Deep Learning 과정

Regularization

Gunhee Kim

Computer Science and Engineering

서 울 대 학 교

SEOUL NATIONAL UNIVERSITY

Outline

- Parameter Norm Penalties
  - L2/L1 Regularization
- Data augmentation
- Early Stopping
- Ensemble Methods
- Dropout
- Meta-learning Frameworks

Regularization

Any modification we make to a ML algorithm that is intended to reduce its generalization error but not its training error

Several strategy

- Extra constraints on a machine learning algorithm
- Extra terms in the objective (based on prior knowledge)
- Ensemble methods (combine multiple hypotheses that explain the training data)

Parameter Norm Penalties

Basic form

$$\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) + \alpha\Omega(\boldsymbol{\theta})$$

- $J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y})$: original objective
- $\Omega(\boldsymbol{\theta})$: a parameter norm penalty
- $\alpha \in [0, \infty)$ a hyperparameter that weights the relative contribution of the penalty

Meaning

- Decreasing $\tilde{J}$: decrease both the original objective J on the training data + some measure of the size of parameter $\boldsymbol{\theta}$
- Different choice of $\Omega(\boldsymbol{\theta})$ results in a different solution

L2 Regularization

Drive the weights closer to the origin by adding the term

$$\Omega(\boldsymbol{\theta}) = \frac{1}{2}||\boldsymbol{w}||_2^2$$

- Also known as *ridge regression* or *Tikhonov regularization*

Then the objective $\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} + J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y})$

- Then the gradient is

$$\nabla_{\boldsymbol{w}}\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = \alpha\boldsymbol{w} + \nabla_{\boldsymbol{w}}J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y})$$

- A single gradient step

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \epsilon(\alpha\boldsymbol{w} + \nabla_{\boldsymbol{w}}J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}))$$

$$\boldsymbol{w} \leftarrow (1 - \epsilon\alpha)\boldsymbol{w} - \epsilon\nabla_{\boldsymbol{w}}J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y})$$

Multiplicatively shrink the weight vector by a constant factor on each step

L1 Regularization

Another option: Penalize the nonzero elements

$$\Omega(\boldsymbol{\theta}) = \alpha||\boldsymbol{w}||_1$$

The objective $\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = \alpha||\boldsymbol{w}||_1 + J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y})$

- Then the gradient is

$$\nabla_{\boldsymbol{w}}\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = \alpha\text{sign}(\boldsymbol{w}) + \nabla_{\boldsymbol{w}}J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y})$$

- A regularization effect to each component is a constant factor α with a $\text{sign}(w_i)$, instead of scaling with each w_i in L2

Norm Penalties for Neural Networks

L2 regularization (weight decay) is a common practice

Constraining the norm of each column of the weight matrix of each layer

- Not for the entire matrix
- Prevents any one hidden unit from having very large weights
- A separate α for each column

L1 regularization is only used if having a strong reason

Parameter Typing or Sharing

Sometimes from knowledge of domain, certain parameters should be close to another

Use norm penalty to encourage this

$$\Omega(\boldsymbol{\theta}) = ||\boldsymbol{w}^{(A)} - \boldsymbol{w}^{(B)}||_2^2$$

Parameter sharing: force sets of parameters to be equal

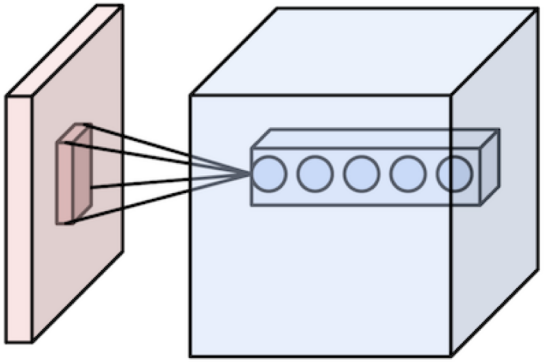
- Popular in practice (especially CNNs)
- Model components share a unique set of parameters

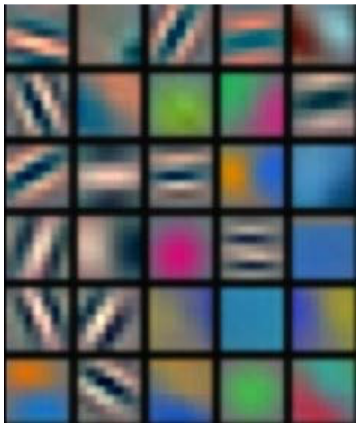
Parameter Sharing in CNNs

Significantly reduction in memory footprint (i.e. model parameters)

Parameter sharing constraints the neurons in each depth slide to use the same weights

- Total number of weights: 30 x 75 = **2,250**





30 Examples of trained weights of size [5x5x3]

Use the same filter across all spatial location!

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Data Augmentation

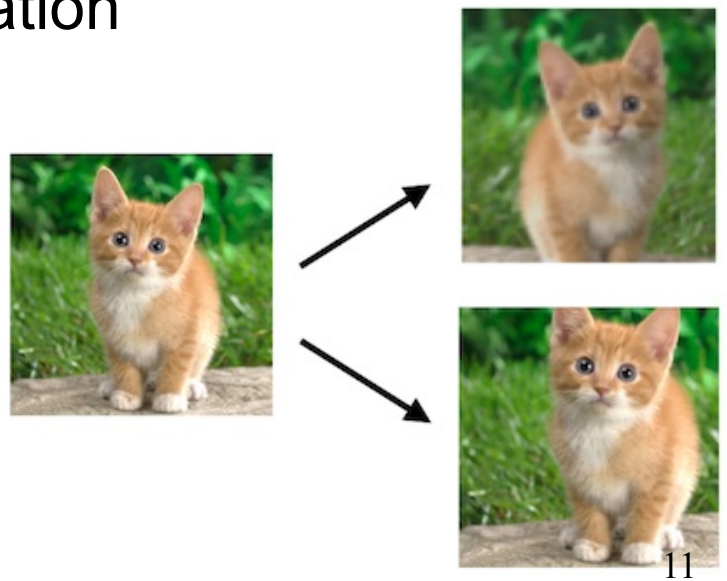
The best way to make ML model generalize better:
More training data

Create fake data from training data!

- For a training sample $(\boldsymbol{x}, y)$, make some transformation $(\boldsymbol{x}', y)$

Very effective for image classification

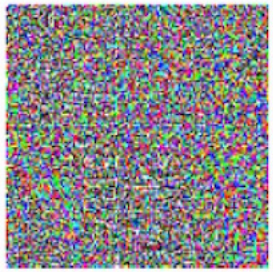
- Images are high-dimensional and have an enormous variety of factors of variation
- (Partial) translating by a few pixels, rotating, scaling, and flipping



Noise injection

Neural Networks are not robust against noise

$+ .007 \times$



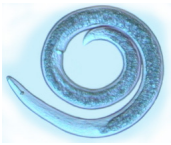
$=$

$\boldsymbol{x}$

$\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$

$\boldsymbol{x} + \epsilon\,\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$

$y =$"panda"
w/ 57.7%
confidence



"nematode"
w/ 8.2%
confidence

"gibbon"
w/ 99.3 %
confidence

Noise injection

Injecting noise in the input can be seen a form of data augmentation

- Highly effective
- Can be seen as regularization

Different ways of noise injection

- A random noise to input
- Noise injection to parameters (or models) (~ Tikhonov regularization)
- Noise at the output targets (e.g. label smoothing)

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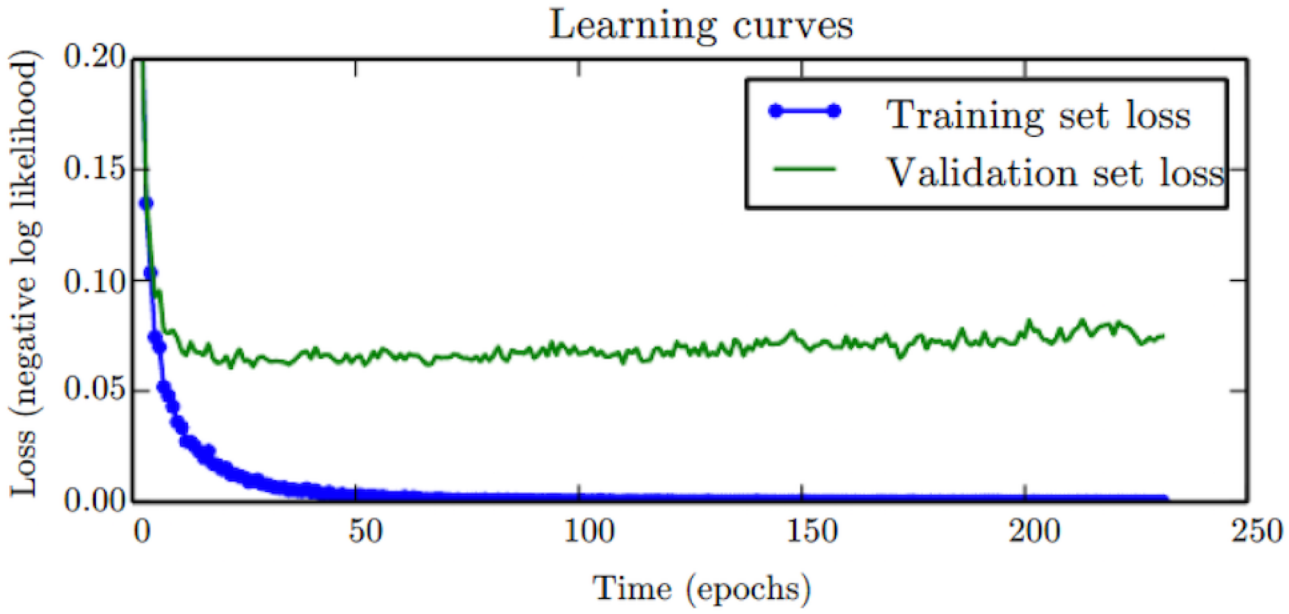
Early Stopping

A conventional learning cover (negative log-likelihood)

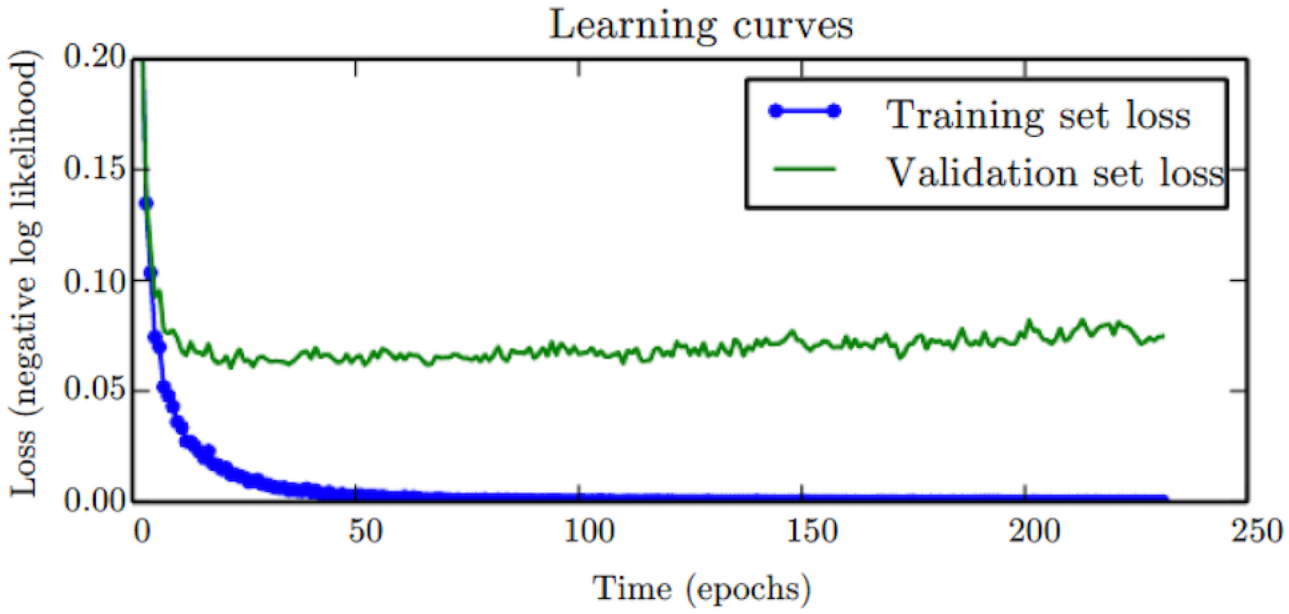
- e.g. Maxout network on MNIST
- The training objective decreases consistently over time
- The validation loss forms an asymmetric U-shaped curve



Early Stopping

Idea: use the parameters at the minimum validation error

- Maintain a copy of model parameters every iteration
- Additional cost is negligible (+ occasional slow writes)
- A kind of hyperparameter selection algorithm (training time)



Properties of Early Stopping

A very unobstrusive form of regularization

- No change in training procedure, objective, etc.
- Can be used jointly with other regularization

Another strategy for using all of the training data

- Early stopping requires a validation set (could seem wasteful)
- Learning the model with training data w/o validation set first + Continue training using all data until the validation loss falls below the training loss

Regularization effect (decreasing generalization error) + reduction of training time

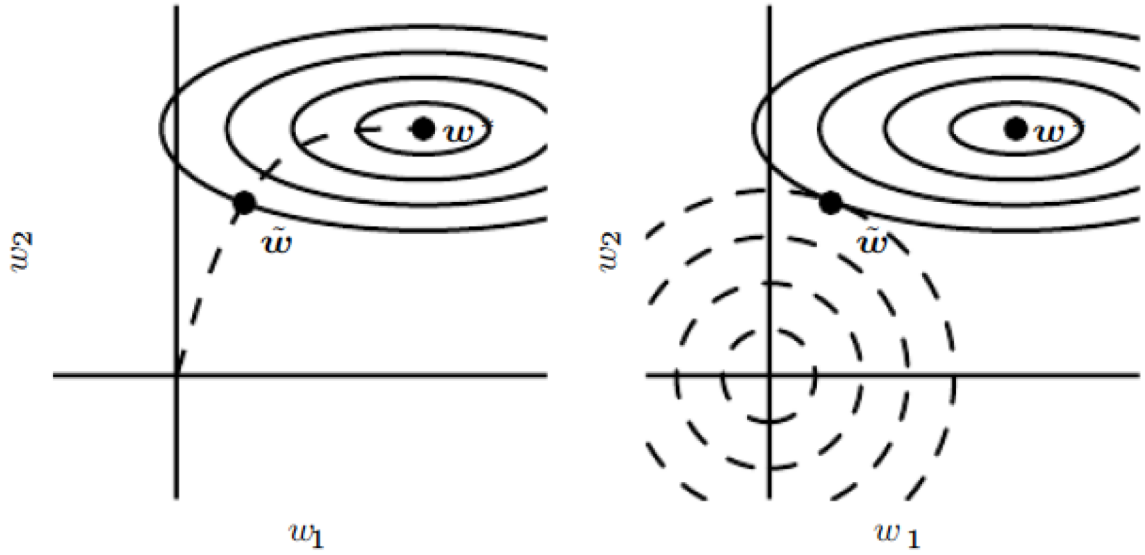
Early Stopping as a Regularizer

Restrict an optimization procedure to a relatively small volume of parameter space from initial parameter $\boldsymbol{\theta}_0$

- A SGD with a learning rate ϵ and τ training iterations
- $\epsilon\tau$: the volume of parameter space reachable from $\boldsymbol{\theta}_0$

The trajectory taken by SGD beginning from the origin

- Stop at $\tilde{\boldsymbol{w}}$ rather than stopping real minimum $\boldsymbol{w}^*$



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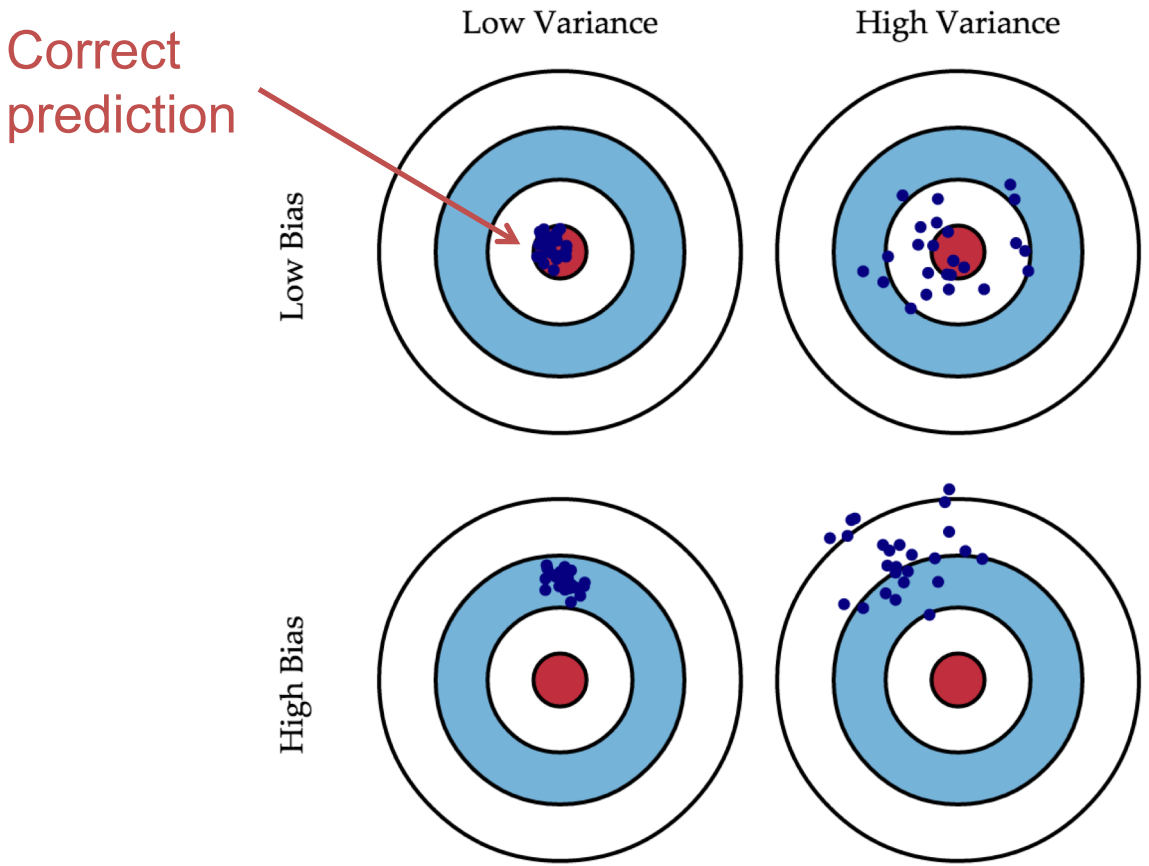
Bias and Variance

Two sources of error in an estimator: bias and variance

(Test Error) = (Bias) + (Variance)



Low bias: predicted well

Low variance: Stable

Bagging (Bootstrap Aggregating)

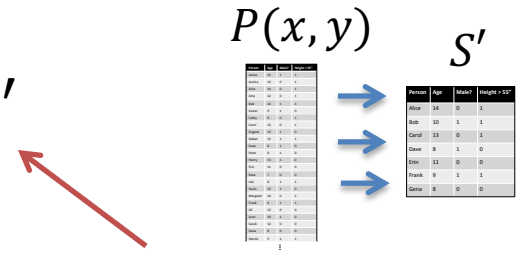
Goal: reduce variance

Variance reduces linearly
Bias unchanged

Expected Error = **Variance** + Bias

Ideal setting: many training sets S'

- Train model using each S'
- Average predictions



Bootstrapping

In practice: Resample S' with replacement ($|S'| = S$)

- cf. Jackknife: Given a sample of size N, generate $N - 1$ sets by ignoring one observation at each time

"Bagging Predictors" [Leo Breiman, 1994]
http://statistics.berkeley.edu/sites/default/files/tech-reports/421.pdf

Bagging (Bootstrap Aggregation)

Given: Training Set S

Bagging: Generate many bootstrap samples S'

Repeat M times

- Sampled with replacement from S ($|S'| = S$)
- Train minimally regularized classifier (ex. DT) on S'

Final predictor: Combine M predictors

- Voting for classification problems
- Averaging for estimation problems
- Averaging reduces variance

Ensemble Methods for Neural Networks

Highly recommended!

- Model averaging is an extremely powerful and reliable for reducing generalization error

NNs reach a wide variety of solution points

- Never obtain the same solution at each running
- random initialization, random selection of minibatches, different hyperparameter setting, …

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Dropout

A method of making bagging practical for ensembles of very many large NNs

- An inexpensive approximation to training and evaluating a bagged ensemble of exponentially many NNs

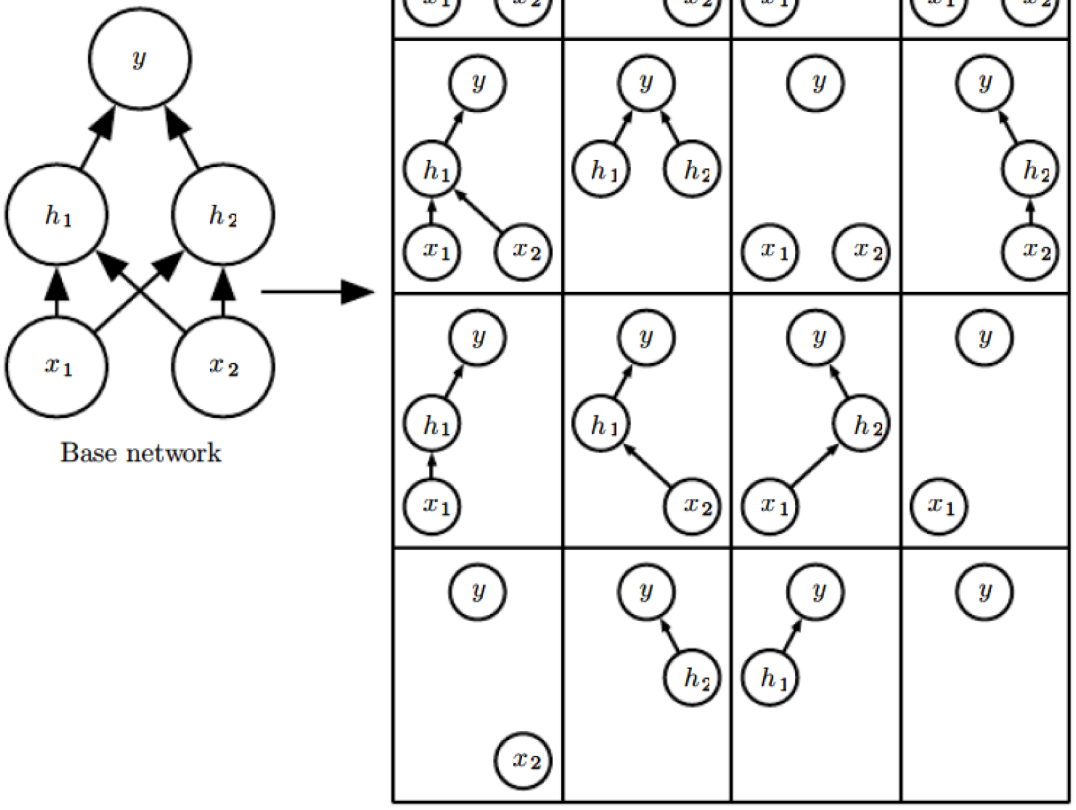
Suppose that we have a big NN model and optimize it with a minibatch-based learning algorithm (e.g. SGD)

- For each minibatch, randomly sample a different binary mask to apply to all of the input and hidden units in the network
- In other words, randomly drop the output of units to zero
- e.g. dropout rate 0.5 for hidden units and 0.2 for input nodes
- Then use learning algorithm as usual

Dropout

A base network with two input and two hidden units

16 possible subsets



Ignore the ones with no input or no paths to output

Properties of Dropout

Comparison with Bagging

- In dropout, the models share parameters
- With each minibatch, a different subset of parameter is updated
- In bagging, the models are all independent

Dropout is very effective and highly recommended

- More effective than other regularizers
  (e.g. weight decay, sparsity)

Computationally very cheap

No limitation on model types or training procedures (e.g. CNNs, RNNs, and RBMs)

Properties of Dropout

Increase the size of the model to offset the regularizer

- Dropout reduces the effective capacity of a model

Do not use Dropout with very few training examples

Key insights

- Training a network with stochastic behavior and making predictions by averaging over multiple stochastic decisions
- Dropout power arises from that masking noise is applied to hidden units

Other relatives: dropconnect, batch normalization

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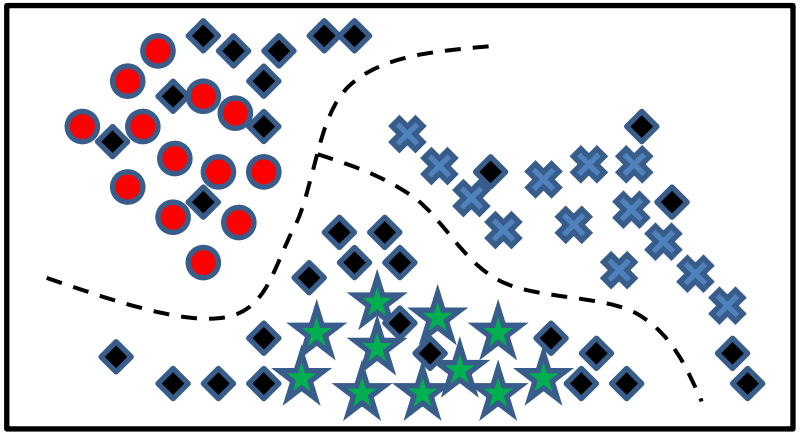
Semi-supervised Learning

Use unlabeled data to augment a small labeled sample to improve learning

- Labeled data can be rare or expensive, while unlabeled data is much cheaper
- Model the generative process too
- One of active research areas



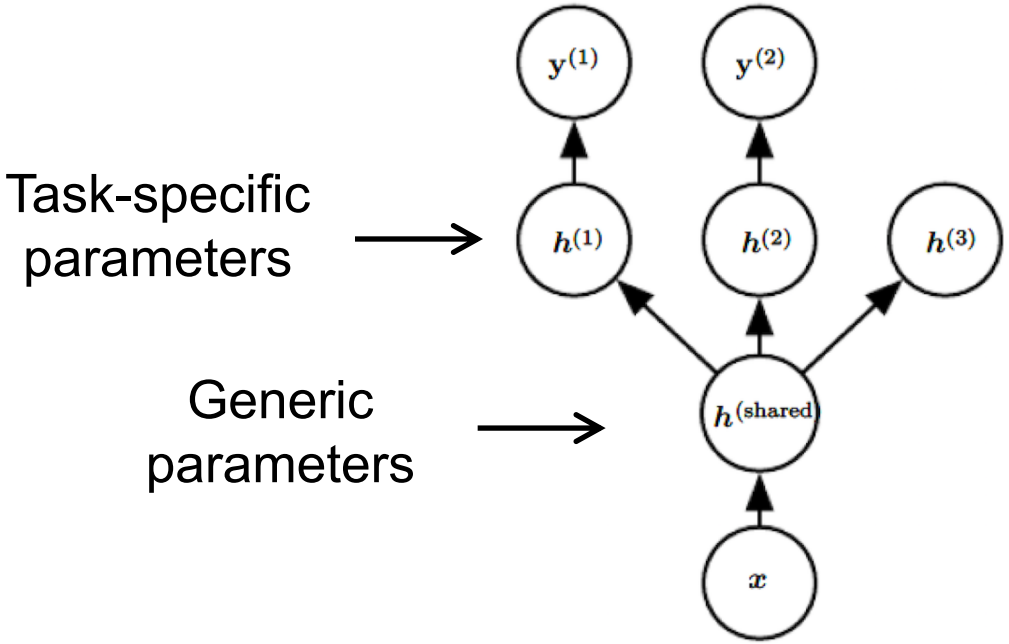
Semi-supervised learning

Multi-task Learning

Learn multiple-related problems together at the same time

- e.g. Image classification and object detection

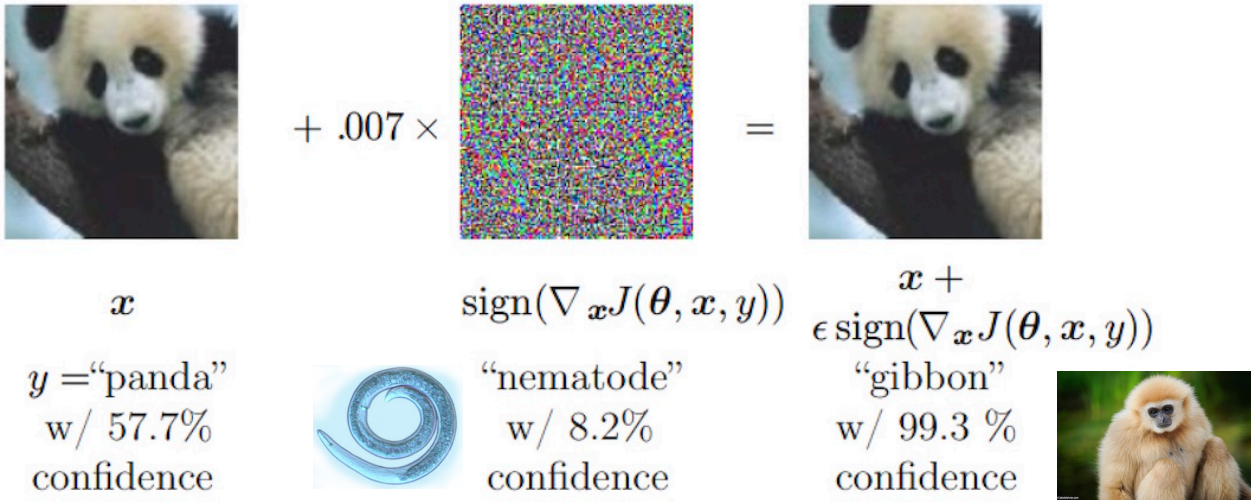
Two different supervised tasks (predicting $\boldsymbol{y}^{(i)}$), while sharing input $\boldsymbol{x}$ and some mid-level representation $\boldsymbol{h}^{(\text{shared})}$



Adversarial Training

Adversarial examples

- Human cannot tell the difference with the original example
- However, the network can make highly different predictions



Adversarial training: training on adversarially perturbed examples

- Purely linear models do not resist them