From Feature Selection to Instance-wise Feature Acquisition[1]

Tutorial @ SDM 2024

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Tutorial Objectives

- Contrast feature selection to feature acquisition, and introduce related nomenclature
- Overview state–of–the–art and summarize research progress on this area
- Draw connections to recent trends in machine learning (e.g., model interpretability, fairness)
- Identify challenges and opportunities for future work

Tutorial Outline

- Introduction
  - Typical machine learning problem
  - Feature selection and variants
  - Applications and main challenges
- Online/Streaming feature selection
  - Problem definition
  - Main idea & methods
  - Variants (e.g., streaming data, feature interactions, group feature selection)
- Instance–wise feature acquisition
  - Problem definition
  - Static approaches
  - Dynamic methods
- Advanced Topics
  - Model interpretability
  - Incorporating fairness constraints
  - Dealing with structure (e.g., Bayesian network classification, hierarchical classification)

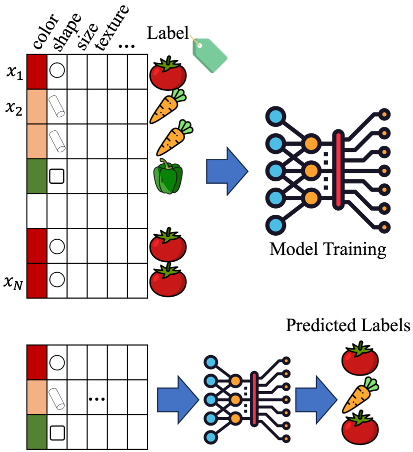
Relevant Tutorials

- Explaining Machine Learning Predictions: State–of–the–art, Challenges, Opportunities [at NeurIPS 2020]
  - Focused on post hoc explainability, and discusses among others how features contribute towards a prediction
  - `https://explainml-tutorial.github.io/neurips20`
- Subset Selection in Machine Learning: Theory, Applications, and Hands On [at AAAI 2021]
  - Focused on the theoretical underpinnings of subset selection and discussed related applications, such as active and human assisted learning
  - `https://explainml-tutorial.github.io/aaai21`

Introduction

Typical Machine Learning Problem

- Training set $\mathcal{D}$ consisting of $(\boldsymbol{x}, y)$ pairs
  - Features $\boldsymbol{x}$ are usually represented as fixed–length numeric feature vectors
  - Labels y are typically modeled as integers
- Goal: Learn function $f : \boldsymbol{x} \rightarrow y$ so the label(s) of unseen instances can be predicted
  - A loss function (e.g., zero–one) is selected
  - The empirical risk is then minimized



Feature Selection

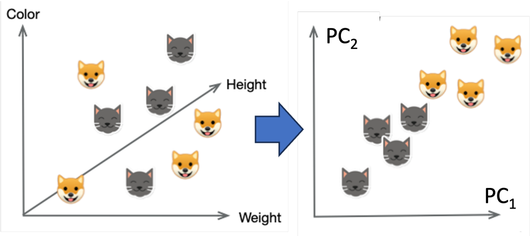
- There are many "characteristics" that can help us recognize a cat from a dog, e.g.,
  - Overall size
  - Existence of whiskers
  - Shape of ears
  - *etc*
- Feature selection: select small subset of elements in $\boldsymbol{x}$ that can be used to derive a good model
  - Features must be "as good as possible" wrt some criterion C
  - Sparse wrt to $\boldsymbol{x}$

Benefits of Feature Selection

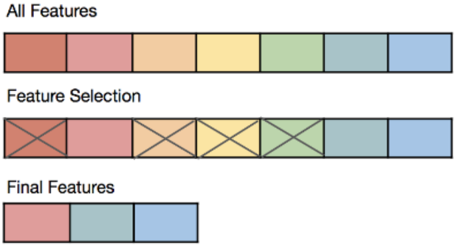
- As the number of features becomes large:
  - Learning models tend to overfit
  - High storage requirements and computational costs
  - Distances lose meaning
- This is where feature selection comes in
  - Remove irrelevant and redundant features
  - Enhance generalization performance
  - Increase computational efficiency (i.e., speed up the learning process)
  - Decrease memory storage
  - Improve model interpretability

Feature Selection Variants

- Dimensionality reduction (e.g., Principal Component Analysis)



- Standard (offline) supervised feature selection



Dimensionality Reduction

- Project original high dimensional features to new feature space with low dimensionality
- Newly constructed feature space is usually (non)linear combination of original features

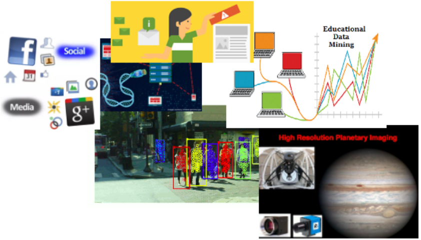
Standard (Offline) Supervised Feature Selection [GE03]

- Feature subsets evaluated wrt information content, predictive accuracy of a given classifier or both
  - Filter methods: independent of learning algorithm
  - Wrapper methods: iteratively assess quality of selected features based on classifier's learning performance
  - Embedded methods: embed feature selection into learning algorithm
- Smallest feature subset satisfying constraint is maintained

Training: all candidate features are available upfront
Testing: same final selected features used for classification

Applications

- Webspam page detection (16 million features) [WCP06]
- Educational data mining for predicting student performance (> 29 million features) [SNMR$^+$10]
- Hot topics detection in social media
- Bionformatics (full set of features is hard to acquired due to high cost of wet lab experiments)
- Planetary imaging, online visual tracking, etc



Main Challenges

- Exhaustive search over the entire feature space is computationally expensive in high–dimensional settings
- Data instances and/or features may not be available in advance (e.g., online/streaming setings) or may be missing
- In practise (e.g., medicine and criminal justice) features have an associated cost
  - Acquisition (e.g., medical tests, evidence collection)
  - Privacy (e.g., revealing personally identifiable information)
  - Fairness (e.g., may amplify bias)
  - Energy consumption (e.g., communication, storage, or computational cost)
- Concept/distribution drift
- Feature dependencies (e.g., multi–collinearity, group structure, multiview settings)
- Predictive power of different feature subsets may vary by subgroups of data instances (e.g., prognosis for different subpopulations)

Online/Streaming Feature Selection

Problem Definition [HZL+18]

- Also known as incremental feature selection
- Goal: choose subset of features from larger set of potentially redundant features without access to full feature space in advance

Training:	features arrive one at a time/batches
Testing:	same final selected features used for classification

- Representative methods can be categorized as threshold–based or rough set theory–based

Threshold–based Streaming Feature Selection

- Newly arriving feature is selected if specific constraint is satisfied
- Representative methods include:
  - Grafting [PLT03]
  - Alpha–investing [ZFSU05]
  - OSFS / Fast–OSFS [WYD^{+}12]
  - SAOLA [YWDP16]
  - OSSFS–DD [ZZYW22]

Scalable and Accurate OnLine Approach (SAOLA) [YWDP16]

- Features are categorized into four disjoint groups:
  - irrelevant: $P(C = c_i | S = s, F_i = f_i) = P(C = c_i | S = s)$ for all $S \subseteq F \setminus \{F_i\}$
  - strongly relevant: if above condition not met
  - redundant: has Markov blanket M (i.e., $P(F_i | M, Y) = P(F_i | M)$ for all $Y \in F \setminus (M\{\cup F_i\}))$ within F
  - non–redundant: $P(C = c_i | S = s, F_i = f_i) \neq P(C = c_i | S = s)$ for some $S \subset F \setminus \{F_i\}$

Scalable and Accurate OnLine Approach (SAOLA) [YWDP16]

- Goal: At each step t_i, maintain minimum size feature subset $S^*_{t_i}$ that maximizes predictive classification performance
- Key steps:
  - Determine relevance of feature F_i to class label C
    - If $P(C|F_i) = P(C)$, then discard F_i
    - Else, check if F_i is redundant wrt already selected features
  - If F_i is relevant and not redundant, add it to the selected feature subset
  - Pruning step: find the subset ζ that maximizes the probability $P(C|\zeta)$

Scalable and Accurate OnLine Approach (SAOLA) [YWDP16]

- Maintaining minimum size feature subset at each step requires examining all possible feature subsets
  - Does not scale with number of features
  - Therefore, problem is rewritten in terms of mutual information
- Mutual information between features is computed online using pairwise comparisons based on heuristics
  - Mutual information between features conditioned on all feature subsets need not be computed

Scalable and Accurate OnLine Approach (SAOLA) [YWDP16]

ALGORITHM 1: The SAOLA Algorithm.

```
1:  Input: F_i: predictive features, C: the class attribute;
    δ: a relevance threshold (0 ≤ δ < 1),
    S*_{t_{i-1}}: the selected feature set at time t_{i-1};
    Output: S*_{t_i}: the selected feature set at time t_i;
2:  repeat
3:    get a new feature F_i at time t_i;
4:    /*Solve Eq.(2)*/
5:    if I(F_i;C) ≤ δ then
6:      Discard F_i;
7:      Go to Step 21;
8:    end if
9:    for each feature Y ∈ S*_{t_{i-1}} do
10:     /*Solve Eq.(3)*/
11:     if I(Y;C) > I(F_i;C) & I(F_i;Y) ≥ I(F_i;C) then
12:       Discard F_i;
13:       Go to Step 21;
14:     end if
15:     /*Solve Eq.(4)*/
16:     if I(F_i;C) > I(Y;C) & I(F_i;Y) ≥ I(Y;C) then
17:       S_{t*_{i-1}} = S_{t*_{i-1}} - Y;
18:     end if
19:   end for
20:   S*_{t_i} = S_{t*_{i-1}} ∪ F_i;
21: until no features are available
22: Output S*_{t_i};
```

Steps 5–8: Determine the **relevance** of feature F_i to class label C

Step 12: And never consider it again!

Steps 11–14: Determine whether F_i should be retained given the current feature set $S^*_{t_{i-1}}$

Steps 16–18: Check if some features within $S^*_{t_{i-1}}$ can be removed due to the inclusion of new feature F_i

Online Streaming Feature Selection (OSFS) [WYD+12]

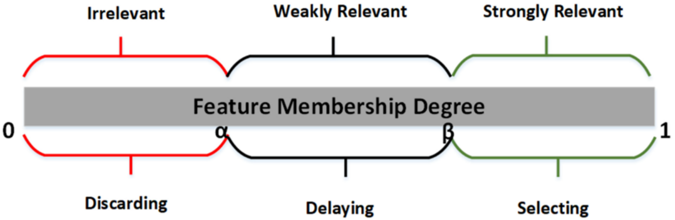
- Goal: find optimal subset comprising non–redundant and strongly relevant features
  - Features are categorized into four disjoint groups
  - Unlike SAOLA, uses G^2 test to measure conditional independence
- Alternating two–step process
  - Relevance analysis: determine if streaming feature is relevant, and if so, add to candidate feature set and Markov blanket of class label C
  - Redundancy analysis: identify and remove redundant features in Markov blanket of class label C
    - Key insight: if a feature is marked redundant, it remains redundant even if some features within its Markov blanket are removed later on
  - Stopping criteria (prediction accuracy, maximum number of iterations, all features examined)

Online Streaming Feature Selection (OSFS) [WYD+12]

- Redundancy analysis re–examines relevance of each feature in candidate set wrt class label every time a new feature is added (time–consuming)
- Fast OSFS:
  - If current streaming feature (as opposed to each and every feature) is relevant but redundant, remove it from candidate feature set
  - Else, add current feature in candidate feature set, and check redundancy of each feature in candidate set wrt subsets that include newly added feature

Streaming Feature Selection via Dynamic Decision [ZZYW22]

- In online streaming feature selection, discarded features are never considered again
  - For weakly relevant features making a decision (selecting or discarding) immediately is risky
- $\forall$ new arriving feature f_t
  - If strongly relevant, add it into the candidate feature subset S_C
  - If irrelevant, discard it immediately
  - If weakly relevant, add it into undetermined feature subset S_U and defer decision



Streaming Feature Selection via Dynamic Decision [ZZYW22]

- Compute membership score, $\gamma_f(d) \in [0, 1]$, between feature f and the decision class d using Normalized Mutual Information
  - if $\beta \leq \gamma_f(d) \leq 1$, f is strongly relevant to d
  - if $\alpha < \gamma_f(d) < \beta$, f is weakly relevant to d
  - if $0 \leq \gamma_f(d) \leq \alpha$, then f is irrelevant to d
- But how to choose proper thresholds of α and β?
  - Assume normally distributed data, and features arriving at random
  - Membership scores in the whole feature space are also normally distributed with mean value μ and standard deviation σ
  - Set $\alpha = \mu - \sigma$ and β
- Without knowledge of the entire feature space the thresholds cannot be set a–priori
- Thankfully, the mean and standard deviation can be dynamically updated $\forall f_t$
  - $\mu_t = \mu_{t-1} + \frac{\gamma_t - \mu_{t-1}}{t}$ and $\sigma_t = \sqrt{\frac{(t-2)*\sigma_{t-1}^2 + (\gamma_t - \mu_{t-1})(\gamma_t - \mu_t)}{t-1}}$

Streaming Feature Selection via Dynamic Decision [ZZYW22]

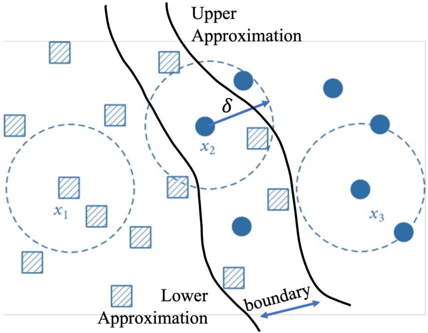
- Feature redundancy
  - Two features f_1 and f_2 must contain some common information if $I(f_1, f_2; d) < I(f_1; d) + I(f_2; d)$
  - If additionally $I(f_1, f_2; d) < 2\beta$ remove the feature with the smaller value of $I(f_1; d)$ or $I(f_2; d)$
  - Note: For each new feature, must check for redundancy between that feature and every feature currently in S_C
- Feature uncertainty
  - f_i is added to S_U if $\alpha < I(f_i; d) < \beta$
  - if $\exists f_j \in S_U$ s.t. $I(f_i, f_j; d) \geq 2\beta$, add both f_i and f_j into S_C
  - Features that don't satisfy this are discarded when S_U reaches a threshold to avoid S_U becoming too large

Rough Set Theory–based Streaming Feature Selection

- Threshold–based streaming feature selection typically require prior information about feature space
- Representative methods include:
  - OFS–Density [ZHLW19a]
  - OFS–A3M [ZHLW19b]

OFS–Density [ZHLW19a]

- Two types of neighborhoods
  - δ neighborhood (set $\{y|(x,y) \leq \delta\}$, where Δ and δ are a distance metric and threshold respectively)
  - k–nearest neighborhood (determined by a fixed number of neighbors)
- Goal is to minimize the size of the boundary region when feature subset B is used



OFS–Density [ZHLW19a]

- New neighborhood relationship is defined
  - All neighbors of x are sorted by distance (nearest to farthest) on feature subset B
  - Pairwise distance between consecutive points in this set is computed
  - For some neighbor x_k (Inflection Point), pairwise distance decreases for the first time
  - The samples between x and x_k are used as the nearest neighbors of x

OFS–Density [ZHLW19a]

- At time t feature f_t arrives, while S_{t-1} is the set of selected candidate features
- The goal is to select features from $S_{t-1} \cup \{f_t\}$ with
  - High correlation
    - Calculate dependency, $\gamma_{f_t}(D)$ of f_t with target class label D
    - Calculate the mean $R(S_{t-1}, D)$ of dependency values $\forall f_j \in S_{t-1}$
    - Discard f_t if the dependency of f_t is less than $R(S_{t-1}, D)$
  - High dependency
    - If $\gamma_{S_{t-1} \cup \{f_t\}}(D) \geq \gamma_{S_t}$ add f_t to S_{t-1}
  - Low redundancy
    - Discard all features f_j in S_t for which $\gamma_{S_t}(D) - \gamma_{S_t - f_j}(D) = 0$
    - In practise, the equality constraint is relaxed to an interval restriction

Sparse Online Learning

- Goal: learn sparse linear classifier from sequence of high–dimensional training instances
- Number of features used by model must be given

Training: data instances arrive sequentially to iteratively update classifier function
Testing: same final selected features used for classification

Online Feature Selection (OFS) [WZHJ13]

- Setting: Binary classification, where each data instance $\mathbf{x}_t$ is to be classified by a linear function $sgn(\mathbf{w}^\top \mathbf{x}_t)$.
  - Full vector is available for each data instance
- Goal: design effective strategy for OFS under constraint that classifier w_t has at most B nonzero elements, $||\boldsymbol{w}_t|| \leqslant B$
  - At most B features of $\mathbf{x}_t$ are used for classification
  - Simply truncating features with small weights can lead to many misclassifications

Online Feature Selection (OFS) [WZHJ13]

Algorithm 3 OFS via Sparse Projection. (**OFS**)

1: **Input**
- λ: regularization parameter
- η: step size
- B: the number of selected features

2: **Initialization**
- $\mathbf{w}_1 = 0$

3: **for** $t = 1, 2, \ldots, T$ **do**
4: Receive $\mathbf{x}_t$
5: Make prediction $\text{sgn}(\mathbf{w}_t^\top \mathbf{x}_t)$
6: Receive y_t
7: **if** $y_t \mathbf{w}_t^\top \mathbf{x}_t \leq 1$ **then**
8: $\widetilde{\mathbf{w}}_{t+1} = (1 - \lambda\eta)\mathbf{w}_t + \eta y_t \mathbf{x}_t$
9: $\widehat{\mathbf{w}}_{t+1} = \min\{1, \frac{\frac{1}{\sqrt{\lambda}}}{\|\widetilde{\mathbf{w}}_{t+1}\|_2}\}\widetilde{\mathbf{w}}_{t+1}$
10: $\mathbf{w}_{t+1} = Truncate(\widehat{\mathbf{w}}_{t+1}, B)$
11: **else**
12: $\mathbf{w}_{t+1} = (1 - \lambda\eta)\mathbf{w}_t$
13: **end if**
14: **end for**

- A linear classifier $\mathbf{w}_t$ is trained online with at most B non–zero elements
- When a training instance $(\mathbf{x}_t, y_t)$ is misclassified, the classifier is first updated by online gradient descent and then projected to a $L1$ ball to ensure that the norm of the classifier is bounded
- If $\widehat{\mathbf{w}}_{t+1}$ has more than B non–zero elements, only the B elements with the largest absolute weight are retained

Online Feature Selection (OFS) [WZHJ13]

- Challenge: Although only B weights are non–zero, every attribute in $\mathbf{x}_t$ must be measured and computed
- Solution: B out of all d attributes are randomly selected for a number of training data instances, while for the remaining data instances, the B attributes for which the classifier $\mathbf{w}_t$ has non–zero values are selected

```
for t = 1, 2, ..., T do
  Sample Z_t from a Bernoulli distribution with probability ε.
  if Z_t = 1 then
    Randomly choose B attributes C_t from [d]
  else
    Choose the attributes that have non-zero values
    in w_t, i.e., C_t = {i : [w_t]_i ≠ 0}
  end if
  Receive x̃_t by only requiring the attributes in C_t
  Make prediction sgn(w_t^⊤ x̃_t)
  Receive y_t
  if y_t w_t^⊤ x̃_t ≤ 1 then
    Compute x̂_t as
```

$$[\widehat{\mathbf{x}}_t]_i = \frac{[\widetilde{\mathbf{x}}_t]_i}{\frac{B}{d}\epsilon + I([\mathbf{w}_t]_i \neq 0)(1-\epsilon)}, i = 1, \ldots, d$$

```
    w̃_{t+1} = w_t + y_t η x̂_t
    ŵ_{t+1} = min{1, R / ||w̃_{t+1}||_2} w̃_{t+1}
    w_{t+1} = Truncate(ŵ_{t+1}, B)
  else
    w_{t+1} = w_t
  end if
end for
```

Second–order Online Feature Selection (SOFS) [WHMY17]

- Main drawback for OFS is its linear time complexity wrt feature dimensionality
- Goal: improve performance and time complexity using second–order online learning techniques
- Main idea: use confidence–weighted (CW) method [DCP08]
  - Assume that weight vector of linear classifier follows Gaussian distribution
  - Based on observed training example $(\mathbf{x}^t, y^t)$, CW updates mean vector and covariance matrix of Gaussian distribution
  - Ensure that probability of correct prediction on observed training example is bigger than specified threshold τ while staying close to previous distribution

$$(\hat{\boldsymbol{\mu}}^{t+1}, \Sigma^{t+1}) = \arg\min_{\boldsymbol{\mu},\Sigma} \mathsf{D}_{\mathsf{KL}}(\mathcal{N}(\boldsymbol{\mu}, \Sigma), \mathcal{N}(\boldsymbol{\mu}^t, \Sigma^t))$$
$$\text{s.t. } \Pr[y^t sgn(\mathbf{w} \cdot \mathbf{x}^t) \geqslant 0] \geqslant \tau$$

Second–order Online Feature Selection (SOFS) [WHMY17]

- Kullback–Leibler (KL) divergence can be easily computed in terms of mean vectors and covariance matrices
- Solve optimization problem with adaptive regularization of the prediction function (AROW) for each new observed training example [CKD13]
- Update most confident B weight variables, whose covariance values Σ_{jj} are among the B smallest
- MeanHeap–based implementation to store B smallest diagonal values of covariance matrix Σ^t
- SOFS has linear time complexity wrt average number of nonzero features per instance

Group–SAOLA [YWDP16]

- Goal: select (in an online manner) feature groups which are sparse at the levels of both features and groups simultaneously
  - Extension of SAOLA for streaming features arriving in groups
- Feature groups appear in a sequential order, one at a time
  - Must optimize selections within each group, as well as between groups

Group–SAOLA [YWDP16]

- Extends notion of relevance to groups:
  - irrelevant: $I(C; G_i) = 0$
    - simplified as $I(C; F_i) \leq \delta, \forall F_i \in G_i$
  - redundant: $I(C; G_i | G \setminus G_i) = 0$
    - simplified as $I(F_j; C) > I(F_i; C)$ and $I(F_j; F_i) \geq I(F_i; C)$ $\forall F_i \in G_i, \exists F_j \in G_j$, where $G_j \in \Psi_{t_i}$, the set of groups selected at time t_{i-1}
- Defines intra–group feature redundancy
  - redundant: $I(C; F_i | S) = 0$ for some $S \subset G_i \setminus \{F_i\}$
    - simplified as $I(Y; C) > I(F_i; C)$ and $I(F_i; Y) \geq I(F_i; C)$ for some $Y \in G_i$

Group–SAOLA [YWDP16]

/*Evaluate irrelevant groups*/
if $\forall F_i \in G_i, I(F_i;C) \leq \delta$ **then**
  Discard G_i;
  Go to Step 39;
end if

Determine the **relevance** of group G_i to class label C

/*Evaluate feature redundancy in G_i*/
for j=1 to $|G_i|$ **do**
  if $\exists Y \in \{G_i - \{F_j\}\}, I(Y;C) > I(F_j;C)$ & $I(Y;F_j) \geq I(F_j;C)$ **then**
    Remove F_j from G_i;
    Continue;
  end if
  /*Otherwise*/
  if $I(F_j;C) > I(Y;C)$ & $I(F_j;Y) \geq I(Y;C)$ **then**
    Remove Y from G_i;
  end if
end for

Identify **redundant** features **within** group G_i

/*Evaluate group redundancy in $\{\Psi_{t_{i-1}} \cup G_i\}$*/
for j=1 to $|\Psi_{t_{i-1}}|$ **do**
  if $\exists F_k \in G_j \subset \Psi_{t_{i-1}}, \exists F_i \in G_i, I(F_i;C) > I(F_k;C)$ & $I(F_i;F_k) \geq I(F_k;C)$ **then**
    Remove F_k from G_j;
  end if
  /*Otherwise*/
  if $I(F_k;C) > I(F_i;C)$ & $I(F_k;F_i) \geq I(F_i;C)$ **then**
    Remove F_i from G_i;
  end if
  if G_j is empty **then**
    $\Psi_{t_{i-1}} = \Psi_{t_{i-1}} - G_j$;
  end if
  if G_i is empty **then**
    Break;
  end if
end for

Identify **redundant** groups and features from the currently selected groups

Instance–wise Feature Selection

Problem Definition

- Informative features may vary by data instance (e.g., heart failure prognosis across subpopulations [KLA+15])
- Ease of interpretation of popular but complex machine learning models
- Goal: identify small number of relevant features that explain machine learning model output for each data instance individually during testing

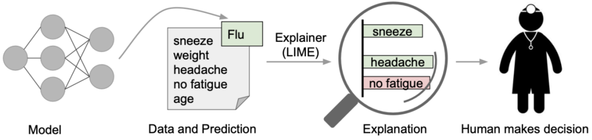
Training: all candidate features are available upfront
Testing: different (fixed or varying) number of features are selected for each data instance and used for model interpretation

Instance–wise Feature Selection

- Representative methods include:
  - SHAP [LL17]
  - L2X [CSWJ18]
  - INVASE [YJVdS18]
  - Mixture of Deep Neural Networks [XW19]
  - Instance–wise Feature Grouping [MWZ+20]
  - GroupFS [XLTW22]
  - DIWIFT [LCZ+23]
- Challenges:
  - Access to all features of test instance is needed before selecting relevant subset
  - Scalability issues for large feature spaces

A Unified Approach to Interpreting Model Predictions [LL17]

- Numerous model interpretability methods, but unclear how they are related or how to choose one over another



- Goal: unified framework for interpreting predictions
  - new class of additive feature importance measures unifying six existing methods
  - theoretical results showing the existence of a unique solution for this class with a set of desirable properties

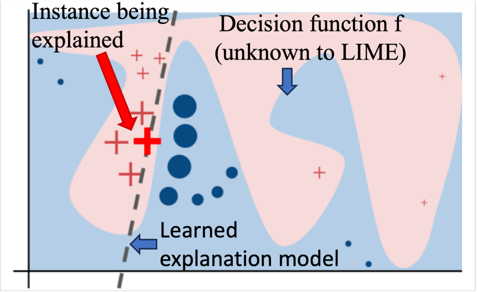
Figure source: LIME [RSG16]

A Unified Approach to Interpreting Model Predictions [LL17]

- Let f be the prediction model to be explained, and g the explanation model
- Explanation models use simplified vectors x' that map to the original instances through a mapping function $x = h_x(x')$
  - Local methods (e.g., LIME [RSG16]) explain $f(x), \forall$ data instance x
    - Try to ensure $g(z') \approx f(h_x(z'))$ whenever $z' \approx x'$
- Additive feature attribution methods use a linear function of binary variables, i.e., $g(z') = \phi_0 + \sum_{i=1}^{M} \phi_i z'_i$, where $z' \in \{0, 1\}$, M is the number of simplified input features, and $\phi \in \mathbb{R}$, as explanation model
  - Each feature i is attributed effect ϕ_i
  - The effects of all feature attributions are summed up to approximate $f(x)$

Example Additive feature attribution method: LIME [LL17]

- LIME samples instances, gets predictions using f, and weighs them by the proximity to the instance being explained
- Interprets individual model predictions by locally approximating f



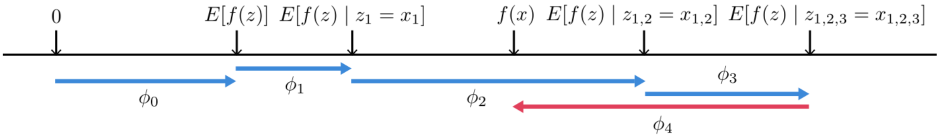
- Mapping h_x depends on input type
  - For bag of words, converts a vector of 1's or 0's into word counts if $x' = 1$, or 0 if $x' = 0$
  - For images, a set of super pixels is used; if $x' = 1$ the super pixel's original value is used, and the average of neighboring pixels is used otherwise

Classic Shapley Value Estimation [LL17]

- Shapley regression
  - Feature importance for linear models in the presence of multicollinearity
  - Model is trained on all feature subsets $S \subseteq F$
  - Importance value represents the effect on the model prediction of including that feature
  - Computationally expensive!
- Shapley sampling
  - Sampling approximations
  - Approximating the effect of removing a variable from the model by integrating over samples from the training dataset
  - Eliminates the need to retrain the model and allows fewer than $2^{|F|}$ differences to be computed
- Quantitative input influence
  - Nearly identical to Shapley sampling values

SHAP (SHapley Additive exPlanation) Values [LL17]

- Shapley values of a conditional expectation function of model f
  - Obtained by solving for the only one possible explanation model g
- Mapping, $h_x(z') = z_S$, where z_S has missing values for features not in the set S
  - Since most models cannot handle arbitrary patterns of missing input values, $f(z_S)$ is approximated with $E[f(z)|z_S]$



- Sample explanation of how to get from the base value $E[f(z)]$ (if we did not know any features to the current output), using feature x_1, features x_1 and x_2 etc
- When the model is non–linear or features are not independent, the order in which features are added to the expectation matters
  - SHAP values arise from averaging the ϕ values across all possible orderings!

SHAP (SHapley Additive exPlanation) Values [LL17]

- Why only one possible explanation model g?
  - Two properties in addition to local accuracy
    - Missingness: constrains features where $x'_i = 0$ to have no attributed impact
    - Consistency: if a model changes so that some simplified input's contribution increases (or stays the same regardless of the other inputs), that input's attribution does not decrease
  - Values $\phi_i(f, x) = \sum_{z' \subseteq x'} \frac{|z'|!(M - |z'| - 1)!}{M!}[f_x(z') - f_x(z' \setminus i)]$ derived using combined cooperative game theory
    - $|z'|$ is the number of non–zero entries in z', and $z' \subseteq x'$ represents all z' vectors where the non–zero entries are a subset of the non–zero entries in x'
- Exact computation of SHAP values is challenging
  - Model–agnostic approximation methods (Shapley sampling and Kernel SHAP)
  - Model–type–specific approximation methods (Max SHAP, Deep SHAP)
  - Feature independence and model linearity to simplify the computation of expected values

Learning to Explain (L2X) [CSWJ18]

- Goal: maximize mutual information between response variable of model and selected features, as function of choice of selection rule

$$\max_{\mathcal{E}} I(X_S; Y) \quad \text{subject to} \quad S \sim \mathcal{E}(X)$$

  - Hyperparameter k : represents number of explaining features
  - Applicable to classification/regression
- Solution: variational approximation
  - Derive lower bound on mutual information
  - Approximate model distribution conditioned on feature subset by rich family of functions

Learning to Explain (L2X) [CSWJ18]

- Relaxed problem

$$\max_{\mathcal{E},\mathbb{Q}} \mathbb{E}\left[\log \mathbb{Q}_S(Y|X_S)\right] \quad \text{subject to} \quad S \sim \mathcal{E}(X)$$

- Main idea:
  - Continuous approximation of feature subset sampling leads to

$$\max_{\theta,\alpha} \mathbb{E}_{X,Y,\zeta}\left[\log g_\alpha(V(\theta,\zeta) \odot X, Y)\right],$$

    where g_α is neural network that approximates model conditional distribution and θ parameterizes explainer
  - Learned explainer maps each data instance X to weight vector $w_\theta(X)$
  - Features X for specific data instance ranked based on $w_\theta(X)$
  - Keep k features with largest weights for explanation

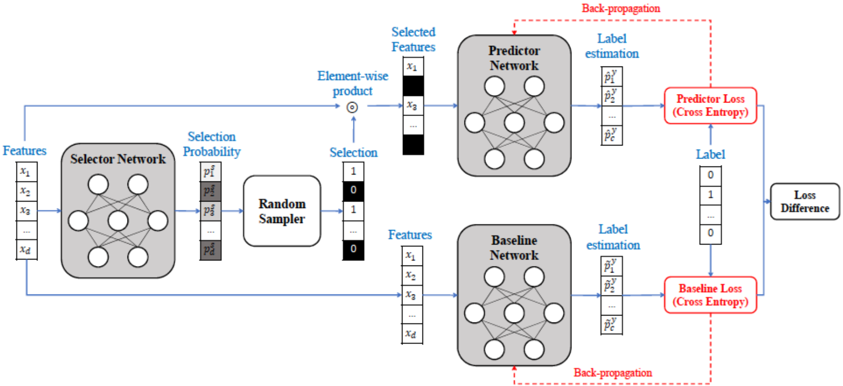
INstance-wise VAriable SElection (INVASE) [YJVdS18]

- Goal: minimize KL divergence between conditional distributions $Y|X$ and $Y|X_S$ inducing sparsity using an ℓ_0 penalty term

$$\min_{S(\cdot)} \mathbb{E}_{\mathbf{x}\sim p_X}\left[\mathsf{KL}(Y|\mathbf{X}=\mathbf{x} \;||\; Y|\mathbf{X}^{S(\mathbf{x})}=\mathbf{x}^{S(\mathbf{x})}) + \lambda||S(\mathbf{x})||\right]$$

- Solution: actor–critic architecture with three neural networks
  - Use baseline network for variance reduction
  - Use predictor network to provide reward to selector network

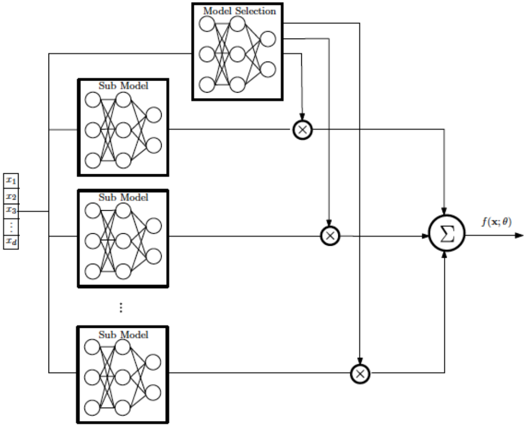
INstance-wise VAriable SElection (INVASE) [YJVdS18]



- Different number of relevant variables are selected for each data instance
- Can be used also for feature selection and prediction tasks

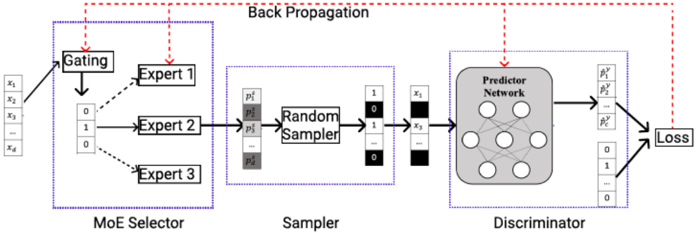
Mixture of Deep Neural Networks [XW19]

- L2X and INVASE do not constrain search space for each data instance
- Mixture of Deep Neural Networks [XW19] limits number of possible relevant feature subsets to K
  - Each data instance $\mathbf{x}$ has unique relevant feature subset
  - Identify which model (model selector neural network) out of K (feature subset selector neural networks) data instance comes from
  - Select most relevant feature subject based on model sensitivity's magnitude



Group FS [XLTW22]

- Each data instance may be associated with different set of relevant features
- Hard to understand feature importance pattern for entire data distribution
- INVASE + K–means:
  - Train instance–wise feature selector for each data instance
  - Apply K–means clustering to all feature selectors
  - Assigned cluster center is group–wise feature selector
- Mixture of Experts selector:



DIWIFT [LCZ+23]

- Feature–level influence function: influence of perturbation $(\mathbf{x}_i, y_i) \to (\mathbf{x}_i + \boldsymbol{\delta}_i, y_i)$ on loss
- Base pre–trained model w/o feature selection
- Self–attention network outputs instance–wise feature selection probabilities
- Compute influence function