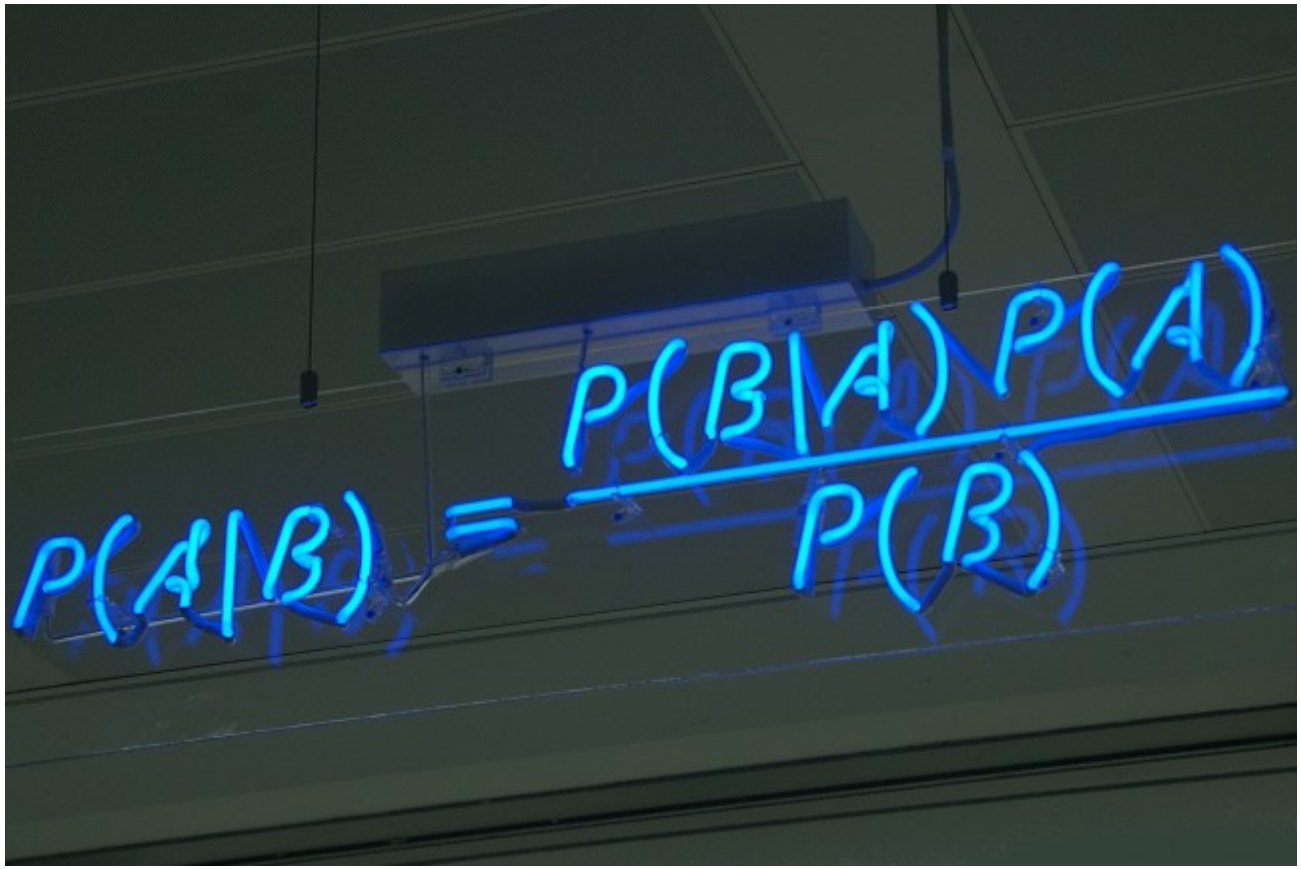
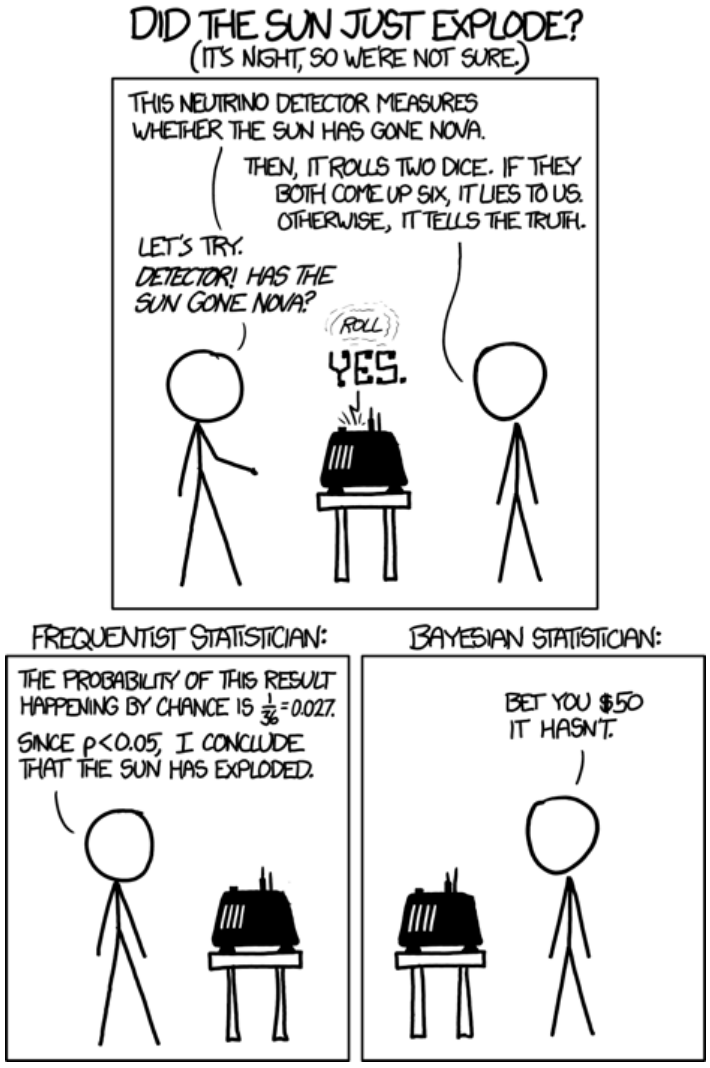
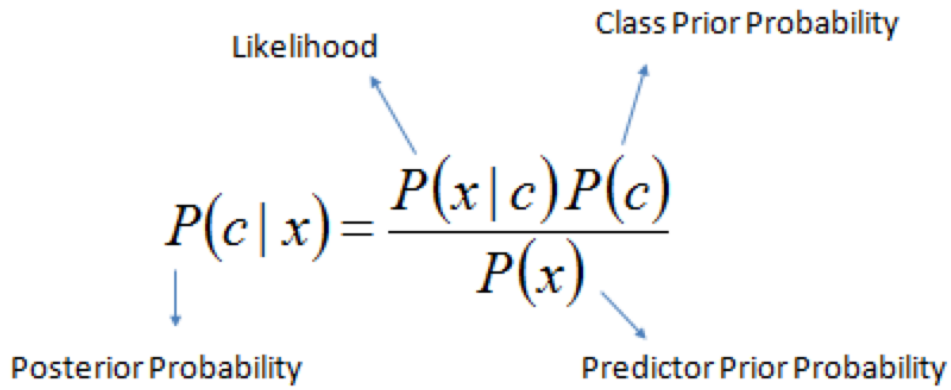
# Bayesian Learning




DID THE SUN JUST EXPLODE?
(IT'S NIGHT, SO WE'RE NOT SURE.)
THIS NEUTRINO DETECTOR MEASURES WHETHER THE SUN HAS GONE NOVA.
THEN, IT ROLLS TWO DICE. IF THEY BOTH COME UP SIX, IT LIES TO US. OTHERWISE, IT TELLS THE TRUTH.
LET'S TRY.
DETECTOR! HAS THE SUN GONE NOVA?
ROLL
YES.
FREQUENTIST STATISTICIAN:
THE PROBABILITY OF THIS RESULT HAPPENING BY CHANCE IS 1/36 = 0.027.
SINCE p<0.05, I CONCLUDE THAT THE SUN HAS EXPLODED.
BAYESIAN STATISTICIAN:
BET YOU $50 IT HASN'T.

## Bayes' rule

Rule for updating the probability of a hypothesis $c$ given data $x$




$P(c|x)$is the posterior probability of class (target) given predictor (attribute).
$P(c)$is the *prior* probability of class: what you believed before you saw the evidence $x$
$P(x|c)$is the *likelihood* of seeing that evidence if your class is correct
$P(x)$is the prior probability of predictor (*marginal likelihood*): the likelihood of the evidence $x$ under any circumstance

**Example**

- Prior $P(exploded)$: the sun has an estimated lifespan of 10 billion years, $P(exploded) = \frac{1}{4.38x10^{13}}$
- Likelihood that detector lies: $P(lie) = \frac{1}{36}$

$$P(exploded|yes) = \frac{P(yes|exploded)P(exploded)}{P(yes)}$$
$$= \frac{(1 - P(lie))P(exploded)}{P(exploded)(1 - P(lie)) + P(lie)(1 - P(exploded))}$$
$$= \frac{1}{1.25226x10^{12}}$$

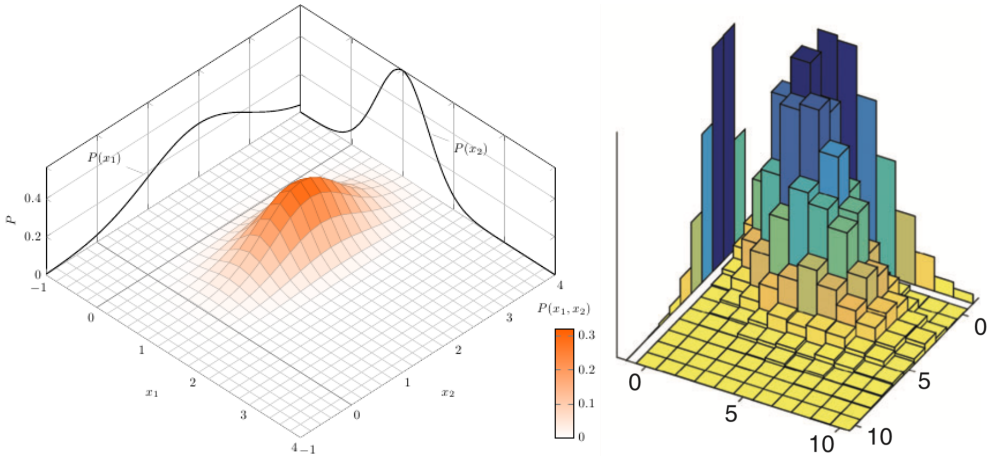
**Example 2**

- What is the probability of having HIV if a 99% accurate test returns positive?
- Prior $P(H)$ : 0.003

$$
\begin{aligned}
P(H|yes) &= \frac{P(yes|H)P(H)}{P(yes)} \\
&= \frac{(1 - P(wrong))P(H)}{P(H)(1 - P(wrong)) + P(wrong)(1 - P(H))} \\
&= \frac{0.99 * 0.003}{0.003 * 0.99 + 0.01 * 0.997} \\
&= 0.2295
\end{aligned}
$$

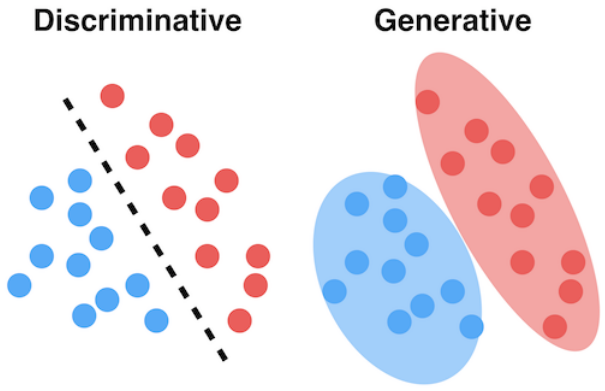
# Bayesian models

- Are easily updatable with new data points ('turning the crank')
  - Previous posterior $P(c|x)$becomes new prior $P(c)$, then apply Bayes' rule on new data $x$
  - e.g. collect new data from the detector, update probabilities
- They learn the joint distribution $P(x, y) = P(x|y)P(y)$
  - Either continuous (left) or discrete (right)



# Bayesian models are generative

- The joint distribution represents the training data for a particular class
- You can sample a *new* point **x** with high predicted likelihood $P(x, c)$: that new point will be very similar to the training points
- Hence, you can generate new (likely) points according to the same distribution: *generative model*
    - You can generate examples that are *fake* but that are very close to the other training examples of the same class
    - There also exist generative neural networks (e.g. GANs) that can do this very accurately for text, images, ...



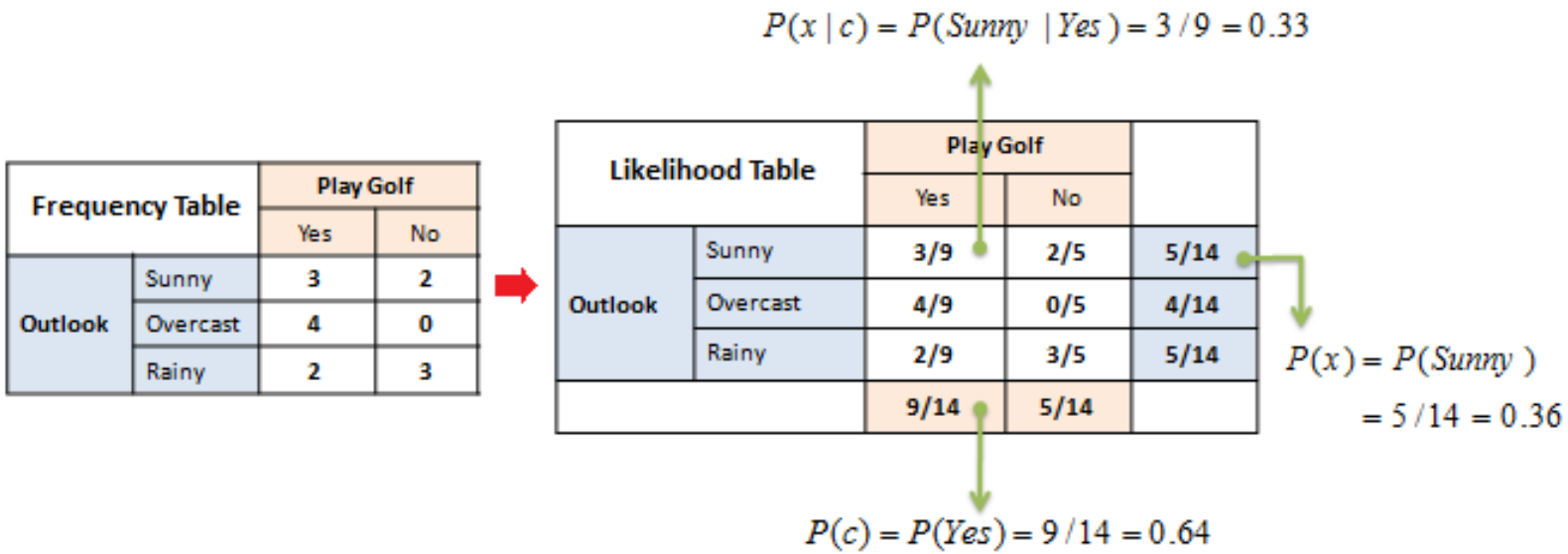
## Naive Bayes Classifier

- Predict the probability that a point belongs to a certain class, using Bayes' Theorem

$$P(c|\mathbf{x}) = \frac{P(\mathbf{x}|c)P(c)}{P(\mathbf{x})}$$

- Problem: since $\mathbf{x}$ is a vector, $P(\mathbf{x}|c)$can be very complex
- Naively assumes that all features are conditionally independent from each other, in which case:
  $P(\mathbf{x}|c) = P(x_1|c) \times P(x_2|c) \times \ldots \times P(x_n|c)$
- Very fast: only needs to extract statistics from each feature.

Example. True or not? Your friend will play golf if weather is sunny.




Posterior Probability: $P(c \mid x) = P(Yes \mid Sunny) = 0.33 \times 0.64 \div 0.36 = 0.60$

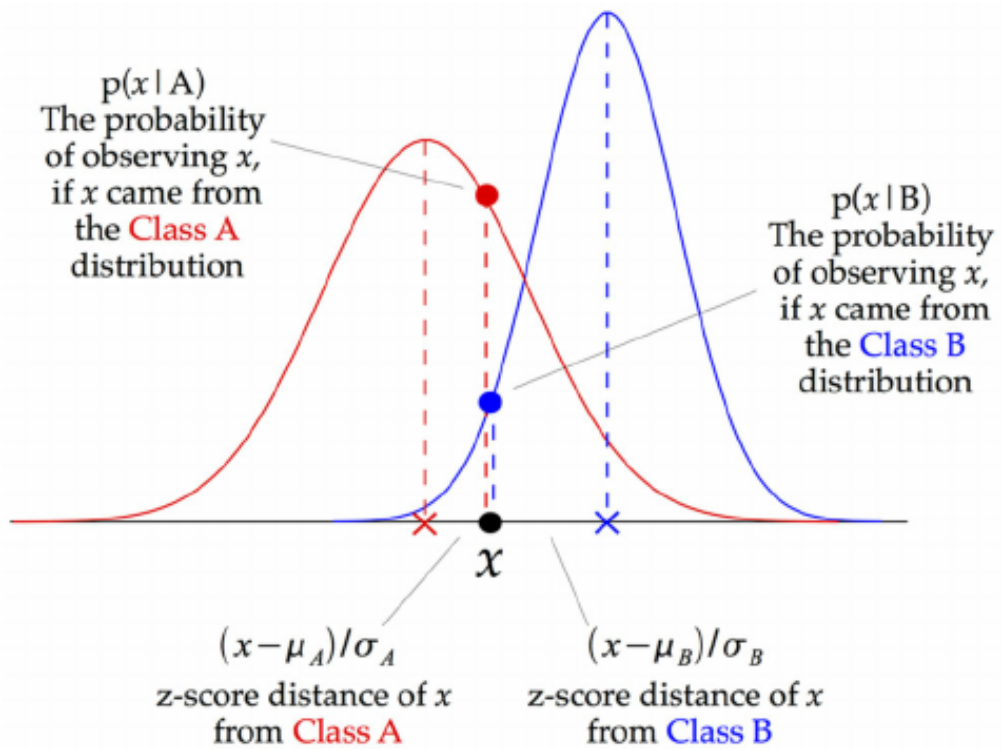
Compute the posterior for every class and predict the class with highest probability

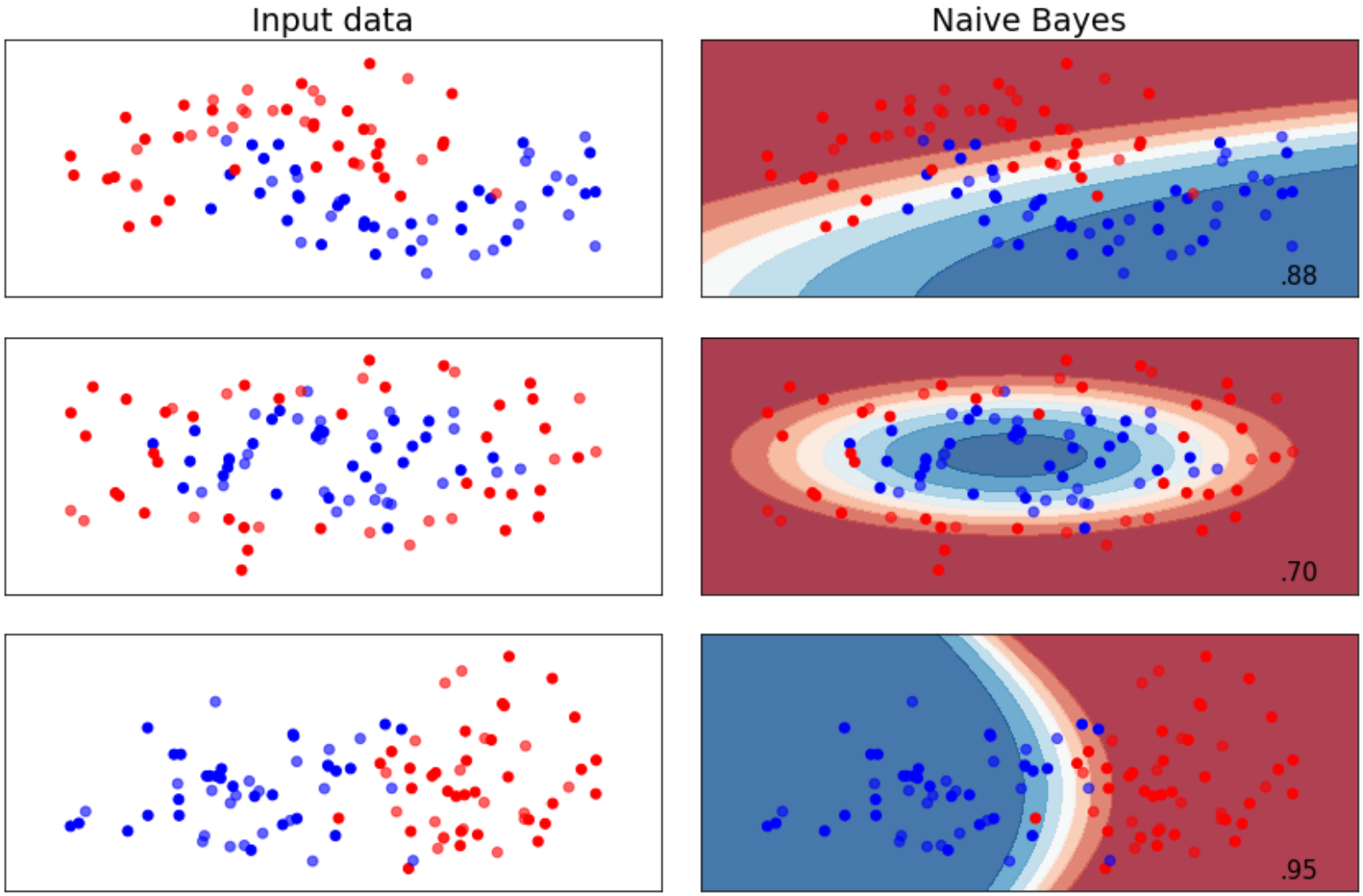
## On numeric data

- We need to fit a distribution over the data points
- GaussianNB: Computes mean $\mu_c$ and standard deviation $\sigma_c$ of the feature values per class (red and blue):

$$p(x = v \mid c) = \frac{1}{\sqrt{2\pi\sigma_c^2}} e^{-\frac{(v-\mu_c)^2}{2\sigma_c^2}}$$

- Prediction are made using Bayes' theorem, by computing the joint probability given all features, and calculating the posterior:
  $p(c \mid \mathbf{x}) = \frac{p(c)\ p(\mathbf{x}|c)}{p(\mathbf{x})}$



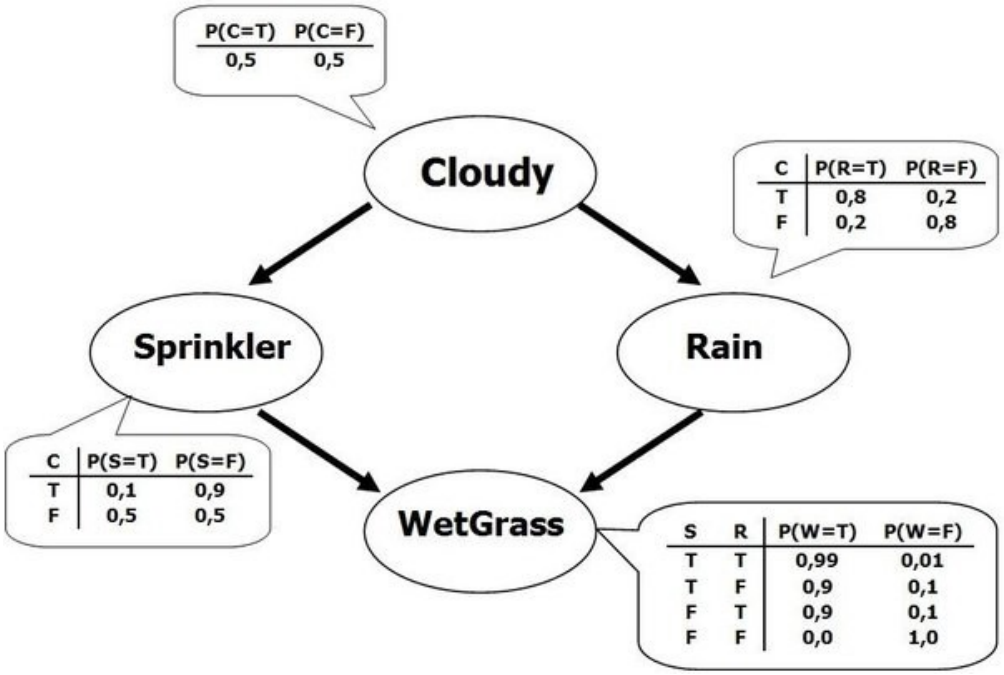

Input data
Naive Bayes
.88
.70
.95

Other Naive Bayes classifiers:

- BernoulliNB
    - Assumes binary data
    - Feature statistics: Number of non-zero entries per class
- MultinomialNB
    - Assumes count data
    - Feature statistics: Average value per class
    - Mostly used for text classification (bag-of-words data)

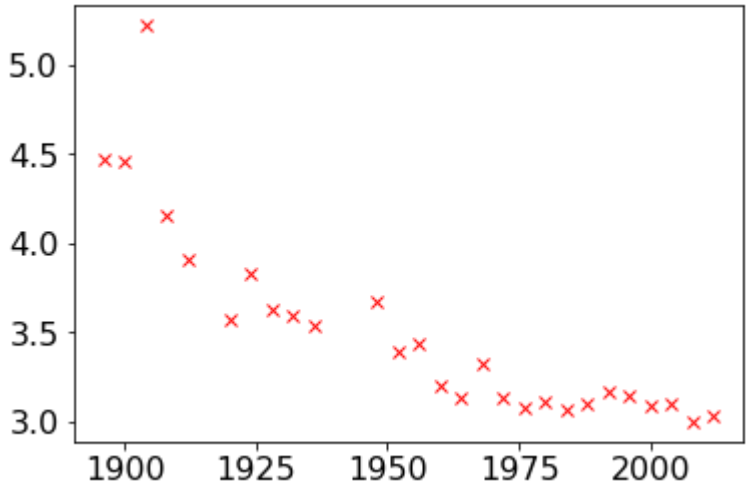
# Bayesian Networks

- A *Bayesian Network* is a directed acyclic graph representing variables as nodes and conditional dependencies as edges.
- If an edge $(A, B)$connects random variables A and B, then $P(B|A)$is a factor in the joint probability distribution
    - We must know $P(B|A)$for all values of $B$ and $A$
- The graph structure can be designed manually or learned (hard!)



# Linear regression and basis expansions (recap)

Let's look at a the following regression problem



Let's first try to fit a linear model

$$y = f(\mathbf{x}_i) = \mathbf{x}_i^\top \mathbf{w} + b$$

In this case (with one input feature):

$$y = w_1 \cdot x_1 + b \cdot 1$$

We can solve this via linear algebra. To obtain a matrix we add a $x_0 = 1$column to represent the bias $b$. Hence, each vector $\mathbf{x}_i = [1, x_i.]$

We can do this for the entire data set to form a design matrix $\mathbf{X}$,

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix},$$

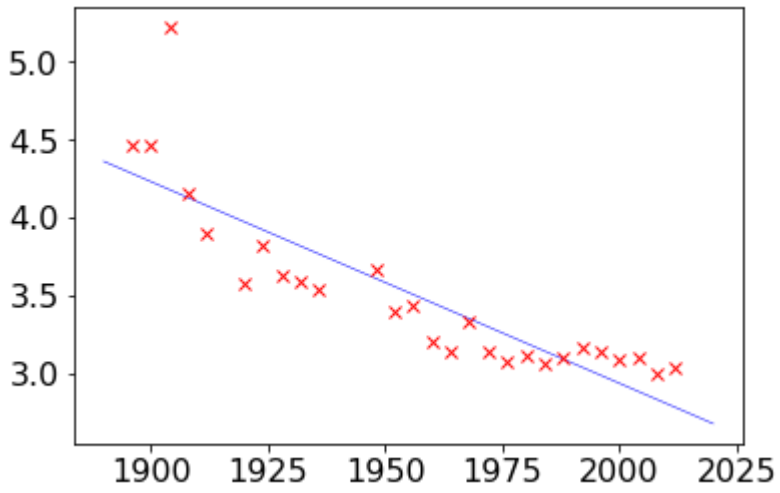
In `numpy` this is done and solved with the following commands:

```
X = np.hstack((np.ones_like(x), x))
w = np.linalg.solve(np.dot(X.T, X), np.dot(X.T, y))
```

```
w: [[28.895 -0.013]]
```

With $w = [w_0, w_1,]$we can now fit the function

$$y = w_1 x + w_0 = -0.013x + 28.895$$

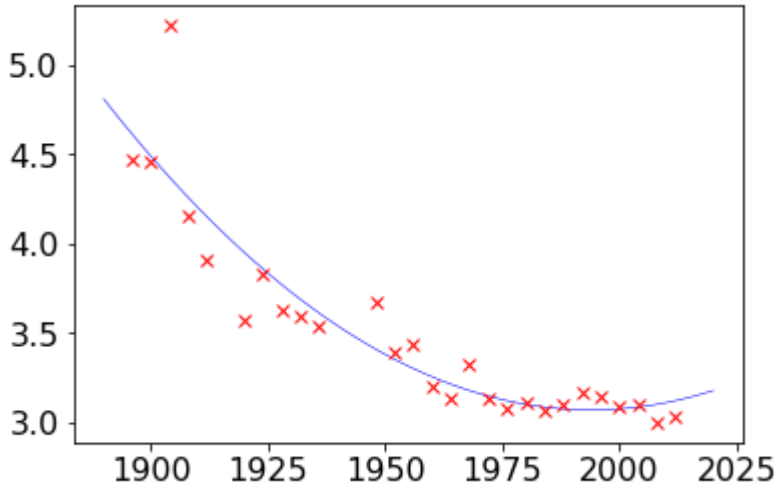


The linear model isn't a very good fit, let's try fitting a 2nd degree polynomial (quadratic model). This can be done by adding more *basis functions*.
Firstly, we need to create a new design matrix that contains the quadratic basis,

$$\mathbf{\Phi} = \begin{bmatrix} \mathbf{1} & \mathbf{x} & \mathbf{x}^2 \end{bmatrix}$$

```
Phi = np.hstack([np.ones(x.shape), x, x**2])
w = np.linalg.solve(np.dot(Phi.T, Phi), np.dot(Phi.T, y))
```

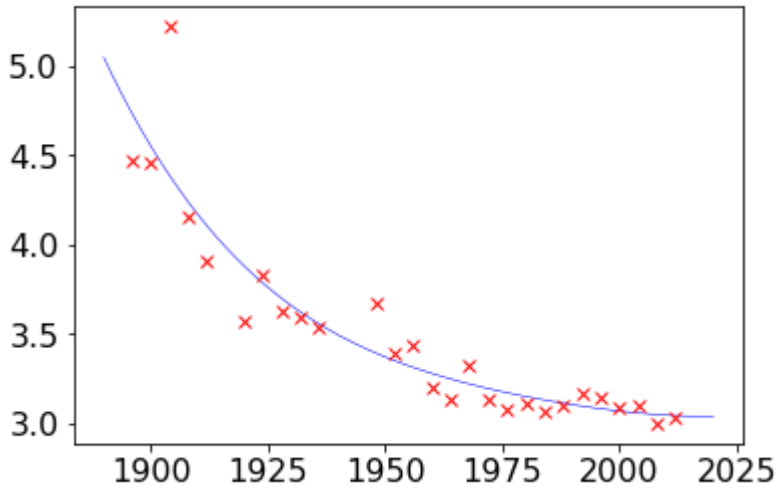
```
w: [[643.642  -0.643   0.   ]]
```



Repeating up to degree 6 gives us:

```
Phi = np.hstack([np.ones(x.shape), x, x**2, x**3, x**4, x**5, x**6])
w = np.linalg.solve(np.dot(Phi.T, Phi), np.dot(Phi.T, y))
```

```
w: [[55403.877   -58.241    -0.018     0.        -0.         0.         0.
]]
```

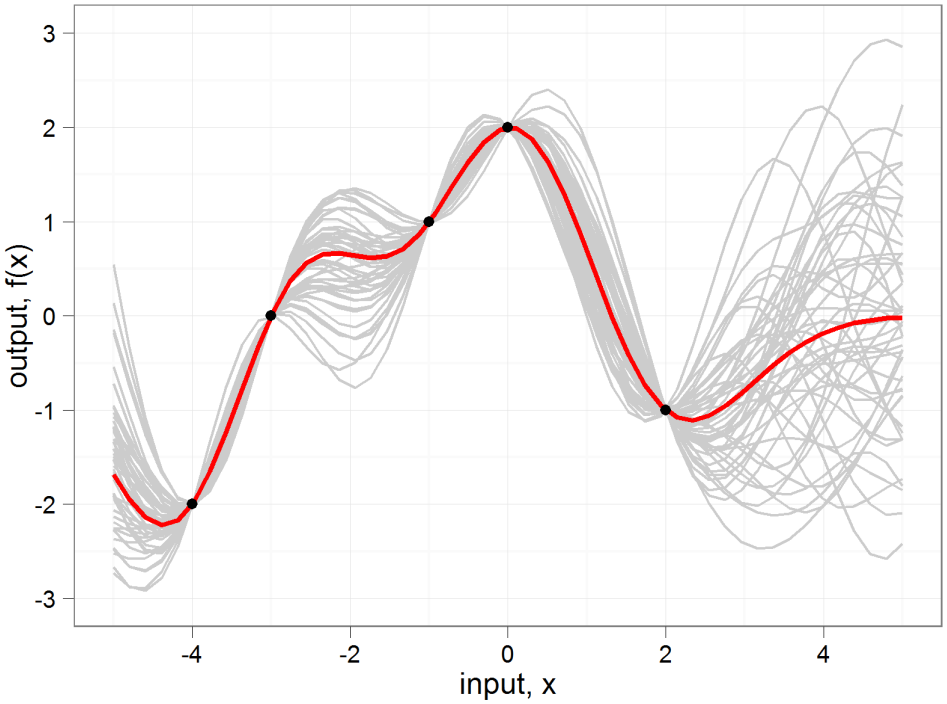


## There must be a better way

- We would like a probability for predictions instead of just one value
    - We should be more certain about predictions close to the training points
    - We need a probabilistic version of regression
- How do we know the optimal degree?
    - Ideally, I don't want to specify this up front, and consider *every possible function* that matches our data, with however many parameters are involved (i.e. a non-parametric model).
    - A *Gaussian process* learns a *distribution* on this set of functions

# Gaussian processes

Learn a probability distribution of possible base functions, update this distribution based on new data.



# Probabilistic interpretation of regression

When there are more observations than unknowns (overdetermined systems), we cannot perfectly fit

$$y = w_1 x + w_0$$

This issue can be solved by assuming that the data is inherently uncertain, and modeling it explictly by introducing a slack variable (http://en.wikipedia.org/wiki/Slack_variable), $\epsilon_i$, known as noise.

For each observation we now have the equation

$$y_i = w_1 x_i + w_0 + \epsilon_i .$$

The slack variable represents the difference between our actual prediction and the true observation. This is also known as the *residual*.

We now have an additional $n$ variables to estimate, one for each data point, $\{\epsilon_i\}$. With the original $w_1$ and $w_0$ we now have $n + 2$ parameters to be estimated from $n$ observations (underdetermined system).

However, we can make assumptions about the noise distribution, i.e. that the slack variables are distributed according to a probability density. One often assumes Gaussian noise:

$$\epsilon_i \sim \mathcal{N}(0, \sigma^2),$$

with zero mean and variance $\sigma^2$.

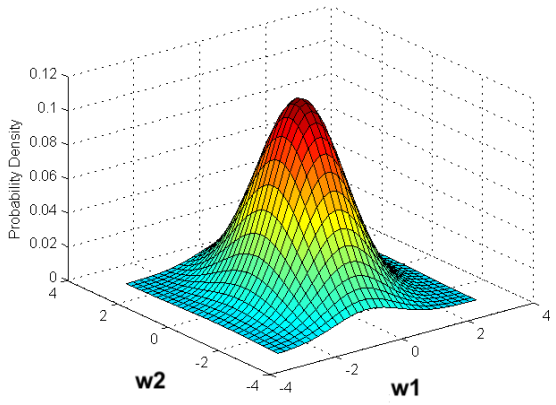
# Bayesian prior

In the Bayesian approach, we also assume a *prior distribution* for the parameters, **w**:

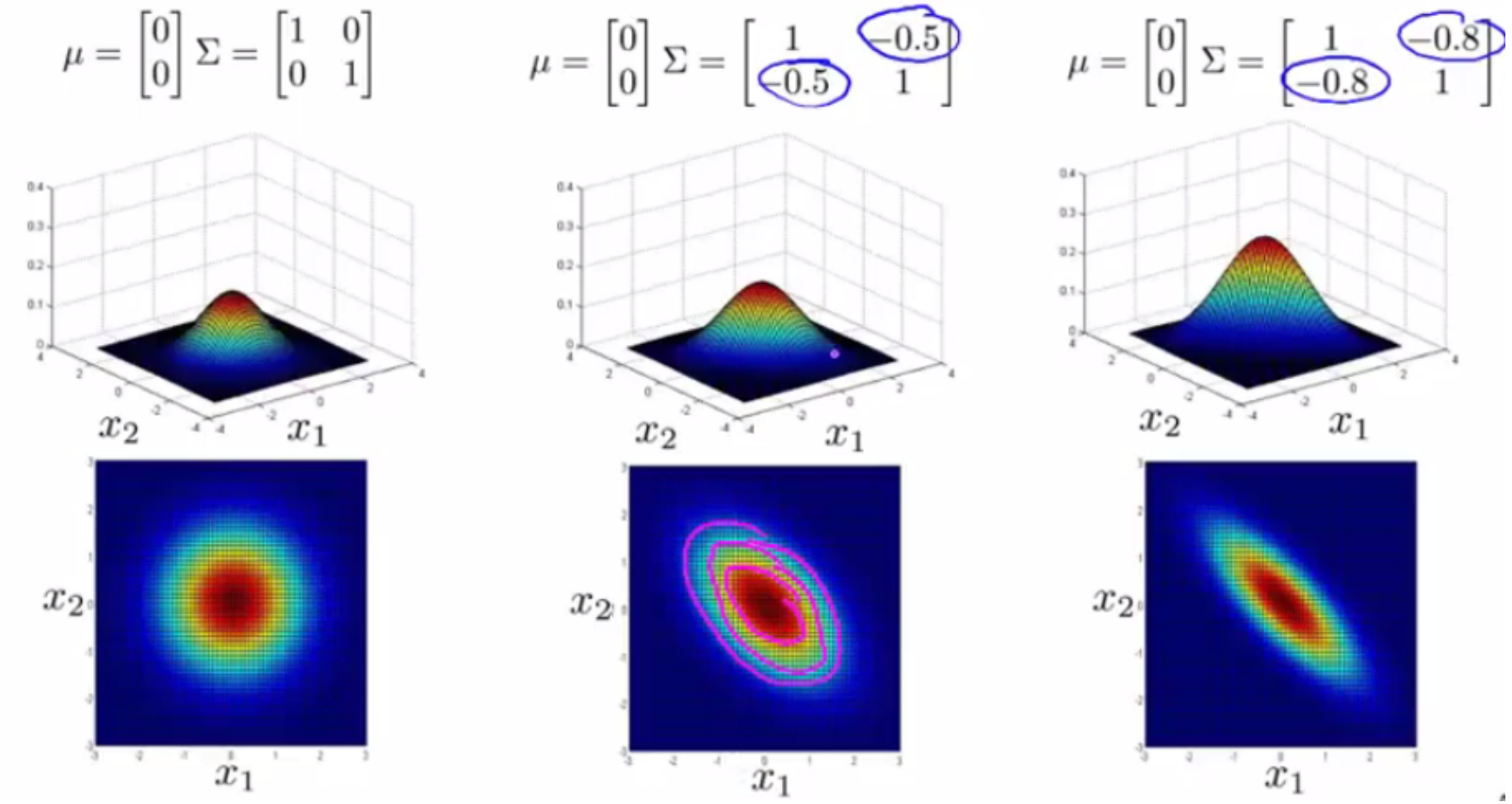
$$\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \alpha\mathbf{I})$$

I.e, each element of the parameters vector, $w_i$, was drawn from a Gaussian density with variance $\alpha$

$$w_i \sim \mathcal{N}(0, \alpha)$$



- $\alpha\mathbf{I}$ is the *covariance matrix*
- Our prior is typically $\alpha\mathbf{I}$ (left), but later we will learn the actual distribution of $w$ given data
- Some examples:



Gaussian process hyper-parameters:

- breadth of the prior (alpha)
- degree of the basis functions (degree)
- noise level (sigma^2)

```
alpha = 4.
degree = 5
sigma2 = 0.01
```

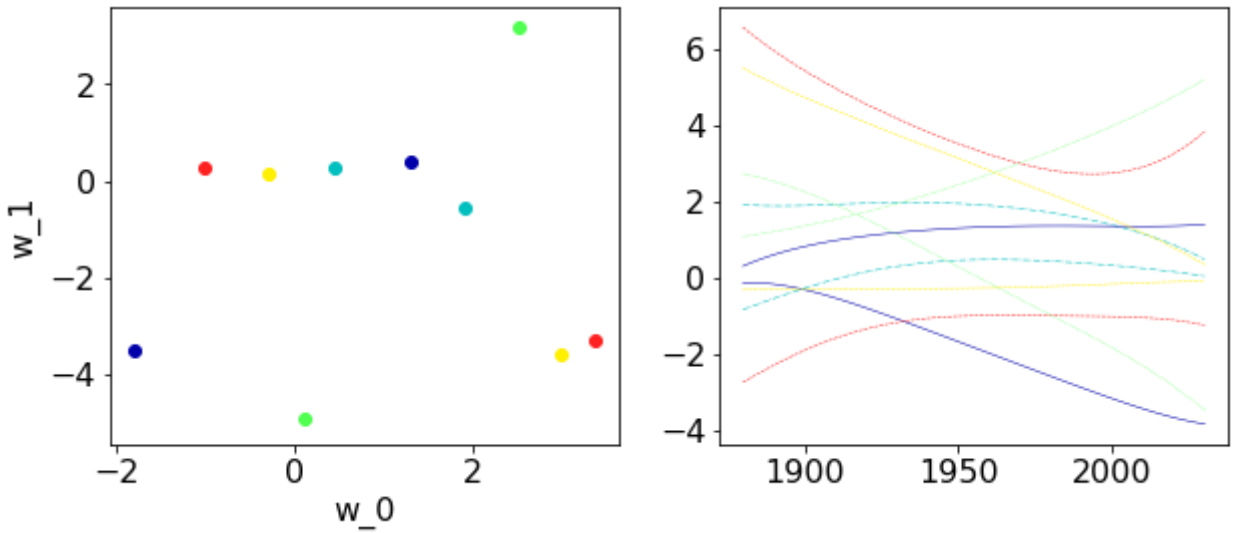
Now we can sample from the prior distribution (e.g. 100 points) to see what form we are imposing on the functions *a priori* (before seeing any data).

```
x_pred = np.linspace(1880, 2030, 100)[:, None] # sample
Phi_pred = polynomial(x_pred, degree=degree, loc=loc, scale=scale) # pre
dict
```

## Weight Space View

With the parameters $w$ (left) are drawn independently from a Gaussian density $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \alpha\mathbf{I})$our prediction function $f(\mathbf{x})$(right) becomes $f(\mathbf{x}) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x})$.

In `numpy` we can sample from the prior density to obtain a vector $\mathbf{w}$ using the function `np.random.normal` and combine these parameters with our basis to create some samples of what $f(\mathbf{x})$looks like. This is a sample from the *space* of possible models.



## Function space view

We can also generate examples of $f$ directly.

We know that if $\mathbf{w}$ is sampled from a multivariate Gaussian with covariance $\alpha\mathbf{I}$ and zero mean, then assuming that the design matrix (with basis expansion) $\mathbf{\Phi}$ is deterministic, then the vector $\mathbf{f}$ will also be distributed according to a zero mean multivariate normal as follows,

$$\mathbf{f} \sim \mathcal{N}(\mathbf{0}, \alpha\mathbf{\Phi}\mathbf{\Phi}^\top).$$

For ease of notation, we define the covariance matrix as

$$\mathbf{K} = \alpha\mathbf{\Phi}\mathbf{\Phi}^\top.$$

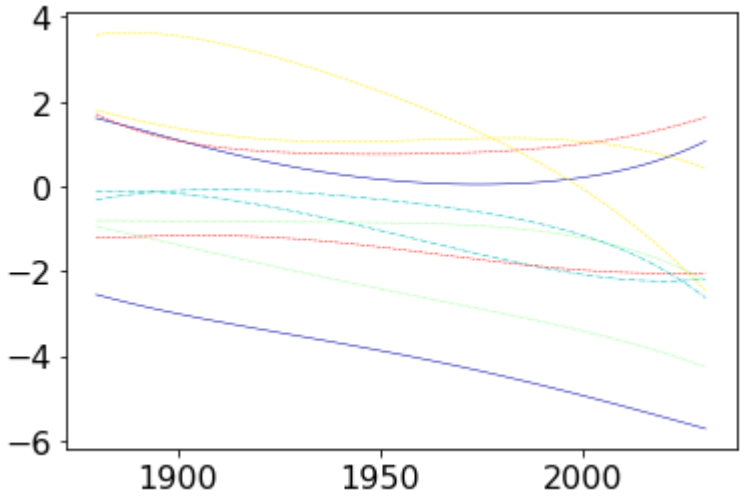
Hence

$$\mathbf{f} \sim \mathcal{N}(\mathbf{0}, \mathbf{K})$$

What happens if we sample $\mathbf{f}$ directly from this density, rather than first sampling $\mathbf{w}$ and then multiplying by $\mathbf{\Phi}$?

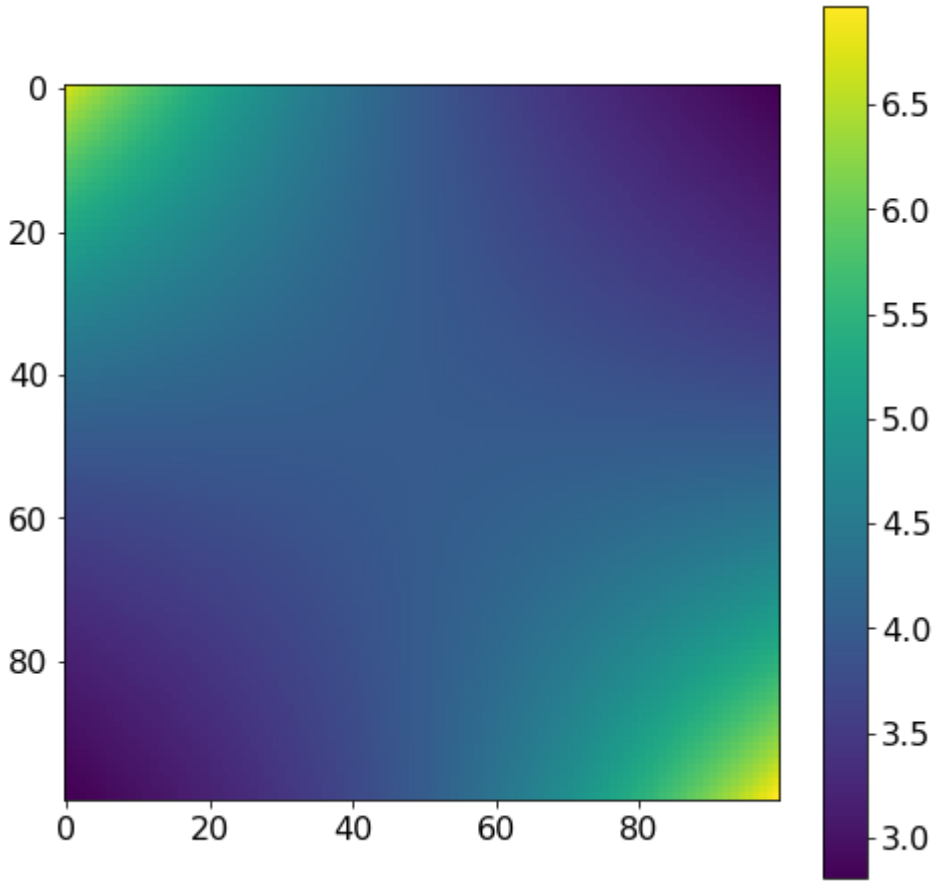
Let's try this.

We can use `np.random.multivariate_normal` for sampling from a multivariate normal with covariance given by $\mathbf{K}$ and zero mean,

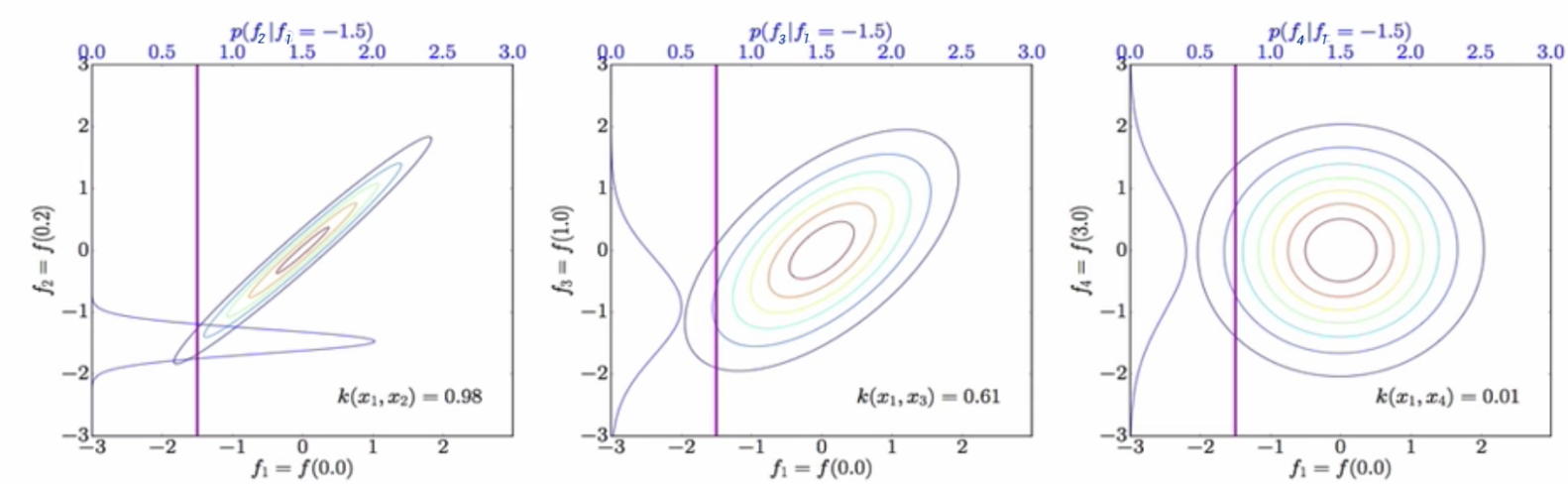


These look very similar! Indeed, they are effectively drawn from the same multivariate normal density.

We can also visualize the covariance matrix $\mathbf{K}$ for polynomial functions:



Understanding covariances



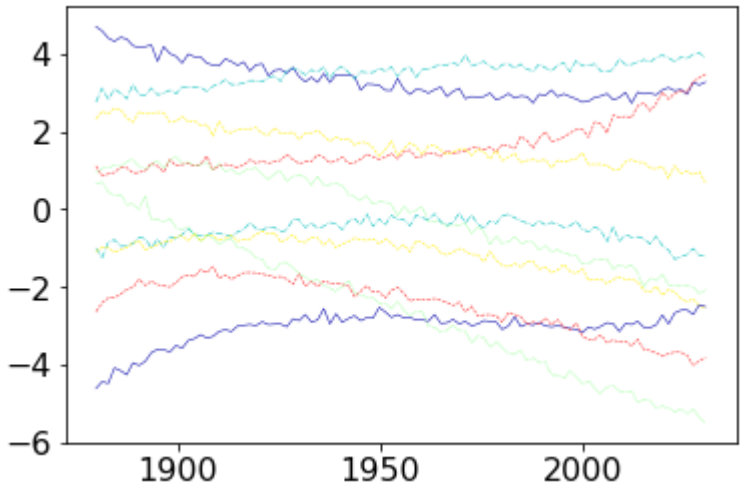

Left: If two variables $f_i$ covariate strongly, knowing about $f_1$ tells us a lot about $f_2$

Right: If covariance is 0, knowing $f_1$ tells us nothing about $f_2$ (the conditional and marginal distributions are the same)

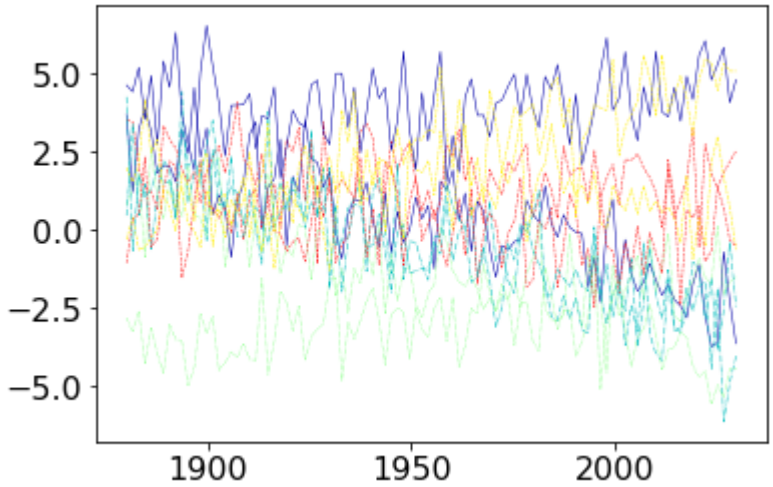
# Noisy functions

We normally add Gaussian noise to obtain our observations:

$$\mathbf{y} = \mathbf{f} + \boldsymbol{\epsilon}$$



We can also increase the variance of the noise



# Gaussian Process

- Usually, we want our functions to be *smooth*: if two points are similar, the predictions should be similar.
- In a Gaussian process we can do this by specifying the *covariance function* directly, rather than *implicitly* through a basis matrix and a prior over parameters.

The RBF (Gaussian) covariance function (or *kernel*) is specified by

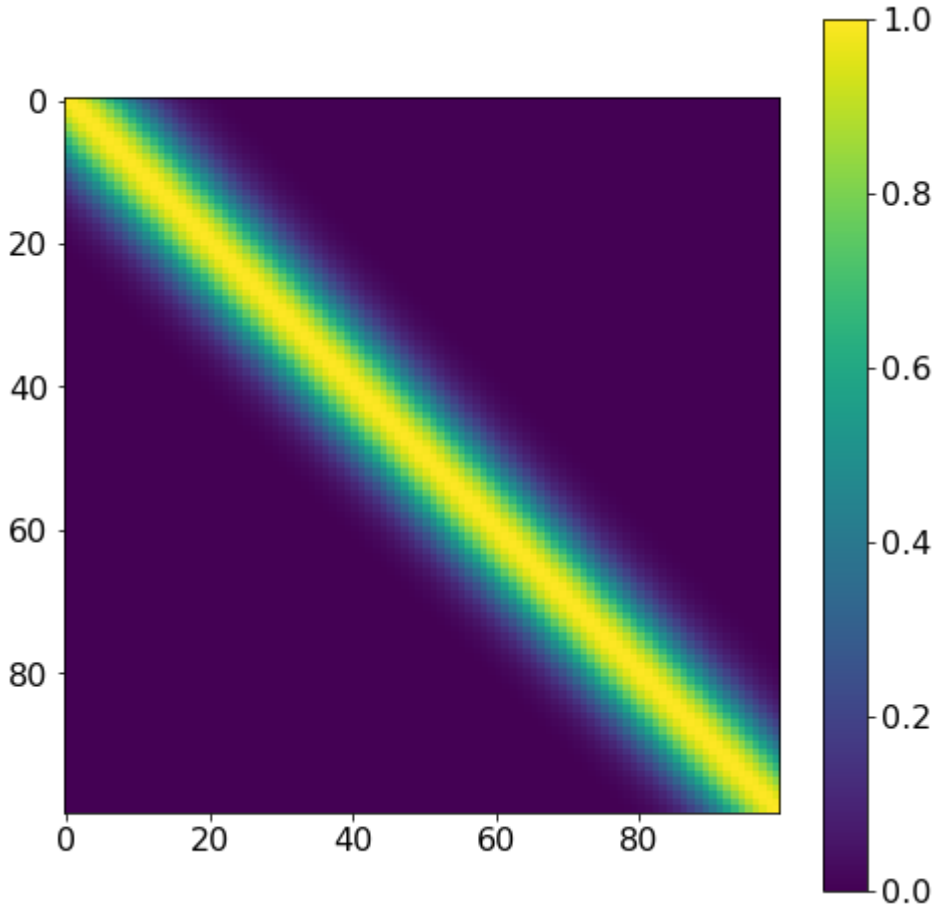
$$k(\mathbf{x}, \mathbf{x}') = \alpha \exp\left( -\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2} \right).$$

where $\|\mathbf{x} - \mathbf{x}'\|^2$ is the squared distance between the two input vectors

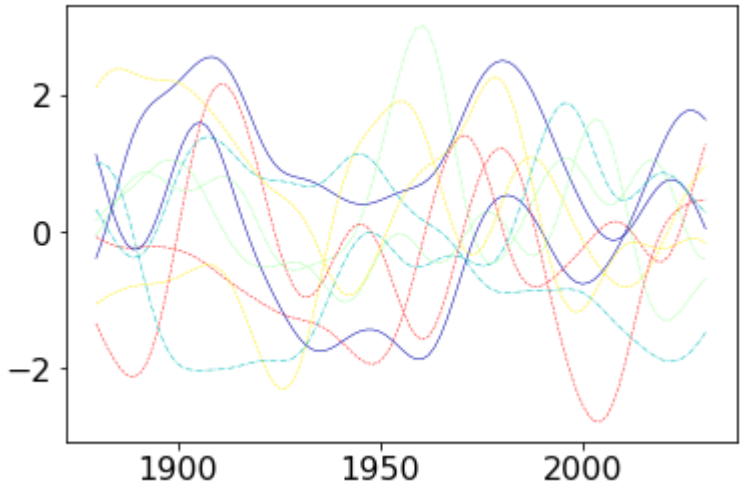
$$\|\mathbf{x} - \mathbf{x}'\|^2 = (\mathbf{x} - \mathbf{x}')^\top (\mathbf{x} - \mathbf{x}')$$

and the length parameter $l$ controls the smoothness of the function and $\alpha$ the vertical variation.

Let's build the covariance matrix for the RBF function:



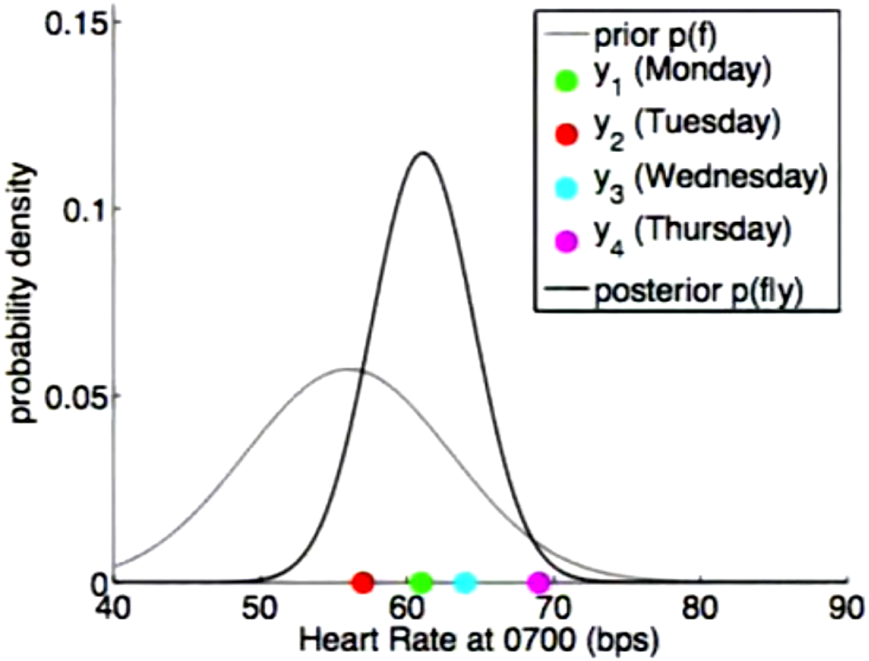
Finally, we can sample functions with this kernel (covariance matrix)



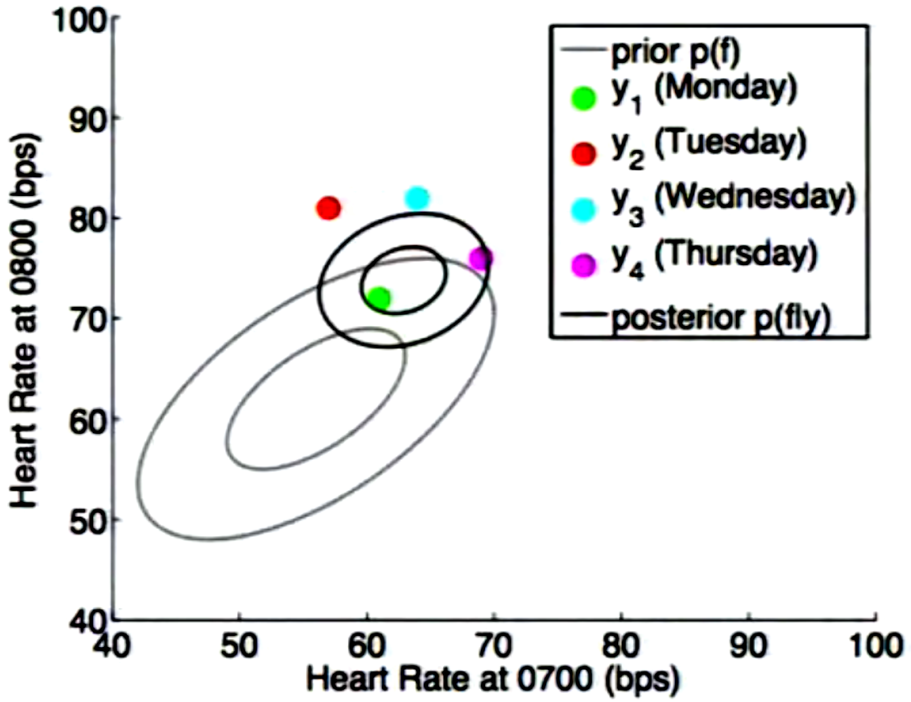

These are our priors. We now need to learn a (posterior) distribution, given data $X$

# Gaussian process intuition

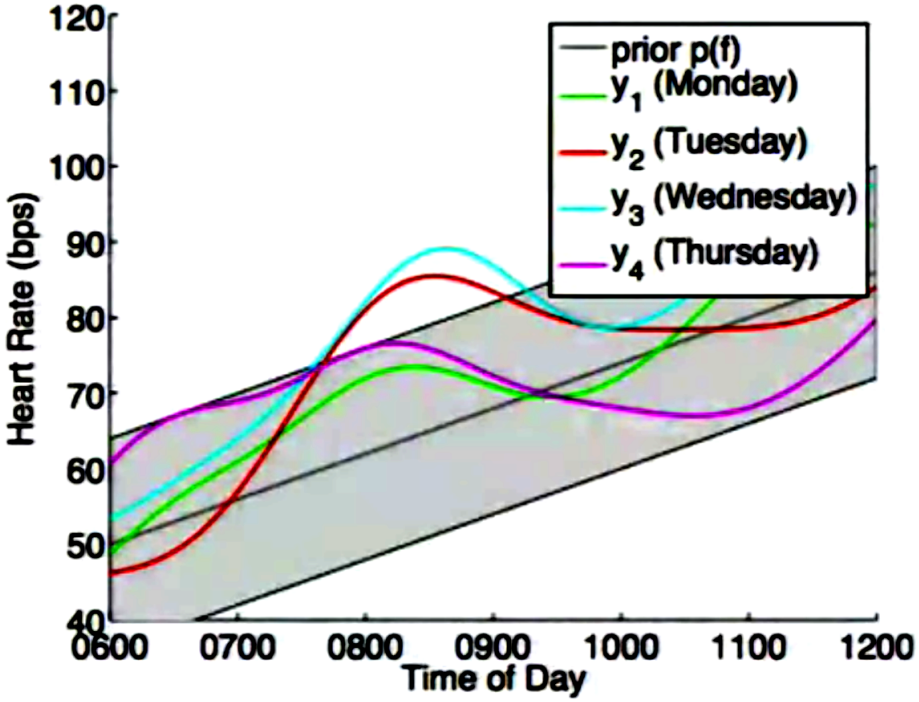
Univariate Gaussians: distributions over real-valued variables



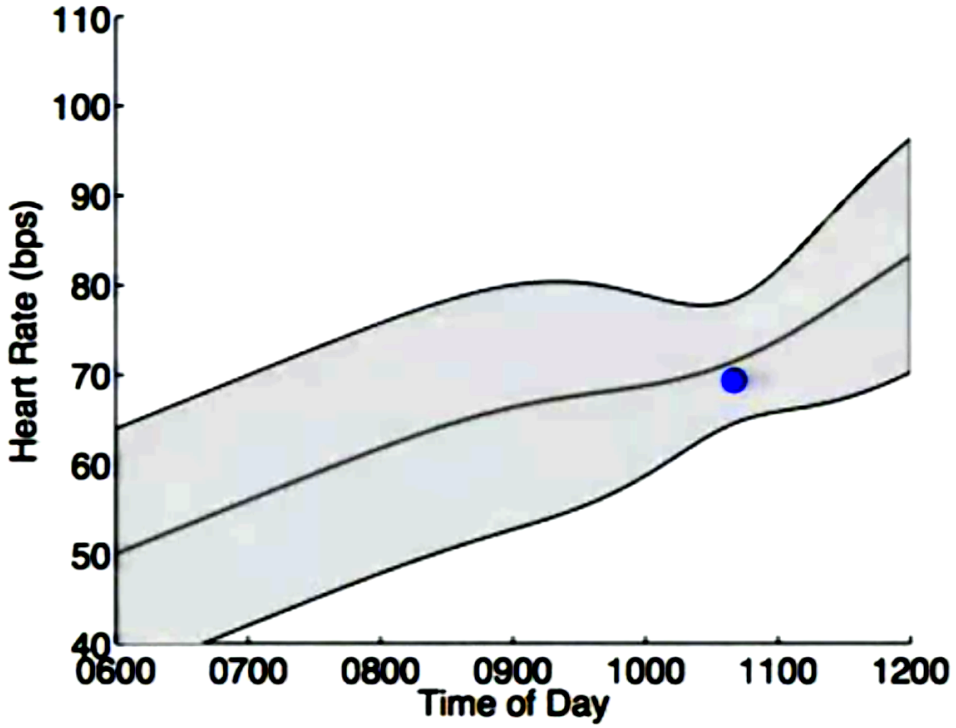
Multi-variate Gaussians: pairs (triplets,...) of real valued variables



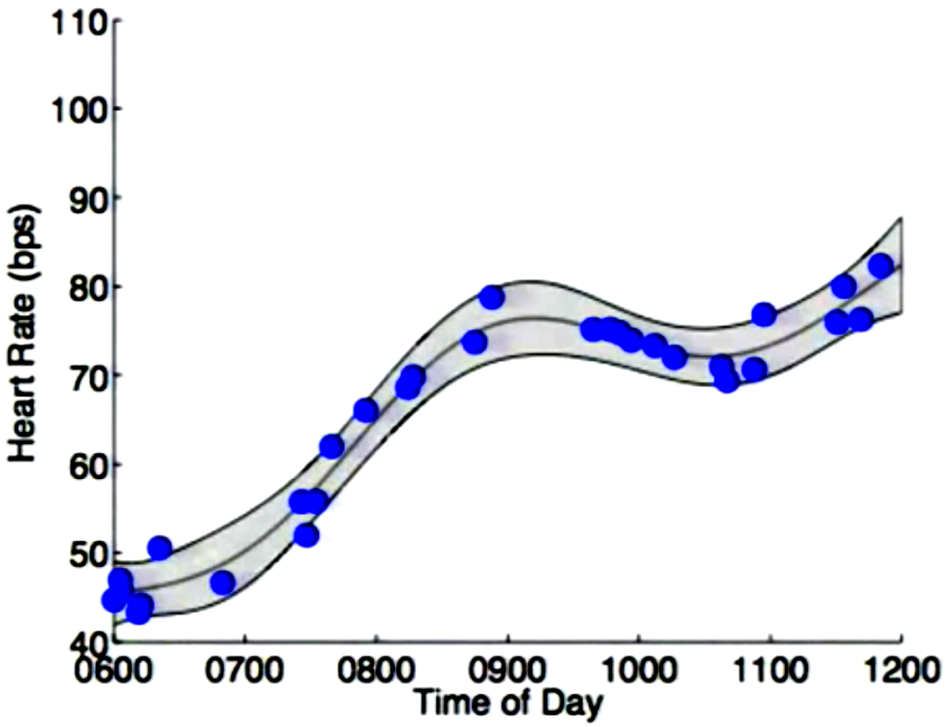
Gaussian processes: functions of infinite numbers of real values variables



Posterior probability after observation 1



Posterior probability after many observations



# Gaussian process optimization

The Gaussian process perspective assumes that $P(X)$(marginal likelihood) of the data is a joint Gaussian density with a covariance given by $\mathbf{K}$.

The model likelihood (posterior) then becomes:

$$p(\mathbf{y}|\mathbf{X}) = \frac{1}{(2\pi)^{\frac{n}{2}}|\mathbf{K}|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}\mathbf{y}^{\top}\left(\mathbf{K}+\sigma^{2}\mathbf{I}\right)^{-1}\mathbf{y}\right)$$

The input data $\mathbf{X}$ updates the covariance matrix $\mathbf{K}$, whose elements are computed through the covariance function (or kernel), $k(\mathbf{x}, \mathbf{x}')$

Hence, the negative log likelihood (the objective function) is given by,

$$E(\theta) = \frac{1}{2}\log|\mathbf{K}| + \frac{1}{2}\mathbf{y}^\top\left(\mathbf{K} + \sigma^2\mathbf{I}\right)^{-1}\mathbf{y}$$

where the *parameters* of the model are also embedded in the covariance function, they include the parameters of the kernel (such as lengthscale and variance), and the noise variance, $\sigma^2$.

Can be solved using the *Cholesky Decomposition*

- Is *cubic* in the number of data points AND the number of features: $\mathcal{O}(n^3 d^3)$

```
class GP():
    def __init__(self, X, y, sigma2, kernel, **kwargs):
        self.K = compute_kernel(X, X, kernel, **kwargs)
        self.X = X
        self.y = y
        self.sigma2 = sigma2
        self.kernel = kernel
        self.kernel_args = kwargs
        self.update_inverse()

    def update_inverse(self):
        # Precompute the inverse covariance and some quantities of inter
est
        ## NOTE: Not the correct *numerical* way to compute this! For ea
se of use.
        self.Kinv = np.linalg.inv(self.K+self.sigma2*np.eye(self.K.shape
[0]))
        # the log determinant of the covariance matrix.
        self.logdetK = np.linalg.det(self.K+self.sigma2*np.eye(self.K.sh
ape[0]))
        # The matrix inner product of the inverse covariance
        self.Kinvy = np.dot(self.Kinv, self.y)
        self.yKinvy = (self.y*self.Kinvy).sum()


    def log_likelihood(self):
        # use the pre-computes to return the likelihood
        return -0.5*(self.K.shape[0]*np.log(2*np.pi) + self.logdetK + se
lf.yKinvy)

    def objective(self):
        # use the pre-computes to return the objective function
        return -self.log_likelihood()
```

# Making predictions

The model makes predictions for $\mathbf{f}$ that are unaffected by future values of $\mathbf{f}^*$.
If we think of $\mathbf{f}^*$ as test points, we can still write down a joint probability density over the training observations, $\mathbf{f}$ and the test observations, $\mathbf{f}^*$.

This joint probability density will be Gaussian, with a covariance matrix given by our covariance function, $k(\mathbf{x}_i, \mathbf{x}_j)$

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}^* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^\top & \mathbf{K}_{*,*} \end{bmatrix}\right)$$

where $\mathbf{K}$ is the covariance computed between all the training points,
$\mathbf{K}_*$ is the covariance matrix computed between the training points and the test points,
$\mathbf{K}_{*,*}$ is the covariance matrix computed between all the tests points and themselves.

# Conditional Density

Just as in naive Bayes, we defined the joint density (although there it was over both the labels and the inputs, $p(\mathbf{y}, \mathbf{X})$and now we need to define *conditional* distributions that answer particular questions of interest.

We will need the *conditional density* for making predictions.

$$\mathbf{f}^*|\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}_f, \mathbf{C}_f)$$

with a mean given by

$$\boldsymbol{\mu}_f = \mathbf{K}_*^\top \left[\mathbf{K} + \sigma^2\mathbf{I}\right]^{-1}\mathbf{y}$$

and a covariance given by

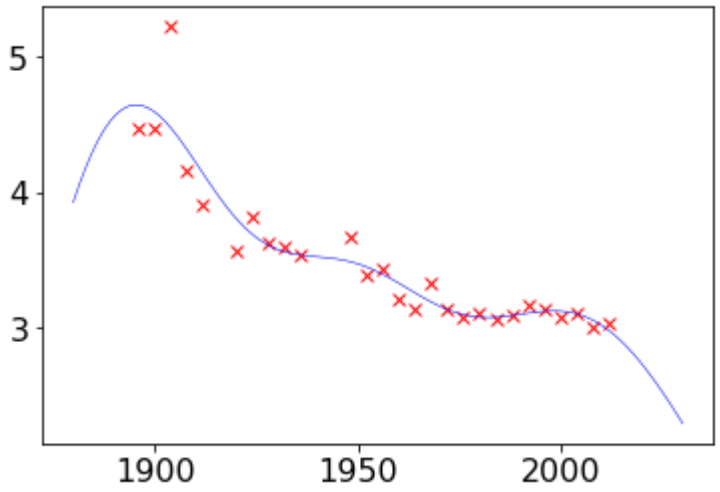
$$\mathbf{C}_f = \mathbf{K}_{*,*} - \mathbf{K}_*^\top \left[\mathbf{K} + \sigma^2\mathbf{I}\right]^{-1}\mathbf{K}_*.$$

Let's compute what those posterior predictions are for the olympic marathon data.

We can now get the mean and covariance:

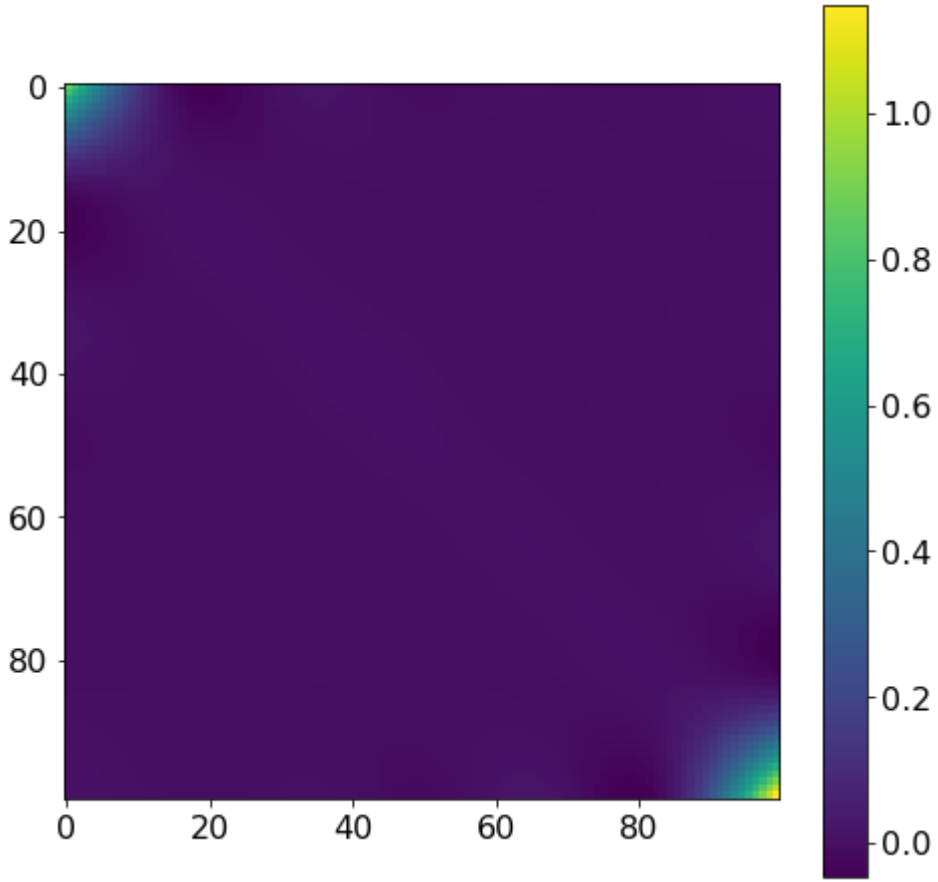
```
model = GP(x, y, sigma2, exponentiated_quadratic, variance=16.0, lengths
cale=32)
mu_f, C_f = model.posterior_f(x_pred)
```

Plot the mean:



The covariance looks like this:

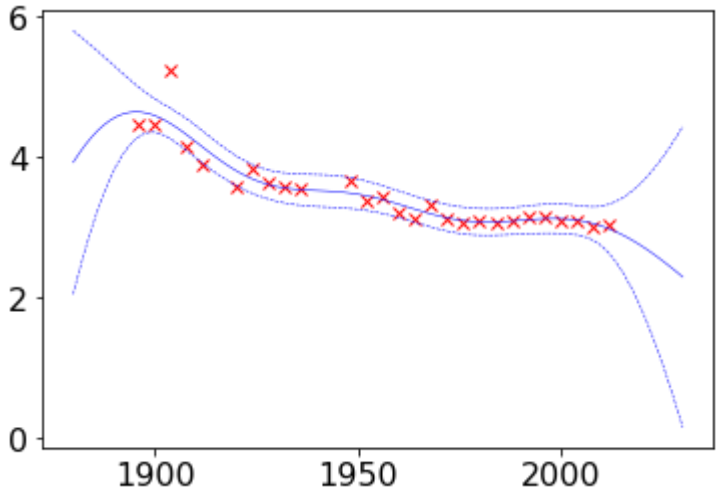
- Look along the diagonal
- High variance at the beginning and the end



Hence, we get:

- High uncertainty and the beginning and the end
- Very low uncertainty in the middle

```
var_f = np.diag(C_f)[:, None]
std_f = np.sqrt(var_f)
```



# Gaussian Processes with GPy

- `GPyRegression`
- Generate a kernel first
    - State the dimensionality of your input data
    - Variance and lengthscale are optional, default = 1

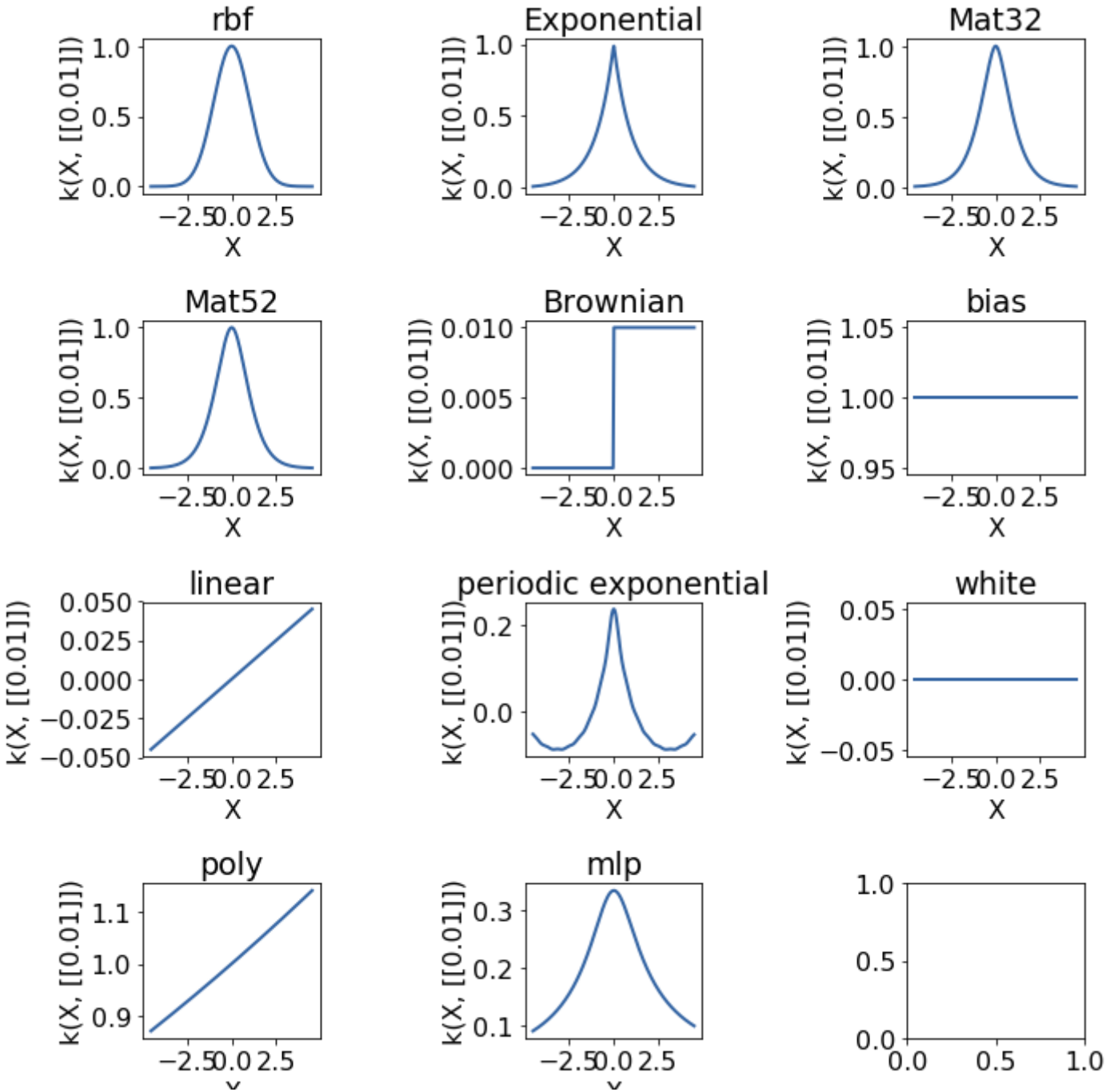
      ```
      kernel = GPy.kern.RBF(input_dim=1, variance=1., lengthscal
      e=1.)
      ```

    - Other kernels:

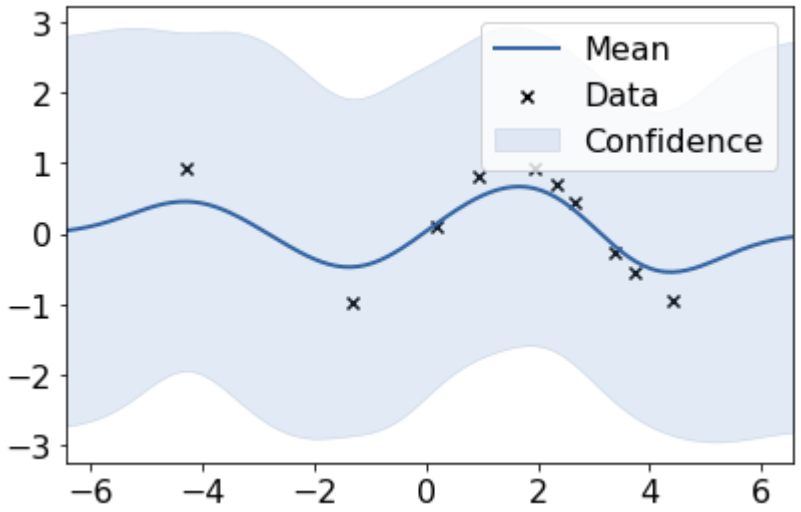
      ```
      GPy.kern.BasisFuncKernel?
      ```

- Build model:

  ```
  m = GPy.models.GPRegression(X,Y,kernel)
  ```

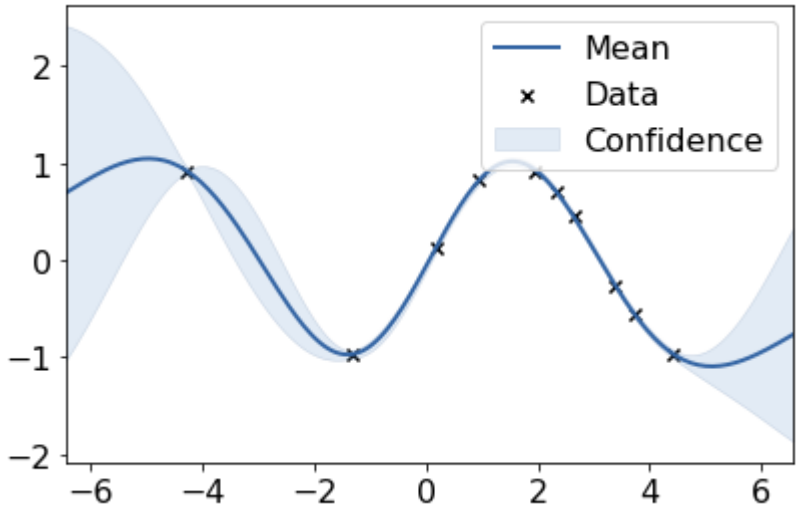

rbf
Exponential
Mat32
Mat52
Brownian
bias
linear
periodic exponential
white
poly
mlp
k(X, [[0.01]])
X

Build the untrained GP. The shaded region corresponds to ~95% confidence intervals (i.e. +/- 2 standard deviation)

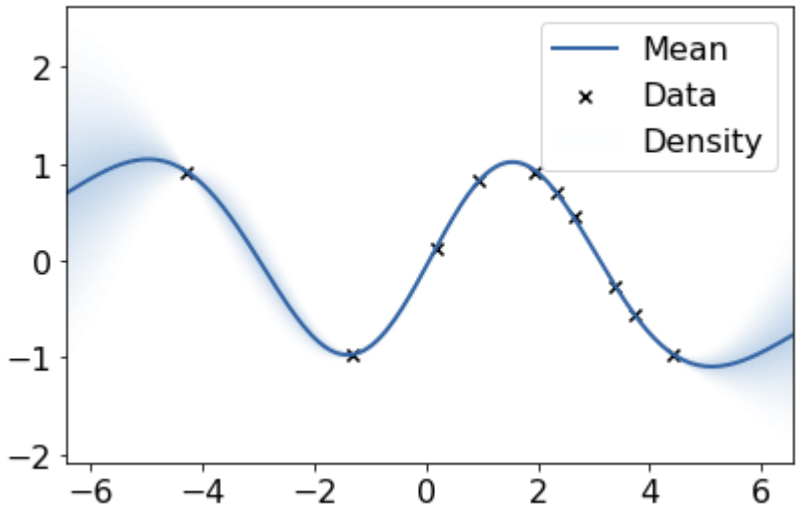


Train the model (optimize the parameters): maximize the likelihood of the data. Best to optimize with a few restarts: the optimizer may converges to the high-noise solution. The optimizer is then restarted with a few random initialization of the parameter values.

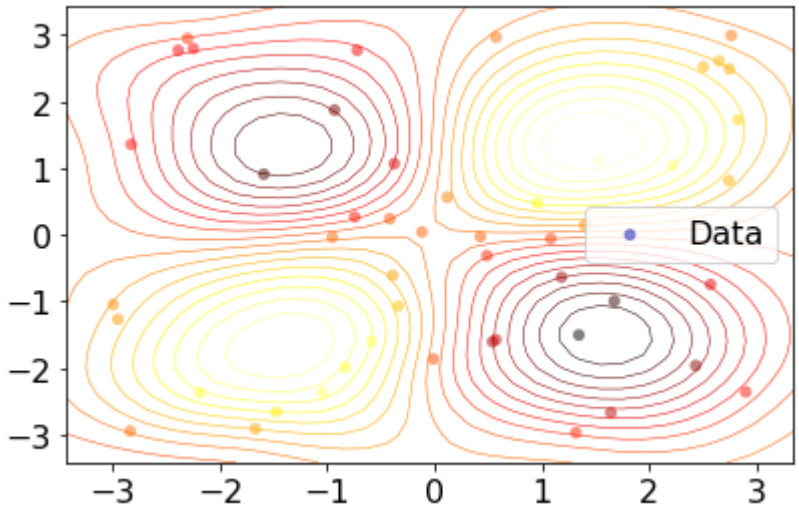
```
Optimization restart 1/3, f = -2.456493488261967
Optimization restart 2/3, f = -0.13080144014056394
Optimization restart 3/3, f = -2.456493488261998
```



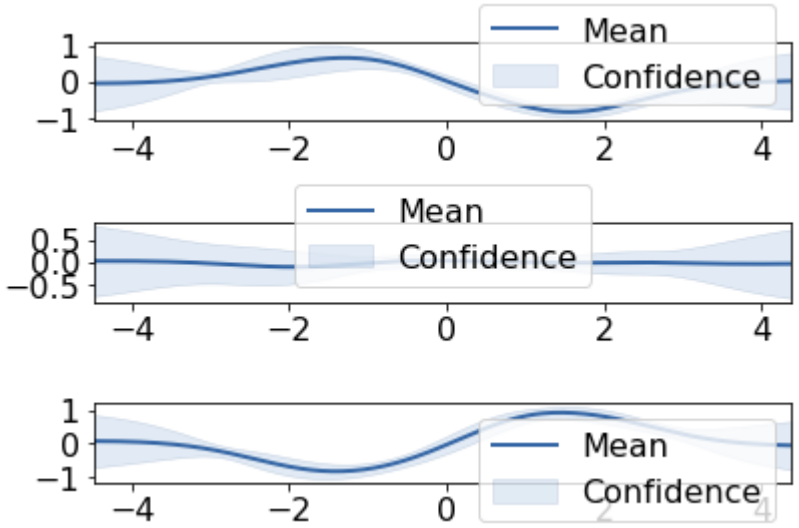
You can also plot densities



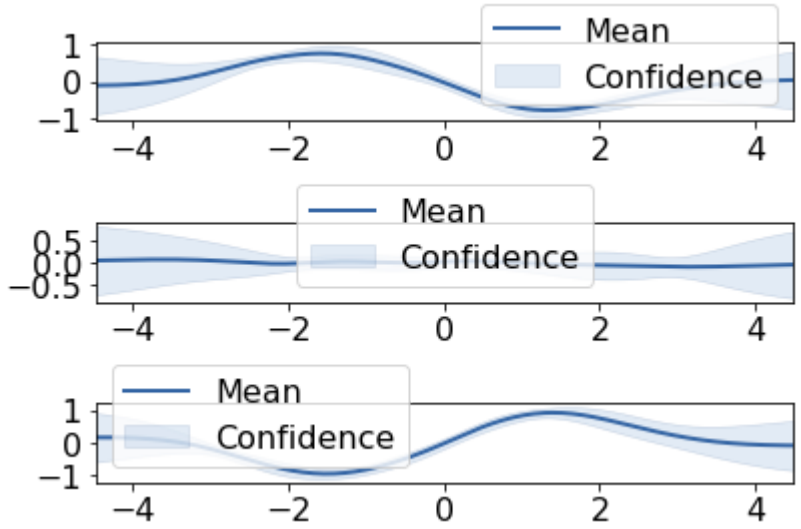
You can also show results in 2D



We can plot 2D slices using the `fixed_inputs` argument to the plot function. `fixed_inputs` is a list of tuples containing which of the inputs to fix, and to which value.



For vertical slices, simply fix the other input: `fixed_inputs=[(0,y)]`

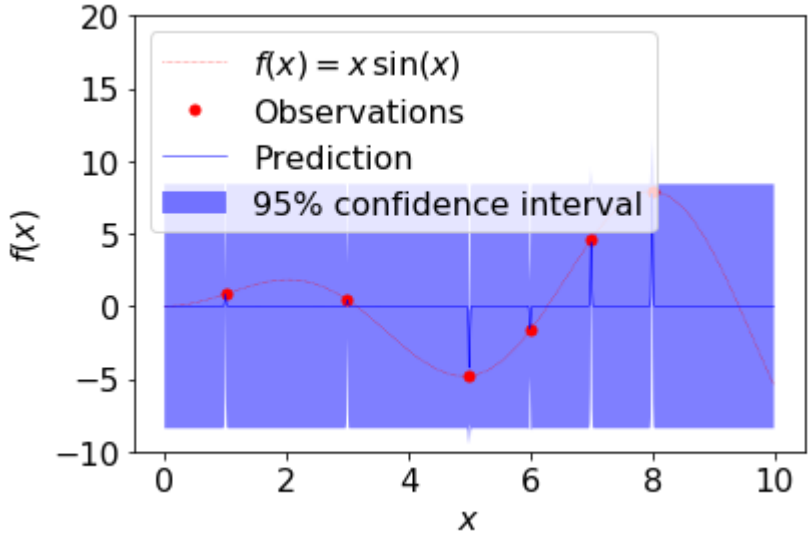


# Gaussian Processes with scikit-learn

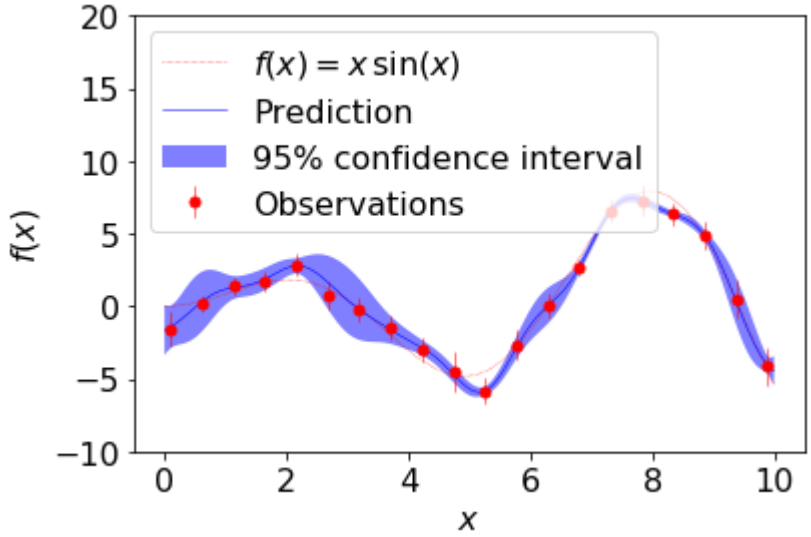
- `GaussianProcessRegressor`
- Hyperparameters:
    - `kernel`: kernel specifying the covariance function of the GP
        - Default: "1.0 * RBF(1.0)"
        - Typically leave at default. Will be optimized during fitting
    - `alpha`: regularization parameter
        - Tikhonov regularization of the assumed covariance between the training points.
        - Adds a (small) value to the diagonal of the kernel matrix during fitting.
        - Larger values:
            - correspond to increased noise level in the observations
            - also reduce potential numerical issues during fitting
        - Default: 1e-10
    - `n_restarts_optimizer`: number of restarts of the optimizer
        - Default: 0. Best to do at least a few iterations.
        - Optimizer finds the kernel's parameters which maximize the log-marginal likelihood
- Retrieve predictions and confidence interval after fitting:

```
y_pred, sigma = gp.predict(x, return_std=True)
```

Example


$f(x) = x\sin(x)$
Observations
Prediction
95% confidence interval
$f(x)$
$x$
20
15
10
5
0
−5
−10
0
2
4
6
8
10

Example with noisy data



# Gaussian processes: Conclusions

The advantages of Gaussian processes are:

- The prediction interpolates the observations (at least for regular kernels).
- The prediction is probabilistic (Gaussian) so that one can compute empirical confidence intervals.
- Versatile: different kernels can be specified.

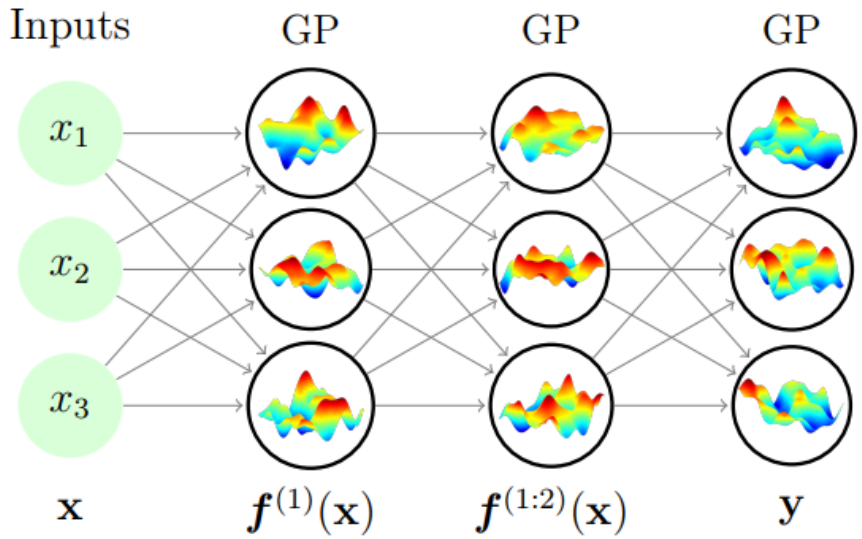
The disadvantages of Gaussian processes include:

- They are not sparse, i.e., they use the whole samples/features information to perform the prediction.
- They lose efficiency in high dimensional spaces – namely when the number of features exceeds a few dozens.

# Gaussian processes and neural networks

- You can prove that a Gaussian process is equivalent to a neural network with one layer and an infinite number of nodes
- You can build *deep Gaussian Processes* by constructing layers of GPs

A net with nonparametric activation functions corresponding to a 3-layer deep GP

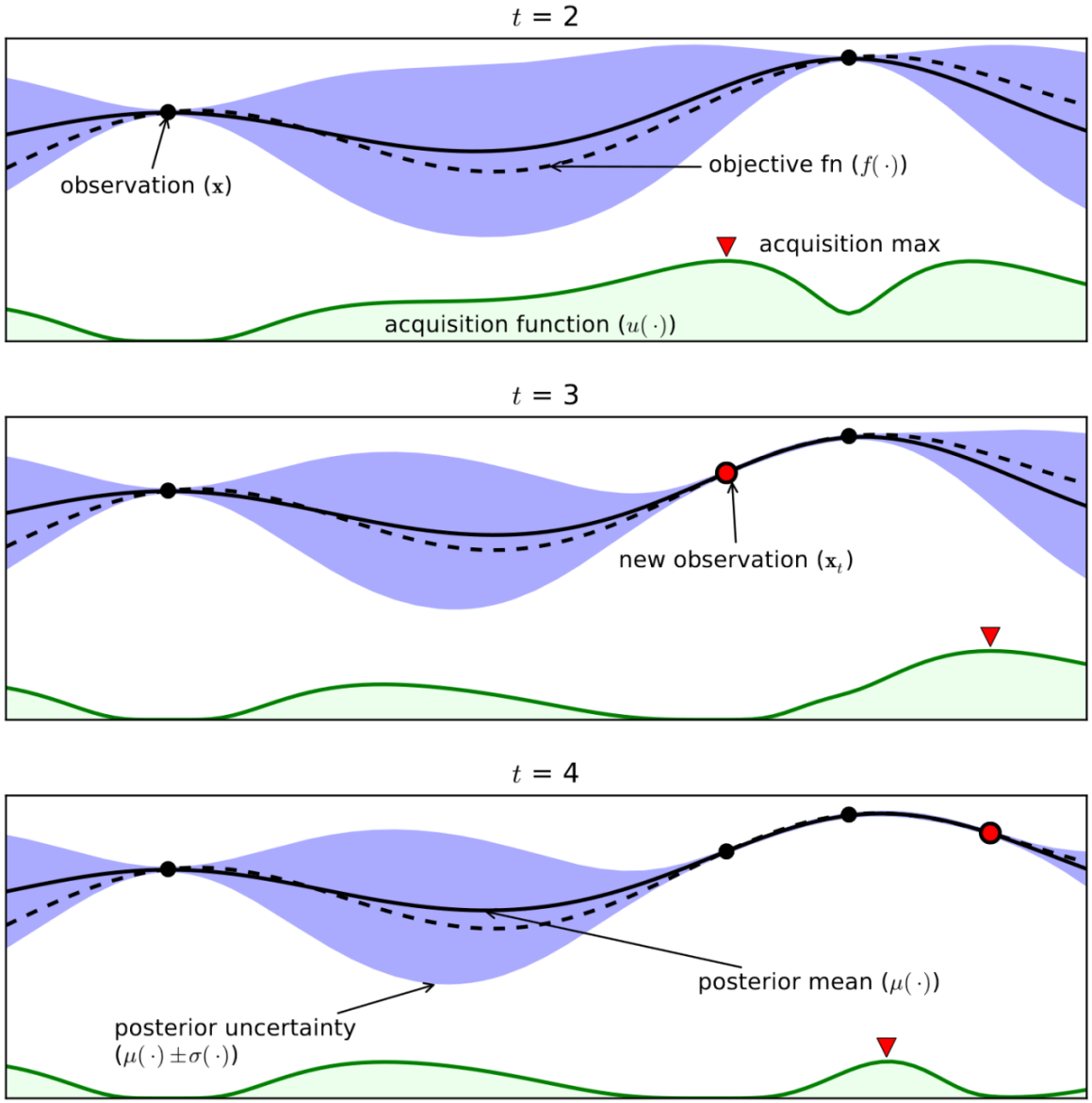


# Bayesian optimization

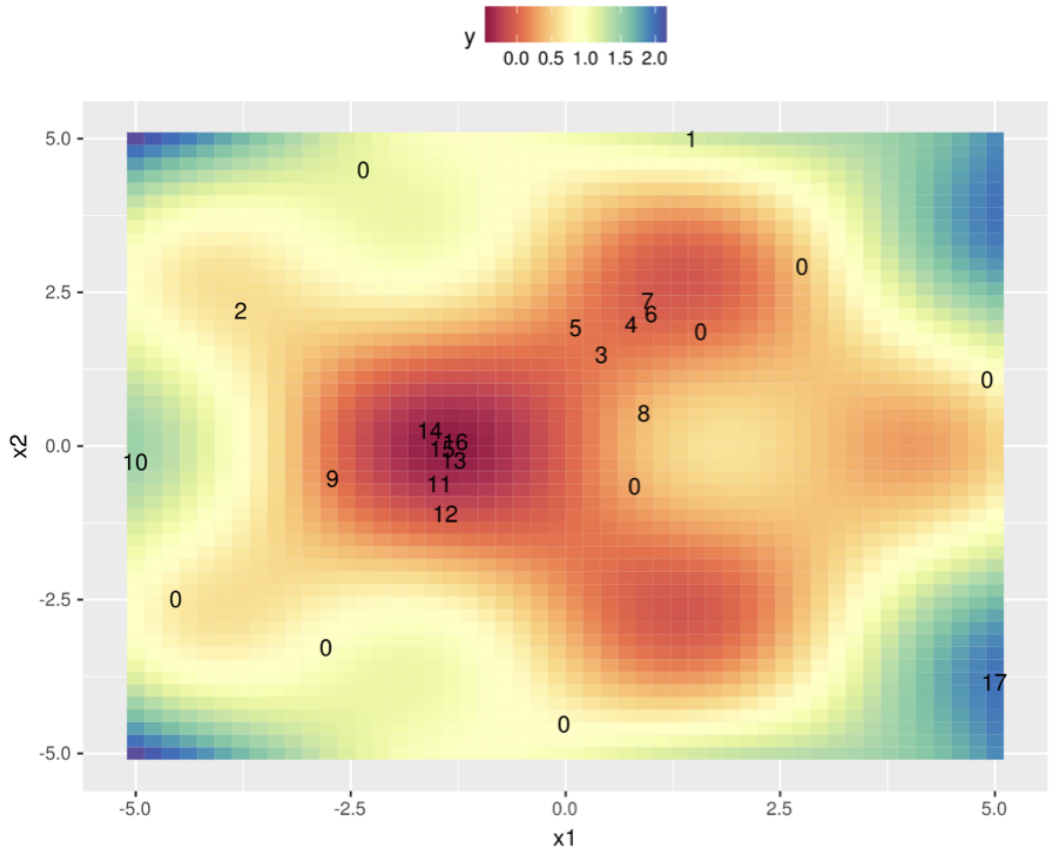
- The incremental updates you can do with Bayesian models allow a more effective way to optimize functions
    - E.g. to optimize the hyperparameter settings of a machine learning algorithm/pipeline
- After a number of random search iterations we know more about the performance of hyperparameter settings on the given dataset
- We can use this data to train a model, and predict which other hyperparameter values might be useful
    - More generally, this is called model-based optimization
    - This model is called a *surrogate model*
- This is often a probabilistic (e.g. Bayesian) model that predicts confidence intervals for all hyperparameter settings
- We use the predictions of this model to choose the next point to evaluate
- With every new evaluation, we update the surrogate model and repeat

## Example (see figure):

- Consider only 1 continuous hyperparameter (X-axis)
    - You can also do this for many more hyperparameters
- Y-axis shows cross-validation performance
- Evaluate a number of random hyperparameter settings (black dots)
    - Sometimes an initialization design is used
- Train a model, and predict the expected performance of other (unseen) hyperparameter values
    - Mean value (black line) and distribution (blue band)
- An *acquisition function* (green line) trades off maximal expected performace and maximal uncertainty
    - Exploitation vs exploration
- Optimal value of the asquisition function is the next hyperparameter setting to be evaluated
- Repeat a fixed number of times, or until time budget runs out


$t$ = 2
observation ($\mathbf{x}$)
objective fn ($f(\cdot)$)
acquisition max
acquisition function ($u(\cdot)$)
$t$ = 3
new observation ($\mathbf{x}_t$)
$t$ = 4
posterior mean ($\mu(\cdot)$)
posterior uncertainty
($\mu(\cdot) \pm \sigma(\cdot)$)

In 2 dimensions:



# Surrogate models

- Surrogate model can be anything as long as it can do regression and is probabilistic
- Gaussian Processes are commonly used
    - Smooth, good extrapolation, but don't scale well to many hyperparameters (cubic)
    - Sparse GPs: select ‘inducing points’ that minimize info loss, more scalable
    - Multi-task GPs: transfer surrogate models from other tasks
- Random Forests
    - A lot more scalable, but don't extrapolate well
    - Often an interpolation between predictions is used instead of the raw (step-wise) predictions
- Bayesian Neural Networks:
    - Expensive, sensitive to hyperparameters

# Acquisition Functions

- When we have trained the surrogate model, we ask it to predict a number of samples
    - Can be simply random sampling
    - Better: *Thompson sampling*
        - fit a Gaussian distribution (a mixture of Gaussians) over the sampled points
        - sample new points close to the means of the fitted Gaussians
- Typical acquisition function: *Expected Improvement*
    - Models the predicted performance as a Gaussian distribution with the predicted mean and standard deviation
    - Computes the *expected* performance improvement over the previous best configuration $\mathbf{X}^+$:

$$EI(X) := \mathbb{E}\left[\max\{0, f(\mathbf{X}^+) - f_{t+1}(\mathbf{X})\}\right]$$

    - Computing the expected performance requires an integration over the posterior distribution, but has a closed form solution (http://ash-aldujaili.github.io/blog/2018/02/01/ei/).

# Bayesian Optimization: conclusions

- More efficient way to optimize hyperparameters
- More similar to what humans would do
- Harder to parallellize
- Choice of surrogate model depends on your search space
    - Very active research area
    - For very high-dimensional search spaces, random forests are popular