Multi-Objective Optimization and Learning

Outline

- Part 1: Multi-Objective Optimization (多目标优化)
  - Introduction
  - Multi-Objective Evolutionary Algorithms
- Part 2: Multi-Objective Learning
  - Introduction
  - Diverse and Accurate Ensemble Learning Algorithm
  - Class Imbalance Learning

Multi-Objective Optimization

- ❖ What is Multi-Objective Optimization
- ❖ Pareto Dominance

Multi-Objective Optimization (MOO)

- Compared to “optimisation” that we have seen previously:
  - More than one objective to be optimised, with or without constraints.

$$\min/\max\ F(\boldsymbol{x}) = (f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \dots, f_m(\boldsymbol{x}))$$

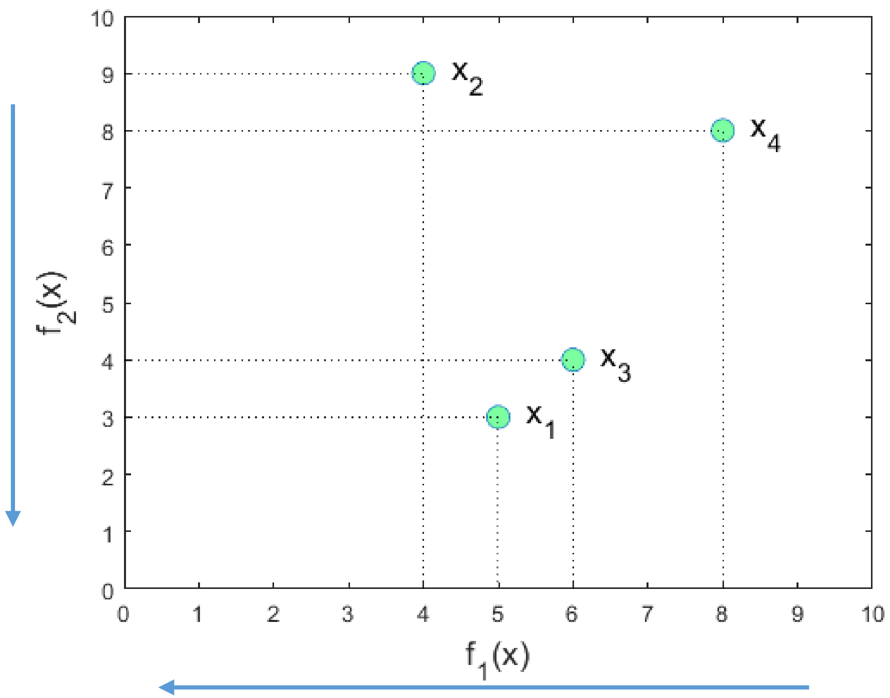
$$s.t.\ g_j(\boldsymbol{x}) \geq 0, \qquad j = 1,2,\dots,J$$

$$h_k(\boldsymbol{x}) = 0, \qquad k = 1,2,\dots,K$$

$$\underbrace{x_i^{(L)}}_{\text{Lower bound}} \leq x_i \leq \underbrace{x_i^{(U)}}_{\text{Upper bound}}, i = 1,2,\dots,n$$

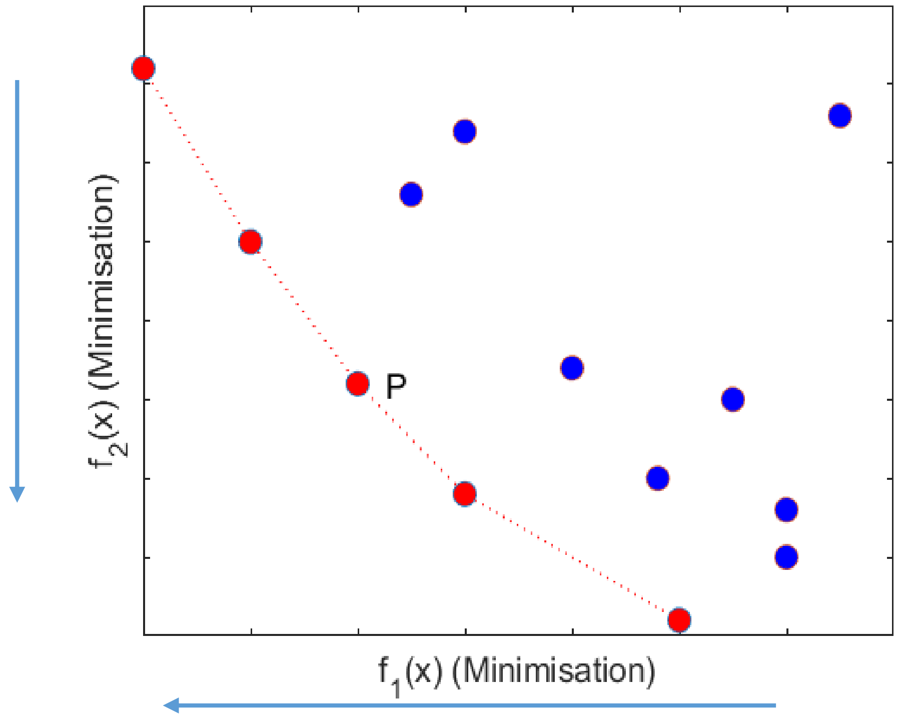
- *$\boldsymbol{x}$ is a vector of continuous, discrete or mixed variables.*
- *”s.t.” stands for “subject to”.*

Pareto (帕雷托) Dominance



- x_a **dominates** $\boldsymbol{x}_b$ if
  - Solution $\boldsymbol{x}_a$ is no worse than $\boldsymbol{x}_b$ in all objectives.
  - Solution $\boldsymbol{x}_a$ is strictly better than $\boldsymbol{x}_b$ in at least one objective.
  - Denote as $\boldsymbol{x}_a \leq \boldsymbol{x}_b$, if minimisation.
- $\boldsymbol{x}_a$ dominates $\boldsymbol{x}_b \Leftrightarrow \boldsymbol{x}_b$ is dominated by $\boldsymbol{x}_a$
- [Question] Can you tell if
  - $\boldsymbol{x}_2$ dominates $\boldsymbol{x}_1$?
    - [Answer] Not comparable.
  - $\boldsymbol{x}_1$ dominates $\boldsymbol{x}_3$?
    - [Answer] Yes.
  - $\boldsymbol{x}_4$ dominates $\boldsymbol{x}_2$?
    - [Answer] Not comparable.

Pareto Front



Pareto optimal: *red points*
Pareto optimal front*: dashed red curve*

- Among a set of solutions P, the **non-dominated solution set** is a set of solutions that are not dominated by any member of P.
- The non-dominated set of the entire feasible decision space is called the **Pareto-optimal set**.
- The boundary defined by the set of all point mapped from the Pareto optimal set is called the **Pareto optimal front**.

Pareto Optimal Solutions

- Pareto optimal set in the decision space (决策空间).
- Pareto optimal front in the objective space (目标空间).

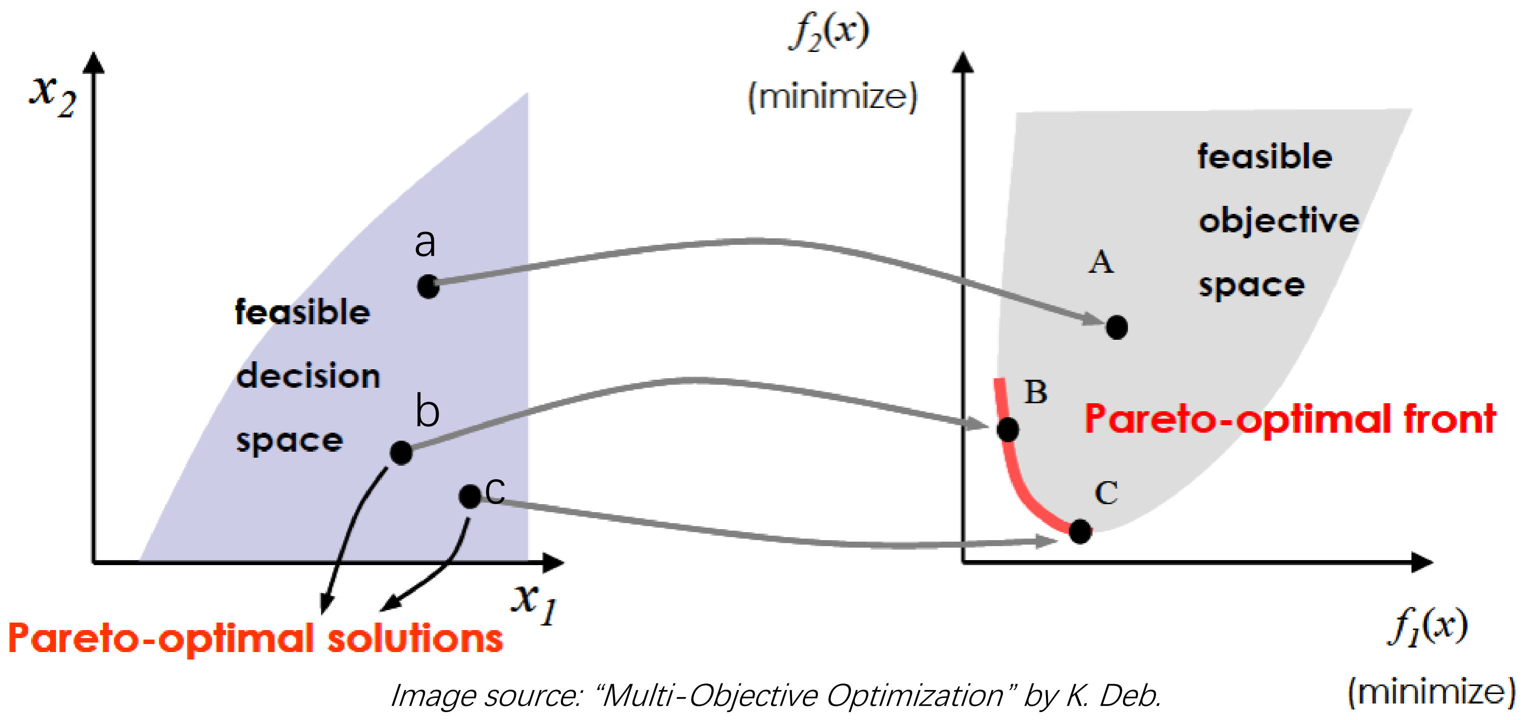


Image source: "Multi-Objective Optimization" by K. Deb.

Main Goals of MOO

1. To find a set of solutions as close as possible to the Pareto optimal front (convergence 收敛性).
2. To find a set of solutions as diverse as possible (diversity 多样性).

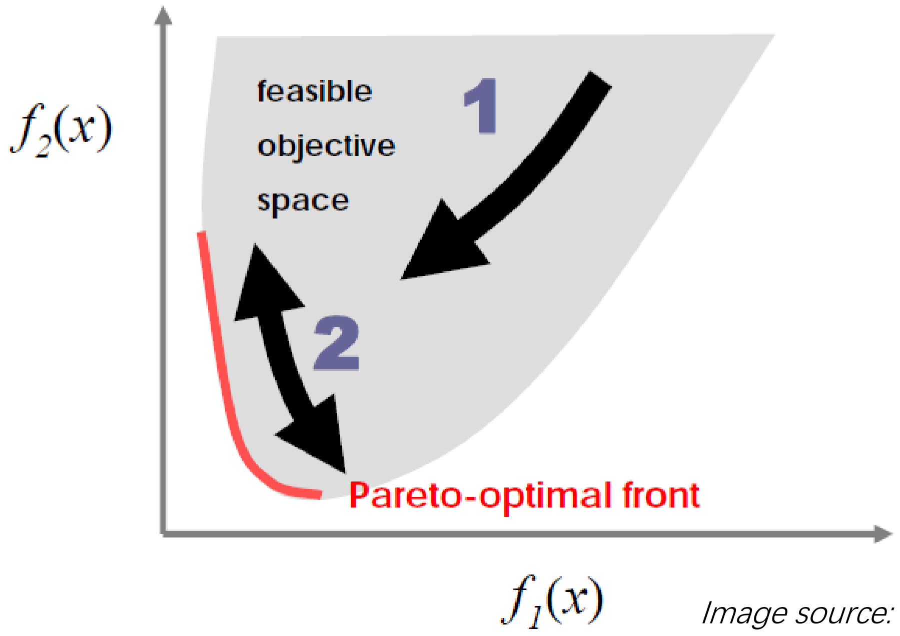


Image source: "Multi-Objective Optimization" by K. Deb.

Pareto Dominance Relation

- Reflexive?
  - No. Any solution x does not dominate itself.
- Symmetric?
  - No. $\boldsymbol{x}_a \preceq \boldsymbol{x}_b \nRightarrow \boldsymbol{x}_b \preceq \boldsymbol{x}_a$.
- Antisymmetric?
  - No.
- Transitive?
  - Yes. If $\boldsymbol{x}_a \preceq \boldsymbol{x}_b$ and $\boldsymbol{x}_b \preceq \boldsymbol{x}_c$ then $\boldsymbol{x}_a \preceq \boldsymbol{x}_c$.
- $\boldsymbol{x}_a \npreceq \boldsymbol{x}_b \nRightarrow \boldsymbol{x}_b \preceq \boldsymbol{x}_a$.

Antisymmetric Relation: A binary relation R *is antisymmetric iff:*
If $R(a,b)$ *and* $R(b,a)$ *then* $a = b$.

How to Solve a MOO Problem?

- Straightforward solution: Convert it to a single-objective problem.
  - ➢The weighted sum approach.
- Provide several solutions, “approach” (逼近) the solutions to the Pareto front, then select a solution from the set.
  - ➢Non-trivial, depends on the decision maker’s experience.
- Provide several solutions, a decision maker selects an area of solutions, then apply local search.
  - ➢Non-trivial, depends on the decision maker’s experience.

Convert to Single Objective

- It’s straightforward:
  - Build a single objective using a weighted sum of objectives:

$$Combined\ Objective = \alpha * f_1 + (1 - \alpha) * f_2$$

  - It seems to be a very simple method!

- [Questions]
  1. What the value α should be?
  2. If you don’t know the exact value, how to decide/compute the value of α?
     - There exist various methods for setting α.

Weakness

- We don't know the exact weights in many cases. Though there are various methods for computing the weights, they also have weakness:
  - Rely on the assumption of convexity/differentiability.
  - Require knowledge of bounds of the objective values.
  - The solution highly depends on the choice of weights.

  ⇒Search in the solution space involves search in the weight space.

- We get only one solution given a set of weights.
  - Unable to provide different trade-off to the decision maker.
  - We don't really know other possible trade-off among objectives.

Multi-Objective Evolutionary Algorithms (MOEAs)

- ❖ Introduction to MOEAs
- ❖ Non-dominated Sorting GA (NSGA II)

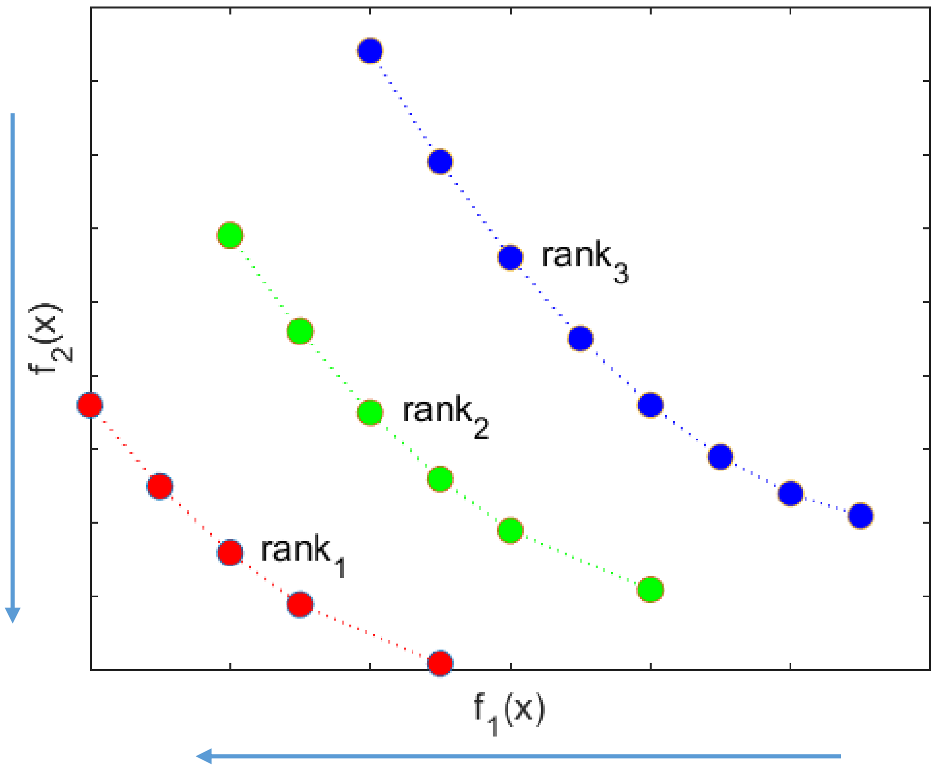
Advantages of MOEAs

- They can provide a set of non-dominated solutions in a single run without requiring the set of weights.
- They do not require the objective functions to be convex, smooth, or even continuous (fewer assumptions).
- They can handle nonlinear constraints.
- They can deal with uncertainty and dynamics better than others.

Multi-Objective Evolutionary Algorithms (MOEAs)

- ❖ Introduction to MOEAs
- ❖ Non-dominated Sorting GA (NSGA II)

Key Ingredient of NSGA II: *Non-dominated Sorting*

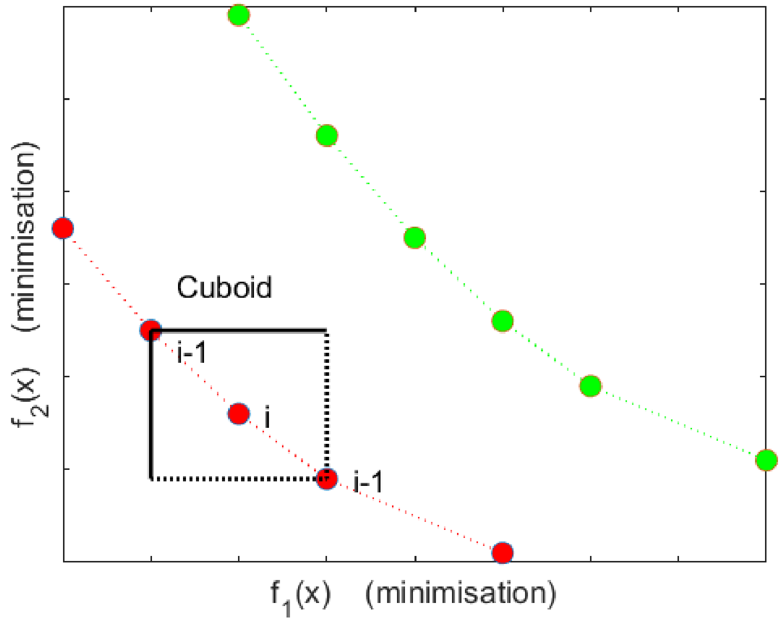


- Classify the solutions into a number of mutually exclusive non-dominated sets.

- $F = \bigcup_{i=1}^{3} rank_i$

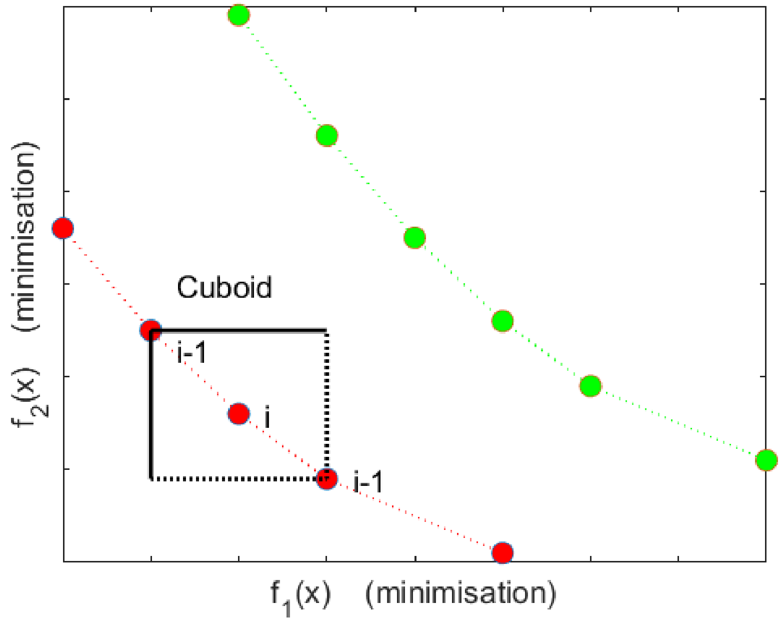
Comparing Solutions

- **Crowding tournament selection**
  - Assume that every solution has a non-domination rank and a local crowding distance.
  - A solution x_a *wins a tournament against another solution* x_b
    - If the solution x_a has a better rank.
    - If they have the same rank but solution x_a has a larger crowding distance than solution x_b.



Crowding Distance

- **Determine Crowding Distance**
  - Denotes half of the perimeter of the enclosing cuboid with the nearest neighbouring solutions in the same rank.
  - Estimation of the largest cuboid enclosing a particular solution (density estimation).
  - *Example (Figure on right)*:
    - The crowding distance of the i^{th} solution in its front (red) is the average side-length of the cuboid (box).



Non-dominated Sorting GA [1]

Step 1	$R_t = P_t \cup Q_t$	combine parent and children population
	$\mathcal{F} = \texttt{fast-nondominated-sort}(R_t)$	$\mathcal{F} = (\mathcal{F}_1, \mathcal{F}_2, \ldots)$, all non-dominated fronts of R_t
Step 2	until $\lvert P_{t+1} \rvert < N$	till the parent population is filled
	$\texttt{crowding-distance-assignment}(\mathcal{F}_i)$	calculate crowding distance in $\mathcal{F}_i$
	$P_{t+1} = P_{t+1} \cup \mathcal{F}_i$	include i-th non-dominated front in the parent pop
Step 3	$\text{Sort}(P_{t+1}, \geq_n)$	sort in descending order using $\geq_n$
	$P_{t+1} = P_{t+1}[0:N]$	choose the first N elements of P_{t+1}
Step 4	$Q_{t+1} = \texttt{make-new-pop}(P_{t+1})$	use selection,crossover and mutation to create a new population Q_{t+1}
	$t = t + 1$	

Non-dominated Sorting GA [1]

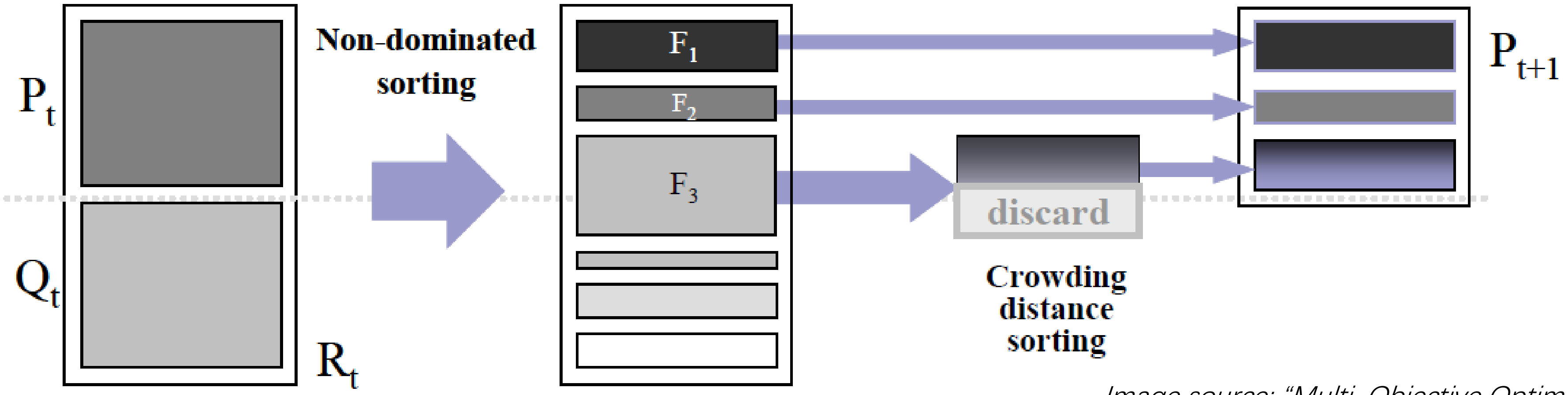
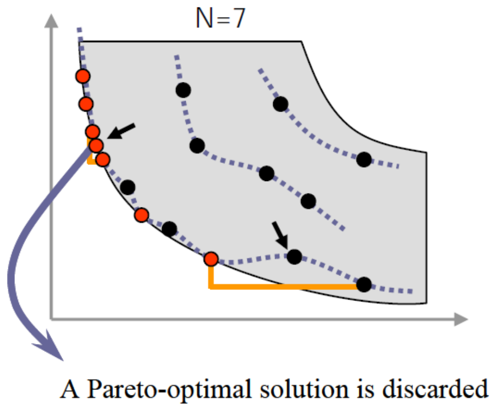


Image source: "Multi-Objective Optimization" by K. Deb.

Non-dominated Sorting GA

- **Advantages**
  - The diversity among non-dominated solutions is maintained using the crowding procedure: No extra diversity control is needed.
  - Elitism protects an already found Pareto-optimal solution from being deleted.
- **Disadvantages**
  - When there are more than *N* members in the first nondominated set, some Pareto-optimal solutions may be discarded.



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Multi-Objective Learning

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- ❖ Diverse and Accurate Ensemble Learning Algorithm
- ❖ Class Imbalance Learning
- ❖ Multi-Objective Ensemble Learning
- ❖ Conclusion

An Example Error Function

- Negative correlation learning defines a simple error function for each network i as follows (N is the size of training set):

$$\varepsilon_i = \frac{1}{N}\sum_{n=1}^{N}\left(\frac{1}{2}(F_i(x_n) - y_n)^2 + \lambda p_i(x_n)\right)$$

where $p_i(x_n) = (F_i(x_n) - F(x_n))\sum_{j \neq i}(F_j(x_n) - F(x_n))$.

Where are Multiple Objectives?

- There are many methods for learning diverse and accurate ensembles, e.g., boosting, bagging, negative correlation learning, etc.
- In general: Accuracy + λ Diversity
- We would like to maximize both the accuracy of each individual learners and the diversity among individuals.
- These are in essence two separate criteria/objectives.

Multi-objective Learning

- Multi-objective learning treats accuracy and diversity as two separate but key objectives in learning.
- Multi-objective optimization algorithms, such as multi-objective evolutionary algorithms (MOEAs), are used as learning algorithms.
- The result from such an MOEA is a non-dominated set of solutions (i.e., learners), which ideally form the ensemble we are interested.
    - A Chandra and X. Yao, ``Ensemble learning using multi-objective evolutionary algorithms,'' Journal of Mathematical Modelling and Algorithms, 5(4):417-445, December 2006.

Flexibility and Generality

- Multi-objective learning offers a highly flexible and general framework for considering different requirements in learning.
- For example, we can include an additional regularization term, as an additional objective [6]. Thus, three objectives are optimised:
    1. objective of performance;
    2. objective of diversity;
    3. objective of regularisation.

$$
\begin{aligned}
e_i \quad = \quad & \frac{1}{M}\sum_{n=1}^{N}(f_i(\mathbf{x}_n) - y_n)^2 - \\
& \frac{\lambda}{M}\sum_{n=1}^{N}(f_i(\mathbf{x}_n) - f_{ens}(\mathbf{x}_n))^2 + \alpha_i \mathbf{w}_i^T \mathbf{w}_i.
\end{aligned}
$$

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Diverse and Accurate Ensemble Learning Algorithm (DIVACE)

- Two objectives:
  - **Accuracy**:

$$\min \mathrm{err}_k = \frac{1}{N}\sum_{i=1}^{N}\left(f_k^i - o^i\right)^2$$

  - **Diversity**:

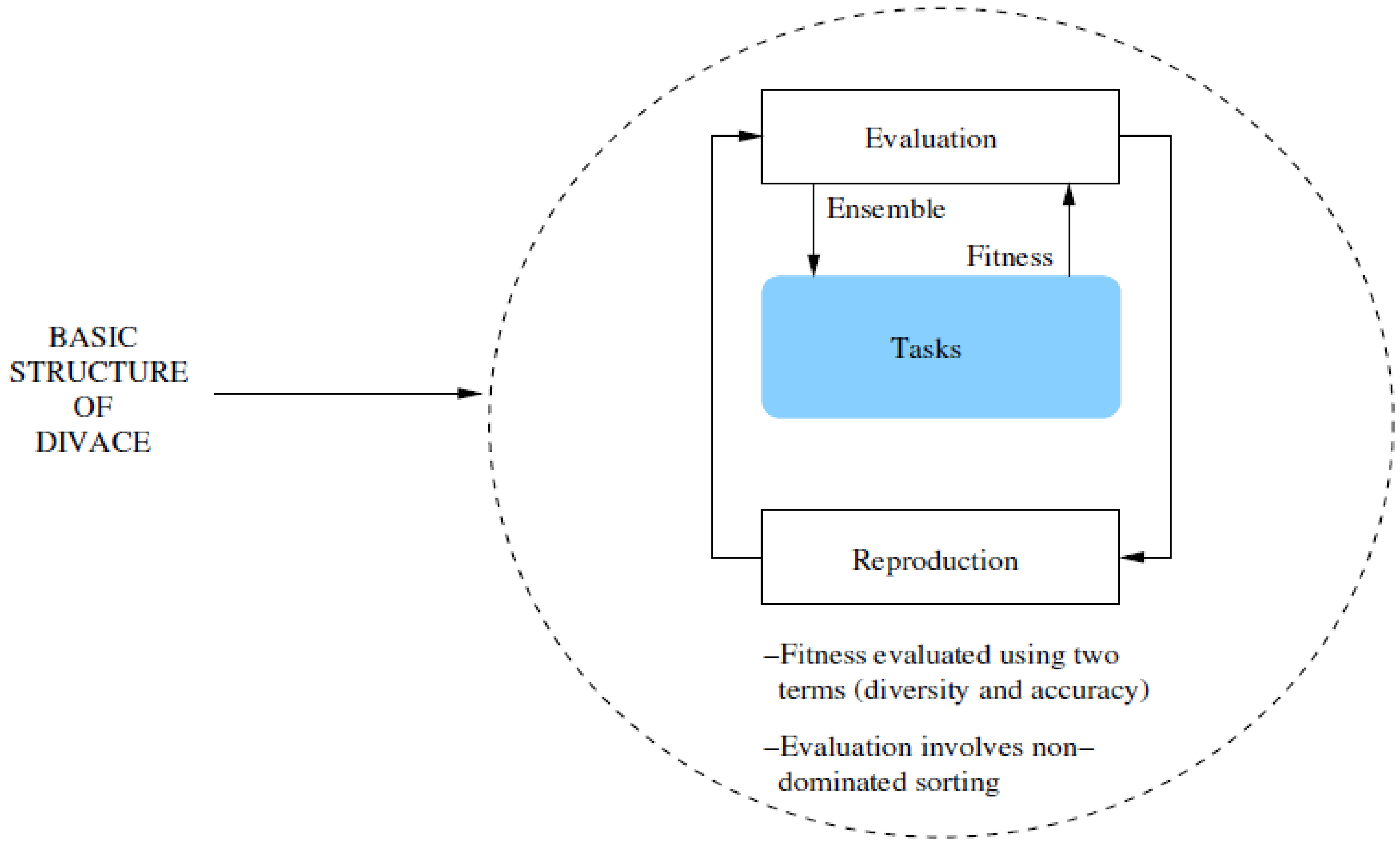
$$\min \mathrm{corr}_k = \sum_{i=1}^{N}\left(f_k^i - f^i\right)\left[\sum_{j\neq k, j=1}^{M}\left(f_j^i - f^i\right)\right]$$

❑ f^i is the ensemble's output for a training sample i;

❑ f_k^i is the k^{th} base learner's output for a training sample i;

❑ o^i is the desired output (true value) for a training sample i.

DIVACE: Basic Structure



DIVACE: Main Steps [5]

1. Initialize a random population of *M* networks, initialize the weights to uniformly distributed random values in the range of $(0,1)$.
2. Apply Back-Propagation (BP) to all individuals in the population.
3. Repeat the following until stopping condition(s) is(are) met:
   1) Evaluate the population in accordance with the two objective functions and label the $S_{NonDominated}$ using the non-dominate sorting algorithm.
   2) If there $|S_{NonDominated}| < 3$, then a repair rule is used [5].
   3) Delete all dominated individuals from the population.
   4) Repeat the following until population size is M:
      - *i. Self-adaptive crossover operator updates itself.*
      - *ii. Select 3 parents uniformly at random from the population.*
      - *iii. Perform crossover (similar to Differential Evolution).*
      - *iv. Perform mutation (additive Gaussian noise).*
      - *v. Apply BP to child and add it to the population.*

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Class Imbalance Learning

- Class imbalance learning refers to learning from imbalanced data sets, in which some classes of examples (minority) are highly under-represented comparing to other classes (majority).

- Learning difficulty: poor generalization on the minority class.

- Learning objective: obtaining a classifier that will provide high accuracy for the minority class without severely jeopardizing the accuracy of the majority class.

Multi-class Imbalance Learning

- Multi-class imbalance: there are more than two classes with uneven class distributions.
  - E.g. In software defect prediction: there are different types of defects.
- Most existing imbalance learning techniques are only designed for and tested in two-class scenarios.
- Existing methods are not effective or even cause a negative effect when there is more than one minority/majority class.

  - S. Wang and X. Yao, “Multi-Class Imbalance Problems: Analysis and Potential Solutions,” IEEE Transactions on Systems, Man and Cybernetics, Part B, 42(4):1119-1130, August 2012.

Multi-objective Class Imbalance Learning [5]

- Multi-objective learning treats single-class performance as separate objectives.

- Multi-objective optimization algorithms, such as multi-objective evolutionary algorithms (MOEAs), are used as learning algorithms.

- The result from such an MOEA is a non-dominated set of solutions (i.e., learners), which ideally form an ensemble we are interested.

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Multi-objective Ensemble Learning

- Multi-objective ensemble learning does improve the performance of single-objective learning.
- The use of different measures as separate objectives helped to increase the diversity in the ensemble and improve ensemble learning performance.
- The ensembles did well even on those performance measures that were not used in multi-objective learning, which provides an evidence demonstrating the robustness of the result.

Software Effort Estimation (SEE)

- Problem description:
  - Estimation of the effort required to develop a software project (e.g., in person-hours). <- Very useful to you for succeeding in CSE!
  - Based on features such as
    - functional size (numerical),
    - required reliability (ordinal),
    - programming language (categorical),
    - development type (categorical),
    - team expertise (ordinal), etc.
- Importance:
  - Main factor influencing project cost.
  - Overestimation vs. underestimation.

Machine Learning in SEE

- Uses completed projects as training examples for creating SEE models, e.g.,
  - Multilayer Perceptrons (MLPs).
  - Radial Basis Function networks (RBFs).
  - Regression Trees (RTs).

- Can be used as decision support tools.

Different Performance Measures in SEE

- Several different performance measures are used in SEE.

Mean Magnitude of the Relative Error:

$$MMRE = \frac{1}{T}\sum_{i=1}^{T} MRE_i,$$

where $MRE_i = |\hat{y}_i - y_i|/y_i$; $\hat{y}_i$ is the predicted effort; and y_i is the actual effort.

Percentage of estimations within 25% of the actual values:

$$PRED(25) = \frac{1}{T}\sum_{i=1}^{T} \begin{cases} 1, & \text{if } MRE_i \leq \frac{25}{100} \\ 0, & \text{otherwise} \end{cases}.$$

Logarithmic Standard Deviation:

$$LSD = \sqrt{\frac{\sum_{i=1}^{T}\left(e_i + \frac{s^2}{2}\right)^2}{T-1}},$$

where s^2 is an estimator of the variance of the residual e_i and $e_i = \ln y_i - \ln \hat{y}_i$.

Current Situation

- There is no universally agreed single performance measure.
- The relationship among different measures in SEE is not well understood.
- Existing SEE approaches use at most one measure during the learning procedure. It is unclear whether a model/learner trained using one measure would still perform well under a different measure.
- Many papers did not even report the measure they used in training!

SEE by Multi-objective Learning

- How about viewing SEE as a multi-objective learning problem?

- Each performance measure is considered explicitly as a separate objective in learning.

But Why?

- A multi-objective algorithm can be used to create SEE models that are generally good in terms of all objective measures, and present different trade-offs among these measures.
- These different trade-offs can help us to understand to what extent different measures behave differently and what the relationship among these measures is.
- They help to enhance the robustness of the models.

Some Research Questions

1. What is the relationship among different performance measures for SEE?
2. Can we use different performance measures as a source of diversity to create SEE ensembles? In particular, can that improve on the performance measures used as objectives with respect to a standard learning algorithm for the same type of base model?
3. Is it possible to outperform the state-of-the-art?

Ensemble Member Selection

- Sometimes it is unnecessary to include the entire set of classifiers found by MOEAs in an ensemble. A subset would be sufficient, or even better.
  - X. Yao and Y. Liu, "Making use of population information in evolutionary artificial neural networks," IEEE Transactions on Systems, Man and Cybernetics, Part B: Cybernetics, 28(3):417-425, June 1998.
- There are various methods in the literature for selecting a diverse subset of classifiers from a large set
  - U. Bhowan, M. Johnston, M. Zhang and X. Yao, ``Reusing Genetic Programming for Ensemble Selection in Classification of Unbalanced Data,'' IEEE Transactions on Evolutionary Computation, 18(6):893-908, December 2014.

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Concluding Remarks for Multi-Objective Learning

- Multi-objective learning fits naturally with ensembles.

- There are different forms of multi-objective learning, e.g., different objectives.

Reading Materials for This Lecture

[1] Deb, K., Pratap. A, Agarwal, S., and Meyarivan, T. (2002). A fast and elitist multiobjective genetic algorithm: NSGA-II. *IEEE Transaction on Evolutionary Computation*, 6(2), 181-197.

[2] H. Wang and X. Yao, Objective Reduction Based on Nonlinear Correlation Information Entropy, *Soft Computing*, June 2016, Volume 20, Issue 6, pp 2393–2407.

[3] Y. Yuan, H. Xu, B. Wang and X. Yao, A New Dominance Relation Based Evolutionary Algorithm for Many-Objective Optimization, *IEEE Transactions on Evolutionary Computation*, 20(1):16-37, February 2016.

[4] K. Praditwong and X. Yao, A New Multi-objective Evolutionary Optimisation Algorithm: The Two-Archive Algorithm, *Proc. of the 2006 International Conference on Computational Intelligence and Security (CIS'2006),* 3-6/11/2006, Ramada Pearl Hotel, Guangzhou, China. IEEE Press, Volume 1, pp.286-291.

[5] A Chandra and X. Yao, ``Ensemble learning using multi-objective evolutionary algorithms,'' Journal of Mathematical Modelling and Algorithms, 5(4):417-445, December 2006.

[6] H. Chen and X. Yao, ``Multiobjective Neural Network Ensembles based on Regularized Negative Correlation Learning,'' IEEE Transactions on Knowledge and Data Engineering, 22(12):1738-1751, December 2010.

[7] L. L. Minku and X. Yao, ``Software Effort Estimation as a Multi-objective Learning Problem,'' ACM Transactions on Software Engineering and Methodology, 22(4), Article No. 35, October 2013, 32 pages.

[8] Z. Gong, H. Chen, B. Yuan and X. Yao, "Multiobjective Learning in the Model Space for Time Series Classification," IEEE Transactions on Cybernetics, online on 23 January 2018.

[9] Minku, L. L., White, A. P., & Yao, X. (2010). The impact of diversity on online ensemble learning in the presence of concept drift. *IEEE Transactions on Knowledge and Data Engineering*, *22*(5), 730-742.

[10] Oza, N. C., & Russell, S. (2001, August). Experimental comparisons of online and batch versions of bagging and boosting. In *Proceedings of the seventh ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 359-364). ACM.