Environmental Data Science

CAMBRIDGE UNIVERSITY PRESS

RESEARCH ARTICLE

Supplement: Identifying climate models based on their daily output using machine learning

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S1. Overview

- Section S2: Technical details and CNN layout
- Section S3: Bootstrap testing
- Section S4: Training evolution and test reliability of the CNN
- Section S6: Additional temperature maps
- Section S6: Models used and model families

Table S1. *Overview of classifiers, classification type, bias corrections, out-of-sample frameworks, and presented results.*

Classifier	Type	Bias correction	Out-of-sample	Results
Log. reg.	Binary	global mean	temporal	Fig 1a
Log. reg.	Binary	global mean	temporal and dataset	Fig 2a
Log. reg.	Binary	global mean	temporal(1)	Fig S1a
CNN	Binary	global mean	temporal and dataset	Fig 2b
CNN	Binary	seasonal cycle and global mean	temporal and dataset	Fig 2c
CNN	Binary	seasonal cycle and global mean	temporal(1)	Fig S1b
CNN	Multi-class	seasonal cycle and global mean	temporal	Fig 3
CNN	Mulit-class	seasonal cycle and global mean	temporal(2)	Fig 4

(1) Training data from 100 random bootstrap samples
(2) Using test samples from the end-of-century period 2091-2100

S2. Technical details and CNN layout

We train the classifiers on a full node of the University of Vienna Institute for Meteorology and Geophysics *Jet* Linux cluster. It has 40 Intel Xeon Gold 6148 CPUs with 2.40GHz and a total of 755GB of memory. The logistic regression classifier is implemented using Pythons scikit-learn library (https://scikit-learn.org), the convolutional neural network is implemented using tensorflows keras library (https://keras.io/). Table S3 details the layers of the convolutional neural network used.

Table S2. *Summary of layers for the convolutional neural network. The convolutional layers use the rectified linear unit as activation function, the dense layer uses softmax.*

Layer	Properties	Output shape	Nr. parameters
Input	-	(72, 144, 1)	0
Convolutional	Depth: 128; Size: 5; Strides: 2	(36, 72, 128)	3’328
Max. pooling	Size: 4	(9, 18, 128)	0
Convolutional	Depth: 64; Size: 3; Strides: 1	(9, 18, 64)	73’792
Max. pooling	Size: 2	(4, 9, 64)	0
Convolutional	Depth: 64; Size: 3; Strides: 1	(4, 9, 64)	36’928
Max. pooling	Size: 2	(2, 4, 64)	0
Convolutional	Depth: 32; Size: 2; Strides: 1	(4, 9, 32)	8’224
Max. pooling	Size: 2	(1, 2, 32)	0
Flatten	-	(64)	0
Dense	-	(2 / 47)	130 / 3’055

S3. Bootstrap testing

In the main manuscript each classifier is trained on one realisation of randomly drawn training samples. To investigate the robustness of the results under different training samples we perform two bootstrap tests, one for the logistic regression classifier and one for the convolutional neural network. For both cases the classifier is trained on all models (i.e., the test samples are only temporally out-of-sample) as training individual classifiers for each model in addition to bootstrapping is computationally not feasible.

For both cases we re-train the classifier 100 times, based on the random bootstrap samples. Figure S1 shows the distribution of probabilities for the test samples from each model similar to figure 2 in the main manuscript. For the logistic regression classifier only the minimum/maximum range is affected by the bootstrapping (green uncertainty ranges), indicating that the method is mostly robust when using different training samples. For the convolutional neural network the interquarile range can also be somewhat affected when basing training on different samples. However, the uncertainty is overall rather small and does not change any of the conclusions from the main paper.

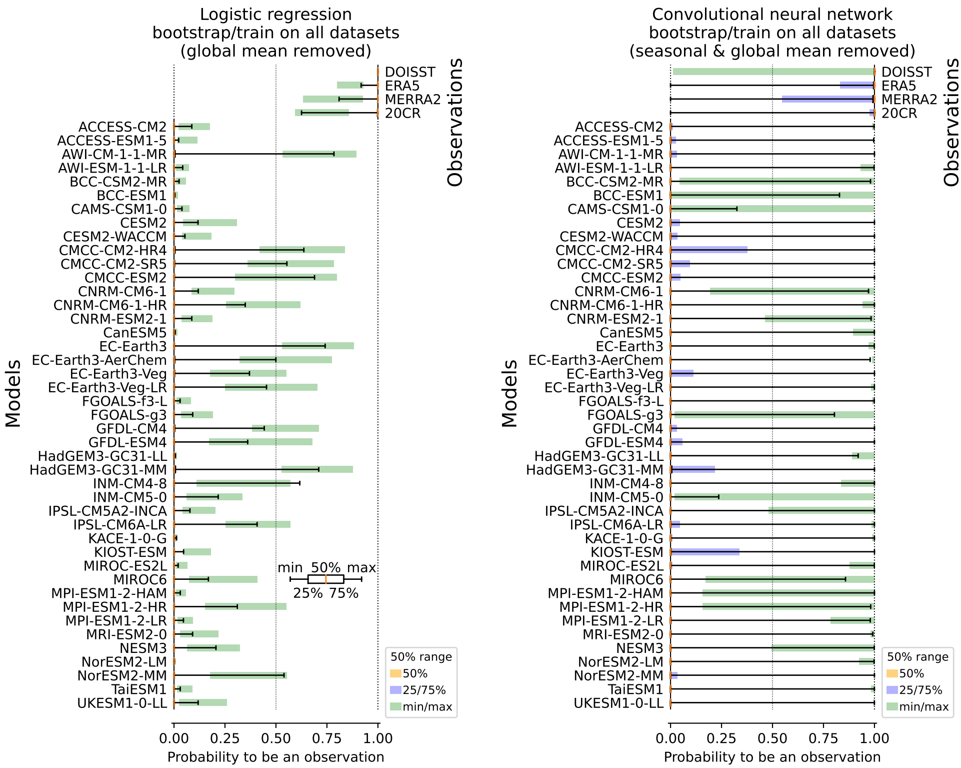

Figure S1. *Distribution of predicted probabilities for the test set in a bootstrap setting. One boostrap sample is plotted as boxes similar to figure 2 in the main manuscript. The shadings give the 50 % uncertainty range in the total range (green), the interquartile range (blue), and the median (yellow). Note that the median uncertainty does not show in any case. (left) Results for a logistic regression classifier using data with the global mean removed. (right) Results for a convolutional neural network using data with the mean seasonal cycle and the global mean removed.*

S4. Training evolution and test reliability of the CNN

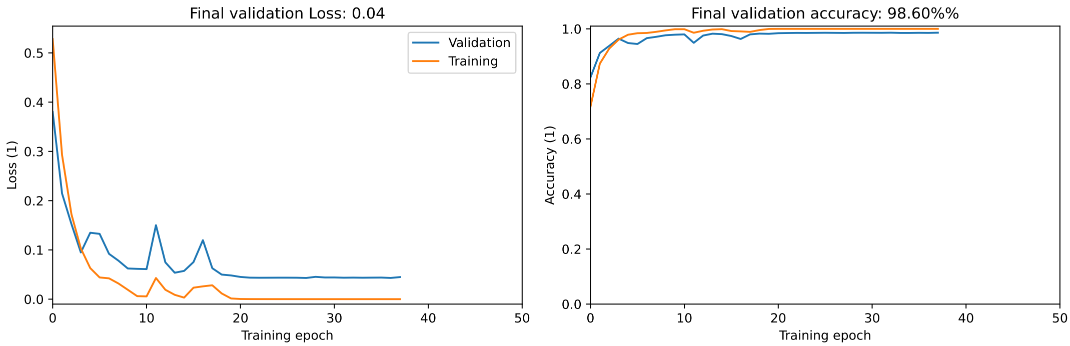

Figure S2. *Training and validation loss (left) and accuracy (right) evolution of the convolutional neural network during the training process for separating models and observations with the seasonal mean cycle and the global mean removed. Training is interrupted before the maximum of 50 epochs by the use of an early stopping algorithm monitoring validation loss.*

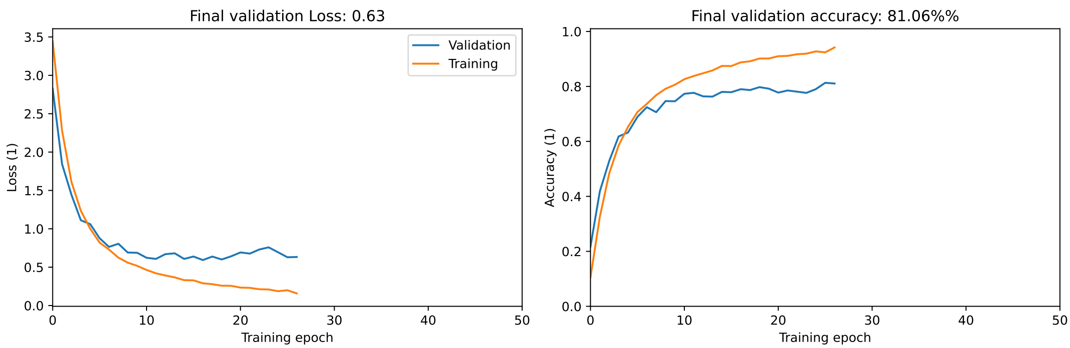

Figure S3. *Similar to figure S2 but for the training process of separating 47 datasets.*

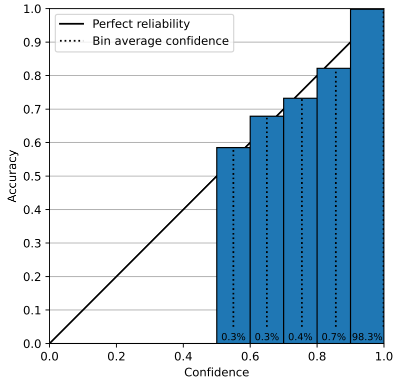

Figure S4. *Reliability diagram for the logistic regression classifiers used in figure 2a. The x-axis is binned by the confidence assigned to the samples, the numbers at the bottom of each bar give the fraction of samples within each bin, and the dashed vertical lines give the average of all confidence values within each bin. The y-axis gives the average accuracy across samples in each bin (i.e., correct samples divided by total samples). For perfect reliability the average confidence should be equal to the average accuracy (i.e., the vertical dashed lines should coincide with the solid 1:1 line).*

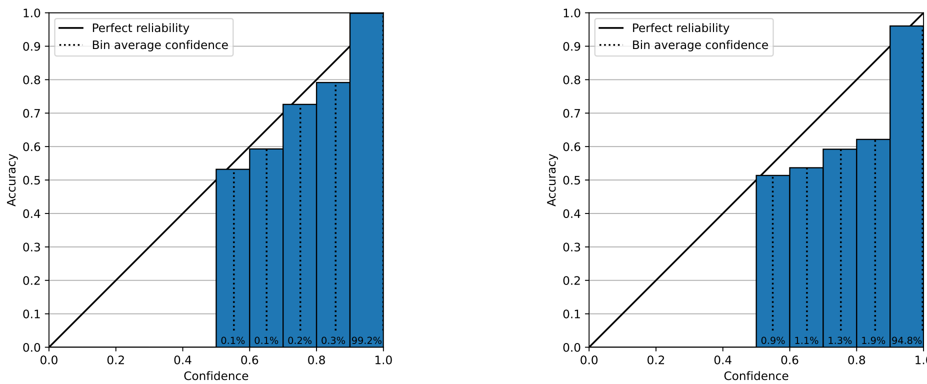

Figure S5. *Similar to figure S4 but for the convolutional neural network classifiers used in (left) figure 2b and (right) figure 2c..*

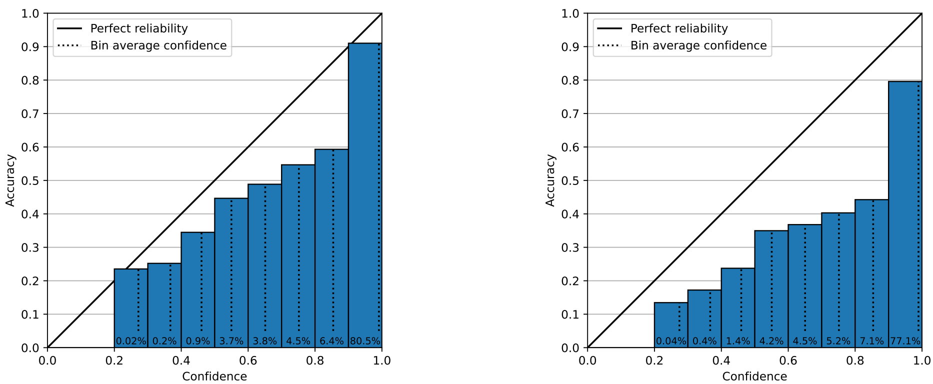

Figure S6. *Similar to figure S5 but for the multi-class case shown in (left) figure 3 with test samples from the period 2005-2014 and (right) figure 4 with test samples from the period 2091-2100.*

S5. Additional temperature maps

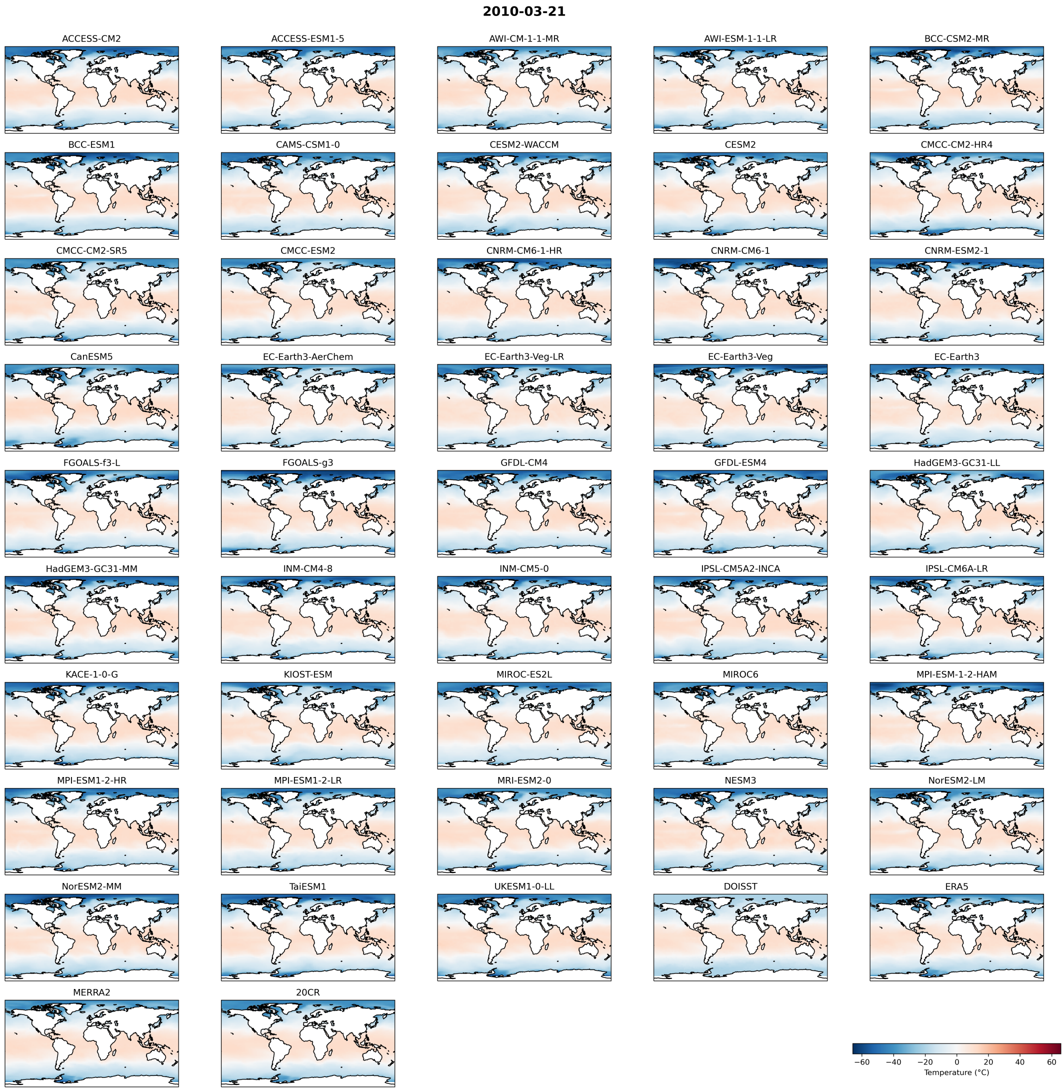

Figure S7. *Maps of temperature with the global mean removed for an example day (March 21st 2010) from each of the 43 models and four observational datasets.*

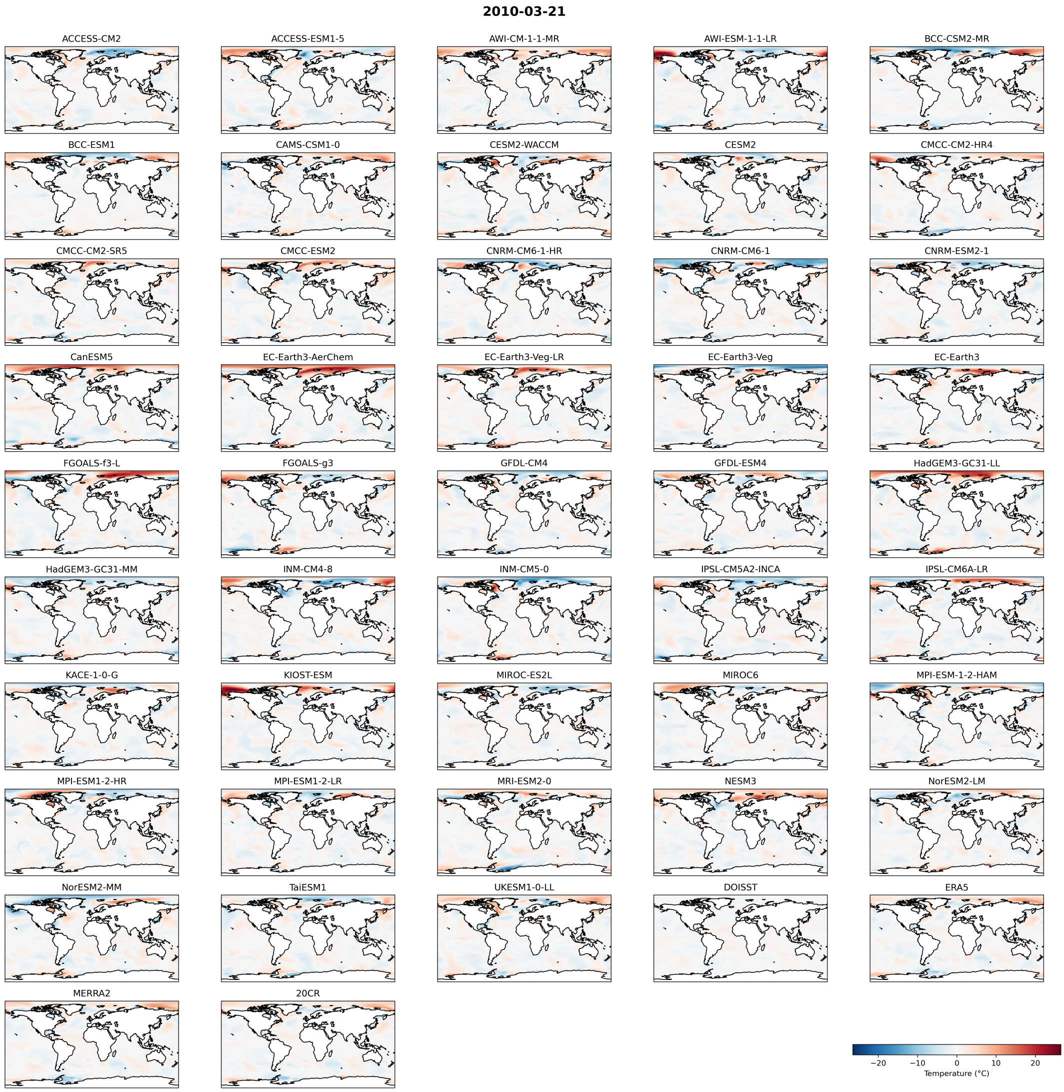

Figure S8. *Maps of temperature with the seasonal cycle and the global mean removed for an example day (March 21st 2010) from each of the 43 models and four observational datasets.*

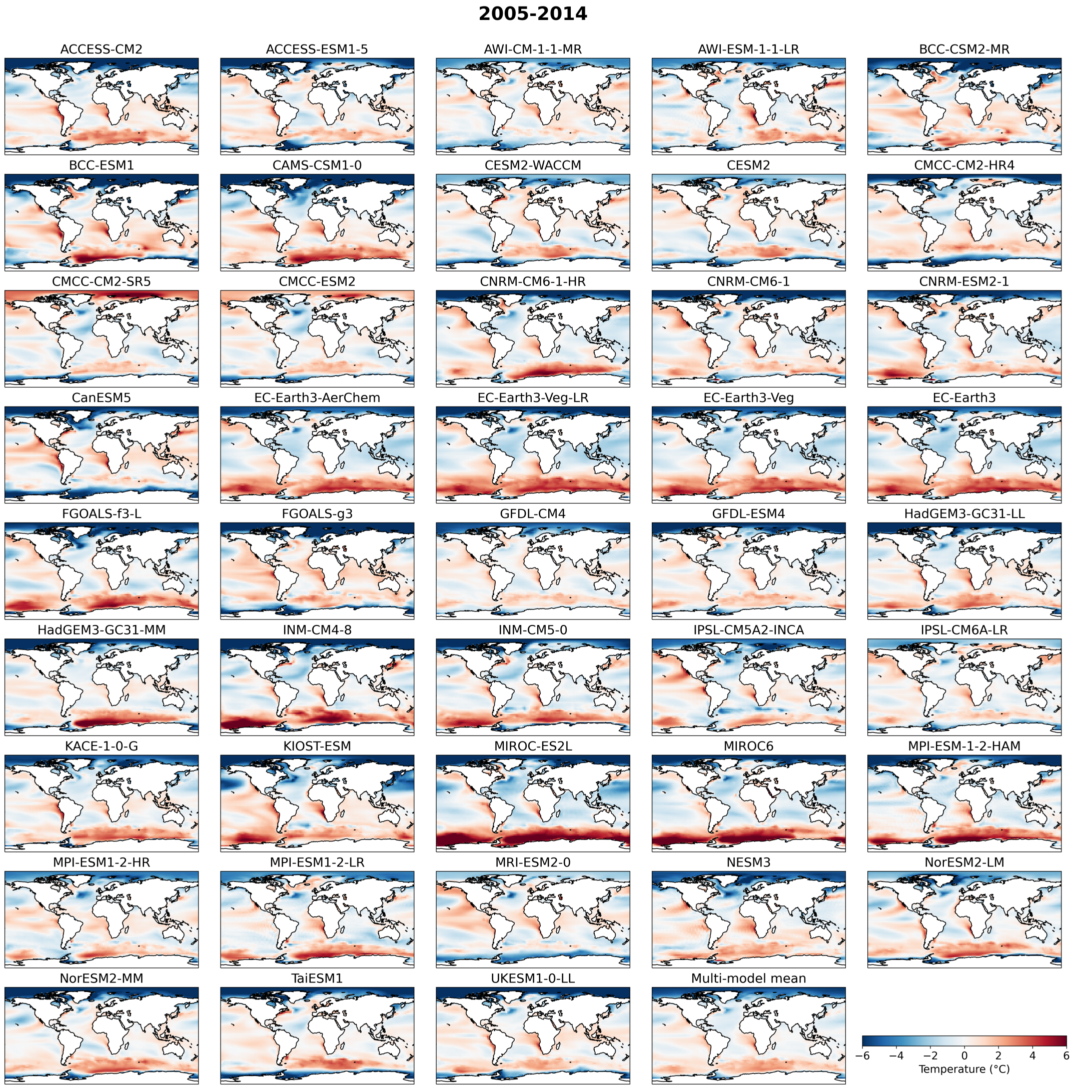

Figure S9. *Climatological mean temperature difference from each of the 43 models to the mean over the four observational datasets in the period 2005-2014. The climatologies are calculated from daily data with the global mean removed. The multi-model mean plot in the last panel is identical to figure 1b in the main manuscript and is only shown here for easier comparison.*

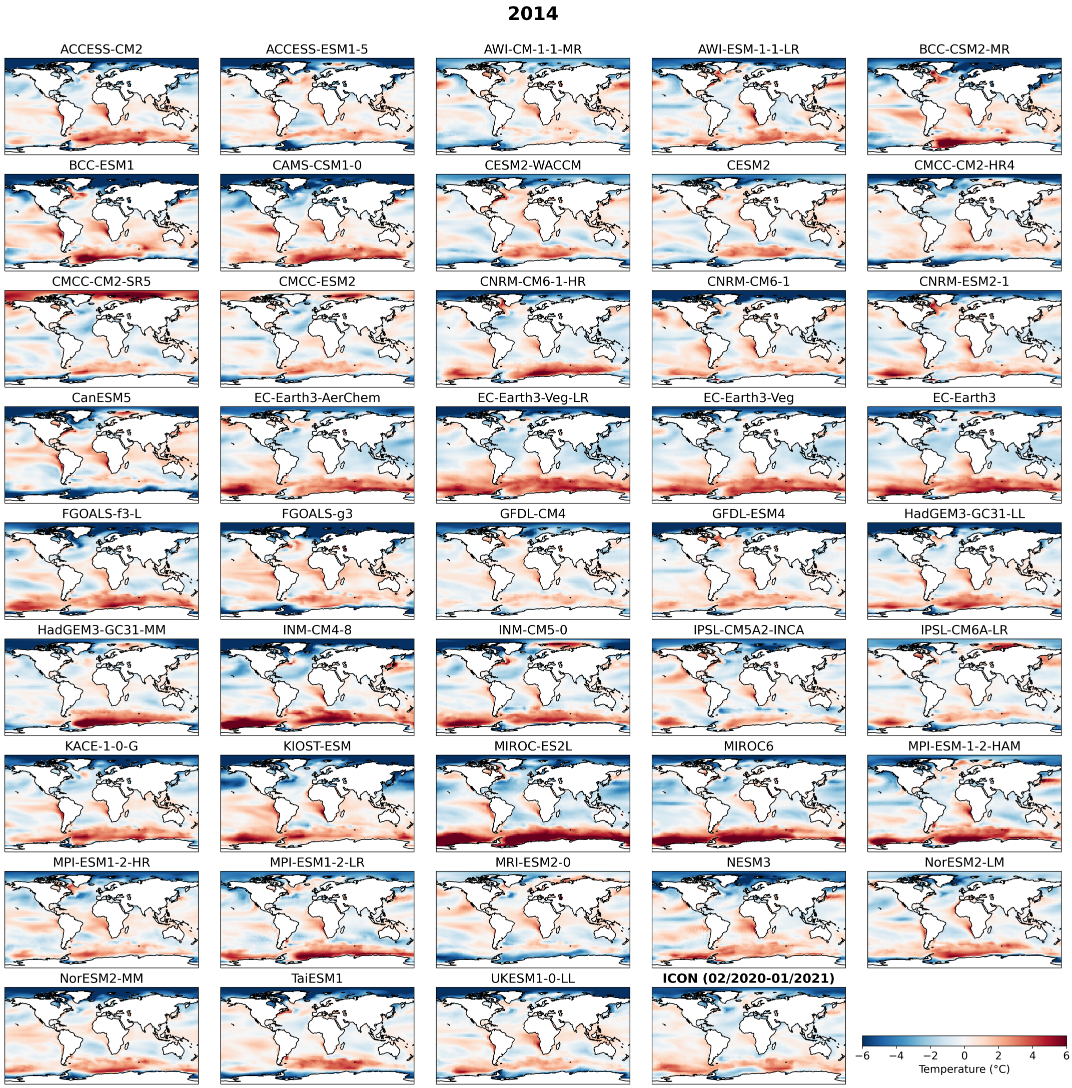

Figure S10. *Similar to figure S9 but for only one year (2014) and including differences for ICON in the period February 2020 to January 2021. Note that for the observations the year 2014 is used in all cases.*

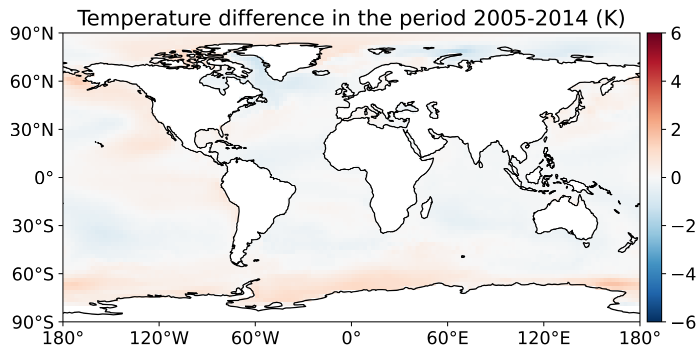

Figure S11. *Climatological mean, multi-model mean temperature difference to the mean over the four observational datasets in the period 2005-2014. The climatologies are calculated from daily data with the seasonal cycle and the global mean removed.*

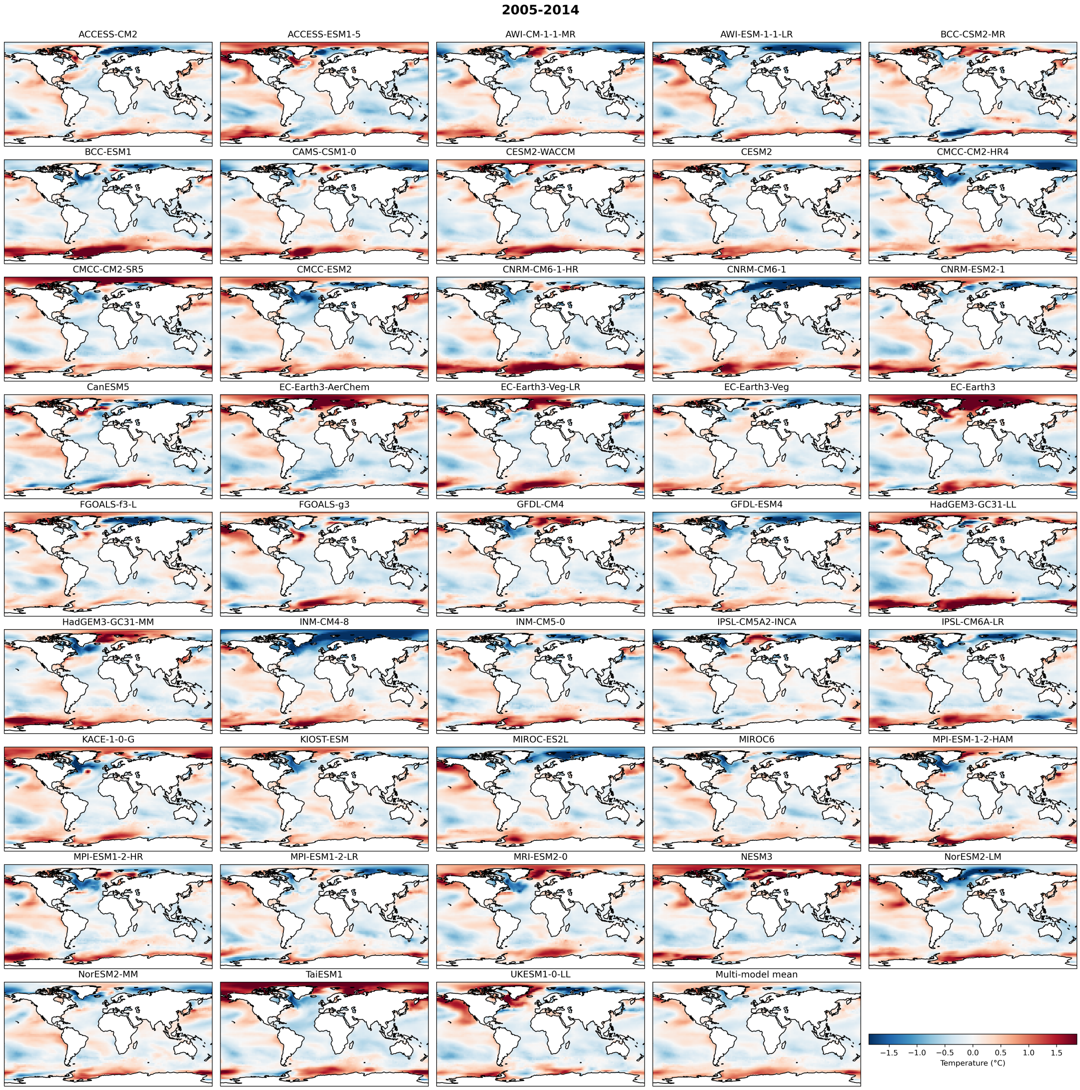

Figure S12. *Climatological temperature difference from each of the 43 models to the four observational datasets in the period 2005-2014. The climatologies are calculated from daily data with the seasonal cycle and the global mean removed. The multi-model mean plot (last panel) is simular to figure S11 except for the colormap range and is shown for easier comparison to the individual models.*

S6. Models used and model families

Table S3. *List of datasets used in this study and related properties.*

	Dataset ID	Variant	Family	Type	Future run
1	DOISST	-	observation	observation	no
2	ERA5	-	observation	observation	no
3	MERRA2	-	observation	observation	no
4	20CR	-	observation	observation	no
5	ACCESS-CM2	r1i1p1f1	ACCESS	model	yes
6	ACCESS-ESM1-5	r1i1p1f1	ACCESS	model	yes
7	AWI-CM-1-1-MR	r1i1p1f1	AWI	model	yes
8	AWI-ESM-1-1-LR	r1i1p1f1	AWI	model	no
9	BCC-CSM2-MR	r1i1p1f1	BCC	model	yes
10	BCC-ESM1	r1i1p1f1	BCC	model	no
11	CAMS-CSM1-0	r2i1p1f1	CAMS-CSM1-0	model	yes
12	CESM2-WACCM	r1i1p1f1	CESM	model	no
13	CESM2	r1i1p1f1	CESM	model	no
14	CMCC-CM2-HR4	r1i1p1f1	CMCC	model	no
15	CMCC-CM2-SR5	r1i1p1f1	CMCC	model	yes
16	CMCC-ESM2	r1i1p1f1	CMCC	model	yes
17	CNRM-CM6-1-HR	r1i1p1f2	CNRM	model	yes
18	CNRM-CM6-1	r1i1p1f2	CNRM	model	yes
19	CNRM-ESM2-1	r1i1p1f2	CNRM	model	yes
20	CanESM5	r1i1p1f1	CanESM5	model	yes
21	EC-Earth3-AerChem	r1i1p1f1	EC-Earth	model	no
22	EC-Earth3-Veg-LR	r1i1p1f1	EC-Earth	model	no
23	EC-Earth3-Veg	r1i1p1f1	EC-Earth	model	yes
24	EC-Earth3	r1i1p1f1	EC-Earth	model	yes
25	FGOALS-f3-L	r1i1p1f1	FGOALS	model	no
26	FGOALS-g3	r1i1p1f1	FGOALS	model	yes
27	GFDL-CM4	r1i1p1f1	GFDL	model	yes
28	GFDL-ESM4	r1i1p1f1	GFDL	model	yes
29	HadGEM3-GC31-LL	r1i1p1f3	HadGEM	model	yes
30	HadGEM3-GC31-MM	r1i1p1f3	HadGEM	model	yes
31	INM-CM4-8	r1i1p1f1	INM	model	yes
32	INM-CM5-0	r1i1p1f1	INM	model	yes
33	IPSL-CM5A2-INCA	r1i1p1f1	IPSL	model	no
34	IPSL-CM6A-LR	r1i1p1f1	IPSL	model	yes
35	KACE-1-0-G	r1i1p1f1	KACE-1-0-G	model	yes
36	KIOST-ESM	r1i1p1f1	KIOST-ESM	model	yes
37	MIROC-ES2L	r1i1p1f2	MIROC	model	yes
38	MIROC6	r1i1p1f1	MIROC	model	yes
39	MPI-ESM-1-2-HAM	r1i1p1f1	MPI	model	no
40	MPI-ESM1-2-HR	r1i1p1f1	MPI	model	yes
41	MPI-ESM1-2-LR	r1i1p1f1	MPI	model	yes
42	MRI-ESM2-0	r1i1p1f1	MRI-ESM2-0	model	yes
43	NESM3	r1i1p1f1	NESM3	model	yes
44	NorESM2-LM	r1i1p1f1	NorESM2	model	yes
45	NorESM2-MM	r1i1p1f1	NorESM2	model	yes
46	TaiESM1	r1i1p1f1	TaiESM1	model	yes
47	UKESM1-0-LL	r1i1p1f2	HadGEM	model	yes
48	ICON	dpp0066	ICON	model	no

Table S4. *List of reference links for the historical datasets used in this study. The numbering corresponds to table S3.*

	Further information
1	https://www.ncei.noaa.gov/products/optimum-interpolation-sst
2	https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-single-levels
3	https://disc.gsfc.nasa.gov/datasets/M2T1NXSLV_5.12.4/summary
4	https://psl.noaa.gov/data/20thC_Rean/
5	https://furtherinfo.es-doc.org/CMIP6.MPI-M.MPI-ESM-1-2-HAM.historical.none.r1i1p1f1
6	https://furtherinfo.es-doc.org/CMIP6.CAMS.CAMS-CSM1-0.historical.none.r2i1p1f1
7	https://furtherinfo.es-doc.org/CMIP6.INM.INM-CM5-0.historical.none.r1i1p1f1
8	https://furtherinfo.es-doc.org/CMIP6.CSIRO-ARCCSS.ACCESS-CM2.historical.none.r1i1p1f1
9	https://furtherinfo.es-doc.org/CMIP6.KIOST.KIOST-ESM.historical.none.r1i1p1f1
10	https://furtherinfo.es-doc.org/CMIP6.CCCma.CanESM5.historical.none.r1i1p1f1
11	https://furtherinfo.es-doc.org/CMIP6.MOHC.UKESM1-0-LL.historical.none.r1i1p1f2
12	https://furtherinfo.es-doc.org/CMIP6.MPI-M.MPI-ESM1-2-HR.historical.none.r1i1p1f1
13	https://furtherinfo.es-doc.org/CMIP6.MOHC.HadGEM3-GC31-MM.historical.none.r1i1p1f3
14	https://furtherinfo.es-doc.org/CMIP6.MRI.MRI-ESM2-0.historical.none.r1i1p1f1
15	https://furtherinfo.es-doc.org/CMIP6.CSIRO.ACCESS-ESM1-5.historical.none.r1i1p1f1
16	https://furtherinfo.es-doc.org/CMIP6.CAS.FGOALS-f3-L.historical.none.r1i1p1f1
17	https://furtherinfo.es-doc.org/CMIP6.NCC.NorESM2-MM.historical.none.r1i1p1f1
18	https://furtherinfo.es-doc.org/CMIP6.EC-Earth-Consortium.EC-Earth3-Veg-LR.historical.none.r1i1p1f1
19	https://furtherinfo.es-doc.org/CMIP6.AWI.AWI-ESM-1-1-LR.historical.none.r1i1p1f1
20	https://furtherinfo.es-doc.org/CMIP6.IPSL.IPSL-CM5A2-INCA.historical.none.r1i1p1f1
21	https://furtherinfo.es-doc.org/CMIP6.AS-RCEC.TaiESM1.historical.none.r1i1p1f1
22	https://furtherinfo.es-doc.org/CMIP6.MIROC.MIROC6.historical.none.r1i1p1f1
23	https://furtherinfo.es-doc.org/CMIP6.IPSL.IPSL-CM6A-LR.historical.none.r1i1p1f1
24	https://furtherinfo.es-doc.org/CMIP6.NOAA-GFDL.GFDL-ESM4.historical.none.r1i1p1f1
25	https://furtherinfo.es-doc.org/CMIP6.EC-Earth-Consortium.EC-Earth3.historical.none.r1i1p1f1
26	https://furtherinfo.es-doc.org/CMIP6.CNRM-CERFACS.CNRM-ESM2-1.historical.none.r1i1p1f2
27	https://furtherinfo.es-doc.org/CMIP6.NIMS-KMA.KACE-1-0-G.historical.none.r1i1p1f1
28	https://furtherinfo.es-doc.org/CMIP6.NCC.NorESM2-LM.historical.none.r1i1p1f1
29	https://furtherinfo.es-doc.org/CMIP6.AWI.AWI-CM-1-1-MR.historical.none.r1i1p1f1
30	https://furtherinfo.es-doc.org/CMIP6.NCAR.CESM2.historical.none.r1i1p1f1
31	https://furtherinfo.es-doc.org/CMIP6.EC-Earth-Consortium.EC-Earth3-AerChem.historical.none.r1i1p1f1
32	https://furtherinfo.es-doc.org/CMIP6.CNRM-CERFACS.CNRM-CM6-1-HR.historical.none.r1i1p1f2
33	https://furtherinfo.es-doc.org/CMIP6.EC-Earth-Consortium.EC-Earth3-Veg.historical.none.r1i1p1f1
34	https://furtherinfo.es-doc.org/CMIP6.BCC.BCC-CSM2-MR.historical.none.r1i1p1f1
35	https://furtherinfo.es-doc.org/CMIP6.NCAR.CESM2-WACCM.historical.none.r1i1p1f1
36	https://furtherinfo.es-doc.org/CMIP6.CAS.FGOALS-g3.historical.none.r1i1p1f1
37	https://furtherinfo.es-doc.org/CMIP6.CMCC.CMCC-CM2-SR5.historical.none.r1i1p1f1
38	https://furtherinfo.es-doc.org/CMIP6.MPI-M.MPI-ESM1-2-LR.historical.none.r1i1p1f1
39	https://furtherinfo.es-doc.org/CMIP6.NUIST.NESM3.historical.none.r1i1p1f1
40	https://furtherinfo.es-doc.org/CMIP6.BCC.BCC-ESM1.historical.none.r1i1p1f1
41	https://furtherinfo.es-doc.org/CMIP6.NOAA-GFDL.GFDL-CM4.historical.none.r1i1p1f1
42	https://furtherinfo.es-doc.org/CMIP6.CMCC.CMCC-ESM2.historical.none.r1i1p1f1
43	https://furtherinfo.es-doc.org/CMIP6.CMCC.CMCC-CM2-HR4.historical.none.r1i1p1f1
44	https://furtherinfo.es-doc.org/CMIP6.INM.INM-CM4-8.historical.none.r1i1p1f1
45	https://furtherinfo.es-doc.org/CMIP6.MIROC.MIROC-ES2L.historical.none.r1i1p1f2
46	https://furtherinfo.es-doc.org/CMIP6.CNRM-CERFACS.CNRM-CM6-1.historical.none.r1i1p1f2
47	https://furtherinfo.es-doc.org/CMIP6.MOHC.HadGEM3-GC31-LL.historical.none.r1i1p1f3
48	https://easy.gems.dkrz.de/DYAMOND/NextGEMS/Models/c1_icon_dpp0066.html

Table S5. *List of reference links for the future model runs used in this study. The numbering corresponds to table S3.*

	Further information
1	-
2	-
3	-
4	-
5	-
6	https://furtherinfo.es-doc.org/CMIP6.CAMS.CAMS-CSM1-0.ssp585.none.r2i1p1f1
7	https://furtherinfo.es-doc.org/CMIP6.INM.INM-CM5-0.ssp585.none.r1i1p1f1
8	https://furtherinfo.es-doc.org/CMIP6.CSIRO-ARCCSS.ACCESS-CM2.ssp585.none.r1i1p1f1
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19	-
20	-
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27	https://furtherinfo.es-doc.org/CMIP6.NIMS-KMA.KACE-1-0-G.ssp585.none.r1i1p1f1
28	https://furtherinfo.es-doc.org/CMIP6.NCC.NorESM2-LM.ssp585.none.r1i1p1f1
29	https://furtherinfo.es-doc.org/CMIP6.AWI.AWI-CM-1-1-MR.ssp585.none.r1i1p1f1
30	-
31	-
32	https://furtherinfo.es-doc.org/CMIP6.CNRM-CERFACS.CNRM-CM6-1-HR.ssp585.none.r1i1p1f2
33	https://furtherinfo.es-doc.org/CMIP6.EC-Earth-Consortium.EC-Earth3-Veg.ssp585.none.r1i1p1f1
34	https://furtherinfo.es-doc.org/CMIP6.BCC.BCC-CSM2-MR.ssp585.none.r1i1p1f1
35	-
36	https://furtherinfo.es-doc.org/CMIP6.CAS.FGOALS-g3.ssp585.none.r1i1p1f1
37	https://furtherinfo.es-doc.org/CMIP6.CMCC.CMCC-CM2-SR5.ssp585.none.r1i1p1f1
38	https://furtherinfo.es-doc.org/CMIP6.MPI-M.MPI-ESM1-2-LR.ssp585.none.r1i1p1f1
39	https://furtherinfo.es-doc.org/CMIP6.NUIST.NESM3.ssp585.none.r1i1p1f1
40	-
41	https://furtherinfo.es-doc.org/CMIP6.NOAA-GFDL.GFDL-CM4.ssp585.none.r1i1p1f1
42	https://furtherinfo.es-doc.org/CMIP6.CMCC.CMCC-ESM2.ssp585.none.r1i1p1f1
43	-
44	https://furtherinfo.es-doc.org/CMIP6.INM.INM-CM4-8.ssp585.none.r1i1p1f1
45	https://furtherinfo.es-doc.org/CMIP6.MIROC.MIROC-ES2L.ssp585.none.r1i1p1f2
46	https://furtherinfo.es-doc.org/CMIP6.CNRM-CERFACS.CNRM-CM6-1.ssp585.none.r1i1p1f2
47	https://furtherinfo.es-doc.org/CMIP6.MOHC.HadGEM3-GC31-LL.ssp585.none.r1i1p1f3
48	