CPSC 440/540: Advanced Machine Learning

Mixtures, EM, KDE

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Last Time: Gaussian Mixtures

- Mixture of k Gaussians: per-class parameters $\pi_c \in \mathbb{R}$, $\mu_c \in \mathbb{R}^d$, $\Sigma_c \in \mathbb{R}^{d \times d}$,

$$p(x \mid \mu, \Sigma, \pi) = \sum_{c=1}^{k} \pi_c \underbrace{p(x \mid \mu_c, \Sigma_c)}_{\text{PDF of Gaussian } c}.$$

- Latent variable representation: $z^i \sim \text{Categorical}(\pi)$, $x^i \mid z^i \sim \mathcal{N}(\mu_c, \Sigma_c)$.
    - Can't observe z^i, but leads to an ancestral sampling algorithm.
- Responsibilities: our "posterior estimate" for which component a point came from:

$$\mathbf{R} \in \mathbb{R}^{n \times k}, \qquad r_c^i = p(z^i = c \mid x^i) = \frac{\pi_c p(x^i \mid \mu_c, \Sigma_c)}{\sum_{c'=1}^{k} \pi_{c'} p(x^i \mid \mu_{c'}, \Sigma_{c'})}.$$

Learning Mixture Models with Imputation

- Mixture of Gaussian parameters are $\{\pi_c, \mu_c, \Sigma_c\}_{c=1}^k$.
  - Unfortunately, NLL is non-convex.
  - Various optimization methods are used in practice.

- If we treat the z^i as parameters, we get a simple algorithm for decreasing NLL:
  1. Given the clusters z^i, find the most likely parameters.
     - Optimize $p(\mathbf{X} \mid \pi, \mu, \Sigma, \mathbf{z})$ in terms of the $\{\pi_c, \mu_c, \Sigma_c\}_{c=1}^k$.
     - Set π_c based on frequency of seeing $z^i = c$.
     - Set μ_c to the mean of examples in cluster c.
     - Set Σ_c to the covariance of examples in cluster c.
  2. Given the parameters, find the most likely clusters.
     - For each example i, compute responsibility $r_c^i = p(z^i = c \mid x^i, \pi_c, \mu_c, \Sigma_c)$.
     - Set z^i to the the argmax of r_c^i over c.

- Connection to Gaussian discriminant analsysis (GDA), using clusters z^i as labels:
  - Step 1 above is the learning step in GDA, Step 2 above is the prediction step in GDA.

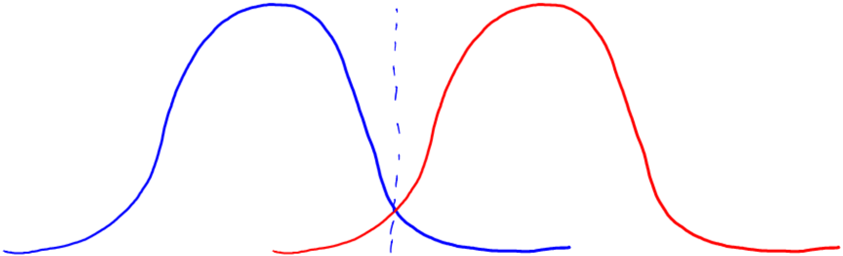
Special Case of K-Means

- Algorithm from the previous slide is a generalization of k-means clustering.
- Apply the algorithm assuming $\pi_c = 1/k$ and $\Sigma_c = I$ for all c:
  1. Given the clusters z^i, find the most likely parameters.
     - Sets μ_c to the mean of examples in cluster c.
  2. Given the parameters, find the most likely clusters.
     - Sets z^i to the closest mean of example i.
- As with k-means, initialization matters for mixture of Gaussians.
  - May need to do multiple random restarts, or clever initializations like k-means++.

K-Means vs. Mixture of Gaussians

- K-means can be viewed as fitting mixture of Gaussians (same π_c and Σ_c).
  - But variable Σ_c in general mixture of Gaussians allows non-convex clusters.

With same covariance, clusters are convex.



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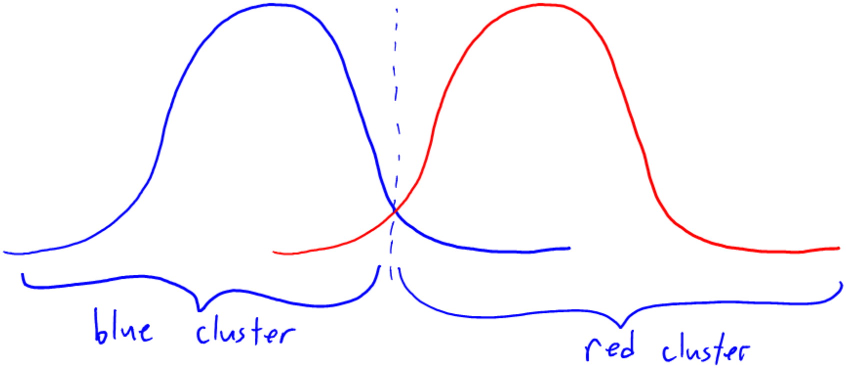

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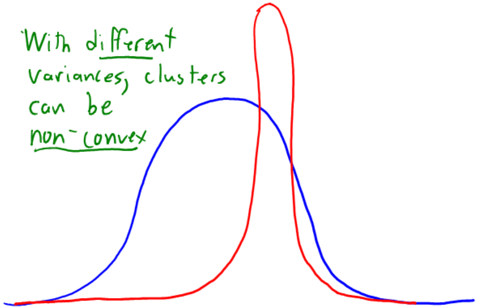

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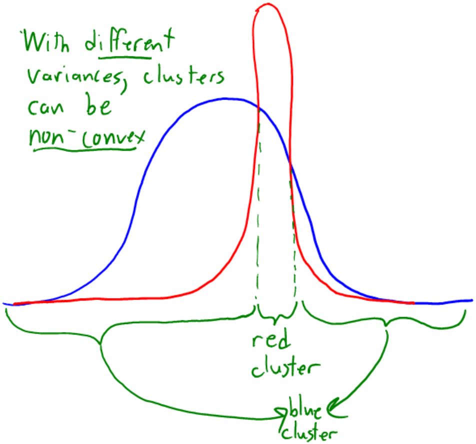

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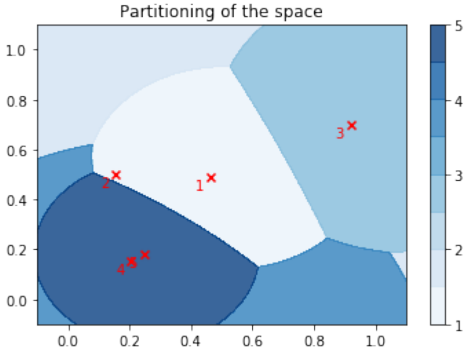

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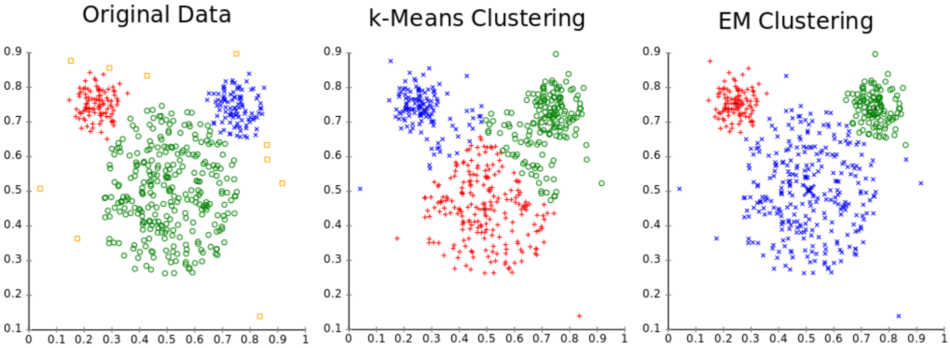


https://en.wikipedia.org/wiki/K-means_clustering

Digression: MLE does not exist

bonus!

- For mixture of Gaussian, there is no MLE.
- You can make the likelihood arbitrarily large:
  - Set $\mu_c = x^i$ for a particular i and c, and make $\Sigma_c \to 0$.
  - It is common for optimizers to converge to models with degenerate clusters.
    - Empty or covariance is not positive definite.
- It is common to remove empty clusters and use a regularized update,

$$\Sigma_c = \frac{1}{\sum_{i=1}^n r_c^i} \sum_{i=1}^n r_c^i (x^i - \mu_c)(x^i - \mu_c)^T + \lambda I,$$

which corresponds to MAP estimation with an L1-regularizer on Θ diagonals.

  - The MAP estimate exists under this and other usual priors on Σ_c.

Outline

1. Mixture of Gaussians
2. Mixture of Bernoullis
3. Expectation Maximization
4. Advanced Mixtures
5. Kernel Density Estimation

Previously: Product of Bernoullis

- We previously considered density estimation with discrete variables,

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

- We considered a product of Bernoullis:

$$p(x^i \mid \theta) = \prod_{j=1}^{d} p(x^i_j \mid \theta_j).$$

  Easy to fit but strong independence assumption:
  - Knowing x^i_j tells you nothing about x^i_k.

- A more-powerful model is a mixture of Bernoullis.

Mixture of Bernoullis

- Consider a coin flipping scenario where we have two coins:
  - Coin 1 has $\theta_1 = 0.5$ (fair) and coin 2 has $\theta_2 = 1$ (biased).

- Half the time we flip coin 1, and otherwise we flip coin 2:

$$
\begin{aligned}
p(x^i = 1 \mid \theta_1, \theta_2) &= \pi_1\, p(x^i = 1 \mid \theta_1) + \pi_2\, p(x^i = 1 \mid \theta_2) \\
&= \frac{1}{2}\theta_1 + \frac{1}{2}\theta_2 = \frac{\theta_1 + \theta_2}{2}
\end{aligned}
$$

- With one variable this mixture model is not very interesting:
  - It's equivalent to flipping one coin with $\theta = 0.75$.

- But with multiple variables, mixture of Bernoullis can model dependencies...

Mixture of Independent Bernoullis

- Consider a mixture of a product of Bernoullis:

$$p(x \mid \theta_1, \theta_2) = \frac{1}{2} \underbrace{\prod_{j=1}^{d} p(x_j \mid \theta_{1j})}_{\text{first set of Bernoullis}} + \frac{1}{2} \underbrace{\prod_{j=1}^{d} p(x_j \mid \theta_{2j})}_{\text{second set of Bernoulli}} .$$

- Conceptually, we now have two sets of coins:
  - Half the time we throw the first set, half the time we throw the second set.

- With $d = 4$ we could have $\theta_1 = \begin{bmatrix} 0 & 0.7 & 1 & 1 \end{bmatrix}$ and $\theta_2 = \begin{bmatrix} 1 & 0.7 & 0.8 & 0 \end{bmatrix}$.
  - Half the time we have $p(x_3^i = 1) = 1$ and half the time it's 0.8.

- Have we gained anything?

Mixture of Independent Bernoullis

- Example from the previous slide: $\theta_1 = \begin{bmatrix} 0 & 0.7 & 1 & 1 \end{bmatrix}$ and $\theta_2 = \begin{bmatrix} 1 & 0.7 & 0.8 & 0 \end{bmatrix}$.
- Here are some samples from this model:

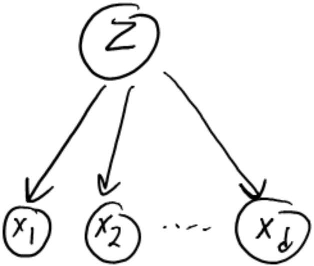
$$\mathbf{X} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

- Unlike product of Bernoullis, notice that features in samples are not independent.
    - In this example knowing $x_1 = 1$ tells you that $x_4 = 0$.

- This model can capture dependencies: $\underbrace{p(x_4 = 1 \mid x_1 = 1)}_{0} \neq \underbrace{p(x_4 = 1)}_{0.5}$.

Mixture of Independent Bernoullis

- Drawing the mixture of Bernoullis as a DAG:



- Since we do not know z, there are dependencies between x_j.
  - But features are independent if we know z.

- This is the same graph as naive Bayes, with cluster z instead of class y.
  - If you see one spammy word, it makes other spammy words more likely.

Mixture of Independent Bernoullis

- General mixture of independent Bernoullis:

$$p(x^i \mid \Theta) = \sum_{c=1}^{k} \pi_c p(x^i \mid \theta_c) = \sum_{c=1}^{k} \pi_c \prod_{j=1}^{d} \theta_{cj},$$

  where Θ contains all the model parameters.
  - Θ has k values of π_c and $k \times d$ values of θ_{cj}.

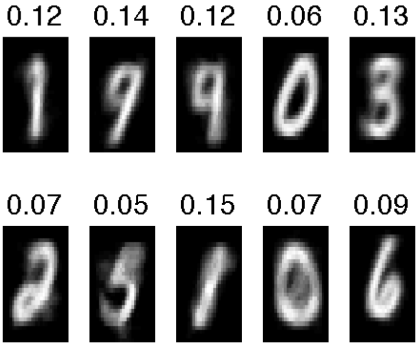
- Mixture of Bernoullis can model dependencies between variables
  - Individual mixtures act like clusters of the binary data.
  - Knowing cluster of one variable gives information about other variables.

- With k large enough, mixture of Bernoullis can model any binary distribution.
  - Hopefully with $k \ll 2^d$.

Mixture of Independent Bernoullis

- Plotting parameters θ_c with 10 mixtures trained on MNIST digits (with "EM"):

(numbers above images are mixture coefficients π_c)

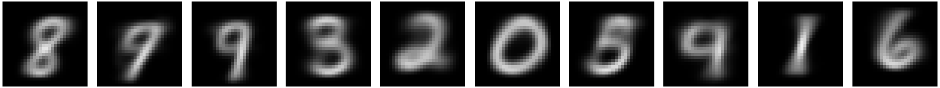


http://pmtk3.googlecode.com/svn/trunk/docs/demoOutput/bookDemos/%2811%29-Mixture_models_and_the_EM_algorithm/mixBerMnistEM.html

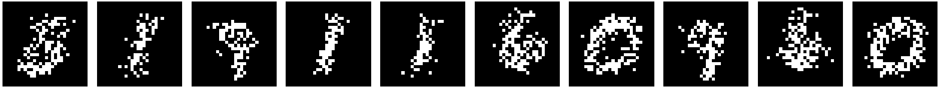
- Remember this is unsupervised: it hasn't been told there are ten digits.
  - You could use this model to "fill in" missing parts of an image.

Mixture of Bernoullis on Digits with $k > 10$

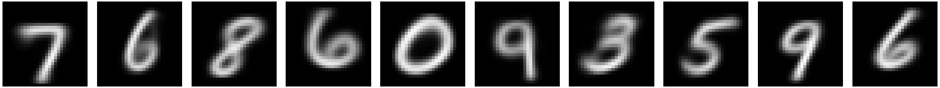
- Parameters of a mixture of Bernoulli model fit to MNIST with $k = 10$:



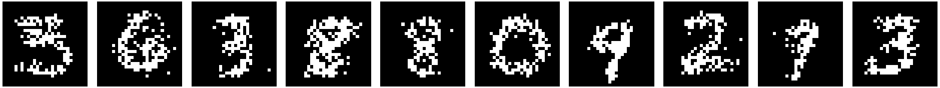
- Samples better than product of Bernoullis (but no within-cluster dependency):



- You get a better model with $k > 10$. First 10 components with $k = 50$:



- Samples from the $k = 50$ model (can have more than one "type" of a number):



Outline

Big Picture: Training and Inference

- Many possible mixture model inference tasks:
  - Generate samples.
  - Measure likelihood of test examples $\tilde{x}$.
    - To detect outliers, for example.
  - Compute probability that test example belongs to cluster c.
  - Compute marginal or conditional probabilities.
  - "Fill in" missing parts of a test example.

- Mixture model training phase:
  - Input is a matrix X, number of clusters k, and form of individual distributions.
  - Output is mixture proportions π_c and parameters of components.
    - The θ_c for Bernoulli, and the $\{\mu_c, \Sigma_c\}$ for Gaussians.
    - And maybe the responsibilities r_c^i or cluster assignments z^i.

Fitting a Mixture of Bernoullis: Imputation of z^i

- Imputation approach to ftting mixture of Bernoullis if we view z^i as parameters:
  1. Find the most likely cluster z^i for each example i,
  $$z^i \in \arg\max_c p(z^i = c \mid x^i, \Theta).$$
  2. Update the mixture probabilities as proportion of examples in cluster,
  $$\pi_c = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}(z^i = c).$$
  3. Update the product of Bernoullis based on examples in cluster,
  $$\theta_{cj} = \frac{\sum_{i=1}^{n} \mathbb{1}(z^i = c) x_j^i}{\sum_{i=1}^{n} \mathbb{1}(z^i = c)}.$$
- You can think of this as doing exact assignments to the z^i variables.

Fitting a Mixture of Bernoullis: Expectation Maximization

- Expectation maximization (EM) approach to ftting mixture of Bernoulli:
  1. Find the responsibility of cluster z^i for each example i
     $$r_c^i = p(z^i = c \mid x^i, \Theta).$$
  2. Update the mixture probabilities as proportion of examples cluster is responsible for,
     $$\pi_c = \frac{1}{n}\sum_{i=1}^{n} r_c^i.$$
  3. Update the product of Bernoullis based on examples cluster is responsible for,
     $$\theta_{cj} = \frac{\sum_{i=1}^{n} r_c^i x_j^i}{\sum_{i=1}^{n} r_c^i}.$$
- You can think of this as doing probabilistic assignment to the z^i variables.

Fitting a Mixture of Gaussians: Expectation Maximization

- Expectation maximization (EM) approach to ftting mixture of Gaussians:
  1. Find the responsibility of cluster z^i for each example i
  $$r_c^i = p(z^i = c \mid x^i, \Theta).$$
  2. Update the mixture probabilities as proportion of examples cluster is responsible for,
  $$\pi_c = \frac{1}{n}\sum_{i=1}^n r_c^i.$$
  3. Update the Gaussian based on examples cluster is responsible for,
  $$\mu_c = \frac{1}{\sum_{i=1}^n r_c^i}\sum_{i=1}^n r_c^i x^i, \quad \Sigma_c = \frac{1}{\sum_{i=1}^n r_c^i}\sum_{i=1}^n r_c^i (x^i - \mu_c)(x^i - \mu_c)^T.$$
- Video: `https://www.youtube.com/watch?v=B36fzChfyGU`

Expectation Maximization vs. Imputation

- The imputation method is optimizing $p(x^i, z^i \mid \Theta)$ in terms of z^i and Θ.
  - So we're optimizing z^i as well as Θ.
    - $p(x^i, z^i \mid \Theta)$ is called the complete-data likelihood.
- Expectation maximization (EM) is optimizing $p(x^i \mid \Theta)$ in terms of Θ.
  - So we're integrating over z^i values while optimizing Θ.
    - $p(x^i \mid \Theta)$ is the usual likelihood, marginalizing over the z^i.
- EM is a general algorithm for parameter learning with missing data.
  - For mixtures, the "missing" data is the z^i variables.
  - But EM can be used for any probabilistic model where we have missing data.

Expectation Maximization: General Form

- With data X and hidden values Z, the general EM uses iterations of the form

$$\Theta^{t+1} \in \underset{\Theta}{\arg\max} \sum_{Z} p(Z \mid X, \Theta^t) \log p(X, Z \mid \Theta)$$
$$\equiv \underset{\Theta}{\arg\max}\, \mathbb{E}_{Z \mid X, \Theta^t}[\log p(X, Z \mid \Theta)].$$

- Summing/integrating over all possible hidden values Z may be hard.
  - But in many cases this simplifies due to conditional independence assumptions.

- For mixture models, the EM iteration simplifies to (see notes on webpage)

$$\sum_{i=1}^{n} \sum_{z^i=1}^{k} \underbrace{p(z^i \mid x^i, \Theta^t)}_{\text{responsibility}} \underbrace{\log p(x^i, z^i \mid \Theta)}_{\text{complete-data log-lik}},$$

so summing over k^n possible clusterings turns into sum over nk terms.

"E-Step" and "M-Step" for Mixture Models

- For mixture models, EM is often written as two steps:
  1. E-step: compute responsibilities r_c^i for all i and c for current Θ^t.
  2. M-step: optimize the weighted "complete-data" log-likelihood

$$\Theta^{t+1} \in \operatorname*{arg\,max}_{\Theta} \sum_{i=1}^{n} \sum_{z^i=1}^{k} r_c^i \log p(x^i, z^i \mid \Theta).$$

- For other models, there may not be separate "E-steps" and "M-steps."

- EM is most useful when complete-data log-likelihood is easy to optimize.

- Most common case: complete-data log-likelihood is in an exponential family.
  - Mixture of Bernoullis, mixture of Gaussians, and many other cases.
  - In this case the M-step is a weighted combination of the sufficient statistics.

Expectation Maximization Algorithm: Properties

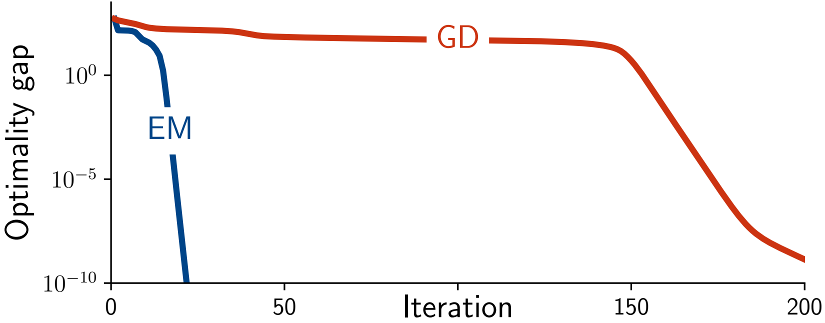
- EM monotonically increases likelihood, $p(X \mid \Theta^{t+1}) \geq p(X \mid \Theta^{t})$.
  - This is useful for debugging: if likelihood decreases you have a bug.
- EM doesn't need a step size, unlike many learning algorithms.
- EM tends to satisfy constraints automatically.
  - Unlike gradient descent, don't need to worry about constraints on π_c and Σ_c.
    - Assuming you have a prior to avoid degenerate situations where MLE does not exist.
- EM iterations are parameterization independent.
  - Get the same performance under any re-parameterization of the problem.
- EM is notorious for converging to bad local optima.
  - Not really the algorithm's fault: we typically apply EM to hard problems.

Expectation Maximization Algorithm: Properties

- EM converges to a stationary point under weak assumptions.
- EM is at least as fast as gradient descent (with a constant step size).
  - In the worst case, for differentiable problems.
  - EM can also be used for non-differentiable likelihoods.
- EM converges faster as entropy of hidden variables decreases.
  - If value of hidden variables is "obvious", it converges very fast.
- And EM can be arbitrarily faster than gradient descent.
- Mark has a bunch of more detailed material on the EM algorithm here:
  - `https://www.cs.ubc.ca/~schmidtm/Courses/440-W22/L34.5.pdf`

Expectation Maximization vs. Gradient Descent

- Expectation maximization vs. gradient for fitting mixture of 2 Gaussians:



- Show video.

Outline

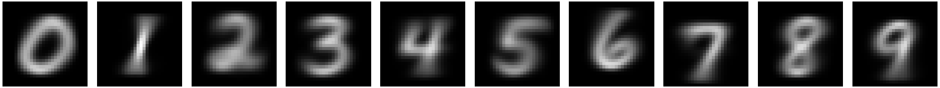
Combining Mixture Models with Other Models

bonus!

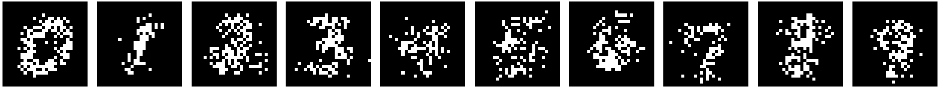
- We can use mixtures in generative classifiers.
  - Model $p(x \mid y)$ as a mixture instead of simple Gaussian or product of Bernoullis.
    - VQNB from Assignment 2 fits a mixture of Bernoullis for each class.
- We can do mixture of more-complicated distributions:
  - Mixture of categoricals (can model arbitrary categorical vectors).
  - Mixture of student t distributions.
    - Not exponential family, so no simple closed-form update of parameters.
  - Mixture of Markov chains for rain data (later).
  - Mixture of DAGs/UGMs (could be tree-structured for easy inference).
    - Captures both clusters and dependencies between variables in clusters.
- We can add features to mixture models for supervised learning:
  - Mixture of experts: have k regression/classification models.
    - Each model can be viewed as a "expert" for a cluster of x^i values.

Less-Naive Bayes on Digits

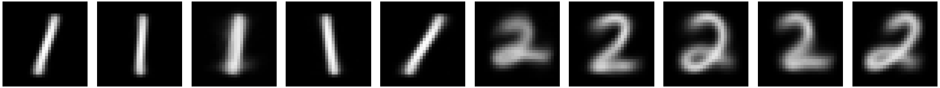
- Naive Bayes θ_c values (independent Bernoullis for each class):



- One sample from each class:



- Generative classifier with mixture of 5 Bernoullis for each class (digits 1 and 2):



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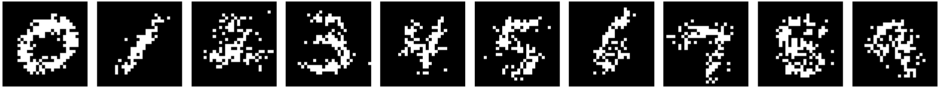


- Would get less noisy samples and more variation with mixture of graphical models.

Dirichlet Process

bonus!

- Non-parametric Bayesian methods allow us to consider infinite mixture model,

$$p(x \mid \Theta) = \sum_{c=1}^{\infty} \pi_c p(x \mid \Theta_c).$$

- Common choice for prior on π values is Dirichlet process:
  - Also called "Chinese restaurant process" and "stick-breaking process".
  - For finite datasets, only a fixed number of clusters have $\pi_c \neq 0$.
  - But don't need to pick number of clusters; it grows with data size.

- Gibbs sampling in Dirichlet process mixture model in action: `https://www.youtube.com/watch?v=0Vh7qZY9sPs`

Dirichlet Process

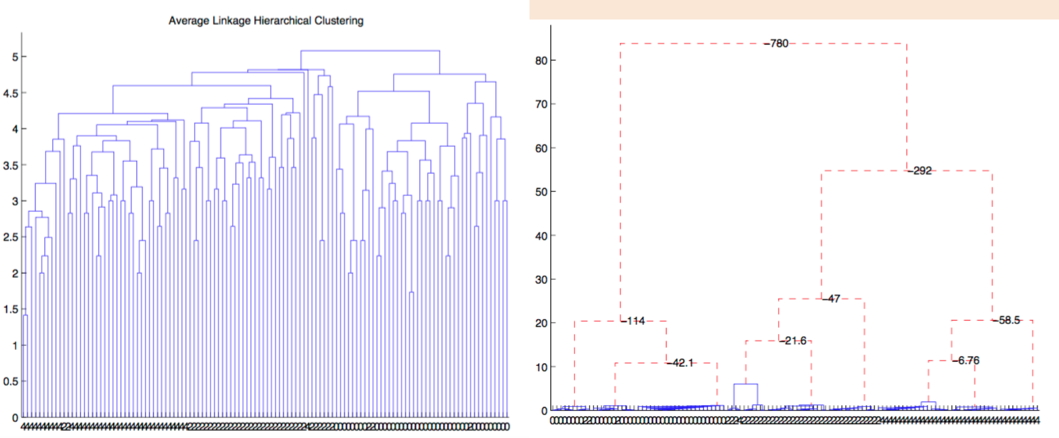
bonus!

- Slides giving more details on Dirichelt process mixture models:
  - `https://www.cs.ubc.ca/labs/lci/mlrg/slides/NP.pdf`
- We could alternately put a prior on number of clusters k:
  - Allows more flexibility than Dirichlet process as a prior.
  - Needs "trans-dimensional" MCMC to sample models of different sizes.
- There are a variety of interesting variations on Dirichlet processes
  - Beta process ("Indian buffet process").
  - Hierarchical Dirichlet process.
  - Polya trees.
  - Infinite hidden Markov models.

Bayesian Hierarchical Clustering

bonus!

- Hierarchical clustering of $\{0, 2, 4\}$ digits using classic and Bayesian method:

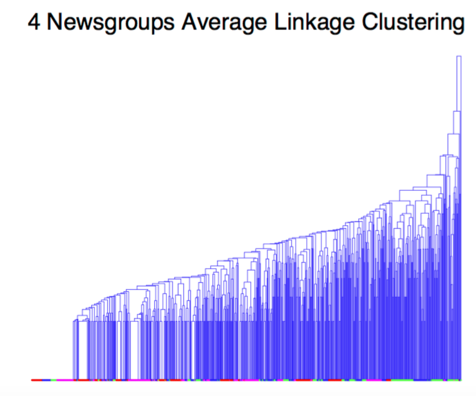


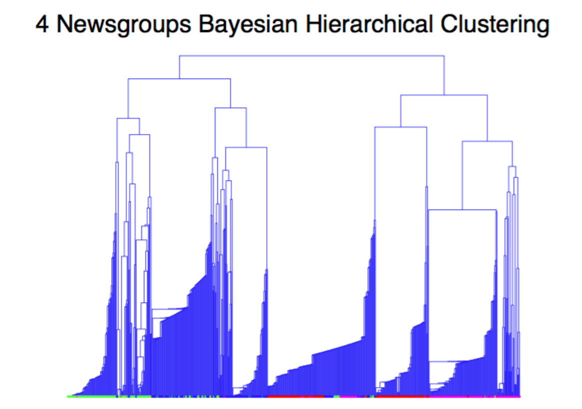
http://www2.stat.duke.edu/~kheller/bhcnew.pdf (y-axis represents distance between clusters)

Bayesian Hierarchical Clustering

bonus!

- Hierarchical clustering of newgroups using classic and Bayesian method:





http://www2.stat.duke.edu/~kheller/bhcnew.pdf (y-axis represents distance between clusters)

Continuous Mixture Models

bonus!

- We can also consider mixture models where z^i is continuous,

$$p(x^i) = \int_{z^i} p(z^i)p(x^i \mid z^i = c)dz^i.$$

- Unfortunately, computing the integral might be hard.

- Special case is if both probabilities are Gaussian (conjugate).
  - Leads to probabilistic PCA and factor analysis (OCEAN model in psychology).
  - My old material:
    `https://www.cs.ubc.ca/~schmidtm/Courses/540-W19/L17.5.pdf`.
- Another special case is scale mixtures of Gaussians
  - Where $p(x^i \mid z^i)$ is Gaussian and $p(z^i)$ is a gamma prior on variance (conjugate).
  - Can represent many distributions in this form, like Laplace and student t.
  - Leads to EM algorithms for fitting Laplace and student t..

Outline

Non-Parametric Mixtures: Kernel Density Estimation

- A common non-parametric mixture model centers one cluster on each example:

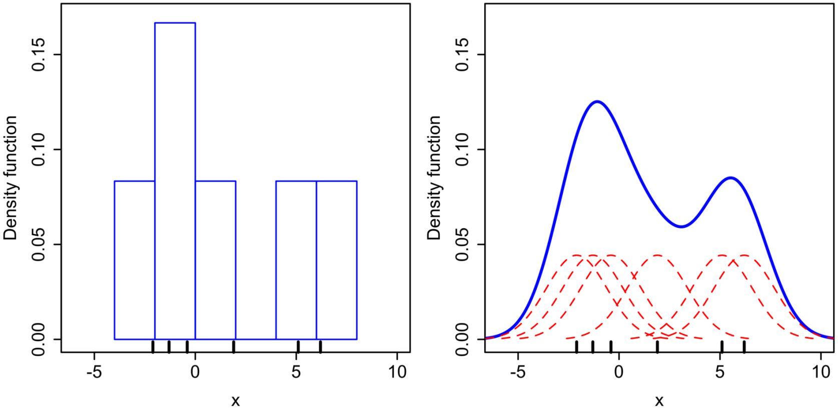
$$p(x^i) = \frac{1}{n}\sum_{j=1}^{n} p(x^i \mid x^j, \sigma^2 I).$$

- This is called kernel density estimation (KDE) or the Parzen window method.
  - Common choice is a Gaussian centered on each example ("mixture of n Gaussians").
  - Scale σ^2 is viewed as a hyper-parameter.

- By fixing mean/covariance/k, no parameters to learn (except σ^2).
  - And most inference tasks (except decoding) are easy but slow (depend on n).
  - Many variations exist, see bonus slides for generalizations.
    - Tends to work great in low dimensions and badly in high dimensions.

Histogram vs. Kernel Density Estimator

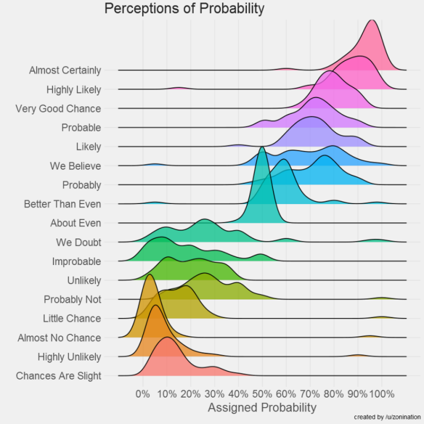
- You can think of a kernel density estimate as a continuous histogram:



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

Kernel Density Estimator for Visualization

- Visualization of people's opinions about what "likely" and other words mean.

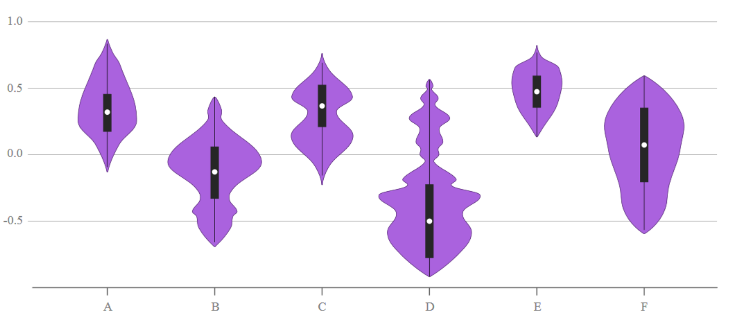


http://blog.revolutionanalytics.com/2017/08/probably-more-probably-than-probable.html

Violin Plot: Added KDE to a Boxplot

bonus!

- Violin plot adds KDE to a boxplot:

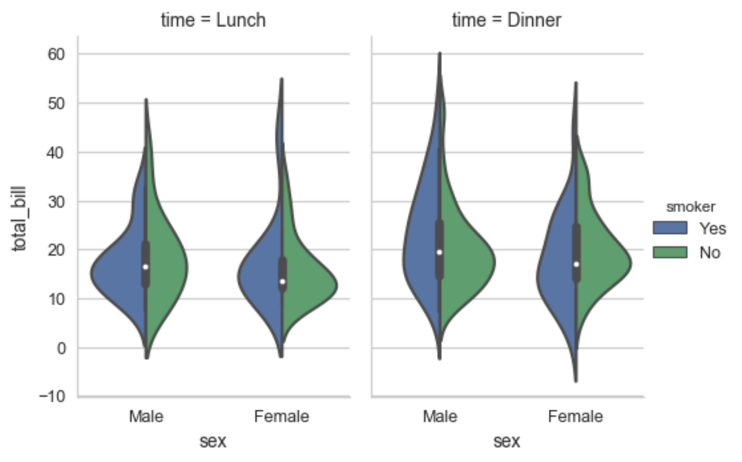


https://datavizcatalogue.com/methods/violin_plot.html

Violin Plot: Added KDE to a Boxplot

bonus!

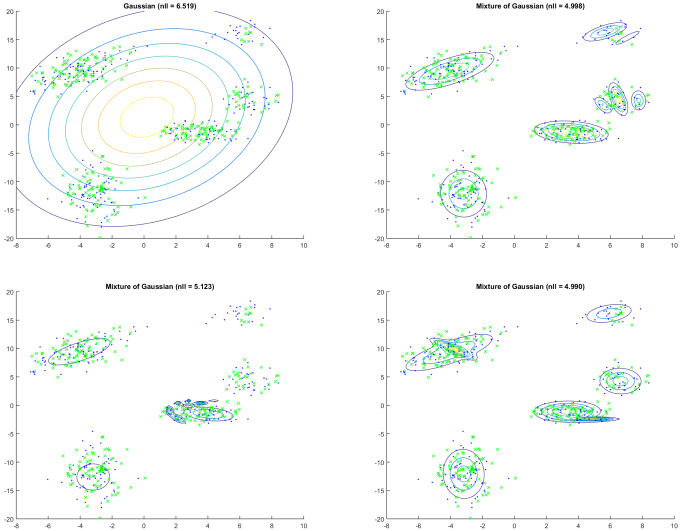
- Violin plot adds KDE to a boxplot:



https://seaborn.pydata.org/generated/seaborn.violinplot.html

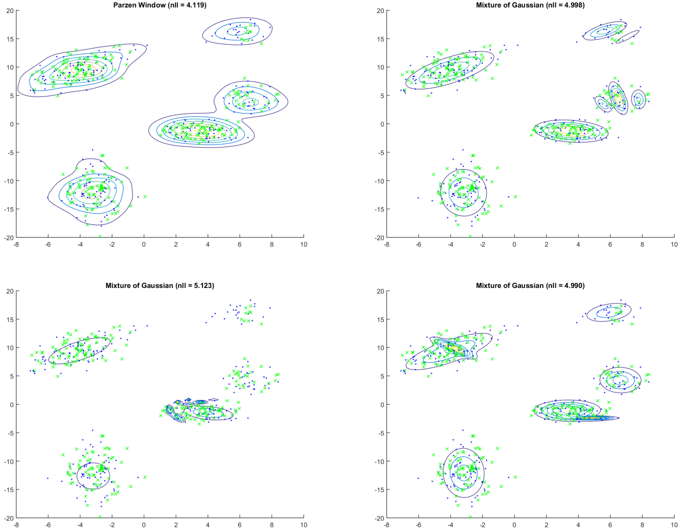
KDE vs. Mixture of Gaussian

- Multivariate vs mixture of Gaussians (different EM initializations):



KDE vs. Mixture of Gaussian

- Kernel density estimation vs mixture of Gaussians (different EM initializations):



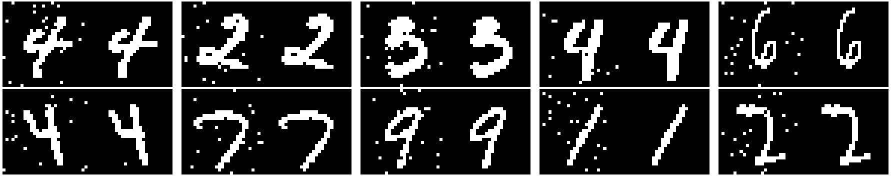
Mean-Shift Clustering

bonus!

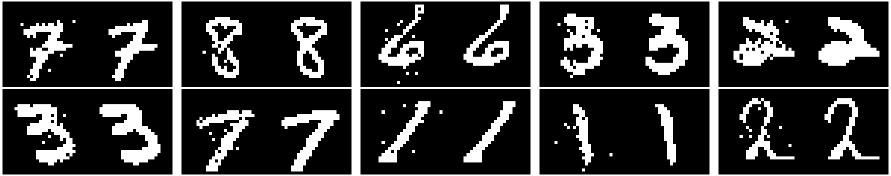
- Mean-shift clustering uses KDE for clustering:
  - Define a KDE on the training examples, and then for test example $\hat{x}$:
    - Run gradient descent to maximize $p(x)$ starting from $\hat{x}$.
  - Clusters are points that reach same local minimum.
- https://spin.atomicobject.com/2015/05/26/mean-shift-clustering
- Not sensitive to initialization, no need to choose k, can find non-convex clusters.
- Similar to density-based clustering from 340.
  - But doesn't require uniform density within cluster.
  - And can be used for vector quantization.
- "The 5 Clustering Algorithms Data Scientists Need to Know":
  - https://towardsdatascience.com/the-5-clustering-algorithms-data-scientists-need-to-know-a36d136ef68

Kernel Density Estimation on Digits

- Samples from a KDE model of digits:
  - Sample is on the left, right is the closest image from the training set.



- KDE just samples a training example then adds noise.
  - Usually makes more sense for continuous data that is densely packed.
- A variation with a location-specific variance (diagonal Σ instead of $\sigma^2 I$):



Summary

- Mixture of Bernoullis can model dependencies between discrete variables.
  - Unsupervised version of naive Bayes; can model arbitrary binary distributions.
- Learning by alternating imputing z^i and fitting full model...or more commonly,
- Expectation maximization: algorithm for optimization with hidden variables.
  - Instead of imputation, works with "soft" assignments to nuisance variables.
  - Maximizes log-likelihood, weighted by all imputations of hidden variables.
  - Simple and intuitive updates for fitting mixtures models.
  - Appealing properties as an optimization algorithm, but only finds local optimum.
- Kernel density estimation: Non-parametric density estimation method.
  - Center a mixture on each datapoint (smooth variation on histograms).
  - Used for data visualization and low-dimensional density estimation.
  - Basis of mean-shift clustering.

- Next time: measuring defense in the NBA.

Avoiding Underflow when Computing Responsibilities

bonus!

- Computing responsibility may underflow for high-dimensional x^i, due to $p(x^i \mid z^i = c, \Theta^t)$.

- Usual ML solution: do all but last step in log-domain.

$$\log r_c^i = \log p(x^i \mid z^i = c, \Theta^t) + \log p(z^i = c \mid \Theta^t) \\ - \log\left(\sum_{c'=1}^{k} p(x^i \mid z^i = c', \Theta^t) p(z^i = c' \mid \Theta^t)\right).$$

- To compute last term, use "log-sum-exp" trick.

Log-Sum-Exp Trick

bonus!

- To compute $\log(\sum_i \exp(v_i))$, set $\beta = \max_i\{v_i\}$ and use:

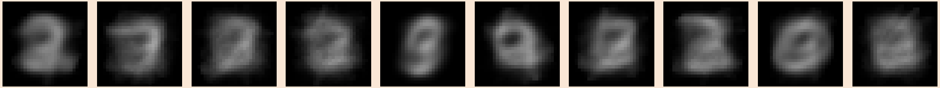
$$\begin{aligned}
\log(\sum_c \exp(v_i)) &= \log(\sum_i \exp(v_i - \beta + \beta)) \\
&= \log(\sum_i \exp(v_i - \beta)\exp(\beta)) \\
&= \log(\exp(\beta))\sum_i \exp(v_i - \beta)) \\
&= \log(\exp(\beta)) + \log(\sum_i \exp(v_i - \beta)) \\
&= \beta + \log(\sum_i \underbrace{\exp(v_i - \beta)}_{\leq 1}).
\end{aligned}$$

- Avoids overflows due to computing $\exp$ operator.

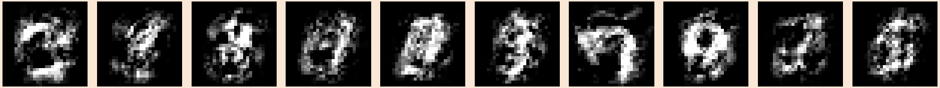
Mixture of Gaussians on Digits

bonus!

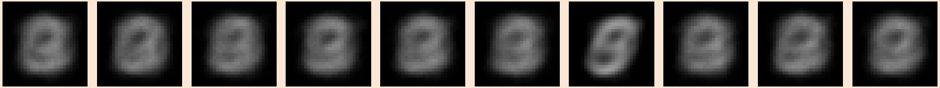
- Mean parameters of a mixture of Gaussians with $k = 10$:



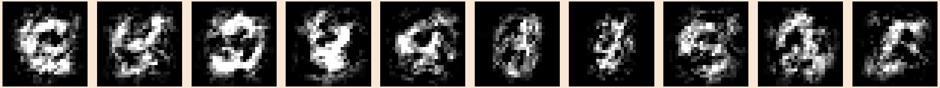
- Samples:



- 10 components with $k = 50$ (might need a better initialization):



- Samples:



EM for MAP Estimation

bonus!

- We can also use EM for MAP estimation. With a prior on Θ our objective is:

$$\underbrace{\log p(X \mid \Theta) + \log p(\Theta)}_{\text{what we optimize in MAP}} = \log\left(\sum_Z p(X, Z \mid \Theta)\right) + \log p(\Theta).$$

- EM iterations take the form of a regularized weighted "complete" NLL,

$$\Theta^{t+1} \in \operatorname*{arg\,max}_{\Theta} \left\{ \underbrace{\sum_Z p(Z \mid X, \Theta^t) \log p(X, Z \mid \Theta)} + \log p(\Theta) \right\},$$

- Now guarantees monotonic improvement in MAP objective.
  - Has a closed-form solution for mixture of exponential families with conjugate priors.

- For mixture of Gaussians with $-\log p(\Theta_c) = \lambda \mathrm{Tr}(\Theta_c)$ for precision matrices Θ_c:
  - Closed-form solution that satisfies positive-definite constraint (no $\log|\Theta|$ needed).

Generative Mixture Models and Mixture of Experts

bonus!

- Classic generative model for supervised learning uses

$$p(y^i \mid x^i) \propto p(x^i \mid y^i)p(y^i),$$

and typically $p(x^i \mid y^i)$ is assumed Gaussian (LDA) or independent (naive Bayes).

- But we could allow more flexibility by using a mixture model,

$$p(x^i \mid y^i) = \sum_{c=1}^{k} p(z^i = c \mid y^i)p(x^i \mid z^i = c, y^i).$$

- Another variation is a mixture of discriminative models (like logistic regression),

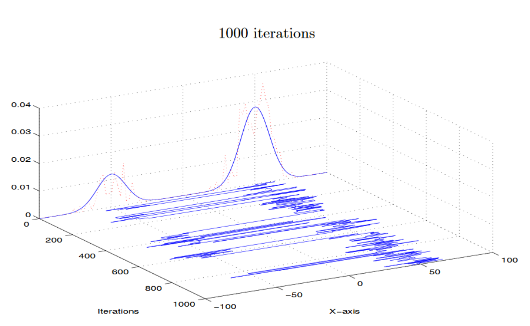
$$p(y^i \mid x^i) = \sum_{c=1}^{k} p(z^i = c \mid x^i)p(y^i \mid z^i = c, x^i).$$

- Called a “mixture of experts” model:
    - Each regression model becomes an “expert” for certain values of x^i.

Mixtures as Proposals in Metropolis-Hastings

bonus!

- Suppose we want to sample from a multi-modal distribution:



http://www.cs.ubc.ca/~arnaud/stat535/slides10.pdf

- With random walk proposals, we stay in one mode for a long time.
- We could instead use mixture model as a proposal in Metropolis-Hastings.
  - Proposal could be a mixture between random walk and "mode jumping".

General Kernel Density Estimation

bonus!

- The 1D kernel density estimation (KDE) model uses

$$p(x^i) = \frac{1}{n}\sum_{j=1}^{n} k_\sigma \underbrace{(x^i - x^j)}_{r},$$

where the PDF k is called the "kernel" and parameter σ is the "bandwidth".

- In the previous slide we used the (normalized) Gaussian kernel,

$$k_1(r) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{r^2}{2}\right), \quad k_\sigma(r) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{r^2}{2\sigma^2}\right).$$

- Note that we can add a "bandwith" (standard deviation) σ to any PDF k_1, using

$$k_\sigma(r) = \frac{1}{\sigma}k_1\left(\frac{r}{\sigma}\right),$$

from the change of variables formula for probabilities ($|\frac{d}{dr}\left[\frac{r}{\sigma}\right]| = \frac{1}{\sigma}$).

- Under common choices of kernels, KDEs can model any continuous density.

Efficient Kernel Density Estimation

bonus!

- KDE with the Gaussian kernel is slow at test time:
  - We need to compute distance of test point to every training point.
- A common alternative is the Epanechnikov kernel,

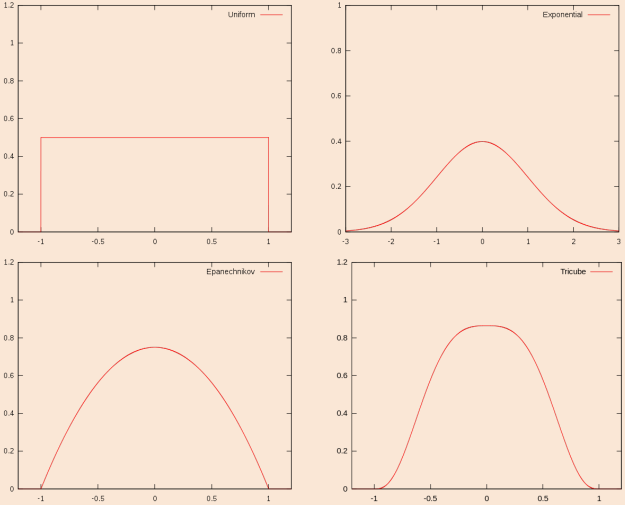
$$k_1(r) = \frac{3}{4}\left(1 - r^2\right)\mathcal{I}\left[|r| \leq 1\right].$$

- This kernel has two nice properties:
  - Epanechnikov showed that it is asymptotically optimal in terms of squared error.
  - It can be much faster to use since it only depends on nearby points.
    - You can use hashing to quickly find neighbours in training data.
- It is non-smooth at the boundaries but many smooth approximations exist.
  - Quartic, triweight, tricube, cosine, etc.
- For low-dimensional spaces, we can also use the fast multipole method.

Visualization of Common Kernel Functions

bonus!

Histogram vs. Gaussian vs. Epanechnikov vs. tricube:



https://en.wikipedia.org/wiki/Kernel_%28statistics%29

Multivariate Kernel Density Estimation

bonus!

- The multivariate kernel density estimation (KDE) model uses

$$p(x^i) = \frac{1}{n}\sum_{j=1}^{n} k_A(\underbrace{x^i - x^j}_{r}),$$

- The most common kernel is a product of independent Gaussians,

$$k_I(r) = \frac{1}{(2\pi)^{\frac{d}{2}}}\exp\left(-\frac{\|r\|^2}{2}\right).$$

- We can add a bandwith matrix A to any kernel using

$$k_A(r) = \frac{1}{|A|}k_1(A^{-1}r) \qquad \text{(generalizes } k_\sigma(r) = \frac{1}{\sigma}k_1\left(\frac{r}{\sigma}\right)\text{)},$$

  and in Gaussian case we get a multivariate Gaussian with $\Sigma = AA^T$.

- To reduce number of parameters, we typically:
  - Use a product of independent distributions and use $A = \sigma I$ for some σ.