Gaussian Process Regression & Gaussian Mixture Models

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Today's Roadmap

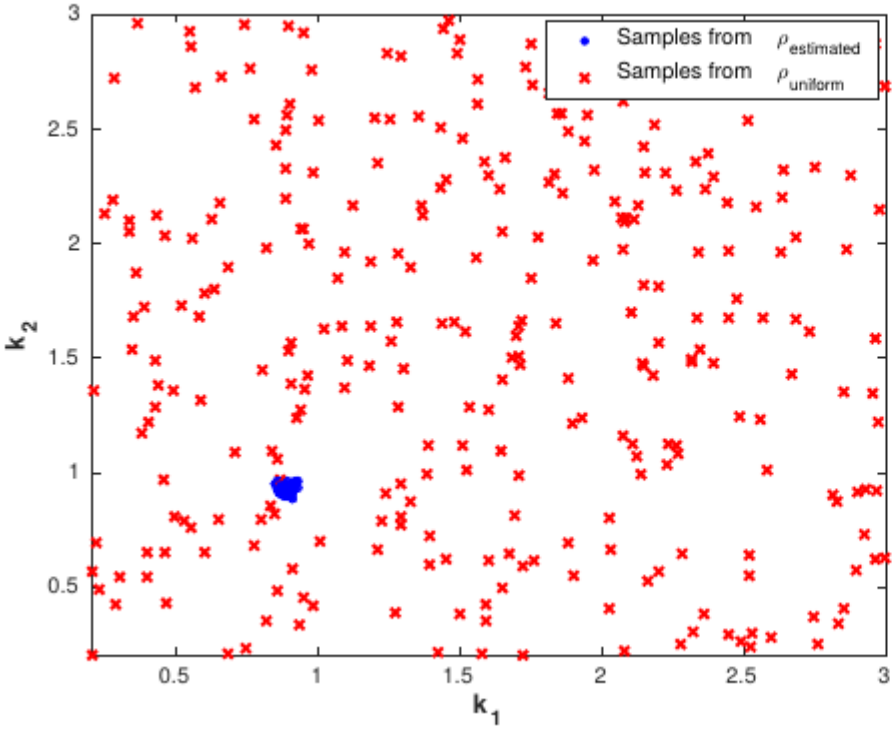
I. Introduction to Gaussian Process Regression (II)

- Predictions using noisy observations
- Estimating the Hyper-parameters
- More on Kernels

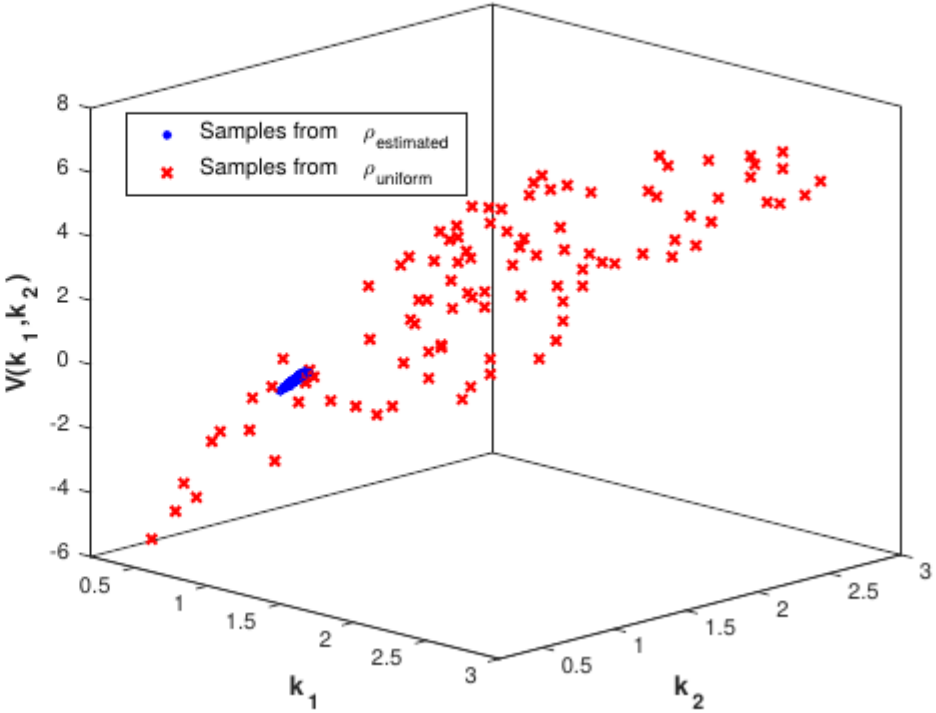
II. Gaussian Mixture Models

- The basic idea
- The Expectation Maximization Algorithm (EM)

Recall: Want to solve Dynamic Models on high-dimensional, irregularly-shaped state-spaces



Blue: ergodic set.
Red: Computational domain



Blue: Value function, evaluated on ergodic set
Red: Value function, evaluated on the entire comp. domain

Recall: Building an ML Algorithm

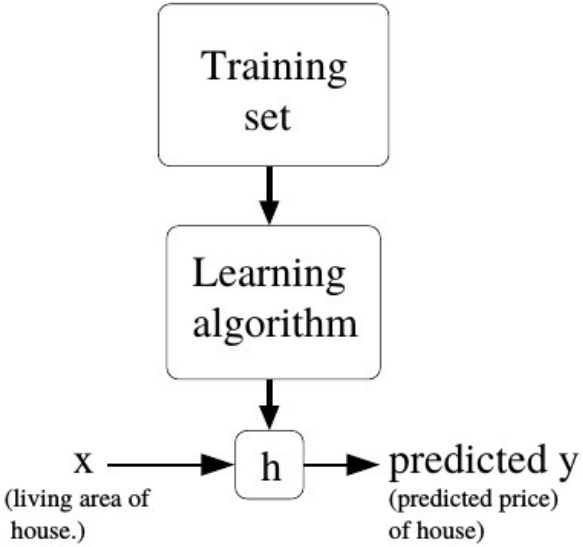
cf. Andrew Ng's ML course http://cs229.stanford.edu/

x(i): "input" variables, also called input features.

y(i): "output" / target variable that we are trying to predict (price).

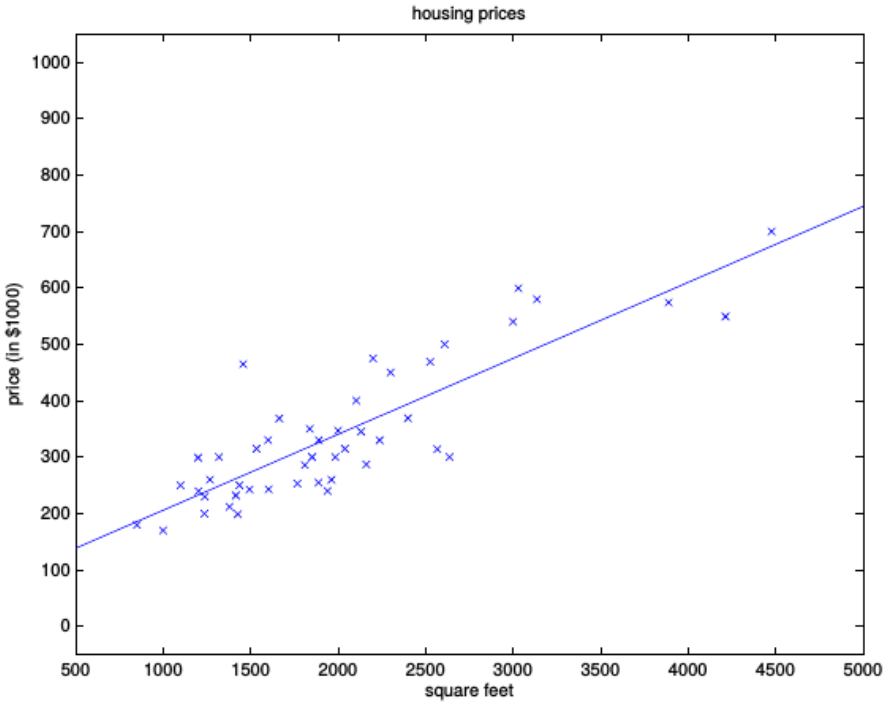
Training example:
a pair (x(i) , y(i)).

Training set:
a list of m training examples {(x(i), y (i)); i = 1, . . . , m}



→ To perform supervised learning, we must decide how we're going to represent **functions/hypotheses *h*** in a computer.

Recall: Building an ML Algorithm (II)



Model / Hypothesis:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

θ_i's: parameters

Cost Function:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

→ Minimize J(θ) in order to obtain the coefficients θ.

Recall: Building an ML Algorithm (III)

All Models are wrong, but some models are useful – (Box & Draper (1987), p.424)

In General: Machine learning (e.g., supervised) in 3 Steps:

- Choose a **model** $h(x|\theta)$.
- Define a **cost function** $J(\theta|x)$.
- **Optimization procedure** to find θ^* that minimizes $J(\theta)$.

Computationally, we need:
data, linear algebra, statistics tools, and optimization routines.

Recall – Predictions using noise-free observations

Suppose we observe a training set

$$D = \{(x_i, f_i), i = 1 : N\}$$

where $\mathbf{f_i = f(x_i)}$ **is the noise-free observation** of the function evaluated at x_i.

Given a test set $\mathbf{X}_*$ of size $N \times D$, we want to predict the function outputs $\mathbf{f}_*$.

If we ask the GP to predict f(x) for a value of x that it has already seen, we want the GP to return the answer f(x) with no uncertainty.

→ In other words, it should act as an interpolator of the training data. This will only happen if we assume the observations are noiseless.

Recall: Joint Gaussian distributions

see, e.g., Rasmussen et al. (2005), Murphy (2012)

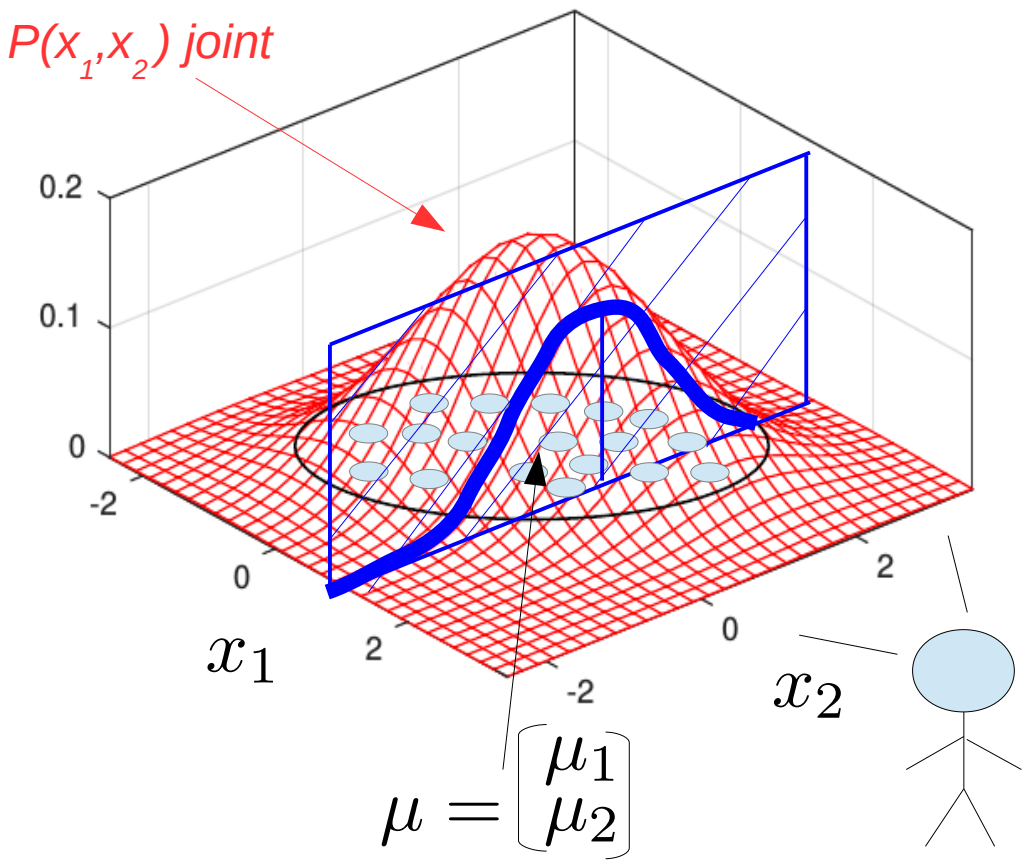
$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \sim N\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right)$$

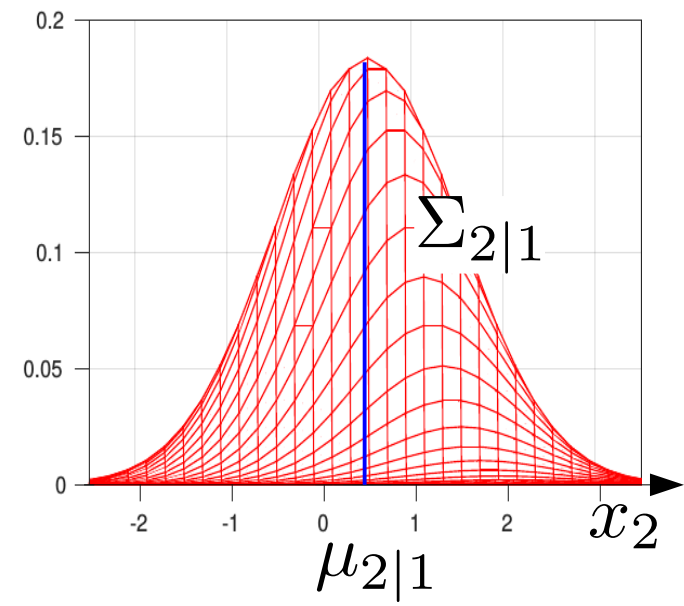
Mean

Covariance

Conditional distribution

$$P(x_2 | X_1 = x_1)$$





Recall: From Joint to Conditional distributions

see, e.g., Murphy (2012), chapter 4.

Theorem 4.3.1 (Marginals and conditionals of an MVN). *Suppose* $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$ *is jointly Gaussian with parameters*

$$\boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix}, \quad \boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1} = \begin{pmatrix} \boldsymbol{\Lambda}_{11} & \boldsymbol{\Lambda}_{12} \\ \boldsymbol{\Lambda}_{21} & \boldsymbol{\Lambda}_{22} \end{pmatrix} \tag{4.67}$$

Two "blocks" of vectors

Then the marginals are given by

$$\begin{aligned} p(\mathbf{x}_1) &= \mathcal{N}(\mathbf{x}_1 | \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11}) \\ p(\mathbf{x}_2) &= \mathcal{N}(\mathbf{x}_2 | \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22}) \end{aligned} \tag{4.68}$$

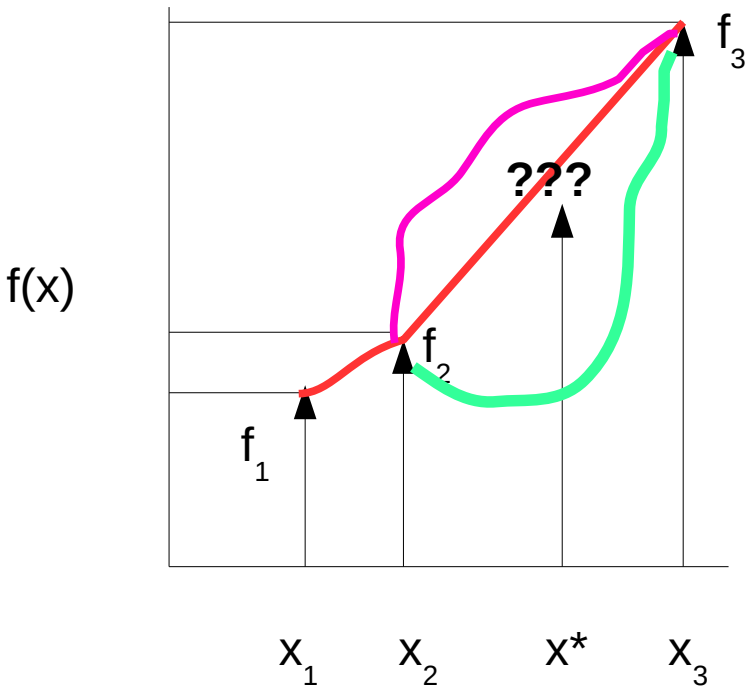
and the posterior conditional is given by

$$\boxed{\begin{aligned} p(\mathbf{x}_1 | \mathbf{x}_2) &= \mathcal{N}(\mathbf{x}_1 | \boldsymbol{\mu}_{1|2}, \boldsymbol{\Sigma}_{1|2}) \\ \boldsymbol{\mu}_{1|2} &= \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2) \\ &= \boldsymbol{\mu}_1 - \boldsymbol{\Lambda}_{11}^{-1}\boldsymbol{\Lambda}_{12}(\mathbf{x}_2 - \boldsymbol{\mu}_2) \\ &= \boldsymbol{\Sigma}_{1|2}\left(\boldsymbol{\Lambda}_{11}\boldsymbol{\mu}_1 - \boldsymbol{\Lambda}_{12}(\mathbf{x}_2 - \boldsymbol{\mu}_2)\right) \\ \boldsymbol{\Sigma}_{1|2} &= \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21} = \boldsymbol{\Lambda}_{11}^{-1} \end{aligned}} \tag{4.69}$$

This Theorem allows you to go from joint to conditional distributions.

Observations → Interpolation (II)

We assume that **f's (the height) are Gaussian distributed**, with **zero – mean** and some **covariance matrix K**.



$$\begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{11}, K_{12}, K_{13} \\ K_{21}, K_{22}, K_{23} \\ K_{31}, K_{32}, K_{33} \end{bmatrix} \right)$$

Note: f_1 and f_2 should probably be more correlated, as they are nearby (compared to f_1 and f_3), e.g.,

$$\sim N\left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1, 0.7, 0.2 \\ 0.7, 1, 0.6 \\ 0.2, 0.6, 1 \end{bmatrix} \right)$$

Covariance matrix **constructed** by some "**measure of similarity**", i.e., a **kernel function** (parametric ansatz), such as "squared exponential". Parameters can be obtained e.g. via MLE (later).

$$\kappa(x, x') = \sigma_f^2 \exp(-\frac{1}{2\ell^2}(x - x')^2)$$

σ_f^2 – controls vertical variation.

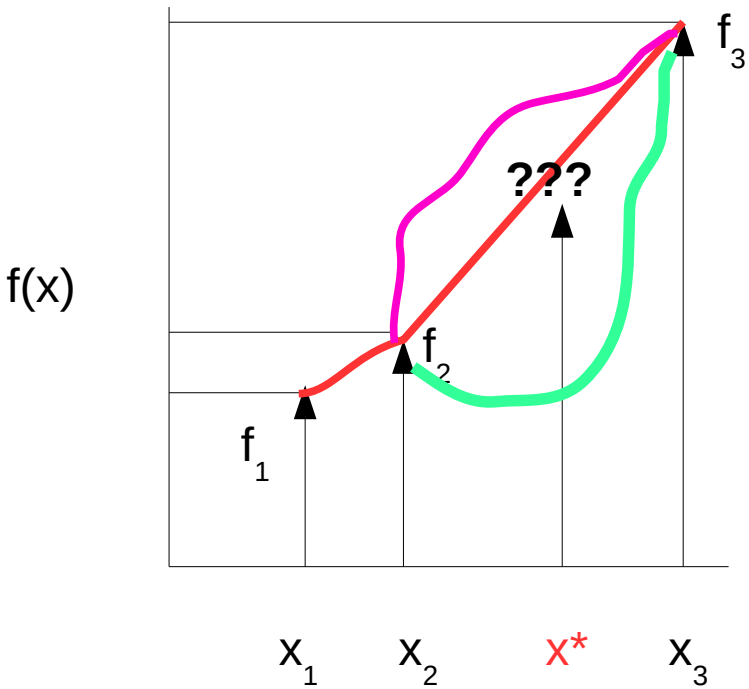
ℓ – controls horizontal length scale.

Remember: Observations → Interpolation

Given data D = { (x_1,f_1), (x_2,f_2), (x_3,f_3)} → **$f(x^*) = f_*$** ?

→ Assume $f \sim N(0, K(\cdot,\cdot))$

→ Assume $f(x^*) \sim N(0, K(x^*,x^*))$



3d-Covariance K from the training data

$$\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_* \end{pmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{11}, K_{12}, K_{13}, K_{1*} \\ K_{21}, K_{22}, K_{23}, K_{2*} \\ K_{31}, K_{32}, K_{33}, K_{3*} \\ K_{*1}, K_{*2}, K_{*3}, K_{**} \end{bmatrix} \right)$$

→ **Joint distribution over f and f_* .**

→ **We need the conditional of f_* given f.**

→ In this example, we "cut" in 3 dimensions.

→ What is left is a 1-dimensional Gaussian, i.e., the Gaussian for f_*

$$K(x_1, x_*) = K_{1*}$$

Recall – Predictions using noise-free observations (II)

By definition of the GP, the joint distribution has the following form:

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{pmatrix}, \begin{pmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right)$$

where $\mathbf{K} = \kappa(\mathbf{X}, \mathbf{X})$ is $N \times N$, $\mathbf{K}_* = \kappa(\mathbf{X}, \mathbf{X}_*)$

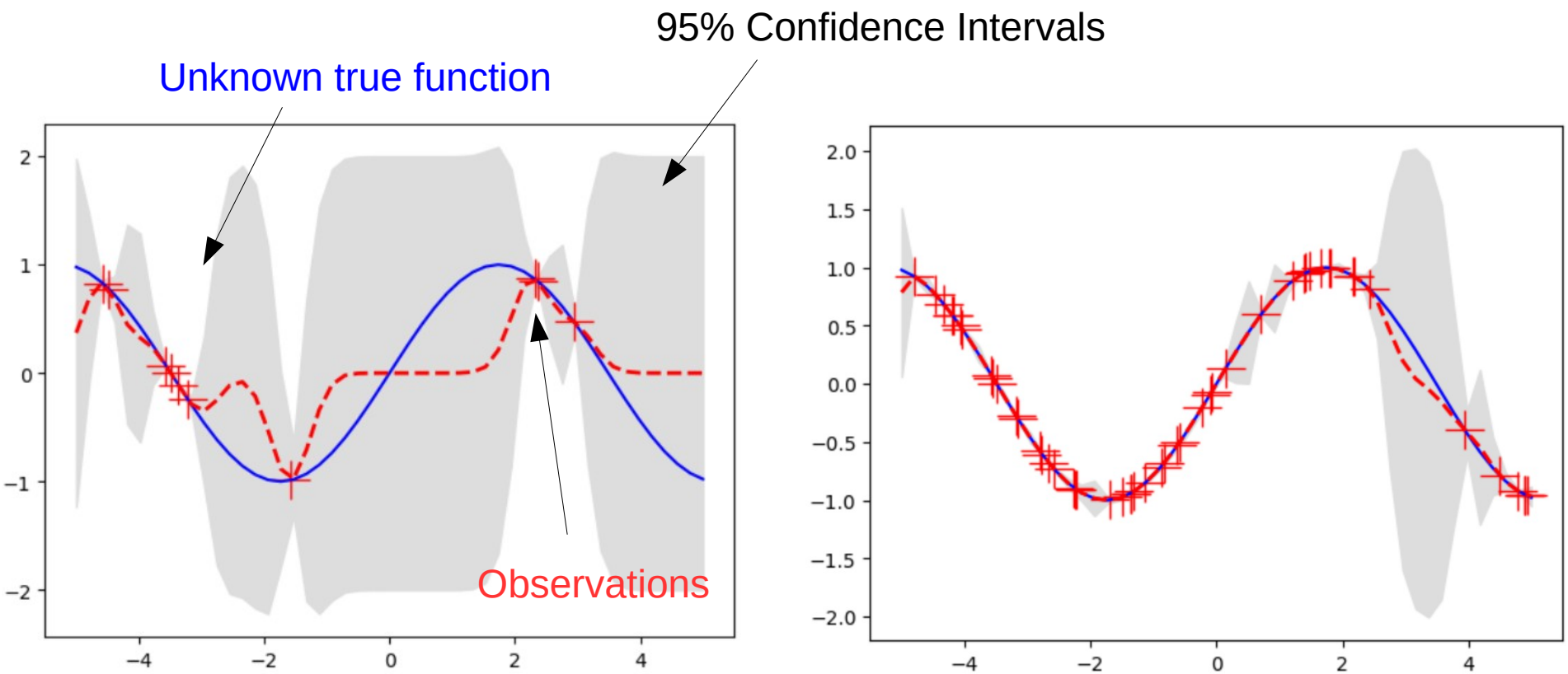
and where $\mathbf{K}_{**} = \kappa(\mathbf{X}_*, \mathbf{X}_*)$ is $N_* \times N_*$

By the standard rules for conditioning Gaussians, the posterior has the following form

$$\begin{aligned} p(\mathbf{f}_* | \mathbf{X}_*, \mathbf{X}, \mathbf{f}) &= \mathcal{N}(\mathbf{f}_* | \boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*) \\ \boldsymbol{\mu}_* &= \boldsymbol{\mu}(\mathbf{X}_*) + \mathbf{K}_*^T \mathbf{K}^{-1} (\mathbf{f} - \boldsymbol{\mu}(\mathbf{X})) \\ \boldsymbol{\Sigma}_* &= \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{K}_* \end{aligned}$$

Illustration of noiseless GPR prediction

Note: if you don't fix the seed, these pictures vary every time you run of the code.



10 Training Points **50 Training Points**

We see that the model perfectly interpolates the training data, and that the predictive uncertainty increases as we move further away from the observed data.

cf. global_solution_yale19/Lecture_5/code/1d_gp_example.py

Illustration of noiseless GPR prediction (II)

- We use a squared exponential kernel, aka Gaussian kernel or RBF kernel.
- In *1d*, this is given by

$$\kappa(x, x') = \sigma_f^2 \exp(-\frac{1}{2\ell^2}(x - x')^2)$$

- Here *l* controls the horizontal length scale over which the function varies, and σ_f controls the vertical variation.
- On the right panel, we showed predictions from the posterior, $p(f_* | X_*, X, f)$.
- We see that the model perfectly interpolates the training data, and that the predictive uncertainty increases as we move further away from the observed data.

The parameters in the Kernel

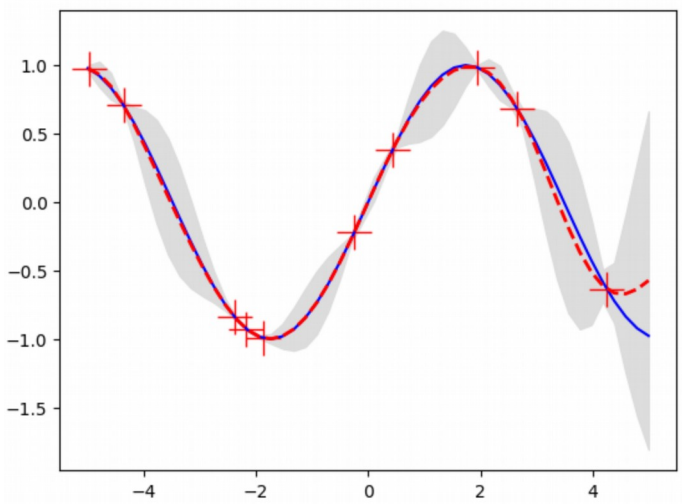
cf. global_solution_yale19/Lecture_5/code/1d_gp_example.py

$$\kappa(x, x') = \sigma_f^2 \exp(-\frac{1}{2\ell^2}(x - x')^2)$$

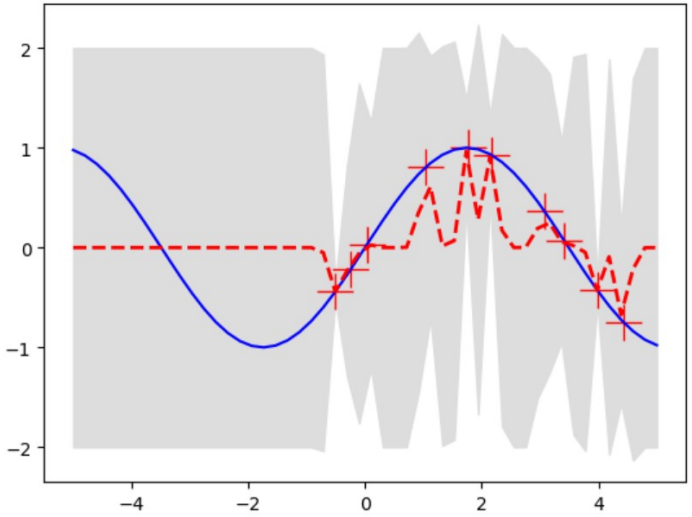
Let $\sigma_f^2 = 1$

→ **Tuning the parameters by hand is not a good idea in general (in particular in high-dimensional settings)**.

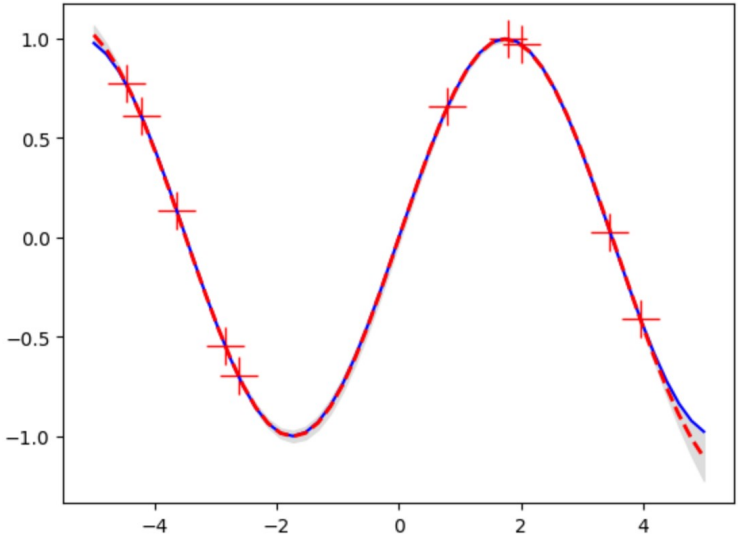
***l*² = 1.0**



***l*² = 0.01**



***l*² = 10.0**



GPR with noisy data

- In empirical setups, measurement noise may arise from our inability to control all the influential factors or from irreducible (aleatory) uncertainties.

- In computer simulations, measurement uncertainty may stem from quasi-random stochasticity, or chaotic behavior.

- Now let us consider the case where what we observe is a noisy version of the underlying function

$$y = f(x) + \epsilon, \text{ where } \epsilon \sim \mathcal{N}(0, \sigma_y^2)$$

GPR with noisy data (II)

- In this case (presence of noise), the model is not required to interpolate the data, but it must come "close" to the observed data.

- The covariance of the observed noisy responses is

$$\mathrm{cov}\left[y_p, y_q\right] = \kappa(\mathbf{x}_p, \mathbf{x}_q) + \sigma_y^2 \delta_{pq}$$

where $\delta_{pq} = \mathbb{I}(p = q)$

- The second matrix is diagonal because we assumed the noise terms were independently added to each observation.

The GPR with noisy data (III)

- The joint density of the observed data and the latent, noise-free function on the test points is given by

Noise in the diagonal, rest is as before.

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{pmatrix} \mathbf{K}_y & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix}\right)$$

Latent function.

- where we are assuming the mean is zero, for notational simplicity.

- Hence the posterior predictive density is

$$\begin{aligned} p(\mathbf{f}_*|\mathbf{X}_*, \mathbf{X}, \mathbf{y}) &= \mathcal{N}(\mathbf{f}_*|\boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*) \\ \boldsymbol{\mu}_* &= \mathbf{K}_*^T \mathbf{K}_y^{-1} \mathbf{y} \\ \boldsymbol{\Sigma}_* &= \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}_y^{-1} \mathbf{K}_* \end{aligned}$$

Prediction at a single test point

In the case of a single test input, this simplifies as follows

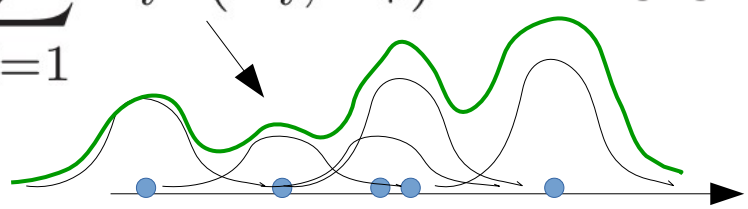
$$p(f_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) \quad = \quad \mathcal{N}(f_*|\mathbf{k}_*^T\mathbf{K}_y^{-1}\mathbf{y}, k_{**} - \mathbf{k}_*^T\mathbf{K}_y^{-1}\mathbf{k}_*)$$

where $\mathbf{k}_* \;=\; [\kappa(\mathbf{x}_*, \mathbf{x}_1), \ldots, \kappa(\mathbf{x}_*, \mathbf{x}_N)]$

and where $k_{**} \;=\; \kappa(\mathbf{x}_*, \mathbf{x}_*)$ (=1)

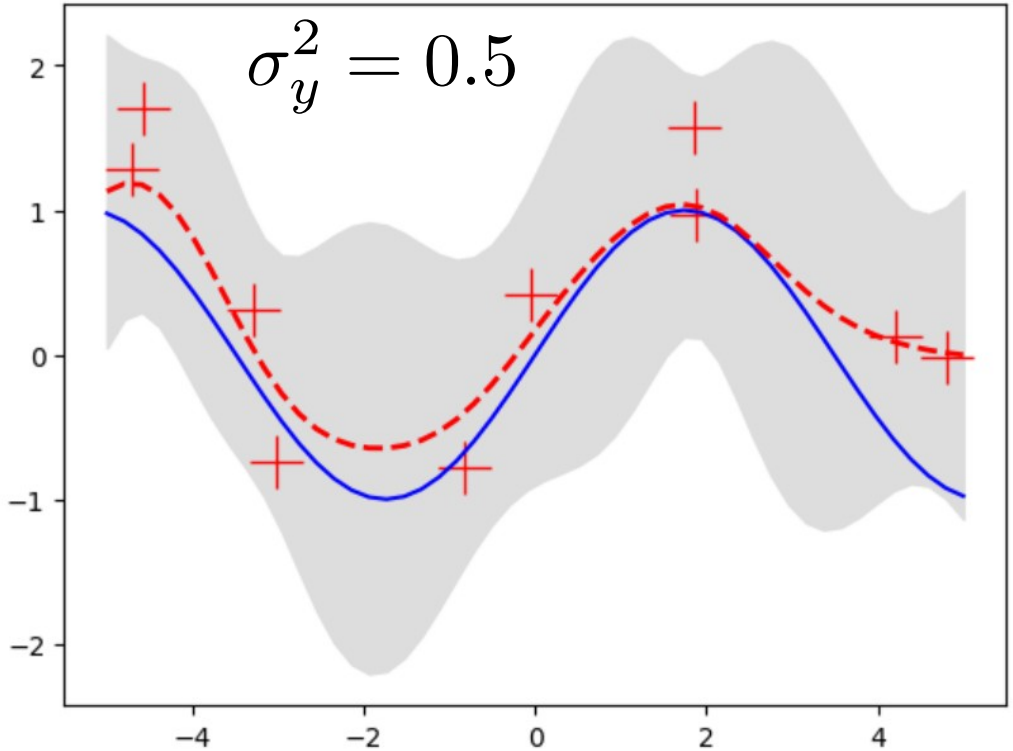
Again, we can write the posterior mean as expansion of basis functions

$$\overline{f}_* = \underbrace{\mathbf{k}_*^T}_{1 \times N}\underbrace{\mathbf{K}_y^{-1}}_{N \times N}\underbrace{\mathbf{y}}_{N \times 1} = \sum_{i=1}^{N} \alpha_i \kappa(\mathbf{x}_i, \mathbf{x}_*) \quad \text{where } \boldsymbol{\alpha} = \underbrace{\mathbf{K}_y^{-1}\mathbf{y}}_{\text{from training data}}$$



Some Plots

cf. global_solution_yale19/Lecture_5/code/1d_gp_example.py



- Even in the regions where you have data, there is still uncertainty.
- In the noise-free version of GPR, the uncertainty is 0 at observation points.
- But we still have the same properties as before: where we have data, we are more certain compared to the case where we have no data.

Noise improves numerical stability

- It is common to use small noise even if there is not any in the data.
- Cholesky fails when covariance is close to being semi-positive definite.
- Adding a small noise improves numerical stability.
- It is known as the “jitter” or as the “nugget” in this case.

“Learning” the kernel parameters

- To estimate the kernel parameters, we could use exhaustive search over a discrete grid of values, with validation loss as an objective, but this can be quite slow.
- Here we consider an empirical Bayes approach, which will allow us to use continuous optimization methods, which are much faster.
- In particular, we will maximize the marginal likelihood.

"Learning" the kernel parameters (II)

Marginal likelihood $p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}|\mathbf{f},\mathbf{X})p(\mathbf{f}|\mathbf{X})d\mathbf{f}$

Since $p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|\mathbf{0},\mathbf{K})$

and $p(\mathbf{y}|\mathbf{f}) = \prod_i \mathcal{N}(y_i|f_i,\sigma_y^2)$

the (log-) marginal likelihood is given by

$$\boxed{\log p(\mathbf{y}|\mathbf{X}) = \log \mathcal{N}(\mathbf{y}|\mathbf{0},\mathbf{K}_y) = -\frac{1}{2}\mathbf{y}\mathbf{K}_y^{-1}\mathbf{y} - \frac{1}{2}\log|\mathbf{K}_y| - \frac{N}{2}\log(2\pi)}$$

1st term: data fit term
2nd term: a model complexity term
3rd term: a constant.

Maximizing the the marginal likelihood

- Let the kernel parameters (also called hyper-parameters) be denoted by $\boldsymbol{\theta}$

- One can show that the following holds.

$$\begin{aligned}\frac{\partial}{\partial \theta_j} \log p(\mathbf{y}|\mathbf{X}) &= \frac{1}{2}\mathbf{y}^T \mathbf{K}_y^{-1} \frac{\partial \mathbf{K}_y}{\partial \theta_j} \mathbf{K}_y^{-1}\mathbf{y} - \frac{1}{2}\mathrm{tr}(\mathbf{K}_y^{-1}\frac{\partial \mathbf{K}_y}{\partial \theta_j}) \\ &= \frac{1}{2}\mathrm{tr}\left((\boldsymbol{\alpha}\boldsymbol{\alpha}^T - \mathbf{K}_y^{-1})\frac{\partial \mathbf{K}_y}{\partial \theta_j}\right)\end{aligned}$$

where $\boldsymbol{\alpha} = \mathbf{K}_y^{-1}\mathbf{y}$

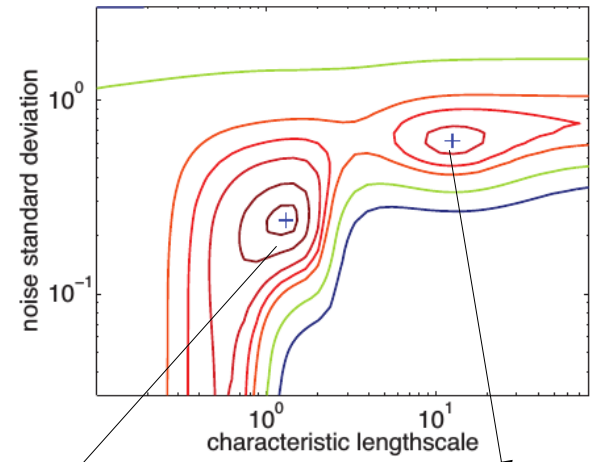
Computational complexity:

- It takes $O(N^3)$ time to compute $\mathbf{K}_y^{-1}$

- $O(N^2)$ time per hyper-parameter to compute the gradient.

Careful: Different optima correspond to different interpretations/believes

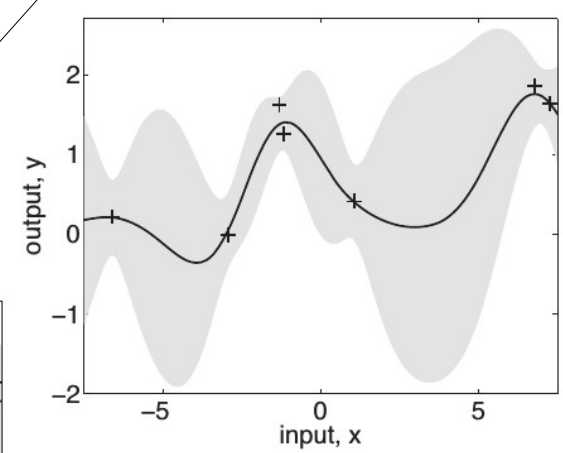
Fig. 5.5 of (Rasmussen and Williams 2006).

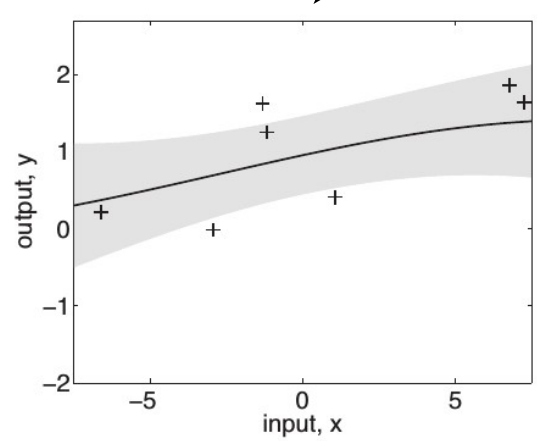


- We use the SE kernel

$$\kappa_y(x_p, x_q) = \sigma_f^2 \exp(-\frac{1}{2\ell^2}(x_p - x_q)^2) + \sigma_y^2 \delta_{pq}$$

- with $\sigma_f^2 = 1$
- We plot $\log p(\mathbf{y}|\mathbf{X}, \ell, \sigma_y^2)$ (where X and y are the 7 data points shown) as we vary ℓ and σ_y^2.
- The two local optima are indicated by +.
- The bottom left optimum corresponds to a low-noise, short-length scale solution.
- The top right optimum corresponds to a high-noise, long-length scale solution.
- With only 7 data points, there is not enough evidence to confidently decide which is more reasonable.





An example: noise and optimization

https://scikit-learn.org/stable/auto_examples/gaussian_process/plot_gpr_noisy_targets.html
global_solution_yale19/Lecture_5/code/GPR_scikit_noise.py

```
import numpy as np
from matplotlib import pyplot as plt

from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF, ConstantKernel as C

np.random.seed(1)


def f(x):
    """The function to predict."""
    return x * np.cos(x)*np.sin(x)

# ----------------------------------------------------------------------
# Mesh the input space for evaluations of the real function, the prediction and
# its MSE
x = np.atleast_2d(np.linspace(0, 10, 1000)).T

# Instantiate a Gaussian Process model
kernel = C(1.0, (1e-3, 1e3)) * RBF(10, (1e-2, 1e2))

# now the noisy case
X = np.linspace(0.1, 9.9, 20)
X = np.atleast_2d(X).T

# Observations and noise
y = f(X).ravel()
dy = 0.5 + 1.0 * np.random.random(y.shape)
noise = np.random.normal(0, dy)
y += noise

# Instantiate a Gaussian Process model
gp = GaussianProcessRegressor(kernel=kernel, alpha=dy ** 2,
                              n_restarts_optimizer=10)

# Fit to data using Maximum Likelihood Estimation of the parameters
gp.fit(X, y)

# Make the prediction on the meshed x-axis (ask for MSE as well)
y_pred, sigma = gp.predict(x, return_std=True)

# Plot the function, the prediction and the 95% confidence interval based on
# the MSE
plt.figure()
plt.plot(x, f(x), 'r:', label=u'$f(x) = x\,\sin(x)$')
plt.errorbar(X.ravel(), y, dy, fmt='r.', markersize=10, label=u'Observations')
plt.plot(x, y_pred, 'b-', label=u'Prediction')
plt.fill(np.concatenate([x, x[::-1]]),
         np.concatenate([y_pred - 1.9600 * sigma,
                        (y_pred + 1.9600 * sigma)[::-1]]),
         alpha=.5, fc='b', ec='None', label='95% confidence interval')
plt.xlabel('$x$')
plt.ylabel('$f(x)$')
plt.ylim(-10, 20)
plt.legend(loc='upper left')

plt.show()
```

A multi-d example

global_solution_yale19/Lecture_5/code/scikit_multi-d.py

```
import numpy as np
from matplotlib import pyplot as plt
import cPickle as pickle
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF, ConstantKernel as C


np.random.seed(1)


# Test function
def f(x):
    """The 2d function to predict."""
    return np.sin(x[0]) * np.cos(x[1])


# generate training data
n_sample = 100  #points
dim = 2        #dimensions

X = np.random.uniform(-1., 1., (n_sample, dim))
y = np.sin(X[:, 0:1]) * np.cos(X[:, 1:2]) + np.random.randn(n_sample, 1) * 0.005

# Instantiate a Gaussian Process model
kernel = C(1.0, (1e-3, 1e3)) * RBF(10, (1e-2, 1e2))
gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)

# Fit to data using Maximum Likelihood Estimation of the parameters
gp.fit(X, y)

# Make the prediction on the meshed x-axis / training points
y_pred, sigma = gp.predict(X, return_std=True)

#Compute MSE
mse = 0.0
n_sample_test=50
Xtest1 = np.random.uniform(-1., 1., (n_sample_test, dim))
y_pred1, sigma = gp.predict(Xtest1, return_std=True)
for g in range(len(Xtest1)):
    delta = abs(y_pred1[g] - f(Xtest1[g]))
    mse +=  delta

mse = mse/len(y_pred)
print("......................")
print(" The MSE is ", mse[0])
print("......................")
```

A multi-d example (II)

global_solution_yale19/Lecture_5/code/scikit_multi-d.py

```
#-----------------------------------------------------------------------

# Important -- save the model to a file
with open('2d_model.pcl', 'wb') as fd:
    pickle.dump(gp, fd, protocol=pickle.HIGHEST_PROTOCOL)
    print("data written to disk")


# Load the model and do predictions
with open('2d_model.pcl', 'rb') as fd:
    gm = pickle.load(fd)
    print("data loaded from disk")

# generate training data
n_test = 50
dim = 2
Xtest = np.random.uniform(-1., 1., (n_test, dim))
y_pred_test, sigma_test = gm.predict(Xtest, return_std=True)

MSE2 = 0
for a in range(len(Xtest)):
    delta = abs(y_pred_test[a] - f(Xtest[a]))
    MSE2 +=delta


MSE2 = MSE2/len(Xtest)
print("......................")
print(" The MSE 2 is ", MSE2[0])
print("......................")
#-----------------------------------------------------------------------
```

More on Kernels

http://www.gaussianprocess.org/gpml/chapters/RW4.pdf
See also e.g. “The Kernel Cookbook”: https://www.cs.toronto.edu/~duvenaud/cookbook/
https://scikit-learn.org/stable/modules/gaussian_process.html#kernels-for-gaussian-processes

- Our prior beliefs about the response are encoded in our choice of the mean and covariance functions.
- The choice of an appropriate kernel is based on assumptions such as smoothness and likely patterns to be expected in the data.
- A sensible assumption is usually that the correlation between two points decays with distance between the points according to some power function.
- The choice of kernel determines almost all the generalization properties of a GP model.
- **You are the expert on your modeling problem - so you're the person best qualified to choose the kernel!**

Stationary versus non-stationary Kernels

Two categories of kernels can be distinguished:

- **Stationary kernels**:
  They depend only on the distance of two data points and not on their absolute values
  $k(x_i, x_j) = k(d(x_i, x_j))$ and are thus invariant to translations in the input space

  Stationary kernels can further be subdivided into isotropic and anisotropic kernels, where isotropic kernels are also invariant to rotations in the input space.

- **Non-stationary kernels**:
  They depend also on the specific values of the data points.

Squared Exponential Kernel

The SE kernel has become the **de-facto default kernel** for GPs.

$$k_{\mathrm{SE}}(x, x') = \sigma^2 \exp\left(-\frac{(x - x')^2}{2\ell^2}\right)$$

This is probably because it has some nice properties:

- It is universal, and you can integrate it against most functions that you need to.
- Every function in its prior has infinitely many derivatives.
- It also has only two parameters:
  - The **lengthscale ℓ** determines the length of the 'wiggles' in your function. In general, **you won't be able to extrapolate more than ℓ units away from your data**.
  - The output **variance σ^2** determines the average distance of your function away from its mean. Every kernel has this parameter out in front; it's just a scale factor.

Pitfalls for the SE kernel

- Most people who set up a GP regression (or classification) model end up using the SE kernel.

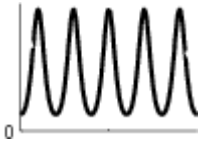
- They are a quick-and-dirty solution that will probably work pretty well for interpolating smooth functions when N is a multiple of D, and when there are no 'kinks' in your function.

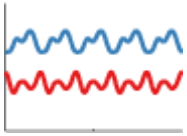
- If your function happens to have a discontinuity or is discontinuous in its first few derivatives (for example, the abs() function), then either your **length-scale** will end up being **extremely short**, and your posterior mean will become zero almost everywhere, or your posterior mean will have 'ringing' effects.

- Even if there are no hard discontinuities, the length-scale will usually end up being determined by the smallest 'wiggle' in your function - so you might end up failing to extrapolate in smooth regions if there is even **a small non-smooth** region in your data.

- If your data is more than two-dimensional, it may be hard to detect this problem. One indication is if the length-scale chosen by maximum marginal likelihood never stops becoming smaller as you add more data. This is a classic sign of **model misspecification**.

Periodic Kernel





$$k_{\mathrm{Per}}(x, x') = \sigma^2 \exp\left(-\frac{2\sin^2(\pi|x - x'|/p)}{\ell^2}\right)$$

- The periodic kernel allows one to model functions which repeat themselves exactly.

- Its parameters are easily interpretable:

  - The period ***p*** simply determines the **distance between repetitions** of the function.

  - The **length-scale ℓ** determines the length-scale function in the same way as in the SE kernel.

Matérn kernel

- The **Matérn kernel** is a stationary kernel and a generalization of the RBF kernel.
- It has an additional parameter ν which controls the smoothness of the resulting function. It is parameterized by a length-scale parameter $\ell > 0$, which can either be a scalar (isotropic variant of the kernel) or a vector with the same number of dimensions as the inputs (anisotropic variant of the kernel).
- The kernel is given by:

$$k(x_i, x_j) = \sigma^2 \frac{1}{\Gamma(\nu) 2^{\nu-1}} \left(\gamma \sqrt{2\nu} d(x_i/l, x_j/l) \right)^{\nu} K_\nu \left(\gamma \sqrt{2\nu} d(x_i/l, x_j/l) \right)$$

Matérn kernel (II)

- As $\nu \rightarrow 0$, the Matérn kernel converges to the RBF kernel.
- When $\nu = 1/2$, the Matérn kernel becomes identical to the absolute exponential kernel.

$$k_{\mathrm{mat}}(x, x') = \sigma^2 \left(1 + \sqrt{3} \sum_{i=1}^{l} \frac{(x_i - x_i')^2}{\ell_i^2}\right) \exp\left(-\sqrt{3} \sum_{i=1}^{l} \frac{(x_i - x_i')^2}{\ell_i^2}\right)$$

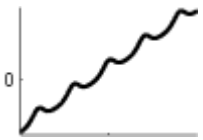
- This are popular choices for learning functions that are not infinitely differentiable (as assumed by the RBF kernel) but at least once ($\nu = 3/2$) (if $\nu = 5/2$, the kernel is twice differentiable).

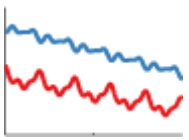
Combining/Adding Kernels

- Roughly speaking, adding two kernels can be thought of as an **OR** operation.

  → If you add together two kernels, then the resulting kernel will have high value if either of the two base kernels have a high value.

- **Linear plus Periodic Kernel**





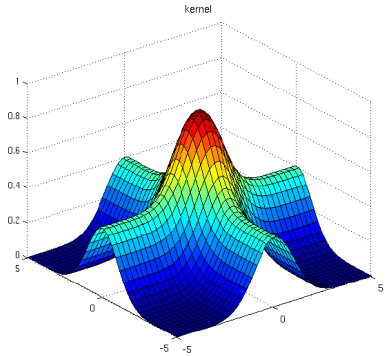
  - A linear kernel plus a periodic results in functions which are periodic with increasing mean as we move away from the origin.

- **Adding across dimensions**

  - Adding kernels which each depend only on a single input dimension results in a prior over functions which are a sum of one-dimensional functions, one for each dimension. That is, the function f(x,y) is simply a sum of two functions $f_x(x) + f_y(y)$

  - These kernels have the form:

$$k_{\text{additive}}(x, y, x', y') = k_x(x, x') + k_y(y, y')$$



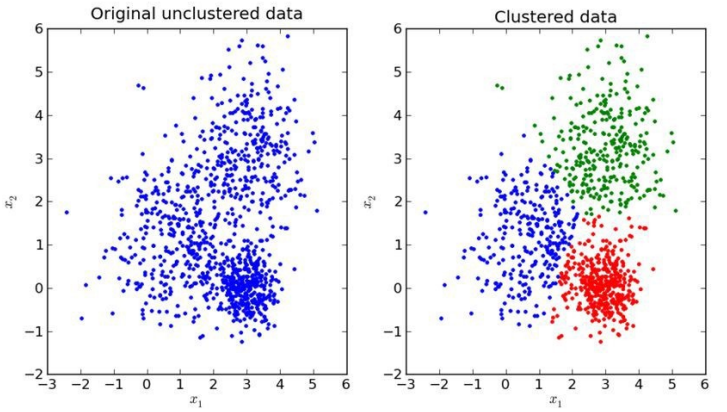
Automatically choosing Kernels

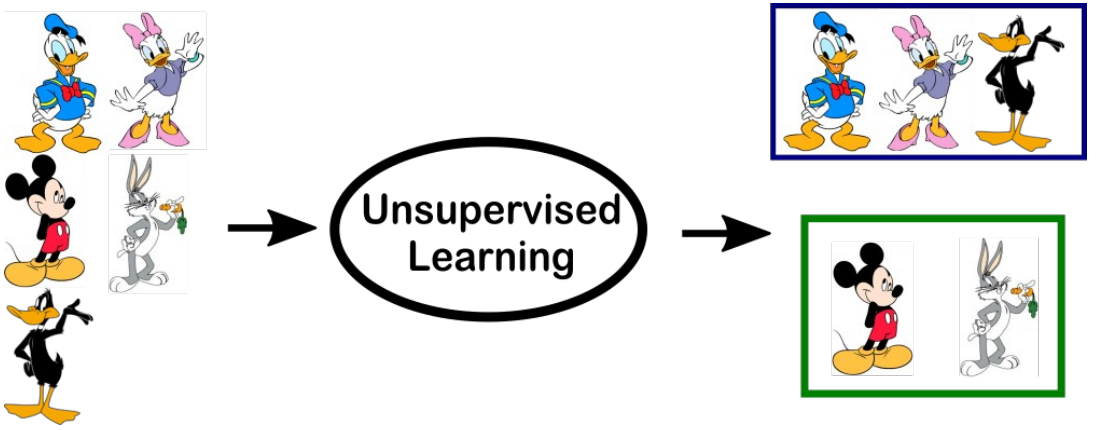
- Sometimes, it is not obvious which kernel is appropriate for your problem.
- In fact, you might decide that choosing the kernel is one of the main difficulties in doing inference
- Just as you don't know what the true parameters are, you also don't know what the true kernel is.
- Probably, you should try out a few different kernels at least, and compare their marginal likelihood on your training data.
- Automatic ways:
  - https://arxiv.org/abs/1302.4922
    (Structure Discovery in Nonparametric Regression through Compositional Kernel Search)
  - https://github.com/jamesrobertlloyd/gp-structure-search

II. Gaussian Mixture Models (GMM)

Recall: Unsupervised Machine Learning

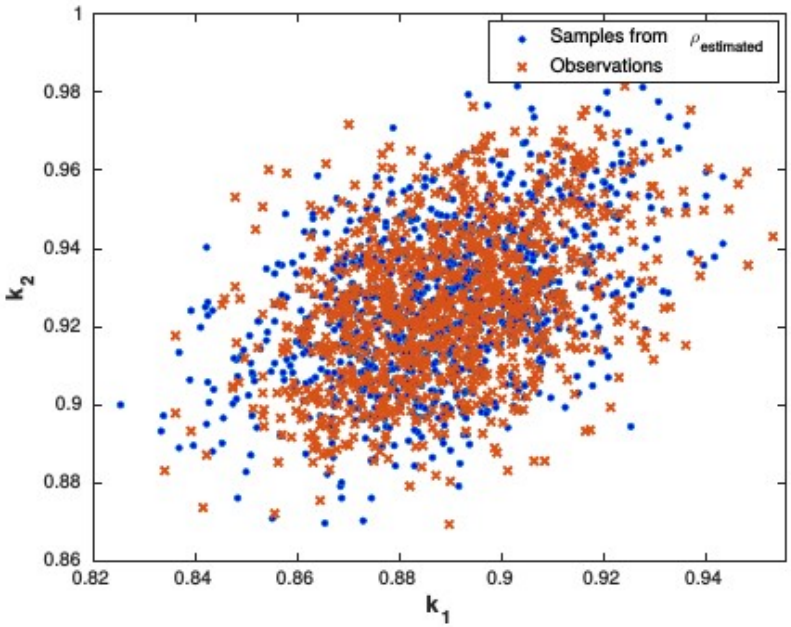
- Learning “what normally happens”.
- No output.
- Clustering: Grouping similar instances.
- Example applications:
  - Customer segmentation.
  - Image compression: Color quantization.
  - Bioinformatics: Learning motifs.

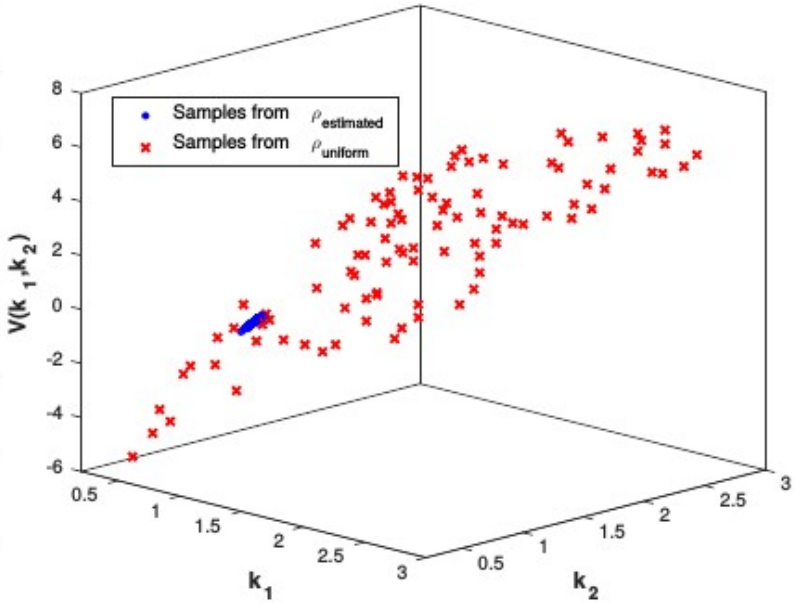




Motivation – Ergodic Sets

Den Haan and Marcet (1994), Judd et al. (2010, and Maliar and Maliar (2015), Scheidegger & Bilionis (2017)





$$V(\mathbf{k}) = \max_{\mathbf{I},\mathbf{c},\mathbf{l}} \left(u(\mathbf{c},\mathbf{l}) + \beta \mathbb{E}\left\{ V_{next}(\mathbf{k}^+) \right\} \right),$$

$$s.t.$$

$$k_j^+ = (1-\delta)\cdot k_j + I_j + \varepsilon_j, \quad j = 1,\ldots,D$$

$$\Gamma_j = \frac{\zeta}{2} k_j \left(\frac{I_j}{k_j} - \delta \right)^2, \quad j = 1,\ldots,D$$

$$\sum_{j=1}^{D} \left\{ c_j + I_j - \delta \cdot k_j \right\} = \sum_{j=1}^{D} \left\{ f(k_j,l_j) - \Gamma_j \right\},$$

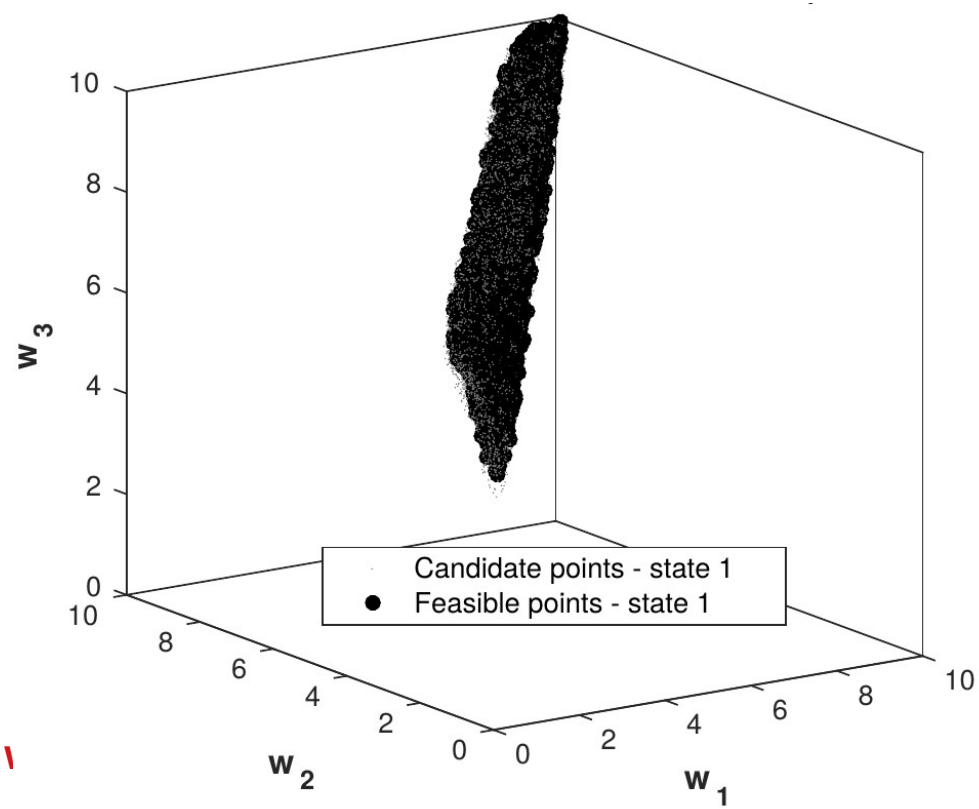
→ Simulate the Model (cf. Lecture 6)

Motivation – Feasible Sets

see, e.g., Abreu et al. (1986/1990), Fernandes & Phelan (2000)

See, e.g., dynamic incentive problems:

- Domain of interest is high-dimensional.
- Irregularly-shaped.
- You need to approximate Value- and Policy functions on such a domain.
- In the multi-d setting, if you use grid-based methods, you spend way more than 99% of your resources in vain.



→ Q: **How can we represent such sets?**

→ Q: **How can we generate "observations" from such sets?**

→ One way to do so are **Mixture of Gaussians** (see, e.g., Bishop (2006)).

→ Approximate the set in a probabilistic fashion.

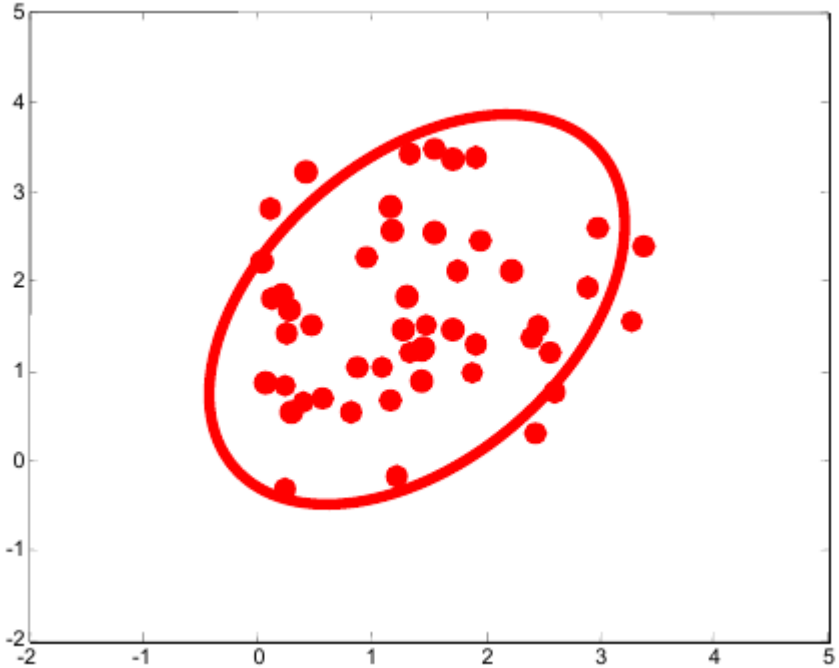
Recall Multivariate Gaussians

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

Maximum Likelihood estimates given by:

$$\hat{\mu} = \frac{1}{N} \sum_i x^{(i)}$$

$$\hat{\Sigma} = \frac{1}{N} \sum_i (x^{(i)} - \hat{\mu})^T (x^{(i)} - \hat{\mu})$$



Mixture of Gaussians – the basic idea

Consult e.g. the books by Bishop (2006) or Murphy (2012) for more details.

- Figure: plots of the 'old faithful' data.

- The blue curves show contours of constant probability density.

- On the left is a single Gaussian distribution which has been fitted to the data using maximum likelihood.

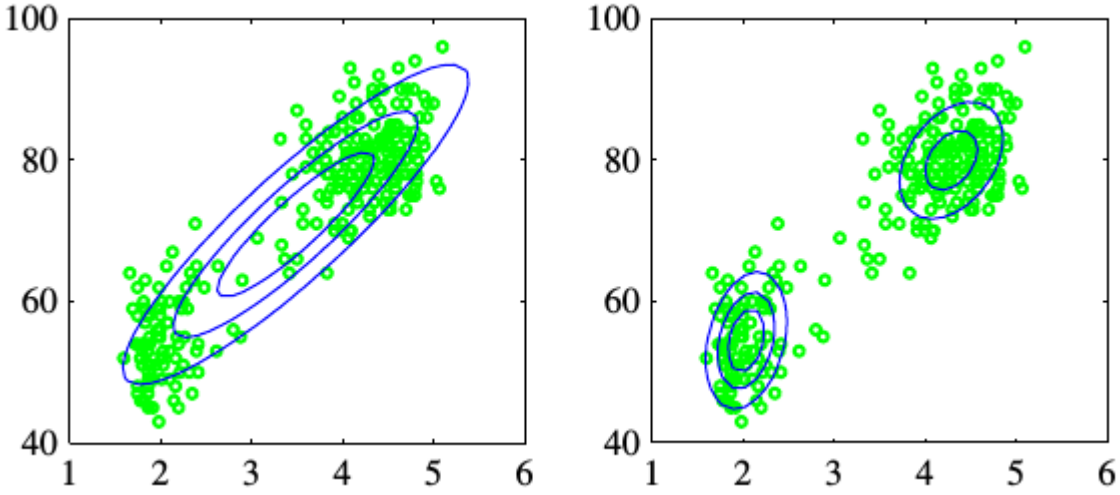
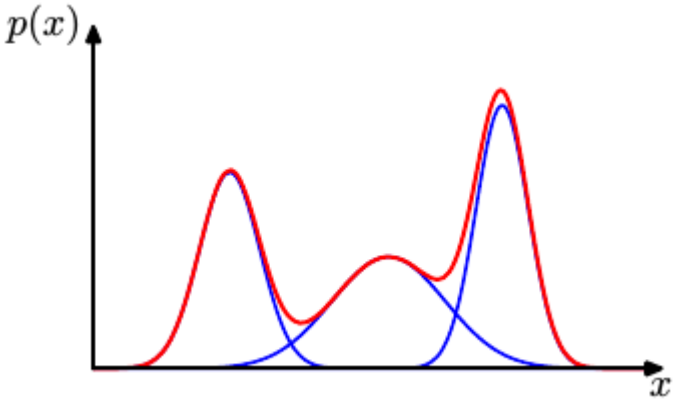


Fig. From Bishop (2006)

→ Note that this distribution fails to capture the two clumps in the data and indeed places much of its probability mass in the central region between the clumps where the data are relatively sparse.

- On the right the distribution is given by a linear combination of two Gaussians which has been fitted to the data, and which gives a better representation of the data.

GMM basics



- Example of a Gaussian mixture distribution p(x) in one dimension showing three Gaussians (each scaled by a coefficient) in blue and their sum in red.

→ Linear combinations of Gaussians can give rise to very complex densities.

→ By using a sufficient number of Gaussians and adjusting their means covariances as well as the coefficients in the linear combination, almost and density can be approximated with arbitrary accuracy.

→ k latent variables.

Superposition of Gaussians

- Formally, a GMM is: $$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \textbf{(A)}$$
- Each Gaussian density $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ is called a component of the mixture.
- It has its own mean μ_k and covariance Σ_k .
- π_k : mixing coefficients.

→ If we integrate both sides of **(A)** with respect to x, and note that both p(x) and the individual Gaussian components are normalized, one obtains:

$$\boxed{\sum_{k=1}^{K} \pi_k = 1. \qquad 0 \leqslant \pi_k \leqslant 1.}$$

$$\left(p(\mathbf{x}) \geqslant 0 \quad \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \geqslant 0 \right)$$

Superposition of Gaussians (II)

- We therefore see that the mixing coefficients satisfy the requirements to be probabilities.

- From the sum and product rules, the marginal density is given by

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(k)p(\mathbf{x}|k) \longleftrightarrow \pi_k = p(k)$$

- This is equivalent say that $\pi_k = p(k)$ as the prior probability of picking the k-th component.

- The density $N(x|\mu_k, \Sigma_k) = p(x|k)$ can be viewed as the probability of x conditioned on k.

→ One can think of p(x|k) as the pdf of cluster k (latent class labels).

Responsibilities: Posterior Distribution of Cluster Labels

- The posterior probabilities *p(k|x)* are also known as *responsibilities*

$$
\begin{aligned}
\gamma_k(\mathbf{x}) &\equiv p(k|\mathbf{x}) \\
&= \frac{p(k)p(\mathbf{x}|k)}{\sum_l p(l)p(\mathbf{x}|l)} \\
&= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_l \pi_l \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_l, \boldsymbol{\Sigma}_l)}
\end{aligned}
$$

- This represents the posterior probability that point i belongs to cluster k.
- This is sometimes known as soft clustering.
- We can represent the amount of uncertainty in the cluster assignment by using $1 - \max_k \gamma_k(\mathbf{x})$.

The likelihood

- The form of the Gaussian mixture distribution is governed by the parameters **π, μ** and **Σ**, where we have used the notation **π** ≡ $\{\pi_1, \ldots, \pi_k\}$, **μ** ≡ $\{\mu_1, \ldots, \mu_k\}$, **Σ** ≡ $\{\Sigma_1, \ldots \Sigma_k\}$.

- One way to set the values of these parameters is to use **maximum likelihood**.

- The log of the likelihood function is given by

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

where $X = \{x_1, \ldots, x_N\}$.

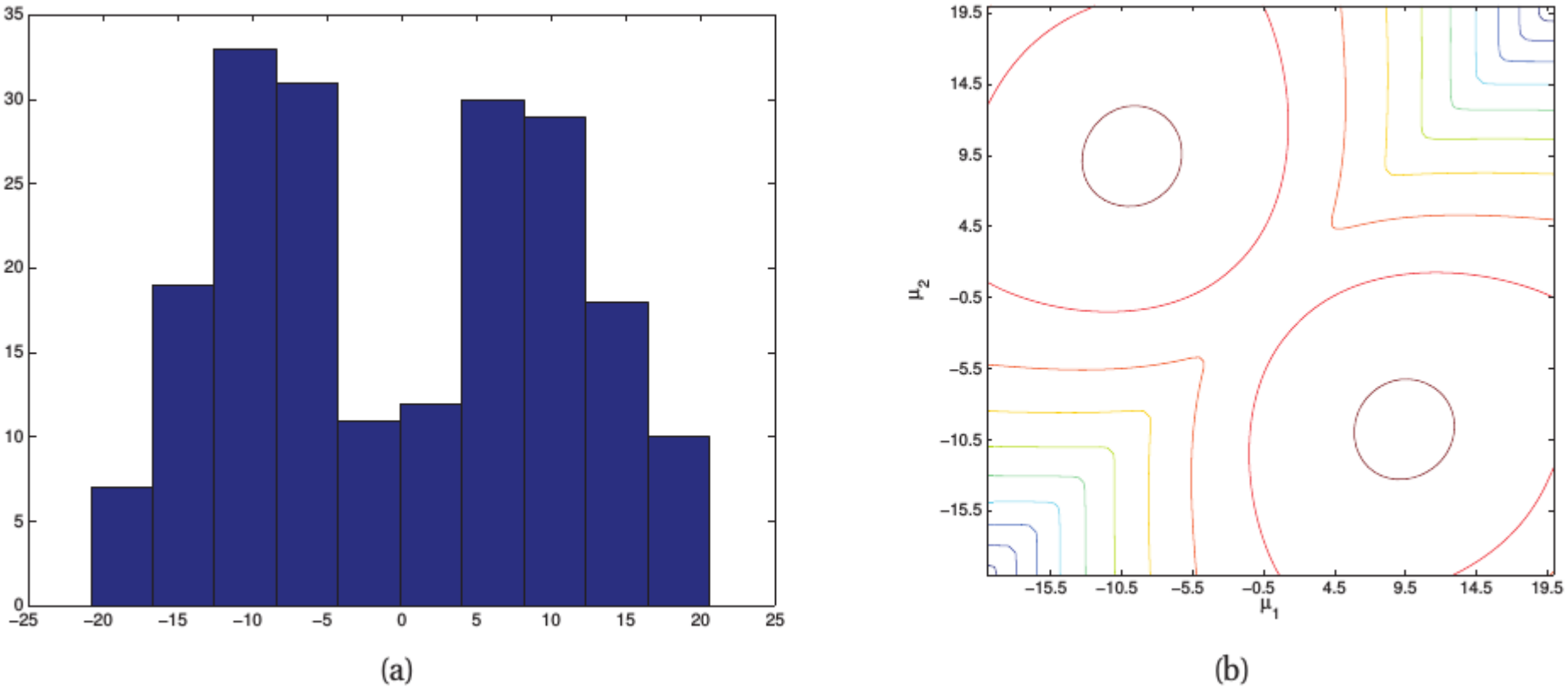
Problems with optimizing the likelihood

- The situation is now much more complex than with a single Gaussian, due to the presence of the summation over k inside the logarithm.
- As a result, the maximum likelihood solution for the parameters no longer has a closed-form analytical solution.
- One approach to maximizing the likelihood function is to use iterative numerical optimization techniques.
- Gradient methods could be used but are painful to implement.

→ Non-convex optimization problem! (multiple optima possible)

Unidentifiability

Fig. From Murphy (2012)



Left panel: N = 200 data points sampled from a mixture of 2 Gaussians in 1d, with $\pi_k = 0.5$, $\sigma_k = 5$, $\mu_1 = -10$ and $\mu_2 = 10$.

Right panel: Likelihood surface $p(D|\mu_1, \mu_2)$, with all other parameters set to their true values.

→ We see the two symmetric modes, reflecting the unidentifiability of the parameters.

Examplein 1d

Observations $x_1 \ldots x_n$

- K=2 Gaussians with unknown μ, σ^2
- Estimation trivial if we know the source of each observation

$$\mu_b = \frac{x_1 + x_2 + \ldots + x_{n_b}}{n_b}$$

$$\sigma_b^2 = \frac{(x_1 - \mu_1)^2 + \ldots + (x_n - \mu_n)^2}{n_b}$$

Example: Expectation Maximization in 1d

see, e..g., Dempster et al. (1977)

Observations $x_1 \ldots x_n$

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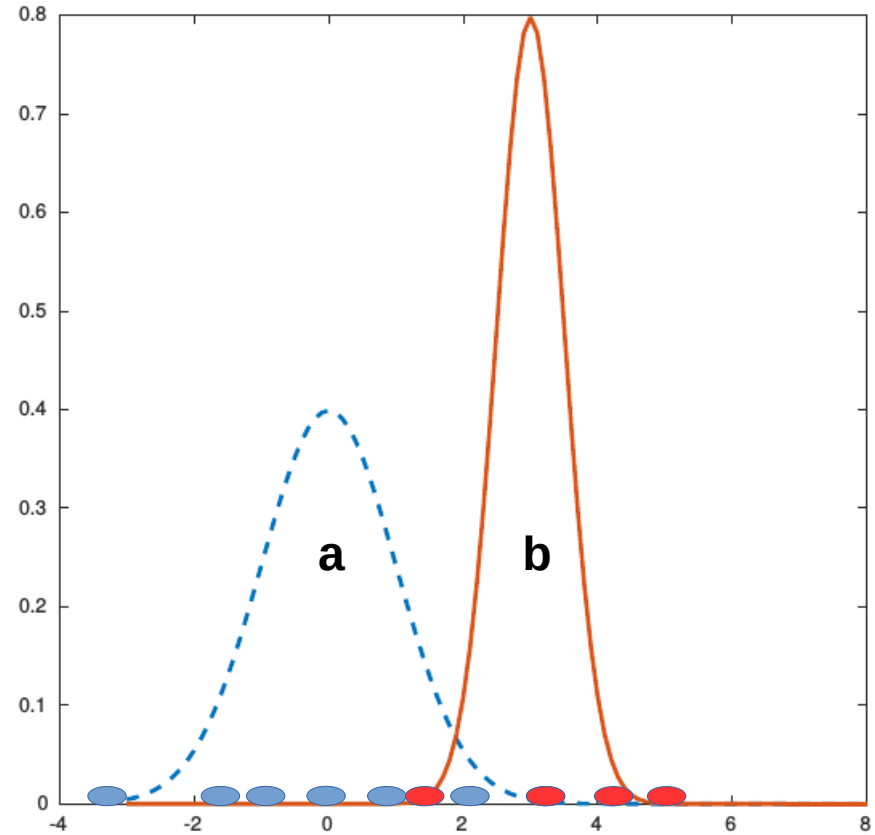


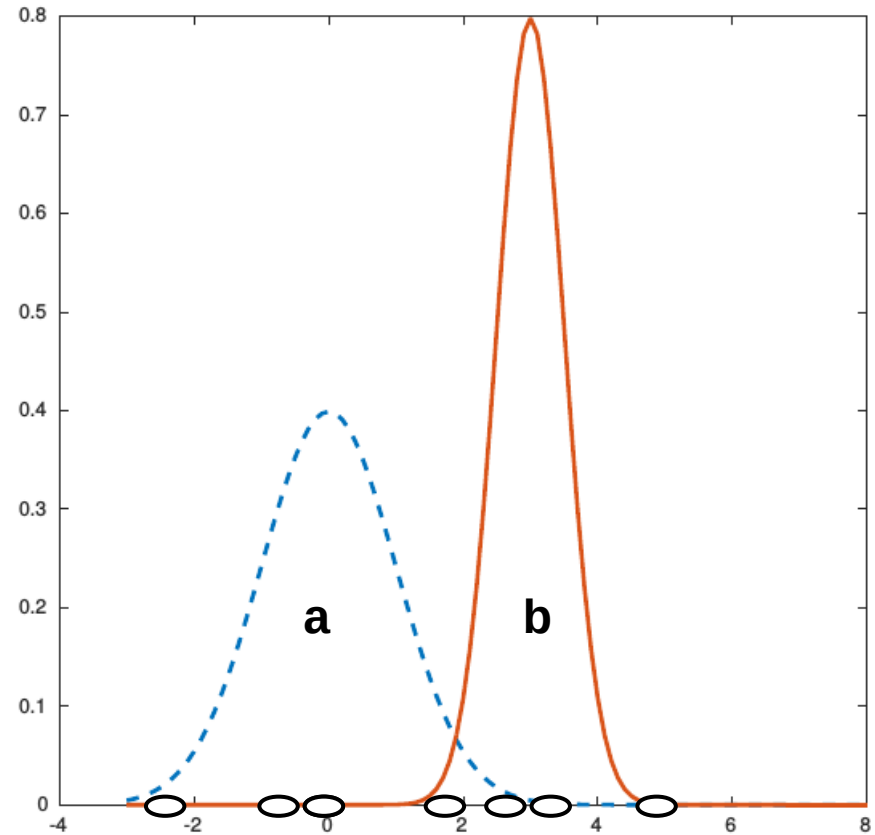
Example: Expectation Maximization in 1d (II)

- What if we don’t know the source?
- If we knew parameters of the Gaussians (μ, σ^2)

Example: Expectation Maximization in 1d (II)

- What if we don't know the source?
- If we knew parameters of the Gaussians (μ, σ^2)

→ can guess whether point is more likely to be a or b.

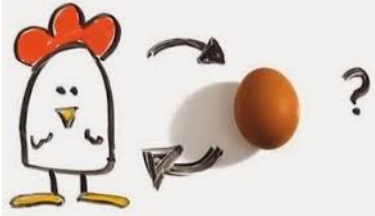


$$P(b \mid x_i) = \frac{P(x_i \mid b)P(b)}{P(x_i \mid b)P(b) + P(x_i \mid a)P(a)}$$

$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left(-\frac{(x_i - \mu_b)^2}{2\sigma_b^2}\right)$$

EM Algorithm (in 1d)

see, e..g., Dempster et al. (1977), Bishop (2006), Murphy (2012) and references therein for details.



A fundamental problem:

→ we need (μ_a, σ_a^2) and (μ_b, σ_b^2) to guess the source of the points.

→ we need to know the source to estimate (μ_a, σ_a^2) and (μ_b, σ_b^2).

EM algorithm

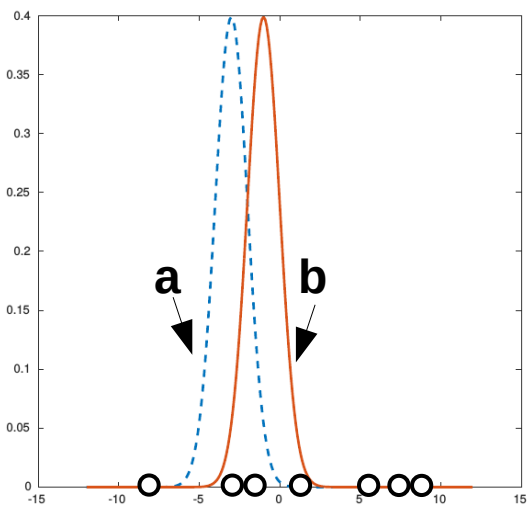
1. **start** with two randomly placed Gaussians (μ_a, σ_a^2) and (μ_b, σ_b^2).

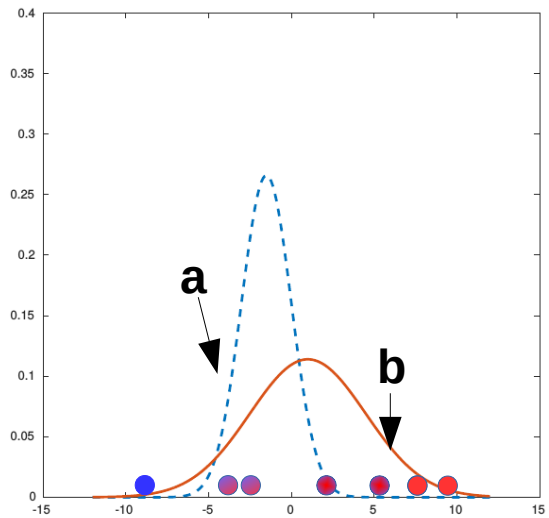
2. **E(xpectation)-step**:
   - for each point: $P(b|x_i)$ = does it look like it came from b?

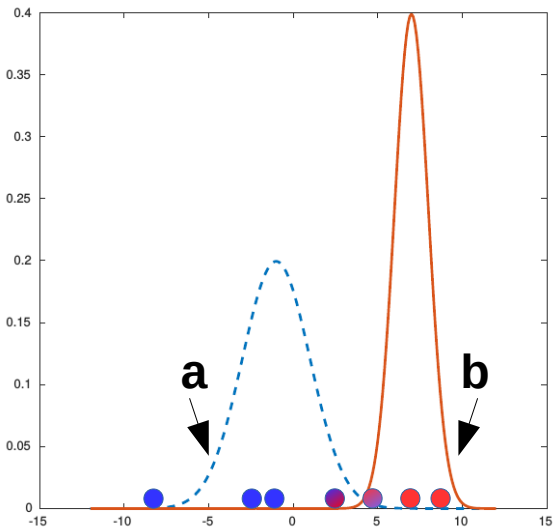
3. **M(maximization)-step**:
   - adjust (μ_a, σ_a^2) and (μ_b, σ_b^2) to fit points assigned to them.

4. **Iterate until convergence.**

EM in 1d







$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left(-\frac{(x_i-\mu_b)^2}{2\sigma_b^2}\right)$$

$$b_i = P(b \mid x_i) = \frac{P(x_i \mid b)P(b)}{P(x_i \mid b)P(b) + P(x_i \mid a)P(a)}$$

$$a_i = P(a \mid x_i) = 1 - b_i$$

$$\mu_b = \frac{b_1 x_1 + b_2 x_2 + \ldots + b_n x_{n_b}}{b_1 + b_2 + \ldots + b_n}$$

$$\sigma_b^2 = \frac{b_1(x_1-\mu_1)^2 + \ldots + b_n(x_n-\mu_n)^2}{b_1 + b_2 + \ldots + b_n}$$

$$\mu_a = \frac{a_1 x_1 + a_2 x_2 + \ldots + a_n x_{n_b}}{a_1 + a_2 + \ldots + a_n}$$

$$\sigma_a^2 = \frac{a_1(x_1-\mu_1)^2 + \ldots + a_n(x_n-\mu_n)^2}{a_1 + a_2 + \ldots + a_n}$$

→ We could also estimate priors:

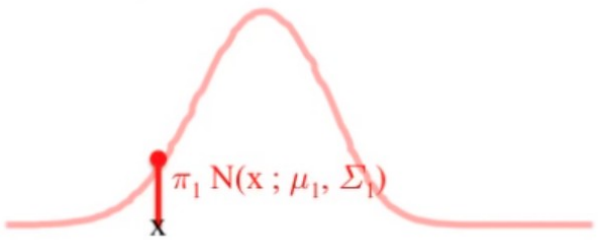
$P(b) = (b_1 + b_2 + \ldots b_n) / n$

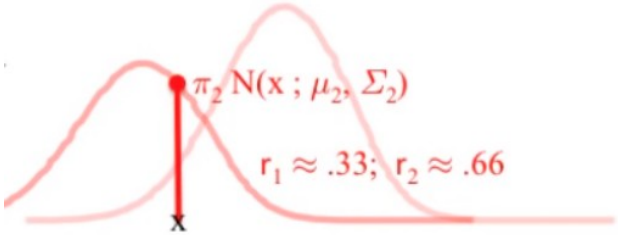
$P(a) = 1 - P(b)$

EM in the multidimensional case

- Start with parameters describing each cluster
- Mean μ_c, Covariance Σ_c, "size" π_c
- **E-step ("Expectation"):**
  - For **each observation/point x_i**
  - Compute "r_{ic}", the probability that it belongs to cluster c.
    - Compute its probability under model c.
    - Normalize to sum to one (over clusters c).

$$r_{ic} = \frac{\pi_c \mathcal{N}(x_i \; ; \; \mu_c, \Sigma_c)}{\sum_{c'} \pi_{c'} \mathcal{N}(x_i \; ; \; \mu_{c'}, \Sigma_{c'})}$$





  - If x_i is very likely under the c-th Gaussian, it gets high weight.
  - Denominator just makes r's sum to one.

EM in the multidimensional case

- **M-step ("Maximization step"):**
  - For each cluster (Gaussian) z=c
  - Update its parameters using the (weighted) data points

$$N_c = \sum_i r_{ic}$$

Total responsibility allocated to cluster c

$$\pi_c = \frac{N_c}{N}$$

Fraction of total assigned to cluster c

$$\underbrace{\mu_c = \frac{1}{N_c} \sum_i r_{ic} x_i}_{\text{Weighted mean of assigned data}}$$

$$\underbrace{\Sigma_c = \frac{1}{N_c} \sum_i r_{ic} (x_i - \mu_c)^T (x_i - \mu_c)}_{\text{Weighted covariance of assigned data (use new weighted means here)}}$$

Expectation-Maximization: Summary

- Likelihood of the data

$$P(x_1, ..., x_N) = \Pi_{i=1}^{N} \sum_{k=1}^{K} P(x_i|k)P(k)$$

- Each step increases the log-likelihood of our model

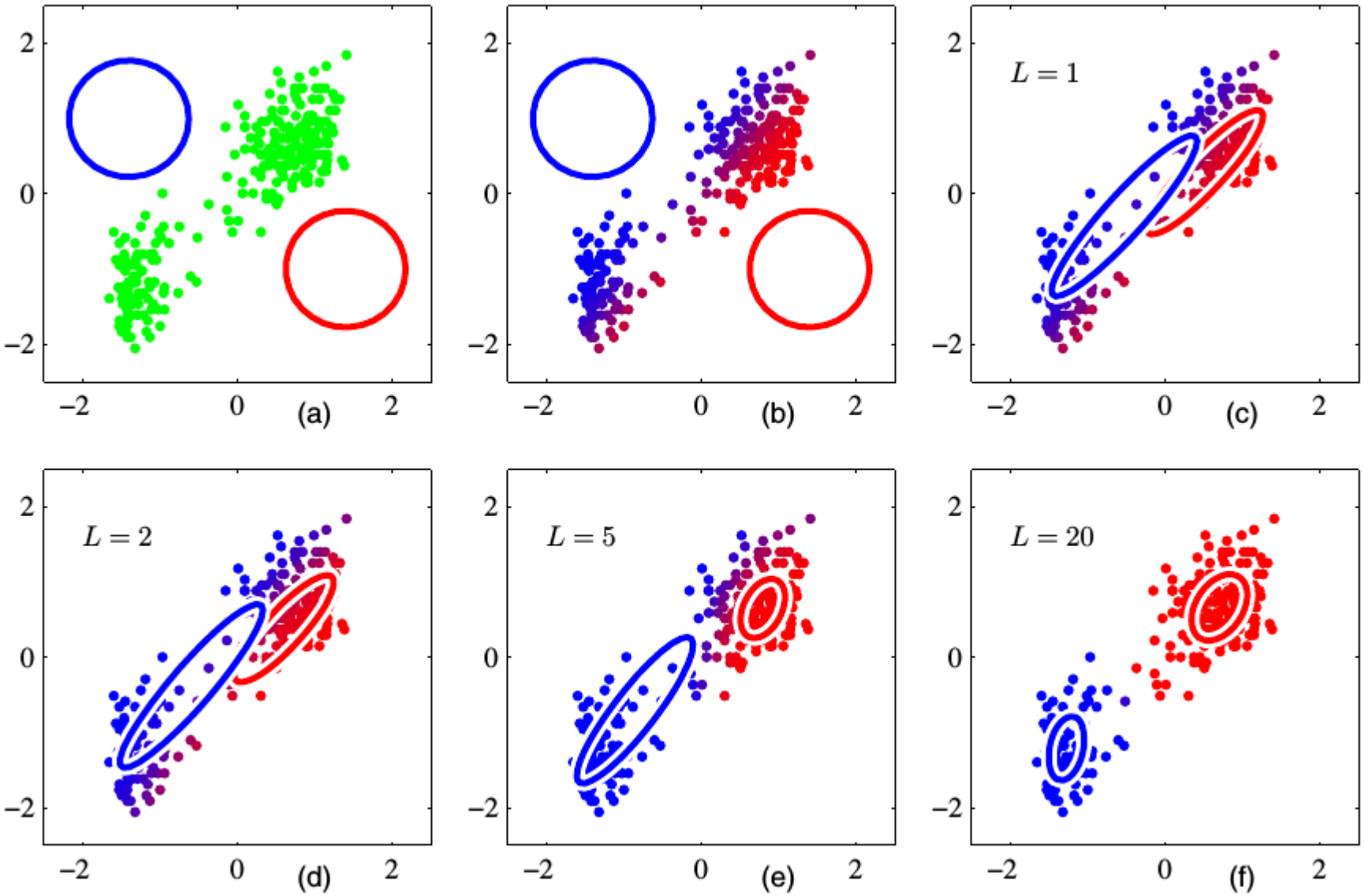
$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

- Iterate until convergence
  - Convergence guaranteed – another ascent method.

- Cannot discover k.

Gaussian mixture models:d>1

See Bishop (2006) for details



Bayesian Information Criterion (BIC)

See, e.g., Alpaydın (2014), MIT Press

- How to pick k?
- Probabilistic model: L = $\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$
  - Tries to "fit" the data (maximize likelihood)
- Choose k that makes L as large as possible?
  - K = n: each data point has its own "source"
  - may not work well for new data points
- Split points into training set **T** and validation set **V**
  - for each k: fit parameters of **T**
  - measure likelihood of **V**
  - sometimes still best when k = n
- "Occam's razor":
  - Pick the "simplest" of all models that fits the data.
  - Assess, e.g., via Bayes Information Criterion (BIC): **$\max_p$ { *L* – 1/2 p*log(n) }**
  - *L*: Likelihood; p: # Parameters in the model – how simple is the model.

About the EM Algorithm

Some good things about EM:

- no learning rate (step-size) parameter.
- automatically enforces parameter constraints.
- very fast for low dimensions.
- each iteration guaranteed to improve likelihood.

Some bad things about EM:

- can get stuck in local minima.
- can be slower than conjugate gradient (especially near convergence).
- requires expensive inference step.
- is a maximum likelihood/MAP (maximum a posterior) method.

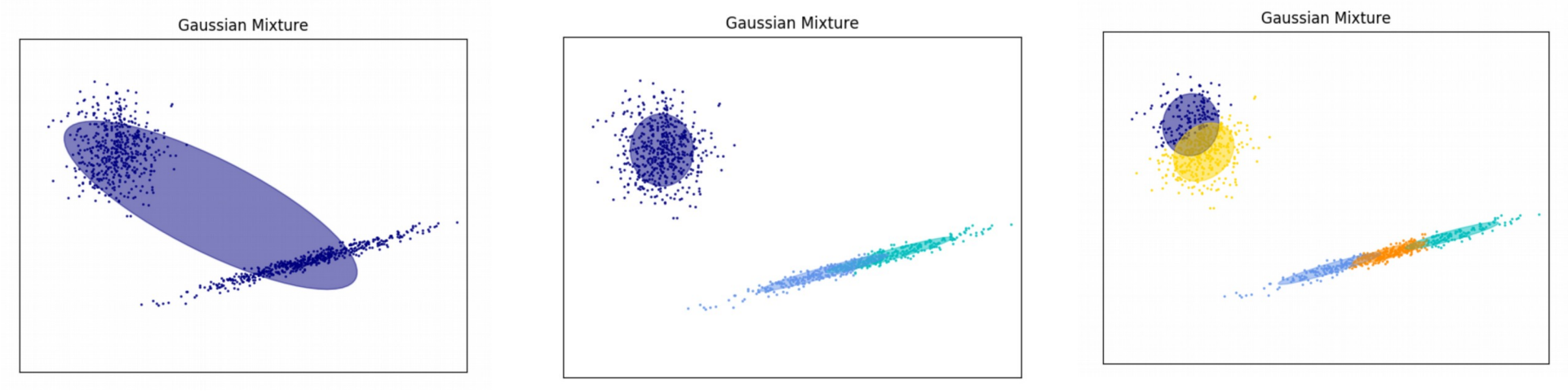
Hands-on example 1

https://scikit-learn.org/stable/modules/mixture.html
global_solution_yale19/Lecture_5/code/GMM_scikit_example.py

- Plot the confidence ellipsoids of a mixture of two Gaussians obtained with Expectation Maximization (GaussianMixture class)

- The model has access to 1, 3, and 5 components with which to fit the data. Note that the Expectation Maximization model will necessarily use ALL components

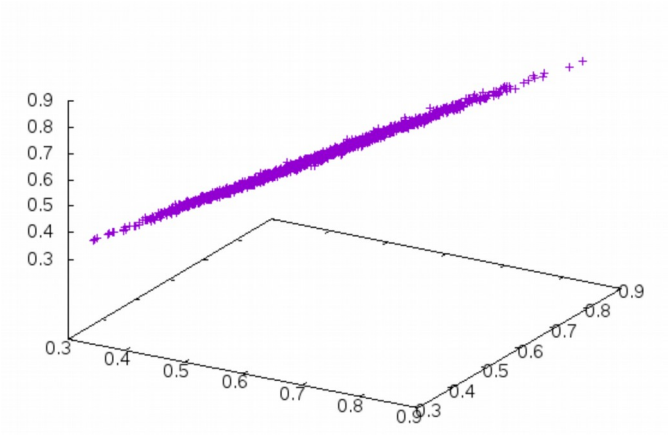
- In the 5-component example, we can see that the Expectation Maximization model splits some components arbitrarily, because it is trying to fit too many components.



Hands-on example 2

global_solution_yale19/Lecture_5/code/code/BGMM_data
cf. https://papers.ssrn.com/sol3/papers.cfm?abstract_id=3282487

- We simulate a bunch of data (e.g., an ergodic set).
  - Its in a text file (**ergodic_data.txt – 3 dimensions**)



- We apply GMM (**build_density.py**)

- We can sample data from the fitted GMM model (**sample.py**)