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Kriging-based metamodeling with qualitative variables to design grassed buffer zones in small agricultural catchment

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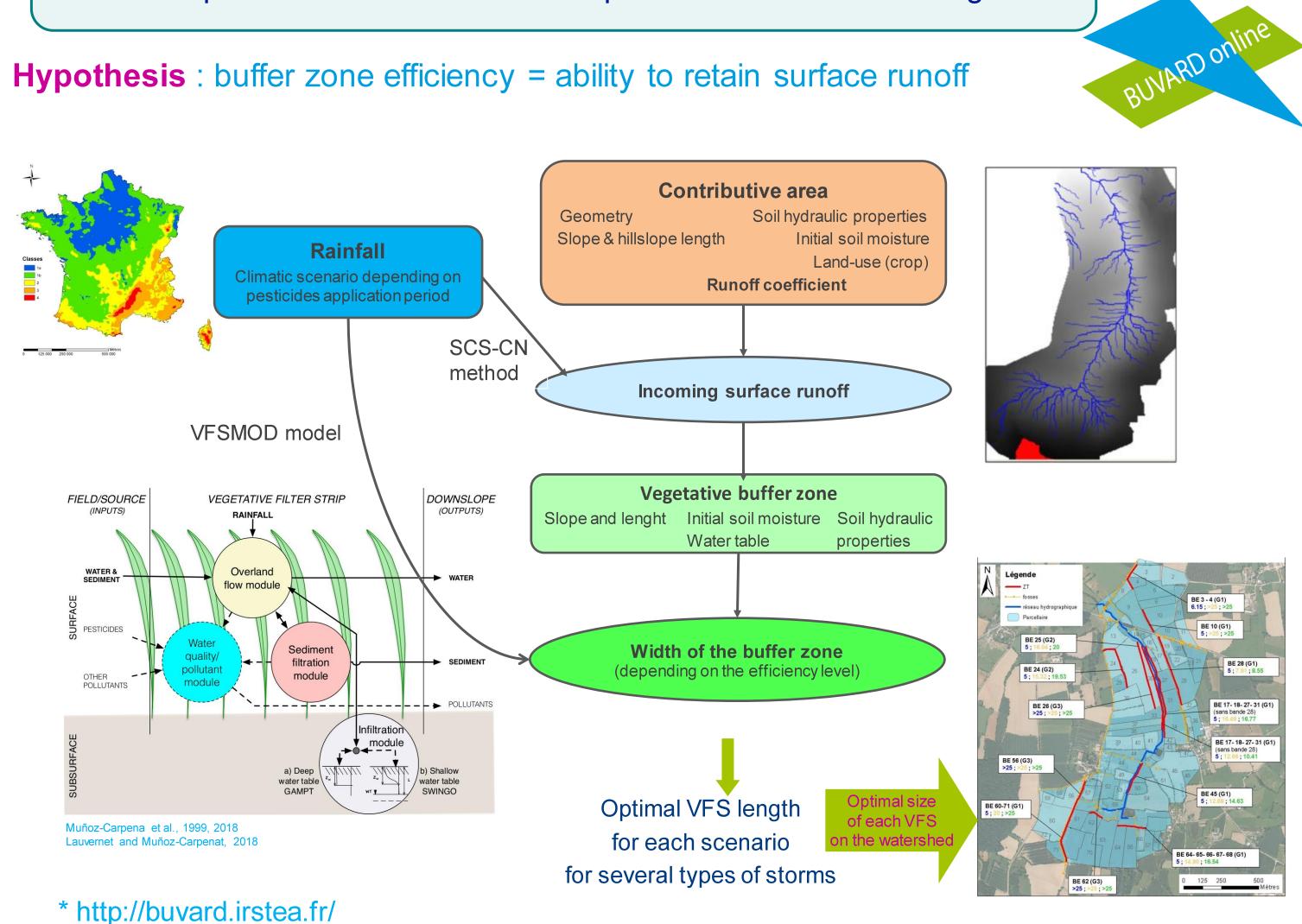
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Objectives

- Buffer strips are identified as the BMP of Choice for Runoff Mitigation to limit contamination of surface water by pesticides.
- Their efficiency strongly depends on soil, agronomic and climatic conditions and they need to be optimized by considering appropriate sizing.
- → Irstea developed a complete/complex toolkit to design site-specific VFS by simulating their efficiency to limit runoff transfers: BUVARD (Carluer et al., 2017).
- This tool is based on quantitative and qualitative variables
- Need for a simpler and efficient tool for end-users
- → A metamodel of BUVARD = methodological challenges for operational purposes

The toolkit BUVARD*

BUffer strip for runoff Attenuation and pesticides Retention Design tool





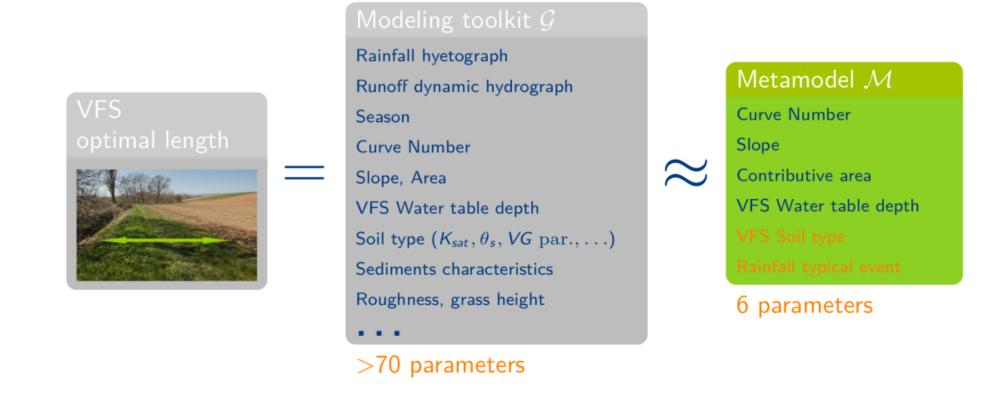


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Methods for building the metamodel

Why metamodeling BUVARD?

- Simple to use but still based on physics
- Able to evaluate an output of the toolchain at any point of the domain
- Allows evaluating sensitivity indices at smaller numerical cost
- Can be easily coupled/integrated in hydrological modeling frameworks



BUT: How to deal with qualitative/categorical variables (type of soil, type of rainfall event), that are typical in water quality modeling?

Stochastic method? Gaussian Processes / Kriging

The relation between points is expressed by a covariance structure between the obs.

→ Need for an adapted cov. kernel

Deterministic method? GAM (Generalized Additive Model)

The relation between points is assumed to be deterministic and explicit

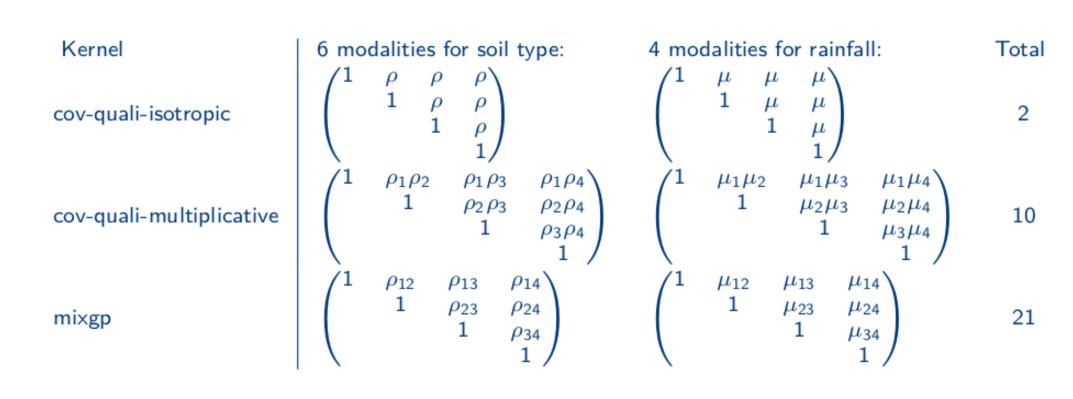
→ Ok with qualit. var.

Gaussian Processes with mixed variables:

- Hyp. = the deterministic output of the model is the realization of a GP
- The GP Z is conditioned by points from the model simulations (still a GP)
- Several options to deal with categ. var.:
- one GP per modalities couple
- adapting the covariance kernel by progressive complexity

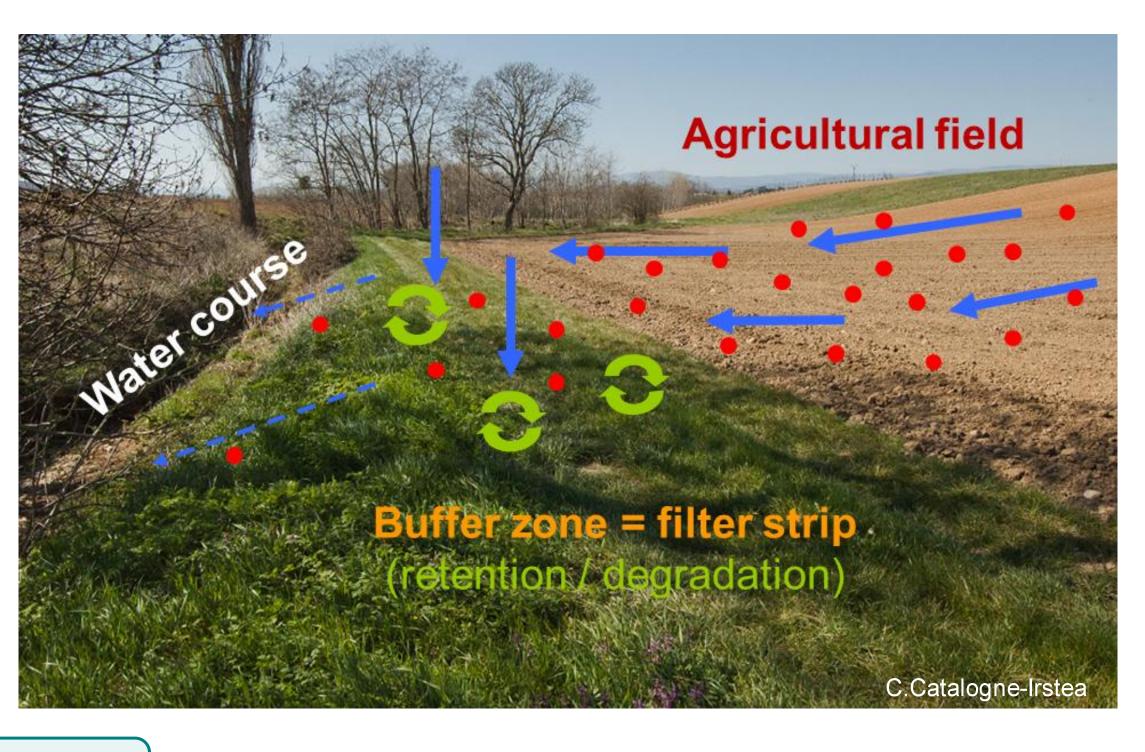
$Cov(W(x), W(x')) = c(x, x') = \sigma$	$^{2}R(\theta,x,x')$
$R(\theta, x, x') = \prod R_k(\theta_k)$	(x_k, x_k')
$R(\theta,x,x') = \prod_{j=1}^J au_j \prod_{k=1}^K au_j$	$_{=1}$ $R_k(\theta_k,x_k,x_k')$
corr. fun. of quali factor j $ au_{j,z_{ij},z_{hj}} = ho_{ij} ho_{hj}1\left[z_{ij} eq z_{hj} ight]$	corr. fun. of
$r_{J},z_{ij},z_{hj} = p_{ij}p_{hj} + [z_{ij} \neq z_{hj}]$	quanti. factor
c(x-x')=	$\sigma^2 \exp -\left(\frac{(x-x')}{x}\right)$

Z(x) = m(x) + W(x)



Sampling of the most influent and the most accessible input parameters

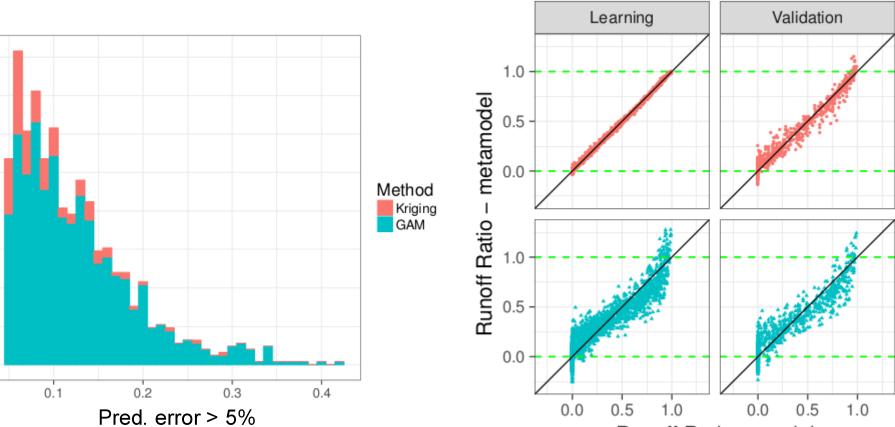
Sampling range	
[63,99]	
[2% , 20%]	
[25 , 300]	
[0.5 , 4]	
Summer/Winter, short/long	
clo, scl, SIL, CLO, SCL, SAL	



Results

- Comparison of two methods : Kriging & Generalized Additive Model
- Kriging was adapted to qualitative variables with adapted covariance model

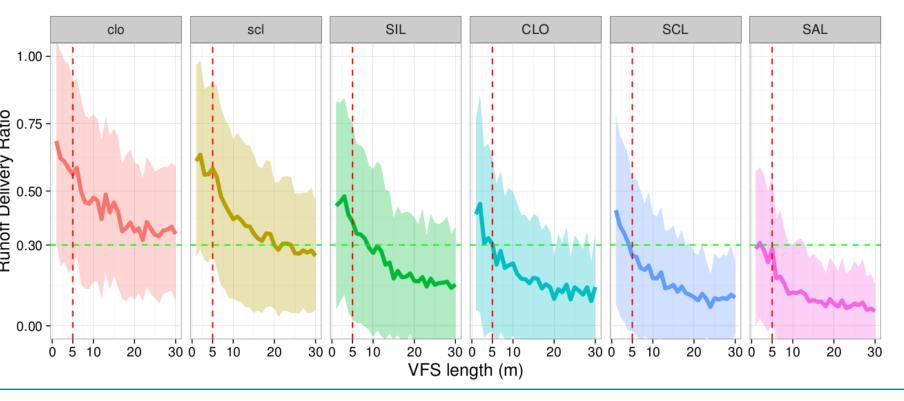
Output variable is the Runoff Delivery Ratio = Runout/Runin: efficiency = 100%; RDR = 1 efficiency = 0%



Kriging $R^2 2 = 0.96$ Kriging is very efficient with qualitative variables

GAM $R^2 = 0.84$

- cov quali multiplicative and mixgp give the best prediction and are similar Still some prediction
- error due to the plateau High sensitivity of RDR to the Curve Number
- Uncertainty analysis: Average efficiency and uncertainty on large sample simulations (24 000)



- > a very large variability of optimal length / type of soil
- possibility to quantify uncertainty of the results

Conclusion

- Qualitative variables were properly taken into account by the GP adaptation
- Good quality of prediction (94 % of variance) but some bad predictions
- The optimal VFS length is very sensitive to the Curve Number
- MM is a promising tool to test the toolkit to perform UA and GSA at low cost **Limitations and perspectives:**
- On larger ranges (Curve Number in p.), the current MM is not satisfying (due to a large plateau of null values of the output variable)
- Continue testing and compare methods on :
 - prediction uncertainty
 - sensitivity of prediction quality to the sampling size
 - global sensitivity analysis (Sobol)

Ref. Carluer, N et al. 2017. Defining context-specific scenarios to design vegetated buffer zones that limit pesticide transfer via surface runoff. Sci. Of Total Env., 575. // Munoz-Carpena, R.; Lauvernet, C. & Carluer, N., 2018. Shallow water table effects on water, sediment, and pesticide transport in vegetative filter strips -- Part 1: nonuniform infiltration and soil water redistribution. Hydrol. Earth System Sci., 22. // Lauvernet, C. & Munoz-Carpena, R. 2018. Part 2: model coupling, application, factor importance, and uncertainty. Hydrol. Earth System Sci., 22. // Chen, Wang & Yang, 2013, Stochastic Kriging with Qualitative factors. WSC '13 Proceedings. // Panodou & Roustant, 2017 mixgp R package: Kriging models for mixed data.





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