CS-E4820 Machine Learning: Advanced Probabilistic Methods (spring 2021)

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Exercise 4, due on Tuesday February 16th at 23:00.

Problem 1: ML-II for a linear model

Fit the Bayesian linear parameter model to a given data 'ex4_1_data.txt' using the ML II approach. Optimize the hyperparameters α and β using grid search. Complete the template given below with your own code. Make predictions for the test data using the fitted model and compute the mean squared error for test data. Also plot the data and the fitted model.

[1]:
```
        # Starter code for problems 1 and 2.
        # NOTE: variables defined in this cell are used in code templates for␣
↪problem 1 and 2.
        import numpy as np
        import matplotlib.pyplot as plt

        # INITIALIZATION
        # Load the observations
        data = np.loadtxt('/coursedata/ex4_1_data.txt')
        x_obs = data[:,0]
        y_obs = data[:,1]

        # Training data
        N_train = 40
        x_train = x_obs[:N_train]
        y_train = y_obs[:N_train]

        # Validation data
        N_valid = 10
        x_valid = x_obs[N_train:N_train+N_valid]
        y_valid = y_obs[N_train:N_train+N_valid]

        # Testing data
        N_test = 10
        x_test = x_obs[N_train+N_valid:]
        y_test = y_obs[N_train+N_valid:]


        x_range = (-5, 5) # Possible values of x are in this range

        # Basis function parameters
        num_basis_functions = 11
        centers = np.linspace(x_range[0], x_range[1], num_basis_functions)
```

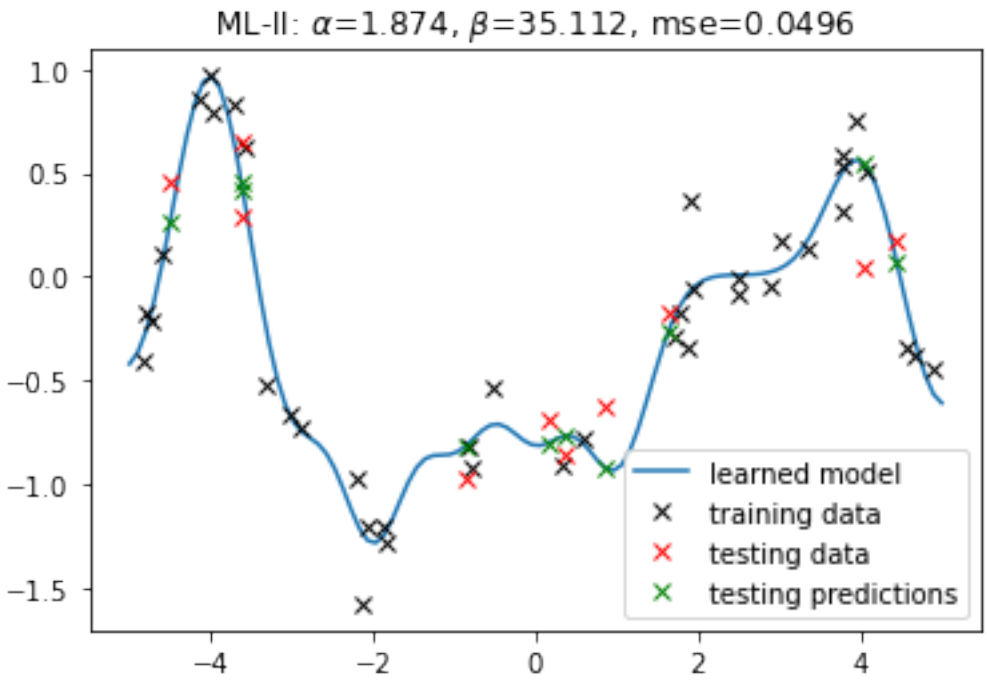
```
        lambdaval = 0.17
        # You can use here assume the correct basis function centers and lambda ...
        def rbf(x, centers, lambdaval):
        # Radial Basis Function output for input x
        #
        # Inputs:
        # x : input points (one-dimensional array)
        # centers : basis function centers (one-dimensional array)
        # lambdaval : basis function width (scalar)
        #
        # Output:
        # Radial Basis Functions evaluated at x (two-dimensional array with len(x)
        #                                        rows and len(centers) columns)
        d = x[:,np.newaxis] - centers[np.newaxis,:]
        y = np.exp(-0.5 * (d ** 2) / lambdaval)
        return y
```

[2]:

```
        # Template for problem 1
        def bayesian_linear_regression(phi_x, y, alpha, beta):
        # Bayesian linear parameter model
        #
        # Inputs:
        # phi_x : the basis function applied to x-data (two-dimensional array)
        # y : y-data (one-dimensional array)
        # alpha : the precision of the weight prior distribution (scalar)
        # beta : the precision of the assumed gaussian noise (scalar)
        #
        # Output:
        # the posterior mean, the posterior covariance, the log marginal likelihood

        N, B = phi_x.shape


        # Add here code to compute:
        # m = ? # EXERCISE: the posterior mean of w
        # S = ? # EXERCISE: the posterior covariance of w
        # S_inv = ? # EXERCISE: the inverse of S


        ### BEGIN SOLUTION
        S_inv = alpha * np.eye(B) + beta * np.dot(phi_x.T, phi_x)
        S = np.linalg.inv(S_inv)
        d = beta * np.dot(phi_x.T, y)
        m = np.dot(S, d)
```

```
        ### END SOLUTION

        # Note: This is a corrected version of equation 18.1.19 from Barbers book
        d = beta * np.dot(phi_x.T, y)
        log_likelihood = 0.5 * (-beta * np.dot(y, y) + d @ S @ d + np.log(np.
↪linalg.det(2 * np.pi * S)) +
        B * np.log(alpha) + N * np.log(beta) - N * np.log(2 * np.pi))
        return m, S, log_likelihood

        # Specify possible values for the alpha and beta parameters to test
        alphas = np.logspace(-3, 3, 100)
        betas = np.logspace(-3, 3, 100)

        # Grid search over possible values of alpha and beta
        best_log_likelihood = -np.inf # optimal parameter values maximize the␣
↪log likelihood
        for alpha in alphas:
        for beta in betas:
        # Use here functions rbf and bayesian_linear_regression to compute the
        # log marginal likelihood for given alpha and beta

        # What are the optimal values of alpha and beta, that maximize the␣
↪marginal likelihood?

        # best_alpha = ? # EXERCISE
        # best_beta = ? # EXERCISE

        # Fit the model one more time using the optimal alpha and beta and the␣
↪training data
        # to get m for the optimal model

        # best_m = ? # EXERCISE

        ### BEGIN SOLUTION
        phi = rbf(x_train, centers, lambdaval)
        m, S, log_likelihood = bayesian_linear_regression(phi, y_train, alpha,␣
↪beta)
        if log_likelihood > best_log_likelihood:
        best_alpha = alpha
        best_beta = beta
        best_m = m
        best_log_likelihood = log_likelihood
        ### END SOLUTION

        # Compute the final regression function
        x_coord = np.linspace(x_range[0], x_range[1], 100)
```

```
        # Compute the predicted values for inputs in x_coord using best_m
        # y_mean = ? # EXERCISE

        ### BEGIN SOLUTION
        y_mean = np.dot(rbf(x_coord, centers, lambdaval), best_m)
        ### END SOLUTION

        # Plot the final learned regression function, together with the samples
        plt.plot(x_coord, y_mean, label="learned model")
        plt.plot(x_train, y_train, 'kx', label="training data")
        plt.plot(x_test, y_test, 'rx', label="testing data")

        # Make predictions for inputs in the test data, so that you get
        # predictions 'y_pred' for inputs in x_test.
        # y_pred = ? #EXERCISE

        ### BEGIN SOLUTION
        y_pred = np.dot(rbf(x_test, centers, lambdaval), best_m)
        ### END SOLUTION

        # print(y_pred)

        # Plot the predictions
        plt.plot(x_test, y_pred, 'gx', label="testing predictions")

        # Compute the mean squared prediction error for the test data.
        # mse_test = ???

        ### BEGIN SOLUTION
        mse_test = np.mean((y_pred - y_test) ** 2)
        ### END SOLUTION

        plt.legend()
        plt.title("ML-II: $\\alpha$=%.3f, $\\beta$=%.3f, mse=%.4f" %
        (best_alpha, best_beta, mse_test))
        plt.show()
```



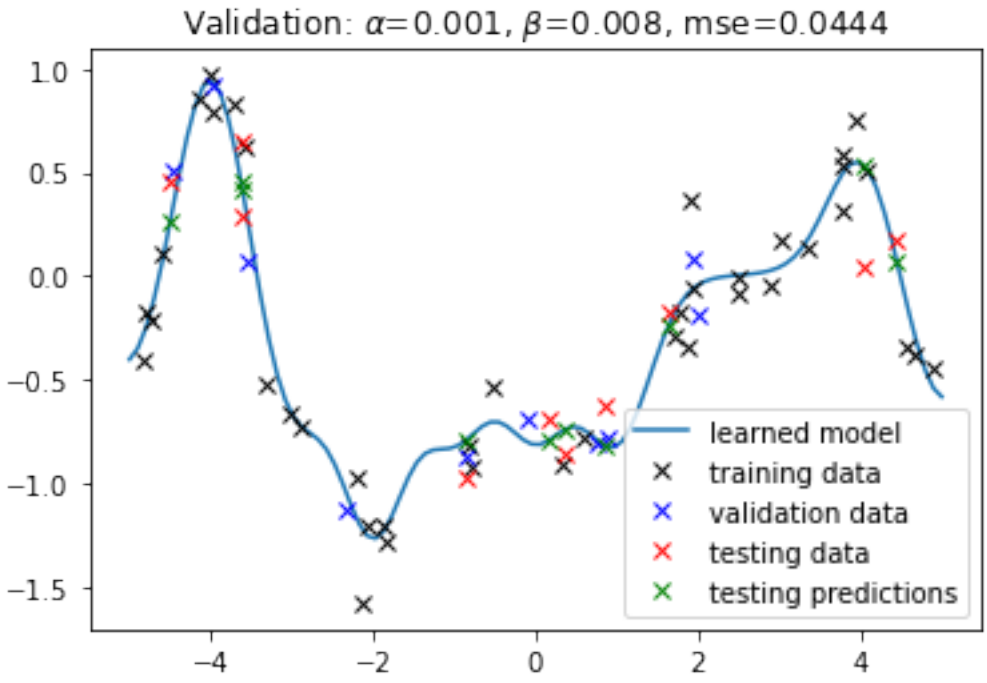
Problem 2: Optimizing hyperparameters with validation set

As in problem 1, fit the Bayesian linear parameter model to a given data 'ex4_1_data.txt', but optimize the hyperparameters α and β by dividing the training data into training and validation sets, and selecting the values of α and β that minimize the mean squared error for the validation set. Make predictions for the test data using the fitted model and compute the mean squared error for test data. Plot the data and the fitted model.

[3]:
```
        # Template for problem 2
        # Specify possible values for the alpha and beta parameters to test
        alphas = np.logspace(-3, 3, 100)
        betas = np.logspace(-3, 3, 100)

        # Grid search over possible values of alpha and beta
        mse_valid = np.zeros((len(alphas), len(betas)))
        for a, alpha in enumerate(alphas):
        for b, beta in enumerate(betas):

        # Use here functions rbf and bayesian_linear_regression to fit the
        # model and compute the prediction error (using mean squared error)
        # for the validation data

        ### BEGIN SOLUTION
        phi = rbf(x_train, centers, lambdaval)
```

```
        m, S, log_likelihood = bayesian_linear_regression(phi, y_train, alpha,␣
↪beta)
        y_pred_valid = np.dot(rbf(x_valid, centers, lambdaval), m)
        mse_valid[a, b] = np.mean((y_pred_valid - y_valid) ** 2)
        ### END SOLUTION

        # What are the optimal values of alpha and beta, that minimize the␣
↪prediction error in the validation data?
        # best_alpha = ? #EXERCISE
        # best_beta = ?  #EXERCISE

        ### BEGIN SOLUTION
        (best_a, best_b) = np.unravel_index(np.argmin(mse_valid), mse_valid.
↪shape)
        best_alpha = alphas[best_a]
        best_beta = betas[best_b]
        ### END SOLUTION

        # Fit the model one more time using the optimal alpha and beta and all␣
↪data
        # available for model fitting (both training and validation sets)
        # best_m = ? #EXERCISE

        ### BEGIN SOLUTION
        best_m, _, _ = bayesian_linear_regression(phi, y_train, best_alpha,␣
↪best_beta)
        ### END SOLUTION

        x_coord = np.linspace(x_range[0], x_range[1], 100)

        # Compute the predicted values for inputs in x_coord using best_m
        # y_mean = ? #EXERCISE

        ### BEGIN SOLUTION
        y_mean = np.dot(rbf(x_coord, centers, lambdaval), best_m)
        ### END SOLUTION

        # Plot the final learned regression function, together with the samples
        plt.plot(x_coord, y_mean, label="learned model")
        plt.plot(x_train, y_train, 'kx', label="training data")
        plt.plot(x_valid, y_valid, 'bx', label="validation data")
        plt.plot(x_test, y_test, 'rx', label="testing data")

        # Make predictions for inputs in the test data, so that you get
        # predictions 'y_pred' for inputs in x_test.
        # y_pred = ? ? # EXERCISE
```

```
        ### BEGIN SOLUTION
        y_pred = np.dot(rbf(x_test, centers, lambdaval), best_m)
        ### END SOLUTION

        # Plot the predictions
        plt.plot(x_test, y_pred, 'gx', label="testing predictions")

        # Compute the mean squared prediction error for the test data.
        # mse_test = ? # EXERCISE

        ### BEGIN SOLUTION
        mse_test = np.mean((y_pred - y_test) ** 2)
        ### END SOLUTION

        plt.legend()
        plt.title("Validation: $\\alpha$=%.3f, $\\beta$=%.3f, mse=%.4f" %
        (best_alpha, best_beta, mse_test))
        plt.show()
```



Problem 3: Poisson regression with Laplace approximation

Poisson regression can be used to model count data. A Poisson regression model can be defined as

$$y_i \mid \boldsymbol{\theta} \sim \text{Poisson}(\exp(\boldsymbol{\theta}^T \mathbf{x}_i)) \tag{1}$$

$$\theta \sim \mathcal{N}(\mathbf{0}, \alpha^{-1}\mathbf{I}) \tag{2}$$

where y_i are the observed counts, $\mathbf{x}_i$ the related covariates, $i = 1, \ldots, N$, and $\boldsymbol{\theta}^T$ are the regression weights. In this exercise, we approximate the posterior $p(\boldsymbol{\theta} \mid \mathbf{y})$ using the Laplace approximation. We will do this in two steps. In the first step we will derive the gradient $-\nabla \log p(\boldsymbol{\theta} \mid \mathbf{y})$ and in the second step we will write Laplace approximation. And finally, we will look compare the true density with the laplace approximation.

(a) Derive the gradient $-\nabla \log p(\boldsymbol{\theta} \mid \mathbf{y})$ and the Hessian $\mathbf{H} = -\nabla\nabla \log p(\boldsymbol{\theta} \mid y)$ needed for the Laplace approximation.

(b) Write the Laplace approximation as the density of a Gaussian distribution. What is the mean and the covariance matrix of this distribution?

(c) Compare the Laplace approximation to the true posterior (computed using numerical integration), in a case where we have one-dimensional covariates only. Use data given in the file 'ex4_4_data.txt' and hyperparameter value $\alpha = 10^{-2}$. Plot the two posteriors and the true value $\theta = \pi/4$ used to generate the data. Also plot the data with the regression line $\hat{y}_i = \exp(\hat{\theta} x_i)$ using the MAP estimate $\hat{\boldsymbol{\theta}}$. The code template below at the end of the notebook will help with this.

Solution

(a) The negative log posterior is given by

$$E(\boldsymbol{\theta}) = -\log p(\boldsymbol{\theta}|\mathbf{y}) = -\sum_i \left(y_i \cdot \boldsymbol{\theta}^T \mathbf{x}_i - \exp(\boldsymbol{\theta}^T \mathbf{x}_i) - \log y_i! \right) + \frac{\alpha}{2} \boldsymbol{\theta}^T \boldsymbol{\theta}.$$

Note that in the current context, E stands for *energy* (a term which derives from physics), **not** expectation. The gradient with respect to the parameters $\boldsymbol{\theta}$ is then

$$\frac{\partial E}{\partial \boldsymbol{\theta}} = -\sum_i \left(y_i \mathbf{x}_i - \mathbf{x}_i \exp(\boldsymbol{\theta}^T \mathbf{x}_i) \right) + \alpha \boldsymbol{\theta}$$

and the Hessian

$$\mathbf{H} = \frac{\partial^2 E}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T} = +\sum_i \mathbf{x}_i \mathbf{x}_i^T \exp(\boldsymbol{\theta}^T \mathbf{x}_i) + \alpha \mathbf{I}.$$

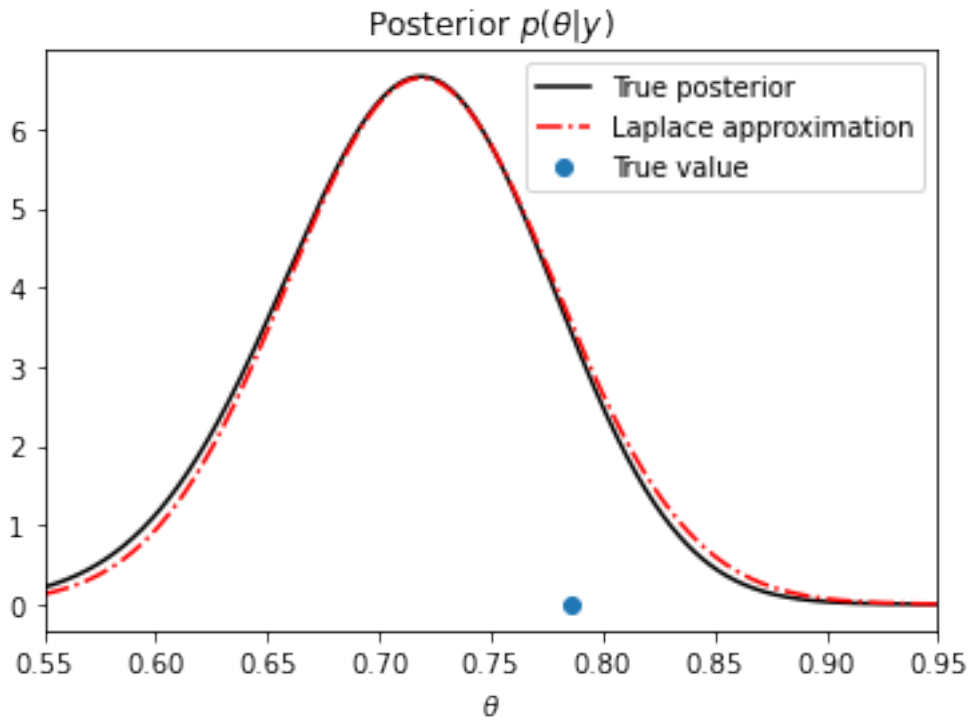
(b) The Laplace approximation is a Gaussian density $\mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}^*, \mathbf{S})$, where the mean $\boldsymbol{\theta}^*$ is the value of the parameter for which the gradient of the log posterior is 0, and the covariance matrix $\mathbf{S} = \mathbf{H}^{-1}|_{\boldsymbol{\theta}^*}$ is the inverse of the Hessian evaluated at $\boldsymbol{\theta}^*$.

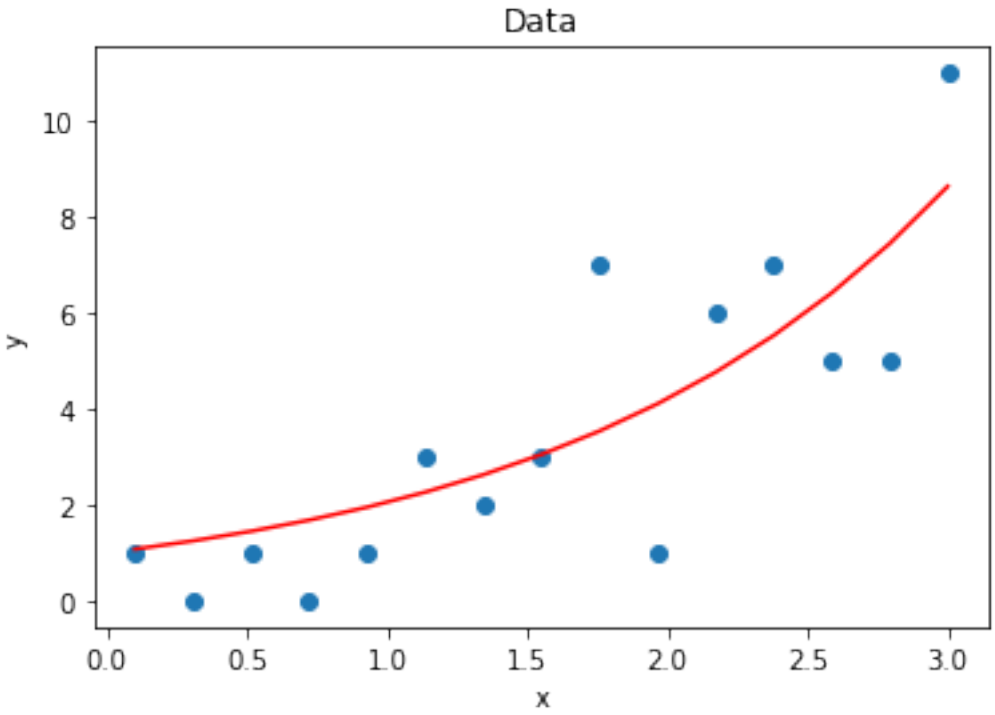
(c) Run the 3(c) solution code to see the plots.

[4]:
```
# Template for problem 3(c)
```

```
        # NOTE: starter code at the begining of the notebook and function␣
↪'bayesian_linear_regression'
        #       is required to run this cell

        import numpy as np
        import matplotlib.pyplot as plt
        from scipy.special import factorial
        from scipy.stats import norm

        # get some data
        data = np.loadtxt('/coursedata/ex4_4_data.txt')
        x = data[:,0]
        y = data[:,1]

        theta_true = np.pi / 4 # true parameter used to generate the data
        alpha = 1e-2 # prior's parameter

        # compute Laplace approximation
        theta_lapl = 0.5 # initial
        # iterate to optimum with newton's method to find the MAP estimate for␣
↪theta
        for iter in range(100):
        # compute gradient
        # grad = ???

        ### BEGIN SOLUTION
        grad = - np.dot(x, y) + np.dot(x, np.exp(x * theta_lapl)) + alpha *␣
↪theta_lapl
        ### END SOLUTION

        # compute Hessian
        # H = ???

        ### BEGIN SOLUTION
        H = np.dot(x, x * np.exp(x * theta_lapl)) + alpha
        ### END SOLUTION


        theta_lapl = theta_lapl - grad / H # do newton step

        # compute Hessian at optimum
        # H = ???

        ### BEGIN SOLUTION
        H = np.dot(x, x * np.exp(x * theta_lapl)) + alpha
        ### END SOLUTION
        print(H)
```

```
        difference = theta_lapl - theta_true

        # plot posterior densities
        theta = np.linspace(0.55, 0.95, 1000)
        post_true = np.zeros(len(theta))
        for i in range(len(theta)):
        # log posterior:
        post_true[i] = (np.dot(y, x * theta[i]) - np.sum(np.exp(x * theta[i]) -
        np.log(factorial(y))) - 0.5*alpha*np.dot(theta[i], theta[i]))

        M = np.amax(post_true)
        post_true = np.exp(post_true-M) / np.sum(np.exp(post_true-M)) /␣
↪(theta[1]-theta[0]) # normalize

        # compute approximative density at the points 'theta'
        # Hint: you can use norm.pdf from scipy.stats
        # post_laplace = ???


        ### BEGIN SOLUTION
        post_laplace = norm.pdf(theta,theta_lapl,np.sqrt(1/H))
        ### END SOLUTION

        plt.figure(1)
        plt.plot(theta, post_true, '-k', label="True posterior")
        plt.plot(theta, post_laplace, '-.r', label="Laplace approximation")
        plt.plot(theta_true, 0, 'o', label="True value")
        plt.xlim(0.55, 0.95)
        plt.xlabel('$\\theta$')
        plt.title('Posterior $p(\\theta|y)$')
        plt.legend()

        plt.figure(2)
        plt.plot(x, y, 'o', x, np.exp(theta_lapl*x), '-r')
        plt.xlabel('x')
        plt.ylabel('y')
        plt.title('Data')
        plt.show()
```


Posterior $p(\theta|y)$
True posterior
Laplace approximation
True value
0
1
2
3
4
5
6
0.55
0.60
0.65
0.70
0.75
0.80
0.85
0.90
0.95
θ


Data
0
2
4
6
8
10
y
0.0
0.5
1.0
1.5
2.0
2.5
3.0
x