Machine Learning, One in Depth: Gaussian Mixture Models

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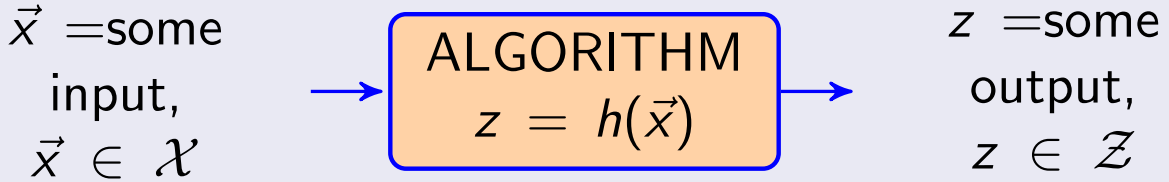
Outline

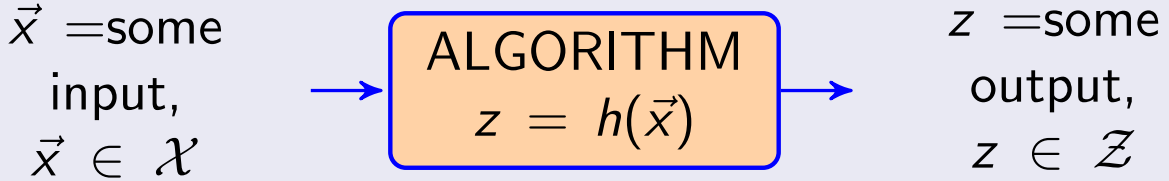
Goal of most software:



CLASSIFIER: $\mathcal{Z} = \{\text{set of all class labels}\}$
(person names; object tags; sequence of words; sequence of phonemes)

REGRESSOR: $\mathcal{Z} = \{\text{real numbers or vectors}\}$
(person's age; tomorrow's stock price; second-language fluency rating; positions of tongue, velum, and glottis)

Goal of most software:



Old School:

DESIGN: Try to figure out $z = h(\vec{x})$ in your brain, then write a program to implement $z = h(\vec{x})$.

TEST: Try it on some examples. How'd you do?

Goal of most software:

$\vec{x}$ =some input, $\vec{x} \in \mathcal{X}$ → ALGORITHM $z = h(\vec{x})$ → z =some output, $z \in \mathcal{Z}$

Machine Learning:

DESIGN: Figure out some parameterized function class $z = h(\vec{x}, \vec{\theta})$ that's sufficiently general s.t., for some parameter vector $\vec{\theta}$, $h(\cdot)$ will fit the data.

TRAIN: Learn $\vec{\theta}$ from a training dataset $\mathcal{D} = \{(x_1, z_1), \ldots, (x_n, z_n)\}$

TEST: Try it on some examples. How'd you do?

Outline

Today's Function Class: Gaussian Mixture Models (GMM)

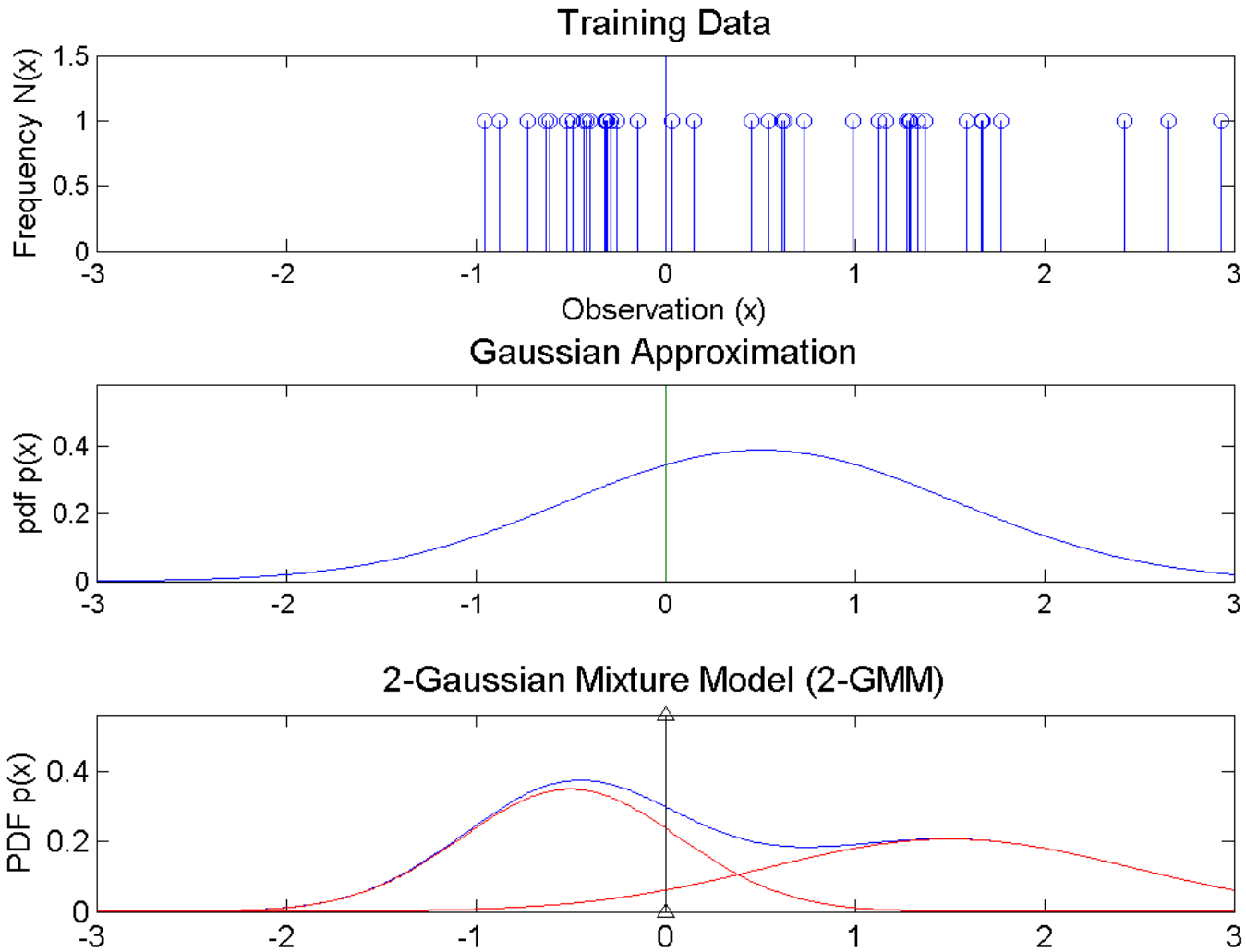
$$h(\vec{x}) = E\left[z|\vec{x}\right], \quad \text{or} \quad \arg\max p(\vec{x}|z), \quad \text{or something like that}$$

$$p(\vec{x}|z) = \sum_{k=1}^{K} c_k \mathcal{N}\left(\vec{x}|\vec{\mu}_k, \Sigma_k\right)$$

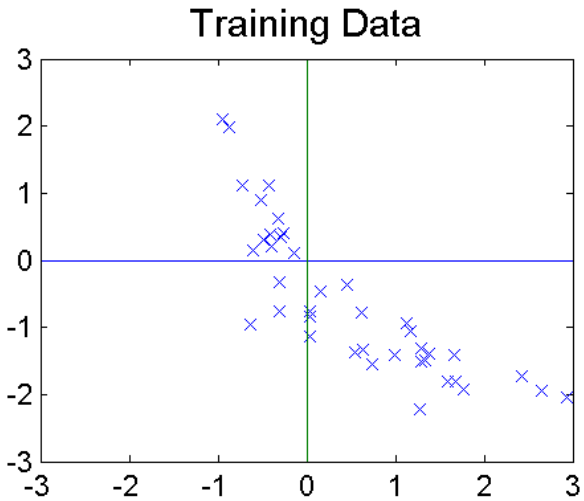
$$\mathcal{N}\left(\vec{x}|\vec{\mu}_k, \Sigma_k\right) = \frac{1}{\sqrt{\det(2\pi\Sigma_k)}} e^{-\frac{1}{2}(\vec{x}-\vec{\mu}_k)^T \Sigma_k^{-1}(\vec{x}-\vec{\mu}_k)}$$

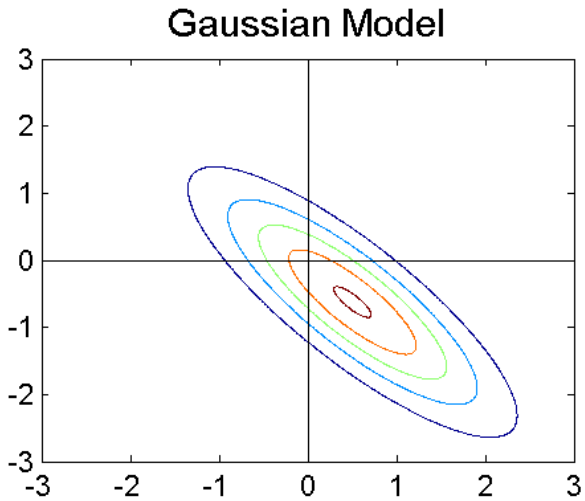
$$\begin{aligned} c_k &= k^{\text{th}} \text{ mixture weight} \\ \vec{\mu}_k &= k^{\text{th}} \text{ mean vector} \\ \Sigma_k &= k^{\text{th}} \text{ covariance matrix} \end{aligned}$$

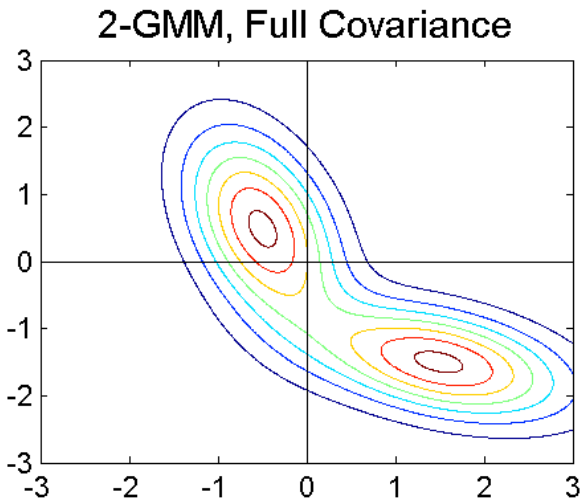
Example: 1-D

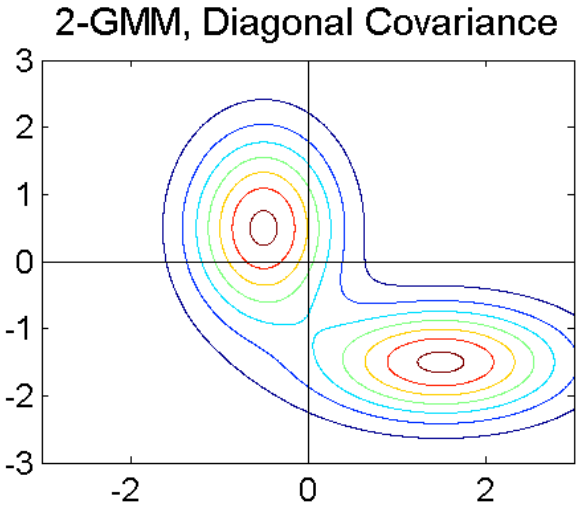

Training Data
Frequency N(x)
1.5
1
0.5
0
-3
-2
-1
0
1
2
3
Observation (x)
Gaussian Approximation
pdf p(x)
0.4
0.2
0
-3
-2
-1
0
1
2
3
2-Gaussian Mixture Model (2-GMM)
PDF p(x)
0.4
0.2
0
-3
-2
-1
0
1
2
3

Example: 2-D


Training Data
3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3


Gaussian Model
3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3


2-GMM, Full Covariance
3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3


2-GMM, Diagonal Covariance
3
2
1
0
-1
-2
-3
-2
0
2

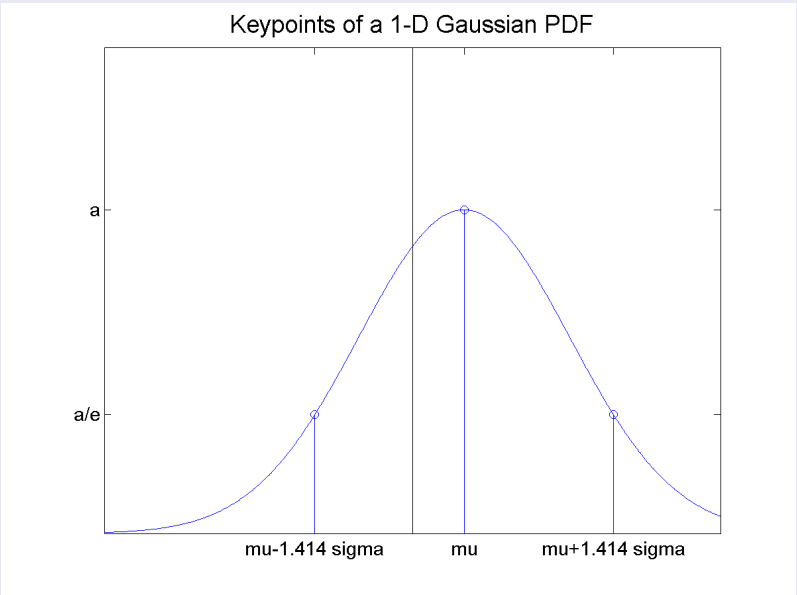
Outline

1-D Gaussian you learned in probability class

Formula

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}}$$

Picture



2-D Gaussian w/Diagonal Covariance

Definitions

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}, \quad \vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad \vec{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$

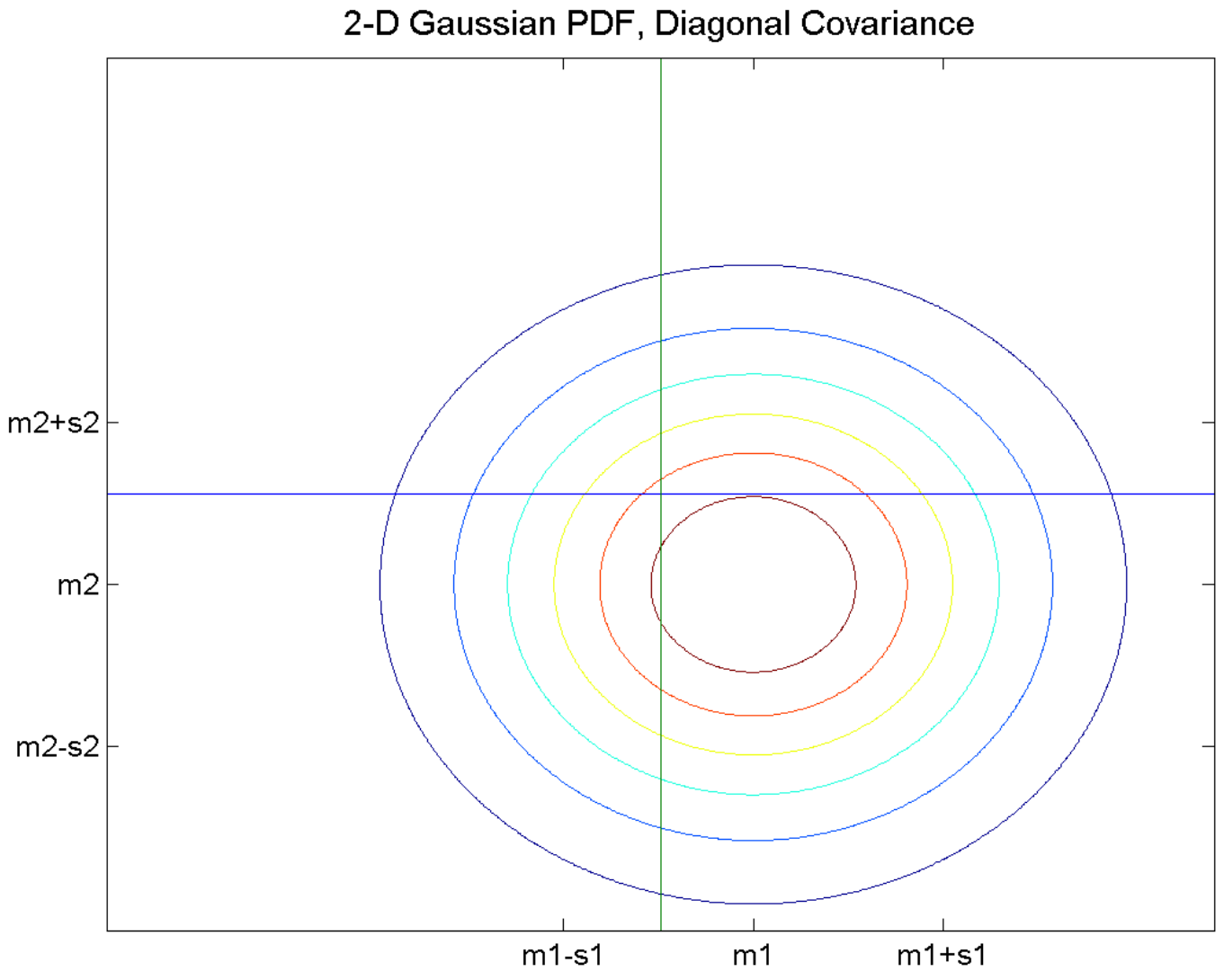
A few facts about linear algebra

$$\det(\Sigma) = \sigma_2^2 \sigma_2^2, \quad \Sigma^{-1} = \begin{bmatrix} \frac{1}{\sigma_1^2} & 0 \\ 0 & \frac{1}{\sigma_2^2} \end{bmatrix}$$

Formula

$$\frac{1}{\sqrt{\det(2\pi\Sigma)}} e^{-\frac{1}{2}(\vec{x}-\vec{\mu})^T \Sigma^{-1}(\vec{x}-\vec{\mu})} = \prod_{j=1}^{2} \frac{1}{\sqrt{2\pi\sigma_j^2}} e^{-\frac{1}{2}\frac{(x_j-\mu_j)^2}{\sigma_j^2}}$$

2D Gaussian, Diagonal Covariance (contour plot)



2-D Gaussian w/Full Covariance (Non-Diagonal)

First useful fact about linear algebra:
Every non-trivial covariance matrix is "positive definite," meaning that it has non-negative eigenvalues...

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \rho_{12} \\ \rho_{21} & \sigma_2^2 \end{bmatrix} = [\vec{v}_1, \vec{v}_2] \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} [\vec{v}_1, \vec{v}_2]^T$$

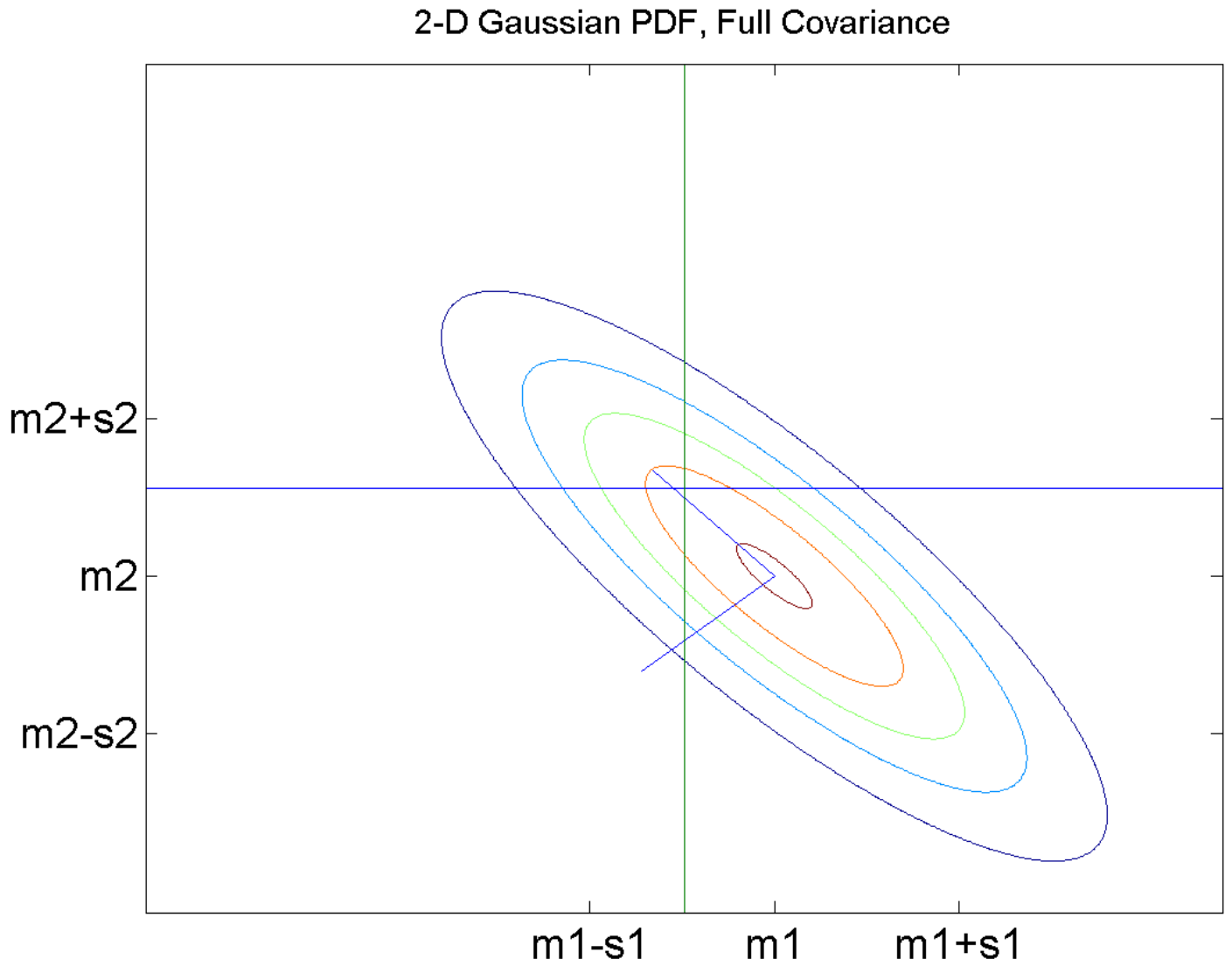
...which specify the determinant and the inverse

$$\det(\Sigma) = \lambda_1 \lambda_2, \quad \Sigma^{-1} = [\vec{v}_1, \vec{v}_2] \begin{bmatrix} \frac{1}{\lambda_1} & 0 \\ 0 & \frac{1}{\lambda_2} \end{bmatrix} [\vec{v}_1, \vec{v}_2]^T$$

Formula

$$\frac{1}{\sqrt{\det(2\pi\Sigma)}} e^{-\frac{1}{2}(\vec{x}-\vec{\mu})^T \Sigma^{-1} (\vec{x}-\vec{\mu})} = \prod_{j=1}^{2} \frac{1}{\sqrt{2\pi\lambda_j}} e^{-\frac{1}{2} \frac{(\vec{v}_j^T \vec{x} - \vec{v}_j^T \vec{\mu})^2}{\lambda_j}}$$

2D Gaussian, Full Covariance (contour plot)



Outline

Maximum Likelihood Estimation of a Gaussian Model

Maximize the Likelihood

- Given some data $\mathcal{D} = \{\vec{x}_1, \ldots, \vec{x}_n\}$
- Find $\vec{\theta} = \begin{bmatrix} \vec{\mu} \\ \Sigma \end{bmatrix}$ to maximize $p(\mathcal{D}|\vec{\theta}) = \prod_{i=1}^{n} p(\vec{x}_i|\vec{\theta})$

Maximize the Log Likelihood

$$\vec{\theta} = \arg\max \log p(\mathcal{D}|\vec{\theta}) = \arg\max \sum_{i=1}^{n} \log p(\vec{x}_i|\vec{\theta})$$

$$= \arg\max \sum_{i=1}^{n} -\frac{1}{2}\left((\vec{x}_i - \vec{\mu})^T \Sigma^{-1} (\vec{x}_i - \vec{\mu}) + \log\det(2\pi\Sigma)\right)$$

ML Estimate of Mean = "Sample Mean"

$$\vec{\mu}_{ML} = \frac{1}{n}\sum_{i=1}^{n}\vec{x}_i$$

ML Estimate of Covariance = "Sample Covariance"

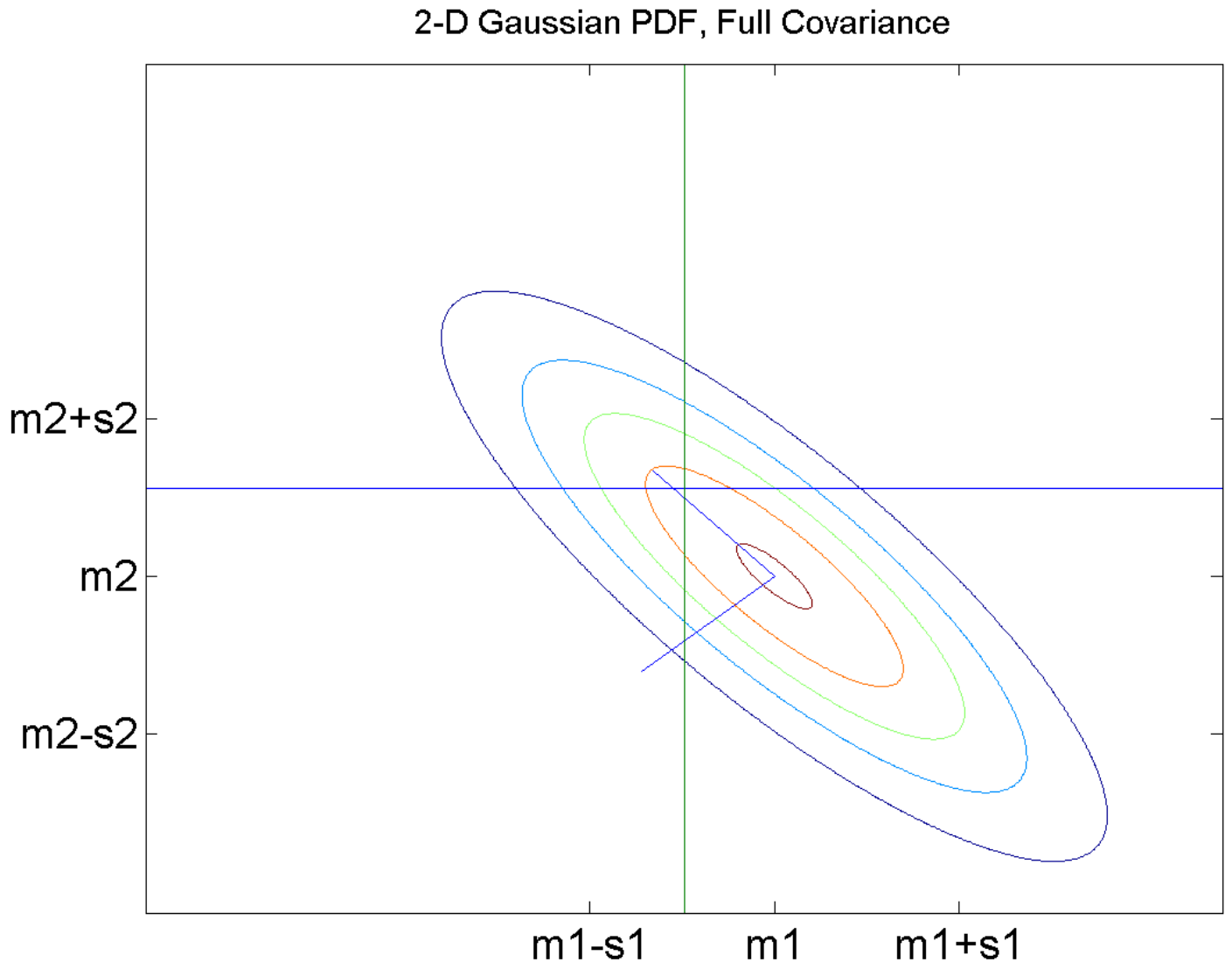
$$\Sigma_{ML} = \frac{1}{n}\sum_{i=1}^{n}(\vec{x}_i - \vec{\mu})(\vec{x}_i - \vec{\mu})^T$$

. . . which is just the matrix way of saying that. . .

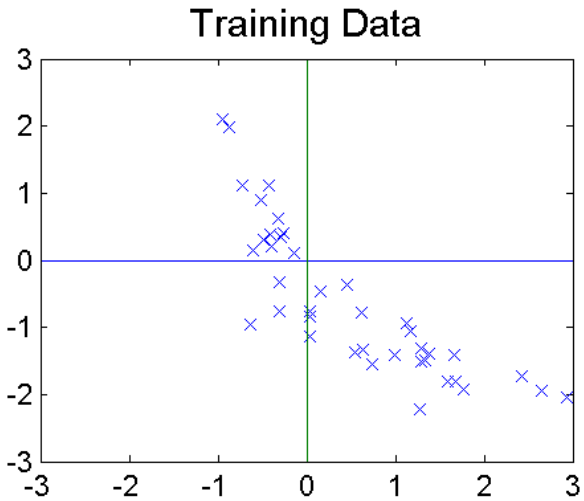
$$\sigma^2_{j,ML} = \frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \mu_j)^2$$

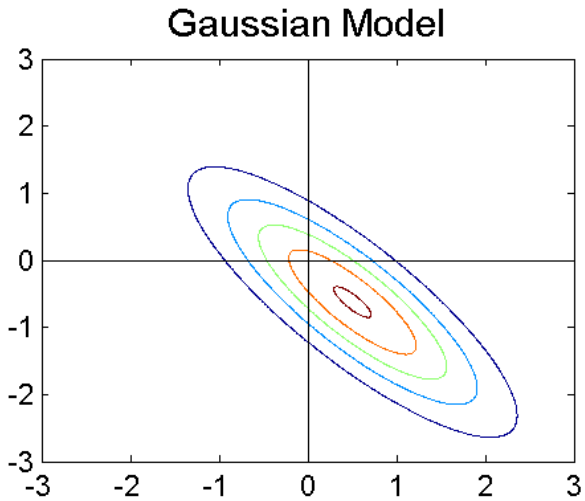
$$\rho_{jk,ML} = \frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \mu_j)(x_{ik} - \mu_k)$$

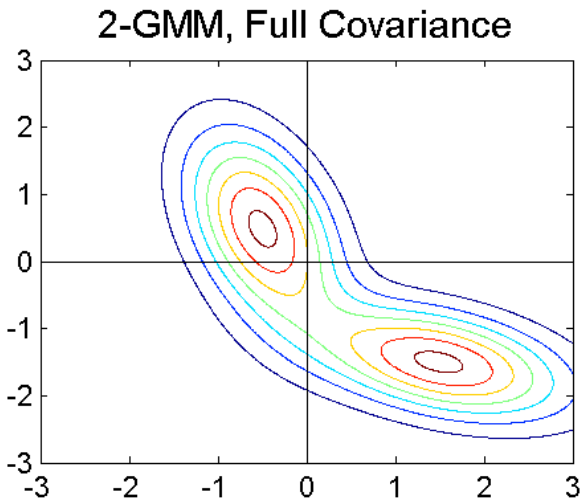
2D Gaussian, Full Covariance (contour plot)

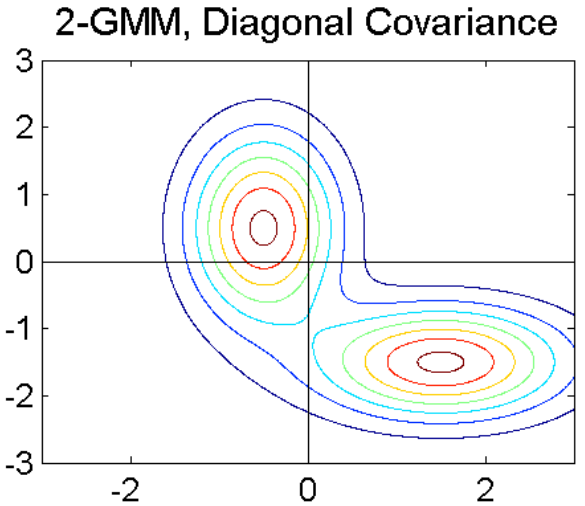


. . . and now, let's learn a Gaussian Mixture Model









GMM Definition

$$p(\vec{x}) = \sum_{k=1}^{K} c_k \mathcal{N}(\vec{x}|\vec{\mu}_k, \Sigma_k)$$

Parameter Vector

$$\vec{\theta} = [c_1, c_2, \vec{\mu}_1, \vec{\mu}_2, \Sigma_1, \Sigma_2]^T$$

Maximum Likelihood Estimation

$$\vec{\theta}_{ML} = \arg\max \log p(\mathcal{D}|\vec{\theta})$$

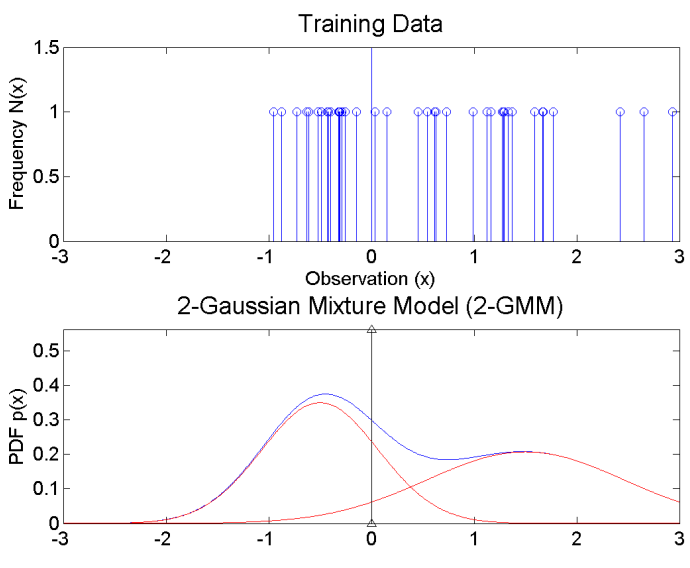
$$= \arg\max \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} c_k \mathcal{N}(\vec{x}|\vec{\mu}_k, \Sigma_k) \right)$$

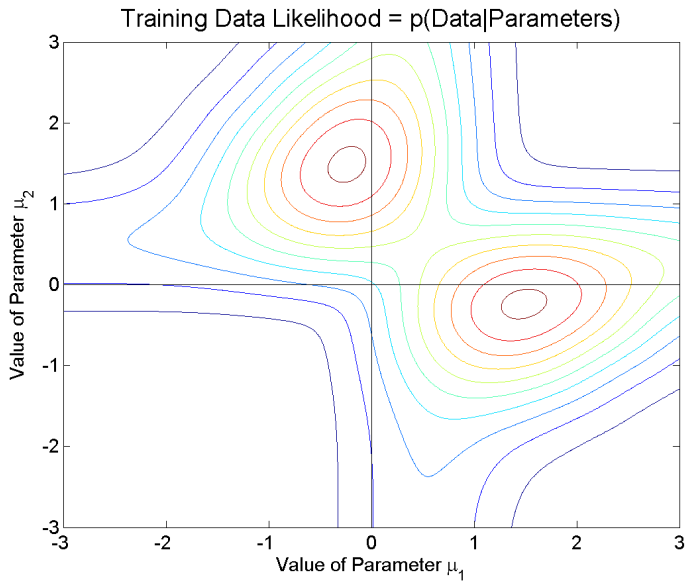
GMMs are Different: There's No Single Best Solution

Example

Swap $c_1 \leftrightarrow c_2$, and $\vec{\mu}_1 \leftrightarrow \vec{\mu}_2$, and $\Sigma_1 \leftrightarrow \Sigma_2$, then $p(\mathcal{D}|\vec{\theta})$ is unchanged!!

Example Pictures: Symmetry of a 2-GMM Under Swap



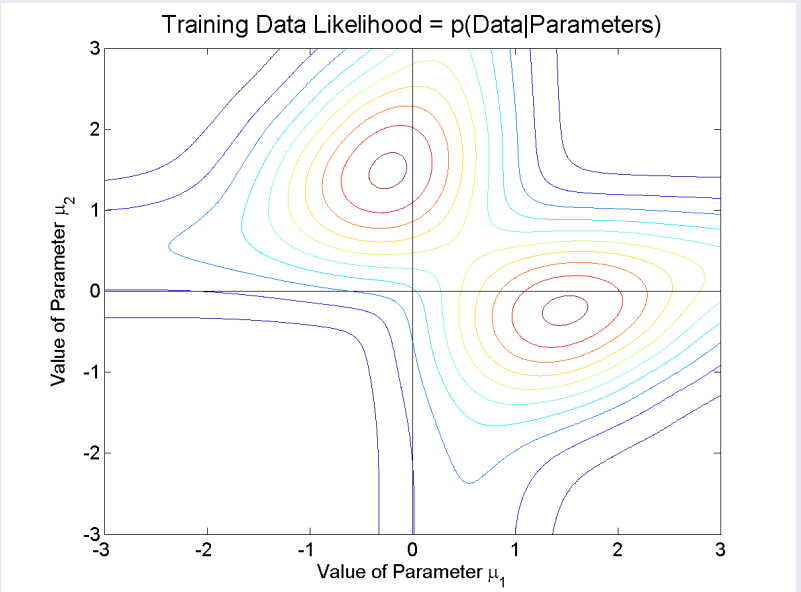


No Global Optimum⇒ Find a Local Optimum

Local Optimum: Algorithm Pseudocode

1. Start with initial guess $\vec{\theta}$
2. Find some $\hat{\theta}$ such that $p(\mathcal{D}|\hat{\theta}) > p(\mathcal{D}|\vec{\theta})$
3. Repeat until $\vec{\theta}$ stops changing

Local Optimum: Algorithm Picture



Find a Local Optimum: Gradient Ascent

Gradient Ascent: Algorithm Definition

$$\hat{\theta} = \vec{\theta} + \eta \nabla_{\vec{\theta}} \log p(\mathcal{D}|\vec{\theta})$$

Practical Issues

- Guaranteed to work if η is small enough
- Problem: what's a good value of η?
  - η too large$\Rightarrow$ $\hat{\theta}$ jumps right over the local optimum
  - η too small$\Rightarrow$gradient ascent takes a very long time to converge
- Usual approach: choose $\eta = 0.002$ and cross your fingers
  - If $\vec{\theta}$ eventually stops changing: Hooray! You found a local optimum!
  - If $\vec{\theta}$ never stops changing: Reduce η and try again.

Find a Local Optimum: Expectation Maximization (EM)

EM: Algorithm Definition

$$\hat{\theta} = \arg\max Q(\vec{\theta}, \hat{\theta}),$$

where $Q(\vec{\theta}, \hat{\theta})$ is some function chosen so that

$$\begin{array}{lcl} Q(\vec{\theta}, \hat{\theta}) & & \text{has a global optimum} \\ Q(\vec{\theta}, \hat{\theta}) & \leq & \log p(\mathcal{D}|\hat{\theta}) \quad \text{for all values of } \hat{\theta} \end{array}$$

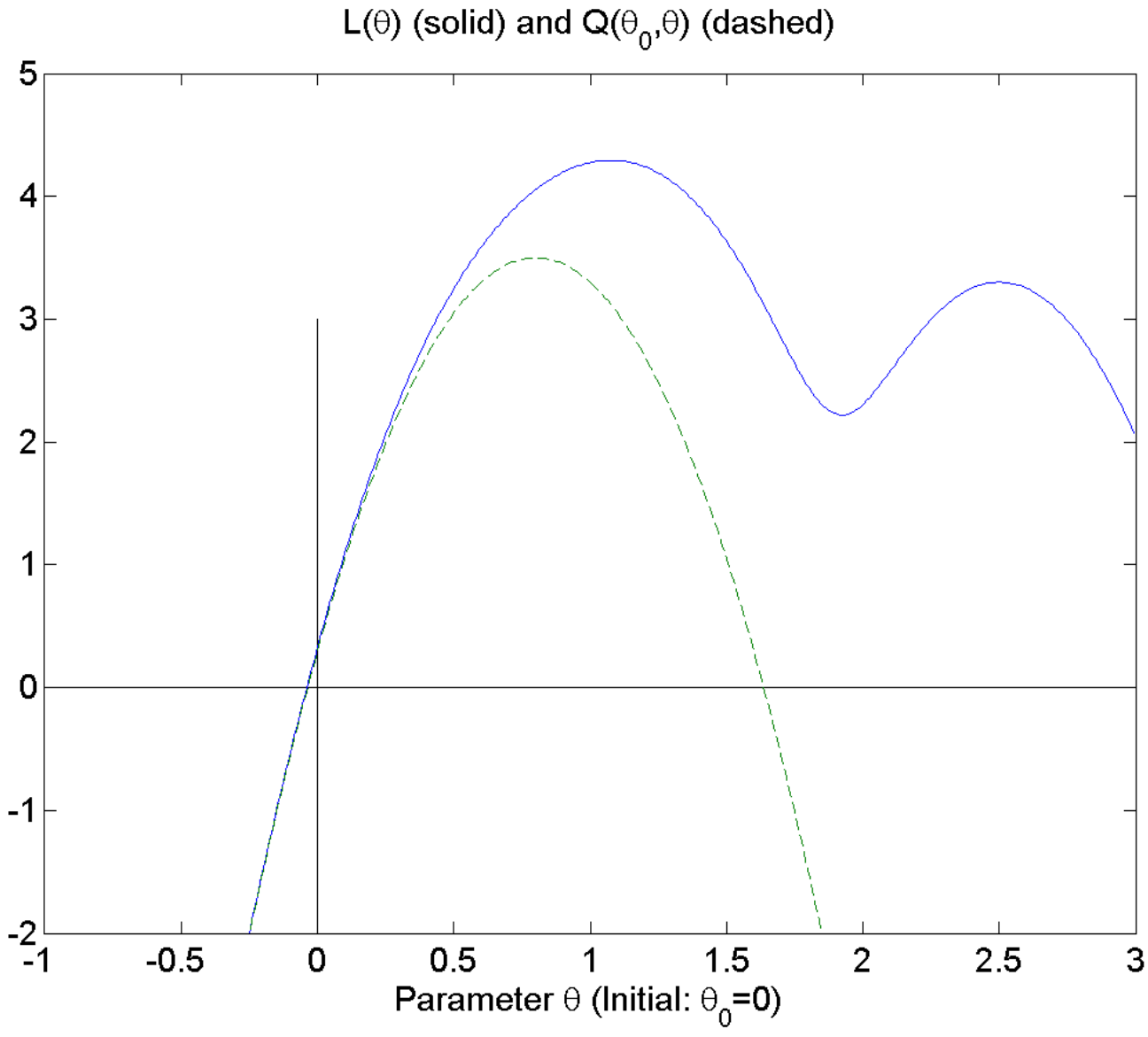
and at the starting point $\hat{\theta} = \vec{\theta}$,

$$Q(\vec{\theta}, \vec{\theta}) = \log p(\mathcal{D}|\vec{\theta}) \quad \text{and} \quad \nabla_{\hat{\theta}} Q(\vec{\theta}, \hat{\theta}) = \nabla_{\hat{\theta}} \log p(\mathcal{D}|\hat{\theta})$$

Practical Issues

- PROBLEM: Can we find such a Q function?
- ANSWER: For GMM and HMM, yes. For most other models, no.

Find a Local Optimum: Expectation Maximization (EM)



EM Algorithm for the GMM

E-Step: Expected frequency of each Gaussian

$$\gamma_i(k) = \Pr\left\{k^{\text{th}} \text{ Gaussian} | \vec{x}_i\right\} = \frac{c_k \mathcal{N}(\vec{x}_i | \vec{\mu}_k, \Sigma_k)}{\sum_{\ell=1}^{K} c_\ell \mathcal{N}(\vec{x}_i | \vec{\mu}_\ell, \Sigma_\ell)}$$

$$n_k = E\left[\#\text{ occurrences } k^{\text{th}} \text{ Gaussian}\right] = \sum_{i=1}^{n} \gamma_i(k)$$

M-Step: Parameters that Maximize the Q Function

$$\hat{c}_k = \frac{n_k}{n}, \quad \hat{\mu}_k = \frac{1}{n_k} \sum_{i=1}^{n} \gamma_i(k) \vec{x}_i$$

$$\hat{\Sigma}_k = \frac{1}{n_k} \sum_{i=1}^{n} \gamma_i(k)(\vec{x}_i - \hat{\mu}_k)(\vec{x}_i - \hat{\mu}_k)^T$$

Outline

Classifying with a GMM

TRAINING a GMM Classifier

GIVEN: $\mathcal{D}_1 = \{\vec{x}_1, \ldots \vec{x}_n\}$ examples of class $z = +1$,

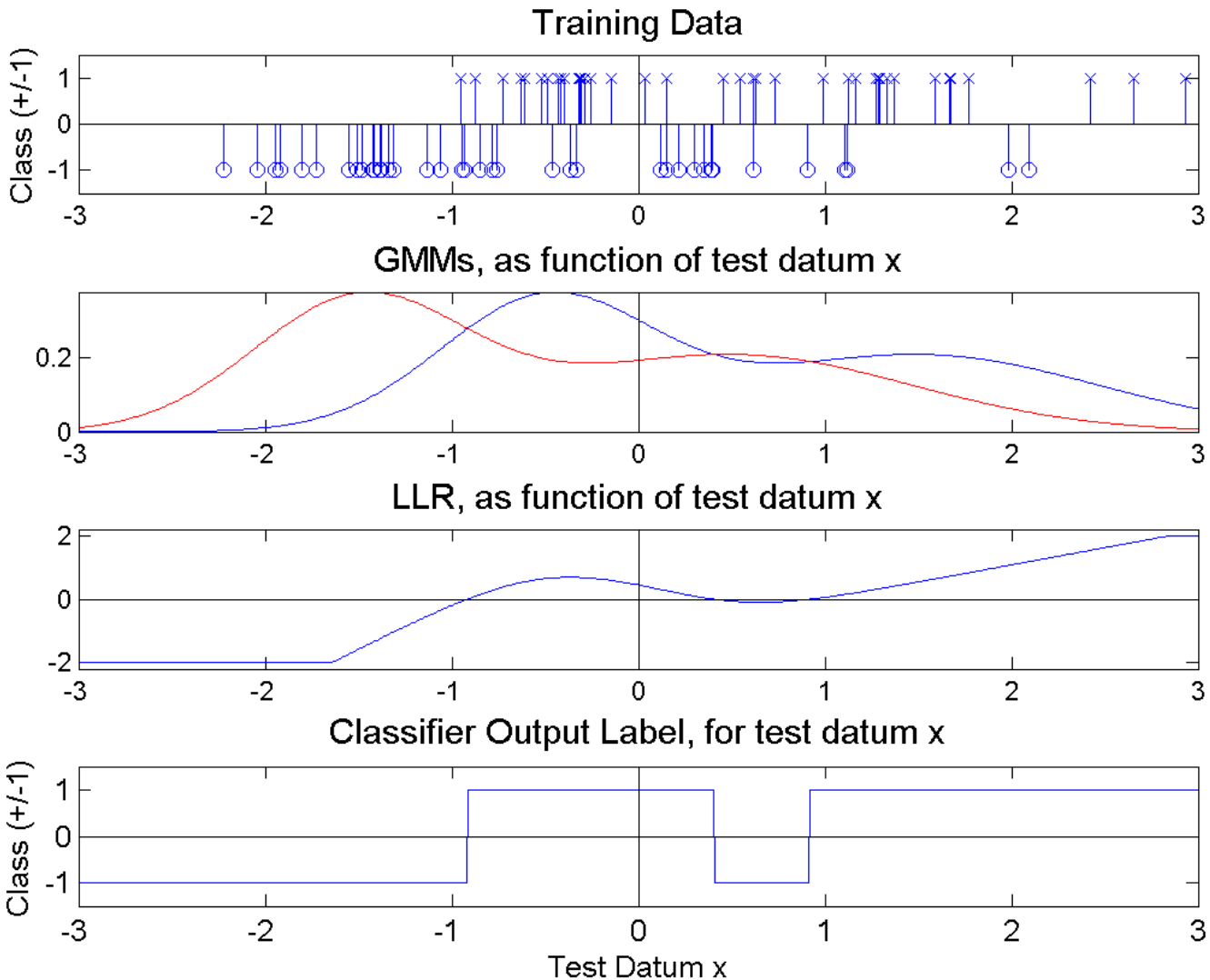
GIVEN: $\mathcal{D}_{-1} = \{\vec{x}_{n+1}, \ldots \vec{x}_{2n}\}$ examples of class $z = -1$,

LEARN: $p(\vec{x}|z) = \sum_{k=1}^{K} c_{zk} \mathcal{N}(\vec{x}|\vec{\mu}_{zk}, \Sigma_{zk})$

TESTING a GMM Classifier

$$LLR = \log \frac{p(\vec{x}|z=+1)p(z=+1)}{p(\vec{x}|z=-1)p(z=-1)}$$

$$h(\vec{x}) = \begin{cases} +1 & \text{if } LLR > 0 \\ -1 & \text{if } LLR < 0 \end{cases}$$


Training Data
Class (+/-1)
GMMs, as function of test datum x
LLR, as function of test datum x
Classifier Output Label, for test datum x
Class (+/-1)
Test Datum x

Outline

The EM Mismatch Problem

TRAINING Criterion: Maximum Likelihood

LOG LIKELIHOOD: $\mathcal{L}(\vec{x}_i, \vec{\theta}) = \log p(\vec{x}_i|\vec{\theta})$

TESTING Criterion: Minimum Classification Error

CLASSIFICATION ERROR: $\ell(\vec{x}_i, \vec{\theta}) = \begin{cases} 1 & h(\vec{x}_i) \neq z_i \\ 0 & h(\vec{x}_i) = z_i \end{cases}$

MISMATCH

Maximum likelihood training might not minimize classification error. The lab has a striking example of this.

Minimum Classification Error (MCE) Training

(1) Write classification error as a function of $\vec{\theta}$

$z_i \in \{-1, +1\}$ is the correct label of $\vec{x}_i$.

$$\begin{aligned} E_n &= \frac{1}{n}(\#\text{ for which } LLR(\vec{x}_i) \text{ and } z_i \text{ have opposite signs}) \\ &= \frac{1}{n}\sum_{i=1}^{n} u\left(z_i LLR(\vec{x}_i)\right) \end{aligned}$$

where $u(b) = \begin{cases} 1 & b > 0 \\ 0 & b < 0 \end{cases}$ is the unit step function.

Minimum Classification Error (MCE) Training

(2) Approximate with a differentiable function

$$\tilde{E}_n = \frac{1}{n} \sum_{i=1}^{n} \sigma \left(z_i LLR(\vec{x}_i) \right)$$

where $\sigma(b) = 1/(1 + e^{-b})$ is called the logistic function, and is a differentiable approximation of the unit step function:

- $\lim_{b \to \infty} \sigma(b) = 1$
- $\lim_{b \to -\infty} \sigma(b) = 0$
- $\sigma(0) = \frac{1}{2}$

Minimum Classification Error (MCE) Training

(3) Gradient Descent

$$\hat{\theta} = \vec{\theta} - \eta \nabla_{\vec{\theta}} \tilde{E}_n$$

Practical Issues

- From this point on, MCE training looks exactly like training a neural net!
- So let's take a break, then talk about how to train neural nets.

Outline

Key Points: GMM

MACHINE LEARNING: Instead of writing a set of if-then statements to figure out the right label, we create a function $h(\vec{x}, \vec{\theta})$, then learn the parameter vector from data.

GMM: a GMM is a universal approximator, meaning that, as $K \to \infty$, a GMM can represent any real-world probability distribution.

Gaussians: maximum likelihood training of a Gaussian is just the sample mean and sample covariance.

Training a GMM is harder, because there's no global optimum. EM algorithm efficiently computes a local optimum.

Testing: if $LLR > 0$, call it class 1, otherwise call it class -1. MCE training explicitly minimizes classification error.

Outline

Regression with a GMM

TRAINING a GMM Regression

GIVEN: $\mathcal{D} = \{(\vec{x}_1, \vec{z}_1), \ldots (\vec{x}_n, \vec{z}_n)\}$

LEARN: $p\left(\begin{bmatrix} \vec{x} \\ \vec{z} \end{bmatrix}\right) =$

$$\sum_{k=1}^{K} c_k \mathcal{N}\left(\begin{bmatrix} \vec{x} \\ \vec{z} \end{bmatrix} | \begin{bmatrix} \vec{\mu}_{x,k} \\ \vec{\mu}_{z,k} \end{bmatrix}, \begin{bmatrix} \Sigma_{xx,k} & \Sigma_{xz,k} \\ \Sigma_{zx,k} & \Sigma_{zz,k} \end{bmatrix}\right)$$

TESTING a GMM Regression

$$\vec{z}(\vec{x}) = E\left[\vec{z} | \vec{x}\right] = \sum_{k=1}^{K} \gamma_{\vec{x}}(k) \left(\vec{\mu}_{z,k} + \Sigma_{zx,k}\Sigma_{xx,k}^{-1}(\vec{x} - \vec{\mu}_{x,k})\right)$$