# Advanced Machine Learning
# Lecture 21

## Repetition

06.02.2017

Bastian Leibe
RWTH Aachen
http://www.vision.rwth-aachen.de/

leibe@vision.rwth-aachen.de

# Announcements

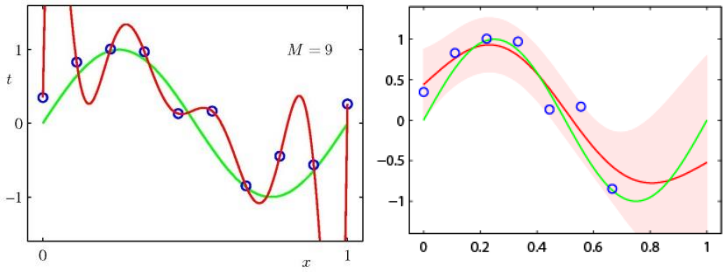
- Today, I'll summarize the most important points from the lecture.
  - It is an opportunity for you to ask questions…
  - …or get additional explanations about certain topics.
  - *So, please do ask.*
- Today's slides are intended as an index for the lecture.
  - But they are not complete, won't be sufficient as only tool.
  - Also look at the exercises – they often explain algorithms in detail.
- Exam procedure
  - Closed-book exam, the core exam time will be 2h.
  - We will send around an announcement with the exact starting times and places by email.

# This Lecture: *Advanced Machine Learning*

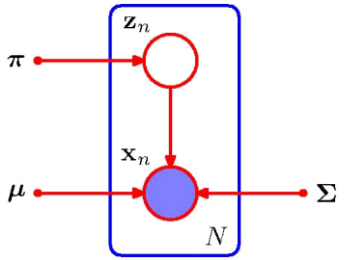


- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

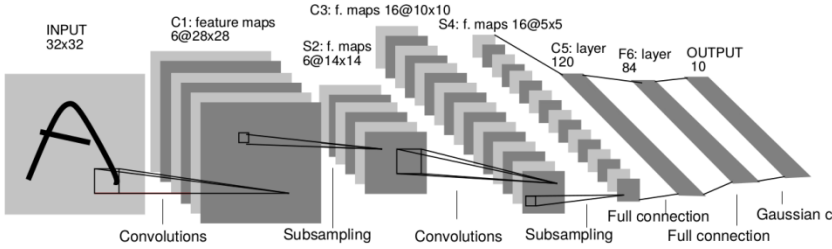
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC



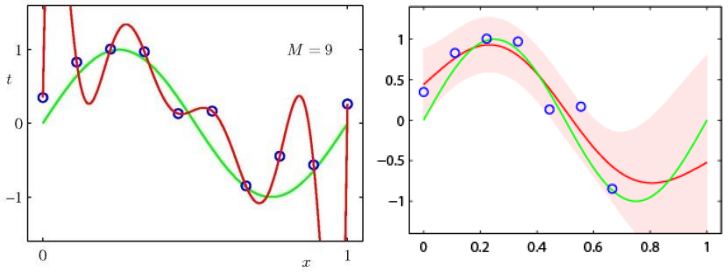

- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



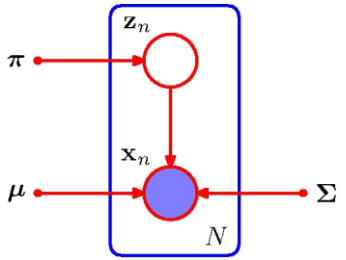
# This Lecture: *Advanced Machine Learning*

- **Regression Approaches**
  - **Linear Regression**
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

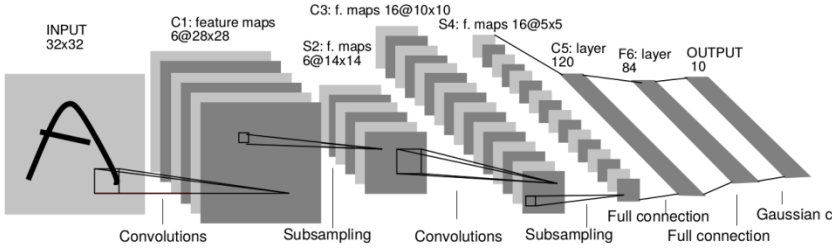
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- **Approximate Inference**
  - Sampling Approaches
  - MCMC




- **Deep Learning**
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



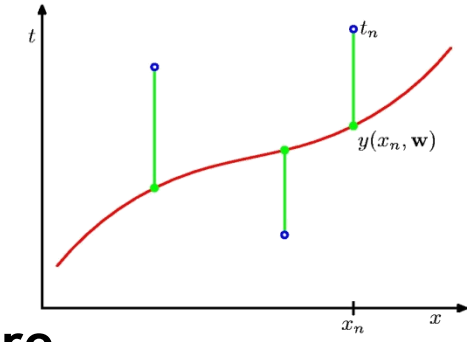
# Recap: Regression

- Learning to predict a continuous function value
  - Given: training set $\mathbf{X} = \{x_1, \ldots, x_N\}$ with target values $\mathbf{T} = \{t_1, \ldots, t_N\}$.

  $\Rightarrow$ Learn a continuous function $y(x)$ to predict the function value for a new input $x$.

- Define an error function $E(\mathbf{w})$ to optimize
  - E.g., sum-of-squares error

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$




  - Procedure: Take the derivative and set it to zero

$$\frac{\partial E(\mathbf{w})}{\partial w_j} = \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\} \frac{\partial y(x_n, \mathbf{w})}{\partial w_j} \stackrel{!}{=} 0$$



Image source: C.M. Bishop, 2006

# Recap: Least-Squares Regression

$$\mathbf{x}_i^T \mathbf{w} + w_0 = t_i, \quad \forall i = 1, \ldots, n$$

- **Setup**
  - **Step 1: Define** $\tilde{\mathbf{x}}_i = \begin{pmatrix} \mathbf{x}_i \\ 1 \end{pmatrix}, \quad \tilde{\mathbf{w}} = \begin{pmatrix} \mathbf{w} \\ w_0 \end{pmatrix}$
  - **Step 2: Rewrite** $\tilde{\mathbf{x}}_i^T \tilde{\mathbf{w}} = t_i, \quad \forall i = 1, \ldots, n$
  - **Step 3: Matrix-vector notation**

$$\tilde{\mathbf{X}}^T \tilde{\mathbf{w}} = \mathbf{t} \quad \text{with} \quad \tilde{\mathbf{X}} = [\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_n], \quad \mathbf{t} = [t_1, \ldots, t_n]^T$$

  - **Step 4: Find least-squares solution**

$$\|\tilde{\mathbf{X}}^T \tilde{\mathbf{w}} - \mathbf{t}\|^2 \rightarrow \min$$

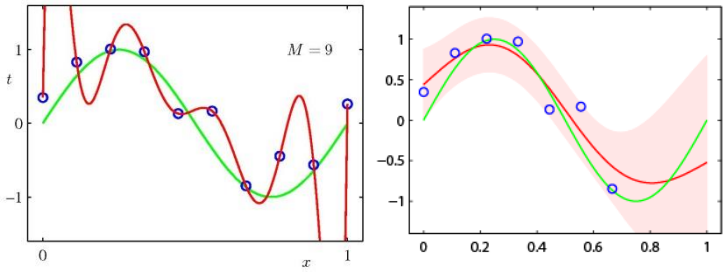
  - **Solution:** $\tilde{\mathbf{w}} = (\tilde{\mathbf{X}} \tilde{\mathbf{X}}^T)^{-1} \tilde{\mathbf{X}} \mathbf{t}$

# This Lecture: *Advanced Machine Learning*

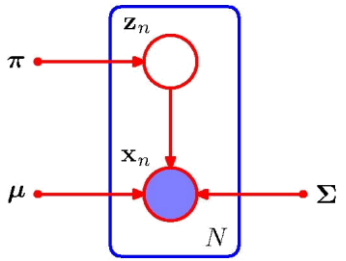


- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

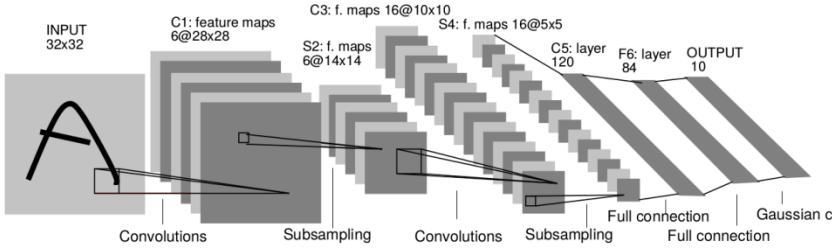
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC




- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Regularization

- Problem: Overfitting
  - Many parameters & little data ⇒ tendency to overfit to the noise
  - Side effect: The coefficient values get very large.

- Workaround: Regularization
  - Penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

  - Here we've simply added a quadratic regularizer, which is simple to optimize

$$\|\mathbf{w}\|^2 = \mathbf{w}^T\mathbf{w} = \cancel{w_0^2} + w_1^2 + \ldots + w_M^2$$

  - The resulting form of the problem is called Ridge Regression.
  - (*Note*: $w_0$ is often omitted from the regularizer.)

# Recap: Probabilistic Regression

- **First assumption:**
  - Our target function values $t$ are generated by adding noise to the ideal function estimate:

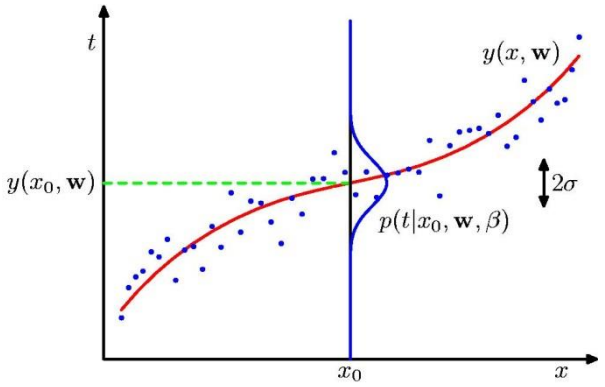
$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon$$

Target function value — Noise — Regression function — Input value — Weights or parameters

- **Second assumption:**
  - The noise is Gaussian distributed.

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$

Mean — Variance ($\beta$ precision)



# Recap: Probabilistic Regression

- Given
  - Training data points: $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
  - Associated function values: $\mathbf{t} = [t_1, \ldots, t_n]^T$

- Conditional likelihood (assuming i.i.d. data)

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|y(\mathbf{x}_n, \mathbf{w}), \beta^{-1}) = \prod_{n=1}^{N} \mathcal{N}(t_n|\underbrace{\mathbf{w}^T \phi(\mathbf{x}_n)}, \beta^{-1})$$

Generalized linear regression function

$\Rightarrow$ Maximize w.r.t. $\mathbf{w}$, $\beta$

# Recap: Maximum Likelihood Regression

$$\nabla_{\mathbf{w}} \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n)) \phi(\mathbf{x}_n)$$

- **Setting the gradient to zero:**

$$0 = -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n)) \phi(\mathbf{x}_n)$$

$$\Leftrightarrow \sum_{n=1}^{N} t_n \phi(\mathbf{x}_n) = \left[ \sum_{n=1}^{N} \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right] \mathbf{w}$$

$$\Leftrightarrow \mathbf{\Phi t} = \mathbf{\Phi \Phi}^T \mathbf{w} \qquad \mathbf{\Phi} = [\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)]$$

$$\Leftrightarrow \mathbf{w}_{\mathrm{ML}} = (\mathbf{\Phi \Phi}^T)^{-1} \mathbf{\Phi t}$$

Same as in least-squares regression!

$\Rightarrow$ *Least-squares regression is equivalent to Maximum Likelihood under the assumption of Gaussian noise.*

# Recap: Role of the Precision Parameter

- Also use ML to determine the precision parameter $\beta$:

$$\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \frac{N}{2}\log\beta - \frac{N}{2}\log(2\pi)$$

- Gradient w.r.t. $\beta$:

$$\nabla_\beta \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = -\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \frac{N}{2}\frac{1}{\beta}$$

$$\frac{1}{\beta_{\text{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2$$

$\Rightarrow$ *The inverse of the noise precision is given by the residual variance of the target values around the regression function.*

# Recap: Predictive Distribution

- Having determined the parameters $\mathbf{w}$ and $\beta$, we can now make predictions for new values of $\mathbf{x}$.

$$p(t|\mathbf{X}, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1})$$

- This means
  - Rather than giving a point estimate, we can now also give an estimate of the estimation uncertainty.

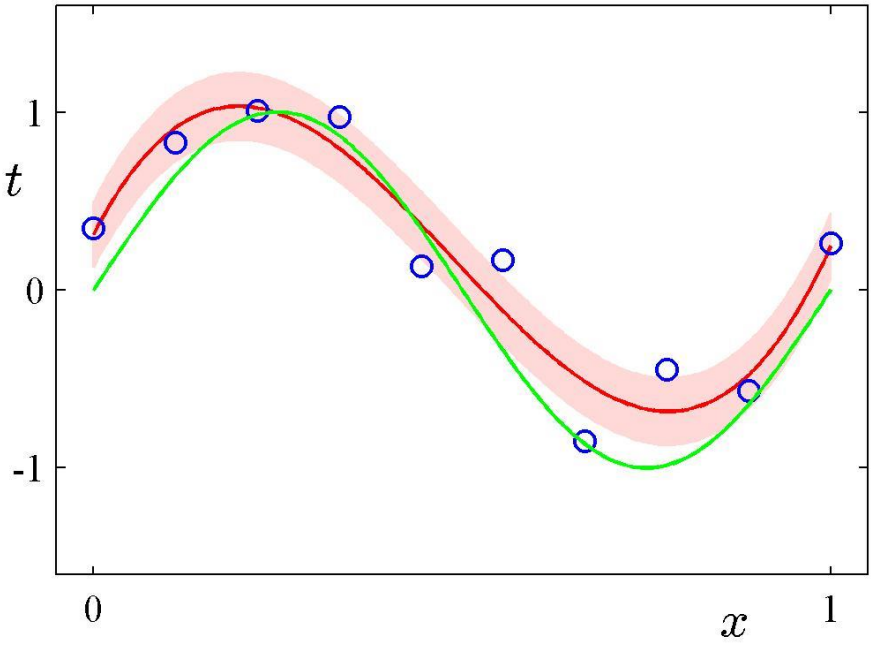




Image source: C.M. Bishop, 2006

# Recap: Maximum-A-Posteriori Estimation

- Introduce a prior distribution over the coefficients $\mathbf{w}$.
  - For simplicity, assume a zero-mean Gaussian distribution

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right\}$$

  - New hyperparameter $\alpha$ controls the distribution of model parameters.

- Express the posterior distribution over $\mathbf{w}$.
  - Using Bayes' theorem:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \beta, \alpha) \propto p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

  - We can now determine $\mathbf{w}$ by maximizing the posterior.
  - This technique is called maximum-a-posteriori (MAP).

# Recap: MAP Solution

- **Minimize the negative logarithm**

$$-\log p(\mathbf{w}|\mathbf{X},\mathbf{t},\beta,\alpha) \propto -\log p(\mathbf{t}|\mathbf{X},\mathbf{w},\beta) - \log p(\mathbf{w}|\alpha)$$

$$-\log p(\mathbf{t}|\mathbf{X},\mathbf{w},\beta) = \frac{\beta}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n,\mathbf{w}) - t_n\}^2 + \text{const}$$

$$-\log p(\mathbf{w}|\alpha) = \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \text{const}$$

- **The MAP solution is therefore**

$$\arg\min_{\mathbf{w}} \frac{\beta}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n,\mathbf{w}) - t_n\}^2 + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w}$$

⇒ ***Maximizing the posterior distribution is equivalent to minimizing the regularized sum-of-squares error*** **(with $\lambda = \frac{\alpha}{\beta}$).**

# Recap: MAP Solution (2)

$$\nabla_{\mathbf{w}} \log p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \beta, \alpha) = -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n)) \phi(\mathbf{x}_n) + \alpha \mathbf{w}$$

- **Setting the gradient to zero:**

$$0 = -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n)) \phi(\mathbf{x}_n) + \alpha \mathbf{w}$$

$$\Leftrightarrow \sum_{n=1}^{N} t_n \phi(\mathbf{x}_n) = \left[ \sum_{n=1}^{N} \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right] \mathbf{w} + \frac{\alpha}{\beta} \mathbf{w}$$

$$\Leftrightarrow \mathbf{\Phi t} = \left( \mathbf{\Phi \Phi}^T + \frac{\alpha}{\beta} \mathbf{I} \right) \mathbf{w} \qquad \mathbf{\Phi} = [\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)]$$

$$\Leftrightarrow \mathbf{w}_{\text{MAP}} = \left( \mathbf{\Phi \Phi}^T + \frac{\alpha}{\beta} \mathbf{I} \right)^{-1} \mathbf{\Phi t}$$

**Effect of regularization:**
**Keeps the inverse well-conditioned**

# Recap: Bayesian Curve Fitting

- Given
  - Training data points: $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
  - Associated function values: $\mathbf{t} = [t_1, \ldots, t_n]^T$
  - Our goal is to predict the value of $t$ for a new point $\mathbf{x}$.

- Evaluate the predictive distribution

$$p(t|x, \mathbf{X}, \mathbf{t}) = \int \underbrace{p(t|x, \mathbf{w})}\underbrace{p(\mathbf{w}|\mathbf{X}, \mathbf{t})} d\mathbf{w}$$

What we just computed for MAP

  - Noise distribution – again assume a Gaussian here

$$p(t|x, \mathbf{w}) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$

  - Assume that parameters $\alpha$ and $\beta$ are fixed and known for now.

# Recap: Bayesian Curve Fitting

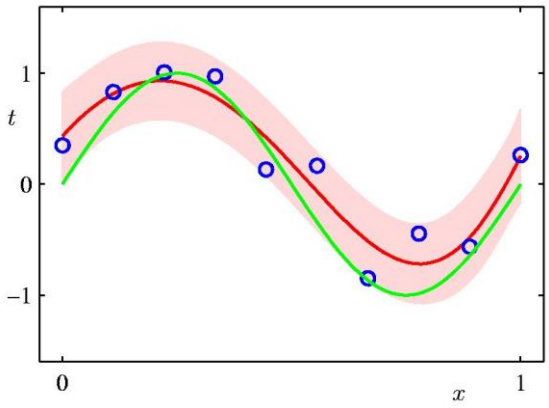
- Under those assumptions, the posterior distribution is a Gaussian and can be evaluated analytically:

$$p(t|x, \mathbf{X}, \mathbf{t}) = \mathcal{N}(t|m(x), s^2(x))$$

  - where the mean and variance are given by

$$m(x) = \beta\phi(x)^T \mathbf{S} \sum_{n=1}^{N} \phi(\mathbf{x}_n) t_n$$

$$s(x)^2 = \beta^{-1} + \phi(x)^T \mathbf{S} \phi(x)$$

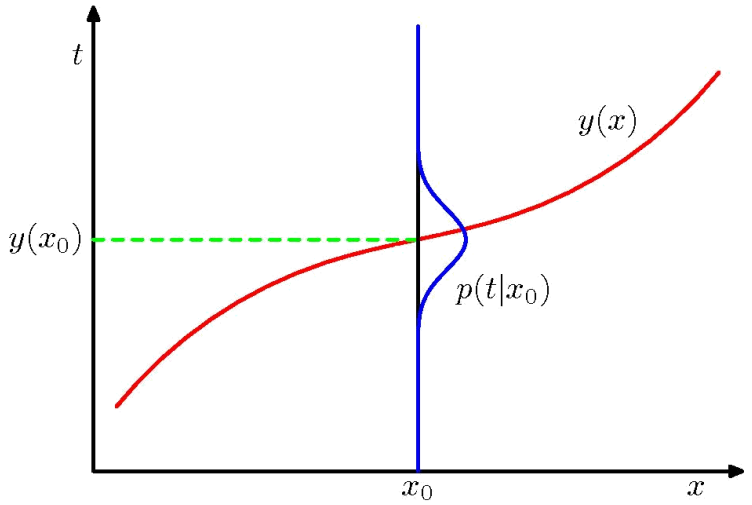



  - and S is the regularized covariance matrix

$$\mathbf{S}^{-1} = \alpha\mathbf{I} + \beta \sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^T$$


Image source: C.M. Bishop, 2006

# Recap: Loss Functions for Regression




Mean prediction

- **Optimal prediction**
  - Minimize the expected loss

$$\mathbb{E}[L] = \iint L(t, y(\mathbf{x}))p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

  - Under squared loss, the optimal regression function is the mean $\mathbb{E}[t|\mathbf{x}]$ of the posterior $p(t|\mathbf{x})$ ("mean prediction").
  - For generalized linear regression function and squared loss:

$$y(\mathbf{x}) = \int t\mathcal{N}(t|\mathbf{w}^T\phi(\mathbf{x}), \beta^{-1})\mathrm{d}t = \mathbf{w}^T\phi(\mathbf{x})$$



Slide adapted from Stefan Roth



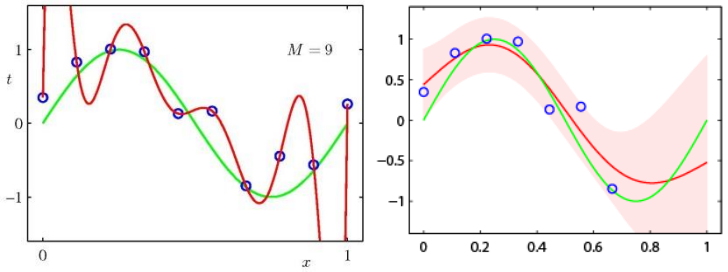


Image source: C.M. Bishop, 2006

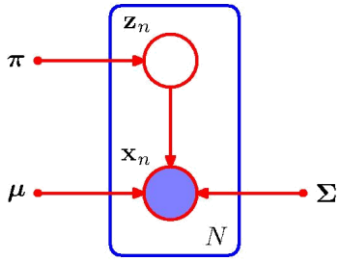
# This Lecture: *Advanced Machine Learning*

- **Regression Approaches**
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

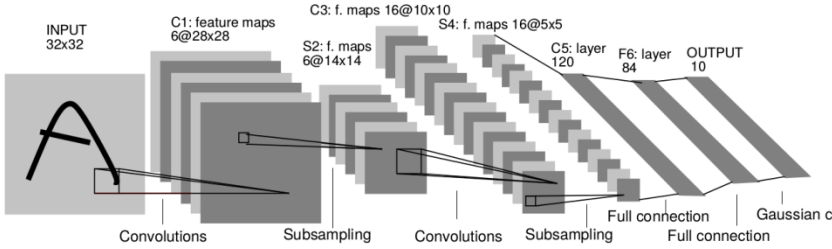
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- **Approximate Inference**
  - Sampling Approaches
  - MCMC




- **Deep Learning**
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Loss Functions for Regression

- The squared loss is not the only possible choice
  - Poor choice when conditional distribution $p(t|\mathbf{x})$ is multimodal.

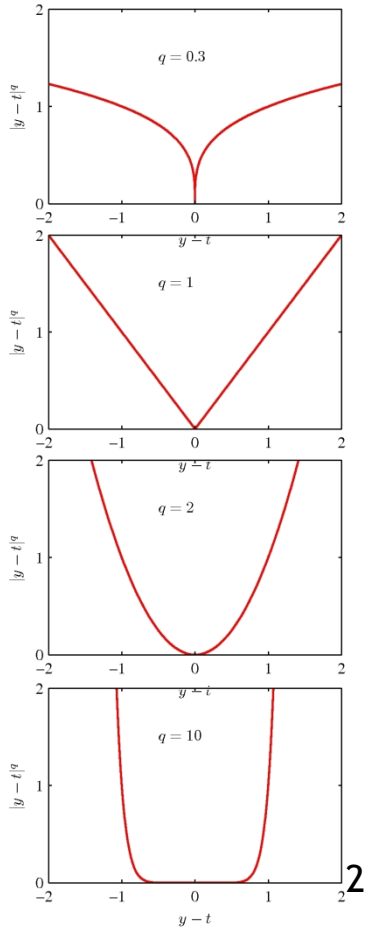
- Simple generalization: Minkowski loss

$$L(t, y(\mathbf{x})) = |y(\mathbf{x}) - t|^q$$

  - Expectation

$$\mathbb{E}[L_q] = \iint |y(\mathbf{x}) - t|^q p(\mathbf{x}, t) \mathrm{d}\mathbf{x} \mathrm{d}t$$

- Minimum of $\mathbb{E}[L_q]$ is given by
  - Conditional mean for $q = 2$,
  - Conditional median for $q = 1$,
  - Conditional mode for $q = 0$.



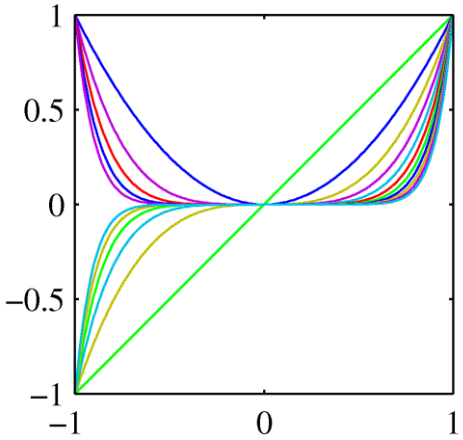
# Recap: Linear Basis Function Models

- Generally, we consider models of the following form

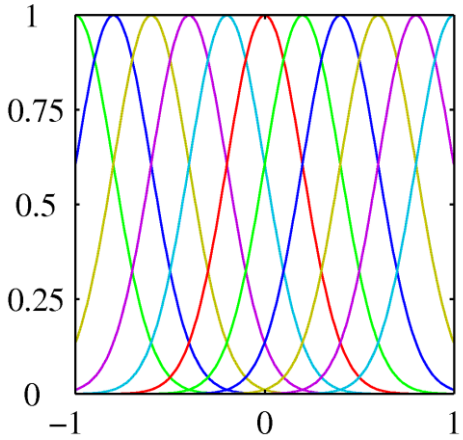
$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

  - where $\phi_j(\mathbf{x})$ are known as *basis functions*.
  - In the simplest case, we use linear basis functions: $\phi_d(\mathbf{x}) = x_d$.

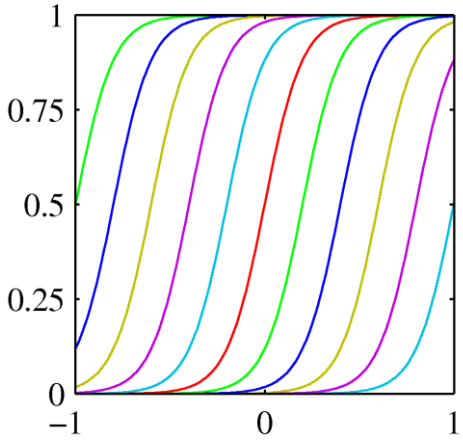
- Other popular basis functions




Polynomial




Gaussian

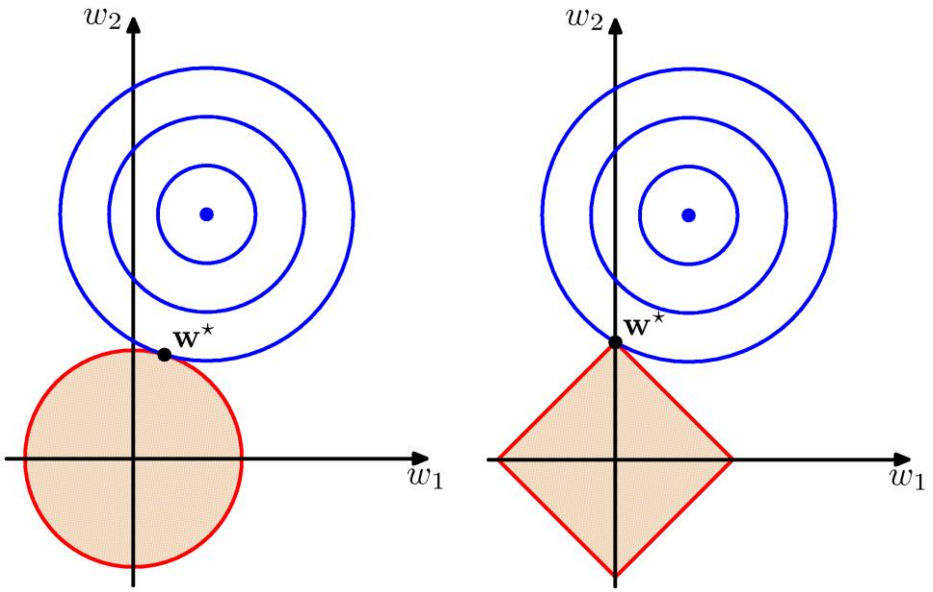



Sigmoid

# Recap: Regularized Least-Squares

- Consider more general regularization functions
  - "$L_q$ norms":

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$




- Effect: Sparsity for $q \leq 1$.
  - Minimization tends to set many coefficients to zero


Image source: C.M. Bishop, 2006

# Recap: The Lasso

- $L_1$ regularization ("The Lasso")

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \lambda\sum_{j=1}^{M}|w_j|$$

  - The solution will be sparse (only few coefficients non-zero)
  - The $L_1$ penalty makes the problem non-linear.

  $\Rightarrow$ There is no closed-form solution.

- Interpretation as Bayes Estimation
  - We can think of $|w_j|^q$ as the log-prior density for $w_j$.

- Prior for Lasso ($q = 1$):
  - Laplacian distribution

$$p(\mathbf{w}) = \frac{1}{2\tau}\exp\{-|\mathbf{w}|/\tau\} \quad \text{with} \quad \tau = \frac{1}{\lambda}$$

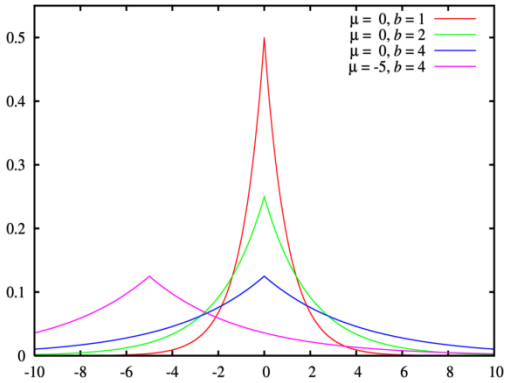
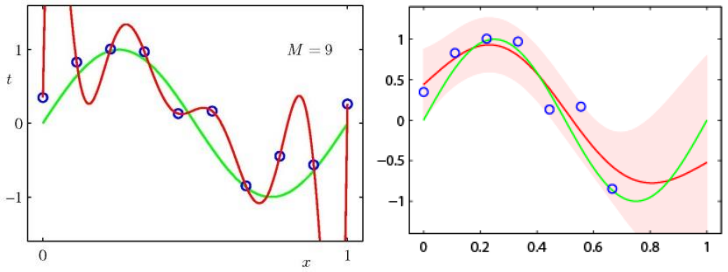



Image source: Wikipedia

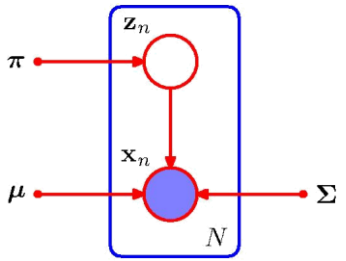
# This Lecture: *Advanced Machine Learning*

- **Regression Approaches**
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

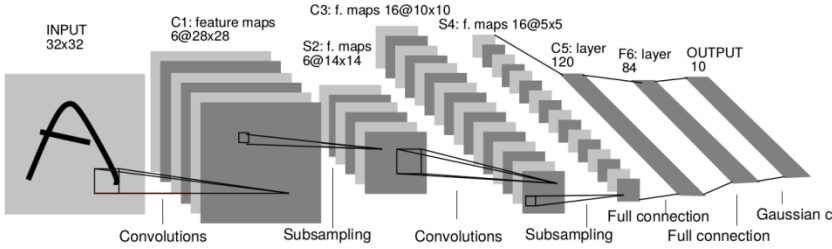
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- **Approximate Inference**
  - Sampling Approaches
  - MCMC




- **Deep Learning**
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



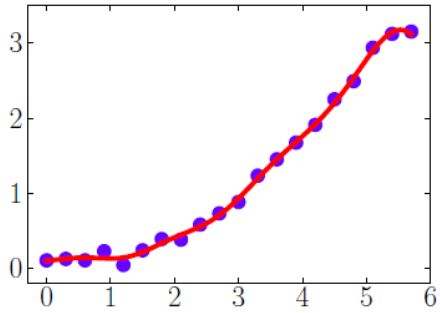
# Recap: Kernel Ridge Regression

- **Dual definition**
  - Instead of working with $\mathbf{w}$, substitute $\mathbf{w} = \mathbf{\Phi}^T\mathbf{a}$ into $J(\mathbf{w})$ and write the result using the kernel matrix $\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^T$:

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}^T\mathbf{K}\mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T\mathbf{K}\mathbf{a}$$

  - Solving for $\mathbf{a}$, we obtain

$$\mathbf{a} = (\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{t}$$




- **Prediction for a new input $\mathbf{x}$:**
  - Writing $\mathbf{k}(\mathbf{x})$ for the vector with elements $k_n(\mathbf{x}) = k(\mathbf{x}_n, \mathbf{x})$

$$y(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x}) = \mathbf{a}^T\mathbf{\Phi}\phi(\mathbf{x}) = \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{t}$$

$\Rightarrow$ ***The dual formulation allows the solution to be entirely expressed in terms of the kernel function $k(\mathbf{x},\mathbf{x}')$.***


Image source: Christoph Lampert

# Recap: Properties of Kernels

- **Theorem**
  - ***Let*** $k$: $\mathcal{X} \times \mathcal{X} \to \mathbb{R}$ ***be a positive definite kernel function. Then there exists a Hilbert Space*** H ***and a mapping*** $\varphi : \mathcal{X} \to \mathcal{H}$ ***such that***

$$k(x, x') = \langle (\phi(x), \phi(x') \rangle_{\mathcal{H}}$$

  - **where** $\langle . \ , \ . \rangle_{\mathcal{H}}$ ***is the inner product in*** H.
- **Translation**
  - **Take *any* set** $\mathcal{X}$ **and *any* function** $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
  - **If** $k$ **is a positive definite kernel, then we can use** $k$ **to learn a classifier for the elements in** $\mathcal{X}$**!**
- **Note**
  - $\mathcal{X}$ **can be any set, e.g.** $\mathcal{X}$ **= *"all videos on YouTube"* or** $\mathcal{X}$ **= *"all permutations of* {1, . . . , *k*}", or** $\mathcal{X}$ **= *"the internet"*.**





Slide credit: Christoph Lampert

# Recap: The "Kernel Trick"

**Any algorithm that uses data only in the form of inner products can be *kernelized*.**

- How to kernelize an algorithm
  - Write the algorithm only in terms of inner products.
  - Replace all inner products by kernel function evaluations.

$\Rightarrow$ The resulting algorithm will do the same as the linear version, but in the (hidden) feature space $\mathcal{H}$.

  - Caveat: working in $\mathcal{H}$ is not a guarantee for better performance. A good choice of $k$ and model selection are important!



Slide credit: Christoph Lampert

# Recap: How to Check if a Function is a Kernel

- **Problem:**
  - Checking if a given $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ fulfills the conditions for a kernel is difficult:
  - We need to prove or disprove

$$\sum_{i,j=1}^{n} t_i k(x_i, x_j) t_j \geq 0$$

for any set $x_1, \ldots, x_n \in \mathcal{X}$ and any $\mathbf{t} \in \mathbb{R}^n$ for any $n \in N$.

- **Workaround:**
  - It is easy to construct functions $k$ that are positive definite kernels.

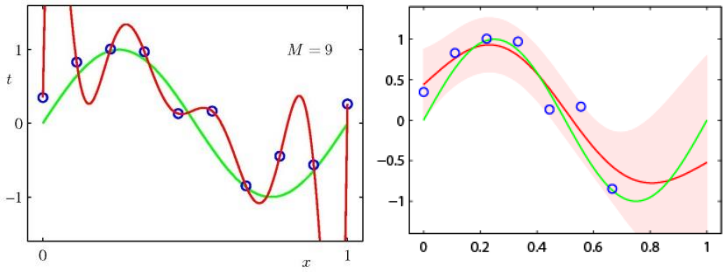


Slide credit: Christoph Lampert

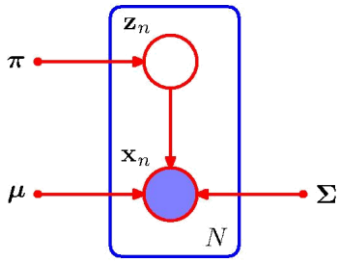
# This Lecture: *Advanced Machine Learning*

- **Regression Approaches**
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

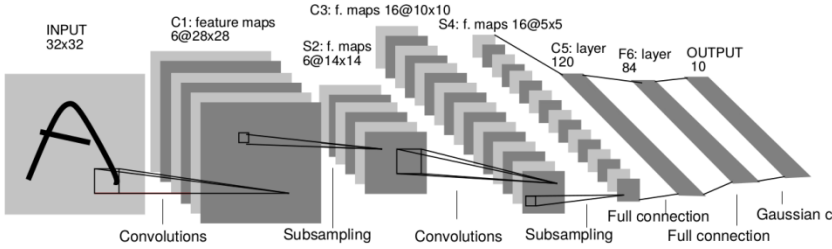
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- **Approximate Inference**
  - Sampling Approaches
  - MCMC




- **Deep Learning**
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Gaussian Process

- Gaussian distribution
  - Probability distribution over scalars / vectors.
- Gaussian process (generalization of Gaussian distrib.)
  - Describes properties of functions.
  - Function: Think of a function as a long vector where each entry specifies the function value $f(\mathbf{x}_i)$ at a particular point $\mathbf{x}_i$.
  - Issue: How to deal with infinite number of points?
    - If you ask only for properties of the function at a finite number of points…
    - Then inference in Gaussian Process gives you the same answer if you ignore the infinitely many other points.
- Definition
  - A Gaussian process (GP) is a collection of random variables any finite number of which has a joint Gaussian distribution.



Slide credit: Bernt Schiele

# Recap: Gaussian Process

- A Gaussian process is completely defined by
  - Mean function $m(\mathbf{x})$ and

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})]$$

  - Covariance function $k(\mathbf{x},\mathbf{x}')$

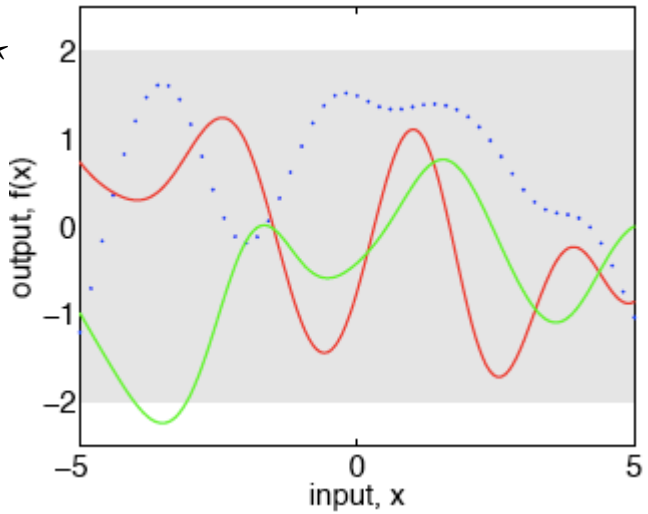
$$k(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x})(f(\mathbf{x}') - m(\mathbf{x}'))]$$

  - We write the Gaussian process (GP)

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$

# Recap: GPs Define Prior over Functions

- **Distribution over functions:**
  - Specification of covariance function implies distribution over functions.
  - I.e. we can draw samples from the distribution of functions evaluated at a (finite) number of points.
  - Procedure
    - We choose a number of input points $X_\star$
    - We write the corresponding covariance matrix (e.g. using SE) element-wise:
      $$K(X_\star, X_\star)$$
    - Then we generate a random Gaussian vector with this covariance matrix:
      $$f_\star \sim \mathcal{N}(\mathbf{0}, K(X_\star, X_\star))$$




Example of 3 functions sampled

Image source: Rasmussen & Williams, 2006

# Recap: Prediction with Noise-free Observations

- **Assume our observations are noise-free:**

$$\{(\mathbf{x}_n, f_n) \mid n = 1, \ldots, N\}$$

  - **Joint distribution of the training outputs $\mathbf{f}$ and test outputs $\mathbf{f}_\star$ according to the prior:**

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}_\star \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X, X) & K(X, X_\star) \\ K(X_\star, X) & K(X_\star, X_\star) \end{bmatrix}\right)$$

  - **Calculation of posterior corresponds to conditioning the joint Gaussian prior distribution on the observations:**

$$\mathbf{f}_\star | X_\star, X, \mathbf{f} \sim \mathcal{N}(\bar{\mathbf{f}}_\star, \mathrm{cov}[\mathbf{f}_\star]) \qquad \bar{\mathbf{f}}_\star = \mathbb{E}[\mathbf{f}_\star | X, X_\star, \mathbf{t}]$$

  - **with:**

$$\begin{aligned} \bar{\mathbf{f}}_\star &= K(X_\star, X)K(X, X)^{-1}\mathbf{f} \\ \mathrm{cov}[\mathbf{f}_\star] &= K(X_\star, X_\star) - K(X_\star, X)K(X, X)^{-1}K(X, X_\star) \end{aligned}$$

# Recap: Prediction with Noisy Observations

- Joint distribution of the observed values and the test locations under the prior:

$$\begin{bmatrix} \mathbf{t} \\ \mathbf{f}_\star \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X,X)+\sigma_n^2 I & K(X,X_\star) \\ K(X_\star,X) & K(X_\star,X_\star) \end{bmatrix}\right)$$

  - Calculation of posterior corresponds to conditioning the joint Gaussian prior distribution on the observations:

$$\mathbf{f}_\star | X_\star, X, \mathbf{t} \sim \mathcal{N}(\bar{\mathbf{f}}_\star, \mathrm{cov}[\mathbf{f}_\star]) \qquad \bar{\mathbf{f}}_\star = \mathbb{E}[\mathbf{f}_\star | X, X_\star, \mathbf{t}]$$

  - with:

$$\bar{\mathbf{f}}_\star = K(X_\star,X)\left(K(X,X)+\sigma_n^2 I\right)^{-1}\mathbf{t}$$

$$\mathrm{cov}[\mathbf{f}_\star] = K(X_\star,X_\star) - K(X_\star,X)\left(K(X,X)+\sigma_n^2 I\right)^{-1}K(X,X_\star)$$

⇒ This is the key result that defines Gaussian process regression!

- Predictive distribution is Gaussian whose mean and variance depend on test points $X_*$ and on the kernel $k(\mathbf{x},\mathbf{x}')$, evaluated on $X$.

# Recap: GP Regression Algorithm

- **Very simple algorithm**

**input**: $X$ (inputs), $\mathbf{y}$ (targets), $k$ (covariance function), $\sigma_n^2$ (noise level), $\mathbf{x}_*$ (test input)

2: $L := \text{cholesky}(K + \sigma_n^2 I)$

$\boldsymbol{\alpha} := L^\top \backslash (L \backslash \mathbf{y})$ } predictive mean eq. (2.25)

4: $\bar{f}_* := \mathbf{k}_*^\top \boldsymbol{\alpha}$

$\mathbf{v} := L \backslash \mathbf{k}_*$ } predictive variance eq. (2.26)

6: $\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$

$\log p(\mathbf{y}|X) := -\frac{1}{2}\mathbf{y}^\top \boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{n}{2}\log 2\pi$ eq. (2.30)

8: **return**: $\bar{f}_*$ (mean), $\mathbb{V}[f_*]$ (variance), $\log p(\mathbf{y}|X)$ (log marginal likelihood)

- **Based on the following equations (Matrix inv. ↔ Cholesky fact.)**

$$\bar{f}_\star = \mathbf{k}_\star^T \left(K + \sigma_n^2 I\right)^{-1} \mathbf{t}$$

$$\text{cov}[f_\star] = k(\mathbf{x}_\star, \mathbf{x}_\star) - \mathbf{k}_\star^T \left(K + \sigma_n^2 I\right)^{-1} \mathbf{k}_\star$$

$$\log p(\mathbf{t}|X) = -\frac{1}{2}\mathbf{t}^T \left(K + \sigma_n^2 I\right)^{-1} \mathbf{t} - \frac{1}{2}\log|K + \sigma_n^2 I| - \frac{N}{2}\log 2\pi$$



Image source: Rasmussen & Williams, 2006

# Recap: Computational Complexity

- Complexity of GP model
  - Training effort: $\mathcal{O}(N^3)$ through matrix inversion
  - Test effort: $\mathcal{O}(N^2)$ through vector-matrix multiplication
- Complexity of basis function model
  - Training effort: $\mathcal{O}(M^3)$
  - Test effort: $\mathcal{O}(M^2)$
- Discussion
  - If the number of basis functions $M$ is smaller than the number of data points $N$, then the basis function model is more efficient.
  - However, advantage of GP viewpoint is that we can consider covariance functions that can only be expressed by an infinite number of basis functions.
  - Still, exact GP methods become infeasible for large training sets.

# Recap: Bayesian Model Selection for GPs

- Goal
  - Determine/learn different parameters of Gaussian Processes
- Hierarchy of parameters
  - Lowest level
    - $\mathbf{w}$ – e.g. parameters of a linear model.
  - Mid-level (hyperparameters)
    - $\theta$ – e.g. controlling prior distribution of $\mathbf{w}$.
  - Top level
    - Typically discrete set of model structures $\mathcal{H}_i$.
- Approach
  - Inference takes place one level at a time.



Slide credit: Bernt Schiele

# Recap: Model Selection at Lowest Level

- Posterior of the parameters $\mathbf{w}$ is given by Bayes' rule

$$p(\mathbf{w}|\mathbf{t}, X, \theta, \mathcal{H}_i) = \frac{p(\mathbf{t}|X, \mathbf{w}, \theta, \mathcal{H}_i)p(\mathbf{w}|\theta, X, \mathcal{H}_i)}{p(\mathbf{t}|X, \theta, \mathcal{H}_i)}$$

$$= \frac{p(\mathbf{t}|X, \mathbf{w}, \mathcal{H}_i)p(\mathbf{w}|\theta, \mathcal{H}_i)}{p(\mathbf{t}|X, \theta, \mathcal{H}_i)}$$

- with
  - $p(\mathbf{t}|X, \mathbf{w}, \mathcal{H}_i)$ likelihood and
  - $p(\mathbf{w}|\theta, \mathcal{H}_i)$ prior parameters $\mathbf{w}$,
  - Denominator (normalizing constant) is independent of the parameters and is called marginal likelihood.

$$p(\mathbf{t}|X, \theta, \mathcal{H}_i) = \int p(\mathbf{t}|X, \mathbf{w}, \mathcal{H}_i)p(\mathbf{w}|\theta, \mathcal{H}_i)d\mathbf{w}$$



Slide credit: Bernt Schiele

# Recap: Model Selection at Mid Level

- Posterior of parameters $\theta$ is again given by Bayes' rule

$$p(\theta|\mathbf{t}, X, \mathcal{H}_i) = \frac{p(\mathbf{t}|X, \theta, \mathcal{H}_i)p(\theta|X, \mathcal{H}_i)}{p(\mathbf{t}|X, \mathcal{H}_i)} = \frac{p(\mathbf{t}|X, \theta, \mathcal{H}_i)p(\theta|\mathcal{H}_i)}{p(\mathbf{t}|X, \mathcal{H}_i)}$$

- where
  - The marginal likelihood of the previous level $p(\mathbf{t}\,|\,X,\theta,\mathcal{H}_i)$ plays the role of the likelihood of this level.
  - $p(\theta\,|\,\mathcal{H}_i)$ is the hyperprior (prior of the hyperparameters)
  - Denominator (normalizing constant) is given by:

$$p(\mathbf{t}|X, \mathcal{H}_i) = \int p(\mathbf{t}|X, \theta, \mathcal{H}_i)p(\theta|\mathcal{H}_i)d\theta$$



Slide credit: Bernt Schiele

# Recap: Model Selection at Top Level

- At the top level, we calculate the posterior of the model

$$p(\mathcal{H}_i|\mathbf{t}, X) = \frac{p(\mathbf{t}|X, \mathcal{H}_i)p(\mathcal{H}_i)}{p(\mathbf{t}|X)}$$

- where
  - Again, the denominator of the previous level $p(\mathbf{t}\,|\,X, \mathcal{H}_i)$ plays the role of the likelihood.
  - $p(\mathcal{H}_i)$ is the prior of the model structure.
  - Denominator (normalizing constant) is given by:

$$p(\mathbf{t}|X) = \sum_i p(\mathbf{t}|X, \mathcal{H}_i)p(\mathcal{H}_i)$$



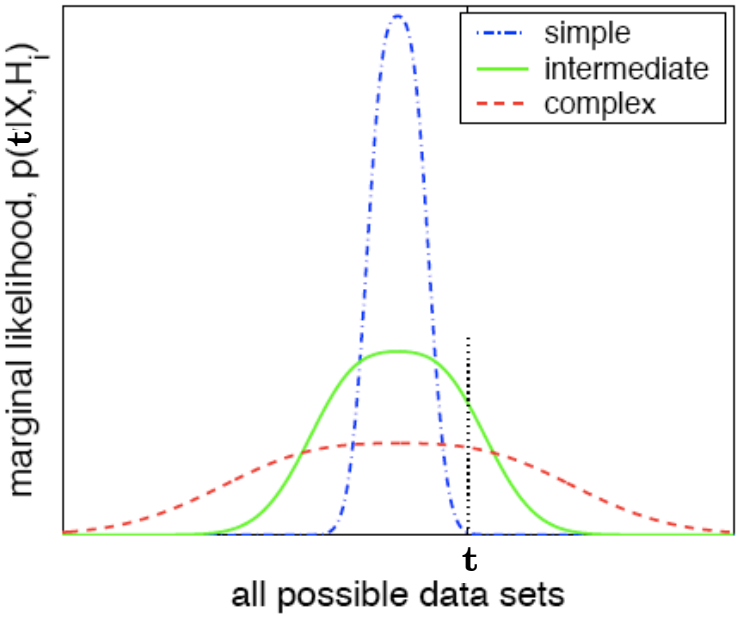
Slide credit: Bernt Schiele

# Recap: Bayesian Model Selection

- Discussion
  - Marginal likelihood is main difference to non-Bayesian methods

$$p(\mathbf{t}|X, \mathcal{H}_i) = \int p(\mathbf{t}|X, \theta, \mathcal{H}_i) p(\theta|\mathcal{H}_i) d\theta$$

  - It automatically incorporates a trade-off between the model fit and the model complexity:
    - A simple model can only account for a limited range of possible sets of target values – if a simple model fits well, it obtains a high marginal likelihood.
    - A complex model can account for a large range of possible sets of target values – therefore, it can never attain a very high marginal likelihood.





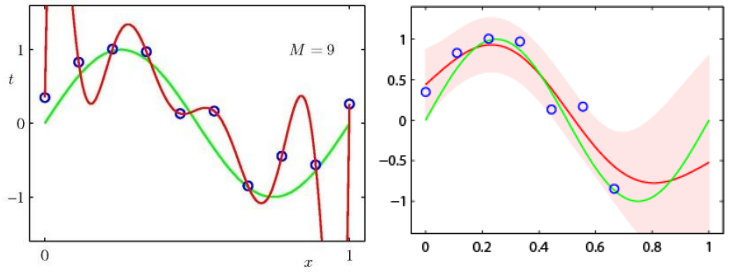
Slide credit: Bernt Schiele
Image source: Rasmussen & Williams, 2006

# This Lecture: *Advanced Machine Learning*

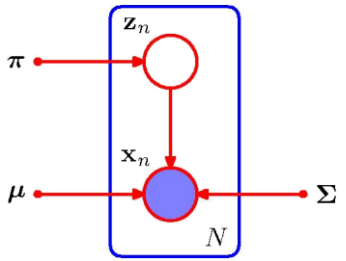


- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

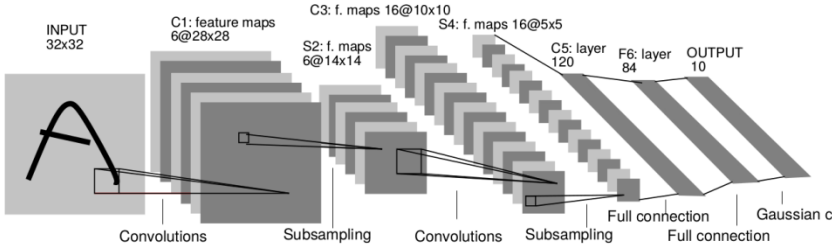
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC



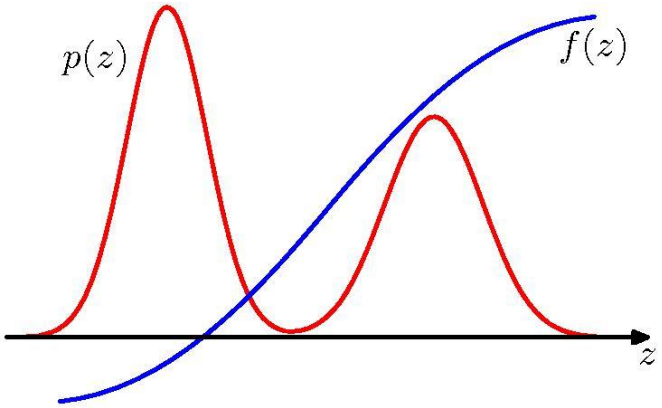

- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Sampling Idea

- **Objective:**
  - Evaluate expectation of a function $f(\mathbf{z})$ w.r.t. a probability distribution $p(\mathbf{z})$.

$$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z}$$




- **Sampling idea**
  - Draw $L$ independent samples $\mathbf{z}^{(l)}$ with $l = 1,\ldots,L$ from $p(\mathbf{z})$.
  - This allows the expectation to be approximated by a finite sum

$$\hat{f} = \frac{1}{L}\sum_{l=1}^{L} f(\mathbf{z}^l)$$

  - As long as the samples $\mathbf{z}^{(l)}$ are drawn independently from $p(\mathbf{z})$, then

$$\mathbb{E}[\hat{f}] = \mathbb{E}[f]$$

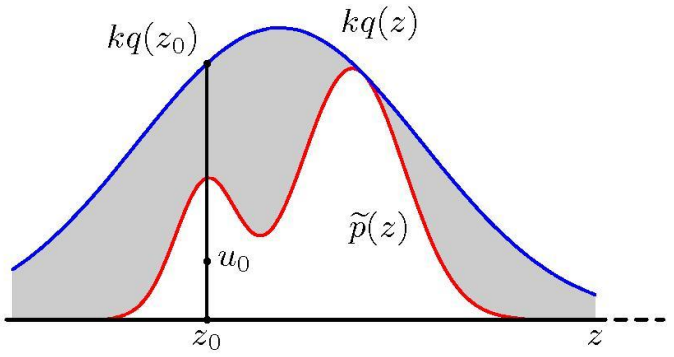
⇒ **Unbiased estimate, independent of the dimension of $\mathbf{z}$!**

# Recap: Rejection Sampling

- **Assumptions**
  - Sampling directly from $p(\mathbf{z})$ is difficult.
  - But we can easily evaluate $p(\mathbf{z})$ (up to some norm. factor $Z_p$):

$$p(\mathbf{z}) = \frac{1}{Z_p}\tilde{p}(\mathbf{z})$$

- **Idea**
  - We need some simpler distribution $q(\mathbf{z})$ (called proposal distribution) from which we can draw samples.
  - Choose a constant $k$ such that: $\forall z : kq(z) \geq \tilde{p}(z)$
- **Sampling procedure**
  - Generate a number $z_0$ from $q(z)$.
  - Generate a number $u_0$ from the uniform distribution over $[0, kq(z_0)]$.
  - If $u_0 > \tilde{p}(z_0)$ reject sample, otherwise accept.



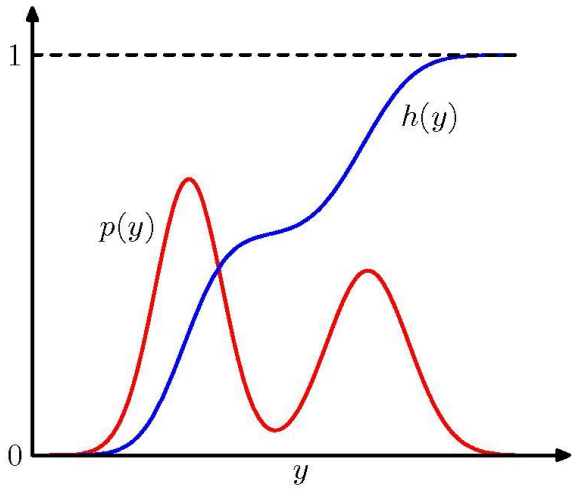
# Recap: Sampling from a pdf

- In general, assume we are given the pdf $p(\mathbf{x})$ and the corresponding cumulative distribution:

$$F(x) = \int_{-\infty}^{x} p(z)dz$$

- To draw samples from this pdf, we can invert the cumulative distribution function:

$$u \sim Uniform(0,1) \Rightarrow F^{-1}(u) \sim p(x)$$






Slide credit: Bernt Schiele





Image source: C.M. Bishop, 2006

# Recap: Importance Sampling

- Approach
  - Approximate expectations directly
    (but does not enable to draw samples from $p(\mathbf{z})$ directly).
  - Goal: $$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z}$$
- Idea
  - Use a proposal distribution $q(\mathbf{z})$ from which it is easy to sample.
  - Express expectations in the form of a finite sum over samples $\{\mathbf{z}^{(l)}\}$ drawn from $q(\mathbf{z})$.

$$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z} = \int f(\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}q(\mathbf{z})d\mathbf{z}$$

$$\simeq \frac{1}{L}\sum_{l=1}^{L}\underbrace{\frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}}f(\mathbf{z}^{(l)})$$

Importance weights

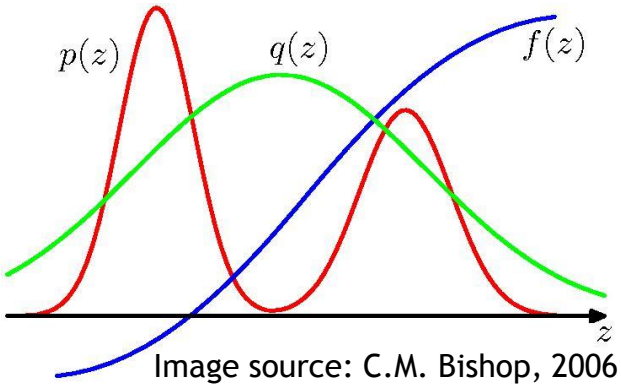



Image source: C.M. Bishop, 2006



Slide adapted from Bernt Schiele

# Recap: Sampling-Importance-Resampling

- Motivation: Avoid having to determine the constant $k$.
- Two stages
  - Draw L samples $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(L)}$ from $q(\mathbf{z})$.
  - Construct weights using importance weighting

$$w_l = \frac{\tilde{r}_l}{\sum_m \tilde{r}_m} = \frac{\frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}}{\sum_m \frac{\tilde{p}(\mathbf{z}^{(m)})}{\tilde{q}(\mathbf{z}^{(m)})}}$$

    and draw a second set of samples $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(L)}$ with probabilities given by the weights $w^{(1)}, \ldots, w^{(L)}$.

- Result
  - The resulting $L$ samples are only approximately distributed according to $p(\mathbf{z})$, but the distribution becomes correct in the limit $L \to \infty$.

# Recap: MCMC – Markov Chain Monte Carlo

- Overview
  - Allows to sample from a large class of distributions.
  - Scales well with the dimensionality of the sample space.
- Idea
  - We maintain a record of the current state $\mathbf{z}^{(\tau)}$
  - The proposal distribution depends on the current state: $q(\mathbf{z} \mid \mathbf{z}^{(\tau)})$
  - The sequence of samples forms a Markov chain $\mathbf{z}^{(1)}$, $\mathbf{z}^{(2)}$,...
- Approach
  - At each time step, we generate a candidate sample from the proposal distribution and accept the sample according to a criterion.
  - Different variants of MCMC for different criteria.

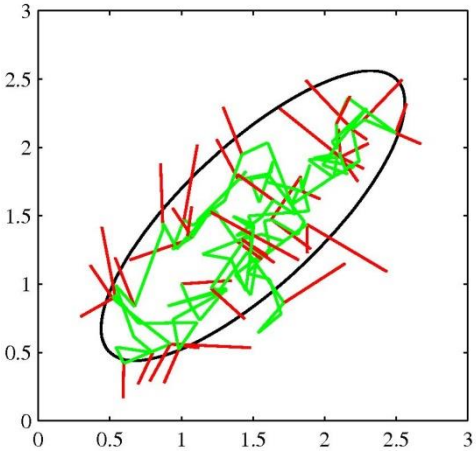



Image source: C.M. Bishop, 2006

# Recap: Markov Chains – Properties

- **Invariant distribution**
  - A distribution is said to be invariant (or stationary) w.r.t. a Markov chain if each step in the chain leaves that distribution invariant.
  - Transition probabilities:

$$T\left(\mathbf{z}^{(m)}, \mathbf{z}^{(m+1)}\right) = p\left(\mathbf{z}^{(m+1)} | \mathbf{z}^{(m)}\right)$$

  - For homogeneous Markov chain, distribution $p^*(\mathbf{z})$ is invariant if:

$$p^\star(\mathbf{z}) = \sum_{\mathbf{z}'} T\left(\mathbf{z}', \mathbf{z}\right) p^\star(\mathbf{z}')$$

- **Detailed balance**
  - Sufficient (but not necessary) condition to ensure that a distribution is invariant:

$$p^\star(\mathbf{z}) T\left(\mathbf{z}, \mathbf{z}'\right) = p^\star(\mathbf{z}') T\left(\mathbf{z}', \mathbf{z}\right)$$

  - A Markov chain which respects *detailed balance* is reversible.



Slide credit: Bernt Schiele

# Recap: Detailed Balance

- **Detailed balance means**
  - If we pick a state from the target distribution $p(\mathbf{z})$ and make a transition under $T$ to another state, it is just as likely that we will pick $\mathbf{z}_A$ and go from $\mathbf{z}_A$ to $\mathbf{z}_B$ than that we will pick $\mathbf{z}_B$ and go from $\mathbf{z}_B$ to $\mathbf{z}_A$.
  - It can easily be seen that a transition probability that satisfies detailed balance w.r.t. a particular distribution will leave that distribution invariant, because

$$\begin{aligned}\sum_{\mathbf{z}'} p^\star(\mathbf{z}')T(\mathbf{z}',\mathbf{z}) &= \sum_{\mathbf{z}'} p^\star(\mathbf{z})T(\mathbf{z},\mathbf{z}') \\ &= p^\star(\mathbf{z})\sum_{\mathbf{z}'} p(\mathbf{z}'|\mathbf{z}) = p^\star(\mathbf{z})\end{aligned}$$

# Recap: MCMC – Metropolis Algorithm

- **Metropolis** algorithm [Metropolis et al., 1953]
  - Proposal distribution is symmetric: $q(\mathbf{z}_A|\mathbf{z}_B) = q(\mathbf{z}_B|\mathbf{z}_A)$
  - The new candidate sample $\mathbf{z}^*$ is accepted with probability

$$A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{p}(\mathbf{z}^\star)}{\tilde{p}(\mathbf{z}^{(\tau)})}\right)$$

  ⇒ New candidate samples always accepted if $\tilde{p}(\mathbf{z}^\star) \geq \tilde{p}(\mathbf{z}^{(\tau)})$.
  - The algorithm sometimes accepts a state with lower probability.

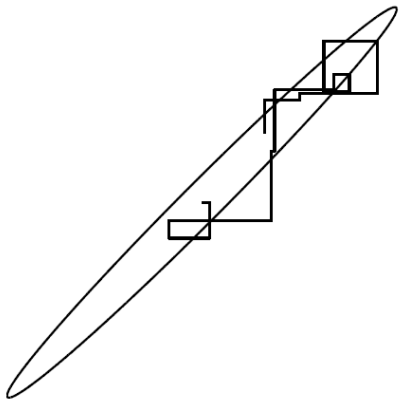
- **Metropolis-Hastings** algorithm
  - Generalization: Proposal distribution not necessarily symmetric.
  - The new candidate sample $\mathbf{z}^*$ is accepted with probability

$$A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{p}(\mathbf{z}^\star) q_k(\mathbf{z}^{(\tau)}|\mathbf{z}^\star)}{\tilde{p}(\mathbf{z}^{(\tau)}) q_k(\mathbf{z}^\star|\mathbf{z}^{(\tau)})}\right)$$

  - where $k$ labels the members of the set of considered transitions.

# Recap: Gibbs Sampling

- Approach
  - MCMC-algorithm that is simple and widely applicable.
  - May be seen as a special case of Metropolis-Hastings.
- Idea
  - Sample variable-wise: replace $\mathbf{z}_i$ by a value drawn from the distribution $p(z_i | \mathbf{z}_{\setminus i})$.
    - This means we update one coordinate at a time.
  - Repeat procedure either by cycling through all variables or by choosing the next variable.
- Properties
  - The algorithm always accepts!
  - Completely parameter free.
  - Can also be applied to subsets of variables.





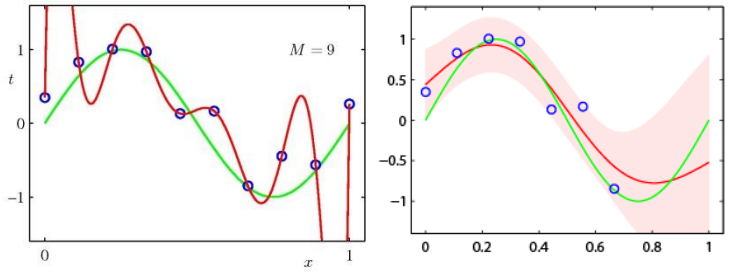
Slide adapted from Bernt Schiele

# This Lecture: *Advanced Machine Learning*

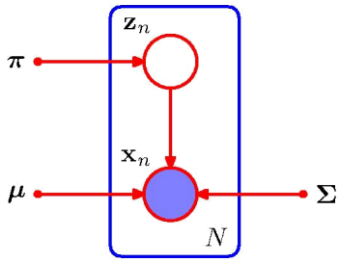


- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

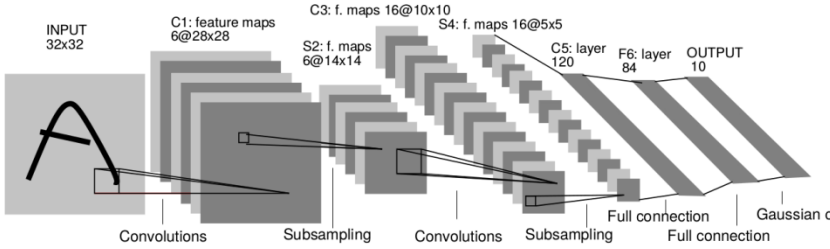
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC




- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Linear Discriminant Functions

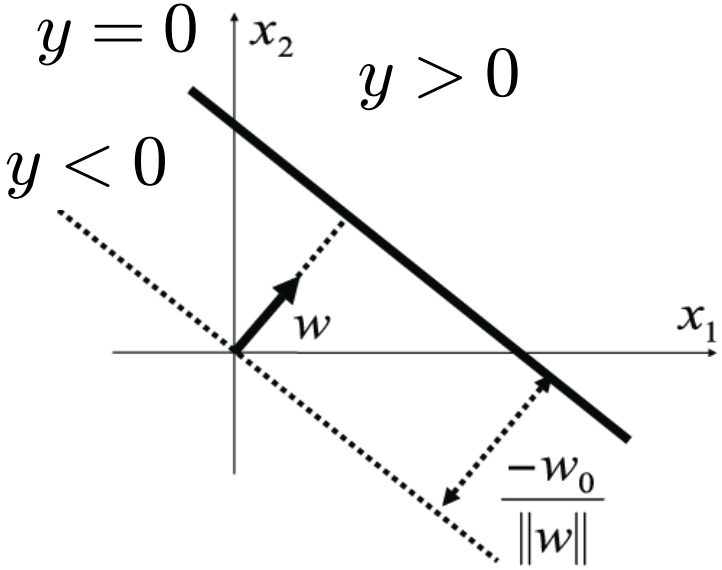
- **Basic idea**
  - Directly encode decision boundary
  - Minimize misclassification probability directly.

- **Linear discriminant functions**

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

weight vector

"bias" (= threshold)




  - $\mathbf{w}$, $w_0$ define a hyperplane in $\mathbb{R}^D$.
  - If a data set can be perfectly classified by a linear discriminant, then we call it linearly separable.

# Recap: Generalized Linear Discriminants

- Extension with non-linear basis functions
  - Transform vector $\mathbf{x}$ with $M$ nonlinear basis functions $\phi_j(\mathbf{x})$:

$$y_k(\mathbf{x}) = g\left(\sum_{j=1}^{M} w_{kj}\phi_j(\mathbf{x}) + w_{k0}\right)$$

  - Basis functions $\phi_j(\mathbf{x})$ allow non-linear decision boundaries.
  - Activation function $g(\cdot)$ bounds the influence of outliers.
  - Disadvantage: minimization no longer in closed form.

- Notation

$$y_k(\mathbf{x}) = g\left(\sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})\right) \qquad \text{with } \phi_0(\mathbf{x}) = 1$$

# Recap: Gradient Descent

- Iterative minimization
  - Start with an initial guess for the parameter values $w_{kj}^{(0)}$.
  - Move towards a (local) minimum by following the gradient.
- Basic strategies
  - "Batch learning"

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

  - "Sequential updating"

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

where $$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

# Recap: Gradient Descent

- Example: Quadratic error function

$$E(\mathbf{w}) = \sum_{n=1}^{N} \left( y(\mathbf{x}_n; \mathbf{w}) - \mathbf{t}_n \right)^2$$

- Sequential updating leads to delta rule (=LMS rule)

$$\begin{aligned} w_{kj}^{(\tau+1)} &= w_{kj}^{(\tau)} - \eta \left( y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn} \right) \phi_j(\mathbf{x}_n) \\ &= w_{kj}^{(\tau)} - \eta \delta_{kn} \phi_j(\mathbf{x}_n) \end{aligned}$$

  - where

$$\delta_{kn} = y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn}$$

⇒ Simply feed back the input data point, weighted by the classification error.

# Recap: Probabilistic Discriminative Models

- Consider models of the form

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = y(\boldsymbol{\phi}) = \sigma(\mathrm{w}^T\boldsymbol{\phi})$$

with $$p(\mathcal{C}_2|\boldsymbol{\phi}) = 1 - p(\mathcal{C}_1|\boldsymbol{\phi})$$

- This model is called **logistic regression**.

- Properties
  - Probabilistic interpretation
  - But discriminative method: only focus on decision hyperplane
  - Advantageous for high-dimensional spaces, requires less parameters than explicitly modeling $p(\boldsymbol{\phi}|\mathcal{C}_k)$ and $p(\mathcal{C}_k)$.

# Recap: Logistic Sigmoid

- **Properties**
  - **Definition:** $\sigma(a) = \frac{1}{1 + \exp(-a)}$
  - **Inverse:** $a = \ln\left(\frac{\sigma}{1-\sigma}\right)$ **"logit" function**
  - **Symmetry property:**
    $$\sigma(-a) = 1 - \sigma(a)$$
  - **Derivative:** $\frac{d\sigma}{da} = \sigma(1-\sigma)$

# Recap: Logistic Regression

- Let's consider a data set $\{\phi_n, t_n\}$ with $n = 1, \ldots, N$, where $\phi_n = \phi(\mathbf{x}_n)$ and $t_n \in \{0, 1\}$, $\mathbf{t} = (t_1, \ldots, t_N)^T$.

- With $y_n = p(\mathcal{C}_1|\phi_n)$, we can write the likelihood as

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} \{1 - y_n\}^{1-t_n}$$

- Define the error function as the negative log-likelihood

$$\begin{aligned} E(\mathbf{w}) &= -\ln p(\mathbf{t}|\mathbf{w}) \\ &= -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\} \end{aligned}$$

  - This is the so-called cross-entropy error function.

# Recap: Gradient of the Error Function

- Gradient for logistic regression

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n)\boldsymbol{\phi}_n$$

- This is the same result as for the Delta (=LMS) rule

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta(y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn})\phi_j(\mathbf{x}_n)$$

- We can use this to derive a sequential estimation algorithm.
  - However, this will be quite slow…
  - More efficient to use 2nd-order Newton-Raphson ⇒ IRLS

# Recap: Iteratively Reweighted Least Squares

- Result of applying Newton-Raphson to logistic regression

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - (\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi})^{-1}\mathbf{\Phi}^T(\mathbf{y}-\mathbf{t})$$

$$= (\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi})^{-1}\left\{\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi}\mathbf{w}^{(\tau)} - \mathbf{\Phi}^T(\mathbf{y}-\mathbf{t})\right\}$$

$$= (\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{R}\mathbf{z}$$

$$\text{with} \quad \mathbf{z} = \mathbf{\Phi}\mathbf{w}^{(\tau)} - \mathbf{R}^{-1}(\mathbf{y}-\mathbf{t})$$

- Very similar form to pseudo-inverse (normal equations)
  - But now with non-constant weighing matrix $\mathbf{R}$ (depends on $\mathbf{w}$).
  - Need to apply normal equations iteratively.

$\Rightarrow$ Iteratively Reweighted Least-Squares (IRLS)

# Recap: Softmax Regression

- Multi-class generalization of logistic regression
  - In logistic regression, we assumed binary labels $t_n \in \{0, 1\}$
  - Softmax generalizes this to $K$ values in 1-of-$K$ notation.

$$\mathbf{y}(\mathbf{x}; \mathbf{w}) = \begin{bmatrix} P(y=1|\mathbf{x}; \mathbf{w}) \\ P(y=2|\mathbf{x}; \mathbf{w}) \\ \vdots \\ P(y=K|\mathbf{x}; \mathbf{w}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x})} \begin{bmatrix} \exp(\mathbf{w}_1^\top \mathbf{x}) \\ \exp(\mathbf{w}_2^\top \mathbf{x}) \\ \vdots \\ \exp(\mathbf{w}_K^\top \mathbf{x}) \end{bmatrix}$$

  - This uses the softmax function

$$\frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

  - Note: the resulting distribution is normalized.

# Recap: Softmax Regression Cost Function

- **Logistic regression**
  - Alternative way of writing the cost function

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$

$$= -\sum_{n=1}^{N}\sum_{k=0}^{1} \{\mathbb{I}(t_n = k)\ln P(y_n = k|\mathbf{x}_n;\mathbf{w})\}$$

- **Softmax regression**
  - Generalization to $K$ classes using indicator functions.

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} \left\{\mathbb{I}(t_n = k)\ln \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^{K}\exp(\mathbf{w}_j^\top \mathbf{x})}\right\}$$

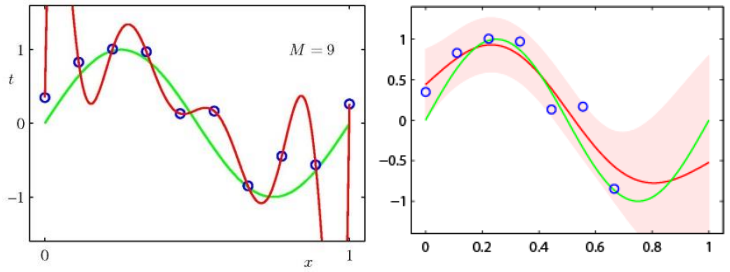
$$\nabla_{\mathbf{w}_k} E(\mathbf{w}) = -\sum_{n=1}^{N} [\mathbb{I}(t_n = k)\ln P(y_n = k|\mathbf{x}_n;\mathbf{w})]$$

# This Lecture: *Advanced Machine Learning*

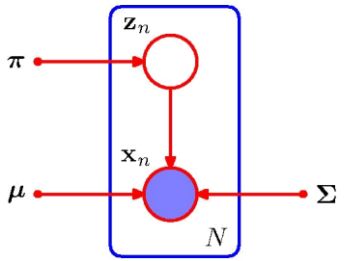


- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

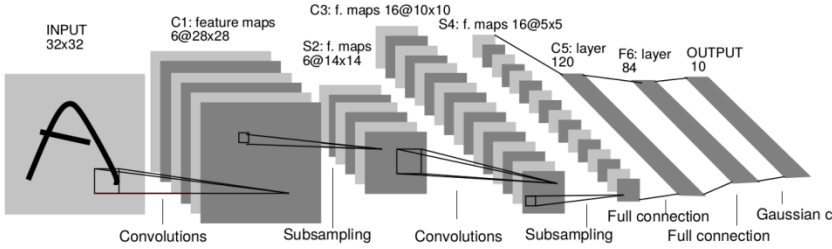
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC

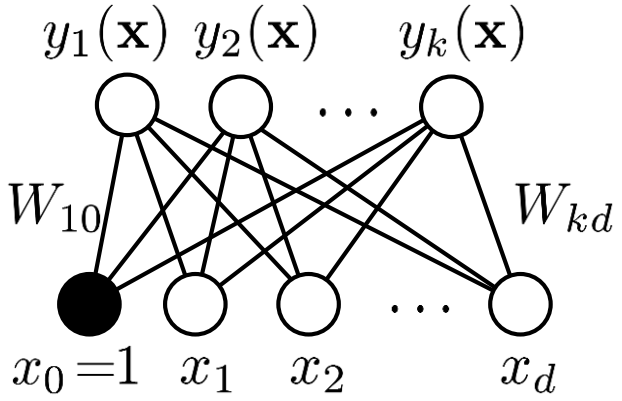



- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Perceptrons

- One output node per class




Output layer

*Weights*

Input layer

- Outputs
  - Linear outputs

$$y_k(\mathbf{x}) = \sum_{i=0}^{d} W_{ki} x_i$$

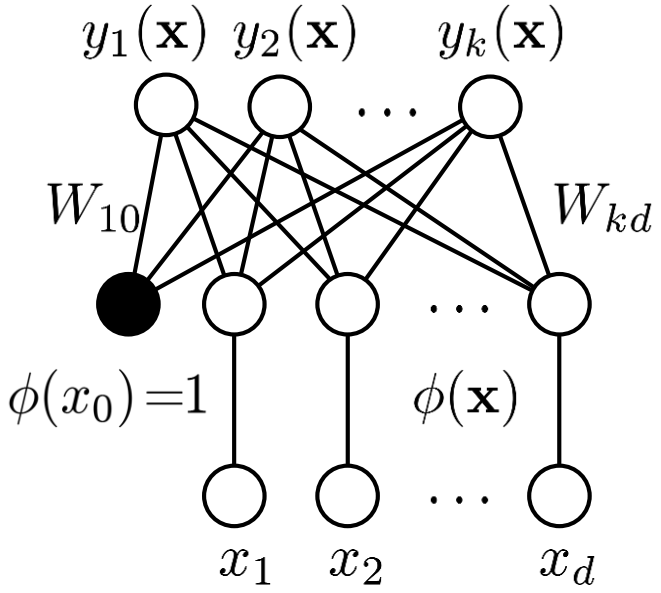
With output nonlinearity

$$y_k(\mathbf{x}) = g\left(\sum_{i=0}^{d} W_{ki} x_i\right)$$

$\Rightarrow$ Can be used to do multidimensional linear regression or multiclass classification.

# Recap: Non-Linear Basis Functions

- **Straightforward generalization**




Output layer

*Weights*

Feature layer

*Mapping (fixed)*

Input layer

- **Outputs**
  - **Linear outputs**

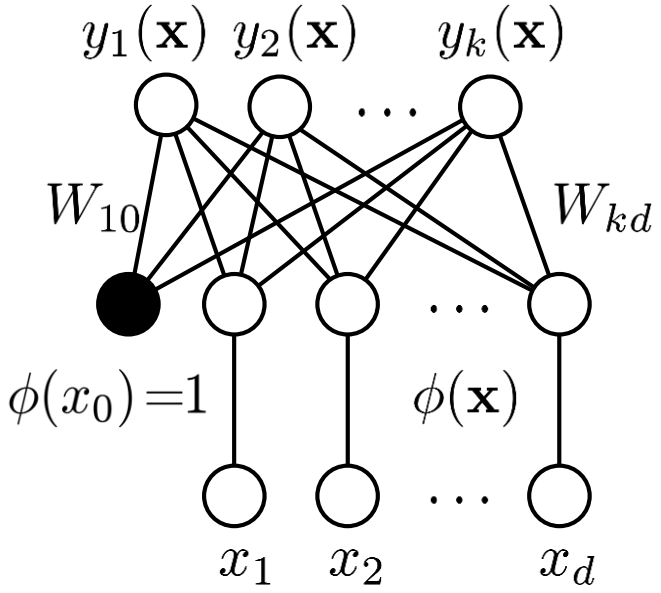
$$y_k(\mathbf{x}) = \sum_{i=0}^{d} W_{ki}\phi(x_i)$$

**with output nonlinearity**

$$y_k(\mathbf{x}) = g\left(\sum_{i=0}^{d} W_{ki}\phi(x_i)\right)$$

# Recap: Non-Linear Basis Functions

- Straightforward generalization




Output layer

*Weights*

Feature layer

*Mapping (fixed)*

Input layer

- Remarks
  - Perceptrons are generalized linear discriminants!
  - Everything we know about the latter can also be applied here.
  - Note: feature functions $\phi(\mathbf{x})$ are kept fixed, not learned!

# Recap: Perceptron Learning

- Process the training cases in some permutation
  - If the output unit is correct, leave the weights alone.
  - If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
  - If the output unit incorrectly outputs a one, subtract the input vector from the weight vector.
- Translation

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left( y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn} \right) \phi_j(\mathbf{x}_n)$$

  - This is the Delta rule a.k.a. LMS rule!

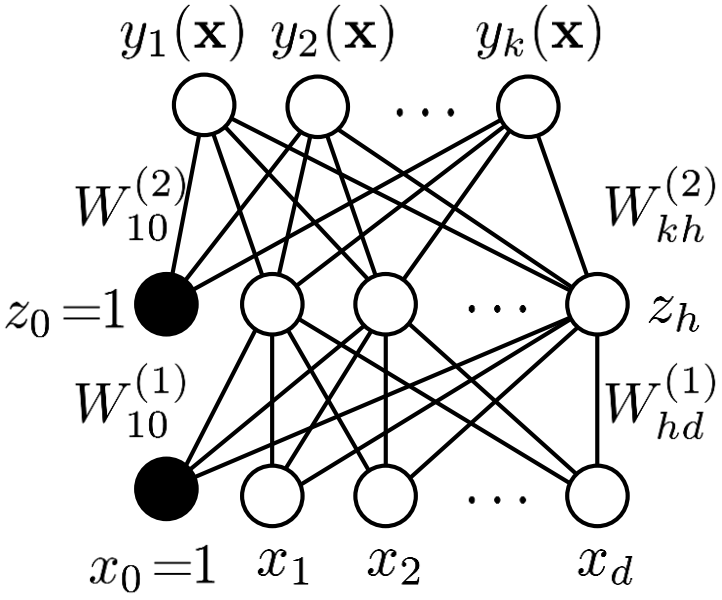
$\Rightarrow$ Perceptron Learning corresponds to 1st-order (stochastic) Gradient Descent of a quadratic error function!

# Recap: Loss Functions

- We can now also apply other loss functions
  - $L_2$ loss ⇒ Least-squares regression
    $$L(t, y(\mathbf{x})) = \sum_n (y(\mathbf{x}_n) - t_n)^2$$
  - $L_1$ loss: ⇒ Median regression
    $$L(t, y(\mathbf{x})) = \sum_n |y(\mathbf{x}_n) - t_n|$$
  - Cross-entropy loss ⇒ Logistic regression
    $$L(t, y(\mathbf{x})) = -\sum_n \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$
  - Hinge loss ⇒ SVM classification
    $$L(t, y(\mathbf{x})) = \sum_n [1 - t_n y(\mathbf{x}_n)]_+$$
  - Softmax loss ⇒ Multi-class probabilistic classification
    $$L(t, y(\mathbf{x})) = -\sum_n \sum_k \left\{ \mathbb{I}(t_n = k) \ln \frac{\exp(y_k(\mathbf{x}))}{\sum_j \exp(y_j(\mathbf{x}))} \right\}$$

# Recap: Multi-Layer Perceptrons

- **Adding more layers**




**Output layer**

**Hidden layer**

**Input layer**

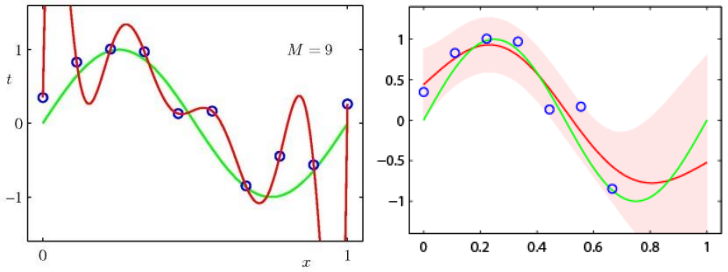
- **Output**

$$y_k(\mathbf{x}) = g^{(2)}\left(\sum_{i=0}^{h} W_{ki}^{(2)} g^{(1)}\left(\sum_{j=0}^{d} W_{ij}^{(1)} x_j\right)\right)$$

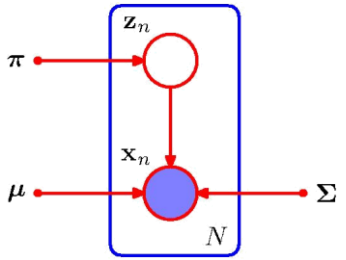
# This Lecture: *Advanced Machine Learning*

- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

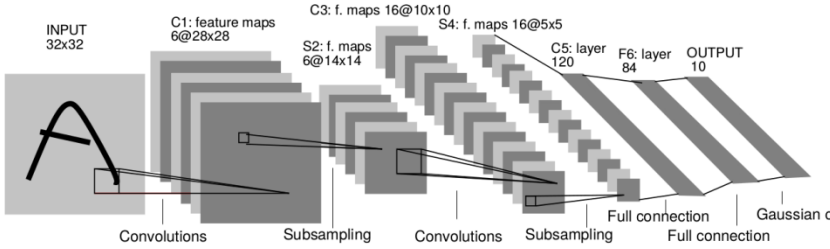
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC




- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Learning with Hidden Units

- How can we train multi-layer networks efficiently?
  - Need an efficient way of adapting all weights, not just the last layer.

- Idea: Gradient Descent
  - Set up an error function

$$E(\mathbf{W}) = \sum_n L(t_n, y(\mathbf{x}_n; \mathbf{W})) + \lambda \Omega(\mathbf{W})$$

with a loss $L(\cdot)$ and a regularizer $\Omega(\cdot)$.

  - E.g., $L(t, y(\mathbf{x}; \mathbf{W})) = \sum_n (y(\mathbf{x}_n; \mathbf{W}) - t_n)^2$ — $L_2$ loss

$$\Omega(\mathbf{W}) = ||\mathbf{W}||_F^2$$

$L_2$ regularizer ("weight decay")

$\Rightarrow$ Update each weight $W_{ij}^{(k)}$ in the direction of the gradient $\frac{\partial E(\mathbf{W})}{\partial W_{ij}^{(k)}}$

# Recap: Gradient Descent

- Two main steps
  1. Computing the gradients for each weight
  2. Adjusting the weights in the direction of the gradient

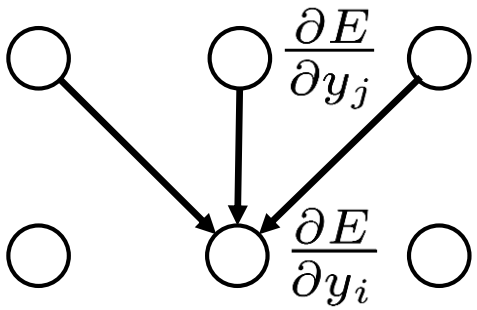
- We consider those two steps separately
  - Computing the gradients: Backpropagation
  - Adjusting the weights: Optimization techniques

# Recap: Backpropagation Algorithm

- **Core steps**
  1. **Convert the discrepancy between each output and its target value into an error derivate.**
  2. **Compute error derivatives in each hidden layer from error derivatives in the layer above.**
  3. **Use error derivatives *w.r.t.* activities to get error derivatives *w.r.t.* the incoming weights**

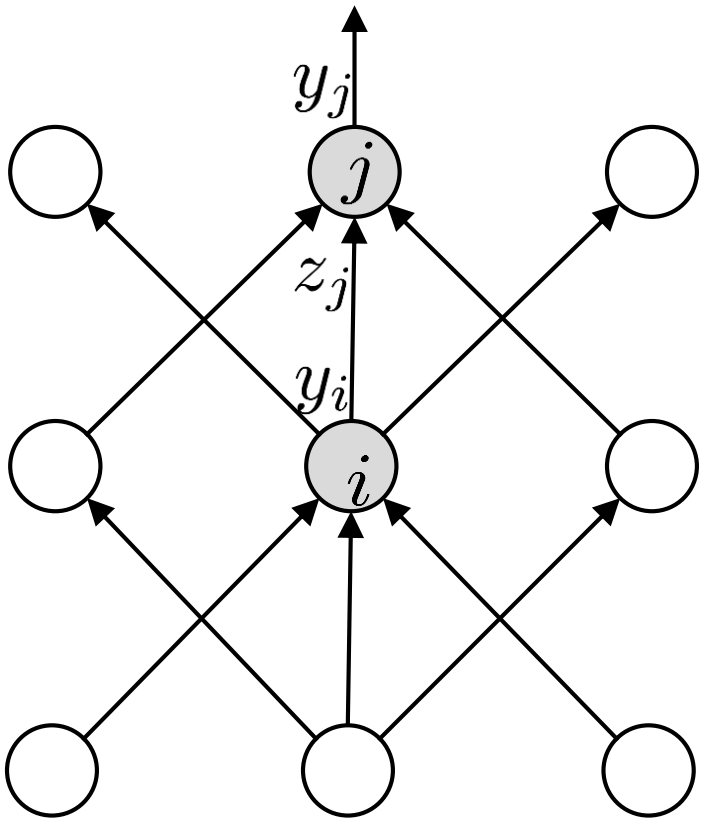
$$E = \frac{1}{2} \sum_{j \in output} (t_j - y_j)^2$$

$$\frac{\partial E}{\partial y_j} = -(t_j - y_j)$$




$$\frac{\partial E}{\partial y_j} \longrightarrow \frac{\partial E}{\partial w_{ik}}$$

# Recap: Backpropagation Algorithm




$$\frac{\partial E}{\partial z_j} = \frac{\partial y_j}{\partial z_j}\frac{\partial E}{\partial y_j} = y_j(1-y_j)\frac{\partial E}{\partial y_j}$$

$$\frac{\partial E}{\partial y_i} = \sum_j \frac{\partial z_j}{\partial y_i}\frac{\partial E}{\partial z_j} = \sum_j w_{ij}\frac{\partial E}{\partial z_j}$$

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}}\frac{\partial E}{\partial z_j} = y_i\frac{\partial E}{\partial z_j}$$

- **Efficient propagation scheme**
  - $y_i$ **is already known from forward pass! (Dynamic Programming)**

  $\Rightarrow$ **Propagate back the gradient from layer** $j$ **and multiply with** $y_i$**.**

# Recap: MLP Backpropagation Algorithm

- **Forward Pass**

$$\mathbf{y}^{(0)} = \mathbf{x}$$

$$\text{for } k = 1, \ldots, l \text{ do}$$

$$\mathbf{z}^{(k)} = \mathbf{W}^{(k)} \mathbf{y}^{(k-1)}$$

$$\mathbf{y}^{(k)} = g_k(\mathbf{z}^{(k)})$$

$$\text{endfor}$$

$$\mathbf{y} = \mathbf{y}^{(l)}$$

$$E = L(\mathbf{t}, \mathbf{y}) + \lambda \Omega(\mathbf{W})$$

- **Backward Pass**

$$\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{y}} = \frac{\partial}{\partial \mathbf{y}} L(\mathbf{t}, \mathbf{y}) + \lambda \frac{\partial}{\partial \mathbf{y}} \Omega$$

$$\text{for } k = l, l\text{-}1, \ldots, 1 \text{ do}$$

$$\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{z}^{(k)}} = \mathbf{h} \odot g'(\mathbf{y}^{(k)})$$

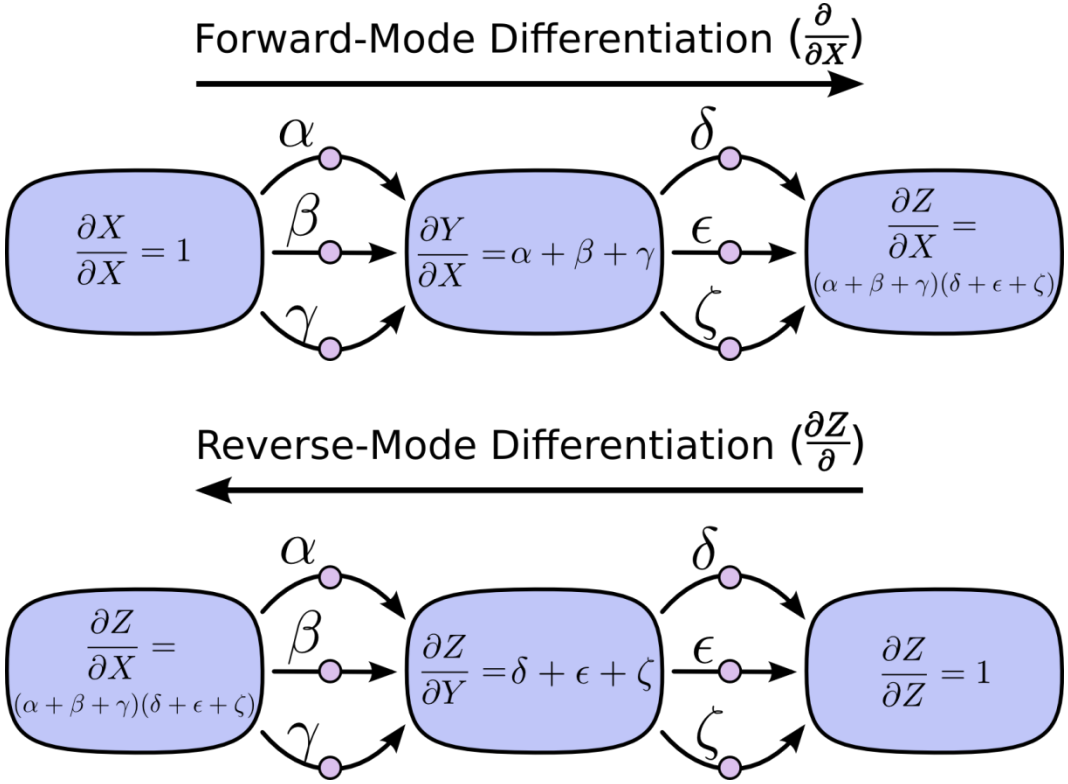
$$\frac{\partial E}{\partial \mathbf{W}^{(k)}} = \mathbf{h} \mathbf{y}^{(k-1)\top} + \lambda \frac{\partial \Omega}{\partial \mathbf{W}^{(k)}}$$

$$\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{y}^{(k-1)}} = \mathbf{W}^{(k)\top} \mathbf{h}$$

$$\text{endfor}$$

- **Notes**
  - For efficiency, an entire batch of data $\mathbf{X}$ is processed at once.
  - $\odot$ denotes the element-wise product

# Recap: Computational Graphs




Apply operator $\frac{\partial}{\partial X}$ to every node.

Apply operator $\frac{\partial Z}{\partial}$ to every node.

- Forward differentiation needs one pass per node. Reverse-mode differentiation can compute all derivatives in one single pass.

$\Rightarrow$ Speed-up in $\mathcal{O}(\#\text{inputs})$ compared to forward differentiation!

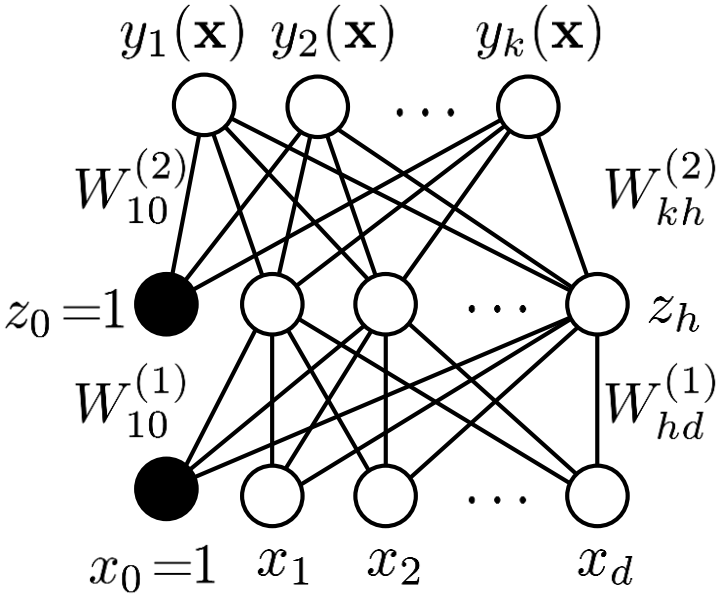


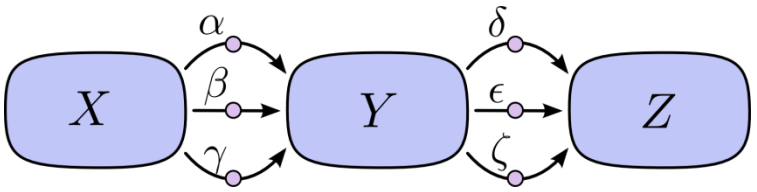
Slide inspired by Christopher Olah

Image source: Christopher Olah, colah.github.io

# Recap: Automatic Differentiation

- Approach for obtaining the gradients




  - Convert the network into a computational graph.
  - Each new layer/module just needs to specify how it affects the forward and backward passes.
  - Apply reverse-mode differentiation.

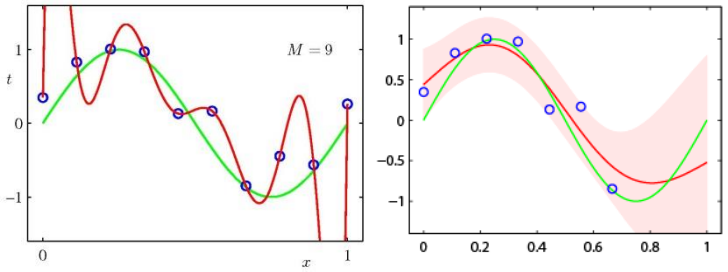
$\Rightarrow$ Very general algorithm, used in today's Deep Learning packages


Image source: Christopher Olah, colah.github.io

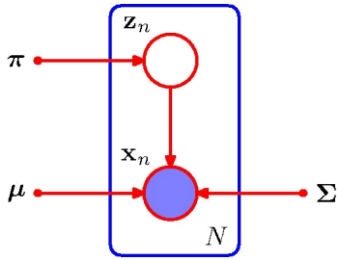
# This Lecture: *Advanced Machine Learning*

- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

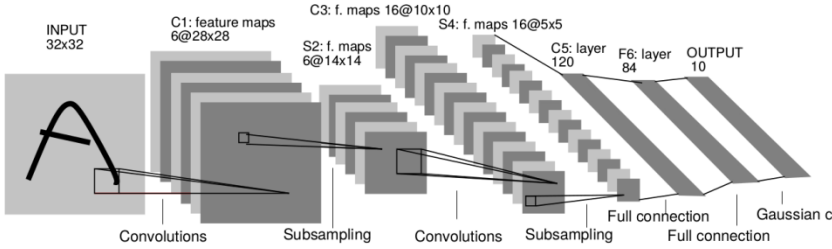
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC

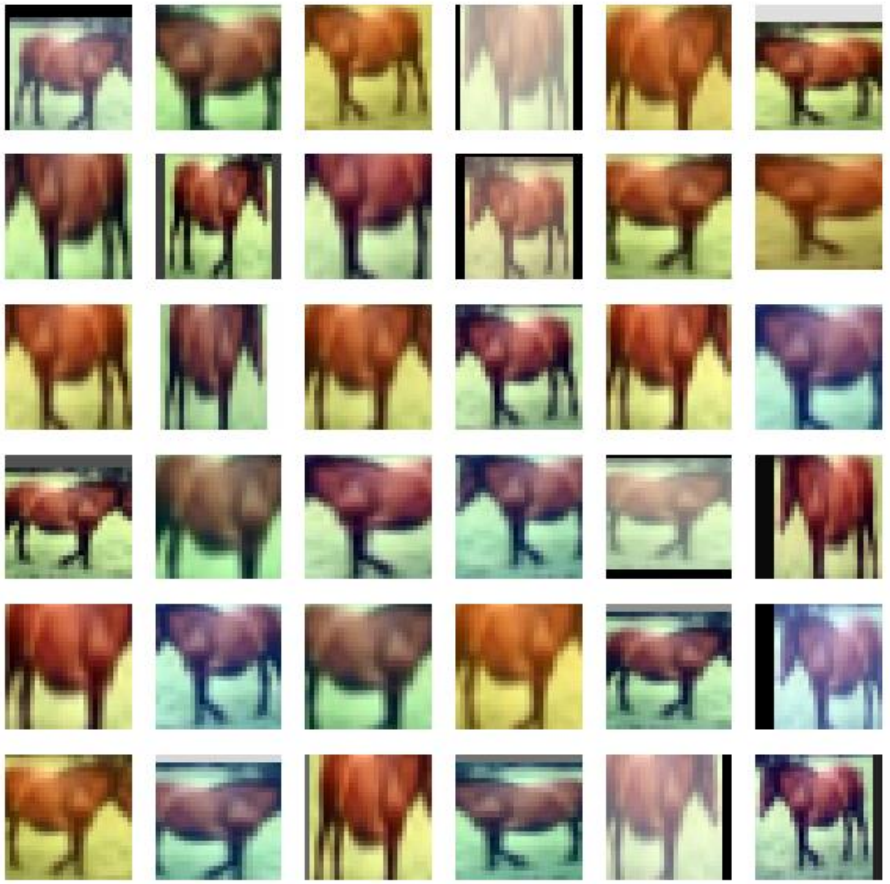



- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Data Augmentation

- Effect
  - Much larger training set
  - Robustness against expected variations
- During testing
  - When cropping was used during training, need to again apply crops to get same image size.
  - Beneficial to also apply flipping during test.
  - Applying several ColorPCA variations can bring another ~1% improvement, but at a significantly increased runtime.

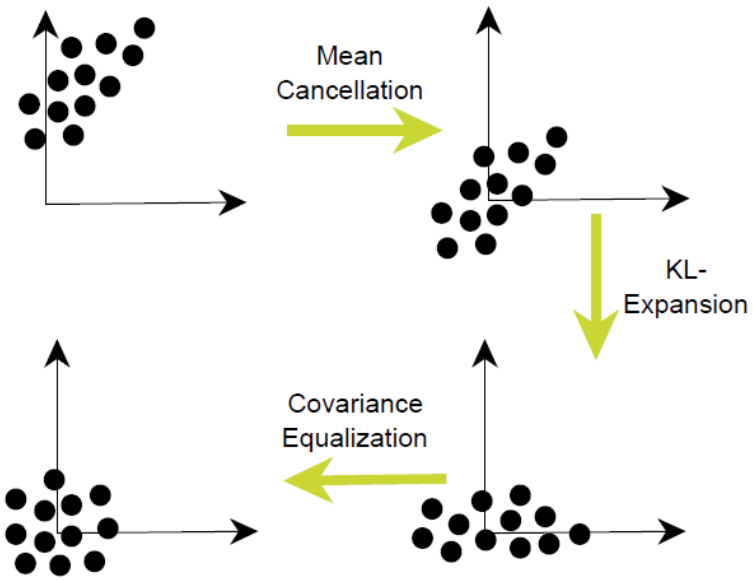


Augmented training data (from one original image)


Image source: Lucas Beyer

# Recap: Normalizing the Inputs

- Convergence is fastest if
  - The mean of each input variable over the training set is zero.
  - The inputs are scaled such that all have the same covariance.
  - Input variables are uncorrelated if possible.



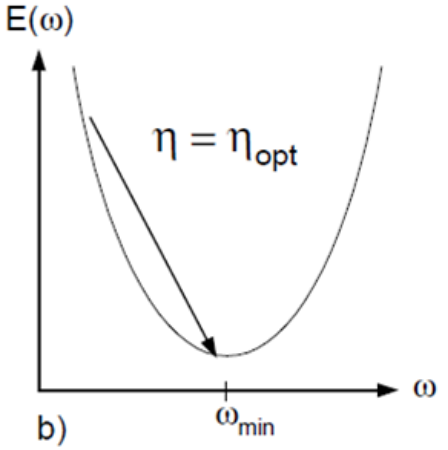

- Advisable normalization steps (for MLPs)
  - Normalize all inputs that an input unit sees to zero-mean, unit covariance.
  - If possible, try to decorrelate them using PCA (also known as Karhunen-Loeve expansion).


Image source: Yann LeCun et al., Efficient BackProp (1998)

# Recap: Choosing the Right Learning Rate

- Convergence of Gradient Descent
  - Simple 1D example

$$W^{(\tau-1)} = W^{(\tau)} - \eta \frac{\mathrm{d}E(W)}{\mathrm{d}W}$$




  - What is the optimal learning rate $\eta_{\mathrm{opt}}$?
  - If $E$ is quadratic, the optimal learning rate is given by the inverse of the Hessian

$$\eta_{\mathrm{opt}} = \left( \frac{\mathrm{d}^2 E(W^{(\tau)})}{\mathrm{d}W^2} \right)^{-1}$$

  - Advanced optimization techniques try to approximate the Hessian by a simplified form.
  - *If we exceed the optimal learning rate, bad things happen!*

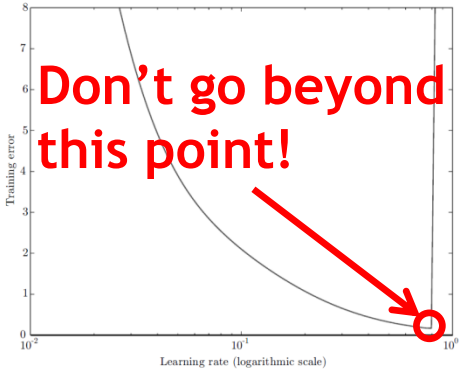
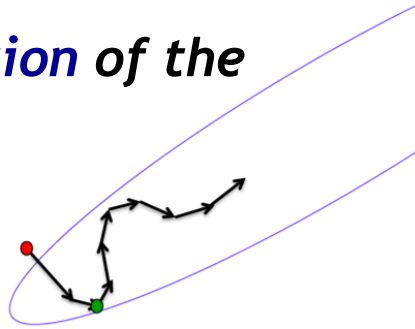




Image source: Yann LeCun et al., Efficient BackProp (1998)

# Recap: Advanced Optimization Techniques

- Momentum
  - *Instead of using the gradient to change the position of the weight "particle", use it to change the velocity.*
  - Effect: dampen oscillations in directions of high curvature



  - Nesterov-Momentum: Small variation in the implementation
- RMS-Prop
  - *Separate learning rate for each weight: Divide the gradient by a running average of its recent magnitude.*
- AdaGrad
- AdaDelta
- Adam

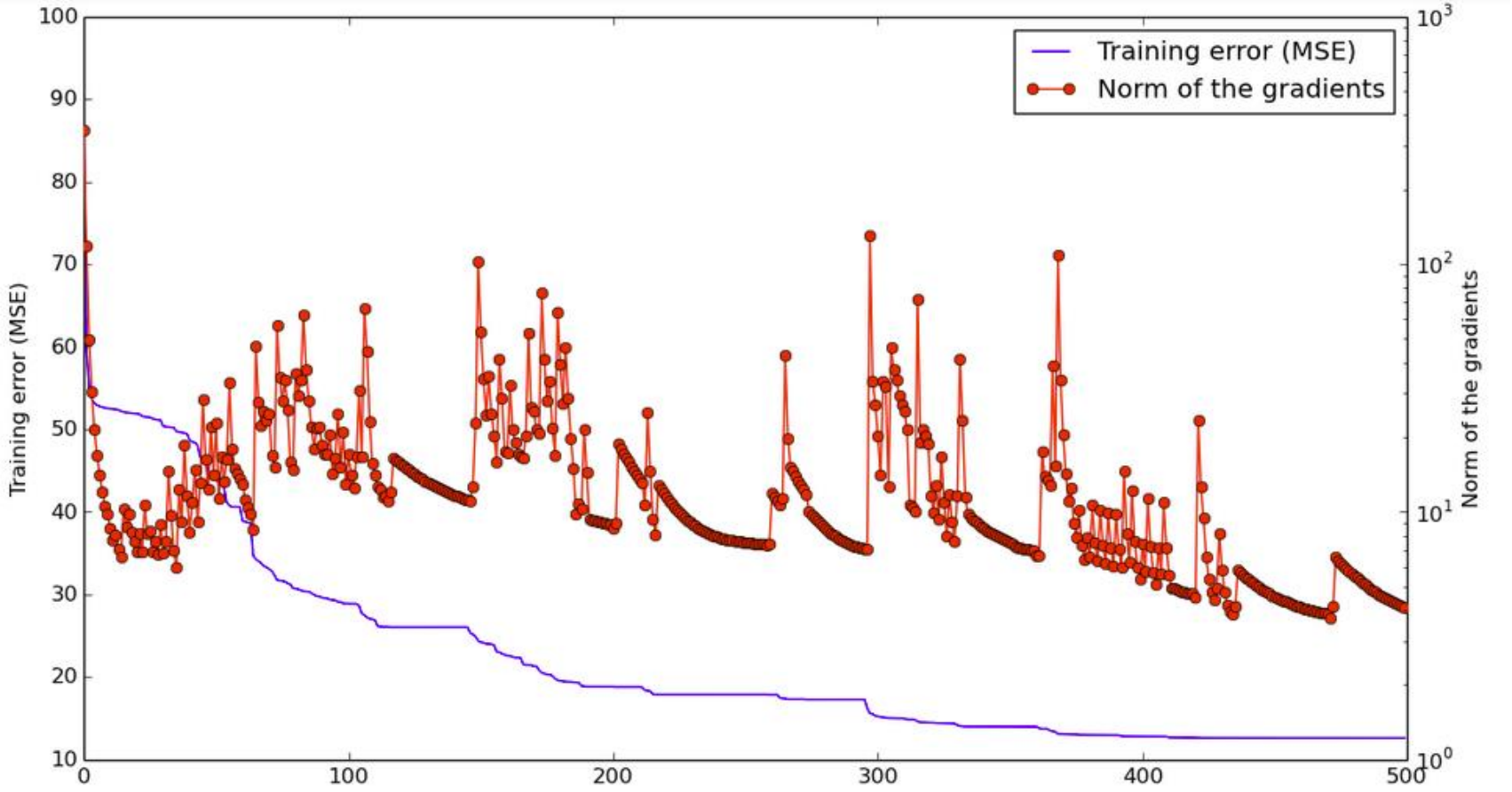
} Some more recent techniques, work better for some problems. Try them.



Image source: Geoff Hinton

# Recap: Patience

- Saddle points dominate in high-dimensional spaces!

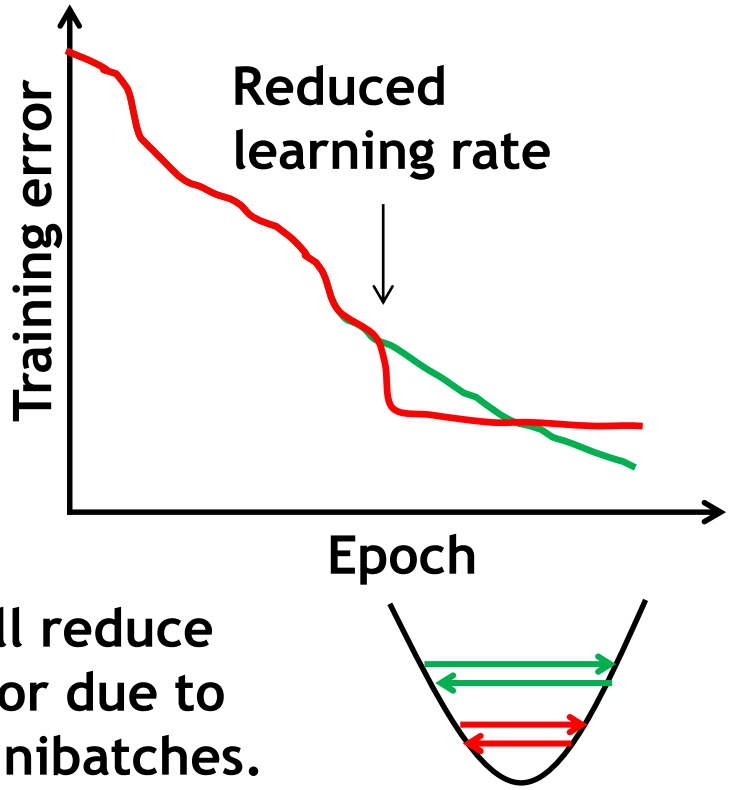



⇒ Learning often doesn't get stuck, you just may have to wait...


Image source: Yoshua Bengio

# Recap: Reducing the Learning Rate

- Final improvement step after convergence is reached
  - Reduce learning rate by a factor of 10.
  - Continue training for a few epochs.
  - Do this 1-3 times, then stop training.




- Effect
  - Turning down the learning rate will reduce the random fluctuations in the error due to different gradients on different minibatches.



- *Be careful: Do not turn down the learning rate too soon!*
  - Further progress will be much slower after that.

# Recap: Glorot Initialization [Glorot & Bengio, '10]

- **Variance of neuron activations**
  - Suppose we have an input $X$ with $n$ components and a linear neuron with random weights $W$ that spits out a number $Y$.
  - We *want the variance of the input and output of a unit to be the same*, therefore $n\ \mathrm{Var}(W_i)$ should be 1. This means

$$\mathrm{Var}(W_i) = \frac{1}{n} = \frac{1}{n_{\mathrm{in}}}$$

  - Or for the backpropagated gradient

$$\mathrm{Var}(W_i) = \frac{1}{n_{\mathrm{out}}}$$

  - As a compromise, Glorot & Bengio propose to use

$$\mathrm{Var}(W) = \frac{2}{n_{\mathrm{in}} + n_{\mathrm{out}}}$$

$\Rightarrow$ Randomly sample the weights with this variance. That's it.

# Recap: He Initialization

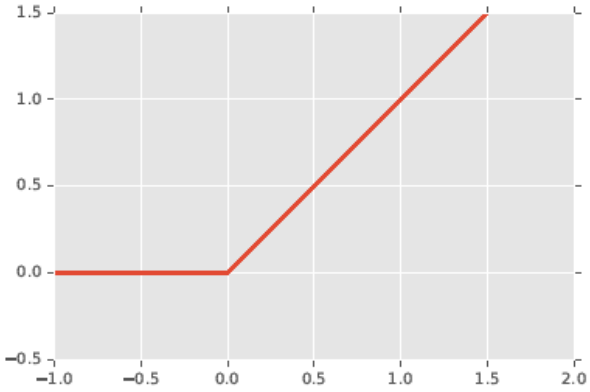
[He et al., '15]

- Extension of Glorot Initialization to ReLU units
  - Use Rectified Linear Units (ReLU)

$$g(a) = \max\{0, a\}$$

  - Effect: gradient is propagated with a constant factor

$$\frac{\partial g(a)}{\partial a} = \begin{cases} 1, & a > 0 \\ 0, & \text{else} \end{cases}$$




- Same basic idea: Output should have the input variance
  - However, the Glorot derivation was based on tanh units, linearity assumption around zero does not hold for ReLU.
  - He et al. made the derivations, proposed to use instead

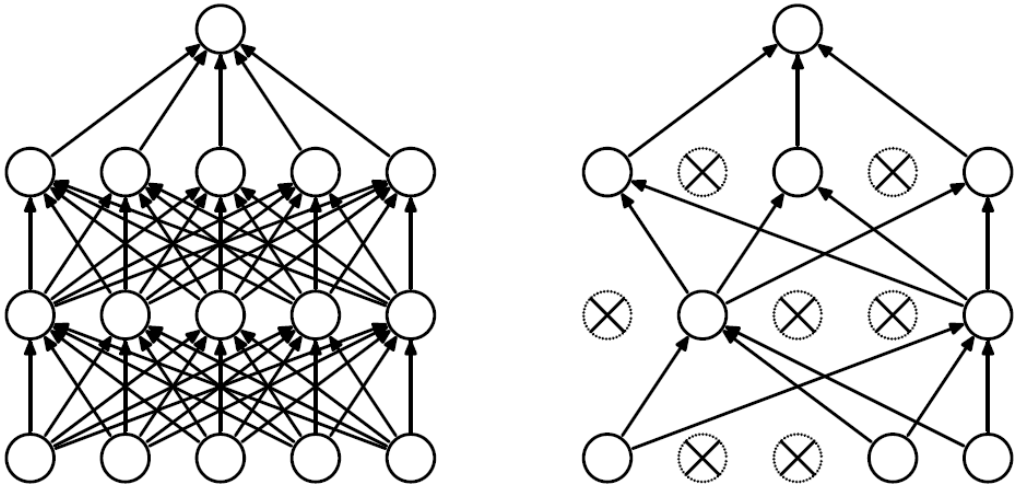
$$\mathrm{Var}(W) = \frac{2}{n_{\text{in}}}$$

# Recap: Batch Normalization [Ioffe & Szegedy '14]

- Motivation
  - Optimization works best if all inputs of a layer are normalized.
- Idea
  - Introduce intermediate layer that centers the activations of the previous layer per minibatch.
  - I.e., perform transformations on all activations and undo those transformations when backpropagating gradients
- Effect
  - Much improved convergence

# Recap: Dropout

[Srivastava, Hinton '12]



(a) Standard Neural Net (b) After applying dropout.

- Idea
  - Randomly switch off units during training.
  - Change network architecture for each data point, effectively training many different variants of the network.
  - When applying the trained network, multiply activations with the probability that the unit was set to zero.

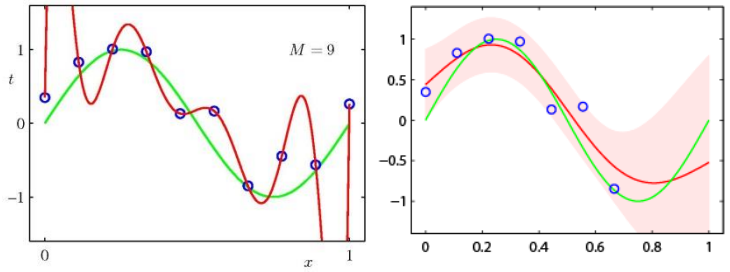
  ⇒ Greatly improved performance

# This Lecture: *Advanced Machine Learning*

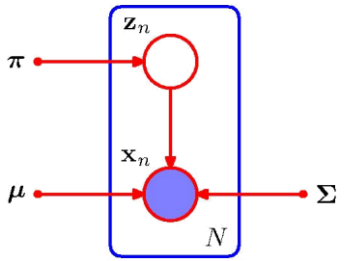


- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

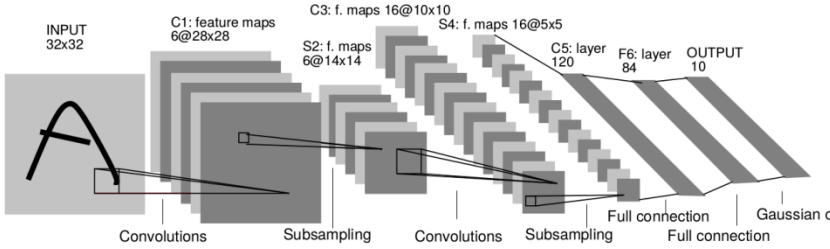
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- Approximate Inference
  - Sampling Approaches
  - MCMC




- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



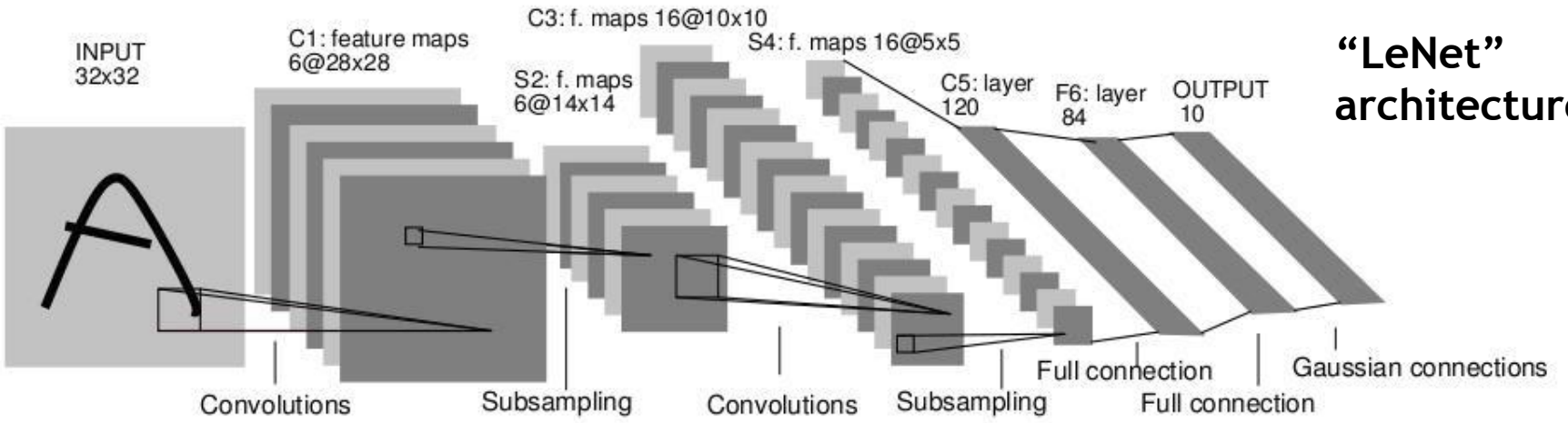
# Recap: ImageNet Challenge 2012

- ImageNet
  - ~14M labeled internet images
  - 20k classes
  - Human labels via Amazon Mechanical Turk


[Deng et al., CVPR'09]

- Challenge (ILSVRC)
  - 1.2 million training images
  - 1000 classes
  - Goal: Predict ground-truth class within top-5 responses
  - Currently one of the top benchmarks in Computer Vision

# Recap: Convolutional Neural Networks




"LeNet" architecture

- Neural network with specialized connectivity structure
  - Stack multiple stages of feature extractors
  - Higher stages compute more global, more invariant features
  - Classification layer at the end

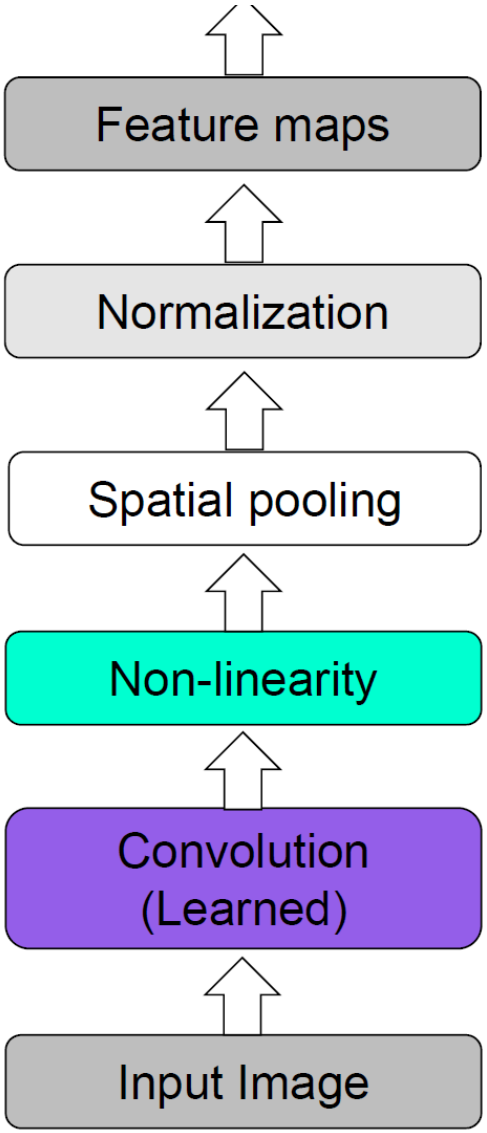
Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, Gradient-based learning applied to document recognition, Proceedings of the IEEE 86(11): 2278–2324, 1998.



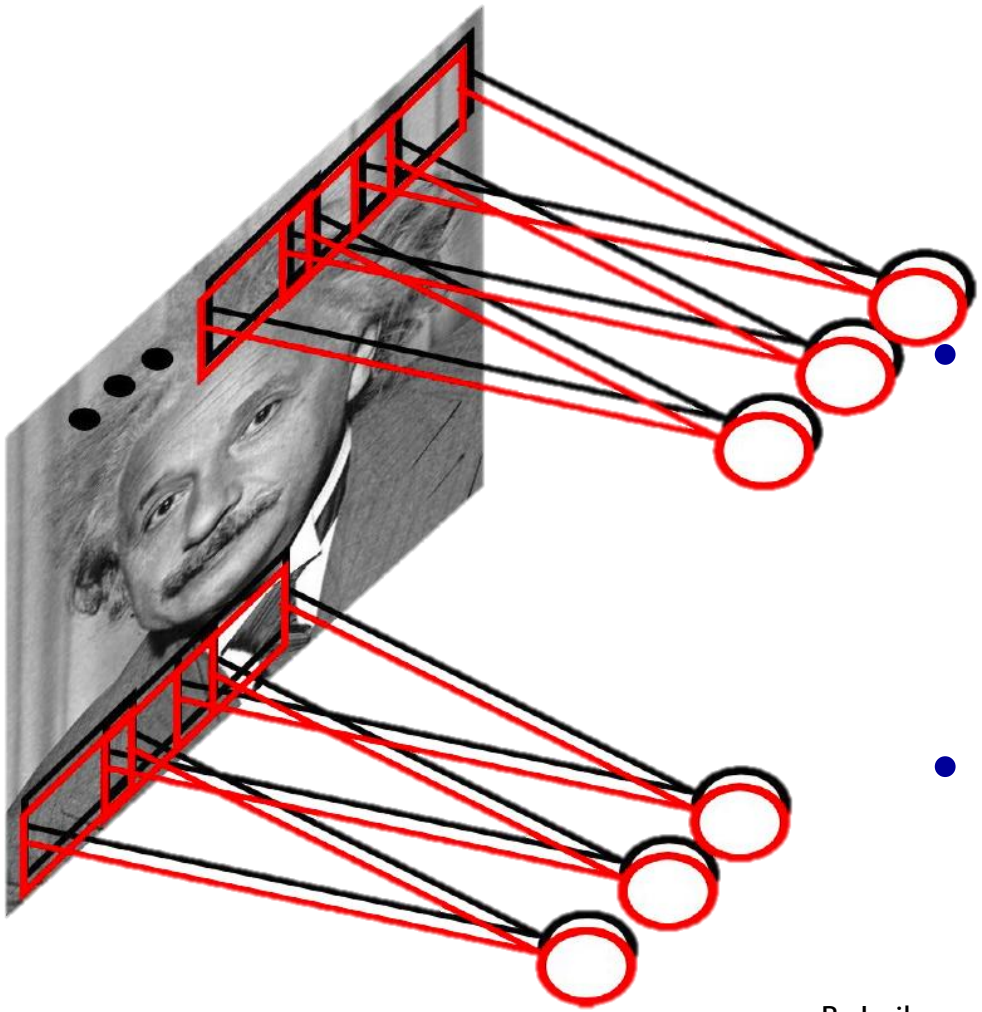
Slide credit: Svetlana Lazebnik

# Recap: CNN Structure

- **Feed-forward feature extraction**
  1. Convolve input with learned filters
  2. Non-linearity
  3. Spatial pooling
  4. (Normalization)
- **Supervised training of convolutional filters by back-propagating classification error**



# Recap: Intuition of CNNs



- **Convolutional net**
  - Share the same parameters across different locations
  - Convolutions with learned kernels
- **Learn *multiple* filters**
  - E.g. 1000×1000 image
    100 filters
    10×10 filter size

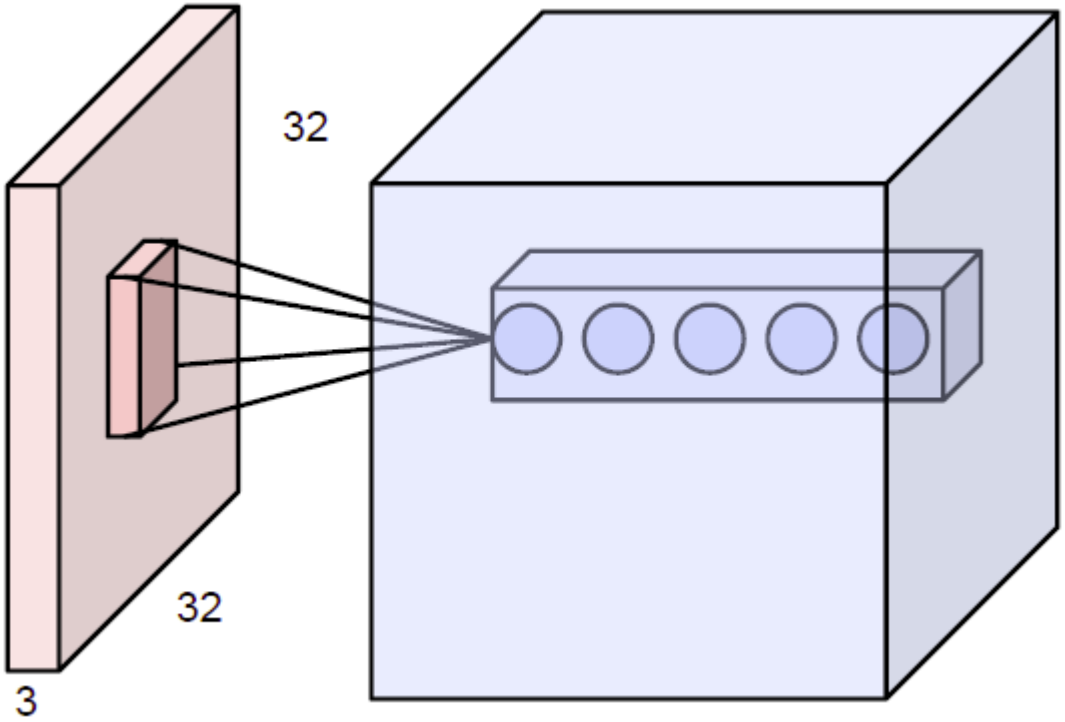
  ⇒ only 10k parameters
- **Result: Response map**
  - size: 1000×1000×100
  - Only memory, not params!

Slide adapted from Marc'Aurelio Ranzato

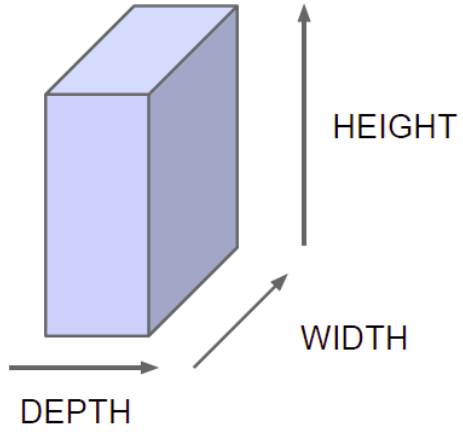


Image source: Yann LeCun

# Recap: Convolution Layers




Naming convention:

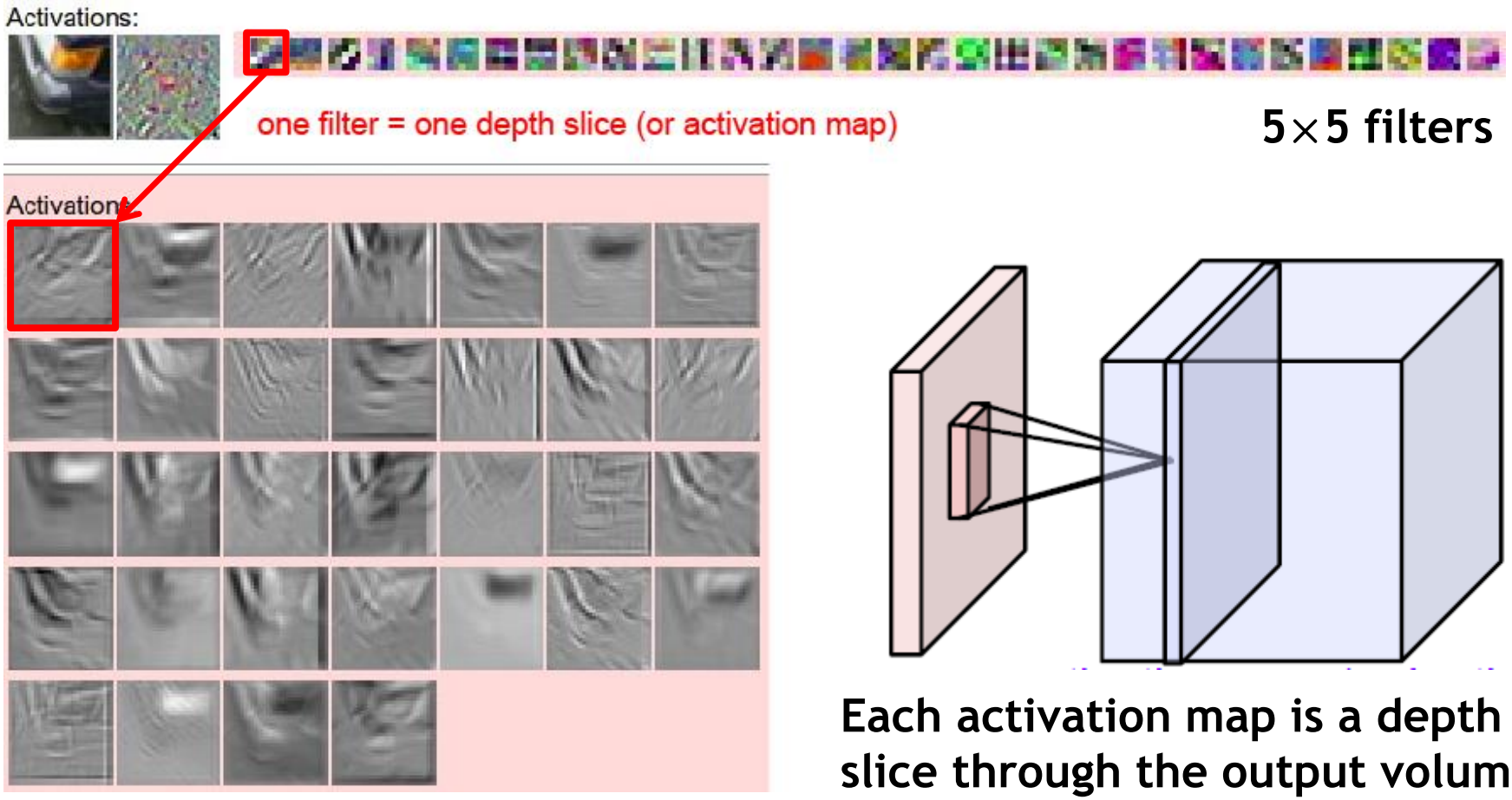



- All Neural Net activations arranged in 3 dimensions
  - Multiple neurons all looking at the same input region, stacked in depth
  - Form a single [1×1×depth] depth column in output volume.



Slide credit: FeiFei Li, Andrej Karpathy

# Recap: Activation Maps

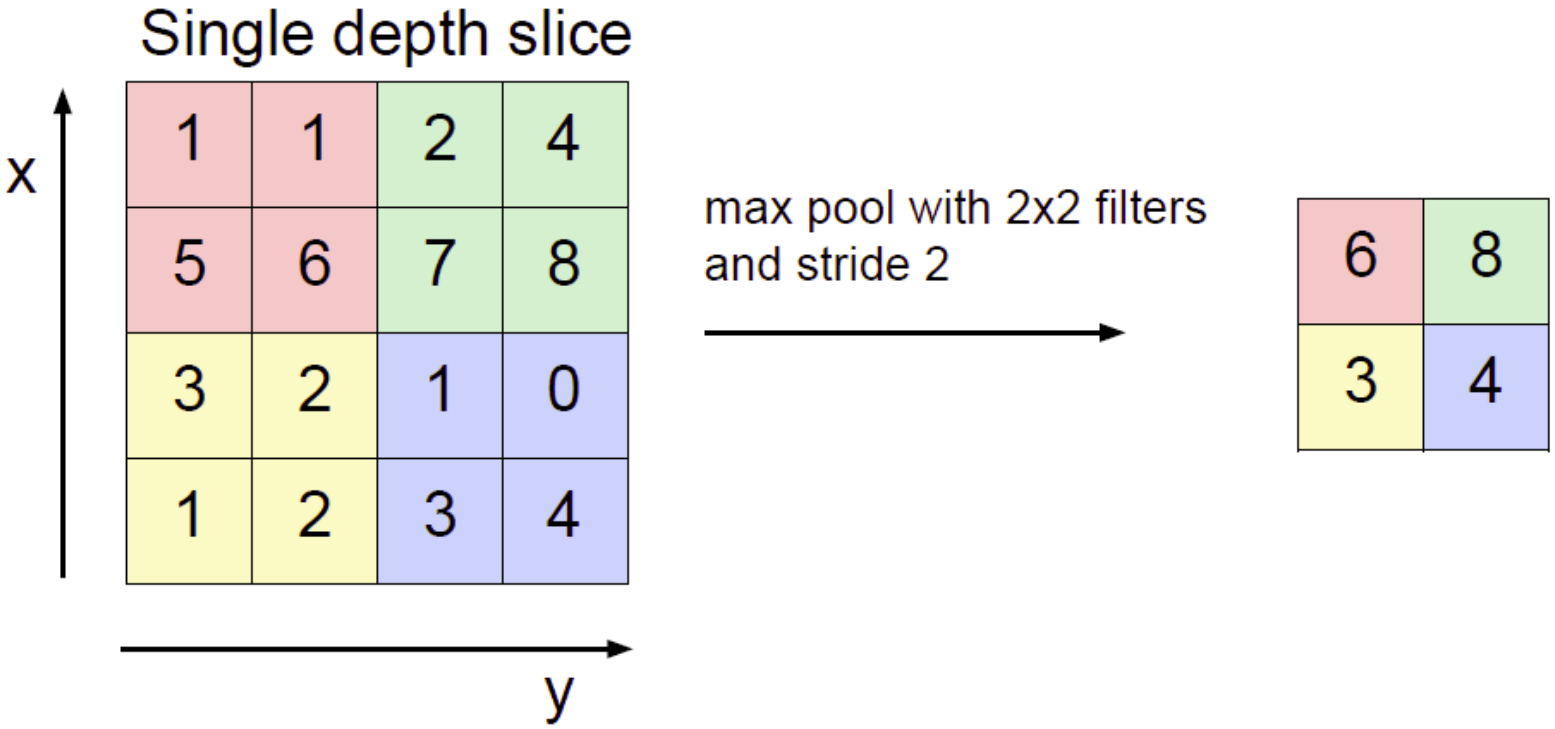



5×5 filters



Each activation map is a depth slice through the output volume.

# Recap: Pooling Layers

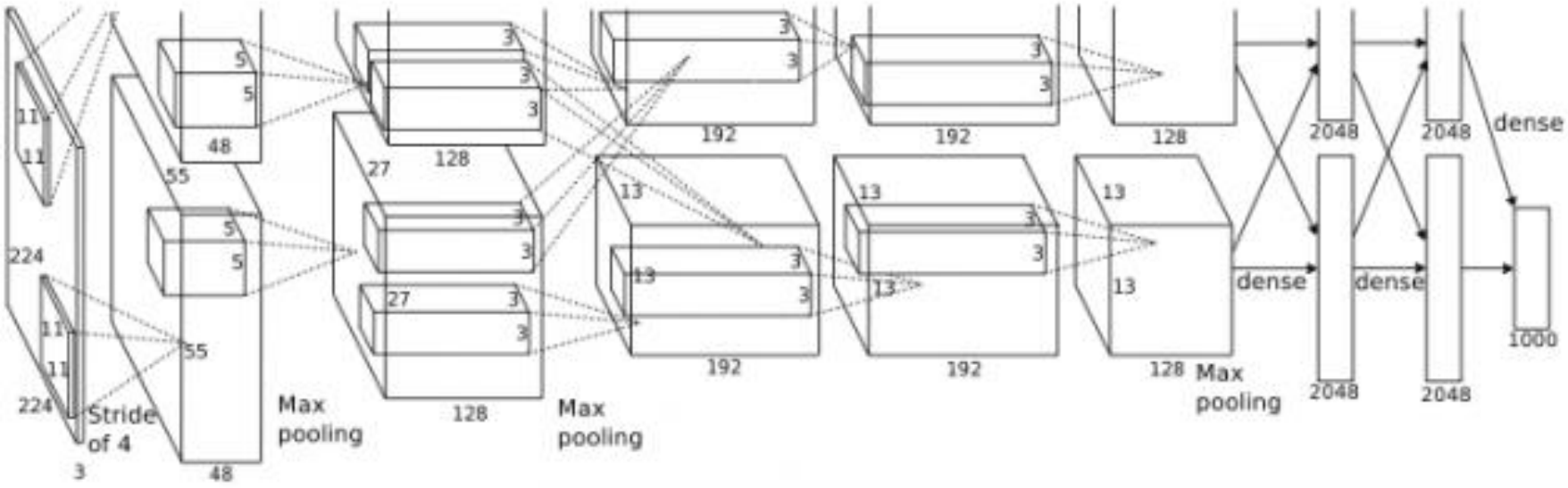



- **Effect:**
  - **Make the representation smaller without losing too much information**
  - **Achieve robustness to translations**



Slide adapted from FeiFei Li, Andrej Karpathy

# Recap: AlexNet (2012)




- Similar framework as LeNet, but
  - Bigger model (7 hidden layers, 650k units, 60M parameters)
  - More data ($10^6$ images instead of $10^3$)
  - GPU implementation
  - Better regularization and up-to-date tricks for training (Dropout)

A. Krizhevsky, I. Sutskever, and G. Hinton, ImageNet Classification with Deep Convolutional Neural Networks, NIPS 2012.



Image source: A. Krizhevsky, I. Sutskever and G.E. Hinton, NIPS 2012

# Recap: VGGNet (2014/15)

- Main ideas
  - Deeper network
  - Stacked convolutional layers with smaller filters (+ nonlinearity)
  - Detailed evaluation of all components
- Results
  - Improved ILSVRC top-5 error rate to 6.7%.

| ConvNet Configuration | | | | | |
|---|---|---|---|---|---|
| A | A-LRN | B | C | D | E |
| 11 weight layers | 11 weight layers | 13 weight layers | 16 weight layers | 16 weight layers | 19 weight layers |
| input (224 × 224 RGB image) | | | | | |
| conv3-64 | conv3-64<br>**LRN** | conv3-64<br>**conv3-64** | conv3-64<br>conv3-64 | conv3-64<br>conv3-64 | conv3-64<br>conv3-64 |
| maxpool | | | | | |
| conv3-128 | conv3-128 | conv3-128<br>**conv3-128** | conv3-128<br>conv3-128 | conv3-128<br>conv3-128 | conv3-128<br>conv3-128 |
| maxpool | | | | | |
| conv3-256<br>conv3-256 | conv3-256<br>conv3-256 | conv3-256<br>conv3-256 | conv3-256<br>conv3-256<br>**conv1-256** | conv3-256<br>conv3-256<br>**conv3-256** | conv3-256<br>conv3-256<br>conv3-256<br>**conv3-256** |
| maxpool | | | | | |
| conv3-512<br>conv3-512 | conv3-512<br>conv3-512 | conv3-512<br>conv3-512 | conv3-512<br>conv3-512<br>**conv1-512** | conv3-512<br>conv3-512<br>**conv3-512** | conv3-512<br>conv3-512<br>conv3-512<br>**conv3-512** |
| maxpool | | | | | |
| conv3-512<br>conv3-512 | conv3-512<br>conv3-512 | conv3-512<br>conv3-512 | conv3-512<br>conv3-512<br>**conv1-512** | conv3-512<br>conv3-512<br>**conv3-512** | conv3-512<br>conv3-512<br>conv3-512<br>**conv3-512** |
| maxpool | | | | | |
| FC-4096 | | | | | |
| FC-4096 | | | | | |
| FC-1000 | | | | | |
| soft-max | | | | | |

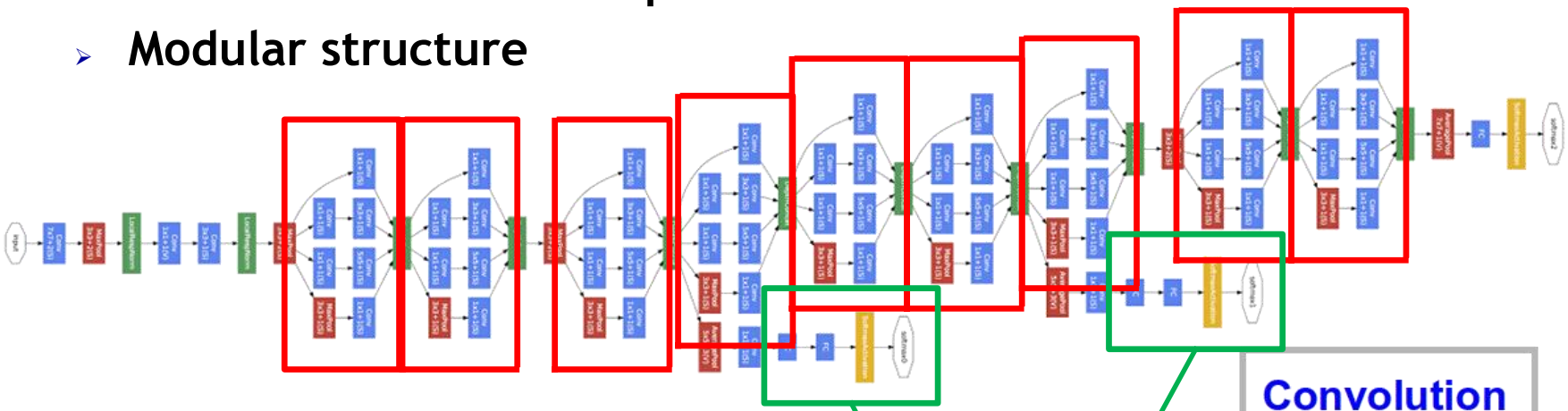
**Mainly used**



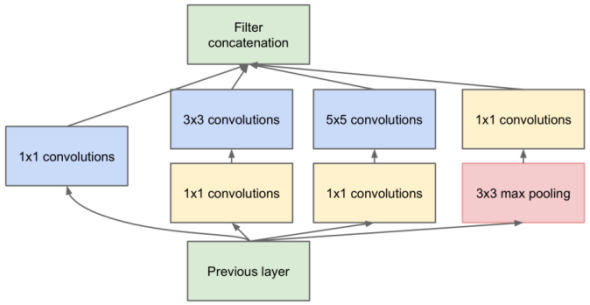
Image source: Simonyan & Zisserman

# Recap: GoogLeNet (2014)

- Ideas:
  - Learn features at multiple scales
  - Modular structure



Inception module + copies




(b) Inception module with dimension reductions

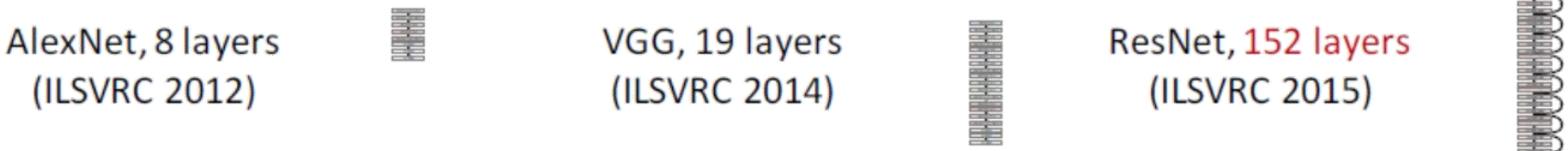
Convolution
Pooling
Softmax
Other

Auxiliary classification outputs for training the lower layers (deprecated)

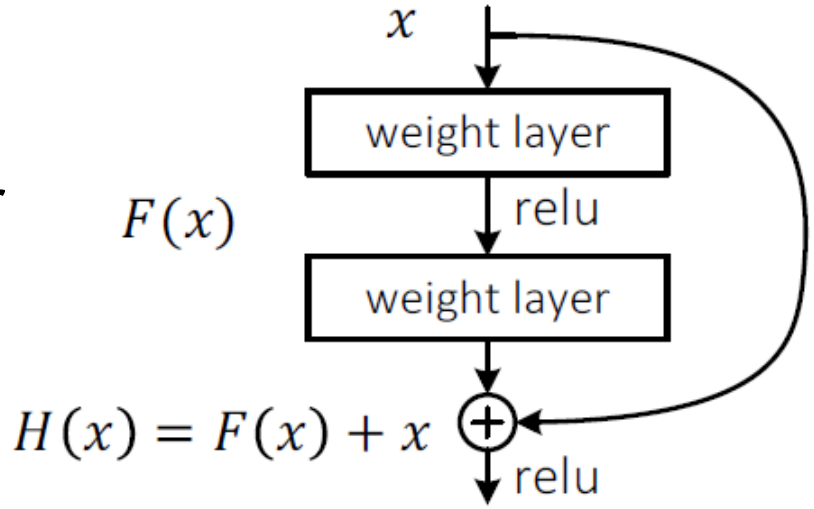


Image source: Szegedy et al.

# Recap: Residual Networks




- **Core component**
  - **Skip connections bypassing each layer**
  - **Better propagation of gradients to the deeper layers**
  - **This makes it possible to train (much) deeper networks.**



# Recap: Transfer Learning with CNNs


1. Train on ImageNet

2. If small dataset: fix all weights (treat CNN as fixed feature extractor), retrain only the classifier

I.e., replace the Softmax layer at the end


3. If you have a medium sized dataset, "finetune" instead: use the old weights as initialization, train the full network or only some of the higher layers.

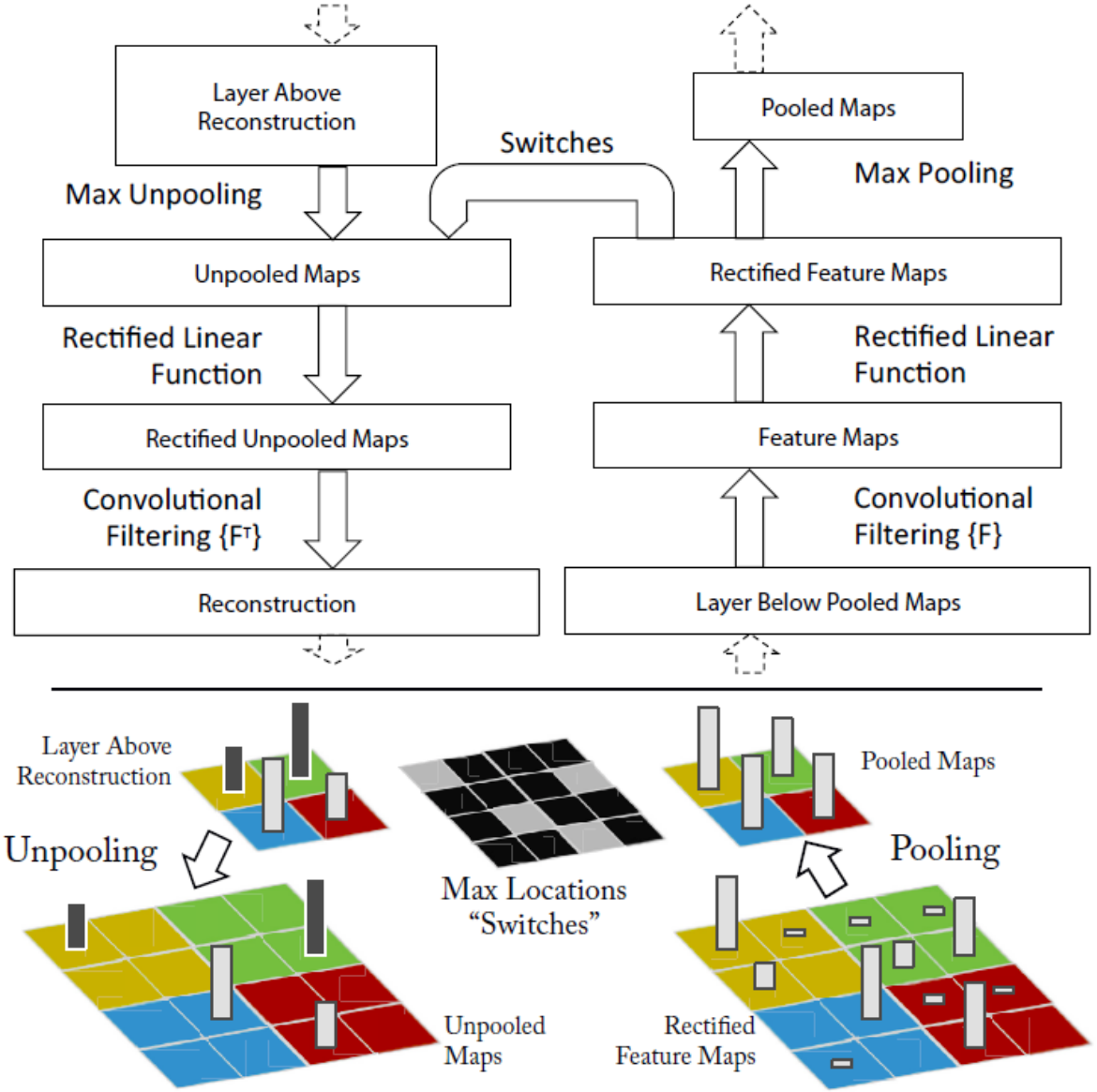
Retrain bigger part of the network



Slide credit: Andrej Karpathy

# Recap: Visualizing CNNs

DeconvNet

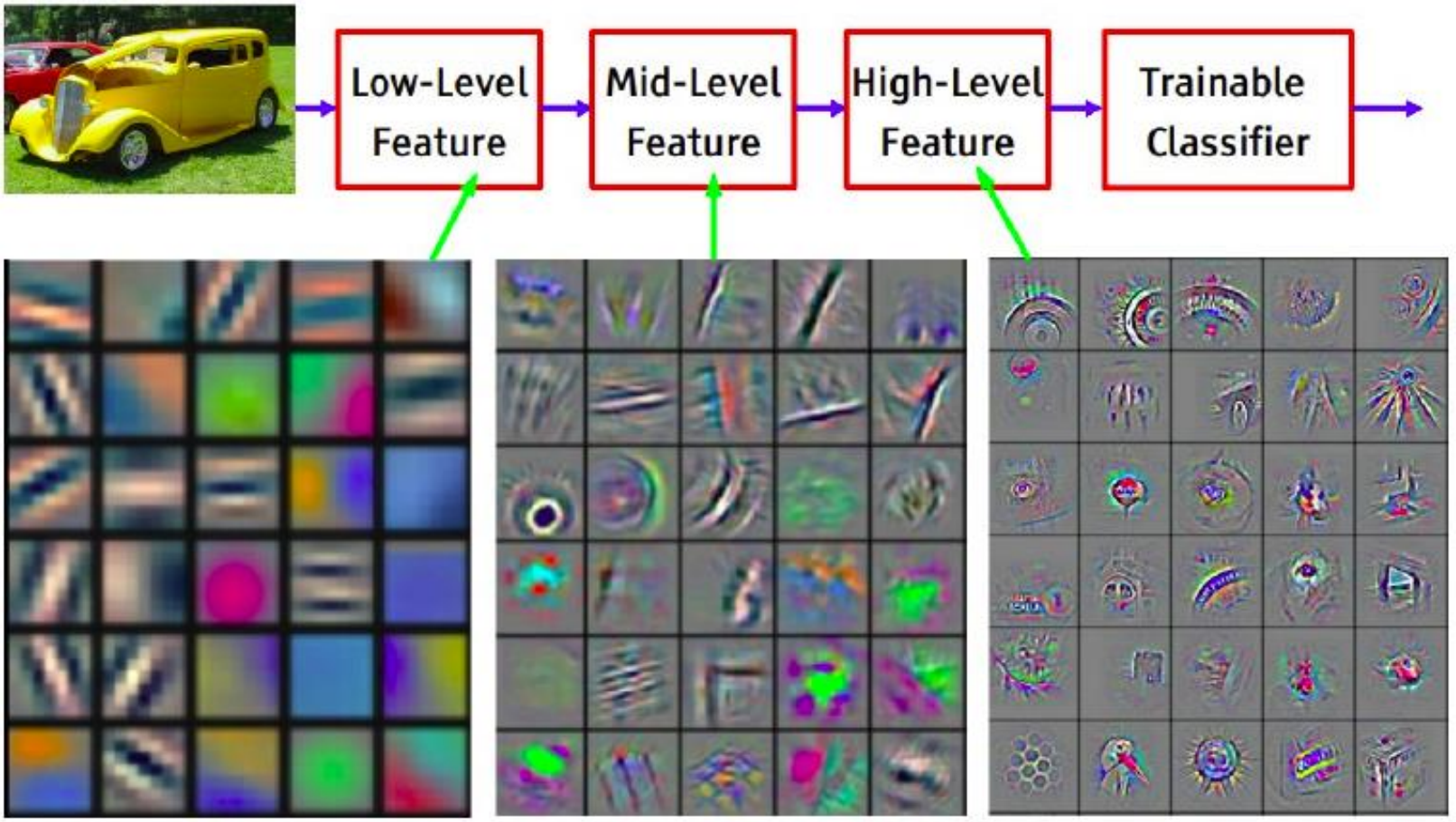



ConvNet



Image source: M. Zeiler, R. Fergus

# Recap: Visualizing CNNs

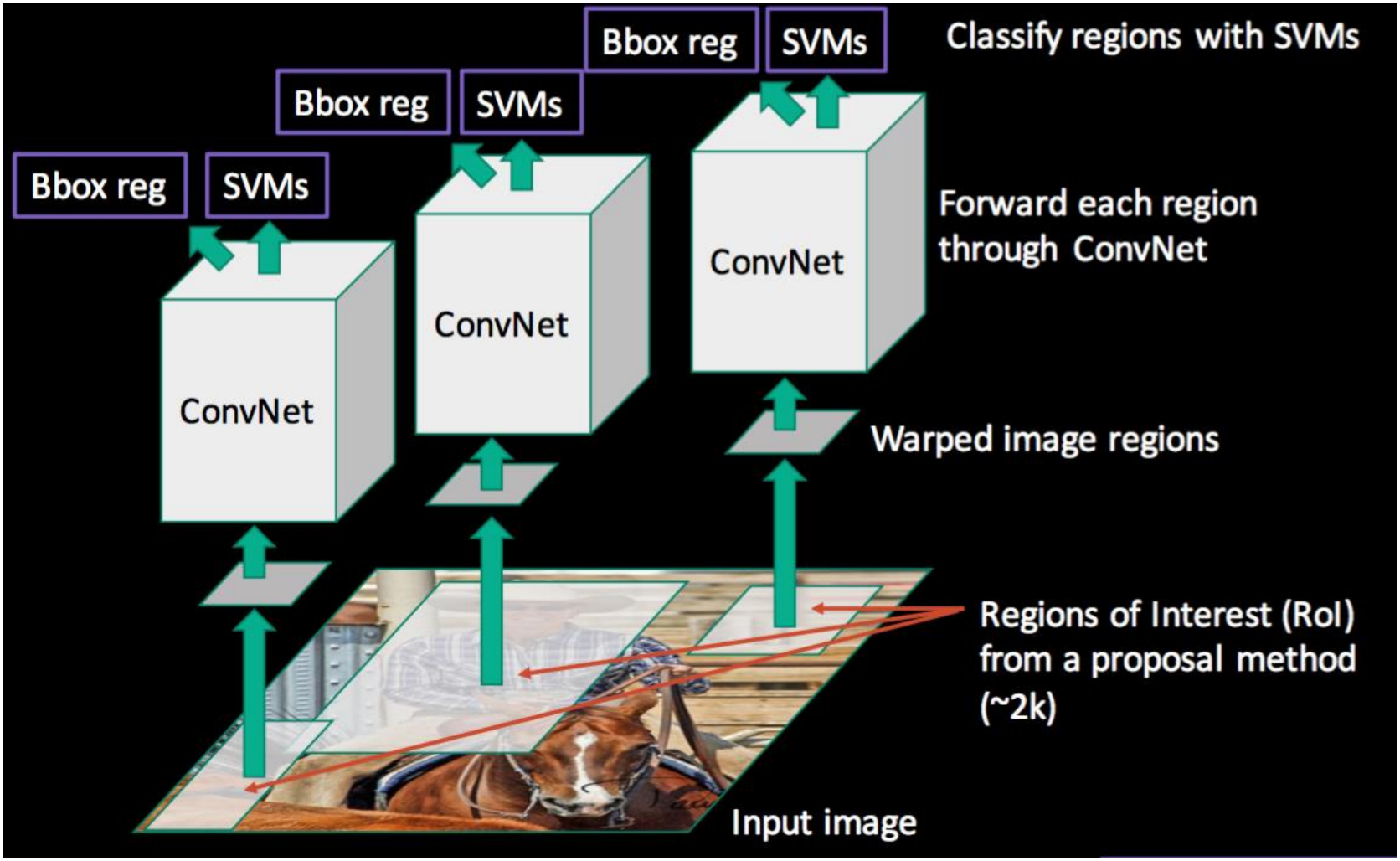



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]



Slide credit: Yann LeCun

# Recap: R-CNN for Object Deteection



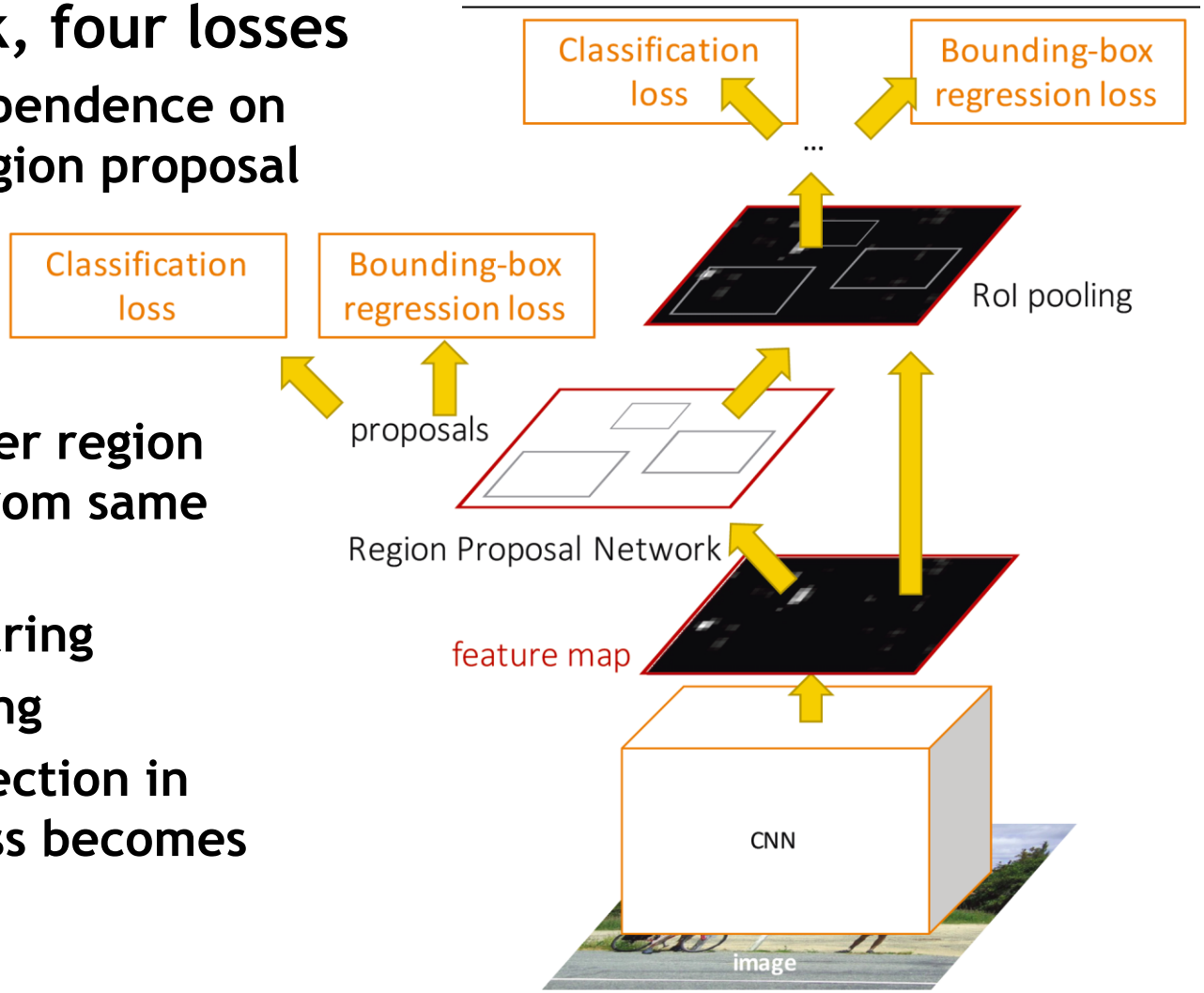



Slide credit: Ross Girshick

# Recap: Faster R-CNN

- One network, four losses
  - Remove dependence on external region proposal algorithm.
  - Instead, infer region proposals from same CNN.
  - Feature sharing
  - Joint training

⇒ Object detection in a single pass becomes possible.



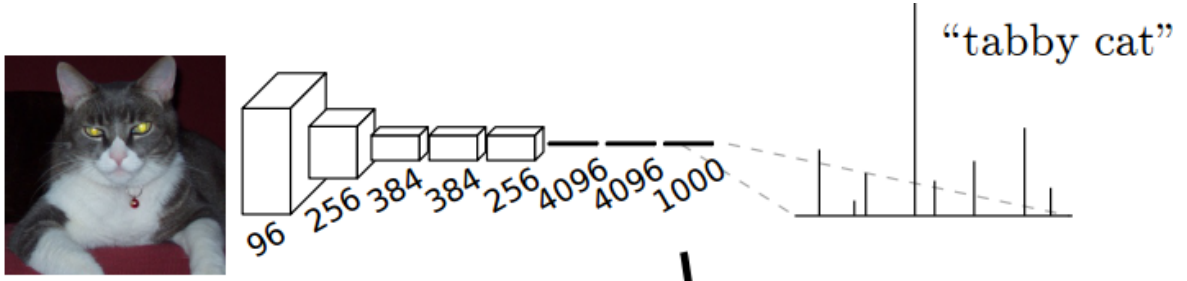




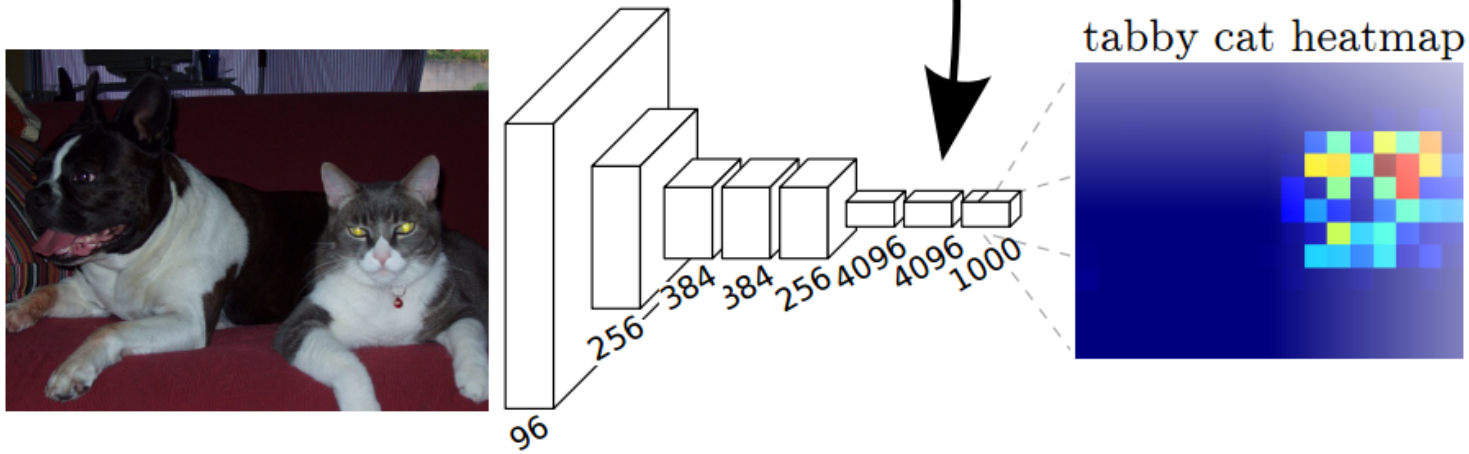

Slide credit: Ross Girshick

# Recap: Fully Convolutional Networks

- CNN




- FCN



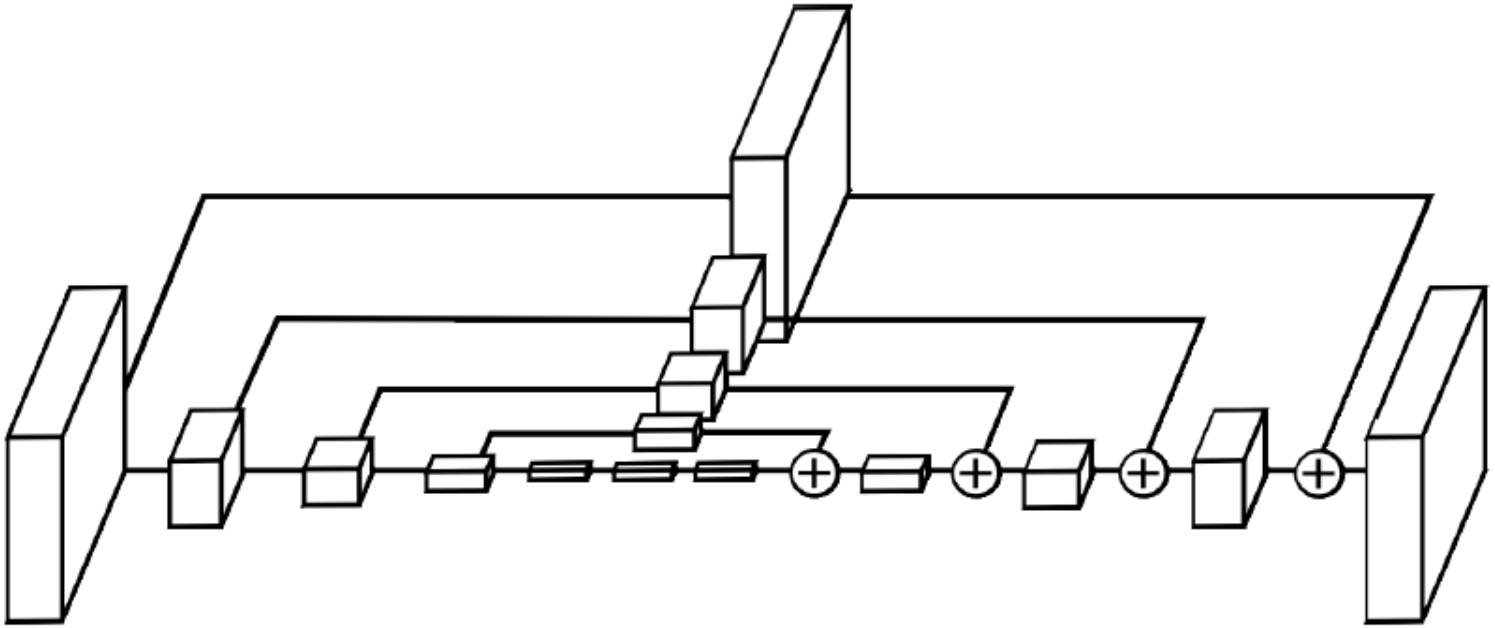

- Intuition
  - Think of FCNs as performing a sliding-window classification, producing a heatmap of output scores for each class





Image source: Long, Shelhamer, Darrell

# Recap: Image Segmentation Networks



- Encoder-Decoder Architecture
  - Problem: FCN output has low resolution
  - Solution: perform upsampling to get back to desired resolution
  - Use skip connections to preserve higher-resolution information





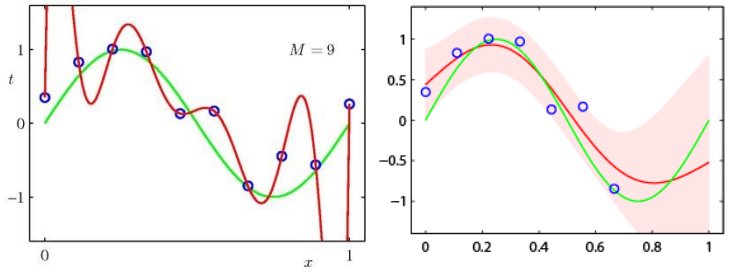
Image source: Newell et al.

# This Lecture: *Advanced Machine Learning*

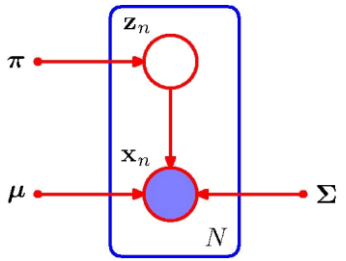


- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

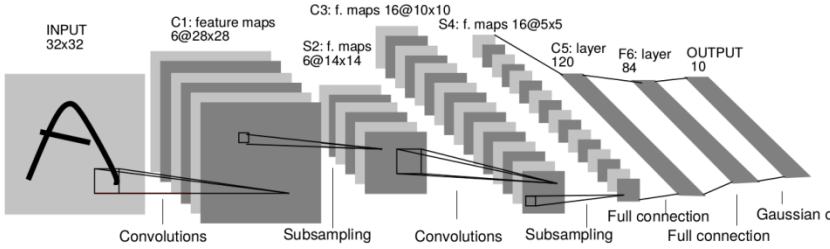
$$f : \mathcal{X} \rightarrow \mathbb{R}$$



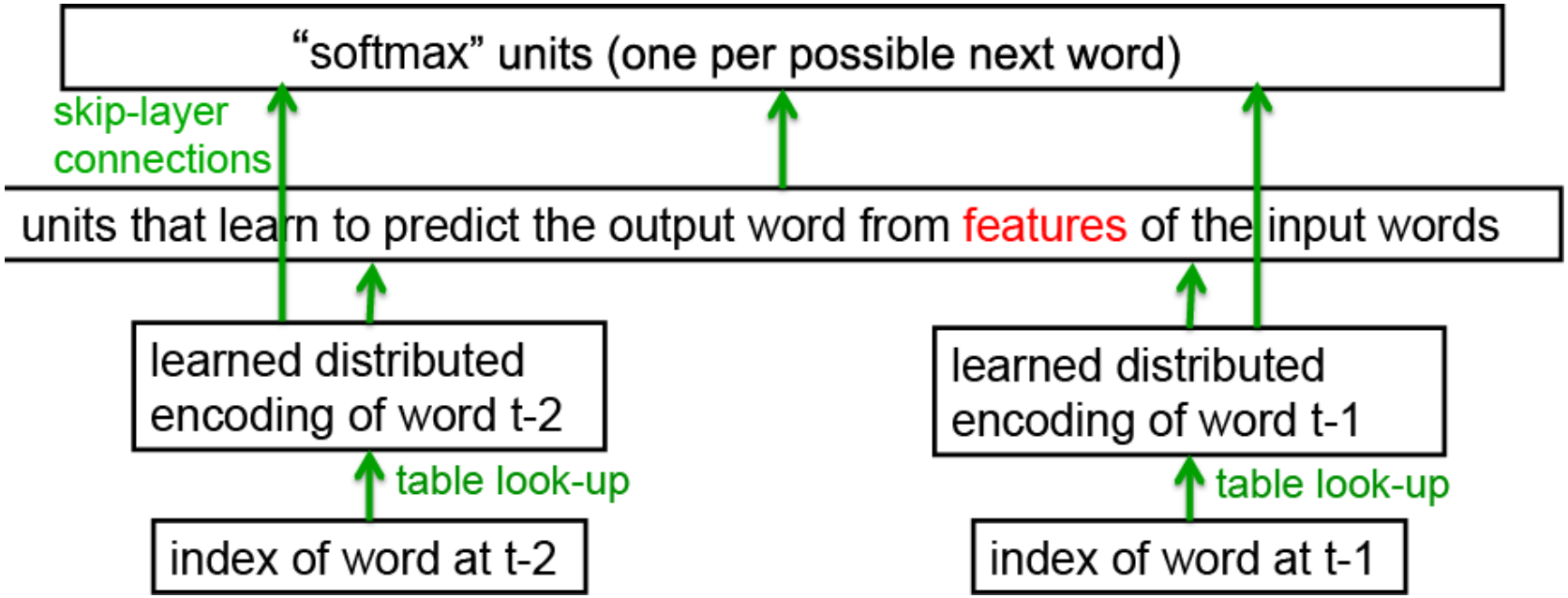

- Approximate Inference
  - Sampling Approaches
  - MCMC




- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Neural Probabilistic Language Model




- **Core idea**
  - **Learn a shared distributed encoding (word embedding) for the words in the vocabulary.**

Y. Bengio, R. Ducharme, P. Vincent, C. Jauvin, A Neural Probabilistic Language Model, In JMLR, Vol. 3, pp. 1137-1155, 2003.

# Recap: word2vec

- Goal
  - Make it possible to learn high-quality word embeddings from huge data sets (billions of words in training set).
- Approach
  - Define two alternative learning tasks for learning the embedding:
    - "Continuous Bag of Words" (CBOW)
    - "Skip-gram"
  - Designed to require fewer parameters.

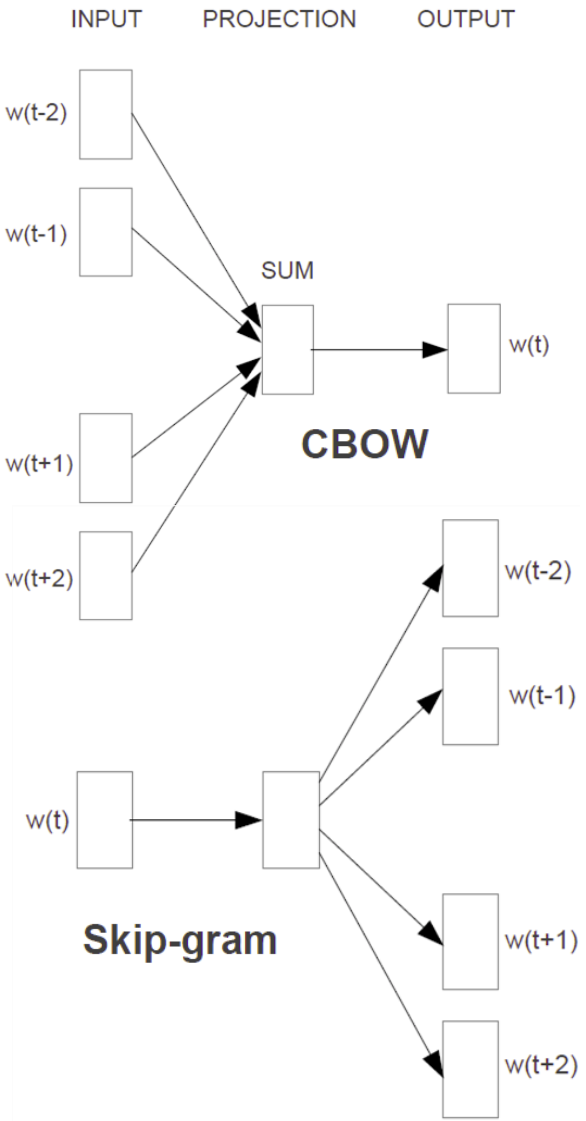




Image source: Mikolov et al., 2015

# Recap: word2vec CBOW Model

- Continuous BOW Model
  - Remove the non-linearity from the hidden layer
  - Share the projection layer for all words (their vectors are averaged)

⇒ Bag-of-Words model
(order of the words does not matter anymore)

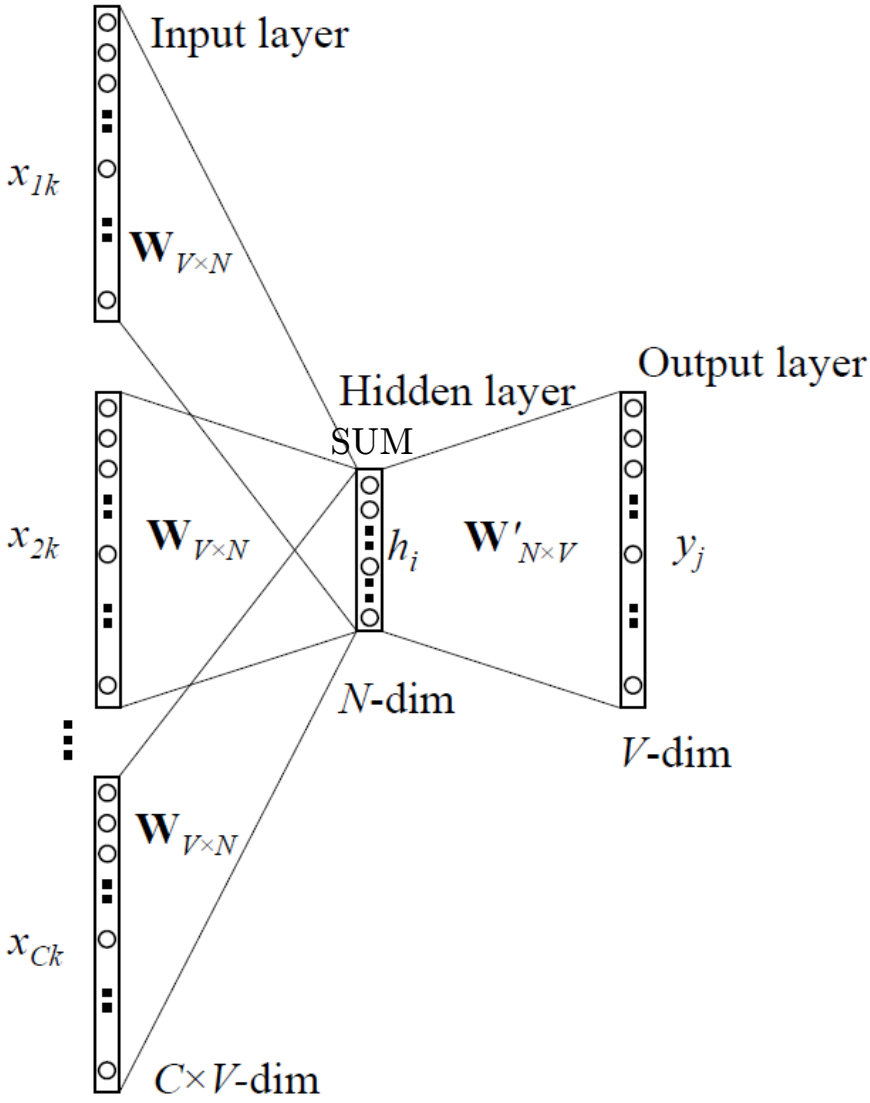
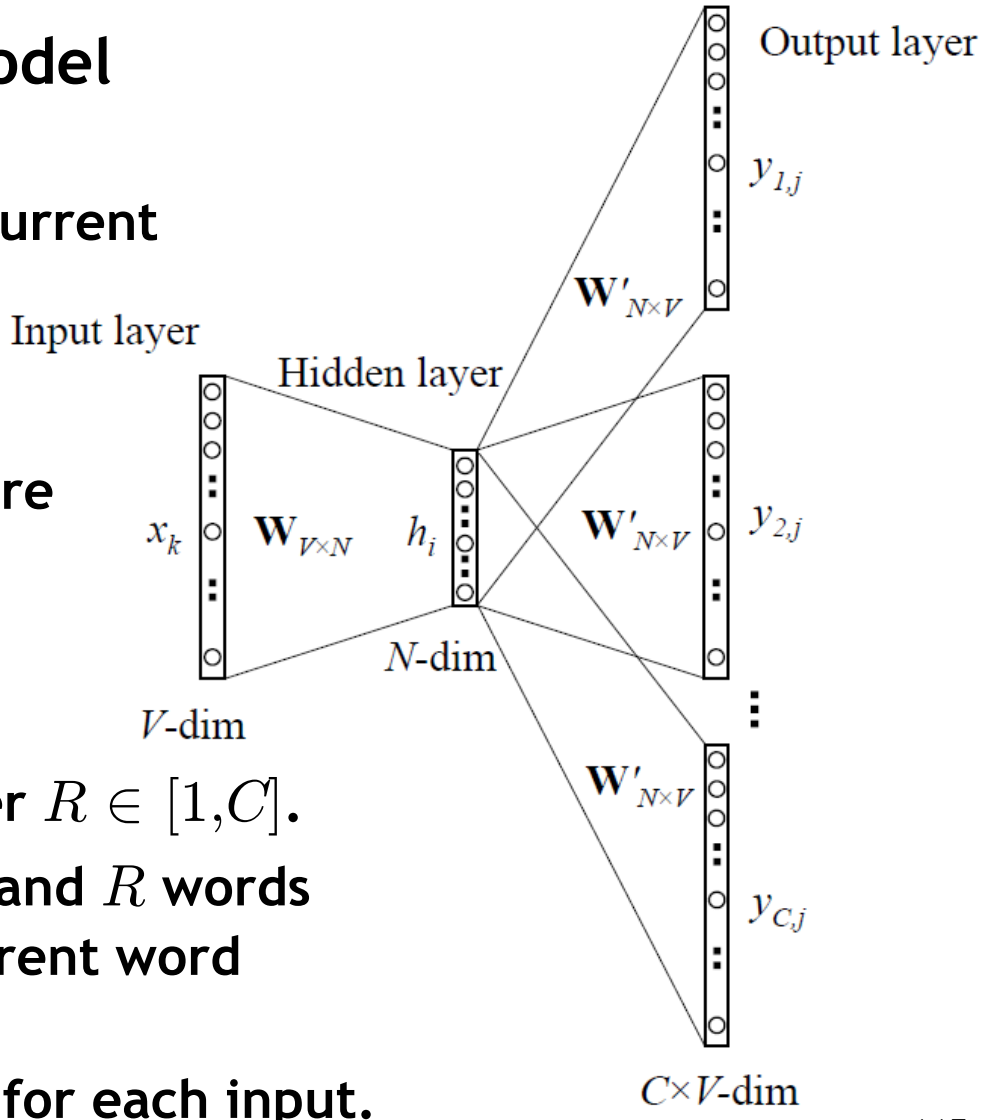




Image source: Xin Rong, 2015

# Recap: word2vec Skip-Gram Model

- Continuous Skip-Gram Model
  - Similar structure to CBOW
  - Instead of predicting the current word, predict words within a certain range of the current word.
  - Give less weight to the more distant words




- Implementation
  - Randomly choose a number $R \in [1,C]$.
  - Use $R$ words from history and $R$ words from the future of the current word as correct labels.

$\Rightarrow R+R$ word classifications for each input.


Image source: Xin Rong, 2015

# Problems with 100k-1M outputs

- **Weight matrix gets huge!**
  - Example: CBOW model
  - One-hot encoding for inputs

  ⇒ Input-hidden connections are just vector lookups.

  - This is not the case for the hidden-output connections!
  - State h is not one-hot, and vocabulary size is 1M.

  ⇒ $\mathbf{W}'_{N\times V}$ has $300\times 1\text{M}$ entries
- **Softmax gets expensive!**
  - Need to compute normalization over 100k-1M outputs

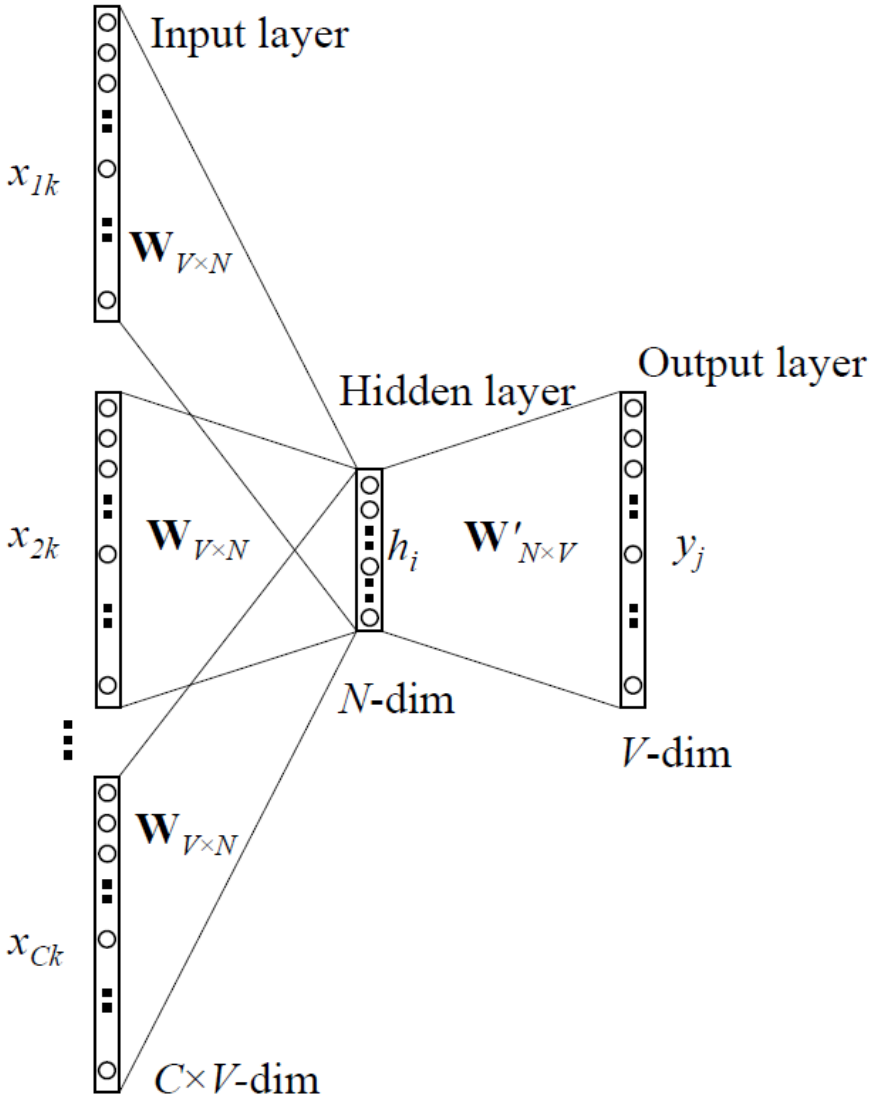
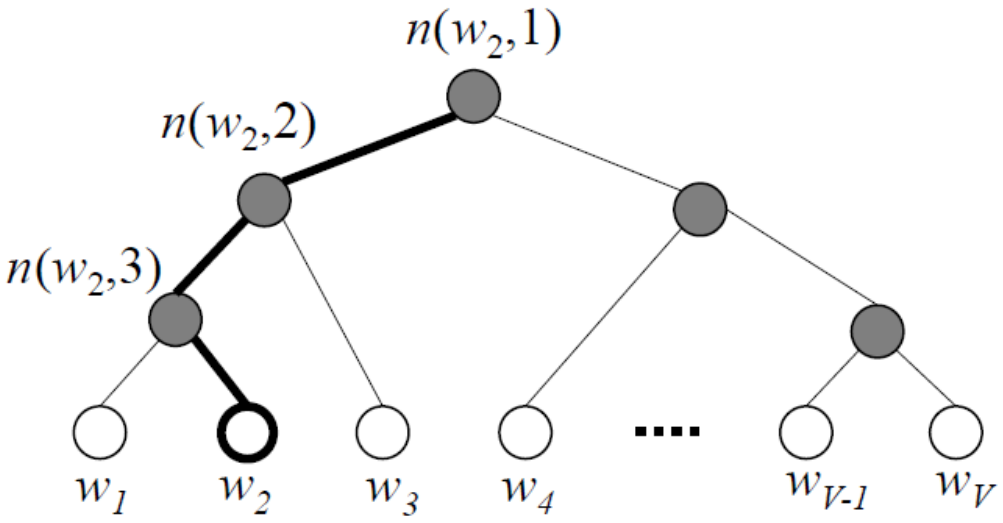




Image source: Xin Rong, 2015

# Recap: Hierarchical Softmax



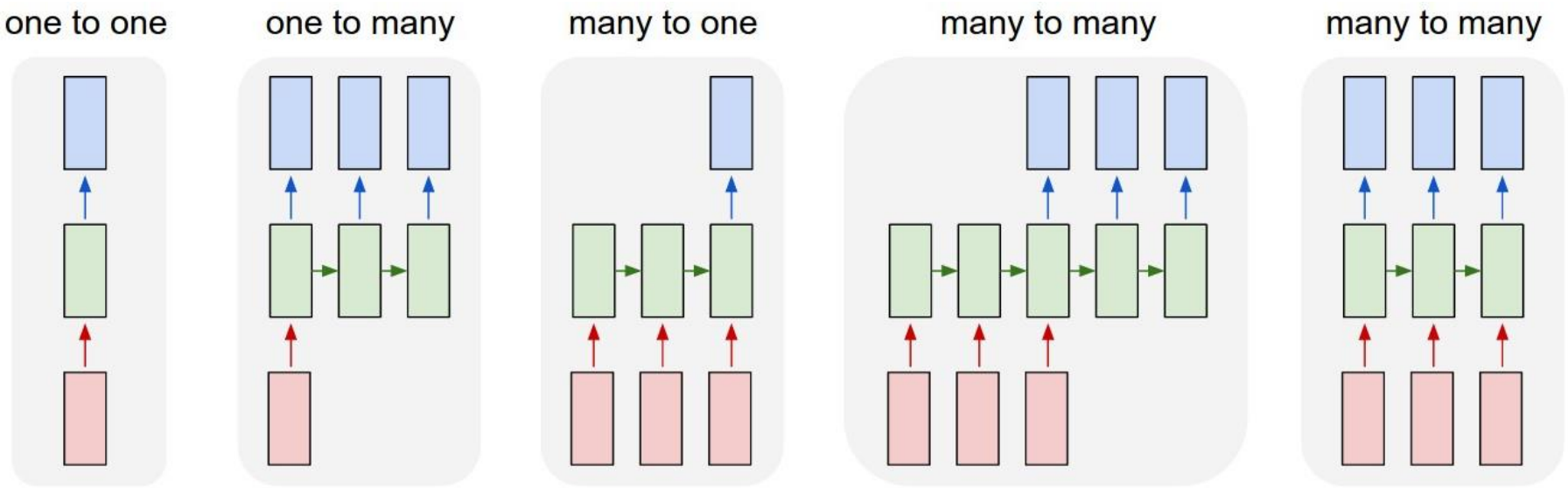

- **Idea**
  - Organize words in binary search tree, words are at leaves
  - Factorize probability of word $w_0$ as a product of node probabilities along the path.
  - Learn a linear decision function $y = v_{n(w,j)} \cdot h$ at each node to decide whether to proceed with left or right child node.

  $\Rightarrow$ Decision based on output vector of hidden units directly.



Image source: Xin Rong, 2015

# Recap: Recurrent Neural Networks

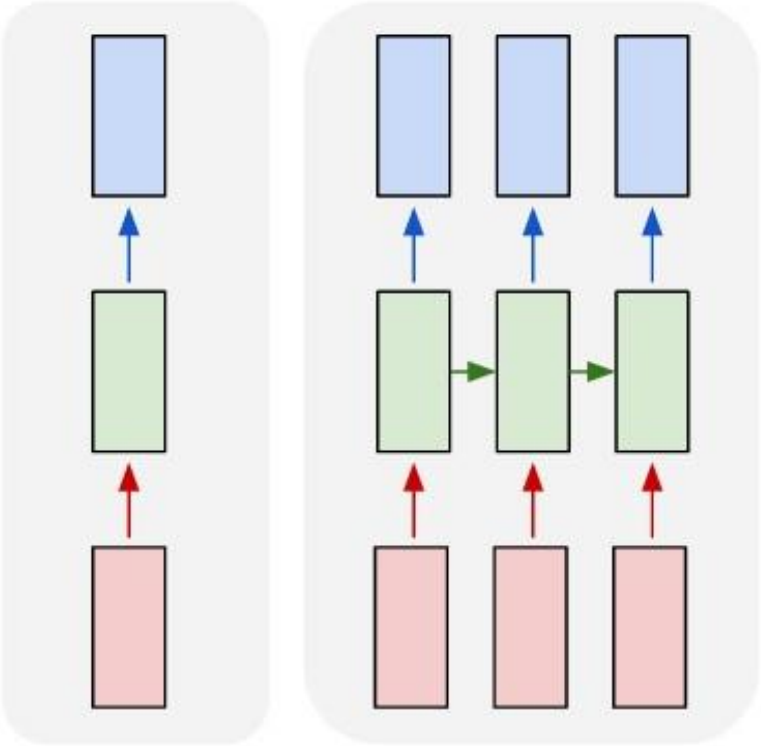



- Up to now
  - Simple neural network structure: 1-to-1 mapping of inputs to outputs
- Recurrent Neural Networks
  - Generalize this to arbitrary mappings


Image source: Andrej Karpathy

# Recap: Recurrent Neural Networks (RNNs)

- RNNs are regular NNs whose hidden units have additional connections over time.
  - You can unroll them to create a network that extends over time.
  - When you do this, keep in mind that the weights for the hidden are shared between temporal layers.

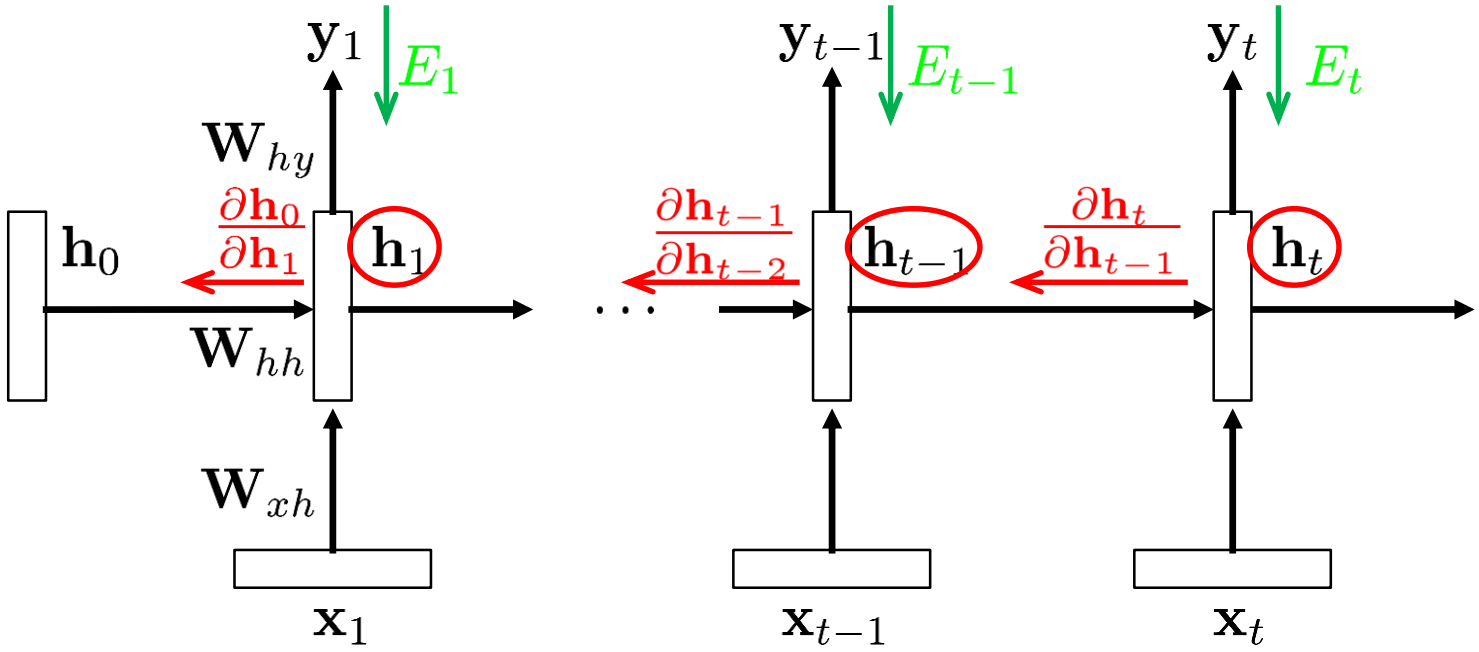


- RNNs are very powerful
  - With enough neurons and time, they can compute anything that can be computed by your computer.



Image source: Andrej Karpathy

# Recap: Backpropagation Through Time (BPTT)




- **Configuration**

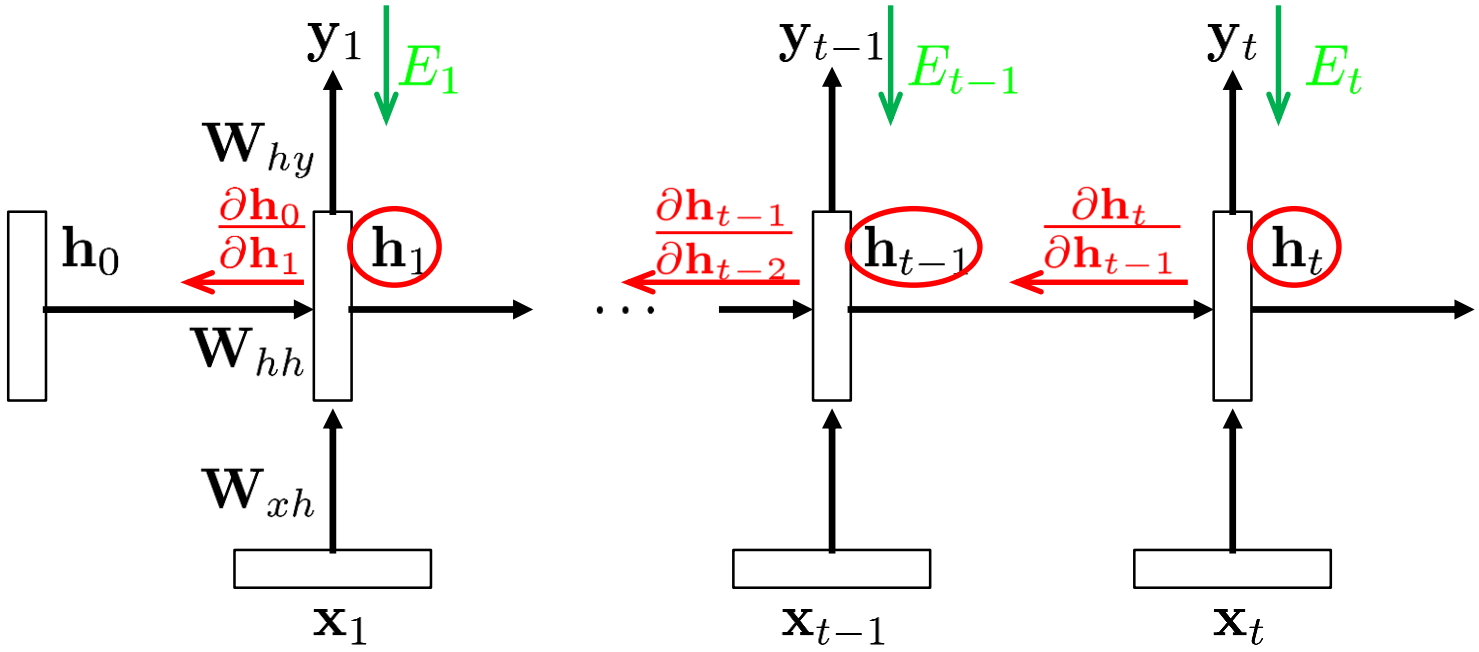
$$\mathbf{h}_t = \sigma\left(\mathbf{W}_{xh}\mathbf{x}_t + \mathbf{W}_{hh}\mathbf{h}_{t-1} + b\right)$$

$$\hat{\mathbf{y}}_t = \text{softmax}\left(\mathbf{W}_{hy}\mathbf{h}_t\right)$$

- **Backpropagated gradient**
  - **For weight $w_{ij}$:**

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left( \frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

# Recap: Backpropagation Through Time (BPTT)

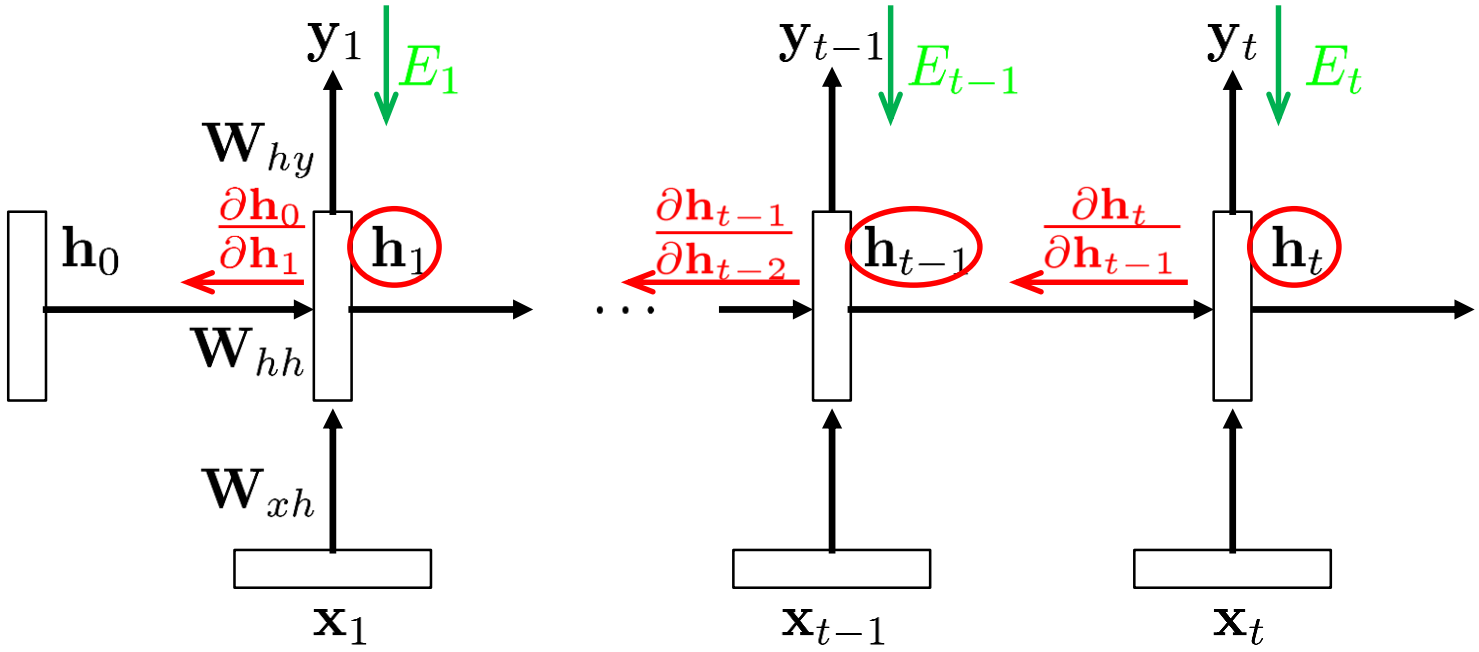



- **Analyzing the terms**
  - **For weight $w_{ij}$:**

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \leq k \leq t} \left( \frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

  - **This is the "immediate" partial derivative (with $\mathbf{h}_{k-1}$ as constant)**

# Recap: Backpropagation Through Time (BPTT)




- **Analyzing the terms**
  - **For weight $w_{ij}$:**

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \leq k \leq t} \left( \frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

  - **Propagation term:**

$$\frac{\partial h_t}{\partial h_k} = \prod_{t \geq i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}}$$

# Recap: Backpropagation Through Time (BPTT)

- **Summary**
  - **Backpropagation equations**

$$E = \sum_{1 \leq t \leq T} E_t$$

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \leq k \leq t} \left( \frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

$$\frac{\partial h_t}{\partial h_k} = \prod_{t \geq i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \prod_{t \geq i > k} \mathbf{W}_{hh}^{\top} diag\left(\sigma'(\mathbf{h}_{i-1})\right)$$

  - **Remaining issue: how to set the initial state $\mathbf{h}_0$?**

**$\Rightarrow$ Learn this together with all the other parameters.**

# Recap: Exploding / Vanishing Gradient Problem

- **BPTT equations:**

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \leq k \leq t} \left( \frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

$$\frac{\partial h_t}{\partial h_k} = \prod_{t \geq i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \prod_{t \geq i > k} \mathbf{W}_{hh}^\top diag\left(\sigma'(\mathbf{h}_{i-1})\right)$$

$$= \left(\mathbf{W}_{hh}^\top\right)^l$$

(if $t$ goes to infinity and $l = t - k$.)

⇒ We are effectively taking the weight matrix to a high power.

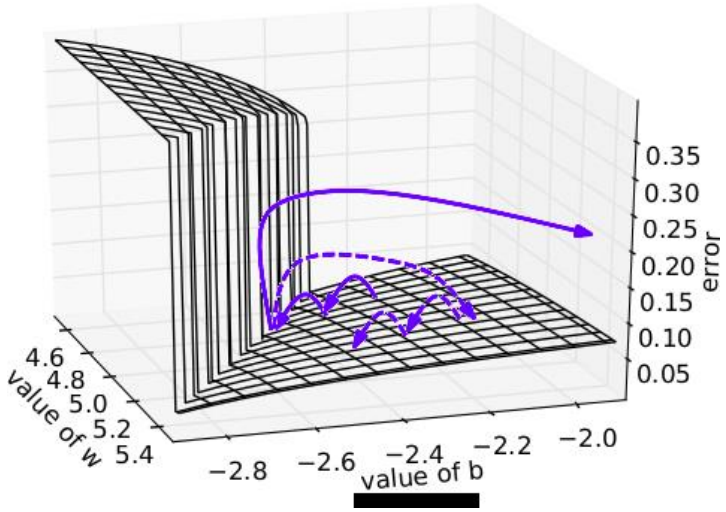
- The result will depend on the eigenvalues of $\mathbf{W}_{hh}$.
  - Largest eigenvalue > 1 ⇒ Gradients *may* explode.
  - Largest eigenvalue < 1 ⇒ Gradients *will* vanish.
  - This is very bad...

# Recap: Gradient Clipping

- Trick to handle exploding gradients
  - If the gradient is larger than a threshold, clip it to that threshold.

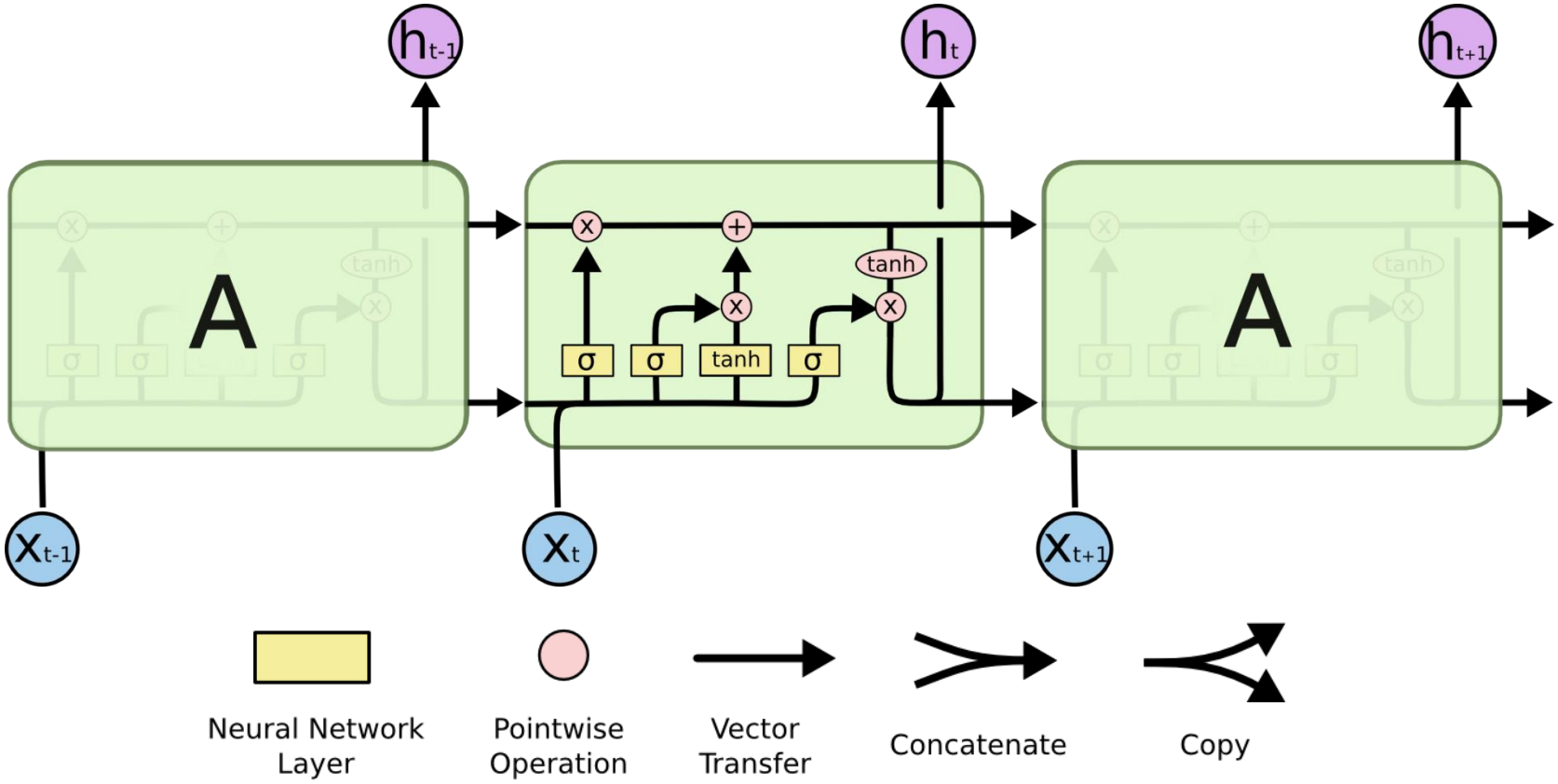
**Algorithm 1** Pseudo-code

$$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$$
$$\textbf{if } \|\hat{\mathbf{g}}\| \geq threshold \textbf{ then}$$
$$\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|}\hat{\mathbf{g}}$$
$$\textbf{end if}$$




  - This makes a big difference in RNNs

# Recap: Long Short-Term Memory (LSTM)



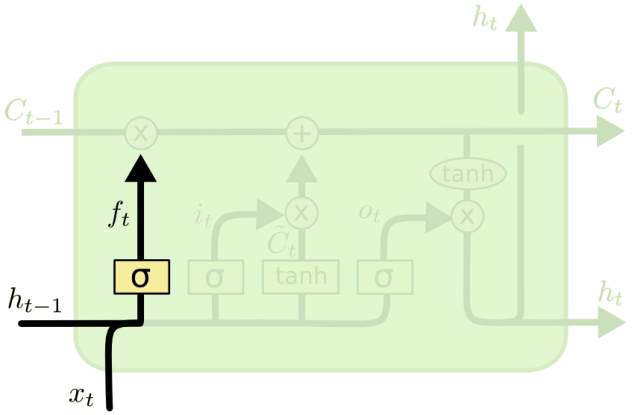

- LSTMs
  - Inspired by the design of memory cells
  - Each module has 4 layers, interacting in a special way.



Image source: Christopher Olah, http://colah.github.io/posts/2015-08-Understanding-LSTMs/

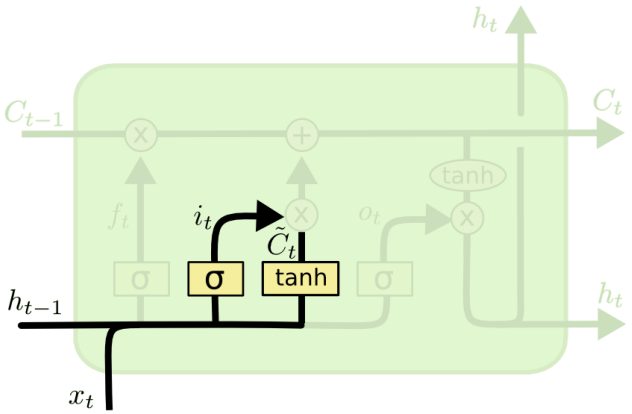
# Recap: Elements of LSTMs

- **Forget gate** layer
  - Look at $\mathbf{h}_{t-1}$ and $\mathbf{x}_t$ and output a number between $0$ and $1$ for each dimension in the cell state $\mathbf{C}_{t-1}$.
    - 0: completely delete this,
    - 1: completely keep this.




$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

- **Update gate** layer
  - Decide what information to store in the cell state.
  - Sigmoid network (**input gate** layer) decides which values are updated.
  - tanh layer creates a vector of new candidate values that could be added to the state.



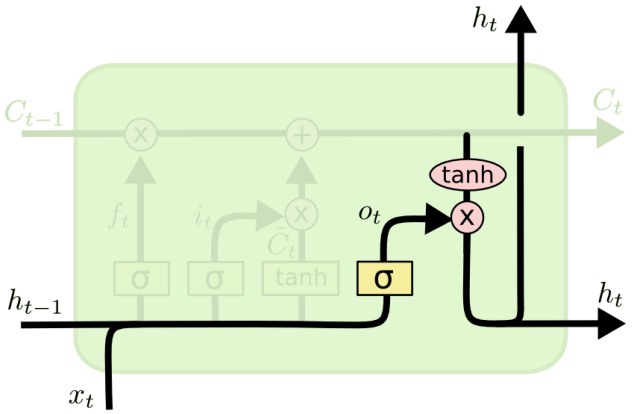

$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$

Source: Christopher Olah, http://colah.github.io/posts/2015-08-Understanding-LSTMs/

# Recap: Elements of LSTMs

- **Output gate** layer
  - Output is a filtered version of our gate state.
  - First, apply sigmoid layer to decide what parts of the cell state to output.
  - Then, pass the cell state through a tanh (to push the values to be between -1 and 1) and multiply it with the output of the sigmoid gate.




$$o_t = \sigma\left(W_o\left[h_{t-1}, x_t\right] + b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

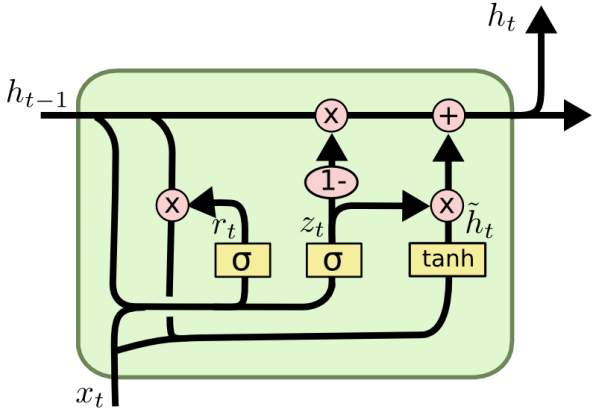




Source: Christopher Olah, http://colah.github.io/posts/2015-08-Understanding-LSTMs/

# Recap: Gated Recurrent Units (GRU)

- Simpler model than LSTM
  - Combines the forget and input gates into a single update gate $z_t$.
  - Similar definition for a reset gate $r_t$, but with different weights.
  - In both cases, merge the cell state and hidden state.




$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$

$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$

$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$

$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

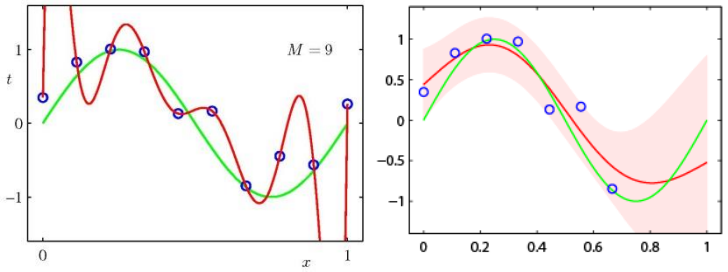
- Empirical results
  - Both LSTM and GRU can learn much longer-term dependencies than regular RNNs
  - GRU performance similar to LSTM (no clear winner yet), but fewer parameters.

Source: Christopher Olah, http://colah.github.io/posts/2015-08-Understanding-LSTMs/

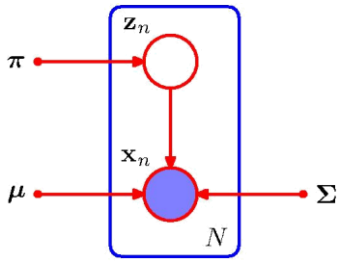
# This Lecture: *Advanced Machine Learning*

- **Regression Approaches**
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

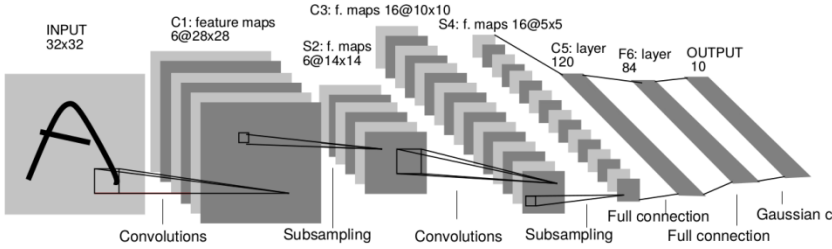
$$f : \mathcal{X} \rightarrow \mathbb{R}$$




- **Approximate Inference**
  - Sampling Approaches
  - MCMC

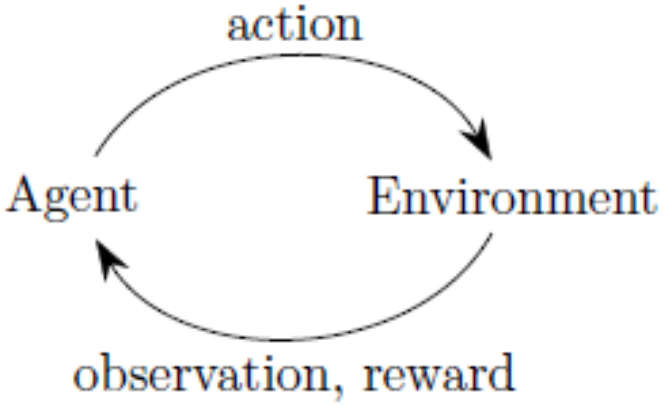



- **Deep Learning**
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, ResNets, RNNs, Deep RL, etc.



# Recap: Reinforcement Learning

- **Motivation**
  - General purpose framework for decision making.
  - Basis: Agent with the capability to interact with its environment
  - Each action influences the agent's future state.
  - Success is measured by a scalar reward signal.
  - Goal: select actions to maximize future rewards.




  - Formalized as a partially observable Markov decision process (POMDP)





Slide adapted from: David Silver, Sergey Levine

# Recap: Reward vs. Return

- **Objective of learning**
  - We seek to maximize the expected return $G_t$ as some function of the reward sequence $R_{t+1}, R_{t+2}, R_{t+3}, \ldots$
  - Standard choice: expected discounted return

$$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \ldots = \sum_{k=0}^{\infty} \gamma^k R_{t+k+1}$$

  where $0 \leq \gamma \leq 1$ is called the discount rate.

- **Difficulty**
  - We don't know which past actions caused the reward.

  $\Rightarrow$ Temporal credit assignment problem

# Recap: Policy

- **Definition**
  - A policy determines the agent's behavior
  - Map from state to action $\pi: \mathcal{S} \rightarrow \mathcal{A}$
- **Two types of policies**
  - Deterministic policy: $a = \pi(s)$
  - Stochastic policy: $\pi(a|s) = \Pr\{A_t = a | S_t = s\}$
- **Note**
  - $\pi(a|s)$ denotes the probability of taking action $a$ when in state $s$.

# Recap: Value Function

- Idea
  - Value function is a prediction of future reward
  - Used to evaluate the goodness/badness of states
  - And thus to select between actions
- Definition
  - The value of a state $s$ under a policy $\pi$, denoted $v_\pi(s)$, is the expected return when starting in $s$ and following $\pi$ thereafter.

$$v_\pi(s) = \mathbb{E}_\pi[G_t | S_t = s] = \mathbb{E}_\pi\left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \,\middle|\, S_t = s\right]$$

  - The value of taking action $a$ in state $s$ under a policy $\pi$, denoted $q_\pi(s,a)$, is the expected return starting from $s$, taking action $a$, and following $\pi$ thereafter.

$$q_\pi(s,a) = \mathbb{E}_\pi[G_t | S_t = s, A_t = a] = \mathbb{E}_\pi\left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \,\middle|\, S_t = s, A_t = a\right]$$

# Recap: Optimal Value Functions

- **Bellman optimality equations**
  - For the optimal state-value function $v_*$:

$$v_*(s) = \max_{a \in \mathcal{A}(s)} q_{\pi_*}(s,a)$$

$$= \max_{a \in \mathcal{A}(s)} \sum_{s',r} p(s',r|s,a)[r + \gamma v_*(s')]$$

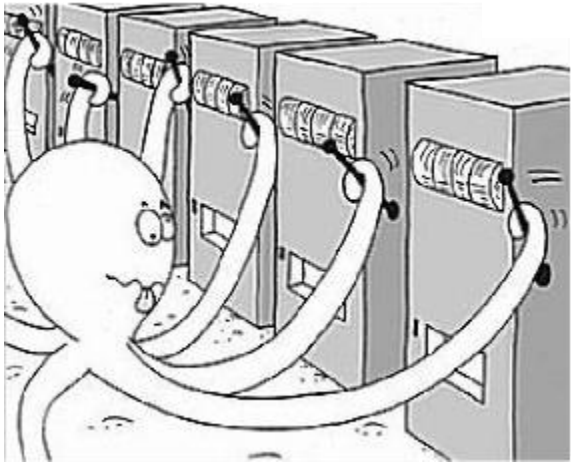
  - $v_*$ is the unique solution to this system of nonlinear equations.
  - For the optimal action-value function $q_*$:

$$q_*(s,a) = \sum_{s',r} p(s',r|s,a)\left[r + \gamma \max_{a'} q_*(s',a')\right]$$

  - $q_*$ is the unique solution to this system of nonlinear equations.

$\Rightarrow$ If the dynamics of the environment $p(s',r|s,a)$ are known, then in principle one can solve those equation systems.

# Recap: Exploration-Exploitation Trade-off



- Example: N-armed bandit problem
  - Suppose we have the choice between $N$ actions $a_1, \ldots, a_N$.
  - If we knew their value functions $q_*(s, a_i)$, it would be trivial to choose the best.
  - However, we only have estimates based on our previous actions and their returns.
- We can now
  - Exploit our current knowledge
    - And choose the greedy action that has the highest value based on our current estimate.
  - Explore to gain additional knowledge
    - And choose a non-greedy action to improve our estimate of that action's value.



Image source: research.microsoft.com

# Recap: TD-Learning

- **Policy evaluation (the prediction problem)**
  - For a given policy $\pi$, compute the state-value function $v_\pi$.
- **One option: Monte-Carlo methods**
  - Play through a sequence of actions until a reward is reached, then backpropagate it to the states on the path.

$$V(S_t) \leftarrow V(S_t) + \alpha[G_t - V(S_t)]$$

**Target: the actual return after time $t$**

- **Temporal Difference Learning – TD($\lambda$)**
  - Directly perform an update using the estimate $V(S_{t+\lambda+1})$.

$$V(S_t) \leftarrow V(S_t) + \alpha[\underbrace{R_{t+1} + \gamma V(S_{t+1})}_{} - V(S_t)]$$

**Target: an estimate of the return (here: TD(0))**

# Recap: SARSA – On-Policy TD Control

- **Idea**
  - Turn the TD idea into a control method by always updating the policy to be greedy w.r.t. the current estimate
- **Procedure**
  - Estimate $q_\pi(s,a)$ for the current policy $\pi$ and for all states $s$ and actions $a$.
  - TD(0) update equation

$$Q(S_t,A_t) \leftarrow Q(S_t,A_t) + \alpha[R_{t+1} + \gamma Q(S_{t+1},A_{t+1}) - Q(S_t,A_t)]$$

  - This rule is applied after every transition from a nonterminal state $S_t$.
  - It uses every element of the quintuple $(S_t, A_t, R_{t+1}, S_{t+1}, A_{t+1})$.

$\Rightarrow$ ***Hence, the name SARSA.***



Image source: Sutton & Barto

# Recap: Q-Learning – Off-Policy TD Control

- **Idea**
  - Directly approximate the optimal action-value function $q_*$, independent of the policy being followed.

- **Procedure**
  - TD(0) update equation

$$Q(S_t, A_t) \leftarrow Q(S_t, A_t) + \alpha \left[ R_{t+1} + \gamma \max_a Q(S_{t+1}, a) - Q(S_t, A_t) \right]$$

  - Dramatically simplifies the analysis of the algorithm.
  - All that is required for correct convergence is that all pairs continue to be updated.



Image source: Sutton & Barto

# Recap: Deep Q-Learning

- **Idea**
  - Optimal Q-values should obey Bellman equation

$$Q_*(s,a) = \mathbb{E}\left[r + \gamma \max_{a'} Q(s',a') \,|s,a\right]$$

  - Treat the right-hand side $r + \gamma \max_{a'} Q(s',a',\mathbf{w})$ as a target
  - Minimize MSE loss by stochastic gradient descent

$$L(\mathbf{w}) = \left(r + \gamma \max_{a'} Q(s',a',\mathbf{w}) - Q(s,a,\mathbf{w})\right)^2$$

  - This converges to $Q_*$ using a lookup table representation.

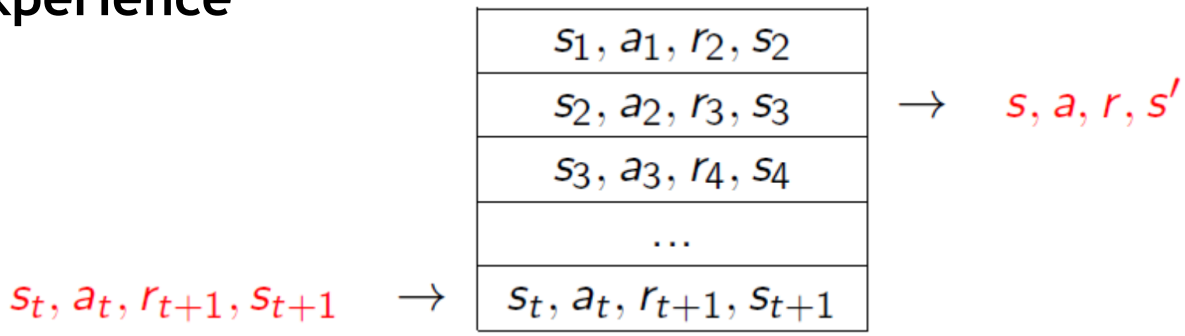
  - Unfortunately, it diverges using neural networks due to
    - Correlations between samples
    - Non-stationary targets



Slide adapted from David Silver

# Recap: Deep Q-Networks (DQN)

- **Adaptation: Experience Replay**
  - To remove correlations, build a dataset from agent's own experience



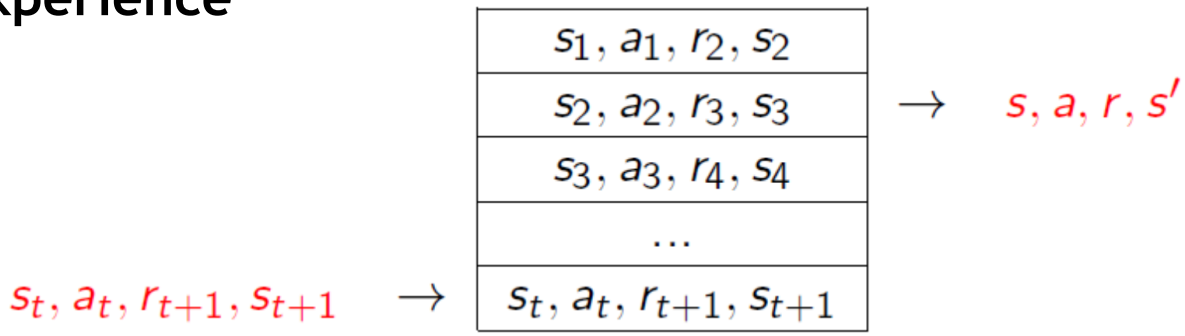

  - Perform minibatch updates to samples of experience drawn at random from the pool of stored samples
    - $(s, a, r, s') \sim U(D)$ where $D = \{(s_t, a_t, r_{t+1}, s_{t+1})\}$ is the dataset
  - Advantages
    - Each experience sample is used in many updates (more efficient)
    - Avoids correlation effects when learning from consecutive samples
    - Avoids feeback loops from on-policy learning



Slide adapted from David Silver

# Recap: Deep Q-Networks (DQN)

- **Adaptation: Experience Replay**
  - To remove correlations, build a dataset from agent's own experience




  - Sample from the dataset and apply an update

$$L(\mathbf{w}) = \left(r + \gamma \max_{a'} Q(s', a', \mathbf{w}^-) - Q(s, a, \mathbf{w})\right)^2$$

  - To deal with non-stationary parameters $\mathbf{w}^-$, are held fixed.
    - Only update the target network parameters every $C$ steps.
    - I.e., clone the network $Q$ to generate a target network $\hat{Q}$.

    $\Rightarrow$ Again, this reduces oscillations to make learning more stable.

# Recap: Policy Gradients

- **How to make high-value actions more likely**
  - **The gradient of a stochastic policy $\pi(s, \mathbf{u})$ is given by**

$$\frac{\partial L(\mathbf{u})}{\partial \mathbf{u}} = \frac{\partial}{\partial \mathbf{u}} \mathbb{E}_\pi [r_1 + \gamma r_2 + \gamma^2 r_3 + \ \ldots \mid \pi(\cdot, \mathbf{u})]$$

$$= \mathbb{E}_\pi \left[ \frac{\partial \log \pi(a|s, \boldsymbol{u})}{\partial \boldsymbol{u}} Q_\pi(s, a) \right]$$

  - **The gradient of a deterministic policy $a = \pi(s)$ is given by**

$$\frac{\partial L(\mathbf{u})}{\partial \mathbf{u}} = \mathbb{E}_\pi \left[ \frac{\partial Q_\pi(s, a)}{\partial a} \frac{\partial a}{\partial \mathbf{u}} \right]$$

  **if $a$ is continuous and $Q$ is differentiable.**

# Recap: Deep Policy Gradients (DPG)

- DPG is the continuous analogue of DQN
  - Experience replay: build data-set from agent's experience
  - Critic estimates value of current policy by DQN

$$L_{\mathbf{w}}(\mathbf{w}) = \left(r + \gamma Q(s', \pi(s', \mathbf{u}^-), \mathbf{w}^-) - Q(s, a, \mathbf{w})\right)^2$$

  - To deal with non-stationarity, targets $\mathbf{u}^-, \mathbf{w}^-$ are held fixed
  - Actor updates policy in direction that improves Q

$$\frac{\partial L_{\mathbf{u}}(\mathbf{u})}{\partial \mathbf{u}} = \frac{\partial Q(s, a, \mathbf{w})}{\partial a} \frac{\partial a}{\partial \mathbf{u}}$$

  - In other words critic provides loss function for actor.

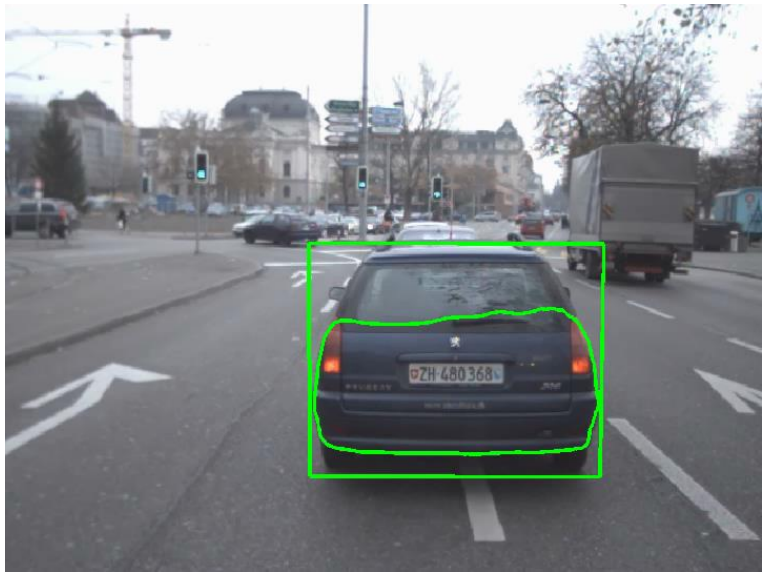


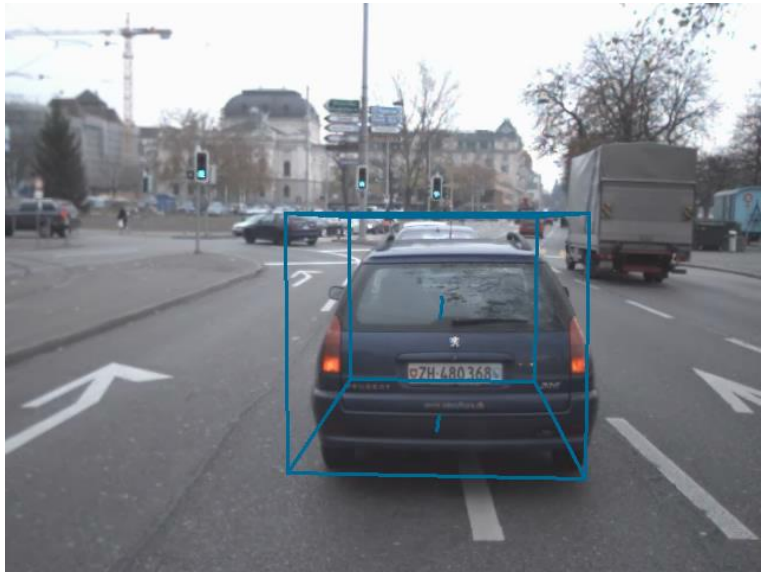
Slide credit: David Silver

# Any Questions?

*So what can you do with all of this?*

# Robust Object Detection & Tracking





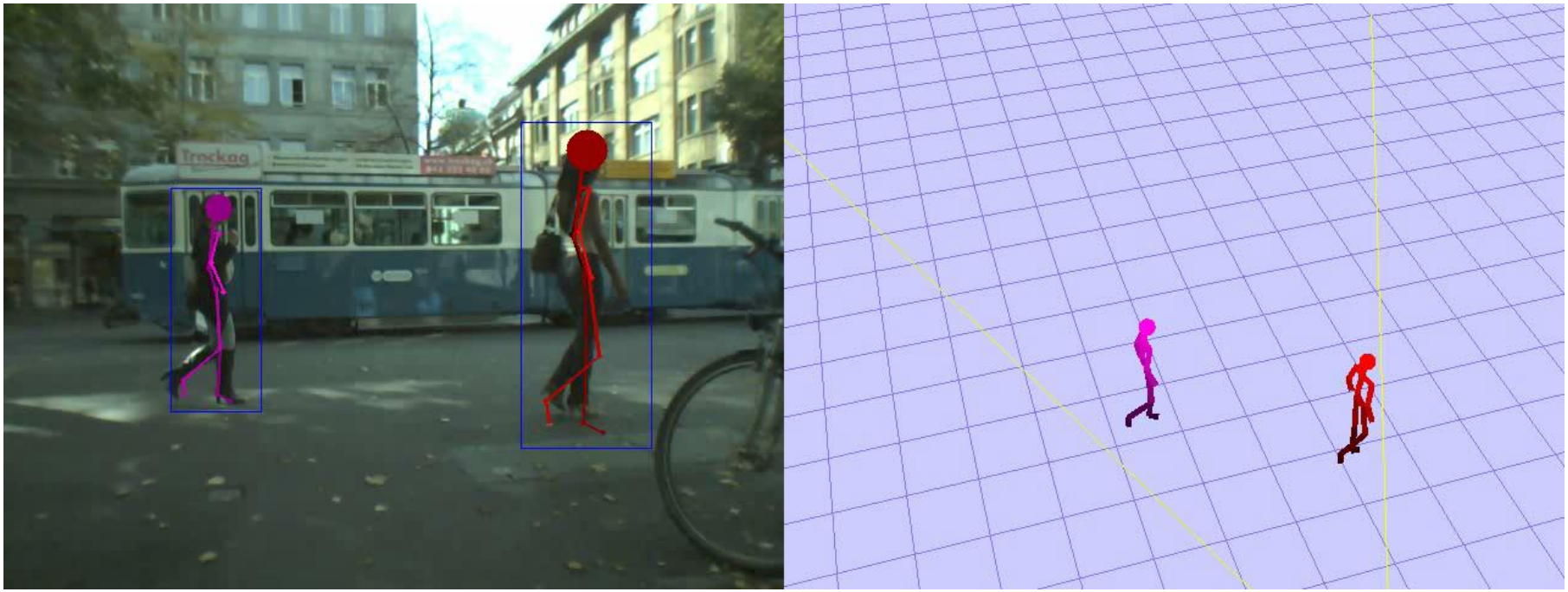
# Applications for Driver Assistance Systems

# Mobile Tracking in Densely Populated Settings




[D. Mitzel, B. Leibe, ECCV'12]

# Articulated Multi-Person Tracking



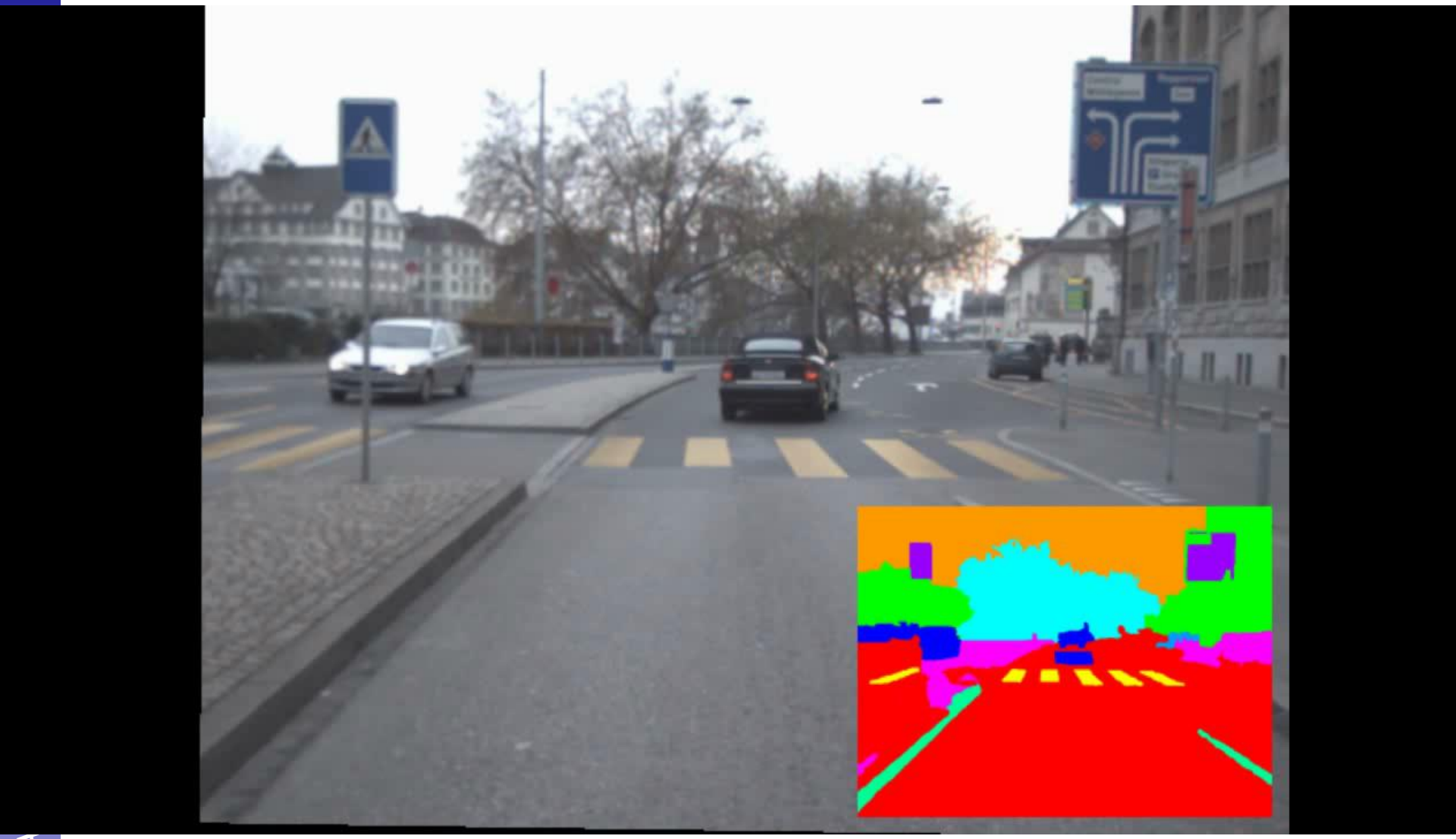
- Multi-Person tracking
  - Recover trajectories and solve data association
- Articulated Tracking
  - Estimate detailed body pose for each tracked person





[Gammeter, Ess, Jaeggli, Schindler, Leibe, Van Gool, ECCV'08]

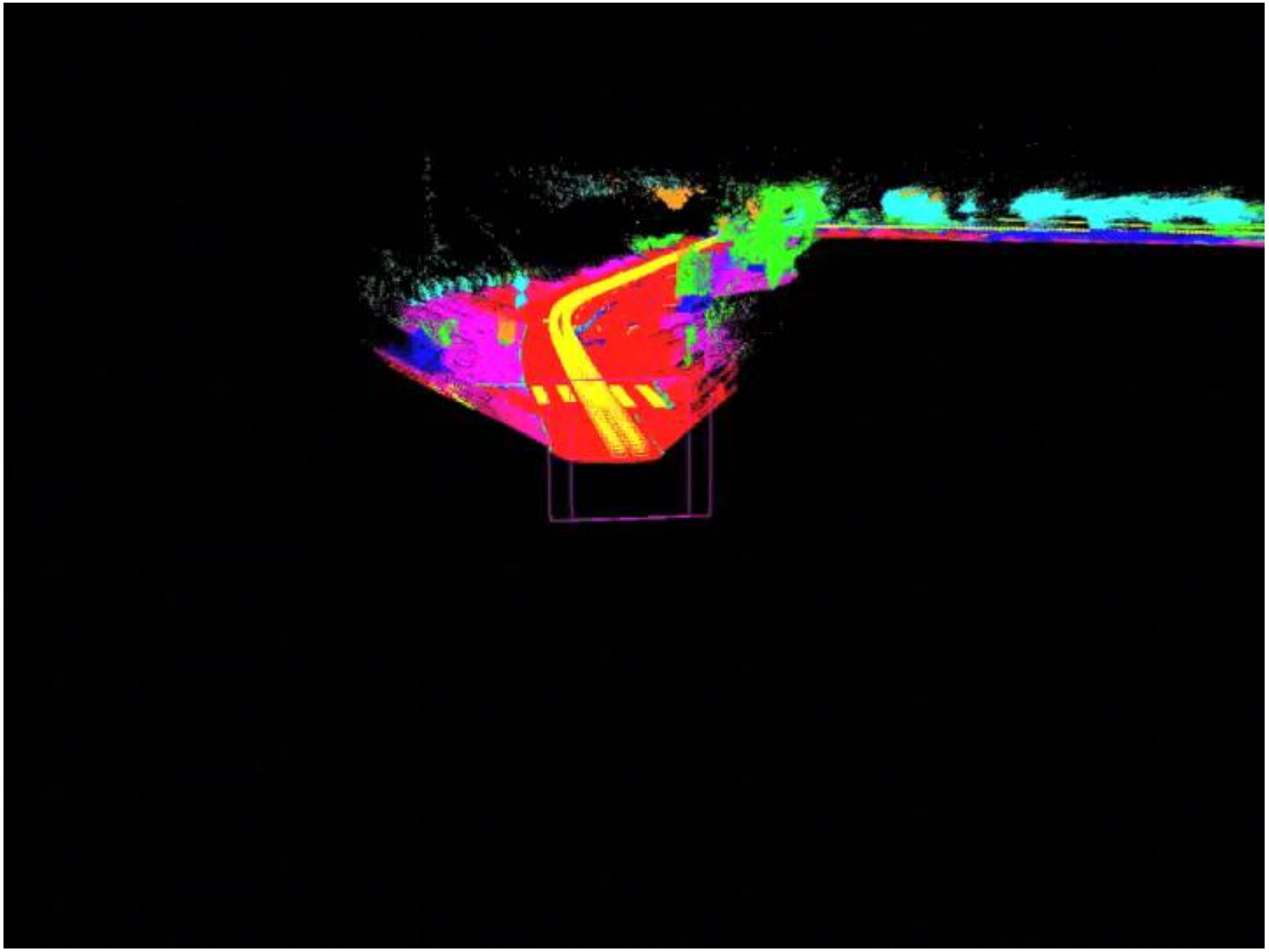
# Semantic 2D-3D Scene Segmentation





[G. Floros, B. Leibe, CVPR'12]

# Integrated 3D Point Cloud Labels





[G. Floros, B. Leibe, CVPR'12]

# Any More Questions?

*Good luck for the exam!*