# Regularization in Deep Learning

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Seminar "Introduction to Deep Learning"

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January 13, 2017

# Structure

# What is regularization?

*Regularization is any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error*

[Goodfellow et al., 2016]

# Concept of overfitting

- Goal of model: perform well on unobserved input data
- Two competing tasks:

↓Train error vs. ↓Gap between train and test ($\widehat{=}$ generalization) error
↓Underfitting vs. ↓Overfitting

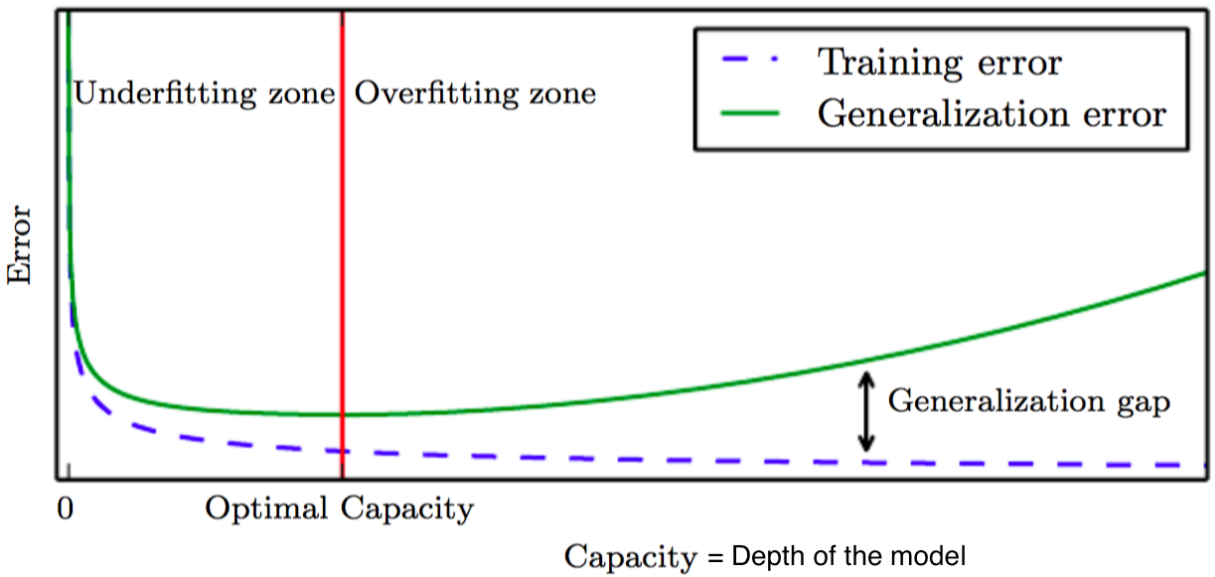



**Figure:** [Goodfellow et al., 2016]

- Generalization gap depends on ratio: $\frac{\text{complexity of the model}}{\#\text{train data}} \widehat{=} \frac{\text{depth of the net}}{\#\text{train data}}$

# Illustration of overfitting

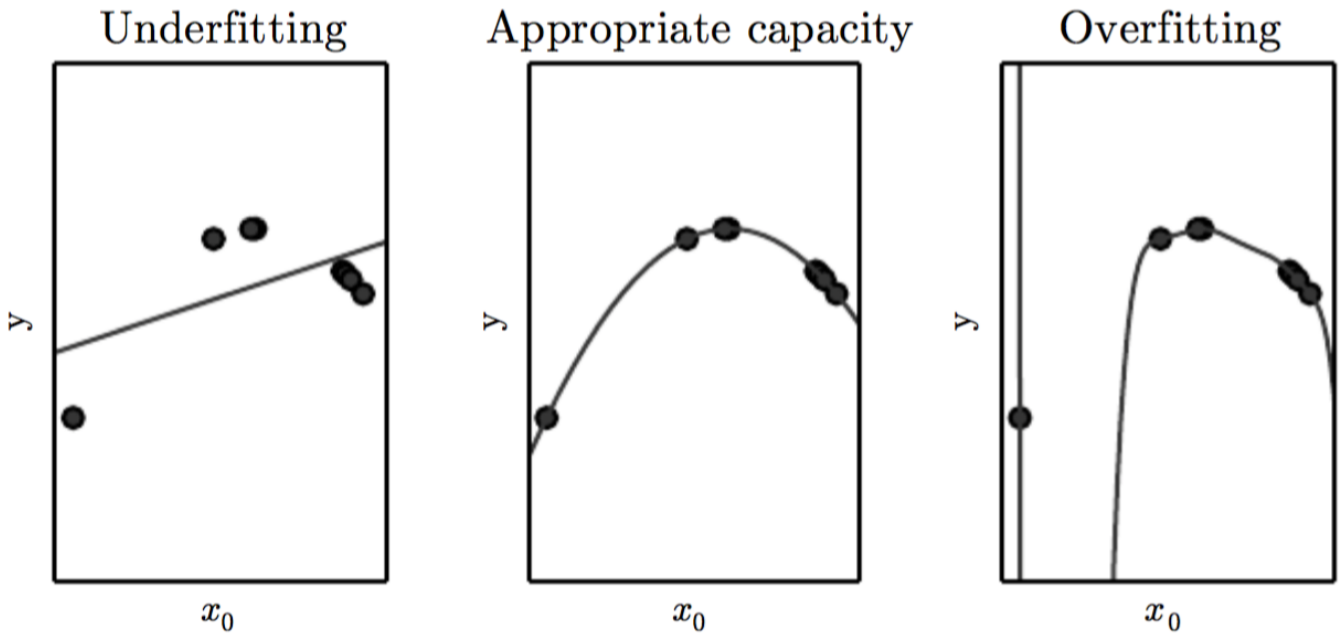



**Figure:** [Goodfellow et al., 2016]

with capacity $\widehat{=}$ model complexity $\widehat{=}$ depth of net $\widehat{=}$ number of updates $m$

# Structure

# Basic concept

- Limit capacity of model $\rightarrow$ limit expression of its parameters
- Penalize the model for large parameters
- Add penalty $\Omega(\theta)$ on the parameter norm such that:

$$\tilde{J}(\theta; X, y) = J(\theta; X, y) + \alpha\Omega(\theta), \text{ with } \alpha \geq 0 \tag{1}$$

- Linear models: parameters $\theta \mathrel{\widehat{=}}$ coefficients $\beta$
- Neural networks: parameters $\theta \mathrel{\widehat{=}}$ weights $\omega$
- No penalization of biases $b$:
  - Less data required for fitting $b$ than $\omega$
  - One bias per unit, n weights per unit (in vanilla net)
  - Possible consequence of bias-regularization: underfitting

# $L^2$-penalization // the superstar

- Analogue to **ridge regression**: $\Omega(\theta) = \frac{1}{2}||\omega||_2^2$ such that

$$\tilde{J}(\theta; X, y) = \alpha\omega^T\omega + J(\theta; X, y) \tag{2}$$

with gradient:

$$\nabla_\omega \tilde{J}(\theta; X, y) = \alpha\omega + \nabla_\omega J(\theta; X, y) \tag{3}$$

- Most popular regularizer
- One weight update using gradient descent:

$$\begin{aligned} &\omega^{m+1} \leftarrow \omega^m - \gamma(\nabla_\omega \tilde{J}(\theta; X, y)) = (1 - \gamma\alpha)\omega^m - \gamma\nabla_\omega J(\omega; X, y) \\ &\Rightarrow \text{Shrinkage of } \omega \text{ in each iteration} \end{aligned} \tag{4}$$

- Therefore termed **weight decay** in neural net applications

# Discovering the effect of weight decay I

1. Quadratic Taylor-approximation of unregularized $J(\theta)$ with $\theta = \omega$ at minimum $\omega^* = \mathit{argmin}_\omega J(\omega)$:

$$\begin{aligned}\hat{J}(\theta) &= J(\omega^*) + \frac{1}{1!}\frac{\partial J(\omega^*)}{\partial \omega}(\omega - \omega^*) + \frac{1}{2!}\frac{\partial^2 J(\omega^*)}{\partial \omega \partial \omega}(\omega - \omega^*)^2 \\ &= J(\omega^*) + \frac{1}{2}(\omega - \omega^*)^T H(\omega - \omega^*)\end{aligned} \tag{5}$$

   with $H$ being the positive-semidefinite Hessian of J at $\omega^*$
2. The minimum of $\hat{J}$ occurs where its first derivatives equal 0:

$$\nabla_\omega \hat{J}(\omega) = H(\omega - \omega^*) = 0 \tag{6}$$

3. Transform into regularized version:

$$\begin{aligned}H(\tilde{\omega} - \omega^*) + \alpha\tilde{\omega} = 0 \Leftrightarrow (H + \alpha I)\tilde{\omega} = H\omega^* \\ \tilde{\omega} = (H + \alpha I)^{-1} H\omega^*\end{aligned} \tag{7}$$

# Discovering the effect of weight decay II

4. Apply eigendecomposition as H is real and symmetric, such that $H = Q\Lambda Q^T$:

$$\begin{aligned} \tilde{\omega} &= Q(\Lambda + \alpha I)^{-1}\Lambda Q^T \omega^* \\ &\Rightarrow \text{collapses to } \omega^* \text{ for } \alpha = 0 \end{aligned} \tag{8}$$

   Where
   - $\Lambda = diag(\lambda_1, ..., \lambda_d)$ with $\lambda_i \widehat{=}$ eigenvalue i of $H$
   - $Q \widehat{=}$ orthonormal basis of eigenvectors $v_i, i = 1, ..., d$

5. Effect on weight $i$:

$$\begin{aligned} \tilde{\omega}_i &= v_i \frac{\lambda_i}{\lambda_i + \alpha} v_i^T \omega_i^* \overset{v_i v_i^T = 1}{=} \frac{\lambda_i}{\lambda_i + \alpha} \omega_i^* \\ &\Rightarrow \textbf{ rescaling of } \omega^* \text{ with eigenvalues of the Hessian} \end{aligned} \tag{9}$$

# Discovering the effect of weight decay III

6. $\lambda_i$ resembles sensitivity of $J$ on $\omega_i$ // importance of $\omega_i$
   - $\tilde{\omega}_i = \frac{\lambda_i}{\lambda_i+\alpha}\omega_i^*$
   - $\lambda_i \gg \alpha$ : high $\lambda_i \rightarrow$ high curvature $\rightarrow$ important weight $\rightarrow$ low shrinkage of update
   - $\lambda_i \ll \alpha$ : small $\lambda_i \rightarrow$ low curvature $\rightarrow \omega_i^m$ "unnecessary" weight $\rightarrow$ heavy shrinkage

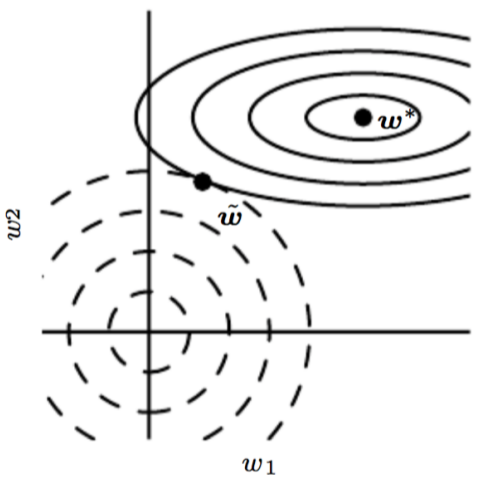



**Figure:** [Goodfellow et al., 2016]

# $L^1$-penalization // the eradicator

- Analogue to **lasso regression**: $\Omega(\theta) = ||\omega||_1$ such that

$$\tilde{J}(\theta; X, y) = \alpha||\omega||_1 + J(\theta; X, y) \tag{10}$$

leading to gradient:

$$\nabla_\omega \tilde{J}(\theta; X, y) = \alpha sign(\omega) + \nabla_\omega J(\theta; X, y) \tag{11}$$

- Harder penalization: shrinks weights **and** sets some to 0
- Creates **sparse** models and is therefore used for **feature selection**

# Understanding $L^1$-penalization I

- Taylor-approximation 2.0 of $\hat{J}(\theta)$
  - Assumption: uncorrelated inputs $\rightarrow H = diag(H_{1,1}, ..., H_{n,n}), H_{i,i} > 0$
  - $L^1$ regularized objective function:

$$\hat{J}(\theta; X, y) = J(\omega^*; X, y) + \sum_i \left[ \frac{1}{2} H_{i,i} (\omega_i - \omega_i^*)^2 + \alpha |\omega_i| \right] \tag{12}$$

- Solution of the minimization problem:

$$\tilde{\omega}_i = sign(\omega_i^*) max \left[ |\omega_i^*| - \frac{\alpha}{H_{i,i}}, 0 \right] \tag{13}$$

with two possible situations given $\omega_i^* > 0$:

  - High $H_{i,i} \rightarrow$ high curvature $\rightarrow$ low penalization of "necessary" weight $\rightarrow$ weight is just shrinked $\rightarrow 0 < \tilde{\omega}_i < \omega_i^*$
  - Low $H_{i,i} \rightarrow$ low curvature $\rightarrow$ hard penalization of "unnecessary" weight $\rightarrow \omega_i^* \leq \frac{\alpha}{H_{i,i}} \rightarrow \tilde{\omega}_i = 0$

# Understanding $L^1$-penalization II

- Compare both methods with $\lambda_i = H_{i,i}$ and $\omega_i^* > 0$:

$$\tilde{\omega}_i^{L^2} = \frac{H_{i,i}}{H_{i,i} + \alpha}\omega_i^* \quad \text{vs.} \quad \tilde{\omega}_i^{L^1} = max\left[|\omega_i^*| - \frac{\alpha}{H_{i,i}}, 0\right] \tag{14}$$

**$L^2$-penalization solely shrinks weights towards 0 and $L^1$-penalization furthermore eradicates weights**

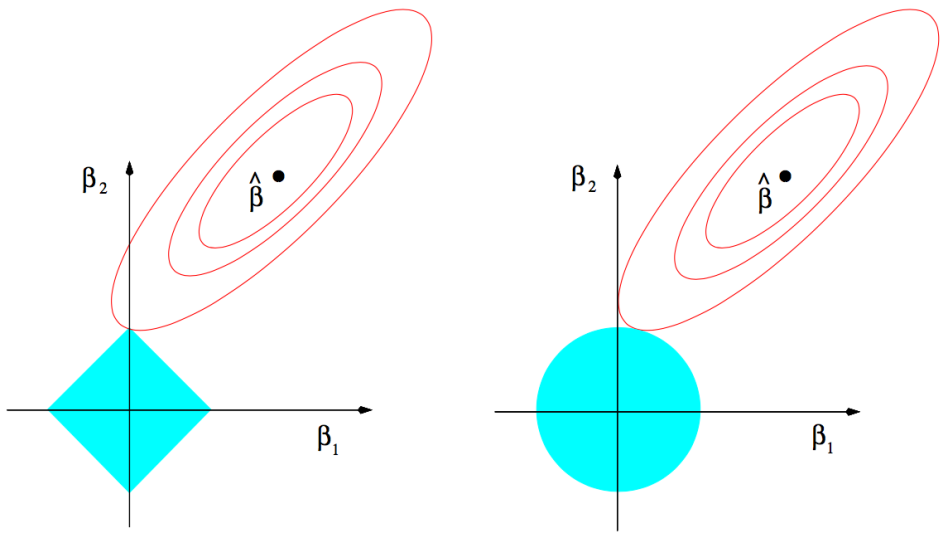



**Figure:** [Hastie et al., 2009]

# Max-norm-penalization // the underdog

- Direct approach to restrict weights
- Absolute upper bound for norm of incoming weight vector at each neuron:

$$||\omega_j||_2 \leq c \text{ for } \textit{neuron}_j \text{ where } \omega_j = (\omega_{1,j}, ..., \omega_{n,j})^T$$

- Empirical finding: $c \approx 4$
- Originated in matrix factorization applications, not in machine learning [Shen et al., 2014]
- Gained popularity as it performs well in combination with **dropout**
- R Implementation of all methods in `h2o.deeplearning()` from package `h2o`. In `caret` solely implementation of weight decay

# Structure

# Basic concept

- Recap: low generalization because high ratio $\frac{\text{complexity of the model}}{\#\text{train data}}$
- Increase train data $\rightarrow$ improve robustness $\rightarrow$ better generalization
- Limited data supply $\rightarrow$ create fake data
- Increase variation in inputs **without** changing the labels
- Link to **Noise Injection**

# Application

- Image and Object recognition:
  Rotation / Scaling / Pixel translation / Flipping / Noise Injection / Vignetting / Color Casting / Lens Distortion / Injection of random negatives
  - R implementation in `imager` and `OpenImageR`
  - See [Wu et al., 2015] for deeper insights
- Speech recognition:
  Speed augmentation / Vocal Tract Perturbation [Cui et al., 2015]

# Graphic Examples

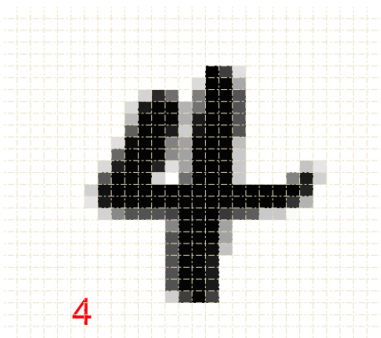
**(a)** Original

**(b)** Color

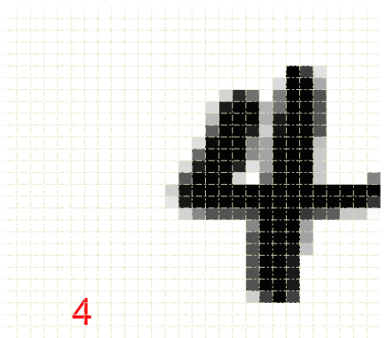
**(c)** Rotate

**(d)** Horizontal Stretch

**Figure:** [Wu et al., 2015]




**(a)** Original




**(b)** Moved

# Structure

# Basic concept

- Goal: find optimal number of iterations $m^*$
- Stop algorithm early // before generalization error increases

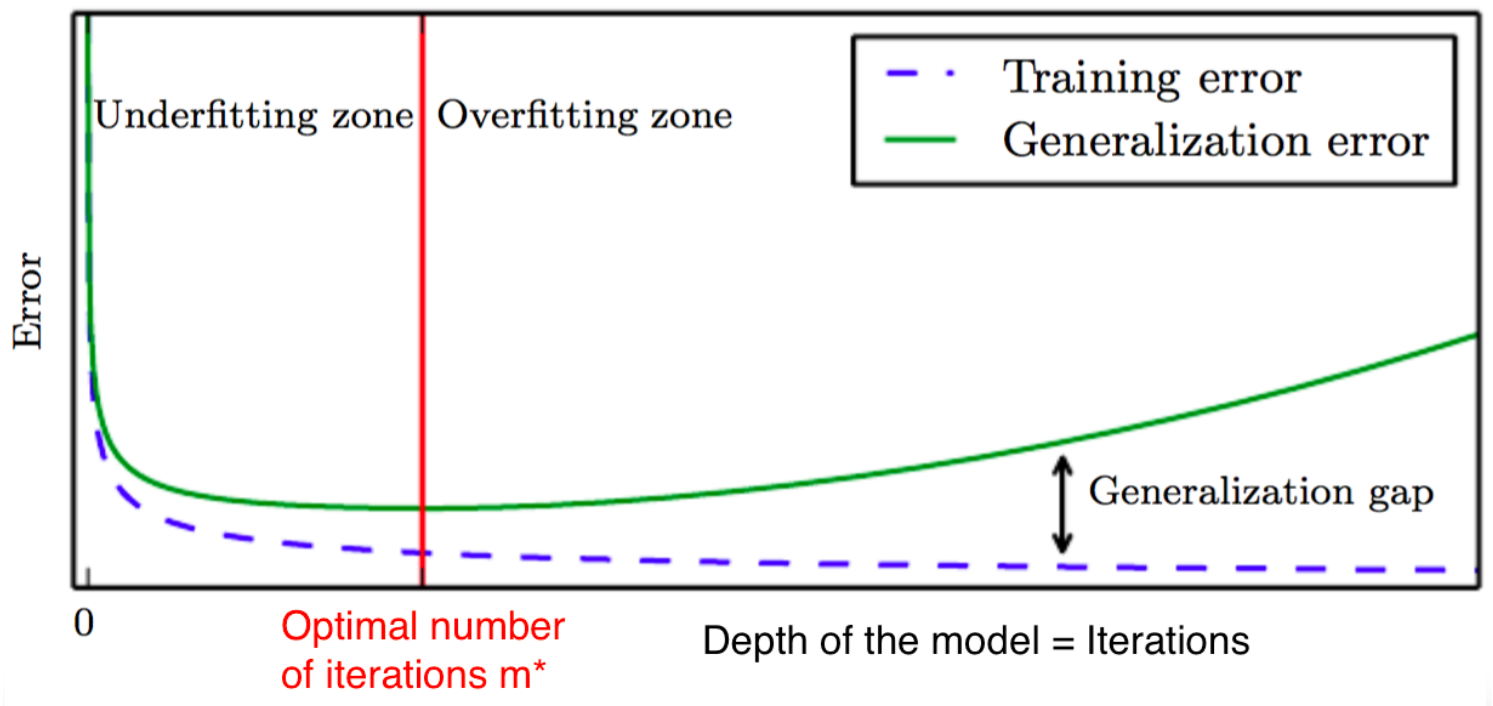



**Figure:** [Goodfellow et al., 2016]

# How to early stopping

- Split train data: $data^{train} = data^{subtrain} + data^{validation}$
- Monitor the error rate on the $data^{validation}$ in steps $n$ and stop the algorithm when it stops decreasing
- Store copy of model parameters after each error-improving step
- Use them as final parameters when there is no improvement after a range of steps $p$ ("patience")
- R implementation: `h2o.deeplearning` with option `stopping_rounds`, disabled in `mlr`

# Strengths and weaknesses

| Strengths | Weaknesses |
|---|---|
| Effective and simple | Periodical evaluation of $data^{validation}$-error |
| Applicable to almost any model without adjustment | Temporary copy of $\theta^*$ |
| Combinable with other regularization methods | Less data for training $\rightarrow$ include $data^{validation}$ afterwards:<br>1. determine $m^*$, retrain with whole $data^{train}$<br>2. determine $\theta^*$, continue training with $data^{train}$ while $\text{Error}(\theta, data^{train}) < \text{Error}(\theta^*, data^{validation})$ |

# Early stopping as weight decay I

- [Goodfellow et al., 2016] proof (under some assumptions) this relation of early stopping's optimal iterations $m$ and weight decay's penalization parameter $\alpha$:

$$m \approx \frac{1}{\gamma\alpha} \Leftrightarrow \alpha \approx \frac{1}{m\gamma}$$

- Small $\alpha \mathrel{\widehat{=}}$ low penalization $\Rightarrow$ high $m \mathrel{\widehat{=}}$ deep model
- Recap weight decay: weights corresponding to directions of high curvature (high $\lambda_i$) are less regularized by weight decay than directions of low curvature (low $\lambda_i$)
- Weights from the first case learn early relative to the latter

# Early stopping as weight decay II

- Graphic interpretation:

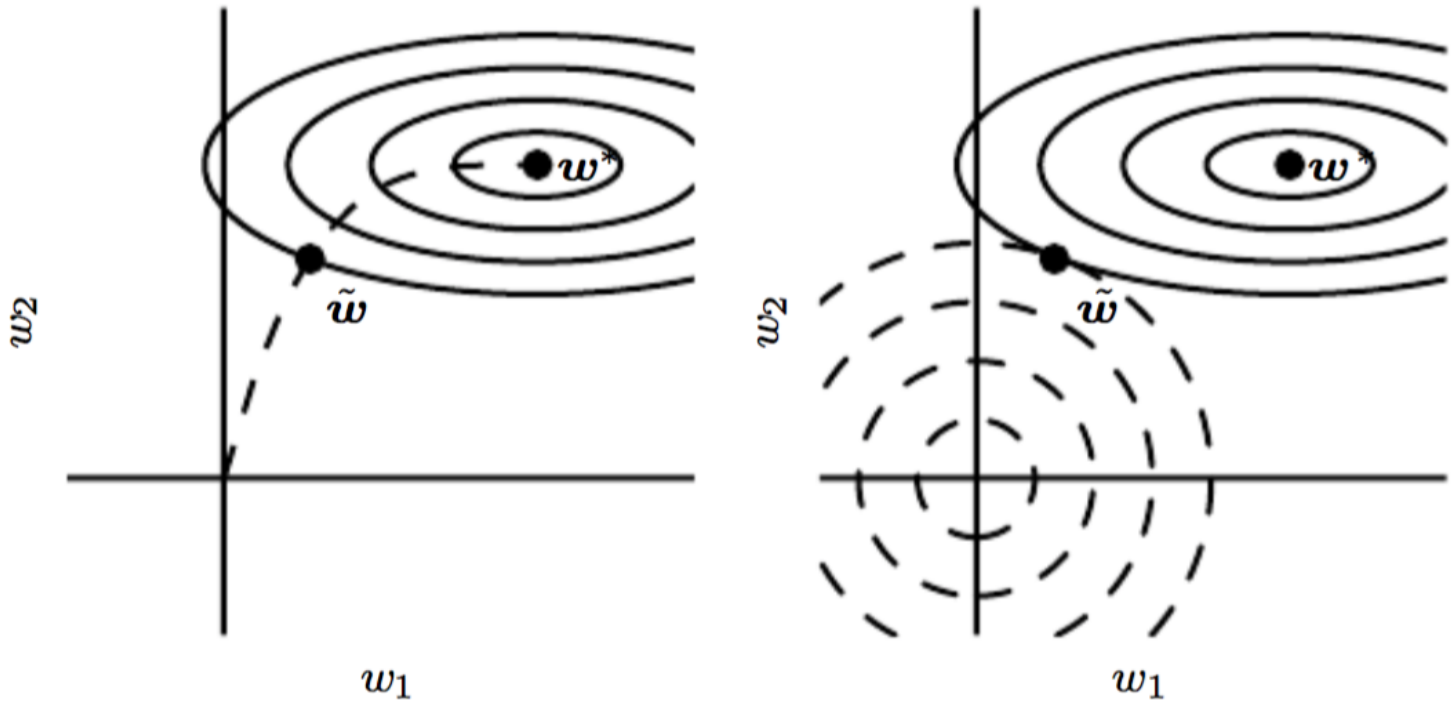



**Figure:** Optimization path in early stopping (left) and weight decy (right) after [Goodfellow et al., 2016]

# Structure

# Basic concept

- Combining several models trained on same task $\rightarrow$ reduce generalization error
- Vote of **ensemble** of models is then averaged for prediction
- Different models will make different errors
- Shortcomings of one ensemble member balanced by the **comittee**
- Methods differ in the way the ensemble is constructed
- Popular examples: **Bagging** and **Boosting**

# Illustration Ensemble Learning

Assume: $k$ models with $\epsilon_i \sim N(0, v)$, $\mathbb{E}[\epsilon_i, \epsilon_j] = c$ and $\mathbb{E}[\epsilon_{ensemble}] = \frac{1}{k}\sum_{i=1}^{k} \epsilon_i$

$$
\begin{aligned}
MSE_{ensemble} &= \mathbb{E}\left[\left(\frac{1}{k}\sum_{i=1}^{k}\epsilon_i\right)^2\right] = \frac{1}{k^2}\sum_{i=1}^{k}\left[\mathbb{E}[\epsilon_i^2] + \sum_{i\neq j}\mathbb{E}\left[\epsilon_i, \epsilon_j\right]\right] \\
&= \frac{1}{k^2}\sum_{i=1}^{k}\left[\mathbb{E}[\epsilon_i^2] + (k-1)\mathbb{E}\left[\epsilon_i, \epsilon_j\right]\right] = \frac{1}{k^2}k\left[v + (k-1)c\right] \\
&= \frac{1}{k}v + \frac{k-1}{k}c
\end{aligned}
\tag{15}
$$

- Perfectly correlated models: $c = v \rightarrow MSE_{ensemble|c=v} = v$
- Perfectly uncorrelated models: $c = 0 \rightarrow MSE_{ensemble|c=0} = \frac{1}{k}v$

# Illustration Bagging (bootstrap aggregation)

- Construct $k$ learners on $k$ data subsets drawn with replacement from original train data set
- Here: "digit 8 detector"

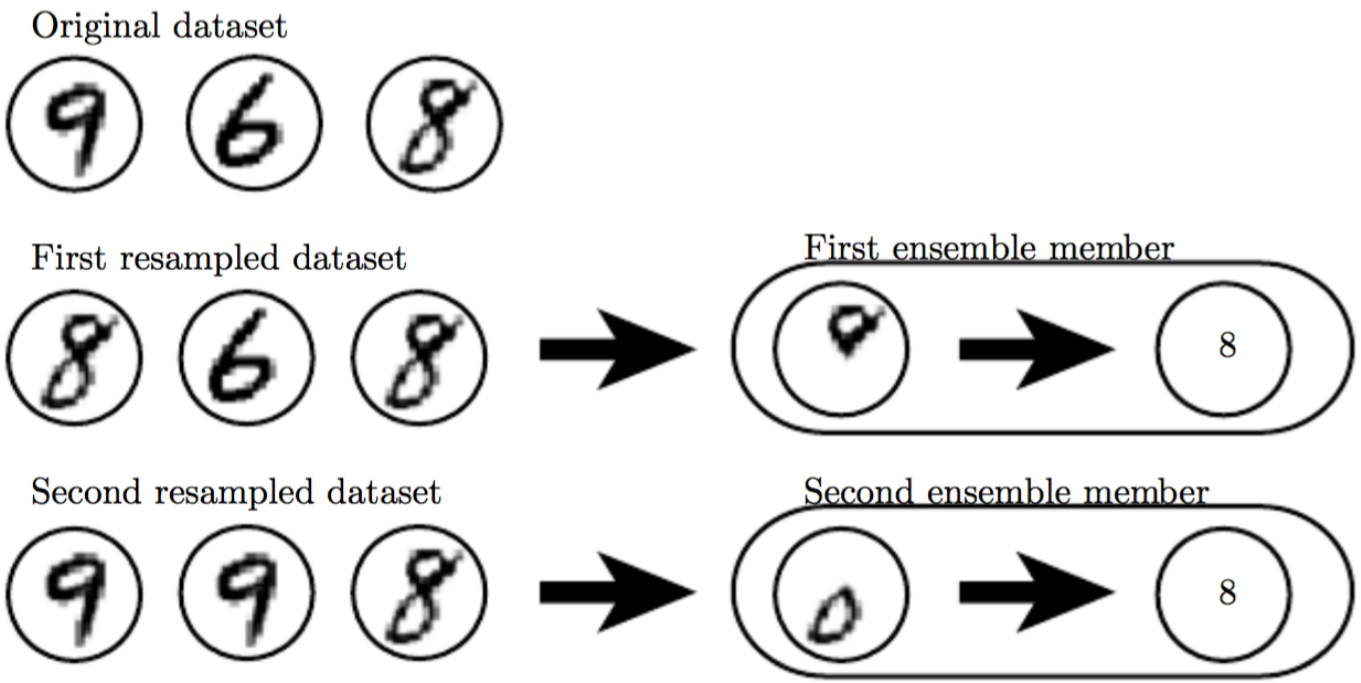



**Figure:** [Goodfellow et al., 2016]

# Structure

# Basic concept

- Problem: overfitting, low generalization
- Idea: force net to generalize by randomly dropping units during training
- Units hindered from relying on each other
- Train ensemble of "thinned sub-nets" and use their collective vote for prediction
- Extensive parameter sharing amongst sub-nets
- Each sub-net solely trained on single train data point

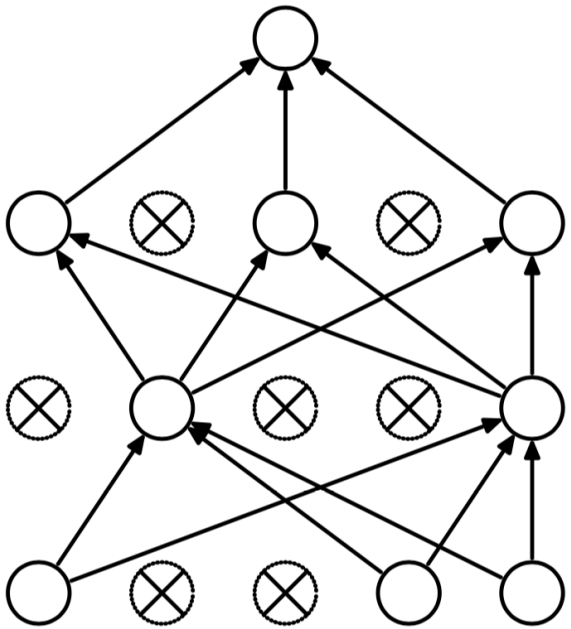


**Figure:**
[Srivastava et al., 2014]

# What happens internally?

- Sample from $2^d$ possible models that share parameters for computational feasibility where $d \widehat{=} \#$ units
- Sub-net with objective function $J(\theta, \mu)$ depends on mask $\mu$ that randomly determines in/exclusion of units and is trained on one randomly sampled train data point $(y^{(i)}, X^{(i)})$
- Mask $\mu$ is vector of length $d$ with $\mu = (\mu_1, ..., \mu_d)$, $\mu_l = \{0; 1\}$ and $P(\mu_l = 1) = p$
- Weights of sub-nets are shared through iterations

# Recap: train net using stochastic gradient descent

- $m \widehat{=}$ # iterations $\widehat{=}$ # data points from shuffled train sample
- $K \widehat{=}$ # parameters $\theta_j$ to be estimated
- $\gamma \widehat{=}$ learning rate of the algorithm
- $J(\theta)_i \widehat{=}$ objective function for iteration $i$

**Algorithm 1** stochastic gradient descent update

1: randomly shuffle train sample
2: **repeat**
3: **for** $i = 1, ..., m$ **do**
4: **for** $j = 1, .., K$ **do**
5: $\theta_j^{(i+1)} = \theta_j^{(i)} - \gamma \frac{\partial J(\theta)_i}{\partial \theta_j}$
6: **end for**
7: **end for**
8: **until** stop criterion is reached

# Train net using stochastic gradient descent and dropout

- $m \widehat{=}$ # iterations $\widehat{=}$ # data points randomly drawn with replacement $\widehat{=}$ # "thinned" subnets
- $K \widehat{=}$ # parameters $\theta_j$ to be estimated
- $\gamma \widehat{=}$ learning rate of the algorithm
- $J(\theta, \mu)_i \widehat{=}$ objective function for "thinned"sub-net $i$ depending on $\mu$

**Algorithm 2** stochastic gradient descent update dropout

randomly draw $m$ train data points from the train sample with replacement
**repeat**
  **for** $i = 1, ..., m$ **do**
    randomly draw mask $\mu$ for sub-net $i$
    **for** $j = 1, .., K$ **do**
      $\theta_j^{(i+1)} = \theta_j^{(i)} - \gamma \frac{\partial J(\theta, \mu)_i}{\partial \theta_j}$
    **end for**
  **end for**
**until** stop criterion is reached

# Test phase / deployment of dropout net

- Models output **probability distributions**: $p(y = y_j|x, \mu)$
- Bagging: arithmetic mean: $\tilde{p}_{ensemble}(y = y_j|x) = \frac{1}{k}\sum_{i=1}^{k} p^{(i)}(y = y_j|x)$
- Dropout: more robust weighting via geometric mean:

$$\tilde{p}_{ensemble}(y = y_j|x) = \sqrt[2^d]{\prod_{\mu} p(y = y_j|x, \mu)} \text{ with } p(y = y_j|x, \mu) > 0$$

re-normalize for prediction:

$$p_{ensemble}(y = y_j|x) = \frac{\tilde{p}_{ensemble}(y = y_j|x)}{\sum_j \tilde{p}_{ensemble}(y = y_j|x)} \tag{16}$$

- Approximation of geometric mean by [Hinton et al., 2012]: **weight scaling rule**

# Test Dropout Net - Weight Scaling Rule

Approximate $p_{ensemble}$ by inspection of the **complete model**:
$\rightarrow$ multiply shared weights of the trained model coming out of unit $i$ by $p$

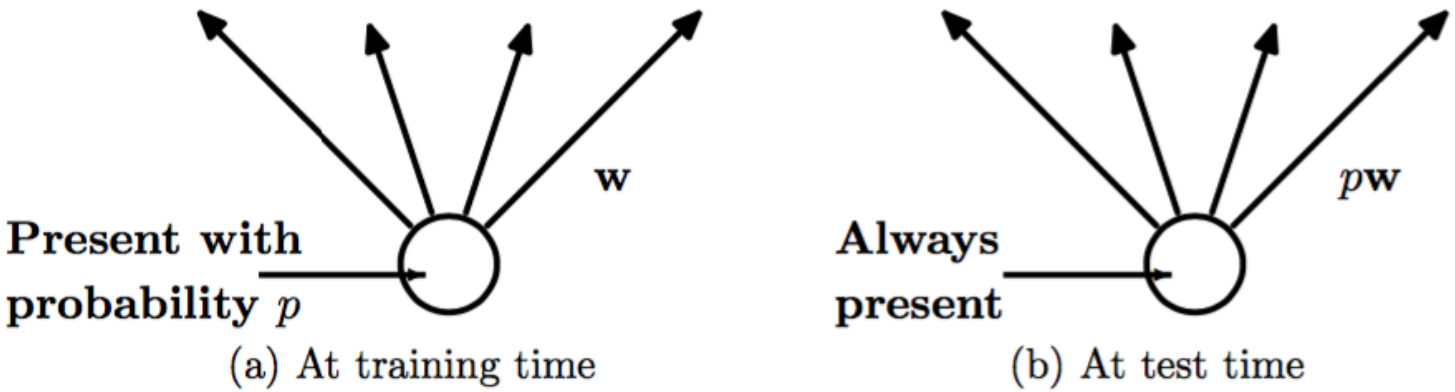



**Figure:** [Goodfellow et al., 2016]

[Goodfellow et al., 2016] show this can be proven to be **exact** for many classes of nets (e.g. Vanilla network with Softmax output layer)

# Bagging vs. Dropout

| | Bagging | Dropout |
|---|---|---|
| Train data | train data points drawn with replacement | |
| Basic Idea | model averaging | |
| # models | $k$ | possibly $2^d$ |
| Prediction | atrithmetic mean | geometric mean |
| Parameters | k independent models | parameter sharing |
| Train method | each model to convergence | each sub-net trained on single randomly sampled train data point restricted by $\mu$ |

# Notes on hyperparameters using dropout

Heuristics by [Srivastava et al., 2014]:

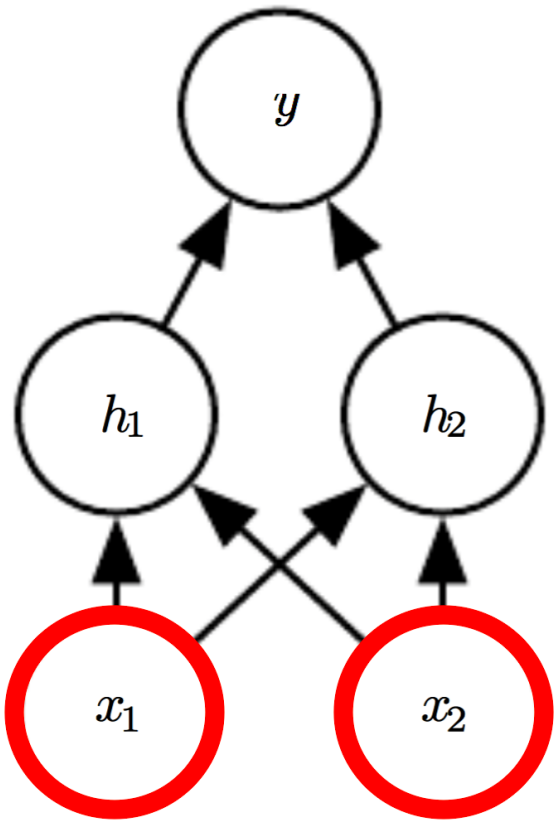
| Parameter | Description | Rule of thumb |
|---|---|---|
| Network size | Dropout rate reduces capacity of net/ number of hidden units | n/p |
| Learning rate | Dropout introduces lot of noise in the model: gradients cancel each other | 10-100 $\times$ standard $\gamma$ |
| Dropout rate | Probability of retaining a unit and $p = \pi$ in $\mu_q \sim Bernoulli(\pi)$ | $p = 0.8$ for inputs $p = 0.5$ for hidden units |
| Regularization | Combination with other regularization methods. **Max-norm-regularization** performs especially well | Max-norm-regularization |

R implementation: `h2o` and `deepnet`

# Structure

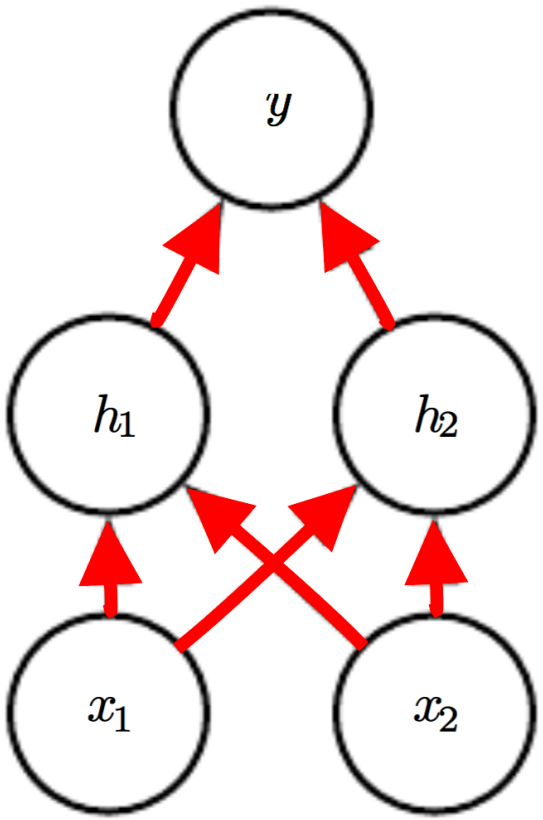
# Variations of Noise Injection

1. Inputs



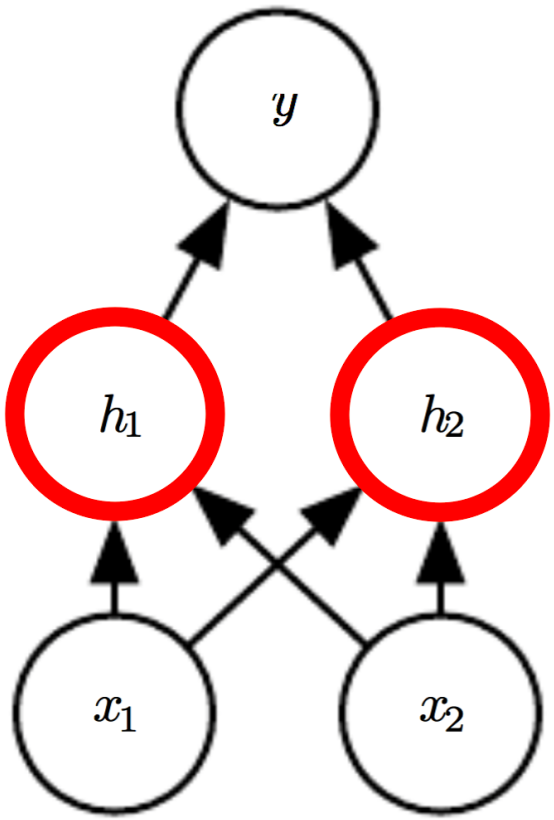
# Variations of Noise Injection

1. Inputs
2. Weights



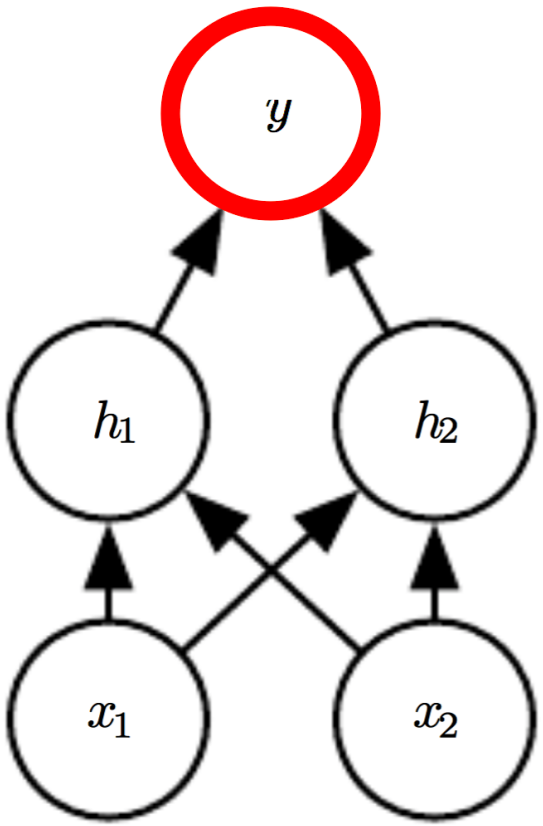
# Variations of Noise Injection

1. Inputs
2. Weights
3. Hidden units



# Variations of Noise Injection

1. Inputs
2. Weights
3. Hidden units
4. Outputs



# Noisy inputs

- Part of the data set augmentation strategy to amplify train data
- [Bishop, 1995] proofs: addition of noise on inputs with small variance is equivalent to norm penalty on the weights

# Noisy weights

- Regression setting, minimize MSE: $J = \mathbb{E}_{p(x,y)}[(\hat{y}(x) - y)^2]$
- Perturbation on weights such that $\tilde{\omega} = \omega + \epsilon_\omega$ with $\epsilon_\omega \sim \mathcal{N}(0, \eta\mathcal{I})$
- [Hochreiter et al., 1995] proof:

$$\nabla_\omega \tilde{J}_\omega = \nabla_\omega J + \eta \mathbb{E}_{p(x,y)} \left[ H^2 \right]$$

- Intuition:
  - Penalization of high levels of the Hessian
  - Weights pushed to areas with "flatter" minima
  - "Perfect" minima cannot be found because of noise, but approximations lie in a "flat" region
  - Weights more insensitive to variation as neighbor weights similarly low

# Noisy hidden units

- Dropout-mask $\mu$ can be interpreted as noise added to the hidden units in each SGD step
- Units cannot rely on each other and therefore have to diversify
- Not just simple addition of white noise to inputs
- Adaptive and intelligent destruction of information
- Optimisation strategy Batch Normalization applies noise to improve optimization which has regularizing side effect
- Illustrational examples
  - Focus on nose in face recogniton
  - Metaphor with eyes: blind spots vs. blurred vision

# Noisy outputs

- Idea: incorporate mesaure errors on the output labels
- Most known method: **label smoothing**
- Assume model with softmax output function and $k$ labels
- Originally: hard targets $y_j = \{0, 1\}$
- Relax them to softer targets $y_j = \{\frac{\epsilon}{k-1}, 1-\epsilon\}$
- Widely known and applied strategy

# Structure

# Basic concept

- Artificially construct data that only differ little from originals but confuse the net
- Use this **adversarial training data** to further train the model and enhance its performance

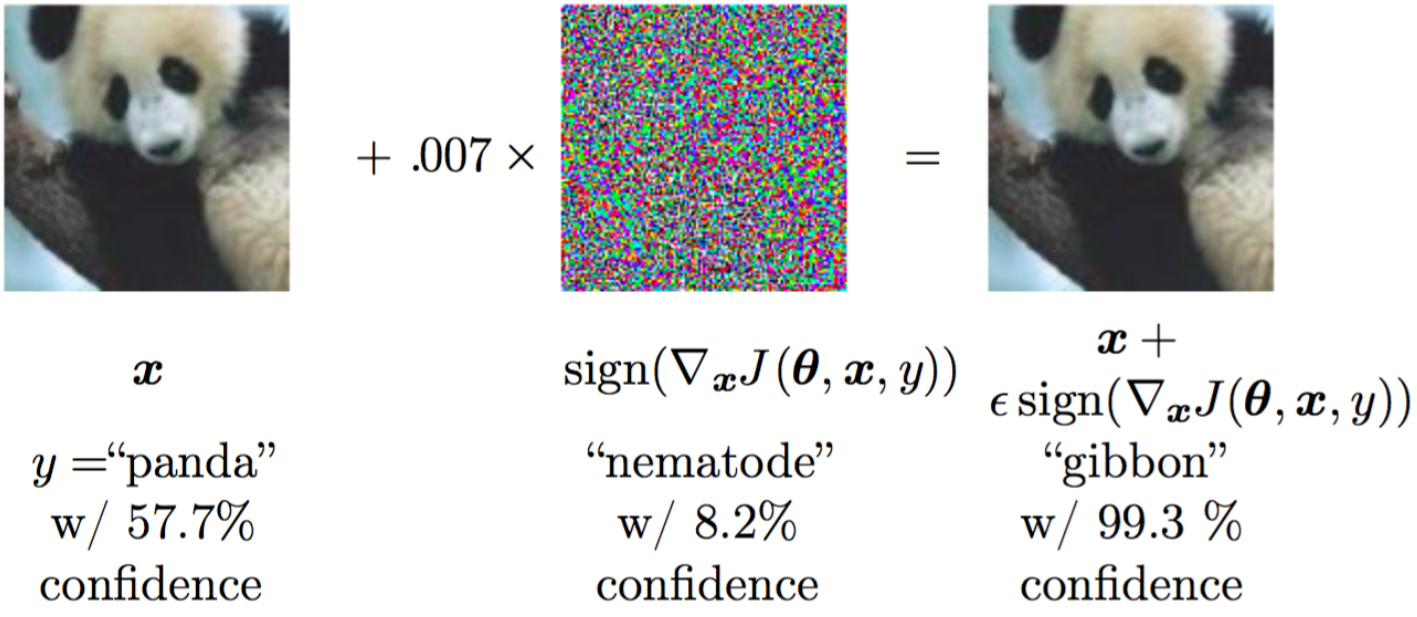



**Figure:** [Goodfellow et al., 2016]

# Structure

# About the data

- MNIST data set by Yann le Cun
- Easy access using package `darch`
- 70K images of handwritten digits in $28 \times 28$ pixels format
- Split in 60K train and 10K test data
- Classification task with 10 classes
- One of most popular benchmark data sets for image recognition

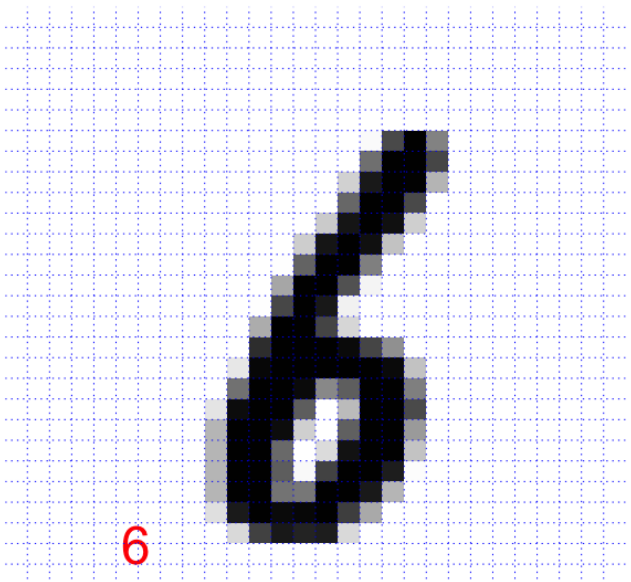



**Figure:** Example image

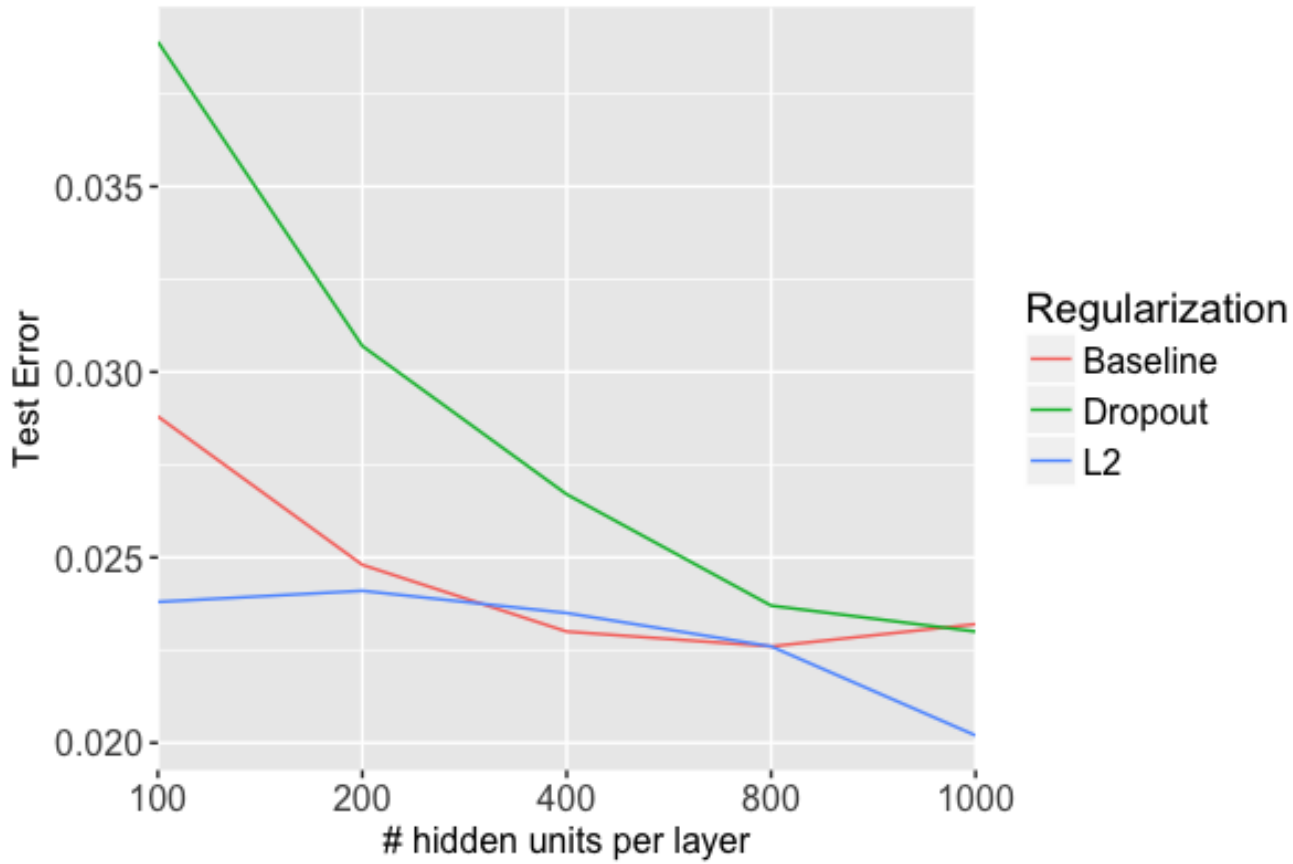
# About the model

- Neural net created using function `deeplearning` from package `h2o` called via `mlr`
- Feed-forward net with specifications:

| | |
|---|---|
| Activation function | Rectifier |
| Epochs | 10 |
| # hidden layer | 2 |
| Loss funtion | Cross entropy |
| Learning rate | 0.001 |
| Error measure | Mean misclassification error |

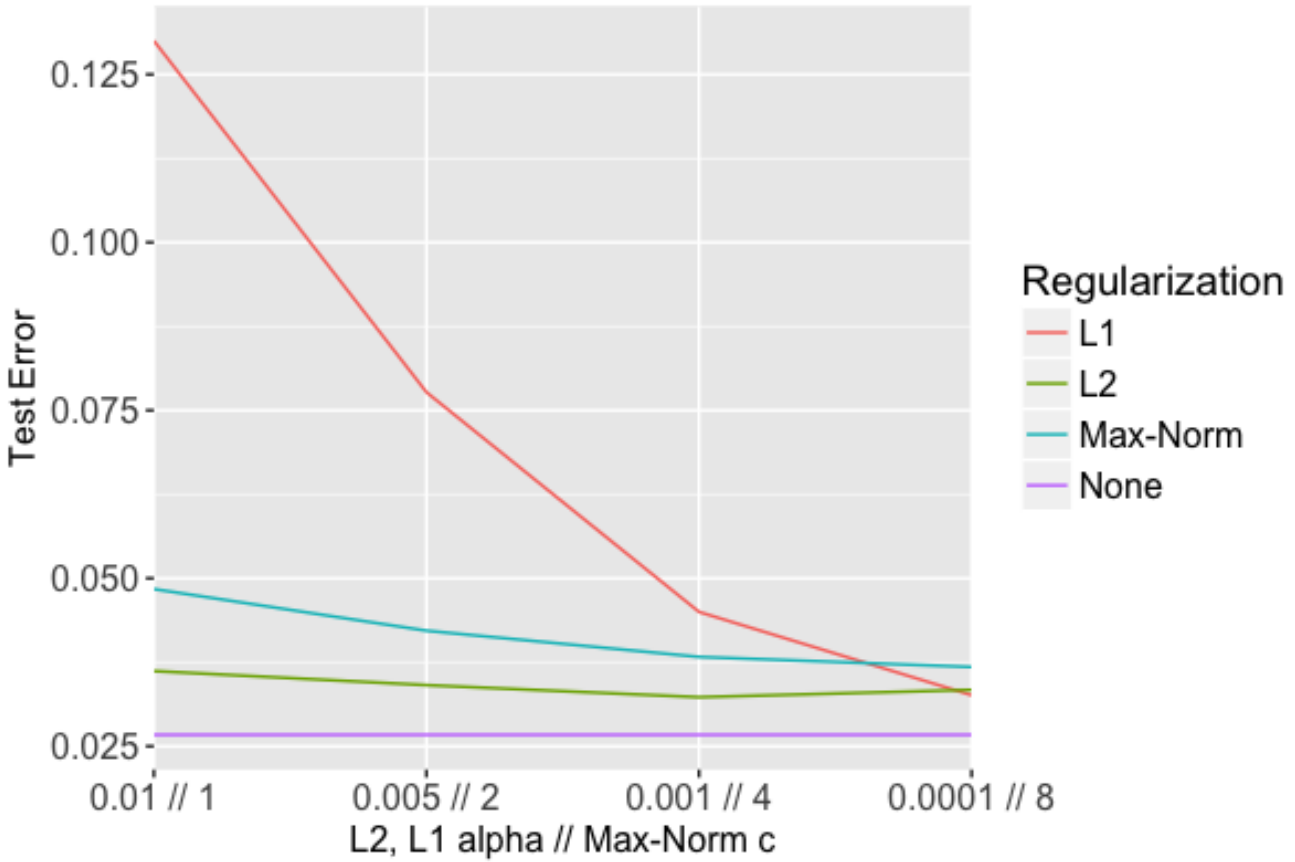
# Structure

# Performance with varying net-size




- 2-layer neural net with varying # hidden units
- Dropout with $p_{\text{hidden\_units}} = 0.5$ and $p_{\text{input\_units}} = 0.8$
- $L^2$-Regularization with penalization rate $\alpha = .001$

# Dropout combined with further regularization




- 2-layer net with 400 hidden units each
- $\Rightarrow$ Max-Norm seems **not to** work best combined with Dropout

# Dataset augmentation

- Train model on three data sets:
  - Small stratified subset with 30K images
  - Original train set with 60K images
  - Vertically augmented data set with 180K images
- Evaluate on same test sample with 10K images

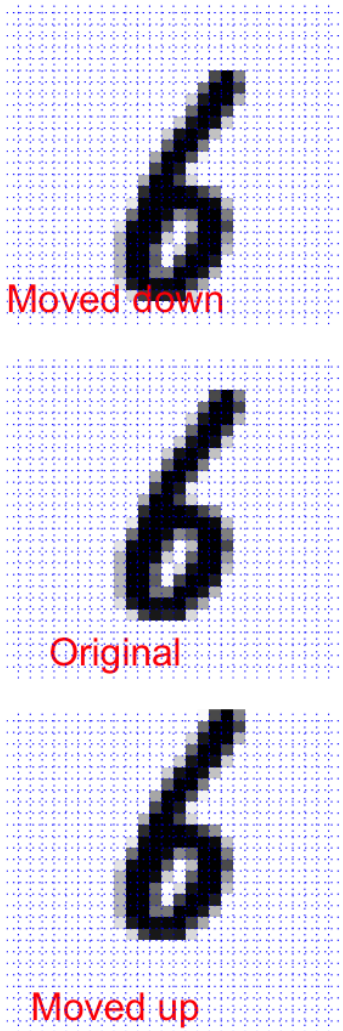



**Figure:** Augmented digit

# Dataset augmentation

- Train model on three data sets:
  - Small stratified subset with 30K images
  - Original train set with 60K images
  - Vertically augmented data set with 180K images
- Evaluate on same test sample with 10K images

| | 30K | 60K | 180K |
|---|---|---|---|
| Baseline | 3.26 % | 2.53 % | 2.20 % |
| Dropout | 4.80 % | 3.67 % | 3.60% |
| L2 | 3.23 % | 2.39 % | 2.05 % |

# Structure

# Current research on regularization

- Dense-sparse-dense neural nets by [Han et al., 2016]
- Shakeout by [Kang et al., 2016]
- Eigenvalue decay by [Ludwig et al., 2014]
- Drop-connect by [Wan et al., 2013]

# Thank you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# Appendix 1: weight decay as early stopping I

- Quadratically approximate $J(\theta)$ at minimal optimal value $\omega^*$ and $\theta = \omega$:

$$\hat{J}(\theta) = J(\omega^*) + \frac{1}{2}(\omega - \omega^*)H(\omega - \omega^*)^T$$

with $H$ being the Hessian of $J$ at $\omega^*$ leading to gradient:

$$\nabla_\omega \hat{J}(\omega) = H(\omega - \omega^*)$$

- Examine the gradient descent update on $\hat{J}$ assuming $\omega^{(0)} = 0$ :

$$\omega^{(m)} \leftarrow \omega^{(m-1)} - \gamma \nabla_\omega \hat{J}(\omega^{(m-1)})$$
$$\omega^{(m)} \leftarrow \omega^{(m-1)} - \gamma H(\omega^{(m-1)} - \omega^*) \mid -\omega^*$$
$$\omega^{(m)} - \omega^* \leftarrow (I - \gamma H)(\omega^{(m-1)} - \omega^*)$$

# Appendix 1: weight decay as early stopping II

- Eigendecompose $H = Q\Lambda Q^T$ such that:

$$\omega^{(m)} - \omega^* \leftarrow (I - \gamma Q\Lambda Q^T)(\omega^{(m-1)} - \omega^*)$$
$$Q^T(\omega^{(m)} - \omega^*) \leftarrow (I - \gamma\Lambda)Q^T(\omega^{(m-1)} - \omega^*)$$

- Assuming $\omega^0 = 0$ and $\gamma$ such that $|1 - \gamma\lambda_i| < 1$ leads to:

$$Q^T\omega^{(m)} = [I - (I - \gamma\Lambda)^{(m)}]Q^T\omega^*$$

- Recap the formula from the $L^2$ penalization:

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

and rearrange it to:

$$Q^T\tilde{\omega} = [I - (\Lambda + \alpha I)^{-1}\alpha]Q^T\omega^*$$

- $\Rightarrow$ weight decay = early stopping if $\gamma, m, \alpha$ chosen such that:

$$(I - \gamma\Lambda)^{(m)} = (\Lambda + \alpha I)^{-1}\alpha$$

# Appendix 1: weight decay as early stopping III

- Examine the effect for one weight $\tilde{\omega}_i$:

$$(1-\gamma\lambda_i)^{(m)} = (\lambda_i+\alpha)^{-1}\alpha|log()$$

$$mlog(1+(-\gamma\lambda_i)) = log(\frac{\alpha}{\lambda_i+\alpha}) = -log(1+\frac{\lambda_i}{\alpha})$$

use series expansion for $log(1+x)$ assuming $|\gamma\lambda_i| \ll 1$ and $|\frac{\lambda_i}{\alpha}| \ll 1$ :

$$\Rightarrow m \approx \frac{1}{\gamma\alpha} \Leftrightarrow \alpha \approx \frac{1}{m\gamma}$$

- Recap weight decay: weights corresponding to directions of high curvature (high $\lambda_i$, required correction) are less regularized by weight decay than directions of low curvature (low $\lambda_i$, "unnecessary" update)
- Weights from the first case learn early relative to the latter

# Appendix 1: weight decay as early stopping IV

- Graphic interpretation:

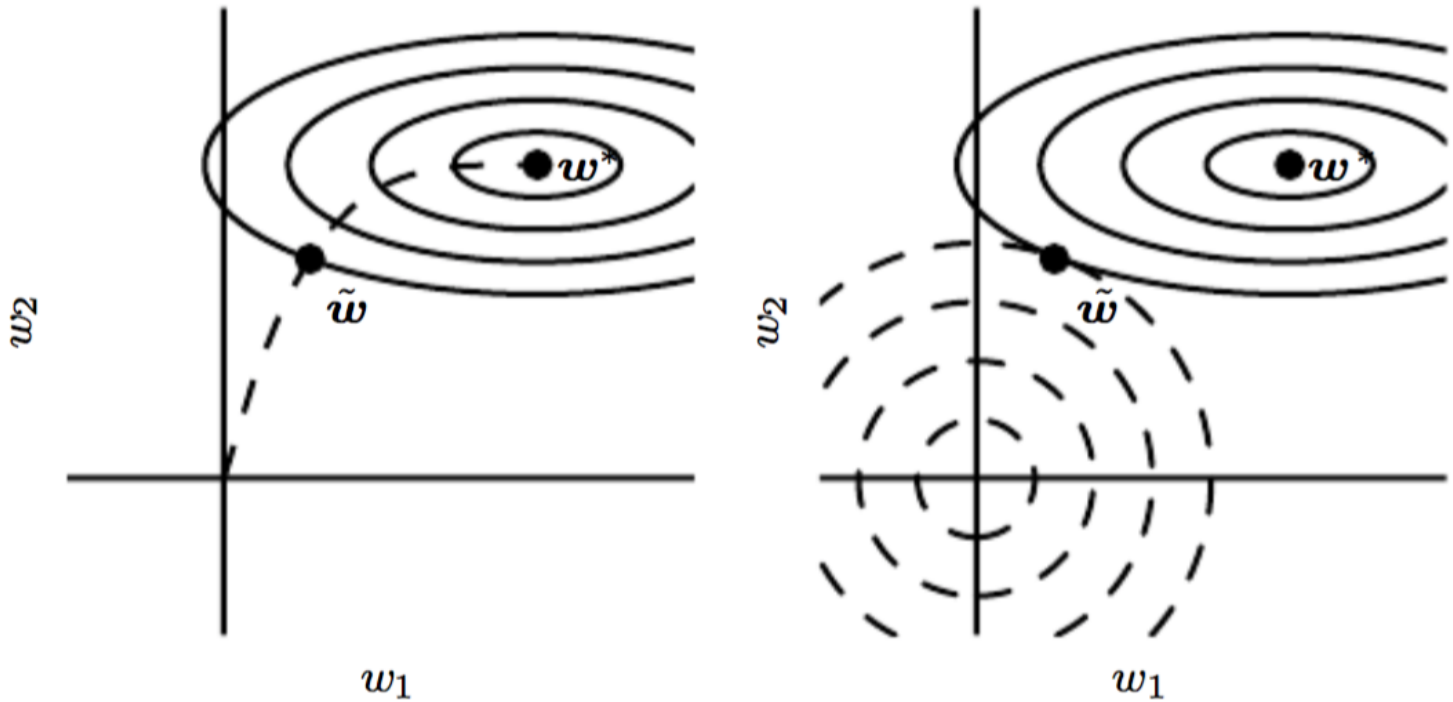


**Figure:** [Goodfellow et al., 2016]

# Appendix 2: formal algorithm early stopping

Set $\theta_0 \widehat{=}$ initial parameters, $n \widehat{=}$ step size, $p \widehat{=}$ patience, $v \widehat{=}$ validation set error

**Algorithm 3** Early stopping meta algorithm

Initialize $\theta^* \leftarrow \theta \leftarrow \theta_0$ and $m, j \leftarrow 0$ and $v \leftarrow \infty$ and $m^* \leftarrow m$
**while** $j < p$ **do**
    run update algorithm for $\theta$ n times
    $m \leftarrow m + n$ and $v' \leftarrow J(\theta, data^{validation})$
    **if** $v' < v$ **then**
        $j \leftarrow 0$ and $\theta^* \leftarrow \theta$ and $m^* \leftarrow m$ and $v \leftarrow v'$
    **else**
        $j \leftarrow j + 1$
    **end if**
**end while**
optimal parameters are $\theta^*$ and optimal number of iterations is $m^*$

# Appendix 3: illustration geometric mean in dropout

| | $P(y = y_1\|x)$ | $P(y = y_2\|x)$ | $P(y = y_3\|x)$ | $\sum$ |
|---|---|---|---|---|
| Model 1 | 0.20 | 0.70 | 0.10 | 1.00 |
| Model 2 | 0.10 | 0.80 | 0.10 | 1.00 |
| Model 3 | 0.05 | 0.90 | 0.05 | 1.00 |
| Model 4 | 0.05 | 0.90 | 0.05 | 1.00 |
| **Model 5** | **0.80** | **0.10** | **0.10** | **1.00** |
| Arithmetic mean | 0.24 | 0.68 | 0.08 | 1.00 |
| Geometric mean | 0.13 | 0.54 | 0.08 | 0.75 |
| Re-normalized | 0.18 | 0.72 | 0.10 | 1.00 |

$$mean_{arithmetic}(x_1, ..., x_n) = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$mean_{geometric}(x_1, ..., x_n) = \sqrt[n]{\prod_{i=1}^{n} x_i} \text{ with } x_i > 0 \forall i = 1, .., n$$