Probabilistic models - Bayesian Methods

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Parametric Family of Densities

- A **parametric family of densities** is a set

$$\{p(y \mid \theta) : \theta \in \Theta\},$$

  - where $p(y \mid \theta)$ is a density on a **sample space** $\mathcal{Y}$, and
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  - θ is a **parameter** in a [finite dimensional] **parameter space** Θ**.**
- This is the common starting point for a treatment of classical or Bayesian statistics.
- In this lecture, whenever we say "density", we could replace it with "mass function." (and replace integrals with sums).

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- But instead of θ, we have data $\mathcal{D}$: $y_1, \ldots, y_n$ sampled i.i.d. from $p(y \mid \theta)$.
- Statistics is about how to get by with $\mathcal{D}$ in place of θ.

Point Estimation

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- **Maximum likelihood estimators** are consistent and efficient under reasonable conditions.

Example of Point Estimation: Coin Flipping

- Parametric family of mass functions:

$$p(\text{Heads} \mid \theta) = \theta,$$

  for $\theta \in \Theta = (0, 1)$.

Coin Flipping: MLE

- Data $\mathcal{D} = (H, H, T, T, T, T, T, H, \ldots, T)$, assumed i.i.d. flips.
  - n_h: number of heads
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- As usual, it is easier to maximize the log-likelihood function:

$$\begin{aligned} \hat{\theta}_{\text{MLE}} &= \underset{\theta \in \Theta}{\arg\max} \log L_{\mathcal{D}}(\theta) \\ &= \underset{\theta \in \Theta}{\arg\max} \left[n_h \log \theta + n_t \log(1-\theta) \right] \end{aligned}$$

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$\hat{\theta}_{\text{MLE}}$ is the empirical fraction of heads.

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- The prior reflects our belief about θ, **before seeing any data**.

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  1. A parametric family of densities
  $$\{p(\mathcal{D} \mid \theta) \mid \theta \in \Theta\}.$$
  2. A **prior distribution** $p(\theta)$ on parameter space Θ.
- Putting the pieces together, we get a joint density on θ and $\mathcal{D}$:
$$p(\mathcal{D}, \theta) = p(\mathcal{D} \mid \theta)p(\theta).$$

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- The posterior represents the **rationally updated belief** about θ, after seeing $\mathcal{D}$.

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- Where $\propto$ means we've dropped factors that are independent of θ.

Coin Flipping: Bayesian Model

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- One convenient choice would be a distribution from the Beta family

Coin Flipping: Beta Prior

- **Prior:**

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\begin{aligned}
\theta &\sim \text{Beta}(\alpha, \beta) \\
p(\theta) &\propto \theta^{\alpha-1}(1-\theta)^{\beta-1}
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Figure by Horas based on the work of Krishnavedala (Own work) [Public domain], via Wikimedia Commons
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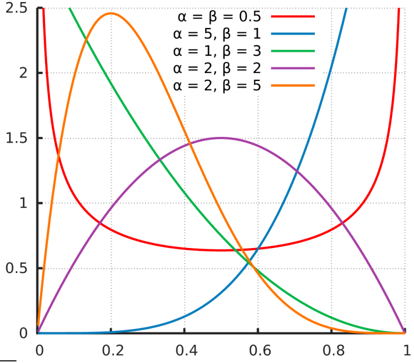

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- **Mode of Beta distribution:**

$$\arg\max_{\theta} p(\theta) = \frac{h-1}{h+t-2}$$

for $h, t > 1$.

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- **Interpretation**:
  - Prior initializes our counts with h heads and t tails.
  - Posterior increments counts by observed n_h and n_t.

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- The beta family is conjugate to the coin-flipping (i.e. Bernoulli) model.

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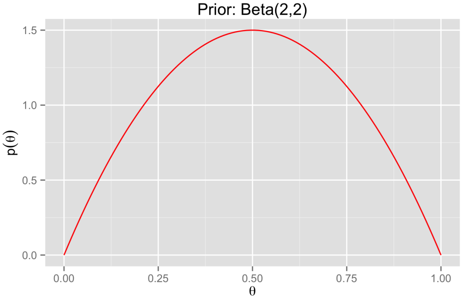

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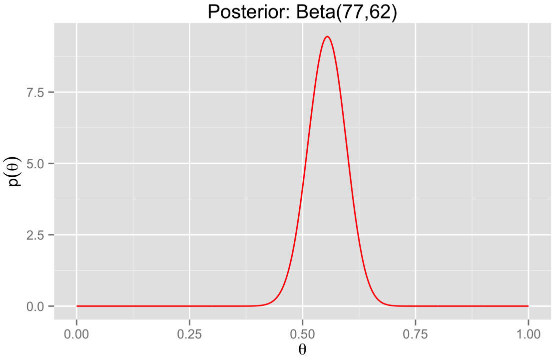
- **Posterior distribution:** $\theta \mid \mathcal{D} \sim \textbf{Beta}(77, 62)$:



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- Common options:
  - **posterior mean** $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}]$
  - **maximum a posteriori (MAP) estimate** $\hat{\theta} = \arg\max_\theta p(\theta \mid \mathcal{D})$
    - Note: this is the **mode** of the posterior distribution

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- Extract a **credible set** for θ (a Bayesian confidence interval).
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- Select a point estimate using **Bayesian decision theory**:
  - Choose a loss function.
  - Find action **minimizing expected risk w.r.t. posterior**

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- Ingredients:
  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
  - **Action space** $\mathcal{A}$.
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- A **Bayes action** a^* is an action that minimizes posterior risk:

$$
r(a^*) = \min_{a \in \mathcal{A}} r(a)
$$

Bayesian Point Estimation

- General Setup:
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Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \quad \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \quad \Rightarrow$ posterior mode
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- Optimal decision depends on the loss function and the posterior distribution.
- We will derive the square loss case next.

Bayesian Point Estimation: Square Loss

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- The **Bayes action** for **square loss** is the posterior mean.

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    - **family of distributions**, indexed by Θ, and
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  - For decision making, we need a **loss function**.

Conditional Probability Modeling

- **Input space** $\mathcal{X}$
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- A **parametric family of conditional densities** is a set

$$\{p(y \mid x, \theta) : \theta \in \Theta\},$$

  - where $p(y \mid x, \theta)$ is a density on **outcome space** $\mathcal{Y}$ for each x in **input space** $\mathcal{X}$, and
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- This is the common starting point for either classical or Bayesian regression.

Classical treatment: Likelihood Function

- **Data:** $\mathcal{D} = (y_1, \ldots, y_n)$
- The probability density for our data $\mathcal{D}$ is

$$p(\mathcal{D} \mid x_1, \ldots, x_n, \theta) = \prod_{i=1}^{n} p(y_i \mid x_i, \theta).$$

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$$p(\mathcal{D} \mid x_1, \ldots, x_n, \theta) \quad = \quad \prod_{i=1}^{n} p(y_i \mid x_i, \theta).$$

- For fixed $\mathcal{D}$, the function $\theta \mapsto p(\mathcal{D} \mid x, \theta)$ is the **likelihood function**:

$$L_{\mathcal{D}}(\theta) = p(\mathcal{D} \mid x, \theta),$$

where $x = (x_1, \ldots, x_n)$.

Maximum Likelihood Estimator

- The **maximum likelihood estimator (MLE)** for θ in the family $\{p(y \mid x, \theta) \mid \theta \in \Theta\}$ is

$$\hat{\theta}_{\text{MLE}} = \underset{\theta \in \Theta}{\arg\max}\, L_{\mathcal{D}}(\theta).$$

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- The corresponding prediction function is

$$\hat{f}(x) = p(y \mid x, \hat{\theta}_{\text{MLE}}).$$

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- Input space $\mathcal{X} = \mathbf{R}^d$ Outcome space $\mathcal{Y} = \mathbf{R}$

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- Each θ corresponds to a prediction function,
  - i.e. the conditional distribution function $p(y \mid x, \theta)$.

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- We may want to use
  - $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}, x]$ (the posterior mean estimate)
  - $\hat{\theta} = \text{median}[\theta \mid \mathcal{D}, x]$
  - $\hat{\theta} = \arg\max_{\theta \in \Theta} p(\theta \mid \mathcal{D}, x)$ (the MAP estimate)
- depending on our loss function.

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- Having set our Bayesian model, how do we predict a distribution on y for input x?
- We don't need to make a discrete selection from the hypothesis space: we **maintain uncertainty**.

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- In the frequentist approach, we choose $\hat{\theta} \in \Theta$, and predict

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- In the Bayesian approach, we integrate out over Θ w.r.t. $p(\theta \mid \mathcal{D})$ and predict with

$$p(y \mid x, \mathcal{D}) = \int p(y \mid x; \theta) p(\theta \mid \mathcal{D}) \, d\theta$$

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- $x \mapsto \arg\max_{y \in \mathcal{Y}} p(y \mid x, \mathcal{D})$, to minimize expected 0/1 loss
- Each of these can be derived from $p(y \mid x, \mathcal{D})$.

Example in 1-Dimension: Setup

- Input space $\mathcal{X} = [-1, 1]$ Output space $\mathcal{Y} = \mathbf{R}$
- Given x, the world generates y as

$$y = w_0 + w_1 x + \varepsilon,$$

where $\varepsilon \sim \mathcal{N}(0, 0.2^2)$.

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- Written another way, the **conditional probability model** is

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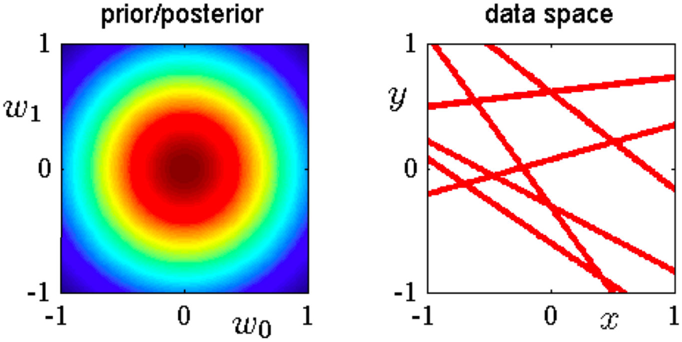
- What's the parameter space? $\mathbf{R}^2$.
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2} I\right)$

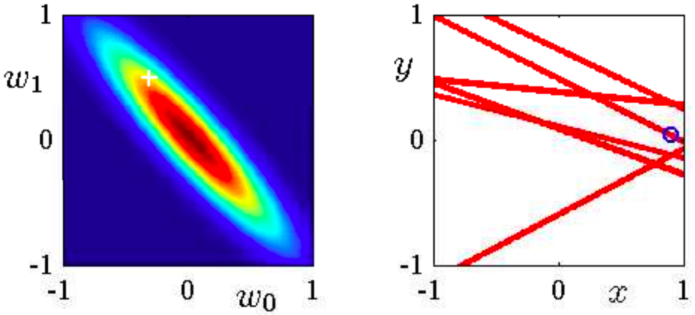
Example in 1-Dimension: Prior Situation

- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$ (Illustrated on left)



- On right, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}\left(0, \frac{1}{2}I\right)$.

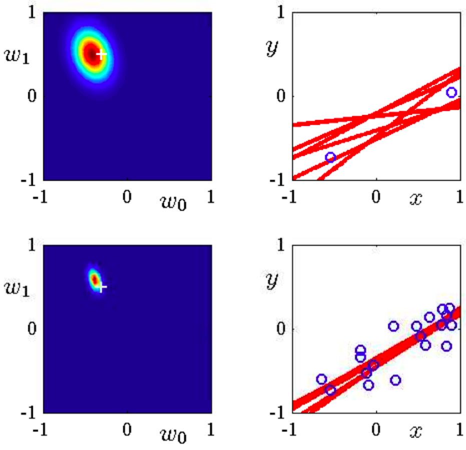
Bishop's PRML Fig 3.7



- On left: posterior distribution; white cross indicates true parameters
- On right:
  - blue circle indicates the training observation
  - red lines, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w|\mathcal{D})$ (posterior)

Bishop's PRML Fig 3.7

Example in 1-Dimension: 2 and 20 Observations



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Closed Form for Posterior

- Model:

$$w \sim \mathcal{N}(0, \Sigma_0)$$

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$$
\begin{array}{rcl}
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y_i \mid x, w & \text{i.i.d.} & \mathcal{N}(w^T x_i, \sigma^2)
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- **Posterior Variance** Σ_P gives us a natural **uncertainty measure.**

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which is of course the ridge regression solution.

Connection the MAP to Ridge Regression

- The **Posterior density** on w for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

$$p(w \mid \mathcal{D}) \quad \propto \quad \underbrace{\exp\left(-\frac{\lambda}{2\sigma^2}\|w\|^2\right)}_{\textbf{prior}} \underbrace{\prod_{i=1}^{n} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right)}_{\textbf{likelihood}}$$

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- Which is the ridge regression objective.

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- Given a new input point x_{new}, how do we predict y_{new} ?

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- For Gaussian regression, predictive distribution has closed form.

Closed Form for Predictive Distribution

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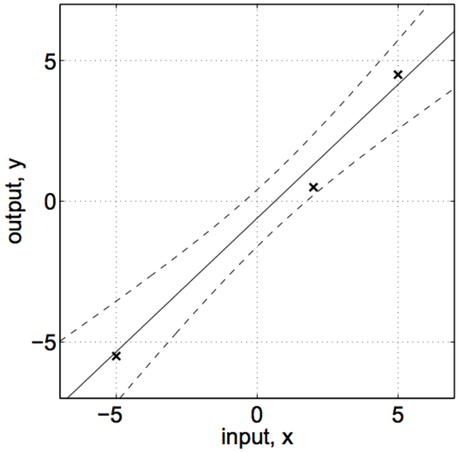
Bayesian Regression Provides Uncertainty Estimates

- With predictive distributions, we can give mean prediction with error bands:



Rasmussen and Williams' *Gaussian Processes for Machine Learning*, Fig.2.1(b)

Motivation

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- Many real-world problems have more than two classes.
  - Document classification (over 10 classes)
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- What are some potential issues when we have a large number of classes?
  - Computation cost
  - Class imbalance
  - Different cost of errors

Today's lecture

- How to *reduce* multiclass classification to binary classification?
  - We can think of binary classifier or linear regression as a black box. Naive ways:
  - E.g. multiple binary classifiers produce a binary code for each class (000, 001, 010)
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- How do we *generalize* binary classification algorithm to the multiclass setting?
  - We also need to think about the loss function.
- Example of very large output space: structured prediction.
  - Multi-class: Mutually exclusive class structure.
  - Text: Temporal relational structure.

One-vs-All / One-vs-Rest

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

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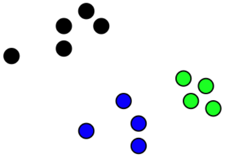
- Majority vote:

$$h(x) = \underset{i \in \{1, \ldots, k\}}{\arg\max}\, h_i(x)$$

- Ties can be broken arbitrarily.

OvA: 3-class example (linear classifier)

<1-> Consider a dataset with three classes:



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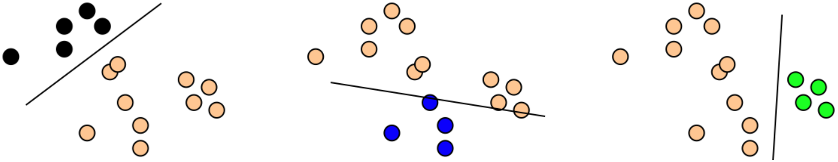

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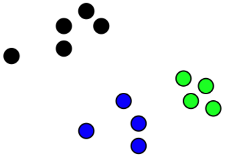

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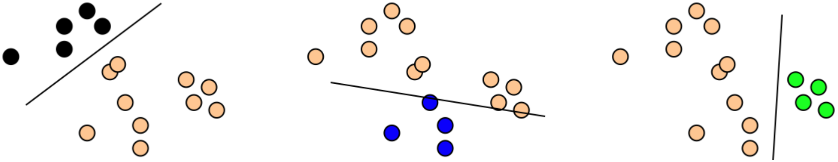

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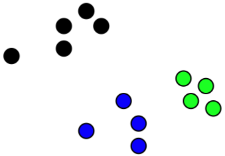

Assumption: each class is linearly separable from the rest.

Ideal case: only target class has positive score.

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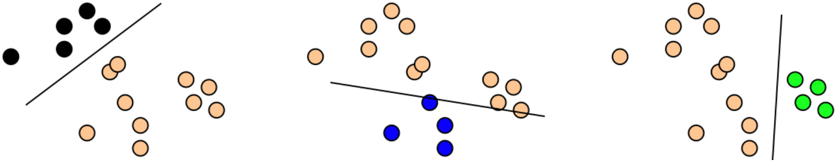

OvA: 4-class non linearly separable example

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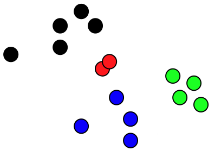

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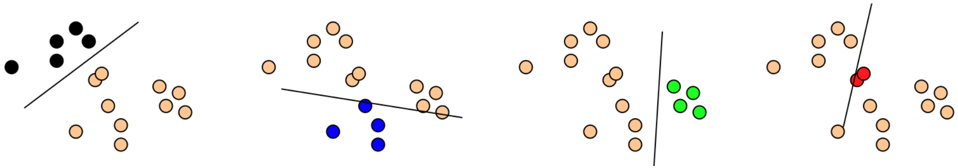

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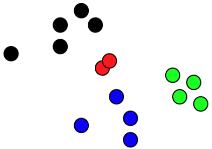
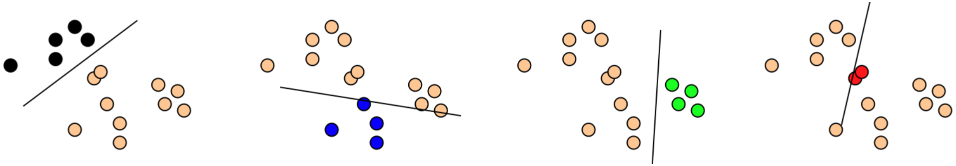


Cannot separate red points from the rest.
Which classes might have low accuracy?

Train OvA classifiers:



All vs All / One vs One / All pairs

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Prediction

- Majority vote (each class gets $k-1$ votes)

$$h(x) = \underset{i \in \{1,\ldots,k\}}{\arg\max} \sum_{j \neq i} \underbrace{h_{ij}(x) i < j}_{\text{class } i \text{ is } +1} - \underbrace{h_{ji}(x) j < i}_{\text{class } i \text{ is -1}}$$

- Tournament
- Ties can be broken arbitrarily.

AvA: four-class example

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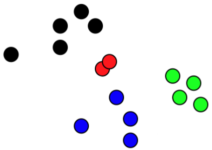
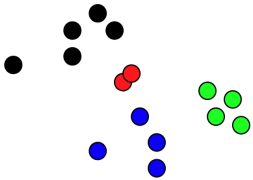


What's the decision region for the red class?



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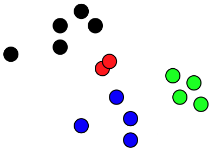

Assumption: each pair of classes are linearly separable.
More expressive than OvA.

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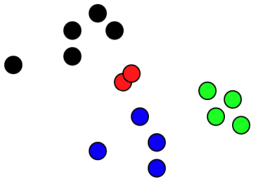

OvA vs AvA

		OvA	AvA
computation	train	$O(k\qquad\qquad)$	$O(k^2\qquad\qquad)$
	test	$O(k\qquad)$	$O(k^2\qquad)$

OvA vs AvA

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computation	train	$O(kB_{\text{train}}(n))$	$O(k^2 B_{\text{train}}(n/k))$
	test	$O(kB_{\text{test}})$	$O(k^2 B_{\text{test}})$

challenges

OvA vs AvA

		OvA	AvA
computation	train	$O(kB_{\text{train}}(n))$	$O(k^2 B_{\text{train}}(n/k))$
	test	$O(kB_{\text{test}})$	$O(k^2 B_{\text{test}})$
challenges	train	class imbalance	small training set
	test	calibration / scale tie breaking	

Lack theoretical justification but simple to implement and works well in practice (when # classes is small).

Code word for labels

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Key idea: Encode labels as binary codes and predict the code bits directly.

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OvA encoding:

class	h_1	h_2	h_3	h_4
1	1	0	0	0
2	0	1	0	0
3	0	0	1	0
4	0	0	0	1

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Key idea: Encode labels as binary codes and predict the code bits directly.
OvA encoding:

class	h_1	h_2	h_3	h_4
1	1	0	0	0
2	0	1	0	0
3	0	0	1	0
4	0	0	0	1

OvA uses k bits to encode each label, what's the minimal number of bits you can use?

Error correcting output codes (ECOC)

Example: 8 classes, 6-bit code

class	h_1	h_2	h_3	h_4	h_5	h_6
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Training Binary classifier h_i:

- +1: classes whose i-th bit is 1
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Code design Want good binary classifiers.

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- Computationally more efficient than OvA (a special case of ECOC). Better for large k.
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  - In plain words, if rows are far from each other, ECOC is robust to errors.
- Trade-off between code distance and binary classification performance.
- Nice theoretical results [Allwein et al., 2000] (also incoporates AvA).

Review

Reduction-based approaches:

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Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA
- Key is to design "natural" binary classification problems without large computation cost.

But,

- Unclear how to generalize to extremely large # of classes.
- ImageNet: >20k labels; Wikipedia: >1M categories.

Next, generalize previous algorithms to multiclass settings.

Binary Logistic Regression

- Given an input x, we would like to output a classification between (0,1).

$$f(x) = sigmoid(z) = \frac{1}{1+\exp(-z)} = \frac{1}{1+\exp(-w^\top x - b)}. \tag{1}$$

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- Another way to view: one class has $(+w, +b)$ and the other class has $(-w, -b)$.

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- Gradient: $\frac{\partial L}{\partial z} = f - y$. Recall: MSE loss.

Comparison to OvA

- **Base Hypothesis Space**: $\mathcal{H} = \{h : \mathcal{X} \to \mathrm{R}\}$ (score functions).
- **Multiclass Hypothesis Space** (for k classes):

$$\mathcal{F} = \left\{ x \mapsto \arg\max_i h_i(x) \mid h_1, \ldots, h_k \in \mathcal{H} \right\}$$

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- OvA objective: $h_i(x) > 0$ for x with label i and $h_i(x) < 0$ for x with all other labels.
- At test time, to predict (x, i) correctly we only need

$$h_i(x) > h_j(x) \qquad \forall j \neq i. \tag{4}$$

Multiclass Perceptron

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Given a multiclass dataset $= (x, y)$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
  for $(x, y) \in$ **do**
    $\hat{y} = \arg\max_{y' \in} w_{y'}^T x$;
    if $\hat{y} \neq y$ **then** `// We've made a mistake`
      $w_y \leftarrow w_y + x$; `// Move the target-class scorer towards` x
      $w_{\hat{y}} \leftarrow w_{\hat{y}} - x$; `// Move the wrong-class scorer away from` x
    end
  end
end

Rewrite the scoring function

- Remember that we want to scale to very large # of classes and reuse algorithms and analysis for binary classification
  - $\Longrightarrow$ a single weight vector is desired
- How to rewrite the equation such that we have one w instead of k?

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$$w_i^T x = w^T \psi(x, i) \tag{5}$$
$$h_i(x) = h(x, i) \tag{6}$$

  - Encode labels in the feature space.
  - Score for each label $\to$ score for the "*compatibility*" of a label and an input.

The Multivector Construction

How to construct the feature map ψ?

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- What if we stack w_i's together $(x \in^2, = 1, 2, 3)$

$$w = \left(\underbrace{-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_1}, \underbrace{0, 1}_{w_2}, \underbrace{\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_3} \right)$$

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- And then do the following: $\Psi : \mathrm{R}^2 \times \{1, 2, 3\} \to \mathrm{R}^6$ defined by

$$\begin{aligned}
\Psi(x, 1) &:= (x_1, x_2, 0, 0, 0, 0) \\
\Psi(x, 2) &:= (0, 0, x_1, x_2, 0, 0) \\
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- Then $\langle w, \Psi(x, y) \rangle = \langle w_y, x \rangle$, which is what we want.

Rewrite multiclass perceptron

Multiclass perceptron using the multivector construction.

Given a multiclass dataset $= (x, y)$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
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Exercise: What is the base binary classification problem in multiclass perceptron?

Features

Toy multiclass example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}$
- $\mathcal{Y} = \{\text{NOUN,VERB,ADJECTIVE,} \ldots\}$.

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How to construct the feature vector?

- Multivector construction: $w \in^{d \times k}$—doesn't scale.
- Directly design features for each class.

$$\Psi(x,y) = (\psi_1(x,y), \psi_2(x,y), \psi_3(x,y), \ldots, \psi_d(x,y)) \tag{7}$$

- Size can be bounded by d.

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Sample training data:

`The boy grabbed the apple and ran away quickly .`

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- E.g., $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \ldots)$
- After training, what's w_1, w_2, w_3, w_4?
- No need to include features unseen in training data.

Feature templates: implementation

- Flexible, neighboring words, suffix/prefix.
- "Read off" features from the training data.
- Often sparse—efficient in practice, NLP problems.
- Can use a hash function: template $\rightarrow 1, 2, \ldots, d$.

Review

Ingredients in multiclass classification:

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- Represent labels in the input space $\Longrightarrow$ single weight vector.

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We've seen

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- Very simple idea. Was popular in NLP for structured prediction (tagging, parsing).

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- Very simple idea. Was popular in NLP for structured prediction (tagging, parsing).

Next,

- How to generalize SVM to the multiclass setting.
- Concept check: Why might one prefer SVM / perceptron?

Margin for Multiclass

Binary

- Margin for (,):

$$w^T \tag{8}$$

- Want margin to be large and positive (w^T has same sign as)

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Multiclass

- Class-specific margin for $(,)$:

$$h(,) - h(,y). \tag{9}$$

- Difference between scores of the correct class and each other class
- Want margin to be large and positive for all $y \neq$.

Multiclass SVM: separable case

Binary

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{10}$$

$$\text{s.t.} \quad \underbrace{w^T}_{\text{margin}} \geqslant 1 \quad \forall (,) \in \tag{11}$$

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Multiclass As in the binary case, take 1 as our target margin.

$$m_{n,y}(w) \quad \underbrace{\langle w, \Psi(,)\rangle}_{\text{score of correct class}} - \underbrace{\langle w, \Psi(,y)\rangle}_{\text{score of other class}} \tag{12}$$

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{13}$$

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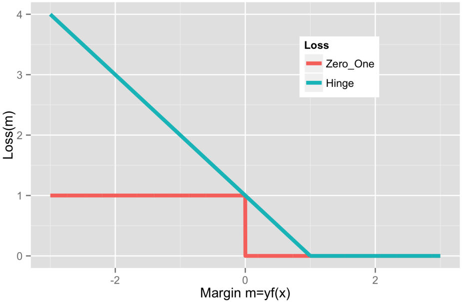
Exercise: write the objective for the non-separable case

Recap: hingle loss for binary classification

- Hinge loss: a convex upperbound on the 0-1 loss

$$\ell_{\text{hinge}}(y, \hat{y}) = \max(0, 1 - yh(x)) \tag{15}$$



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$$\implies \Delta(y, \hat{y}) \leqslant \Delta(y, \hat{y}) - \langle w, \Psi(x, y) - \Psi(x, \hat{y}) \rangle \qquad \text{When are they equal?} \tag{19}$$

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- Generalized hinge loss:

$$\ell_{\text{hinge}}(y, x, w) \max_{y' \in} \Delta(y, y') - \left\langle w, \Psi(x, y) - \Psi(x, y') \right\rangle \tag{20}$$

Multiclass SVM with Hinge Loss

- Recall the hinge loss formulation for binary SVM (without the bias term):

$$\min_{w \in \mathrm{R}^d} \frac{1}{2}||w||^2 + C \sum_{n=1}^{N} \max\left(0, 1 - \underbrace{w^T}_{\text{margin}}\right).$$

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- The multiclass objective:

$$\min_{w \in \mathrm{R}^d} \frac{1}{2}||w||^2 + C \sum_{n=1}^{N} \max_{y' \in} \Delta(y, y') - \underbrace{\left\langle w, \Psi(x, y) - \Psi(x, y') \right\rangle}_{\text{margin}}$$

  - $\Delta(y, y')$ as target margin for each class.
  - If margin $m_{n,y'}(w)$ meets or exceeds its target $\Delta(, y')$ $\forall y \in$, then no loss on example n.

Recap: What Have We Got?

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- Problem: Multiclass classification $\mathcal{Y} = \{1, \ldots, k\}$
- Solution 1: One-vs-All
  - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathrm{R}$.
  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
  - Gave simple example where this fails for linear classifiers

Recap: What Have We Got?

- Problem: Multiclass classification $\mathcal{Y} = \{1, \ldots, k\}$
- Solution 1: One-vs-All
  - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathrm{R}$.
  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
  - Gave simple example where this fails for linear classifiers
- Solution 2: Multiclass loss
  - Train one model: $h(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}$.
  - Prediction involves solving $\arg\max_{y \in \mathcal{Y}} h(x, y)$.

Does it work better in practice?

- Paper by Rifkin & Klautau: "In Defense of One-Vs-All Classification" (2004)
  - Extensive experiments, carefully done
    - albeit on relatively small UCI datasets
  - Suggests one-vs-all works just as well in practice
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  - Extensive experiments, carefully done
    - albeit on relatively small UCI datasets
  - Suggests one-vs-all works just as well in practice
    - (or at least, the advantages claimed by earlier papers for multiclass methods were not compelling)
- Compared
  - many multiclass frameworks (including the one we discuss)
  - one-vs-all for SVMs with RBF kernel
  - one-vs-all for square loss with RBF kernel (for classification!)
- All performed roughly the same

Why Are We Bothering with Multiclass?

- The framework we have developed for multiclass
  - compatibility features / scoring functions
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- The framework we have developed for multiclass
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- Generalizes to situations where k is very large and one-vs-all is intractable.
- Key idea is that we can generalize across outputs y by using features of y.

Example: Part-of-speech (POS) Tagging

- Given a sentence, give a part of speech tag for each word:

x	$\underbrace{\text{[START]}}_{x_0}$	$\underbrace{\text{He}}_{x_1}$	$\underbrace{\text{eats}}_{x_2}$	$\underbrace{\text{apples}}_{x_3}$
y	$\underbrace{\text{[START]}}_{y_0}$	$\underbrace{\text{Pronoun}}_{y_1}$	$\underbrace{\text{Verb}}_{y_2}$	$\underbrace{\text{Noun}}_{y_3}$

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- $\mathcal{P} = \{\text{START}, \text{Pronoun}, \text{Verb}, \text{Noun}, \text{Adjective}\}$
- $\mathcal{Y} = \mathcal{P}^n$, $n = 1, 2, 3, \ldots$[Part of speech sequence of any length]

Multiclass Hypothesis Space

- Discrete output space: $\mathcal{Y}(x)$
  - Very large but has structure, e.g., linear chain (sequence labeling), tree (parsing)
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- Multiclass hypothesis space

$$\mathcal{F} = \left\{ x \mapsto \underset{y \in \mathcal{Y}}{\arg\max}\, h(x, y) \mid h \in \mathcal{H} \right\}$$

- Final prediction function is an $f \in \mathcal{F}$.
- For each $f \in \mathcal{F}$ there is an underlying compatibility score function $h \in \mathcal{H}$.

Structured Prediction

- Part-of-speech tagging

x:	he	eats	apples
y:	pronoun	verb	noun

- Multiclass hypothesis space:

$$h(x,y) = w^T \Psi(x,y) \tag{21}$$

$$\mathcal{F} = \left\{ x \mapsto \arg\max_{y \in \mathcal{Y}} h(x,y) \mid h \in \mathcal{H} \right\} \tag{22}$$

- A special case of multiclass classification
- How to design the feature map Ψ? What are the considerations?

Unary features

- A **unary feature** only depends on
  - the label at a single position, y_i, and x
- Example:

$$
\begin{aligned}
\phi_1(x, y_i) &= \mathbb{1}[x_i = \text{runs}]\mathbb{1}[y_i = \text{Verb}] \\
\phi_2(x, y_i) &= \mathbb{1}[x_i = \text{runs}]\mathbb{1}[y_i = \text{Noun}] \\
\phi_3(x, y_i) &= \mathbb{1}[x_{i-1} = \text{He}]\mathbb{1}[x_i = \text{runs}]\mathbb{1}[y_i = \text{Verb}]
\end{aligned}
$$

Markov features

- A **markov feature** only depends on
  - two adjacent labels, y_{i-1} and y_i, and x
- Example:

$$\begin{aligned}\theta_1(x, y_{i-1}, y_i) &= \mathbb{1}[y_{i-1} = \text{Pronoun}]\mathbb{1}[y_i = \text{Verb}] \\ \theta_2(x, y_{i-1}, y_i) &= \mathbb{1}[y_{i-1} = \text{Pronoun}]\mathbb{1}[y_i = \text{Noun}]\end{aligned}$$

- Reminiscent of Markov models in the output space
- Possible to have higher-order features

Local Feature Vector and Compatibility Score

- At each position i in sequence, define the **local feature vector** (unary and markov):

$$\begin{aligned}\Psi_i(x, y_{i-1}, y_i) &= (\phi_1(x, y_i), \phi_2(x, y_i), \ldots, \\ &\quad \theta_1(x, y_{i-1}, y_i), \theta_2(x, y_{i-1}, y_i), \ldots)\end{aligned}$$

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- And **local compatibility score** at position i: $\langle w, \Psi_i(x, y_{i-1}, y_i)\rangle$.

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- And **local compatibility score** at position i: $\langle w, \Psi_i(x, y_{i-1}, y_i)\rangle$.
- The compatibility score for (x, y) is the sum of local compatibility scores:

$$\sum_i \langle w, \Psi_i(x, y_{i-1}, y_i)\rangle = \left\langle w, \sum_i \Psi_i(x, y_{i-1}, y_i)\right\rangle = \langle w, \Psi(x, y)\rangle, \tag{23}$$

where we define the **sequence feature vector** by

$$\Psi(x, y) = \sum_i \Psi_i(x, y_{i-1}, y_i). \qquad \text{decomposable}$$

Structured perceptron

Given a dataset $= (x, y)$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
  for $(x, y) \in$ **do**
    $\hat{y} = \arg\max_{y' \in (x)} w^T \psi(x, y')$;
    if $\hat{y} \neq y$ **then** `// We've made a mistake`
      $w \leftarrow w + \Psi(x, y)$; `// Move the scorer towards` $\psi(x, y)$
      $w \leftarrow w - \Psi(x, \hat{y})$; `// Move the scorer away from` $\psi(x, \hat{y})$
    end
  end
end

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    end
  end
end

Identical to the multiclass perceptron algorithm except the $\arg\max$ is now over the structured output space (x).

Structured hinge loss

- Recall the generalized hinge loss

$$\ell_{\text{hinge}}(y, \hat{y}) \max_{y' \in (x)} \Delta(y, y') + \left\langle w, \Psi(x, y') - \Psi(x, y) \right\rangle \tag{24}$$

- What is $\Delta(y, y')$ for two sequences?

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- What is $\Delta(y, y')$ for two sequences?
- **Hamming loss** is common:

$$\Delta(y, y') = \frac{1}{L} \sum_{i=1}^{L} \mathbb{1}[y_i \neq y_i']$$

where L is the sequence length.

Structured SVM

Exercise:

- Write down the objective of structured SVM using the structured hinge loss.
- Stochastic sub-gradient descent for structured SVM (similar to HW3 P3)
- Compare with the structured perceptron algorithm

The argmax problem for sequences

Problem To compute predictions, we need to find $\arg\max_{y \in \mathcal{Y}(x)} \langle w, \Psi(x, y) \rangle$, and $|\mathcal{Y}(x)|$ is exponentially large.

Figure by Daumé III. A course in machine learning. Figure 17.1.

The argmax problem for sequences

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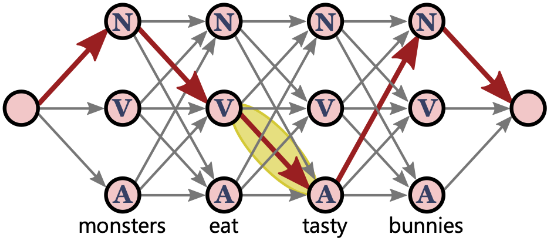
Solution Dynamic programming (similar to the Viterbi algorithm)



What's the running time?

Figure by Daumé III. A course in machine learning. Figure 17.1.

Conditional random field (CRF)

- Recall that we can write logistic regression in a general form:

$$p(y|x) = \frac{1}{Z(x)} \exp(w^\top \psi(x, y)).$$

- Z is normalization constant: $Z(x) = \sum_{y \in Y} \exp(w^\top \psi(x, y))$.

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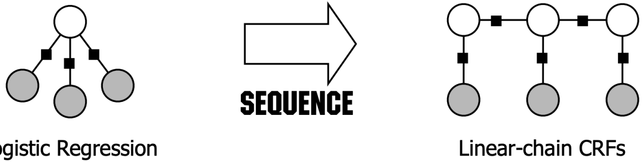
- Example: linear chain $\{y_t\}$
- We can incorporate unary and Markov features: $p(y|x) = \frac{1}{Z(x)} \exp(\sum_t w^\top \psi(x, y_t, y_{t-1}))$



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- We can draw samples in the output space.

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- Compared to Structured SVM, CRF has a probabilistic interpretation.
- We can draw samples in the output space.
- How do we learn w? Maximum log likelihood, and regularization term: $\lambda \|w\|^2$
- Loss function:

$$
\begin{aligned}
l(w) &= -\frac{1}{N} \sum_{i=1}^{N} \log p(y^{(i)} | x^{(i)}) + \frac{1}{2} \lambda \|w\|^2 \\
&= -\frac{1}{N} \sum_{i} \sum_{t} \sum_{k} w_k \psi_k (y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N} \sum_{i} \log Z(x^{(i)}) + \frac{1}{2} \sum_{k} \lambda w_k^2
\end{aligned}
$$

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- Loss function:

$$l(w) = -\frac{1}{N}\sum_i \sum_t \sum_k w_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N}\sum_i \log Z(x^{(i)}) + \frac{1}{2}\sum_k \lambda w_k^2$$

- Gradient:

$$\frac{\partial l(w)}{\partial w_k} = -\frac{1}{N}\sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) \tag{25}$$

$$+\frac{1}{N}\sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'}\psi_{k'}(x^{(i)}, y'_t, y'_{t-1})) + \sum_k \lambda w_k \tag{26}$$

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- What is $\frac{1}{N}\sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)})$?

Conditional random field (CRF)

- What is $\frac{1}{N}\sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)})$?
- It is the expectation $\psi_k(x^{(i)}, y_t, y_{t-1})$ under the empirical distribution $\tilde{p}(x, y) = \frac{1}{N}\sum_i \mathbb{1}[x = x^{(i)}]\mathbb{1}[y = y^{(i)}]$.

Conditional random field (CRF)

- What is $\frac{1}{N}\sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_t, y'_{t-1}))$?

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- It is the expectation of $\psi_k(x^{(i)}, y'_t, y'_{t-1})$ under the model distribution $p(y'_t, y'_{t-1}|x)$.

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- To compute the gradient, we need to infer expectation under the model distribution $p(y|x)$.
- Compare the learning algorithms: in structured SVM we need to compute the argmax, whereas in CRF we need to compute the model expectation.
- Both problems are NP-hard for general graphs.

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- In general graphs, we rely on approximate inference (e.g. loopy belief propagation).

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- Semantic segmentation
  Relationship between pixels, e.g. a grass pixel is likely to be next to another grass pixel, and a sky pixel is likely to be above a grass pixel.
- Multi-label learning
  An image may contain multiple class labels, e.g. a bus is likely to co-occur with a car.

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- Generalize binary classification algorithms using multiclass loss
  - Multi-class perceptron, multi-class logistics regression, multi-class SVM
- Structured prediction: Structured SVM, CRF. Data containing structure. Extremely large output space. Text and image applications.