# DS-UA 301
# Advanced Topics in Data Science
# *Advanced Techniques in ML and Deep Learning*

**LECTURE 3**

**Parijat Dube**

# Today’s Agenda

- ML performance metrics
  - Algorithmic
  - System-level
- ML performance improvement techniques
  - Regularization techniques
  - Data augmentation
  - Input scaling

# Performance Metrics

- Accuracy, Loss
- Precision, Recall, F score
- Confusion matrix
- Training time, inference time
- Training cost
- Memory requirement

# Accuracy, Precision, Recall, Specificity

| | | True value | |
|---|---|---|---|
| | | Positive | Negative |
| Predicted value | Positive | true positive (tp) | false positive (fp) |
| | Negative | false negative (fn) | true negative (tn) |

$$\text{Accuracy} = \frac{tp + tn}{tp + tn + fp + fn}$$

$$\text{Precision} = \frac{tp}{tp + fp}$$

False discovery rate = 1-Precision

$$\text{Recall} = \frac{tp}{tp + fn}$$

Sensitivity, True positive rate

$$\text{True negative rate} = \frac{tn}{tn + fp}$$

Specificity

False positive rate = 1-Specificity

Balanced accuracy = $(Sensitivity + Specificity)/2$

Considers all entries in the confusion matrix
Value lies between 0 (worst classifier) and 1 (best classifier)

# Performance metrics of a binary classifier

Consider the outcome of a test to detect presence of a radioactive element in drinking water. Given 1000 samples of drinking water from different geographies the test results are summarized as follows (with positive being the sample has radioactive element present or is contaminated). The test results are summarized in the contingency table on the right. Based on the test outcome answer following questions.

1. How many samples did the test correctly classified ?
2. What is the chance (in percentage) that a sample identified as not contaminated is in fact contaminated ?
3. What is the chance (in percentage) that a sample identified as contaminated is in fact contaminated ?
4. What is the precision, recall, and specificity for this test ?

| | | True value | |
|---|---|---|---|
| | | Radioactive present | Radioactive absent |
| Test outcome | Radioactive present | 100 | 300 |
| | Radioactive absent | 250 | 350 |

# An Example AI System

- AI-assisted tumor diagnosis for cancer detection
- “The firm’s deep-learning tool was able to correctly distinguish metastatic cancer 99% of the time, a greater accuracy rate than human pathologists.”
- 99% sounds great. What does this actually mean ?

# An Example AI System (contd.)

- Test data for performance evaluation:
  - 1,000,000 tumors in total
  - 999,000 out of 1,000,000 are *actually* benign (Actual Negatives)
  - 1,000 out of 1,000,000 are *actually* malignant (Actual Positives)

Imbalanced dataset

- Vendor's performance
  - Accuracy = 99%
  - Precision = 9.02%
  - Recall = 99%
- How many tumors did the system correctly classify (i.e. both True Positives or True Negatives) out of all the tumors? 99%
- What is the chance that a tumor identified by the system as malignant is *in fact* malignant"? 9%

| | | Actual Result | |
|---|---|---|---|
| | | Malignant *(Positive)* | Benign *(Negative)* |
| Predicted Result | Malignant *(Positive)* | 990<br>True positive | 9,990<br>False positive |
| | Benign *(Negative)* | 10<br>False negative | 989,010<br>True negative |

# Importance of Context

- Prioritizing Precision vs Recall depends on problem context
- **Recall should be optimized over precision** when there is a **high cost associated with a False Negative, i.e. system predicts benign when tumor is in fact malignant**.
- **Precision should be optimized over recall** when there is a **high cost associated with a False Positive, i.e. spam detection.**

# Balancing Precision and Recall

- F1 score: Harmonic mean of precision and recall; measure of classifier accuracy

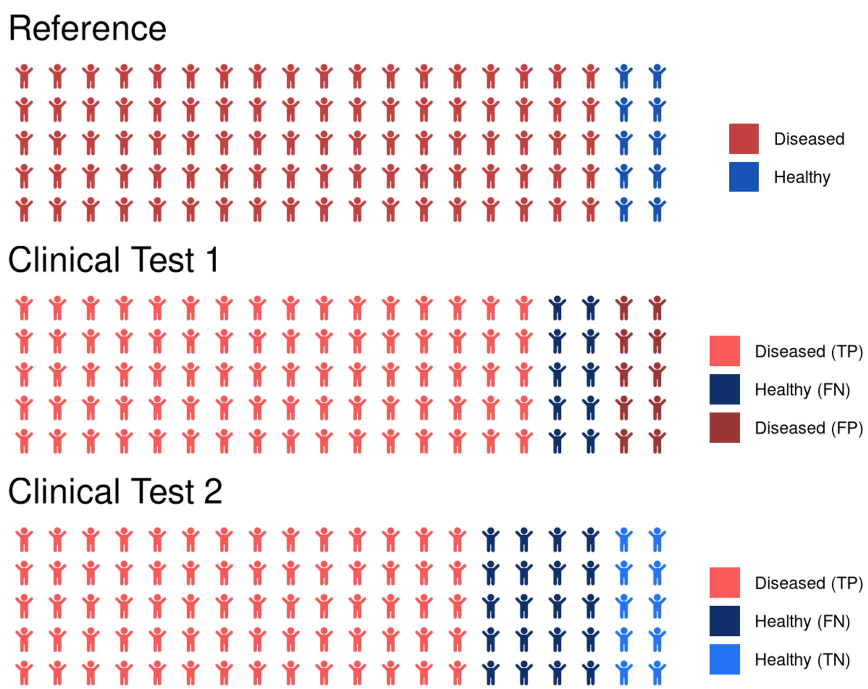
$$F_1 = \frac{2}{\mathrm{recall}^{-1} + \mathrm{precision}^{-1}} = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}} = \frac{\mathrm{tp}}{\mathrm{tp} + \frac{1}{2}(\mathrm{fp} + \mathrm{fn})}.$$

- $F_\beta$ $score$: $\beta = 1$ $is$ $F1$ $score$; recall is considered β times as important as precision

$$F_\beta = (1 + \beta^2) \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\beta^2 \cdot \mathrm{precision} + \mathrm{recall}}$$

# Precision and Recall

True negatives are not accounted in Precision and Recall
Metrics work in situations where the correct identification of negative class is not important




**Confusion matrix for the first test**

| Prediction/Reference | Diseased | Healthy |
|---|---|---|
| Diseased | TP = 80 | FP = 10 |
| Healthy | FN = 10 | TN = 0 |

**Confusion matrix for the second test**

| Prediction/Reference | Diseased | Healthy |
|---|---|---|
| Diseased | TP = 70 | FP = 0 |
| Healthy | FN = 20 | TN = 10 |

If we prefer Test 1 with higher F1 score
➔ No one healthy is identified as healthy (Specificity = 0%)

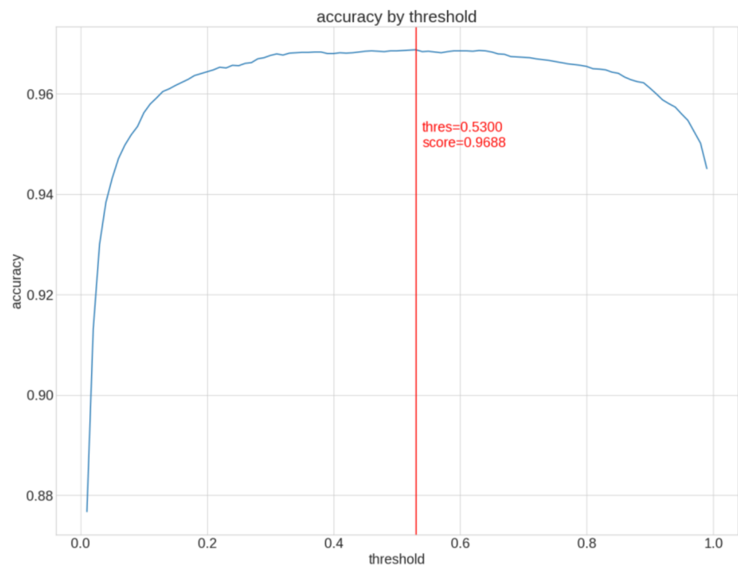
**Comparison of the two tests**

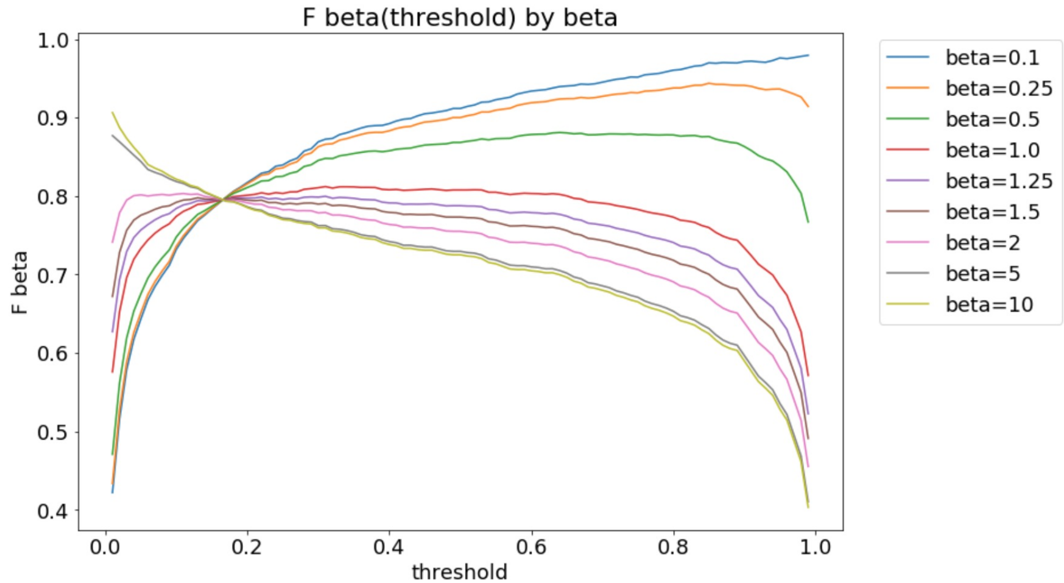
Let us compare the performance of the two tests:

| Measure | Test 1 | Test 2 |
|---|---|---|
| Sensitivity (Recall) | 88.9% | 77.7% |
| Specificity | 0% | 100% |
| Precision | 88.9% | 100% |
| F1 score | 0.889 | 0.87 |

# Performance dependence on positive class threshold

- Classifier gives prediction score (the probability of belonging to positive class) and then we apply a threshold on the score to predict the class
- Metrics like accuracy, precision, recall, Fbeta score are all calculated on the predicted classes and not on prediction scores
    - Metric value depends on the threshold



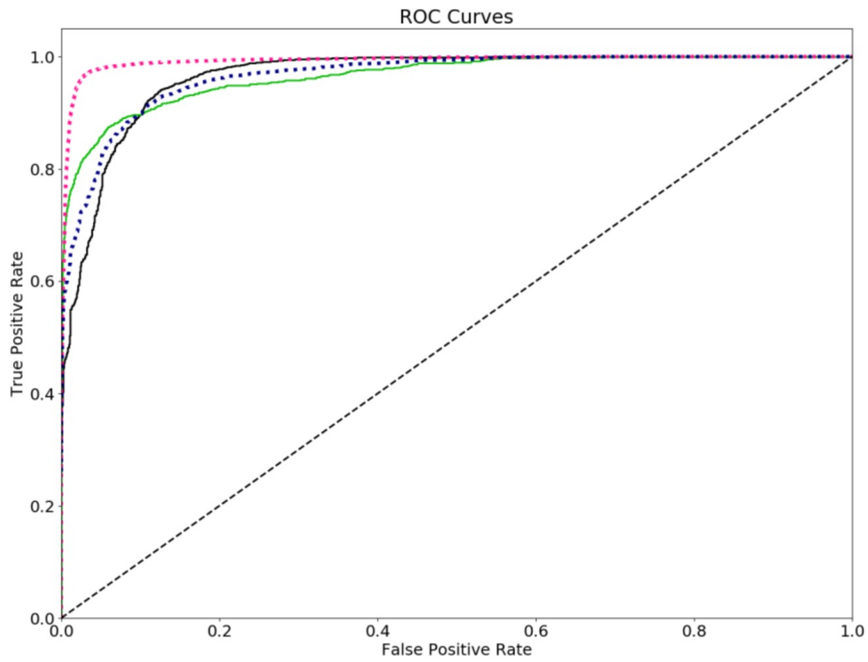
# Performance dependence on positive class threshold

| ID | Actual | Prediction Probability | >0.6 | >0.7 | > 0.8 | Metric |
|---|---|---|---|---|---|---|
| 1 | 0 | 0.98 | 1 | 1 | 1 | |
| 2 | 1 | 0.67 | 1 | 0 | 0 | |
| 3 | 1 | 0.58 | 0 | 0 | 0 | |
| 4 | 0 | 0.78 | 1 | 1 | 0 | |
| 5 | 1 | 0.85 | 1 | 1 | 1 | |
| 6 | 0 | 0.86 | 1 | 1 | 1 | |
| 7 | 0 | 0.79 | 1 | 1 | 0 | |
| 8 | 0 | 0.89 | 1 | 1 | 1 | |
| 9 | 1 | 0.82 | 1 | 1 | 1 | |
| 10 | 0 | 0.86 | 1 | 1 | 1 | |
| | | | 0.75 | 0.5 | 0.5 | TPR |
| | | | 1 | 1 | 0.66 | FPR |
| | | | 0 | 0 | 0.33 | TNR |
| | | | 0.25 | 0.5 | 0.5 | FNR |

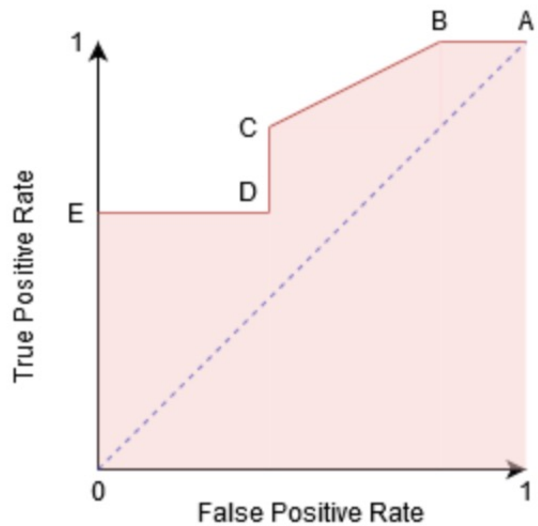
- The metrics change with the changing threshold values.
- Which threshold to choose?

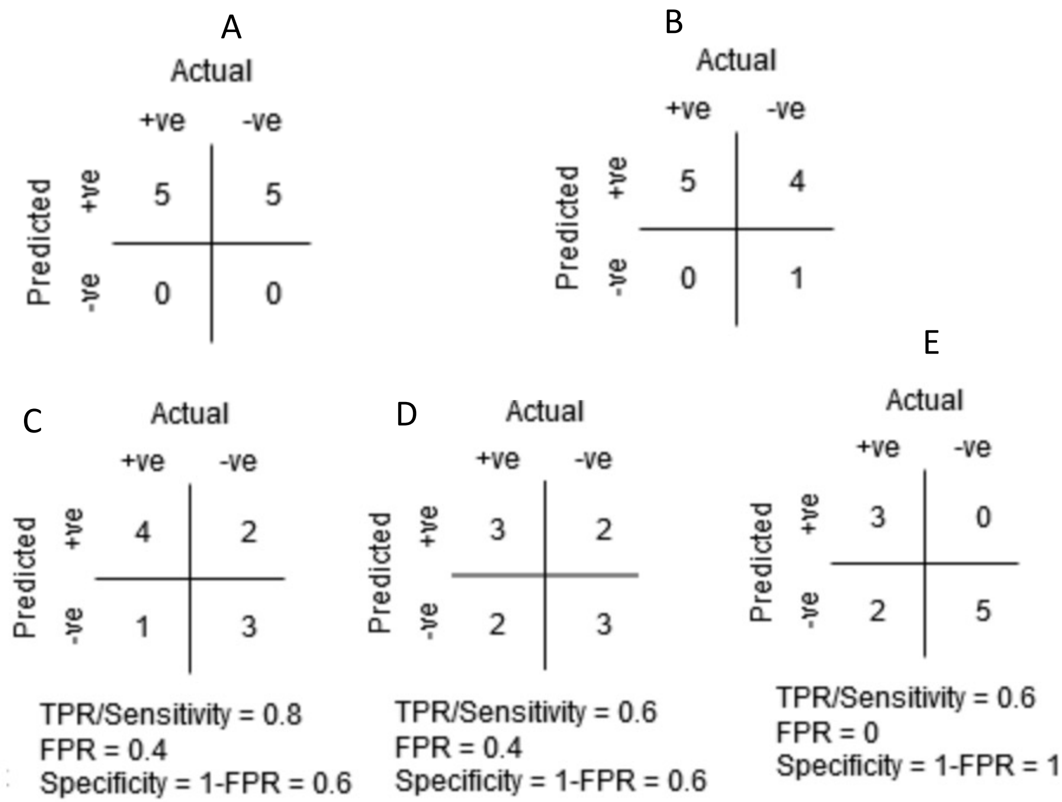
# Receiver Operating Characteristics (ROC)

- Plots True positive rate (Recall) vs False positive rate at different thresholds



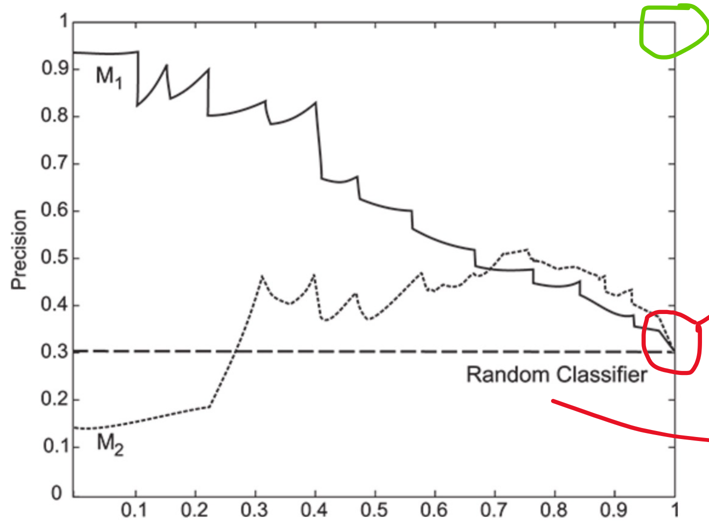
# AUC-ROC




https://www.analyticsvidhya.com/blog/2020/06/auc-roc-curve-machine-learning/

# Precision Recall Curve (PRC)




Perfect classifier

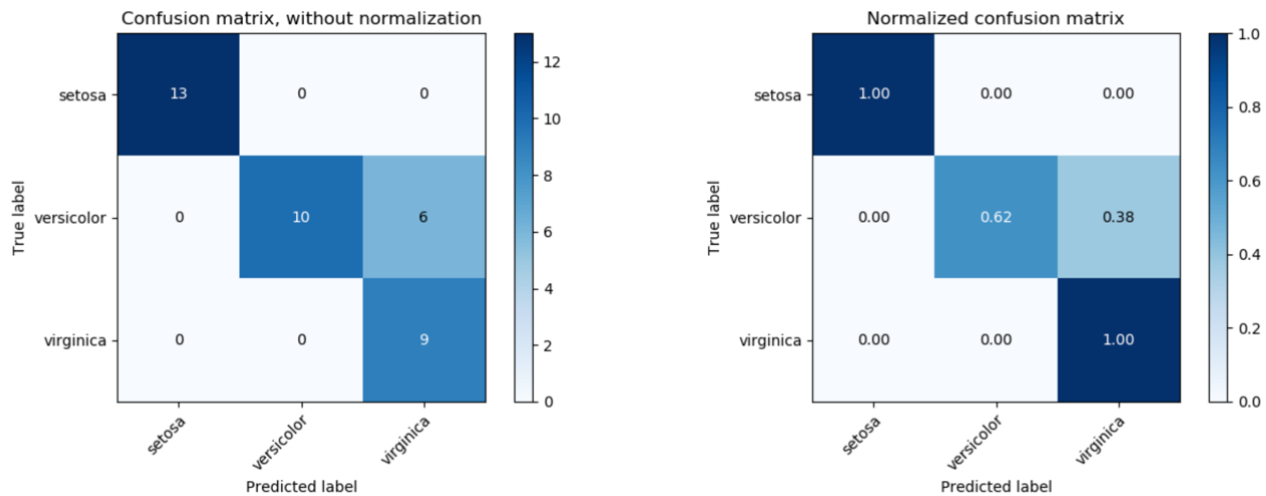
Lowest score threshold
Recall =1, Precision : $\alpha$ :

Recall = p (positive class probability)

- Sensitive to skew factor $\alpha = P/(P+N)$;
- Recall monotonically declines as score threshold increases
- Precision may increase or decrease for the same value of recall
- Random basesline in PR curve depends on the skew; ROC it's the fixed diagonal line independent of skew
- AUC-PR of random classifier = $\alpha$ ; of perfect classifier = 1

https://neptune.ai/blog/f1-score-accuracy-roc-auc-pr-auc

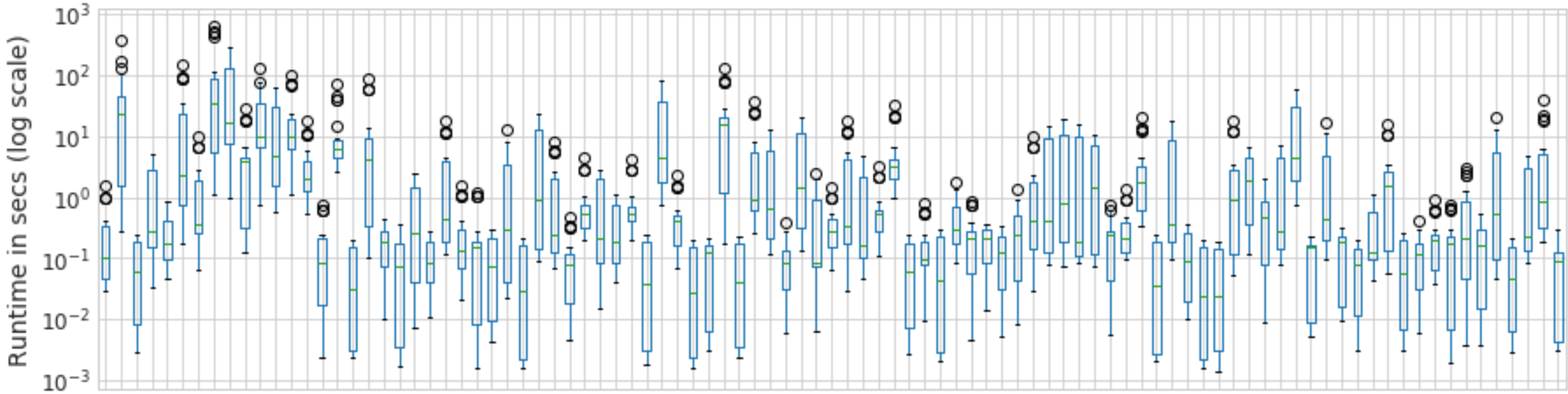
# Confusion matrix example




- Heat map visualization
- Not symmetric: *versicolor* confused with *virginica* not vice-versa
- Prediction is most accurate for *setosa* and *virginica*
- Helps calculate Precision and Recall for multiclass classification

# Runtime: ML

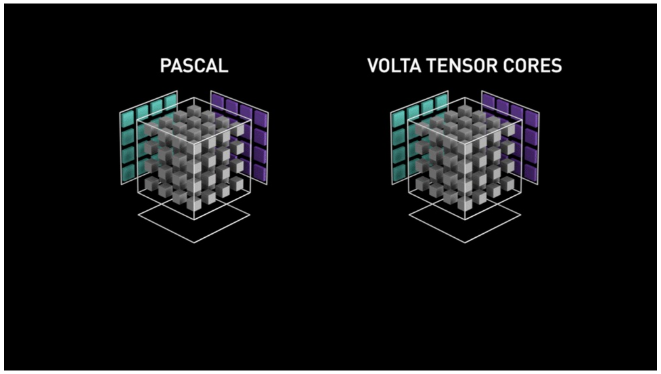
95 OpenML datasets, 7 classification algorithms, fit time

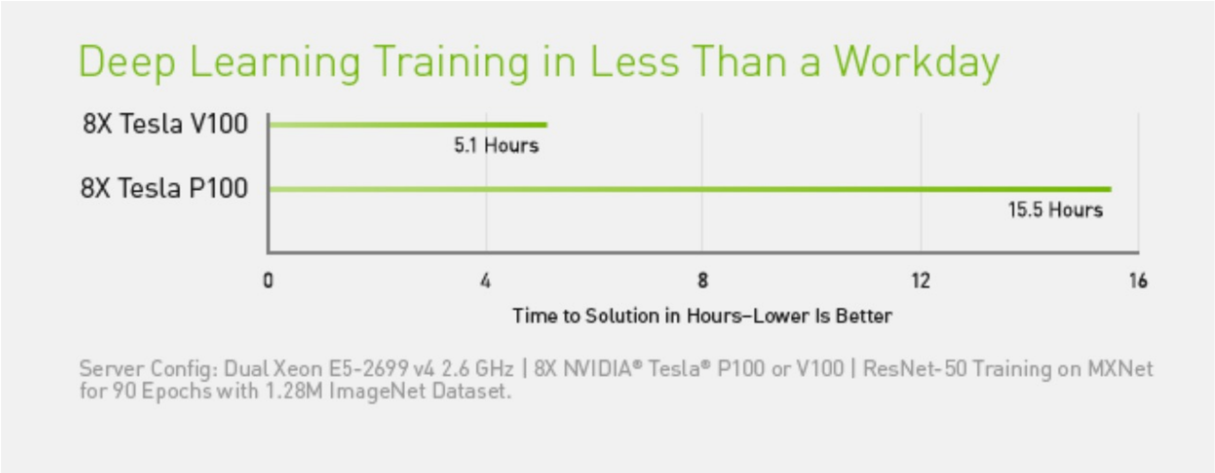



- For the same dataset, depending on the choice of classifier, the runtime can differ by orders of magnitude
- Runtime has both algorithmic, dataset, and system level dependency
- Runtime depends on how the model scales with different features of input: training data size, linear separability, complexity (number of output classes for classification problems), algorithmic hyperparameters, statistical meta-features of data (mean size per class, log number of features)

# DL Training Time

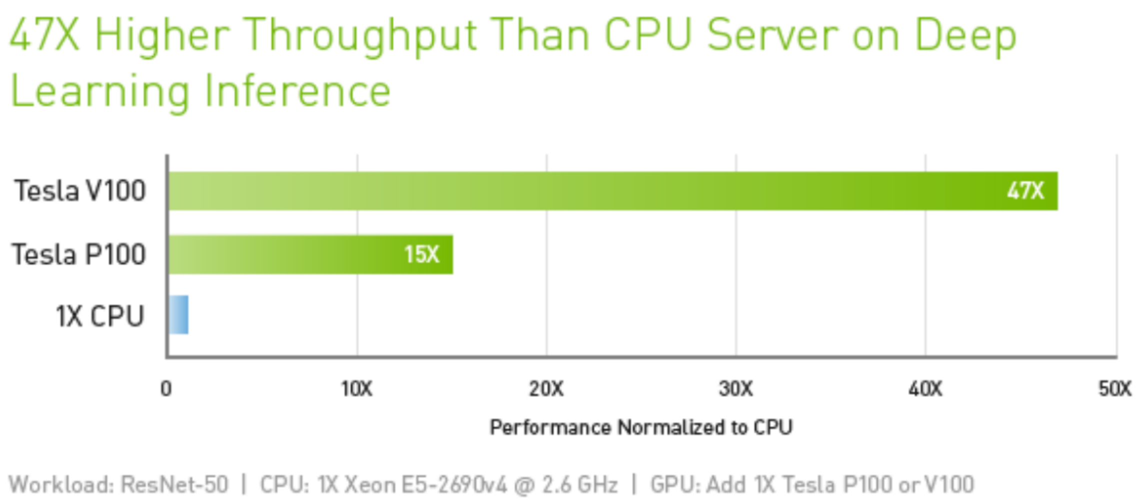
- DL performance is closely tied to the hardware
  - compute power, memory, network
  - Tesla V100: 640 tensor cores (> 100 TFLOPS), 16 GB
  - NVIDIA NVLink: 300 GB/s
  - Volta optimized CUDA libraries




- 32x faster training throughput than a CPU
- 24 faster inference throughput than a CPU

# DL Inference Throughput

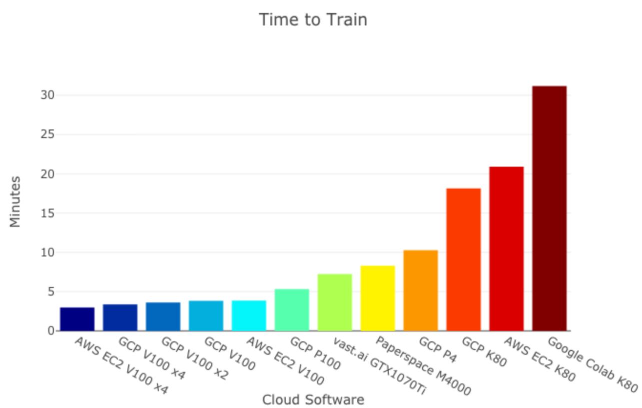


# Training time and cost: An example

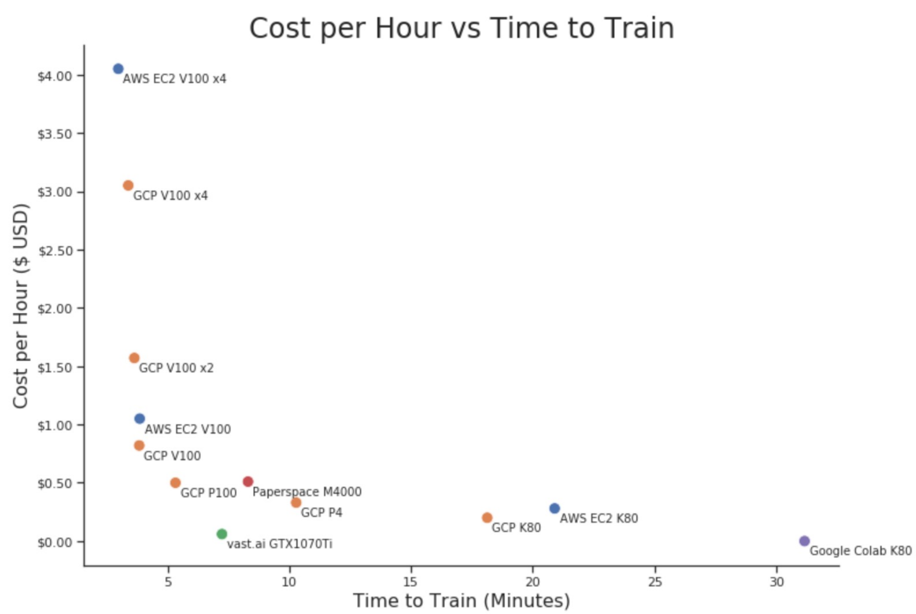
| Cloud Service | NVIDIA GPU | CPUs | GPU RAM | CPU RAM | Cost Per Hour | Wall Time | Cost to Train |
|---|---|---|---|---|---|---|---|
| Google Colab | K80 | 1 | 12 | 13 | 0.00 | 31.17 | 0.000 |
| Google Cloud Compute Engine | P100 | 6 | 16 | 20 | 0.50 | 5.32 | 0.044 |
| Google Cloud Compute Engine | K80 | 6 | 12 | 17 | 0.20 | 18.13 | 0.060 |
| Google Cloud Compute Engine | V100 | 8 | 16 | 20 | 0.82 | 3.83 | 0.052 |
| Google Cloud Compute Engine | P4 | 4 | 8 | 26 | 0.33 | 10.28 | 0.057 |
| Google Cloud Compute Engine | V100 x 2 | 8 | 32 | 30 | 1.57 | 3.63 | 0.095 |
| Google Cloud Compute Engine | V100 x 4 | 8 | 64 | 30 | 3.05 | 3.38 | 0.172 |
| AWS EC2 | K80 (p2.xlarge) | 4 | 12 | 61 | 0.28 | 20.90 | 0.098 |
| AWS EC2 | K80 x 8 (p2.8xlarge) | 32 | 96 | 488 | 2.35 | 16.12 | 0.631 |
| AWS EC2 | V100 (p3.2xlarge) | 8 | 16 | 61 | 1.05 | 3.85 | 0.067 |
| AWS EC2 | V100 x 4 (p3.8xlarge) | 64 | 128 | 488 | 4.05 | 2.97 | 0.200 |
| vast.ai | GTX 1070 Ti | 4 | 8.1 | 16 | 0.06 | 7.23 | 0.008 |
| Paperspace | Quadro M4000 | 8 | 8 | 30 | 0.51 | 8.30 | 0.071 |

- Training time and cost are important when doing DL on cloud
- While runtime (Wall Time) is mostly governed by GPU type, different cloud platforms show differences (18.13 on GCP vs 20.90 on AWS EC2)
- GCP is cheaper than AWS EC2 for same GPU (compare cost with 1 K80 and 1 V100)
- Job does not scale linearly with increasing compute

# Training time and cost tradeoffs







# What Performance Metrics are Important ?

- Depends on the use case
- Model deployment on edge devices: model size is very important; model should fit into device (limited) memory
- Model deployment as a cloud service: model robustness, de-biasing, inference time
- Model development and training: training time, training cost, accuracy
- Instead of a single performance objective, performance optimization of ML models is often a *multi-objective problem*

# Multi-objective optimization

- Example: Control complexity of the model while minimizing MSE
- Control complexity:
  - Improve model Interpretability: In general, the lower the complexity, the easier it is to understand the model.
  - Prevent overfitting
- Scalarized multiobjective learning $\min f = E + \lambda\Omega$
- Pareto based multiobjective learning

$$\min \{f_1, f_2\}$$
$$f_1 = E$$
$$f_2 = \Omega.$$

$$\Omega = \sum_{i=1}^{M} w_i^2$$

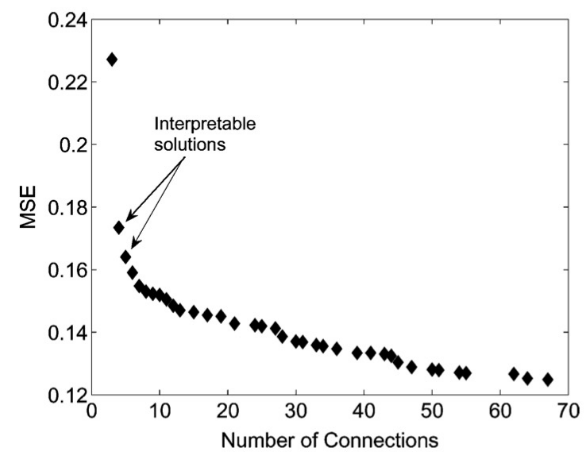
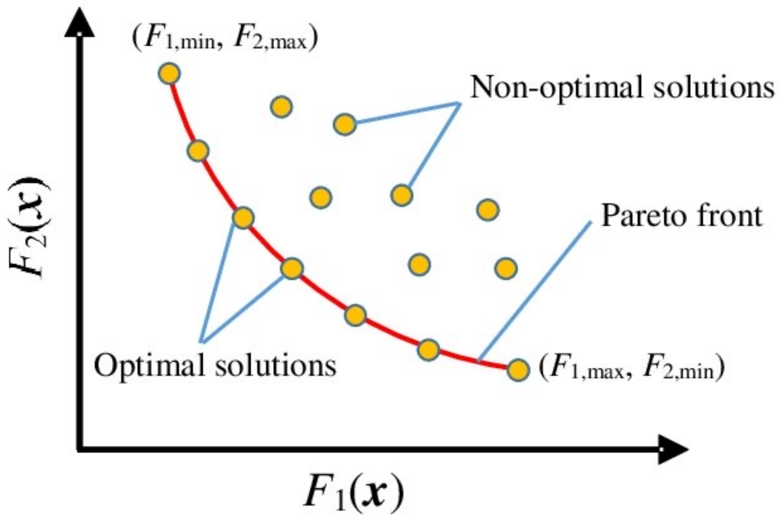



Fig. 9. Typical Pareto-front obtained for the diabetes data composed of 37 solutions.

# Pareto front

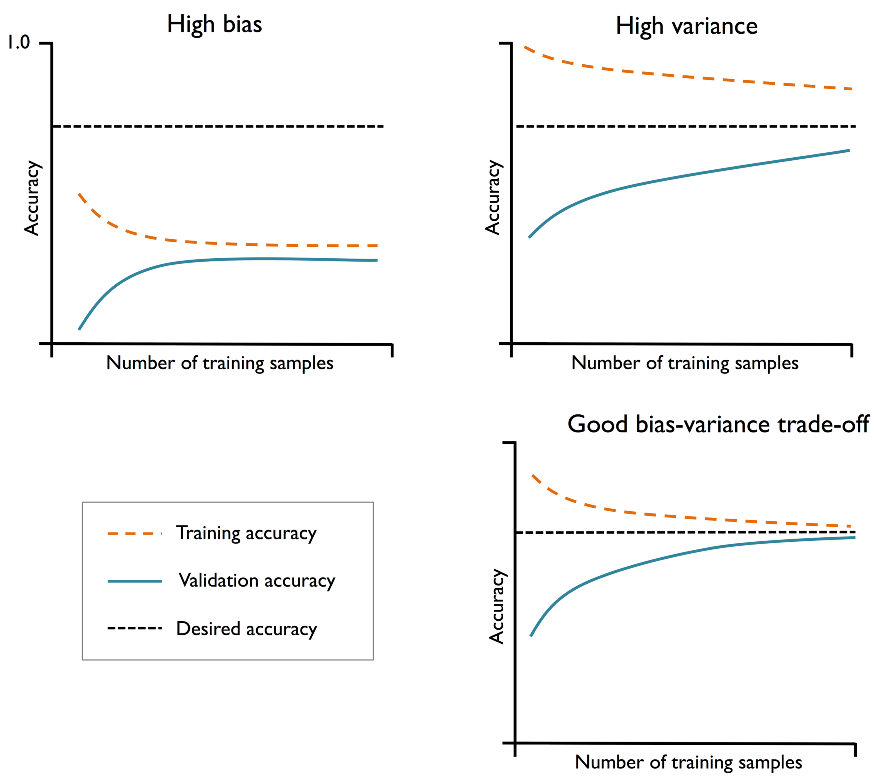


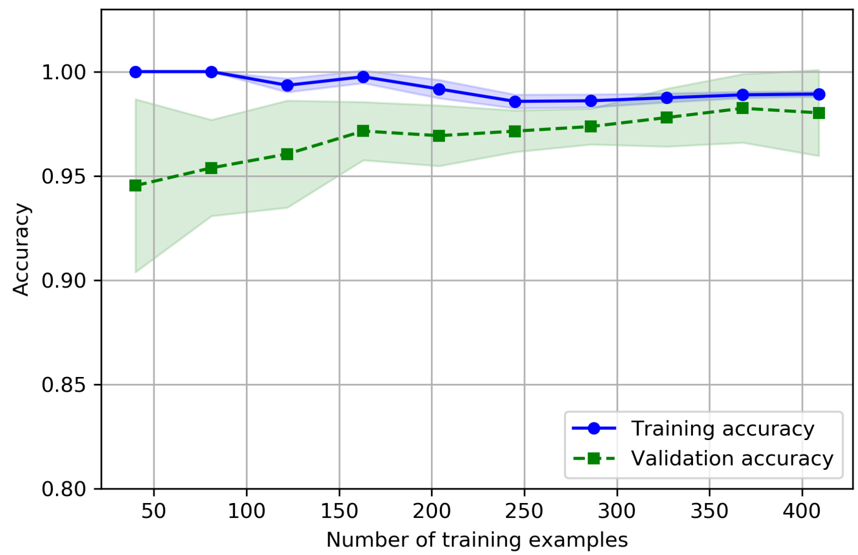

A solution x_1 is said to dominate x_2 if

x_1 is better or equal to x_2 in all objectives

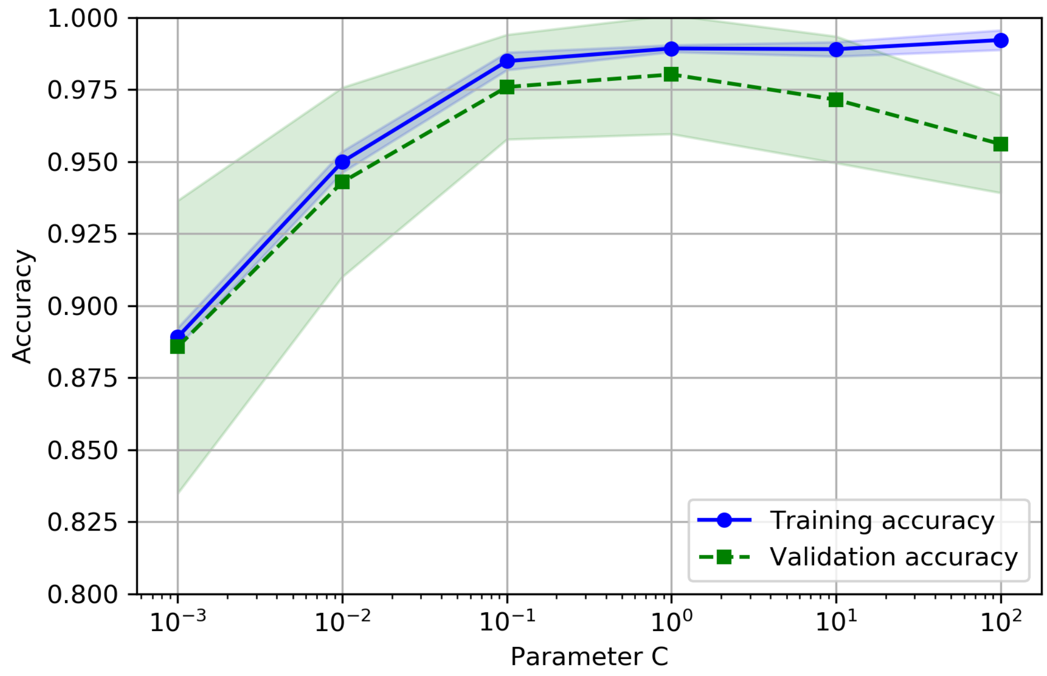
x_1 is **strictly** better than x_2 in at least one objective

# Diagnosing bias and variance problems with learning curve



# Addressing over- and under-fitting with validation curves



# Reading List

- **Model Selection**
  - Sebastian Raschka. Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning. 2018
- **Practical ML**
  - Pedro Domingos, A few useful things to Know about machine Learning
  - Jeff Dale, *Best Deals in Deep Learning Cloud Providers, medium article*
- **Precision-Recall**
  - Jesse Davis, Mark Godarich The Relationship Between Precision-Recall and ROC Curves, ICML 2006
  - Blog. The case against precision as a model selection criterion
  - Blog. Beyond Accuracy: Precision and Recall
- **Application Paper**
  - A prediction model of outcome of SARS-CoV-2 pneumonia based on laboratory findings

# Code Links

- Model Selection: Underfitting, Overfitting, and the Bias-Variance Tradeoff

https://dustinstansbury.github.io/theclevermachine/bias-variance-tradeoff

- Methods for testing linear separability in Python
  http://www.tarekatwan.com/index.php/2017/12/methods-for-testing-linear-separability-in-python/#fnref-102-6
- Jupyter notebook comparing cloud providers
  https://www.kaggle.com/discdiver/best-values-in-deep-learning-cloud-providers/