CPSC 540: Machine Learning

Mixture Models, Density Estimation, Factor Analysis

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Winter 2016

Admin

- Assignment 2:
  - 1 late day to hand it in now.
- Assignment 3:
  - Posted, due on Feburary 23. Start early.
  - Some additional hints will be added.

Multiple Kernel Learning

- Last time we discussed kernelizing L2-regularized linear models,

$$\underset{w \in \mathbb{R}^d}{\text{argmin}}\, f(Xw, y) + \frac{\lambda}{2}\|w\|^2 \Leftrightarrow \underset{z \in \mathbb{R}^n}{\text{argmin}}\, f(Kz, y) + \frac{\lambda}{2}\|z\|_K^2,$$

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  - Defines a valid kernel and is convex if f is convex.
  - Group L1-regularization of parameters associated with each kernel.
    - Selects a sparse set of kernels.
  - Hiearchical kernel learning:
    - Use structured sparsity to search through exponential number of kernels.

Unconstrained and Smooth Optimization

- For typical unconstrained/smooth optimization of ML problems,

$$\operatorname*{argmin}_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w^T x_i) + \frac{\lambda}{2}\|w\|^2.$$

we discussed several methods:

- Gradient method:
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- Coordinate optimization:
  - Faster than gradient method if iteration cost is $O(n)$.
- Stochastic subgradient:
  - Iteration cost is $O(d)$ but sublinear convergence rate.
  - SAG/SVRG improve to linear rate for finite datasets.

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  - Dual optimzation for smoothing strongly-convex problems.
- With a few more tricks, you can almost always beat subgradient methods:
  - Chambolle-Pock: min-max problems.
  - ADMM: for "simple" regularized composed with affine function like $\|Ax\|_1$.
  - Frank-Wolfe: for nuclear-norm regularization.
  - Mirror descent: for probability-simplex constraints.

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- Major issues:
  - Synchronization: we can't wait for the slowest machine.
  - Communication: it's expensive to transfer across machines.
- "Embarassingly" parallel solution:
  - Split data across machines, each machine computes gradient of their subset.
- Fancier methods (key idea is usually that you just make step-size smaller):
  - Asyncronous stochastic gradient.
  - Parallel coordinate optimization.
  - Decentralized gradient.

Last Time: Density Estimation

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  - Unsuperivsed task of estimating $p(x)$.
- It can also be used for supervised learning:
  - Generative models estimate joint distribution over feature and labels,

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  - Special cases:
    - Naive Bayes models $p(x^i|y^i)$ as product of independent distributions.
    - Linear discriminant analysis models $p(x^i|y^i)$ as a multivariate Gaussian.
  - Currently unpopular, but may be coming back:
    - We believe that most human learning is unsupervised.

Last Time: Independent vs. General Discrete Distributions

- We considered density estimation with discrete variables,

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

and considered two extreme appraoches:

- Product of independent distributions:

$$p(x) = \prod_{j=1}^{d} p(x_j).$$

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- General discrete distribution:

$$p(x) = \theta_x.$$

No assumptions but hard to fit:

- Parameter vector θ_x for each possible x.

- What lies between these extremes?

Mixture of Bernoullis

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- With 0.5 probability we look coin 1, otherwise we look at coin 2:

$$\begin{aligned} p(x = 1|\theta_1, \theta_2) &= p(z = 1)p(x = 1|\theta_1) + p(z = 2)p(x = 1|\theta_2) \\ &= 0.5\theta_1 + 0.5\theta_2, \end{aligned}$$

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  where z is the choice of coin we flip.
- This is called a mixture model:
  - The probability is a convex combination ("mixture") of probabilities.
- Here we get a Bernoulli with $\theta = 0.75$, but other mixtures are more interesting...

Mixture of Independent Bernoullis

- Consider a mixture of the product of independent Bernoullis:

$$p(x) = 0.5 \prod_{j=1}^{d} p(x_j|\theta_{1j}) + 0.5 \prod_{j=1}^{d} p(x_j|\theta_{2j}).$$

- E.g., $\theta_1 = \begin{bmatrix}\theta_{11} & \theta_{12} & \theta_{13}\end{bmatrix} = \begin{bmatrix}0 & 0.7 & 1\end{bmatrix}$ and $\theta_2 = \begin{bmatrix}1 & 0.7 & 0.8\end{bmatrix}$.
- Conceptually, we now have two *sets* of coins:
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- Product of independent distributions is special case where $\theta_{1j} = \theta_{2j}$ for all j:
  - We haven't lost anything by taking a mixture.
- But mixtures can model dependencies between variables x_j:
  - If you know x_j, it tells you something about which mixture x_k comes from.
  - E.g., if $\theta_1 = \begin{bmatrix}0 & 0 & 0\end{bmatrix}$ and $\theta_2 = \begin{bmatrix}1 & 1 & 1\end{bmatrix}$, seeing $x_j = 1$ tells you $x_k = 1$.

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- General mixture of independent Bernoullis:

$$p(x) = \sum_{c=1}^{k} p(z = c)p(x|z = c),$$

where every thing is conditioned on θ_c values and

1. We have likelihood $p(x|z = c)$ of x if it came from cluster c.
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- We typically model $p(z = c)$ using a categorical distribution.
- With k large enough, we can model any discrete distribution.
  - Though k may not be much smaller than 2^d in the worst case.
- An important quantity is the responsibility,

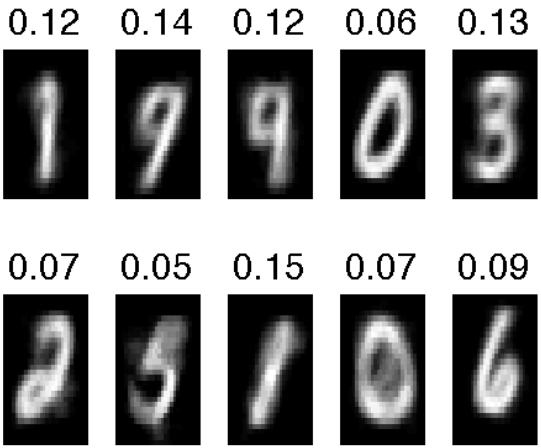
$$p(z = c|x) = \frac{p(x|z = c)p(z = c)}{\sum_{c'} p(x|z = c')p(z' = c)},$$

the probability that x came from mixture c.

- The responsibilities are often interpreted as a probabilistic clustering.

Mixture of Independent Bernoullis

Plotting mean vectors θ_c with 10 mixtures trained on MNIST:
(hand-written images of the the numbers 0 through 9)



(pause)

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- Even with 1 variable there are many possible distributions.
- Most common is the Gaussian (or "normal") distribution:

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

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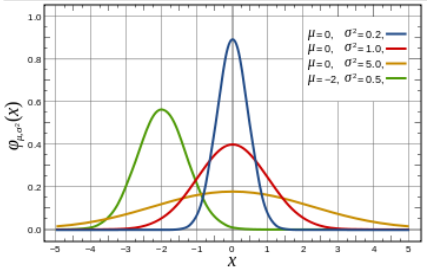
  - Data might actually follow Gaussian.
  - Analytics properties: symmetry, closed-form solution for μ and σ:
    - Maximum likelihood for mean is $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x^i$.
    - Maximum likelihood for variance is $\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x^i - \hat{\mu})^2$ (for $n > 1$).



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

Alternatives to Univariate Gaussian

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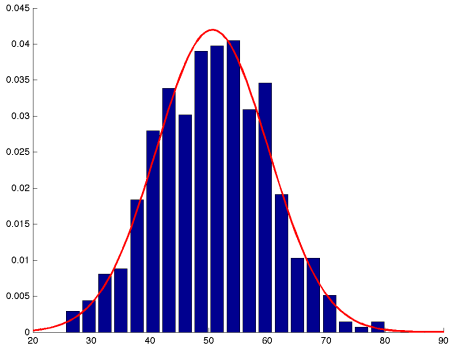
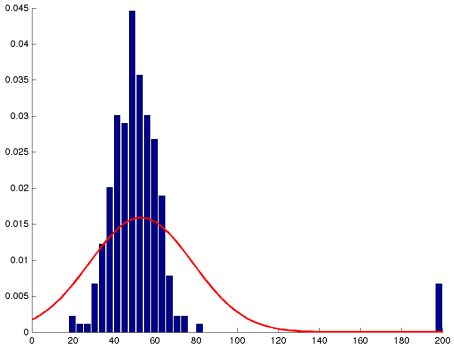
  - Negative log-likelihood is a quadratic function of μ,

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

so as with least squares distribution is not robust to outliers.





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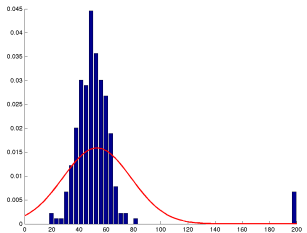
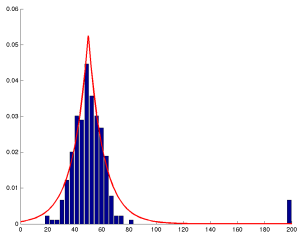
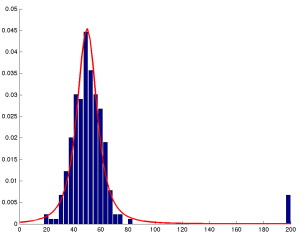

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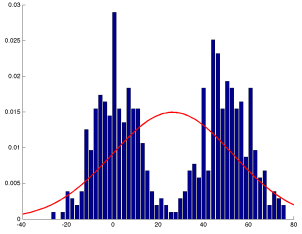

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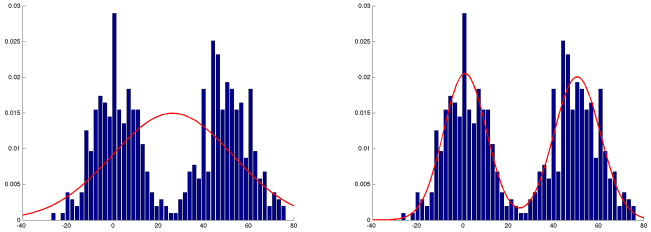

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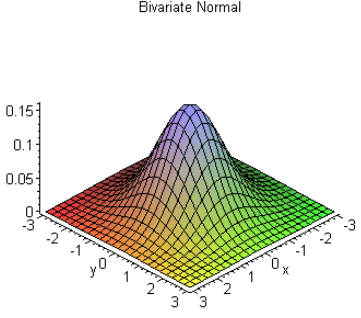

http://personal.kenyon.edu/hartlaub/MellonProject/Bivariate2.html

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- Why the multivariate Gaussian?
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    - Closed-form MLE but unimodal and not robust to outliers.
  - Closed under some common operations:
    - Products of Gaussians PDFs is Gaussian:

$$p(x_1|\mu_1,\Sigma_1)p(x_2|\mu_2,\Sigma_2) = p(\tilde{x}|\tilde{\mu},\tilde{\Sigma}).$$

    - Marginal distributions $p(x_S|\mu,\Sigma)$ are Gaussians.
    - Conditional distributions $p(x_S|x_{-S},\mu,\Sigma)$ are Gaussians.

Product of Independent Gaussians

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with $\mu = (\mu_1, \mu_2, \ldots, \mu_d)$ and Σ diagonal with elements σ_j.

- This follows from

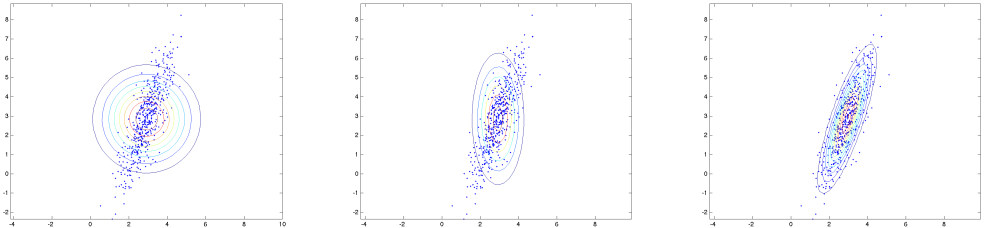
$$p(x|\mu, \Sigma) = p(x_j|\mu_j, \sigma_j^2) \propto \prod_{j=1}^{d} \exp\left(-\frac{(x_j - \mu_j)^2}{2\sigma_j^2}\right)$$

$$= \exp\left(-\frac{1}{2}\sum_{j=1}^{d} -\frac{(x_j - \mu_j)^2}{\sigma_j^2}\right) \qquad (e^a e^b = e^{a+b})$$

$$= \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right) \quad \text{(definition of } \Sigma\text{)}.$$

Product of Independent Gaussians

- What is the effect of diagonal Σ in the independent Gaussian model?
  - If $\Sigma = \alpha I$ the level curves are circles (1 parameter).
  - If $\Sigma = D$ (diagonal) they axis-aligned ellipses (d parameters).
  - If Σ is dense they do not need to be axis-aligned ($d(d+1)/2$ parameters). (by symmetry, we need to estimate upper-triangular part of Σ)



Maximum Likelihood Estimation in Multivariate Gaussians

- With a multivariate Gaussian we have

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

so up to a constant our negative log-likelihood is

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- Noting that $\sum_{i=1}^{n}\mu = n\mu$ and pre-multiplying by Σ we get $\mu = \frac{1}{n}\sum_{i=1}^{n}x^i$.
  - So μ should be the average, and it doesn't depend on Σ.

Maximum Likelihood Estimation in Multivariate Gaussians

- Re-parameterizing in terms of precision matrix $\Theta = \Sigma^{-1}$ we have

$$\begin{aligned}
&\frac{1}{2}\sum_{i=1}^{n}(x^i-\mu)^T\Sigma^{-1}(x^i-\mu)+\frac{n}{2}\log|\Sigma| \\
=&\frac{1}{2}\sum_{i=1}^{n}\mathsf{Tr}\left((x^i-\mu)^T\Theta(x^i-\mu)\right)+\frac{n}{2}\log|\Theta^{-1}| && (y^TAy=\mathsf{Tr}(y^TAy) \\
=&\frac{1}{2}\sum_{i=1}^{n}\mathsf{Tr}((x^i-\mu)(x^i-\mu)^T\Theta)-\frac{n}{2}\log|\Theta| && (\mathsf{Tr}(AB)=\mathsf{Tr}(BA))
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- Changing trace/sum and using sample covariance $S=\frac{1}{n}\sum_{i=1}^{n}(x^i-\mu)(x^i-\mu)^T$,

$$\begin{aligned}
=&\frac{1}{2}\mathsf{Tr}\left(\sum_{i=1}^{n}(x^i-\mu)(x^i-\mu)^T\Theta\right)-\frac{n}{2}\log|\Theta| \quad (\sum_i \mathsf{Tr}(A_iB)=\mathsf{Tr}(\sum_i A_iB)) \\
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Maximum Likelihood Estimation in Multivariate Gaussians

- So the NLL in terms of the precision matrix Θ is

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- Weird-looking but has nice properties:
  - $\text{Tr}(S\Theta)$ is linear function of Θ, with $\nabla_\Theta \text{Tr}(S\Theta) = S$.
  - Negative log-determinant is strictly-convex and has $\nabla_\Theta \log|\Theta| = \Theta^{-1}$. (generalization of $\nabla \log|x| = 1/x$ for for $x > 0$.

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- The constraint $\Sigma \succ 0$ means we need empirical covariance $S \succ 0$.
  - If S is not invertible, NLL is unbounded below and no MLE exists.

Bonus Slide: Comments on Positive-Definiteness

- If we define centered vectors $\tilde{x}^i = x^i - \mu$ then empirical covariance is

$$S = \frac{1}{n}\sum_{i=1}^{n}(x^i - \mu)(x^i - \mu)^T = \sum_{i=1}^{n}\tilde{x}^i(\tilde{x}^i)^T = \tilde{X}^T\tilde{X} \succeq 0,$$

  so S is positive semi-definite but not positive-definite by construction.
- If data has noise, it will be positive-definite with n large enough.
- For $\Theta \succ 0$, note that for an upper-triangular T we have

$$\log|T| = \log(\mathsf{prod}(eig(T))) = \log(\mathsf{prod}(\mathsf{diag}(T))) = \mathsf{Tr}(\log(\mathsf{diag}T)),$$

  where we've used Matlab notation.
- So to compute $\log|\Theta|$ for $\Theta \succ 0$, use Cholesky to turn into upper-triangular.
  - Bonus: Cholesky will fail if $\Theta \succ 0$ is not true, so it checks constraint.

MAP Estimation in Multivariate Gaussian

- We typically don't regularize μ, but you could add an L2-regularizer $\frac{\lambda}{2}\|\mu\|^2$.
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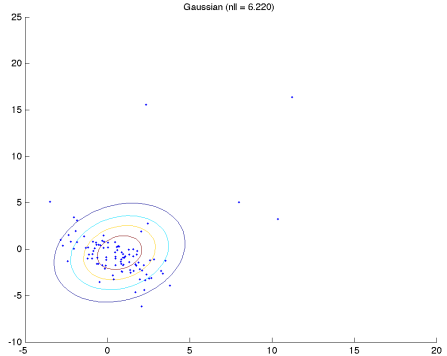
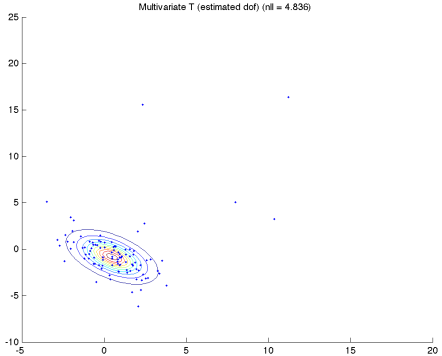
where we are using the element-wise L1-norm.

  - Gives sparse Θ and introduces independences.
    - E.g., if it makes Θ diagonal then all variables are independent.
  - Can solve very large instances with proximal-Newton and other tricks.

Alternatives to Multivariate Gaussian

- Why not the multivariate Gaussian distribution?
  - Still not robust, may want to consider multivariate Laplace or multivariate T.





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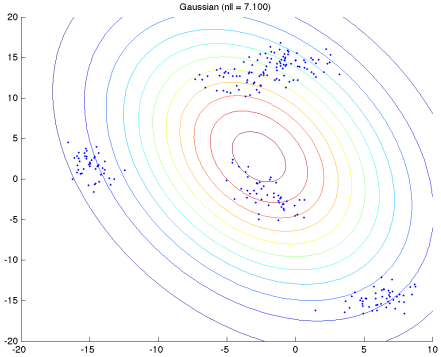
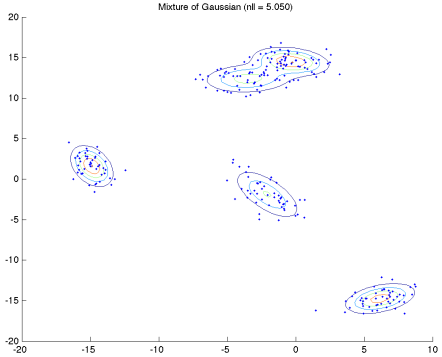
- Why not the multivariate Gaussian distribution?
  - Still not robust, may want to consider multivariate Laplace of multivariate T.
  - Still unimodal, may want to consider mixture of Gaussians.





(pause)

Learning with Hidden Values

- We often want to learn when some variables unobserved/missing/hidden/latent.
- For example, we could have a dataset

$$X = \begin{bmatrix} N & 33 & 5 \\ F & 10 & 1 \\ F & ? & 2 \\ M & 22 & 0 \end{bmatrix}, y = \begin{bmatrix} -1 \\ +1 \\ -1 \\ ? \end{bmatrix}.$$

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- Missing values are very common in real datasets.
- Heuristic approach:
  1. Imputation: replace each ? with the most likely value.
  2. Estimation: fit model with these imputed values.
- Sometimes you alternate between these two steps ("hard EM").
  - EM algorithm is a more theoretically-justified version of this.

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  - Hide the labels of all the "2" examples: not MAR.
- If you are not MAR, you need to model why data is missing.

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- Missing at random: fact that variable is missing does not depend on its value.

- Netx time: EM algorithm for hidden varialbles and probabilistic PCA.