CPSC 440: Machine Learning

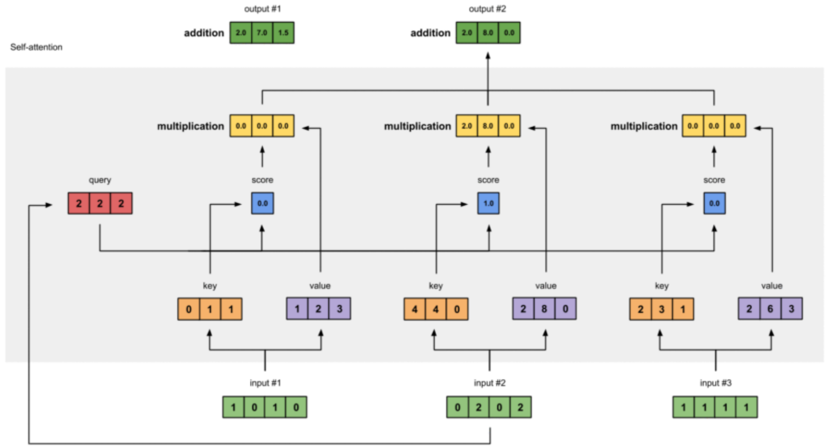
Gaussians

Winter 2022

Last Time: Attention and Transformers

- We discussed attention in RNNs:
  - Re-weight encoder states into context vector at each time.

- We discuss transformer networks:
  - Include "self-attention" layers.
    - Use attention mechanism between all input values.
  - Outperform CNNs/RNNs on many applications.
    - Many details/heuristics needed to make transformers work.
  - Basis of modern self-supervised language models like BERT and GPT-3.
    - Use BERT as pre-training for language models.



https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-models-with-attention/
https://towardsdatascience.com/illustrated-self-attention-2d627e33b20a

OpenAI's GPT-3

- One of the most widely-used methods is GPT-3:
  - Recent "massive number of parameters" NLP model.
    - Full version has 175 billion parameters.
  - Often works well in new applications with little or no "fine-tuning" on the application (pre-training does almost everything).
  - Basis for many modern language applications.
  - See the paper for a starting point on where we are (and are not) in terms of language understanding.

Language Models are Few-Shot Learners

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Abstract

Recent work has demonstrated substantial gains on many NLP tasks and benchmarks by pre-training on a large corpus of text followed by fine-tuning on a specific task. While typically task-agnostic in architecture, this method still requires task-specific fine-tuning datasets of thousands or tens of thousands of examples. By contrast, humans can generally perform a new language task from only a few examples or from simple instructions – something which current NLP systems still largely struggle to do. Here we show that scaling up language models greatly improves task-agnostic, few-shot performance, sometimes even reaching competitiveness with prior state-of-the-art fine-tuning approaches. Specifically, we train GPT-3, an autoregressive language model with 175 billion parameters, 10x more than any previous non-sparse language model, and test its performance in the few-shot setting. For all tasks, GPT-3 is applied without any gradient updates or fine-tuning, with tasks and few-shot demonstrations specified purely via text interaction with the model. GPT-3 achieves strong performance on many NLP datasets, including translation, question-answering, and cloze tasks, as well as several tasks that require on-the-fly reasoning or domain adaptation, such as unscrambling words, using a novel word in a sentence, or performing 3-digit arithmetic. At the same time, we also identify some datasets where GPT-3's few-shot learning still struggles, as well as some datasets where GPT-3 faces methodological issues related to training on large web corpora. Finally, we find that GPT-3 can generate samples of news articles which human evaluators have difficulty distinguishing from articles written by humans. We discuss broader societal impacts of this finding and of GPT-3 in general.

https://arxiv.org/pdf/2005.14165.pdf

More Applications

- Generating memes:
  - https://github.com/alpv95/Dank-Learning
- Generating Wikipedia articles:
  - https://arxiv.org/pdf/1801.10198.pdf
- Talking with historical figures:
  - https://www.besttechie.com/aiwriter-uses-openai-to-simulate-conversations-with-historical-figures/
- Generating music:
  - https://magenta.tensorflow.org/music-transformer
- Writing code:
  - https://copilot.github.com
- Generating video game content:
  - https://play.aidungeon.io/main/home

End of Part 2 (“Categorical Variables”): Key Concepts

- We discussed categorical density estimation.
  - Model the proportion of times different categories appear.
  - Categorical θ_c parameterization and unnormalized probabilities $\tilde{\theta}_c$.
  - Sampling using the cumulative distribution function (CDF).
- We discussed Monte Carlo for approximating expectations.
  - Generate samples from a model.
  - Compute the average function value on the samples.
- We discussed conjugate priors.
  - For a given likelihood, a prior that leads to posterior in “family” of prior.
  - Conjugate prior for categorical distribution is the Dirichlet distribution.
    - Dirichlet gives a “probability over discrete probabilities”.

End of Part 2 ("Categorical Variables"): Key Concepts

- We reviewed standard conditional independence assumptions:
  - Data is IID [given parameters].
  - Data is independent of hyper-parameters given parameters.
  - Discriminative models assume parameters are independent of features.
- We discussed Bayesian learning:
  - Instead of using a single parameter, sum/integrate over all parameters.
  - Prediction using the posterior predictive distribution.
    - And possibly a cost function for Bayesian decision theory.
  - Very-strong protection against overfitting.
- We discussed empirical Bayes:
  - Optimize hyper-parameters using the marginal likelihood.
  - Can optimize a large number of hyper-parameters, without a validation set.
- We discussed hierarchical Bayes:
  - Putting a prior on the prior, which we used to model non-IID grouped data.

End of Part 2 (“Categorical Variables”): Key Concepts

- We discussed multi-class classification.
  - Categorical generalization of sigmoid function is the softmax function.
- We discussed multi-class neural networks.
  - Put softmax on the last layer.
  - Other layers can stay the same, and the same tricks are used/needed.
- We discussed “what have we learned”.
  - Layers in CNNs seem to be doing something sensible.
  - But ML models are easily fooled in various ways.
  - And ML models can have harmful biases.

End of Part 2 (“Categorical Variables”): Key Concepts

- We discussed recurrent neural networks (RNNs).
  - Use tied parameters across time to model sequences of different lengths.
    - Makes vanishing/exploding gradient and “forgetting” problems worse.
  - Sequence-to-sequence handles output sequences of unknown lengths.
  - Multi-modal learning considers input and output of different formats.
- We discussed long short term memory (LSTM) models.
  - Include memory cells that are read/written/cleared with gates.
  - Allows modeling longer-range dependencies than standard RNNs.
- We discussed attention.
  - Allows decoder to access information from all encoding steps.
- We discussed transformers.
  - “Fully-connected” attention that forms basis for many modern methods.

Next Topic: Gaussian Density Estimation

Motivating Problem: Cell Phone Battery Life

- Consider modeling battery life between charges:
  - It makes sense to view this as a continuous quantity.
    - Rather than a fixed set of values, the battery life could be any real number.

- Reviews/advertisements will often advertise estimates:

If you want the longest battery life, the iPhone 13 Pro Max is the one to get. In our battery test, the iPhone 13 Pro Max streamed a continuous video at full screen brightness for a whopping **20 hours and 18 minutes**. Nov 11, 2021

https://www.businessinsider.com › ... › Tech › Smartphones

iPhone 13 Pro Max Review: Longest Battery Life and Biggest ...

- We want to find the full distribution over charging times.
  - So we can solve real-world problems like:
    - “If I have not charged for 18 hours, what is the probability I will make it to 21 hours?”

General Problem: Continuous Density Estimation

- We can view this as density estimation with a continuous variable:
  - Input: 'n' IID samples of continous values x^1, x^2, x^3,…, x^n from a population.
  - Output: model of probability density for any real number 'x'.
- Continuous density estimation as a picture:

X =

Battery Life
20h18m00s
16h53m42s
21h03m50s
17h33m13s
27h46m28s

p(x = 20h18m02s) = 0.8

- Watch out: we are estimating the density here, not the probability.
  - We could have $p(x) > 1$.
  - You would get probabilities for doing integrals of the density over intervals.

Other Applications

- Other applications where continuous density estimation is useful:
  - Modeling sizes (size of food grown in field, birthweight of babies).
  - Modeling times or control values in a manufacturing process.
  - Modeling stock variations or income distributions.
  - Modeling continuous medical measurements (blood pressure).
  - Modeling grades.

- Even with 1 variable there are many possible distributions.
  - More complicated than binary/categorical.

- We first consider the simple case were we assume data is Gaussian.
  - Also known as a "normal" distribution.

Univariate Gaussian

- The Gaussian probability density has the form:

$$p(x^i \mid \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x^i-\mu)^2}{2\sigma^2}\right)$$

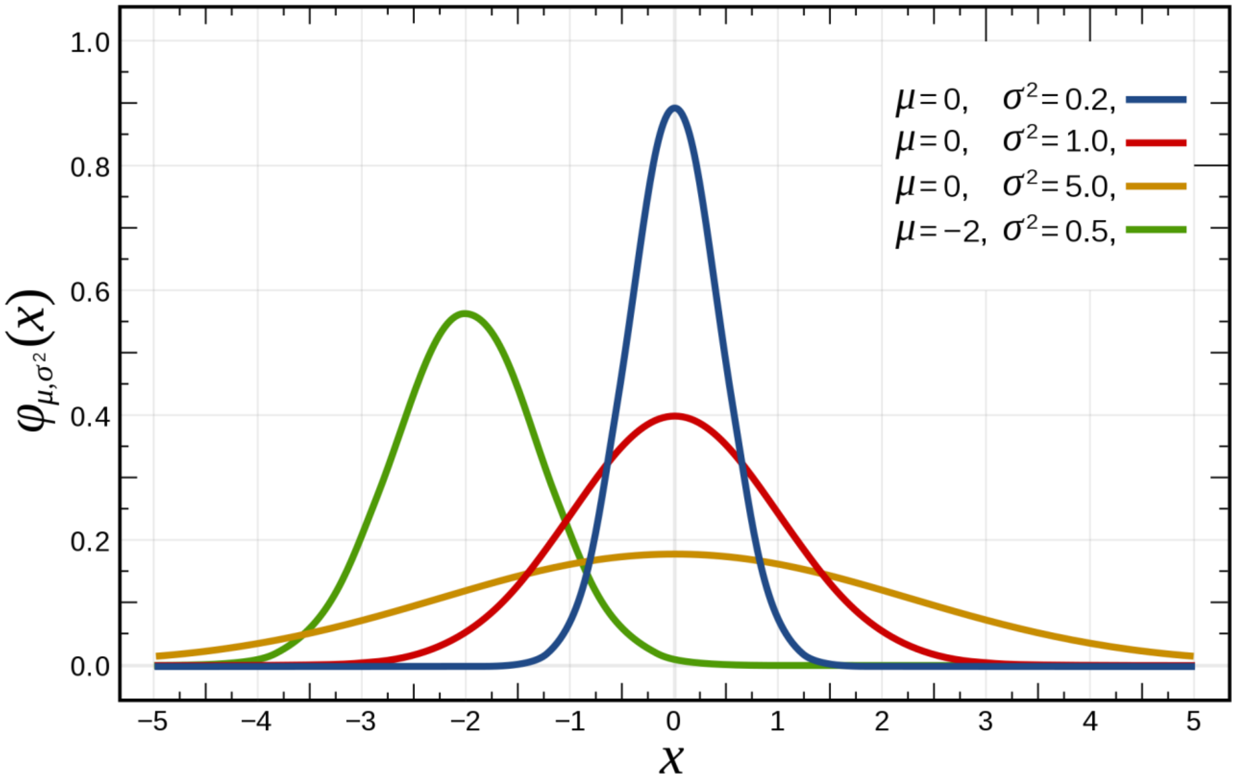
  - The mean parameter μ can be any real number.
  - The standard deviation σ can be any positive number.
    - We call σ^2 the variance.
    - Gaussians are also known as normal distributions.

- If we assume x^i follows a Gaussian distribution, we often write:

$$x^i \sim \mathcal{N}(\mu, \sigma^2)$$

"x^i is generated from a normal distribution with mean μ and variance σ^2"

Univariate Gaussian



- Mean parameter μ controls location of center of density.
- Variance parameter σ^2 controls how spread out density is.
  - As $\sigma \to 0$ you get a "spike" at the mean, as $\sigma \to \infty$ you get uniform.

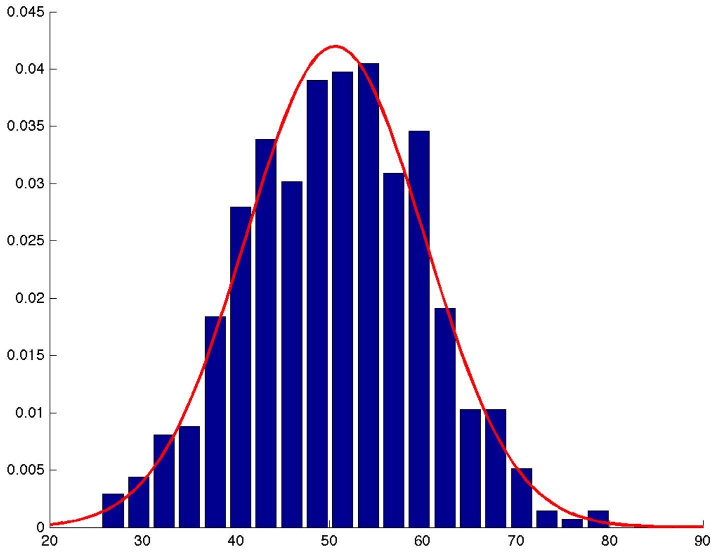
https://en.wikipedia.org/wiki/Normal_distribution

Motivation for Gaussian

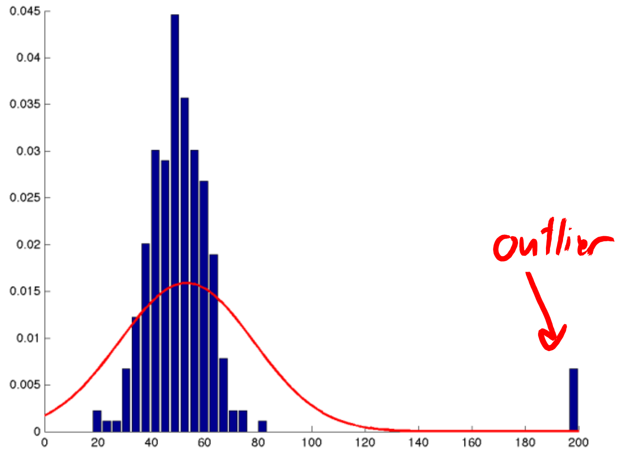
- Why use the Gaussian distribution?
  - Data might actually follow Gaussian.
    - Good justification if true, but usually false.
  - Central limit theorem: many sums of random variables converge* to Gaussian.
    - Usually a bad justification: does not imply data distribution converges to a Gaussian.
      - You would have to argue that your data comes from an asymptotic process where CLT applies.
  - Distribution with maximum entropy that fits mean and variance of data.
    - "Makes the least assumptions" while matching the mean and variance of data.
      - We will discuss this later when we discuss the "exponential family".
    - But for complicated problems, just matching means and variances is not enough.
  - Makes many computations and doing theory much easier.
    - The same reason we use a lot of the common distributions.
    - Sometimes Gaussians are "good enough to be useful".
    - Gaussians are common "building blocks" in more-advanced methods.

Motivations for not using Gaussians

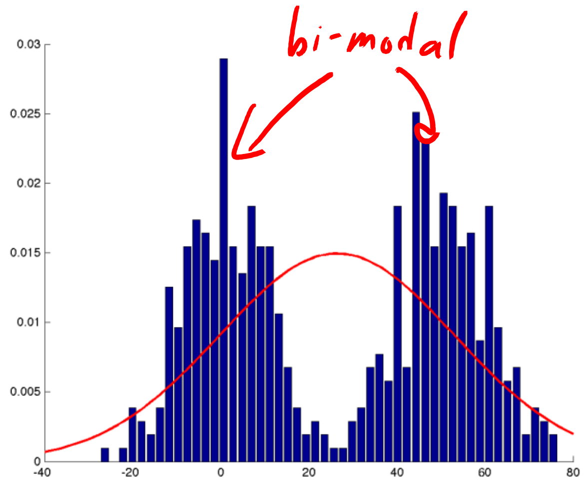
- Histogram of x^i values with red line being MLE Gaussian density:



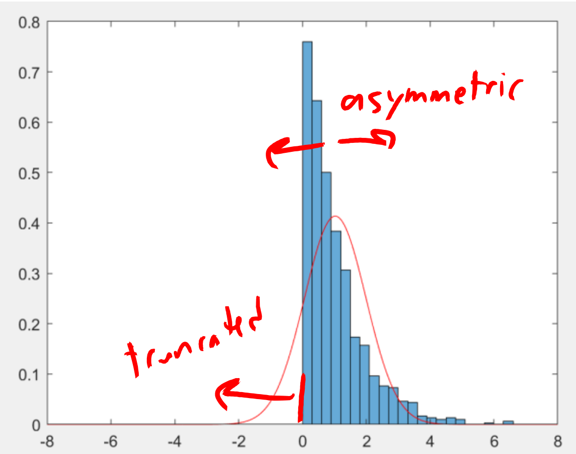
Symmetric around mean, untruncated, no outliers, uni-modal =>



Sensitive to outliers



Cannot model multiple modes



assumes symmetric and not truncated

- Grades usually have all these issues.

Next Topic: Gaussian Inference and Learning

Inference in Univariate Gaussians

- Decoding: find 'x' that maximizes the PDF p(x | μ, σ^2).
  - The decoding is given by the mean μ.
- Computing likelihood of an IID dataset:

$$p(X \mid \mu, \sigma^2) = \prod_{i=1}^{n} p(x^i \mid \mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x^i-\mu)^2}{2\sigma^2}\right) = \frac{1}{(\sigma\sqrt{2\pi})^n} \prod_{i=1}^{n} \exp\left(-\frac{(x^i-\mu)^2}{2\sigma^2}\right)$$

$$= \frac{1}{(\sigma\sqrt{2\pi})^n} \exp\left(-\frac{\sum_{i=1}^{n}(x^i-\mu)^2}{2\sigma^2}\right)$$

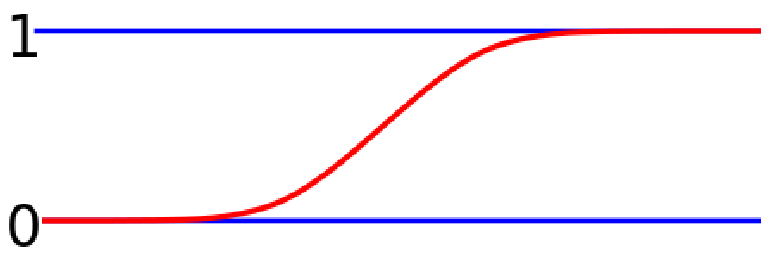
  - Not that the likelihood is a density and not a probability.
- Computing probability that an 'x' lies in an interval:

$$\text{prob}(a \leq x \leq b \mid \mu, \sigma^2) = \int_a^b p(x \mid \mu, \sigma^2)dx = \underbrace{\text{prob}(x \leq b \mid \mu, \sigma^2)}_{\text{CDFs}} - \underbrace{\text{prob}(x \leq a \mid \mu, \sigma^2)}_{\text{CDFs}}$$

  - If a=b this is zero, so any 'x' has probability zero.

Cumulative Distribution Function (CDF)

- We often use F(c) = prob(x ≤ c) = $\int_{-\infty}^{c} p(x)$ to denote the CDF.
  - F(c) is between 0 and 1, giving proportion of times ‘x’ is below ‘c’.
  - F(c) monotonically increases with ‘c’.



- The Gaussian CDF is given by: $F(c) = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{c-\mu}{\sigma\sqrt{2}}\right)\right]$
  - Where the “error function” erf is computed numerically and given by:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$$

Sampling with the Inverse CDF ("Quantile") Function

- How can we sample from a continuous density?
- We want to write a function that takes a uniform sample and:
  - 50% of the time it returns a sample in the region where F(c)= 50%.
  - 25% of the time it returns a sample in the region where F(c) = 25%.
  - 75% of the time it returns a sample in the region where F(c) = 75%.
  - 10% of the time it returns a sample in the region where F(c) = 10%.
  - And so on, so the CDF F(c) divides up the interval [0,1].
- The function we want is the inverse of the CDF F^{-1} ("quantile" function):
  - $F^{-1}(u) = c$ for the unique 'c' where $F(c) = u$.
  - Allows sampling from Gaussians and using Monte Carlo with Gaussians.

Inverse Transform Method (Exact 1D Sampling)

- Inverse transform method for exact sampling of a continuous density in 1D:
  1. Sample 'u' uniformly between 0 and 1.
  2. Return $F^{-1}(u)$.

- For Gaussians, we have $F^{-1}(u) = \mu + \sigma\sqrt{2}\,\mathrm{erf}^{-1}(2u - 1)$.
  - Formula will convert uniform 'u' values into sample from a Gaussian.
  - To sample a N(0,1) distribution as in the "randn()" function, use "sqrt(2)*erfinv(2*rand()-1)".

- Showing that CDF of samples has CDF we want to sample from (for invertible 'F'):

$$
\begin{aligned}
\mathrm{prob}(\text{sample} \leq c) &= \mathrm{prob}(F^{-1}(u) \leq c) && \text{(sample is given by } F^{-1}(u)\text{)} \\
&= \mathrm{prob}(F(F^{-1}(u)) \leq F(c)) && \text{(apply strictly-monotonic 'F' to inequality)} \\
&= \mathrm{prob}(u \leq F(c)) && \text{(F and } F^{-1} \text{ are inverses)} \\
&= F(c) && \text{(}\mathrm{prob}(u \leq y) = y \text{ for uniform 'u')}
\end{aligned}
$$

  - So after the inverse transform, we have the CDF of the distribution we want.
- Video on pseudo-randomness and inverse-transform sampling.

MLE for Univariate Gaussian

- We showed that the likelihood for 'n' IID examples is given by:

$$p(X \mid \mu, \sigma^2) = \frac{1}{(\sigma\sqrt{2\pi})^n} \exp\left(-\frac{\sum_{i=1}^{n}(x^i-\mu)^2}{2\sigma^2}\right)$$

- To compute the MLE, minimize the NLL (which is convex):

$$-\log p(X \mid \mu, \sigma^2) = n \log \sigma + \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x^i-\mu)^2 + \text{constant}$$

- Setting derivative with respect to μ to 0 gives MLE of: $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x^i$
  - So MLE for the mean is the mean of the samples.
- Plugging in $\hat{\mu}$ and setting derivative with respect to σ to 0 gives: $\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x^i-\hat{\mu})^2$
  - So MLE for the variance is the variance of the samples.
    - Unless all x^i are equal (then NLL is not bounded below and MLE does not exist).

Conjugate Prior and Posterior for Mean

- For fixed variance, conjugate prior for mean is Gaussian.

If each $x^i \sim \mathcal{N}(\mu, \sigma^2)$ and $\mu \sim \mathcal{N}(m, v)$, then $\mu \mid x^1, x^2, \dots, x^n \sim \mathcal{N}(\tilde{m}, \tilde{v})$

where $\tilde{m} = \frac{vn}{vn + \sigma^2}\hat{\mu}_{MLE} + \frac{\sigma^2}{vn + \sigma^2} m$ and $\tilde{v} = \left(\frac{n}{\sigma^2} + \frac{1}{v}\right)^{-1}$

  - "Self conjugacy" is a **very special** property (a key to usefulness of Gaussians).
    - Derived by using '∝' and "completing the square" in exponent (see notes on webpage).
  - Formulas look a bit weird, but consider $\tilde{m}$ and $\tilde{v}$ change as 'n' grows:
    - As 'n' grows posterior mean $\tilde{m}$ converges from prior mean m towards MLE.
    - As 'n' grows posterior variance $\tilde{v}$ converges from prior variance v down to 0.
  - MAP estimate is given by $\tilde{m}$ (it has the highest PDF of the posterior).
  - Posterior predictive is also given by a Gaussian (not obvious, see notes linked on webpage).
    - With mean $\tilde{m}$ and variance $\tilde{v} + \sigma^2$.
    - For complicated Bayeisan inference tasks, can use Monte Carlo by sampling from Gaussian posterior.

- We will come back to MAP/Bayes estimation for variance later.

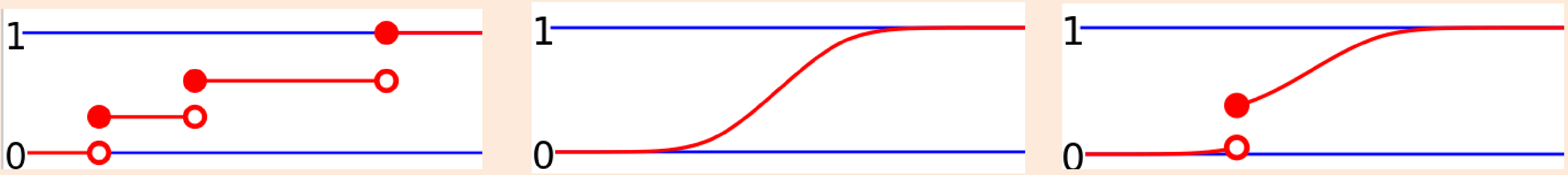
Summary

- Gaussian density estimation:
  - Modeling continuous variable samples, assuming it follows a Gaussian.
  - We use Gaussians because they have lots of nice properties.
  - But Gaussians assume symmetric, no outliers, no truncation, uni-modal.
- Mean and variance parameterization of Gaussians:
  - Mean specifies center of distribution.
  - Variance specifies spread of distribution.
- Inverse transform method for sampling:
  - Apply the “inverse” of the CDF to uniform samples to generate samples.
- MLE and MAP for Gaussians:
  - MLE is given by mean and variance of samples.
  - Conjugate prior for mean is another Gaussian.
    - MAP moves between mean of samples and prior mean.
    - Posterior predictive is also Gaussian in this case.

- Next time: more about Gaussians than you ever wanted to know.

Cumulative Distribution Function (CDF)

- CDF can be used for discrete and continuous variables (and mixed).



- We can generalize the quantile function to non-invertible case.

https://en.wikipedia.org/wiki/Cumulative_distribution_function

Quantile Function – Non-Invertible Case

- If the CDF 'F' is not invertible, we define the quantile F^{-1} as:

$$F^{-1}(u) = \inf\{c \mid F(c) \geq u\}$$

- "Smallest value 'c' such that F(c) is bigger than u."
  - See notes on max and argmax if you have not seen 'inf' before.
    - It's a variant on 'min' that is defined in more cases.

- If 'F' is invertible at this 'c', this gives the usual inverse.
  - But this more-general definition handles non-invertible points.
    - For example, the CDF is not invertible for categorical variables at the "jumps" in CDF.
      - Many values of 'u' are mapped to by the same 'c'.