**1. Початковий простір пошуку гіперпараметрів**

Table S1. Hyperparameter space for RF

|  |  |
| --- | --- |
| Hyperparameter | Values |
| # estimators | 200, 300, 400, 500, 600, 700 |
| max depth | 10, 20, 30, 40, 50, 60 |
| min samples leaf | 1, 3, 6, 9, 12, 15 |
| min samples split | 2, 4, 6, 8, 10, 12, 14, 16 |
| bootstrap | True, False |
| max features | 'log2', 'sqrt', 1.0, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2 |

Table S2. Hyperparameter space for GB

|  |  |
| --- | --- |
| Hyperparameter | Values |
| # estimators | 100, 200, 250, 300, 350, 400, 450, 500, 550, 600 |
| max depth | 15, 20, 25, 30, 35, 40, 45 |
| min samples leaf | 1, 2, 3, 4, 5, 6, 7 |
| min samples split | 2, 3, 4, 5, 6, 7 |
| learning rate | [10-3; 10-1] |
| max features | 'log2', 'sqrt', 1.0, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1 |

Table S3. Hyperparameter space for SVR

|  |  |
| --- | --- |
| Hyperparameter | Values |
| kernel | linear, poly, rbf, sigmoid |
| degree\* | 2, 3, 4, 5, 6 |
| C0 | [0; 5] |
| Tolerance | [10-5; 10-2] |
| C | [10-2; 10] |
| Epsilon | [10-4; 1] |

\* for poly kernel only

Table S4. Hyperparameter space for XGB

|  |  |
| --- | --- |
| Hyperparameter | Values |
| booster | gbtree, gblinear, dart |
| max depth\* | 3, 4, 5, 6, 7 |
| min split loss\* | [0; 5] |
| min child weight\* | [0; 5] |
| subsample\* | 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 |
| сolsample by tree\* | 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 |
| # estimators | 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700 |
| learning rate | [10-5; 10-2] |
| L1 | [10-8; 1] |
| L2 | [10-8; 1] |

\* for all boosters except gblinear

Table S5. Hyperparameter space for DNN

|  |  |
| --- | --- |
| Hyperparameter | Values |
| hidden layers configuration | Pipe, Trapezium, Triangle, Butterfly, Fir |
| # nodes for first hidden layer | 10 |
| # hidden layers | 5 |
| batch size | 25 |
| activation function | ReLu, sigmoid, tanh, SELU, ELU |
| optimizer | SGD, RMSprop, Adam, Adadelta, Adagrad, Adamax, Nadam, Ftrl |
| learning rate | [10-5; 10-2] |
| # epochs | 1000 |
| weight initializer | XavierNormal, XavierUniform, HeNormal, HeUniform, RandomNormal, RandomUniform |
| Regularizer | None, L1, L2 |
| RegRate\* | 10-5, 10-4, 10-3, 10-2, 10-1 |
| DropoutNeeded | True, False |
| DropRate\*\* | 0.2, 0.3, 0.4, 0.5 |
| LayerNormNeed | True, False |

\* for Regularizer ≠ None

\*\* for DropoutNeeded = True

**2. Обрані (раціональні) параметри за метрикою MRE [Варіант який виходить в альбомному форматі для RF]**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | | Visual Model | | | | | | | | |
| EfficientNet  (Class\*) | EfficientNet  (Pre-Class\*\*) | EfficientNet  (Pre-Class:PC\*\*\*) | MobileNet  (Class) | MobileNet  (Pre-Class) | MobileNet  (Pre-Class:PC) | NASNet  (Class) | NASNet  (Pre-Class) | NASNet  (Class:PCA) |
| Hyperparameter | # estimators | 750 | 900 | 460 | 450 | 460 | 500 | 395 | 750 | 1175 |
| max depth | 35 | 40 | 54 | 20 | 50 | 85 | 59 | 10 | 70 |
| min samples leaf | 3 | 4 | 4 | 4 | 3 | 5 | 2 | 2 | 2 |
| min samples split | 2 | 2 | 1 | 1 | 1 | 3 | 1 | 1 | 1 |
| max features | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| bootstrap | False | False | True | False | False | False | False | False | False |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | | ResNet  (Class) | ResNet  (Pre-Class) | Xception  (Class) | Xception (Pre-Class) | YOLO  (L)ʹ | YOLO  (L+M)ʹʹ | YOLO  (2FL:PC)ʹʹʹ | YOLO  (FL:PC)ʹʹʹʹ |
| Hyperparameter | # estimators | 640 | 367 | 640 | 820 | 960 | 650 | 475 | 425 |
| max depth | 40 | 38 | 90 | 48 | 75 | 70 | 45 | 45 |
| min samples leaf | 4 | 2 | 2 | 4 | 4 | 2 | 3 | 10 |
| min samples split | 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| bootstrap | 0.5 | sqrt | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| max features | False | False | False | False | False | False | False | False |

\* if use class layer

\*\* if use layer before class layer

\*\*\* if use layer before class layer + PCA

ʹ Global average pooled features from the last backbone layer; ʹʹ Concatenation of global average pooled features from the middle and last backbone layers; ʹʹʹ Concatenation of embeddings from two different YOLO feature maps; ʹʹʹʹ Intermediate YOLO feature maps converted into embeddings (before detection head).

Table S6. Chosen hyperparameter combinations for RF models **[варіант в форматі А4]**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Visual Model | Hyperparameter | | | | | |
| # estimators | max depth | min sample split | min sample leaf | max features | bootstrap |
| EfficientNetC\* | 750 | 35 | 3 | 2 | 0.2 | False |
| EfficientNetP\*\* | 900 | 40 | 4 | 2 | 0.2 | False |
| EfficientNetP:PC\*\*\* | 460 | 54 | 4 | 1 | 1 | True |
| MobileNetC | 450 | 20 | 4 | 1 | 0.1 | False |
| MobileNetP | 460 | 50 | 3 | 1 | 0.05 | False |
| MobileNetP:PC | 500 | 85 | 5 | 3 | 0.5 | False |
| NASNetC | 395 | 59 | 2 | 1 | 0.2 | False |
| NASNetC:PC | 1175 | 70 | 2 | 1 | 0.4 | False |
| NASNetP | 750 | 10 | 2 | 1 | 0.1 | False |
| ResNetC | 640 | 40 | 4 | 2 | 0.4 | False |
| ResNetP | 367 | 38 | 2 | 1 | sqrt | False |
| XceptionC | 640 | 90 | 2 | 1 | 0.2 | False |
| XceptionP | 820 | 48 | 4 | 1 | 0.1 | False |
| YOLO (L)ʹ | 960 | 75 | 4 | 1 | 0.4 | False |
| YOLO2 (L+M)ʹʹ | 650 | 70 | 2 | 1 | 0.2 | False |
| YOLO (2FL:PC)ʹʹʹ | 475 | 45 | 3 | 1 | 0.5 | False |
| YOLO (FL:PC)ʹʹʹʹ | 425 | 45 | 10 | 1 | 0.5 | False |

\* if use class layer

\*\* if use layer before class layer

\*\*\* if use layer before class layer + using Principal Component Analysis

ʹ Global average pooled features from the last backbone layer

ʹʹ Concatenation of global average pooled features from the middle and last backbone layers

ʹʹʹ Concatenation of embeddings from two different YOLO feature maps

ʹʹʹʹ Intermediate YOLO feature maps converted into embeddings (before detection head)

Table S7. Chosen hyperparameter combinations for GB models

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Visual Model | Hyperparameter | | | | | |
| # estimators | max depth | min sample split | min sample leaf | max features | learning rate |
| EfficientNetC | 750 | 20 | 7 | 11 | 0.1 | 3.4e-02 |
| EfficientNetP | 750 | 50 | 6 | 9 | 0.3 | 4.2e-02 |
| EfficientNetP:PC | 680 | 25 | 4 | 15 | 1 | 3.9e-02 |
| MobileNetC | 1100 | 40 | 10 | 3 | sqrt | 1.0e-02 |
| MobileNetP | 890 | 50 | 12 | 2 | sqrt | 1.4e-02 |
| MobileNetP:PC | 575 | 60 | 4 | 12 | 0.6 | 2.8e-02 |
| NASNetC | 850 | 70 | 13 | 15 | 0.3 | 4.8e-02 |
| NASNetC:PC | 675 | 80 | 11 | 13 | 0.4 | 3.8e-02 |
| NASNetP | 650 | 67 | 5 | 3 | 0.1 | 1.3e-02 |
| ResNetC | 700 | 55 | 8 | 1 | 0.4 | 1.1e-01 |
| ResNetP | 640 | 85 | 3 | 7 | sqrt | 2.3e-02 |
| XceptionC | 470 | 25 | 2 | 6 | sqrt | 5.2e-02 |
| XceptionP | 760 | 75 | 10 | 4 | 0.1 | 2.9e-02 |
| YOLO (L) | 1160 | 75 | 2 | 8 | 0.1 | 3.9e-02 |
| YOLO2 (L+M) | 900 | 54 | 3 | 6 | 0.2 | 2.3e-02 |
| YOLO (2FL:PC) | 750 | 55 | 4 | 7 | 0.4 | 1.9e-02 |
| YOLO (FL:PC) | 850 | 55 | 2 | 10 | 0.7 | 1.2e-02 |

Table S8. Chosen hyperparameter combinations for SVR models

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Visual Model | Hyperparameter | | | | |
| kernel | C0 | Tolerance | C | Epsilon |
| EfficientNetC | linear | 7.79 | 6.9e-06 | 2.5 | 2.2e-05 |
| EfficientNetP | linear | 8.29 | 3.0e-05 | 2.6 | 3.5e-05 |
| EfficientNetP:PC | linear | 10.57 | 8.4e-04 | 13.7 | 2.9e-04 |
| MobileNetC | rbf | 6.80 | 3.9e-04 | 10.9 | 9.6e-05 |
| MobileNetP | linear | 6.54 | 4.9e-04 | 6.7 | 7.1e-05 |
| MobileNetP:PC | linear | 7.31 | 5.2e-04 | 4.6e-03 | 8.7e-04 |
| NASNetC | linear | 6.60 | 4.9e-04 | 4.6 | 1.5e-04 |
| NASNetC:PC | rbf | 7.17 | 5.5e-03 | 11.7 | 1.5e-04 |
| NASNetP | linear | 5.31 | 6.5e-04 | 5.9 | 2.6e-05 |
| ResNetC | linear | 6.66 | 4.2e-03 | 2.3 | 5.4e-05 |
| ResNetP | linear | 6.65 | 1.3e-04 | 5.2 | 1.4e-04 |
| XceptionC | rbf | 8.27 | 7.2e-03 | 13.8 | 3.5e-04 |
| XceptionP | linear | 11.24 | 2.5e-03 | 9.1 | 3.8e-04 |
| YOLO (L) | rbf | 12.61 | 2.4e-03 | 6.9 | 5.6e-05 |
| YOLO2 (L+M) | rbf | 8.30 | 1.9e-04 | 9.2 | 1.4e-05 |
| YOLO (FL) | linear | 8.62 | 5.3e-04 | 7.9 | 1.6e-05 |
| YOLO (FL:PC) | rbf | 11.5 | 2.3e-05 | 4.6 | 6.3e-06 |
| YOLO (2FL) | linear | 9.18 | 3.9e-03 | 2.2 | 2.4e-04 |
| YOLO (2FL:PC) | rbf | 7.04 | 2.7e-03 | 2.6 | 2.5e-04 |

Table S9. Chosen hyperparameter combinations for XGB models

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Visual Model | Hyperparameter | | | | | | | | | |
| booster | max depth | min split loss | min child weight | sub  sample | сolsample bytree | # estimators | learning rate | L1 | L2 |
| EfficientNetC | gblinear | 3 | -- | -- | -- | -- | 1080 | 1.1e-01 | 1.8e-07 | 8.4e-04 |
| EfficientNetP | gblinear | 3 | -- | -- | -- | -- | 1150 | 3.2e-01 | 3.8e-08 | 2.6e-03 |
| EfficientNetP:PC | gblinear | 3 | -- | -- | -- | -- | 1640 | 1.6e-01 | 5.9e-09 | 1.4e-02 |
| MobileNetC | gblinear | 3 | -- | -- | -- | -- | 1040 | 7.0e-02 | 5.7e-07 | 3.1e-03 |
| MobileNetP | gblinear | 3 | -- | -- | -- | -- | 600 | 1.4e-01 | 6.1e-08 | 1.9e-02 |
| MobileNetP:PC | gblinear | 3 | -- | -- | -- | -- | 1150 | 7.4e-02 | 1.0e-08 | 1.0e-01 |
| NASNetC | gblinear | 3 | -- | -- | -- | -- | 1050 | 2.6e-01 | 9.9e-09 | 2.3e-03 |
| NASNetC:PC | gblinear | 3 | -- | -- | -- | -- | 800 | 3.8e-02 | 5.0e-09 | 1.4e-02 |
| NASNetP | gblinear | 3 | -- | -- | -- | -- | 700 | 6.9e-02 | 8.5e-09 | 6.1e-02 |
| ResNetC | gbtree | 8 | 7.9e-03 | 5.7e-01 | 0.4 | 0.9 | 825 | 2.2e-02 | 1.9e-08 | 3.3e-03 |
| ResNetP | gblinear | 6 | -- | -- | -- | -- | 500 | 4.4e-01 | 1.1e-08 | 1.5e-02 |
| XceptionC | gblinear | 3 | -- | -- | -- | -- | 550 | 2.0e-01 | 1.4e-06 | 1.7e-04 |
| XceptionP | gblinear | 3 | -- | -- | -- | -- | 390 | 2.2e-01 | 3.7e-06 | 9.9e-02 |
| YOLO (L) | gblinear | 3 | -- | -- | -- | -- | 520 | 9.4e-02 | 4.7e-05 | 2.0e-02 |
| YOLO2 (L+M) | gblinear | 3 | -- | -- | -- | -- | 650 | 1.7e-01 | 8.1e-09 | 1.9e-02 |
| YOLO (2FL:PC) | gbtree | 5 | 6.4e-02 | 3.6 | 0.9 | 0.5 | 1275 | 8.1e-03 | 1.9e-08 | 4.9e-03 |
| YOLO (FL:PC) | gbtree | 2 | 3.2e-01 | 2.5 | 0.8 | 0.9 | 525 | 3.5e-02 | 2.1e-08 | 6.7e-03 |

Table S10. Chosen hyperparameter combinations for DNN models

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Visual Model | Hyperparameter | | | | | | | | |
| learning  rate | optimizer | activ. func. | w.  init. | Regul. | RegRate | Drop.  Need. | Drop  Rate | LayerNorm. |
| EfficientNetC | 3.0e-03 | Adam | ELU | HN | None | -- | False | -- | True |
| EfficientNetP | 1.4e-03 | Adamax | SELU | RN | L2 | 1.0e-03 | False | -- | True |
| EfficientNetP:PC | 1.4e-04 | Nadam | SELU | RU | L2 | 1.0e-03 | False | -- | True |
| MobileNetC | 2.4e-03 | Nadam | SELU | RN | L2 | 1.7e-03 | True | 0.5 | True |
| MobileNetP | 2.8e-03 | Nadam | ELU | RN | None | -- | False | -- | False |
| MobileNetP:PC | 1.3e-04 | Adam | tanh | RU | L2 | 6.4e-04 | True | 0.4 | False |
| NASNetC | 1.4e-04 | Adamax | sigmoid | XU | None | -- | False | -- | False |
| NASNetC:PC | 3.9e-04 | Nadam | tanh | RU | None | -- | False | -- | True |
| NASNetP | 4.4e-04 | Nadam | SELU | RU | None | -- | False | -- | True |
| ResNetC | 3.3e-04 | Adamax | ELU | RN | L2 | 2.2e-03 | False | -- | True |
| ResNetP | 1.1e-03 | Nadam | ReLu | HN | None | -- | False | -- | True |
| XceptionC | 1.5e-04 | Adamax | ReLu | HU | L1 | 9.7e-04 | False | -- | True |
| XceptionP | 2.1e-04 | Nadam | sigmoid | XN | L2 | 8.5e-04 | False | -- | True |
| YOLO (L) | 5.2e-05 | Adam | tanh | RU | None | -- | False | -- | True |
| YOLO2 (L+M) | 6.9e-04 | Adam | SELU | RU | None | -- | False | -- | True |
| YOLO (2FL:PC) | 4.1e-04 | Adam | sigmoid | XN | L1 | 1.3e-04 | True | 0.2 | True |
| YOLO (FL:PC) | 4.3e-04 | RMSprop | ELU | XU | L1 | 5.4e-05 | False | -- | True |