Supplemental materials: Performance-weighted-voting model: an ensemble machine learning method for cancer type classification using whole-exome sequencing mutation

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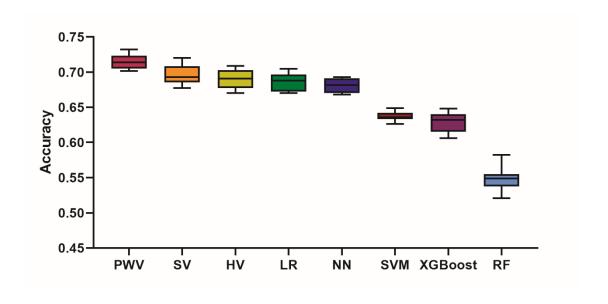


Figure S1. The predictive performance of the performance-weighted-voting model compared with the other models. Hard-voting model (HV, yellow box), soft-voting model (SV, orange box) and performance-weighted-voting model (PWV, violet red box) were introduced compared with the five weak classifiers. Each model was trained and predicted 10 times independently.

Table S1: The precision, recall and F1-score of the eight models.

| | | BLCA | BRCA | GBM | HNSC | KIRC | LGG | LIHC | LUAD | LUSC | PRAD | SKCM | STAD | THCA | UCEC |
|---------------------------------|-----------|------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Logistic Regression | precision | $72\%^{a} \pm 5\%^{b}$ | $61\% \pm 3\%$ | $60\% \pm 4\%$ | 56% ± 5% | 85% ± 3% | $88\% \pm 2\%$ | $71\% \pm 4\%$ | $74\% \pm 4\%$ | $73\% \pm 5\%$ | $46\% \pm 5\%$ | $94\% \pm 2\%$ | $66\% \pm 6\%$ | $70\% \pm 5\%$ | $79\% \pm 4\%$ |
| | recall | $61\% \pm 4\%$ | $66\% \pm 3\%$ | $63\% \pm 5\%$ | $58\% \pm 5\%$ | $69\% \pm 6\%$ | $82\% \pm 3\%$ | $58\% \pm 6\%$ | $59\% \pm 4\%$ | $70\% \pm 4\%$ | $70\% \pm 5\%$ | $79\% \pm 3\%$ | $49\% \pm 6\%$ | $92\% \pm 1\%$ | $76\% \pm 5\%$ |
| | F1-score | $66\% \pm 3\%$ | $63\% \pm 2\%$ | $61\% \pm 4\%$ | $57\% \pm 4\%$ | $76\% \pm 4\%$ | $85\% \pm 2\%$ | $64\% \pm 4\%$ | $65\% \pm 3\%$ | $72\% \pm 4\%$ | $56\% \pm 3\%$ | $86\% \pm 2\%$ | $56\% \pm 4\%$ | $79\% \pm 3\%$ | $77\% \pm 3\%$ |
| | | | | | | | | | | | | | | | |
| SVM | precision | $64\% \pm 2\%$ | $44\% \pm 3\%$ | $68\% \pm 6\%$ | $52\% \pm 3\%$ | $89\% \pm 3\%$ | $94\% \pm 2\%$ | $70\% \pm 8\%$ | $78\% \pm 7\%$ | $65\% \pm 5\%$ | $41\% \pm 4\%$ | $98\% \pm 2\%$ | $67\% \pm 8\%$ | $76\% \pm 5\%$ | $86\% \pm 5\%$ |
| | recall | $54\% \pm 3\%$ | $66\% \pm 5\%$ | $48\% \pm 6\%$ | $50\% \pm 4\%$ | $61\% \pm 6\%$ | $79\% \pm 3\%$ | $46\% \pm 5\%$ | $44\% \pm 5\%$ | $71\% \pm 4\%$ | $77\% \pm 6\%$ | $76\% \pm 3\%$ | $40\% \pm 5\%$ | $94\% \pm 2\%$ | $68\% \pm 5\%$ |
| | F1-score | $58\% \pm 2\%$ | 52% ± 3% | 56% ± 6% | $51\% \pm 2\%$ | $72\% \pm 5\%$ | $86\% \pm 2\%$ | 55% ± 5% | $56\% \pm 4\%$ | 68% ± 4% | 53% ± 3% | $85\% \pm 2\%$ | $49\% \pm 4\%$ | $84\% \pm 4\%$ | $76\% \pm 4\%$ |
| Random Forest | precision | 65% ± 6% | $71\% \pm 4\%$ | $41\% \pm 6\%$ | $64\% \pm 4\%$ | 79% ± 5% | $74\% \pm 8\%$ | $64\% \pm 5\%$ | $73\% \pm 5\%$ | $45\% \pm 4\%$ | $36\% \pm 4\%$ | $68\% \pm 7\%$ | 53% ± 12% | $34\% \pm 6\%$ | 80% ± 7% |
| | recall | $54\% \pm 7\%$ | $45\% \pm 3\%$ | $47\% \pm 6\%$ | $29\% \pm 5\%$ | $69\% \pm 7\%$ | $82\% \pm 2\%$ | $39\% \pm 5\%$ | $33\% \pm 6\%$ | $83\% \pm 4\%$ | $29\% \pm 8\%$ | $76\% \pm 3\%$ | $10\% \pm 4\%$ | $99\% \pm 1\%$ | $67\% \pm 3\%$ |
| | F1-score | $59\% \pm 6\%$ | $55\% \pm 3\%$ | $43\% \pm 5\%$ | $39\% \pm 5\%$ | $73\% \pm 6\%$ | $78\% \pm 5\%$ | $48\% \pm 5\%$ | $45\% \pm 6\%$ | $58\% \pm 3\%$ | $32\% \pm 5\%$ | $71\% \pm 5\%$ | $17\% \pm 6\%$ | $51\% \pm 6\%$ | $73\% \pm 5\%$ |
| | precision | 68% ± 6% | 56% ± 2% | 46% ± 5% | 55% ± 4% | 82% ± 6% | 87% ± 3% | 65% ± 5% | 61% ± 5% | 59% ± 5% | 39% ± 5% | 86% ± 2% | 50% ± 7% | $74\% \pm 4\%$ | $80\% \pm 4\%$ |
| XGBoost | recall | 58% ± 6% | $67\% \pm 3\%$ | $41\% \pm 6\%$ | 51% ± 5% | 69% ± 6% | $85\% \pm 3\%$ | 52% ± 6% | 52% ± 5% | 61% ± 5% | $67\% \pm 4\%$ | $76\% \pm 3\%$ | $32\% \pm 5\%$ | $77\% \pm 3\%$ | $73\% \pm 4\%$ |
| | F1-score | $62\% \pm 5\%$ | $61\% \pm 2\%$ | $43\% \pm 5\%$ | $52\% \pm 4\%$ | $75\% \pm 6\%$ | $86\% \pm 2\%$ | $57\% \pm 5\%$ | $56\% \pm 3\%$ | $60\% \pm 4\%$ | $49\% \pm 5\%$ | $81\% \pm 2\%$ | $39\% \pm 4\%$ | $75\% \pm 3\%$ | $76\% \pm 2\%$ |
| | precision | 67% ± 4% | 64% ± 3% | 57% ± 3% | 57% ± 5% | 85% ± 3% | 90% ± 3% | 67% ± 5% | 67% ± 4% | $70\% \pm 4\%$ | $45\% \pm 4\%$ | 93% ± 2% | 60% ± 5% | $76\% \pm 5\%$ | 80% ± 5% |
| Neural Network | recall | 60% ± 5% | $63\% \pm 3\%$ | $60\% \pm 4\%$ | 54% ± 3% | $70\% \pm 6\%$ | $82\% \pm 3\%$ | $58\% \pm 4\%$ | 58% ± 4% | $73\% \pm 4\%$ | $72\% \pm 4\%$ | $81\% \pm 2\%$ | 52% ± 5% | $90\% \pm 2\%$ | $74\% \pm 6\%$ |
| | F1-score | $63\% \pm 4\%$ | $64\% \pm 2\%$ | $58\% \pm 3\%$ | $55\% \pm 3\%$ | $76\% \pm 4\%$ | $86\% \pm 2\%$ | $62\% \pm 3\%$ | $62\% \pm 2\%$ | $71\% \pm 3\%$ | $55\% \pm 3\%$ | $86\% \pm 1\%$ | $56\% \pm 4\%$ | $83\% \pm 3\%$ | $77\% \pm 3\%$ |
| | precision | 72% ± 5% | 61% ± 5% | 59% ± 5% | 58% ± 5% | $88\% \pm 4\%$ | 90% ± 2% | 75% ± 5% | $74\% \pm 4\%$ | 67% ± 7% | $45\% \pm 4\%$ | 94% ± 3% | $71\% \pm 7\%$ | $72\% \pm 5\%$ | 86% ± 5% |
| Hard-Voting | recall | $63\% \pm 5\%$ | $67\% \pm 3\%$ | $60\% \pm 7\%$ | $56\% \pm 4\%$ | $69\% \pm 5\%$ | $82\% \pm 3\%$ | $59\% \pm 6\%$ | 55% ± 5% | $76\% \pm 4\%$ | $74\% \pm 6\%$ | $79\% \pm 2\%$ | $45\% \pm 6\%$ | $93\% \pm 1\%$ | $77\% \pm 4\%$ |
| | F1-score | $67\% \pm 4\%$ | $64\% \pm 2\%$ | $59\% \pm 5\%$ | $57\% \pm 3\%$ | $78\% \pm 4\%$ | $86\% \pm 2\%$ | $66\% \pm 4\%$ | $63\% \pm 3\%$ | $71\% \pm 4\%$ | $56\% \pm 3\%$ | $86\% \pm 2\%$ | $55\% \pm 5\%$ | $81\% \pm 3\%$ | $81\% \pm 3\%$ |
| Soft-Voting | precision | $71\% \pm 4\%$ | 61% ± 4% | 59% ± 5% | 58% ± 5% | 88% ± 3% | 89% ± 2% | 74% ± 5% | 73% ± 6% | 69% ± 6% | $46\% \pm 4\%$ | 94% ± 3% | 67% ± 6% | 73% ± 6% | 86% ± 5% |
| | recall | $63\% \pm 5\%$ | $68\% \pm 2\%$ | $59\% \pm 6\%$ | $56\% \pm 4\%$ | $70\% \pm 6\%$ | $83\% \pm 3\%$ | $59\% \pm 5\%$ | $57\% \pm 6\%$ | $75\% \pm 5\%$ | $73\% \pm 4\%$ | $80\% \pm 2\%$ | $46\% \pm 6\%$ | $93\% \pm 2\%$ | $76\% \pm 4\%$ |
| | F1-score | $67\% \pm 4\%$ | $64\% \pm 2\%$ | $59\% \pm 5\%$ | $57\% \pm 3\%$ | $78\% \pm 4\%$ | $86\% \pm 2\%$ | $65\% \pm 4\%$ | $64\% \pm 2\%$ | $72\% \pm 4\%$ | $56\% \pm 3\%$ | $86\% \pm 2\%$ | $54\% \pm 4\%$ | $82\% \pm 4\%$ | $81\% \pm 3\%$ |
| Performance- Weighted-Voting | precision | $72\% \pm 4\%$ | 69% ± 2% | 61% ± 4% | 58% ± 4% | 88% ± 2% | 91% ± 3% | 62% ± 4% | 73% ± 5% | $74\% \pm 5\%$ | $48\% \pm 4\%$ | 94% ± 2% | $60\% \pm 6\%$ | 80% ± 3% | $85\% \pm 4\%$ |
| | recall | $65\% \pm 5\%$ | $62\% \pm 2\%$ | $66\% \pm 7\%$ | $59\% \pm 4\%$ | $72\% \pm 7\%$ | $83\% \pm 3\%$ | $69\% \pm 4\%$ | $60\% \pm 4\%$ | $71\% \pm 3\%$ | $78\% \pm 5\%$ | $81\% \pm 2\%$ | $57\% \pm 7\%$ | $93\% \pm 2\%$ | $79\% \pm 4\%$ |
| | F1-score | $68\% \pm 3\%$ | $66\% \pm 2\%$ | $63\% \pm 5\%$ | $60\% \pm 3\%$ | $79\% \pm 5\%$ | $87\% \pm 2\%$ | $65\% \pm 2\%$ | $66\% \pm 3\%$ | $72\% \pm 2\%$ | $60\% \pm 3\%$ | $87\% \pm 2\%$ | $58\% \pm 4\%$ | $86\% \pm 2\%$ | $82\% \pm 3\%$ |

^a The average number of 10 repeats

^b The standard deviation of 10 repeats

Table S2: 52 misclassification cases that received the same predictions from five classifiers

| Case ID | Cancer Type | Performance-weighted-voting |
|------------------------------|-------------|-----------------------------|
| TCGA-FD-A3B7 | BLCA | BRCA |
| TCGA-XF-AAMH | BLCA | LIHC |
| TCGA-A7-A0CH | BRCA | THCA |
| TCGA-A2-A25F | BRCA | THCA |
| TCGA-76-6193 | GBM | BRCA |
| TCGA-26-1442 | GBM | LGG |
| TCGA-06-5417 | GBM | LGG |
| TCGA-32-4208 | GBM | LGG |
| TCGA-14-4157 | GBM | LGG |
| TCGA-CR-7368 | HNSC | BLCA |
| TCGA-MT-A7BN | HNSC | GBM |
| TCGA-CR-7371 | HNSC | LUSC |
| TCGA-DQ-5629 | HNSC | LUSC |
| TCGA-CR-7370 | HNSC | LUSC |
| TCGA-CN-6020 | HNSC | LUSC |
| TCGA-CR-7398 | HNSC | LUSC |
| TCGA-CV-A45W | HNSC | LUSC |
| TCGA-CV-5443 | HNSC | PRAD |
| TCGA-HD-A634 | HNSC | PRAD |
| TCGA-BP-5010 | KIRC | GBM |
| TCGA-BP-5199 | KIRC | UCEC |
| TCGA-VM-A8C9 | LGG | BRCA |
| TCGA-HT-8110 | LGG | GBM |
| TCGA-TM-A7C3 | LGG | GBM |
| TCGA-QH-A6CX | LGG | GBM |
| TCGA-DU-7292 | LGG | GBM |
| TCGA-WJ-A86L | LIHC | HNSC |
| TCGA-XR-A8TG | LIHC | HNSC |
| TCGA-LG-A9QC | LIHC | KIRC |
| TCGA-DD-A4NA | LIHC | LGG |
| TCGA-97-8177 | LUAD | GBM |
| TCGA-55-A57B | LUAD | LGG |
| TCGA-L9-A743 | LUAD | LUSC |
| TCGA-55-8301 | LUAD | LUSC |
| TCGA-69-8255 | LUAD | LUSC |
| TCGA-22-4605 | LUSC | HNSC |
| TCGA-63-6202 | LUSC | LUAD |
| TCGA-HC-A9TH | PRAD | BRCA |
| TCGA-J9-A8CL | PRAD | BRCA |
| TCGA-EJ-7125 | PRAD | LGG |
| TCGA-KK-A6E7 | PRAD | LGG |
| TCGA-KK-A6E/ | PRAD | THCA |
| TCGA-EJ-A8FU TCGA-FW-A3I3 | SKCM | GBM |
| TCGA-FW-A313 TCGA-FS-A1ZU | SKCM | PRAD |
| TCGA-CG-5722 | STAD | BRCA |
| TCGA-CG-5722 TCGA-D7-6518 | STAD | BRCA |
| TCGA-BR-A4J9 | STAD | BRCA |
| TCGA-BR-8592 | STAD | BRCA |
| TCGA-BR-8592 TCGA-D7-8573 | STAD | LIHC |
| | STAD | LUSC |
| TCGA-VQ-A8PJ | | |
| TCGA P5 A5OE | UCEC | BRCA |
| TCGA-B5-A5OE | UCEC | HNSC |