Supplementary material 1

This document describes the 78 additional derived spectral indices/features in addition to the nine primary bands of Landsat-8 (OLI) imagery used in the study.

Table S1: Water indices as features derived from Landsat 8 OLI used in the study. https://custom-scripts.sentinel-hub.com/custom-scripts/landsat-8/indexdb/

Description	Indices	formula
Blue-wide Dynamic Range Vegetation Index	BWDRVI	0.1*NIR-BLUE/0.1*NIR+BLUE
Chlorophyll Index Green	Clgreen	(NIR/GREEN) - 1
Chlorophyll Vegetation index	CVI	$NIR*RED/GREEN^2$
Coloration index	CI	(RED – BLUE)/RED
Corrected Transformed Vegetation Index	CTVI	(((RED-GREEN)/(RED+GREEN)+0.5)/ Abs(((RED-GREEN)/(RED+GREEN)+0.5)))*sqrt(abs(((RED-GREEN)/(RED+GREEN)+0.5))
Difference NIR/Green Difference	GDVI	(NIR-GREEN)
Differenced Vegetation Index MSS	DVIMSS	2.4*NIR - RED
Enhanced Vegetation Index	EVI	2.5*((NIR-RED)/((NIR+6*RED-7.5*BLUE)+1)
Enhanced Vegetation Index 2	EVI2	2.4*((NIR-RED)/(NIR+RED + 1))
Enhanced Vegetation Index 2-2	EVI2-2	2.5*((NIR-RED)/(NIR+2.4*RED + 1))
NIR-Green NDVI	GNDVI_1	(NIR-GREEN)/(NIR+GREEN)
NIR-Red NDVI	GNDVI_2	(NIR-RED)/(NIR+RED)
NIR-SWIR1 NDVI	GNDVI_3	(NIR-SWIR1)/(NIR+SWIR1)
NIR-SWIR2 NDVI	GNDVI_4	(NIR-SWIR2)/(NIR+SWIR2)
Normalized Difference Water Index with NIR, SWIR1 & SWIR2	GNDVI_5	(NIR-SWIR1)/(NIR+SWIR2)
Normalized Difference Water Index with SWIR2 & SWIR1	GNDVI_6	(NIR-SWIR2)/(NIR+SWIR1)
Normalized Difference Water Index with SWIR1 & SWIR2	NDVI	(NIR-RED)/(NIR+RED)
Normalized Difference NIR/SWIR1 Modified Normalized Difference Vegetation Index	$MNDWI_1$	(GREEN – SWIR1)/(GREEN + SWIR1)
Normalized Difference NIR/SWIR2 Modified Normalized Difference Vegetation Index	$MNDWI_2$	(GREEN – SWIR2)/(GREEN + SWIR2)
Normalized Difference NIR/SWIR1 SWIR2 Modified Normalized Difference Vegetation Index	$MNDWI_3$	(GREEN – SWIR1)/(GREEN + SWIR2)
Normalized Difference NIR/SWIR2 SWIR1 Modified Normalized Difference Vegetation Index	$MNDWI_4$	(GREEN – SWIR2)/(GREEN + SWIR1)
New Water Index	NWI	(BLUE – (NIR+SWIR1+SWIR2))/BLUE + (NIR+SWIR1+SWIR2))
RED SWIR1 band difference	TWI_1	RED – SWIR1

RED SWIR2 band difference	TWI_2	RED – SWIR2
Algal Bloom Index	ABI	(RED – BLUE) * (GREEN-BLUE)/(RED-BLUE) – NIR – BLUE) *(GREEN-BLUE)/(NIR-BLUE)
Floating Algae Index	FAI	(NIR-RED) +(RED-SWIR1)*(λ_{nir} - λ_{red})/(λ_{swir} - λ_{red}) Where, λ_{red} = 662 nm, λ_{nir} = 835 nm, λ_{swir} = 1648 nm.
Automated water extraction index with SWIR1	$AWEI_1$	(4 * (GREEN – SWIR1) - (0.25 * NIR + 2.75 * SWIR1))
Automated water extraction index with SWIR1	$AWEI_2$	(4 * (GREEN – SWIR2) - (0.25 * NIR + 2.75 * SWIR2))
Automated water extraction index with SWIR2 & SWIR1	$AWEI_3$	(4 * (GREEN – SWIR1) - (0.25 * NIR + 2.75 * SWIR2))
Automated water extraction index with SWIR1 & SWIR2	$AWEI_4$	(4 * (GREEN – SWIR2) - (0.25 * NIR + 2.75 * SWIR1))
Automated water extraction index for urban background	$AWEI_{nsh}$	GREEN + BLUE+0.25+1.5(NIR+SWIR1)-0.25*SWIR2)
Normalized difference index from NIR and GREEN + BLUE	GBNDVI	(NIR-(GREEN+BLUE))/ (NIR+(GREEN+BLUE))
Normalized difference index of three bands	GRNDVI	(NIR-(GREEN+RED))/(NIR+(GREEN+RED))
Normalized difference index from NIR and BLUE	BNDVI	(NIR-BLUE)/(NIR+BLUE)
Two Band ratio	Gossan	SWIR1/RED
Normalized difference index of four bands	GARI	(NIR-(GREEN-(BLUE-RED)))/(NIR-(GREEN+(BLUE-RED)))
Norm G	Norm G	G/(NIR+R+G)
Norm NIR	Norm NIR	NIR/(NIR+R+G)
Norm R	Norm R	R/(NIR+R+G)
Normalized difference index from GREEN and BLUE	PPR	(GREEN - BLUE)/(GREEN + BLUE)
Normalized difference index from GREEN and RED	PVR	(GREEN - RED)/(GREEN + RED)
Intensity	I	(1/30.5)(RED + GREEN + BLUE)
Two Band ratio	Laterite	SWIR1/SWIR2
Hue	H	arctan((2RED – GREEN - BLUE)/30.5(GREEN -BLUE))
Log of two band ratio	LogR	Log(NIR/RED)
	mCRIG	$(BLUE^{-1} – GREEN^{-1})$*NIR
Mid-infrared vegetation index	MVI	NIR/SWIR1
	MSRNir/Red	(NIR/RED)-1/sqrt((NIR/RED)+1))
Normalized difference index from NIR^2 and RED	NLI	$(NIR^2-RED)/(NIR^2+RED)$
Normalized difference index from (SWIR1 and SWIR2)	NDSI	(SWIR1 – SWIR2)/(SWIR1 + SWIR2)
Normalized difference index from (NIR and (GREEN + RED + BLUE)	PNDVI	(NIR-(GREEN+RED+BLUE)) /(NIR+(GREEN+RED+BLUE))
Normalized difference index from (NIR and (RED + BLUE)	RBNDVI	(NIR-(RED+BLUE)) / (NIR+(RED+BLUE))

Shape index	IF	(2*RED-GREEN-BLUE)/GREEN-BLUE
Two Band ratio	SR550/670	GREEN/RED
"	SR860/550	NIR/GREEN
"	SRSWIR1/NIR	SWIR1/NIR
"	SRSWIR2/NIR	SWIR2/NIR
"	DVI	NIR/RED
"	RGR	RED/GREEN
"	WRI_1	(GREEN + RED)/(NIR+SWIR1)
"	WRI_2	(GREEN + RED)/(NIR+SWIR2)
Two band averages		(RED+NIR)/2
"		(GREEN+NIR)/2
"		(BLUE+NIR)/2
"		(RED+GREEN)/2
"		(RED+BLUE)/2
"		(GREEN+BLUE)/2
Three bands average		(BLUE+GREEN+RED)/3
"		(BLUE+GREEN+NIR)/3
"		(GREEN+RED+NIR)/3
"		(BLUE+RED+NIR)/3
Four band averages		(BLUE+GREEN+RED+NIR)/4
Surface Algal Bloom Index	SABI	(NIR-RED)/(BLUE+GREEN)
Three Band Algorithm	3BDA-like (KIVU)	(BLUE-RED)/GREEN

Supplementary material 2

ML Models hyperparameter tuning result for the three water quality parameters; Chl-a, TDS and Turbidity were shown in Figure S1 - Figure S12, Figure S13 - Figure S24, Figure S25 – Figure S36, respectively.

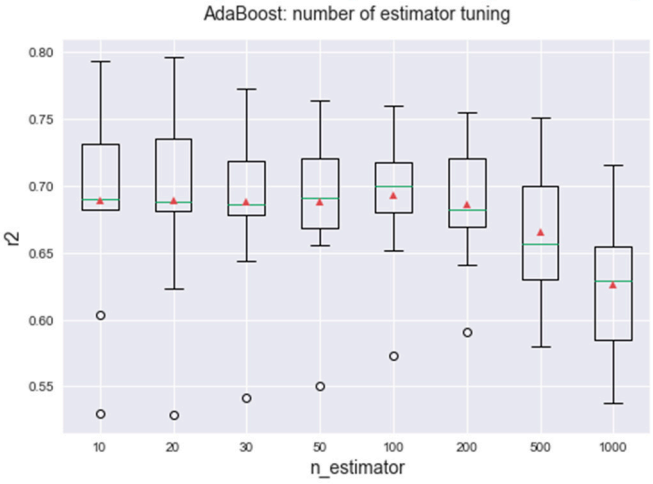

Figure S1: AdaBoost number of estimator tuning for Chl-a

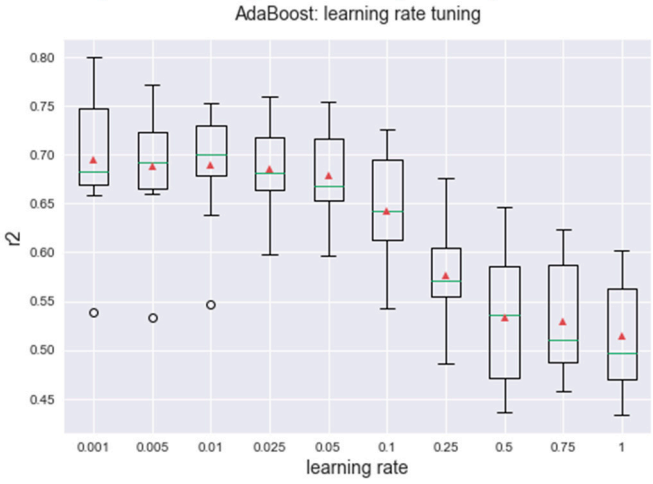

Figure S2: AdaBoost learning rate tuning for Chl-a

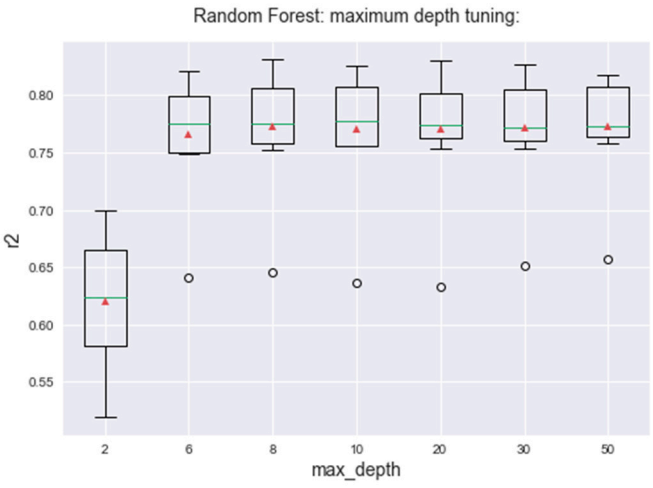

Figure S3: Random Forest maximum depth tuning for Chl-a

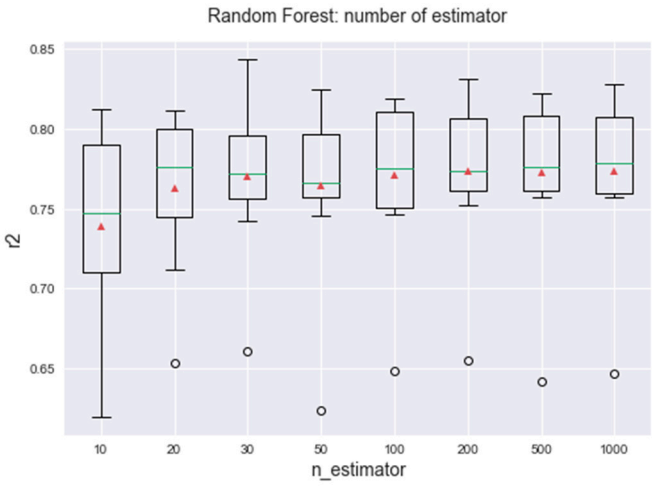

Figure S4: Random Forest number of estimator tuning for Chl-a

Figure S5: SVR c regularization tuning for Chl-a

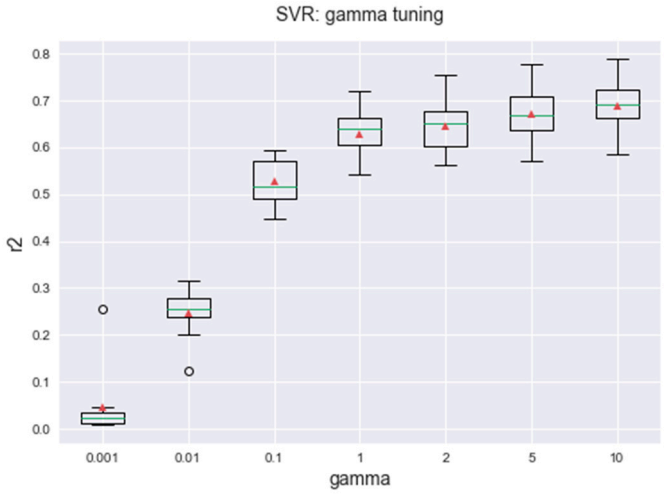

Figure S6: SVR gamma tuning for Chl-a

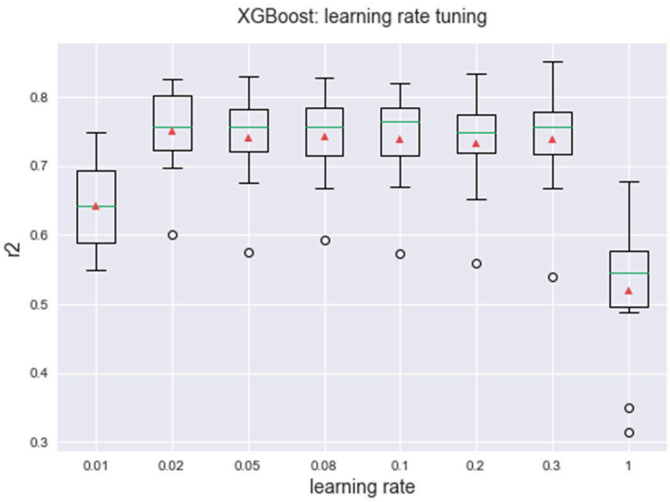

Figure S7: XGBoost learning rate tuning for Chl-a

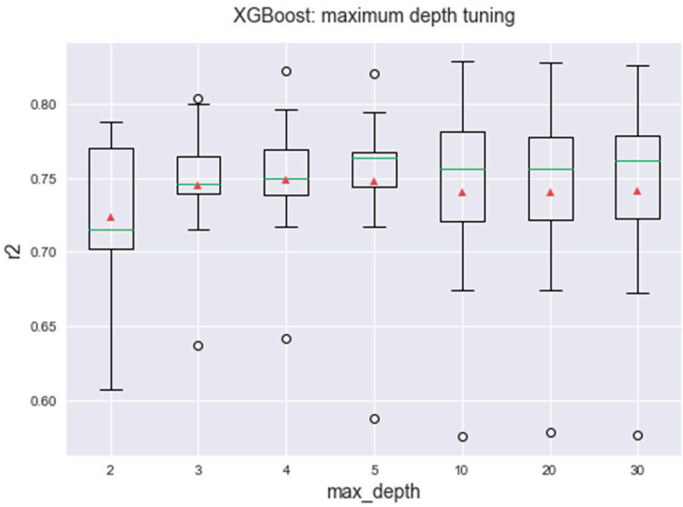

Figure S8: XGBoost maximum depth tuning for Chl-a

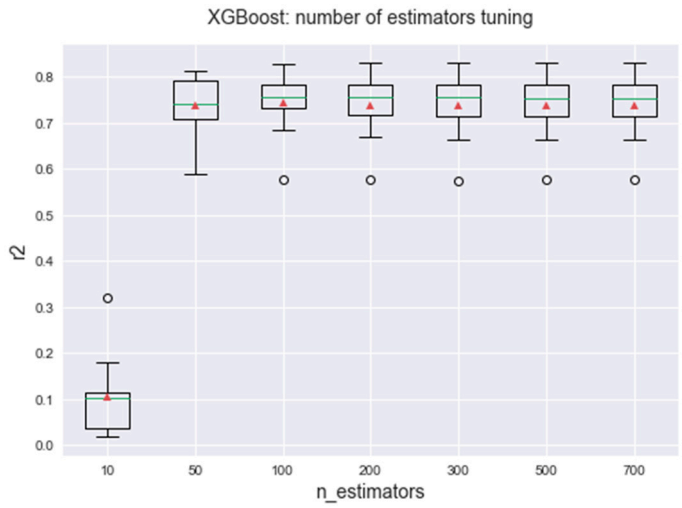

Figure S9: GradBoost number of estimator tuning result for Chl-a

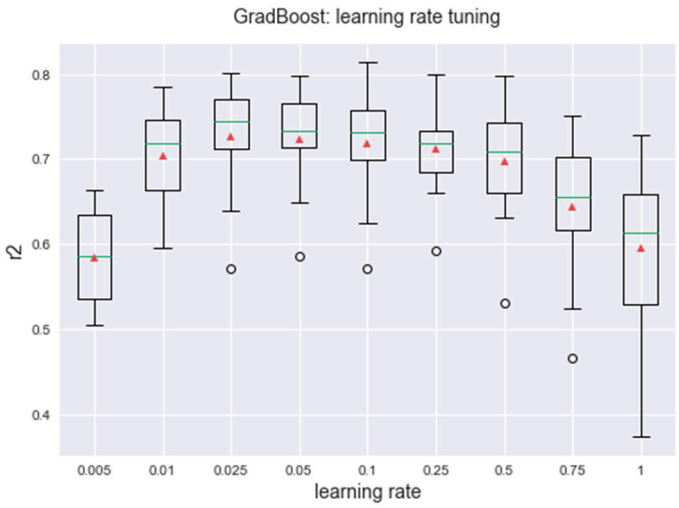

Figure S10: XGBoost learning rate tuning for Chl-a

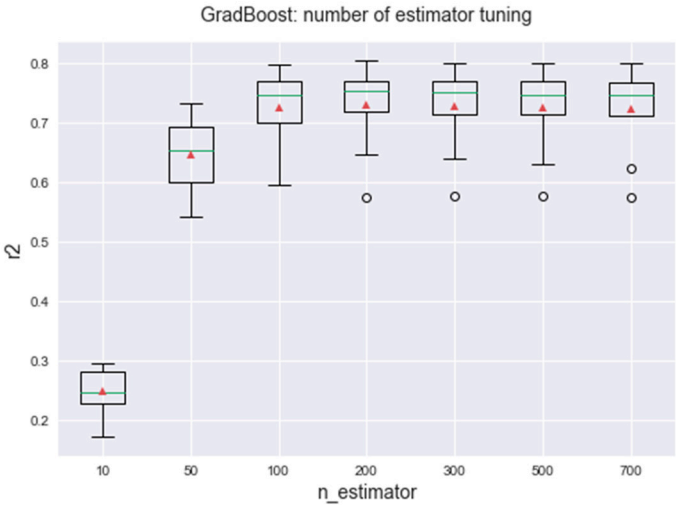

Figure S11: GradBoost number of estimator tuning for Chl-a

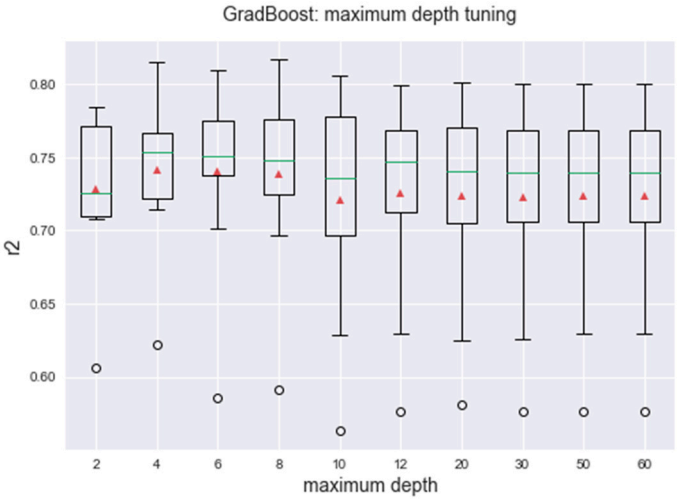

Figure S12: GradBoost maximum depth tuning for Chl-a

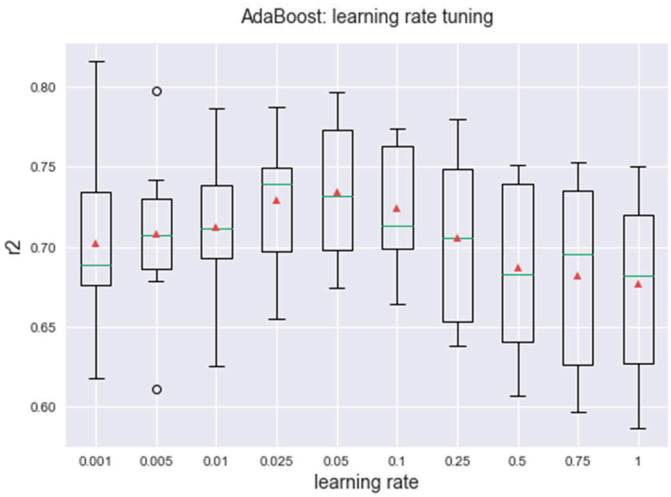

Figure S13: AdaBoost learning rate tuning for TDS

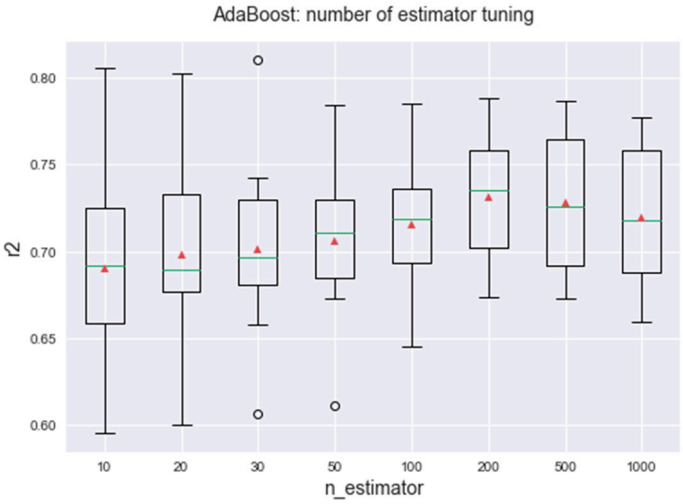

Figure S14: AdaBoost number of estimator tuning for TDS

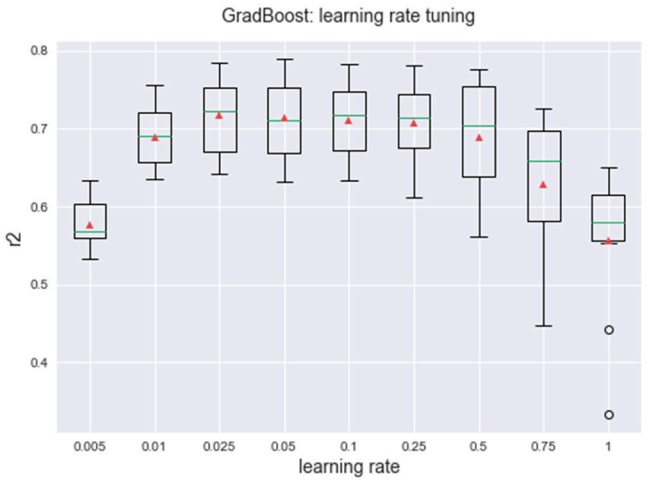

Figure S15: GradBoost learning rate tuning for TDS

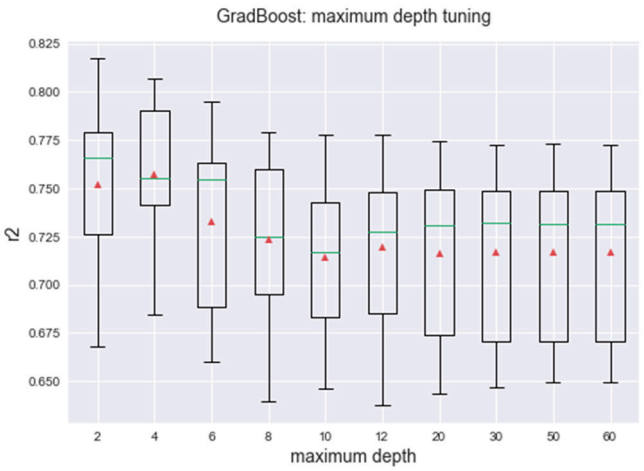

Figure S16: GradBoost maximum depth tuning for TDS

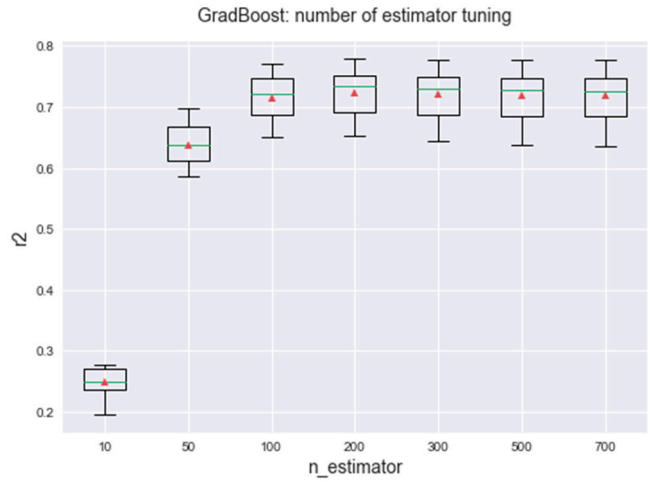

Figure S17: GradBoost number of estimator tuning for TDS

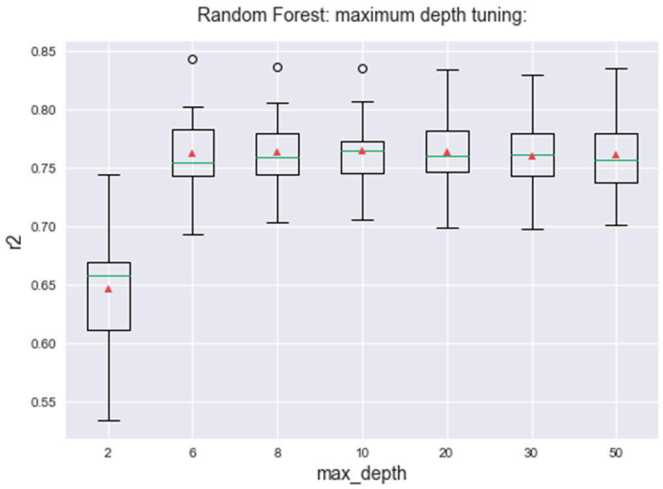

Figure S18: Random Forest maximum depth tuning for TDS

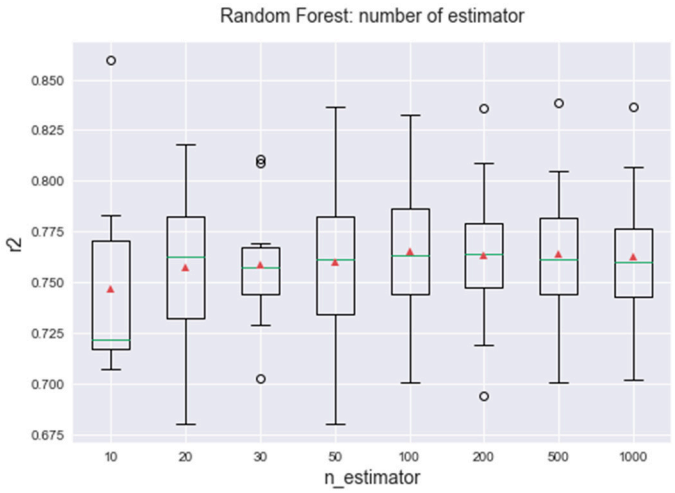

Figure S19: Random Forest number of estimator tuning for TDS

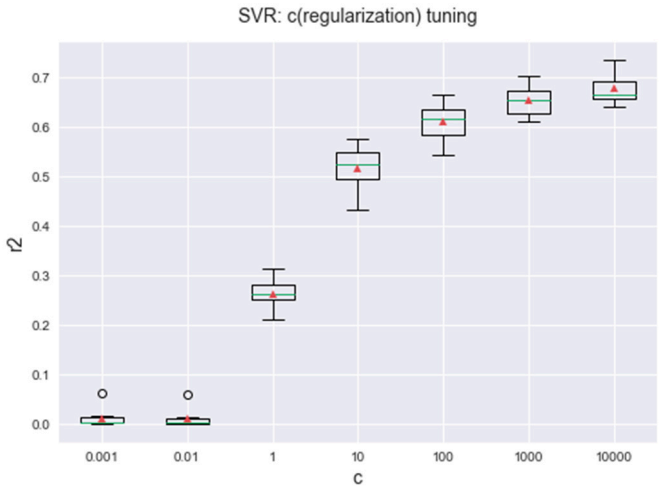

Figure S20: SVR c regularization tuning for TDS

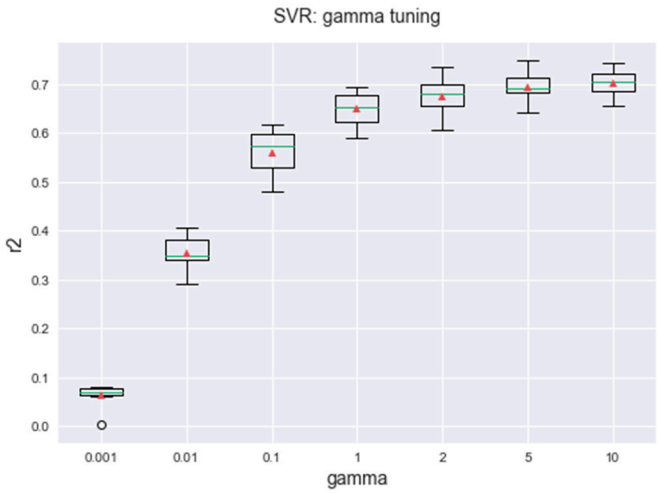

Figure S20: SVR gamma tuning for TDS

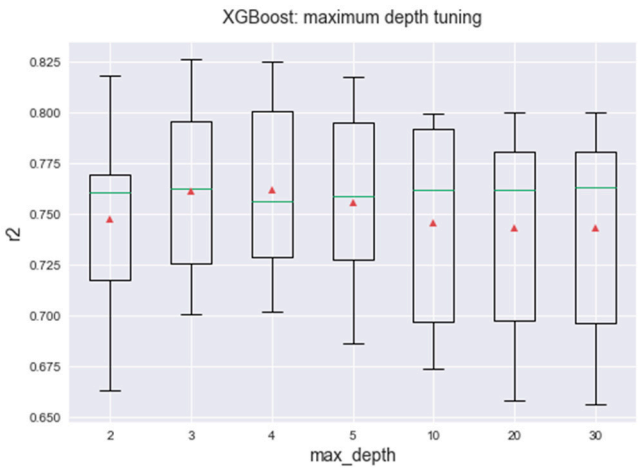

Figure S21: XGBoost maximum depth tuning for TDS

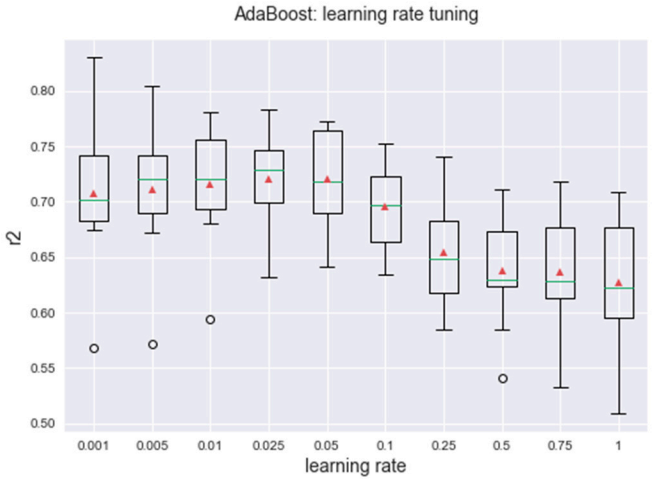

Figure S22: AdaBoost learning rate tuning for TUR

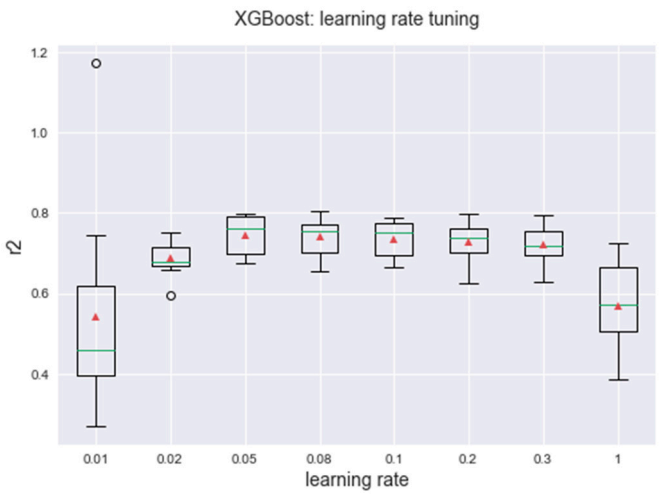

Figure S22: XGBoost learning rate tuning for TDS

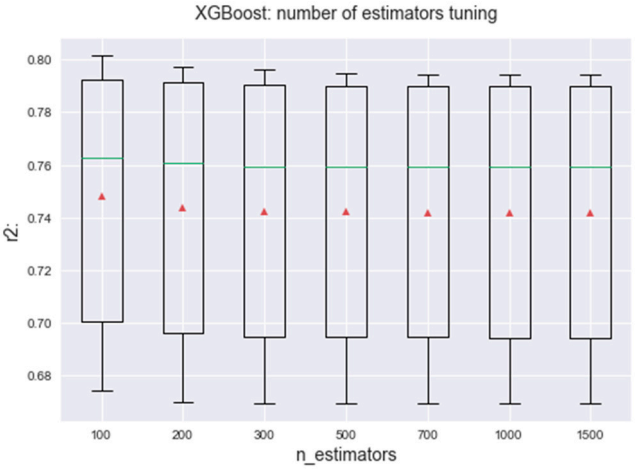

Figure S24: XGBoost number of estimator tuning for TDS

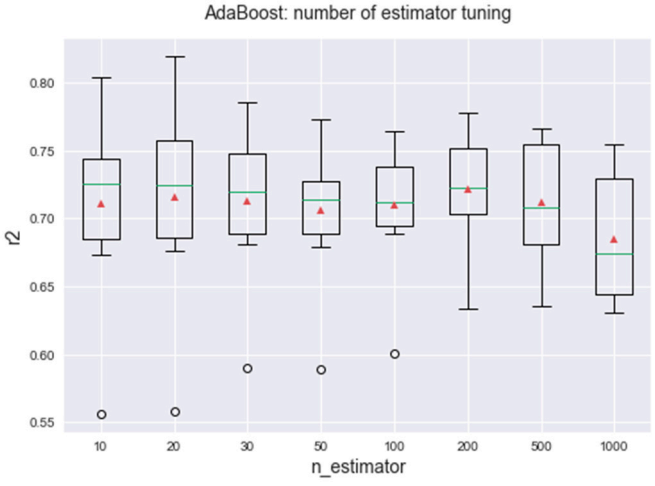

Figure S26: GradBoost number of estimator tuning for TUR

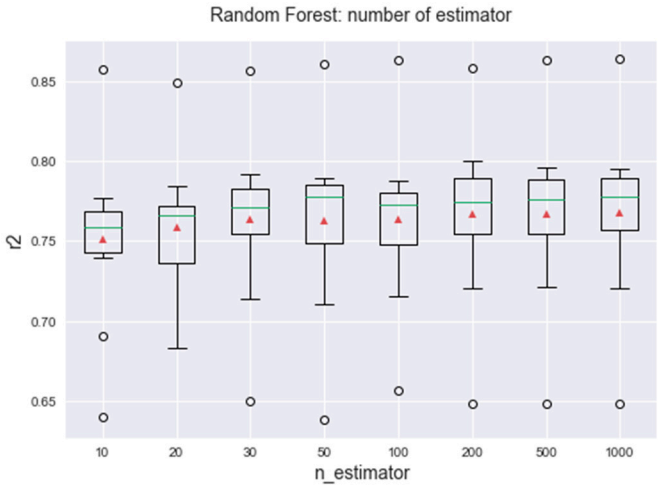

Figure S23: Random Forest number of estimator tuning for TUR

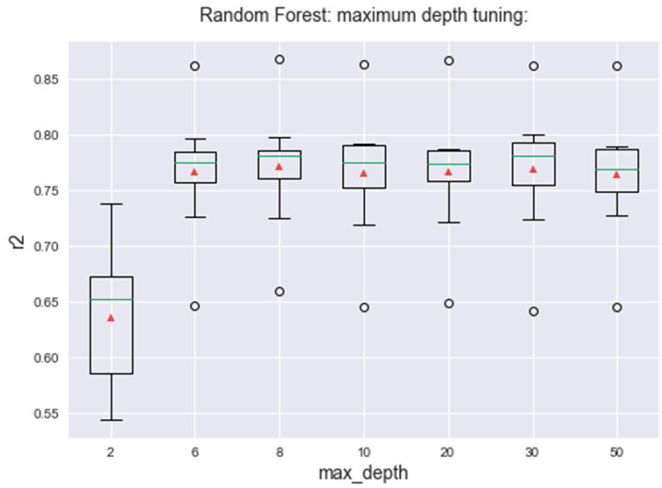

Figure S28: Random Forest maximum depth tuning for TUR

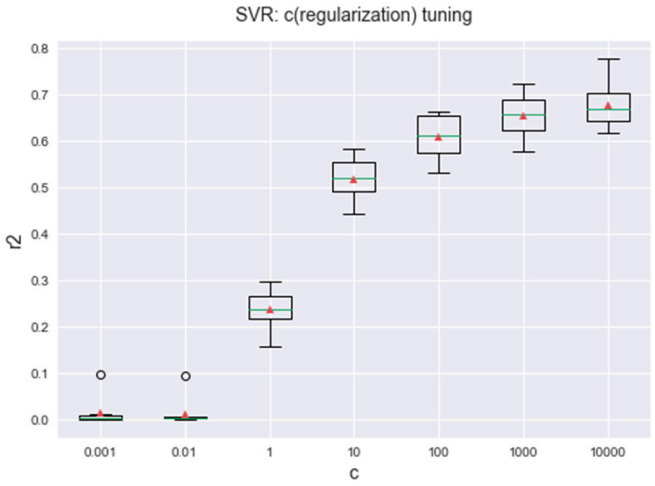

Figure S29: SVR c regularization tuning for TUR

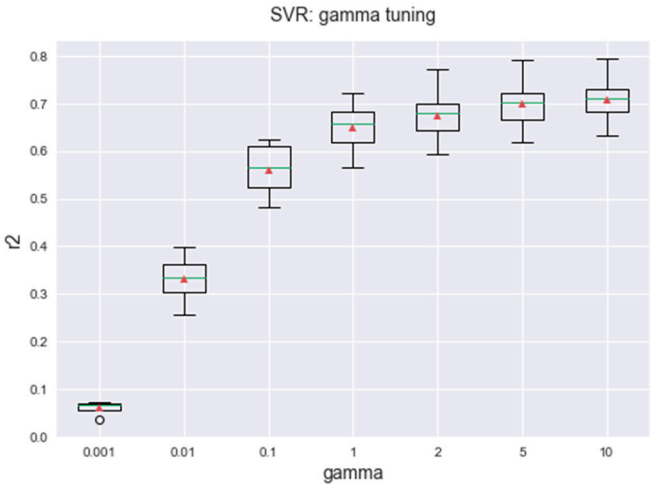

Figure S30: SVRgamma tuning for TUR

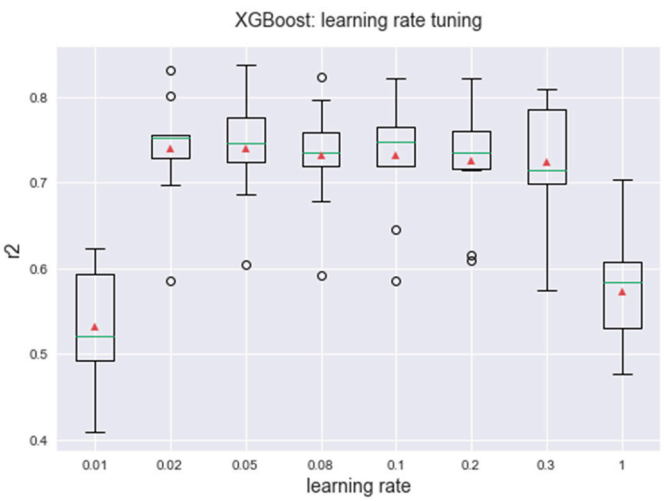

Figure S241: XGBoost learning rate tuning for TUR

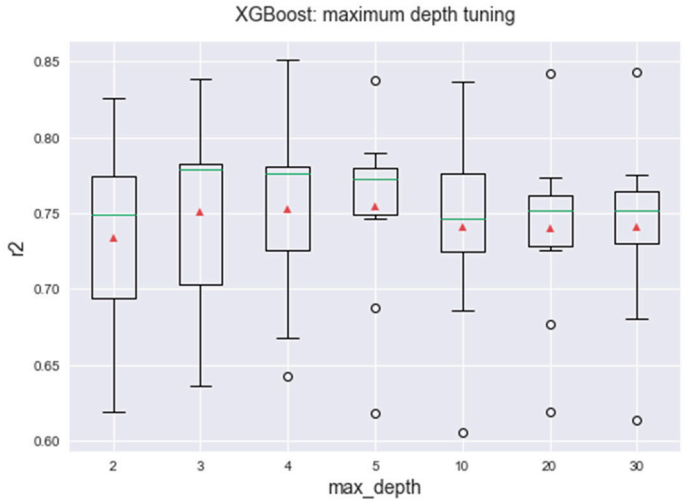

Figure S32: XGBoost maximum depth tuning for TUR

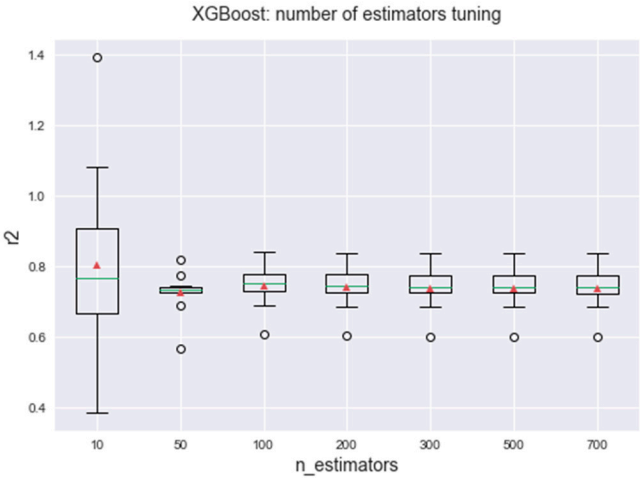

Figure S253: XGBoost number of estimator tuning for TUR

Figure S34: GradBoost learning rate tuning for TUR

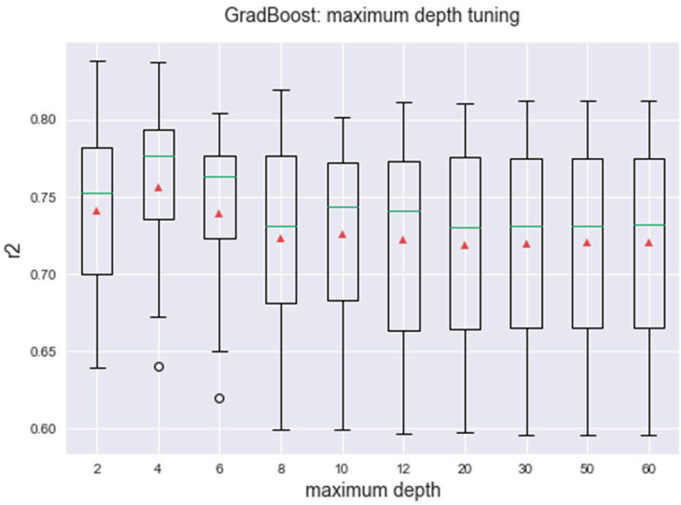

Figure S265: GradBoost maximum depth tuning for TUR

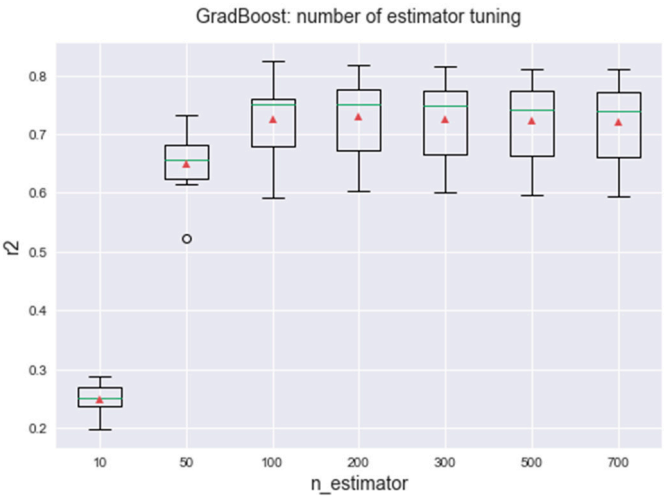

Figure S36: GradBoost number of estimator tuning for TUR