COMS 4721: Machine Learning for Data Science

Lecture 1, 1/12/2021

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OVERVIEW

This class will cover model-based techniques for extracting information from data with an end-task in mind. Such tasks include:

- predicting an unknown "output" given its corresponding "input"
- uncovering information within the data to better understand it
- data-driven recommendation, grouping, classification, ranking, etc.

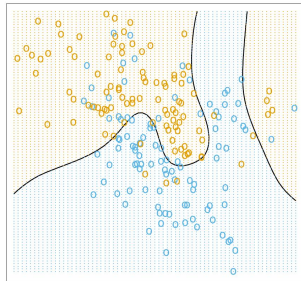There are a few ways we can divide up the material as we go along, e.g.,

supervised learning	unsupervised learning
probabilistic models	non-probabilistic models
modeling approach	optimization techniques

We'll adopt the first method and work in the second two along the way.
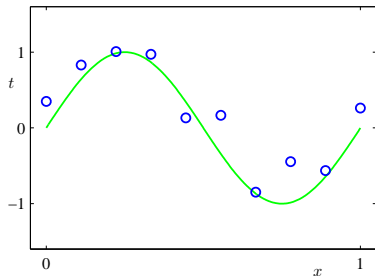
(a) Regression

(b) Classification

Regression: Using set of inputs, predict real-valued output.

Classification: Using set of inputs, predict a discrete label (aka class).

EXAMPLE CLASSIFICATION PROBLEM

Given a set of inputs characterizing an item, assign it a label.
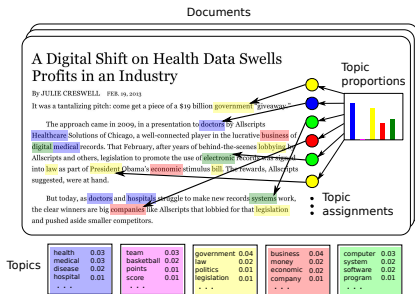
Is this spam?

hi everyone,

i saw that close to my hotel there is a pub with bowling (it's on market between 9th and 10th avenue). meet there at 8:30?
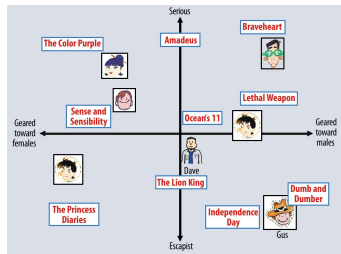
What about this?

Enter for a chance to win a trip to Universal Orlando to celebrate the arrival of Dr. Seuss's The Lorax on Movies On Demand on August 21st! Click here now!

(c) topic modeling

(d) recommendations[1]

With unsupervised learning our goal is often to uncover structure in the data. This helps with predictions, recommendations, efficient data exploration.

[1] Figure from Koren, Y., Robert B., and Volinsky, C.. "Matrix factorization techniques for recommender systems." Computer 42.8 (2009): 30-37.

Goal: Learn the dominant topics from a set of news articles.

The New York Times

|				
music band songs rock album jazz pop song singer night	book life novel story books man stories love children family	art museum show exhibition artist artists paintings painting century works	game knicks nets points team season play games night coach	show film television movie series says life man character know
theater play production show stage street broadway director musical directed	clinton bush campaign gore political republican dole presidential senator house	stock market percent fund investors funds companies stocks investment trading	restaurant sauce menu food dishes street dining dinner chicken served	budget tax governor county mayor billion taxes plan legislature fiscal

DATA MODELING
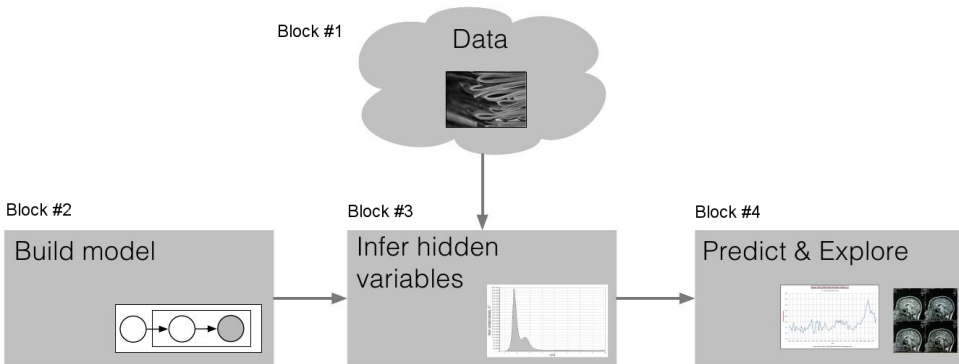
- ▶ Supervised vs. unsupervised: Blocks #1 and #4

- ▶ Probabilistic vs. non-probabilistic: Primarily Block #2 (Some Block #3)

- ▶ Model development (Block #2) vs. Optimization techniques (Block #3)

GAUSSIAN DISTRIBUTION (MULTIVARIATE)

Gaussian density in d dimensions

- ▶ Block #1: Data $x_1, \ldots, x_n$. Each $x_i \in \mathbb{R}^d$
- ▶ Block #2: An i.i.d. Gaussian model
- ▶ Block #3: Maximum likelihood
- ▶ Block #4: Leave undefined
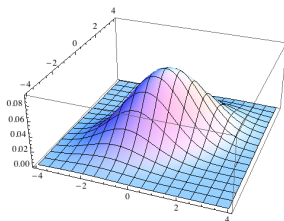
The density function is

$$p(x|\mu, \Sigma) := \frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{\det(\Sigma)}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

The central moments are:

$$\mathbb{E}[x] = \int_{\mathbb{R}^d} x\, p(x|\mu, \Sigma)dx = \mu,$$

$$\text{Cov}(x) = \mathbb{E}[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^T] = \mathbb{E}[xx^T] - \mathbb{E}[x]\mathbb{E}[x]^T = \Sigma.$$

Probabilistic Models

- ► A *probabilistic model* is a set of probability distributions, $p(x|\theta)$.
- ► We pick the *distribution family* $p(\cdot)$, but don't know the parameter θ.

Example: Model data with a Gaussian distribution $p(x|\theta)$, $\theta = \{\mu, \Sigma\}$.

The i.i.d. assumption

Assume data is *independent and identically distributed (iid)*. This is written

$$x_i \overset{iid}{\sim} p(x|\theta), \quad i = 1, \ldots, n.$$

Writing the density as $p(x|\theta)$, then the *joint* density decomposes as

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

BLOCK #3: MAXIMUM LIKELIHOOD ESTIMATION

Maximum Likelihood approach

We now need to find θ. *Maximum likelihood* seeks the value of θ that maximizes the likelihood function:

$$\hat{\theta}_{\text{ML}} := \arg \max_{\theta} \; p(x_1, \ldots, x_n | \theta),$$

This value best explains the data according to the chosen distribution family.

Maximum Likelihood equation

The analytic criterion for this maximum likelihood estimator is:

$$\nabla_{\theta} \prod_{i=1}^{n} p(x_i | \theta) = 0.$$

Simply put, the maximum is at a peak. There is no "upward" direction.

Logarithm trick

Calculating $\nabla_\theta \prod_{i=1}^{n} p(x_i|\theta)$ can be complicated. We use the fact that the logarithm is monotonically increasing on $\mathbb{R}_+$, and the equality

$$\ln\Big(\prod_i f_i\Big) = \sum_i \ln(f_i).$$

Consequence: Taking the logarithm does not change the *location* of a maximum or minimum:

$$\max_y \, \ln g(y) \neq \max_y g(y) \qquad \text{The \textit{value} changes.}$$

$$\arg\max_y \, \ln g(y) = \arg\max_y g(y) \qquad \text{The \textit{location} does not change.}$$

Maximum likelihood and the logarithm trick

$$\hat{\theta}_{\text{ML}} = \arg \max_{\theta} \prod_{i=1}^{n} p(x_i|\theta) = \arg \max_{\theta} \ln\Big(\prod_{i=1}^{n} p(x_i|\theta)\Big) = \arg \max_{\theta} \sum_{i=1}^{n} \ln p(x_i|\theta)$$

To then solve for $\hat{\theta}_{\text{ML}}$, find

$$\nabla_\theta \sum_{i=1}^{n} \ln p(x_i|\theta) = \sum_{i=1}^{n} \nabla_\theta \ln p(x_i|\theta) = 0.$$

Depending on the choice of the model, we will be able to solve this

1. analytically (via a simple set of equations)
2. numerically (via an iterative algorithm using different equations)
3. approximately (typically when #2 converges to a local optimal solution)

EXAMPLE: MULTIVARIATE GAUSSIAN MLE

Block #2: Multivariate Gaussian data model

Model: Set of all Gaussians on $\mathbb{R}^d$ with unknown mean $\mu \in \mathbb{R}^d$ and covariance $\Sigma \in \mathbb{S}_{++}^d$ (positive definite $d \times d$ matrix).

We assume that $x_1, \ldots, x_n$ are i.i.d. $p(x|\mu, \Sigma)$, written $x_i \overset{iid}{\sim} p(x|\mu, \Sigma)$.

Block #3: Maximum likelihood solution

We have to solve the equation

$$\sum_{i=1}^{n} \nabla_{(\mu, \Sigma)} \ln p(x_i|\mu, \Sigma) = 0$$

for μ and Σ. (Try doing this without the log to appreciate it's usefulness.)

EXAMPLE: GAUSSIAN MEAN MLE

First take the gradient with respect to μ.

$$
\begin{aligned}
0 &= \nabla_\mu \sum_{i=1}^n \ln \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\left(-\frac{1}{2}(x_i - \mu)^T \Sigma^{-1} (x_i - \mu)\right) \\
&= \nabla_\mu \sum_{i=1}^n -\frac{1}{2} \ln(2\pi)^d |\Sigma| - \frac{1}{2}(x_i - \mu)^T \Sigma^{-1} (x_i - \mu) \\
&= -\frac{1}{2} \sum_{i=1}^n \nabla_\mu \left(x_i^T \Sigma^{-1} x_i - 2\mu^T \Sigma^{-1} x_i + \mu^T \Sigma^{-1} \mu\right) = \Sigma^{-1} \sum_{i=1}^n (x_i - \mu)
\end{aligned}
$$

Since Σ is positive definite, the only solution is

$$
\sum_{i=1}^n (x_i - \mu) = 0 \qquad \Rightarrow \qquad \hat\mu_{\text{ML}} = \frac{1}{n} \sum_{i=1}^n x_i
$$

Since this solution is independent of Σ, it doesn't depend on $\hat\Sigma_{\text{ML}}$.

EXAMPLE: GAUSSIAN COVARIANCE MLE

Now take the gradient with respect to Σ.

$$
\begin{aligned}
0 &= \nabla_\Sigma \sum_{i=1}^{n} -\frac{1}{2}\ln(2\pi)^d|\Sigma| - \frac{1}{2}(x_i - \mu)^T \Sigma^{-1}(x_i - \mu) \\
&= -\frac{n}{2}\nabla_\Sigma \ln|\Sigma| - \frac{1}{2}\nabla_\Sigma \mathrm{trace}\Big(\Sigma^{-1}\sum_{i=1}^{n}(x_i - \mu)(x_i - \mu)^T\Big) \\
&= -\frac{n}{2}\Sigma^{-1} + \frac{1}{2}\Sigma^{-2}\sum_{i=1}^{n}(x_i - \mu)(x_i - \mu)^T
\end{aligned}
$$

Solving for Σ and plugging in $\mu = \hat{\mu}_{\mathrm{ML}}$,

$$
\hat{\Sigma}_{\mathrm{ML}} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu}_{\mathrm{ML}})(x_i - \hat{\mu}_{\mathrm{ML}})^T.
$$

EXAMPLE: GAUSSIAN MLE (SUMMARY)

Thus, if we have data $x_1, \ldots, x_n$ in $\mathbb{R}^d$ that we hypothesize is i.i.d. Gaussian, the maximum likelihood values of the mean and covariance matrix are

$$\hat{\mu}_{\text{ML}} = \frac{1}{n} \sum_{i=1}^{n} x_i, \quad \hat{\Sigma}_{\text{ML}} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \hat{\mu}_{\text{ML}})(x_i - \hat{\mu}_{\text{ML}})^T.$$

Are we done? There are many assumptions/issues with this approach that makes finding the "best" parameter values not a complete victory.

- ▶ We made a model assumption (multivariate Gaussian).
- ▶ We made an i.i.d. assumption.
- ▶ We assumed that maximizing the likelihood is the best thing to do.

    Comment: We often use θ_{ML} to make predictions about x_{new} (Block #4).
    How does θ_{ML} generalize to x_{new}?
    If $x_{1:n}$ don't "capture the space" well, θ_{ML} can *overfit* the data.