Diagnostics for Posterior Predictive

Contents


```
import numpy as np
np.set_printoptions(precision=3)
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
sns.set(rc={"figure.dpi":100, "savefig.dpi":300})
sns.set_context("notebook")
sns.set_style("ticks")

import scipy
import scipy.stats as st
import urllib.request
import os

def download(
    url : str,
    local_filename : str = None
):
    """Download a file from a url.

    Arguments
    url            -- The url we want to download.
    local_filename -- The filemame to write on. If not
                      specified
    """
    if local_filename is None:
        local_filename = os.path.basename(url)
    urllib.request.urlretrieve(url, local_filename)
```

Objectives

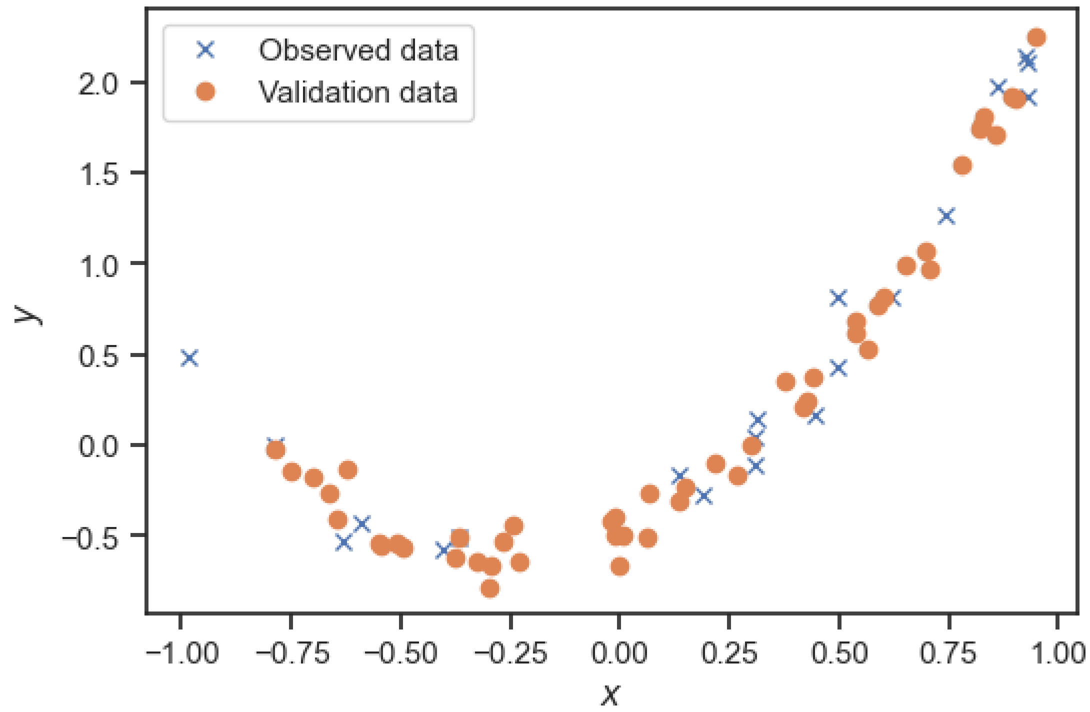
- To introduce measures that quantify how good the posterior predictive distribution is.

Example (Quadratic)

We start with our quadratic synthetic example because we know that our model is adequate. You will see how the standarized errors will turn out perfect.

```
np.random.seed(12345)

num_obs = 20
x = -1.0 + 2 * np.random.rand(num_obs)
w0_true = -0.5
w1_true = 1.0
w2_true = 2.0
sigma_true = 0.1

true_func = lambda x: (
    w0_true
    + w1_true * x
    + w2_true * x ** 2
)

observe_func = lambda x: (
    true_func(x)
    + sigma_true * np.random.randn(x.shape[0])
)

y = observe_func(x)

num_valid = 50
x_valid = -1.0 + 2 * np.random.rand(num_valid)
y_valid = observe_func(x_valid)

fig, ax = plt.subplots()
ax.plot(x, y, 'x', label='Observed data')
ax.plot(x_valid, y_valid, 'o', label='Validation data')
ax.set_xlabel('$x$')
ax.set_ylabel('$y$')
plt.legend(loc='best');
```

Notice how the true and observed functions are generated here, and how y is formed and plotted



Let’s copy paste again our previous code.

> **Note**
>
> In general, it is a bad idea to copy paste your code from notebook to notebook. This can introduce bugs that are very hard to fix. The best approach would be to put all our code in a text file, say `regression.py` and then import everything from the file. We will try this out in the homework assignment.

```
def get_polynomial_design_matrix(x, degree):
    """Return the polynomial design matrix of ``degree`` evaluated at ``x``.

    Arguments:
    x      -- A 2D array with only one column.
    degree -- An integer greater than zero.
    """
    assert isinstance(x, np.ndarray), 'x is not a numpy array.'
    assert x.ndim == 2, 'You must make x a 2D array.'
    assert x.shape[1] == 1, 'x must be a column.'
    cols = []
    for i in range(degree+1):
        cols.append(x ** i)
    return np.hstack(cols)

def get_fourier_design_matrix(x, L, num_terms):
    """Fourier expansion with ``num_terms`` cosines and sines.

    Arguments:
    x          --  A 2D array with only one column.
    L          --  The "length" of the domain.
    num_terms  --  How many Fourier terms do you want.
                   This is not the number of basis
                   functions you get. The number of basis functions
                   is 1 + num_terms / 2. The first one is a constant.
    """
    assert isinstance(x, np.ndarray), 'x is not a numpy array.'
    assert x.ndim == 2, 'You must make x a 2D array.'
    assert x.shape[1] == 1, 'x must be a column.'
    N = x.shape[0]
    cols = [np.ones((N, 1))]
    for i in range(int(num_terms / 2)):
        cols.append(np.cos(2 * (i+1) * np.pi / L * x))
        cols.append(np.sin(2 * (i+1) * np.pi / L * x))
    return np.hstack(cols)

def get_rbf_design_matrix(x, x_centers, ell):
    """Radial basis functions design matrix.

    Arguments:
    x        --  The input points on which you want to evaluate the
                 design matrix.
    x_center --  The centers of the radial basis functions.
    ell      --  The lengthscale of the radial basis function.
    """
    assert isinstance(x, np.ndarray), 'x is not a numpy array.'
    assert x.ndim == 2, 'You must make x a 2D array.'
    assert x.shape[1] == 1, 'x must be a column.'
    N = x.shape[0]
    cols = [np.ones((N, 1))]
    for i in range(x_centers.shape[0]):
        cols.append(np.exp(-(x - x_centers[i]) ** 2 / ell))
    return np.hstack(cols)

def plot_posterior_predictive(
    model,
    xx,
    phi_func,
    phi_func_args=(),
    y_true=None
):
    """Plot the posterior predictive separating
    aleatory and espitemic uncertainty.

    Arguments:
    model    -- A trained model.
    xx       -- The points on which to evaluate
                the posterior predictive.
    phi_func -- The function to use to compute
                the design matrix.

    Keyword Arguments:
    phi_func_args -- Any arguments passed to the
                     function that calculates the
                     design matrix.
    y_true        -- The true response for plotting.
    """
    Phi_xx = phi_func(
        xx[:, None],
        *phi_func_args
    )
    yy_mean, yy_measured_std = model.predict(
        Phi_xx,
        return_std=True
```

```
    )

    sigma = np.sqrt(1.0 / model.alpha_)
    yy_std = np.sqrt(yy_measured_std ** 2 - sigma**2)
    yy_le = yy_mean - 2.0 * yy_std
    yy_ue = yy_mean + 2.0 * yy_std
    yy_lae = yy_mean - 2.0 * yy_measured_std
    yy_uae = yy_mean + 2.0 * yy_measured_std

    fig, ax = plt.subplots()
    ax.plot(xx, yy_mean, 'r', label="Posterior mean")
    ax.fill_between(
        xx,
        yy_le,
        yy_ue,
        color='red',
        alpha=0.25,
        label="95% epistemic credible interval"
    )
    ax.fill_between(
        xx,
        yy_lae,
        yy_le,
        color='green',
        alpha=0.25
    )
    ax.fill_between(
        xx,
        yy_ue,
        yy_uae,
        color='green',
        alpha=0.25,
        label="95% epistemic + aleatory credible interval"
    )
    ax.plot(x, y, 'kx', label='Observed data')
    if y_true is not None:
        ax.plot(xx, y_true, "--", label="True response")
    ax.set_xlabel('$x$')
    ax.set_ylabel('$y$')
    plt.legend(loc="best");

def plot_posterior_samples(
    model,
    xx,
    phi_func,
    phi_func_args=(),
    num_samples=10,
    y_true=None,
    nugget=1e-6
):
    """Plot posterior samples from the model.

    Arguments:
    model    -- A trained model.
    xx       -- The points on which to evaluate
                the posterior predictive.
    phi_func -- The function to use to compute
                the design matrix.

    Keyword Arguments:
    phi_func_args -- Any arguments passed to the
                     function that calculates the
                     design matrix.
    num_samples   -- The number of samples to take.
    y_true        -- The true response for plotting.
    nugget        -- A small number to add the covariance
                     if it is not positive definite
                     (numerically).
    """
    Phi_xx = phi_func(
        xx[:, None],
        *phi_func_args
    )
    m = model.coef_
    S = model.sigma_
    w_post = st.multivariate_normal(
        mean=m,
        cov=S + nugget * np.eye(S.shape[0])
    )
    fig, ax = plt.subplots()
    for _ in range(num_samples):
        w_sample = w_post.rvs()
        yy_sample = Phi_xx @ w_sample
        ax.plot(xx, yy_sample, 'r', lw=0.5)
    ax.plot([], [], "r", lw=0.5, label="Posterior samples")
    ax.plot(x, y, 'kx', label='Observed data')
    ax.plot(xx, yy_true, label='True response surface')
```

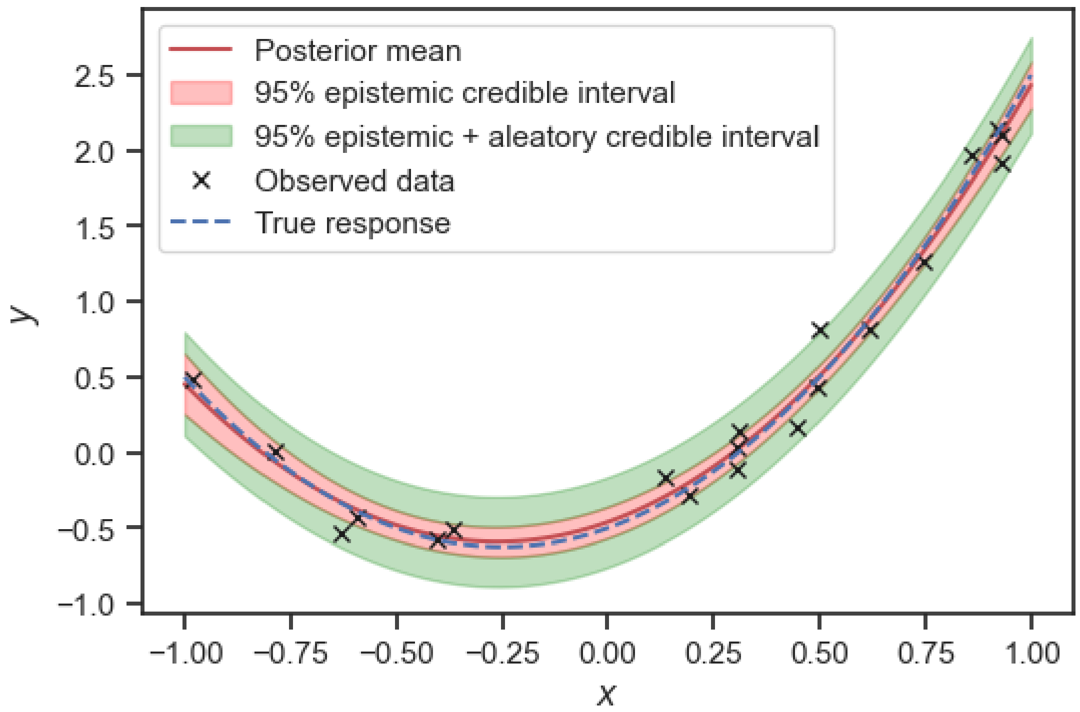
```
    ax.set_xlabel('$x$')
    ax.set_ylabel('$y$')
    plt.legend(loc="best");
```

Let's fit the model using automatic relevance determination:

```
from sklearn.linear_model import ARDRegression

# Parameters
degree = 4

# Design matrix
Phi = get_polynomial_design_matrix(x[:, None], degree)

# Fit
model = ARDRegression(
    fit_intercept=False
).fit(Phi, y)
```

Let's visualize the resulting model:

```
xx = np.linspace(-1, 1, 100)

plot_posterior_predictive(
    model,
    xx,
    get_polynomial_design_matrix,
    phi_func_args=(degree,),
    y_true=true_func(xx)
)
```

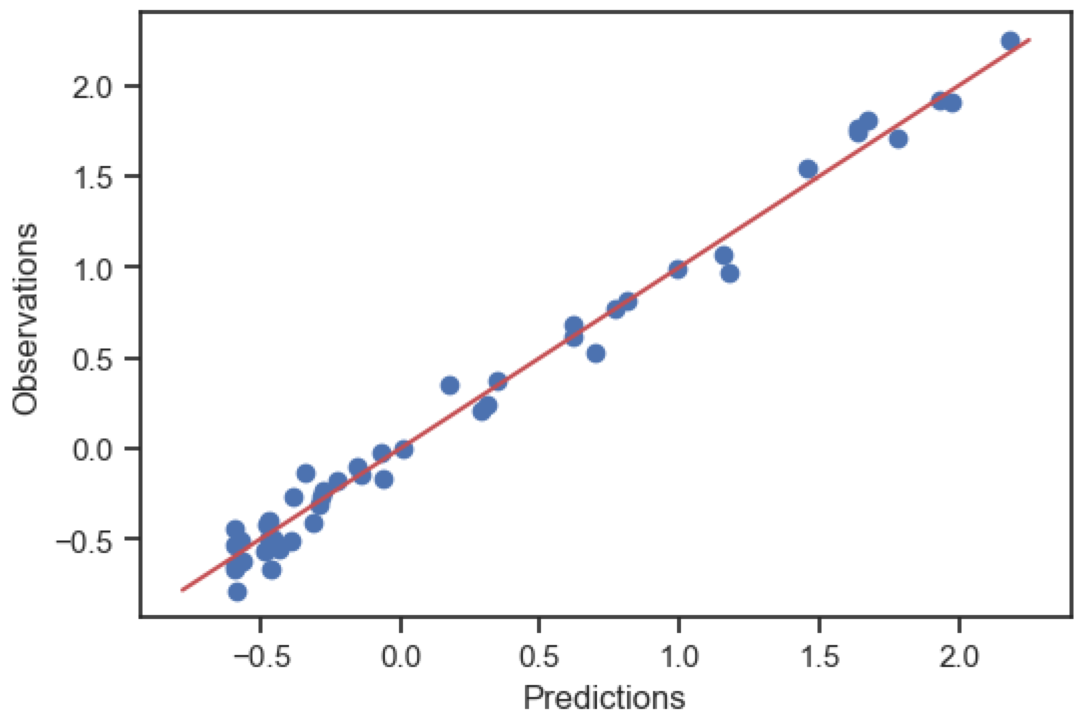


And now let's make predictions on the validation data:

```
Phi_valid = get_polynomial_design_matrix(
    x_valid[:, None],
    degree
)
y_predict, y_std = model.predict(
    Phi_valid,
    return_std=True
)
```

First, let's do the observations vs predictions plot:

```
fig, ax = plt.subplots()
ax.plot(y_predict, y_valid, 'o')
yys = np.linspace(
    y_valid.min(),
    y_valid.max(),
    100)
ax.plot(yys, yys, 'r-')
ax.set_xlabel('Predictions')
ax.set_ylabel('Observations');
```



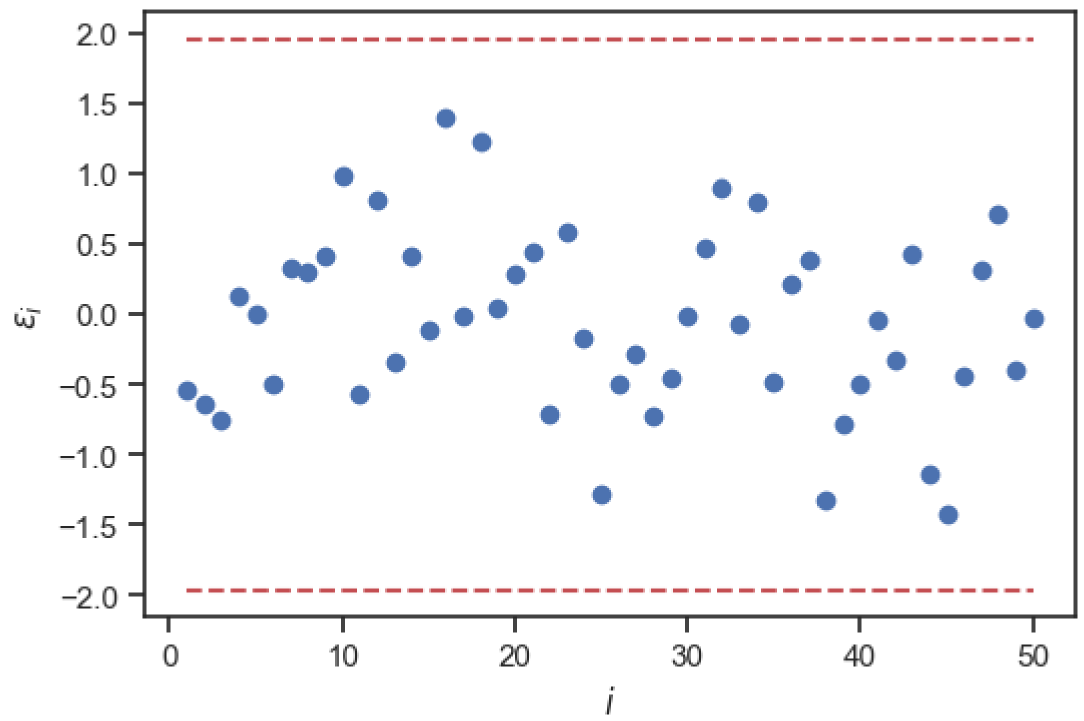
It's okay. However, notice that the predictions do not fall on the red line because there is a little bit of noise on the observations.

Let's now compute the standarized errors:

```
eps = (y_valid - y_predict) / y_std
```

Remember, that if the model is correct, the standarized errors must follow a standard normal. There are various ways to check this. First, let's just plot them:

```
idx = np.arange(1, eps.shape[0] + 1)

fig, ax = plt.subplots()
ax.plot(idx, eps, 'o', label='Standarized errors')
ax.plot(idx, 1.96 * np.ones(eps.shape[0]), 'r--')
ax.plot(idx, -1.96 * np.ones(eps.shape[0]), 'r--')
ax.set_xlabel('$i$')
ax.set_ylabel('$\epsilon_i$');
```



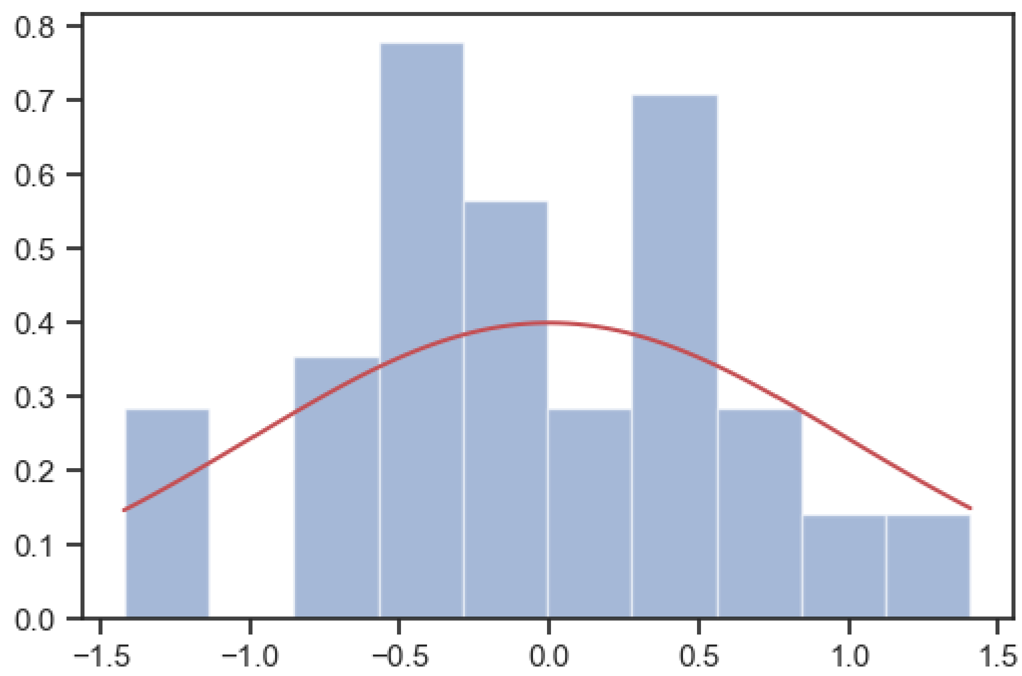
credible interval here determined by +/- 2*sigma

Notice that the majority of the standarized errors fall within the 95% central credible interval for $N(0,1)$. This is an indication that the model is good.

The other plot we can do is the histogram of the standarized errors compared to the probability density of the standard normal:

What if you wanted to get the samples from the posterior? You would have to do a little bit of manual work to translate the posterior weights and their variance back to the original values... because the built-ins that we are using are taking an approach that subtracts off the mean before performing the computations

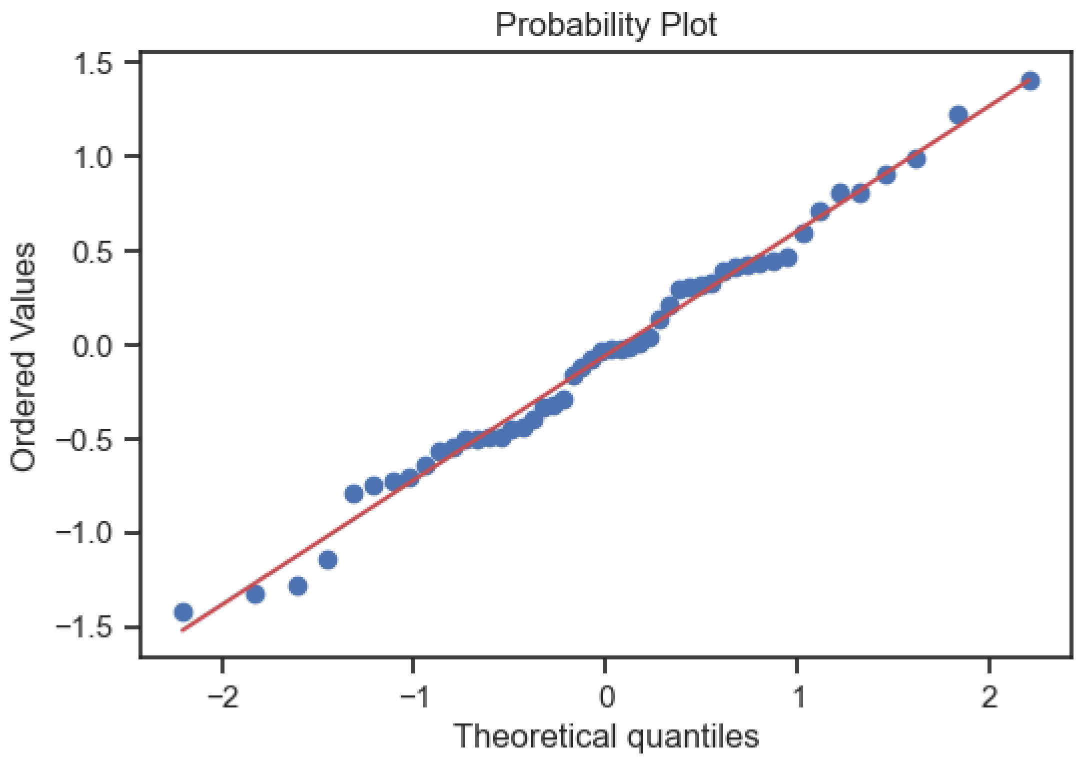
```
import scipy.stats as st

fig, ax = plt.subplots()
ax.hist(eps, alpha=0.5, density=True)
ee = np.linspace(eps.min(), eps.max(), 100)
ax.plot(ee, st.norm.pdf(ee), 'r');
```



Not perfect, but a pretty good fit.

The final diagnostic is the so call quantile-quantile plot. This compares the empirical quantiles of the standarized errors (computed by building and inverting the empirical cummulative distribution function, see Lecture 9). Here is how to do it:

```
fig, ax = plt.subplots()
st.probplot(eps, dist=st.norm, plot=ax);
```



This is also indicative of a pretty good fit.

Questions

- Rerun the code blocks above with a large number of training observations, say 100. Did the diagnosics improve or are they the same?
- Keep the number of training observations to 100 and change the validation points to 1000. How do the diagnostics look like now?
- Let's now try a model that is not adequate for the data. Set the polynomial degree to 1 and rerun everything. How do the diagnostics look like now?

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