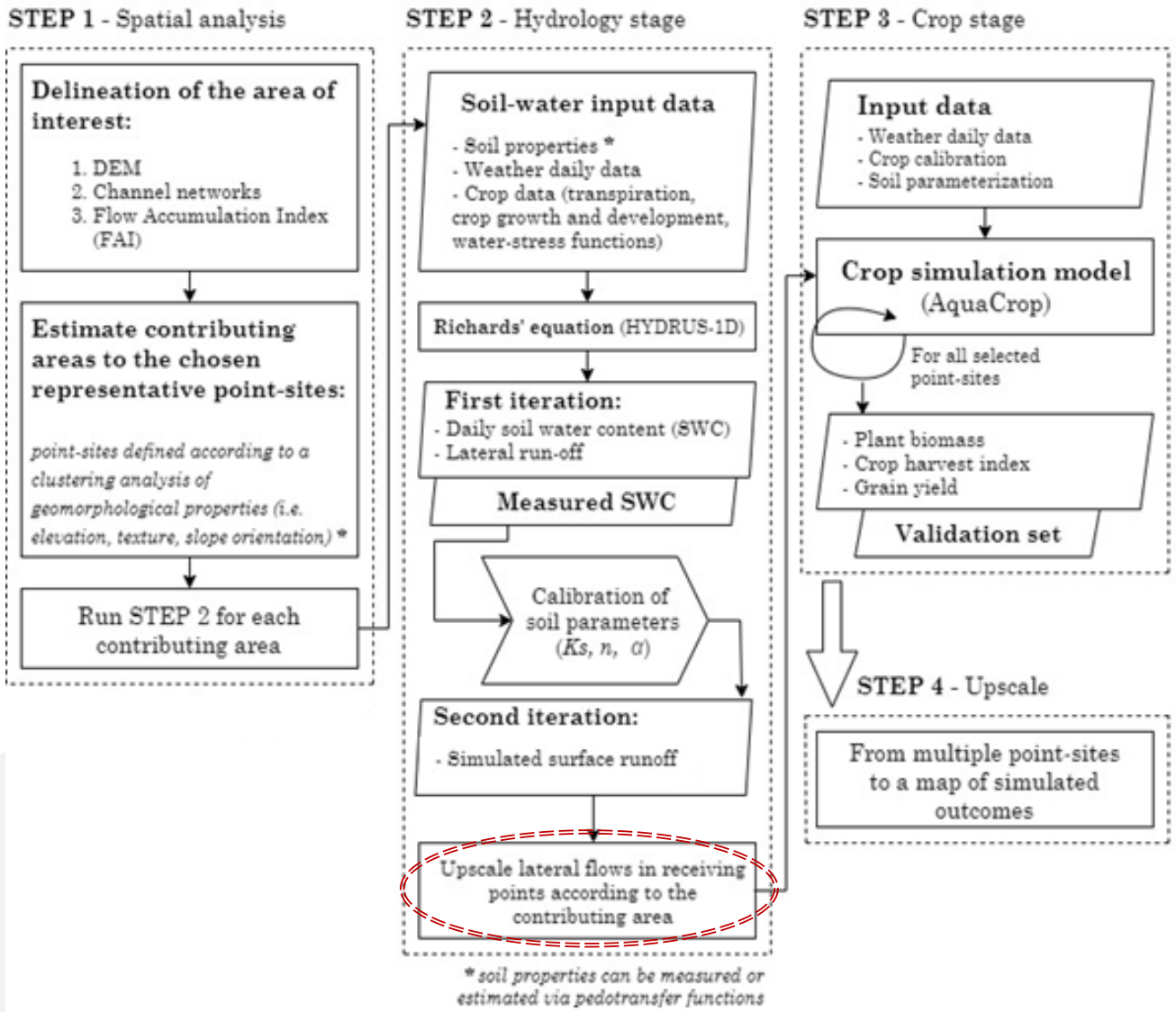


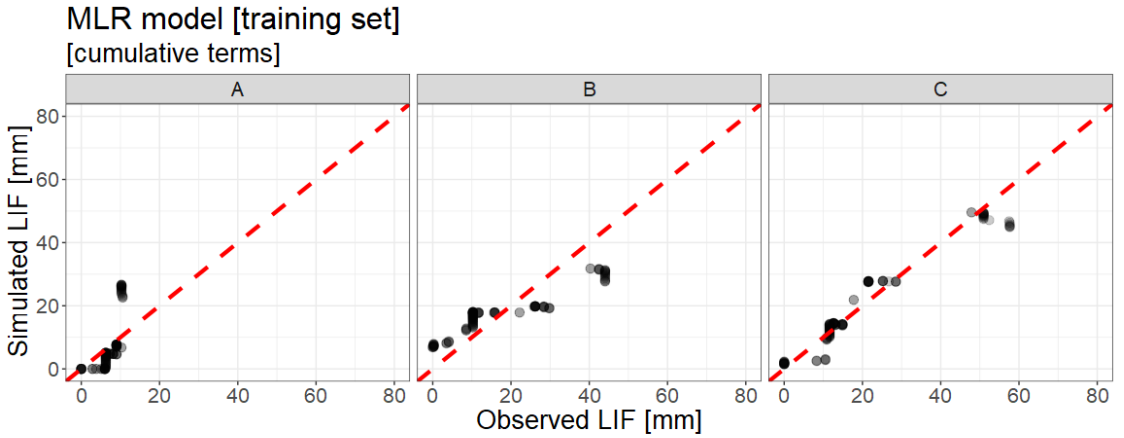
	Zone	Catchment-1 *2019/20*	Catchment-2 *2019/21*	Average *2019-21*
SWC [mm]	A	209.36 (39.6) c	327.46 (22.3) c	257.36 (67.1) c
	B	237.36 (34.4) b	352.06 (10.9) a	269.66 (60.7) b
	C	269.37 (63.1) a	343.41 (12.6) b	299.65 (67.4) a
LIF_n [mm]	A	0.08 (0.46) b	0.21 (1.22) b	0.13 (0.9) b
	B	0.31 (1.52) ab	0.41 (2.3) b	0.35 (1.8) b
	C	0.42 (2.09) a	1.11 (3.3) a	0.70 (2.7) a
$CUM.LIF_n$ [mm]	A	6.98 (3.9) b	4.43 (6.1) c	6.15 (5.5) c
	B	17.88 (15.7) a	16.75 (15.3) b	18.52 (15.8) b
	C	19.76 (16.9) a	34.45 (27.3) a	25.77 (22.9) a

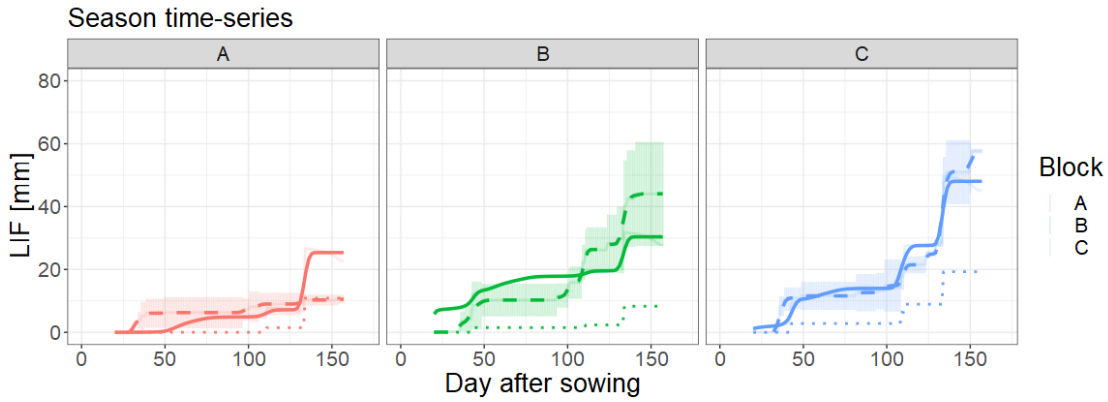
Methodological design



Upscaling methods – "MLR"



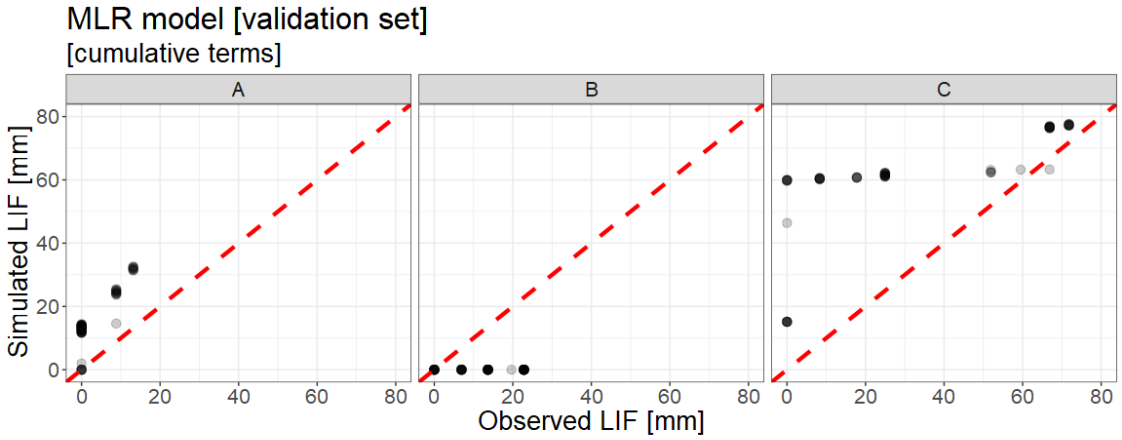


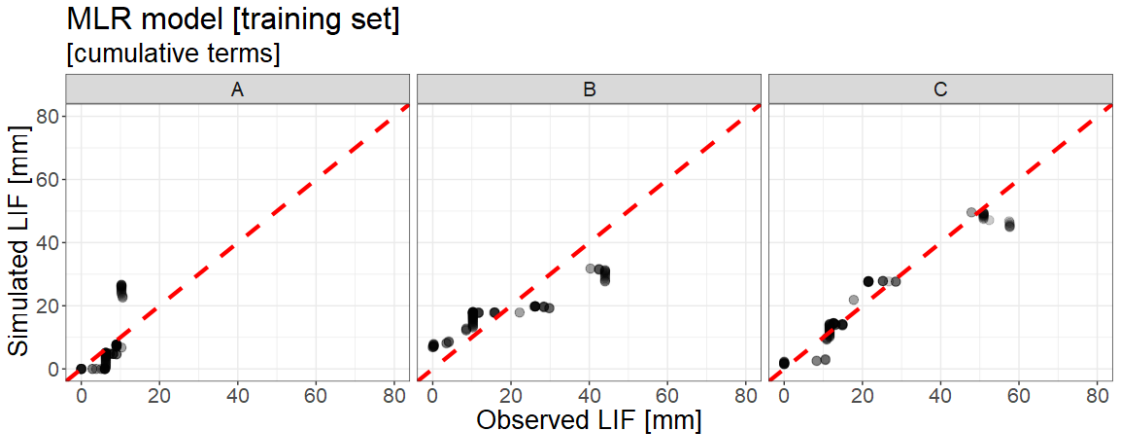


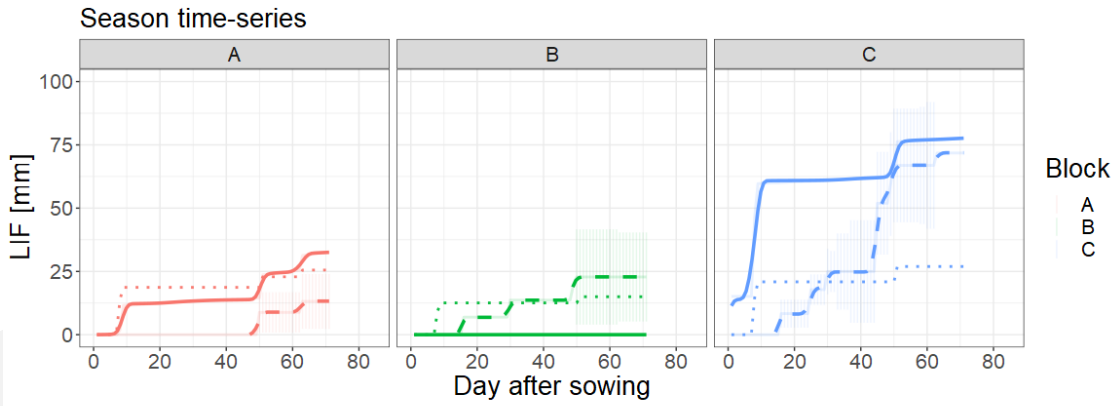
R-sq=0.78 (training)

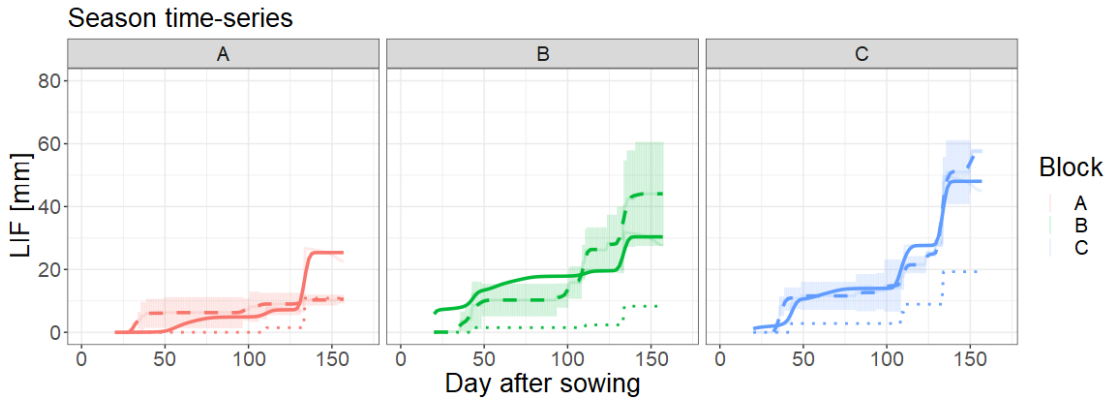
MLR model

(RMSE=21 mm; R-sq=0.78 (training); R-sq=0.48 (testing); Pearson=0.68; d-Willmott index=0.7)



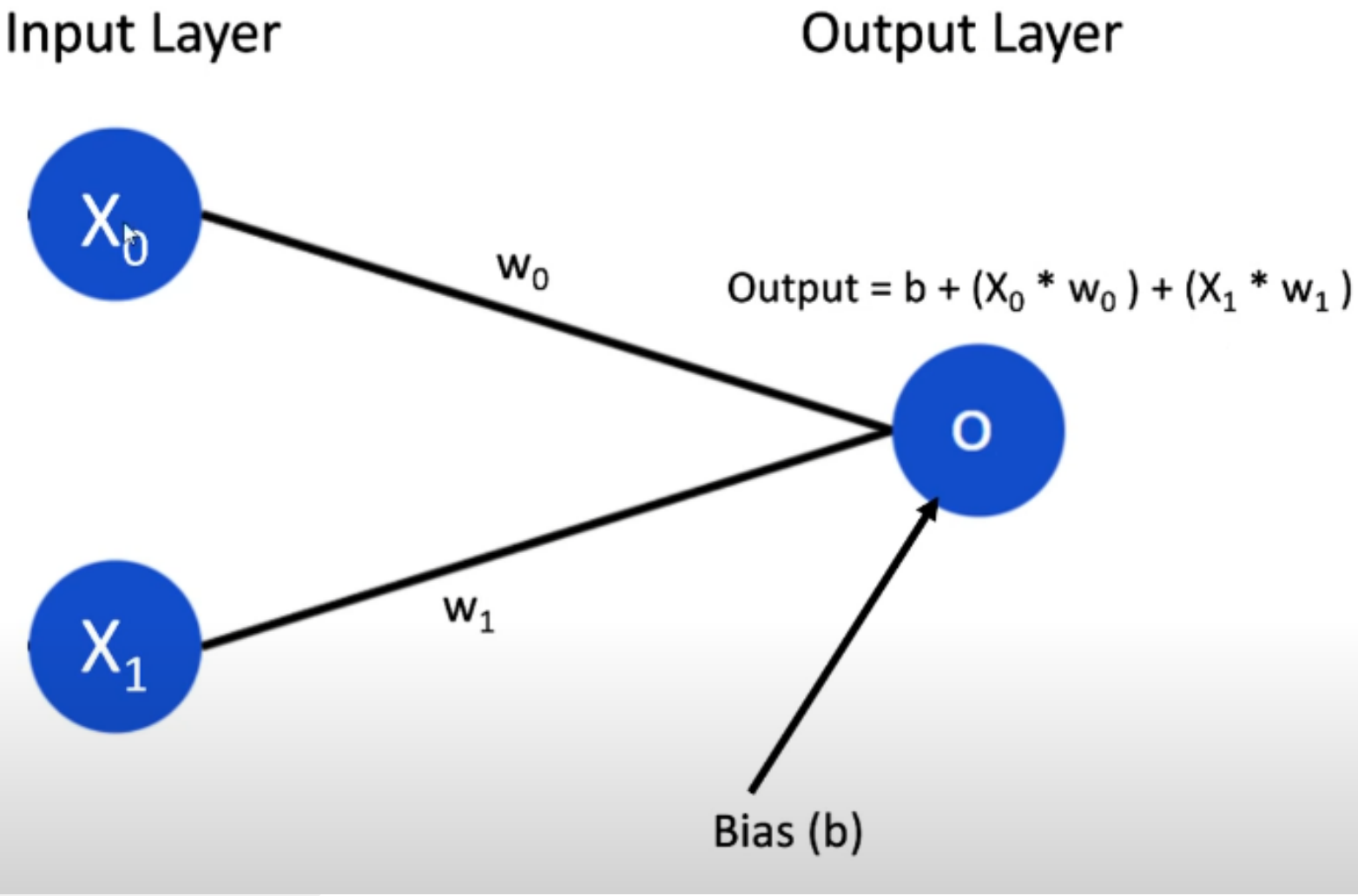






MLR -> ANN

Neural network with no hidden layers is just a linear model

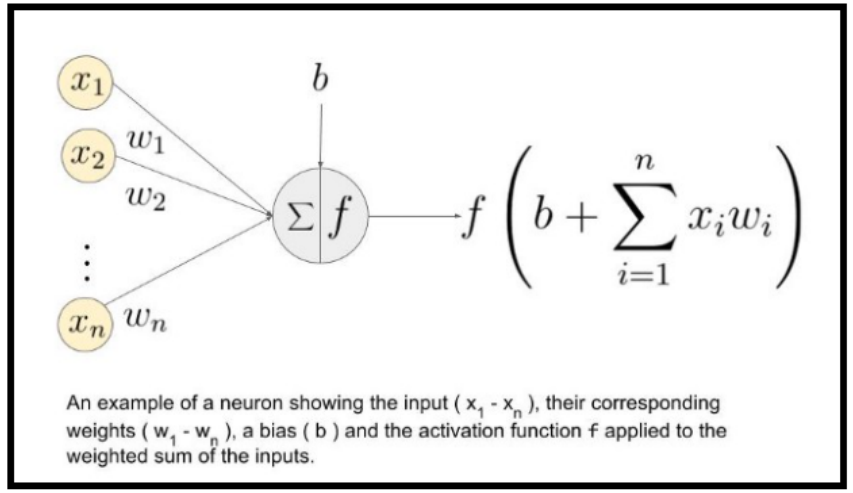


MLR -> ANN

MLR

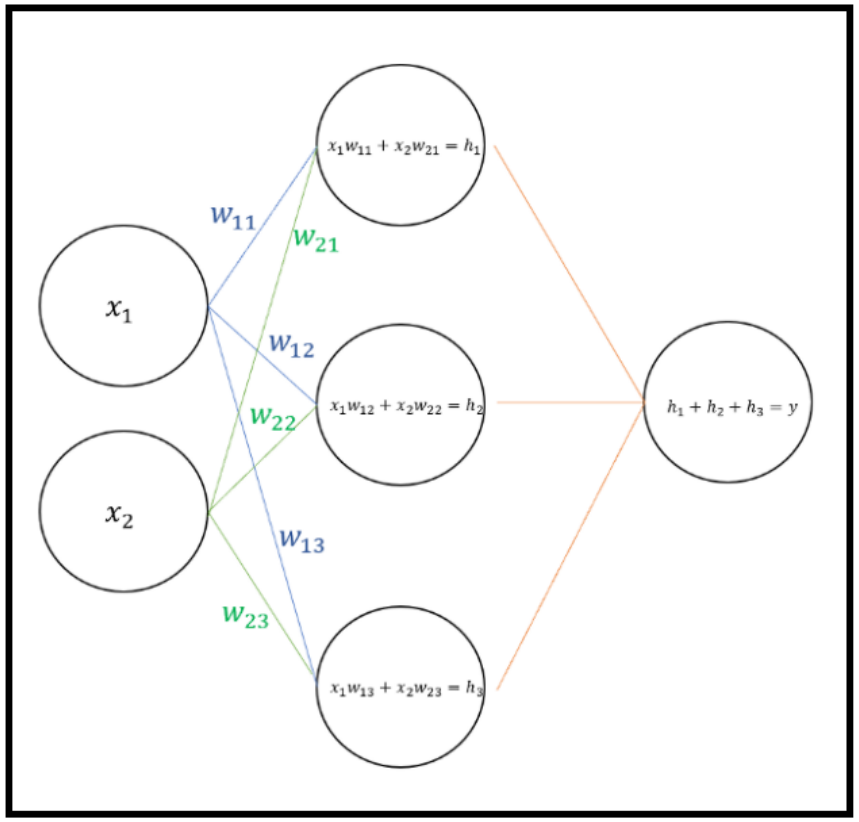
$$y_{pi} = X_i \beta_p + e_{p_i}.$$

The simplest ANN (single neuron)



An example of a neuron showing the input (x_1 - x_n), their corresponding weights (w_1 - w_n), a bias (b) and the activation function f applied to the weighted sum of the inputs.

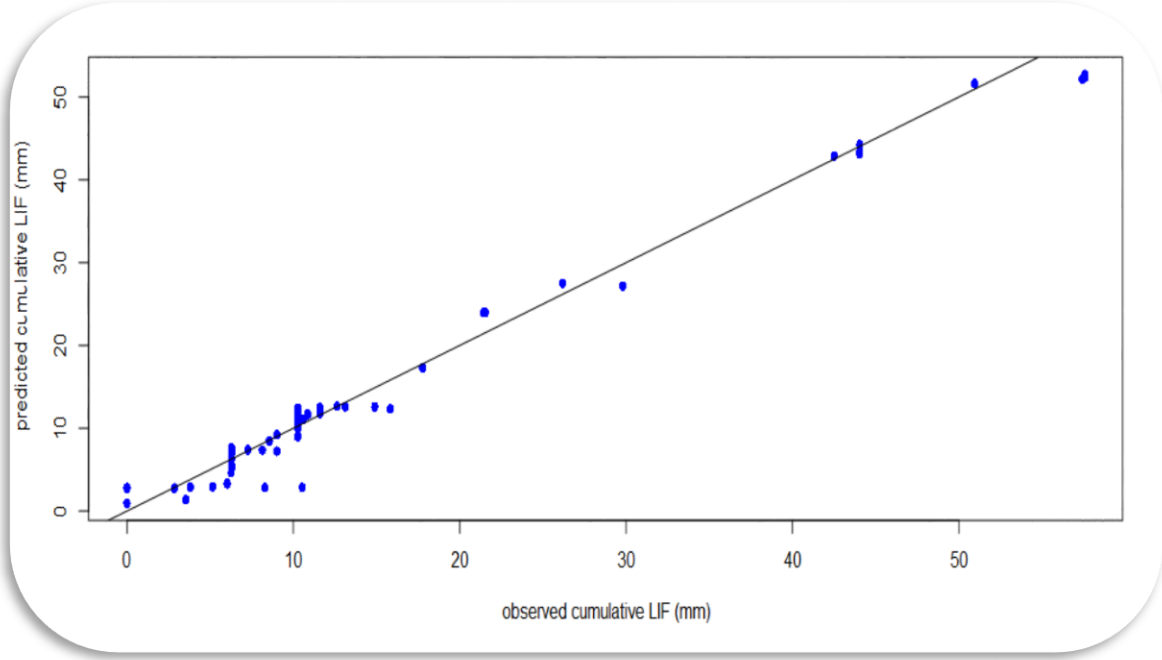
ANN w/3 neurons

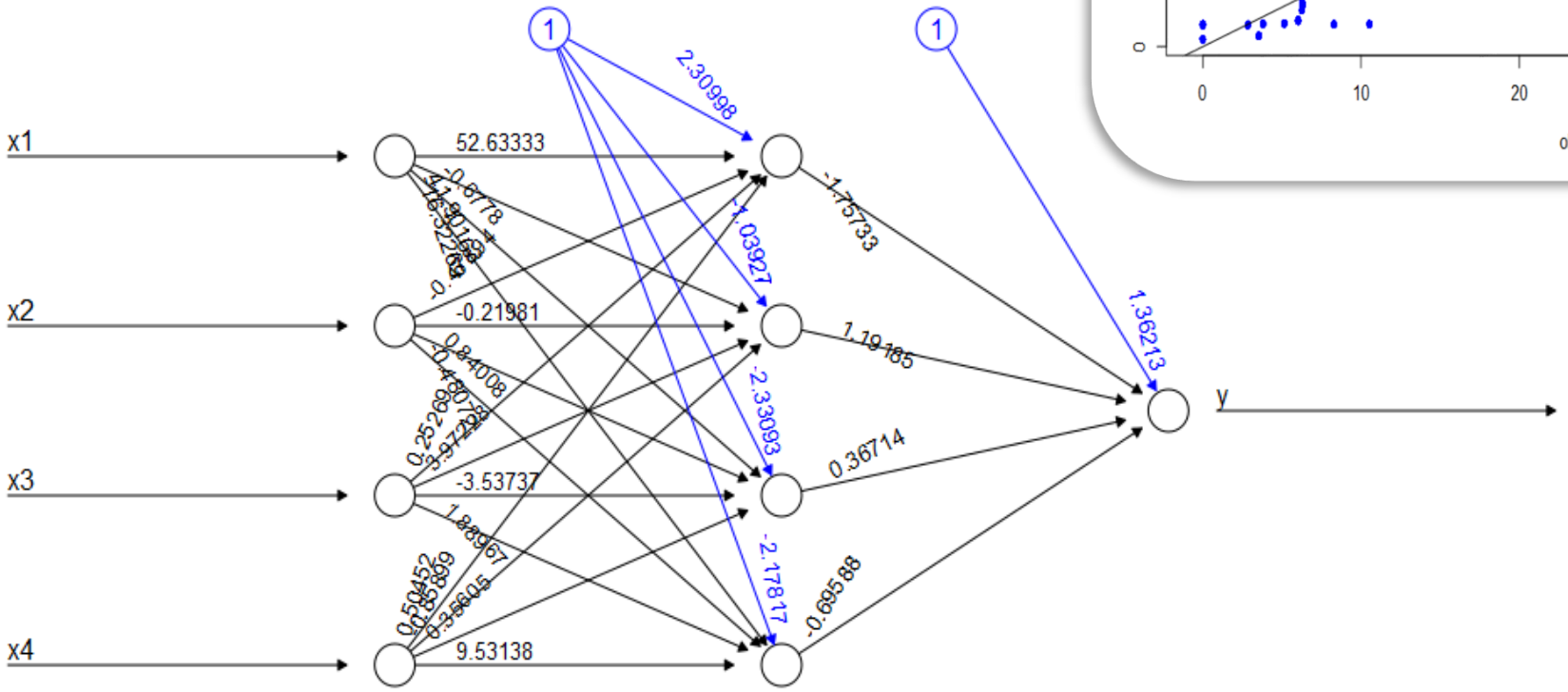


$$[x_1 \quad x_2] \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix} = \begin{bmatrix} x_1 w_{11} + x_2 w_{21} \\ x_1 w_{12} + x_2 w_{22} \\ x_1 w_{13} + x_2 w_{23} \end{bmatrix}' = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix}'$$

ANN – random initialization

(RMSE=3 mm; R-sq=0.93)

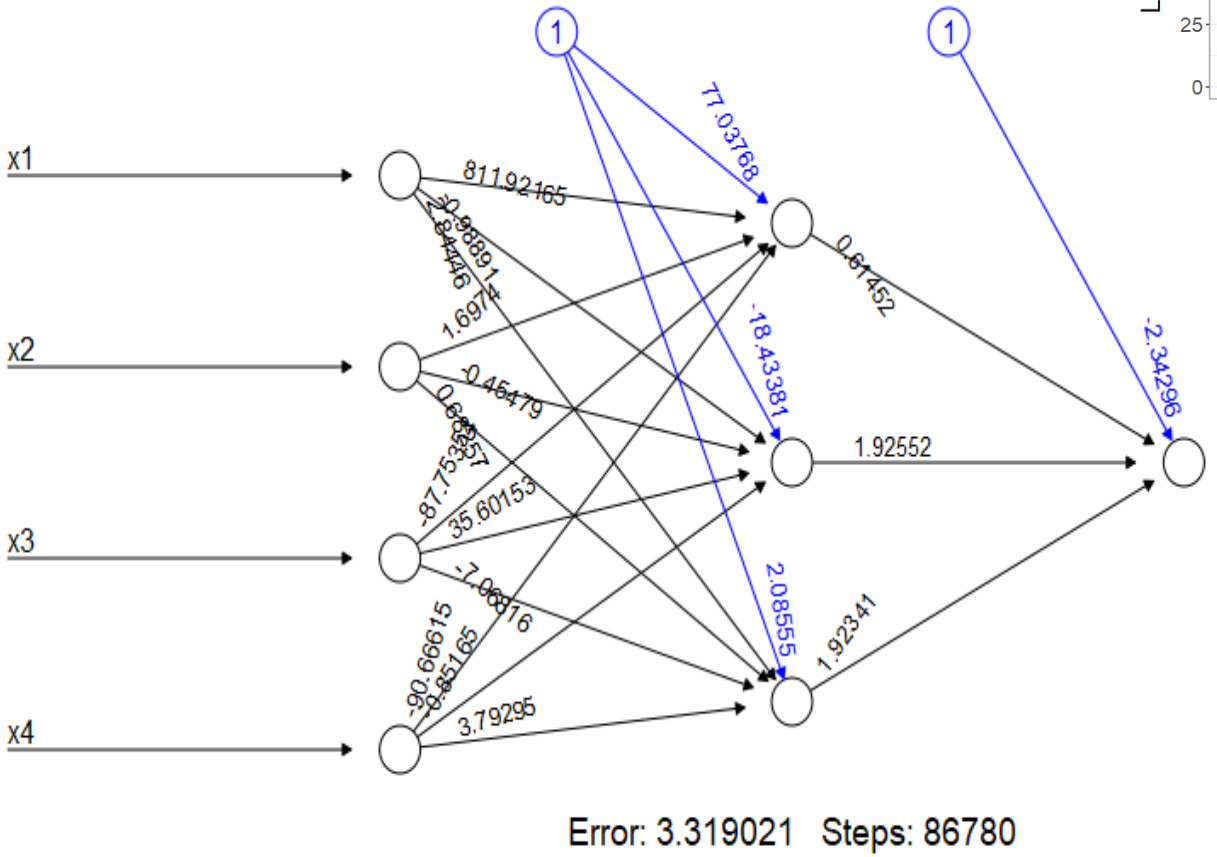


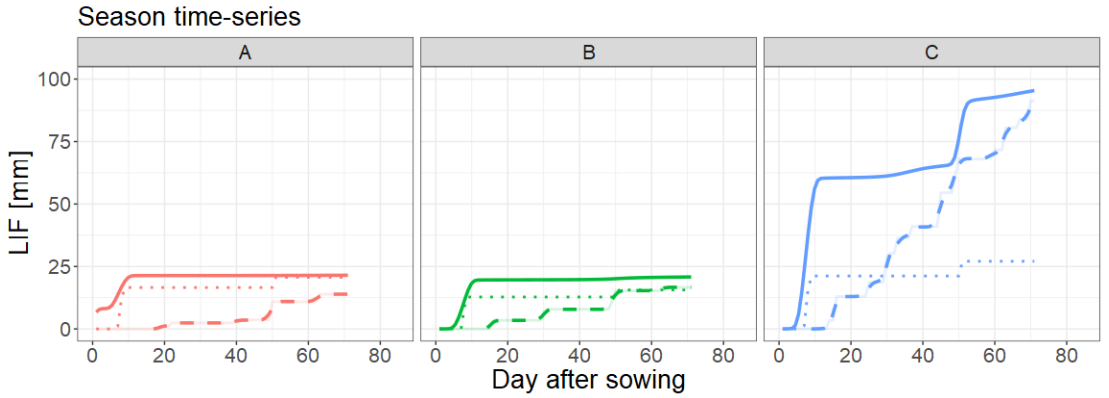


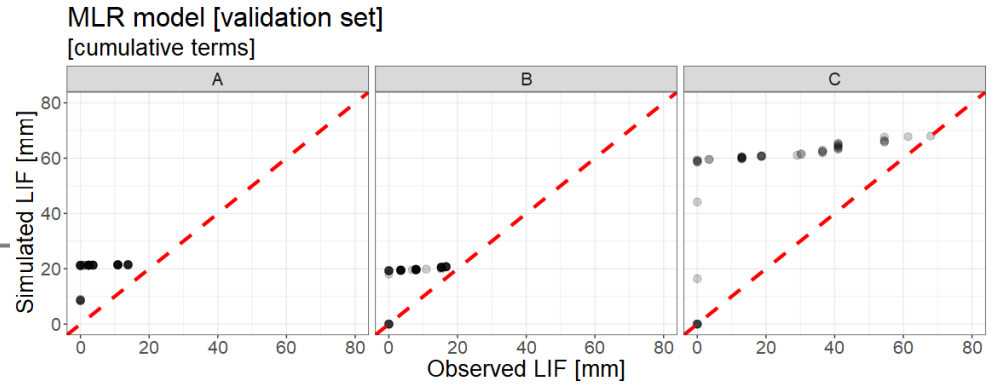
Error: 0.195424 Steps: 1369

ANN – 1st/2nd year sets [train/test]

(RMSE=21 mm; R-sq=0.76; Pearson=0.86; d-Willmott index=0.83)

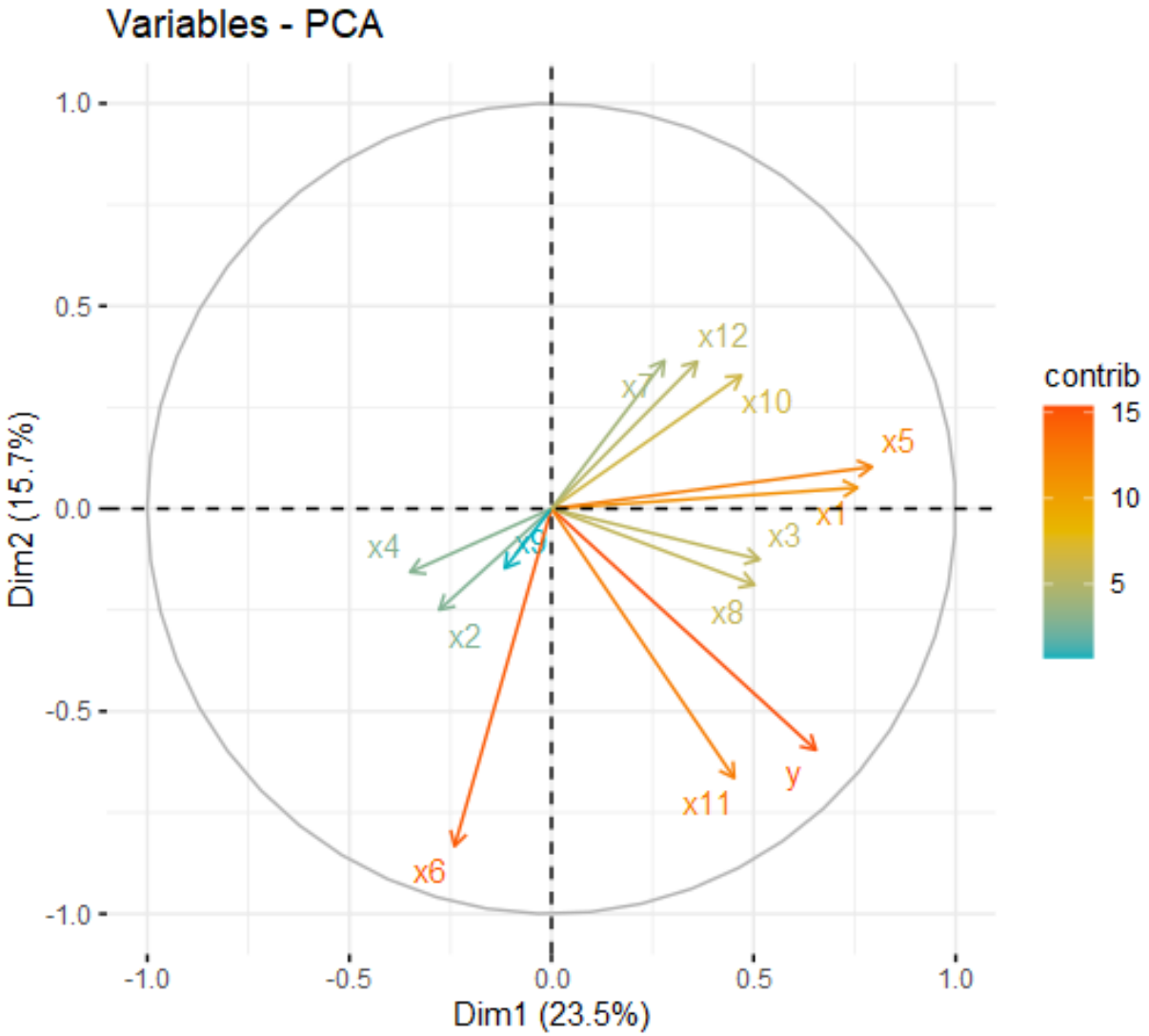






ANN – 1st/2nd year sets [train/test] + X_n (??)

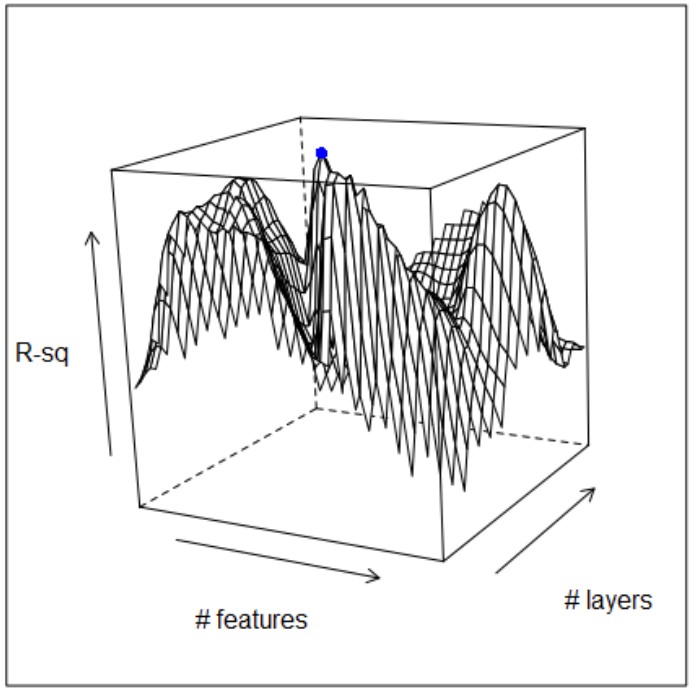
(RMSE=??; R-sq=??; Pearson=??; d-Willmott index=??)



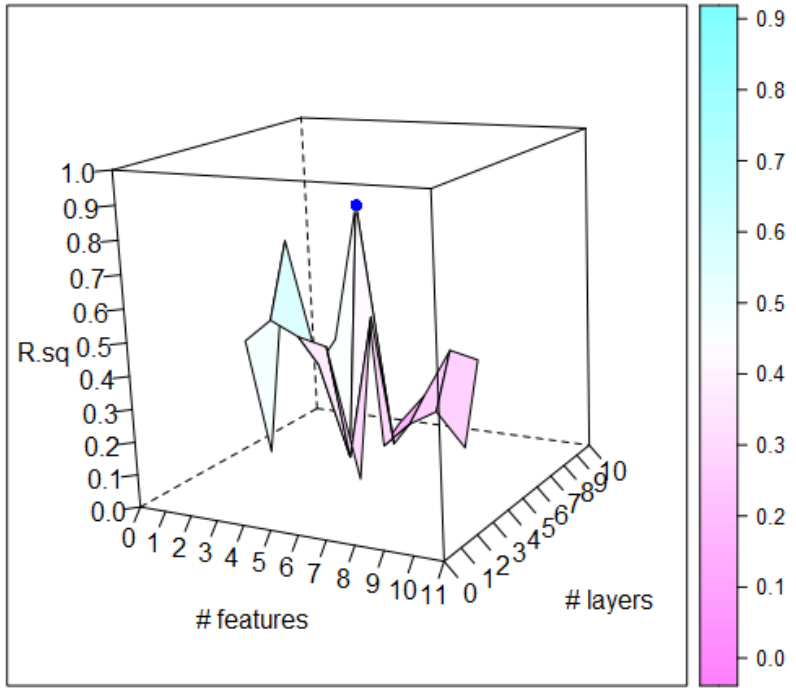
ANN – 1st/2nd year sets [train/test] -> *X1 + X3 + X5 + X6 + X10 + X11*

(*Train RMSE=7.9 mm; Test RMSE=9.1 mm*)

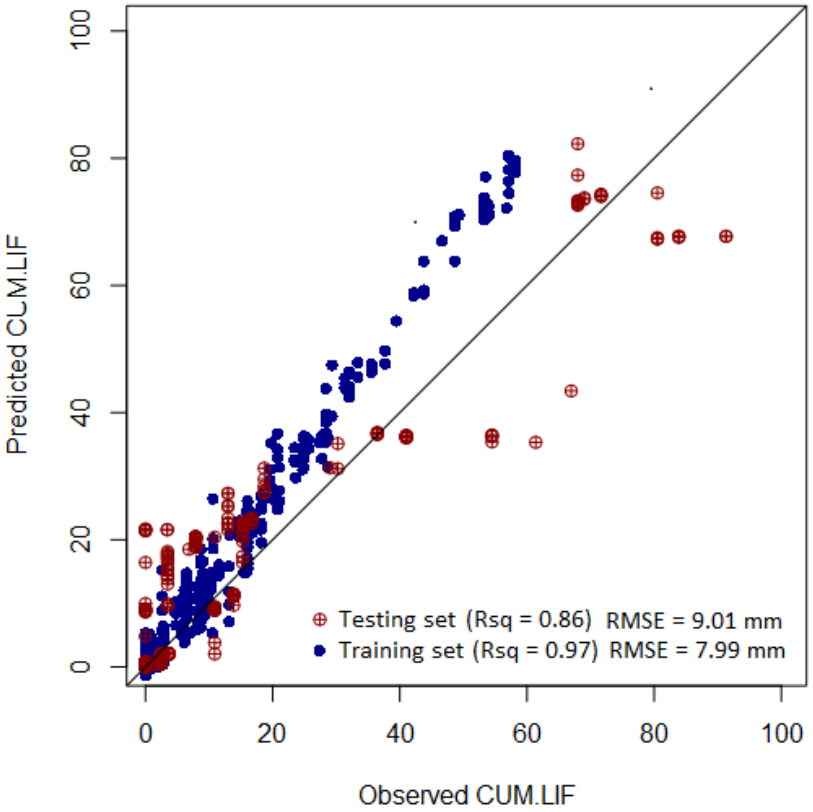
A) **ANN R-sq surface plot**



B) **ANN structure and performance assessment**



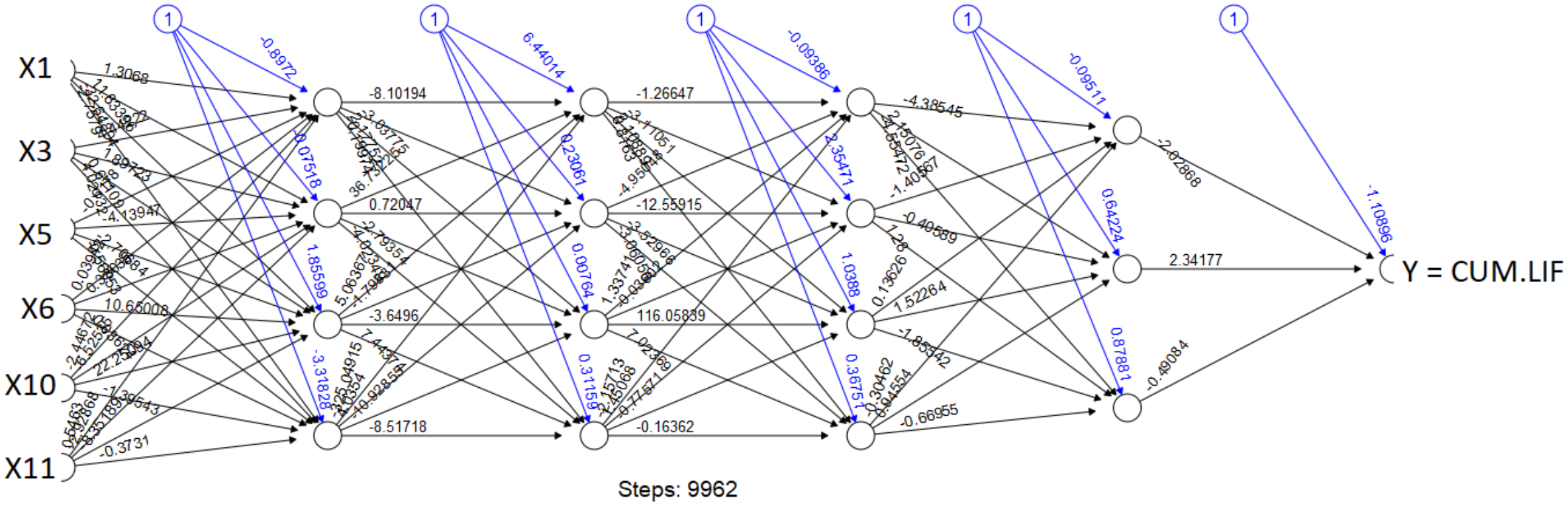
C)



- static multi-layer feedforward network;
- 6 input features;
- 4 hidden layers (w/logistic transformations);
- 3-4 neurons per layer [4,4,4,3]

ANN – 1st/2nd year sets [train/test] -> *X1 + X3 + X5 + X6 + X10 + X11*

(RMSE=9.8 mm; R-sq=0.86; Pearson=0.93; d-Willmott index=0.95)



Best performing **ANN structure**:

- static multi-layer feedforward network;
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ANN – 1st/2nd year sets [train/test] -> *X1 + X3 + X5 + X6 + X10 + X11*

(RMSE=9.8 mm; R-sq=0.86; Pearson=0.93; d-Willmott index=0.95)

```
data=data.frame(CVUT.LIF$Zone,                    #Zone
                CVUT.LIF$Year,                    #Year
                CVUT.LIF$DAS,                     #DAS
                CVUT.LIF$LIF.C.CUM,               #y
                CVUT.LIF$HYD.10min.CUM,           #x1
                CVUT.LIF$DAR.off,                 #x2
                normalize(CVUT.LIF$FAI),          #x3
                CVUT.LIF$slope,                   #x4
                CVUT.LIF$SR.contribution,         #x5
                CVUT.LIF$CC,                      #x6
                CVUT.LIF$Ks.10min.surface,        #x7
                CVUT.LIF$DAR.off.c,               #x8
                CVUT.LIF$DAPre,                   #x9
                CVUT.LIF$K.sat,                   #x10
                CVUT.LIF$P.CUM,                   #x11
                CVUT.LIF$satunsat                 #x12
                )
```

Best performing ANN structure:

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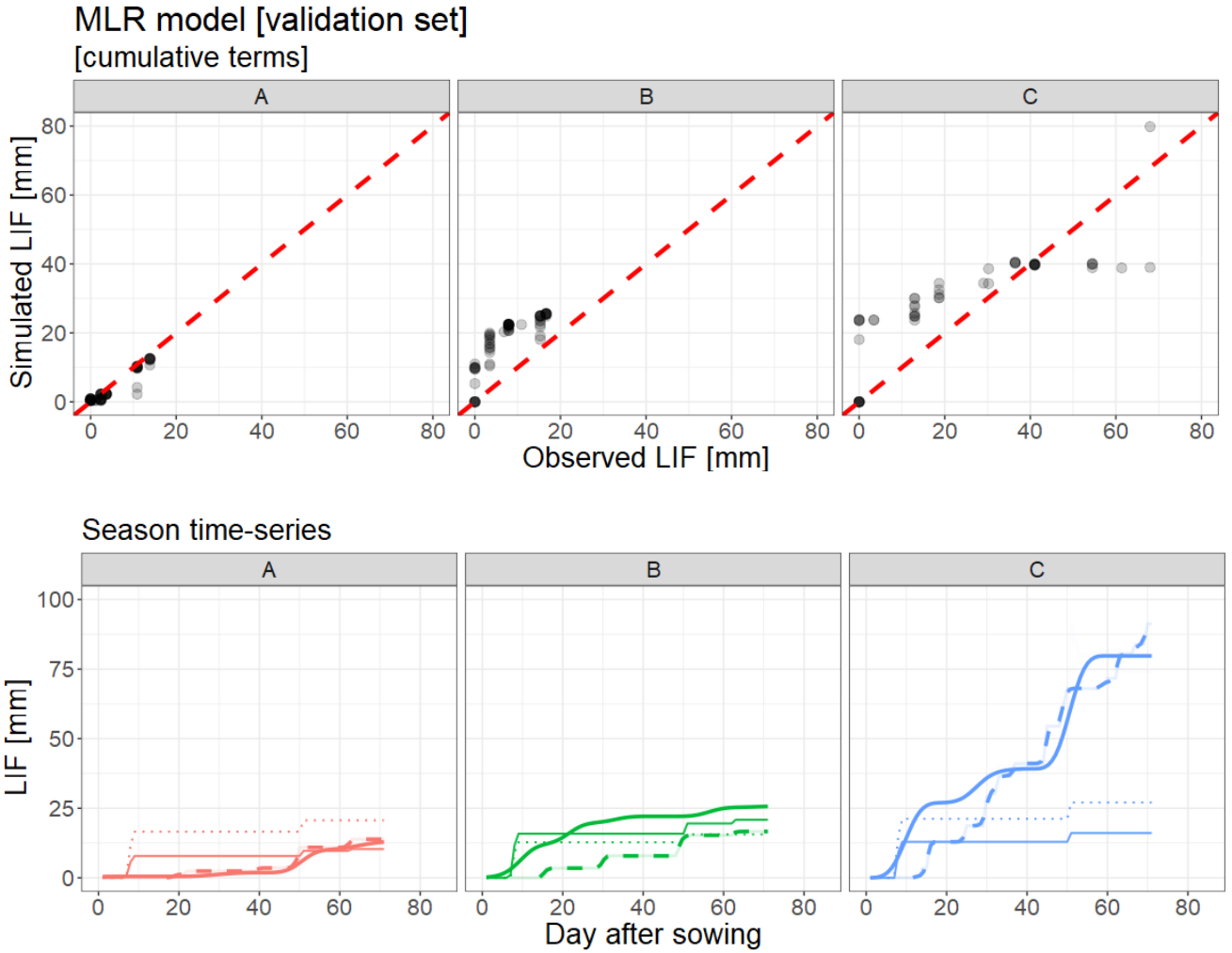

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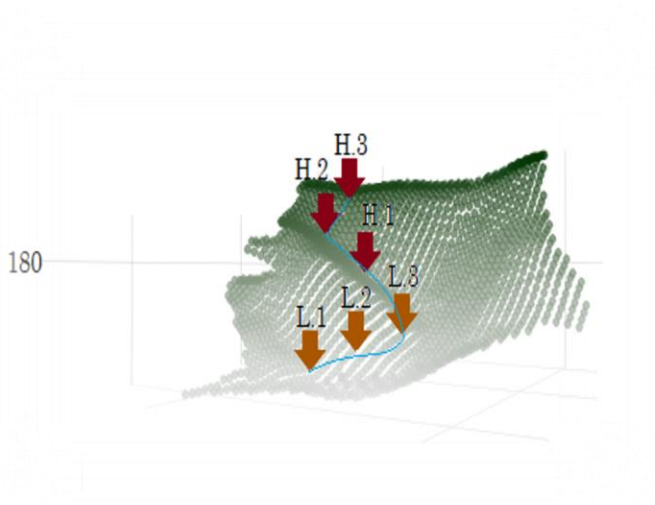
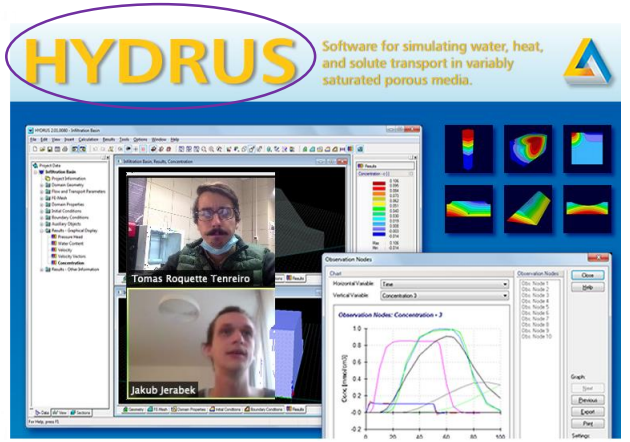
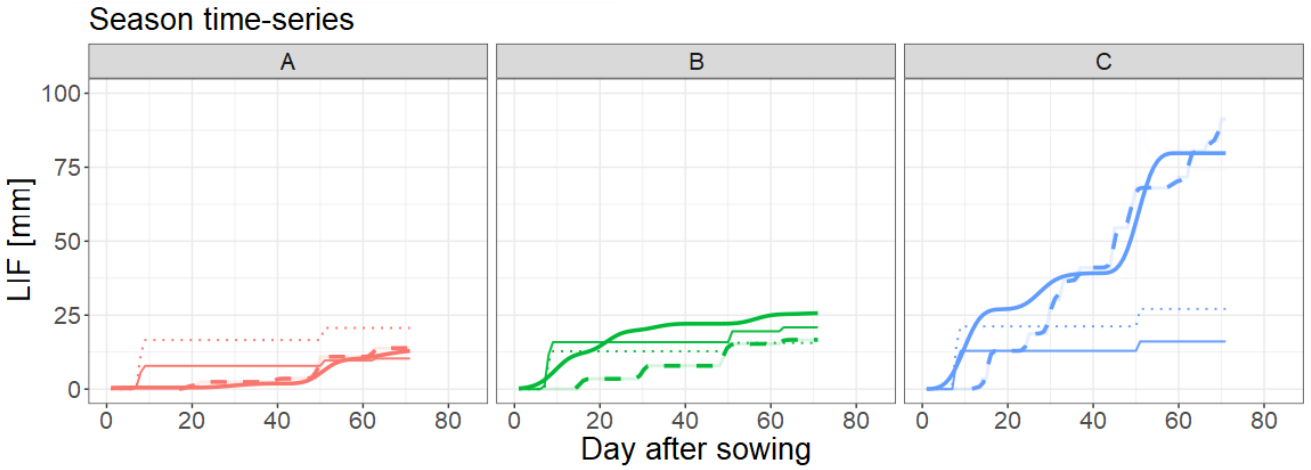
(RMSE=9.8 mm; R-sq=0.86; Pearson=0.93; d-Willmott index=0.95)

```
data=data.frame(CVUT.LIF$Zone,                  #Zone
                CVUT.LIF$Year,                  #Year
                CVUT.LIF$DAS,                   #DAS
                CVUT.LIF$LIF.C.CUM,             #y
                CVUT.LIF$HYD.10min.CUM,         #x1
                CVUT.LIF$DAR.off,               #x2
                normalize(CVUT.LIF$FAI),        #x3
                CVUT.LIF$slope,                 #x4
                CVUT.LIF$SR.contribution,       #x5
                CVUT.LIF$CC,                    #x6
                CVUT.LIF$Ks.10min.surface,      #x7
                CVUT.LIF$DAR.off.c,             #x8
                CVUT.LIF$DAPre,                 #x9
                CVUT.LIF$K.sat,                 #x10
                CVUT.LIF$P.CUM,                 #x11
                CVUT.LIF$satunsat               #x12
                )
```







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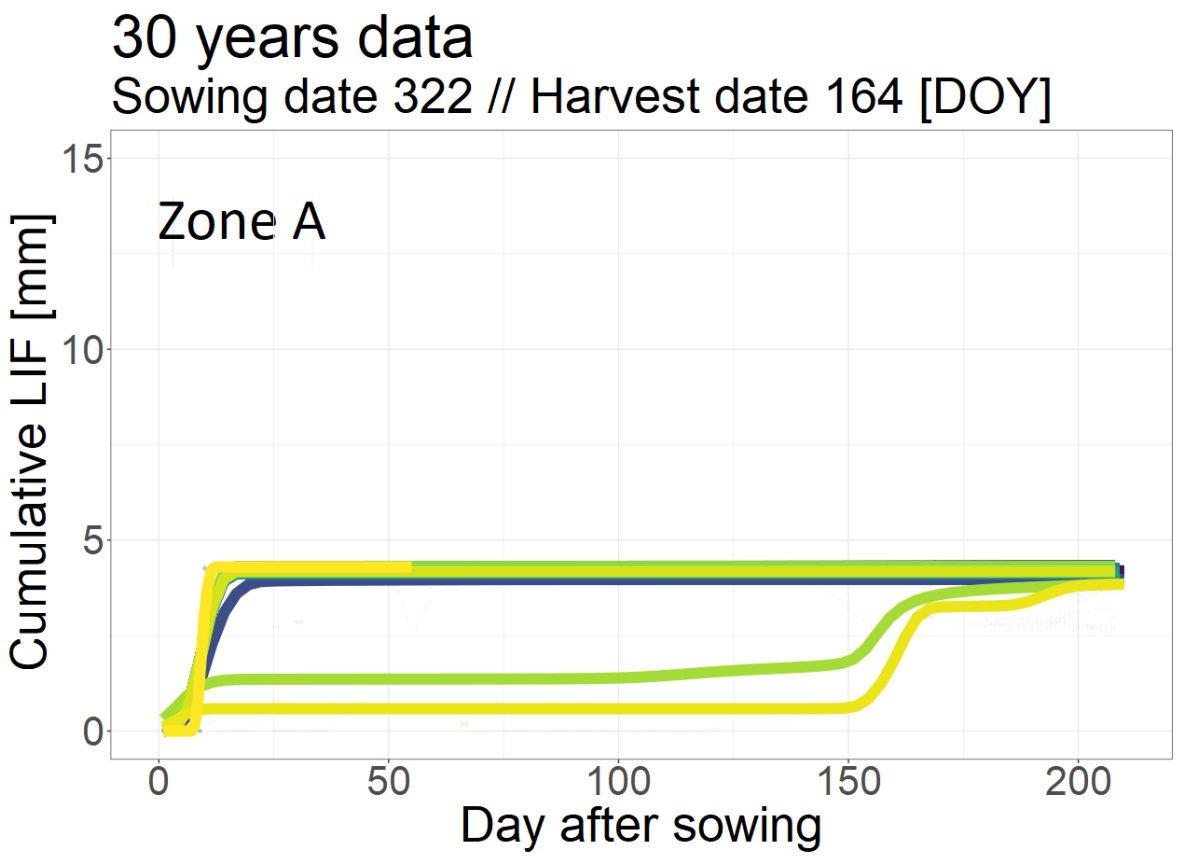
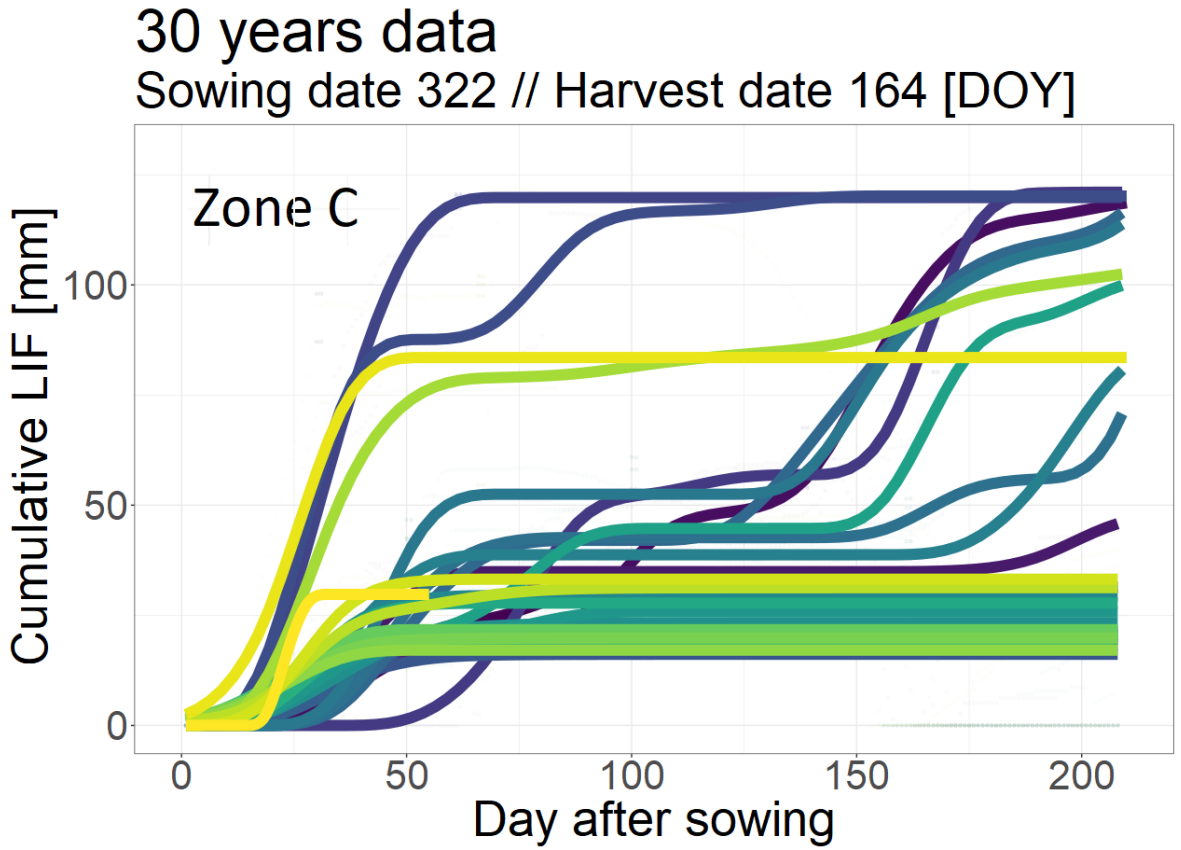
ANN $X1 + X3 + X5 + X6 + X10 + X11$

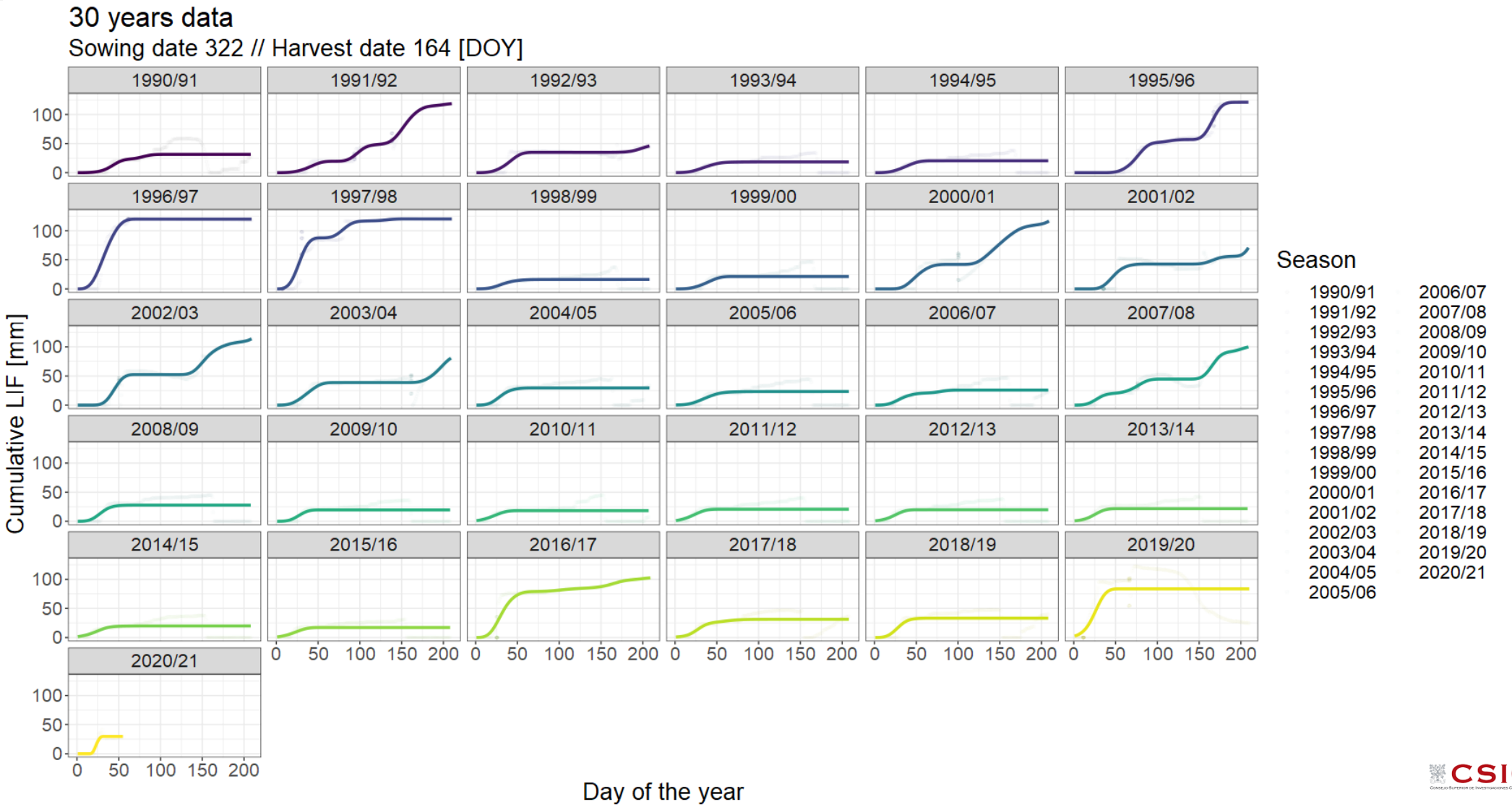
Lateral inflow in cumulative terms (CUM.LIF) predicted by the ANN for a sequence of 30 years





ANN – 1st/2nd year sets [train/test] -> *X1 + X3 + X5 + X6 + X10 + X11*

Lateral inflow in cumulative terms (CUM.LIF) predicted by the ANN for a sequence of 30 years



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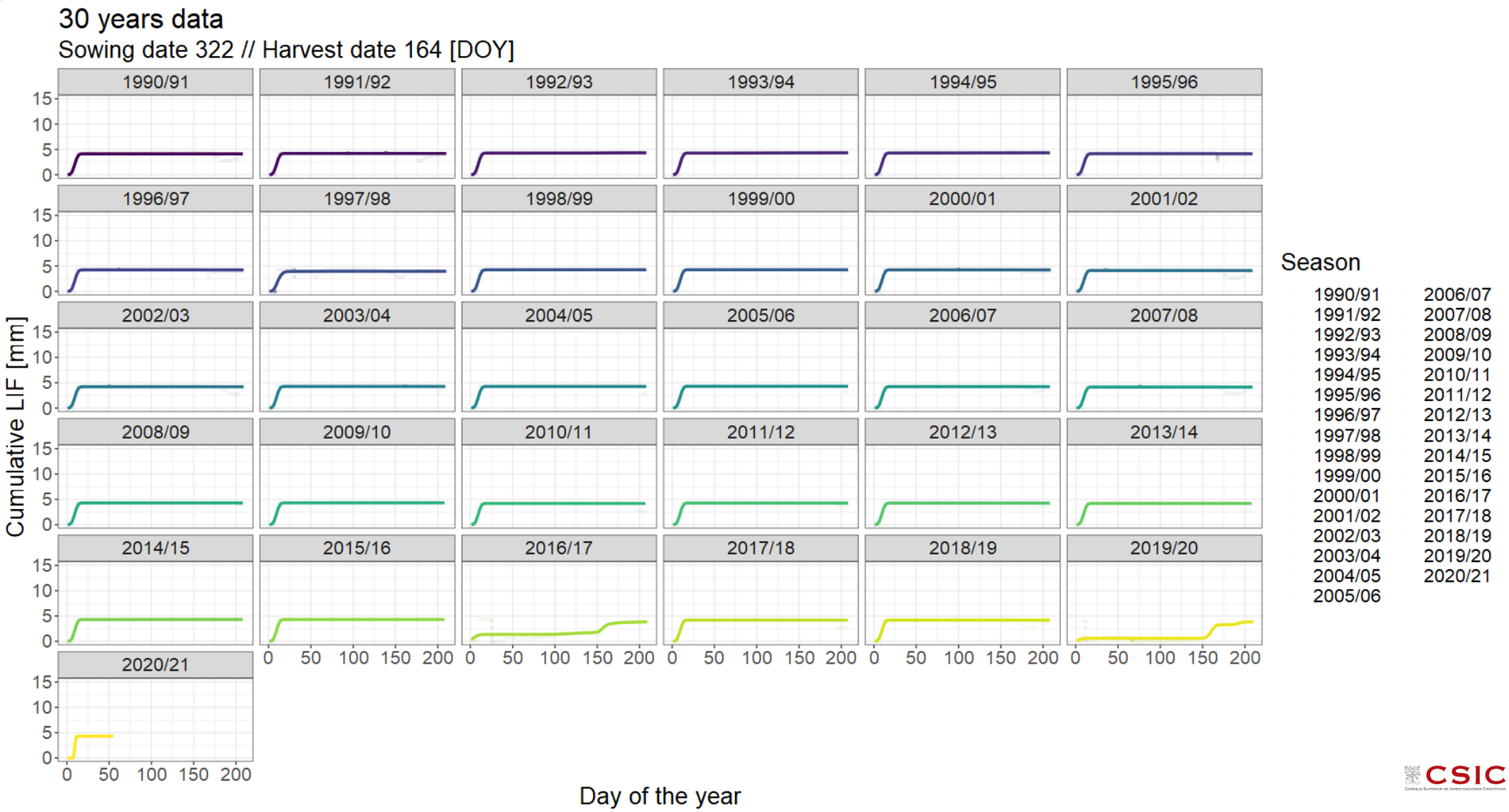
Lateral inflow in cumulative terms (CUM.LIF) predicted by the ANN for a sequence of 30 years



ANN – 1st/2nd year sets [train/test] -> *X1 + X3 + X5 + X6 + X10 + X11*

(RMSE=9.8 mm; R-sq=0.86; Pearson=0.93; d-Willmott index=0.95)

Post-prediction inference correction ??

Wang, S., McCormick, T. H., & Leek, J. T. (2020).
Methods for correcting inference based on outcomes predicted by machine learning.
Proceedings of the National Academy of Sciences, *117*(48), 30266-30275.