### Project discussion, 22 May: Mandatory but ungraded. We split into 6

sub-classes. The purpose is to make sure your project is on track, good progress and good goals. **The discussion following your presentation is the most important.** 

Each group gives a ~10 min presentation by all members (each person talks for ~2 min, ~1 slide)

- 1) Motivation & background, which data?
- 2) small Example,
- 3) final outcome, (focused on method and data)
- 4) difficulties,

Timing: There are upto 8 Groups in each sub-class, thus we have 15 min in total/group, with 2 min/person 10min presentation time/group. The discussion following a presentation might be the most important.

### June 5, 5-8pm: Poster and Pizza

### **Generative Models**

Given training data, generate new samples from same distribution



Addresses density estimation, a core problem in unsupervised learning **Several flavors:** 

- Explicit density estimation: explicitly define and solve for p<sub>model</sub>(x)
- Implicit density estimation: learn model that can sample from p<sub>model</sub>(x) w/o explicitly defining it



Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.



Optimizing posterior p(x|y)

You can also optimize the evidence (type II likelihood) p(x)

$$\begin{aligned}
\rho(x_{1}, x_{2}, x_{3}) &= \rho(x_{2}, x_{3} | x_{1}) \rho(x_{1}) \\
&= p(x_{3} | x_{2}, x_{2}) \rho(x_{2} | x_{1}) \rho(x_{1}) \\
&= \frac{1}{11} \rho(x_{n} | x_{1}, x_{n-1}), \quad N=J
\end{aligned}$$

# Fully visible belief network

Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

Then maximize likelihood of training data

# Fully visible belief network

Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

Then maximize

 $P(x_i) P(x_2|\lambda_i) P(x_3|x_i)$ 

# PixeIRNN [van der Oord et al. 2016]

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

Drawback: sequential generation is slow!



# PixeICNN [van der Oord et al. 2016]

Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region

Training: maximize likelihood of training images

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$

Softmax loss at each pixel



# **PixelRNN** and **PixelCNN**

#### Pros:

- Can explicitly compute likelihood p(x)
- Explicit likelihood of training data gives good evaluation metric
- Good samples

#### Con:

- Sequential generation => slow

#### Improving PixelCNN performance

- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc...

#### See

- Van der Oord et al. NIPS 2016
- Salimans et al. 2017 (PixelCNN++)

#### Some background first: Autoencoders Unsupervised approach for learning a lower-dimensional feature representati from unlabeled training data Encoder: 4-layer conv Decoder: 4-layer upconv z usually smaller than x Originally: Linear + Input data (dimensionality reduction) nonlinearity (sigmoid) Later: Deep, fully-connected Q: Why dimensionality Later: Rel U CNN reduction? A: Want features to Features zcapture meaningful factors of variation in data Encoder Input data x

Reconstructed data

## Some background first: Autoencoders



Reconstructed data



Encoder: 4-layer conv Decoder: 4-layer upconv



After training, throw away decoder

# Some background first: Autoencoders



Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data. Can we generate new images from an autoencoder?

Variational Bayes summary

Bayes  $p(x|y) = \frac{p(y|x)p(y)}{p(x)}$ 

Optimizing posterior p(x|y)

You can also optimize the evidence (type II likelihood) p(y)

Bishop Ch 10 Approximate inference

Observations  $X = [x_1, \dots, x_N]$ 

With latent parameter  $Z = [z_1, ..., z_N]$ 

And probability p(X, Z)

We like to find an approximation to p(X, Z) and the evidence p(Z)A good guess is a factorized distribution  $p(X, Z) = \prod_{n=1}^{N} z_n$ 

# Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data  $\{x^{(i)}\}_{i=1}^N$  is generated from underlying unobserved (latent) representation **z** 



We want to estimate the true parameters  $\theta^*$  of this generative model.

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian.

Conditional p(x|z) is complex (generates image) => represent with neural network

#### How to train the model?

Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

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

Q: What is the problem with this?

Intractable!

# Variational Autoencoders: Intractability

Data likelihood: 
$$p_{\theta}(x) = \int p_{\theta}(z) p_{\theta}(x|z) dz$$

Intractible to compute p(x|z) for every z!

Posterior density also intractable:  $p_{\theta}(z|x) = p_{\theta}(x|z)p_{\theta}(z)/p_{\theta}(x)$ 

Solution: In addition to decoder network modeling  $p_{\theta}(x|z)$ , define additional encoder network  $q_{\phi}(z|x)$  that approximates  $p_{\theta}(z|x)$ 

Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize

#### Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data  $~\{x^{(i)}\}_{i=1}^N$  is generated from underlying unobserved (latent) representation  ${\bf z}$ 



### Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic





# Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)})\right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})}\right] \quad (Bayes' \text{ Rule})$$

$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})}\right] \quad (Multiply \text{ by constant}) \quad Optimized by constant) \quad Optimized by constant \quad Optimized by constant \quad Optimized by constant \quad Optimized by constant \quad Optimized by constant) \quad Optimized by constant \quad Optimized by const$$



### Variational Autoencoders: Generating Data!

#### Use decoder network. Now sample z from prior!

#### Data manifold for 2-d z

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### Markov models, Bishop 13.1

n=1



#### First order Markov chain



### Markov models, Bishop 13.1



State Space model



X<sub>R+1</sub>=M<sub>R</sub> X<sub>R</sub> + S<sub>R</sub>

YR = HRXR + VR

Sha N(O, Qhe)

### Product of Gaussians=Gaussian:



### The Model

State equation

Consider the discrete, linear system,

$$\mathbf{\underline{x}}_{k+1} = \mathbf{\underline{M}}_k \mathbf{x}_k + \mathbf{w}_k, \quad k = 0, 1, 2, \dots,$$
(1)

where

- $\mathbf{x}_k \in \mathbb{R}^n$  is the state vector at time  $t_k$
- $\mathbf{M}_k \in \mathbb{R}^{n \times n}$  is the state transition matrix (mapping from time  $t_k$  to  $t_{k+1}$ ) or model
- { $\mathbf{w}_k \in \mathbb{R}^n$ ; k = 0, 1, 2, ...} is a white, Gaussian sequence, with  $\mathbf{w}_k \sim N(\mathbf{0}, \mathbf{Q}_k)$ , often referred to as model error
- $\mathbf{Q}_k \in \mathbb{R}^{n \times n}$  is a symmetric positive definite covariance matrix (known as the model error covariance matrix).

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Some of the following slides are from: Sarah Dance, University of Reading

The Observations

Measurement equation

We also have discrete, linear observations that satisfy

$$\mathbf{y}_{k} = \mathbf{H}_{k}\mathbf{x}_{k} + \mathbf{v}_{k}, \ k = 1, 2, 3, \dots,$$
 (2)

where

- y<sub>k</sub> ∈ ℝ<sup>p</sup> is the vector of actual measurements or observations at time t<sub>k</sub>
- H<sub>k</sub> ∈ ℝ<sup>n×p</sup> is the observation operator. Note that this is not in general a square matrix.
- { $\mathbf{v}_k \in \mathbb{R}^p$ ; k = 1, 2, ...} is a white, Gaussian sequence, with  $\mathbf{v}_k \sim N(\mathbf{0}, \mathbf{R}_k)$ , often referred to as observation error.
- $\mathbf{R}_k \in \mathbb{R}^{p \times p}$  is a symmetric positive definite covariance matrix (known as the observation error covariance matrix).

We assume that the initial state,  $\mathbf{x}_0$  and the noise vectors at each step,  $\{\mathbf{w}_k\}$ ,  $\{\mathbf{v}_k\}$ , are assumed mutually independent.

### The Prediction and Filtering Problems

We suppose that there is some uncertainty in the initial state, i.e.,

$$\mathbf{x}_0 \sim N(0, \mathbf{P}_0)$$
 (3)

with  $\mathbf{P}_0 \in \mathbb{R}^{n \times n}$  a symmetric positive definite covariance matrix.

The problem is now to compute an improved estimate of the stochastic variable  $\mathbf{x}_k$ , provided  $\mathbf{y}_1, \dots \mathbf{y}_j$  have been measured:

$$\widehat{\mathbf{x}}_{k|j} = \widehat{\mathbf{x}}_{k|y_1,\dots,y_j}.$$
(4)

- When j = k this is called the filtered estimate.
- When j = k 1 this is the one-step predicted, or (here) the predicted estimate.

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- The Kalman filter (Kalman, 1960) provides estimates for the linear discrete prediction and filtering problem.
- We will take a minimum variance approach to deriving the filter.
- We assume that all the relevant probability densities are Gaussian so that we can simply consider the mean and covariance.
- Rigorous justification and other approaches to deriving the filter are discussed by Jazwinski (1970), Chapter 7.

Prediction

Xn~ N(xn, Pen)

$$\boldsymbol{x}_{k+1|k} = \boldsymbol{M}_k \boldsymbol{x}_k + \boldsymbol{\delta}_k = \boldsymbol{x}'_k + \boldsymbol{\delta}_k$$

X 11/2

 $\mathbf{x}'_{k} \sim \mathcal{N}(\mathcal{M}, \mathcal{K}_{k}, \mathcal{M}, \mathcal{M}_{k}, \mathcal{M}_{k})$  $\boldsymbol{\delta}_{k} \sim \mathcal{N}(\boldsymbol{c}, \boldsymbol{Q})$  $x_{k+1|k} \sim$ 

 $\widehat{x}_{k+1|k}$ =  $P_{k+1|k} =$ 

### **Prediction step**

We first derive the equation for one-step prediction of the mean using the state propagation model (1).



The one step prediction of the covariance is defined by,

$$\mathbf{P}_{k+1|k} = \mathbb{E}\left[ (\mathbf{x}_{k+1} - \widehat{\mathbf{x}}_{k+1|k}) (\mathbf{x}_{k+1} - \widehat{\mathbf{x}}_{k+1|k})^T | \mathbf{y}_1, \dots \mathbf{y}_k \right].$$
(6)

Exercise: Using the state propagation model, (1), and one-step prediction of the mean, (5), show that

$$\mathbf{P}_{k+1|k} = \mathbf{M}_k \mathbf{P}_{k|k} \mathbf{M}_k^T + \mathbf{Q}_k.$$
(7)



#### Filtering Step

At the time of an observation, we assume that the update to the mean may be written as a linear combination of the observation and the previous estimate:

$$\widehat{\mathbf{x}}_{k|k} = \widehat{\mathbf{x}}_{k|k-1} + \mathbf{K}_k(\mathbf{y}_k - \mathbf{H}_k \widehat{\mathbf{x}}_{k|k-1}),$$
(8)

where  $\mathbf{K}_k \in \mathbb{R}^{n \times p}$  is known as the Kalman gain and will be derived shortly.



But first we consider the covariance associated with this estimate:

$$\mathbf{P}_{k|k} = \mathbb{E}\left[ (\mathbf{x}_k - \widehat{\mathbf{x}}_{k|k}) (\mathbf{x}_k - \widehat{\mathbf{x}}_{k|k})^T | \mathbf{y}_1, \dots \mathbf{y}_k \right].$$
(9)

Using the observation update for the mean (8) we have,

$$\begin{aligned} \mathbf{x}_{k} - \widehat{\mathbf{x}}_{k|k} &= \mathbf{x}_{k} - \widehat{\mathbf{x}}_{k|k-1} - \mathbf{K}_{k}(\mathbf{y}_{k} - \mathbf{H}_{k}\widehat{\mathbf{x}}_{k|k-1}) \\ &= \mathbf{x}_{k} - \widehat{\mathbf{x}}_{k|k-1} - \mathbf{K}_{k}(\mathbf{H}_{k}\mathbf{x}_{k} + \mathbf{v}_{k} - \mathbf{H}_{k}\widehat{\mathbf{x}}_{k|k-1}), \\ &\text{replacing the observations with their model equivalent,} \\ &= (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})(\mathbf{x}_{k} - \widehat{\mathbf{x}}_{k|k-1}) - \mathbf{K}_{k}\mathbf{v}_{k}. \end{aligned}$$
(10)

Thus, since the error in the prior estimate,  $\mathbf{x}_k - \hat{\mathbf{x}}_{k|k-1}$  is uncorrelated with the measurement noise we find

$$\mathbf{P}_{k|k} = (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})\mathbb{E}\left[(\mathbf{x}_{k} - \widehat{\mathbf{x}}_{k|k-1})(\mathbf{x}_{k} - \widehat{\mathbf{x}}_{k|k-1})^{T}\right](\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})^{T} + \mathbf{K}_{k}\mathbb{E}\left[\mathbf{v}_{k}\mathbf{v}_{k}^{T}\right]\mathbf{K}_{k}^{T}.$$
(11)

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# Simplification of the a posteriori error covariance formula

Using this value of the Kalman gain we are in a position to simplify the Joseph form as

$$\mathbf{P}_{k|k} = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_{k|k-1} (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)^T + \mathbf{K}_k \mathbf{R}_k \mathbf{K}_k^T = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_{k|k-1}.$$
(15)

Exercise: Show this.

Note that the covariance update equation is independent of the actual measurements: so  $\mathbf{P}^{k|k}$  could be computed in advance.



### Summary of the Kalman filter

#### Prediction step

Mean update: Covariance update:

$$\widehat{\mathbf{x}}_{k+1|k} = \mathbf{M}_k \widehat{\mathbf{x}}_{k|k} \\ \mathbf{P}_{k+1|k} = \mathbf{M}_k \mathbf{P}_{k|k} \mathbf{M}_k^T + \mathbf{Q}_k$$

#### Observation update step

Mean update: Kalman gain: Covariance update:

$$\begin{split} \widehat{\mathbf{x}}_{k|k} &= \widehat{\mathbf{x}}_{k|k-1} + \mathbf{K}_{k}(\mathbf{y}_{k} - \mathbf{H}_{k}\widehat{\mathbf{x}}_{k|k-1}) \\ \mathbf{K}_{k} &= \mathbf{P}_{k|k-1}\mathbf{H}_{k}^{T}(\mathbf{H}_{k}\mathbf{P}_{k|k-1}\mathbf{H}^{T} + \mathbf{R}_{k})^{-1} \\ \mathbf{P}_{k|k} &= (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})\mathbf{P}_{k|k-1}. \end{split}$$



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### Bayes' Theorem for Gaussian Variables, Lecture 3

Given

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$$
$$p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1})$$

we have

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathrm{T}})$$
  
$$p(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\Sigma}\{\mathbf{A}^{\mathrm{T}}\mathbf{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\}, \boldsymbol{\Sigma})$$

where

$$\boldsymbol{\Sigma} = (\boldsymbol{\Lambda} + \mathbf{A}^{\mathrm{T}} \mathbf{L} \mathbf{A})^{-1}$$

$$p(\boldsymbol{x}_k|\boldsymbol{y}_k,\boldsymbol{x}_{k|k-1}) = p(\boldsymbol{y}_k|\boldsymbol{x}_k)p(\boldsymbol{x}_k|\boldsymbol{x}_{k|k-1})$$

$$\boldsymbol{P}_{k}^{-1} =$$

$$\boldsymbol{P}_{k} = (\mathbf{I} - \mathbf{K}\mathbf{H}_{k})\boldsymbol{P}_{k|k-1}$$

$$\boldsymbol{K} = \boldsymbol{P}_{k|k-1}\boldsymbol{H}_{k}^{T} (\boldsymbol{H}_{k} \boldsymbol{P}_{k|k-1}\boldsymbol{H}_{k}^{T} + \boldsymbol{R}_{k})^{-1}$$

The Woodbury matrix identity is<sup>[4]</sup>

$$(A+UCV)^{-1}=A^{-1}-A^{-1}Uig(C^{-1}+VA^{-1}Uig)^{-1}VA^{-1},$$