CPSC 540: Machine Learning

Multivariate Gaussians

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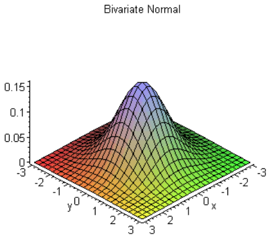
Last Time: Multivariate Gaussian



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

- The multivariate normal/Gaussian distribution models PDF of vector x^i as

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

  where $\mu \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d \times d}$ and $\Sigma \succ 0$.
- Motivated by CLT, maximum entropy, computational properties.
- Diagonal Σ implies independence between variables.

MLE for Multivariate Gaussian (Mean Vector)

- With a multivariate Gaussian we have

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

  so up to a constant our negative log-likelihood for n examples x^i is

$$\frac{1}{2}\sum_{i=1}^n (x^i-\mu)^\top\Sigma^{-1}(x^i-\mu) + \frac{n}{2}\log|\Sigma|.$$

- This is a strongly-convex quadratic in μ, setting gradient to zero gives

$$\mu = \frac{1}{n}\sum_{i=1}^n x^i,$$

  which is the unique solution (strong-convexity is due to $\Sigma \succ 0$).
    - MLE for μ is the average along each dimension, and it doesn't depend on Σ.

MLE for Multivariate Gaussians (Covariance Matrix)

- To get MLE for Σ we re-parameterize in terms of precision matrix $\Theta = \Sigma^{-1}$,

$$\frac{1}{2}\sum_{i=1}^{n}(x^i-\mu)^\top\Sigma^{-1}(x^i-\mu)+\frac{n}{2}\log|\Sigma|$$

$$=\frac{1}{2}\sum_{i=1}^{n}(x^i-\mu)^\top\Theta(x^i-\mu)+\frac{n}{2}\log|\Theta^{-1}| \qquad \text{(ok because } \Sigma \text{ is invertible)}$$

$$=\frac{1}{2}\sum_{i=1}^{n}\mathrm{Tr}\left((x^i-\mu)^\top\Theta(x^i-\mu)\right)+\frac{n}{2}\log|\Theta|^{-1} \qquad \text{(scalar } y^\top Ay = \mathrm{Tr}(y^\top Ay))$$

$$=\frac{1}{2}\sum_{i=1}^{n}\mathrm{Tr}((x^i-\mu)(x^i-\mu)^\top\Theta)-\frac{n}{2}\log|\Theta| \qquad (\mathrm{Tr}(ABC)=\mathrm{Tr}(CAB))$$

- Where the trace $\mathrm{Tr}(A)$ is the sum of the diagonal elements of A.
  - That $\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB)$ when dimensions match is the cyclic property of trace.

MLE for Multivariate Gaussians (Covariance Matrix)

- From the last slide we have in terms of precision matrix Θ that

$$=\frac{1}{2}\sum_{i=1}^{n}\mathsf{Tr}((x^i-\mu)(x^i-\mu)^\top\Theta)-\frac{n}{2}\log|\Theta|$$

- We can exchange the sum and trace (trace is a linear operator) to get,

$$=\frac{1}{2}\mathsf{Tr}\left(\sum_{i=1}^{n}(x^i-\mu)(x^i-\mu)^\top\Theta\right)-\frac{n}{2}\log|\Theta|$$

$$\sum_i \mathsf{Tr}(A_iB)=\mathsf{Tr}\left(\sum_i A_iB\right)$$

$$=\frac{n}{2}\mathsf{Tr}\left(\left(\underbrace{\frac{1}{n}\sum_{i=1}^{n}(x^i-\mu)(x^i-\mu)^\top}_{\text{sample covariance `}S\text{'}}\right)\Theta\right)-\frac{n}{2}\log|\Theta|.$$

$$\left(\sum_i A_iB\right)=\left(\sum_i A_i\right)B$$

MLE for Multivariate Gaussians (Covariance Matrix)

- So the NLL in terms of the precision matrix Θ and sample covariance S is

$$f(\Theta) = \frac{n}{2}\text{Tr}(S\Theta) - \frac{n}{2}\log|\Theta|, \text{ with } S = \frac{1}{n}\sum_{i=1}^{n}(x^i - \mu)(x^i - \mu)^\top$$

- Weird-looking but has nice properties:
  - $\text{Tr}(S\Theta)$ is linear function of Θ, with $\nabla_\Theta \text{Tr}(S\Theta) = S$.
    (it's the matrix version of an inner-product $s^\top\theta$)
  - Negative log-determinant is strictly-convex and has $\nabla_\Theta \log|\Theta| = \Theta^{-1}$.
    (generalizes $\nabla \log|x| = 1/x$ for for $x > 0$).
- Using these two properties the gradient matrix has a simple form:

$$\nabla f(\Theta) = \frac{n}{2}S - \frac{n}{2}\Theta^{-1}.$$

MLE for Multivariate Gaussians (Covariance Matrix)

- Gradient matrix of NLL with respect to Θ is

$$\nabla f(\Theta) = \frac{n}{2}S - \frac{n}{2}\Theta^{-1}.$$

- The MLE for a given μ is obtained by setting gradient matrix to zero, giving

$$\Theta = S^{-1} \quad \text{or} \quad \Sigma = S = \frac{1}{n}\sum_{i=1}^{n}(x^i - \mu)(x^i - \mu)^\top.$$

- The constraint $\Sigma \succ 0$ means we need positive-definite sample covariance, $S \succ 0$.
  - If S is not invertible, NLL is unbounded below and no MLE exists.
  - This is like requiring "not all values are the same" in univariate Gaussian.
    - In d-dimensions, you need d linearly-independent x^i values.

- For most distributions, the MLEs are not the sample mean and covariance.

MAP Estimation in Multivariate Gaussian (Covariance Matrix)

- A classic regularizer for Σ is to add a diagonal matrix to S and use

$$\Sigma = S + \lambda I,$$

  which satisfies $\Sigma \succ 0$ by construction (eigenvalues at least λ).

- This corresponds to a regularizer that penalizes diagonal of the precision,

$$\begin{aligned} f(\Theta) &= \mathrm{Tr}(S\Theta) - \log|\Theta| + \lambda \mathrm{Tr}(\Theta) \\ &= \mathrm{Tr}(S\Theta + \lambda\Theta) - \log|\Theta| \\ &= \mathrm{Tr}((S + \lambda I)\Theta) - \log|\Theta|. \end{aligned}$$

- L1-regularization of diagonals of inverse covariance.
    - But doesn't set to exactly zero as it must be positive-definite.

Graphical LASSO

- A popular generalization called the graphical LASSO,

$$f(\Theta) = \text{Tr}(S\Theta) - \log|\Theta| + \lambda\|\Theta\|_1.$$

  where we are using the element-wise L1-norm.

- Gives sparse off-diagonals in Θ.
  - Can solve very large instances with proximal-Newton and other tricks ("QUIC").

- It's common to draw the non-zeroes in Θ as a graph.
  - Has an interpretation in terms on conditional independence (we'll cover this later).
  - Examples: `https://normaldeviate.wordpress.com/2012/09/17/high-dimensional-undirected-graphical-models`

Closedness of Multivariate Gaussian

- Multivariate Gaussian has nice properties of univariate Gaussian:
  - Closed-form MLE for μ and Σ given by sample mean/variance.
  - Central limit theorem: mean estimates of random variables converge to Gaussians.
  - Maximizes entropy subject to fitting mean and covariance of data.

- A crucial computation property: Gaussians are closed under many operations.
  1. Affine transformation: if $p(x)$ is Gaussian, then $p(Ax + b)$ is a Gaussian[1].
  2. Marginalization: if $p(x, z)$ is Gaussian, then $p(x)$ is Gaussian.
  3. Conditioning: if $p(x, z)$ is Gaussian, then $p(x \mid z)$ is Gaussian.
  4. Product: if $p(x)$ and $p(z)$ are Gaussian, then $p(x)p(z)$ is proportional to a Gaussian.

- Most continuous distributions don't have these nice properties.

[1] Could be degenerate with $|\Sigma| = 0$ dependending on A.

Affine Property: Special Case of Shift

- Assume that random variable x follows a Gaussian distribution,

$$x \sim \mathcal{N}(\mu, \Sigma).$$

- And consider an shift of the random variable,

$$z = x + b.$$

- Then random variable z follows a Gaussian distribution

$$z \sim \mathcal{N}(\mu + b, \Sigma),$$

  where we've shifted the mean.

Affine Property: General Case

- Assume that random variable x follows a Gaussian distribution,

$$x \sim \mathcal{N}(\mu, \Sigma).$$

- And consider an affine transformation of the random variable,

$$z = Ax + b.$$

- Then random variable z follows a Gaussian distribution

$$z \sim \mathcal{N}(A\mu + b, A\Sigma A^\top),$$

although note we might have $|A\Sigma A^\top| = 0$.

Marginalization of Gaussians

- Consider partitioning multivariate Gaussian variables into two sets,

$$\begin{bmatrix} x \\ z \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_x \\ \mu_z \end{bmatrix}, \begin{bmatrix} \Sigma_{xx} & \Sigma_{xz} \\ \Sigma_{zx} & \Sigma_{zz} \end{bmatrix}\right),$$

so our dataset would be something like

$$X = \begin{bmatrix} | & | & | & | \\ x_1 & x_2 & z_1 & z_2 \\ | & | & | & | \end{bmatrix}.$$

- If I want the marginal distribution $p(x)$, I can use the affine property,

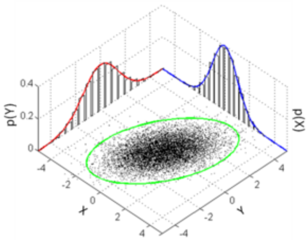
$$x = \underbrace{\begin{bmatrix} I & 0 \end{bmatrix}}_{A} \begin{bmatrix} x \\ z \end{bmatrix} + \underbrace{0}_{b},$$

to get that

$$x \sim \mathcal{N}(\mu_x, \Sigma_{xx}).$$

Marginalization of Gaussians

- In a picture, ignoring a subset of the variables gives a Gaussian:



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

- This seems less intuitive if you use usual marginalization rule:

$$p(x) = \int_{z_1}\int_{z_2}\cdots\int_{z_d} \frac{1}{(2\pi)^{\frac{d}{2}}\left|\begin{bmatrix}\Sigma_{xx} & \Sigma_{xz}\\ \Sigma_{zx} & \Sigma_{zz}\end{bmatrix}\right|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}\left(\begin{bmatrix}x\\ z\end{bmatrix} - \begin{bmatrix}\mu_x\\ \mu_z\end{bmatrix}\right)\begin{bmatrix}\Sigma_{xx} & \Sigma_{xz}\\ \Sigma_{zx} & \Sigma_{zz}\end{bmatrix}^{-1}\left(\begin{bmatrix}x\\ z\end{bmatrix} - \begin{bmatrix}\mu_x\\ \mu_z\end{bmatrix}\right)\right) dz_d dz_{d-1}\dots dz_1.$$

Conditioning in Gaussians

- Consider partitioning multivariate Gaussian variables into two sets,

$$\begin{bmatrix} x \\ z \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_x \\ \mu_z \end{bmatrix}, \begin{bmatrix} \Sigma_{xx} & \Sigma_{xz} \\ \Sigma_{zx} & \Sigma_{zz} \end{bmatrix}\right).$$

- The conditional probabilities are also Gaussian,

$$x \mid z \sim \mathcal{N}(\mu_{x \mid z}, \Sigma_{x \mid z}),$$

where

$$\mu_{x \mid z} = \mu_x + \Sigma_{xz}\Sigma_{zz}^{-1}(z - \mu_z), \quad \Sigma_{x \mid z} = \Sigma_{xx} - \Sigma_{xz}\Sigma_{zz}^{-1}\Sigma_{zx}.$$

- "For any fixed z, the distribution of x is a Gaussian".
  - Notice that if $\Sigma_{xz} = 0$ then x and z are independent ($\mu_{x \mid z} = \mu_x$, $\Sigma_{x \mid z} = \Sigma_x$).
  - We previously saw the special case where Σ is diagonal (all variables independent).

Product of Gaussian Densities

- Let $f_1(x)$ and $f_2(x)$ be Gaussian PDFs defined on variables x.
  - Let (μ_1, Σ_1) be parameters of f_1 and (μ_2, Σ_2) for f_2.
- The product of the PDFs $f_1(x)f_2(x)$ is proportional to a Gaussian density,

$$\text{covariance of} \quad \Sigma = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}.$$

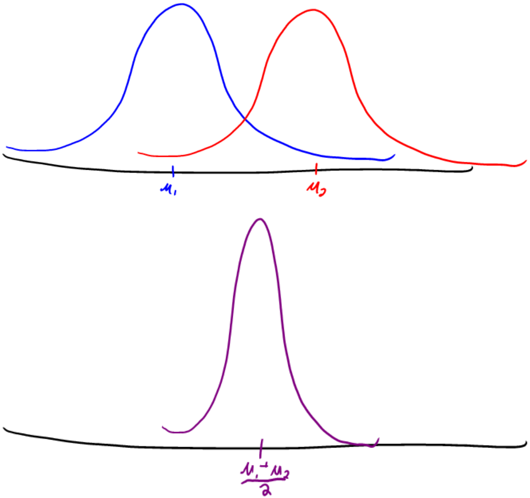
$$\text{mean of } \mu = \Sigma\Sigma_1^{-1}\mu_1 + \Sigma\Sigma_2^{-1}\mu_2,$$

  although this density may not be normalized (may not integrate to 1 over all x).

- But if we can write a probability as $p(x) \propto f_1(x)f_2(x)$ for 2 Gaussians, then p is a Gaussian with the above mean/covariance.
  - Can be to derive MAP estimate if f_1 is likelihood and f_2 is prior.
  - Can be used in Gaussian Markov chains models (later).

Product of Gaussian Densities

- If $\Sigma_1 = I$ and $\Sigma_2 = I$ then product has $\Sigma = \frac{1}{2}I$ and $\mu = \frac{\mu_1+\mu_2}{2}$.

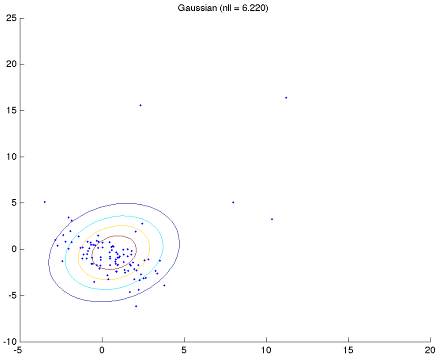


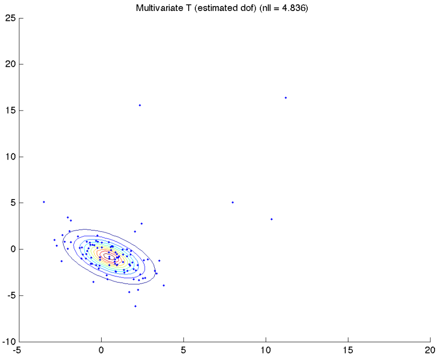
Properties of Multivariate Gaussians

- A multivariate Gaussian "cheat sheet" is here:
  - https://ipvs.informatik.uni-stuttgart.de/mlr/marc/notes/gaussians.pdf
- For a careful discussion of Gaussians, see the playlist here:
  - `https://www.youtube.com/watch?v=TC0ZAX3DA88&t=2s&list=PL17567A1A3F5DB5E4&index=34`

Problems with Multivariate Gaussian

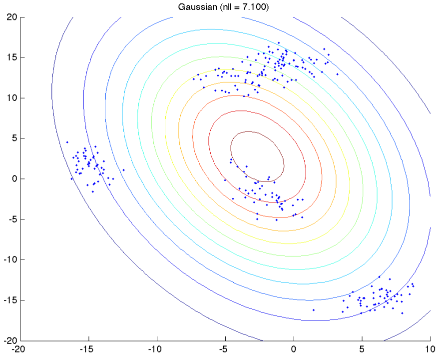
- Why not the multivariate Gaussian distribution?
  - Still not robust, may want to consider multivariate Laplace or multivariate T.
    - These require numerical optimization to compute MLE/MAP.





Problems with Multivariate Gaussian

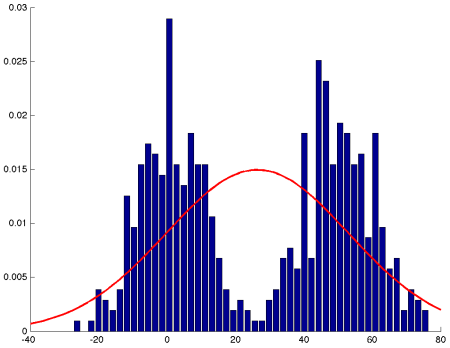
- Why not the multivariate Gaussian distribution?
  - Still not robust, may want to consider multivariate Laplace of multivariate T.
  - Still unimodal, which often leads to very poor fit.



Outline

1 Gaussian for Multi-Modal Data

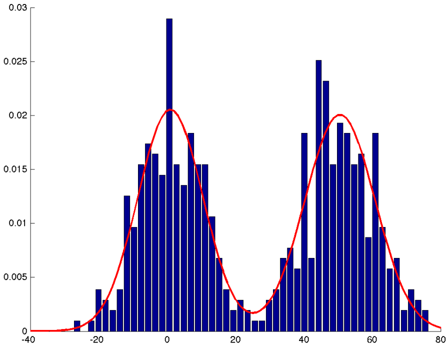
- Major drawback of Gaussian is that it's uni-modal.
    - It gives a terrible fit to data like this:



- If Gaussians are all we know, how can we fit this data?

2 Gaussians for Multi-Modal Data

- We can fit this data by using two Gaussians



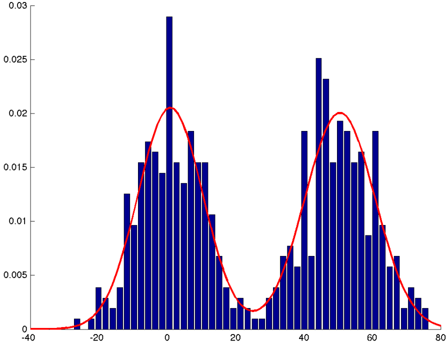
- Half the samples are from Gaussian 1, half are from Gaussian 2.

Mixture of Gaussians

- Our probability density in this example is given by

$$p(x^i \mid \mu_1, \mu_2, \Sigma_1, \Sigma_2) = \frac{1}{2} \underbrace{p(x^i \mid \mu_1, \Sigma_1)}_{\text{PDF of Gaussian 1}} + \frac{1}{2} \underbrace{p(x^i \mid \mu_2, \Sigma_2)}_{\text{PDF of Gaussian 2}},$$

  - We need the (1/2) factors so it still integrates to 1.

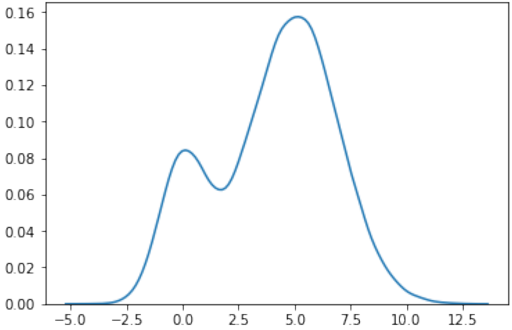


Mixture of Gaussians

- If data comes from one Gaussian more often than the other, we could use

$$p(x^i \mid \mu_1, \mu_2, \Sigma_1, \Sigma_2, \pi_1, \pi_2) = \pi_1 \underbrace{p(x^i \mid \mu_1, \Sigma_1)}_{\text{PDF of Gaussian 1}} + \pi_2 \underbrace{p(x^i \mid \mu_2, \Sigma_2)}_{\text{PDF of Gaussian 2}},$$

where π_1 and π_2 and are non-negative and sum to 1.

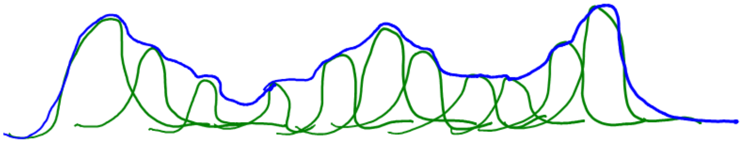


Mixture of Gaussians

- In general we might have a mixture of k Gaussians with different weights.

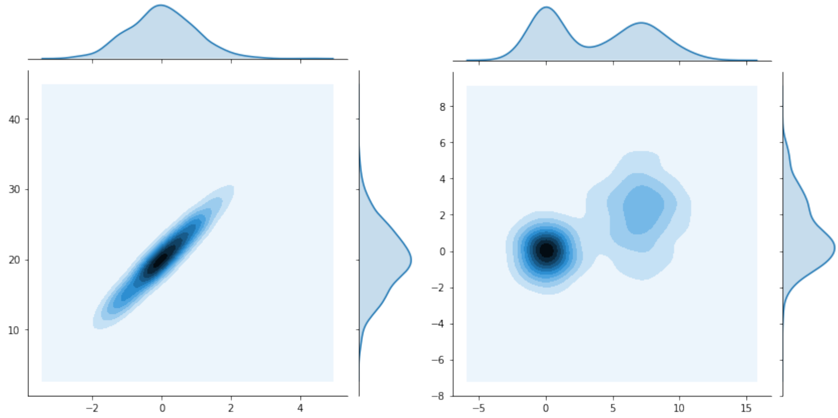
$$p(x \mid \mu, \Sigma, \pi) = \sum_{c=1}^{k} \pi_c \underbrace{p(x \mid \mu_c, \Sigma_c)}_{\text{PDF of Gaussian } c},$$

  - Where the π_c are non-negative and sum to 1.
  - We can use it to model complicated densities with Gaussians (like RBFs).
    - "Universal approximator": can model any continuous density on compact set.



Mixture of Gaussians

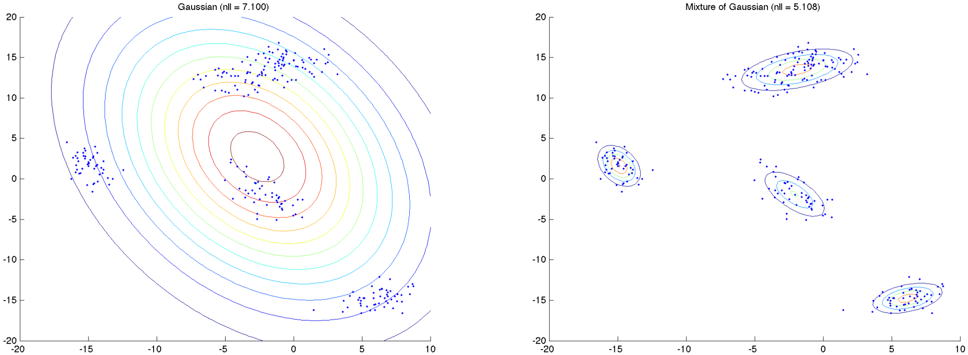
- Gaussian vs. mixture of 2 Gaussian densities in 2D:



- Marginals will also be mixtures of Gaussians.

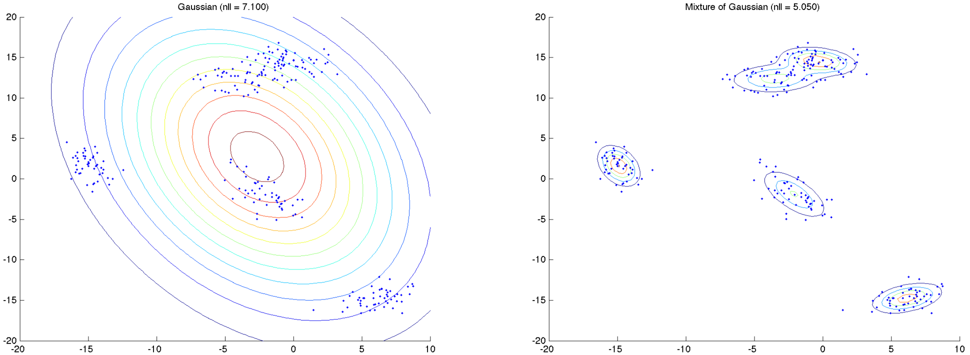
Mixture of Gaussians

- Gaussian vs. Mixture of 4 Gaussians for 2D multi-modal data:



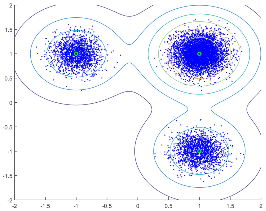
Mixture of Gaussians

- Gaussian vs. Mixture of 5 Gaussians for 2D multi-modal data:



Mixture of Gaussians

- Given parameters $\{\pi_c, \mu_c, \Sigma_c\}$, we can sample from a mixture of Gaussians using:
  1. Sample cluster c based on prior probabilities π_c (categorical distribution).
  2. Sample example x based on mean μ_c and covariance Σ_c.



- We usually fit these models with expectation maximization (EM):
  - EM is a general method for fitting models with hidden variables.
  - For mixture of Gaussians: we treat cluster c as a hidden variable.

Summary

- Multivariate Gaussian generalizes univariate Gaussian for multiple variables.
  - Closed-form MLE given by sample mean and covariance.
  - Closed under affine transformations, marginalization, conditioning, and products.
  - But unimodal and not robust.
- Mixture of Gaussians writes probability as convex comb. of Gaussian densities.
  - Can model arbitrary continuous densities.
- Next time: dealing with missing data.

Positive-Definiteness of Θ and Checking Positive-Definiteness

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

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

  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

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

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