IFT 6085 Probability refresher

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Jan 25, 2013

Probabilities in AI

- Probabilities allow us to be explicit about uncertainties:
- Instead of representing *values*, we can "keep all options open" by defining a distribution over alternatives.
- Example: Instead of setting '$x = 4$', define all of: $p(x = 1), p(x = 2), p(x = 3), p(x = 4), p(x = 5)$
- Benefits:
  1. Robustness (let modules tell each other their whole state of knowledge)
  2. Measure of uncertainty ("errorbars")
  3. Multimodality (keep ambiguities around)
- We can still express '$x = 4$' as a special case.

Random variables

- The only relevant information about random variable is its distribution: ("A random variable is (i) not random, (ii) not a variable.")
- $p(x)$ is a distribution if

$$p(x) \geq 0 \quad \text{and} \quad \sum_x p(x) = 1$$

- Notational quirks:
  - p is usually heavily overloaded. The argument decides. For example, in "$p(x, y) = p(x)p(y)$" each p means something different!
  - Sometimes we write X for the RV and x for the values it can take on.
  - Another common notation is $p(X = x)$.
  - $\sum_x \ldots$ refers to the sum over all values that x can take on.
- For continuous x, replace $\sum$ by $\int$ (up to some measure theoretic "glitches", that we can usually safely ignore)
- Some use the term "density" or "probability density function (pdf)" to refer to continuous $p(\cdot)$.

Summarizing properties

- Any relevant properties of RVs are just properties of their distributions.
- Mean:

$$\mu = \sum_x p(x)x = E[x]$$

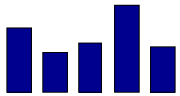
- Variance:

$$\sigma^2 = \sum_x p(x)(x - \mu)^2 = E[(x - \mu)^2]$$

- (Standard deviation: $\sigma = \sqrt{\sigma^2}$)

Some useful distributions (1d)

Discrete

- **Bernoulli:** $p^x(1-p)^{1-x}$ where x is 0 or 1.
- **Discrete distribution**:  (also known as "multinoulli")
- **Binomial**, **Multinomial**: Sum over Bernoulli/Discrete. (Sometimes "multinomial" is used to refer to a discrete distribution, too...)
- **Poisson**: $p(k) = \frac{\lambda^k \exp(-\lambda)}{k!}$

Continuous

- **Uniform**: 
- **Gaussian (1d)**: $p(x) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$

How to represent discrete values

- A very useful way to represent a variable that takes one out of K values:
- As a K-vector with $(K-1)$ 0's, and one 1 at position k

$$\mathbf{x} = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

- This is known as **one-of-K encoding**, **one-hot encoding**, or as **orthogonal encoding**.
- Note that we can interpret $\mathbf{x}$ itself as a probability distribution.

Some useful distributions (1d)

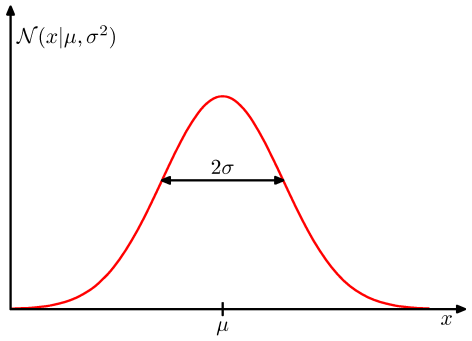
- Using a one-hot encoding allows us to write the discrete distribution compactly as

$$p(\mathbf{x}) = \prod_k \mu_k^{x_k}$$

where μ_k is the probability for state k.

- This can greatly simply maximum likelihood calculations (see below).

The Gaussian (1d)



$$p(x) = \mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

Multiple variables

- The **joint distribution** $p(x, y)$ of two variables x and y also satisfies
$$p(x, y) > 0 \text{ and } \sum_{x,y} p(x, y) = 1,$$
- Likewise, we can write
$$p(\boldsymbol{x}) > 0 \text{ and } \sum_{\boldsymbol{x}} p(\boldsymbol{x}) = 1,$$
for vector $\boldsymbol{x}$
- For discrete RVs, the joint is a *table* (or a higher-dimensional *array*).
- Everything else stays the same.

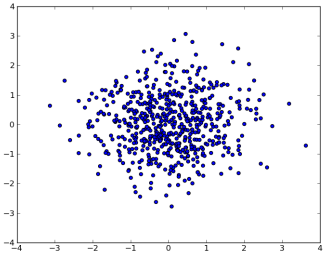
Conditionals, marginals

- Everything one may want to know about a random vector can be derived from the joint distribution.
- **Marginal distributions**:
$$p(x) = \sum_{y} p(x, y) \quad \text{and} \quad p(y) = \sum_{x} p(x, y)$$
- Imagine collapsing tables.
- **Conditional distributions**:
$$p(y|x) = \frac{p(x, y)}{p(x)} \quad \text{and} \quad p(x|y) = \frac{p(x, y)}{p(y)}$$
- Think of conditional as a family of distributions, "indexed" by the conditioning variable. (We could write $p(y|x)$ also as $p_x(y)$).

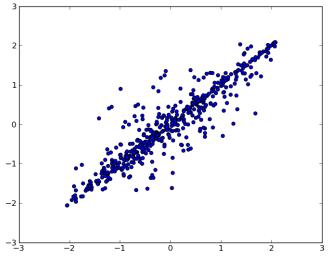
Summarizing properties, correlation

- Mean:
$$\boldsymbol{\mu} = \sum_{\boldsymbol{x}} p(\boldsymbol{x})\boldsymbol{x} = E[\boldsymbol{x}]$$
- Covariance:
$$\operatorname{cov}(x_i, x_j) = E[(x_i - \mu_i)(x_j - \mu_j)]$$
- Covariance matrix:
$$\Sigma_{ij} = \operatorname{cov}(x_i, x_j) \quad (\Sigma = \sum_{\boldsymbol{x}} p(\boldsymbol{x})(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^{\mathrm{T}})$$
- The correlation coefficient:
$$\operatorname{corr}(x_i, x_j) = \frac{\operatorname{cov}(x_i, x_j)}{\sqrt{\sigma_i^2 \sigma_j^2}}$$
- Two variables for which the covariance is zero are called **uncorrelated**.

Correlation example

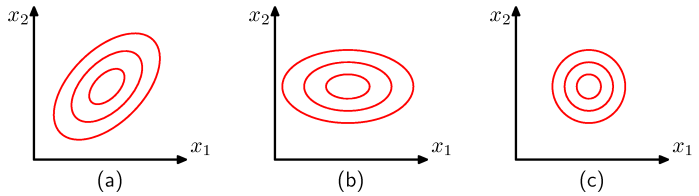


uncorrelated



correlated

The multivariate Gaussian



$$p(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{D}{2}}|\Sigma|^{\frac{1}{2}}} \exp\Big(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathrm{T}}\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\Big)$$

A fundamental formula

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

- This can be generalized to more variables ("chainrule of probability").
- A special case is **Bayes' rule:**

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

Independence and conditional independence

- Two RVs are called **independent**, if

$$p(x,y) = p(x)p(y)$$

- Captures our intuition of "dependence". In particular, note that this definition implies

$$p(y|x) = p(y)$$

- Independence implies uncorrelatedness, but not vice versa!
- Related: Two RVs are called **conditionally independent**, given a third variable z, if

$$p(x,y|z) = p(x|z)p(y|z)$$

- (Note that these concepts are just a property of the joint.)

Independence is useful

- Say, we have some variables, $x1, x2, \ldots, x_K$
- Even just defining their joint (let alone doing computations with it) is hopeless for large K !
- But what if all the x_i are independent?
- Then we need to specify just K probabilities, because *the joint is the product.*
- A more sophisticated version of this idea, using *conditional independence*, is the basis for the area of *graphical models*.

Maximum likelihood

- Another useful property of independence.
- Task: Given a set of data points

$$(x_1, \ldots, x_N)$$

  build a model of the data-generating process.
- Approach: Fit a parametric distribution $p(x; \boldsymbol{w})$ with some parameters $\boldsymbol{w}$ to the data.
- How? Maximize the probability of "seeing" the data under your model!

Maximum likelihood

- This is easy if examples are independent and identically distributed ("**iid**"):

$$p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N; \boldsymbol{w}) = \prod_i p(\boldsymbol{x}_i; \boldsymbol{w})$$

- Instead of maximizing probability, we may maximize log-probability, because the log function is monotonic.
- So we may maximize:

$$L(\boldsymbol{w}) := \log \prod_i p(\boldsymbol{x}_i; \boldsymbol{w}) = \sum_i \log p(\boldsymbol{x}_i; \boldsymbol{w})$$

- Thus each example $\boldsymbol{x}_i$ contributes an additive component to the objective.

Gaussian example

- What is the ML-estimate of the mean of a Gaussian?
- We need to maximize

$$L(\mu) = \sum_i \log p(x_i; \mu) = \sum_i \big(-\frac{1}{2\sigma^2}(x_i - \mu)^2 \big) - \text{const.}$$

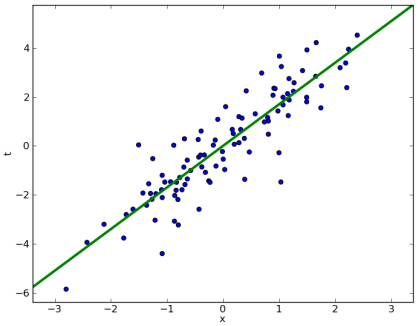
- The derivative is:

$$\frac{\partial L(\mu)}{\partial \mu} = \frac{1}{\sigma^2} \sum_i (x_i - \mu) = \frac{1}{\sigma^2} \big(\sum_i x_i - N\mu \big)$$

- By setting to zero, we get:

$$\mu = \frac{1}{N} \sum_i x_i$$

Linear regression



$$\mathbf{x} \rightarrow \mathbf{t}$$

- Given two *real-valued* observations $\mathbf{x}$ and $\mathbf{t}$, learn to predict $\mathbf{t}$ from $\mathbf{x}$.
- This is a *supervised learning* problem.

Linear regression

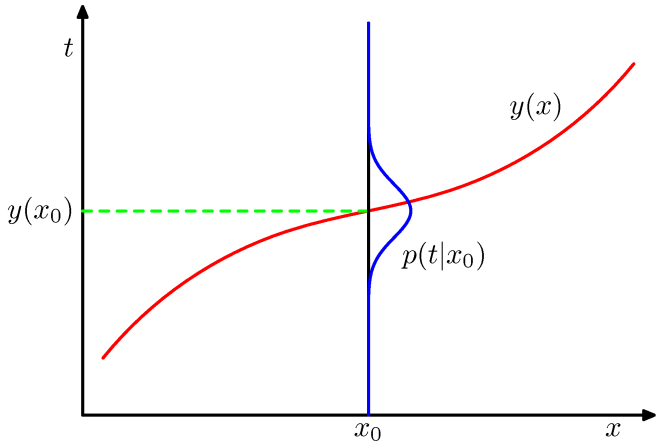
- We can define linear regression as a probabilistic model, if we make the following assumption:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon$$

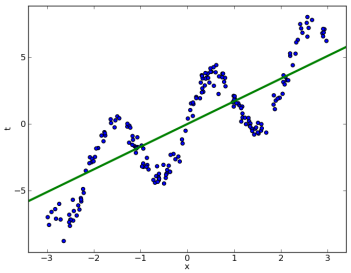
- In words, we assume there is a true, underlying function $y(\mathbf{x}, \mathbf{w})$, and the function values we observe are corrupted by *additive Gaussian noise.*
- Thus

$$p(t|\mathbf{x}; \mathbf{w}) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \sigma^2)$$

Linear regression



Noise vs. dependencies we don't care about



- Actually, linear regression can work fine also with highly non-Gaussian noise.

Linear regression

- To fit the conditional Gaussian, given training data $\mathcal{D} = \{(\mathbf{x}_n, t_n)\}_{n=1}^N$, we make the iid assumption and get:

$$p(\mathcal{D}) = \prod_n \mathcal{N}(t_n|y(\mathbf{x}_n, \mathbf{w}), \sigma^2)$$

- Using monotonicity of the log, we may again maximize the log-probability (or minimize its negation):

$$\text{minimize} \quad \sum_{n=1}^{N} \left(t_n - \mathbf{w}^{\mathrm{T}}\mathbf{x}_n\right)^2 + \text{const.}$$

Least squares

- To optimize with respect to $\mathbf{w}$, we differentiate:

$$\frac{\partial E}{\partial \mathbf{w}} = -\sum_{n=1}^{N} (t_n - \mathbf{w}^{\mathrm{T}}\mathbf{x}_n)\mathbf{x}_n^{\mathrm{T}}$$

- Setting the derivative to zero:

$$0 = -\sum_{n=1}^{N} t_n \mathbf{x}_n^{\mathrm{T}} + \mathbf{w}^{\mathrm{T}} \left(\sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^{\mathrm{T}}\right)$$

yields the solution

$$\mathbf{w} = \left(\sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^{\mathrm{T}}\right)^{-1} \left(\sum_{n=1}^{N} t_n \mathbf{x}_n^{\mathrm{T}}\right)$$

- (It can be instructional to write down the case for 1-d inputs, if this confuses you)

Least squares

- We can write this more compactly with the following definitions:

$$\mathbf{t} = \begin{pmatrix} t_1 \\ \vdots \\ t_N \end{pmatrix}$$

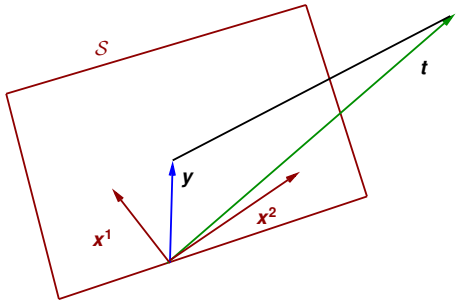
$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_N \end{pmatrix}$$

This allows us to write the the solution as

$$\mathbf{w} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{t}$$

"The normal equations".

Geometrical interpretation



- We can think of the squared error $\sum_n (t_n - \mathbf{w}^{\mathrm{T}}\mathbf{x}_n)^2$ as the squared norm of the difference between two $N-$dimensional vectors $\mathbf{t}$ and $\mathbf{y}$, containing all training-outputs and model-predictions.
- The vector $\mathbf{y}\left(= \mathbf{X}\mathbf{w}\right)$ has to lie in the space $\mathcal{S}$ spanned by the *columns* $\mathbf{x}^j$ of $\mathbf{X}$.
- It is exactly the *orthogonal projection* of $\mathbf{t}$ onto $\mathcal{S}$

Linear classification

$$\mathbf{x} \rightarrow t$$

- A prediciton task, where the outputs, t, are discrete (that is, they can take on one of K values, $\mathcal{C}_1, \ldots, \mathcal{C}_K$), the task is a *classification task*.
- Like linear regression, this is a *supervised learning* problem.

(Multi-class) logistic regression

- Logistic regression defines a probabilistic model over classes given inputs as follows:

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{\exp\left(\mathbf{w}_k^{\mathrm{T}}\mathbf{x}_n\right)}{\sum_{j=1}^{K}\exp\left(\mathbf{w}_j^{\mathrm{T}}\mathbf{x}_n\right)}$$

  where $\mathbf{w}_1, \ldots, \mathbf{w}_K$ are parameters.
- The exp-function ensures positivity, and the normalization that the outputs sum to one.
- (In practice, one usually adds constant "bias"-terms inside the exp's)

Multi-class logistic regression

- Represent discrete one-hot labels row-wise in a matrix $\mathbf{T}$, like we did before for continuous vectors.
- The negative log-likelihood cost, assuming iid training data, can then be written

$$\begin{aligned}
E(\mathbf{W};\mathcal{D}) &= -\log\prod_n p(\mathbf{t}_n|\mathbf{x}_n) \\
&= -\log\prod_n\prod_k p(\mathcal{C}_k|\mathbf{x}_n)^{t_{nk}} \\
&= -\sum_n\sum_k t_{nk}\log p(\mathcal{C}_k|\mathbf{x}_n) \\
&= -\sum_n\sum_k t_{nk}\left(\mathbf{w}_k^{\mathrm{T}}\mathbf{x}_n - \log\sum_{j=1}^{K}\exp\left(\mathbf{w}_j^{\mathrm{T}}\mathbf{x}_n\right)\right) \\
&= -\sum_n\left(\mathbf{w}_{t_n}^{\mathrm{T}}\mathbf{x}_n - \log\sum_{j=1}^{K}\exp\left(\mathbf{w}_j^{\mathrm{T}}\mathbf{x}_n\right)\right)
\end{aligned}$$

Multi-class logistic regression

- In contrast to linear regression, there is no closed-form solution for $\mathbf{W}$.
- But one can use gradient-based optimization to minimize $E(\mathbf{W};\mathcal{D})$ iteratively.
- The gradient with respect to each parameter-vector $\mathbf{w}_k$ is

$$\begin{aligned}
\frac{\partial E(\mathbf{W};\mathcal{D})}{\partial \mathbf{w}_k} &= -\sum_n t_{nk}\mathbf{x}_n - \frac{\exp\left(\mathbf{w}_k^{\mathrm{T}}\mathbf{x}_n\right)}{\sum_j\exp\left(\mathbf{w}_j^{\mathrm{T}}\mathbf{x}_n\right)}\mathbf{x}_n \\
&= \sum_n\left(p(\mathcal{C}_k|\mathbf{x}_n) - t_{nk}\right)\mathbf{x}_n
\end{aligned}$$

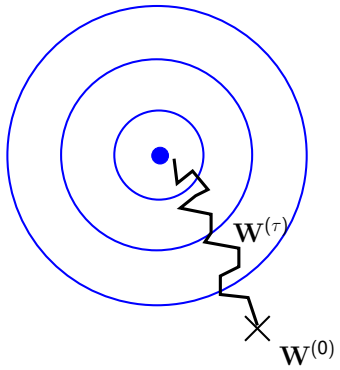
- It can be shown that $E(\mathbf{W};\mathcal{D})$ is convex, so there are no local minima.

Learning with stochastic gradient descent

$$\mathbf{W}^{(\tau+1)} = \mathbf{W}^{(\tau)} - \eta\frac{\partial E_n}{\mathbf{W}}$$

- Here, τ denotes the iteration number, and E_n is the cost contributed by the n^{th} training case (one term in the sum over n).
- Parameters are initialized to some random starting value $\mathbf{W}^{(0)}$.
- η is called **learning rate**, and it is typically set to a small real value (such as, $\eta = 0.001$). It may be reduced as learning progresses.
- It is convenient to think of $\mathbf{W}$ as a vector not a matrix when doing learning. (Think of it in "vectorized" form: $\mathrm{vec}(\mathbf{W})$)

Learning with stochastic gradient descent



- Since the algorithm visits one training-case at a time, it will jitter around an idealized "average path" towards the optimum.
- That's why it's called "stochastic" gradient descent.
- One could use the gradient of the whole sum instead but that is often slower (because of redundancies in the data).

The "logsumexp"-trick

- Expressions like

$$\frac{\exp\left(\mathbf{w}_k^{\mathrm{T}}\mathbf{x}_n\right)}{\sum_{j=1}^{K}\exp\left(\mathbf{w}_j^{\mathrm{T}}\mathbf{x}_n\right)}$$

  are very common but *highly unstable*, because the "exp" in the denominator can cause an under- or overflow.
- Never compute sums $\sum_i \exp(a_i)$ naively.
- Add a constant A to each argument in all exp's, so that even the largest argument is small; then undo the operation after computing the sum!
- Many software packages supply a convenience function "logsumexp" for this purpose:

logsumexp

$$\mathrm{logsumexp}(a1,\ldots,a_K) = \log\left(\sum_i \exp(a_i + A)\right) - A$$
$$\text{with } A = -(\max_i a_i)$$

Random variables and information

- "Probabilities allow us to be explicit about uncertainty". So how can we *measure* uncertainty?
- Idea: Define the *information content*

$$\log\left(\frac{1}{p(x)}\right) = -\log(p(x))$$

  contained in a random event.
- The information content is additive for independent events.
- So if we use $\log_2$ and fair coin tosses, then the information content is measured in *bits* and it exactly fits our intuition.

Entropy

- To measure uncertainty, we define the entropy

$$H(X) = -\sum_x p(x)\log p(x)$$

  which is the average information content.
- For continuous RV:

$$H(X) = -\int_x p(x)\log p(x)dx$$

- The more uniform, the more uncertain. The more "peaky", the more certain.
- Question: Which probability distribution has maximum entropy, given mean and (co)variance(s)?

KL divergence

- Closely related to entropy is the Kullback-Leibler divergence (KL divergence) (or "relative entropy"):

$$\mathrm{KL}(p||q) = \sum_x p(x) \log \left(\frac{p(x)}{q(x)} \right)$$

- The KL divergence measures the dissimilarity between two distributions.
- It is not symmetric.

Mutual Information

- The mutual information between two random variables x, y with joint density $p(x, y)$ is defined as

$$\mathrm{MI}(x, y) = \sum_{x,y} p(x, y) \log \left(\frac{p(x, y)}{p(x)p(y)} \right)$$

- It is the KL divergence between $p(x, y)$ and the joint of two perfectly independent random variables (with marginals $p(x)$ and $p(y)$).
- Thus, MI measures the *dependence* between x and y.
- It is nonnegative, and it is zero iff x and y are independent, in other words iff $p(x, y) = p(x)p(y)$.

The Frequentist – Bayesian debate

- Probability theory tells us how to *calculate* with probabilities.
- As scientists, we may ask how to *interpret* a probabilistic expression, like $p(x = 1) = 0.7$
- There are two common interpretations:
  1. *Frequentist:* "The *relative frequency* of x in a (possibly infinite) population of trials is 0.7"
  2. *Bayesian:* "*I believe* that x is 1 with certainty 0.7"
- The Bayesian view used to be contentious because it is less intuitive.
- But it gives us the freedom to turn model parameters into random variables.

Reading

- A good introduction to most of the concepts discussed in this class can be found in:

  Pattern Recognition and Machine Learning. C. Bishop. Springer, 2006.

- Most drawings were taken from that book.