Introduction to Machine Learning
– Fundamentals of Machine Learning

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Overview

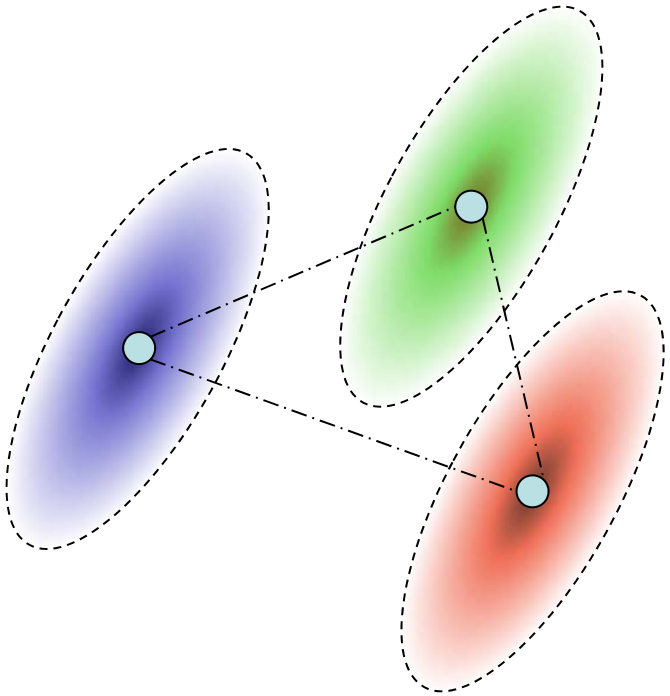
- Fisher discriminative analysis and generative methods
- Bayesian vs. Frequentist view
- Generalization issue
- Denoising autoencoder

FISHER DISCRIMINANT ANALYSIS (FDA) AND REGULARIZATION

Consider Two Statistics

- Between class variance

$$var_B(\mathbf{w}) = \mathbf{w}^\top S_B \mathbf{w}$$



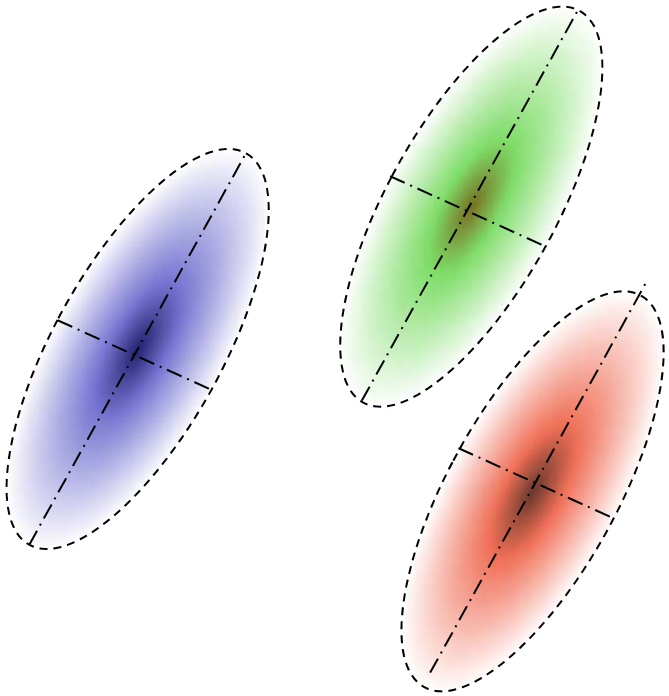
$$S_B = \sum_{c=1}^{C} \frac{N_c}{N} (\mathbf{m}_c - \mathbf{m})(\mathbf{m}_c - \mathbf{m})^\top$$

$$\mathbf{m} = \sum_{i=1}^{N} \frac{1}{N} \mathbf{x}_i \qquad \mathbf{m}_c = \frac{1}{N_c} \sum_{i \in C_c} \mathbf{x}_i$$

Consider Two Statistics

- Within class variance

$$var_W(\mathbf{w}) = \mathbf{w}^\top S_W \mathbf{w}$$



$$S_W = \sum_{c=1}^{C} \frac{N_c}{N} S_c$$

S_c: covariance matrix of each class

$$S_c = \frac{1}{N_c} \sum_{i \in C_c} (\mathbf{x}_i - \mathbf{m}_c)(\mathbf{x}_i - \mathbf{m}_c)^\top \qquad \mathbf{m}_c = \frac{1}{N_c} \sum_{i \in C_c} \mathbf{x}_i$$

Fisher Discriminant Analysis

- Find $\mathbf{w}$ having maximal $var_B(\mathbf{w})$ for give $var_W(\mathbf{w})$

- Total variance:

$$S_T = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \mathbf{m})(\mathbf{x}_i - \mathbf{m})^\top$$

$$S_T = S_W + S_B$$

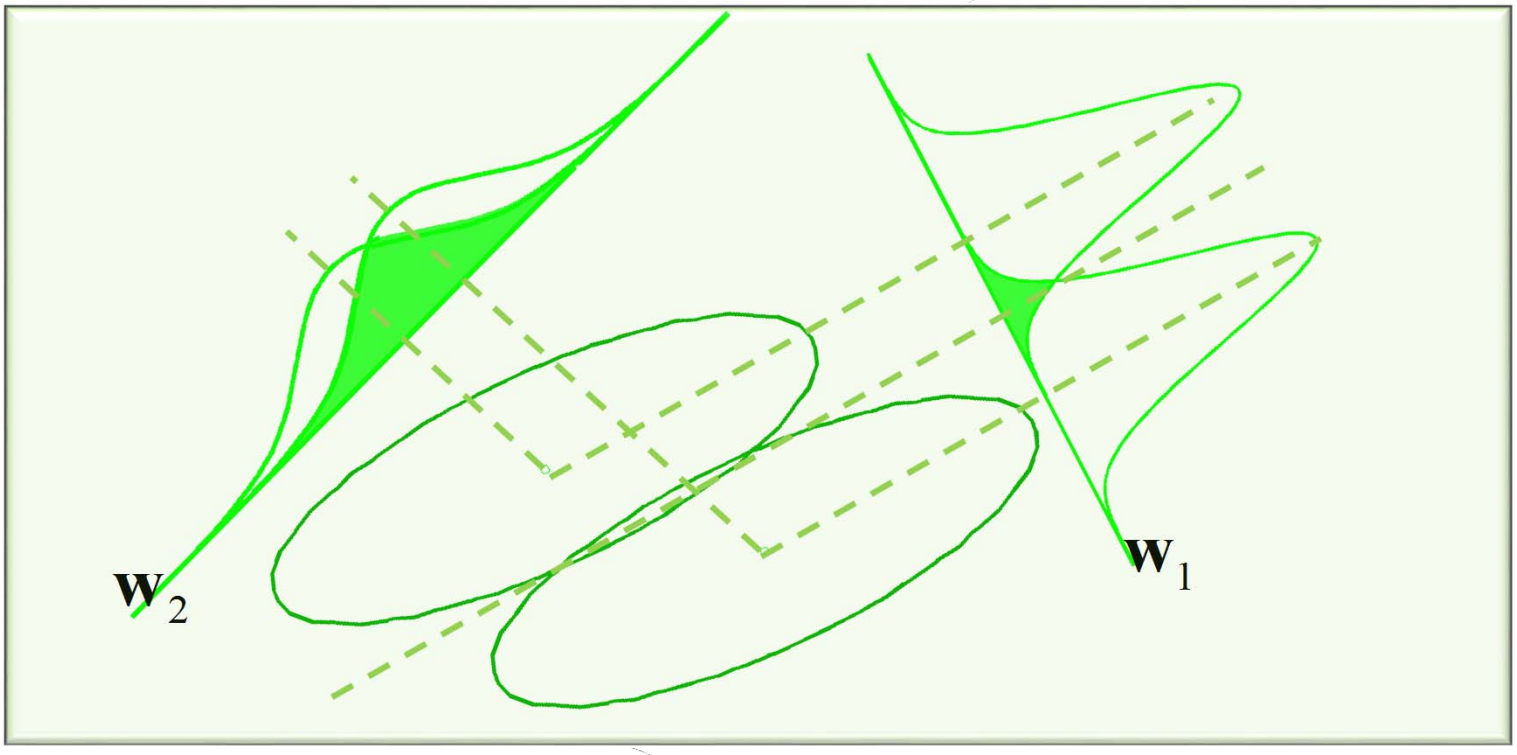
$$var(\mathbf{w}) = var_W(\mathbf{w}) + var_B(\mathbf{w})$$

Fisher Discriminant Analysis

$$\arg\max_{\mathbf{w}} J(\mathbf{w}) = \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}}$$

← Between class covariance

← Within class covariance



Take the Derivative

$$\mathbf{w} = \arg\max_{\mathbf{w}} \frac{var_B(\mathbf{w})}{var_W(\mathbf{w})} = \arg\max \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}}$$

Take the derivative

$$J(\mathbf{w}) = \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}}$$

$$J'(\mathbf{w}) = \frac{1}{(\mathbf{w}^\top S_W \mathbf{w})^2} \left[2S_B \mathbf{w}(\mathbf{w}^\top S_W \mathbf{w}) - 2\mathbf{w}^\top S_W (\mathbf{w} S_B \mathbf{w}) \right] = 0$$

$$S_B \mathbf{w} = \left(\frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}} \right) S_W \mathbf{w} = \lambda S_W \mathbf{w}$$

➔ Generalized eigenvector problem

Quiz 1: Closed Form Solution

- Problem: $S_B \mathbf{w} = \lambda S_W \mathbf{w}$
- For two class problem with $N_1 = N_2$:

$$S_B = \sum_{c=1}^{2} \frac{N_c}{N} (\mathbf{m}_c - \mathbf{m})(\mathbf{m}_c - \mathbf{m})^\top$$

$$= \frac{1}{2} (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^\top$$

- Find the closed form solution:

$$\mathbf{w} = ?$$

Quiz 2: How to solve the generalized eigenvector problem?

- Problem: $S_B\mathbf{w} = \lambda S_W\mathbf{w}$

  Are the solution eigenvalues real? (non-complex)?

  If not, how are these eigenvalues are treated?

Quiz 3: Two different FDAs

- Some papers consider the criterion

$$J_T(\mathbf{w}) = \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_T \mathbf{w}}$$

instead of $J(\mathbf{w}) = \dfrac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}}$

What is the difference?

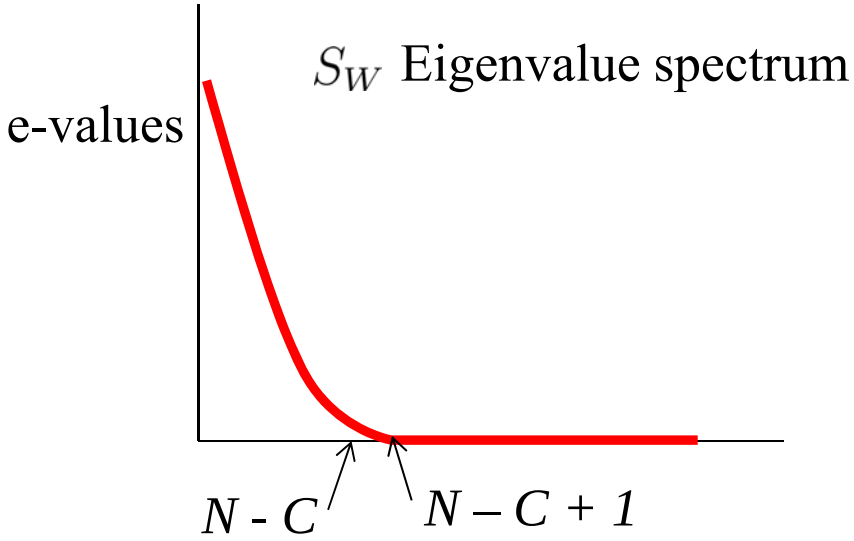
In High Dimensional Space (1/2)

$$D > N$$

$$rank(S_T = S_W + S_B) = N - 1$$

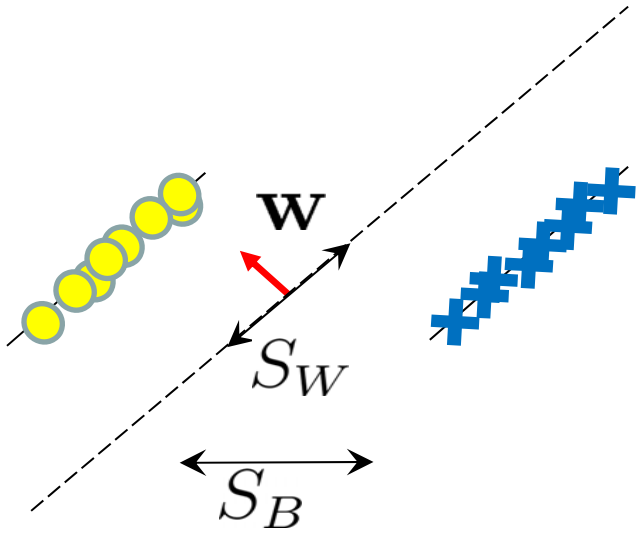
$$rank(S_W) = N - C \longrightarrow S_W\text{: not a full rank matrix}$$

$$rank(S_B) = C - 1$$



In High Dimensional Space (2/2)

- FDA will trivially pick up the null space of S_W as solution.



$$J(\mathbf{w}) = \infty$$

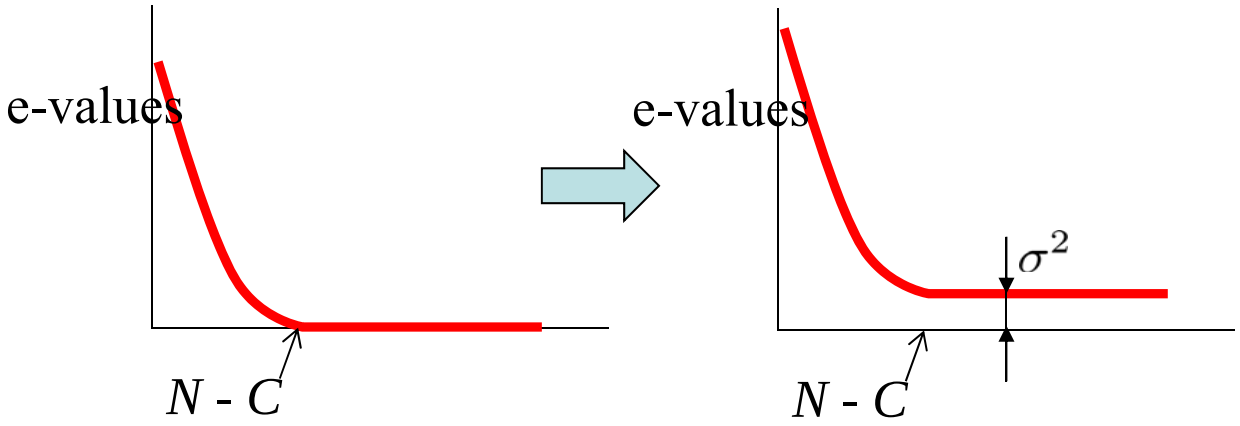
More seriously, the nullspace varies by sampling

➔ Ill-posed problem

Regularization in FDA

- Regularize

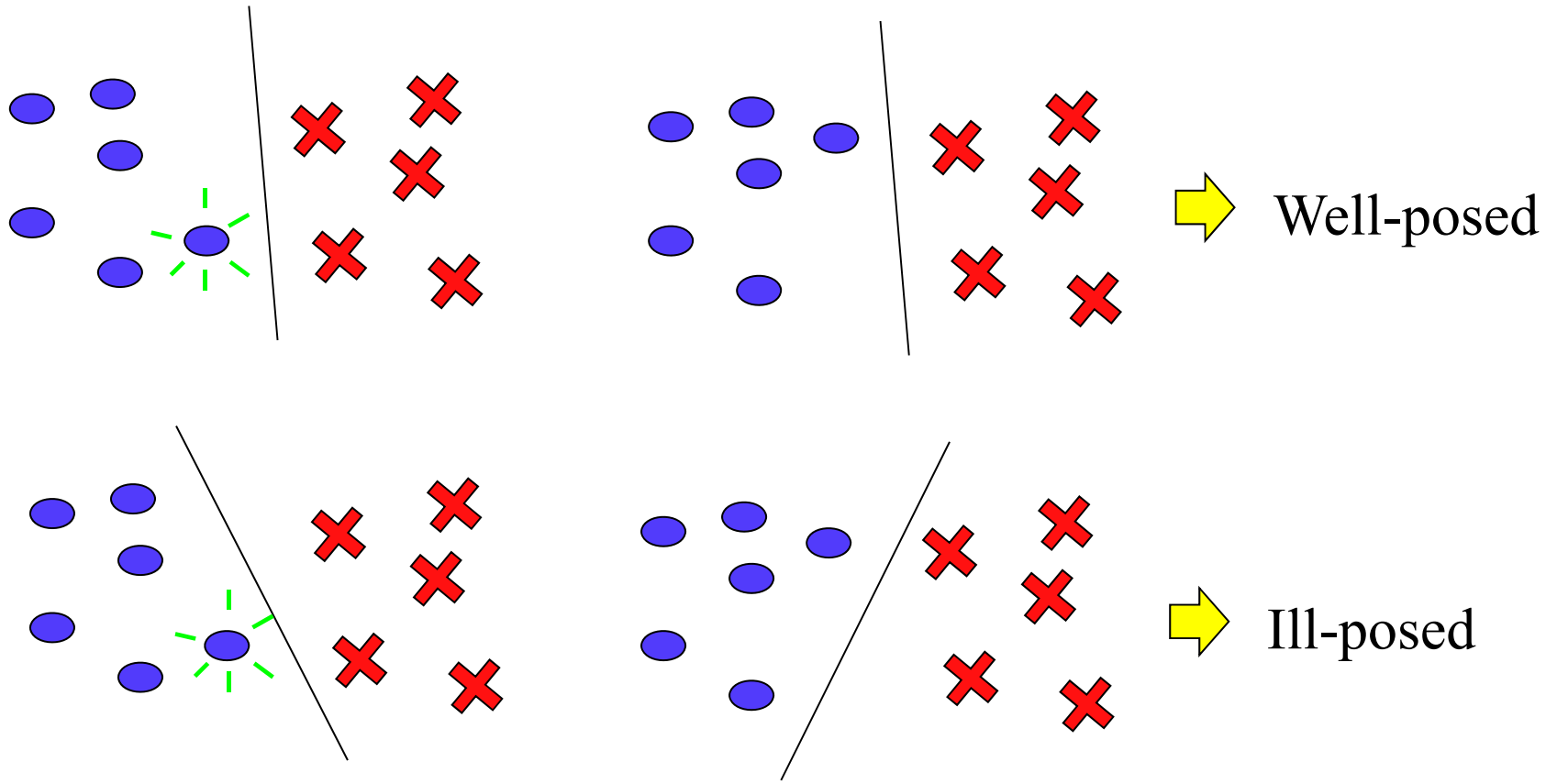
$$S_W \rightarrow S_W + \sigma^2 I$$



The problem becomes well-posed.

New solution: $\mathbf{w} = (S_W + \sigma^2 I)^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$
for two classes

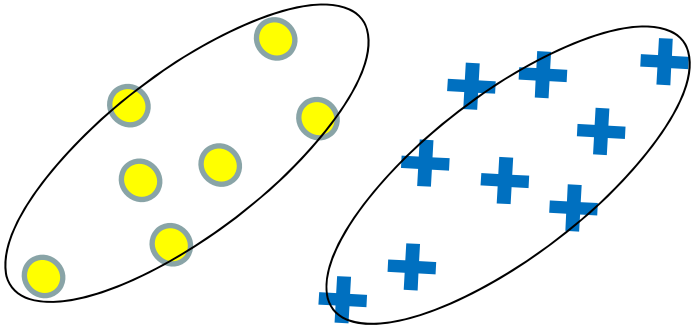
Well-posed Problem vs. Ill-Posed Problem

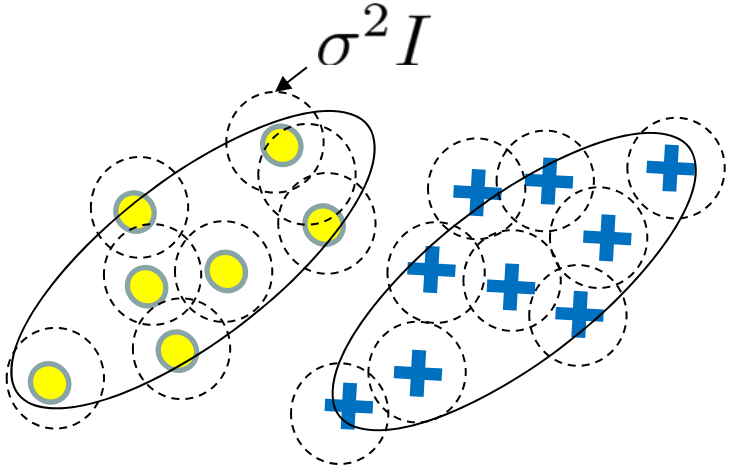


The variation of configuration may come from the sampling variation.

Quiz 4: New S_W with Infinite Data

- If infinite number of data are generated around each datum with isotropic Gaussian





$$S_W = \frac{1}{N} \sum_{c=1}^{C} \sum_{i \in C_c} (\mathbf{x}_i - \mathbf{m}_c)(\mathbf{x}_i - \mathbf{m}_c)^\top$$

$$S_W \rightarrow S_W + \sigma^2 I$$

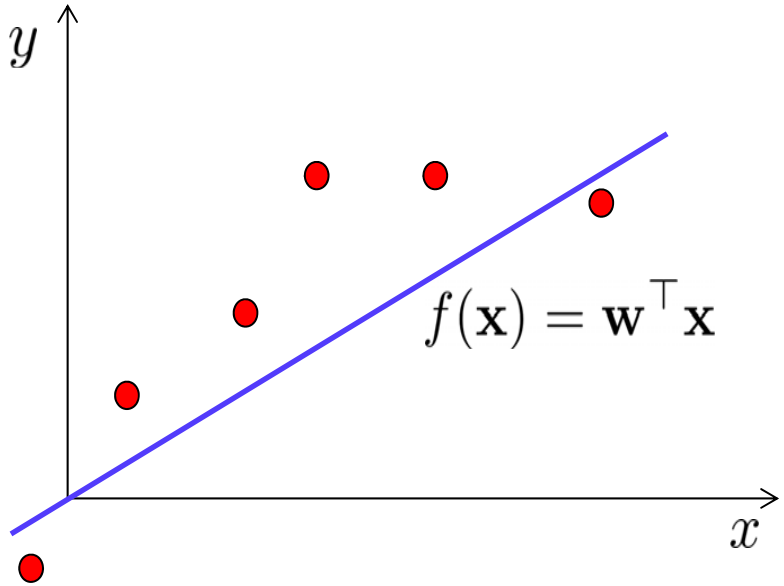
FREQUENTIST VIEW VS. BAYESIAN VIEW

Ridge Regression

- Find $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$, which minimizes

$$J(\mathbf{w}) = \frac{1}{2}\sum_n ||y_n - \mathbf{w}^\top \mathbf{x}_n||^2 + \frac{1}{2}\lambda \mathbf{w}^\top \mathbf{w}$$

$$\left(= ||\mathbf{y} - \mathbf{w}^\top X||^2 + \frac{1}{2}\lambda ||\mathbf{w}||^2 \right) \qquad X = [\mathbf{x}_1, \ldots, \mathbf{x}_N],\ \mathbf{x}_i \in \mathbb{R}^D$$
$$\mathbf{y} = [y_1, \ldots, y_N]^\top$$



Minimizing error + Regularization

Ridge Regression

- Closed form solution
  - Without regularization

$$J(\mathbf{w}) = \frac{1}{2}\sum_n ||y_n - \mathbf{w}^\top \mathbf{x}_n||^2$$

$$\mathbf{w} = (X^T X)^{-1} X^\top \mathbf{y}$$

  - With regularization

$$J(\mathbf{w}) = \frac{1}{2}\sum_n ||y_n - \mathbf{w}^\top \mathbf{x}_n||^2 + \frac{1}{2}\lambda \mathbf{w}^\top \mathbf{w}$$

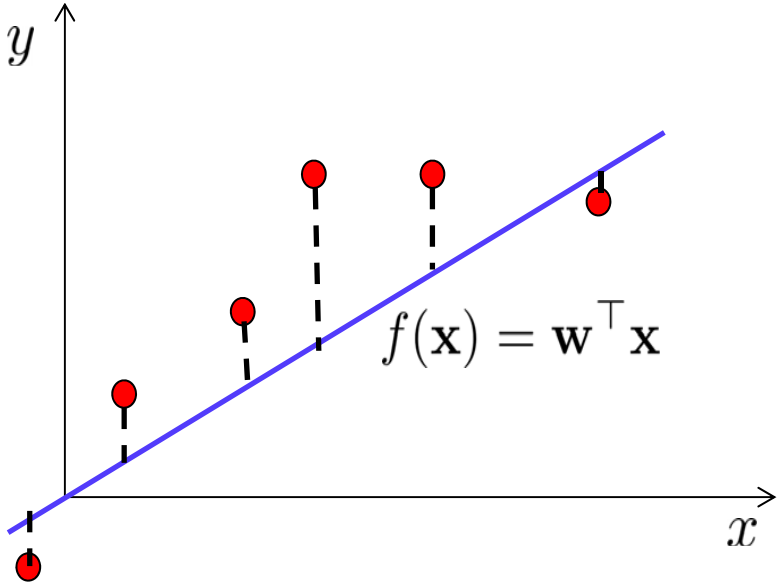
$$\mathbf{w} = (X^\top X + \lambda I)^{-1} X^\top \mathbf{y}$$

1) Frequentists' Point Estimation View

- Minimizing empirical L2 error + penalty

$$L_2 = \sum_n ||y_n - \mathbf{w}^\top \mathbf{x}||^2 \qquad R = \frac{1}{2}\lambda \mathbf{w}^\top \mathbf{w}$$

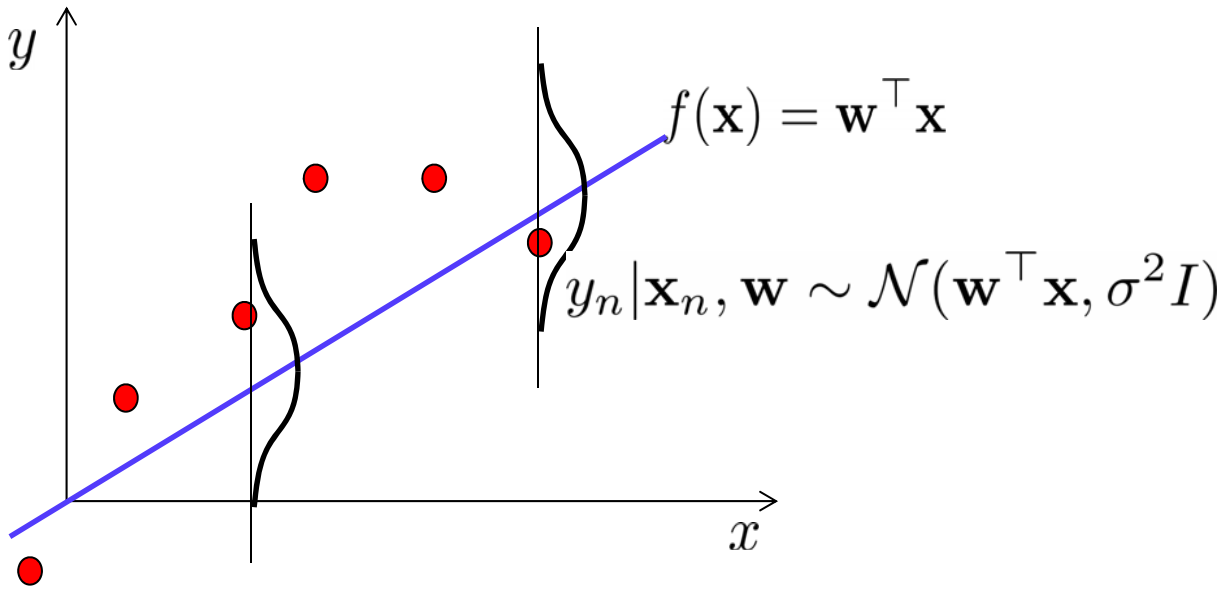
$$\mathbf{w} = (X^\top X)^{-1} X^\top \mathbf{y} \;\rightarrow\; \mathbf{w} = (X^\top X + \lambda I)^{-1} X^\top \mathbf{y}$$



2) Bayesian Inference View (1/3)

- Make a probability model

$$y_n = f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}_n + \epsilon_n, \;\; \epsilon_n \sim \mathcal{N}(0, \sigma^2)$$



$$p(\mathbf{y}|X, \mathbf{w}) = \prod_{n=1}^{N} p(y_n|\mathbf{x}_n, \mathbf{w})$$

2) Bayesian Inference View (2/3)

- Maximizing log likelihood

$$\log p(\mathbf{y}|X,\mathbf{w}) = \sum_{n=1}^{N} \log p(y_n|\mathbf{x}_n,\mathbf{w})$$

$$= -\frac{ND}{2}\log 2\pi\sigma^2 - \sum_{n=1}^{N}\frac{1}{2\sigma^2}||y_n - \mathbf{w}^\top \mathbf{x}_n||^2$$

$$\mathbf{w}_{ML} = (X^\top X)^{-1}X^\top \mathbf{y}$$

2) Bayesian Inference View (3/3)

- Maximizing posterior

With a prior $\mathbf{w} \sim \mathcal{N}(0, \lambda^{-1} I)$

$$\log p(\mathbf{w}|X, \mathbf{y}) \propto -\sum_{n=1}^{N} ||y_n - \mathbf{w}^\top \mathbf{x}_n||^2 - \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w}$$

$$\mathbf{w}_{MAP} = (X^\top X + \lambda I)^{-1} X^\top \mathbf{y}$$ ← Bayesian inference of posterior using linear model

Solving Optimization Problem

- *Machine learning algorithms are optimization problems using training data*
  - Minimizing empirical loss function + regularization term
  - Maximizing likelihood or posterior to estimate parameters
  - In Bayesian inference, marginalization is the main bottleneck. (e.g. through variational approximation, integration problems can be turned into optimization problems)

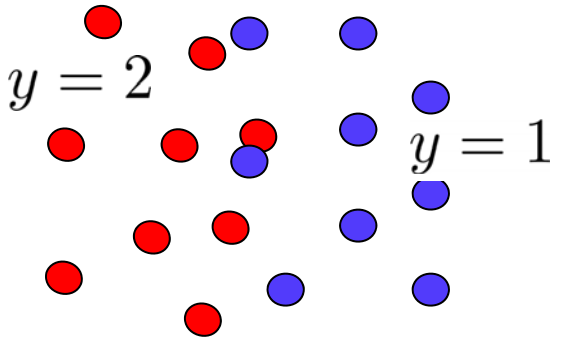
GENERALIZATION ISSUE

Learning

- Data

$$\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^{N} \sim P$$

(Regularity)



- Prediction

$$\mathbf{x} \in \mathbb{R}^D \xrightarrow{\quad y = f(\mathbf{x}) \quad} \begin{array}{l} y \in \{1, 2, \ldots, C\} \\ y \in \mathbb{R} \end{array}$$

- Learning
  - ➢ Learn prediction function $f(\mathbf{x}) \in \mathcal{H}$ from data $\mathcal{D}$
    ($\mathcal{H}$: Hypothesis set/Candidate set)

Quantify the Evaluation

- Measure of quality: expected loss

$$L = \mathbb{E}_P[l(y, f(\mathbf{x}))] \qquad l(y, y'): \text{loss function}$$

- Estimated error

$$\hat{L} = \sum_n l(y_n, f(\mathbf{x}_n)), \quad f(\mathbf{x}) \in \mathcal{H}$$

- Examples
  - Classification $\widehat{L} = \frac{1}{N}\sum_n \mathbb{I}(y_n \neq f(\mathbf{x}_n))$
  - Regression $\widehat{L} = \frac{1}{N}\sum_n ||y_n - f(\mathbf{x}_n)||^2$
  - Clustering $\widehat{L} = \frac{1}{N}\sum_n \min_c ||y_n - f(\mathbf{x}_n)||^2$

Consistent Learner

- $\mathcal{H}$ satisfies $\widehat{L} \underset{N \to \infty}{\to} L$

$$P\{\sup_{f \in \mathcal{H}} (L(f) - \widehat{L}(f)) > \epsilon\} \to 0 \quad \text{for} \quad \epsilon > 0$$

<Uniform convergence>

- Caution:
  - The definition of consistency is *not*

$$\widehat{L}(f) \to L(f) \quad \text{for} \quad f \in \mathcal{H}$$

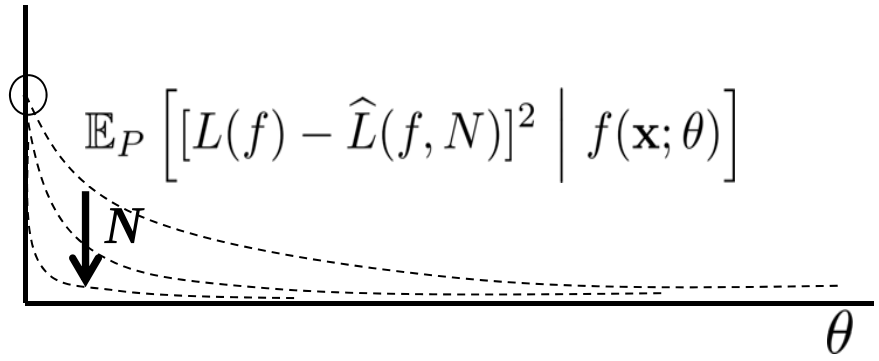
Quiz 1

- Consider a hypothesis set $\mathcal{H}$ which satisfies

$$\mathbb{E}_P\left[[L(f)-\widehat{L}(f,N)]^2 \;\middle|\; f(\mathbf{x};\theta)\right]=\left(\frac{1}{N}\right)^{\theta}$$

$$\mathcal{H}=\{f(\mathbf{x};\theta)|\theta>0\}$$

Explain that learning with $\mathcal{H}$ is not consistent though it satisfies $\widehat{L}(f)\to L(f)$.



What is the possible problem in this case?

Related Terms with Confining $\mathcal{H}$

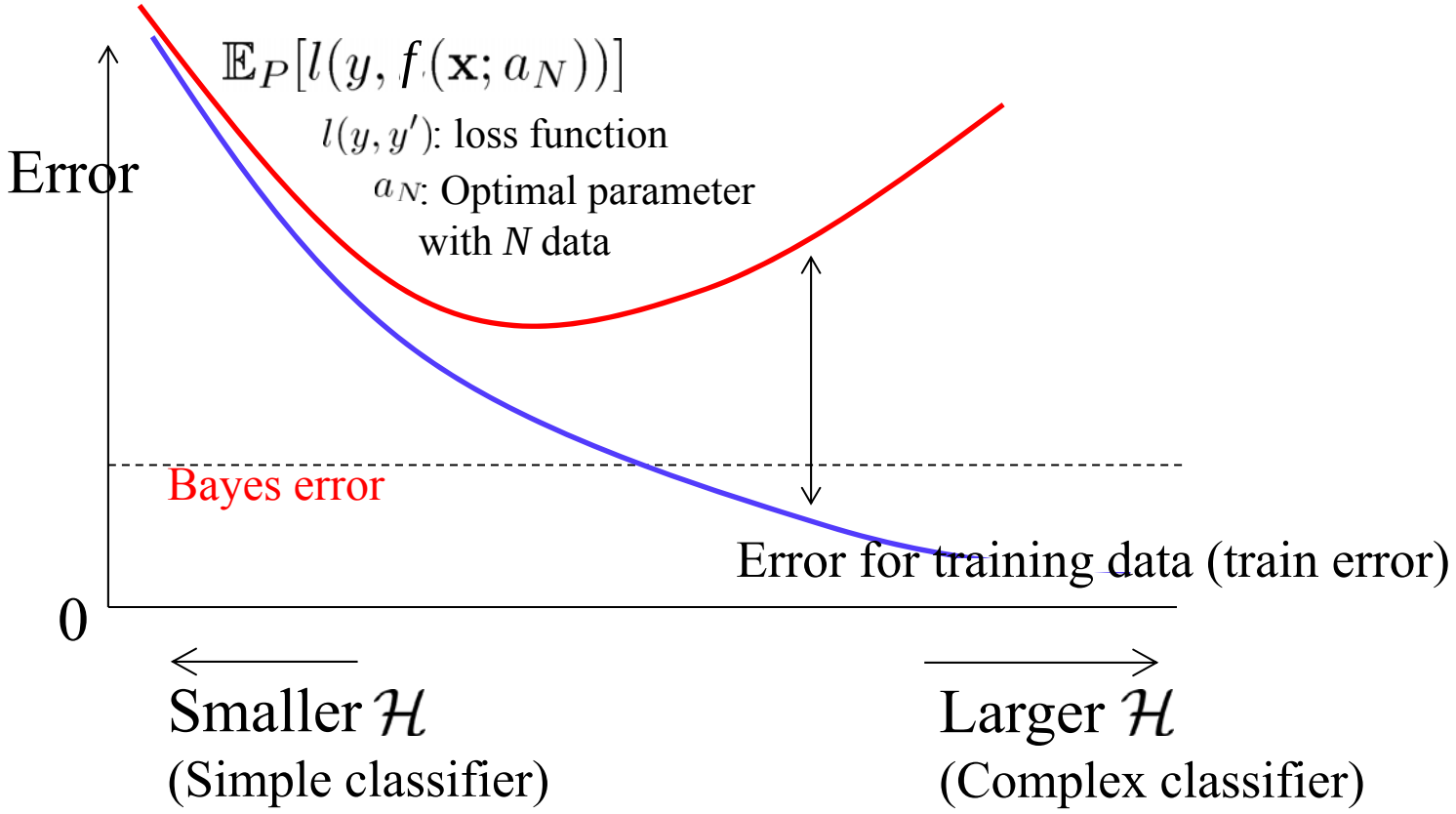
- Linear model →

  VC-dim for classification = Dimensionality + 1
- Small number of parameters
- Large margin
- Regularization
- Bias-Variance trade-off
- Generalization ability, overfitting

➔ Many terms are theoretically connected

Consistency and Bayes Error

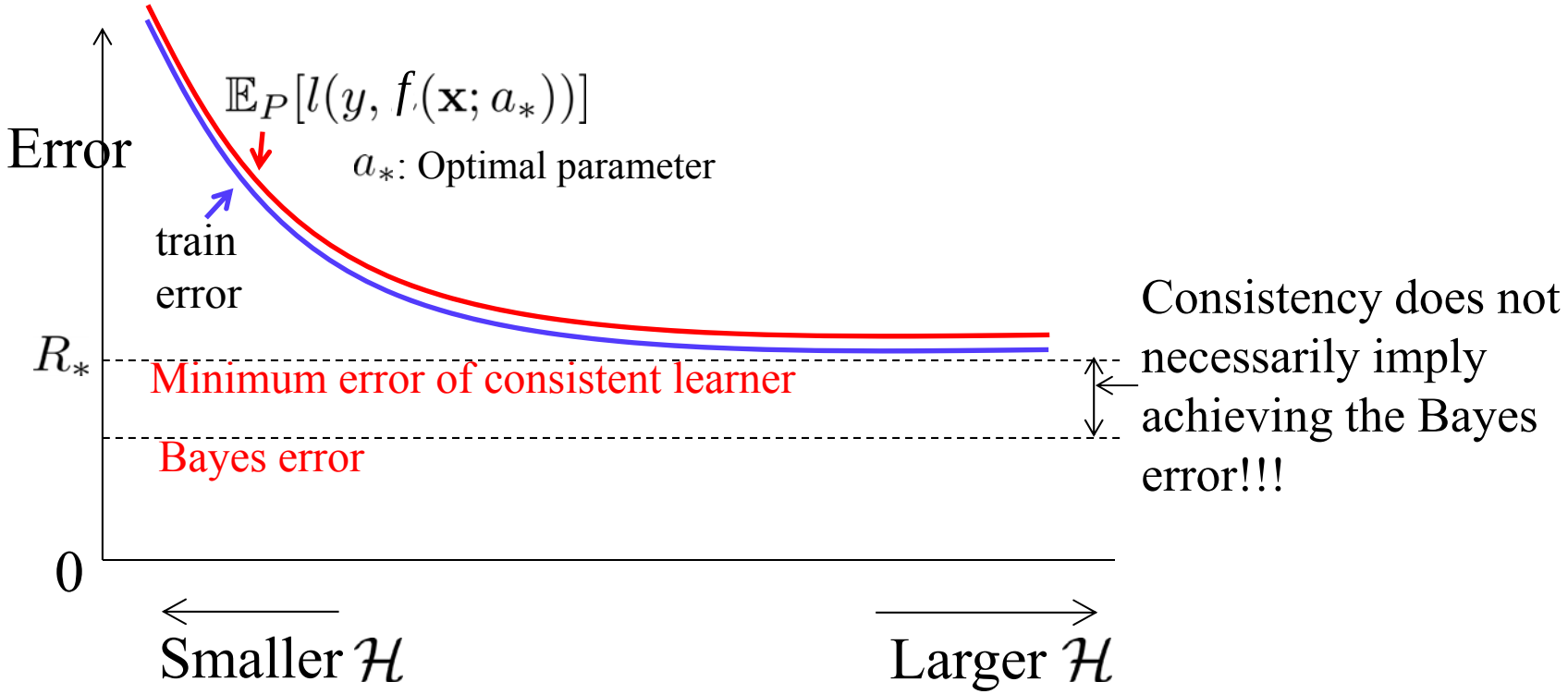
- Minimizing expected error (objective) vs. minimizing estimated error



(For example, a linear classifier with regularization)

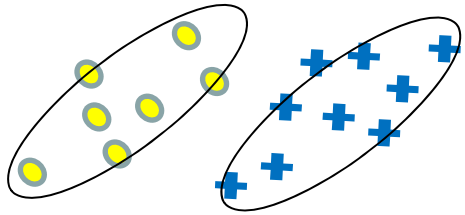
Consistency and Bayes Error

- Consistent learner with many data



(For example, a linear classifier with regularization)

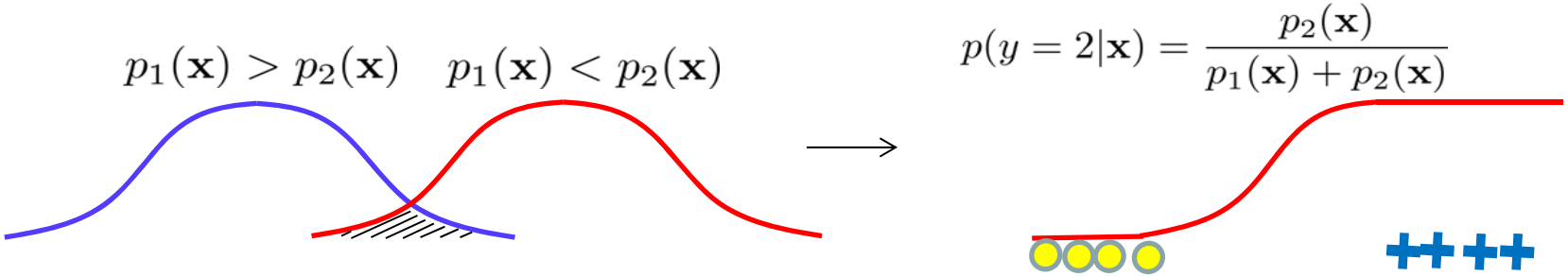
In Terms of the Posterior



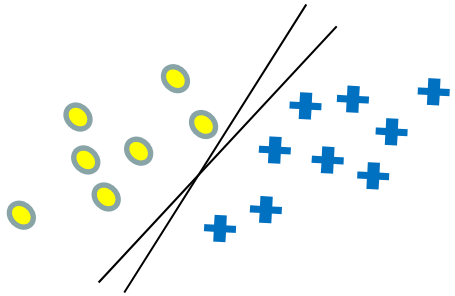
$$p(y=1|\mathbf{x},\mathbf{w},b) = \frac{p_1}{p_1+p_2} = \frac{1}{1+p_2/p_1} = \frac{1}{1+\exp(\mathbf{w}^\top\mathbf{x}-b)}$$

$$p(y=2|\mathbf{x},\mathbf{w},b) = \frac{p_2}{p_1+p_2} = 1-p(y=1|\mathbf{x}) = \frac{\exp(\mathbf{w}^\top\mathbf{x}-b)}{1+\exp(\mathbf{w}^\top\mathbf{x}-b)}$$

- Class-conditional model vs. Posterior model



Logistic Regression



- Starts from the posterior

$$p(\mathbf{y}|X,\mathbf{w},b) = \prod_n p(y_n = 1|\mathbf{x}_n,\mathbf{w},b)$$

$$p(y_n|\mathbf{x}_n,\mathbf{w},b) = \begin{cases} \frac{1}{1+\exp(\mathbf{w}^\top\mathbf{x}-b)}, & y_n = 1 \\ \frac{\exp(\mathbf{w}^\top\mathbf{x}-b)}{1+\exp(\mathbf{w}^\top\mathbf{x}-b)}, & y_n = 2 \end{cases}$$

$$\mathbf{w}, b = \arg\max_{\mathbf{w},b} \ln p(\mathbf{y}|X,\mathbf{w},b)$$

$$\sum_n \mathbb{I}(y_n = 1)\ln p(y_n = 1|\mathbf{x}_n,\mathbf{w},b) + \mathbb{I}(y_n = 2)\ln p(y_n = 2|\mathbf{x}_n,\mathbf{w},b)$$

Learn **w** using posterior model (instead of class-conditional model)

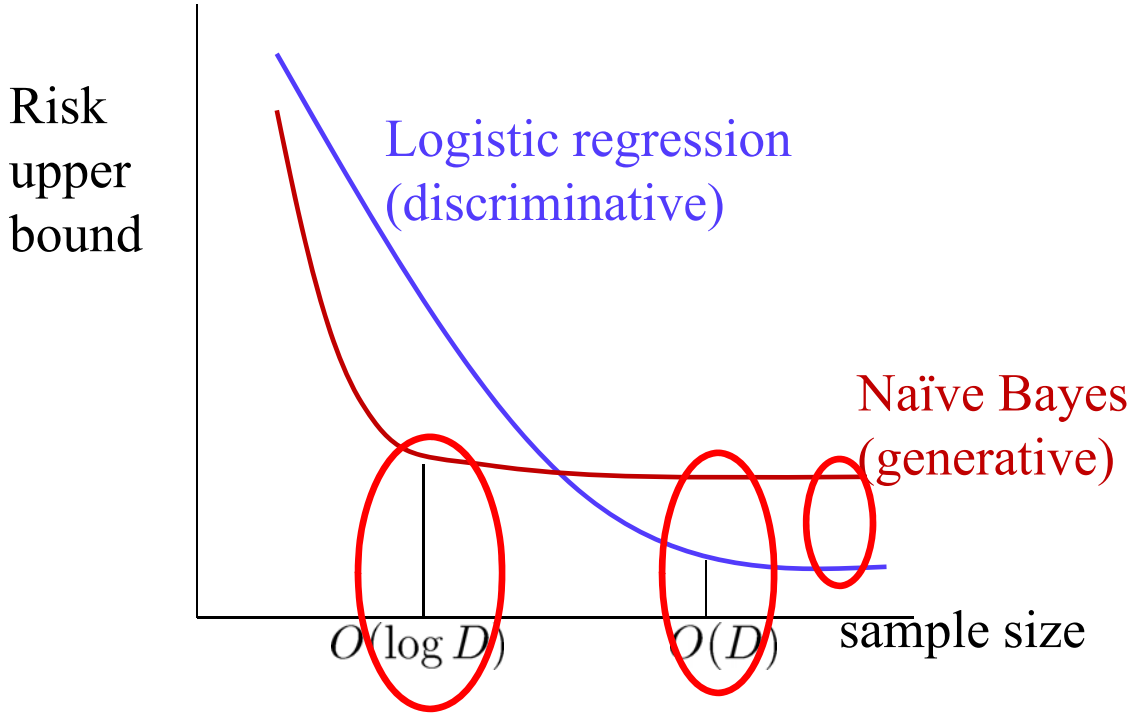
Generative vs. Discriminative Methods

- Generative methods
  - Gaussian class-conditional model
  - Graphical model
  - Restricted Boltzmann Machines

- Discriminative methods
  - Support Vector Machines (SVMs)
  - Logistic regression
  - Artificial Neural Networks

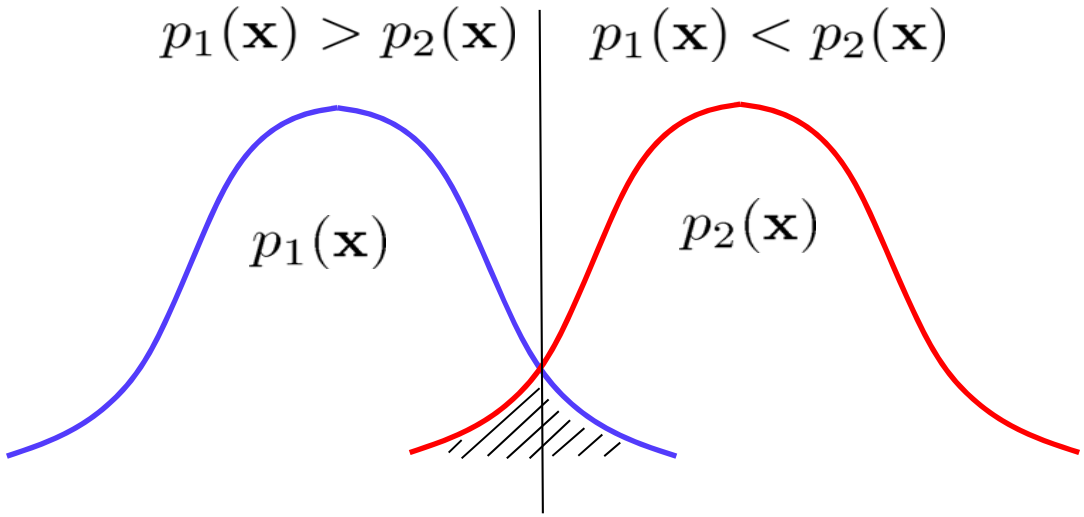
Comparative Study

- Generative & discriminative pair
  - Same number of parameters, same form of *f(x)*



Probabilistic Assumption and Bayes Classification

- Bayes classification produces theoretical minimum error

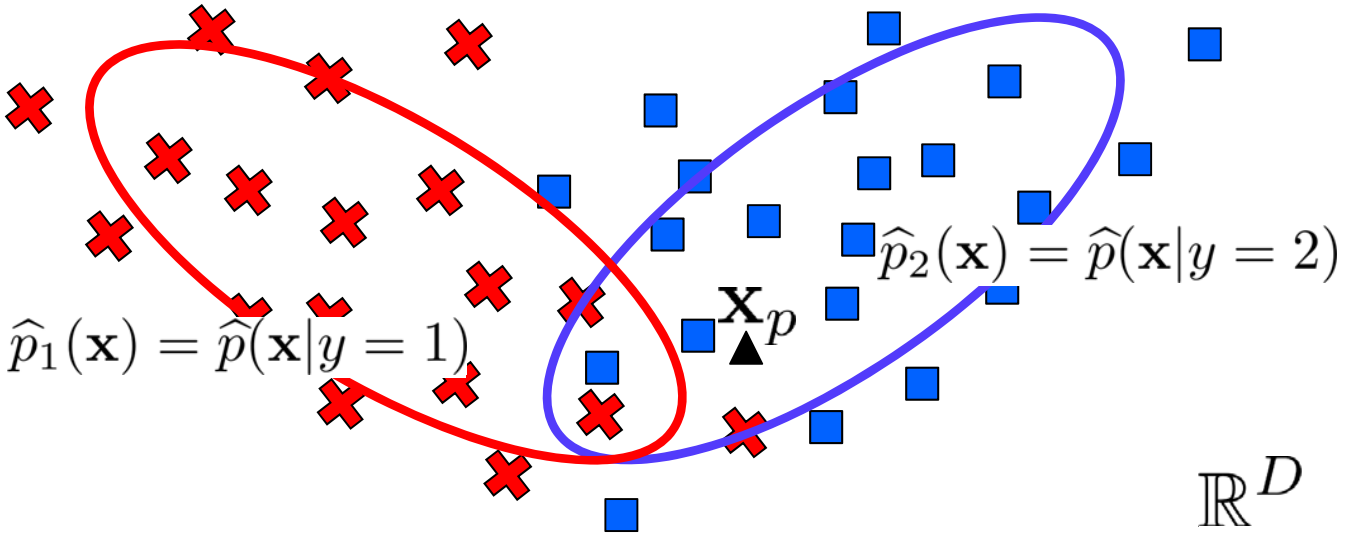


➔ Error:

$$\frac{1}{2}\int \min[p_1, p_2]\, d\mathbf{x}$$

Model + Estimated Parameters

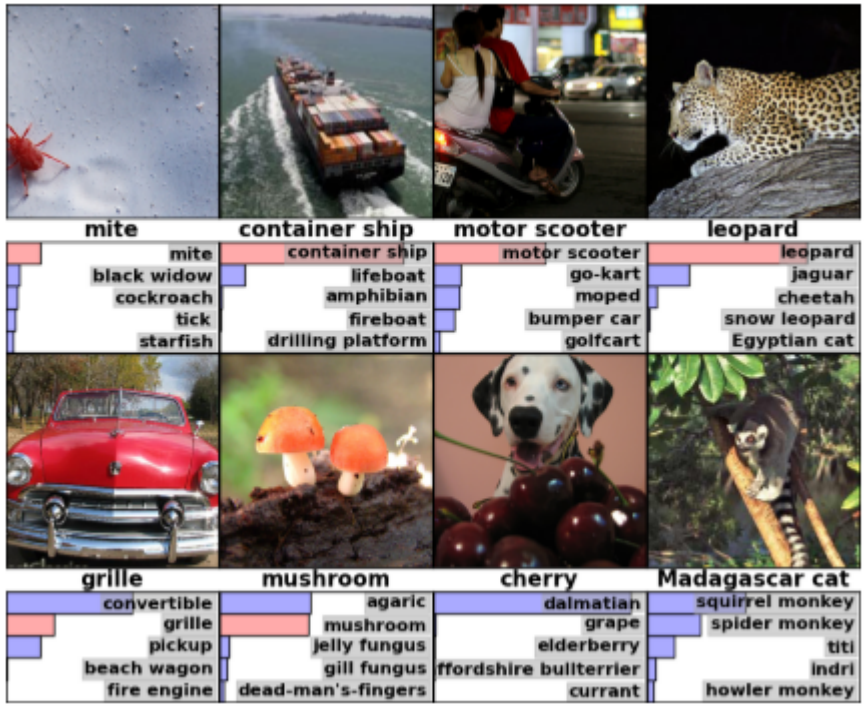
- Ex. Gaussian model



$$\widehat{p}_1(\mathbf{x}_p) \geq \widehat{p}_2(\mathbf{x}_p) \rightarrow y_p = 1$$
$$\widehat{p}_1(\mathbf{x}_p) < \widehat{p}_2(\mathbf{x}_p) \rightarrow y_p = 2$$

AlexNet (2012 NIPS)

- ImageNet Large Scale Visual Recognition Challenge 2010 (ILSVRC2010)



ImageNet Classification with Deep Convolutional Neural Networks

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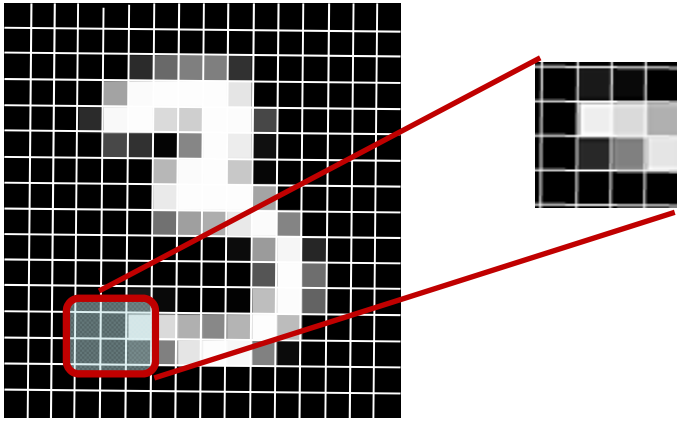
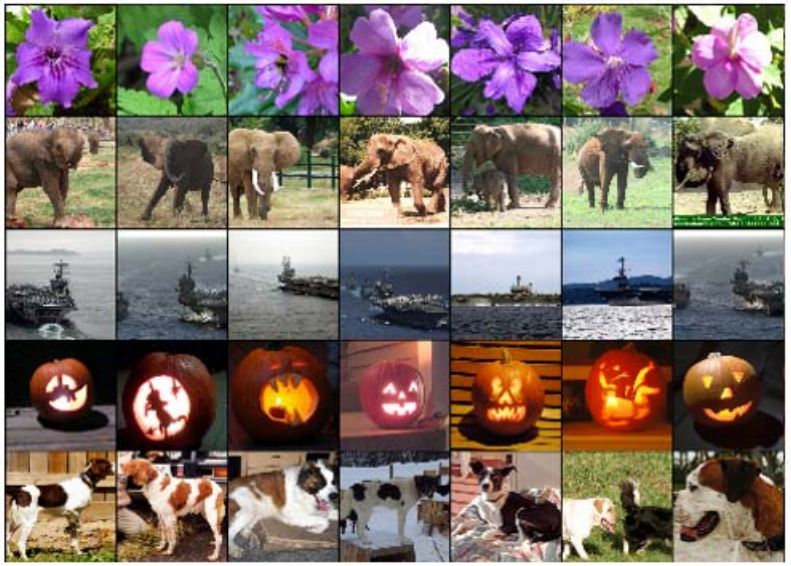
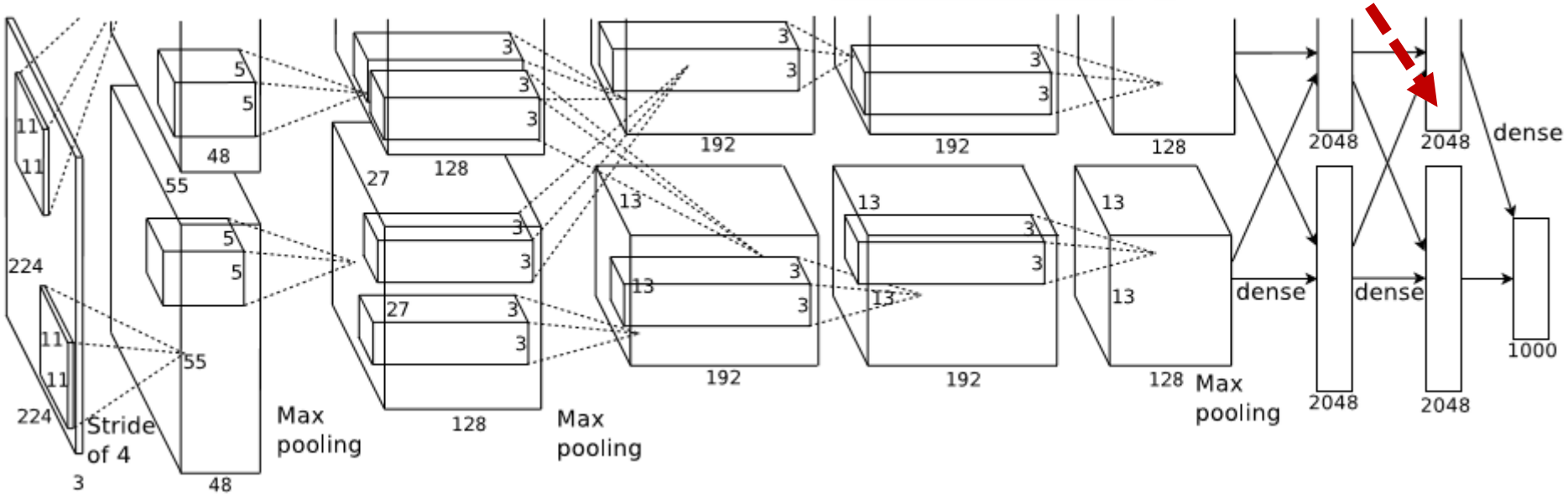
Architecture of AlexNet



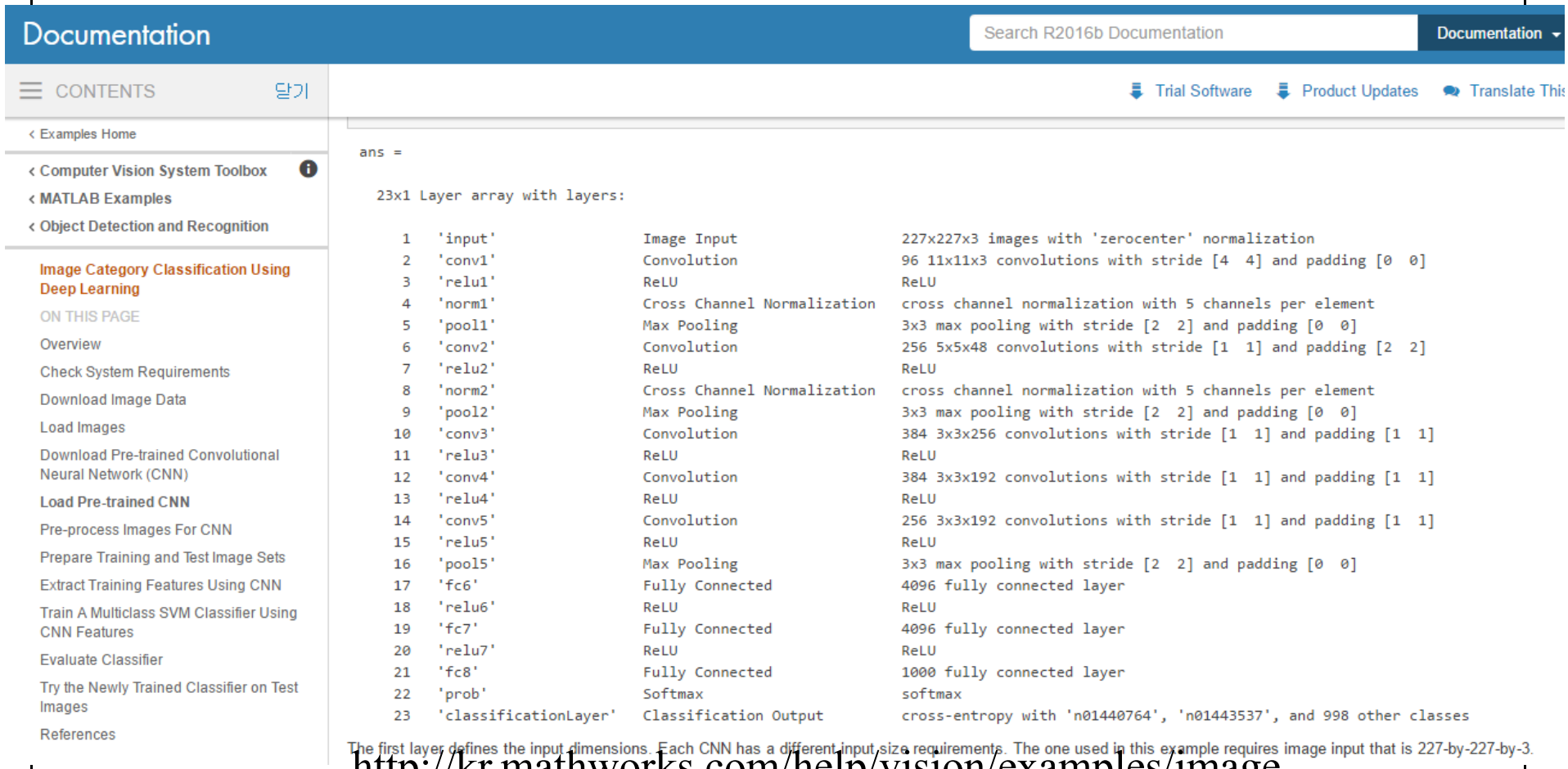




NIPS 2013 Tutorial - Deep Learning for Computer Vision (Rob Fergus)

Matlab Computer Vision System Toolbox

- Image category classification using deep learning



http://kr.mathworks.com/help/vision/examples/image-category-classification-using-deep-learning.html

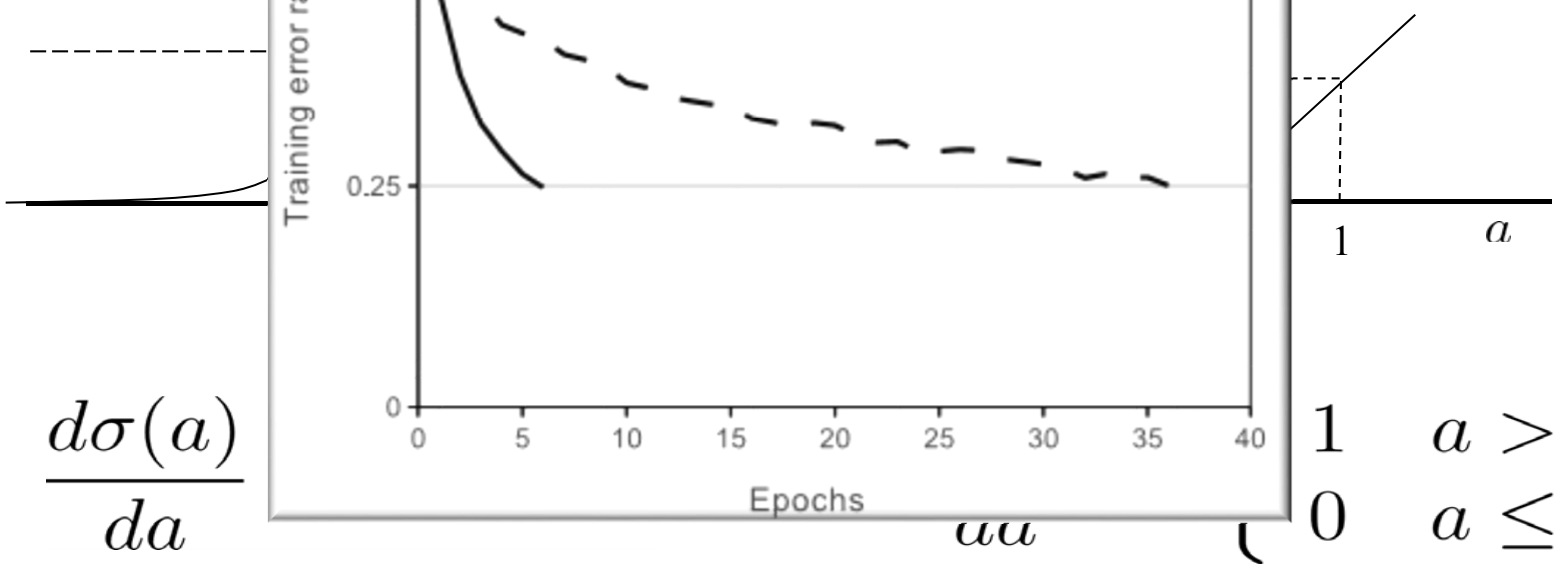
ReLU Activation Function

- Sigmoid
- Rectified Linear Unit

$$\sigma(a) = \frac{1}{1+e^{-a}}$$

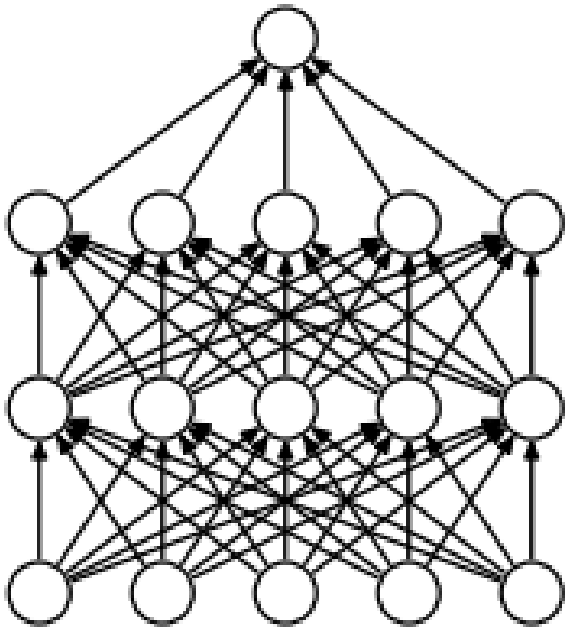
$$\frac{d\sigma(a)}{da} = \sigma(a)(1-\sigma(a))$$

$$\max\{0, a\}$$

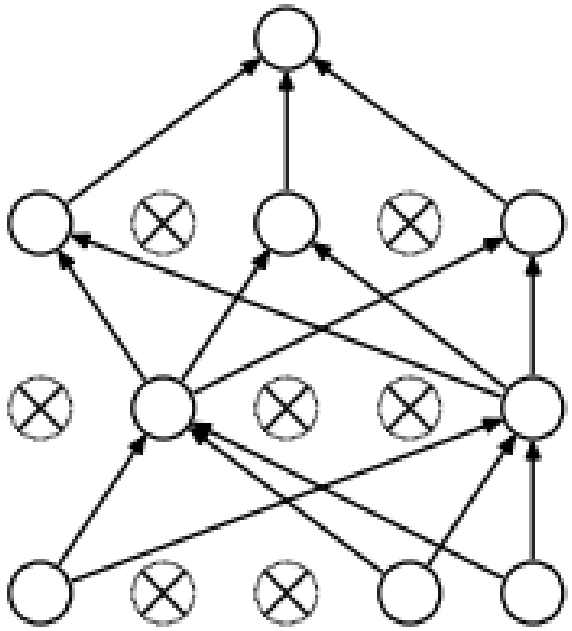


$$\frac{d}{da}\max\{0, a\} = \begin{cases} 1 & a > 0 \\ 0 & a \leq 0 \end{cases}$$

Dropout



(a) Standard Neural Net



(b) After applying dropout.

Srivastava et al. (2014) Dropout: A Simple Way to Prevent Neural Networks from Overfitting, *JMLR*

GPGPU

- GTX 580, 3G memory

Deep Autoencoder Using RBM as Pretraining Procedure

- Science, Vol. 313 no. 5786 pp. 504-507
  - We introduce this pretraining procedure for binary data, generalize it to real-valued data, and show that it works well for a variety of data sets

the optical properties of the SRR constituent materials are identical for all configurations. The blue bars in Fig. 1 summarize the measured SHG signals. For excitation of the *LC* resonance in Fig. 1A (horizontal incident polarization), we find an SHG signal that is 500 times above the noise level. As expected for SHG, this signal closely scales with the square of the incident power (Fig. 2A). The polarization of the SHG emission is nearly vertical (Fig. 2B). The small angle with respect to the vertical is due to deviations from perfect mirror symmetry of the SRRs (see electron micrographs in Fig. 1). Small detuning of the *LC* resonance toward smaller wavelength (i.e., to 1.3-μm wavelength) reduces the SHG signal strength from 100% to 20%. For excitation of the Mie resonance with vertical incident polarization in Fig. 1D, we find a small signal just above the noise level. For excitation of the Mie resonance with horizontal incident polarization in Fig. 1C, a small but significant SHG emission is found, which is again po-

of the nonlinear optical properties of metallic

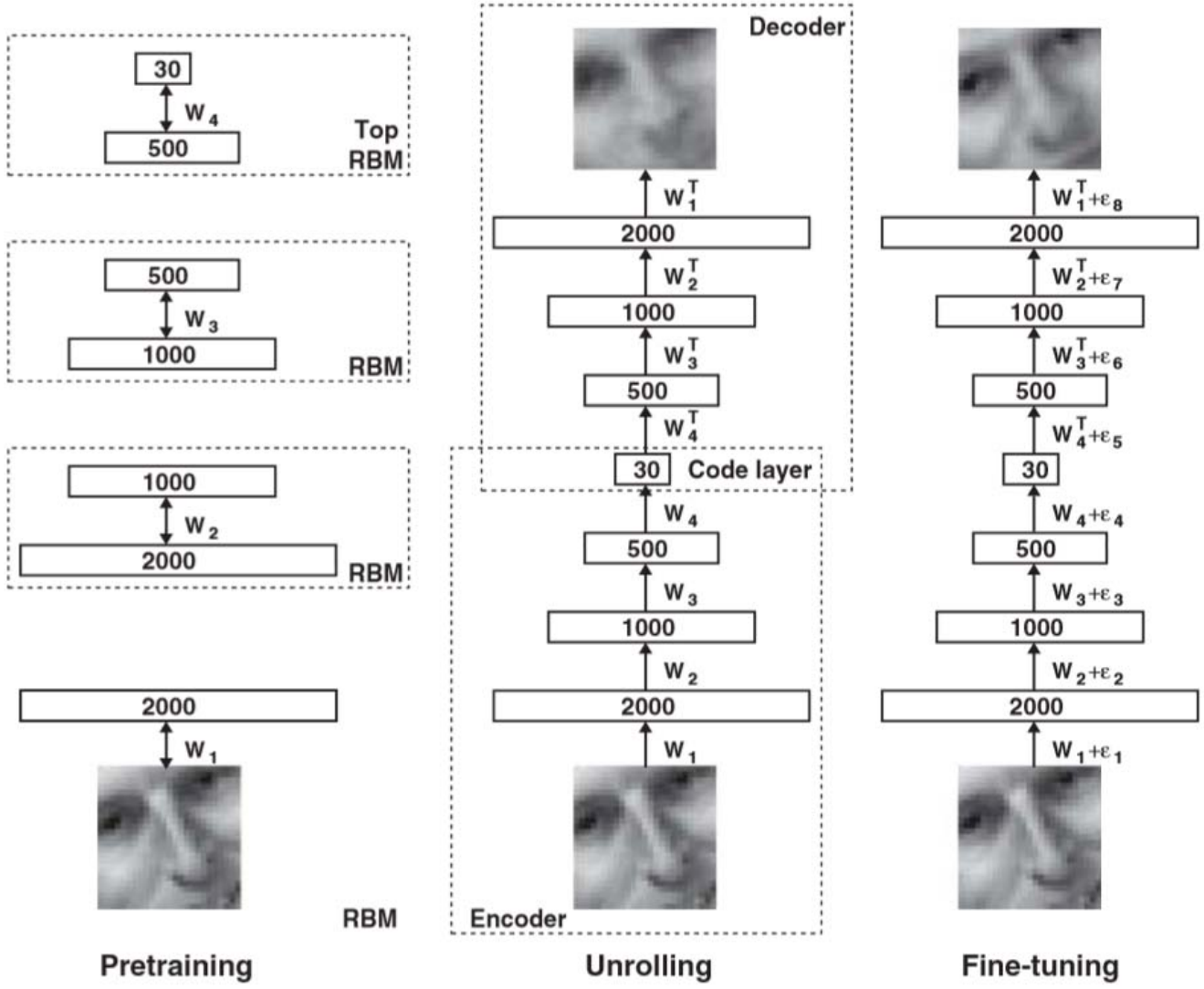
10.1126/science.1129198

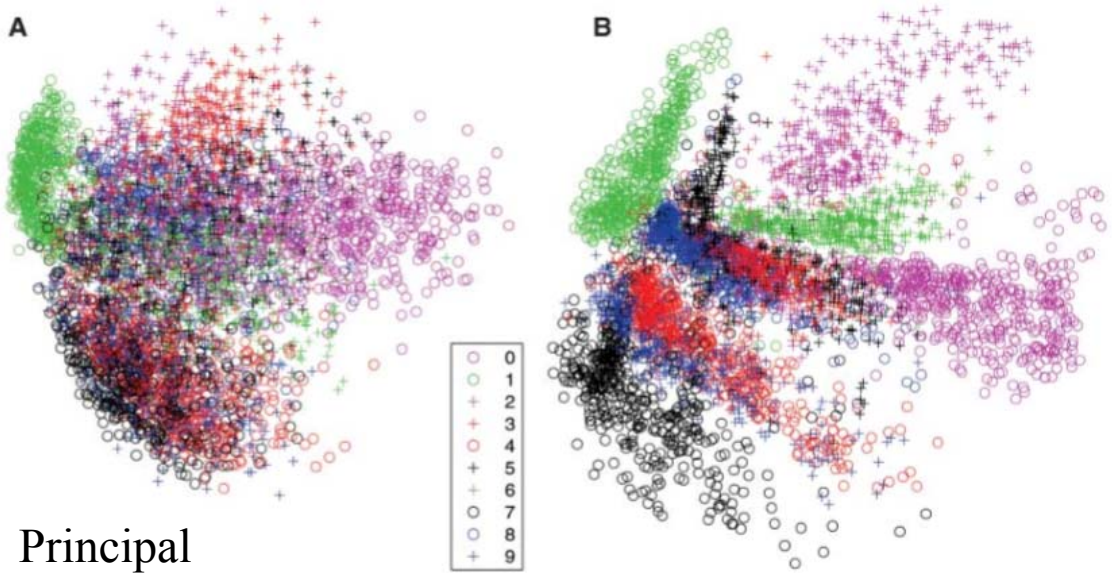
Reducing the Dimensionality of Data with Neural Networks

G. E. Hinton* and R. R. Salakhutdinov

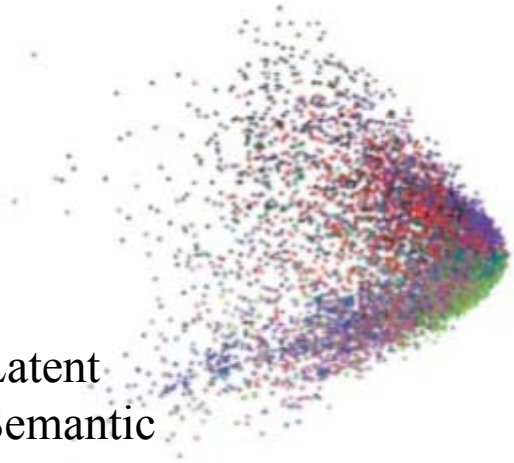
High-dimensional data can be converted to low-dimensional codes by training a multilayer neural network with a small central layer to reconstruct high-dimensional input vectors. Gradient descent can be used for fine-tuning the weights in such "autoencoder" networks, but this works well only if the initial weights are close to a good solution. We describe an effective way of initializing the weights that allows deep autoencoder networks to learn low-dimensional codes that work much better than principal components analysis as a tool to reduce the dimensionality of data.

Dimensionality reduction facilitates the classification, visualization, communication, and storage of high-dimensional data. A simple and widely used method is principal components analysis (PCA), which finds the directions of greatest variance in the data set and represents each data point by its coordinates along each of these directions. We describe a nonlinear generalization of PCA that uses an adaptive, multilayer "encoder" network

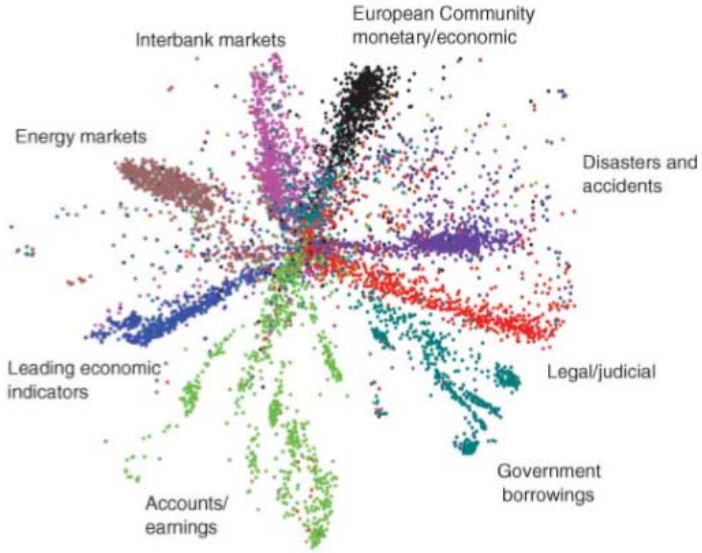

30
W 4
500
Top RBM
500
W 3
1000
RBM
1000
W 2
2000
RBM
2000
W 1
RBM
Pretraining
Decoder
2000
1000
500
30
Code layer
500
1000
2000
Encoder
Unrolling
Fine-tuning



Principal Component Analysis



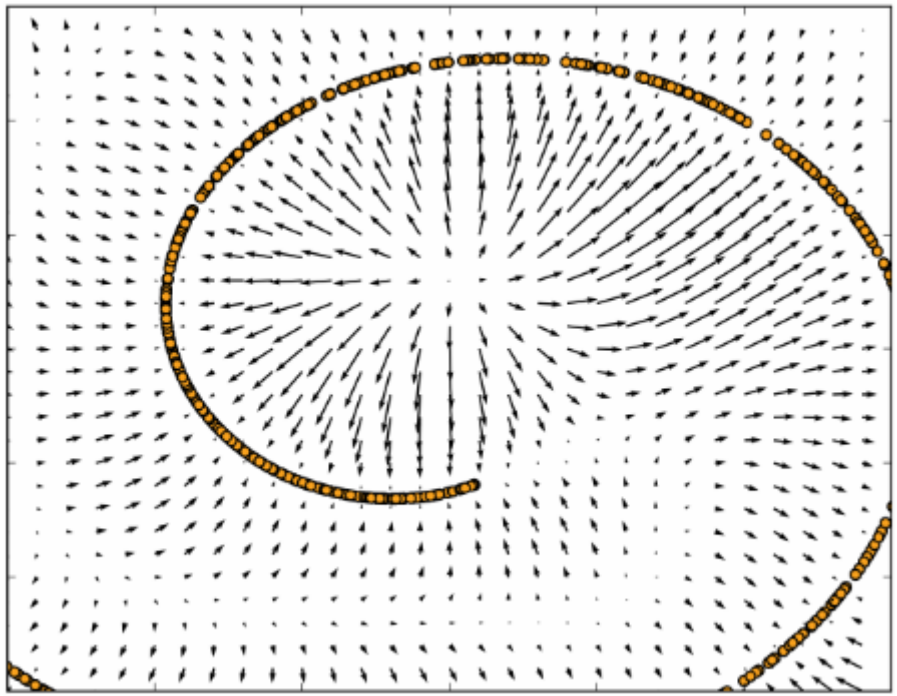
Latent Semantic Analysis

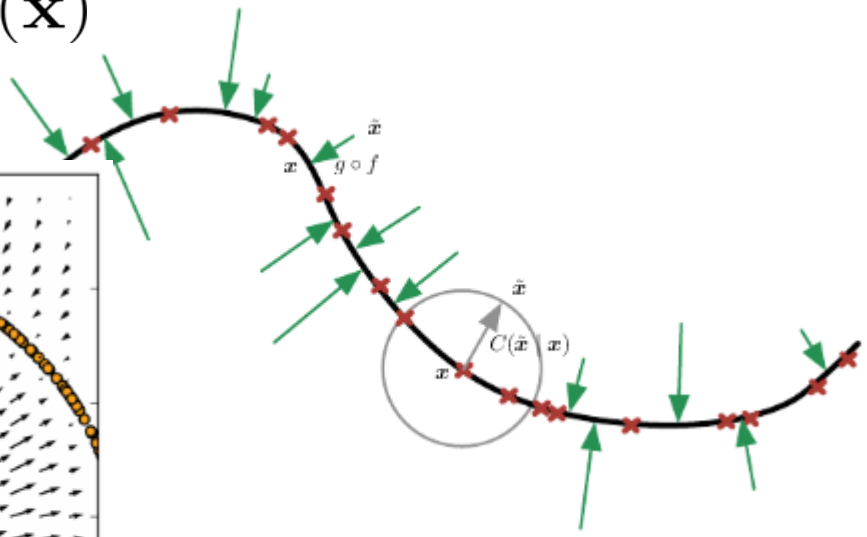


Denoising Autoencoder

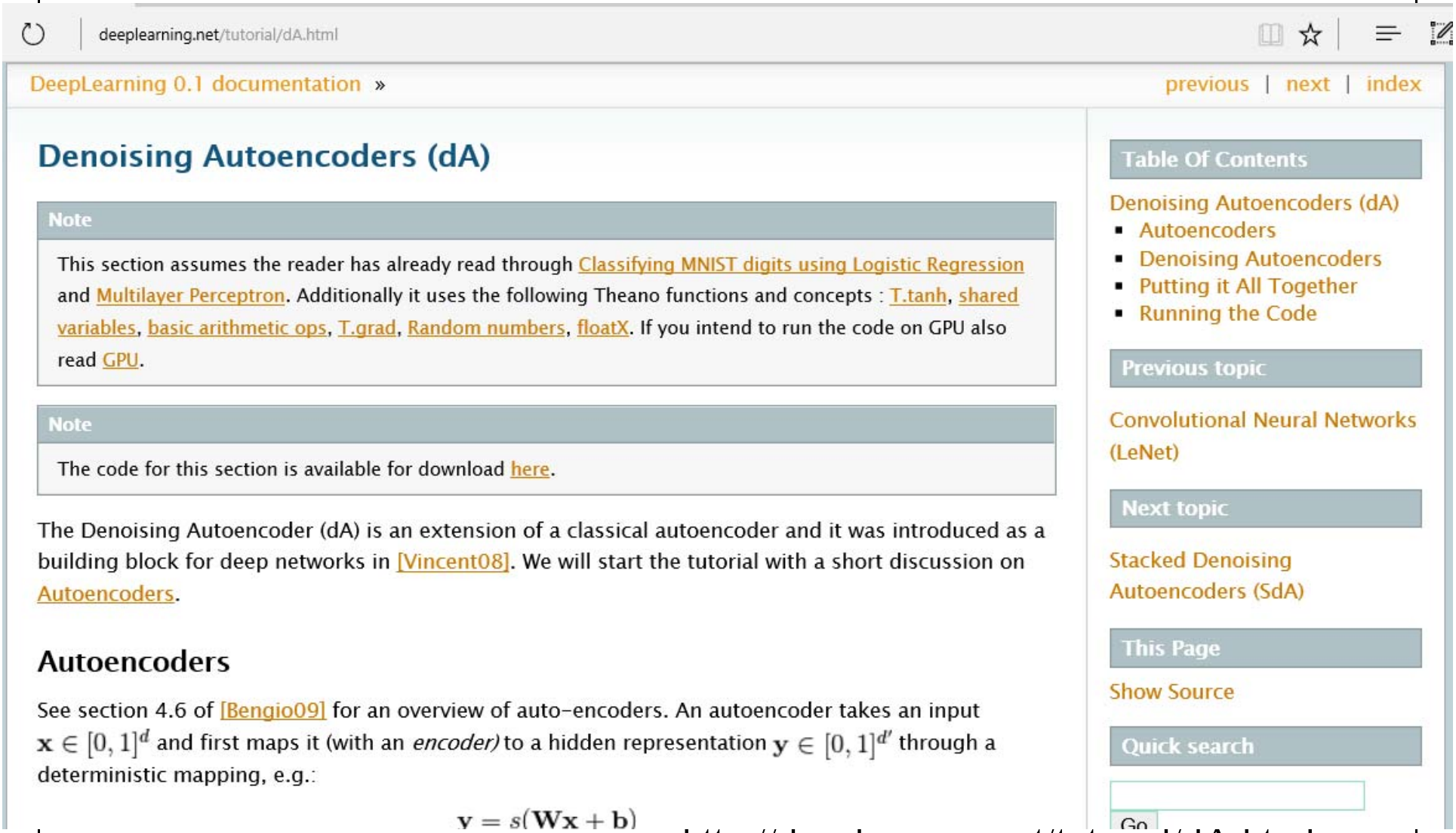
- With Gaussian noise,

  output – input = $\nabla_{\mathbf{x}} \log p(\mathbf{x})$





Theano Tutorial



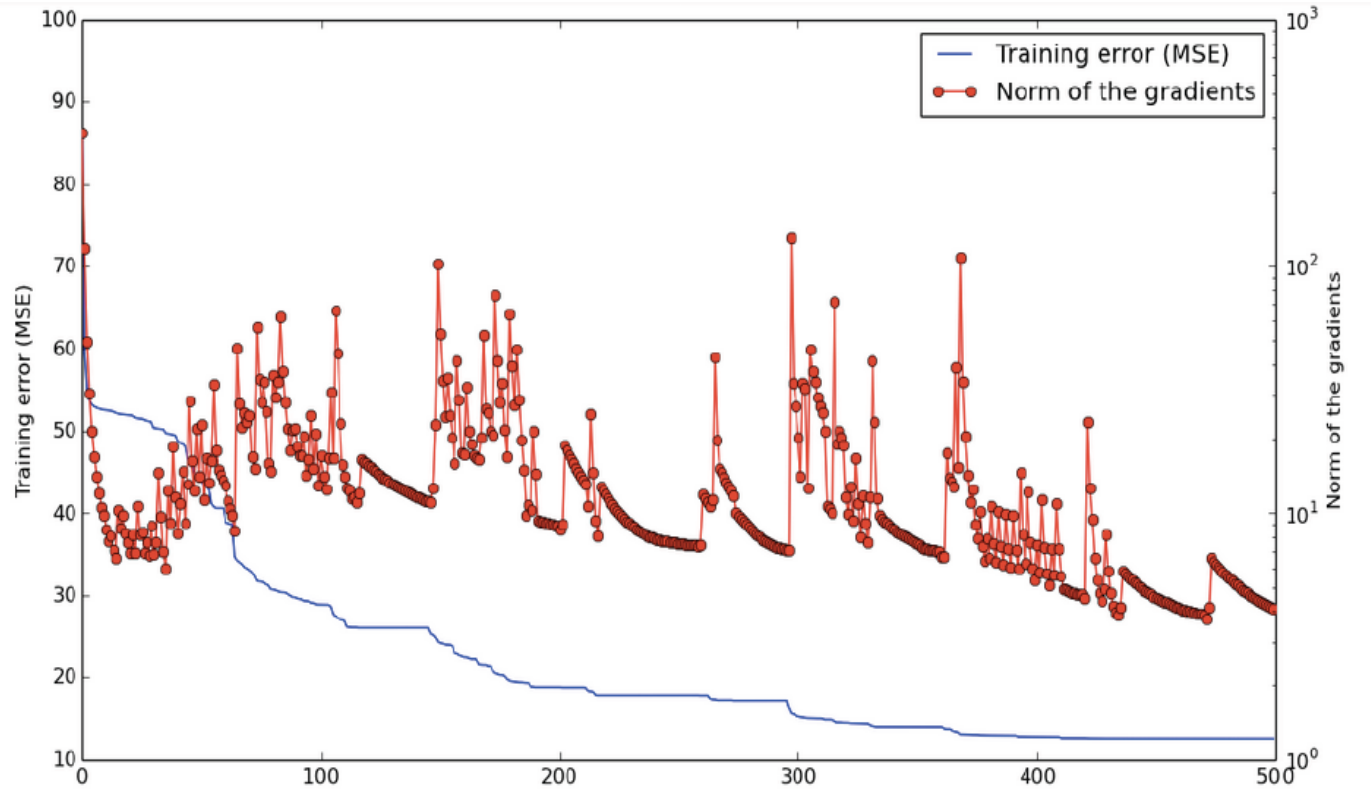
http://deeplearning.net/tutorial/dA.html

What Brought Successes to Deep Learning

- Many data and back propagation (Ruslan Salakhutdinov at NIPS 2013)
- We found a better way to initialize the weights, but that's sort of the minor things. (Geoffrey Hinton, at NIPS 2012 invited talk)
- Multilayer feedforward networks are universal approximators (Kurt Hornik, 1981)
- Deep Belief Networks are compact universal approximators (Yoshua Bengio, 2010)

Local Minima in ANN

- Saddle point analysis

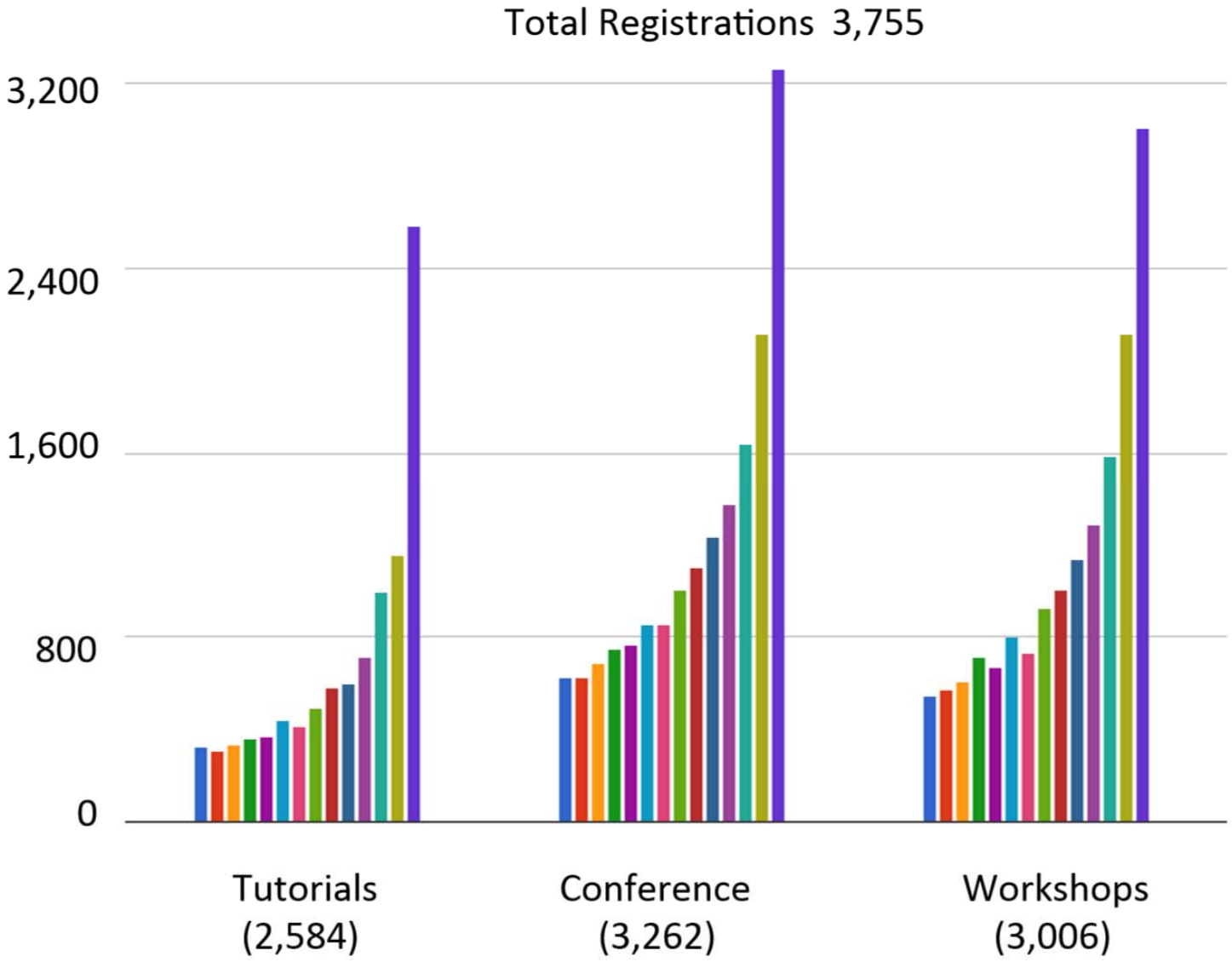


Razvan Pascanu et al. "On the saddle point problem for non-convex optimization." arXiv preprint arXiv:1405.4604 (2014)
Anna Choromanska et al. "The loss surfaces of multilayer networks." arXiv preprint arXiv:1412.0233 (2014)

Machine Learning Conferences

- Neural Information Processing Systems

Neural Information Processing Systems (NIPS) Growth



Neural Information Processing Systems (NIPS 2015)

- Oral talks:15
- Spotlights: 37
- Accepted papers: 403
- Single session: more than 3000 participants are listening to the single presentation.
- 7pm – 12am (5hr) poster session every day

Look at the poster session how it does look ➔

From Neil Lawrence's Blog

The New York Times

December 11, 2015

. . . .

Last month, the Toyota Motor Corporation announced a five-year, billion-dollar investment to create a research center based next to Stanford University to focus on artificial intelligence and robotics.

Also, a formerly obscure academic conference, Neural Information Processing Systems, underway this week in Montreal, has doubled in size since the previous year and has attracted a growing list of brand-name corporate sponsors, including Apple for the first time.

"There is a sellers' market right now — not enough talent to fill the demand from companies who need them," said Terrence Sejnowski, the director of the Computational Neurobiology Laboratory at the Salk Institute for Biological Studies in San Diego. "Ph.D. students are getting hired out of graduate schools for salaries that are higher than faculty members who are teaching them."

Machine Learning Conferences

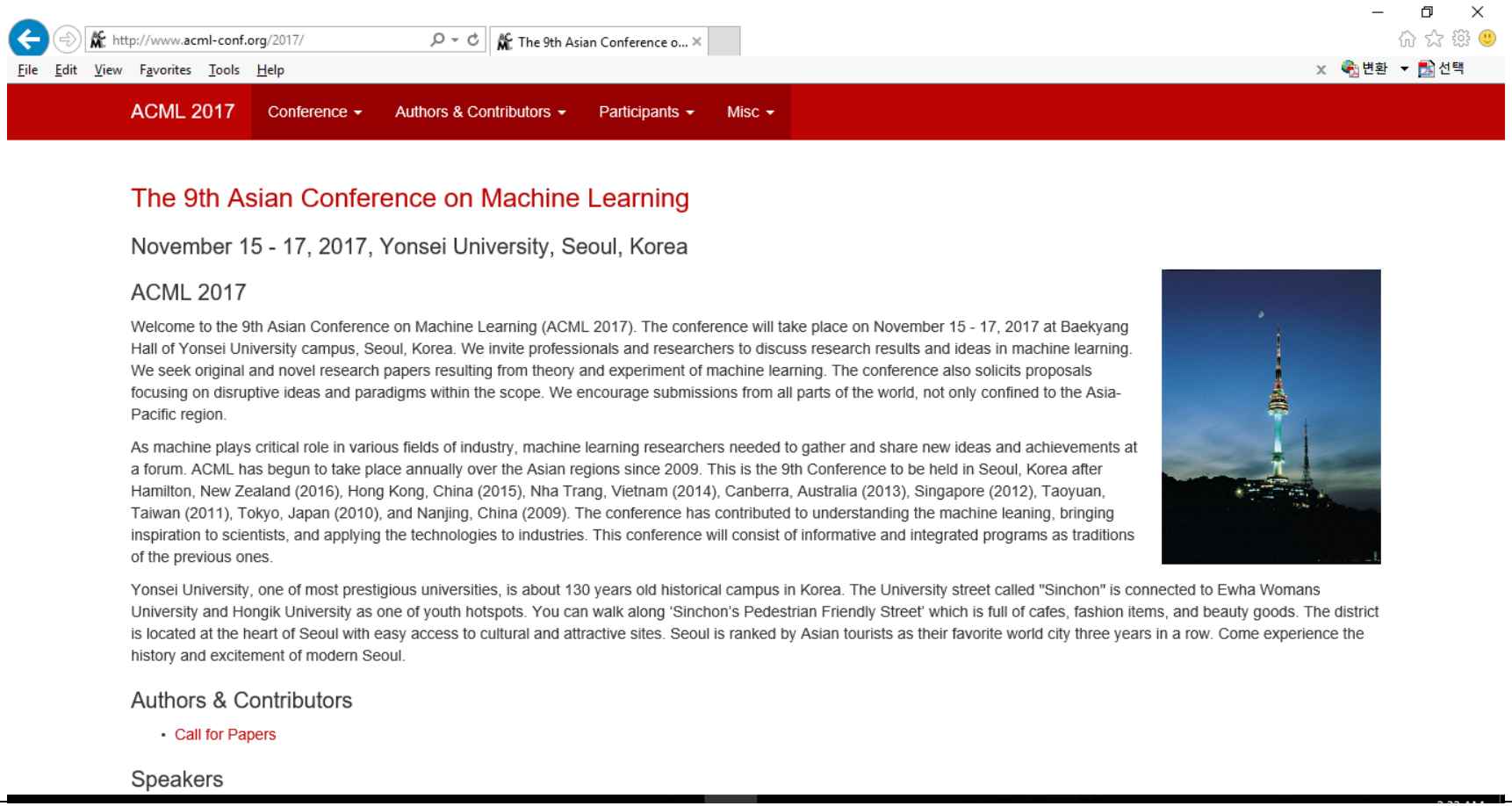
- International Conference on Machine Learning

Machine Learning Conferences

- AI & Statistics (AIStats)
- Association for the Advancement of Artificial Intelligence (AAAI) Conference
- Conference on Uncertainty in Artificial Intelligence (UAI)
- European Conference on Machine Learning (ECML)
- Asian Conference on Machine Learning (ACML)

Asian Conference on Machine Learning (ACML) in Seoul

- http://www.acml-conf.org/2017/
- Nov. 15 - 17 (Wed. – Fri.), 2017



Deep Learning book

Exercises Lectures

The Deep Learning textbook is a resource intended to help students and practitioners enter the field of machine learning in general and deep learning in particular. The online version of the book is now complete and will remain available online for free.

The deep learning textbook can now be pre-ordered on Amazon. Pre-orders should ship on December 16, 2016.

For up to date announcements, join our mailing list.

Citing the book

To cite this book, please use this bibtex entry:

```
@unpublished{Goodfellow-et-al-2016-Book,
    title={Deep Learning},
    author={Ian Goodfellow and Yoshua Bengio and Aaron Courville},
    note={Book in preparation for MIT Press},
    url={http://www.deeplearningbook.org},
    year={2016}
}
```

http://www.deeplearningbook.org/

THANK YOU

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