# Neural Networks

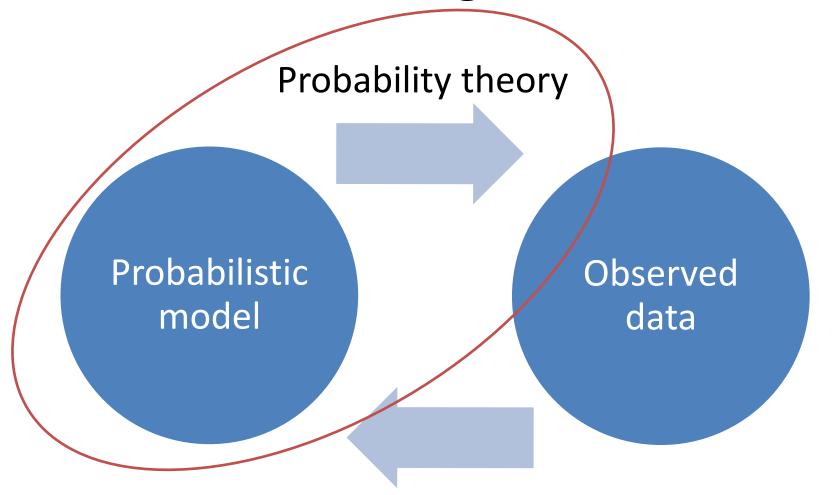
Lecture 2: probability & statistics refresher

Jan Chorowski
Instytut Informatyki
Wydział Matematyki i Informatyki Uniwersytet
Wrocławski
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#### Additional materials

- Murphy, chapter 2
- Goodfellow et al. chapter 3 (the book webpage also hosts slides)
- Slides from LXMLS Summer School: http://lxmls.it.pt/2016/Lecture\_0.pdf

# Statistical modeling and inference



Inference and learning

#### **Definitions**

- $\Omega$  is a **sample space**, e.g. two coin tosses  $\Omega = \{HH, HT, TH, TT\}$
- $A \in 2^{\Omega}$  is an **event**, e.g. "first head"  $\{HH, HT\}$

- $P: 2^{\Omega} \to \mathbb{R}$  is a **probability distributions** if:
  - $-P(A) \ge 0$  for every A
  - $-P(\Omega)=1$
  - $-\operatorname{If} A \cap B = \emptyset \text{ then } P(A \cup B) = P(A) + P(B)$

#### Random Variables

A RV is a mapping  $X: \Omega \to \mathbb{R}$ .

- Discrete RV has countable values:  $\{0,1\}$ ,  $\mathbb{N}$
- Continuous RV has uncountable values: [0,1],  $\mathbb{R}$
- E.g. Binomial distribution X is the number of heads in n tosses. Tosses are independent, each with head probability  $\Theta$ .

$$P(X = k) = P(k) = \binom{n}{k} \Theta^k (1 - \Theta)^{n-k}$$

#### Continuous RV

- A continuous RV X has an associated density function  $f_X(x)$ :
  - $-\forall x f_X(x) \ge 0$
  - $-\int_{-\infty}^{\infty} f_X(x) dx = 1$
  - $-P(a < X < b) = \int_a^b f_X(x) dx$
  - For a continuous RV it is possible that  $f_X(x) > 1!$
- Note: in the later lectures we will drop the distinction between probability P() and probability density f(), using P() in both contexts.

### **Expected values**

• The expected value of a function r of a RV X is:

$$\mathbb{E}[r(X)]_{X \sim P(X)} = \sum_{x} r(x)P(x)$$

$$\mathbb{E}[r(X)]_{X \sim f_X} = \int r(x)f_X(x)dx$$

- Example: the mean value of X is  $\mu = \sum_{x} x P(x)$
- The expectation is linear:

$$-\mathbb{E}[X+c] = \mathbb{E}[X] + c \qquad \mathbb{E}[cX] = c\mathbb{E}[X]$$

$$-\mathbb{E}[X+Y] = \mathbb{E}[X] + \mathbb{E}[Y]$$
 for all RV  $X$  and  $Y$ .

#### Variance

Variance measures the spread of a RV X:

$$\sigma^2 = \operatorname{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2] = \sum_{x} (x - \mathbb{E}[X])^2$$

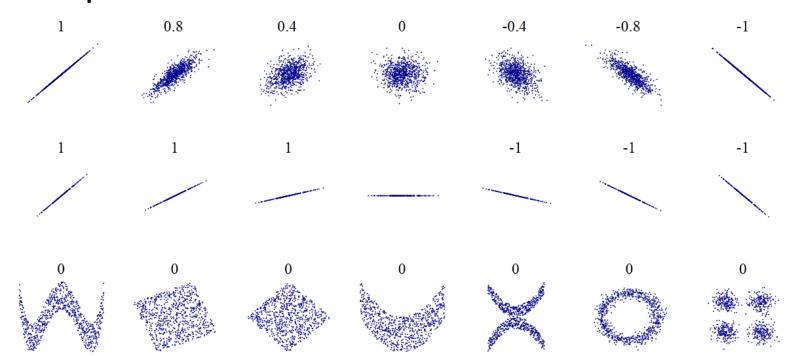
- Standard deviation  $\sigma_X = \sqrt{\text{Var}[X]}$
- The Covariance between X and Y is:  $Cov[X,Y] = \mathbb{E}[(X \mathbb{E}[X])(Y \mathbb{E}[Y])]$
- Properties of variance:
  - $\operatorname{Var}[X c] = \operatorname{Var}[X]$
  - $Var[cX] = c^2 Var[X]$
  - Var[aX + bY] = a<sup>2</sup>Var[X] + b<sup>2</sup>Var[Y] + 2abCov[X, Y]
  - When X and Y are independent:  $Var[aX + bY] = a^{2}Var[X] + b^{2}Var[Y]$

### Correlation

Correlation coefficient is normalized Covariance:

$$\rho_{X,Y} = \frac{\operatorname{Cov}[X,Y]}{\sigma_X \sigma_Y}$$

- $-1 \le \rho_{X,Y} \le 1$
- Independent ⇒ uncorrelated



# Joint probability

- Given two RVs X and Y P(x, y) denotes the event that X = x and Y = y.
- X and Y are independent iff P(x, y) = P(x)P(y)
- Marginal probability:  $P(x) = \sum_{y} P(x, y)$
- Conditional probability (read probability of x given y):

$$P(x|y) = \frac{P(x,y)}{P(y)}$$

# Bayes theorem

$$P(x,y) = P(x|y)P(y) = P(y|x)P(x)$$

$$P(x|y) = \frac{P(y|x)P(x)}{P(y)} = \frac{P(y|x)P(x)}{\sum_{x'} P(x',y)}$$

E.g. compute p(car crash | drunk driving)

# Bayes theorem in action

We want: P(crash|drunk)

Can't get people drunk and send on the road...

$$P(\text{crash}|\text{drunk}) = \frac{P(\text{drunk}|\text{crash})P(\text{crash})}{P(\text{drunk})}$$

That's ethical – we can estimate all need probabilities from police statistics!

#### Bernoulli and Binomial

#### Bernoulli:

-X is binary  $P(X = 1) = \phi, P(X = 0) = 1 - \phi$   $-\mathbb{E}[X] = 0(1 - \phi) + 1\phi = \phi$   $-\operatorname{Var}[X] = (0 - \phi)^2(1 - \phi) + (1 - \phi)^2\phi = \phi(1 - \phi)$ 

#### Binomial:

 $- RV K = sum of n independent Bernoulli(\phi) trials$ 

$$-P(k;\phi,n) = \binom{n}{k} \phi^k (1-\phi)^{n-k}$$

$$-\mathbb{E}[K] = n\phi$$

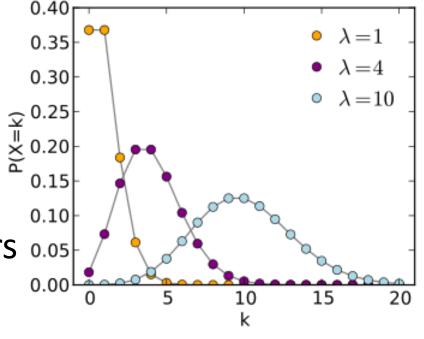
$$-\operatorname{Var}(K) = n\phi(1-\phi)$$

#### Poisson

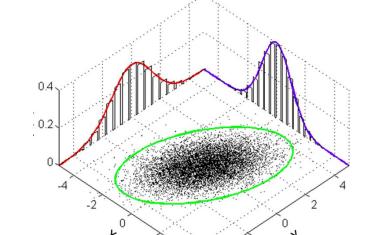
- The count of rare events
- Defined for natural numbers 0.05

• 
$$P(X = k; \lambda) = \frac{\lambda^k}{k!} e^{-\lambda}$$

- $\mathbb{E}[X] = \lambda$
- $Var[X] = \lambda$
- Sum of independent Poissons is Poisson: if  $X \sim \text{Pois}(\lambda_X)$  and  $Y \sim \text{Pois}(\lambda_Y)$  then  $X + Y \sim \text{Pois}(\lambda_X + \lambda_Y)$



### Normal distribution



- $X \sim \mathcal{N}(\mu, \sigma^2)$
- Univariate:

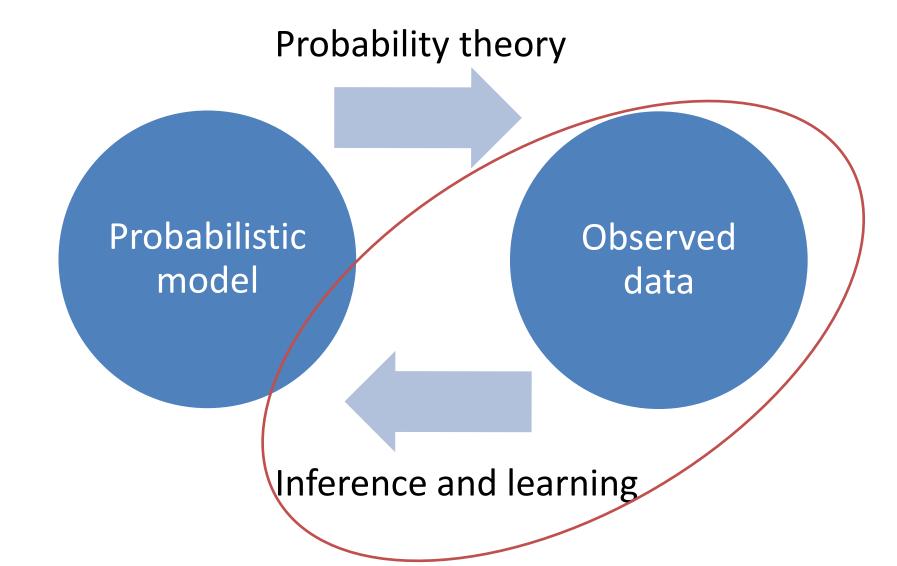
$$P(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}}e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

• Multivariate, *k*-dimensional:

$$P(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{k}{2}} |\Sigma|^{-\frac{1}{2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$

- Mean: μ
- Variance:  $\Sigma$  (in 1D case  $\sigma$ )
- Conditionals, sums, and marginals of Gaussians are Gaussian

# Statistical modeling and inference



#### Statistical Inference

#### Consider the polling problem:

- There exists a population of individuals (e.g. voters).
- The individuals have a voting preference (party A or B).
- We want the fraction of voters that prefer A.
- But we don't want to ask everyone (run an election)!

# Polling

- Choose a sample of eligible voters
- Get the fraction  $\phi$  of A's supporters
- Questions:
  - How are  $\phi$  and  $\bar{\phi}$  related?
  - What is the error  $(\phi \overline{\phi})$
  - How many people to ask to have  $\pm 3$  perc. points accuracy with a high probability?

# Polling model

If the population is very large, we can assume that our poll is a set of n independent Bernoulli( $\phi$ ) trials.

The sample is IID – Independent Identically Distributed.

This corresponds to a binomial distribution:

$$P(k; n, \phi) = \binom{n}{k} \phi^k (1 - \phi)^{n-k}$$

where k is the count of A's supporters among n polled.

### Likelihood

The probability of seeing k supporters is:

$$P(k; n, \phi) = \binom{n}{k} \phi^k (1 - \phi)^{n-k}$$

- Taken as a function  $\mathcal{L}(\phi)$  we call it the likelihood.
- We will estimate the real, unknown  $\phi$  by  $\widehat{\phi}$ , the maximizer of the sample likelihood:

$$\hat{\phi} = \arg \max_{\phi} \mathcal{L}(\phi) = \arg \max_{\phi} P(k; n, \phi)$$

$$= \arg \max_{\phi} \log P(k; n, \phi)$$

$$= \arg \max_{\phi} k \log(\phi) + (n - k) \log(1 - \phi)$$

#### Maximum Likelihood

$$\hat{\phi} = \arg \max_{\phi} ll(\phi)$$

$$= \arg \max_{\phi} k \log \phi + (n - k) \log 1 - \phi$$

At maximum the derivative wrt.  $\phi$  is 0:

$$\frac{\partial ll(\phi)}{\partial \phi} = \frac{k}{\phi} - \frac{n-k}{1-\phi}$$

Solve for  $\hat{\phi}$ :

$$\frac{k}{\hat{\phi}} = \frac{n-k}{1-\hat{\phi}}$$

$$\hat{\phi} = \frac{k}{n}$$

The MLE (Maximum Likelihood Estimator) for  $\hat{\phi}$  is just the sample mean  $\bar{\phi} = \frac{k}{n}!$ 

# Polling accuracy

 $\frac{k}{n} = \bar{\phi}$ , the fraction of A voters in the poll is an estimator for populations' fraction  $\phi$ ! How accurate is  $\bar{\phi}$ ?

- Observation:  $\overline{\phi}$  is an RV!
- It maps polls to results!
- $P\left(\bar{\phi} = \frac{k}{n}\right) = \text{Binomial}(k; n, \phi)$
- $\mathbb{E}[\bar{\phi}] = \mathbb{E}\left[\frac{\sum_{i} \text{trial}_{i}}{n}\right] = \frac{1}{n} \sum_{i} \mathbb{E}[\text{trial}_{i}] = \phi$
- $Var[\bar{\phi}] = Var\left[\frac{1}{n}\sum_{i} trial_{i}\right] = \frac{1}{n^{2}}\sum_{i} Var[trial_{i}] = \frac{\phi(1-\phi)}{n}$

# Desired accuracy

Observation: the higher n, the less variable  $ar{\phi}$ 

We want to find *n* such that:

$$P(\phi - 0.03 \le \bar{\phi} \le \phi + 0.03) \ge 0.95$$

Then we will say that our 95% confidence interval is  $\pm 3\%$  points.

That means, that if we did 100 polls, 95 would return an estimator within 3 perc. points from the true value.

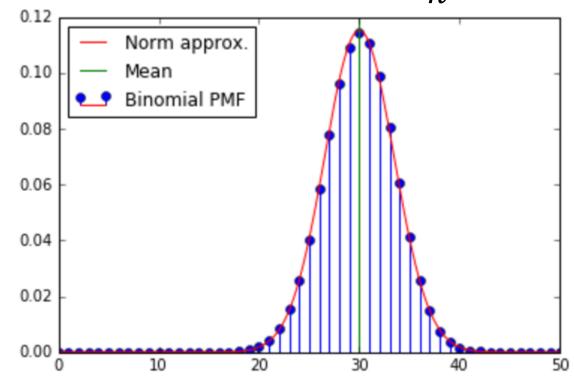
### Gaussian approximation

We want to find *n* such that:

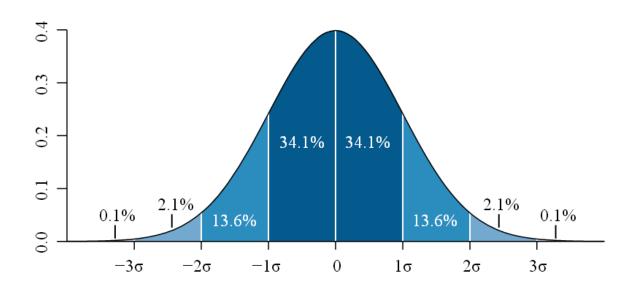
$$P(\phi - 0.03 \le \bar{\phi} \le \phi + 0.03) \ge 0.95$$

We know that  $\mathbb{E}[\bar{\phi}] = \phi$  and  $\mathrm{Var}[\bar{\phi}] = \frac{\phi(1-\phi)}{n}$ .

Approximate with a Gaussian!



#### Gaussian confidence intervals



95% of the Gaussian's pdf lies in the range  $\pm 1.96\sigma$ 

We want that the

$$0.03 = 1.96\sigma = 1.96\sqrt{\text{Var}[\bar{\phi}]}$$

Assume the worse case ( $\phi = .5$ ) and solve for n!

# Bayesian Reasoning

Bayesian methods pose the problem in terms of our beliefs. This allows us to answer additional questions:

- How did my belief about the population change after seeing the poll?
- How to incorporate my prior knowledge?
- How to use small polls?

In Bayesian reasoning we will treat the population's parameter  $\phi$  as yet another RV!

# Bayesian Reasoning

- The probability assigned to  $\phi$  is subjective it expresses *our* uncertainty about the real  $\phi$ .
- We have seen poll results and ...
   we will use the Bayes theorem:

$$P(\phi|poll) = \frac{P(poll|\phi)P(\phi)}{P(poll)}$$

- We know the likelihood term,  $P(poll|\phi)$ .
- We need the prior  $P(\phi)$ !
- We don't need P(poll) it's only a scaling constant!

#### Prior

For convenience we will choose a prior that has a similar formula to the likelihood.

- This is called a *conjugate prior*.

Recall that: 
$$P(k|\phi;n) \propto \phi^k (1-\phi)^{n-k}$$

Choose 
$$P(\phi) \propto \phi^{\alpha-1} (1-\phi)^{\beta-1}$$

– This is the Beta $(\alpha, \beta)$  distribution

The posterior is then:

$$P(\phi|k) \propto P(k|\phi)P(\phi)$$
  
=  $\phi^{k+\alpha-1}(1-\phi)^{n-k+\beta-1}$ 

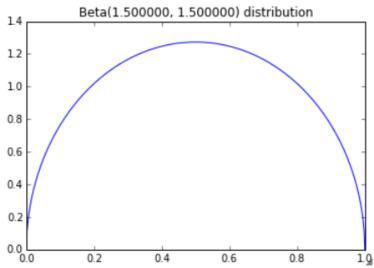
This is just Beta $(k + \alpha, n - k + \beta)$ .

# Bayesian polling

This our prior (Beta(1.5, 1.5))

After seeing one success we update to Beta(2.5, 1.5).

In this case, the prior can be interpreted as *pseudo-counts*.



Posterior after seeing 1 successes and 0 failures Prior pseudo-counts: A=1.500000, B=1.500000 MAP estimate: 0.750000, MLE estimate: 1.000000

