Lecture 5
Regularization in Deep Neural Networks

CMSC 35246: Deep Learning

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  - Norm Penalties (weight decay)

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  - Early Stopping as a form of Regularization

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  - Dropout
  - Other Approaches that have a regularizing effect

Housekeeping

- Quiz scores will be uploaded after class
- Projects:
  - One page proposal due 19 April 23:59
  - Summarize the task of interest and why is it of interest to you
  - Describe the dataset intended for use
  - Roughly: What model do you want to use?
  - What framework do you plan to use?
- Mid Term dates will be announced on Wednesday

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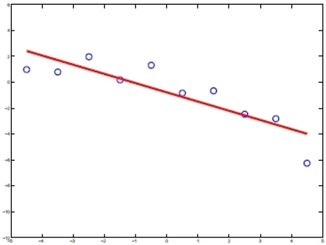
- **More generally:** Any modification to a learning algorithm intended to reduce its generalization error but not its training error

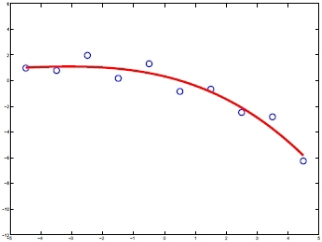
Training Regimes



$$m = 1$$

- **Regime 1 in training:** Model family excludes the true generation process (underfitting, high bias)

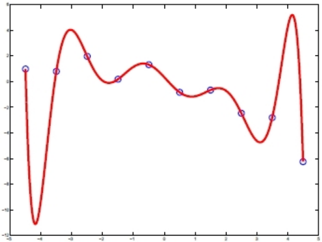
Training Regimes



$$m = 3$$

- **Regime 2 in training:** Model family matches the true generative process

Training Regimes



$$m = 10$$

- **Regime 3 in training:** The generative process is included but many other generating processes as well (overfitting!)

Regularization

Goal of Regularization: Take a model from the third regime to second regime

In Deep Learning

A trend: Use extremely large models (high capacity) and then regularize strongly (try to limit capacity)

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"If you are not in the small-data regime, you should just use a bigger model so that you are in the small-data regime. You should always be in the small-data regime." – David Belanger

Yet another quote

Geoffrey Hinton: "The brain has about 10^{14} synapses and we live for about 10^{9} seconds. So we have a lot more parameters than data."

- Note: $\#$ synapses $\equiv \#$ parameters is problematic, so is the use of seconds as a unit. But the point remains: *Large looking model, small data*

- Open area of research: How do deep learning models generalize with such large models that can "memorize" the data

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- Personal "Conjecture" (feel free to ignore!): A reasonable upper bound on the Kolmogorov Complexity of models with good generalization performance will turn out to be small i.e. they are essentially simple models, not as complex as they seem. Generalization in this case is a result of parsimony.

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- α is the tradeoff parameter
  - $\alpha = 0$ implies no regularization
  - High value of α implies strong regularization

Penalizing the $L2$ norm

- Let's fold in all parameters θ i.e weight matrices, biases etc. into $\mathbf{w}$ (although biases are usually not regularized)

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- The corresponding gradient then is:

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

Penalizing the $L2$ norm

- Familiar gradient update:

$$\mathbf{w} := \mathbf{w} - \epsilon(\alpha \mathbf{w} + \nabla_{\mathbf{w}} J(\mathbf{w}; X, y))$$

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- Let's re-write it:

$$\mathbf{w} := (1 - \epsilon\alpha)\mathbf{w} - \epsilon\nabla_{\mathbf{w}} J(\mathbf{w}; X, y)$$

Update Rule

- Old update rule (without the penalty; seen before!):

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- **Interpretation:** Multiplicatively *shrink* weight vector by a constant factor before performing the usual gradient update
- This is the origin of the terminology *weight decay*

Update Rule for One Weight Matrix

$$\begin{bmatrix} w_{11} & w_{12} & w_{13} & \dots & w_{1n} \\ w_{21} & w_{22} & w_{23} & \dots & w_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \\ w_{n1} & w_{n2} & w_{n3} & \dots & w_{nn} \end{bmatrix} = (1 - \epsilon\alpha) \begin{bmatrix} w_{11} & w_{12} & w_{13} & \dots & w_{1n} \\ w_{21} & w_{22} & w_{23} & \dots & w_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \\ w_{n1} & w_{n2} & w_{n3} & \dots & w_{nn} \end{bmatrix} - \epsilon \nabla_W J(\mathbf{w}; X, y)$$

$\epsilon \nabla_W J(\mathbf{w}; X, y)$ is also a $n \times n$ matrix

A Simple Analysis

$L2$ Penalty: Analysis

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- Note that $\nabla_{\mathbf{w}} J(\mathbf{w}) = H(\mathbf{w} - \mathbf{w}^*)$ (just differentiate the quadratic approximation)

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- To understand what weight decay does, modify above by adding weight decay gradient:

$$\alpha\tilde{\mathbf{w}} + H(\tilde{\mathbf{w}} - \mathbf{w}^*) = 0$$

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- Rearranging, we have:

$$\tilde{\mathbf{w}} = (H + \alpha I)^{-1} H \mathbf{w}^*$$

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- Plug decomposition in above equation and rearrange:

$$\tilde{\mathbf{w}} = Q(\Lambda + \alpha I)^{-1} \Lambda Q^T \mathbf{w}^*$$

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- What is the interpretation of this?

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- What is the interpretation of this?
- Effect of weight decay: Rescale $\mathbf{w}^*$ (the optimal solution for the unregularized objective) along axes defined by the H
- Coordinate of $\mathbf{w}^*$ that is aligned with the ith eigenvector of H is rescaled by $\frac{\lambda_i}{\lambda_i + \alpha}$

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    - Directions which contribute significantly to reducing the objective function value are kept relatively intact

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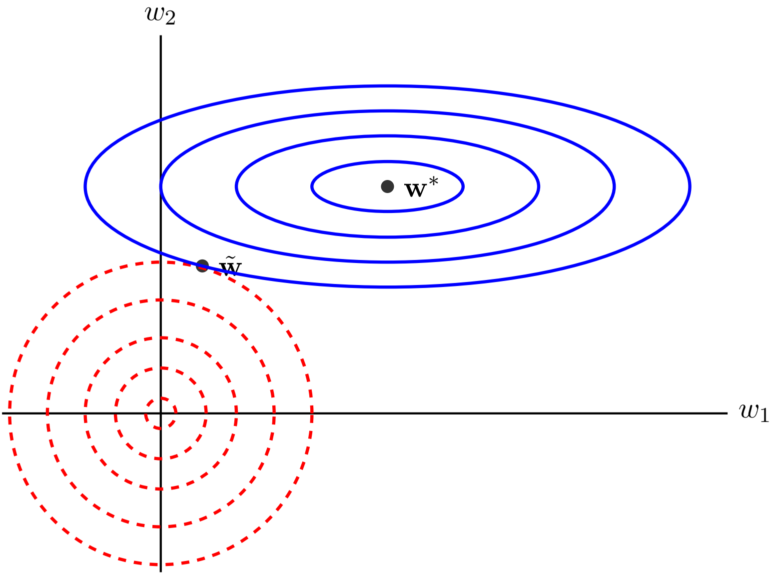
- Directions for which $\lambda_i \ll \alpha$ the $\mathbf{w}_i^*$ coordinate will shrink to nearly zero
- In English:
  - Directions which contribute significantly to reducing the objective function value are kept relatively intact
  - Directions that make little contribution to reducing the objective function value are killed off

$L2$ Penalty: Analysis



$L1$ Weight Decay

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- We penalize the absolute value of parameters

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- Recall the gradient for the $L2$ penalty:

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- Regularization contribution is only a constant α with $sign$ equal to $sign(w_i)$

Simple Analysis

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- Consider the case when $w_i^* > 0 \forall i$
  - When $w_i^* < \frac{\alpha}{H_{i,i}}$, value of regularized objective $w_i = 0$

Simple Analysis

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- Consider the case when $w_i^* > 0 \forall i$
  - When $w_i^* < \frac{\alpha}{H_{i,i}}$, value of regularized objective $w_i = 0$
  - When $w_i^* > \frac{\alpha}{H_{i,i}}$, value of w_i is shifted towards zero by $\frac{\alpha}{H_{i,i}}$

Simple Analysis

$$w_i = sign(w_i^*) \max \left\{ |w_i^*| - \frac{\alpha}{H_{i,i}}, 0 \right\}$$

- Consider the case when $w_i^* > 0 \forall i$
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- Conclusion: $L1$ results in a sparser solution (as compared to $L2$)

Early Stopping

Bagging

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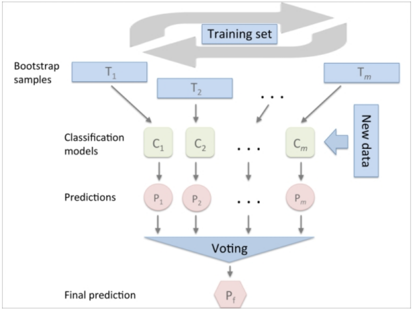

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- The average prediction of the k predictors:

$$\frac{1}{k} \sum_i \epsilon_i$$

Why does Bagging work?

- The expected squared error of the ensemble:

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- Error decreases linearly with ensemble size
- On average the ensemble performs atleast as well as any of its members

Reference

"Bagging Regularizes", Tomaso Poggio, Ryan Rifkin, Sayan Mukherjee, Alex Rakhlin, 2002

Dropout

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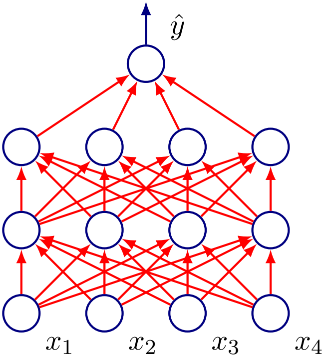

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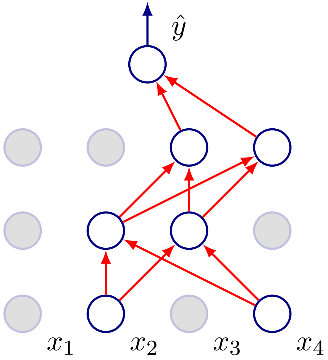

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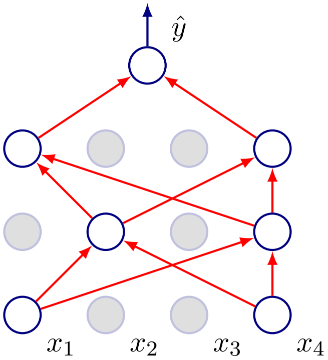

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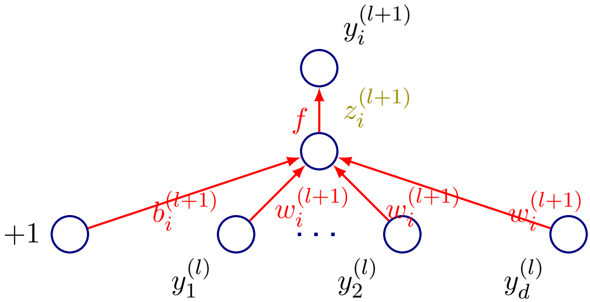
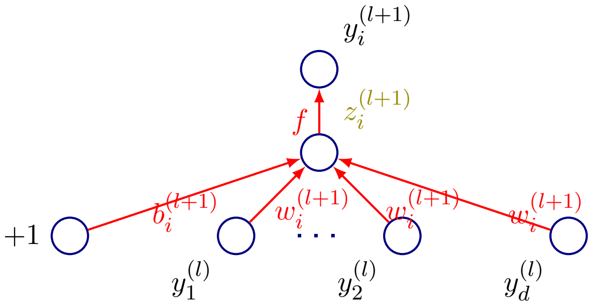


Without Dropout



- $z_i^{(l)} = \mathbf{w}^{(l+1)T}\mathbf{y}^{(l)} + b_i^{(l+1)}$ and $y_i^{(l+1)} = f(z_i^{(l+1)})$

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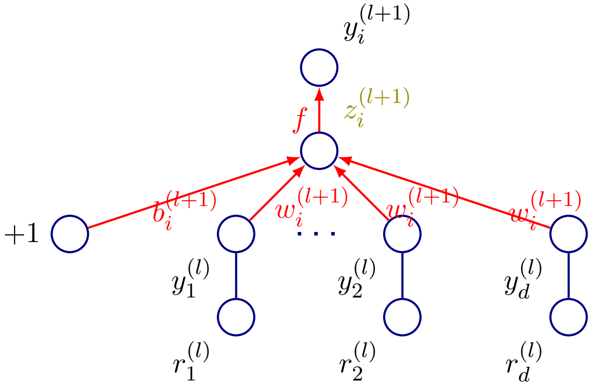

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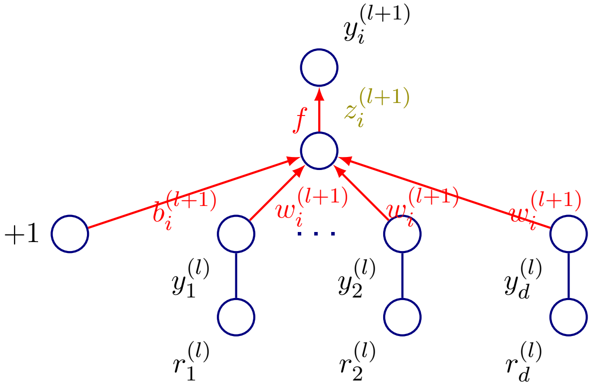

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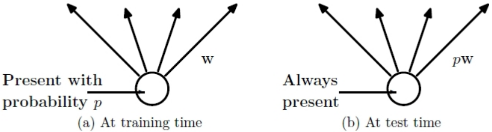

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- We minimize the loss function stochastically under a noise distribution: Minimizing an expected loss function
- During test time, we only want the expected output of each neuron, so weights are scaled down by p

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Why Else does Dropout work?

- Noise injection at input, hidden layers

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- Can also cause shrinkage: Let's see a toy example

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- We now have a expected loss function:

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- Γ scales down weight cost for each w_i by the standard deviation of ith dimension of data

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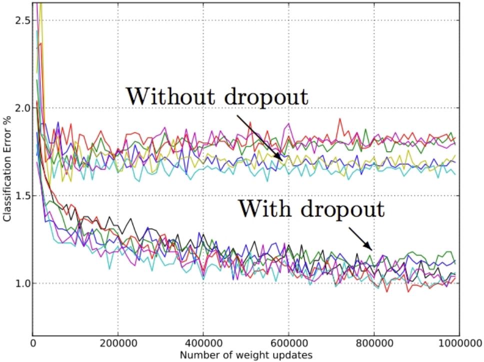
- Another interpretation: When p is close to one all inputs are retained and regularization constant is small

Dropout: Performance

These architectures have 2 to 4 hidden layers with 1024 to 2048 hidden units

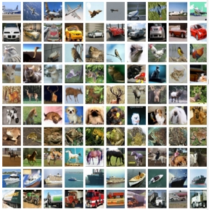


Dropout: Performance

(a) Street View House Numbers (SVHN)

Method	Error %
Binary Features (WDCH) (Netzer et al., 2011)	36.7
HOG (Netzer et al., 2011)	15.0
Stacked Sparse Autoencoders (Netzer et al., 2011)	10.3
KMeans (Netzer et al., 2011)	9.4
Multi-stage Conv Net with average pooling (Sermanet et al., 2012)	9.06
Multi-stage Conv Net + L2 pooling (Sermanet et al., 2012)	5.36
Multi-stage Conv Net + L4 pooling + padding (Sermanet et al., 2012)	4.90
Conv Net + max-pooling	3.95
Conv Net + max pooling + dropout in fully connected layers	3.02
Conv Net + stochastic pooling (Zeiler and Fergus, 2013)	2.80
Conv Net + max pooling + dropout in all layers	2.55
Conv Net + maxout (Goodfellow et al., 2013)	**2.47**
Human Performance	2.0

Table 3: Results on the Street View House Numbers data set.



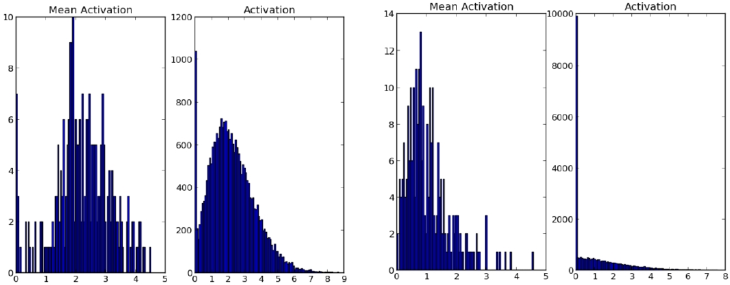
(b) CIFAR-10

Method	CIFAR-10	CIFAR-100
Conv Net + max pooling (hand tuned)	15.60	43.48
Conv Net + stochastic pooling (Zeiler and Fergus, 2013)	15.13	42.51
Conv Net + max pooling (Snoek et al., 2012)	14.98	-
Conv Net + max pooling + dropout fully connected layers	14.32	41.26
Conv Net + max pooling + dropout in all layers	12.61	**37.20**
Conv Net + maxout (Goodfellow et al., 2013)	**11.68**	38.57

Table 4: Error rates on CIFAR-10 and CIFAR-100.

Dropout: A simple way to prevent neural networks from overfitting, N Srivastava, G Hinton, A Krizhevsky, I Sutskever, R Salakhutdinov, JMLR 2014

Dropout: Effect on Sparsity



(a) Without dropout (b) Dropout with $p = 0.5$.

Dropout: A simple way to prevent neural networks from overfitting, N Srivastava, G Hinton, A Krizhevsky, I Sutskever, R Salakhutdinov, JMLR 2014

Why does this make sense?

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  - Shrinkage
- Some motivations:

Motivation

- **Motivation 1:** Ten conspiracies each involving five people is probably a better way to wreak havoc than a conspiracy involving 50 people. If conditions don't change (stationary) and plenty of time for rehearsal, a big conspiracy can work well, but otherwise will "overfit"

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- **Motivation 2:** Comes from a theory for the superiority of sexual reproduction in evolution (Livnat, Papadimitriou, PNAS, 2010).
- Criterion for natural selection may not be individual fitness but mixability. Thus role of sexual reproduction is not just to allow useful new genes to propagate but also to ensure that complex coadaptations between genes are broken.

Dataset Augmentation

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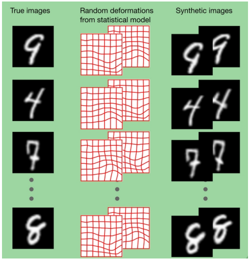

Image Credit: Søren Hauberg

- Warning: Be careful in what transformations you apply to your data

Noise Injection

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- Generally: Noise injection can be much more powerful than penalizing the parameters
- In what other ways can we add noise ?

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- Let the perturbed model be denoted as: $\hat{y}_{\epsilon_W}$

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- Observation: For small η, minimization of J with added noise, is equivalent to minimization of J with an extra regularization term $\eta\mathbb{E}_{p(\mathbf{x},y}[\|\nabla_W \hat{y}\|]$
- This automatically pushes the model into regions where it is relatively insensitive to perturbations in the weights (Hochreiter and Schmidhuber, 1995)

Injecting noise into outputs

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Injecting noise into outputs

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- How can this problem be solved?

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- This is an old idea in Machine Learning going to the early 80s

Multi-Task Learning

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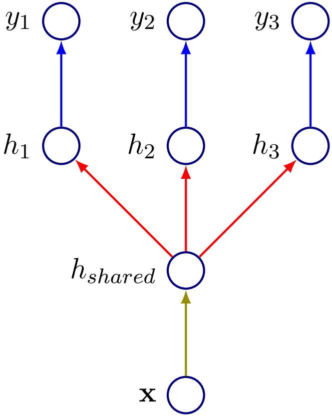

Parameter Sharing

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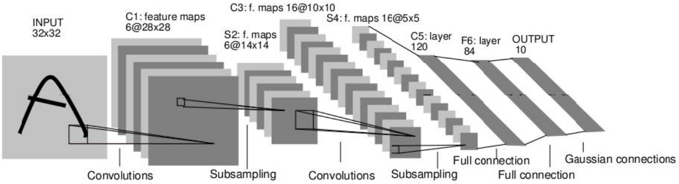
- Popular way to use constraints: Force sets of parameters to be equal



Representational Sparsity

Recap

- Recall parameter penalized objective from earlier:

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- We saw that the $L1$ penalty encouraged parameters to be *sparse*

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- h represents the hidden unit activations

Illustration: Parameter Sparsity

$$\underbrace{\begin{bmatrix} 7 \\ -43 \\ 3 \\ -74 \\ 29 \\ -15 \end{bmatrix}}_{\text{Output, } \mathbf{y}} = \underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 4 \\ 0 & -9 & 0 & 0 & 0 & -3 \\ -1 & 0 & 0 & 0 & -7 & 0 \\ 0 & 0 & 0 & 5 & 5 & -1 \\ 0 & 0 & 0 & -9 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}}_{\text{Parameters, } W} \underbrace{\begin{bmatrix} -1 \\ 5 \\ -7 \\ -4 \\ 6 \\ 3 \end{bmatrix}}_{\text{Input, } \mathbf{x} \text{ or } \mathbf{h}}$$

- Sparsity in parameters (possibly induced by a $L1$ penalty on parameters)

Illustration: Representational Sparsity

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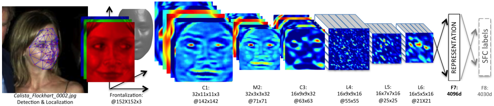
- Efficiently solvable when W is constrained to be orthogonal
- People who have seen sparse coding will recognize this!

Adversarial Training

Motivation

- Since 2014 or so, Deep Neural Networks have matched human performance on some specific tasks:
  - Face recognition (Taigman *et al.*, CVPR 2014)



  - Reading addresses
  - Solving Captchas
  - ...

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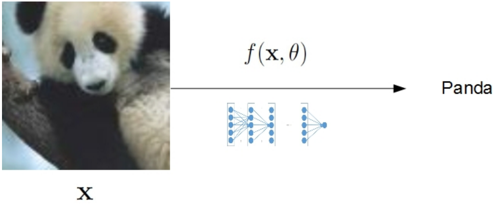

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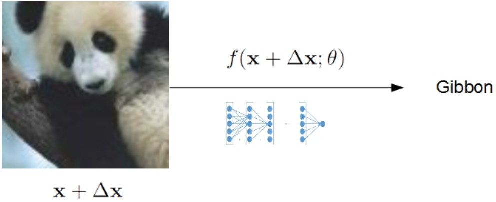

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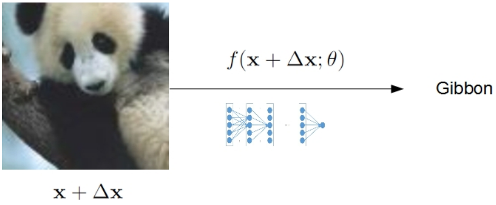

- Obvious optimization problem:

$$\arg\min_{\Delta\mathbf{x}} \|\Delta\mathbf{x}\| \text{ s.t. } f(\mathbf{x} + \Delta\mathbf{x}; \theta) = y_g$$

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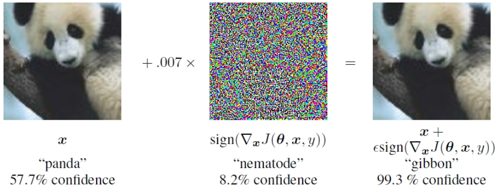

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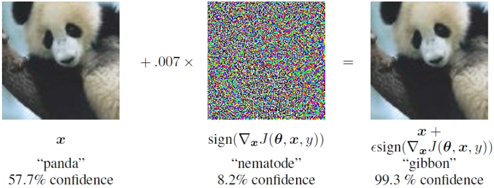

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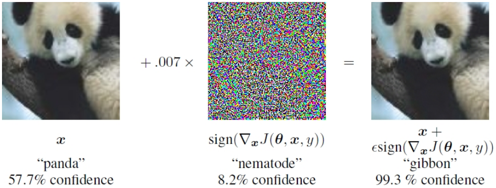

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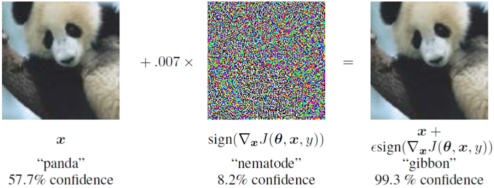

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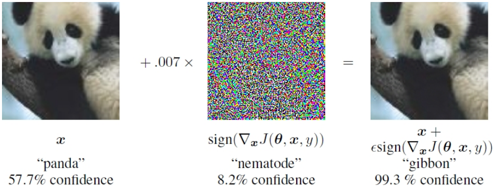

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- Interesting properties: Such examples often generalize across datasets and models (implications for computer security!)
- Not specific to deep networks!
- Designing networks resistant to adversarial attacks is a very active (and important) area of research

Adversarial Training

- Recall the optimization problem

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- A form of regularization like dataset augmentation, robustifying the network to perturbations

Next time

- Optimization Methods for Deep Neural Networks