In [3]:
```
# ============================================================
# Notebook setup: run this before everything
# ============================================================

%load_ext autoreload
%autoreload 2

# Control figure size
figsize=(15, 4.5)

from util import util
import numpy as np
from sklearn.mixture import GaussianMixture
```

```
The autoreload extension is already loaded. To reload it, use:
  %reload_ext autoreload
```

Gaussian Mixture Models

A Deeper Analysis

We'll start by focusing on the scalability issues

We have established that KDE has trouble with:

- Large dimensional datasets
- Large number of training examples

> **Can you make a guess about the root of the problem?**

KDE makes no attempt to "compress" the information from the training data:

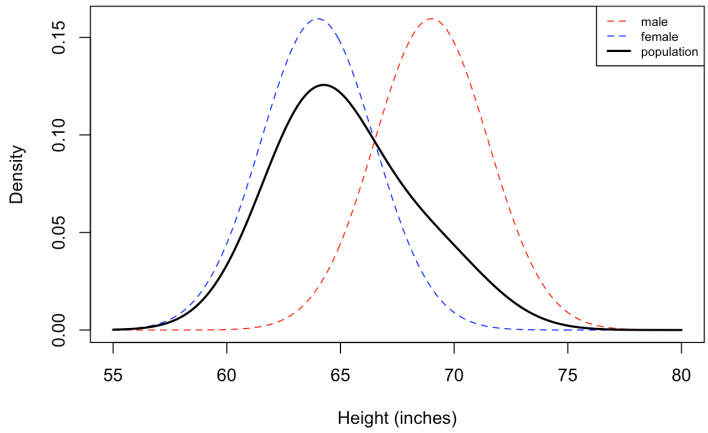
- The size of a KDE models grows directly with the training set size
- In statistical terms, KDE has very little bias and a very large variance

It's time to introduce a new density estimation technique

Gaussian Mixture Models

In particular, we'll now switch to using *Gaussian Mixture Models (GMMs)*

A GMM describes a distribution via a *weighted sum of Gaussian components*



Gaussian Mixture Models

In particular, we'll now switch to using *Gaussian Mixture Models (GMMs)*

A GMM describes a distribution via a *weighted sum of Gaussian components*

- The model size depends on the dimensionality and on #components
- The #components can be chosen, to control the bias/variance trade-off

Formally, we assume data is generated by the following probabilistic model

$$X_Z$$

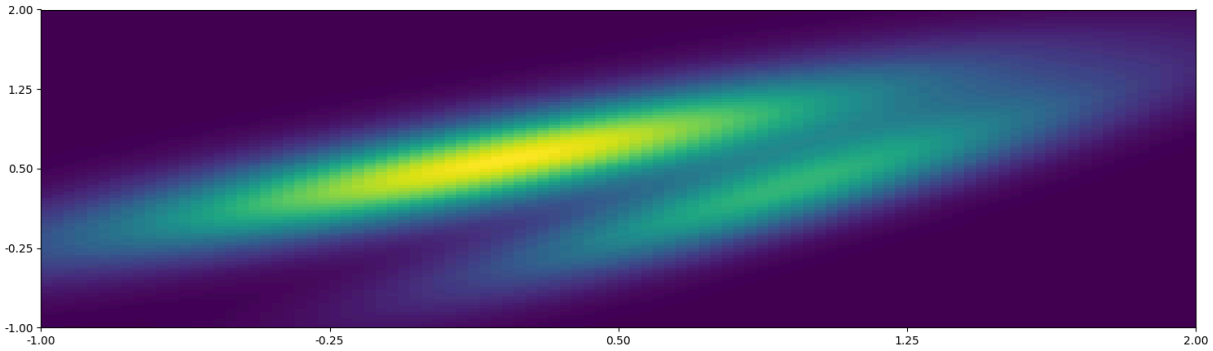
- Z e X_k are both random variables
- Z represents the index of the component that generates the sample
- X_k follows a multivariate Gaussian distribution

In other words, a GMM is *a selection-based ensemble*

A GMM Example

Let's build a (random) GMM in two dimensions so see an example

In [4]:
```
gt = util.generate_gmm_dist(n_components=2, seed=59)
util.plot_density_estimator_2D(gt, xr=np.linspace(-1, 2, 100), yr=np.linspac
```



- Our example has two components, each with its own mean and covariance
- One component is slightly less prevalent than the other

GMM Parameters

The PDF of a GMM is given by:

$$g(x, \mu, \Sigma, \tau) = \sum_{k=1}^{n} \tau_k f(x, \mu_k, \Sigma_k)$$

- f is the PDF of a multivariante Normal distribution
- μ_k is the (vector) mean and Σ_k the covariance matrix for the k-th component
- τ_k corresponds to $P(Z = k)$

We can inspect the values for our example GMM

In [5]:
```
print('tau:', gt.weights)
print('mu', str(gt.mu).replace('\n', ' '))
print('sigma', str(gt.sigma).replace('\n', ' '))
```

```
tau: [0.69756198 0.30243802]
mu [[0.20612642 0.58696692]  [0.94152811 0.3112852 ]]
sigma [array([[0.5610369 , 0.3646768 ],        [0.3646768 , 0.31593376]]), a
rray([[0.29862754, 0.29550211],        [0.29550211, 0.35832187]])]
```

Sampling from GMMs

When we want to *sample* from a GMM

- First we need to sample the Z variable
- Then we sample from the corresponding multivariate distribution

In [6]:
```
train_x, train_z = gt.sample(1000, seed=42)
test_x, test_z = gt.sample(1000, seed=42)
```

Hence, we don't get to now just the sample value

...But also *which of the Gaussian components* it was generated by

In [7]:
```
print('z values :', train_z[:4])
print('x values:', train_x[:4])
```

```
z values : [0 1 1 0]
x values: [[ 0.25595526  0.24144331]
 [ 0.65952904  0.16087875]
 [ 0.50240258  0.11145718]
 [-0.47036887  0.2317656 ]]
```

Training a GMM

We can train a GMM to *approximate other distributions*

The training problem can be formulated in terms of *likelihood maximization*

$$\arg\max_{\mu,\Sigma,\tau} \mathbb{E}_{x\sim X}\left[L(x,\mu,\Sigma,\tau)\right] \tag{1}$$

$$\text{s.t.} \sum_{k=1}^{n} \tau_k = 1 \tag{2}$$

- As usual, the likelihood function L measures how likely it is...
- ...that the training sample $\hat{x}$ is generated by a GMM with parameters μ, Σ, τ

There's more than one issue here

...And the first one is dealing with the expectation

Training a GMM

We can approximate the expectation by using the training set

$$\mathbb{E}_{x\sim X}\left[L(x,\mu,\Sigma,\tau)\right] \simeq \prod_{i=1}^{m} g(x_i,\mu,\Sigma,\tau)$$

Technically, this is just an example of Monte-Carlo estimation

- When used for the likelihood of the training data
- ...This is often called "Empirical Risk Minimization" principle

There are two sub-variants of this approach

- We can use a single large sample (the classical approach)
- ...Or many smaller ones (what we do in cross-validation)

We will stick to the simplest approach (a single training sample)

Training a GMM

Let's put everything together

$$\arg\max_{\mu,\Sigma,\tau} \prod_{i=1}^{m}\sum_{k=1}^{n}\tau_k f(x,\mu_k,\Sigma_k) \tag{3}$$

$$\text{s.t.} \sum_{k=1}^{n}\tau_k = 1 \tag{4}$$

From an optimization point of view, this is *very annoying problem*:

- There's a *constraint*
- There's both *a product and a sum*
- The product cannot be decomposed (μ, Σ, τ appear in every term)

So we'll need to get clever!

An Apparent Overcomplication

We get clever by apparently overcomplicating the problem

In particular, we introduce a random variable Z_i *for each example*

- $Z_i = k$ iff i-th example was drawn from the k-th component
- The Z_i are *latent* since we do not know their value
- We focus on *our* uncertainty, rather than on the uncertainty in the process

When computin the PDF, we take the values of Z_i for granted:

$$\tilde{g}_i(x_i, z_i, \mu, \Sigma, \tau) = \tau_{z_i} f(x, \mu_k, \Sigma_k)$$

- The value z_i is now *an input to* $\tilde{g}_i$
- ...And we can use it as an index to retrieve the correct τ_k
- This alternative PDF is much easier (there is *no sum*)!

An Apparent Overcomplication

The drawback is that we have now uncertainty over *both* X *and all* Z_i

$$\mathbb{E}_{x\sim X,\{z_i\}\sim\{Z_i\}}\left[L(x,z,\mu,\Sigma,\tau)\right]$$

We can deal with X by using the training:s

By doing this we obtain:

$$\mathbb{E}_{x\sim X,\{z_i\}\sim\{Z_i\}}\left[L(x,z,\mu,\Sigma,\tau)\right] \simeq \mathbb{E}_{\{z_i\}\sim\{Z_i\}}\left[\prod_{i=1}^{m}\tilde{g}_i(x_i,z_i,\mu,\Sigma,\tau)\right]$$

- We cannot use the same technique for the Z_i variables
- ...Since we do not have a sample for them (they are latent)!

An Apparent Overcomplication

We can however compute the expectation *in closed form*

- We introduce new variables (to be estimated) $\tilde{\tau}_{i,k}$
- ...which represet the (unknown) distribution of the latent Z_i variables

In particular, $\tilde{\tau}_{i,k}$ corresponds to $P(Z_i = k)$

With the new variable, we can compute the expectation *in closed form*:

$$\mathbb{E}_{\hat{x}\sim X,\hat{z}\sim Z}\left[L(\hat{x},\hat{z},\mu,\Sigma,\tau)\right] \simeq \prod_{i=1}^{m}\prod_{k=1}^{n}\tilde{g}_i(x_i,z_i,\mu,\Sigma,\tau)^{\tau_{i,k}}$$

- Intuitively, we if we sampled Z_i
- ...We would generate $\tilde{\tau}_{i,k}$ samples for each component k
- ...So that the corresponding density is multplied by itself $\tilde{\tau}_{i,k}$ times

An Apparent Overcomplication

The reworked training problem therefore is

$$\arg\max_{\mu,\Sigma,\tau,\tilde{\tau}} \prod_{i=1}^{m}\prod_{k=1}^{n}\tilde{g}_i(x_i,z_i,\mu,\Sigma,\tau)^{\tau_{i,k}} \tag{5}$$

$$\text{s.t.} \sum_{k=1}^{n}\tau_k = 1 \tag{6}$$

$$\sum_{k=1}^{n}\tilde{\tau}_{i,k} = 1 \qquad \forall i = 1..m \tag{7}$$

- We have even more variables (the $\tilde{\tau}_{i,k}$ ones)
- ...But they are statistically related! Each Z_i is drawn from Z
- ...And there's no longer a combination of sums and products

Expectation-Maximization

We can now use the Expectation-Maximization algorithm

The EM algorithm is an optimization method based on *alternating steps*

- In the *expectation* step:
  - We consider μ, Σ, τ as fixed and we optimize over $\tilde{\tau}$
  - ...I.e. we try to estimate how sampling went
  - After this, we compute the expectation over Z (in a symbolic form)
- In the *maximization* step:
  - We use the (symbolic) expectation over Z from before
  - We consider $\tilde{\tau}$ as fixed and we optimize over μ, Σ, τ

The method converges to a local optimum

...And we will not detail it further in this lecture

GMM in Action

There are many implementations and variants of the EM method

We will use the code from scikit-learn:

In [8]:
```
from sklearn.mixture import GaussianMixture

gm = GaussianMixture(n_components=2, random_state=4)
gm.fit(train_x);
```

- The API is the usual one

We need to specify the number of components a priori

- We can tune it using a maximum likelihood approach on a validation set
- ...Or using other criteria (e.g. elbow method)

Inspecting the Results

Let's inspect the learned parameters

In [9]:
```
print('Learned weights', gm.weights_)
print('True weights', gt.weights)
```

```
Learned weights [0.6590098 0.3409902]
True weights [0.69756198 0.30243802]
```

In [10]:
```
print('Learned means', str(gm.means_).replace('\n', ' '))
print('True means', str(gt.mu).replace('\n', ' '))
```

```
Learned means [[0.06974974 0.54625223]  [0.96907679 0.40083217]]
True means [[0.20612642 0.58696692]  [0.94152811 0.3112852 ]]
```

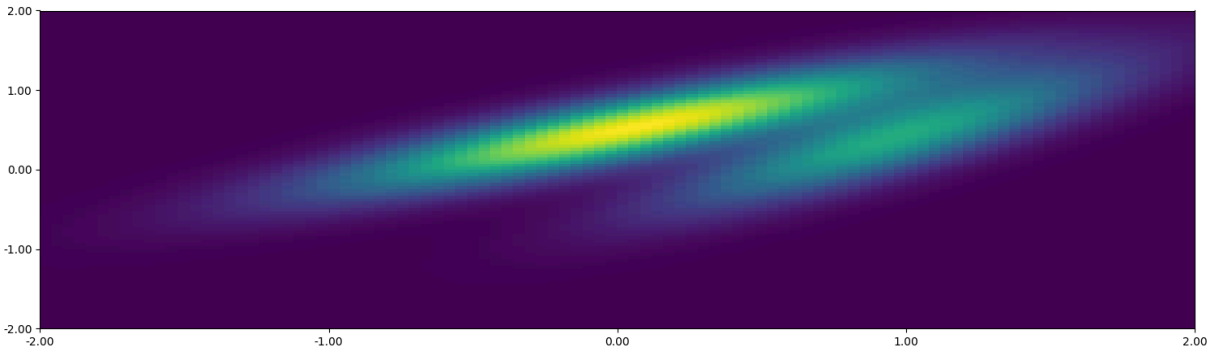
In [11]:
```
print('Learned covariance #1', str(gm.covariances_[0]).replace('\n', ' '))
print('True covariance #1', str(gt.sigma[0]).replace('\n', ' '))
print('Learned covariance #2', str(gm.covariances_[1]).replace('\n', ' '))
print('True covariance #2', str(gt.sigma[1]).replace('\n', ' '))
```

```
Learned covariance #1 [[0.47861885 0.32101492]  [0.32101492 0.28622476]]
True covariance #1 [[0.5610369  0.3646768 ]  [0.3646768  0.31593376]]
Learned covariance #2 [[0.26613038 0.26083955]  [0.26083955 0.34615556]]
True covariance #2 [[0.29862754 0.29550211]  [0.29550211 0.35832187]]
```

Inspecting the Results

Here is the approximated PDF

In [12]:
```
util.plot_density_estimator_2D(gm, xr=np.linspace(-2, 2, 100), yr=np.linspac
```



Which Kind of Prediction

GMMs are very flexible in terms of what they can do

We can use them to *evaluate the (log) density* of a sample:

In [13]:
```
pred_lf = np.exp(gm.score_samples(train_x))
print('Log densities:', pred_lf[:3])
```

```
Log densities: [0.17629181 0.29102933 0.21023248]
```

We can use them to *generate a sample*:

In [14]:
```
pred_x, pred_z = gm.sample(3)
print('Sampled values:', str(pred_x).replace('\n', ' '))
print('Sampled components:', pred_z)
```

```
Sampled values: [[ 0.74060004  0.14883754]  [ 0.31220378 -0.02384664]  [ 0.3
0811268 -0.47618621]]
Sampled components: [1 1 1]
```

More then Densities

GMMs are very flexible in terms of what they can do

We can estimate the *probability that a sample belongs to a component*

In [15]:
```
pred_p = gm.predict_proba(train_x)
print('Probability of belonging to a component:')
print(pred_p[:3])
```

```
Probability of belonging to a component:
[[0.84724085 0.15275915]
 [0.01845649 0.98154351]
 [0.05474391 0.94525609]]
```

- The approach is the same we used to optimize $\tilde{\tau}_{i,k}$ in the expectation step

By picking the maximum probability, we can *assign samples to a component*

In [16]:
```
pred_c = gm.predict(train_x)
print(pred_c[:3])
```

```
[0 1 1]
```

More then Densities

GMMs can certainly act as density estimators

...But can do much more!

- Sampling
- Component assignment
- ...And therefore *clustering*

This is so true that GMM are often presented as a generalization of k-means

And this (partially) addresses the last limitation of KDE

- By choosing certain density estimator
- ...We can obtain additional information in addition to the densities