A TUTORIAL ON CONDITIONAL RANDOM FIELDS

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Contents

The supervised classification problem

Goal: predict *labels* y (aka *classes* or *outputs*) for some *observations* o (aka *data points*, *inputs*).

Examples:

- Predict *translation/part-of-speech tag* for a word.
- Predict *instrument*, *chord*, *notes* played... for a music segment.

Supervised classification:

- Each observation o is supposed to pertain to a **predefined** class $\mathcal{C}_k$: the k-th (**discrete**) class of a classification problem; $k = 1, \cdots, K$.
- This is represented using a label y for each o; $y \in \mathcal{Y}$, e.g. $\mathcal{Y} = \{0, 1\}$, $\mathcal{Y} = \{1, 2, 3, ..., K\}$.

Examples of classes:

- **POS tags:** *noun, verb, adjective...*
- **Music chords:** $C7$, $Gmaj7$, $Fmin7$...

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- **POS tags:** *noun, verb, adjective...*
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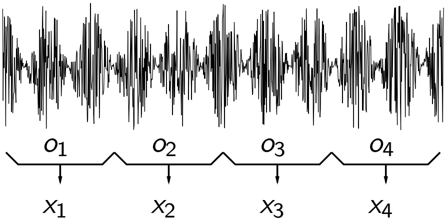
Features

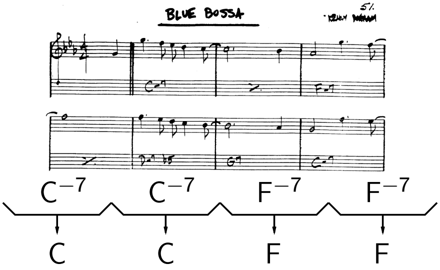
- Classification relies on **features** x: descriptors of some qualities/ attributes of the inputs o. Two types of features:

Continuous features



real-valued: *e.g. MFCC, chroma, tempo...*

Discrete/categorical



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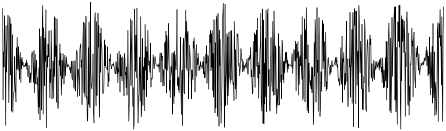

o_1 o_2 o_3 o_4

x_1 x_2 x_3 x_4

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C^{-7} C^{-7} F^{-7} F^{-7}

C C F F

symbolic: *e.g. note/chord played, key...*

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Notations

- o: an input (observation) to be classified; *e.g.: a word, an image, an audio frame/segment...*

- $\mathbf{x} = (x_1, \cdots, x_D)^T$: a D-dimensional column vector (usually in $\mathbb{R}^D$); $\mathbf{x}^T$is a row vector.
- $\mathbf{x}_n$ is a **feature vector** among a collection of N examples $\mathbf{x}_1, \cdots, \mathbf{x}_N$.
- x_{jn} is the j-th **feature coefficient** of $\mathbf{x}_n$; $1 \leq j \leq D$.
- $\mathcal{D} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$: the set of all training feature-vector examples.

Feature functions

Different from features!

Definition

A **feature function** is a real-valued function of both the input space $\mathcal{O}$ (observations) and the output space $\mathcal{Y}$ (target labels), $f_j : \mathcal{O} \times \mathcal{Y} \to \mathbb{R}$, that can be used to compute characteristics of the observations.

- An alternative way to express the characteristics of the observations, in a more **flexible manner**:
  - using output-specific features;
  - describing the **context**.

Example: $f_j(o_i, y_i) = \begin{cases} 1 & \text{if } o_i = \textit{"We"}, \text{ and } y_i = \textit{"noun"} \\ 0 & \text{otherwise} \end{cases}$

Feature functions

- Remarks:
  - Different attributes may thus be considered for different classes.
  - Feature functions are more general than features: one can define
    - $f_j(o, y) \triangleq x_j$;

      or
    - $f_j(o, y) \triangleq \mathbf{x}$.
  - In the following:
    - Feature-function notations will be used only when needed.
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Probabilistic classification

Take decisions based on the MAP rule:

$$\hat{y} = \underset{y \in \mathcal{Y}}{\operatorname{argmax}}\, p(y|\mathbf{x})$$

in order to minimize the error rate (here the expected 0-1 loss).

MAP: *Maximum A Posteriori* probability

→ this is the **Bayes decision rule** (for the 0-1 loss.)

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Generative model based classification

- **Objective**: $\hat{y} = \text{argmax}_y \, p(y|\mathbf{x})$.
- By the **Bayes** rule $p(y|\mathbf{x}) = \frac{p(y,\mathbf{x})}{p(\mathbf{x})} = \frac{p(y)p(\mathbf{x}|y)}{p(\mathbf{x})}$,

$$\hat{y} = \underset{y}{\text{argmax}} \frac{p(y)p(\mathbf{x}|y)}{p(x)} = \underset{y}{\text{argmax}} \, p(y)p(\mathbf{x}|y).$$

- Assuming a fixed prior $p(y)$ (possibly uninformative: $p(y) = \frac{1}{K}$), one is left with:

$$\hat{y} = \underset{y}{\text{argmax}} \, p(\mathbf{x}|y).$$

→ Our decision criterion becomes a **maximum-likelihood** criterion.

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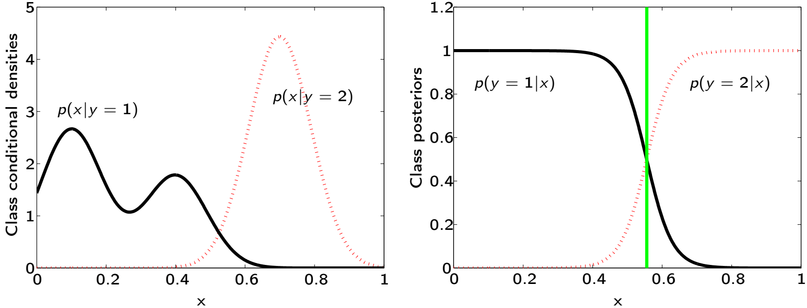

Generated using pmtk3 (?)

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  - Improved robustness to model imperfections, as independence assumptions will be made only among the labels, not the observations.
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Predicting structured-output data

- In many classification tasks the outputs are **structured**, *e.g.:*

Part-of-speech (POS) tagging:
tags follow predefined patterns

John	**saw**	**the**	**big**	**table**
noun	*verb*	*det*	*adj*	*noun*

Linear-chain structure

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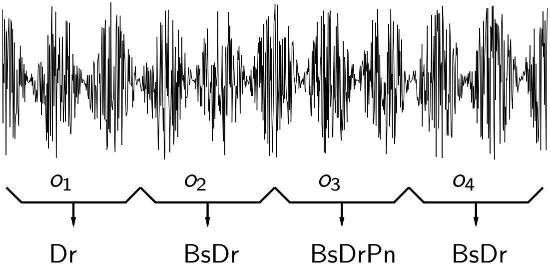
Musical instrument recognition



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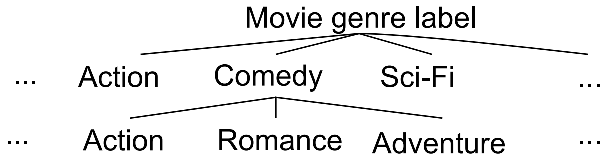
Autotagging tasks:
target tags are correlated (*e.g. comedy*, *romance*, *humour*)



Tree structure

→ Need for predictors able to take advantage of this structure.

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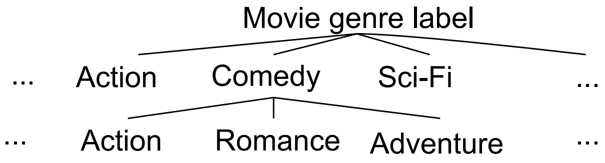

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Predicting sequential data

- In this tutorial, we focus on **sequential data**

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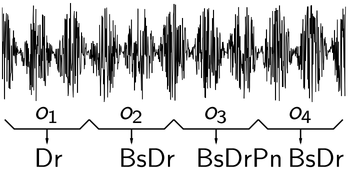
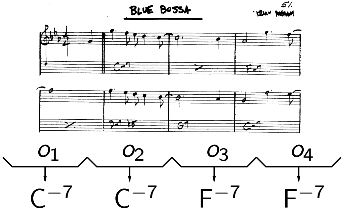
noun	*verb*	*det*	*adj*	*noun*





- Specialized inference algorithms can then be used (**forward-backward** method), which are easier to apprehend.
- More general methods can be used for more general structure (**belief propagation** and extensions), see for *e.g.* (**?**).

More notations

- $\underline{x}$ is a sequence of observations: $\underline{x} = (x_1, \cdots, x_n)$.
- $\underline{y}$ is the corresponding sequence of labels: $\underline{y} = (y_1, \cdots, y_n)$.
- We assume we have a training dataset $\mathcal{D}$ of N (i.i.d) such sequences: $\mathcal{D} = \{(\underline{x}^{(1)}, \underline{y}^{(1)}), \cdots, (\underline{x}^{(N)}, \underline{y}^{(N)})\}$.
- Remarks:
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The CRF model

A discriminative model for structured-output data

CRF model definition

$$p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta}) = \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}},\underline{y})$$

$$= \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \exp \Psi(\underline{\mathbf{x}},\underline{y};\boldsymbol{\theta}); \quad \boldsymbol{\theta} = \{\theta_1, \cdots, \theta_D\}.$$

- $Z(\underline{\mathbf{x}},\boldsymbol{\theta}) = \sum_{\underline{y}} \exp \sum_j \theta_j F_j(\underline{\mathbf{x}},\underline{y})$ is called a **partition function**.
- $\Psi(\underline{\mathbf{x}},\underline{y};\boldsymbol{\theta}) = \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}},\underline{y})$ is called a **potential function**.
- **Remark**: feature functions $F_j(\underline{\mathbf{x}},\underline{y})$ depend on the whole sequence of observations $\underline{\mathbf{x}}$ and labels $\underline{y}$.

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Applications of CRFs

CRF models have proven to be superior to competitors in a variety of application fields.

- They are the state-of-the-art techniques in many **natural language processing** (NLP) tasks (???)

  part-of-speech tagging (POS), named-entity recognition (NER)...

- They have been successfully used for various **computer vision** tasks (?????)

  image labeling, object and gesture recognition, facial expressions...

- Also for **speech analysis** tasks (????)

  speech recognition, speech segmentation, speaker identification...

- And a few applications to **music analysis** (**????**).

  autotagging, musical mood recognition, audio-to-score alignment, beat detection...

- Introduction
- The logistic regression model
  - Model specification
  - Maximum Entropy Modeling
  - Parameter estimation
  - Improvements to the logistic regression model
- Conditional Random Fields (for sequential data)
- Improvements and extensions to original CRFs
- Conclusion
- References

The logistic regression model

Approach: model the **posterior** probabilities of the K classes using linear functions of the inputs $\mathbf{x}$, according to:

$$
\begin{aligned}
\log \frac{P(\mathcal{C}_1|\mathbf{x})}{P(\mathcal{C}_K|\mathbf{x})} &= w_{10} + \mathbf{w}_1^T \mathbf{x} \\
\log \frac{P(\mathcal{C}_2|\mathbf{x})}{P(\mathcal{C}_K|\mathbf{x})} &= w_{20} + \mathbf{w}_2^T \mathbf{x} \\
&\vdots \\
\log \frac{P(\mathcal{C}_{K-1}|\mathbf{x})}{P(\mathcal{C}_K|\mathbf{x})} &= w_{(K-1)0} + \mathbf{w}_{K-1}^T \mathbf{x}
\end{aligned}
$$

Defines a **log-linear** model specified in terms of $K-1$ **log-odds** ($\log \frac{P(\mathcal{C}_k|\mathbf{x})}{P(\mathcal{C}_K|\mathbf{x})}$) or **logit** transformations so that the K probabilities sum to 1.

The logistic regression model

- From $\log \frac{P(\mathcal{C}_k|\mathbf{x})}{P(\mathcal{C}_K|\mathbf{x})} = w_{k0} + \mathbf{w}_k^T \mathbf{x}$; $k = 1, \cdots, K-1$; it is easy to deduce that:

Multiclass logistic regression model

$$P(\mathcal{C}_k|\mathbf{x}) = \frac{\exp(w_{k0} + \mathbf{w}_k^T \mathbf{x})}{1 + \sum_{l=1}^{K-1} \exp(w_{l0} + \mathbf{w}_l^T \mathbf{x})} \; ; \; k = 1, \cdots, K-1,$$

$$P(\mathcal{C}_K|\mathbf{x}) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(w_{l0} + \mathbf{w}_l^T \mathbf{x})}$$

- Remarks
  - The model is a **classification** model (not a regression model!)
  - It is a **discriminative** model as it targets $P(\mathcal{C}_k|\mathbf{x})$ (as opposed to modeling $p(\mathbf{x}|\mathcal{C}_k)$ in **generative** models.)

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Binary classification case

- When $K = 2$

$$
\begin{aligned}
P(\mathcal{C}_1|\mathbf{x}) &= p = \frac{1}{1 + \exp -(w_{10} + \mathbf{w}_1^T \mathbf{x})} \\
P(\mathcal{C}_2|\mathbf{x}) &= 1 - p
\end{aligned}
$$

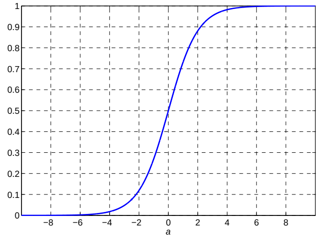
- $p = \dfrac{1}{1 + \exp -a}$; $a = w_{10} + \mathbf{w}_1^T \mathbf{x}$

Logistic sigmoid function

$$
\sigma(a) \stackrel{\Delta}{=} \frac{1}{1 + \exp -a}
$$

The logistic sigmoid function

$$\sigma(a) \triangleq \frac{1}{1+\exp -a}$$



- Properties:

Symmetry: $\sigma(-a) = 1 - \sigma(a)$

Inverse: $a = \log \frac{\sigma}{1-\sigma}$: **logit** function

- The odds $\frac{p}{1-p} \in [0, +\infty]$ hence the **log-odds** $\log \frac{p}{1-p} \in [-\infty, +\infty]$

- Logistic regression models the **log-odds** as **linear functions** of the inputs... ***why is this a good idea?***

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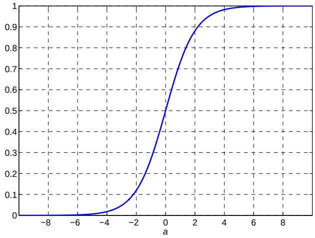

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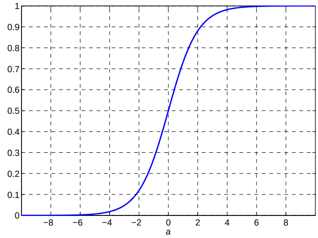

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Maximum Entropy: an introductory example

By (?)

Goal: perform English-to-French translation.

Approach: model an expert translator's approach to decide to translate a particular word, e.g. "*in*".

Method: Use a training dataset to estimate $p(y|o)$: the probability to assign the word (or phrase) y to the observed word "in"; to be used for MAP decision.

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→ Our model should capture these facts to perform accurate predictions.

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Using facts about the data

- *The translator always chooses among {dans, en, à, au cours de, pendant}:*

In terms of statistics

$P(dans) + P(en) + P(à) + P(au\ cours\ de) + P(pendant) = 1$

- How to choose $P(dans)$, ..., $P(pendant)$?
- Safe choice:

In terms of statistics

$P(dans) = P(en) = P(à) = P(au\ cours\ de) = P(pendant) = 1/5$

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Why "uniform"?

- Intuitively: the most uniform model according to our knowledge, the only **unbiased** assumption

- Ancient wisdom:
  - *Occam's razor* (William of Ockham, 1287-1347)*: principle of parsimony: "Nunquam ponenda est pluralitas sine necesitate." [Plurality must never be posited without necessity.]*
  - *Laplace: "when one has no information to distinguish between the probability of two events, the best strategy is to consider them equally likely."*

More facts

- *The translator chooses either "dans" or "en" 30% of the time:*

$$\begin{aligned} P(dans) + P(en) &= 3/10 \\ P(dans) + P(en) + P(à) + P(au\,cours\,de) + P(pendant) &= 1 \end{aligned}$$

- Again many solutions... and a reasonable choice is:

$$\begin{aligned} P(dans) = P(en) &= 3/20 \\ P(à) = P(au\,cours\,de) = P(pendant) &= 7/30 \end{aligned}$$

Even more facts

- *The translator chooses either "dans" or "à" 50% of the time:*

In terms of statistics

$$\begin{aligned} P(dans) + P(en) &= 3/10 \\ P(dans) + P(en) + P(à) + P(au\,cours\,de) + P(pendant) &= 1 \\ P(dans) + P(à) &= 1/2 \end{aligned}$$

$\rightarrow$ *Less intuitive...*

- What does *"uniform"* mean?
- How to determine the *"most uniform"* model subject to the constraints at hand?

Using feature functions

- Need to express the **facts** about the observations in a **flexible way**, to make sure the model will match them:
  - make use of **statistics** of the observations: e.g. *"in"* translates to either *"dans"* or *"en"* with frequency 3/10.
  - allow for using the **context**: e.g. if *"in"* is followed by "*April*" then the translation is *"en"* with frequency 9/10.

→ define **feature functions** to capture these statistics and use them to impose **constraints** to the model.

Example: $f_j(o_i, y_i) = \begin{cases} 1 & \text{if } y_i = \textit{"en"} \text{ and } \textit{"April"} \text{ follows } \textit{"in"} \\ 0 & \text{otherwise} \end{cases}$

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Defining constraints through feature functions

- The training sample can be described in terms of its **empirical** probability distribution $\tilde{p}(o,y)$:

$$\tilde{p}(o,y) \triangleq \frac{1}{N} \times \text{number of times that } (o,y) \text{ occurs in the sample}$$

- $\tilde{\mathbb{E}}(f_j) \triangleq \sum_{o,y} \tilde{p}(o,y) f_j(o,y)$: expected value of f_j w.r.t $\tilde{p}(o,y)$.

- $\mathbb{E}(f_j) \triangleq \sum_{o,y} p(o)p(y|o) f_j(o,y)$: expected v. of f_j w.r.t the **model** $p(o,y)$.

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- The observed statistics (facts) are captured by enforcing:

Constraint equation

$$\mathbb{E}(f_j) = \tilde{\mathbb{E}}(f_j),\ i.e.$$

$$\sum_{o,y} p(o)p(y|o)f_j(o,y) = \sum_{o,y} \tilde{p}(o,y)f_j(o,y)$$

- **Remark**: the constraints cannot be inconsistent since they are extracted from the data.

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Maximum entropy principle

- Now how to implement the idea of **uniform modeling**?
- Among the set $\mathcal{M}$ of probability distributions that satisfy the **constraints**, $\mathbb{E}(f_j) = \tilde{\mathbb{E}}(f_j)$, choose:

Maximum entropy criterion

$$p^*(y|o) = \underset{p(y|o)\in\mathcal{M}}{\operatorname{argmax}} \; H(y|o);$$

$$H(y|o) \triangleq -\sum_{o,y} p(o)p(y|o)\log p(y|o) : \text{ the } \textbf{conditional entropy}$$

- Hint from information theory: the discrete distribution with maximum **entropy** is the **uniform** distribution.

Solving the problem

Primal: $p^*(y|o) = \text{argmax}_{p(y|o)\in\mathcal{M}} H(y|o)$

Constraints: $\mathbb{E}(f_j) = \tilde{\mathbb{E}}(f_j)$ and $\sum_y p(y|o) = 1$

Lagrangian: $L(p, \boldsymbol{\lambda}) \triangleq H(y|o) + \lambda_0 \left(\sum_y p(y|o) - 1\right) + \sum_j \lambda_j \left(\mathbb{E}(f_j) - \tilde{\mathbb{E}}(f_j)\right)$

Equating the derivative of the Lagrangian with 0:

$$p_{\boldsymbol{\lambda}}(y|o) = \frac{1}{Z_{\boldsymbol{\lambda}}(o)} \exp \sum_j \lambda_j f_j(o, y);$$

$Z_{\boldsymbol{\lambda}}(x) = \sum_y \exp\left(\sum_j \lambda_j f_j(o, y)\right)$

The solution is given by the dual optimal: $\boldsymbol{\lambda}^* = \text{argmax}_{\boldsymbol{\lambda}} L(p, \boldsymbol{\lambda})$.

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Compare to the LR model

- Maxent model:

$$p(y=k|o) = \frac{1}{Z_{\boldsymbol{\lambda}}(o)} \exp\left(\sum_j \lambda_{jk} f_j(o,y)\right);$$

$$Z_{\boldsymbol{\lambda}}(o) = \sum_y \exp\left(\sum_j \lambda_{jk} f_j(o,y)\right).$$

- Logistic regression model:

$$\begin{aligned} p(y=k|\mathbf{x}) &= \frac{\exp(w_{k0} + \mathbf{w}_k^T \mathbf{x})}{1 + \sum_{l=1}^{K-1} \exp(w_{l0} + \mathbf{w}_l^T \mathbf{x})} \\ &= \frac{\exp(w'_{k0} + \mathbf{w'}_k^T \mathbf{x})}{\sum_{l=1}^{K} \exp(w'_{l0} + \mathbf{w'}_l^T \mathbf{x})} \\ &= \frac{1}{Z_{\mathbf{w}}(\mathbf{x})} \exp(w'_{k0} + \mathbf{w'}_k^T \mathbf{x}). \end{aligned}$$

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- Using:
  - feature-function: $f_j(o,y) = x_j$; $f_0(o,y) = 1$ and $\mathbf{x} = (x_1, \cdots, x_j, \cdots, x_D)^T$;
  - $w'_{k0} + \mathbf{w}'^{T}_{k}\mathbf{x} = \sum_{j=0}^{D} w'_{kj} f_j(o,y)$;

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- CRF model:

$$p(\underline{y}|\underline{x};\theta) = \frac{1}{Z_{\theta}(\underline{x})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{x}, \underline{y})$$

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Conclusion

The solution to the maximum entropy models has the same parametric form as logistic regression and CRF models.

- It is easily shown that the optimal solution is the **maximum-likelihood** solution in the parametric family $p_{\boldsymbol{\lambda}}(y|\mathbf{x}) = \frac{1}{Z_{\boldsymbol{\lambda}}(\mathbf{x})} \exp(\sum_j \lambda_j x_j)$.
- We've only considered discrete inputs, what about **continuous** inputs?
  - It is found that if the class-conditional densities $p(\mathbf{x}|y)$ are members of the **exponential family** of distributions, then the posterior probabilities are again given by **logistic sigmoids** of a linear function.
  - In particular, the model is optimal with **Gaussian densities** (with a shared covariance matrix).

The logistic regression model is quite well justified in a variety of situations.

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The logistic regression model is quite well justified in a variety of situations.

Fitting the LR models

- Done by **maximum likelihood** estimation; in practice minimizing the **Negative Log-Likelihood** (**NLL**).

- Let θ denote the set of all parameters:
  $\boldsymbol{\theta} = \{w_{10}, \mathbf{w}_1, \cdots, w_{(K-1)0}, \mathbf{w}_{K-1}\}$.

- The **log-likelihood** for the N (i.i.d) feature-vector observations is:

$$L(\mathcal{D}; \boldsymbol{\theta}) \triangleq -\sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i; \boldsymbol{\theta})$$

- To simplify, we focus on the **bi-class** case...

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NLL for bi-class LR

- Let $y_i = 1$ for $\mathcal{C}_1$ observations and $y_i = 0$ for $\mathcal{C}_2$ observations.
- Let $p(\mathbf{x};\boldsymbol{\theta}) \stackrel{\Delta}{=} p(y_i = 1|\mathbf{x}_i;\boldsymbol{\theta})$; hence $p(y_i = 0|\mathbf{x}_i;\boldsymbol{\theta}) = 1 - p(\mathbf{x};\boldsymbol{\theta})$.
- We can write: $p(y|\mathbf{x};\boldsymbol{\theta}) = p(\mathbf{x};\boldsymbol{\theta})^y(1 - p(\mathbf{x};\boldsymbol{\theta}))^{1-y}$.

Negative Log-Likelihood

$$
\begin{aligned}
L(\mathcal{D};\boldsymbol{\theta}) = L(\tilde{\mathbf{w}}) &= -\sum_{i=1}^{N}\{y_i \log p(\mathbf{x}_i;\tilde{\mathbf{w}}) + (1-y_i)\log(1 - p(\mathbf{x}_i;\tilde{\mathbf{w}}))\} \\
&= -\sum_{i=1}^{N}\left\{y_i\tilde{\mathbf{w}}^T\tilde{\mathbf{x}}_i - \log\left(1+\exp(\tilde{\mathbf{w}}^T\tilde{\mathbf{x}}_i)\right)\right\}
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where $\tilde{\mathbf{w}} = (w_0, \mathbf{w})$ and $\tilde{\mathbf{x}}_i = (1, \mathbf{x}_i)$ so that $\tilde{\mathbf{w}}^T\tilde{\mathbf{x}}_i = w_0 + \mathbf{w}^T\mathbf{x}_i$.

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Gradient and Hessian of the NLL

Gradient: $\nabla L(\mathcal{D}; \tilde{\mathbf{w}}) = -\sum_{i=1}^{N} \tilde{\mathbf{x}}_i (y_i - p(\mathbf{x}_i; \tilde{\mathbf{w}}))$

Hessian: $\frac{\partial^2 L(\mathcal{D}; \tilde{\mathbf{w}})}{\partial \tilde{\mathbf{w}} \partial \tilde{\mathbf{w}}^T} = \sum_{i=1}^{N} \tilde{\mathbf{x}}_i \tilde{\mathbf{x}}_i^T p(\mathbf{x}_i; \tilde{\mathbf{w}}) \left(1 - p(\mathbf{x}_i; \tilde{\mathbf{w}})\right)$

→ so the Hessian is **positive semi-definite**,

→ the NLL is **convex** and it has a global minimum.

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$\rightarrow$ so the Hessian is **positive semi-definite**,

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Minimizing the NLL

- By setting the derivatives to zero:

$$\frac{\partial L(\mathcal{D};\tilde{\mathbf{w}})}{\partial w_j} = -\sum_{i=1}^{N} \tilde{x}_{ji}(y_i - p(\mathbf{x}_i;\tilde{\mathbf{w}})) = 0\,;\, 0 \leq j \leq D.$$

Optimization problem

Solve for $\tilde{\mathbf{w}}$ the $D+1$ **non-linear** equations:

$$\sum_{i=1}^{N} y_i \tilde{x}_{ji} = \sum_{i=1}^{N} \tilde{x}_{ji}\, p(\mathbf{x}_i;\tilde{\mathbf{w}})$$

Optimization methods

Objective: Solve $\sum_{i=1}^{N} y_i \tilde{x}_{ji} = \sum_{i=1}^{N} \tilde{x}_{ji} p(\mathbf{x}_i; \tilde{\mathbf{w}})$

Problem: No closed-form solution in general (system of $D+1$ **non-linear** equations).

Solution: use **descent** methods.

Among the many descent algorithms available, two are widely used:

- the **Newton-Raphson** method: fast... but complex (efficient variations exist);
- the **stochastic gradient** descent method (**?**): easy to implement, adapted to large scale problems (*see Appendix*).

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Optimization with the Newton-Raphson method

- To minimize $g(\boldsymbol{\theta})$, consider its second-order Taylor series approximation around $\boldsymbol{\theta}_n$:

$$g(\boldsymbol{\theta}) \approx g(\boldsymbol{\theta}_n) + \nabla g(\boldsymbol{\theta}_n)^T(\boldsymbol{\theta} - \boldsymbol{\theta}_n) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_n)^T H(\boldsymbol{\theta}_n)(\boldsymbol{\theta} - \boldsymbol{\theta}_n);$$

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$$\boldsymbol{\theta}_{n+1} = \boldsymbol{\theta}_n - H(\boldsymbol{\theta}_n)^{-1}\nabla(\boldsymbol{\theta}).$$

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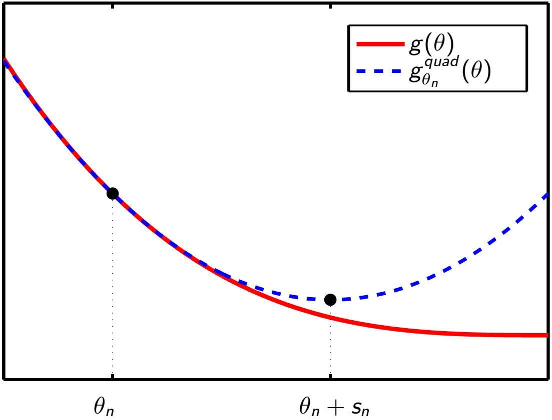
Illustration



Generated using pmtk3 (?)

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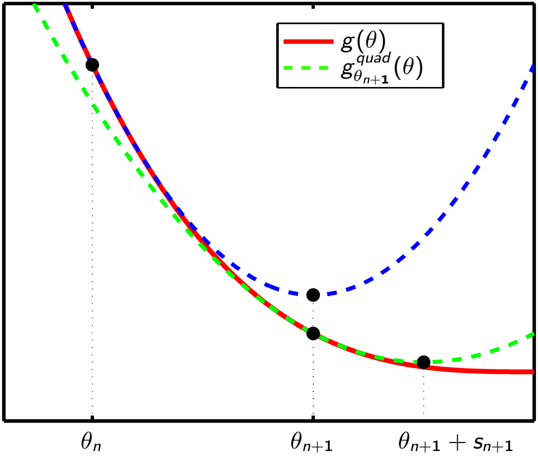

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Optimization with the Newton-Raphson method

Discussion

- Typically the algorithm converges (though overshooting may occur), and convergence speed is quadratic.
- D has to be small enough so that it is not too costly to **recompute** and **store** the inverse Hessian matrix at each iteration.
- Otherwise use **Quasi-Newton methods**:
  - **BFGS** (Broyden, Fletcher, Goldfarb and Shanno) method: approximates the inverse Hessian using successive gradient values.
  - **L-BFGS** (limited memory BFGS) method: stores only a few vectors used to approximate the inverse Hessian.
- Alternatively, use **stochastic gradient learning**:
  - Makes gradient updates based on **one** training example **at a time.**
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Optimization with the Newton-Raphson method

Discussion

- Typically the algorithm converges (though overshooting may occur), and convergence speed is quadratic.
- D has to be small enough so that it is not too costly to **recompute** and **store** the inverse Hessian matrix at each iteration.
- Otherwise use **Quasi-Newton methods**:
  - **BFGS** (Broyden, Fletcher, Goldfarb and Shanno) method: approximates the inverse Hessian using successive gradient values.
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ℓ_2-regularization

- To **avoid overfitting** the complexity of the model should be penalized.
- Similarly to **ridge regression** (?), a quadratic regularization term can be added to the NLL:

Regularized logistic regression problem

$$
\begin{aligned}
\hat{\mathbf{w}} &= \underset{\tilde{\mathbf{w}}}{\operatorname{argmin}}\, L(\mathcal{D}; \tilde{\mathbf{w}}) + \frac{\gamma}{2}||\mathbf{w}||^2 \\
&= \underset{\tilde{\mathbf{w}}}{\operatorname{argmin}} \left\{ -\sum_{i=1}^{N} \left[y_i \tilde{\mathbf{w}}^T \tilde{\mathbf{x}}_i - \log\left(1 + \exp \tilde{\mathbf{w}}^T \tilde{\mathbf{x}}_i\right)\right] + \frac{\gamma}{2}\sum_{j=1}^{D} w_j^2 \right\}
\end{aligned}
$$

$\gamma \geq 0$: complexity parameter controlling the amount of shrinkage; usually tuned by **cross-validation**.

ℓ_2-regularization

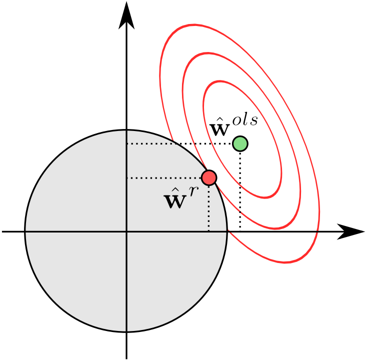
Discussion

Recall that:

$$\hat{\mathbf{w}} = \underset{\tilde{\mathbf{w}}}{\operatorname{argmin}}\, L(\mathcal{D}; \tilde{\mathbf{w}}) + \frac{\gamma}{2}||\mathbf{w}||^2$$

is equivalent to:

$$\begin{cases} \hat{\mathbf{w}} = \operatorname{argmin}_{\tilde{\mathbf{w}}} L(\mathcal{D}; \tilde{\mathbf{w}}) \\ \text{subject to } ||\mathbf{w}||^2 \leq t \end{cases}$$



for some t which has a correspondence to γ.

ℓ_2-regularization
Gradient and Hessian

Gradient: $\nabla L_2(\mathcal{D}; \tilde{\mathbf{w}}) = \nabla L_2(\mathcal{D}; \tilde{\mathbf{w}}) + \gamma \mathbf{w}$

Hessian: $H_2(\tilde{\mathbf{w}}) = H(\tilde{\mathbf{w}}) + \gamma \mathbf{I}_{D+1}$

→ So the Hessian becomes **positive definite**, the NLL is now **strictly convex** and it has a unique global minimum.

→ The previous optimization methods can be straightforwardly adapted by modifying the expressions of the gradient and Hessian.

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ℓ_1-regularization

- Proceed as in the **LASSO** (?), using a ℓ_1-regularization.

ℓ_1-regularized logistic regression problem

$$\begin{aligned}\hat{\mathbf{w}} &= \underset{\tilde{\mathbf{w}}}{\operatorname{argmin}}\, L(\mathcal{D}; \tilde{\mathbf{w}}) + \gamma ||\mathbf{w}||_1 \\ &= \underset{\tilde{\mathbf{w}}}{\operatorname{argmin}}\, L(\mathcal{D}; \tilde{\mathbf{w}}) + \gamma \sum_{j=1}^{D} |w_j|\,;\ \gamma \geq 0.\end{aligned}$$

ℓ_1-regularization

Discussion

- ℓ_1-regularization achieves **feature selection**.

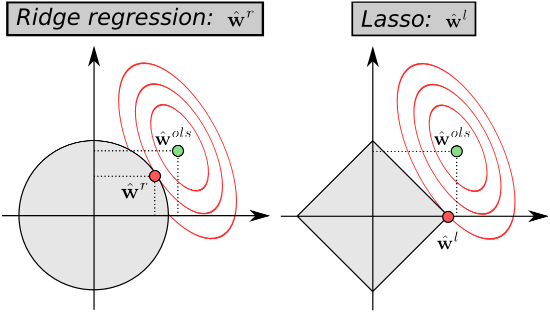

Illustration by Alexandre Gramfort, Telecom ParisTech

ℓ_1-regularization
Discussion

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- The problem is still **concave**, but...
- **Difficulties**:
  - The regularizer is **not differentiable** at zero yielding **non-smooth** optimization problem.

  $\rightarrow$ specific optimization techniques needed (**?**).
  - In configurations with groups of highly correlated features:
    - ℓ_1-regularization tends to select randomly one feature in each group;
    - ℓ_2-regularization tends to yield better prediction performance.

  $\rightarrow$ Consider the **elastic net** model (**?**):

$$L(\mathcal{D}; \tilde{\mathbf{w}}) + \gamma_2 ||\mathbf{w}||_2^2 + \gamma_1 ||\mathbf{w}||_1$$

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Kernel logistic regression (KLR)

- Let $\mathcal{K}$: positive definite kernel and $\mathcal{H}_\mathcal{K}$: the **RKHS** generated by $\mathcal{K}$.
- Let $\phi \in \mathcal{H}_\mathcal{K}$, a feature mapping to $\mathcal{H}_\mathcal{K}$.

KLR model

$$p(y_i|\mathbf{x}_i) = \frac{1}{1 + \exp -g(\mathbf{x}_i)}\ ; \quad g(\mathbf{x}) = w_0 + \mathbf{w}^T\phi(\mathbf{x})$$

KLR model estimation problem:

$$\min_{\tilde{\mathbf{w}}} L(\tilde{\mathbf{w}}) = -\sum_{i=1}^{N}\left[y_i g(\mathbf{x}_i) - \log(1 + \exp g(\mathbf{x}_i))\right]$$

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- By the **representer theorem**: $g(\mathbf{x}) = w_0 + \sum_{i=1}^{N} \alpha_i \mathcal{K}(\mathbf{x}_i, \mathbf{x})$
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KLR vs SVM

- It can be shown that KLR and SVM are quite related (*see Appendix*).
- Very similar prediction performance and optimal margin properties.
- Same refinements are possible: SMO, MKL...

+ Provides well-calibrated **class probabilities.**
+ Naturally generalizes to multi-class problems.

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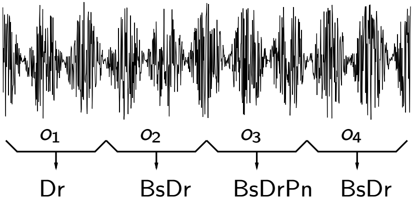
- Introduction
- The logistic regression model
- Conditional Random Fields (for sequential data)
  - Introduction
  - Inference
  - Parameter estimation
- Improvements and extensions to original CRFs
- Conclusion
- References
- Appendix

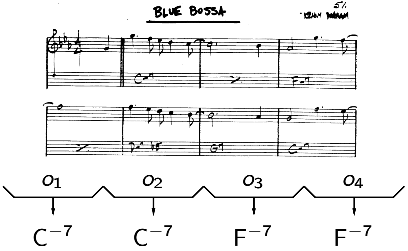
Structured-output data

John	saw	the	big	table
noun	*verb*	*det*	*adj*	*noun*

POS tagging



Musical instrument classification



Chord transcription

Recalling the notations

- $\underline{\mathbf{x}}$ is a sequence of observations: $\underline{\mathbf{x}} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)$.
- $\underline{y}$ is the corresponding sequence of labels: $\underline{y} = (y_1, \cdots, y_n)$.
- We assume we have a training dataset $\mathcal{D}$ of N (i.i.d) such sequences: $\mathcal{D} = \{(\underline{\mathbf{x}}^{(1)}, \underline{y}^{(1)}), \cdots, (\underline{\mathbf{x}}^{(N)}, \underline{y}^{(N)})\}$.
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The CRF model

CRF model definition

$$\begin{aligned} p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta}) &= \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}},\underline{y}) \\ &= \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \exp \Psi(\underline{\mathbf{x}},\underline{y};\boldsymbol{\theta}); \quad \boldsymbol{\theta} = \{\theta_1, \cdots, \theta_D\}. \end{aligned}$$

- $Z(\underline{\mathbf{x}},\boldsymbol{\theta}) = \sum_{\underline{y}} \exp \sum_j \theta_j F_j(\underline{\mathbf{x}},\underline{y})$ is called a **partition function**.
- $\Psi(\underline{\mathbf{x}},\underline{y};\boldsymbol{\theta}) = \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}},\underline{y})$ is called a **potential function**.
- Remarks:
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Defining label constraints

- Without any further assumptions on the structure of $\underline{y}$ the model is hardly usable: one needs to enumerate all possible sequences $\underline{y}$ for:
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→ defines **linear-chain** CRFs: at each position i, $1 \leq i \leq n$, each f_j depends on the **whole observation sequence**, but only on the current and previous labels.

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Examples of such feature functions (for discrete observations):

- *The current observation is "**saw**", the current label is **verb** and the previous is **noun**;*
- *The past 4 observations..., the current label is...*
- *The next observation is...*
- *The current label is...*

Defining label constraints

- For convenience, one can define two types of feature functions:
  - **Observation** (aka **state**) feature functions: $b_j(y_i, \underline{\mathbf{x}}, i)$;
  - **Transition** feature functions: $t_j(y_{i-1}, y_i, \underline{\mathbf{x}}, i)$.
- Hence

$$p(\underline{y}|\underline{\mathbf{x}}; \boldsymbol{\theta}) = \frac{1}{Z(\underline{\mathbf{x}}, \boldsymbol{\theta})} \exp\left\{ \sum_{i=1}^{n} \sum_{j=1}^{D_o} \theta_j b_j(y_i, \underline{\mathbf{x}}, i) + \sum_{i=1}^{n} \sum_{j=1}^{D_t} \theta'_j t_j(y_{i-1}, y_i, \underline{\mathbf{x}}, i) \right\}$$

Connection to HMM

The Hidden Markov Model

$$p_{hmm}(\underline{y}, \underline{\mathbf{x}}) \triangleq \prod_{i=1}^{n} p(y_i|y_{i-1})p(\mathbf{x}_i|y_i) \quad ; \quad \text{where } p(y_1|y_0) \triangleq p(y_1).$$

One can write:

$$\begin{aligned} p_{hmm}(\underline{y}, \underline{\mathbf{x}}) &= \exp\left\{\sum_{i=1}^{n} \log p(y_i|y_{i-1}) + \sum_{i=1}^{n} \log p(\mathbf{x}_i|y_i)\right\} \\ &= \exp\left\{\sum_{i=1}^{n} \sum_{l,q\in\mathcal{Y}} \lambda_{lq}\mathbb{I}(y_i = l)\mathbb{I}(y_{i-1} = q)\right. \\ &\qquad \left. + \sum_{i=1}^{n} \sum_{l\in\mathcal{Y},\mathbf{o}\in\mathcal{X}} \mu_{\mathbf{o}l}\mathbb{I}(y = l)\mathbb{I}(\mathbf{x}_i = \mathbf{o})\right\}; \end{aligned}$$

where $\lambda_{lq} = \log p(y_i = l|y_{i-1} = q)$ and $\mu_{\mathbf{o}l} = \log p(\mathbf{x}_i = \mathbf{o}|y_i = l)$.

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Connection to HMM

- Using the feature functions:
  - $b_j(y_i, \underline{\mathbf{x}}, i) = \mathbb{I}(y = l)\mathbb{I}(\mathbf{x}_i = \mathbf{o})$, where each j indexes a different "$l, \mathbf{o}$ configuration";
  - $t_j(y_{i-1}, y_i, \mathbf{x}, i) = \mathbb{I}(y_i = l)\mathbb{I}(y_{i-1} = q)$, where j indexes a different "l, q configuration";

- also using $p(\underline{y}|\underline{x}) = \frac{p(\underline{y},\underline{x})}{\sum_{\underline{y}'} p(\underline{y}',\underline{x})}$ and letting $Z(\underline{x}) = \sum_{\underline{y}'} p(\underline{y}', \underline{x})$, one gets:

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$\rightarrow$ HMMs are a particular type of linear-chain CRFs.

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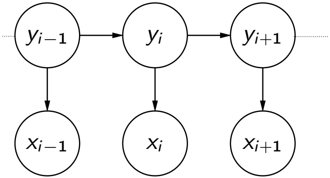

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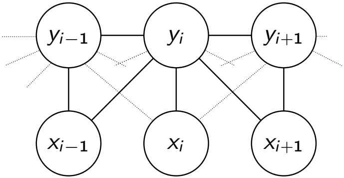

CRF

CRFs have a number of advantages over HMMs, as a consequence of two major differences:

- CRFs are **discriminative models**.
- CRFs are **undirected models**.

Connection to HMM

Advantage of the discriminative nature of CRF

HMM: observation x_i is independent of all other variables given its parent state y_i.

CRF: no assumptions on the dependencies among the observations: only $p(\underline{y}|\underline{\mathbf{x}})$ is modeled.

→ CRFs can safely:

- exploit **overlapping features**;
- account for **long-term dependencies**, considering the whole sequence of observations $\underline{\mathbf{x}}$ at each location i ($i \mapsto b_j(y_i, \underline{\mathbf{x}}, i)$);
- use **transition feature-functions** $t_j(y_{i-1}, y_i, \underline{\mathbf{x}}, i)$.

Using linear-chain CRFs

- **Inference**: given a model $\boldsymbol{\theta}$, how to compute:
  - $\hat{\underline{y}} = \operatorname{argmax}_{\underline{y}} p(\underline{y}|\underline{\mathbf{x}}; \boldsymbol{\theta})$?
  - $Z(\underline{\mathbf{x}}, \boldsymbol{\theta}) = \sum_{\underline{y}} \exp \sum_j \theta_j F_j(\underline{\mathbf{x}}, \underline{y})$ to deduce
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- **Parameter estimation**: given a training dataset
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Decoding the optimal sequence

- **Problem**: solve $\hat{\underline{y}} = \text{argmax}_{\underline{y} \in \mathcal{Y}^n} p(\underline{y}|\underline{\mathbf{x}}; \boldsymbol{\theta})$, with $|\mathcal{Y}|^n$ possible assignments!
- **Solution**: use the **Viterbi** algorithm.
- **Remark**:

$$\hat{\underline{y}} = \underset{\underline{y}}{\text{argmax}}\, p(\underline{y}|\underline{\mathbf{x}}; \boldsymbol{\theta}) = \underset{\underline{y}}{\text{argmax}} \frac{1}{Z(\underline{\mathbf{x}}, \boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}, \underline{y})$$

$$= \underset{\underline{y}}{\text{argmax}} \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}, \underline{y})$$

$$= \underset{\underline{y}}{\text{argmax}} \sum_{i=1}^{n} \sum_{j=1}^{D} \theta_j f_j(y_{i-1}, y_i, \underline{\mathbf{x}}, i)$$

Decoding the optimal sequence

- **Problem**: solve $\hat{\underline{y}} = \text{argmax}_{\underline{y} \in \mathcal{Y}^n} p(\underline{y}|\underline{x}; \boldsymbol{\theta})$, with $|\mathcal{Y}|^n$ possible assignments!
- **Solution**: use the **Viterbi** algorithm.
- Remark:

$$
\begin{aligned}
\hat{\underline{y}} = \underset{\underline{y}}{\text{argmax}}\, p(\underline{y}|\underline{x}; \boldsymbol{\theta}) &= \underset{\underline{y}}{\text{argmax}} \frac{1}{Z(\underline{x}, \boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{x}, \underline{y}) \\
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\end{aligned}
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\end{aligned}$$

Decoding the optimal sequence

Let: $g_i(y_{i-1}, y_i) \triangleq \sum_{j=1}^{D} \theta_j f_j(y_{i-1}, y_i, \underline{\mathbf{x}}, i)$; then:

$$\hat{y} = \underset{\underline{y}}{\operatorname{argmax}} \sum_{i=1}^{n} \sum_{j=1}^{D} \theta_j f_j(y_{i-1}, y_i, \underline{\mathbf{x}}, i) = \underset{\underline{y}}{\operatorname{argmax}} \sum_{i=1}^{n} g_i(y_{i-1}, y_i).$$

Let $\delta_m(s)$ be the optimal "intermediate score" where at time step m the label value is s:

$$\delta_m(s) \triangleq \max_{\{y_1,\cdots,y_{m-1}\}} \left[\sum_{i=1}^{m-1} g_i(y_{i-1}, y_i) + g_m(y_{m-1}, s) \right]$$

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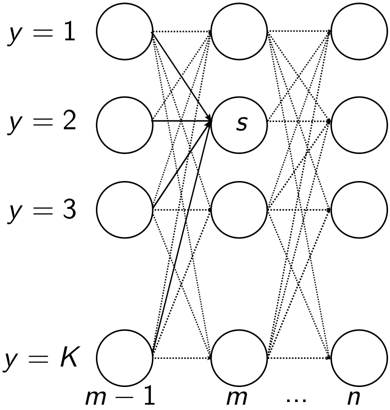
Decoding the optimal sequence

Trellis representation

$$\delta_m(s) \triangleq \max_{\{y_1,\cdots,y_{m-1}\}} \left[\sum_{i=1}^{m-1} g_i(y_{i-1}, y_i) + g_m(y_{m-1}, s) \right]$$



Decoding the optimal sequence

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$$\text{So: } \delta_{m-1}(y_{m-1}) \triangleq \max_{\{y_1,\cdots,y_{m-2}\}} \left[\sum_{i=1}^{m-2} g_i(y_{i-1}, y_i) + g_{m-1}(y_{m-2}, y_{m-1}) \right]$$

$$= \max_{\{y_1,\cdots,y_{m-2}\}} \sum_{i=1}^{m-1} g_i(y_{i-1}, y_i).$$

$$\delta_m(s) = \max_{y_{m-1} \in \mathcal{Y}} [\delta_{m-1}(y_{m-1}) + g_m(y_{m-1}, s)].$$

Decoding the optimal sequence

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Decoding the optimal sequence

- Thus, the intermediate scores $\delta_m(s)$ can be efficiently computed using:

Viterbi recursion

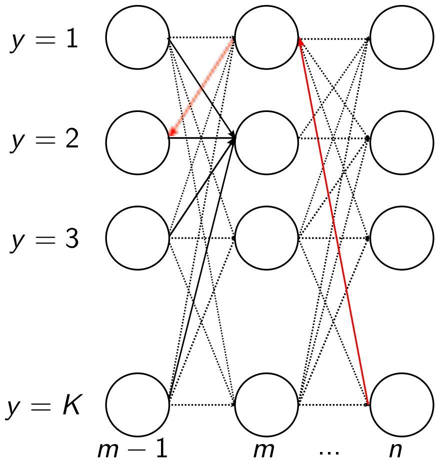
$$\delta_m(s) = \max_{y_{m-1} \in \mathcal{Y}} \left[\delta_{m-1}(y_{m-1}) + g_m(y_{m-1}, s)\right] ;\ 1 \leq m \leq n$$

- As we proceed we need to keep track of the selected predecessor of s, at each time step m.
- We use $\psi_m(s)$ for this purpose.

Decoding the optimal sequence

Backtracking

$$y_m^* = \psi_{m+1}(y_{m+1}^*); \quad m = n-1, n-2, \cdots, 1.$$



Viterbi decoding

The algorithm

Initialization:

$$\delta_1(s) = g_1(y_0, s); \ \forall s \in \mathcal{Y}; \ y_0 = \text{start}$$
$$\psi_1(s) = \text{start}$$

Recursion: $\forall s \in \mathcal{Y}; \ 1 \leq m \leq n$

$$\delta_m(s) = \max_{y \in \mathcal{Y}} \left[\delta_{m-1}(y) + g_m(y, s)\right]$$
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Termination:

$$\delta_n(y_n^*) = \max_{y \in \mathcal{Y}} \delta_n(y)$$
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Path backtracking:

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Complexity of Viterbi decoding

Remarks on the computational cost:

- $O(K^2 n)$ in the worst case; $K = |\mathcal{Y}|$.
- In practice: $O(\mathcal{T} K n)$, where $\mathcal{T}$: average number of possible "transitions" between labels y.
- Can be reduced using **beam search**: exploring a subset of possible labels at each time position (**?**).

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Computing the partition function $Z(\underline{\mathbf{x}}, \boldsymbol{\theta})$

The sum-product problem

Recall the CRF model:

$$p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta}) = \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \prod_{i=1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}})\,;$$

$$M_i(y_{i-1}, y_i, \underline{\mathbf{x}}) = \exp\left(\sum_{j=1}^{D} \theta_j f_j(y_{i-1}, y_i, \underline{\mathbf{x}}, i)\right);$$

$Z(\underline{\mathbf{x}}, \boldsymbol{\theta}) = \sum_{\underline{y} \in \mathcal{Y}^n} \prod_{i=1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}})$: intractable as is...

$\rightarrow$ use the **forward-backward** method: reduces **complexity** from $O(K^n)$ to $O(nK^2)$.

The forward-backward method

- Defining $\alpha_m(y_m) = \sum_{y_{m-1}} M_m(y_{m-1}, y_m)\alpha_{m-1}(y_{m-1})$; $2 \leq m \leq n$, it is easily shown[1] that:

At the end of the sequence

$$Z(\underline{x}, \theta) = \sum_{y_n \in \mathcal{Y}} \alpha_n(y_n).$$

- Alternatively, defining $\beta_m(y_m) = \sum_{y_{m+1}} M_{m+1}(y_m, y_{m+1})\beta_{m+1}(y_{m+1})$; $1 \leq m \leq n-1$ and $\beta_n(y_n) = 1$, one gets:

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$$Z(\underline{x}, \theta) = \sum_{y_1 \in \mathcal{Y}} M_1(y_0, y_1)\beta_1(y_1).$$

[1] *See Appendix for more details*

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Marginal probability

$$p(y_{m-1}, y_m|\underline{\mathbf{x}}) = \sum_{\underline{y} \backslash \{y_{m-1}, y_m\}} p(\underline{y}|\mathbf{x})$$

Marginal probability by forward-backward

$$p(y_{m-1}, y_m|\underline{\mathbf{x}}) = \frac{1}{Z(\underline{\mathbf{x}})} \alpha_{m-1}(y_{m-1}) M_m(y_{m-1}, y_m, \underline{\mathbf{x}}) \beta_m(y_m).$$

More details in the appendix.

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More details in the appendix.

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Negative log-likelihood (NLL)

- Given training data $\mathcal{D} = \{(\underline{\mathbf{x}}^{(1)}, \underline{y}^{(1)}), \cdots, (\underline{\mathbf{x}}^{(N)}, \underline{y}^{(N)})\}$, the NLL is:

$$
\begin{aligned}
L(\mathcal{D};\boldsymbol{\theta}) &= -\sum_{q=1}^{N} \log p(\underline{y}^{(q)} | \underline{\mathbf{x}}^{(q)}; \boldsymbol{\theta}) \\
&= \sum_{q=1}^{N} \left\{ \log Z(\underline{\mathbf{x}}^{(q)}; \boldsymbol{\theta}) - \sum_{i=1}^{n_q} \sum_{j=1}^{D} \theta_j f_j(y_{i-1}^{(q)}, y_i^{(q)}, \underline{\mathbf{x}}^{(q)}, i) \right\} \\
&= \sum_{q=1}^{N} \left\{ \log Z(\underline{\mathbf{x}}^{(q)}; \boldsymbol{\theta}) - \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}^{(q)}, \underline{y}^{(q)}) \right\}.
\end{aligned}
$$

- $L(\mathcal{D};\boldsymbol{\theta})$ is **convex** $\rightarrow$ gradient-descent will converge to global minimum.

NLL gradient

Gradient:
$$\frac{\partial L(\mathcal{D};\boldsymbol{\theta})}{\partial \theta_k} = \sum_{q=1}^{N} \left\{ \frac{\partial}{\partial \theta_k} \log Z(\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta}) - F_k(\underline{\mathbf{x}}^{(q)}, \underline{y}^{(q)}) \right\}.$$

$$\begin{aligned}
\frac{\partial}{\partial \theta_k} \log Z(\underline{\mathbf{x}};\boldsymbol{\theta}) &= \frac{1}{Z(\underline{\mathbf{x}};\boldsymbol{\theta})} \sum_{\underline{y}\in\mathcal{Y}^n} \frac{\partial}{\partial \theta_k} \left[\exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}, \underline{y}) \right] \\
&= \frac{1}{Z(\underline{\mathbf{x}};\boldsymbol{\theta})} \sum_{\underline{y}\in\mathcal{Y}^n} F_k(\underline{\mathbf{x}}, \underline{y}) \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}, \underline{y}) \\
&= \sum_{\underline{y}\in\mathcal{Y}^n} F_k(\underline{\mathbf{x}}, \underline{y}) \frac{\exp \sum_j \theta_j F_j(\underline{\mathbf{x}}, \underline{y})}{Z(\underline{\mathbf{x}};\boldsymbol{\theta})} \\
&= \sum_{\underline{y}\in\mathcal{Y}^n} F_k(\underline{\mathbf{x}}, \underline{y}) p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta}) \\
&= \mathbb{E}_{p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta})} \left[F_k(\underline{\mathbf{x}}, \underline{y}) \right].
\end{aligned}$$

NLL gradient

Gradient: $$\frac{\partial L(\mathcal{D};\boldsymbol{\theta})}{\partial \theta_k} = \sum_{q=1}^{N} \left\{ \frac{\partial}{\partial \theta_k} \log Z(\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta}) - F_k(\underline{\mathbf{x}}^{(q)}, \underline{y}^{(q)}) \right\}.$$

$\frac{\partial}{\partial \theta_k} \log Z(\underline{\mathbf{x}};\boldsymbol{\theta}) = \mathbb{E}_{p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta})}\left[F_k(\underline{\mathbf{x}}, \underline{y})\right]$: conditional expectation given $\underline{\mathbf{x}}$.

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Optimality condition

- Setting the derivatives to 0, *i.e.* $\frac{\partial L(\mathcal{D};\boldsymbol{\theta})}{\partial \theta_k} = 0$, yields:

$$\sum_{q=1}^{N} \mathbb{E}_{p(\underline{y}|\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta})} \left[F_k(\underline{\mathbf{x}}^{(q)}, \underline{y}) \right] = \sum_{q=1}^{N} F_k(\underline{\mathbf{x}}^{(q)}, \underline{y}^{(q)});\ 1 \leq k \leq D$$

- No closed-form solution: numerical optimization is again needed.
- Need to compute $\mathbb{E}_{p(\underline{y}|\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta})} \left[F_k(\underline{\mathbf{x}}^{(q)}, \underline{y}) \right]$ efficiently.

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Efficient gradient computation

$$\mathbb{E}_{p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta})}\left[F_k(\underline{\mathbf{x}},\underline{y})\right] = \sum_{\underline{y}\in\mathcal{Y}^n} F_k(\underline{\mathbf{x}},\underline{y})p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta})$$
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$$= \sum_{i=1}^{n}\sum_{y_{i-1},y_i\in\mathcal{Y}^2} f_k(y_{i-1},y_i,\underline{\mathbf{x}})p(y_{i-1},y_i|\underline{\mathbf{x}};\boldsymbol{\theta})$$

$p(y_{i-1},y_i|\underline{\mathbf{x}};\theta)$ is the **marginal probability** which thanks to the **forward-backward** algorithm is obtained by:

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Optimization

Many **algorithms** are available (see ??):

- Generalized iterative scaling (?): original algorithm, slow convergence, suboptimal.
- Conjugate gradient (?): faster convergence, better quality.
- **L-BFGS** (?): fast convergence, scalable; a good option, most used.
- Stochastic gradient: suboptimal, simple, online, **large-scale applications**.

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Regularization

Using ℓ_2-norm

- Redefine the objective function as: $L(\mathcal{D};\boldsymbol{\theta}) = L(\mathcal{D};\boldsymbol{\theta}) + \frac{||\boldsymbol{\theta}||_2^2}{2\sigma^2}$;
  σ^2: a free parameter penalizing large weights (as in **ridge regression**).
- The gradient coefficients become:
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- **Advantages**:
  - The objective becomes **strictly convex**.
  - Shrinkage of θ coefficients is achieved avoiding overfitting and numerical problems.
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Regularization

Using ℓ_2-norm

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Using ℓ_1-norm to perform feature selection

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  $L(\mathcal{D};\boldsymbol{\theta}) = L(\mathcal{D};\boldsymbol{\theta}) + \rho||\boldsymbol{\theta}||_1 = L(\mathcal{D};\boldsymbol{\theta}) + \rho\sum_{j=1}^{D}|\theta_j|$ (as in the LASSO).
- **Advantage:** performs **feature selection**

  in some NLP apps: up to 95% of the features can be discarded without affecting performance! (see **?**).
- **Difficulties**:
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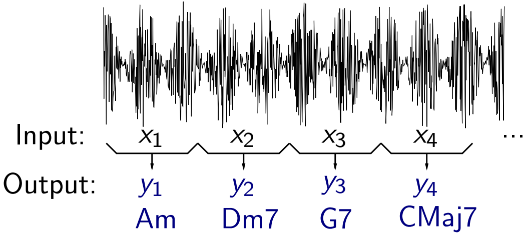
Motivation

Problem: the CRF model does not support **hidden states**.

CRF

$$\mathcal{D} = \{(\underline{\mathbf{x}}^{(i)}, \underline{y}^{(i)})\}_i$$



Hidden-state CRF

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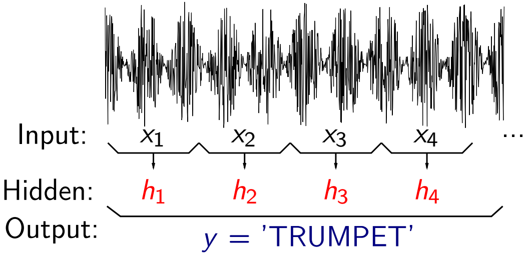

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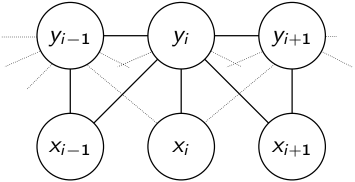

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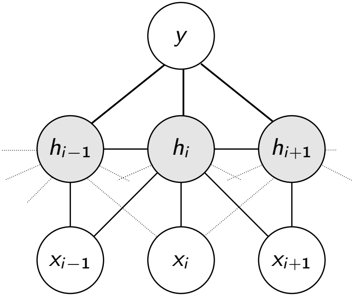

The HCRF model
(?)

- Each sequence of observations $\underline{x} = (x_1, \cdots, x_n)$ is associated with:
  - a unique label y;
  - a sequence of **latent variables** $\underline{h} = (h_1, \cdots, h_n)$, where $h_i \in \mathcal{H}$.

HCRF model definition

$$p(y, \underline{h}|\underline{x}; \boldsymbol{\theta}) = \frac{1}{Z(\underline{x}, \boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{x}, y, \underline{h})$$

$Z(\underline{x}, \boldsymbol{\theta}) = \sum_{y,\underline{h}} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{x}, y, \underline{h})$; $\boldsymbol{\theta} = \{\theta_1, \cdots, \theta_D\}$.

Inference in HCRF

- HCRF model: $p(y, \underline{h}|\underline{\mathbf{x}}; \boldsymbol{\theta}) = \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}, y, \underline{h})$.
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- We have:
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- $Z'(y, \underline{\mathbf{x}}, \theta)$ can be easily computed using forward/backward recursions (as done in CRF).
- To classify new test cases, use:
  $\hat{y} = \text{argmax}_{y\in\mathcal{Y}}\, p(y|\underline{\mathbf{x}}; \theta^*) = \text{argmax}_{y\in\mathcal{Y}} \frac{Z'(y,\underline{\mathbf{x}},\theta)}{\sum_y Z'(y,\underline{\mathbf{x}},\theta)}$.
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Negative log-likelihood

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L(\mathcal{D};\boldsymbol{\theta}) &= -\sum_{q=1}^{N} \log p(y^{(q)}|\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta}) \\
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$L(D;\boldsymbol{\theta})$ is no longer convex $\rightarrow$ convergence to a local minimum.

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NLL gradient

$$\frac{\partial L(\mathcal{D};\boldsymbol{\theta})}{\partial \theta_k} = \sum_{q=1}^{N} \Bigg\{ \sum_{y,\underline{h}} F_k(\underline{\mathbf{x}}^{(q)}, y, \underline{h}) p(y, \underline{h} | \underline{\mathbf{x}}; \boldsymbol{\theta}) - \sum_{\underline{h}} F_k(\underline{\mathbf{x}}^{(q)}, y^{(q)}, \underline{h}) p(\underline{h} | y^{(q)}, \underline{\mathbf{x}}^{(q)}; \boldsymbol{\theta}) \Bigg\}$$

which can be again computed using the **forward-backward** method.

A gradient descent method (L-BFGS) can be again used to solve for $\boldsymbol{\theta}$.

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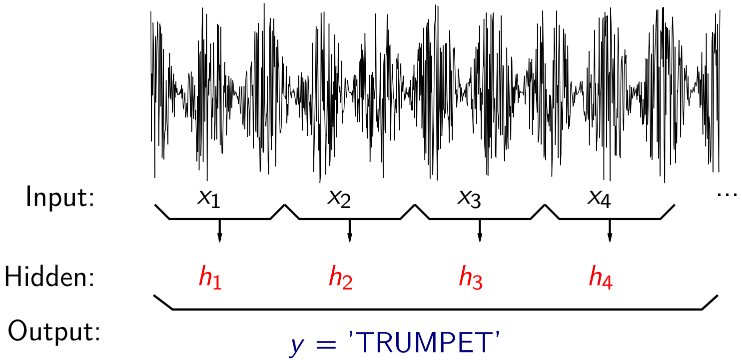
Application to musical instrument classification



Feature functions for HCRF

Following (?)

$$\Psi(\underline{\mathbf{x}}, y, \underline{h}, \boldsymbol{\theta}) = \sum_{i=1}^{N} < \boldsymbol{\theta}(h_i), \mathbf{x}_i > + \sum_{i=1}^{N} \theta(y, h_i) + \sum_{i=1}^{N} \theta(y, h_{i-1}, h_i)$$

- $< \boldsymbol{\theta}(h_i), \mathbf{x}_i >$: compatibility between observation $\mathbf{x}_i$ and hidden state $h_i \in \mathcal{H}$;
- $\theta(y, h_i)$: compatibility between hidden state h_i and label y;
- $\theta(y, h_{i-1}, h_i)$: compatibility between transition $h_{i-1} \leftrightarrow h_i$ and label y.

Evaluation

- Classifying 1-second long segments of solo excerpts of **Cello**, **Guitar**, **Piano**, **Bassoon** and **Oboe.**
- Data:
  - training set: 2505 segments (*i.e. 42');*
  - testing set: 2505 segments.
- Classifiers:
  - ℓ_2-regularized **HCRF** with 3 hidden states;
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- Features: 47 cepstral, perceptual and temporal features.
- Results

Classifier	SVM	HCRF
Average accuracy	75%	76%

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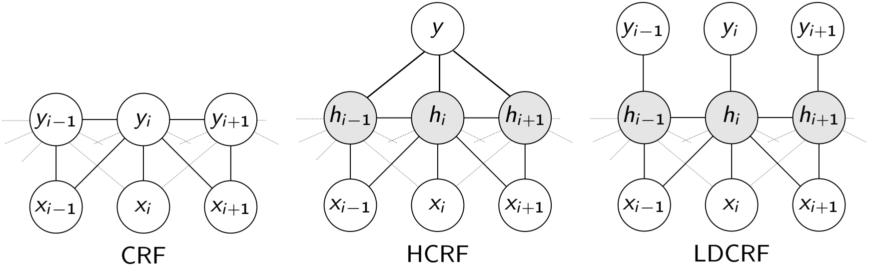
Other extensions

- **LDCRF**: Latent-Dynamic Conditional Random Field (?)

  modeling both hidden-states and structured-outputs.



Other extensions

- **LDCRF**: Latent-Dynamic Conditional Random Field (**?**)

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- **Kernel-CRF** (**??**)

  introducing implicit features to account for (non-linear) interactions between original features.

- **Semi-Markov CRF** (**?**)

  modeling segment-level labels

- **CCRF**: Continuous CRF (**?**)

  modeling continuous labels in a regression setting.

Take-home messages

- CRFs are powerful structured-data prediction models (more flexible than HMMs and other more general Bayesian networks) as they are:
  - **discriminative models**: focus on modeling the target labels;

  $\rightarrow$ can handle a high number of feature functions, including transition features, and account for long-range dependencies.

  - **undirected models**: no need to normalize potentials locally.

  $\rightarrow$ allow for incorporating prior knowledge about constraints and label dependencies in an intuitive way.

- Easily **extendable** with key mechanisms: regularization, sparsity, latent variables, kernels...

- Great potential for various classification tasks (both symbolic and numerically-continuous data).

CRF software packages

Package	Language	Main features	Reference
CRF++	C++	Linear-chain CRF, NLP, L-BFGS optimization	(?)
crfChain	Matlab, C mex	Linear-chain CRF, categorical features, L-BFGS optimization	?
CRFsuite	C++, Python	Linear-chain CRF, NLP, various regularization and optimization methods (L-BFGS), designed for fast training	(?)
HCRF library	C++, Matlab, Python	CRF, HCRF, LDCRF, continuous inputs, L-BFGS optimization	(?)
Mallet	Java	CRF, maxent, HMM, NLP, text feature extraction routines, various optimization methods (L-BFGS)	(?)
Wapiti	C99	Linear-chain CRF, NLP, large label and feature sets, various regularization and optimization methods (L-BFGS, SGD), multi-threaded	(?)

CRF tutorials

- Charles Sutton and Andrew McCallum. **An Introduction to Conditional Random Fields for Relational Learning**. In *Introduction to Statistical Relational Learning*. Edited by Lise Getoor and Ben Taskar. MIT Press, 2006.
- Charles Elkan. **Log-linear Models and Conditional Random Fields**. *Notes for a tutorial at CIKM'08*, October 2008.
- Roman Klinger and Katrin Tomanek. **Classical Probabilistic Models and Conditional Random Fields**. *Algorithm Engineering Report TR07-2-2013*, December 2007.
- Hanna M. Wallach. **Conditional Random Fields: An Introduction**. Technical Report MS-CIS-04-21, Department of Computer and Information Science, University of Pennsylvania, 2004.
- Roland Memisevic. **An Introduction to Structured Discriminative Learning**. Technical Report, University of Toronto, 2006.
- Rahul Gupta. **Conditional Random Fields**. Unpublished report, IIT Bombay, 2006.

Bibliography I

- Conditional Random Fields (for sequential data)
- Improvements and extensions to original CRFs
- Conclusion
- References
- Appendix
  - Optimization with stochastic gradient learning
  - Comparing KLR and SVM
  - The forward-backward method

LR model learning with stochastic gradient descent (SGL)

- **Idea**: make gradient updates based on **one** training example **at a time**
- **Use**: $\frac{\partial L(\mathcal{D};\tilde{\mathbf{w}})}{\partial w_j} = \left(y_i - p(\mathbf{x}_i;\tilde{\mathbf{w}})\right) x_{ji}$

Algorithm

- Initialise $\tilde{\mathbf{w}}$
- Repeat (until convergence)
    - Randomly permute training examples $\mathbf{x}_i$
    - For $i = 1 : N$

      $w_j \leftarrow w_j + t\left(y_{\sigma_i} - p_{\sigma_i}\right) x_{j\sigma_i}$; $j = 1, \cdots, D$

- t : *step size*, to be tuned
- **Complexity of SGL:** $O(NFD)$ per *epoch*; with F the average number of non-zero feature coefficients per example; an *epoch* is a "complete" update using all training examples.

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Support Vector Machines

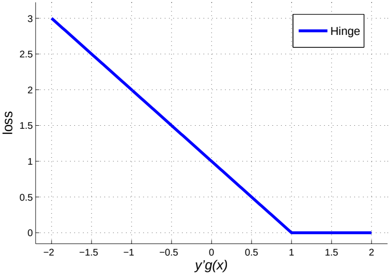
Recalling SVM as a regularized function fitting problem

- The SVM solution, $g(\mathbf{x}) = w_0 + \mathbf{w}^T\phi(\mathbf{x})$, can be found by solving:

$$\min_{\tilde{\mathbf{w}}} \sum_{i=1}^{N} \left[1 - y_i' g(\mathbf{x}_i)\right]_+ + \frac{\gamma}{2} ||g||^2_{\mathcal{H}_\mathcal{K}} \; ; \; y_i' \in \{-1, 1\}$$

Hinge loss

$$\left[1 - y_i' g(\mathbf{x}_i)\right]_+ = \max(0, 1 - y_i' g(\mathbf{x}_i))$$



KLR vs SVM

- Let $y_i' = \begin{cases} 1 & \text{if } y_i = 1 \\ -1 & \text{if } y_i = 0 \end{cases}$
- The negative log-likelihood of the KLR model can then be written as $L(\mathcal{D}; \tilde{\mathbf{w}}) = \sum_{i=1}^{N} \log\left(1 + \exp -y_i' g(\mathbf{x}_i)\right)$.
- Both KLR and SVM solve:

$$\min_{\tilde{\mathbf{w}}} \sum_{i=1}^{N} l(y_i' g(\mathbf{x}_i)) + \frac{\lambda}{2} ||g||^2_{\mathcal{H}_\mathcal{K}};$$

KLR

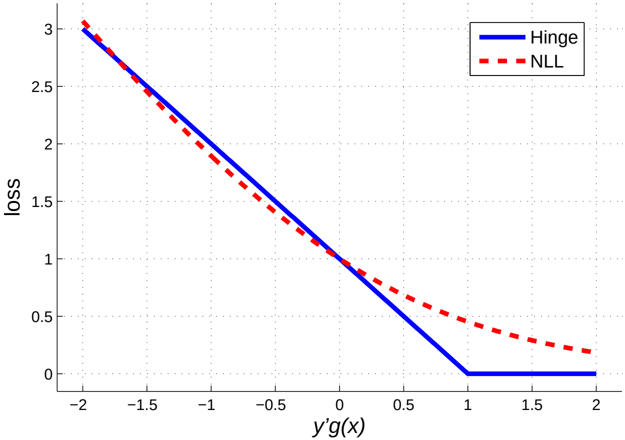
$$l(y_i' g(\mathbf{x}_i)) = \log\left(1 + \exp -y_i' f(\mathbf{x}_i)\right)$$

SVM

$$l(y_i' g(\mathbf{x}_i)) = \left[1 - y_i' f(\mathbf{x}_i)\right]_+$$

KLR vs SVM

Hinge vs negative binomial log-likelihood



The forward recursion

Define α scores as:

$$
\begin{aligned}
\alpha_1(y_1) &= M_1(y_0, y_1) \\
\alpha_2(y_2) &= \sum_{y_1 \in \mathcal{Y}} M_2(y_1, y_2)\alpha_1(y_1) \\
\alpha_3(y_3) &= \sum_{y_2 \in \mathcal{Y}} M_3(y_2, y_3)\alpha_2(y_2) \\
&\vdots \\
\alpha_m(y_m) &= \sum_{y_{m-1}} M_m(y_{m-1}, y_m)\alpha_{m-1}(y_{m-1})\,;\; 2 \leq m \leq n
\end{aligned}
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\boldsymbol{\alpha}_3(y_3) &= \sum_{y_2 \in \mathcal{Y}} M_3(y_2, y_3)\boldsymbol{\alpha}_2(y_2) = \sum_{y_1, y_2} M_3(y_2, y_3) M_2(y_1, y_2) M_1(y_0, y_1) \\
&\vdots \\
\boldsymbol{\alpha}_m(y_m) &= \sum_{y_{m-1}} M_m(y_{m-1}, y_m)\boldsymbol{\alpha}_{m-1}(y_{m-1})\,;\ 2 \leq m \leq n
\end{aligned}
$$

At the end of the sequence

$$
\sum_{y_n \in \mathcal{Y}} \boldsymbol{\alpha}_n(y_n) = \sum_{\underline{y} \in \mathcal{Y}^n} \prod_{i=1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}}) = Z(\underline{\mathbf{x}}, \boldsymbol{\theta}).
$$

The forward recursion

Define $\boldsymbol{\alpha}$ scores as:

$$\boldsymbol{\alpha}_m(y_m) = \sum_{y_{m-1}} M_m(y_{m-1}, y_m)\boldsymbol{\alpha}_{m-1}(y_{m-1})\,;\ 2 \leq m \leq n.$$

At the end of the sequence

$$\sum_{y_n \in \mathcal{Y}} \boldsymbol{\alpha}_n(y_n) = \sum_{\underline{y} \in \mathcal{Y}^n} \prod_{i=1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}}) = Z(\underline{\mathbf{x}}, \boldsymbol{\theta}).$$

Complexity: reduced from $O(K^n)$ to $O(nK^2)$.

The backward recursion

$$\begin{aligned}\beta_m(y_m) &= \sum_{y_{m+1}\in\mathcal{Y}} M_{m+1}(y_m, y_{m+1})\beta_{m+1}(y_{m+1})\,;\ 1 \le m \le n-1 \\ \beta_n(y_n) &= 1\end{aligned}$$

At the beginning of the sequence

$$Z(\underline{x}, \theta) = \sum_{y_1\in\mathcal{Y}} M_1(y_0, y_1)\beta_1(y_1).$$

Marginal probability

$p(y_{m-1}, y_m|\underline{\mathbf{x}}) = \sum_{\underline{y}\backslash\{y_{m-1},y_m\}} p(\underline{y}|\mathbf{x})$;

$\underline{y}\backslash\{y_{m-1}, y_m\} \triangleq \{y_1, \cdots, y_{m-2}, y_{m+1}, \cdots, y_n\}$.

$$p(y_{m-1}, y_m|\underline{\mathbf{x}}) = \frac{1}{Z(\underline{\mathbf{x}})} \sum_{\underline{y}\backslash\{y_{m-1},y_m\}} \prod_{i=1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}})$$

$$= \frac{1}{Z(\underline{\mathbf{x}})} \sum_{\underline{y}\backslash\{y_{m-1},y_m\}} \prod_{i=1}^{m-1} M_i(y_{i-1}, y_i, \underline{\mathbf{x}}) \times M_m(y_{m-1}, y_m, \underline{\mathbf{x}})$$

$$\times \prod_{i=m+1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}})$$

Marginal probability

$p(y_{m-1}, y_m|\underline{\mathbf{x}}) = \sum_{\underline{y}\backslash\{y_{m-1},y_m\}} p(\underline{y}|\underline{\mathbf{x}})$;

$\underline{y}\backslash\{y_{m-1}, y_m\} \stackrel{\Delta}{=} \{y_1, \cdots, y_{m-2}, y_{m+1}, \cdots, y_n\}$.

$$
\begin{aligned}
p(y_{m-1}, y_m|\underline{\mathbf{x}}) &= \frac{1}{Z(\underline{\mathbf{x}})} \sum_{\underline{y}\backslash\{y_{m-1},y_m\}} \prod_{i=1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}}) \\
&= \frac{1}{Z(\underline{\mathbf{x}})} \sum_{\underline{y}\backslash\{y_{m-1},y_m\}} \prod_{i=1}^{m-1} M_i(y_{i-1}, y_i, \underline{\mathbf{x}}) \times M_m(y_{m-1}, y_m, \underline{\mathbf{x}}) \\
&\qquad \times \prod_{i=m+1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}})
\end{aligned}
$$

Marginal probability

$$p(y_{m-1}, y_m|\underline{\mathbf{x}}) = \frac{1}{Z(\underline{\mathbf{x}})} M_m(y_{m-1}, y_m, \underline{\mathbf{x}}) \times \sum_{\{y_1,\dots,y_{m-2}\}} \prod_{i=1}^{m-1} M_i(y_{i-1}, y_i, \underline{\mathbf{x}}) \times \sum_{\{y_{m+1},\dots,y_n\}} \prod_{i=m+1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}})$$

$$p(y_{m-1}, y_m|\underline{\mathbf{x}}) = \frac{1}{Z(\underline{\mathbf{x}})} \alpha_{m-1}(y_{m-1}) M_m(y_{m-1}, y_m, \underline{\mathbf{x}}) \beta_m(y_m).$$