# 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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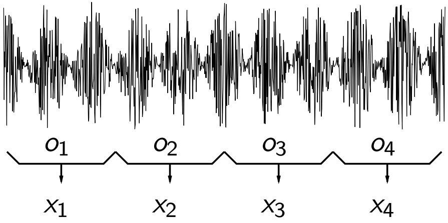
## Features

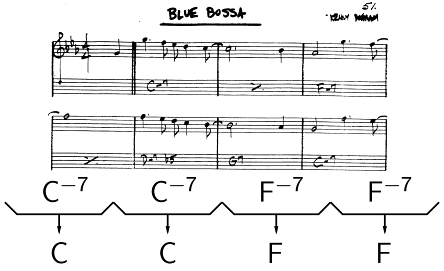
- Classification relies on **features** $x$: descriptors of some qualities/ attributes of the inputs $o$. Two types of features:

**Continuous features**



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

**Discrete/categorical**



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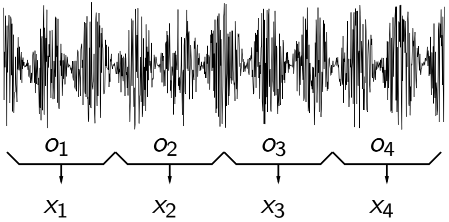

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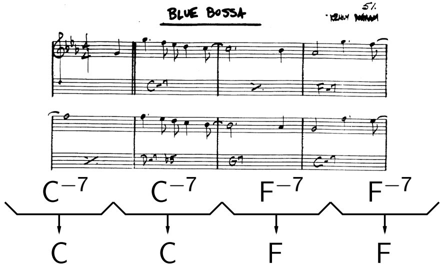

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## Notations

- $o$: 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), $f_j : \mathcal{O} \times \mathcal{Y} \rightarrow \mathbb{R}$, 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**.

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

## Feature functions

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

      or
    - $f_j(o, y) \overset{\Delta}{=} \mathbf{x}$.
  - 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

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## Generative model based classification

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

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

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

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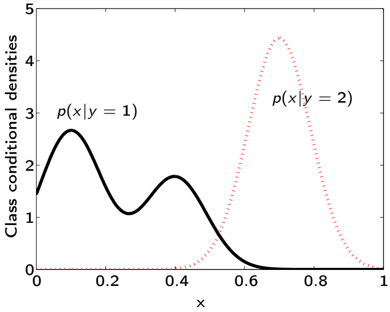

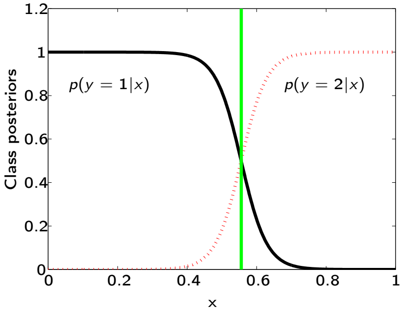

*Generated using pmtk3 (Dunham and Murphy, 2010)*

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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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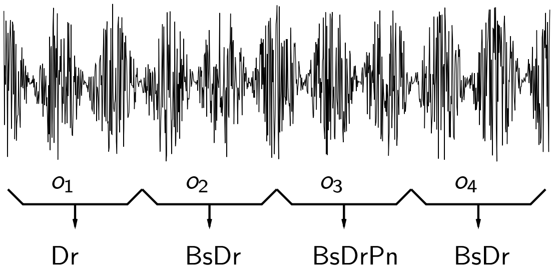
**Musical instrument recognition**



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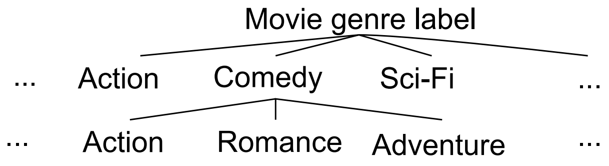
*target tags are correlated* (*e.g. comedy*, *romance*, *humour*)



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

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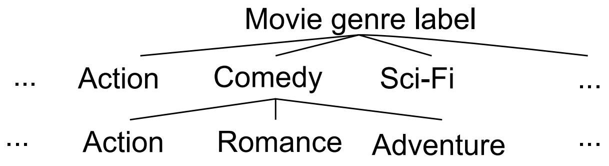

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## Predicting sequential data

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

| | | | | |
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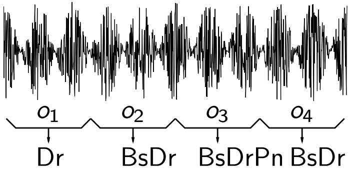

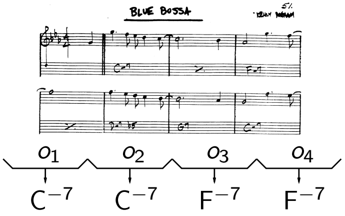

- Specialized inference algorithms can then be used (**forward-backward** method), which are easier to apprehend.
- More general methods can be used for more general structure (**belief propagation** and extensions), see for *e.g.* (Jensen and Nielsen, 2007).

## More 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: $\mathcal{D} = \{(\underline{\mathbf{x}}^{(1)}, \underline{y}^{(1)}), \cdots, (\underline{\mathbf{x}}^{(N)}, \underline{y}^{(N)})\}$.
- Remarks:
  - Observations are no longer assumed to be i.i.d within each sequence.
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## The CRF model

A discriminative model for structured-output data

### CRF model definition

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

- $Z(\underline{\mathrm{x}},\boldsymbol{\theta}) = \sum_{\underline{y}} \exp \sum_j \theta_j F_j(\underline{\mathrm{x}},\underline{y})$ is called a **partition function**.
- $\Psi(\underline{\mathrm{x}},\underline{y};\boldsymbol{\theta}) = \sum_{j=1}^{D} \theta_j F_j(\underline{\mathrm{x}},\underline{y})$ is called a **potential function**.
- **Remark**: feature functions $F_j(\underline{\mathrm{x}},\underline{y})$ depend on the whole sequence of observations $\underline{\mathrm{x}}$ 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 (Taskar et al., 2002; Settles, 2004; Lavergne et al., 2010)

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

- They have been successfully used for various **computer vision** tasks (He et al., 2004; Quattoni et al., 2007; Wang et al., 2006; Morency et al., 2007; Rudovic et al., 2012)

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

- Also for **speech analysis** tasks (Gunawardana et al., 2005; Reiter et al., 2007; Morris and Fosler-Lussier, 2008; Hong, 2010)

  *speech recognition, speech segmentation, speaker identification...*

- And a few applications to **music analysis** (Li, 2011; Schmidt and Kim, 2011; Imbrasaite et al., 2013; Joder et al., 2011).

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

## 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**

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

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

- 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

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

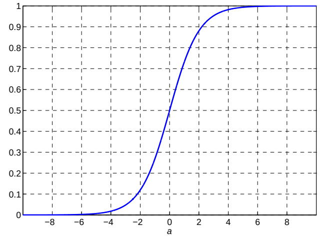
## The logistic sigmoid function

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

- 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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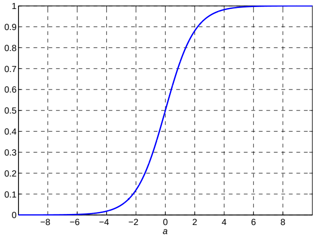

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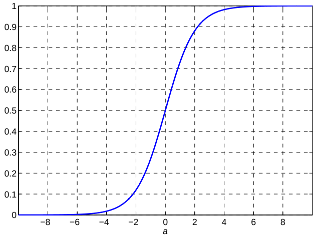

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## Maximum Entropy: an introductory example
By (Berger et al., 1996)

**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.

- The structure of both the ground-truth labels $y$ and the observations $o$ reflect a set of **facts** about the data: the translator's expertise.

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

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$\rightarrow$ Our model should capture these facts to perform accurate predictions.

## Using facts about the data

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

**In terms of statistics**

$P(dans) + P(en) + P(\grave{a}) + P(au\ cours\ de) + P(pendant) = 1$

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

**In terms of statistics**

$P(dans) = P(en) = P(\grave{a}) = P(au\ cours\ de) = P(pendant) = 1/5$

## 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 $P(dans)$, ..., $P(pendant)$?

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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." (Principle of Insufficient Reason)*

## More facts

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

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

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

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

## Even more facts

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

**In terms of statistics**

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

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

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

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: $\boldsymbol{\lambda}^* = \operatorname{argmax}_{\boldsymbol{\lambda}} L(p,\boldsymbol{\lambda})$.

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## Compare to the LR model

- Maxent model:

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

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- 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 $\mathbf{x} = (x_1, \cdots, x_j, \cdots, x_D)^T$;
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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.
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## Fitting the LR models

- Done by **maximum likelihood** estimation; in practice minimizing the **Negative Log-Likelihood (NLL)**.
- Let $\theta$ 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:

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

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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 $p(\mathbf{x};\boldsymbol{\theta}) \overset{\Delta}{=} p(y_i = 1|\mathbf{x}_i;\boldsymbol{\theta})$; 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**

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

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

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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 (Bottou, 2010): 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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  $\nabla g(\boldsymbol{\theta}_n)$ and $H(\boldsymbol{\theta}_n)$ are resp. the **gradient** and **Hessian** of $g(\boldsymbol{\theta})$ at $\boldsymbol{\theta}_n$.

- This approximation is a quadratic function which is minimized by solving:

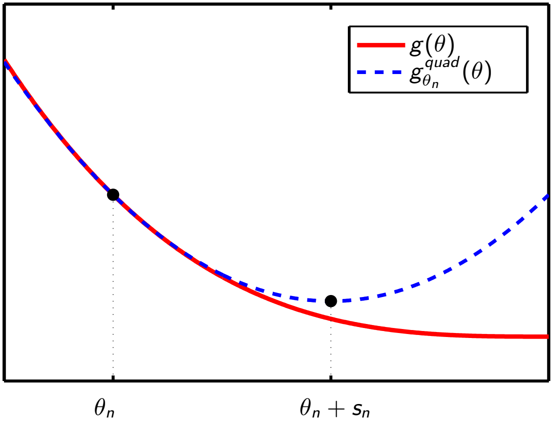
$$\nabla g(\boldsymbol{\theta}_n) + H(\boldsymbol{\theta}_n)(\boldsymbol{\theta} - \boldsymbol{\theta}_n) = 0.$$

Hence the **Newton-Raphson step**

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

## Optimization with the Newton-Raphson method

### Illustration



*Generated using pmtk3 (Dunham and Murphy, 2010)*

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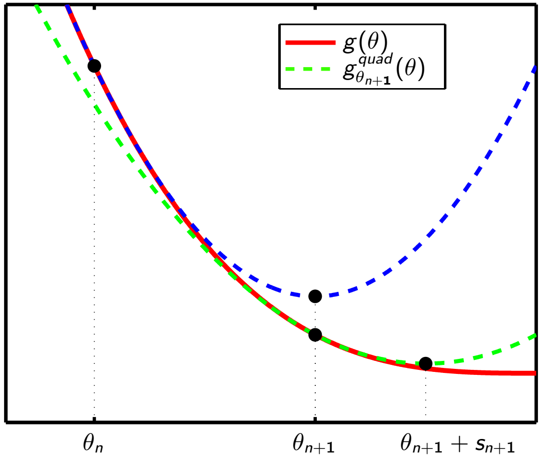

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## Optimization with the Newton-Raphson method

### 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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## $\ell_2$-regularization

- To **avoid overfitting** the complexity of the model should be penalized.
- Similarly to **ridge regression** (Hastie et al., 2009), 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**.

## $\ell_2$-regularization

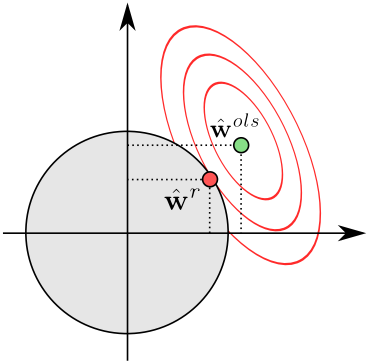
### Discussion

Recall that:

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

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 $\gamma$.

## $\ell_2$-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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## $\ell_1$-regularization

- Proceed as in the **LASSO** (Hastie et al., 2009), using a $\ell_1$-regularization.

**$\ell_1$-regularized logistic regression problem**

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

## $\ell_1$-regularization
### Discussion

- $\ell_1$-regularization achieves **feature selection**.

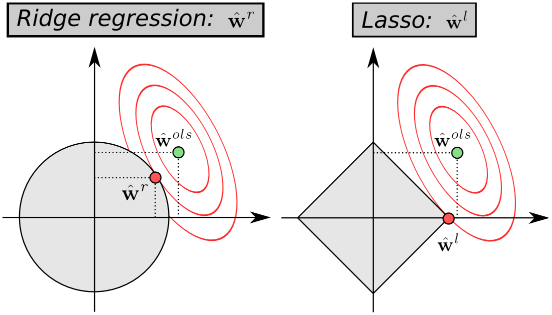

*Illustration by Alexandre Gramfort, Telecom ParisTech*

## $\ell_1$-regularization
### Discussion

- $\ell_1$-regularization achieves **feature selection**.

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

$\rightarrow$ specific optimization techniques needed (Yuan et al., 2010).

  - In configurations with groups of highly correlated features:
    - $\ell_1$-regularization tends to select randomly one feature in each group;
    - $\ell_2$-regularization tends to yield better prediction performance.

$\rightarrow$ Consider the **elastic net** model (Hastie et al., 2009):

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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:

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

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**Regularized KLR model estimation problem:**

$$\min_{\tilde{\mathbf{w}}} L(\tilde{\mathbf{w}}) = -\sum_{i=1}^{N} [y_i g(\mathbf{x}_i) - \log(1 + \exp g(\mathbf{x}_i))] + \frac{\gamma}{2} ||g||^2_{\mathcal{H}_\mathcal{K}}$$

- 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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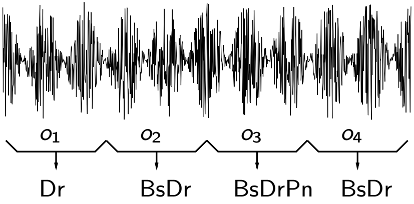
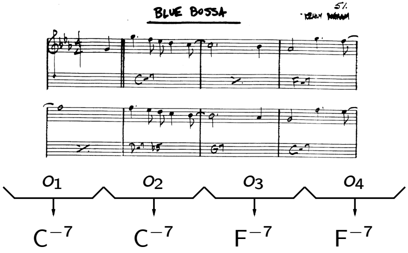
## Structured-output data

| **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: $\mathcal{D} = \{(\underline{\mathbf{x}}^{(1)}, \underline{y}^{(1)}), \cdots, (\underline{\mathbf{x}}^{(N)}, \underline{y}^{(N)})\}$.
- Remarks:
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## The CRF model

**CRF model definition**

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\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}
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- $Z(\underline{\mathbf{x}},\boldsymbol{\theta}) = \sum_{\underline{y}} \exp \sum_j \theta_j F_j(\underline{\mathbf{x}},\underline{y})$ 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**.
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  - CRFs appear to be an extension of logistic regression to structured data.
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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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$$F_j(\underline{x}, \underline{y}) = \sum_{i=1}^{n} f_j(y_{i-1}, y_i, \underline{x}, i) \; ; \quad \text{where } n \text{ is the length of } \underline{x}.$$

$\rightarrow$ 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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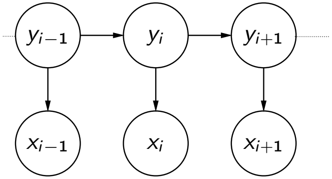
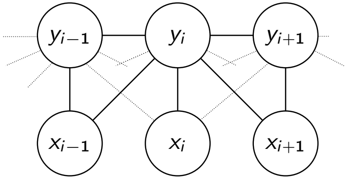


HMM



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.

$\rightarrow$ 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:
  - $\underline{\hat{y}} = \text{argmax}_{\underline{y}}\, p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta})$ ?
  - $Z(\underline{\mathbf{x}},\boldsymbol{\theta}) = \sum_{\underline{y}} \exp \sum_j F_j(\underline{\mathbf{x}},\underline{y})$ to deduce $p(\underline{y}|\underline{\mathbf{x}};\boldsymbol{\theta}) = \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}},\underline{y})$ ?

- **Parameter estimation**: given a training dataset $\mathcal{D} = \{(\underline{\mathbf{x}}^{(1)},\underline{y}^{(1)}),\cdots,(\underline{\mathbf{x}}^{(N)},\underline{y}^{(N)})\}$, how to estimate the optimal $\boldsymbol{\theta}$?

## Using linear-chain CRFs

- **Inference**: given a model $\boldsymbol{\theta}$, how to compute:
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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**:

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

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## 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

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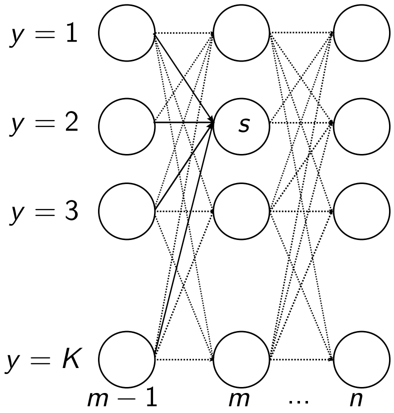

## Decoding the optimal sequence

- The intermediate scores $\delta_m(s)$ can be efficiently computed using[1]:

**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.

[1] *See Appendix for more details.*

## Decoding the optimal sequence

### Viterbi algorithm

**Initialization:**

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

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

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

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## Decoding the optimal sequence

### Backtracking

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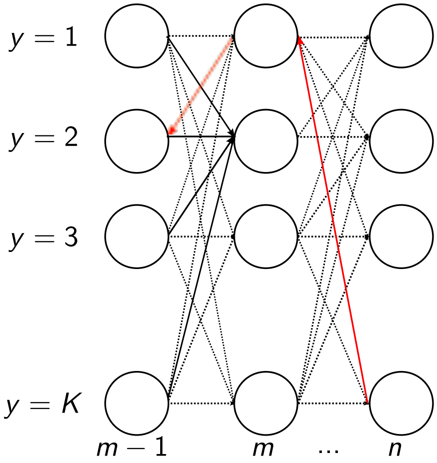

## Complexity of Viterbi decoding

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 (Ortmanns et al., 1996).

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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[2] 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:

**At the beginning of the sequence**

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

[2] *See Appendix for more details*

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## Marginal probability

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

**Marginal probability by forward-backward**

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

*More details in the appendix.*

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*More details in the appendix.*

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

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

$$\frac{\partial L(\mathcal{D};\boldsymbol{\theta})}{\partial\theta_k} = \sum_{q=1}^{N}\left\{\mathbb{E}_{p(\underline{y}|\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta})}\left[F_k(\underline{\mathbf{x}}^{(q)},\underline{y})\right] - F_k(\underline{\mathbf{x}}^{(q)},\underline{y}^{(q)})\right\}.$$

## 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

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

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

$$p(y_{i-1},y_i|\underline{\mathbf{x}}) = \frac{1}{Z(\underline{\mathbf{x}})}\alpha_{i-1}(y_{i-1})M_i(y_{i-1},y_i,\underline{\mathbf{x}})\beta_i(y_i).$$

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

$$p(y_{i-1},y_i|\underline{\mathbf{x}}) = \frac{1}{Z(\underline{\mathbf{x}})}\alpha_{i-1}(y_{i-1})M_i(y_{i-1},y_i,\underline{\mathbf{x}})\beta_i(y_i).$$

## Optimization

Many **algorithms** are available (see Sokolovska, 2010; Lavergne et al., 2010):

- Generalized iterative scaling (Lafferty et al., 2001): original algorithm, slow convergence, suboptimal.
- Conjugate gradient (Wallach, 2002): faster convergence, better quality.
- **L-BFGS** (McCallum, 2002): fast convergence, scalable; a good option, most used.
- Stochastic gradient: suboptimal, simple, online, **large-scale applications**.

## Regularization

### Using $\ell_2$-norm

- Redefine the objective function as: $L(\mathcal{D};\boldsymbol{\theta}) = L(\mathcal{D};\boldsymbol{\theta}) + \frac{||\boldsymbol{\theta}||_2^2}{2\sigma^2}$;
  $\sigma^2$: a free parameter penalizing large weights (as in **ridge regression**).
- The gradient coefficients become:
  $\frac{\partial L(\mathcal{D};\boldsymbol{\theta})}{\partial \theta_k} = \sum_{q=1}^{N} \left\{ \mathbb{E}_{p(\underline{y}|\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta})} \left[ F_k(\underline{\mathbf{x}}^{(q)}, \underline{y}) \right] - F_k(\underline{\mathbf{x}}^{(q)}, \underline{y}^{(q)}) \right\} + \frac{\theta_k}{\sigma^2}$.
- **Advantages**:
  - The objective becomes **strictly convex**.
  - Shrinkage of $\theta$ coefficients is achieved avoiding overfitting and numerical problems.
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## Regularization

### Using $\ell_1$-norm to perform feature selection

- Redefine the objective function as:
  $L(\mathcal{D};\boldsymbol{\theta}) = L(\mathcal{D};\boldsymbol{\theta}) + \rho||\boldsymbol{\theta}||_1 = L(\mathcal{D};\boldsymbol{\theta}) + \rho\sum_{j=1}^{D}|\theta_j|$ (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 Sokolovska, 2010).
- **Difficulties**:
  - The regularizer is **not differentiable** at zero: specific optimization techniques needed (Sokolovska, 2010).
  - In configurations with groups of highly correlated features, tend to select randomly one feature in each group.

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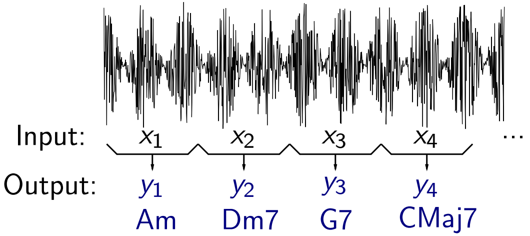
## Motivation

**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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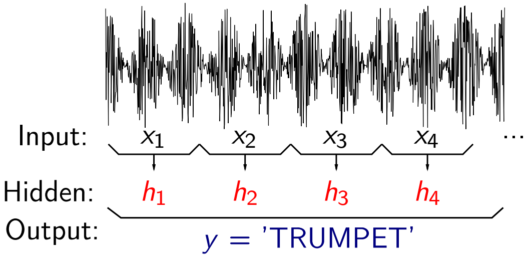

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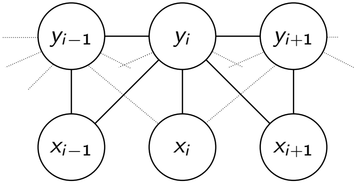

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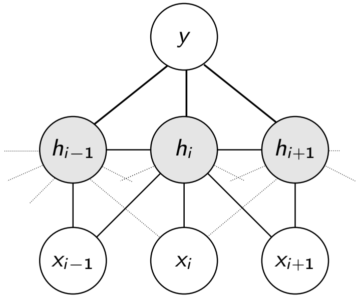

## The HCRF model
(Quattoni et al., 2007)

- Each sequence of observations $\underline{\mathrm{x}} = (\mathrm{x}_1, \cdots, \mathrm{x}_n)$ 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**

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

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

## Inference in HCRF

- HCRF model: $p(y, \underline{h}|\underline{\mathbf{x}}; \boldsymbol{\theta}) = \frac{1}{Z(\underline{\mathbf{x}},\boldsymbol{\theta})} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}, y, \underline{h})$.
- Let $Z'(y, \underline{\mathbf{x}}, \boldsymbol{\theta}) \triangleq \sum_{\underline{h}\in\mathcal{H}^n} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}, y, \underline{h})$: **marginalization** wrt $\underline{h}$.
- We have:
  - $Z(\underline{\mathbf{x}}, \theta) = \sum_y Z'(y, \underline{\mathbf{x}}, \theta)$;
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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:
  $\hat{y} = \text{argmax}_{y\in\mathcal{Y}} p(y|\underline{\mathbf{x}}; \theta^*) = \text{argmax}_{y\in\mathcal{Y}} \frac{Z'(y,\underline{\mathbf{x}},\theta)}{\sum_y Z'(y,\underline{\mathbf{x}},\theta)}$.
- To compute the partition function, use $Z(\underline{\mathbf{x}}, \theta) = \sum_y Z'(y, \underline{\mathbf{x}}, \theta)$.

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## 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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## Negative log-likelihood

$$\begin{aligned}
L(\mathcal{D};\boldsymbol{\theta}) &= -\sum_{q=1}^{N} \log p(y^{(q)}|\underline{\mathbf{x}}^{(q)};\boldsymbol{\theta}) \\
&= \sum_{q=1}^{N} \left\{ \log\left(\sum_{y} Z'(y,\underline{\mathbf{x}}^{(q)},\boldsymbol{\theta})\right) \right. \\
&\qquad \left. - \log\left(\sum_{\underline{h}\in\mathcal{H}} \exp \sum_{j=1}^{D} \theta_j F_j(\underline{\mathbf{x}}^{(q)}, y^{(q)}, \underline{h})\right) \right\}
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$L(D;\boldsymbol{\theta})$ is no longer convex $\rightarrow$ convergence to a local minimum.

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## NLL gradient

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

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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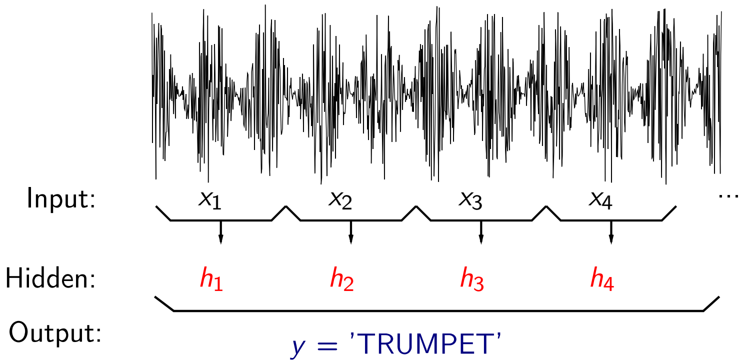
## Application to musical instrument classification



## Feature functions for HCRF

Following (Quattoni et al., 2007)

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

- $< \boldsymbol{\theta}(h_i), \mathbf{x}_i >$: 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:
  - $\ell_2$-regularized **HCRF** with 3 hidden states;
  - **Linear SVM**.
- Features: 47 cepstral, perceptual and temporal features.
- Results

| Classifier | SVM | HCRF |
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| Average accuracy | 75% | 76% |

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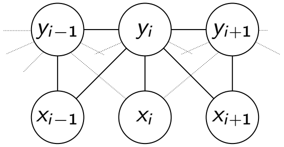
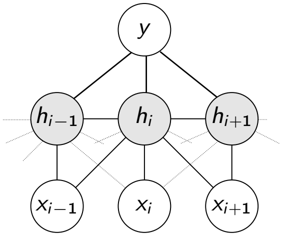
## Other extensions

- **LDCRF**: Latent-Dynamic Conditional Random Field (Sung and Jurafsky, 2009)

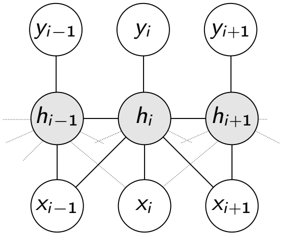
  modeling both hidden-states and structured-outputs.



CRF



HCRF



LDCRF

## Other extensions

- **LDCRF**: Latent-Dynamic Conditional Random Field (Morency et al., 2007)

  modeling both hidden-states and structured-outputs.
- **Kernel-CRF** (Laferty et al., 2004; Altun et al., 2004)

  introducing implicit features to account for (non-linear) interactions between original features.
- **Semi-Markov CRF** (Sarawagi and Cohen, 2005)

  modeling segment-level labels
- **CCRF**: Continuous CRF (Qin and Liu, 2008)

  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;

  → 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.

  → 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 | (Taku-ku, 2003) |
| crfChain | Matlab, C mex | Linear-chain CRF, categorical features, L-BFGS optimization | Schmidt (2008) |
| CRFsuite | C++, Python | Linear-chain CRF, NLP, various regularization and optimization methods (L-BFGS), designed for fast training | (Okazaki, 2007) |
| HCRF library | C++, Matlab, Python | CRF, HCRF, LDCRF, continuous inputs, L-BFGS optimization | (Morency, 2010) |
| Mallet | Java | CRF, maxent, HMM, NLP, text feature extraction routines, various optimization methods (L-BFGS) | (McCallum, 2002) |
| Wapiti | C99 | Linear-chain CRF, NLP, large label and feature sets, various regularization and optimization methods (L-BFGS, SGD), multi-threaded | (Lavergne et al., 2010) |

## 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

Y. Altun, A. Smola, and T. Hofmann. Exponential families for conditional random fields. In *Proceedings of the 20th conference on Uncertainty in artificial intelligence*, volume 0, 2004. URL http://dl.acm.org/citation.cfm?id=1036844.

A. L. Berger, S. A. D. Pietra, and Vincent J. Della Pietra. A Maximum Entropy Approach to Natural Language Processing. *Computational Linguistics*, 22(1), 1996.

L. Bottou. Stochastic Gradient Descent, 2010. URL http://leon.bottou.org/projects/sgd.

M. Dunham and K. P. Murphy. pmtk3: probabilistic modeling toolkit for Matlab/Octave, version 3, 2010. URL https://code.google.com/p/pmtk3/.

A. Gunawardana, M. Mahajan, A. Acero, and J. Platt. Hidden conditional random fields for phone classification. In *Interspeech*, 2005. URL http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.113.8190&rep=rep1&type=pdf.

T. Hastie, R. Tibshirani, and J. H. Friedman. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Springer, 2009. ISBN 0387848576. URL http://books.google.com/books?id=tVIjmNS3Ob8C&pgis=1.

X. He, R. Zemel, and M. Carreira-Perpinan. Multiscale conditional random fields for image labeling. In *IEEE Computer Society Conference on Computer Vision and Pattern Recognition, CVPR*, volume 2, pages 695–702. IEEE, 2004. ISBN 0-7695-2158-4. doi: 10.1109/CVPR.2004.1315232. URL http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=1315232.

W.-T. Hong. Speaker identification using Hidden Conditional Random Field-based speaker models. In *2010 International Conference on Machine Learning and Cybernetics*, pages 2811–2816. IEEE, July 2010. ISBN 978-1-4244-6526-2. doi: 10.1109/ICMLC.2010.5580793. URL http://ieeexplore.ieee.org/xpl/articleDetails.jsp?tp=&arnumber=5580793&contentType=Conference+Publications&searchField=Search_All&queryText=Hidden+Conditional+Random+Fields.

V. Imbrasaite, T. Baltrusaitis, and P. Robinson. Emotion tracking in music using continuous conditional random fields and relative feature representation. In *2013 IEEE International Conference on Multimedia and Expo Workshops (ICMEW)*. IEEE, July 2013. ISBN 978-1-4799-1604-7. doi: 10.1109/ICMEW.2013.6618357. URL http://ieeexplore.ieee.org/articleDetails.jsp?arnumber=6618357.

## Bibliography II

F. V. Jensen and T. D. Nielsen. *Bayesian Networks and Decision Graphs*. Springer, 2007. ISBN 0387682813. URL http://books.google.fr/books/about/Bayesian_Networks_and_Decision_Graphs.html?id=goSLmQq4UBcC&pgis=1.

C. Joder, S. Essid, and G. Richard. A Conditional Random Field Framework for Robust and Scalable Audio-to-Score Matching. *IEEE Transactions on Audio, Speech and Language Processing*, 19(8):2385–2397, 2011.

J. Laferty, Y. Liu, and X. Zhu. Kernel Conditional Random Fields: Representation, Clique Selection, and Semi-Supervised Learning. In *International Conference on Machine Learning*, 2004. URL http://scholar.google.com/scholar?hl=en&btnG=Search&q=intitle:Kernel+Conditional+Random+Fields+:+Representation+,+Clique+Selection+,+and+Semi-Supervised+Learning#5.

J. Lafferty, A. McCallum, and F. Pereira. Conditional random fields: Probabilistic models for segmenting and labeling sequence data. In *Machine learning international workshop then conference*, pages 282–289. Citeseer, 2001. URL http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.23.9849&amp;rep=rep1&amp;type=pdf.

T. Lavergne, O. Cappe, and F. Yvon. Practical very large scale CRFs. In *48th Annual Meeting of the Association for Computational Linguistics (ACL)*, number July, pages 504–513, Uppsala, Sweeden, 2010. URL http://www.aclweb.org/anthology/P10-1052.

C.-X. Li. *Exploiting label correlations for multi-label classification*. Master thesis, UC San Diego, 2011.

A. K. McCallum. Mallet: A machine learning for language toolkit, 2002. URL http://mallet.cs.umass.edu.

L.-P. Morency. HCRF: Hidden- state Conditional Random Field Library, 2010. URL http://sourceforge.net/projects/hcrf/.

L.-P. Morency, A. Quattoni, and T. Darrell. Latent-Dynamic Discriminative Models for Continuous Gesture Recognition. In *2007 IEEE Conference on Computer Vision and Pattern Recognition*, pages 1–8. IEEE, June 2007. ISBN 1-4244-1179-3. doi: 10.1109/CVPR.2007.383299. URL http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumber=4270324.

J. Morris and E. Fosler-Lussier. Conditional Random Fields for Integrating Local Discriminative Classifiers. *TASLP*, 16(3):617–628, 2008. ISSN 1558-7916. doi: 10.1109/TASL.2008.916057. URL http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumber=4451149.

## Bibliography III

N. Okazaki. CRFsuite: a fast implementation of Conditional Random Fields (CRFs), 2007. URL http://www.chokkan.org/software/crfsuite/.

S. Ortmanns, H. Ney, and A. Eiden. Language-model look-ahead for large vocabulary speech recognition. In *Proceeding of Fourth International Conference on Spoken Language Processing. ICSLP '96*, volume 4, pages 2095–2098. IEEE, 1996. ISBN 0-7803-3555-4. doi: 10.1109/ICSLP.1996.607215. URL http://ieeexplore.ieee.org/articleDetails.jsp?arnumber=607215.

T. Qin and T. Liu. Global ranking using continuous conditional random fields. In *Advances in Neural and Information Processing Systems*, 2008. URL http://machinelearning.wustl.edu/mlpapers/paper_files/NIPS2008_0518.pdf.

A. Quattoni, S. Wang, L.-P. Morency, M. Collins, and T. Darrell. Hidden conditional random fields. *IEEE transactions on pattern analysis and machine intelligence*, 29(10):1848–53, Oct. 2007. ISSN 0162-8828. doi: 10.1109/TPAMI.2007.1124. URL http://www.ncbi.nlm.nih.gov/pubmed/17699927.

S. Reiter, B. Schuller, and G. Rigoll. Hidden Conditional Random Fields for Meeting Segmentation. In *Multimedia and Expo, 2007 IEEE International Conference on*, pages 639–642. IEEE, July 2007. ISBN 1-4244-1016-9. doi: 10.1109/ICME.2007.4284731. URL http://ieeexplore.ieee.org/xpl/articleDetails.jsp?tp=&arnumber=4284731&contentType=Conference+Publications&searchField=Search_All&queryText=Hidden+Conditional+Random+Fields.

O. Rudovic, V. Pavlovic, and M. Pantic. Kernel conditional ordinal random fields for temporal segmentation of facial action units. In *Computer Vision - ECCV*, pages 1–10, 2012. URL http://link.springer.com/chapter/10.1007/978-3-642-33868-7_26.

S. Sarawagi and W. Cohen. Semi-markov conditional random fields for information extraction. In *Advances in Neural Information Processing Systems*, 2005. URL http://machinelearning.wustl.edu/mlpapers/paper_files/NIPS2005_427.pdf.

E. Schmidt and Y. Kim. Modeling musical emotion dynamics with conditional random fields. In *International Conference on Music Information Retrieval (ISMIR)*, number Ismir, pages 777–782, Miami, FL, USA, 2011. URL http://music.ece.drexel.edu/files/Navigation/Publications/Schmidt2011c.pdf.

M. Schmidt. crfChain, 2008. URL http://www.di.ens.fr/~mschmidt/Software/crfChain.html.

## Bibliography IV

B. Settles. Biomedical named entity recognition using conditional random fields and rich feature sets. *International Joint Workshop on Natural Language Processing in Biomedicine and its Applications*, 2004. URL `http://dl.acm.org/citation.cfm?id=1567618`.

N. Sokolovska. *Contributions to the estimation of probabilistic discriminative models: semi-supervised learning and feature selection*. PhD thesis, Telecom ParisTech, 2010.

Y.-H. Sung and D. Jurafsky. Hidden Conditional Random Fields for phone recognition. *2009 IEEE Workshop on Automatic Speech Recognition & Understanding*, pages 107–112, Dec. 2009. doi: 10.1109/ASRU.2009.5373329. URL `http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumber=5373329`.

Taku-ku. CRF++, 2003. URL `http://crfpp.googlecode.com/svn/trunk/doc/index.html`.

B. Taskar, P. Abbeel, and D. Koller. Discriminative probabilistic models for relational data. In *Proceedings of the Eighteenth conference on Uncertainty in Artificial Intelligence (UAI02)*, 2002. URL `http://dl.acm.org/citation.cfm?id=2073934`.

H. M. Wallach. *Efficient Training of Conditional Random Fields*. PhD thesis, University of Edinburgh, 2002.

S. B. Wang, A. Quattoni, L.-P. Morency, and D. Demirdjian. Hidden Conditional Random Fields for Gesture Recognition. pages 1521–1527. IEEE Computer Society, 2006. ISBN 0-7695-2597-0. URL `http://portal.acm.org/citation.cfm?id=1153171.1153627`.

G. Yuan, K. Chang, C. Hsieh, and C. Lin. A comparison of optimization methods and software for large-scale l1-regularized linear classification. *The Journal of Machine Learning Research*, 2010. URL `http://dl.acm.org/citation.cfm?id=1953034`.

J. Zhu and T. Hastie. Support vector machines, kernel logistic regression and boosting. *Multiple Classifier Systems*, 2364:16–26, 2002. URL `http://link.springer.com/chapter/10.1007/3-540-45428-4_2`.

## LR model learning with stochastic gradient descent (SGL)

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

Algorithm

```
- Initialise $\tilde{\mathbf{w}}$
- Repeat    (until convergence)
    - Randomly permute training examples $\mathbf{x}_i$
    - For $i = 1 : N$
        $w_j \leftarrow w_j + t\,(y_{\sigma_i} - p_{\sigma_i})\, x_{j\sigma_i}$ ; $j = 1, \cdots, D$
```

- $t$ : *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

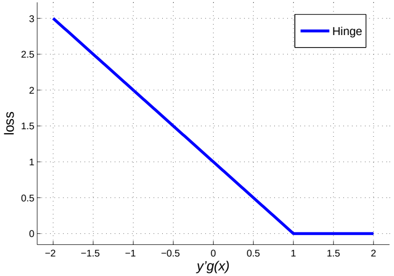
### Recalling SVM as a regularized function fitting problem

- 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**

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



## 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**

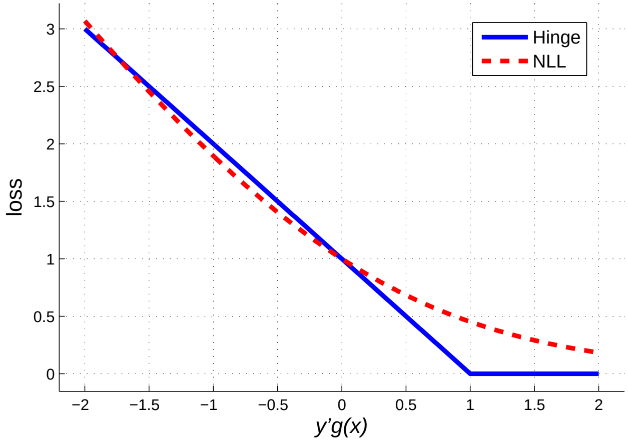
$$l(y'_i g(\mathbf{x}_i)) = \log\left(1 + \exp -y'_i f(\mathbf{x}_i)\right)$$

**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



## Decoding the optimal sequence

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

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

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

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

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

## Viterbi decoding

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

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

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

## Viterbi decoding

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

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

## Viterbi decoding

### The algorithm

**Initialization:**

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

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

$$\begin{aligned}\delta_m(s) &= \max_{y \in \mathcal{Y}} \left[\delta_{m-1}(y) + g_m(y, s)\right]\\ \psi_m(s) &= \operatorname*{argmax}_{y \in \mathcal{Y}} \left[\delta_{m-1}(y) + g_m(y, s)\right]\end{aligned}$$

**Termination:**

$$\begin{aligned}\delta_n(y_n^*) &= \max_{y \in \mathcal{Y}} \delta_n(y)\\ y_n^* &= \operatorname*{argmax}_{y \in \mathcal{Y}} \delta_n(y)\end{aligned}$$

**Path backtracking:**

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

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

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## The forward recursion

Define $\alpha$ scores as:

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

### 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**

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

## Marginal probability

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

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

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

## Marginal probability

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

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& \times \sum_{\{y_{m+1},\dots,y_n\}} \prod_{i=m+1}^{n} M_i(y_{i-1}, y_i, \underline{\mathbf{x}})
\end{aligned}
$$

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