

Machine Learning Workshop 2

Variational Autoencoder

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Outline

- 1 Autoencoders
 - An example to keep in mind
 - Autoencoders
- 2 Variational autoencoder
 - Generative Model
 - Latent variable models
 - Variational Lower Bound
- 3 Experiment
 - Unsupervised Spam Detection
 - Preprocessing
 - Binary Cross Entropy
 - Bernoulli MLP as Decoder
 - Spam Detector

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An example to keep in mind

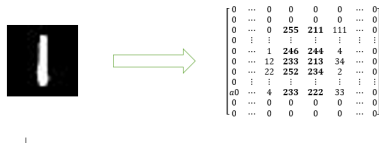


Figure: Conversion of a greyscale image to an matrix

Note: In the workshop, we will mostly work with linear layer, so we also need to flatten the image.

```
from PIL import Image
def image_to_array(image_path):
    with Image.open(image_path) as img:
        image = img.convert()
        array_image = np.asarray(image, np.float)
    return array_image
```

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Autoencoders

Autoencoders are neural networks that are trained to learn how to map their input to their input. Internally, it has a hidden layer h that contains a lossy summary of the relevant features for the task.

Autoencoders

An autoencoder can be seen has a two parts network

- Encoder function: $z = f_{\phi}(x)$
- Decoder function: $\tilde{x} = g_{\theta}(z)$
- ϕ and θ are set of learned parameters

Autoencoders

The simplest autoencoder is a one layer MLP:

$$\begin{aligned}\mathbf{z} &= \text{relu}(\mathbf{W}_{xz}\mathbf{x} + \mathbf{b}_{xz}) \quad [\text{encoder}] \\ \tilde{\mathbf{x}} &= \text{sigmoid}(\mathbf{W}_{zx}\mathbf{z} + \mathbf{b}_{zx}) \quad [\text{decoder}]\end{aligned}\tag{1}$$

Pytorch simple autoencoder

```
class Autoencoder:
    def __init__(self, **kwargs):
        """constructor"""
        pass

    def encoder(self, x):
        pass

    def decoder(self, z):
        pass

    def forward(self, x):
        pass
```

Parameter initialization

$$\begin{aligned}\mathbf{z} &= \text{relu}(\mathbf{W}_{xz}\mathbf{x} + \mathbf{b}_{xz}) \\ \tilde{\mathbf{x}} &= \text{sigmoid}(\mathbf{W}_{zx}\mathbf{z} + \mathbf{b}_{zx})\end{aligned}\tag{2}$$

```
class Autoencoder:
    def __init__(self, x_dim, z_dim):
        # encoder parameters \phi
        self.Wxz = xavier_init(size=[x_dim, z_dim])
        self.bxz = Variable(torch.zeros(z_dim), requires_grad=True)
        # decoder parameters \theta
        self.Wzx = xavier_init(size=[z_dim, x_dim])
        self.bzx = Variable(torch.zeros(x_dim), requires_grad=True)
```

Encoder $f_\phi(x)$

$$\mathbf{z} = \text{relu}(\mathbf{W}_{xz}\mathbf{x} + \mathbf{b}_{xz}) \quad (3)$$

$$\phi = \{\mathbf{W}_{xz}, \mathbf{b}_{xz}\} \quad (4)$$

```
class Autoencoder:
    ...
    def encoder(self, x):
        z = F.relu(self.Wxz @ x + self.bxz.repeat(x.size(0), 1))
        return z
```

Decoder $g_{\theta}(x)$

$$\mathbf{z} = \sigma(\mathbf{W}_{zx}\mathbf{z} + \mathbf{b}_{zx}) \quad (5)$$

$$\theta = \{\mathbf{W}_{zx}, \mathbf{b}_{zx}\} \quad (6)$$

```
class Autoencoder:
    ...
    def decoder(self, z):
        x_recon = F.sigmoid(z @ self.Wzx + self.bzx.repeat(z.size(0), 1))
        return x_recon
```

Forward propagation

$$\begin{aligned} \mathbf{z} &= \text{relu}(\mathbf{W}_{xz}\mathbf{x} + \mathbf{b}_{xz}) \\ \tilde{\mathbf{x}} &= \text{sigmoid}(\mathbf{W}_{zx}\mathbf{z} + \mathbf{b}_{zx}) \end{aligned} \tag{7}$$

```
class Autoencoder:
    ...
    def forward(self, x):
        z = self.encoder(x)
        x_recon = self.decoder(z)
        return x_recon
```

Pytorch simple autoencoder

```
class Autoencoder:
    def __init__(self, x_dim, z_dim):
        # encoder parameters
        Wxz = xavier_init(size=[x_dim, z_dim])
        bxz = Variable(torch.zeros(z_dim), requires_grad=True)
        # decoder parameters
        Wzx = xavier_init(size=[h_dim, x_dim])
        bxz = Variable(torch.zeros(X_dim), requires_grad=True)

    def encoder(self, x):
        z = F.relu(x @ self.Wxz + self.bxz.repeat(x.size(0), 1))
        return z

    def decoder(self, z):
        x_recon = F.sigmoid(z @ self.Wzx + self.bzx.repeat(z.size(0), 1))
        return x_recon

    def forward(self, x):
        z = self.encoder(x)
        x_recon = self.decoder(z)
        return x_recon
```

Autoencoder - Loss Function

If you treat the problem like a *regression*¹, use the mean square error between the input and the reconstruction

$$\mathcal{L} = \sum_{i=1}^d (x_i - \tilde{x}_i)^2 \quad (8)$$

¹If you do regression, you don't have to apply sigmoid in the decoder.

Training Autoencoders

Algorithm 1 Pseudocode for Stochastic Gradient Training

Require: Learning rate η

Require: Initial parameter ω_0

Require: Number of epochs T

for $i = 1$ to T **do**

$X = X^{train}.copy()$ and $Y = Y^{train}.copy()$

while X is not empty **do**

Sample $\{x^{(1)}, \dots, x^{(m)}\}$ from X and $\{y^{(1)}, \dots, y^{(m)}\}$ from Y

Remove samples from X and Y

Compute gradient $\mathbf{g}_t = \frac{1}{m} \nabla_{\omega} \sum_i \mathcal{L}(\tilde{x}^{(i)}, x^{(i)})$

Apply update: $\omega_t = \omega_{t-1} - \eta \cdot \mathbf{g}_t$

end while

end for

Pytorch Stochastic Gradient

```
def train(self, trainloader, num_epochs, learning_rate):

    for epoch in range(num_epochs):
        for inputs, targets in trainloader:
            batch_size = inputs.size(0)
            x_tilde = self.forward(x)

            loss = F.mse_loss(x, x_tilde)

            # Use autograd to compute the derivative of the loss w.r.t
            # all Tensors with requires_grad=True. After calling `loss.backward()`,
            # conv_weight.grad, dense_weight.grad, and dense_bias.grad
            # will be Tensors equal to the gradient of the loss with respect
            # to the filters of the cnn layer, the weight of the fully connected layer, and
            # the bias of the fully connected layer respectively.
            loss.backward()

            # Apply gradient descent to all the leaned parameters
            # The derivative of the loss is giving us the direction
            # where the funtion increase. Thus we go in the
            # opposite direction. Using torch.no_grad() tells pytorch
            # to not include thes operation in the computational graph.
            # Instead, gradient descent is goning to be applied `inplace`.
            with torch.no_grad():
                self.W_xz -= learning_rate * self.W_xz.grad
                self.b_xz -= learning_rate * self.b_xz.grad
                self.W_zx -= learning_rate * self.W_zx.grad
                self.b_zx -= learning_rate * self.b_zx.grad
```

Autoencoders

To summarize

- A neural network encode x in a hidden state z of smaller dimension
- Another neural network decode z to reconstruct x
- A sound loss function could be the mean square error between the input and its reconstruction.
- Both network can be train at the same time with gradient method.

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Generative Models

Represent the probability distribution of either $P(X, Y)$ or $P(X)$. In the case of *density estimation*, we are looking for a representation of

$$x \sim P_{\theta}(X)$$

For example, $x \sim \mathcal{N}(x; \mu_{\text{mle}}, \sigma_{\text{mle}})$

Problem: Most parametric distribution make strong (and often wrong) assumption about the distribution.

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Latent variable models

We can model the distribution of x as a function of a latent variable z

$$p(x) = \int p_{\theta}(x|z)p(z)dz$$

where the distribution of z is chosen. A typical choice for z is

$$z \sim \mathcal{N}(z; \mathbf{0}, \mathbf{I})$$

Then we can train a model to learn a good representation of $p_{\theta}(x|z)$ with stochastic gradient.

Latent variable models

$$p(x) = \int p_{\theta}(x|z)p(z)dz$$

Once we have a good representation of $p_{\theta}(x|z)$, we can sample from $p(x)$ by first sampling

$$z' \sim p(z)$$

and then sampling

$$x' \sim p(x|z')$$

Latent variable models

Problem 1: To learn $p_{\theta}(x|z)$ using stochastic gradient, we need to know a good mapping

$$f : \mathcal{Z} \times \Theta \mapsto \mathcal{X}$$

In other word when we sample $x \sim p(x|z')$ we need to know which x is likely to be generated by this particular z' in order to train the model.

Latent variable models

Solution: the prior of the latent space can be written as

$$p(z) = \int p(z|x)p(x)dx$$

During training, We can sample z by sampling

$$x' \sim p(x)$$

and then

$$z \sim p(z|x')$$

The training set comes from $p(x)$ so we can sample from it. This will reduce the space of the latent variable a lot and allow the model to learn efficiently.

Latent variable models

Problem 2: $p(z|x)$ is intractable.

Solution: use an approximation $q_\phi(z|x)$

To summarize

- Sample $x \sim D_n$
- Sample $z \sim q_\phi(z|x)$
- Sample $\tilde{x} \sim p_\theta(x|z)$

The parameter to learn are ϕ and θ and they should be learn such that the marginal likelihood $p(x)$ is maximized.

Latent variable models

Before looking at how we can train this model efficiently, let's take a closer look at how it works concretely.

Probabilistic Encoder $q_\phi(z|x)$

Example: Gaussian MLP as encoder

- $\mu_z, \log \sigma_z^2 = f(\mathbf{x}; \phi)$
 - $\mathbf{h} = \text{relu}(xW_{xh} + b_{xh})$
 - $\mu = hW_{hz}^{(1)} + b_{hz}^{(1)}$
 - $\log \sigma^2 = hW_{hz}^{(2)} + b_{hz}^{(2)}$
- $q_\phi(z|x) = \mathcal{N}(\mathbf{z}; \mu_z, \sigma_z^2)$
- $\phi = \{W_{hz}^{(1)}, b_{hz}^{(1)}, W_{hz}^{(2)}, b_{hz}^{(2)}, W_{xh}, b_{xh}\}$

```
class VAE:
```

```
...
```

```
def encoder(self, x):
```

```
    # Encoder network. Return the parameter of q(z|x)
```

```
    h = relu(x @ self.Wxh + self.bxh.repeat(x.size(0), 1))
```

```
    mu = h @ self.Whz_mu + self.bhz_mu.repeat(x.size(0), 1)
```

```
    log_var = h @ self.Whz_var + self.bhz_var.repeat(x.size(0), 1)
```

```
    return mu, log_var
```

Sampling $z \sim q_\phi(z|x)$

Example: Sampling z from $q_\phi(z|x)$

- $\mathbf{z} \sim \mathcal{N}(\boldsymbol{\mu}_z, \boldsymbol{\sigma}_z)$
 - $\boldsymbol{\mu}_z, \log \boldsymbol{\sigma}_z^2 = f(\mathbf{x}; \phi)$
 - $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
 - $\mathbf{z} = \boldsymbol{\mu}_z + \boldsymbol{\sigma}_z \odot \boldsymbol{\epsilon}$

```
class VAE:
    ...
    def _sample_z(self, mu, log_var):
        epsilon = Variable(torch.randn(mu.size())).to(self._device)
        sigma = torch.exp(log_var / 2)
        return mu + sigma * epsilon
```

Probabilistic Decoder $p_{\theta}(x|z)$

Example: Gaussian MLP as decoder

- $\mu_x, \log \sigma_x^2 = g(\mathbf{x}; \theta)$
 - $\mathbf{h} = \text{relu}(\mathbf{W}_{zh}\mathbf{x} + \mathbf{b}_{zh})$
 - $\mu_x = W_{hz}^{(1)}\mathbf{h} + \mathbf{b}_{hz}^{(1)}$
 - $\log \sigma_x^2 = W_{hz}^{(2)}\mathbf{h} + \mathbf{b}_{hz}^{(2)}$
- $p_{\theta}(x|z) = \mathcal{N}(x; \mu_x, \log \sigma_x^2)$
- $\theta = \{W_{zh}, b_{zh}, W_{zx}, b_{zx}\}$

```
class VAE:
    ...
    def decoder(self, z):
        # Decoder network. Reconstruct the input from
        # the latent variable z
        h = relu(z @ self.Whx + self.bhx.repeat(x.size(0), 1))
        gamma = h @ self.Whx_mu + self.bhx.repeat(x.size(0), 1)
        return gamma
```

Latent variable models

To summarize

- Sample $x \sim D_n$
- Sample $z \sim q_\phi(z|x)$
- Sample $\tilde{x} \sim p_\theta(x|z)$

The parameter to learn are ϕ and θ and they should be learn such that the marginal likelihood $p(x)$ is maximized.

Outline

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- Autoencoders

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Training VAE

We need $p_{\theta}(x|z)$ to be such that the marginal likelihood $p(x)$ is maximized.

In other word the lost function should be

$$-\log p(x^{(1)}, \dots, x^{(N)}) = -\sum_{i=1}^N \log p(x^{(i)})$$

Kullback-Leibler divergence

$$\mathcal{D}_{KL}[q(x)||p(x)] = \mathbb{E}_{x \sim q(x)}[\log q(x) - \log p(x)] \quad (9)$$

Gibbs' inequality:

$$\mathcal{D}_{KL}[q(x)||p(x)] \geq 0 \quad (10)$$

Training VAE

Now let's compute the Kullback-Leibler divergence \mathcal{D}_{KL} between $p(z|x)$ and $q(z|x)$

$$\begin{aligned}\mathcal{D}_{KL}[q(z|x)||p(z|x)] &= \mathbb{E}_{z \sim q(z|x)} [\log q(z|x) - \log p(z|x)] \\ &= \mathbb{E}_{z \sim q(z|x)} [\log q(z|x) - \log p(x|z) - \log p(z) + \log p(x)] \\ &= \log p(x) + \mathbb{E}_{z \sim q(z|x)} [\log q(z|x) - \log p(z)] - \mathbb{E}_{z \sim q(z|x)} \log p(x|z) \\ &= \log p(x) - \mathcal{D}_{KL}[q(z|x)||p(z|x)] - \mathbb{E}_{z \sim q(z|x)} \log p(x|z)\end{aligned}$$

Training VAE

$$\log p(x) = \mathbb{E}_{z \sim q(z|x)} \log p(x|z) - \mathcal{D}_{KL}[q(z|x)||p(z)] + \mathcal{D}_{KL}[q(z|x)||\log p(z|x)] \quad (11)$$

Because of Gibbs' inequality we have

$$\log p(x) \geq \mathbb{E}_{z \sim q(z|x)} \log p(x|z) - \mathcal{D}_{KL}[q(z|x)||p(z)]$$

Hence, our loss function is

$$\mathcal{L} = \mathbb{E}_{z \sim q(z|x)} \log p(x|z) - \mathcal{D}_{KL}[q(z|x)||p(z)]$$

Solution of $\mathcal{D}_{KL}[q(z|x)||p(z)]$

$$\begin{aligned}\mathcal{D}_{KL}[q_\phi(z|x)||p(z)] &= \int q_\phi(z|x)(\log q_\phi(z|x) - \log p(z))dx \\ &= \int q_\phi(z|x) \log q_\phi(z|x)dx - \int q_\phi(z|x) \log p(z)dx\end{aligned}$$

Training VAE

Suppose $z \in \mathbb{R}^J$ is normal

$$\begin{aligned}\int q(z|x) \log q(z|x) dz &= \int \mathcal{N}(z; \mu, \sigma) \log \mathcal{N}(z; \mu, \sigma) \\ &= -\frac{J}{2} \log 2\pi - \frac{1}{2} \sum_{j=1}^J (1 + \log \sigma_j^2)\end{aligned}\tag{12}$$

$$\begin{aligned}\int q(z|x) \log p(z) dz &= \int \mathcal{N}(z; \mu, \sigma) \log \mathcal{N}(z; 0, I) \\ &= -\frac{J}{2} \log 2\pi - \frac{1}{2} \sum_{j=1}^J (\mu_j^2 + \sigma_j^2)\end{aligned}\tag{13}$$

Training VAE

$$\begin{aligned}\mathcal{D}_{KL}[q(z|x)||p(z)] &= (12) - (13) \\ &= \frac{1}{2} \sum_{j=1}^J \mu_j^2 + \sigma_j^2 - 1 - \log \sigma_j^2\end{aligned}\tag{14}$$

```
def kl_divergence(mu, log_sigma):  
    sigma = torch.exp(log_sigma)  
    return .5 * torch.sum(mu**2 + sigma**2 - 1 - 2*log_sigma, axis=1)
```

VAE Loss Function

$$\begin{aligned}\mathcal{L} &= -\mathbb{E}_{z \sim q(z|x)} \log p(x|z) + \mathcal{D}_{KL}[q(z|x) || p(z)] \\ &= -\log \mathcal{N}(x; \boldsymbol{\mu}_x, \boldsymbol{\sigma}_x) + \frac{1}{2} \sum_{j=1}^J \mu_j^2 + \sigma_j^2 - 1 - \log \sigma_j^2\end{aligned}\tag{15}$$

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Unsupervised Spam Detection

- SMS Spam Collection Data Set²
 - Number of instances: 5574
 - Number of spams: 747 ($\sim 13\%$)
- Spam detection
 - Estimate the distribution of all the text messages
 - Evaluate the density of each text message
 - Text message with low density are classified as spam

²<https://archive.ics.uci.edu/ml/datasets/sms+spam+collection>

Data

- Examples of **non spams**

- *What you doing?how are you?*
- *Ok lar... Joking wif u oni...*
- *Cos i was out shopping wif darren jus now n i called him 2 ask wat present he wan lor. Then he started guessing who i was wif n he finally guessed darren lor.*

- Examples of **spams**

- *FreeMsg: Txt: CALL to No: 86888 & claim your reward of 3 hours talk time to use from your phone now! ubscribe6GBP/ mnth inc 3hrs 16 stop?txtStop*
- *Sunshine Quiz! Win a super Sony DVD recorder if you canname the capital of Australia? Text MQUIZ to 82277. B*
- *URGENT! Your Mobile No 07808726822 was awarded a L2,000 Bonus Caller Prize on 02/09/03! This is our 2nd attempt to contact YOU! Call 0871-872-9758 BOX95QUm*

Performance Metric

$$\begin{aligned} F_1 - \text{Score} &= \left(\frac{\text{recall}^{-1} + \text{precision}^{-1}}{2} \right)^{-1} \\ &= 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} \end{aligned} \tag{16}$$

where

$$\text{precision} = \frac{|\{\text{spams detected}\}|}{|\{\text{spams classified}\}|} \quad \text{recall} = \frac{|\{\text{spams detected}\}|}{|\{\text{spams}\}|}$$

Motivation: Both precision and recall metric are important. Take the harmonic mean between them.

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Preprocessing

- Some terminology
 - Vocabulary: Set of all the word types in the training set $\{w_1, \dots, w_{|\text{Vocabulary}|}\}$.
 - Training corpus: Set of all text messages in the training set $\{x^{(1)}, \dots, x^{(n)}\}$.
 - Bag of words: Vector representation of a sentence.

Bag of words

- $x^{(i)}$ = *What you doing?how are you?* (original sentence)
- $x^{(i)}$ = *what you do how be you* (after preprocessing)
- $x^{(i)}$ = $[0 \dots 0 \ 1 \ 0 \dots 0 \ 2 \ 0 \dots 0]$ (vector representation)

```
x = 'What you doing?how are you?'
```

```
x = preprocess(x)
```

```
print(x)
```

```
>>> 'what you do how be you'
```

```
x = vectorize(x)
```

```
print(x)
```

```
>>> [0 0 0 ... 0 0 0]
```

Bag of words

- Bag of words

- All examples in the corpus have the same length.
- The value of a position in the vector is equal to the frequency of this word in the example.
- $x^{(i)} = [0 \dots 0 \ 1 \ 0 \dots 0 \ 2 \ 0 \dots 0]$

- Binary bag of words

- All examples in the corpus have the same length.
- Each element in the vector is either 0 or 1.
- $x^{(i)} = [0 \dots 0 \ 1 \ 0 \dots 0 \ 1 \ 0 \dots 0]$

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- 1 Autoencoders
 - An example to keep in mind
 - Autoencoders
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 - **Binary Cross Entropy**
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Binary Cross Entropy

Recall that the density of a Bernoulli distribution is given by

$$\text{Bernoulli}(x; \gamma) = \gamma^x (1 - \gamma)^{1-x} \quad (17)$$

where $\gamma \equiv p(x = 1)$.

Binary Cross Entropy

Thus the log-likelihood of a Bernoulli distribution is

$$\log p(x) = x \log \gamma + (1 - x) \log(1 - \gamma) \quad (18)$$

Binary Cross Entropy

If you have binary features, i.e. $x_i \in \{0, 1\}$ for $i = 1, \dots, d$, then the output of the decoder can be interpreted as the parameter of a Bernoulli. Thus the likelihood of the input x can be computed as

$$p(x|z) = \prod_{i=1}^d p(x_i|z) = \prod_{i=1}^d \gamma_i^{x_i} (1 - \gamma_i)^{1-x_i} \quad (19)$$

Note that this works only if $\gamma_i \in (0, 1)$. To ensure it, apply sigmoid element wise on the output of the decoder.

Binary Cross Entropy

And the log-likelihood is given by

$$\log p(x|z) = - \sum_{i=1}^d x_i \log \gamma_i + (1 - x_i) \log(1 - \gamma_i)$$

```
# in pytorch  
functional.binary_cross_entropy(param, x)
```

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Probabilistic Decoder $p_{\theta}(x|z)$

Bernoulli MLP as decoder

- $\gamma = g(z; \theta)$
 - $h = \text{relu}(W_{zh}x + b_{zh})$
 - $\gamma = \sigma(W_{hx}h + b_{hx})$
- $p_{\theta}(x|z) = \text{Bernoulli}(x; \gamma)$
- $\theta = \{W_{zh}, b_{zh}, W_{zx}, b_{zx}\}$

```
class VAE:
    ...
    def decoder(self, z):
        h = relu(self.W_zh @ z + self.b_zh.repeat(x.size(0), 1))
        gamma = self.W_hx @ h + self.b_hx.repeat(x.size(0), 1)
        return gamma
```

Outline

1 Autoencoders

- An example to keep in mind
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Anomaly detection

Algorithm 2 Pseudocode for Batch Gradient Descent

Require: Learning rate ϵ_k

Require: Initial parameter w_0

Require: Number of epochs T

for $i = 1$ to T **do**

 Compute gradient $g_t = \frac{1}{m} \nabla_w \sum_i L(h_{w_{t-1}}(x^{(i)}), y^{(i)})$

 Apply update: $w_t = w_{t-1} - \epsilon g_t$

end for
