Learning and Inference with Dynamical Systems¹

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¹Slides are based from [Bishop, Pattern Recognition and Machine Learning, 2007] 9 .

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Learning and Inference with Dynamical Systems

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- Sets of data points assumed to be independent and identically distributed (i.i.d.) in many popular models
- i.i.d. is not a reasonable assumption for sequential data
 - Measurements of time series, daily values of a currency exchange rate, acoustic features in speech recognition
 - Sequence of nucleotide base pairs along a strand of DNA, sequence of characters in an English sentence

• Markov model:

$$p(x_1,\cdots,x_N)=\prod_{n=1}^N p(x_n|x_1,\cdots,x_{n-1})$$

• Each of the conditional distributions is independent of all previous observations except N most recent

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The first-order Markov Chain

• Homogeneous Markov chain

 \mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3 \mathbf{x}_4

Joint distribution for a sequence of N observations

$$p(x_1, \cdots, x_N) = p(x_1) \prod_{n=2}^N p(x_n | x_{n-1})$$

• From the d-seperation property

$$p(x_n|x_1,\cdots,x_{n-1})=p(x_n|x_{n-1})$$

Given x_{n-1} , x_n is conditionally independent of x_1 , \cdots , x_{n-1} .

D-separation (Pearl, 1988)

Given a directed acyclic graph, two variables a, b and a set of variables C. Any path from a to b is said to be blocked, if it includes a node such that either

 arrows on the path meet either head-to-tail or tail-to-tail at the node in the C (inclusion),



If every path from *a* to *b* is blocked, then, *a* is said to be *d*-separated from *b* by *C*, and *a* is conditionally independent of *b* given *C*.

A higher-order Markov chain



- A higher-order Markov chain
 - Observations are discrete variables having K states
 - first-order: K 1 parameters for each K states $\rightarrow K(K 1)$ parameters
 - *M*th order: $K^M(K-1)$ parameters E.g., p(x|y,z): a second order MC with binary variables (K=2) p(x = 0|y=0, z=0), p(x = 0|y=0, z=1), p(x = 0|y=1, z=0), p(x = 0|y=1, z=1)

Hidden Markov models (HMMs)



- z_n latent variables (discrete) (assumption: $z_{n+1} \perp z_{n-1} | z_n$)
- x_n observed variables
- The joint distribution of the state space model

$$p(x_1, \cdots, x_N, z_1, \cdots, z_N) = p(z_1) \left[\prod_{n=2}^N p(z_n | z_{n-1})\right] \prod_{n=1}^N p(x_n | z_n)$$

The hidden variables make possible to represent a mixture model.

Hidden Markov Models (HMMs)

 Transition probability
 The probability of z_n has the kth value when z_{n-1} has the jth value. Let's denote

$$A_{jk} \equiv p(z_{nk} = 1 | z_{n-1,j} = 1),$$

 $0 \le A_{jk} \le 1$ and $\sum_k A_{jk} = 1$. - Latent variables are *K*-dimensional binary variables.

$$z_n = \{z_{n1}, z_{n2}, \cdots, z_{nK}\}, \text{ e.g.,}$$

 $\{0, 1, \cdots, 0\} \text{ when } z_n = 2.$

$$p(z_n|z_{n-1},A) = \prod_{k=1}^K \prod_{j=1}^K A_{jk}^{z_{n-1,j}z_{nk}}$$
 $p(z_1|\pi) = \prod_{k=1}^K \pi_k^{z_{1k}}$



Hidden Markov Models (HMMs)

• Emission probability (observations)

$$p(x_n|z_n,\phi) = \prod_{k=1}^{K} p(x_n|\phi_k)^{z_{nk}}$$



 ϕ_k is the parameter of the model.

Three hidden models



Samples when p of transition is 5%



HMM applications

- Speech recognition
- Natural language modeling
- Analysis of biological sequences
- On-line handwriting recognition (Handwritten digits)
 - Left-to-right architecture: A_{jk} of A to zero if j > k.
 - On-line data: each digit represented by the trajectory of the pen as a function of time





Bottom: synthetic digits from a left-toright HMM. 16 sequences of 16 stroke (angle) directions.

- We have observed a data set $X = x_1, \cdots, x_N$,
- Determine the parameters of an HMM $\theta=\pi, {\it A}, \phi$
- The likelihood function is $p(X|\theta) = \sum_{Z} p(X, Z|\theta)$
- The maximum likelihood estimate is $\operatorname{argmax}_{\theta} P(X|\theta)$

Expectation maximization algorithm (EM)

- Initial selection for the model parameters: θ^{old}
- E step:
 - Posterior distribution of the latent vars: $p(Z|X, \theta^{old})$
 - A log likelihood function: $p(X, Z|\theta)$

$$Q(\theta, \theta^{old}) = \mathbb{E}_{p(Z|X, \theta^{old})}[\ln p(X, Z|\theta)]$$
$$= \sum_{Z} p(Z|X, \theta^{old}) \ln p(X, Z|\theta)$$

Maximizing the likelihood function: EM

E step:



• The marginal posterior distribution of a latent variable γ and the joint posterior distribution of two successive latent variables ξ

$$\gamma(z_n) = p(z_n|X, \theta^{old})$$

$$\xi(z_{n-1}, z_n) = p(z_{n-1}, z_n|X, \theta^{old})$$

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M step:

• Maximize $Q(\theta, \theta^{old})$ with respect to parameters $\theta = \{\pi, A, \phi\}$, treat $\gamma(z_n)$ and $\xi(z_{n-1}, z_n)$ as constant. By using Lagrange multipliers²

$$\pi_{k} = \frac{\gamma(z_{1k})}{\sum_{j=1}^{K} \gamma(z_{1j})}$$
$$A_{jk} = \frac{\sum_{l=1}^{N} \xi(z_{n-1,j}, z_{nk})}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nl})}$$

That is, the marginals become the parameter of the categorical (multinoulli) distribution.

²http://cs.berkeley.edu/~stephentu/writeups/hmm-baum-welch-derivation.pdf Jaesik Choi(UNIST) Learning and Inference with Dynamical Systems 14 / 39

Lagrangian:

$$\mathcal{L}(\theta, \theta^{old}) = Q(\theta, \theta^{old}) - \lambda_{\pi} \left(\sum_{k=1}^{K} \pi_k - 1 \right) - \sum_{j=1}^{K} \lambda_{A_j} \left(\sum_{k=1}^{K} A_{jk} - 1 \right)$$
$$- \sum_{j=1}^{K} \lambda_{p(\mathbf{x}_n | \phi_j)} \left(\sum_{\mathbf{x}_n} p(\mathbf{x}_n | \phi_j) - 1 \right)$$

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Lagrangian of $Q(\theta, \theta^{old})$

Partial derivative (set to 0):

$$\frac{\partial \mathcal{L}(\theta, \theta^{old})}{\partial A_{jk}} = \sum_{\substack{n=2\\ \partial \text{ of log of transition}}}^{N} \frac{\xi(z_{n-1,j}, z_{nk})}{A_{jk}} - \underbrace{\lambda_{A_j}}_{\partial \text{ of lagrangian term}} = 0$$
$$\implies A_{jk} = \frac{\sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})}{\lambda_{A_j}}$$
$$\frac{\partial \mathcal{L}(\theta, \theta^{old})}{\partial \lambda_{A_j}} = -\left(\sum_{k=1}^{K} A_{jk} - 1\right) = 0$$
$$\implies \lambda_{A_j} = \sum_{k=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})$$

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M step:

• Parameters ϕ_k independent for Gaussian emission densities $p(x|\phi_k) = \mathcal{N}(x|\mu_k, \Sigma_k)$

$$\mu_{k} = \frac{\sum_{n=1}^{N} \gamma(z_{nk}) x_{n}}{\sum_{n=1}^{N} \gamma(z_{nk})}$$
$$\sum_{k} = \frac{\sum_{n=1}^{N} \gamma(z_{nk}) (x_{n} - \mu_{k}) (x_{n} - \mu_{k})^{T}}{\sum_{n=1}^{N} \gamma(z_{nk})}$$

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The Forward-Backward algorithm



 $\bullet\,$ Two-stage message passing algorithm to compute marginals γ and ξ

• Here, we focus on alpha-beta algorithm

$$\alpha(z_n) \equiv p(x_1, \cdots, x_n, z_n) \tag{13.34}$$

$$\beta(z_n) \equiv p(x_{n+1}, \cdots, x_N | z_n)$$
(13.35)

Conditional Independence Properties in HMM

Use $X_{[i,i]} = (x_i, \dots, x_i)$ as a simplied notation, $p(X|z_n) = p(X_{[1,n]}|z_n)p(X_{[n+1,N]}|z_n)$ (13.24) $X_{[1,n]}$ and $X_{[n+1,N]}$ are independent given z_n $p(X_{[1,n-1]}|x_n, z_n) = p(X_{[1,n-1]}|z_n)$ $p(X_{[1,n-1]}|z_{n-1}, z_n) = p(X_{[1,n-1]}|z_{n-1})$ $p(X_{[n+1,N]}|z_n, z_{n+1}) = p(X_{[n+1,N]}|z_{n+1})$ $p(X_{[n+2,N]}|z_{n+1},x_{n+1}) = p(X_{[n+2,N]}|z_{n+1})$ $p(X|z_{n-1}, z_n) = p(X_{[1,n-1]}|z_{n-1}, z_n)p(x_n|z_{n-1}, z_n)p(X_{[n+1,N]}|z_{n-1}, z_n)$ $= p(X_{[1,n-1]}|z_{n-1})p(x_n|z_n)p(X_{[n+1,N]}|z_n)$ $p(x_{N+1}|X_{[1,N]}, z_{N+1}) = p(x_{N+1}|z_{N+1})$ $p(z_{N+1}|z_N, X) = p(z_{N+1}|z_N)$ (13.31)

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The Forward Recursion

Forward recursion for $\alpha(z_n)$



$$\alpha(z_{n}) = \underline{p(X_{[1,n]}|z_{n})}p(z_{n}) = p(x_{n}|z_{n})\underline{p(X_{[1,n-1]}|z_{n})}p(z_{n})$$

$$= \overline{p(x_{n}|z_{n})}\underline{p(X_{[1,n-1]},z_{n})} = p(x_{n}|z_{n})\sum_{z_{n-1}}\underline{p(X_{[1,n-1]},z_{n-1},z_{n})}$$

$$= p(x_{n}|z_{n})\sum_{z_{n-1}}\underline{p(X_{[1,n-1]}|z_{n-1})}p(z_{n}|z_{n-1})\underline{p(z_{n-1})}$$

$$= p(x_{n}|z_{n})\sum_{z_{n-1}}\alpha(z_{n-1})p(z_{n}|z_{n-1}) \qquad (13.36)$$

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The Backward Recursion

k = 1 k = 1 A_{11} A_{12} $p(\mathbf{x}_n | z_{n+1,1})$ k = 2 A_{13} $p(\mathbf{x}_n | z_{n+1,2})$ $\beta(z_{n+1,2})$ $\beta(z_{n+1,3})$ k = 3 n n + 1 $p(\mathbf{x}_n | z_{n+1,3})$

Backward recursion for $\beta(z_n)$

$$\beta(z_n) = \sum_{z_{n+1}} \beta(z_{n+1}) p(x_{n+1}|z_{n+1}) p(z_{n+1}|z_n)$$

$$\beta(z_N) = 1$$

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The Backward Recursion - Derivation

$$\beta(z_n) = p(X_{[n+1,N]}|z_n)$$

$$= \sum_{z_{n+1}} p(X_{[n+1,N]}, z_{n+1}|z_n)$$

$$= \sum_{z_{n+1}} p(X_{[n+1,N]}|\underline{z_n}, z_{n+1}) p(z_{n+1}|z_n)$$

$$= \sum_{z_{n+1}} \frac{p(X_{[n+1,N]}|z_{n+1})}{p(z_{n+1}|z_n)} p(z_{n+1}|z_n)$$

$$= \sum_{z_{n+1}} \frac{p(X_{[n+2,N]}|z_{n+1})}{p(x_{n+1}|z_{n+1})} p(z_{n+1}|z_n).$$

By using the definition of $\beta(z_{n+1})$,

$$=\sum_{z_{n+1}}\beta(z_{n+1})p(x_{n+1}|z_{n+1})p(z_{n+1}|z_n).$$
(13.38)

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Evaluation of $\xi(z_{n-1}, z_n)$

• Using Bayes' theorem

$$\begin{split} \xi(z_{n-1}, z_n) &= p(z_{n-1}, z_n | X) = \frac{p(X, z_{n-1}, z_n)}{p(X)} \\ &= \frac{p(X | z_{n-1}, z_n) p(z_{n-1}, z_n)}{p(X)} \\ &= \frac{p(X_{[1,n-1]} | z_{n-1}) p(x_n | z_n) p(X_{[n+1,N]} | z_n) p(z_n | z_{n-1}) p(z_{n-1})}{p(X)} \\ &= \frac{p(X_{[1,n-1]} | z_{n-1}) p(z_{n-1}) p(x_n | z_n) p(X_{[n+1,N]} | z_n) p(z_n | z_{n-1})}{p(X)} \\ &= \frac{\alpha(z_{n-1}) p(x_n | z_n) \beta(z_n) p(z_n | z_{n-1})}{p(X)} \end{split}$$

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The sum-product algorithm

- Solve the problem of finding local marginals for the hidden variables γ and $\xi.$
- Can be used instead of forward-backward algorithm



Results in

$$\gamma(z_n) = \frac{\alpha(z_n)\beta(z_n)}{p(X)}$$
(13.54)

$$\xi(z_{n-1}, z_n) = \frac{\alpha(z_{n-1})\rho(x_n|z_n)\rho(z_n|z_{n-1})\beta(z_n)}{\rho(X)}$$
(13.43)

Used to solve forward-backward algorithm

$$\alpha(z_n) = p(x_n | z_n) \sum_{z_{n-1}} \alpha(z_{n-1}) p(z_n | z_{n-1})$$
(13.36)

- Probabilities $p(x_n|z_n)$ and $p(z_n|z_{n-1})$ are often significantly less than unity, thus values $\alpha(z_n)$ go to zero exponentially.
- Re-scaled equations

$$\hat{\alpha}(z_n) = p(z_n | X_{[1,n]}) = \frac{\alpha(z_n)}{p(x_1, \cdots, x_n)}$$
(13.55)
$$\hat{\beta}(z_n) = \frac{\beta(z_n)}{p(x_{n+1}, \cdots, x_N | x_1, \cdots, x_n)}$$

• Longer-range effects could be included by adding extra link



• Input and output pairs could be modeled (where u_n is an input value).



• The distribution of the observed variable at a given time step is conditional on the states of latent variables.



Extensions III - Factorial HMM

• Latent variables (e.g., $z_{n-1}^{(1)}$ and $z_{n+1}^{(1)}$) are not d-seperated (connected by a path given observations).



A Linear-Gaussian model

- The general form of algorithms for the LDS are the same as for the HMM
- Continuous latent variables
- Both observed x_n and latent z_n variables Gaussian
 - Joint distribution over all variables, marginals and conditionals are Gaussian
 - The sequence of individually most probable latent variable values is the same as the most probable latent sequence

• Transition and emission probabilities

$$p(z_n|z_{n-1}) = \mathcal{N}(z_n|Az_{n-1}, \Gamma)$$
 (13.75)

$$p(x_n|z_n) = \mathcal{N}(x_n|Cz_n, \Sigma)$$
(13.76)

• The initial latent variable

$$p(z_1) = \mathcal{N}(z_1 | \mu_0, V_0) \tag{13.77}$$

The parameters θ = {A, Γ, C, Σ, μ₀, V₀} determined using maximum likelihood through EM

Inference with Linear Dynamical Systems

- Find the marginal distributions for the latent variables conditional on the observation sequence
- Given the parameters $\theta = \{A, \Gamma, C, \Sigma, \mu_0, V_0\}$, predict the next latent state z_{n+1} and next observation x_{n+1}
- Sum-product algorithm
 - Kalman filter (forward-recursion, α message)
 - Kalman smoother (backward-recursion, β message)



blue: true position green: noisy measurements red inferred posterior Jaesik Choi(UNIST)

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Kalman filtering: Model

Transition model and observation model, params $\theta = \{A, \Gamma, C, \Sigma, \mu_0, P_0\},\$

$$p(z_n|z_{n-1}) = \mathcal{N}(z_n|Az_{n-1}, \Gamma)$$
 (13,75)

$$p(x_n|z_n) = \mathcal{N}(x_n|Cz_n, \Sigma)$$
(13.76)

Initial value:

$$p(z_1) = \mathcal{N}(z_1 | \mu_0, P_0) \tag{13.77}$$

Linear equations expressions:



$$z_n = Az_{n-1} + w_n, \ x_n = Cz_n + v_n, \ z_1 = \mu_0 + u$$

with noise terms:

$$w \sim \mathcal{N}(w|0,\Gamma), \ v \sim \mathcal{N}(v|0,\Sigma), \ u \sim \mathcal{N}(u|0,P_0).$$

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(1)

Normalized marginal distributions:

$$\hat{\alpha}(z_n) = \mathcal{N}(z_n | \mu_n, V_n). \tag{13.84}$$

Recursion equations:

$$c_n\hat{\alpha}(z_n) = p(x_n|z_n) \int \hat{\alpha}(z_{n-1})p(z_n|z_{n-1})dz_{n-1} \qquad (13.85)$$

$$c_{n}\mathcal{N}(z_{n}|\mu_{n}, V_{n}) = \mathcal{N}(x_{n}|Cz_{n}, \Sigma) \underbrace{\int \mathcal{N}(z_{n-1}|\mu_{n-1}, V_{n-1})\mathcal{N}(z_{n}|Az_{n-1}, \Gamma)dz_{n-1}}_{= \mathcal{N}(x_{n}|Cz_{n}, \Sigma) \underbrace{\mathcal{N}(z_{n}|A\mu_{n-1}, P_{n-1})}$$
(13.87)

where $P_{n-1} = AV_{n-1}A^T + \Gamma$.

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$$c_n \mathcal{N}(z_n | \mu_n, V_n) = \mathcal{N}(x_n | Cz_n, \Sigma) \mathcal{N}(z_n | A \mu_{n-1}, P_{n-1})$$

where $P_{n-1} = AV_{n-1}A^T + \Gamma$. Solve the above equations,

$$\mu_n = A\mu_{n-1} + K_n(x_n - CA\mu_{n-1})$$
(13.89)

$$V_n = (I - K_n C) P_{n-1}$$
(13.90)

$$c_n = \mathcal{N}(x_n | CA\mu_{n-1}, CP_{n-1}C^T + \Sigma).$$
(13.91)

where K_n is the Kalman gain matrix:

$$K_n = P_{n-1}C^T(CP_{n-1}C^T + \Sigma)^{-1}$$

[Important] the exponent of a Gaussian distribution is represented by

$$\frac{1}{2}x^{T}\Sigma^{-1}x + x^{T}\Sigma^{-1}\mu + constant = -\frac{1}{2}(x-\mu)^{T}\Sigma^{-1}(x-\mu)$$
 (2.71)

Before filtering

$$p(z_{n-1}|X_{[1,n-1]})$$

Diffusion by transition

$$p(z_n|X_{[1,n-1]}) = \underline{p(z_n|z_{n-1})}p(z_{n-1}|X_{[1,n-1]})$$

Sifted and Narrowed by an observation

$$p(z_n|X_{[1,n]}) = \underline{p(x_n|z_n)}p(z_n|X_{[1,n-1]})$$



- Determine $\theta = \{A, \Gamma, C, \Sigma, \mu_0, V_0\}$ using maximum likelihood
- Expectation maximization
 - E step: $Q(\theta, \theta^{old}) E_{Z|\theta^{old}}[\ln p(X, Z|\theta)]$
 - $\bullet\,$ M step: Maximize with respect to the components of θ

- The marginal distribution of the observed variables is Gaussian use Gaussian mixture as the initial distribution for *z*₁
- Make Gaussian approximation by linearizing around the mean of the predicted distribution
 Extended Kalman filter
- Combining the HMM with a set of linear dynamical systems Switching state space model

Particle filters

Sampling methods



- Needed for dynamical systems which do not have a linear-Gaussian
- Sampling-importance-resampling formalism a sequential Monte Carlo as the particle filter
- Particle filter algorithm: At time step *n*
 - obtained a set of samples and weights
 - observe x_{n+1}
 - evaluate samples and weights for time step n + 1

Recent Advances in Dynamical Systems

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• Automatic Bayesian Covariance Discovery (ABCD, The Automatic Statistician)





The Automatic Statistician, http://www.automaticstatistician.com), 2013

• Automatic Bayesian Covariance Discovery (ABCD, The Automatic Statistician)





• Automatic Bayesian Covariance Discovery (ABCD, The Automatic Statistician)



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13 raw regression datasets



Relational Automatic Bayesian Covariance Discovery with Multiple datasets



http://sail.unist.ac.kr/yunseong/



An automatic report for the dataset : GE Relational version

The Automatic Statistician

Abstract

2.6 Component 6 : A constant. This function applies from 12 Sep 2001 until 15 Sep 2001

This report was produced by the Automatic Bayesian (ABCD) algorithm.

1 Executive summary

The raw data and full model posterior with extrapolations are shown



This component explains 100.0% of the residual variance; this increases the total variance explained from 95.2% to 100.0%. The addition of this component increases the cross validated MAE by 0.67% from 0.87 to 0.87. This component explains residual variance but does not improve MAE which suggests that this component describes very short term patterns, uncorrelated noise or is an artefact of the model or search procedure.



Figure 1: Raw data (left) and model posterior with extrapolation (right)



Recurrent Convolutional Neural Network for EEG analysis

RNN $\mathbf{x}(t) = \sigma \left(\mathbf{W}^{in} \mathbf{u}(t) + \mathbf{W}^{rec} \mathbf{x}(t-1) \right) + \mathbf{b}$

$$\mathbf{RCL} x_{ijk}(t) = \boldsymbol{\sigma} \left(\left(\mathbf{w}_k^{in} \right)^{\mathrm{T}} \mathbf{u}^{(i,j)}(t) + \left(\mathbf{w}_k^{rec} \right)^{\mathrm{T}} \mathbf{x}^{(i,j)}(t-1) + b_k \right)$$



One chunk: Data: 3584,32







Completed • \$10,000 • 379 teams Grasp-and-Lift EEG Detection

lon 29 Jun 2015 – Mon 31 Aug 2015 (4 months ago)



Applying RCL

Layer type	Size	Output shape
Convolutional	256 1×9 filters	(64, 256, 1, 3584)
Max pooling	Pool size 4, stride 4	(64, 256, 1, 896)
RCL	256 1×1 feed-forward filters, 256 1×9 filters, 3 iterations	(64, 256, 1, 896)
Max pooling	Pool size 4, stride 4	(64, 256, 1, 224)
RCL	256 1×1 feed-forward filters, 256 1×9 filters, 3 iterations	(64, 256, 1, 224)
Max pooling	Pool size 4, stride 4	(64, 256, 1, 56)
RCL	256 1×1 feed-forward filters, 256 1×9 filters, 3 iterations	(64, 256, 1, 56)
Max pooling	Pool size 4, stride 4	(64, 256, 1, 14)
RCL	256 1×1 feed-forward filters, 256 1×9 filters, 3 iterations	(64, 256, 1, 14)
Max pooling	Pool size 2, stride 2	(64, 256, 1, 7)
Fully connected	1792×6	(64, 6)





Thank you!

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