Supplementary Information 1

Elemental composition of the habitat water surrounding the *Ifremeria nautilei* communities sampled at hydrothermal-vent sites in the Southwest Pacific

The data presented here are from measurements of 40 seawater samples collected over the *Ifremeria nautilei* communities collected during the Chubacarc expedition (Hourdez & Jollivet 2019). Note that not all of these samples correspond to sites where *Shinkailepas tollmanni* capsules have been collected. All available measurements were used in the manuscript for the PCA. Only 20 of these samples corresponded to locations where *S. tollmanni* capsules were collected, and were used to compare the elemental composition of seawater with that of the larval shells (see Supplementary Information 6).

REFERENCES

Hourdez, S., Jollivet, D., 2019. CHUBACARC cruise, L'Atalante R/V. doi: 10.17600/18001111.

Area	Site Name	Ca (mM/kg)	K (mM/kg)	Mg (mM/kg)	S (mM/kg)	Si (µM/kg)	Fe (µM/kg)	Mn (µM/kg)	Cu (µM/kg)	Zn (µM/kg)	Li (µM/kg)	Al (µM/kg)	B (µM/kg)	Rb (µM/kg)	Sr (µM/kg)	V (µM/kg)	P (µM/kg)	Mo (nM/kg)	U (nM/kg)	Y (nM/kg)
Lau Basin	Tow Cam	10.37	11.19	70.75	29.61	132.94	0.11	0.15	0.06	0.43	26.39	0.44	423.45	1.40	94.33	0.03	3.19	94.70	13.13	1.17
Lau Basin	Tow Cam	10.77	11.45	68.58	29.44	289.99	0.91	2.24	0.07	0.88	33.57	0.75	408.09	1.49	94.68	0.03	3.42	93.20	12.95	0.87
Lau Basin	Tu'i Malila	12.42	12.73	56.79	28.11	716.40	4.70	15.46	0.12	2.16	48.94	0.36	400.40	3.47	99.97	0.03	2.60	85.19	11.78	1.22
Lau Basin	Tu'i Malila	12.87	13.70	60.40	28.83	995.88	1.53	18.95	0.11	1.05	58.44	1.99	417.16	4.39	103.63	0.03	3.32	79.17	11.72	1.38
Lau Basin	ABE	10.08	11.06	52.63	26.98	299.00	0.93	3.27	0.03	0.97	29.08	1.21	423.75	1.53	86.31	0.03	4.58	84.33	11.49	0.95
Mangatolo	Mangatolo Triple Junction	12.04	12.83	60.44	30.43	630.38	15.87	5.81	0.46	40.28	35.48	1.36	423.97	2.74	112.69	0.04	4.90	104.48	12.14	13.23
Mangatolo	Mangatolo Triple Junction	12.22	13.11	60.77	30.47	1105.35	14.14	28.73	0.78	20.94	35.35	1.32	450.78	2.82	103.84	0.03	4.57	138.28	12.33	7.81
Futuna	Fatu Kapa - Aster'X	13.24	14.40	64.82	33.47	298.79	0.86	2.06	0.07	1.47	42.72	0.90	498.16	3.43	104.49	0.04	3.84	97.65	10.37	0.90
Futuna	Fatu Kapa -Stéphanie	13.41	14.03	64.80	33.33	332.17	1.86	4.19	0.10	1.32	40.52	1.09	473.12	3.02	105.03	0.04	4.46	95.95	11.49	0.81
Futuna	Fatu Kapa -Fati Ufu 7	11.70	11.54	52.19	27.42	440.68	3.27	7.18	0.08	1.20	41.26	0.99	416.43	3.22	93.21	0.03	2.94	96.72	12.45	0.93
Futuna	Fatu Kapa -Fati Ufu 9	14.24	12.45	51.71	26.84	517.81	10.28	20.26	0.04	0.75	56.27	0.72	414.13	5.52	97.39	0.03	2.87	88.29	11.55	1.07
Futuna	Kulo Lasi	9.61	10.03	54.13	28.16	107.87	0.01	0.03	0.03	0.60	24.40	0.77	417.48	1.33	91.33	0.03	4.10	90.43	12.63	0.79
North Fiji	Phoenix	11.23	12.18	60.48	30.00	284.37	1.13	2.11	0.01	1.64	28.58	0.69	400.36	1.56	97.67	0.03	3.33	97.30	12.42	0.92
North Fiji	Phoenix	11.26	11.89	60.97	30.06	212.71	0.52	1.53	0.01	0.52	26.87	0.81	421.56	1.51	97.97	0.03	3.69	98.05	13.24	0.97
Manus Basin	FenWay	10.27	11.17	56.27	28.75	189.09	2.45	4.52	0.05	0.41	25.69	1.11	453.28	1.46	92.21	0.04	3.49	88.91	12.12	1.40
Manus Basin	FenWay	10.03	10.89	54.55	27.17	167.42	1.99	3.63	0.11	0.45	27.13	0.77	443.25	1.39	90.13	0.03	3.29	87.19	11.97	1.16
Manus Basin	Solwara 7	9.95	11.06	52.63	26.59	229.26	12.31	11.89	0.07	0.59	29.32	0.89	435.34	1.77	88.48	0.03	3.46	89.66	12.18	1.01
Manus Basin	Solwara 7	10.09	11.77	52.10	26.89	311.33	27.12	21.67	0.02	0.52	31.81	0.89	421.27	2.12	88.75	0.03	3.13	88.16	12.29	0.97
Manus Basin	Solwara 7	10.08	11.20	53.84	27.15	178.32	4.70	4.83	0.05	0.41	25.74	0.45	420.91	1.51	89.59	0.03	3.16	90.58	12.68	0.88
Manus Basin	Solwara 7	9.69	10.85	52.27	26.42	190.97	8.35	7.96	0.06	0.67	27.29	22.84	419.97	1.60	89.42	0.03	3.28	90.96	12.19	0.85
Manus Basin	Solwara 7	9.74	10.79	52.54	26.68	143.85	2.48	2.44	0.02	0.25	25.88	0.63	426.69	1.39	88.35	0.03	2.95	91.19	12.42	0.79
Manus Basin	Solwara 6	9.94	11.35	51.31	25.98	345.13	0.18	31.40	0.02	0.67	31.59	0.74	436.75	2.10	89.26	0.03	3.93	83.17	10.81	1.73
Manus Basin	Solwara 6	9.88	11.44	52.75	26.76	300.54	0.26	26.73	0.04	1.27	30.57	0.93	435.47	1.99	88.00	0.03	4.57	86.87	11.13	1.66
Manus Basin	Solwara 6	9.76	10.71	51.79	26.11	216.40	0.09	12.37	0.03	0.21	30.79	0.47	445.43	1.65	92.22	0.03	3.38	91.46	11.98	1.18
Manus Basin	Solwara 6	9.92	11.79	52.57	26.33	359.53	0.90	34.02	0.15	0.48	32.42	0.75	442.62	2.17	89.07	0.03	3.99	87.48	10.37	1.79
Manus Basin	Solwara 6	9.99	10.90	52.39	27.51	166.44	0.11	6.25	0.05	1.92	24.34	0.41	422.55	1.43	88.92	0.03	3.23	92.83	12.43	1.79
Manus Basin	Solwara 6	10.08	11.08	53.67	27.17	215.61	0.15	12.76	0.04	1.04	26.52	0.42	428.51	1.64	91.18	0.03	3.65	88.12	11.67	1.22
Manus Basin	North Su	10.39	12.96	52.63	26.03	673.76	1.67	21.88	0.04	25.22	47.56	2.01	437.70	3.84	92.02	0.06	4.15	61.00	8.09	2.35
Manus Basin	North Su	10.21	11.90	52.84	25.34	483.66	2.02	14.94	0.04	45.68	40.11	2.02	429.14	3.07	91.67	0.06	3.68	71.41	9.42	2.26
Manus Basin	North Su	10.22	11.63	53.21	25.70	372.66	1.20	11.10	0.04	1.67	36.48	0.80	417.24	2.61	90.58	0.03	3.39	76.15	10.14	1.65
Manus Basin	South Su	9.52	10.80	53.90	26.69	195.39	0.28	2.62	0.07	22.93	25.08	1.48	370.88	1.48	89.68	0.06	2.86	88.92	12.24	1.28
Manus Basin	South Su	9.51	10.80	52.56	26.63	202.32	0.18	2.15	0.05	31.93	25.61	1.50	379.89	1.47	90.20	0.06	2.76	90.53	12.41	1.41
Manus Basin	South Su	9.48	10.61	51.22	24.64	217.31	0.27	5.66	0.04	17.40	26.31	5.17	406.67	1.60	84.41	0.04	2.81	80.86	10.49	1.72
Manus Basin	South Su	9.64	10.64	52.15	26.56	154.31	0.70	1.45	0.06	10.31	26.72	2.69	370.64	1.44	89.70	0.04	2.74	88.65	12.78	1.81
Manus Basin	South Su	10.25	10.82	54.82	27.85	150.79	0.27	1.07	0.07	24.86	23.95	2.02	415.77	1.38	89.19	0.07	3.13	88.71	12.10	0.90
Manus Basin	South Su	10.16	10.92	55.39	27.56	138.18	1.23	0.46	0.04	2.00	23.03	1.04	415.88	1.32	88.76	0.03	2.86	89.93	12.09	0.38
Manus Basin	South Su	9.69	10.66	54.27	27.10	143.31	0.10	0.40	0.04	7.00	24.86	1.13	371.47	1.35	91.47	0.04	2.80	92.36	12.84	1.03
Woodlark Basin	La Scala	9.78	10.48	52.05	25.43	209.28	0.08	6.99	0.05	1.66	34.71	0.64	388.90	1.33	85.40	0.03	2.17	84.80	11.68	0.86
Woodlark Basin	La Scala	9.60	10.50	52.89	26.10	142.21	0.08	1.34	0.04	19.73	26.55	1.08	377.44	1.27	85.43	0.05	2.39	89.72	12.16	0.88
Woodlark Basin	La Scala	9.93	10.70	54.19	26.62	114.08	0.09	0.48	0.04	2.78	24.94	1.02	385.01	1.29	87.31	0.04	2.31	93.39	13.13	0.75

Supplementary Information 2

Geographic classes and distributions of abundances for the entire *Shinkailepas tollmanni* larval shell dataset

A total of 600 individual encapsulated larval shells was sampled and analyzed from 14 hydrothermal sites, separated into areas and regions. Although part of the Lau Basin, the Mangatolo sites were separated in our study due to the large distance between this area and the three other sites from the Lau Basin. For some sites, *Shinkailepas tollmanni* capsules were collected from several spots (referred to as 'bioboxes'), not necessarily from the same chimney.

Table S2-1: Coordinates of the sampling sites.

Area	Site	Coordinates
Manus	Roman Ruins	3°43'39" S, 151°40'51" E
	Fenway	3°43'42" S, 151°40'20" E
	Solwara 8	3°48'49" S, 151°40'27" E
	North Su	3°47'56" S, 152°06'02" E
	South Su	3°48'29" S, 152°06'17" E
Woodlark	La Scala	9°47'57" S, 155°03'10" E
North Fiji	Phoenix	16°57'00" S, 173°55'08" E
Futuna	Kulo Lasi	14°56'28" S, 177°15'33" W
	Fatu Kapa	14°44'15" S, 177°09'58" W
Lau	Tu'i Malila	21°59'21" S, 176°34'06" W
	ABE	20°45'47" S, 176°11'28" W
	Tow Cam	20°19'05" S, 176°08'16" W
Mangatolo	Mangatolo North	15°24'52" S, 174°39'12" W
	Mangatolo South	15°24'57" S, 174°39'20" W

Table S2-2: Number of individual larvae analyzed for each hydrothermal site. Some sites were sampled more than once and the number of larvae for each biobox is indicated in parentheses.

Region	Area	Site	Number of bioboxes	Number of individual larvae
East	Lau	Tow Cam	2	**10** (2+8)
		Tu'i Malila	2	**49** (40+9)
		ABE	2	**73** (38+35)
	Mangatolo	North	1	**50**
		South	1	**24**
	Futuna	Kulo Lasi	1	**46**
		Fatu Kapa	4	**141** (53+21+34+33)
	North Fiji	Phoenix	2	**96** (48+48)
West	Manus	Fenway	1	**19**
		Solwara	2	**44** (16+28)
		South Su	2	**26** (2+24)
		North Su	2	**11** (6+5)
		Roman Ruins	1	**7**
	Woodlark	Scala	1	**4**

Metal abundances in the 600 analyzed shells of *S. tollmanni* encapsulated larvae are presented in **Figure S2-1**. From these, 104 shells presented one or more measurements below the limit of detection (LOD), altogether representing 124 measurements (all elements combined) out of 7800 (1.59%). These measurements corresponded to values of As (33 shells), Cr (30 shells), Cd (30 shells), Sb (30 shells), and Cu (1 shell). We opted to keep these measurements below the LOD for comparison purposes in subsequent data analyses as these low abundances are informative, albeit not quantitative. Their values have been assigned the arbitrary value of 3.85 10^{-8} $\mu g.g^{-1}$ to reflect a much lower value than the rest of the dataset.

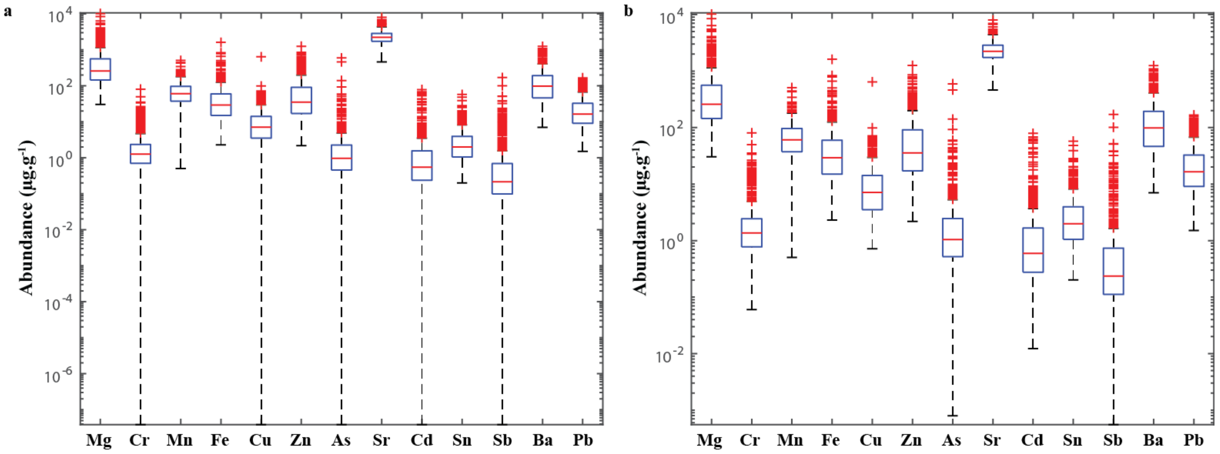

Figure S2-1: Elemental composition of 600 shells of *Shinkailepas tollmanni* encapsulated larvae. **a:** All data, including measurements below the limit of detection. **b:** Same data excluding values below the limit of detection (for Cr, Cu, As, Cd, and Sb).

Parametric statistical comparison between sites was hampered by lack of normality of the data distributions, which is a requirement for MANOVA, as well as homoscedasticity. Data transformation (log and other methods such as cubic root or fourth root) failed to normalize the data, as observed by other studies measuring low-concentration elements (*e.g.*, Gillanders et al., 2001; de Vries et al., 2005). This step was therefore discarded in favor of multivariate classification, described in the main manuscript.

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de Vries, M.C., Gillanders, B.M., Elsdon, T.S., 2005. Facilitation of barium uptake into fish otoliths: influence of strontium concentration and salinity. *Geochimica et Cosmochimica Acta*, 69, 4061–4072. https://doi.org/10.1016/j.gca.2005.03.052.

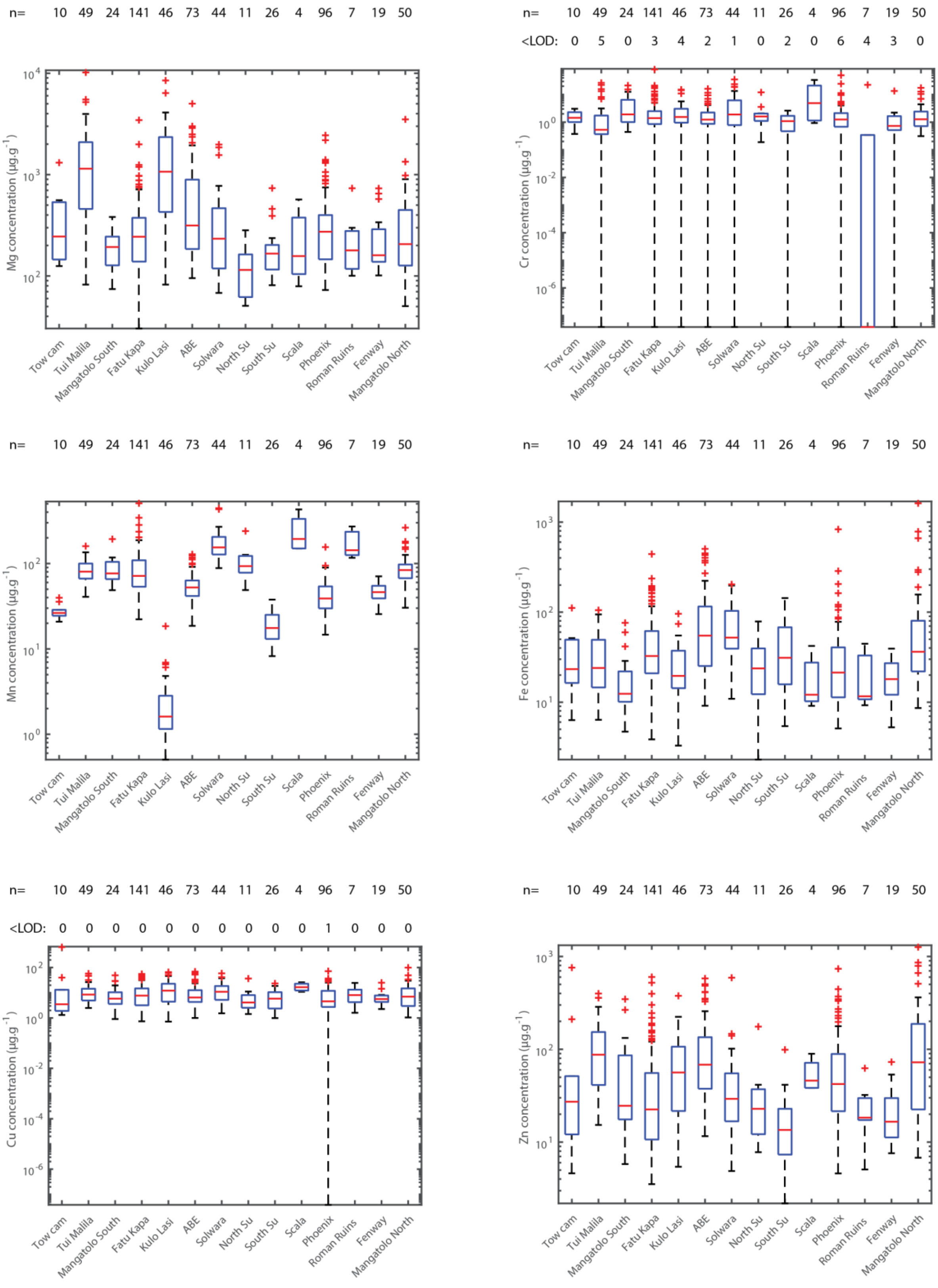
Gillanders, B.M., Sanchez-Jerez, P., Bayle-Sempere, J., Ramos-Espla, A., 2001. Trace elements in otoliths of the two-banded bream from a coastal region in the south-west Mediterranean: are there differences among locations? *Journal of Fish Biology*, 59, 350–363. https://doi.org/10.1111/j.1095-8649.2001.tb00135.x.

Supplementary Information 3

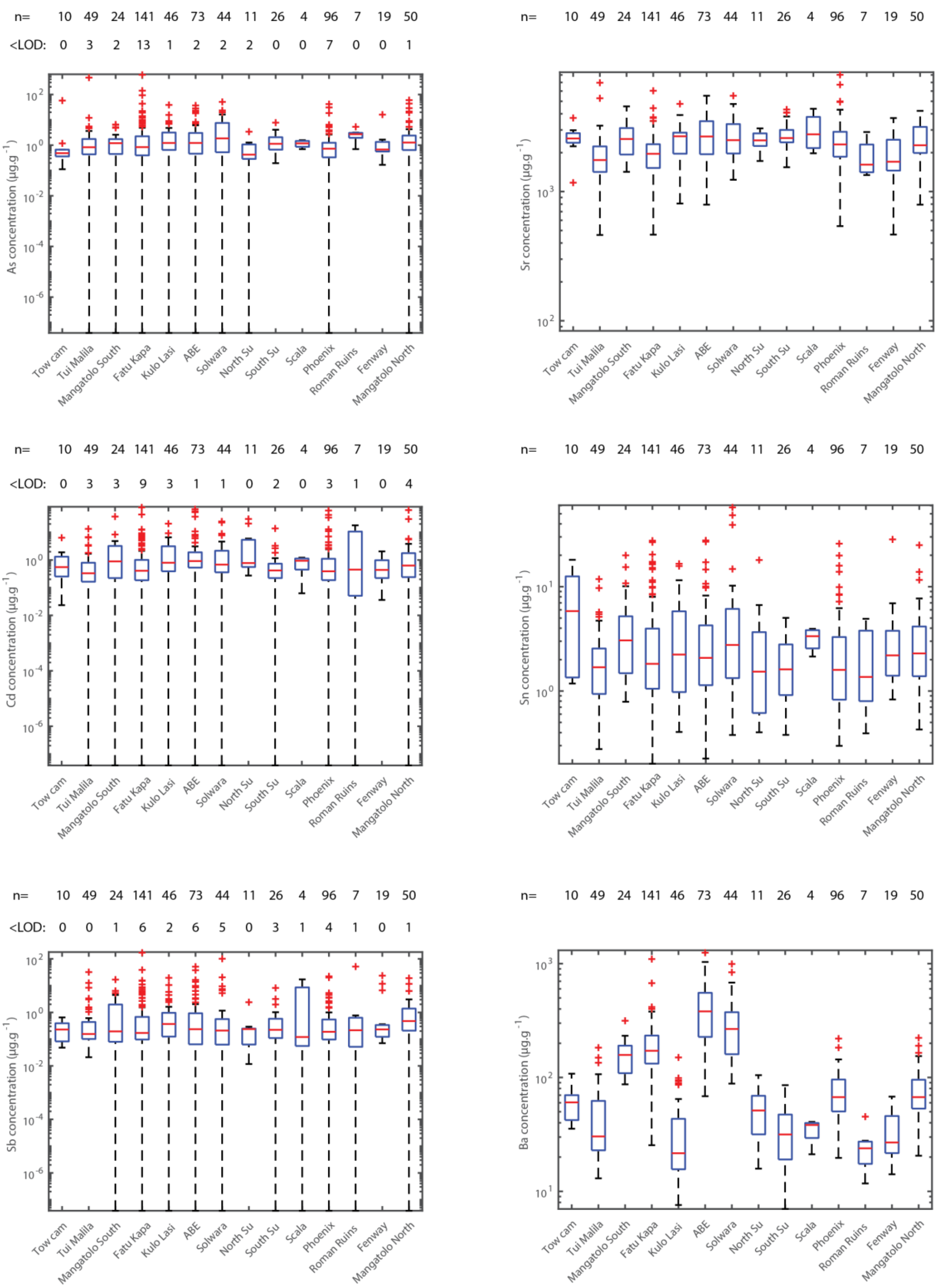
Boxplots for each element measured in the shells of *Shinkailepas tollmanni* encapsulated larvae.

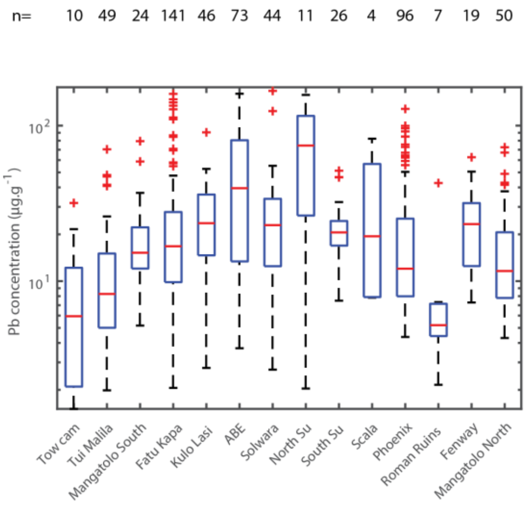
For each element, the number of samples (n) is indicated for all sites. When relevant, the number of values under the limit of detection (LOD) is also indicated. These represent 124 values from the 7800 of the dataset.

Several elements present different distributions between sites; this is the case for Mn, Ba and Pb, with other elements that have less obvious differences such as Mg, Fe, Zn, and Sr. Other elements have relatively similar distributions in all sites: Cr, Cu, As, Sn, Cd, and Sb. Therefore, these last elements do not appear to be promising candidates for discrimination. As five of these six elements are those presenting some values below LOD, we are able to focus on the other elements and use all 600 analysed larval shells for classification, with no values below LOD.



n= 10 49 24 141 46 73 44 11 26 4 96 7 19 50
<LOD: 0 5 0 3 4 2 1 0 2 0 6 4 3 0
<LOD: 0 0 0 0 0 0 0 0 0 0 1 0 0 0
Mg concentration (µg.g⁻¹)
Cr concentration (µg.g⁻¹)
Mn concentration (µg.g⁻¹)
Fe concentration (µg.g⁻¹)
Cu concentration (µg.g⁻¹)
Zn concentration (µg.g⁻¹)
Tow cam
Tui Malila
Mangatolo South
Fatu Kapa
Kulo Lasi
ABE
Solwara
North Su
South Su
Scala
Phoenix
Roman Ruins
Fenway
Mangatolo North


n= 10 49 24 141 46 73 44 11 26 4 96 7 19 50
<LOD: 0 3 2 13 1 2 2 2 0 0 7 0 0 1
As concentration (µg.g^{-1})
Sr concentration (µg.g^{-1})
<LOD: 0 3 3 9 3 1 1 0 2 0 3 1 0 4
Cd concentration (µg.g^{-1})
Sn concentration (µg.g^{-1})
<LOD: 0 0 1 6 2 6 5 0 3 1 4 1 0 1
Sb concentration (µg.g^{-1})
Ba concentration (µg.g^{-1})
Tow cam
Tui Malila
Mangatolo South
Fatu Kapa
Kulo Lasi
ABE
Solwara
North Su
South Su
Scala
Phoenix
Roman Ruins
Fenway
Mangatolo North


n=
10
49
24
141
46
73
44
11
26
4
96
7
19
50
Pb concentration (µg.g⁻¹)
10²
10¹
Tow cam
Tui Malila
Mangatolo South
Fatu Kapa
Kulo Lasi
ABE
Solwara
North Su
South Su
Scala
Phoenix
Roman Ruins
Fenway
Mangatolo North

Supplementary Information 4

Best classification models for *Shinkailepas tollmanni* larval shells elemental fingerprinting

Each model presented in this manuscript refers to the result of a classification method based on several predictors (*i.e.*, variables, here chemical elements). These models can be used as mathematical equations to determine the origin of individual larvae from the composition of its shell.

Model	**Corresponding Figure number**	**Most accurate method**	**Classification success rate**	**Predictors (number)**
All sites	Figure 4	Quadratic Support Vector Machines	70.0%	Mg, Mn, Fe, Zn, Sr, Ba, Pb (7)
Manus/Woodlark	Figure 5a	Trilayered Neural Network	86.5%	Mn, Ba (2)
Sites in East/Woodlark	Figure 5b	Quadratic Support Vector Machines	77.1%	Mg, Mn, Fe, Zn, Sr, Ba, Pb (7)
Areas in East/Woodlark	Figure 5c	Quadratic Support Vector Machines	75.3%	Mg, Mn, Fe, Zn, Sr, Ba, Pb (7)
Sites in Lau	Figure 6a	Linear Discriminant	97.7%	Mn, Ba (2)
Sites in Mangatolo	Figure 6b	Medium Gaussian Support Vector Machines	98.6%	Fe, Ba (2)
Sites in Futuna	Figure 6c	Medium Gaussian Support Vector Machines	100%	Mn, Ba (2)

Short explanations on used methods

To classify data, a support vector machine (SVM) finds the best hyperplane separating all data points of one class (here, site/area) from those of other classes.

Neural networks learn how to classify data using interconnected nodes in a layered structure that resembles a human brain with neurons. Each node transforms input data using single operators and sends the result to the next layer. Each layer learns from the previous one (the first one being the initial training data) according to how its individual nodes are connected and by the weights of those connections.

Discriminant analysis assumes that different classes present data based on different multivariate Gaussian distributions, and estimates the parameters of that distribution for each class. Linear discriminant analysis is also known as the Fisher discriminant.

The best model to classify Lau Basin sites uses Linear Discriminant Analysis, although the distribution of data on both kept variables (Mn and Ba) do not exhibit a normal distribution (one-sample Kolmogorov-Smirnov tests, 5% significance level), also visible on the scatter plot of Figure 6 of the manuscript. However, the distribution of the data from this area presents some overlap between the sites, which tend to reduce the quality of the discrimination of the SVM method. For comparison, Medium Gaussian SVM reached a 97.0% classification success rate on this dataset. Although the difference is minimal, we elected to keep the Linear Discriminant-based model that present better results.

Supplementary Information 5

Details on the larval shell elemental distributions in the Lau area

Some collection sites were sampled several times (bioboxes) in the *Ifremeria* communities to study the variability within site. An example for Lau is given on **Figure S5-1**. We observed no significant difference in the variability at this scale for both Tu'i Malila and ABE. The low number of specimens from Tow Cam (n=10), particularly for biobox 2 (n=2), prevents a reliable interpretation. Still, bioboxes from the same site appear generally similar, and remain different than specimens from other sites.

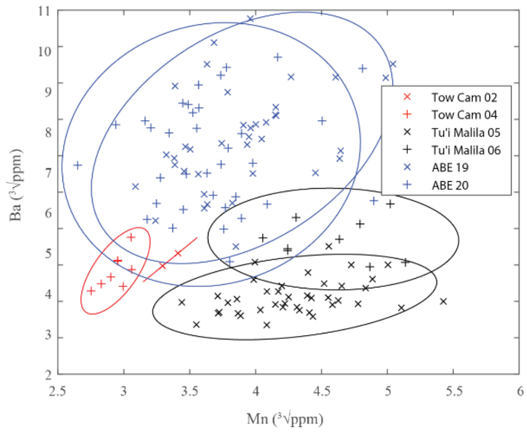


Figure S5-1: Distribution of all larval shell Mn and Ba from Lau for each site and biobox (2 bioboxes at each site).

Supplementary Information 6

Comparison of elemental composition between water and *Shinkailepas tollmanni* larval shells

A total of 20 habitat water samples (out of the 40 indicated in Supplementary Information 1) were collected immediately before sampling *S. tollmanni* capsules. These habitat water samples are from 13 sites, *i.e.* all *S. tollmanni* sampling sites except Solwara 8. Replicates correspond to different bioboxes. Six elements were measured in both the habitat water and the larval shells. The composition of these elements in the shells (n=542) was compared to the composition of habitat water from the corresponding biobox. Due to the large number of larval shells compared to the number of habitat water samples, and because of the individual variability of elemental abundance in shells at the same locality (see **Supplementary Information 3**), we provide the Pearson determination coefficient r^2 and the Spearman correlation coefficient *rho*.

Since hydrothermal fluids are enriched in Mn, we standardized all available concentration data (both waters and shells) by this element to take into account the dilution factor for the hydrothermal fluid in the community water. Results show that most elemental ratios are significantly correlated between shells and water using either the Pearson determination coefficient r^2 or the Spearman correlation coefficient *rho*. Still, correlation coefficients are relatively low. This observation indicates that the elemental composition of larval shells can partially reflect the composition of the hydrothermal environment. Only Fe/Mn was not significantly correlated between shells and water. This might be explained by a fraction of fluid Fe being trapped in the formation of Fe-oxides that are not present in the *S. tollmanni* capsules.

Table S6-1: Correlations of elemental ratios to Mn between habitat water and larval shells.

Elemental ratios	**r^2 Pearson**	**p-value Pearson**	**rho Spearman**	**p-value Spearman**
Mg/Mn	0.492	< 0.001	0.449	< 0.001
Fe/Mn	0.004	0.124	-0.154	< 0.001
Cu/Mn	0.429	< 0.001	0.305	< 0.001
Zn/Mn	0.448	< 0.001	0.256	< 0.001
Sr/Mn	0.641	< 0.001	0.639	< 0.001

As a comparison, we provide also the correlation coefficients for elemental ratios to Ca, commonly reported for carbonates. The Pearson method identifies Fe/Ca and Cu/Ca to have a weak but significant positive correlation between water and shells. However, the Spearman rank correlation method only finds a significant correlation for Fe/Ca.

Table S6-2: Correlations of elemental ratios to Ca between habitat water and larval shells.

Elemental ratios	**r^2 Pearson**	***p-value* Pearson**	***rho* Spearman**	***p-value* Spearman**
Mg/Ca	0,002	0,3	0.015	0.731
Mn/Ca	0,001	0,47	-0.072	0.096
Fe/Ca	0,145	< 0,001	0.580	< 0.001
Cu/Ca	0,022	< 0,001	0.012	0.786
Zn/Ca	0,001	0,42	0.030	0.481
Sr/Ca	0,001	0,57	0.044	0.312

In our manuscript, shell elemental fingerprints were assessed using elemental abundances, not Mn ratios. We tested elemental fingerprints using Mn ratios (not shown here), but observed no improvements of the quality of the models, as Mn is nearly systematically a valid predictor to origin determination.

Supplementary Information 7

Laserogram of acquisition of composition of encapsulated larval shell

A typical laserogram obtained from an Agilent 8900 ICP-MS Triple Quad by the ablation of a *Shinkailepas tollmanni* larval shell with a femtosecond laser ablation system (Novalase SA) is shown on **Figure S7-1**. We present here all the elements used for the classification models, as well as Ca which was used as the internal standard. For each shell ablated, another ablation was performed immediately nearby to analyse the tape on which the samples were deposited. Only a small signal is visible from the tape for Mg and Fe, in significantly lower abundance than in the shell, therefore strongly limiting the potential impact of contamination.

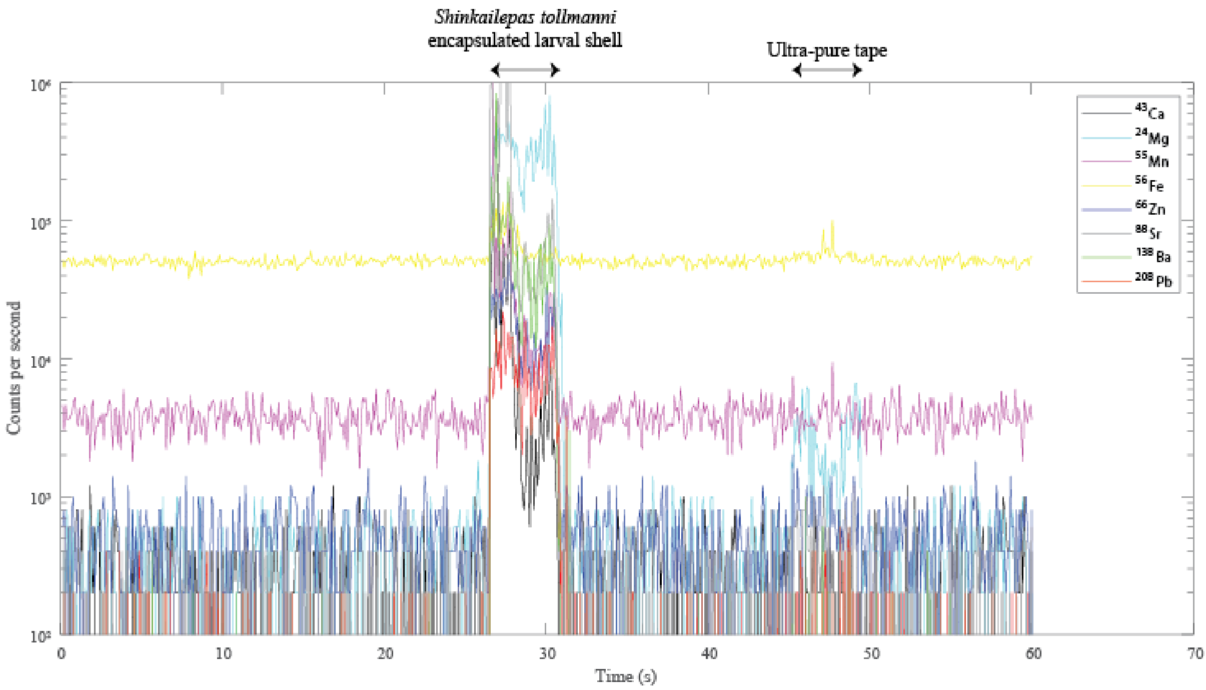


Figure S7-1: Laserogram of a *Shinkailepas tollmanni* encapsulated larval shell and the tape for elements of interest. The positions (in time) of the ablated shell and tape are indicated.

Supplementary Information 8

Matlab scripts and functions for randomization.

This document is composed of ten distinct files, to save each as .m files.

The first one is the script that computes the randomization process of the data to be checked using the user-defined trained classifier, modified from White & Ruttenberg (2007) which was restricted to linear discriminant analysis. This modified version allows running this procedure on any type of classification model saved from the *ClassificationLearner* app from Matlab. To do so, select a trainer classifier from the app, click on “Generate function” (top right corner of the app on Matlab version R2022a), and save it on your computer. The name of that function is to be indicated in the script where indicated.

The code by White & Ruttenberg (2007) used site numbers instead of site names. Since we used site names to train the model, we had to convert site names to site numbers, and site numbers to site names to call the trained classifier. Two functions have been written to perform this task and should be modified according to your data. These two functions are given after the script described above.

The following functions correspond to the trained classifiers generated from our dataset for each of the seven models presented in our manuscript.

References:

White, J.W., Ruttenberg, B.I., 2007. Discriminant function analysis in marine ecology: some oversights and their solutions. *Marine Ecology Progress Series*, 329, 301-305. doi: 10.3354/meps329301.

<u>Script for randomization</u>

```
%This script generates a null expectation for the jack-knife
%reclassification success of a discriminant function analysis by
%randomizing user-provided data

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%Dept. of Ecology, Evolution, and Marine Biology
%University of California, Santa Barbara, CA 93106
%w_white@lifesci.ucsb.edu

%version: last modified March 8, 2007



%Modified by Vincent Mouchi on September 13, 2022


% The initial code by J. Wilson White required numbers as sites. Since we
% used site names to train the model, we had to convert site names to site
% numbers, and site numbers to site names to call the trained classifier.
% Two functions have been written to perform this task (available on
% separate files).

%Output: Vector 'null' containing (in order):
%        Mean of randomized distribution (null(1))
%        Standard deviation of randomized distribution (null(2))
%        Median of randomized distribution (null(3))
%        95% quantile of randomized distribution (null(4))
%        5% quantile of randomized distribution  (null(5))
%        Actual jackknife value (null(6))
%        One-tailed P-value (alpha = 0.05) for actual jackknife value
%        (p(7))



%% To edit
Data=Data_all_sites; % User matrix of data
Group_names=Site_names_all;  % Class names (corresponding to those used for the
trained model)
runs=1000;   % Number of bootstraps desired

% Change also the name of the trained classifier at lines 78 & 108
% Change also the name of the function to convert numbers in sites or
% regions at lines 48, 86 & 112 for class to number, and 78 & 108 for number to
class

%% End edit


nbind=size(Data,1);
Groupid = tollmanni_site2number(Group_names);    %vector Groupid holds group
labels

%%
%Data = Data;              %matrix Data holds raw data
%vars = length(D(1,2:end));      %vars = #columns in Data
g = length(Groupid);           %g = #rows in Data
```

```
rdist=[];

%Begin randomization
disp('Step 1: randomization')
for z=1:runs
    disp(sprintf('Number of iteration: %d',z))
    %Assemble randomized dataset:
    newgroups = randperm(g);
    for b = 1:g %for each sample
        rgroups(b) = Groupid(newgroups(b)); %select random group ID
    end    %end for each sample


%the following loop performs the jackknife
for i=1:nbind %begin jackknifing
    data2=Data;
    group2=rgroups;
    group2(i)=[]; %delete the group ID to be jackknifed out
    data2(i,:)=[]; %delete the data to be jackknifed out
    sample=Data(i,:);

    % Modification here by Vincent Mouchi for classification method %
    [trainedClassifier, validationAccuracy] =
trainClassifierAllSites_70_QuadraticSVM(data2, tollmanni_number2site(group2));
    class(i) = trainedClassifier.predictFcn(sample);
    %class(i)=classify(sample,data2,group2,'linear'); %Matlab's DFA function
    %disp(i)

end %end jackknifing


class_id=tollmanni_site2number(class);

q = 0;  %q is counter for DFA classification success
q = sum(class_id == rgroups) %tabulate correct classifications

dis=q/length(Data(:,1))    %calculate jackknife success rate

rdist(z)=dis;%store success rate in vector 'rdist'
%clear class
end %end randomizations


%% Now calculate observed jackknife success rate for the data:
disp('Step 2: data')
for i=1:nbind
    data2=Data;
    group2=Groupid;
    group2(i)=[];
    data2(i, :) = [];
    sample=Data(i,:);

    % Modification here by Vincent Mouchi for classification method %
    [trainedClassifier, validationAccuracy] =
trainClassifierAllSites_70_QuadraticSVM(data2, tollmanni_number2site(group2));
    class(i) = trainedClassifier.predictFcn(sample);
end
```

```
class_num=tollmanni_site2number(class);

q = 0;
q = sum(class_num == Groupid) %tabulate correct classifications
Uservalue=q/length(Groupid)    %calculate observed jackknife success rate

%% Calculate Pvalue

rdist = sort(rdist); %sort rdist in ascending order

i = 1;
while rdist(i) < Uservalue && i < runs %determine where actual jackknife value
lies in null distribution
    i = i + 1;
end

Pvalue = 1-(i)/runs; %one-tailed P-value based on position of actual jackknife
value in null distribution
if Pvalue == 0
    Pvalue = 1/runs;  %the smallest possible P-value provided is 1/runs
end



null=[mean(rdist) std(rdist) quantile(rdist,0.5) quantile(rdist,0.95)
quantile(rdist,0.05) Uservalue Pvalue];
%Report results
fprintf('\n','Results:','\n')
Mean=null(1)
sd = null(2)
Median = null(3)
Upper95quantile = null(4)
Lower95quantile = null(5)
Observed = Uservalue
P = Pvalue
```

<u>Function to convert site names in numbers</u>

```
function site_number=tollmanni_site2number(site_name)
% Convert the site name from tollmanni data to site number
% site_number=tollmanni_site2number(site_name)
% Input: site_name: cell, name of site
% Output: site_number: integer

for i=1:length(site_name)
if strcmp(site_name(i),'ABE')
    site_number(i)=1;
else
    if strcmp(site_name(i),'Fenway')
        site_number(i)=2;
    else
        if strcmp(site_name(i),'Futuna North')
            site_number(i)=3;
        else
            if strcmp(site_name(i),'Futuna South')
                site_number(i)=4;
            else
                if strcmp(site_name(i),'Mangatolo North')
                    site_number(i)=5;
                else
                    if strcmp(site_name(i),'Mangatolo South')
                        site_number(i)=6;
                    else
                        if strcmp(site_name(i),'North_Su')
                            site_number(i)=7;
                        else
                            if strcmp(site_name(i),'Phoenix')
                                site_number(i)=8;
                            else
                                if strcmp(site_name(i),'Roman_Ruins')
                                    site_number(i)=9;
                                else
                                    if strcmp(site_name(i),'Scala')
                                        site_number(i)=10;
                                    else
                                        if strcmp(site_name(i),'Solwara')
                                            site_number(i)=11;
                                        else
                                            if strcmp(site_name(i),'South_Su')
                                                site_number(i)=12;
                                            else
                                                if strcmp(site_name(i),'Tow cam')
                                                    site_number(i)=13;
                                                else
                                                    if strcmp(site_name(i),'Tui Malila')
                                                        site_number(i)=14;
                                                    end
                                                end
                                            end
                                        end
                                    end
                                end
                            end
                        end
                    end
                end
            end
        end
    end
end
end
end
```

Function to convert site numbers in names

```
function site_name=tollmanni_number2site(site_number)
% Convert the site number from tollmanni data to site name
% site_name=tollmanni_number2site(site_number)
% Output: site_name: cell, name of site
% Input: site_number: integer

for i=1:length(site_number)
if site_number(i)==1
    site_name{i}='ABE';
else
    if site_number(i)==2
        site_name{i}='Fenway';
    else
        if site_number(i)==3
            site_name{i}='Futuna North';
        else
            if site_number(i)==4
                site_name{i}='Futuna South';
            else
                if site_number(i)==5
                    site_name{i}='Mangatolo North';
                else
                    if site_number(i)==6
                        site_name{i}='Mangatolo South';
                    else
                        if site_number(i)==7
                            site_name{i}='North_Su';
                        else
                            if site_number(i)==8
                                site_name{i}='Phoenix';
                            else
                                if site_number(i)==9
                                    site_name{i}='Roman_Ruins';
                                else
                                    if site_number(i)==10
                                        site_name{i}='Scala';
                                    else
                                        if site_number(i)==11
                                            site_name{i}='Solwara';
                                        else
                                            if site_number(i)==12
                                                site_name{i}='South_Su';
                                            else
                                                if site_number(i)==13
                                                    site_name{i}='Tow cam';
                                                else
                                                    if site_number(i)==14
                                                        site_name{i}='Tui Malila';
                                                    end
                                                end
                                            end
                                        end
                                    end
                                end
                            end
                        end
                    end
                end
```

```
                    end
                end
            end
        end
    end
    end
    end
```

__Trained classifier for all sites by Quadratic SVM__

```
function [trainedClassifier, validationAccuracy] =
trainClassifierAllSites_70_QuadraticSVM(trainingData, responseData)
% [trainedClassifier, validationAccuracy] = trainClassifier(trainingData,
% responseData)
% Returns a trained classifier and its accuracy. This code recreates the
% classification model trained in Classification Learner app. Use the
% generated code to automate training the same model with new data, or to
% learn how to programmatically train models.
%
%  Input:
%      trainingData: A matrix with the same number of columns and data type
%       as the matrix imported into the app.
%
%      responseData: A vector with the same data type as the vector
%       imported into the app. The length of responseData and the number of
%       rows of trainingData must be equal.
%
%  Output:
%      trainedClassifier: A struct containing the trained classifier. The
%       struct contains various fields with information about the trained
%       classifier.
%
%      trainedClassifier.predictFcn: A function to make predictions on new
%       data.
%
%      validationAccuracy: A double containing the accuracy as a
%       percentage. In the app, the Models pane displays this overall
%       accuracy score for each model.
%
% Use the code to train the model with new data. To retrain your
% classifier, call the function from the command line with your original
% data or new data as the input arguments trainingData and responseData.
%
% For example, to retrain a classifier trained with the original data set T
% and response Y, enter:
%   [trainedClassifier, validationAccuracy] = trainClassifier(T, Y)
%
% To make predictions with the returned 'trainedClassifier' on new data T2,
% use
%   yfit = trainedClassifier.predictFcn(T2)
%
% T2 must be a matrix containing only the predictor columns used for
% training. For details, enter:
%   trainedClassifier.HowToPredict

warning('off','all')  % Do not display warnings (for trainClassifier)


% Auto-generated by MATLAB on 09-Sep-2022 16:42:26


% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Data transformation: Select subset of the features
% This code selects the same subset of features as were used in the app.
includedPredictorNames = predictors.Properties.VariableNames([true false true true
false true false true false false false true true]);
predictors = predictors(:,includedPredictorNames);
isCategoricalPredictor = isCategoricalPredictor([true false true true false true
false true false false false true true]);

% Train a classifier
% This code specifies all the classifier options and trains the classifier.
template = templateSVM(...
    'KernelFunction', 'polynomial', ...
    'PolynomialOrder', 2, ...
    'KernelScale', 'auto', ...
    'BoxConstraint', 1, ...
    'Standardize', false);
classificationSVM = fitcecoc(...
    predictors, ...
    response, ...
    'Learners', template, ...
    'Coding', 'onevsone', ...
    'ClassNames', {'ABE'; 'Fenway'; 'Futuna North'; 'Futuna South'; 'Mangatolo
North'; 'Mangatolo South'; 'North_Su'; 'Phoenix'; 'Roman_Ruins'; 'Scala';
'Solwara'; 'South_Su'; 'Tow cam'; 'Tui Malila'});

% Create the result struct with predict function
predictorExtractionFcn = @(x) array2table(x, 'VariableNames', predictorNames);
featureSelectionFcn = @(x) x(:,includedPredictorNames);
svmPredictFcn = @(x) predict(classificationSVM, x);
trainedClassifier.predictFcn = @(x)
svmPredictFcn(featureSelectionFcn(predictorExtractionFcn(x)));

% Add additional fields to the result struct
trainedClassifier.ClassificationSVM = classificationSVM;
trainedClassifier.About = 'This struct is a trained model exported from
Classification Learner R2022a.';
trainedClassifier.HowToPredict = sprintf('To make predictions on a new predictor
column matrix, X, use: \n  yfit = c.predictFcn(X) \nreplacing ''c'' with the name
of the variable that is this struct, e.g. ''trainedModel''. \n \nX must contain
exactly 13 columns because this model was trained using 13 predictors. \nX must
contain only predictor columns in exactly the same order and format as your
training \ndata. Do not include the response column or any columns you did not
import into the app. \n \nFor more information, see <a
href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''),
''appclassification_exportmodeltoworkspace'')">How to predict using an exported
model</a>.');
```

```
% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Perform cross-validation
partitionedModel = crossval(trainedClassifier.ClassificationSVM, 'KFold', 5);

% Compute validation predictions
[validationPredictions, validationScores] = kfoldPredict(partitionedModel);

% Compute validation accuracy
validationAccuracy = 1 - kfoldLoss(partitionedModel, 'LossFun', 'ClassifError');
```

Trained classifier for sites from Manus and Woodlark by Trilayered NN

```
function [trainedClassifier, validationAccuracy] =
trainClassifierManusWoodlark_TrilayeredNN(trainingData, responseData)
% [trainedClassifier, validationAccuracy] =
trainClassifierManusWoodlark_TrilayeredNN(trainingData,
% responseData)
% Returns a trained classifier and its accuracy. This code recreates the
% classification model trained in Classification Learner app. Use the
% generated code to automate training the same model with new data, or to
% learn how to programmatically train models.
%
%  Input:
%      trainingData: A matrix with the same number of columns and data type
%       as the matrix imported into the app.
%
%      responseData: A vector with the same data type as the vector
%       imported into the app. The length of responseData and the number of
%       rows of trainingData must be equal.
%
%  Output:
%      trainedClassifier: A struct containing the trained classifier. The
%       struct contains various fields with information about the trained
%       classifier.
%
%      trainedClassifier.predictFcn: A function to make predictions on new
%       data.
%
%      validationAccuracy: A double containing the accuracy as a
%       percentage. In the app, the Models pane displays this overall
%       accuracy score for each model.
%
% Use the code to train the model with new data. To retrain your
% classifier, call the function from the command line with your original
% data or new data as the input arguments trainingData and responseData.
%
% For example, to retrain a classifier trained with the original data set T
% and response Y, enter:
%   [trainedClassifier, validationAccuracy] = trainClassifier(T, Y)
%
% To make predictions with the returned 'trainedClassifier' on new data T2,
% use
%   yfit = trainedClassifier.predictFcn(T2)
%
% T2 must be a matrix containing only the predictor columns used for
% training. For details, enter:
%   trainedClassifier.HowToPredict

% Auto-generated by MATLAB on 14-Nov-2022 10:45:58

warning('off','all')  % Do not display warnings

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Data transformation: Select subset of the features
% This code selects the same subset of features as were used in the app.
includedPredictorNames = predictors.Properties.VariableNames([false false true
false false false false false false false false true false]);
predictors = predictors(:,includedPredictorNames);
isCategoricalPredictor = isCategoricalPredictor([false false true false false
false false false false false false true false]);

% Train a classifier
% This code specifies all the classifier options and trains the classifier.
classificationNeuralNetwork = fitcnet(...
    predictors, ...
    response, ...
    'LayerSizes', [10 10 10], ...
    'Activations', 'relu', ...
    'Lambda', 0, ...
    'IterationLimit', 1000, ...
    'Standardize', true, ...
    'ClassNames', {'Fenway'; 'North_Su'; 'Roman_Ruins'; 'Scala'; 'Solwara';
'South_Su'});

% Create the result struct with predict function
predictorExtractionFcn = @(x) array2table(x, 'VariableNames', predictorNames);
featureSelectionFcn = @(x) x(:,includedPredictorNames);
neuralNetworkPredictFcn = @(x) predict(classificationNeuralNetwork, x);
trainedClassifier.predictFcn = @(x)
neuralNetworkPredictFcn(featureSelectionFcn(predictorExtractionFcn(x)));

% Add additional fields to the result struct
trainedClassifier.ClassificationNeuralNetwork = classificationNeuralNetwork;
trainedClassifier.About = 'This struct is a trained model exported from
Classification Learner R2022a.';
trainedClassifier.HowToPredict = sprintf('To make predictions on a new predictor
column matrix, X, use: \n  yfit = c.predictFcn(X) \nreplacing ''c'' with the name
of the variable that is this struct, e.g. ''trainedModel''. \n \nX must contain
exactly 13 columns because this model was trained using 13 predictors. \nX must
contain only predictor columns in exactly the same order and format as your
training \ndata. Do not include the response column or any columns you did not
import into the app. \n \nFor more information, see <a
href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''),
''appclassification_exportmodeltoworkspace'')">How to predict using an exported
model</a>.');

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Perform cross-validation
partitionedModel = crossval(trainedClassifier.ClassificationNeuralNetwork,
'KFold', 5);

% Compute validation predictions
[validationPredictions, validationScores] = kfoldPredict(partitionedModel);

% Compute validation accuracy
validationAccuracy = 1 - kfoldLoss(partitionedModel, 'LossFun', 'ClassifError');
```

Trained classifier for sites from eastern region and Woodlark by Quadratic SVM

```
function [trainedClassifier, validationAccuracy] =
trainClassifierSitesEasternWoodlark_77_1_QuadraticSVM(trainingData, responseData)
% [trainedClassifier, validationAccuracy] =
trainClassifierSitesEasternWoodlark_77_1_QuadraticSVM(trainingData,
% responseData)
% Returns a trained classifier and its accuracy. This code recreates the
% classification model trained in Classification Learner app. Use the
% generated code to automate training the same model with new data, or to
% learn how to programmatically train models.
%
%  Input:
%      trainingData: A matrix with the same number of columns and data type
%       as the matrix imported into the app.
%
%      responseData: A vector with the same data type as the vector
%       imported into the app. The length of responseData and the number of
%       rows of trainingData must be equal.
%
%  Output:
%      trainedClassifier: A struct containing the trained classifier. The
%       struct contains various fields with information about the trained
%       classifier.
%
%      trainedClassifier.predictFcn: A function to make predictions on new
%       data.
%
%      validationAccuracy: A double containing the accuracy as a
%       percentage. In the app, the Models pane displays this overall
%       accuracy score for each model.
%
% Use the code to train the model with new data. To retrain your
% classifier, call the function from the command line with your original
% data or new data as the input arguments trainingData and responseData.
%
% For example, to retrain a classifier trained with the original data set T
% and response Y, enter:
%   [trainedClassifier, validationAccuracy] = trainClassifier(T, Y)
%
% To make predictions with the returned 'trainedClassifier' on new data T2,
% use
%   yfit = trainedClassifier.predictFcn(T2)
%
% T2 must be a matrix containing only the predictor columns used for
% training. For details, enter:
%   trainedClassifier.HowToPredict

% Auto-generated by MATLAB on 06-Oct-2022 13:16:32

warning('off','all')  % Do not display warnings

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Data transformation: Select subset of the features
% This code selects the same subset of features as were used in the app.
includedPredictorNames = predictors.Properties.VariableNames([true false true true
false true false true false false false true true]);
predictors = predictors(:,includedPredictorNames);
isCategoricalPredictor = isCategoricalPredictor([true false true true false true
false true false false false true true]);

% Train a classifier
% This code specifies all the classifier options and trains the classifier.
template = templateSVM(...
    'KernelFunction', 'polynomial', ...
    'PolynomialOrder', 2, ...
    'KernelScale', 'auto', ...
    'BoxConstraint', 1, ...
    'Standardize', true);
classificationSVM = fitcecoc(...
    predictors, ...
    response, ...
    'Learners', template, ...
    'Coding', 'onevsone', ...
    'ClassNames', {'ABE'; 'Futuna North'; 'Futuna South'; 'Mangatolo North';
'Mangatolo South'; 'Phoenix'; 'Scala'; 'Tow cam'; 'Tui Malila'});

% Create the result struct with predict function
predictorExtractionFcn = @(x) array2table(x, 'VariableNames', predictorNames);
featureSelectionFcn = @(x) x(:,includedPredictorNames);
svmPredictFcn = @(x) predict(classificationSVM, x);
trainedClassifier.predictFcn = @(x)
svmPredictFcn(featureSelectionFcn(predictorExtractionFcn(x)));

% Add additional fields to the result struct
trainedClassifier.ClassificationSVM = classificationSVM;
trainedClassifier.About = 'This struct is a trained model exported from
Classification Learner R2022a.';
trainedClassifier.HowToPredict = sprintf('To make predictions on a new predictor
column matrix, X, use: \n  yfit = c.predictFcn(X) \nreplacing ''c'' with the name
of the variable that is this struct, e.g. ''trainedModel''. \n \nX must contain
exactly 13 columns because this model was trained using 13 predictors. \nX must
contain only predictor columns in exactly the same order and format as your
training \ndata. Do not include the response column or any columns you did not
import into the app. \n \nFor more information, see <a
href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''),
''appclassification_exportmodeltoworkspace'')">How to predict using an exported
model</a>.');

% Extract predictors and response
```

```
% This code processes the data into the right shape for training the
% model.
% Convert input to table
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Perform cross-validation
partitionedModel = crossval(trainedClassifier.ClassificationSVM, 'KFold', 5);

% Compute validation predictions
[validationPredictions, validationScores] = kfoldPredict(partitionedModel);

% Compute validation accuracy
validationAccuracy = 1 - kfoldLoss(partitionedModel, 'LossFun', 'ClassifError');
```

Trained classifier for areas from eastern region and Woodlark by Quadratic SVM

```
function [trainedClassifier, validationAccuracy] =
trainClassifierAreasEastWoodlark75_3_QuadraticSVM(trainingData, responseData)
% [trainedClassifier, validationAccuracy] =
trainClassifierAreasEastWoodlark75_3_QuadraticSVM(trainingData,
% responseData)
% Returns a trained classifier and its accuracy. This code recreates the
% classification model trained in Classification Learner app. Use the
% generated code to automate training the same model with new data, or to
% learn how to programmatically train models.
%
%  Input:
%      trainingData: A matrix with the same number of columns and data type
%       as the matrix imported into the app.
%
%      responseData: A vector with the same data type as the vector
%       imported into the app. The length of responseData and the number of
%       rows of trainingData must be equal.
%
%  Output:
%      trainedClassifier: A struct containing the trained classifier. The
%       struct contains various fields with information about the trained
%       classifier.
%
%      trainedClassifier.predictFcn: A function to make predictions on new
%       data.
%
%      validationAccuracy: A double containing the accuracy as a
%       percentage. In the app, the Models pane displays this overall
%       accuracy score for each model.
%
% Use the code to train the model with new data. To retrain your
% classifier, call the function from the command line with your original
% data or new data as the input arguments trainingData and responseData.
%
% For example, to retrain a classifier trained with the original data set T
% and response Y, enter:
%   [trainedClassifier, validationAccuracy] = trainClassifier(T, Y)
%
% To make predictions with the returned 'trainedClassifier' on new data T2,
% use
%   yfit = trainedClassifier.predictFcn(T2)
%
% T2 must be a matrix containing only the predictor columns used for
% training. For details, enter:
%   trainedClassifier.HowToPredict

% Auto-generated by MATLAB on 06-Oct-2022 11:34:01
warning('off','all')  % Do not display warnings


% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Data transformation: Select subset of the features
% This code selects the same subset of features as were used in the app.
includedPredictorNames = predictors.Properties.VariableNames([true false true
false false true false true false false false true true]);
predictors = predictors(:,includedPredictorNames);
isCategoricalPredictor = isCategoricalPredictor([true false true false false true
false true false false false true true]);

% Train a classifier
% This code specifies all the classifier options and trains the classifier.
template = templateSVM(...
    'KernelFunction', 'polynomial', ...
    'PolynomialOrder', 2, ...
    'KernelScale', 'auto', ...
    'BoxConstraint', 1, ...
    'Standardize', true);
classificationSVM = fitcecoc(...
    predictors, ...
    response, ...
    'Learners', template, ...
    'Coding', 'onevsone', ...
    'ClassNames', {'Futuna'; 'Lau'; 'Mangatolo'; 'North Fiji'; 'Woodlark'});

% Create the result struct with predict function
predictorExtractionFcn = @(x) array2table(x, 'VariableNames', predictorNames);
featureSelectionFcn = @(x) x(:,includedPredictorNames);
svmPredictFcn = @(x) predict(classificationSVM, x);
trainedClassifier.predictFcn = @(x)
svmPredictFcn(featureSelectionFcn(predictorExtractionFcn(x)));

% Add additional fields to the result struct
trainedClassifier.ClassificationSVM = classificationSVM;
trainedClassifier.About = 'This struct is a trained model exported from
Classification Learner R2022a.';
trainedClassifier.HowToPredict = sprintf('To make predictions on a new predictor
column matrix, X, use: \n  yfit = c.predictFcn(X) \nreplacing ''c'' with the name
of the variable that is this struct, e.g. ''trainedModel''. \n \nX must contain
exactly 13 columns because this model was trained using 13 predictors. \nX must
contain only predictor columns in exactly the same order and format as your
training \ndata. Do not include the response column or any columns you did not
import into the app. \n \nFor more information, see <a
href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''),
''appclassification_exportmodeltoworkspace'')">How to predict using an exported
model</a>.');

% Extract predictors and response
% This code processes the data into the right shape for training the
```

```
% model.
% Convert input to table
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Perform cross-validation
partitionedModel = crossval(trainedClassifier.ClassificationSVM, 'KFold', 5);

% Compute validation predictions
[validationPredictions, validationScores] = kfoldPredict(partitionedModel);

% Compute validation accuracy
validationAccuracy = 1 - kfoldLoss(partitionedModel, 'LossFun', 'ClassifError');
```

Trained classifier for sites from Lau by LDA

```
function [trainedClassifier, validationAccuracy] =
trainClassifierLau_97_7_LinearDiscriminant2(trainingData, responseData)
% [trainedClassifier, validationAccuracy] =
trainClassifierLau_97_7_LinearDiscriminant2(trainingData,
% responseData)
% Returns a trained classifier and its accuracy. This code recreates the
% classification model trained in Classification Learner app. Use the
% generated code to automate training the same model with new data, or to
% learn how to programmatically train models.
%
%  Input:
%      trainingData: A matrix with the same number of columns and data type
%       as the matrix imported into the app.
%
%      responseData: A vector with the same data type as the vector
%       imported into the app. The length of responseData and the number of
%       rows of trainingData must be equal.
%
%  Output:
%      trainedClassifier: A struct containing the trained classifier. The
%       struct contains various fields with information about the trained
%       classifier.
%
%      trainedClassifier.predictFcn: A function to make predictions on new
%       data.
%
%      validationAccuracy: A double containing the accuracy as a
%       percentage. In the app, the Models pane displays this overall
%       accuracy score for each model.
%
% Use the code to train the model with new data. To retrain your
% classifier, call the function from the command line with your original
% data or new data as the input arguments trainingData and responseData.
%
% For example, to retrain a classifier trained with the original data set T
% and response Y, enter:
%   [trainedClassifier, validationAccuracy] = trainClassifier(T, Y)
%
% To make predictions with the returned 'trainedClassifier' on new data T2,
% use
%   yfit = trainedClassifier.predictFcn(T2)
%
% T2 must be a matrix containing only the predictor columns used for
% training. For details, enter:
%   trainedClassifier.HowToPredict

% Auto-generated by MATLAB on 15-Nov-2022 11:12:35

warning('off','all')  % Do not display warnings

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Data transformation: Select subset of the features
% This code selects the same subset of features as were used in the app.
includedPredictorNames = predictors.Properties.VariableNames([false false true
false false false false false false false false true false]);
predictors = predictors(:,includedPredictorNames);
isCategoricalPredictor = isCategoricalPredictor([false false true false false
false false false false false false true false]);

% Train a classifier
% This code specifies all the classifier options and trains the classifier.
classificationDiscriminant = fitcdiscr(...
    predictors, ...
    response, ...
    'DiscrimType', 'linear', ...
    'Gamma', 0, ...
    'FillCoeffs', 'off', ...
    'ClassNames', {'ABE'; 'Tow cam'; 'Tui Malila'});

% Create the result struct with predict function
predictorExtractionFcn = @(x) array2table(x, 'VariableNames', predictorNames);
featureSelectionFcn = @(x) x(:,includedPredictorNames);
discriminantPredictFcn = @(x) predict(classificationDiscriminant, x);
trainedClassifier.predictFcn = @(x)
discriminantPredictFcn(featureSelectionFcn(predictorExtractionFcn(x)));

% Add additional fields to the result struct
trainedClassifier.ClassificationDiscriminant = classificationDiscriminant;
trainedClassifier.About = 'This struct is a trained model exported from
Classification Learner R2022a.';
trainedClassifier.HowToPredict = sprintf('To make predictions on a new predictor
column matrix, X, use: \n  yfit = c.predictFcn(X) \nreplacing ''c'' with the name
of the variable that is this struct, e.g. ''trainedModel''. \n \nX must contain
exactly 13 columns because this model was trained using 13 predictors. \nX must
contain only predictor columns in exactly the same order and format as your
training \ndata. Do not include the response column or any columns you did not
import into the app. \n \nFor more information, see <a
href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''),
''appclassification_exportmodeltoworkspace'')">How to predict using an exported
model</a>.');

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});
```

```
predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Perform cross-validation
partitionedModel = crossval(trainedClassifier.ClassificationDiscriminant, 'KFold',
5);

% Compute validation predictions
[validationPredictions, validationScores] = kfoldPredict(partitionedModel);

% Compute validation accuracy
validationAccuracy = 1 - kfoldLoss(partitionedModel, 'LossFun', 'ClassifError');
```

Trained classifier for sites from Futuna by Medium Gaussian SVM

```
function [trainedClassifier, validationAccuracy] =
trainClassifierFutuna_100_MediumGaussianSVM2(trainingData, responseData)
% [trainedClassifier, validationAccuracy] =
trainClassifierFutuna_100_MediumGaussianSVM2(trainingData,
% responseData)
% Returns a trained classifier and its accuracy. This code recreates the
% classification model trained in Classification Learner app. Use the
% generated code to automate training the same model with new data, or to
% learn how to programmatically train models.
%
%  Input:
%      trainingData: A matrix with the same number of columns and data type
%       as the matrix imported into the app.
%
%      responseData: A vector with the same data type as the vector
%       imported into the app. The length of responseData and the number of
%       rows of trainingData must be equal.
%
%  Output:
%      trainedClassifier: A struct containing the trained classifier. The
%       struct contains various fields with information about the trained
%       classifier.
%
%      trainedClassifier.predictFcn: A function to make predictions on new
%       data.
%
%      validationAccuracy: A double containing the accuracy as a
%       percentage. In the app, the Models pane displays this overall
%       accuracy score for each model.
%
% Use the code to train the model with new data. To retrain your
% classifier, call the function from the command line with your original
% data or new data as the input arguments trainingData and responseData.
%
% For example, to retrain a classifier trained with the original data set T
% and response Y, enter:
%   [trainedClassifier, validationAccuracy] = trainClassifier(T, Y)
%
% To make predictions with the returned 'trainedClassifier' on new data T2,
% use
%   yfit = trainedClassifier.predictFcn(T2)
%
% T2 must be a matrix containing only the predictor columns used for
% training. For details, enter:
%   trainedClassifier.HowToPredict

% Auto-generated by MATLAB on 15-Nov-2022 12:21:34

warning('off','all')  % Do not display warnings

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Data transformation: Select subset of the features
% This code selects the same subset of features as were used in the app.
includedPredictorNames = predictors.Properties.VariableNames([false false true
false false false false false false false false true false]);
predictors = predictors(:,includedPredictorNames);
isCategoricalPredictor = isCategoricalPredictor([false false true false false
false false false false false false true false]);

% Train a classifier
% This code specifies all the classifier options and trains the classifier.
classificationSVM = fitcsvm(...
    predictors, ...
    response, ...
    'KernelFunction', 'gaussian', ...
    'PolynomialOrder', [], ...
    'KernelScale', 1.4, ...
    'BoxConstraint', 1, ...
    'Standardize', true, ...
    'ClassNames', {'Futuna North'; 'Futuna South'});

% Create the result struct with predict function
predictorExtractionFcn = @(x) array2table(x, 'VariableNames', predictorNames);
featureSelectionFcn = @(x) x(:,includedPredictorNames);
svmPredictFcn = @(x) predict(classificationSVM, x);
trainedClassifier.predictFcn = @(x)
svmPredictFcn(featureSelectionFcn(predictorExtractionFcn(x)));

% Add additional fields to the result struct
trainedClassifier.ClassificationSVM = classificationSVM;
trainedClassifier.About = 'This struct is a trained model exported from
Classification Learner R2022a.';
trainedClassifier.HowToPredict = sprintf('To make predictions on a new predictor
column matrix, X, use: \n  yfit = c.predictFcn(X) \nreplacing ''c'' with the name
of the variable that is this struct, e.g. ''trainedModel''. \n \nX must contain
exactly 13 columns because this model was trained using 13 predictors. \nX must
contain only predictor columns in exactly the same order and format as your
training \ndata. Do not include the response column or any columns you did not
import into the app. \n \nFor more information, see <a
href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''),
''appclassification_exportmodeltoworkspace'')">How to predict using an exported
model</a>.');

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
```

```
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});

predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];

% Perform cross-validation
partitionedModel = crossval(trainedClassifier.ClassificationSVM, 'KFold', 5);

% Compute validation predictions
[validationPredictions, validationScores] = kfoldPredict(partitionedModel);

% Compute validation accuracy
validationAccuracy = 1 - kfoldLoss(partitionedModel, 'LossFun', 'ClassifError');
```

Trained classifier for sites from Mangatolo by SVM

```
function [trainedClassifier, validationAccuracy] =
trainClassifier_Mangatolo_SVM_98_6(trainingData, responseData)
% [trainedClassifier, validationAccuracy] = trainClassifier(trainingData,
% responseData)
% Returns a trained classifier and its accuracy. This code recreates the
% classification model trained in Classification Learner app. Use the
% generated code to automate training the same model with new data, or to
% learn how to programmatically train models.
%
%  Input:
%      trainingData: A matrix with the same number of columns and data type
%       as the matrix imported into the app.
%
%      responseData: A vector with the same data type as the vector
%       imported into the app. The length of responseData and the number of
%       rows of trainingData must be equal.
%
%
%  Output:
%      trainedClassifier: A struct containing the trained classifier. The
%       struct contains various fields with information about the trained
%       classifier.
%
%      trainedClassifier.predictFcn: A function to make predictions on new
%       data.
%
%      validationAccuracy: A double representing the validation accuracy as
%       a percentage. In the app, the Models pane displays the validation
%       accuracy for each model.
%
% Use the code to train the model with new data. To retrain your
% classifier, call the function from the command line with your original
% data or new data as the input arguments trainingData and responseData.
%
% For example, to retrain a classifier trained with the original data set T
% and response Y, enter:
%   [trainedClassifier, validationAccuracy] = trainClassifier(T, Y)
%
% To make predictions with the returned 'trainedClassifier' on new data T2,
% use
%   [yfit,scores] = trainedClassifier.predictFcn(T2)
%
% T2 must be a matrix containing only the predictor columns used for
% training. For details, enter:
%   trainedClassifier.HowToPredict

% Auto-generated by MATLAB on 01-Apr-2023 12:02:11


% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});
```

```
predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];
classNames = {'Mangatolo North'; 'Mangatolo South'};

% Data transformation: Select subset of the features
% This code selects the same subset of features as were used in the app.
includedPredictorNames = predictors.Properties.VariableNames([false false false
true false false false false false false false true false]);
predictors = predictors(:,includedPredictorNames);
isCategoricalPredictor = isCategoricalPredictor([false false false true false
false false false false false false true false]);

% Train a classifier
% This code specifies all the classifier options and trains the classifier.
classificationSVM = fitcsvm(...
    predictors, ...
    response, ...
    'KernelFunction', 'gaussian', ...
    'PolynomialOrder', [], ...
    'KernelScale', 1.4, ...
    'BoxConstraint', 1, ...
    'Standardize', true, ...
    'ClassNames', classNames);

% Create the result struct with predict function
predictorExtractionFcn = @(x) array2table(x, 'VariableNames', predictorNames);
featureSelectionFcn = @(x) x(:,includedPredictorNames);
svmPredictFcn = @(x) predict(classificationSVM, x);
trainedClassifier.predictFcn = @(x)
svmPredictFcn(featureSelectionFcn(predictorExtractionFcn(x)));

% Add additional fields to the result struct
trainedClassifier.ClassificationSVM = classificationSVM;
trainedClassifier.About = 'This struct is a trained model exported from
Classification Learner R2023a.';
trainedClassifier.HowToPredict = sprintf('To make predictions on a new predictor
column matrix, X, use: \n  [yfit,scores] = c.predictFcn(X) \nreplacing ''c'' with
the name of the variable that is this struct, e.g. ''trainedModel''. \n \nX must
contain exactly 13 columns because this model was trained using 13 predictors. \nX
must contain only predictor columns in exactly the same order and format as your
training \ndata. Do not include the response column or any columns you did not
import into the app. \n \nFor more information, see <a
href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''),
''appclassification_exportmodeltoworkspace'')">How to predict using an exported
model</a>.');

% Extract predictors and response
% This code processes the data into the right shape for training the
% model.
% Convert input to table
inputTable = array2table(trainingData, 'VariableNames', {'column_1', 'column_2',
'column_3', 'column_4', 'column_5', 'column_6', 'column_7', 'column_8',
'column_9', 'column_10', 'column_11', 'column_12', 'column_13'});
```

```
predictorNames = {'column_1', 'column_2', 'column_3', 'column_4', 'column_5',
'column_6', 'column_7', 'column_8', 'column_9', 'column_10', 'column_11',
'column_12', 'column_13'};
predictors = inputTable(:, predictorNames);
response = responseData;
isCategoricalPredictor = [false, false, false, false, false, false, false, false,
false, false, false, false, false];
classNames = {'Mangatolo North'; 'Mangatolo South'};

% Perform cross-validation
partitionedModel = crossval(trainedClassifier.ClassificationSVM, 'KFold', 5);

% Compute validation predictions
[validationPredictions, validationScores] = kfoldPredict(partitionedModel);

% Compute validation accuracy
validationAccuracy = 1 - kfoldLoss(partitionedModel, 'LossFun', 'ClassifError');
```