Learning to Label Graph with Kernel Methods

Hongyu Su

Department of Information and Computer Science
Aalto University, School of Science and Technology
hongyu.su@aalto.fi

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Outline

Ensemble Learning
- Bagging
- Boosting

Multi-Label/Task Classification
- via Single-Task Classifier
- Multi-Task Feature Learning
- Max-Margin Conditional Random Field

What is Ensemble System?

- Classical learning approach
  - Choose a model class (Bayesian, Random Field, Max-Margin, etc.)
  - Fit a single model to training data.
  - Predict on test data.
- An ensemble system
  - Choose a model class
  - Construct multiple models on training data (base learners)
  - Generate predictions on test data (base hypotheses)
  - Combine the predictions
- The idea of *ensemble learning* is to employ multiple learners, that do better than coin-toss, to get more accurate prediction.

Ensemble Methods

- Manipulating the training examples
  - Multiple weak hypotheses are generated by training individual classifier on different datasets obtained from common training data.
  - Bagging: sampling
  - Boosting: reweighting
- Manipulating the output target
  - The output targets are encoded with a bit vector, and individual base learner is trained to predict each of the bit in the code word.
  - Error-correcting code [Ghani, 2000]
- Manipulating the input features: random subspace method [Ho, 1998]
- Modifying the learning parameters

Bootstrap aggregating (bagging) [Breiman, 1994]

- Basic idea: Build different experts and let them vote for the finial prediction
- Sample N training examples from the total N, with replacement. The selecting probability for individual example is $\frac{1}{N}$.
  - Original dataset $\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), (x_5, y_5)\}$
  - Bootstrap dataset $\{(x_1, y_1), (x_3, y_3), (x_3, y_3), (x_5, y_5), (x_5, y_5)\}$

Bootstrap aggregating (bagging)

Algorithm Framework

Algorithm 1 Bagging

Require: Required ensemble size T, Training dataset $S = \{(x_1, y_1), \cdots, (x_N, y_N)\}$

1: **for** $t = 1$**to** T **do**

2: Build a dataset S_t by sampling N items, uniform at random with replacement from S

3: Train a weak hypothesis h_t by S_t, and add it to ensemble collection

4: **end for**

5: For a new testing point (x', y')

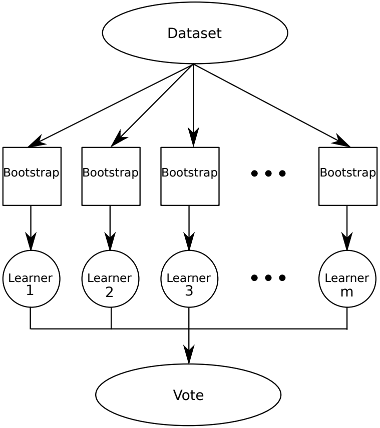
6: Get predictions from ensemble components.

7: Combine predictions to get a finial prediction.

Bootstrap aggregating (bagging) (cont.)

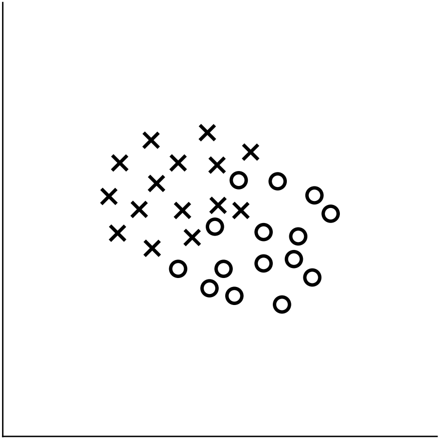
Algorithm Framework

- Diagram



Bootstrap aggregating (bagging)

Example



Bootstrap aggregating (bagging)

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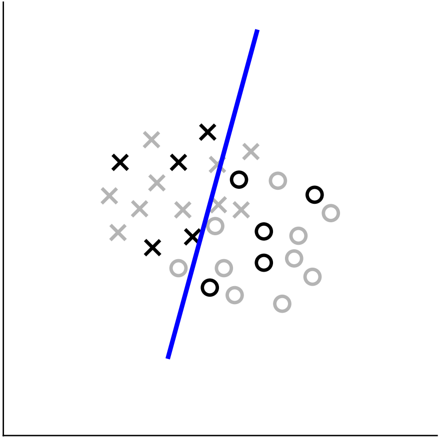
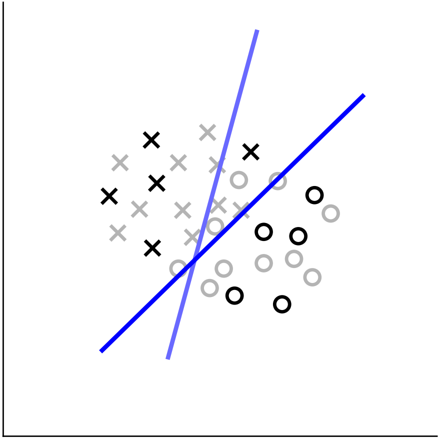


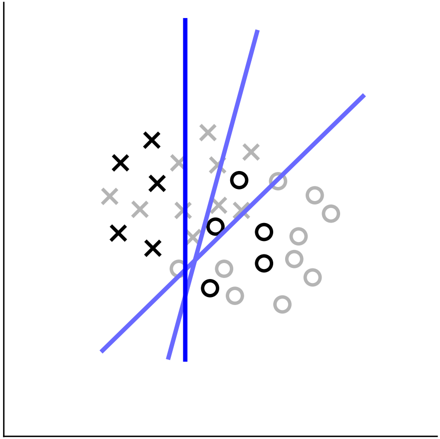
Bootstrap aggregating (bagging)

Example



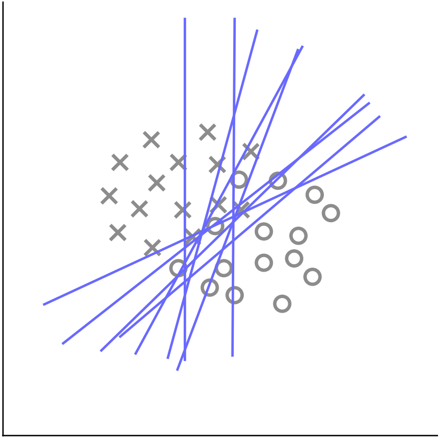
Bootstrap aggregating (bagging)

Example



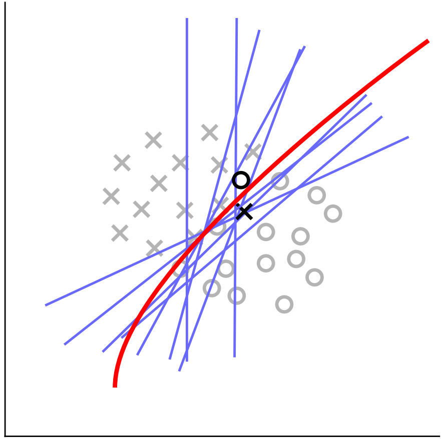
Bootstrap aggregating (bagging)

Example



Bootstrap aggregating (bagging)

Example



Bootstrap aggregating (bagging)

Why bagging works?

- Suppose there are 25 base learners
- Each has an error rate $\eta = 0.35$
- Assume independence among classifiers
- Probability that the ensemble makes a mistake

$$\sum_{i=13}^{25} \binom{25}{i} \eta^i (1-\eta)^{25-i} = 0.06$$

Bootstrap aggregating (bagging)

Bias-Variance Decomposition

- Error of learning algorithm on example x comes from three source
  - Noise, measure error / uncertainty for true label of x
  - Bias, how close/good, is the algorithm to optimal prediction
  - Variance, how much does prediction change if when training data change
- Error can be decomposed as:

$$error(x) = noise(x) + bias(x) + variance(x)$$

- Bias-variance trade-off
  - high bias $\mapsto$ low variance
  - low bias $\mapsto$ high variance

Bootstrap aggregating (bagging) (cont.)

Bias-Variance Decomposition

- Averaging can decrease variance while have the same bias

$$Var(\hat{x}) = \frac{Var(x)}{N}$$

- Bagging can be viewed as averaging.
- Bagging typically helps
  - Over-fitted base model: high variance & low bias
  - Unstable model: highly dependent on training data (decision tree, KNN, etc)

Boosting

- Boosting:
  - Base learner is just better than random prediction(coin toss)
  - Incrementally build an ensemble.
  - Each new model instant emphasizes the training instances that previous model misclassified.
- Adaptive Boosting (Adaboost) (■ See additional material) [Freund, 1992, Schapire and Singer, 1998]
- Boosting can:
  - Reduce variance, like bagging
  - Eliminate the effect the high bias of the weak learner [Freund and Schapire, 1996]

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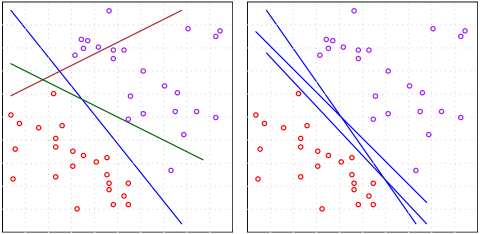
Support Vector Machine Revisit

- Learning Task
  - Single task, binary classification
  - m examples $\{(x_1, y_1), \cdots, (x_m, y_m)\}, x_i \in \mathcal{R}^d, y_i \in \{+, -\}$
- Linear separator of the form $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$
- Principal:*Empirical risk minimization*
  - minimize training error
- Hyperplanes with same empirical risk



Support Vector Machine Revisit

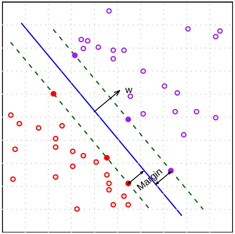
Max-Margin Hyperplane

- Maximum margin hyperplane (hard-Margin).
  - Robustness: small perturbation in training data does not change the classification
  - Performance: a large margin leads to low error on unseen data
- Hard-Margin SVM takes the form:

$$(\mathbf{w}, b) = \underset{\mathbf{w},b}{\mathbf{argmin}} \frac{1}{2}||\mathbf{w}||^2,$$

$$\text{s.t. } y_i\,(\mathbf{w}^T\mathbf{x}_i + b) \geq 1,$$

$$1 \leq i \leq n.$$



Support Vector Machine Revisit

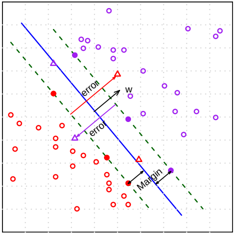
Soft-Margin SVM [Cortes and Vapnik, 1995]

- In practice, training data cannot be perfectly classified by a hyperplane
- Soft-Margin hyperplane allows training points to have smaller margin, subject to a penalty ξ
- Soft-Margin SVM takes the form

$$(\mathbf{w}, b) = \underset{\mathbf{w},b}{\mathbf{argmin}} \left(\frac{1}{2}||\mathbf{w}||^2 + C \sum_{i=1}^{m} \xi_i \right),$$

$$\text{s.t. } y_i \left(\mathbf{w}^T \mathbf{x}_i + b \right) \geq 1 - \xi_i,$$

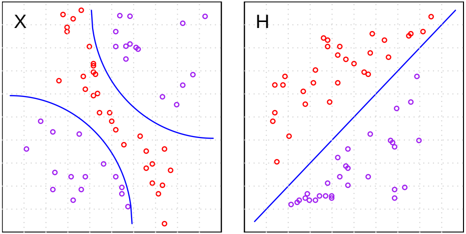
$$\xi_i \geq 0,\ 1 \leq i \leq n.$$



Support Vector Machine Revisit

Non-linear SVM

- Training data is not linear separable.



- Map data to high dimensional space $\mathcal{H}$,
  $\mathbf{x}_i = (x_1, x_2, \cdots, x_n) \xrightarrow{\varphi} \varphi(\mathbf{x}_i) = (\varphi_1, \varphi_2, \cdots, \varphi_k)$.

Support Vector Machine Revisit (cont.)

Non-linear SVM

- Dual is given by

$$
\begin{aligned}
\tilde{\mathcal{L}}(\alpha) &= \sum_{i=1}^{n} \alpha_i - \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j (\varphi(\mathsf{x}_i) \cdot \varphi(\mathsf{x}_j)) \\
&= \sum_{i=1}^{n} \alpha_i - \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathsf{x}_i, \mathsf{x}_j)
\end{aligned}
$$

- kernel trick: mapping observation to inner product space without computing the mappping explicitly.
- Example

Support Vector Machine Revisit (cont.)

Non-linear SVM

- Assume we have variables X and Y in n dimensional feature space $X, Y \in \mathbb{R}^n$

$$\phi(X) = (x_1, \ldots, x_n) \tag{1}$$
$$\phi(Y) = (y_1, \ldots, y_n) \tag{2}$$

Linear kernel corresponds to a dot product denoted by

$$K_{linear}(X, Y) = \phi(X) \cdot \phi(Y) \tag{3}$$
$$= \sum_i^n x_i y_i \tag{4}$$

A more interesting kernel can be constructed by constructing a kernel from two different feature sets $\phi_A(X) \in \mathbb{R}^a$ and

Support Vector Machine Revisit (cont.)

Non-linear SVM

$\phi_B(X) \in \mathbb{R}^b$. We can combine the two feature sets into $a+b$ dimensional vector $\phi_{A,B}(X) = [\phi_A(X), \phi_B(X)]$ and computing the kernel $K_{A,B}(X,Y)$ directly as $\phi_{A,B}(X) \cdot \phi_{A,B}(Y)$.
However, by definition $K_A(X,Y) + K_B(X,Y) = K_{A,B}(X,Y)$.
Thus, we can either concatenate features before hand and then compute a single kernel, or compute the individual kernels and sum them.
By taking an element-wise product $K_A \cdot K_B$ between kernels K_A and K_B we get features of type $\phi_A(X)_i \phi_B(X)_j$ for all $i \in [1, \ldots, a]$ and $j \in [1, \ldots, b]$.
For quadratic kernels, we have

Support Vector Machine Revisit (cont.)

Non-linear SVM

$$
\begin{aligned}
K_{quadratic}(X, Y) &= (K_{linear}(X, Y) + C)^2 && (5)\\
&= \left(\sum_{i}^{n} x_i y_i + C\right)^2 && (6)\\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j y_i y_j + 2\sum_{i=1}^{n} x_i y_i + C^2 && (7)\\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j y_i y_j + \sum_{i=1}^{n} \sqrt{2} x_i \sqrt{2} y_i + C^2 && (8)\\
&= \phi'(X) \cdot \phi'(Y), && (9)
\end{aligned}
$$

where the expanded feature spaces $\phi'(X)$ and $\phi'(Y)$ are

Support Vector Machine Revisit (cont.)

Non-linear SVM

$$\phi'(X) = (x_1x_1, \ldots, x_1x_n, x_2x_1, \ldots, x_nx_n; \sqrt{2}x_1, \ldots, \sqrt{2}x_n, C) \tag{10}$$

$$\phi'(Y) = (y_1y_1, \ldots, y_1y_n, y_2y_1, \ldots, y_ny_n; \sqrt{2}y_1, \ldots, \sqrt{2}y_n, C) \tag{11}$$

Structured Multi-Task Classification

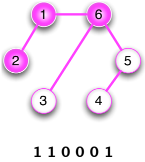
- m training data $\{(x_i, \mathbf{y}_i)\}_{i=1}^m$
- d dimension feature representation for each example $x \in \mathcal{R}^d$
- T targets/labels, $\mathbf{y} \in \{+,-\}^T$
- General form:

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x_{i1}} & \mathbf{x_{i2}} & \dots & \mathbf{x_{id}} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \dots & x_{md} \end{bmatrix}, \quad Y = \begin{bmatrix} y_{11} & y_{12} & \dots & y_{1T} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{y_{i1}} & \mathbf{y_{i2}} & \dots & \mathbf{y_{iT}} \\ \vdots & \vdots & \ddots & \vdots \\ y_{m1} & y_{m2} & \dots & y_{mT} \end{bmatrix}$$

$$x_j = \begin{pmatrix} x_{j1} & x_{j2} & \dots & x_{jm} \end{pmatrix}, \qquad y_j = \begin{pmatrix} ? & ? & \cdots & ? \end{pmatrix}$$

Structured Multi-Task Classification (cont.)

- Output graph: a structure $\mathcal{G} = (E, V)$ on multiple targets
  - A node $v \in V$ corresponds to target/label
  - An edge $e \in E$ represents dependency between pair of targets
- A prediction of multiple targets/labels can be seen as a labeling of the output graph.

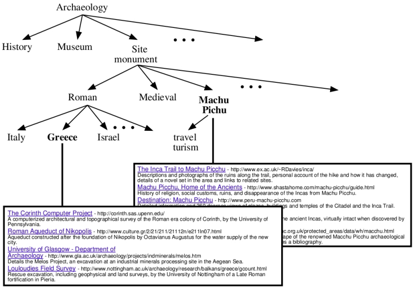


$\mathbf{y} = (y_1, y_2, y_3, y_4, y_5, y_6)$

Application Areas

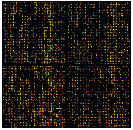
- Hierarchical document classification [Veeramachaneni et al., 2005, Rousu et al., 2006a]

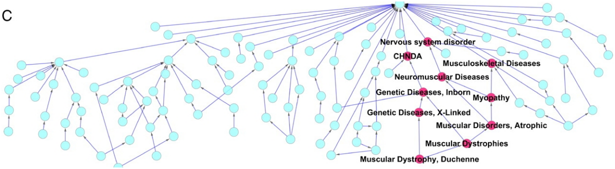
Given news articles x and the classification hierarchy $\mathcal{G}$, predict the multiple categories of the new article.



Application Areas (cont.)

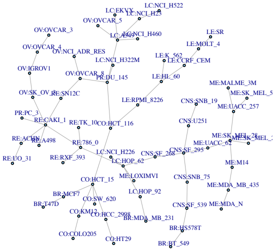
- Medical diagnosis [Huang et al., 2010]
  Given microarray profile of tissue sample x and the disease hierarchy $\mathcal{G}$, predict multiple labels in the hierarchy.



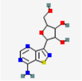


Application Areas (cont.)

- Drug bioactivity prediction [Su et al., 2010]
  Given molecular structure x and relation of cancer cell lines, predict the anti-cancer potentials of the molecules.



$$x \xrightarrow{\textit{predict}} \mathbf{y} = \{y_1, y_2, \cdots, y_{60}\}, y_i \in \{0, 1\}.$$



1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	0	1	1	1	1	0	1	1	1	1
1	1	1	0	1	1	1	0	1	1	1	1	0	1	1
1	1	1	1	1	1	1	1	0	1	1	1	1	1	1

blocks correspond to cell lines

A Collection of Single-Task Classifiers

- Reduce multiple tasks to a a bag of single takes and solved by a collection of single-task classifiers (e.g. SVM)

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{i1} & x_{i2} & \dots & x_{im} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nm} \end{bmatrix}, \quad Y = \begin{bmatrix} y_{11} & y_{12} & \dots & y_{1k} \\ \vdots & \vdots & \ddots & \vdots \\ y_{i1} & y_{i2} & \dots & y_{ik} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n1} & y_{n2} & \dots & y_{nk} \end{bmatrix}$$

$$\{y_1, y_2, \cdots, y_T\} = F(x)$$

- Drawbacks:
  - Train a collection of classifiers separately
  - Assume tasks are independent

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$$\{y_1, \cdots, \cdots, \cdots\} = \{\mathbf{f_1}(\mathbf{x}), \cdots, \cdots, \cdots\}$$

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$$\{\cdots, y_2, \cdots, \cdots\} = \{\cdots, \mathbf{f_2}(\mathbf{x}), \cdots, \cdots\}$$

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$$\{\cdots, \cdots, y_j, \cdots\} = \{\cdots, \cdots, \mathbf{f_j}(\mathbf{x}) \cdots\}$$

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$$\{\cdots, \cdots, \cdots, y_T\} = \{\cdots, \cdots, \cdots, \mathbf{f_T}(\mathbf{x})\}$$

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Multi-Task Feature Learning [Argyriou et al., 2007]

- Sparse dimensionality reduction
  - Sparse PCA
  - Sparse ICA

Multi-Task Feature Learning

- Inspired by sparse modeling.
- Learning multiple related tasks *vs.* learning independently.
- Assumptions:
  - Few data per task, pooling data across related tasks.
  - Common underlying representation across tasks.
  - A small set of shared features across tasks (task relations).

Multi-Task Feature Learning

- Learning Paradigm
  - Task index $t = 1, \cdots, T$
  - m examples for each task $(x_1, y_{t,1}), \cdots, (x_m, y_{t,m}) \in \mathcal{R}^d \times \mathcal{R}$
  - d-dimension features for each example
    $H(x) = h_1(x), \cdots, h_d(x)$
- Predict via a linear function $f_t : \mathcal{R}^d \to \mathcal{R}$ with the form

$$f_t(x) = \sum_{i=1}^{d} a_{i,t} h_i(x)$$

MTL - Coefficient Matrix

- Task specific coefficients can be arranged as a matrix

$$A = \begin{pmatrix} a_{1,1} & \cdots & a_{1,T} \\ \vdots & \ddots & \vdots \\ a_{d,1} & \cdots & a_{d,T} \end{pmatrix}$$

- $a_{i,t}$ reveals feature importance and task organization
- Desiderata
  - a low dimensional data representation shared across tasks (few features)
  - importance of each feature is also preserved across tasks (similar feature weight)

MTL - Regularization

- A should be a matrix with property
  - most elements being zero (sparsity)
  - for task t, $|a_{i,t}|$ being similar (uniformity)
- $(2,1)$-norm regularization

$$||A||_{2,1} = \sum_{i=1}^{d} \sqrt{\sum_{t=1}^{T} a_{i,t}^2}$$

  - first compute l_2 norm of the rows $||\mathbf{a_1}||_2, \cdots, ||\mathbf{a_d}||_2$
  - then compute the sum of result vectors $\sum_{i=1}^{d} ||\mathbf{a_i}||_2$

MTL - Learning Objective

- (2, 1)-norm $||A||_{2,1} = \sum_{i=1}^{d} \sqrt{\sum_{t=1}^{T} a_{i,t}^2}$ to be small
  - small l_2 norm favors uniformity
  - small l_1 norm favors sparsity
- Learning objective function

$$\min \left\{ \sum_{t=1}^{T} \sum_{j=1}^{m} \mathcal{L}(y_{t,j}, \sum_{i=1}^{d} a_{i,t} h_i(x_{t,j})) + \gamma ||A||_{2,1}^2 \right\}$$

  - minimize error ($\mathcal{L}$ is loss function)
  - minimize $||A||_{2,1}^2$
  - the number of features decreases with γ

MTL - Single Task variation

- Single task variation

$$\min \left\{ \sum_{j=1}^{m} \mathcal{L}(y_j, \sum_{i=1}^{d} a_i h_i(x_j)) + \gamma ||\mathbf{a}||_1^2 \right\}$$

  - $||\mathbf{a}_1||$ is l_1 norm, number of non-zero entries of $\mathbf{a}$
  - Many entries will be 0 (sparse model)

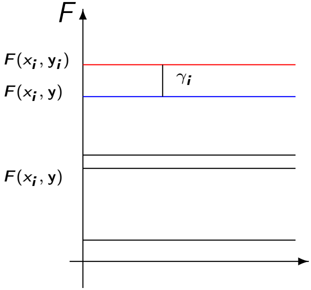
Max-Margin Condition Random Field [Rousu et al., 2006b]

- What is margin
  - Confidence of assigning an example to a label.
- Maximum margin learning
  - Define a compatibility score $F(x_i, \mathbf{y}_i; \mathbf{w})$
  - Define a separation margin for $(x_i, \mathbf{y}_i)$

$$\gamma_i = F(x_i, \mathbf{y}_i; \mathbf{w}) - \max_{\mathbf{y} \neq \mathbf{y}_i} F(x_i, \mathbf{y}; \mathbf{w})$$

  - Maximize the minimum margin

$$\max \min_i \gamma_i$$

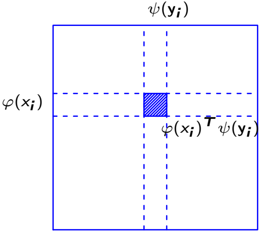


Max-Margin Conditional Random Field

Learning Paradigm

- Learning Paradigm
  - Data from a domain $\mathcal{X} \times \mathcal{Y}$, where $\mathcal{Y} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_k, \mathcal{Y}_j \in \{+1, -1\}$.
    - Training data is given as $\{(x_i, \mathbf{y}_i)\}_{i=1}^n \subset \mathcal{X} \times \mathcal{Y}$.
    - A *pseudo-example* is $(x_i, \mathbf{y})$ where $\mathbf{y}$ is an arbitrary multilabel.
  - Markov network $\mathcal{G} = (\mathcal{E}, \mathcal{V})$ over multiple labels.
- Joint feature map
- Map input and output to a *joint feature map* $\phi(x, \mathbf{y})$:

$$\phi(x, \mathbf{y}) = \varphi(x) \otimes \psi(\mathbf{y}).$$



Max-Margin Conditional Random Field

Compatibility Function

- Model family
  - Exponential family defined on Markov network $\mathcal{G} = (\mathcal{E}, \mathcal{V})$:

$$P(\mathbf{y}|x) = \frac{1}{Z(x, \mathbf{w})} \prod_{e \in \mathcal{E}} \exp(\mathbf{w}_e^T \phi_e(x, \mathbf{y}_e)),$$

    which leads to a log linear model:

$$\log P(\mathbf{y}|x) = \mathbf{w}^T \phi(x_i, \mathbf{y}_i) - \log Z(x, \mathbf{w}).$$

Max-Margin Conditional Random Field (cont.)

Compatibility Function

- Margin-based learning:
  - Use margin-based learning to avoid partition function $Z(\mathbf{w}, x)$
  - Related to odds-ratio learning:

$$\frac{\log P(\mathbf{y}_i|x_i)}{\log P(\mathbf{y}|x_i)} = \mathbf{w}^T\phi(x_i, \mathbf{y}_i) - \mathbf{w}^T\phi(x_i, \mathbf{y})$$

  Maximize the margin between real example $\phi(x_i, \mathbf{y}_i)$ and all the pseudo-example $\phi(x_i, \mathbf{y})$, according to $\ell_\Delta(\mathbf{y}_i, \mathbf{y})$.

- Compatibility Function

$$F(x_i, \mathbf{y}_i; \mathbf{w}) = \mathbf{w}^T\phi(x_i, \mathbf{y}_i)$$

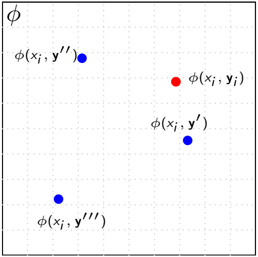
Max-Margin Conditional Random Field

Maximum Margin Learning

- Maximize the margin of difference in compatibility score between correct pair and incorrect pair
- Optimization problem (quadratic programming)

$$(\mathbf{w}) = \underset{w,\xi \geq 0}{\mathbf{argmin}} \left(\frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1}^{n} \xi_i \right)$$

$$\text{s.t. } \mathbf{w}^T \phi(x_i, \mathbf{y}_i) - \mathbf{w}^T \phi(x_i, \mathbf{y}) \geq \ell_\Delta(\mathbf{y}_i, \mathbf{y}) - \xi_i, \ \forall x_i, \mathbf{y}.$$



Max-Margin Conditional Random Field

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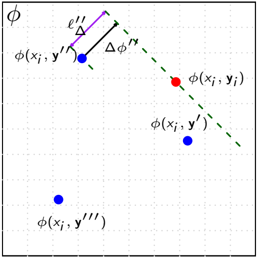
$$\textbf{s.t. } \mathbf{w}^T\phi(x_i,\mathbf{y}_i) - \mathbf{w}^T\phi(x_i,\mathbf{y}) \geq \ell_{\Delta}(\mathbf{y}_i,\mathbf{y}) - \xi_i,\ \forall x_i, \mathbf{y}.$$



Max-Margin Conditional Random Field

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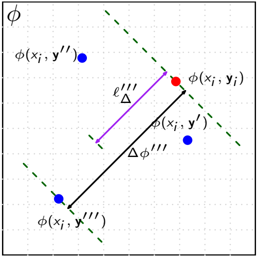
$$

$$
\textbf{s.t. } \mathbf{w}^T \phi(x_i, \mathbf{y}_i) - \mathbf{w}^T \phi(x_i, \mathbf{y}) \geq \ell_\Delta(\mathbf{y}_i, \mathbf{y}) - \xi_i, \ \forall x_i, \mathbf{y}.
$$



Max-Margin Conditional Random Field

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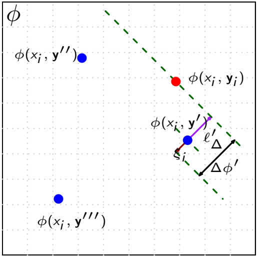
$$\geq \ell_\Delta(\mathbf{y}_i, \mathbf{y}) - \xi_i,\ \forall x_i, \mathbf{y}.$$



- Maximize the margin of difference in compatibility score between correct pair and incorrect pair
- Optimization problem (quadratic programming)

$$(\mathbf{w}) = \underset{w,\xi \geq 0}{\mathbf{argmin}} \left(\frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1}^{n} \xi_i \right)$$

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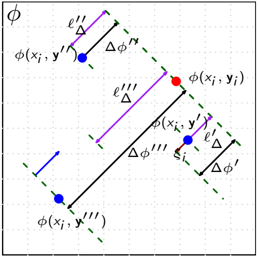

Max-Margin Conditional Random Field

Prediction

- Prediction is made by

$$\mathbf{y}^* = \underset{\mathbf{y} \in \mathcal{Y}}{\mathbf{argmax}}\, \mathbf{w}^T \phi(x_i, \mathbf{y}_i)$$

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