Dropout as Regularization and Bayesian Approximation

Weidong Xu, Zeyu Zhao, Tianning Zhao

Our assigned paper is Improving neural networks by preventing co-adaptation of feature detectors (https://arxiv.org/pdf/1207.0580.pdf). In our tutorial, we also implemented models in the paper Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning (https://arxiv.org/pdf/1506.02142.pdf) to show that dropout can provide model uncertainty.

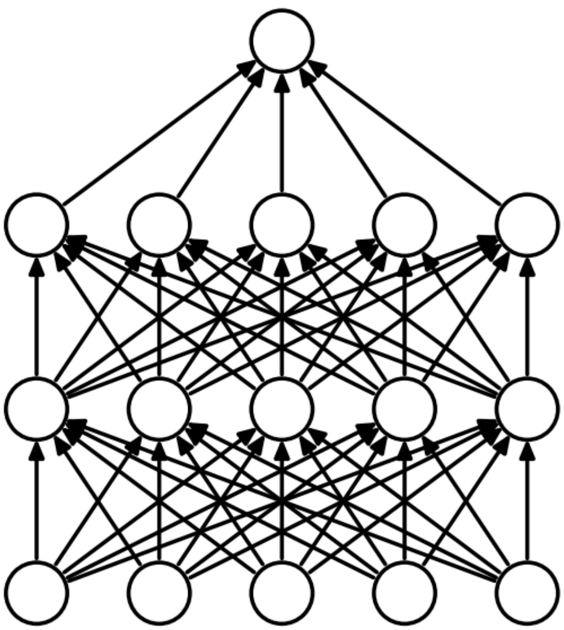
Abstract: This tutorial aims to give readers a complete view of dropout, which includes the implementation of dropout, how to use dropout and why dropout is useful. Basically, dropout can (1) reduce overfitting (so test results will be better) and (2) provide model uncertainty like Bayesian models we see in the class (Bayesian Approximation).

Warning: Some parts of the notebook is very slow to run so we commented them out and provided the saved results. To re-run those parts, you will need to uncomment the code and run with GPU and CUDA support. Except the commented part, this notebook can run without GPU.

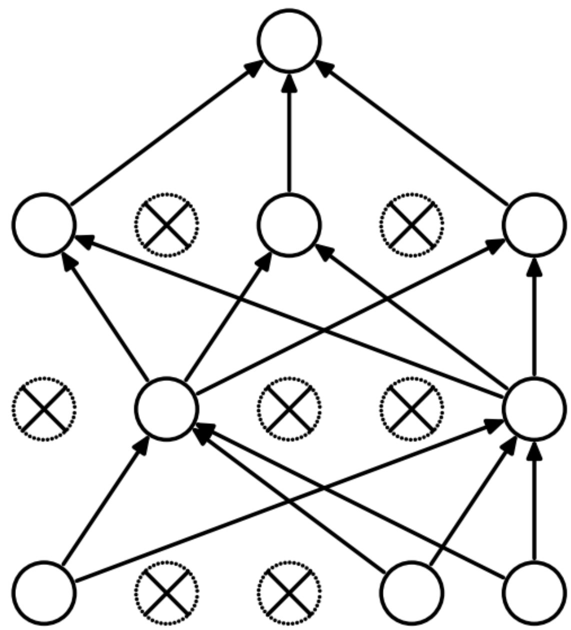
Table of Content:

1. Introduction

Deep neural network is a very powerful tool in machine learning. Multiple non-linear hidden layers enable the model to learn complicated relationships between input and output. However, when the training set is small, there are different parameter settings that would fits training set perfectly, but the one complex parameter setting tends to perform poorly on the test dataset, ie we got the problem of overfitting. One way to solve this problem is by averaging predictions of different neural networks , but this becomes computationally expensive when applied to large datasets. The alternative that makes it possible to train a huge number of different networks in a reasonable time is dropout, which randomly omits some hidden units i.e. feature detectors to prevent co-adaption. The idea of dropout model can be shown as below.



(a) Standard Neural Net



(b) After applying dropout.

ref: Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., & Salakhutdinov, R. (2014). Dropout: A simple way to prevent neural networks from overfitting. The Journal of Machine Learning Research, 15(1), 1929-1958.

2. Model Description

With dropout, the feed-forward operation of neural networks can be described as :

$$
\begin{gathered}
r_j^{(l)} \sim Bernoulli(p), \\
\tilde{y}^{(l)} = r^{(l)} \times y^{(l)}, \\
z_i^{(l+1)} = w_i^{(l+1)} \tilde{y}^{(l)} + b_i^{(l+1)}, \\
y_i^{(l+1)} = f(z_i^{(l+1)})
\end{gathered}
$$

where l is the index the hidden layers of the network, $z^{(l)}$ denote the vector of inputs into layer l, $y^{(l)}$ denote the vector of outputs from layer l ($y^{(0)} = x$ is the input). $w^{(l)}$ and $b^{(l)}$ are the weights and biases at layer l. f is any activation function.

With this, the standard stochastic gradient descent procedure was used for training the dropout neural networks on mini-batches of training cases.

For testing, we use the “mean network” that contains all of the hidden units with their outgoing weights halved instead of averaging over a large number of dropout networks.

3. Dropout Implementation

All our implementations are based on PyTorch. The model training is on GPU and all other tasks are on CPU (so readers with no GPUs can run our notebook). To switch between GPU and CPU, you can add or remove `.cuda()` in the code.

Import libraries

In [1]:
```
import warnings
warnings.filterwarnings("ignore")

import numpy as np
import pandas as pd
import time
import h5py
from scipy.ndimage.interpolation import rotate

import matplotlib
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
import matplotlib.gridspec as gridspec

import seaborn as sns
%matplotlib inline

import torch
import torchvision
from torchvision import datasets
from torchvision import transforms
from torch.autograd import Variable
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
from torch.utils.data.sampler import SubsetRandomSampler

import pymc3 as pm
```

Dropout Implementation

Below is the dropout layer we implemented, based on PyTorch.

We should multiply the dropout output by $\frac{1}{1-p}$ where p is the dropout rate to compensate for the dropped neurons. We implemented a dropout layer below, it should have same functionality as `nn.Dropout` in Pytorch.

We will use `MyDropout` in our first example network to show the implementation works. However, since `nn.Dropout` is more efficient than our implementation, we will use `nn.Dropout` for all remaining networks.

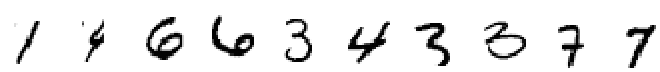
In [2]:
```
class MyDropout(nn.Module):
    def __init__(self, p=0.5):
        super(MyDropout, self).__init__()
        self.p = p
        # multiplier is 1/(1-p). Set multiplier to 0 when p=1 to avoid
 error...
        if self.p < 1:
            self.multiplier_ = 1.0 / (1.0-p)
        else:
            self.multiplier_ = 0.0
    def forward(self, input):
        # if model.eval(), don't apply dropout
        if not self.training:
            return input

        # So that we have `input.shape` numbers of Bernoulli(1-p) samp
les
        selected_ = torch.Tensor(input.shape).uniform_(0,1)>self.p

        # To support both CPU and GPU.
        if input.is_cuda:
            selected_ = Variable(selected_.type(torch.cuda.FloatTensor
), requires_grad=False)
        else:
            selected_ = Variable(selected_.type(torch.FloatTensor), re
quires_grad=False)

        # Multiply output by multiplier as described in the paper [1]
        return torch.mul(selected_,input) * self.multiplier_
```

4. Dropout as Regularization

In this section, we want to show dropout is a kind of regularization techniques for deep neural networks. It can reduce the overfitting and make our network perform better on test set. We will first do a multilayer perceptron (fully connected network) to show dropout works and then do a LeNet (convolutional neural network) to show dropout is also useful for different network architectures.

We use MNIST (as we see in homework) as our sample dataset. This dataset has images of hand written digits and the labels of the ground truth digits. Code cell below loads the dataset and shows 10 training samples.

In [3]:
```
transform = transforms.Compose([transforms.ToTensor(), \
                                transforms.Normalize((0, 0, 0), (1, 1,
 1))])

trainset = datasets.MNIST(root='data/', train=True, download=True, tra
nsform=transform)
testset = datasets.MNIST(root='data/', train=False, transform=transfor
m)

# Visualize 10 image samples in MNIST dataset
trainloader = torch.utils.data.DataLoader(trainset, batch_size=64, shu
ffle=True, num_workers=2)
dataiter = iter(trainloader)
images, labels = dataiter.next()
# plot 10 sample images
_,ax = plt.subplots(1,10)
ax = ax.flatten()
iml = images[0].numpy().shape[1]
[ax[i].imshow(np.transpose(images[i].numpy(),(1,2,0)).reshape(iml,-1),
cmap='Greys') for i in range(10)]
[ax[i].set_axis_off() for i in range(10)]
plt.show()
print('label:',labels[:10].numpy())
print('image data shape:',images[0].numpy().shape)
```



```
label: [1 4 6 6 3 4 3 3 7 7]
image data shape: (1, 28, 28)
```

4.1 Multilayer Perceptron

We first build a multilayer perceptron (MLP), and use the code below to define the network as described in paper [1]. This network has 2 hidden layer with 800 hidden units per hidden layer.

In [4]:
```
class MLP(nn.Module):
    def __init__(self, hidden_layers=[800, 800], droprates=[0, 0]):
        super(MLP, self).__init__()
        self.model = nn.Sequential()
        self.model.add_module("dropout0",MyDropout(p=droprates[0]))
        self.model.add_module("input", nn.Linear(28*28, hidden_layers[
0]))
        self.model.add_module("tanh", nn.Tanh())

        # Add hidden layers
        for i,d in enumerate(hidden_layers[:-1]):
            self.model.add_module("dropout_hidden"+str(i+1), MyDropout
(p=droprates[1]))
            self.model.add_module("hidden"+str(i+1), nn.Linear(hidden_
layers[i], hidden_layers[i+1]))
            self.model.add_module("tanh_hidden"+str(i+1), nn.Tanh())
        self.model.add_module("final",nn.Linear(hidden_layers[-1], 10
))

    def forward(self, x):
        # Turn to 1D
        x = x.view(x.shape[0], 28*28)
        x = self.model(x)
        return x
```

Next, we implement a sklearn-like classifier for training and keep track of the **full test results** after each epoch.

In [5]:

```
class MLPClassifier:
    def __init__(self, hidden_layers=[800, 800], droprates=[0, 0], bat
ch_size=128, max_epoch=10, \
                 lr=0.1, momentum=0):
        # Wrap MLP model
        self.hidden_layers = hidden_layers
        self.droprates = droprates
        self.batch_size = batch_size
        self.max_epoch = max_epoch
        self.model = MLP(hidden_layers=hidden_layers, droprates=dropra
tes)
        self.model.cuda()
        self.criterion = nn.CrossEntropyLoss().cuda()
        self.optimizer = optim.SGD(self.model.parameters(), lr=lr, mom
entum=momentum)
        self.loss_ = []
        self.test_accuracy = []
        self.test_error = []

    def fit(self, trainset, testset, verbose=True):
        # Training, make sure it's on GPU, otherwise, very slow...
        trainloader = torch.utils.data.DataLoader(trainset, batch_size
=self.batch_size, shuffle=True)
        testloader = torch.utils.data.DataLoader(testset, batch_size=l
en(testset), shuffle=False)
        X_test, y_test = iter(testloader).next()
        X_test = X_test.cuda()
```

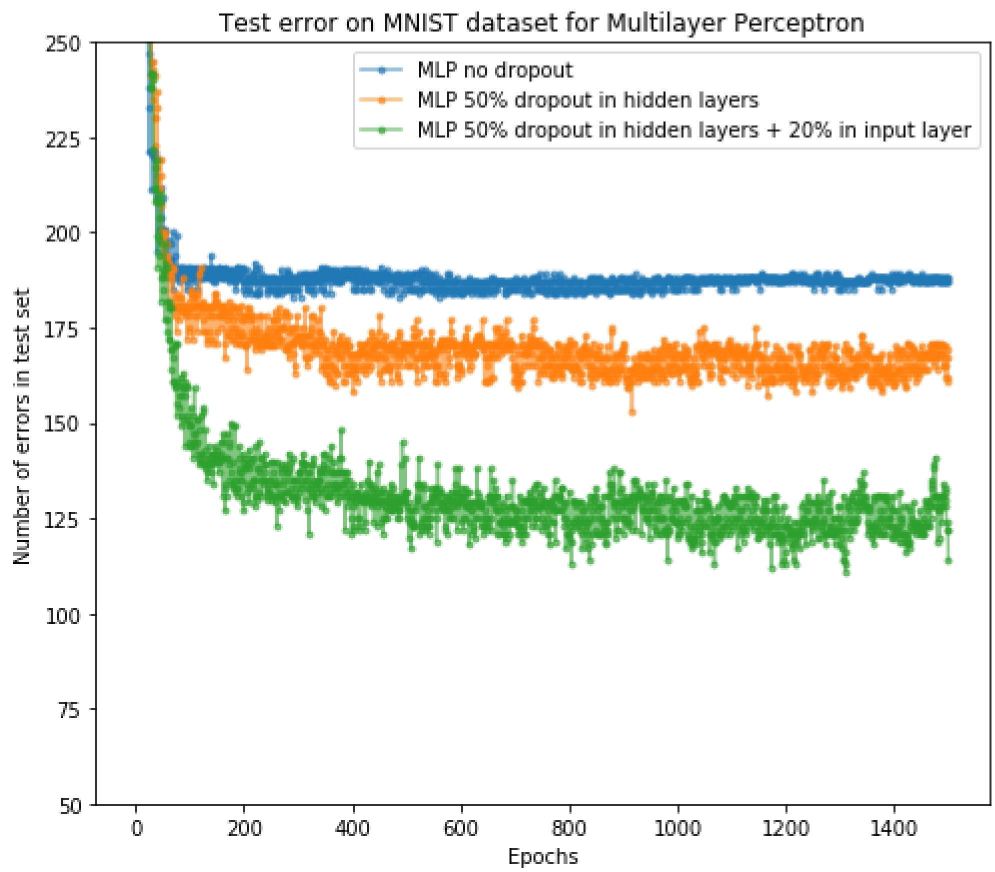
```
        for epoch in range(self.max_epoch):
            running_loss = 0
            for i, data in enumerate(trainloader, 0):
                inputs, labels = data
                inputs, labels = Variable(inputs).cuda(), Variable(lab
els).cuda()
                self.optimizer.zero_grad()
                outputs = self.model(inputs)
                loss = self.criterion(outputs, labels)
                loss.backward()
                self.optimizer.step()
                running_loss += loss.data[0]
            self.loss_.append(running_loss / len(trainloader))
            if verbose:
                print('Epoch {} loss: {}'.format(epoch+1, self.loss_[-
1]))
            y_test_pred = self.predict(X_test).cpu()
            self.test_accuracy.append(np.mean(y_test == y_test_pred))
            self.test_error.append(int(len(testset)*(1-self.test_accur
acy[-1])))
            if verbose:
                print('Test error: {}; test accuracy: {}'.format(self.
test_error[-1], self.test_accuracy[-1]))
        return self

    def predict(self, x):
        # Used to keep all test errors after each epoch
        model = self.model.eval()
        outputs = model(Variable(x))
        _, pred = torch.max(outputs.data, 1)
        model = self.model.train()
        return pred

    def __str__(self):
        return 'Hidden layers: {}; dropout rates: {}'.format(self.hidd
en_layers, self.droprates)
```

Paper [1] tried three networks. One with **no dropout**, one with **dropout in hidden layers** and one with **dropout in both hidden layers and input**. We use the same number of epoches, the same dropout rate as in paper [1]. We define those three networks in the code section below.

In [6]:
```
hidden_layers = [800, 800]

### Below is training code, uncomment to train your own model... ###
### Note: You need GPU to run this section ###
'''
# Define networks
mlp1 = [MLPClassifier(hidden_layers, droprates=[0, 0], max_epoch=300
0),
        MLPClassifier(hidden_layers, droprates=[0, 0.5], max_epoch=300
0),
        MLPClassifier(hidden_layers, droprates=[0.2, 0.5], max_epoch=3
000)]

# Training, set verbose=True to see loss after each epoch.
[mlp.fit(trainset, testset,verbose=False) for mlp in mlp1]

# Save torch models
for ind, mlp in mlp1:
    torch.save(mlp.model, 'mnist_mlp1_'+str(ind)+'.pth')
    # Prepare to save errors
    mlp.test_error = list(map(str, mlp.test_error))

# Save test errors to plot figures
open("mlp1_test_errors.txt","w").write('\n'.join([','.join(mlp.test_er
ror) for mlp in mlp1]))
'''

# Load saved models to CPU
mlp1_models = [torch.load('mnist_mlp1_'+str(ind)+'.pth',map_location={
'cuda:0': 'cpu'}) for ind in [0,1,2]]

# Load saved test errors to plot figures.
mlp1_test_errors = [error_array.split(',') for error_array in open("ml
p1_test_errors.txt","r").read().split('\n')]
mlp1_test_errors = np.array(mlp1_test_errors,dtype='f')
```

After the training, we can plot the number of error predictions on test set after each epoch for all three networks as in paper [1].

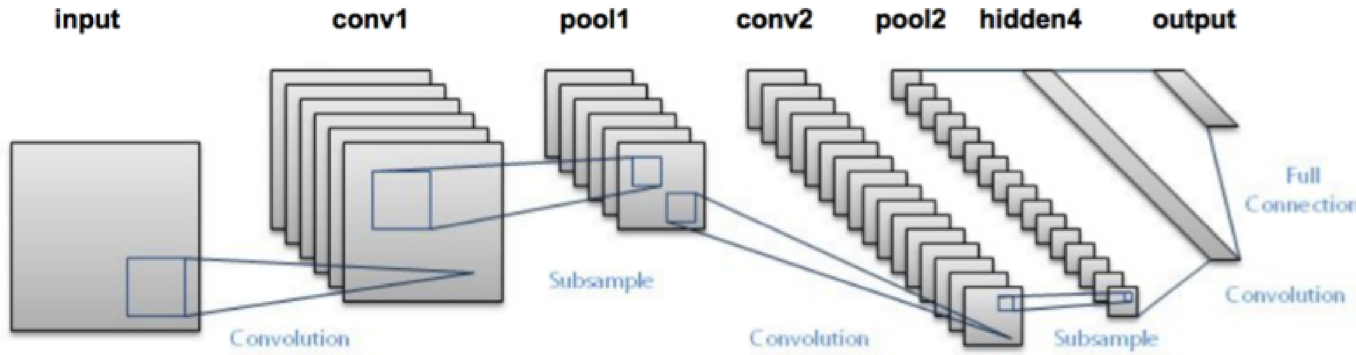
In [7]:
```
labels = ['MLP no dropout',
          'MLP 50% dropout in hidden layers',
          'MLP 50% dropout in hidden layers + 20% in input layer']

plt.figure(figsize=(8, 7))
for i, r in enumerate(mlp1_test_errors):
    plt.plot(range(1, len(r)+1), r, '.-', label=labels[i], alpha=0.6);
plt.ylim([50, 250]);
plt.legend(loc=1);
plt.xlabel('Epochs');
plt.ylabel('Number of errors in test set');
plt.title('Test error on MNIST dataset for Multilayer Perceptron')
plt.show()
```



From the result, we see dropout as regularization is useful and it successfully improves the network accuracy on the test set. In addition, further adding the dropout layer after the input layer will help as well.

4.2 Convolutional Neural Network (LeNet)

Next, we show dropout can improve test performance in convolutional neural networks as well. Here, we implement a simple LeNet for demonstration. The LeNet architecture is shown below.



ref: https://blog.dataiku.com/deep-learning-with-dss (https://blog.dataiku.com/deep-learning-with-dss)

We first calculate the dimension of images after going through convolutional layers and pooling layers since we need to specify in and out dimensions for linear layers in `pytorch`.

In [8]:
```
def caloutdim(hin, kernel_size, stride=1, padding=0, dilation=1):
    return int(np.floor((hin+2*padding-dilation*(kernel_size-1)-1)/str
ide+1))

d = [28]
d.append(caloutdim(d[-1], 5, padding=2))
d.append(caloutdim(d[-1], 2, 2))
d.append(caloutdim(d[-1], 5, padding=2))
d.append(caloutdim(d[-1], 2, 2))
print(d)
```

```
[28, 28, 14, 14, 7]
```

The code cell below defines the LeNet.

In [9]:
```
class Flatten(nn.Module):
    def __init__(self):
        super(Flatten, self).__init__()

    def forward(self, x):
        x = x.view(x.size(0), -1)
        return x

class LeNet(nn.Module):
    def __init__(self, droprate=0.5):
        super(LeNet, self).__init__()
        self.model = nn.Sequential()
        self.model.add_module('conv1', nn.Conv2d(1, 20, kernel_size=5,
 padding=2))
        self.model.add_module('dropout1', nn.Dropout2d(p=droprate))
        self.model.add_module('maxpool1', nn.MaxPool2d(2, stride=2))
        self.model.add_module('conv2', nn.Conv2d(20, 50, kernel_size=5
, padding=2))
        self.model.add_module('dropout2', nn.Dropout2d(p=droprate))
        self.model.add_module('maxpool2', nn.MaxPool2d(2, stride=2))
        self.model.add_module('flatten', Flatten())
        self.model.add_module('dense3', nn.Linear(50*7*7, 500))
        self.model.add_module('relu3', nn.ReLU())
        self.model.add_module('dropout3', nn.Dropout(p=droprate))
        self.model.add_module('final', nn.Linear(500, 10))

    def forward(self, x):
        return self.model(x)
```

Similar as above, we implement a sklearn-like classifier for LeNet.

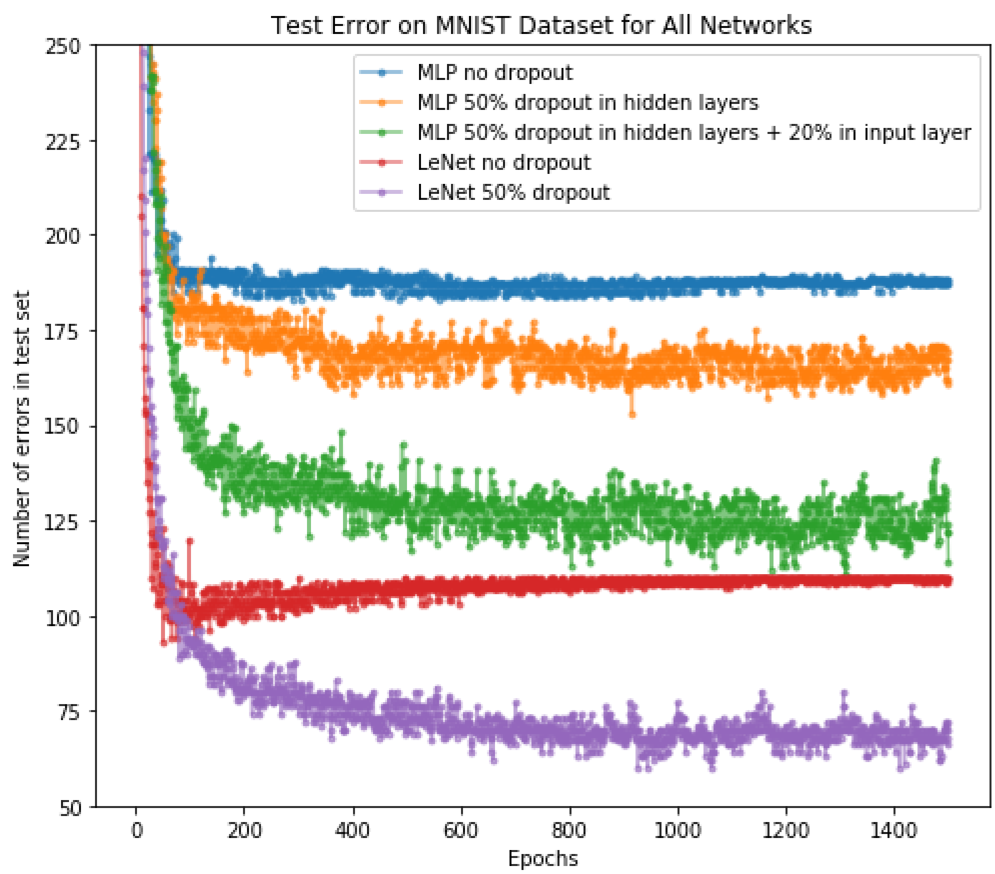
In [10]:
```
class LeNetClassifier:
    def __init__(self, droprate=0.5, batch_size=128, max_epoch=300, lr
=0.01):
        self.batch_size = batch_size
        self.max_epoch = max_epoch
        self.lr = lr
        self.model = LeNet(droprate)
        self.model.cuda()
        self.criterion = nn.CrossEntropyLoss().cuda()
        self.optimizer = optim.SGD(self.model.parameters(), lr=lr)
        self.loss_ = []
        self.test_error = []
        self.test_accuracy = []

    def fit(self, trainset, testset, verbose=True):
        trainloader = torch.utils.data.DataLoader(trainset, batch_size
=self.batch_size, shuffle=True)
        testloader = torch.utils.data.DataLoader(testset, batch_size=l
en(testset), shuffle=False)
        X_test, y_test = iter(testloader).next()
        X_test = X_test.cuda()
        print(self.model)
        for epoch in range(self.max_epoch):
            running_loss = 0
            for i, data in enumerate(trainloader, 0):
                inputs, labels = data
                inputs, labels = Variable(inputs).cuda(), Variable(lab
els).cuda()
                self.optimizer.zero_grad()
                outputs = self.model(inputs)
                loss = self.criterion(outputs, labels)
                loss.backward()
                self.optimizer.step()
                running_loss += loss.data[0]
            self.loss_.append(running_loss / len(trainloader))
            if verbose:
                print('Epoch {} loss: {}'.format(epoch+1, self.loss_[-
1]))
            y_test_pred = self.predict(X_test).cpu()
            self.test_accuracy.append(np.mean(y_test == y_test_pred))
            self.test_error.append(int(len(testset)*(1-self.test_accur
acy[-1])))
            if verbose:
                print('Test error: {}; test accuracy: {}'.format(self.
test_error[-1], self.test_accuracy[-1]))
        return self

    def predict(self, x):
        model = self.model.eval()
        outputs = model(Variable(x))
        _, pred = torch.max(outputs.data, 1)
        model = self.model.train()
        return pred
```

And the training code is below. We load our trained models here.

In [11]:
```
### Below is training code, uncomment to train your own model... ###
### Note: You need GPU and CUDA to run this section ###
'''
# Define networks
lenet1 = [LeNetClassifier(droprate=0, max_epoch=3),
          LeNetClassifier(droprate=0.5, max_epoch=3)]

# Training, set verbose=True to see loss after each epoch.
[lenet.fit(trainset, testset,verbose=False) for lenet in lenet1]

# Save torch models
for ind, lenet in lenet1:
    torch.save(lenet.model, 'mnist_lenet1_'+str(ind)+'.pth')
    # Prepare to save errors
    lenet.test_error = list(map(str, lenet.test_error))

# Save test errors to plot figures
open("lenet1_test_errors.txt","w").write('\n'.join([','.join(lenet.tes
t_error) for lenet in lenet1]))
'''

# Load saved models to CPU
lenet1_models = [torch.load('mnist_lenet1_'+str(ind)+'.pth',map_locati
on={'cuda:0': 'cpu'}) for ind in [0,1]]

# Load saved test errors to plot figures.
lenet1_test_errors = [error_array.split(',') for error_array in
                      open("lenet1_test_errors.txt","r").read().split(
'\n')]
lenet1_test_errors = np.array(lenet1_test_errors,dtype='f')
```

After the training, we can plot the number of error predictions on test set after each epoch for all networks. Here we overlay the LeNet result on the MLP network we just showed.

In [12]:
```
labels = ['MLP no dropout',
          'MLP 50% dropout in hidden layers',
          'MLP 50% dropout in hidden layers + 20% in input layer',
          'LeNet no dropout',
          'LeNet 50% dropout']

plt.figure(figsize=(8, 7))
for i, r in enumerate(mlp1_test_errors.tolist() + lenet1_test_errors.t
olist()):
    plt.plot(range(1, len(r)+1), r, '.-', label=labels[i], alpha=0.6);
plt.ylim([50, 250]);
plt.legend(loc=1);
plt.xlabel('Epochs');
plt.ylabel('Number of errors in test set');
plt.title('Test Error on MNIST Dataset for All Networks')
plt.show()
```



As we can see,

1. Dropout in hidden layers can reduce test errors in standard feedforward network (i.e., MLP); we can further improve the test performance by applying dropout in input layer.
2. LeNet performs better than MLP even without dropout, but overfitting occurs. Dropout significantly improves the test performance, which demonstrates dropout as an effective regularization method in CNNs.

5. Dropout as Bayesian Approximation

It is shown that deep NNs with dropout applied before every weight layer are mathematically equivalent to approximate variational inference in the deep Gaussian process marginalised over its covariance function parameters ([2]).

The related Gaussian process could be described as below:

$$F|X, W_1, b \sim N(0, K(X, X))$$
$$Y|F \sim N(F, \tau^{-1} I_N)$$

Introduing W_1, which is a matrix parameterizing the covariance function K:

$$p(Y|X) = \int p(Y|F)p(F|W_1, b, X)p(W_1)p(b)$$

Introduing W_2, another matrix that get the integration rid of F:

$$p(Y|X) = \int p(Y|X, W_1, W_2, b)p(W_1)p(W_2)p(b)$$

To perform variational inference in our approximate model we need to define a variational distribution $q(W_1, W_2, b) := q(W_1)q(W_2)q(b)$, where $q(W_1)$ and $q(W_2)$ are defined as a Gaussian mixture model with two components, factorized over dimensinality of W_1 and W_2. For example:

$$q(W_1) = \prod_{q=1}^{Q} q(w_q)$$
$$q(w_q) = p_1 N(m_q, \sigma^2 I_K) + (1 - p_1)N(0, \sigma^2 I_K)$$

with some probability p1 ∈ [0, 1], scalar σ > 0 and $m_q \in R^K$

In dropout model, the input was weighted by some weight matrix and then pass into some non-linear function, which is the same as what we did with the parameterizing matrix and covariance function. The output of the non-linear function would be the input of the next hidden layer. When we implement dropout, we actually created a binary vector to decide which hidden unit would be passed to the next layer, which is similar to what we did for the variational inference. With this setup, we update the parameters by minimizing some loss function we choose, just as minimizing KL divergence in Gaussian process approximation.

5.1 Dropout as Bayesian Approximation in Classification Task

Here we use the models (MLP and LeNet) that we trained above for the classification of MNIST digits to demonstrate how we can acquire model uncertainty through dropout.

We evaluate the models on a continuously rotated image of the digit 1 (as shown below).

In [13]:
```
testloader = torch.utils.data.DataLoader(testset, batch_size=len(tests
et), shuffle=False)
X_test, y_test = iter(testloader).next()
X_test = X_test.numpy()
X1 = np.array([rotate(X_test[9978].squeeze(), i, reshape=False) for i
in range(50, 130, 7)])
X1 = X1.reshape(X1.shape[0], 1, X1.shape[1], X1.shape[2])

plt.figure(figsize=(8, 1))

gs = gridspec.GridSpec(1, 12)
gs.update(wspace=0, hspace=0)

for i in range(len(X1)):
    plt.subplot(gs[i])
    plt.imshow(X1.squeeze()[i], cmap='gray');
    plt.axis('off');
```

For each model, we simulate 1000 stochastic forward passes, and visualize distributions of the softmax inputs and the softmax outputs for each of the top classes.

Below is the function doing this simulation.

In [14]:
```
def predict_class(model, X):
    model = model.eval()
    outputs = model(Variable(X))
    _, pred = torch.max(outputs.data, 1)
    model = model.train()
    return pred.numpy()

def predict(model, X, T=1000):
    standard_pred = predict_class(model, X)
    y1 = []
    y2 = []
    for _ in range(T):
        _y1 = model(Variable(X))
        _y2 = F.softmax(_y1, dim=1)
        y1.append(_y1.data.numpy())
        y2.append(_y2.data.numpy())
    return standard_pred, np.array(y1), np.array(y2)
```

5.1.1 MLP 50% dropout in hidden layers + 20% in input layer

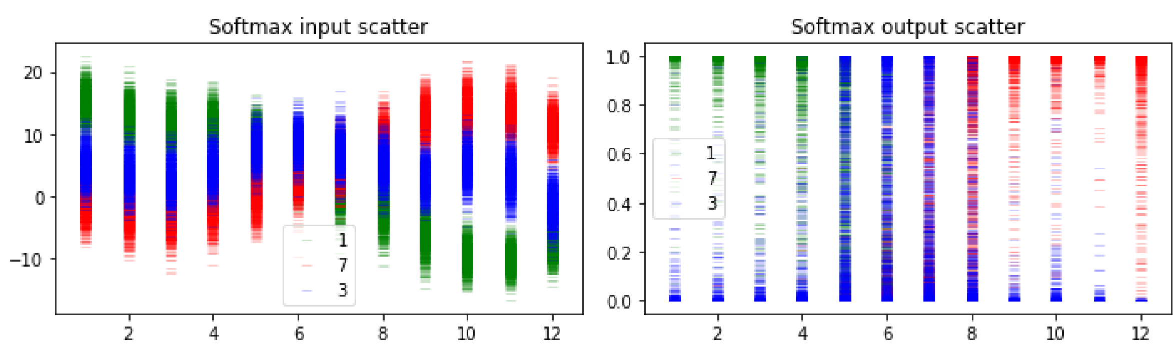
We get this model (50% dropout in hidden layers and 20% dropout in input layer) from section 4.1. First, let's see how well the model does on the rotated digit '1'.

In [15]:
```
model = mlp1_models[2]

# Need to flatten X1 before feeding into MLP
y1_pred, y1_si, y1_so = predict(model, torch.from_numpy(X1.reshape(-1,
784)))
print('Predictions: {}'.format(y1_pred))
```

```
Predictions: [1 1 1 1 1 3 3 7 7 7 7 7]
```

Now let's do simulations to get the uncertainty of the output.

In [16]:
```
plt.figure(figsize=(10, 3))
plt.subplot(1, 2, 1)
plt.scatter(np.tile(np.arange(1, 13), y1_si.shape[0]), y1_si[:, :, 1].
flatten(), \
            color='g', marker='_', linewidth=None, alpha=0.2, label=
'1');
plt.scatter(np.tile(np.arange(1, 13), y1_si.shape[0]), y1_si[:, :, 7].
flatten(), \
            color='r', marker='_', linewidth=None, alpha=0.2, label=
'7');
plt.scatter(np.tile(np.arange(1, 13), y1_si.shape[0]), y1_si[:, :, 3].
flatten(), \
            color='b', marker='_', linewidth=None, alpha=0.2, label=
'3');
plt.title('Softmax input scatter');
plt.legend(framealpha=0.7);

plt.subplot(1, 2, 2)
plt.scatter(np.tile(np.arange(1, 13), y1_so.shape[0]), y1_so[:, :, 1].
flatten(), \
            color='g', marker='_', linewidth=None, alpha=0.2, label=
'1');
plt.scatter(np.tile(np.arange(1, 13), y1_so.shape[0]), y1_so[:, :, 7].
flatten(), \
            color='r', marker='_', linewidth=None, alpha=0.2, label=
'7');
plt.scatter(np.tile(np.arange(1, 13), y1_so.shape[0]), y1_so[:, :, 3].
flatten(), \
            color='b', marker='_', linewidth=None, alpha=0.2, label=
'3');
plt.title('Softmax output scatter');
plt.legend(framealpha=0.7);

plt.tight_layout();
```



5.1.2 LeNet 50% dropout

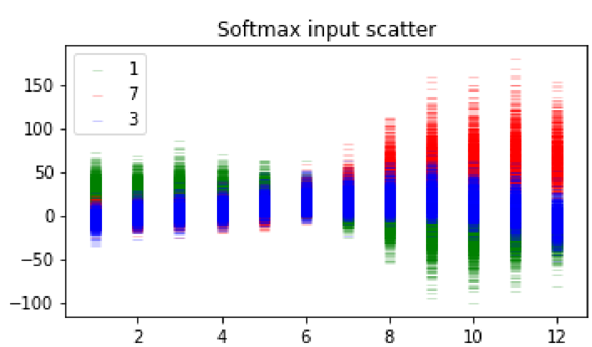
We get this model (50% dropout in hidden layers) from section 4.2. First, let's see how well the model does on the rotated digit '1'.

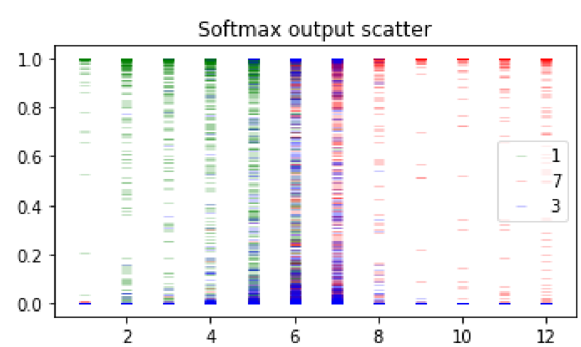
```
In [17]: model = lenet1_models[1]
         y1_pred, y1_si, y1_so = predict(model, torch.from_numpy(X1))
         print('Predictions: {}'.format(y1_pred))
```

```
Predictions: [1 1 1 1 1 1 7 7 7 7 7 7]
```

Now let's do simulations to get the uncertainty of the output.

```
In [18]: plt.figure(figsize=(10, 3))
         plt.subplot(1, 2, 1)
         plt.scatter(np.tile(np.arange(1, 13), y1_si.shape[0]), y1_si[:, :, 1].
         flatten(), \
                     color='g', marker='_', linewidth=None, alpha=0.2, label=
         '1');
         plt.scatter(np.tile(np.arange(1, 13), y1_si.shape[0]), y1_si[:, :, 7].
         flatten(), \
                     color='r', marker='_', linewidth=None, alpha=0.2, label=
         '7');
         plt.scatter(np.tile(np.arange(1, 13), y1_si.shape[0]), y1_si[:, :, 3].
         flatten(), \
                     color='b', marker='_', linewidth=None, alpha=0.2, label=
         '3');
         plt.title('Softmax input scatter');
         plt.legend(framealpha=0.7);

         plt.subplot(1, 2, 2)
         plt.scatter(np.tile(np.arange(1, 13), y1_so.shape[0]), y1_so[:, :, 1].
         flatten(), \
                     color='g', marker='_', linewidth=None, alpha=0.2, label=
         '1');
         plt.scatter(np.tile(np.arange(1, 13), y1_so.shape[0]), y1_so[:, :, 7].
         flatten(), \
                     color='r', marker='_', linewidth=None, alpha=0.2, label=
         '7');
         plt.scatter(np.tile(np.arange(1, 13), y1_so.shape[0]), y1_so[:, :, 3].
         flatten(), \
                     color='b', marker='_', linewidth=None, alpha=0.2, label=
         '3');
         plt.title('Softmax output scatter');
         plt.legend(framealpha=0.7);

         plt.tight_layout();
```





5.1.3 Explanation and Analysis

When the uncertainty envelop of the top class is far away from that of other classes (e.g., the leftmost image), we can make predictions with high confidence. When the uncertainty envelopes for different classes intersect with each other (e.g., the middle input images), the softmax output can be as large as the entire space even though the softmax output can be arbitrarily high.

Although we got different predictions for the middle images, the softmax output scatters show that we make those predictions with high uncertainty. And the softmax output scatters for 2 different networks look similar, although the softmax input scatters look sightly different.

As mentioned by the authors, such uncertainty information can help us obtain higher classification accuracies (not shown in this paper), and help us check whether we correctly specify the model or whether we have enough data.

5.2. Dropout as Bayesian Approximation in Regression Task

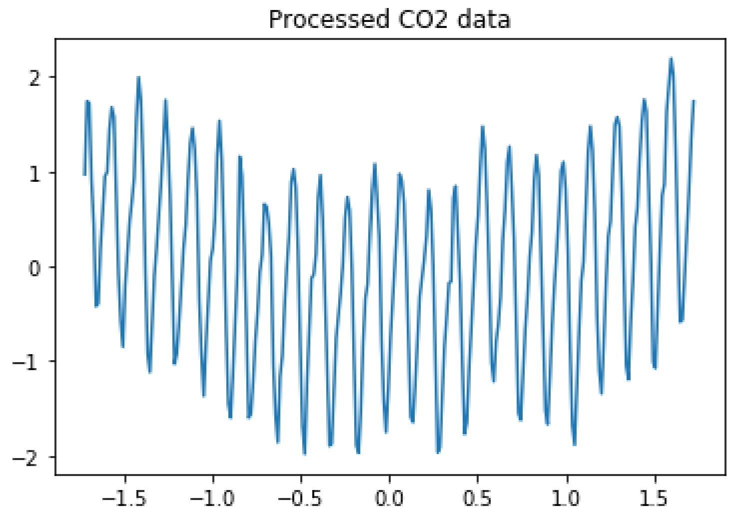
In this part, we show how to use dropout to obtain model uncertainty in regression tasks.

Here we use the CO2 concentrations dataset (example in [2]) for demonstration. We load training set (provided in [2]) and generate test data that is very different from the training set.

In [19]:
```
f = h5py.File('co2_data.h5', 'r')
data_train = np.concatenate((f['data'].value, f['label'].value), axis=
1)
f.close()
X_train = data_train[:, 0].reshape(-1, 1)
y_train = data_train[:, 1].reshape(-1, 1)
print(data_train.shape)

X_test = np.arange(-1.72, 3.51, 0.01).reshape(-1, 1)
```

```
(272, 2)
```

In [20]:
```
plt.plot(data_train[:, 0], data_train[:, 1]);
plt.title('Processed CO2 data');
```



We train a multilayer perceptron with 5 hidden layers, 1024 units in each layer, ReLU/Tanh non-linearities, and dropout with probability 0.2 after each weight layer. As pointed out by Gal et al. (https://arxiv.org/abs/1506.02142), similar results can be obtained when using 4 hidden layers or dropout probability of 0.1.

We define the network with code below.

In [21]:
```
class MLP2(nn.Module):
    def __init__(self, hidden_layers=[1024, 1024, 1024, 1024, 1024], d
roprate=0.2, activation='relu'):
        super(MLP2, self).__init__()
        self.model = nn.Sequential()
        self.model.add_module('input', nn.Linear(1, hidden_layers[0]))
        if activation == 'relu':
            self.model.add_module('relu0', nn.ReLU())
        elif activation == 'tanh':
            self.model.add_module('tanh0', nn.Tanh())
        for i in range(len(hidden_layers)-1):
            self.model.add_module('dropout'+str(i+1), nn.Dropout(p=dro
prate))
            self.model.add_module('hidden'+str(i+1), nn.Linear(hidden_
layers[i], hidden_layers[i+1]))
            if activation == 'relu':
                self.model.add_module('relu'+str(i+1), nn.ReLU())
            elif activation == 'tanh':
                self.model.add_module('tanh'+str(i+1), nn.Tanh())
        self.model.add_module('dropout'+str(i+2), nn.Dropout(p=droprat
e))
        self.model.add_module('final', nn.Linear(hidden_layers[i+1], 1
))

    def forward(self, x):
        return self.model(x)
```

Similar as last section, we implement a sklearn-like regressor for this MLP.

In [22]:
```
class MLP2Regressor:
    def __init__(self, hidden_layers=[1024, 1024, 1024, 1024, 1024], d
roprate=0.2, activation='relu', \
                 max_epoch=1000000, lr=0.0001, weight_decay=1e-6):
        self.max_epoch = max_epoch
        self.lr = lr
        self.model = MLP2(hidden_layers=hidden_layers, droprate=dropra
te, activation=activation)
        self.model.cuda()
        self.criterion = nn.MSELoss().cuda()
        self.optimizer = optim.Adam(self.model.parameters(), lr=lr, we
ight_decay=weight_decay)

    def fit(self, X_train, y_train, verbose=True):
        X = Variable(torch.from_numpy(X_train).type(torch.FloatTensor
)).cuda()
        y = Variable(torch.from_numpy(y_train).type(torch.FloatTensor
)).cuda()
        print(self.model)
        for epoch in range(self.max_epoch):
            self.optimizer.zero_grad()
            outputs = self.model(X)
            loss = self.criterion(outputs, y)
            loss.backward()
            self.optimizer.step()
            if verbose:
                print('Epoch {} loss: {}'.format(epoch+1, loss.data[0
]))
        return self
```

And the training code is below. We load our trained models here.

In [23]:
```
### Below is training code, uncomment to train your own model... ###
### Note: You need GPU and CUDA to run this section ###
'''
# Define networks
mlp2 = [MLP2Regressor(activation='relu'),
        MLP2Regressor(activation='tanh')]

# Training, set verbose=True to see loss after each epoch.
[mlp.fit(X_train, y_train,verbose=False) for mlp in mlp2]

# Save torch models
for ind, mlp in mlp2:
    torch.save(mlp.model, 'co2_mlp2_'+str(ind)+'.pth')
'''

# Load saved models to CPU
mlp2_models = [torch.load('co2_mlp2_'+str(ind)+'.pth',map_location={'c
uda:0': 'cpu'}) for ind in [0,1]]
```

Below is the function doing the simulation for the regressors. Here, we simulate 10000 times. The simulation is very slow since we have many data points.

In [24]:
```
def predict_reg(model, X, T=10000):
    X = Variable(torch.from_numpy(X).type(torch.FloatTensor))
    model = model.train()
    Yt_hat = np.array([model(X).data.numpy() for _ in range(T)]).squee
ze()
    model = model.eval()
    y_pred = model(X).data.numpy()
    model = model.train()
    return y_pred, Yt_hat
```

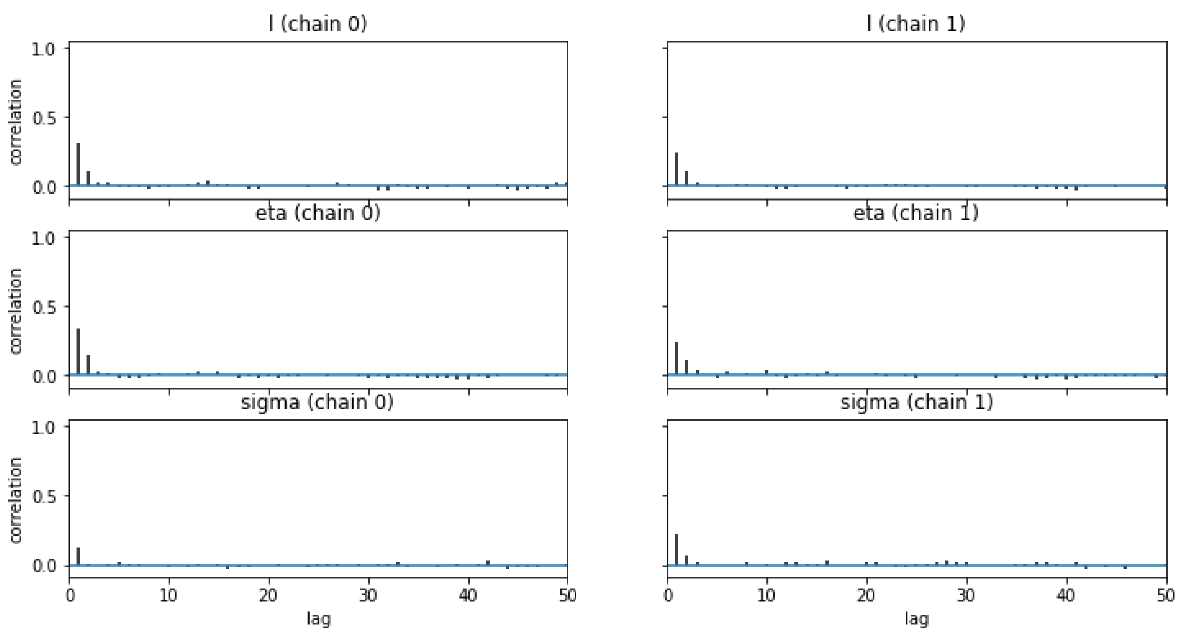
We stored the simulation results and load here. To generate simulation results yourself, uncomment the code below.

In [25]:
```
# Simulation below is very slow. Run with GPU! #
### Uncomment to simulate ###
'''
mlp2_models = [torch.load('co2_mlp2_'+str(ind)+'.pth') for ind in [0,
1]]
y_relu_pred, y_hat = predict_reg(mlp2_models[0], X_test)
y_relu_mc = y_hat.mean(axis=0)
y_relu_mc_std = y_hat.std(axis=0)
y_tanh_pred, y_hat = predict(model, X_test)
y_tanh_mc = y_hat.mean(axis=0)
y_tanh_mc_std = y_hat.std(axis=0)
results = [y_relu_pred,y_relu_mc,y_relu_mc_std,y_tanh_pred,y_tanh_mc,y
_tanh_mc_std]
results = [x.reshape(-1).astype(str).tolist() for x in results]
open("mlp2_sim_results.txt","w").write('\n'.join([','.join(res) for re
s in results]))
'''

# Load saved simulation results
results = [res_array.split(',') for res_array in
                      open("mlp2_sim_results.txt","r").read().split('
\n')]
results = np.array(results,dtype='f')
y_relu_pred,y_relu_mc,y_relu_mc_std,y_tanh_pred,y_tanh_mc,y_tanh_mc_st
d = results
```

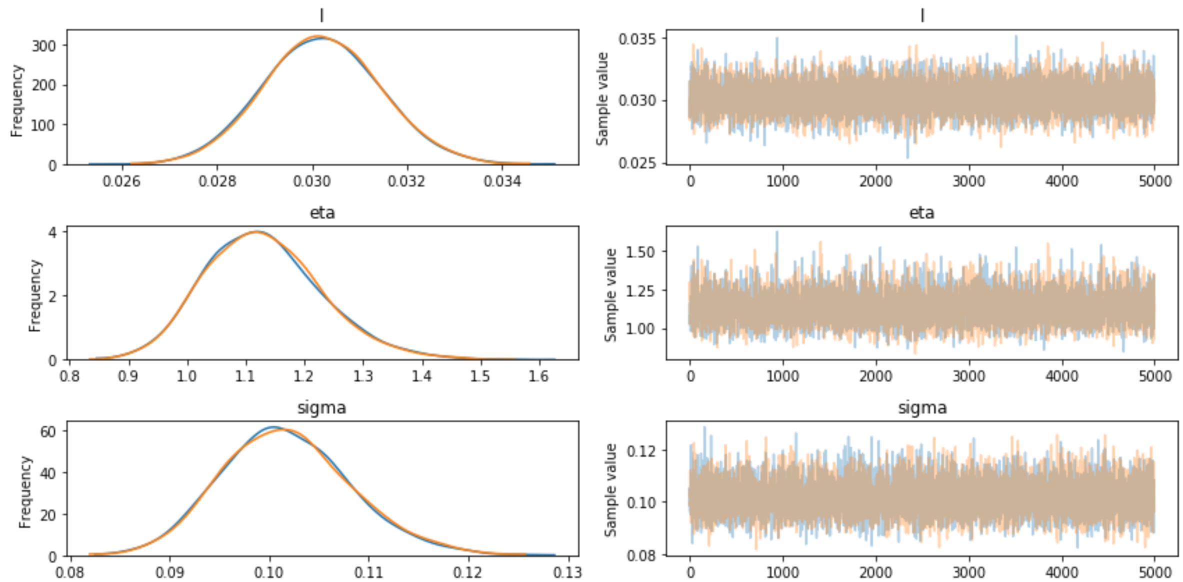
We can compare the uncertainty we get through dropout with the uncertainty we get from a Gaussian process.

In [26]:
```
import pickle

with pm.Model() as gp_model:
    l = pm.HalfCauchy('l', 0.05)
    eta = pm.HalfCauchy('eta', 1)
    sigma = pm.HalfCauchy('sigma', 0.1)
    gp = pm.gp.Marginal(cov_func=(eta ** 2) * pm.gp.cov.ExpQuad(1, l))
    obs = gp.marginal_likelihood('obs', X=X_train, y=y_train.squeeze
(), noise=sigma, is_observed=True)

# Code below trains the GP model, it's very slow. So we load the train
ed model and comment this out
'''
with gp_model:
    step = pm.NUTS(target_accept=0.95)
    trace1 = pm.sample(5000, tune=2000, step=step, njobs=2)
with open(self.'co2_gp.pkl', 'wb') as output:
            pickle.dump((gp_model,trace1), output, protocol=pickle.HIG
HEST_PROTOCOL)
'''
with open('co2_gp.pkl', 'rb') as input_:
    gp_model, trace1 = pickle.load(input_)
```

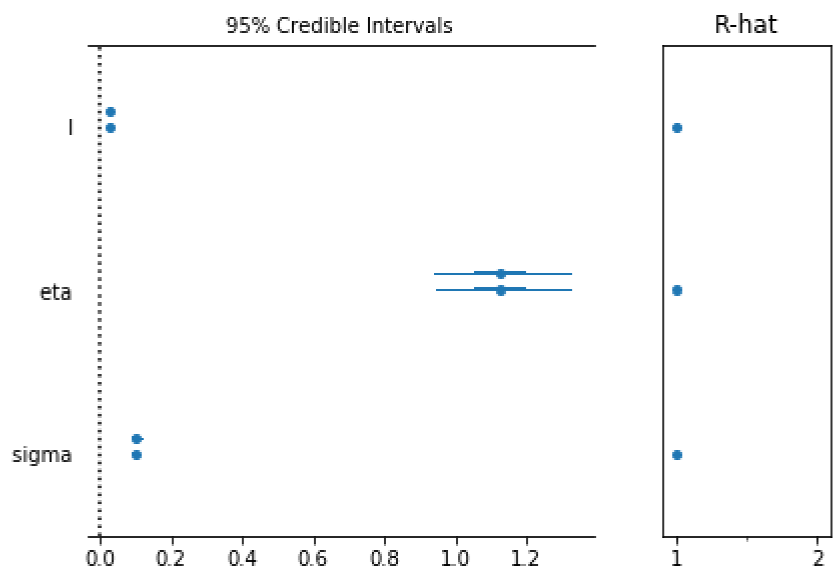
In [27]:
```
pm.autocorrplot(trace1, max_lag=50);
```



In [28]:
```
pm.traceplot(trace1);
```



In [29]:
```
pm.forestplot(trace1);
```

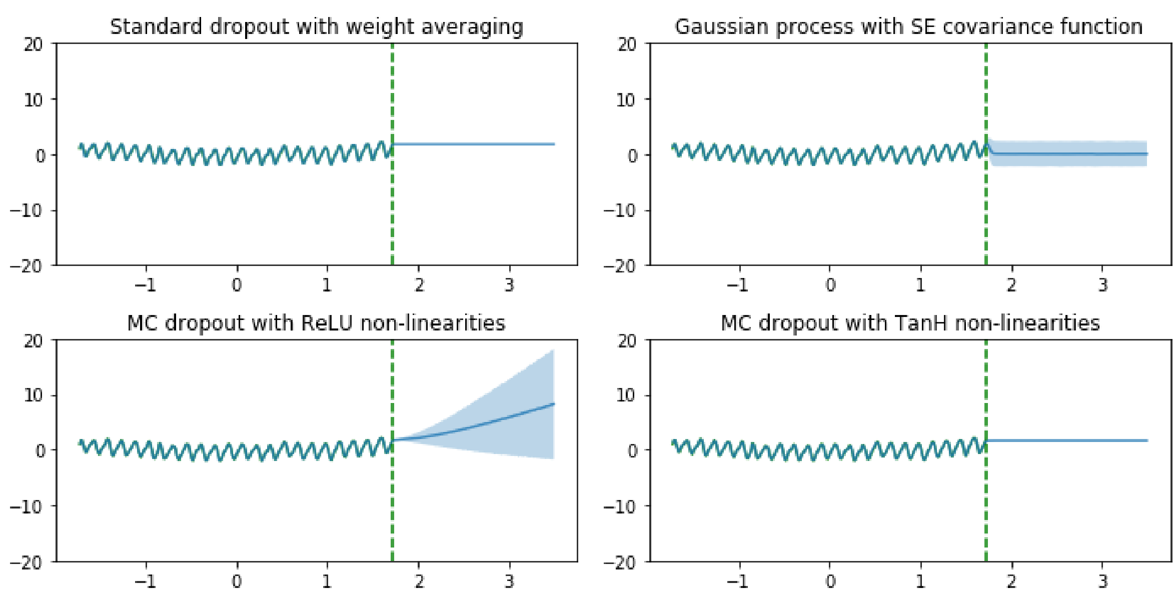


The above tests show the convergence of the model.

In [30]:
```
# PPC below is very slow. So we load saved results #
### Uncomment to simulate ###
'''
with gp_model:
    y_gp = gp.conditional('y_pred', Xnew=X_test, pred_noise=True)
    gp_samples = pm.sample_ppc(trace1, vars=[y_gp], samples=10000)
ppc = gp_samples['y_pred']
y_gp_pred = ppc.mean(axis=0)
y_gp_std = ppc.std(axis=0)
results = [y_gp_pred,y_gp_std]
results = [x.reshape(-1).astype(str).tolist() for x in results]
open("gp_sim_results.txt","w").write('\n'.join([','.join(res) for res
 in results]))
'''

# Load saved PPC results
results = [res_array.split(',') for res_array in
                      open("gp_sim_results.txt","r").read().split('\n'
)]
results = np.array(results,dtype='f')
y_gp_pred,y_gp_std = results
```

Next, we compare those models for regression.

In [31]:
```
plt.figure(figsize=(10, 5))

plt.subplot(2, 2, 1)
plt.plot(X_train.squeeze(), y_train.squeeze(), 'g', alpha=0.8);
plt.plot(X_test.squeeze(), y_tanh_pred, alpha=0.8);
plt.axvline(X_train.squeeze()[-1], color='g',linestyle='--');
plt.title('Standard dropout with weight averaging');
plt.ylim([-20, 20]);

plt.subplot(2, 2, 2)
plt.plot(X_train.squeeze(), y_train.squeeze(), 'g', alpha=0.8);
plt.plot(X_test.squeeze(), y_gp_pred, alpha=0.8);
plt.axvline(X_train.squeeze()[-1], color='g',linestyle='--');
plt.fill_between(X_test.squeeze(), y_gp_pred-2*y_gp_std, y_gp_pred+2*y
_gp_std, alpha=0.3);
plt.title('Gaussian process with SE covariance function');
plt.ylim([-20, 20]);

plt.subplot(2, 2, 3)
plt.plot(X_train.squeeze(), y_train.squeeze(), 'g', alpha=0.8);
plt.plot(X_test.squeeze(), y_relu_mc, alpha=0.8);
plt.axvline(X_train.squeeze()[-1], color='g',linestyle='--');
plt.fill_between(X_test.squeeze(), y_relu_mc-2*y_relu_mc_std, y_relu_m
c+2*y_relu_mc_std, alpha=0.3);
plt.title('MC dropout with ReLU non-linearities');
plt.ylim([-20, 20]);

plt.subplot(2, 2, 4)
plt.plot(X_train.squeeze(), y_train.squeeze(), 'g', alpha=0.8);
plt.plot(X_test.squeeze(), y_tanh_mc, alpha=0.8);
plt.axvline(X_train.squeeze()[-1], color='g',linestyle='--');
plt.fill_between(X_test.squeeze(), y_tanh_mc-2*y_tanh_mc_std, y_tanh_m
c+2*y_tanh_mc_std, alpha=0.3);
plt.title('MC dropout with TanH non-linearities');
plt.ylim([-20, 20]);

plt.tight_layout();
```



As we can see, the dropout network with ReLU non-linearities and the Gaussian process model successfully show the uncertainty for points away from the training data points. The uncertainty estimates are different since they correpond to different Gaussian process covariance functions. The uncertainty of dropout network with Tanh non-linearities doesn't increase far from the data, presumably because Tanh saturates whereas ReLU does not, as explained by in [2]

Reference

[1] Improving neural networks by preventing co-adaptation of feature detectors (https://arxiv.org/pdf/1207.0580.pdf)

[2] Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning (https://arxiv.org/pdf/1506.02142.pdf)