# Neural Network Part 2: Regularization

CS 760@UW-Madison

# Goals for the lecture

you should understand the following concepts

- regularization
- different views of regularization
- norm constraint
- data augmentation
- early stopping
- dropout
- batch normalization

# What is regularization?

- In general: any method to prevent overfitting or help the optimization

- Specifically: additional terms in the training optimization objective to prevent overfitting or help the optimization

# Example: regression using polynomials

$t = \sin(2\pi x) + \epsilon$

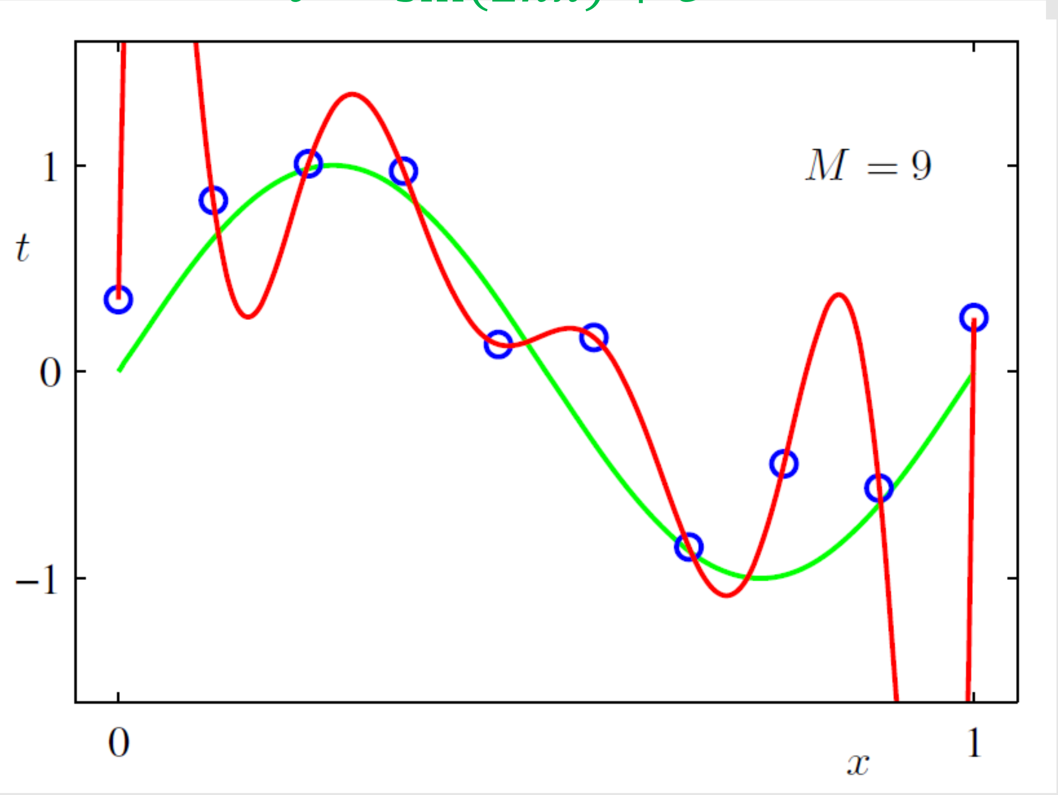



Figure from *Machine Learning and Pattern Recognition*, Bishop

# Example: regression using polynomials

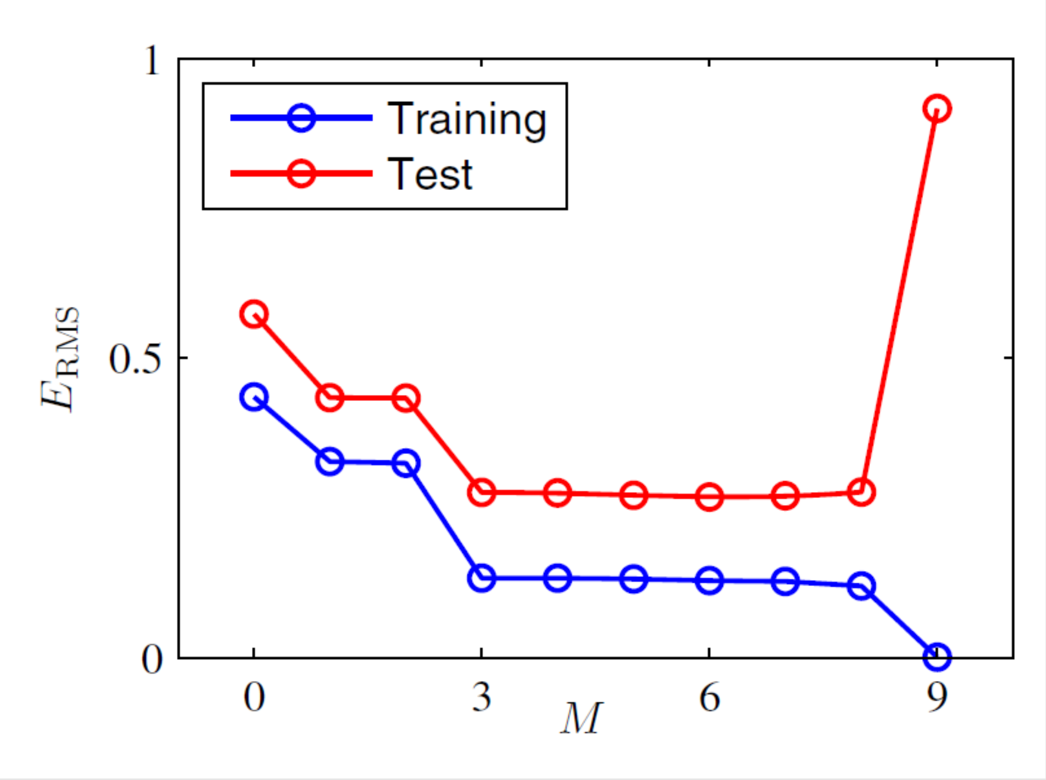



Figure from *Machine Learning and Pattern Recognition*, Bishop

# Overfitting

- Key: empirical loss and expected loss are different

- Smaller the data set, larger the difference between the two
- Larger the hypothesis class, easier to find a hypothesis that fits the difference between the two
  - Thus has small training error but large test error (overfitting)

- Larger data set helps
- Throwing away useless hypotheses also helps (regularization)

# Different views of regularization

# Regularization as hard constraint

- Training objective

$$\min_f \hat{L}(f) = \frac{1}{n}\sum_{i=1}^{n} l(f, x_i, y_i)$$

$$\text{subject to: } f \in \boldsymbol{\mathcal{H}}$$

- When parametrized

$$\min_\theta \hat{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i)$$

$$\text{subject to: } \theta \in \Omega$$

# Regularization as hard constraint

- When $\Omega$ measured by some quantity $R$

$$\min_{\theta} \hat{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i)$$

$$\text{subject to: } R(\theta) \le r$$

- Example: $l_2$ regularization

$$\min_{\theta} \hat{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i)$$

$$\text{subject to: } ||\theta||_2^2 \le r^2$$

# Regularization as soft constraint

- The hard-constraint optimization is equivalent to soft-constraint

$$\min_{\theta} \hat{L}_R(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i) + \lambda^* R(\theta)$$

  for some regularization parameter $\lambda^* > 0$
- Example: $l_2$ regularization

$$\min_{\theta} \hat{L}_R(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i) + \lambda^* ||\theta||_2^2$$

# Regularization as soft constraint

- Showed by Lagrangian multiplier method

$$\mathcal{L}(\theta, \lambda) \coloneqq \hat{L}(\theta) + \lambda[R(\theta) - r]$$

- Suppose $\theta^*$ is the optimal for hard-constraint optimization

$$\theta^* = \underset{\theta}{\operatorname{argmin}} \max_{\lambda \geq 0} \mathcal{L}(\theta, \lambda) \coloneqq \hat{L}(\theta) + \lambda[R(\theta) - r]$$

- Suppose $\lambda^*$ is the corresponding optimal for max

$$\theta^* = \underset{\theta}{\operatorname{argmin}} \mathcal{L}(\theta, \lambda^*) \coloneqq \hat{L}(\theta) + \lambda^*[R(\theta) - r]$$

# Regularization as Bayesian prior

- Bayesian view: everything is a distribution
- Prior over the hypotheses: $p(\theta)$
- Posterior over the hypotheses: $p(\theta \mid \{x_i, y_i\})$
- Likelihood: $p(\{x_i, y_i\}|\theta)$

- Bayesian rule:

$$p(\theta \mid \{x_i, y_i\}) = \frac{p(\theta)p(\{x_i, y_i\}|\theta)}{p(\{x_i, y_i\})}$$

# Regularization as Bayesian prior

- Bayesian rule:

$$p(\theta \mid \{x_i, y_i\}) = \frac{p(\theta)p(\{x_i, y_i\}|\theta)}{p(\{x_i, y_i\})}$$

- Maximum A Posteriori (MAP):

$$\max_{\theta} \log p(\theta \mid \{x_i, y_i\}) = \min_{\theta} \underbrace{-\log p(\theta)}_{\text{Regularization}} \underbrace{-\log p(\{x_i, y_i\} \mid \theta)}_{\text{MLE loss}}$$

# Regularization as Bayesian prior

- Example: $l_2$ loss with $l_2$ regularization

$$\min_{\theta} \hat{L}_R(\theta) = \frac{1}{n}\sum_{i=1}^{n}(f_\theta(x_i) - y_i)^2 + \lambda^* ||\theta||_2^2$$

- Correspond to a normal $p(x \mid y, \theta)$ and a normal prior $p(\theta)$

# Three views

- Typical choice for optimization: soft-constraint

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \lambda R(\theta)$$

- Hard constraint and Bayesian view: conceptual; or used for derivation

- Hard-constraint preferred if
  - Know the explicit bound $R(\theta) \leq r$
  - Soft-constraint causes trapped in a local minima while projection back to feasible set leads to stability

- Bayesian view preferred if
  - Domain knowledge easy to represent as a prior

# Examples of Regularization

# Classical regularization

- Norm penalty
  - $l_2$ regularization
  - $l_1$ regularization

- Robustness to noise
  - Noise to the input
  - Noise to the weights

# $l_2$ regularization

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \frac{\alpha}{2}||\theta||_2^2$$

- Effect on (stochastic) gradient descent
- Effect on the optimal solution

# Effect on gradient descent

- Gradient of regularized objective

$$\nabla \hat{L}_R(\theta) = \nabla \hat{L}(\theta) + \alpha\theta$$

- Gradient descent update

$$\theta \leftarrow \theta - \eta \nabla \hat{L}_R(\theta) = \theta - \eta\, \nabla \hat{L}(\theta) - \eta\alpha\theta = (1 - \eta\alpha)\theta - \eta\, \nabla \hat{L}(\theta)$$

- Terminology: weight decay

# Effect on the optimal solution

- Consider a quadratic approximation around $\theta^*$

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + (\theta - \theta^*)^T \nabla \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

- Since $\theta^*$ is optimal, $\nabla \hat{L}(\theta^*) = 0$

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

$$\nabla \hat{L}(\theta) \approx H(\theta - \theta^*)$$

# Effect on the optimal solution

- Gradient of regularized objective

$$\nabla \hat{L}_R(\theta) \approx H(\theta - \theta^*) + \alpha\theta$$

- On the optimal $\theta_R^*$

$$0 = \nabla \hat{L}_R(\theta_R^*) \approx H(\theta_R^* - \theta^*) + \alpha\theta_R^*$$

$$\theta_R^* \approx (H + \alpha I)^{-1} H\theta^*$$

# Effect on the optimal solution

- The optimal

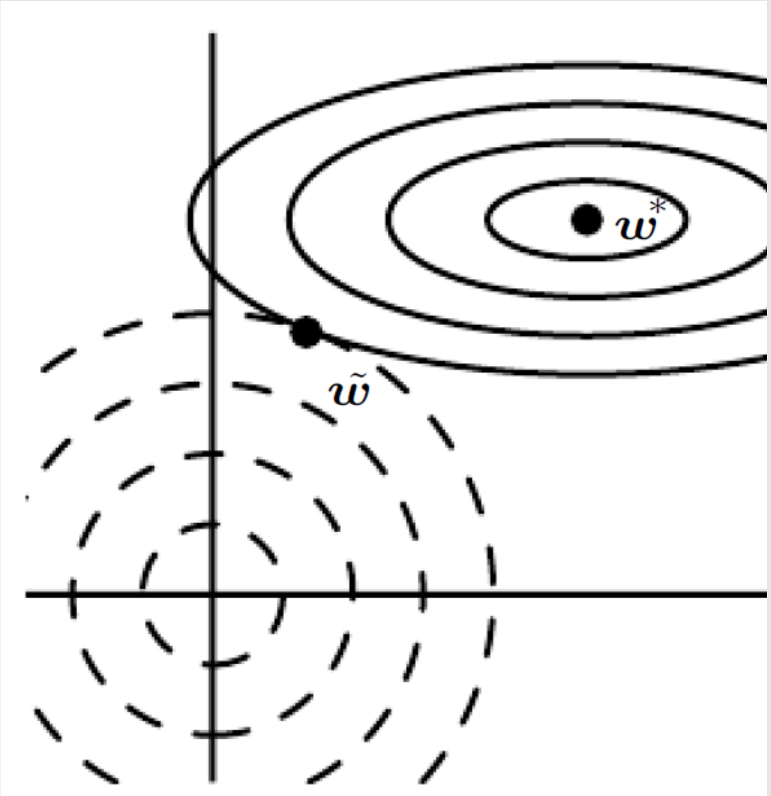
$$\theta_R^* \approx (H + \alpha I)^{-1} H \theta^*$$

- Suppose $H$ has eigen-decomposition $H = Q \Lambda Q^T$ and assume $(\Lambda + \alpha I)^{-1}$ exists:

$$\theta_R^* \approx (H + \alpha I)^{-1} H \theta^* = Q(\Lambda + \alpha I)^{-1} \Lambda Q^T \theta^*$$

- Effect: rescale along eigenvectors of $H$

# Effect on the optimal solution




Notations:

$\theta^* = w^*, \theta_R^* = \widetilde{w}$

Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

# $l_1$ regularization

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \alpha||\theta||_1$$

- Effect on (stochastic) gradient descent
- Effect on the optimal solution

# Effect on gradient descent

- Gradient of regularized objective

$$\nabla \hat{L}_R(\theta) = \nabla \hat{L}(\theta) + \alpha \,\mathrm{sign}(\theta)$$

where $\mathrm{sign}$ applies to each element in $\theta$

- Gradient descent update

$$\theta \leftarrow \theta - \eta \nabla \hat{L}_R(\theta) = \theta - \eta\, \nabla \hat{L}(\theta) - \eta\alpha \,\mathrm{sign}(\theta)$$

# Effect on the optimal solution

- Consider a quadratic approximation around $\theta^*$

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + (\theta - \theta^*)^T \nabla \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

- Since $\theta^*$ is optimal, $\nabla \hat{L}(\theta^*) = 0$

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

# Effect on the optimal solution

- Further assume that $H$ is diagonal and positive $(H_{ii} > 0, \forall i)$
  - not true in general but assume for getting some intuition
- The regularized objective is (ignoring constants)

$$\hat{L}_R(\theta) \approx \sum_i \frac{1}{2} H_{ii}(\theta_i - \theta_i^*)^2 + \alpha\, |\theta_i|$$

- The optimal $\theta_R^*$

$$(\theta_R^*)_i \approx \begin{cases} \max\left\{\theta_i^* - \dfrac{\alpha}{H_{ii}}, 0\right\} & \text{if } \theta_i^* \geq 0 \\ \min\left\{\theta_i^* + \dfrac{\alpha}{H_{ii}}, 0\right\} & \text{if } \theta_i^* < 0 \end{cases}$$

- Compact expression for the optimal $\theta_R^*$

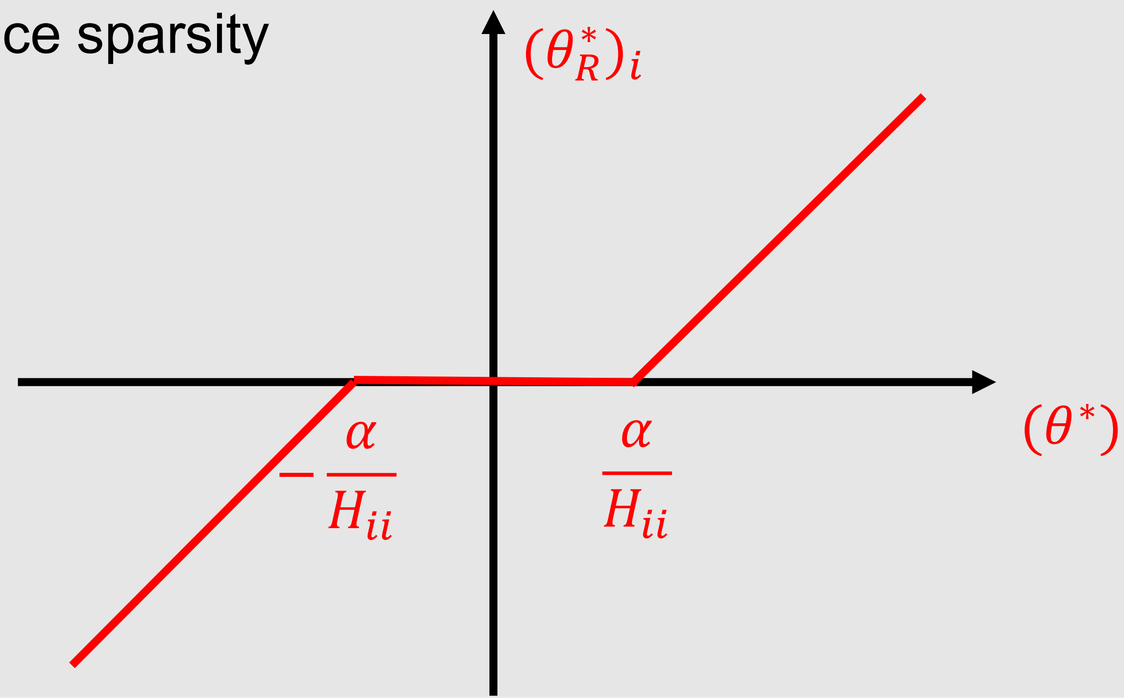
$$(\theta_R^*)_i \approx \operatorname{sign}(\theta_i^*) \max\{|\theta_i^*| - \frac{\alpha}{H_{ii}}, 0\}$$

# Effect on the optimal solution

- The optimal $\theta_R^*$

$$(\theta_R^*)_i \approx \begin{cases} \max\left\{\theta_i^* - \frac{\alpha}{H_{ii}}, 0\right\} & \text{if } \theta_i^* \geq 0 \\ \min\left\{\theta_i^* + \frac{\alpha}{H_{ii}}, 0\right\} & \text{if } \theta_i^* < 0 \end{cases}$$

- Effect: induce sparsity



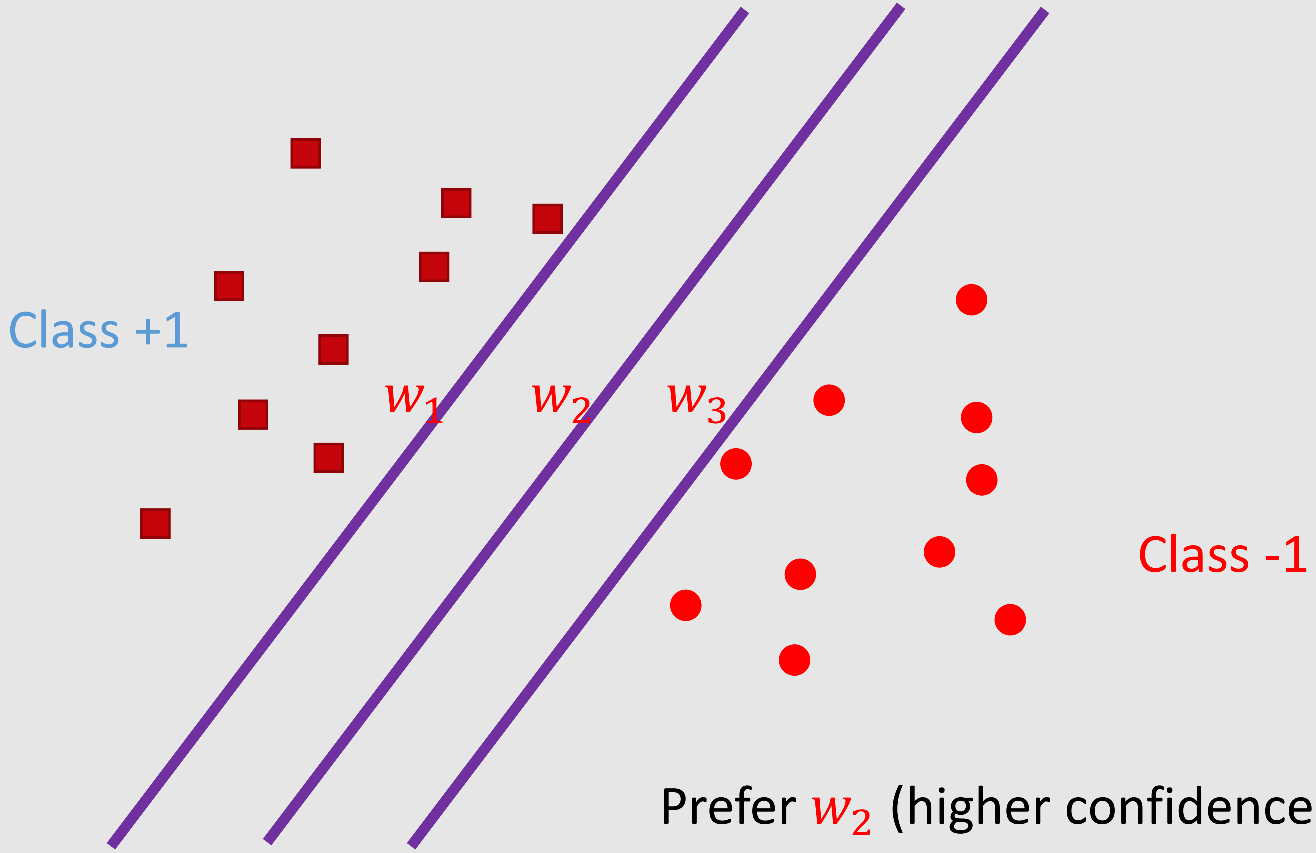
# Bayesian view

- $l_1$ regularization corresponds to Laplacian prior

$$p(\theta) \propto \exp(-\alpha \sum_i |\theta_i|)$$

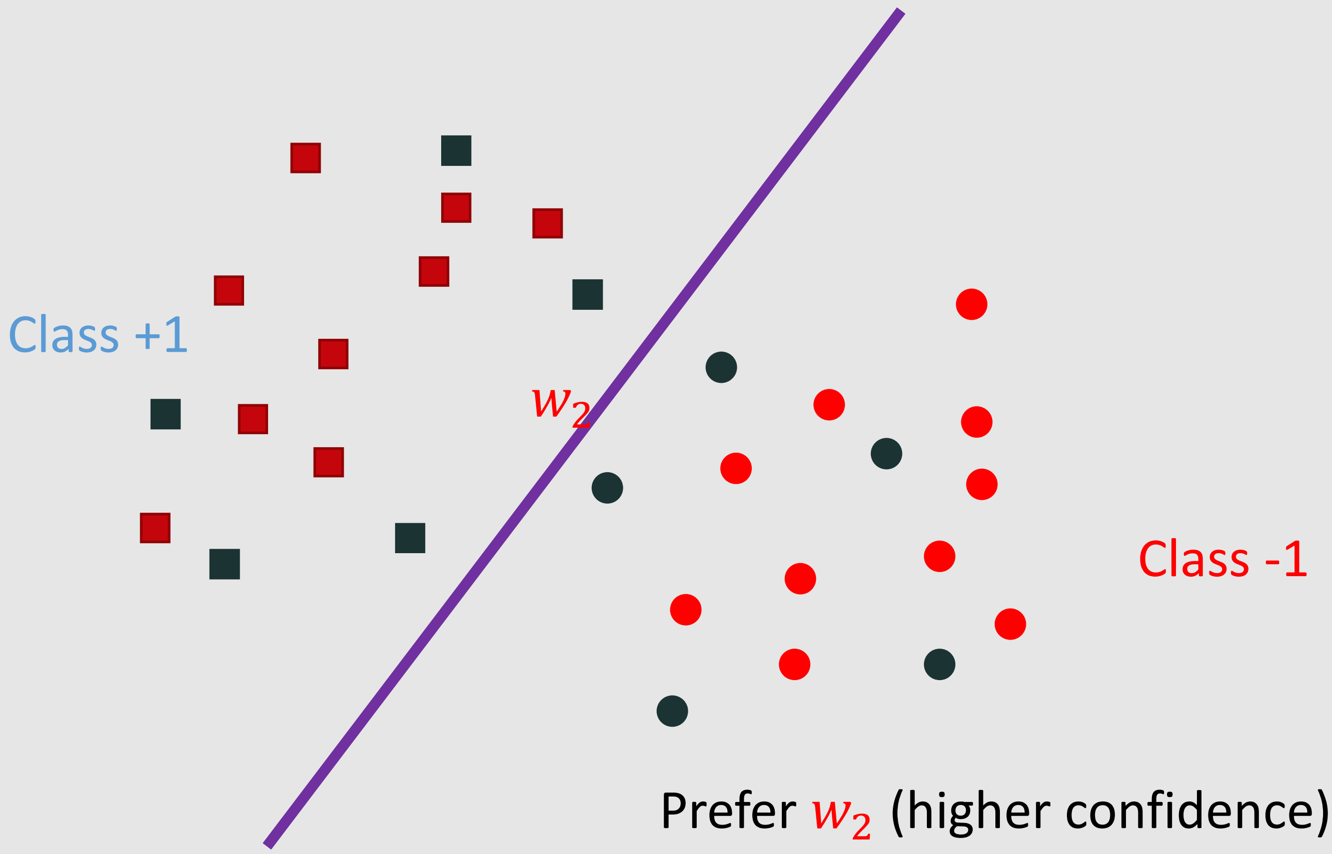
$$-\log p(\theta) = \alpha \sum_i |\theta_i| + \text{constant} = \alpha||\theta||_1 + \text{constant}$$

# Multiple optimal solutions?

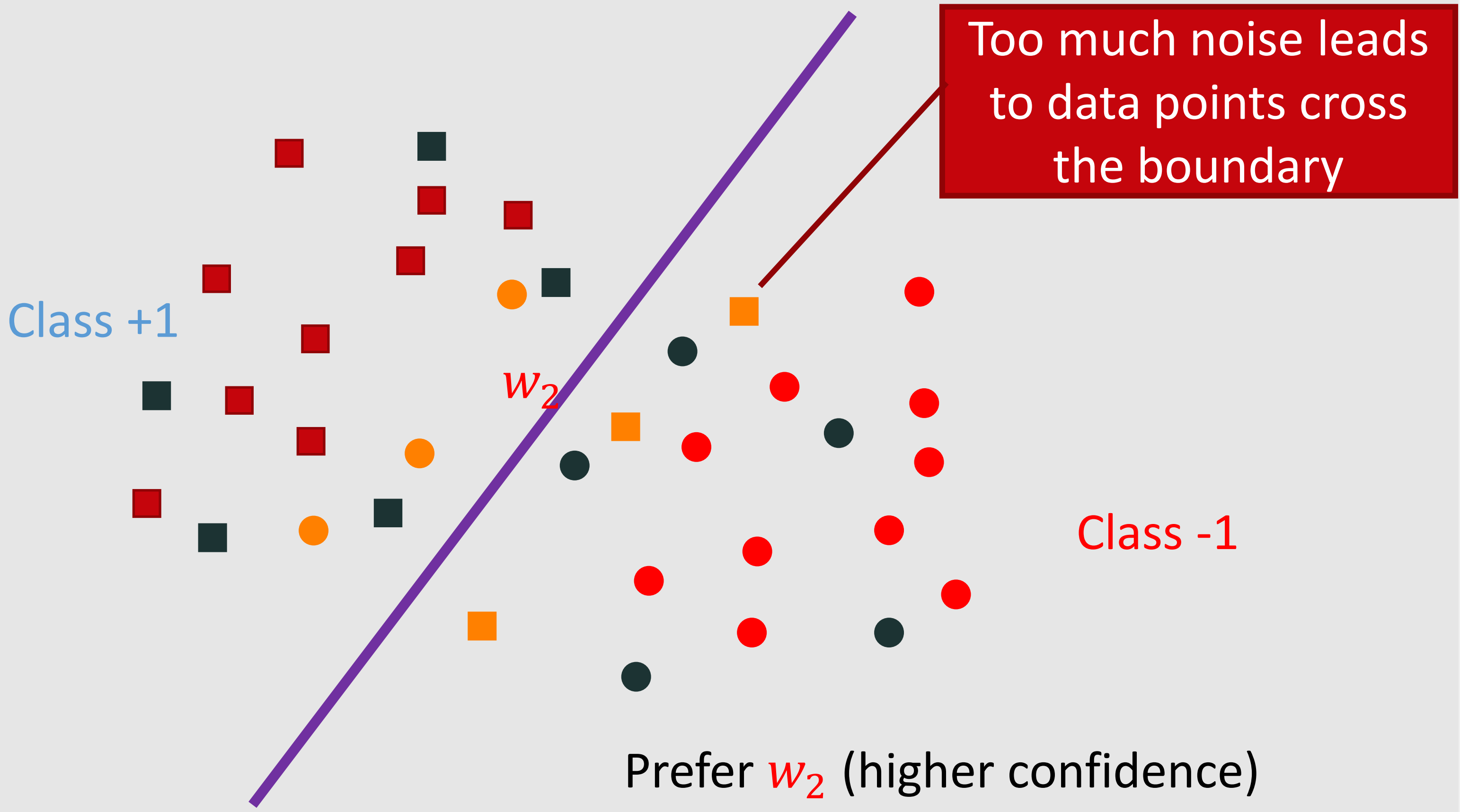



Prefer $w_2$ (higher confidence)

# Add noise to the input



# Caution: not too much noise



# Equivalence to weight decay

- Suppose the hypothesis is $f(x) = w^T x$, noise is $\epsilon \sim N(0, \lambda I)$
- After adding noise, the loss is

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f(x+\epsilon) - y]^2 = \mathbb{E}_{x,y,\epsilon}[f(x) + w^T\epsilon - y]^2$$

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f(x) - y]^2 + 2\mathbb{E}_{x,y,\epsilon}[w^T\epsilon(f(x) - y)] + \mathbb{E}_{x,y,\epsilon}[w^T\epsilon]^2$$

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f(x) - y]^2 + \lambda\left|\left|w\right|\right|^2$$

# Add noise to the weights

- For the loss on each data point, add a noise term to the weights before computing the prediction

$$\epsilon \sim N(0, \eta I),\ w' = w + \epsilon$$

- Prediction: $f_{w'}(x)$ instead of $f_w(x)$
- Loss becomes

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f_{w+\epsilon}(x) - y]^2$$

# Add noise to the weights

- Loss becomes

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f_{w+\epsilon}(x) - y]^2$$

- To simplify, use Taylor expansion
- $f_{w+\epsilon}(x) \approx f_w(x) + \epsilon^T \nabla f_w(x)$
- Plug in
- $L(f) \approx \mathbb{E}[f_w(x) - y]^2 + \eta \underbrace{\mathbb{E}||\nabla f_w(x)||^2}_{\text{Regularization term}}$

# Other types of regularizations

- Data augmentation
- Early stopping
- Dropout
- Batch Normalization

# Data augmentation

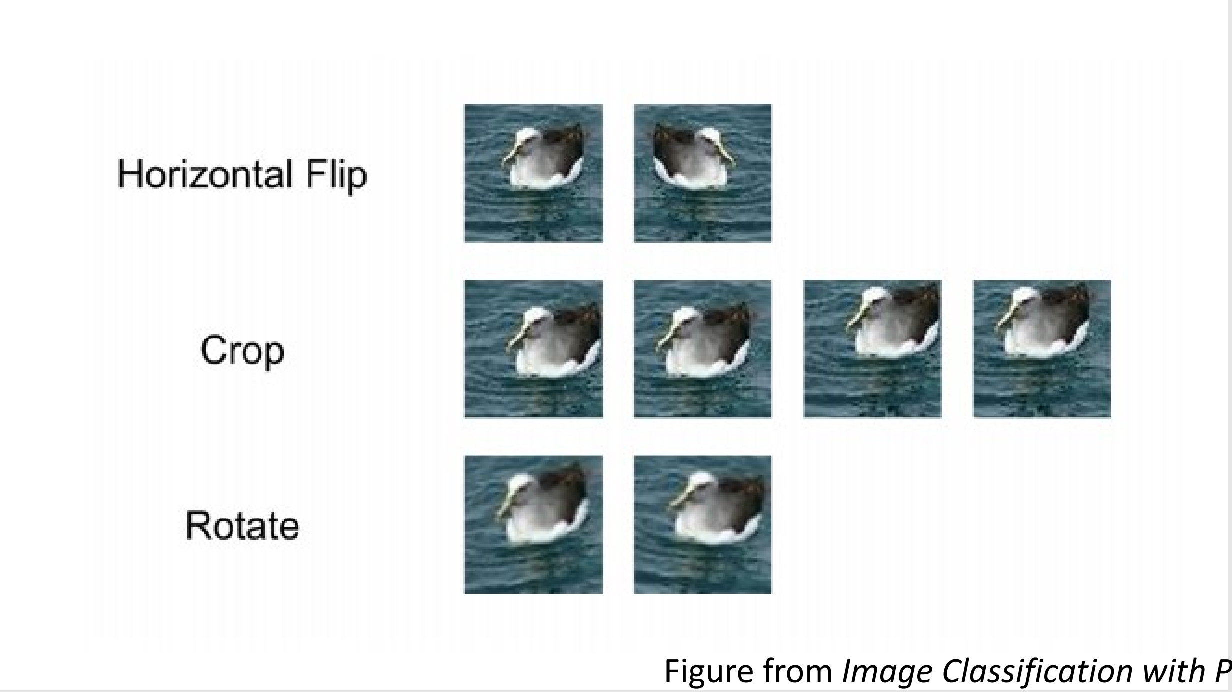



Figure from *Image Classification with Pyramid Representation and Rotated Data Augmentation on Torch 7,* by Keven Wang

# Data augmentation

- Adding noise to the input: a special kind of augmentation

- Be careful about the transformation applied:
  - Example: classifying ‘b’ and ‘d’
  - Example: classifying ‘6’ and ‘9’

# Early stopping

- Idea: don’t train the network to too small training error

- Recall overfitting: Larger the hypothesis class, easier to find a hypothesis that fits the difference between the two

- Prevent overfitting: do not push the hypothesis too much; use validation error to decide when to stop

# Early stopping

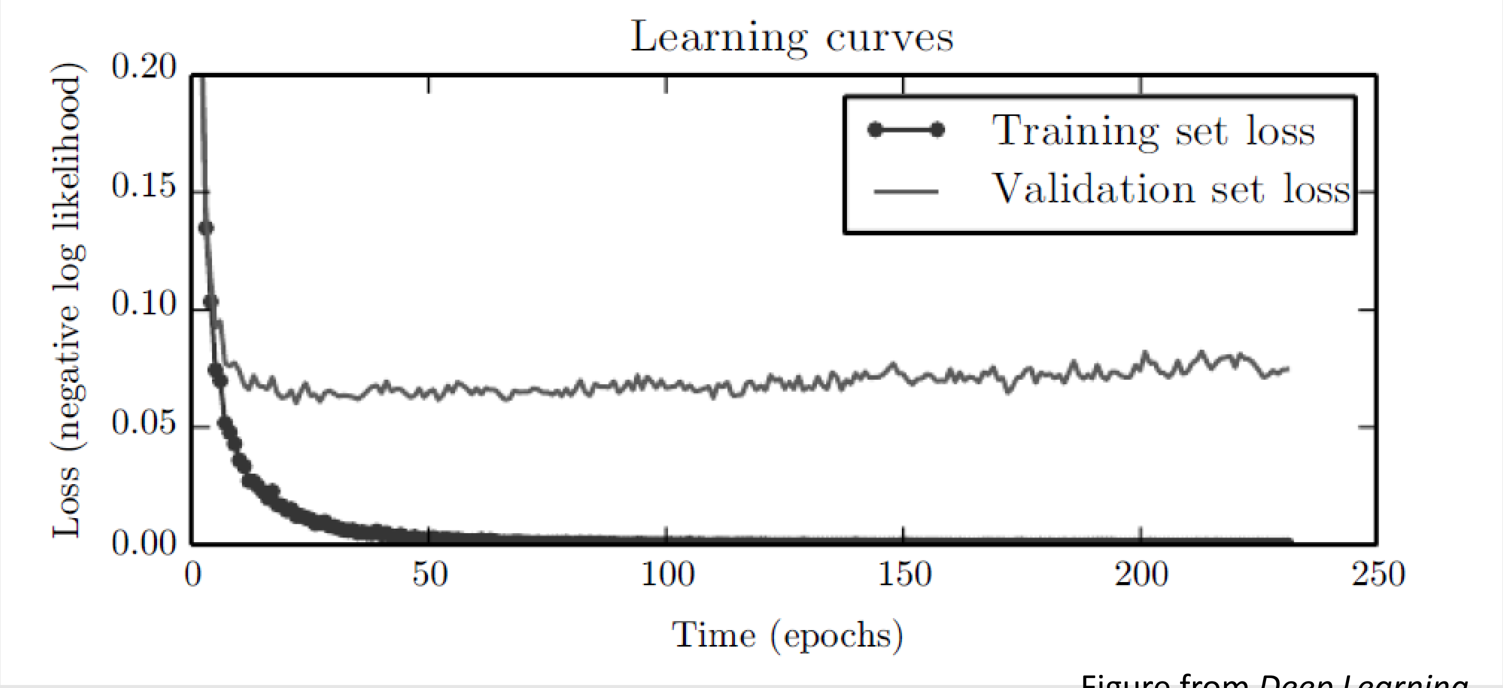



Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

# Early stopping

- When training, also output validation error
- Every time validation error improved, store a copy of the weights
- When validation error not improved for some time, stop
- Return the copy of the weights stored

# Early stopping

- hyperparameter selection: training step is the hyperparameter

- Advantage
  - Efficient: along with training; only store an extra copy of weights
  - Simple: no change to the model/algo

- Disadvantage: need validation data

# Early stopping as a regularizer

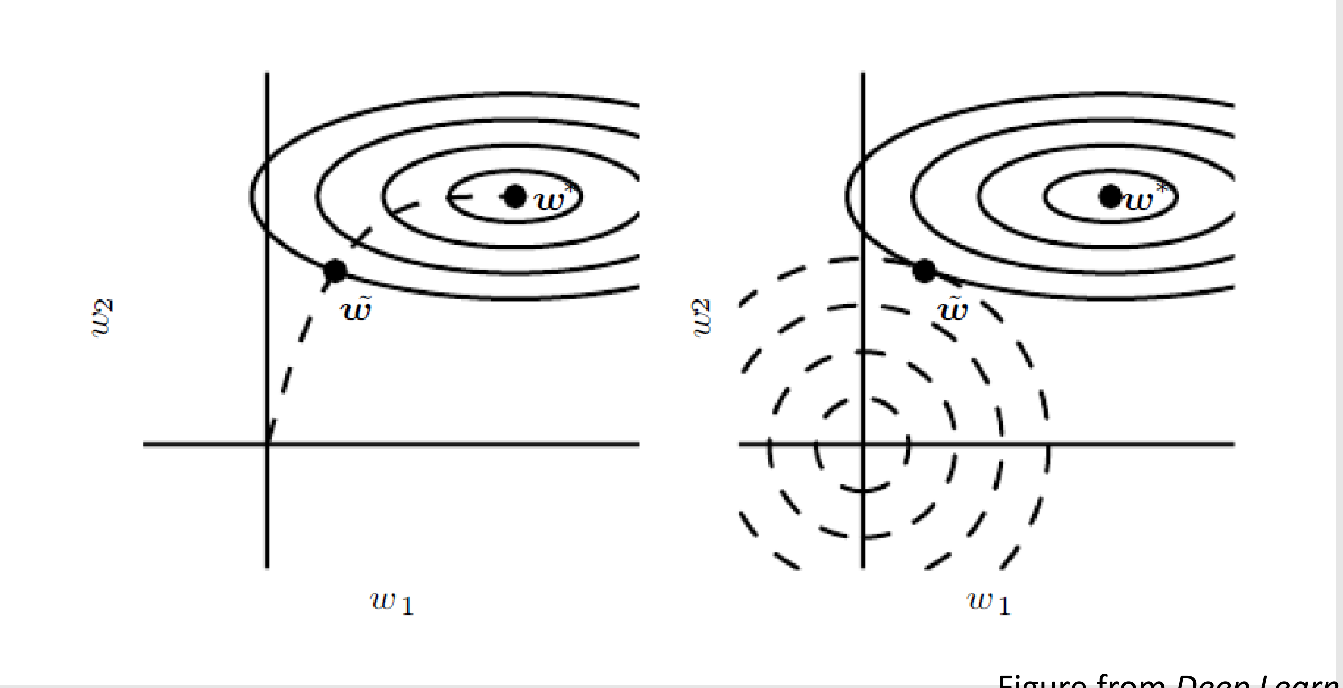



Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

# Dropout

- Randomly select weights to update

- More precisely, in each update step
  - Randomly sample a different binary mask to all the input and hidden units
  - Multiple the mask bits with the units and do the update as usual

- Typical dropout probability: 0.2 for input and 0.5 for hidden units

# Dropout

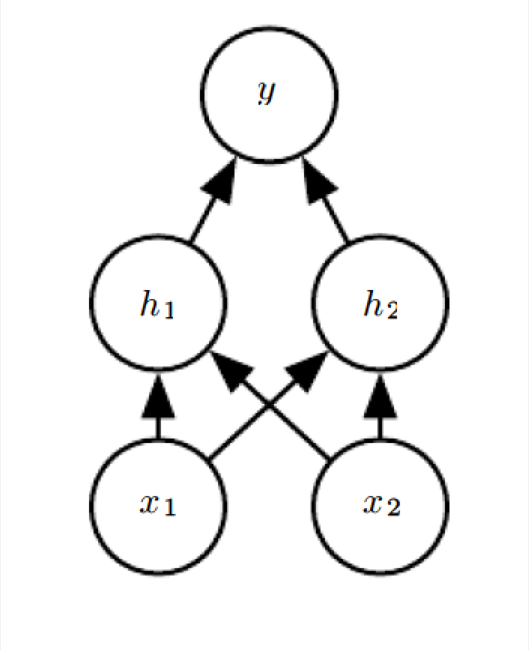



Figure from *Deep Learning*, Goodfellow, Bengio and Courville

# Dropout

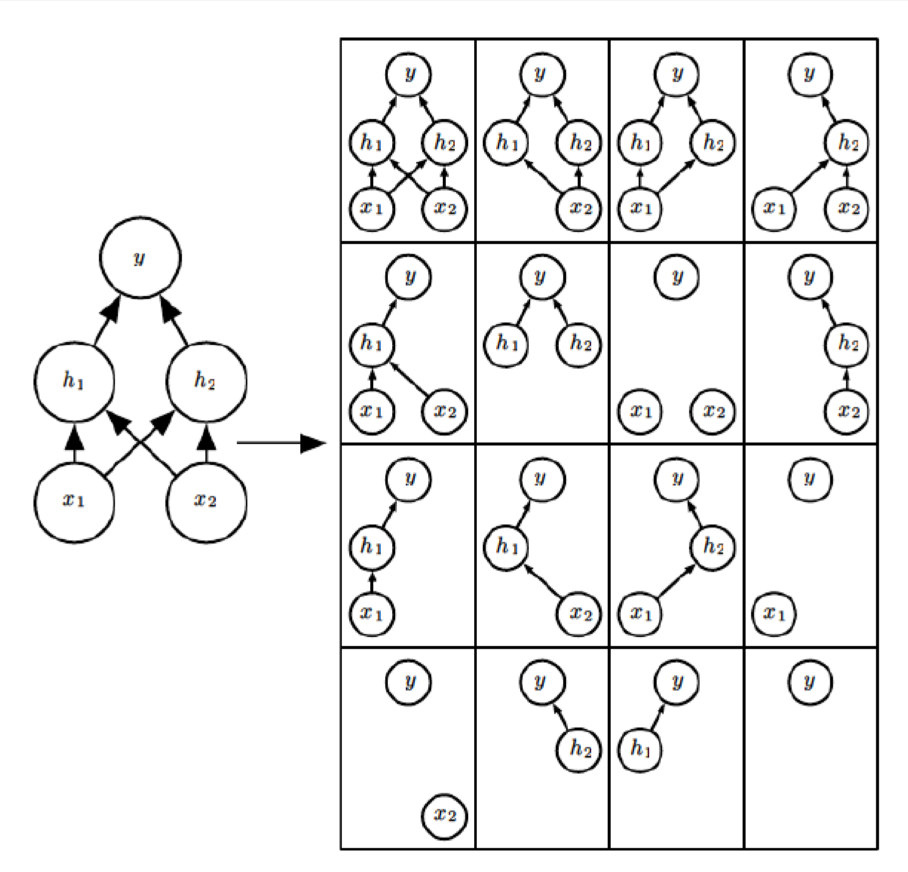



Figure from *Deep Learning*, Goodfellow, Bengio and Courville

# Batch Normalization

- If outputs of earlier layers are uniform or change greatly on one round for one mini-batch, then neurons at next levels can’t keep up: they output all high (or all low) values

- Next layer doesn’t have ability to change its outputs with learning-rate-sized changes to its input weights

- We say the layer has “saturated”

# Another View of Problem

- In ML, we assume future data will be drawn from same probability distribution as training data

- For a hidden unit, after training, the earlier layers have new weights and hence generate input data for this hidden unit from a *new* distribution

- Want to reduce this *internal covariate shift* for the benefit of later layers

**Input:** Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: $\gamma$, $\beta$

**Output:** $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

**Algorithm 1:** Batch Normalizing Transform, applied to activation $x$ over a mini-batch.

# Comments on Batch Normalization

- First three steps are just like standardization of input data, but with respect to only the data in mini-batch.  Can take derivative and incorporate the learning of last step parameters into backpropagation.

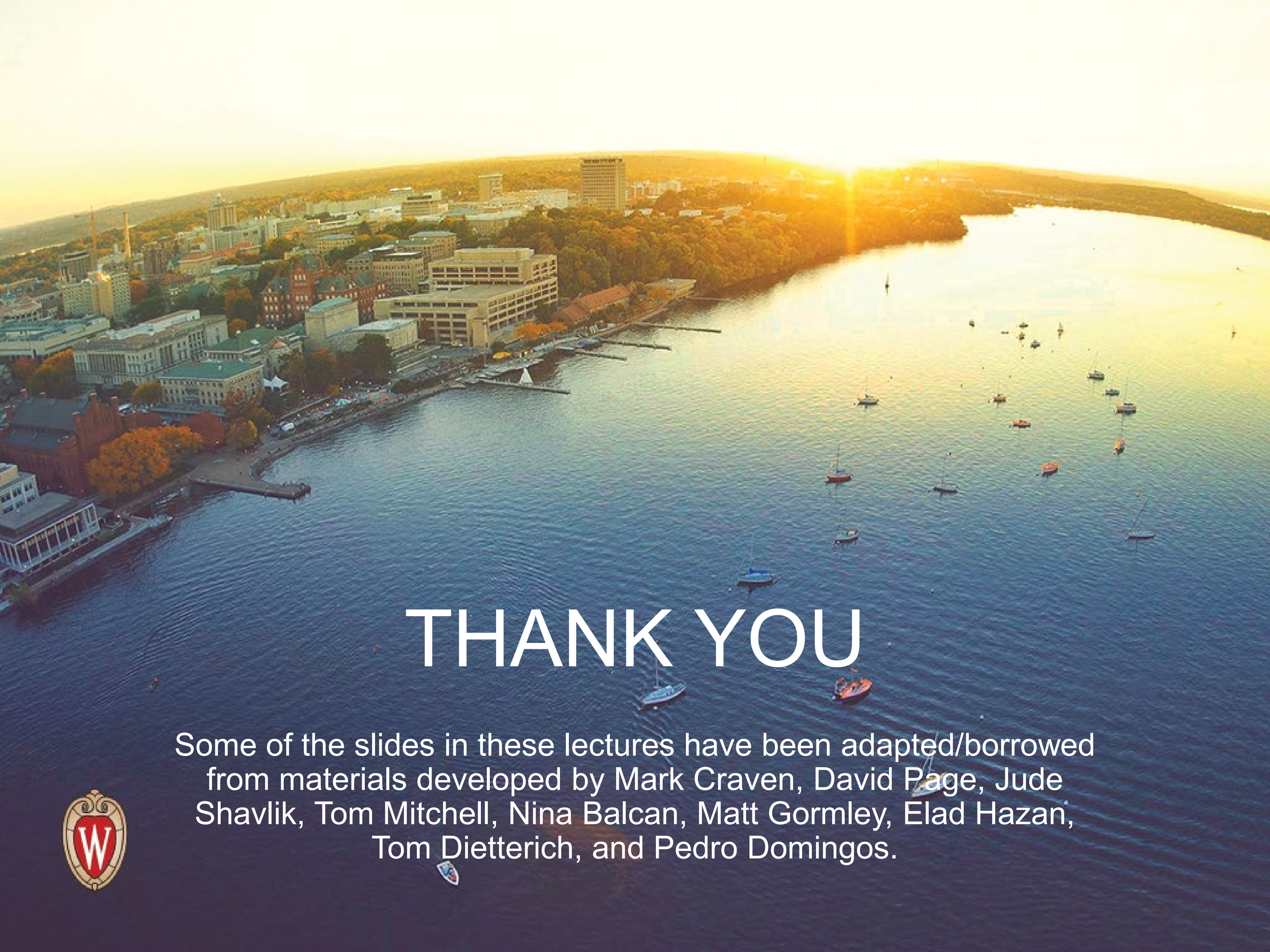
- Note last step can completely un-do previous 3 steps

- But if so this un-doing is driven by the *later* layers, not the *earlier* layers; later layers get to “choose” whether they want standard normal inputs or not

# What regularizations are frequently used?

- $l_2$ regularization
- Early stopping
- Dropout/Batch Normalization

- Data augmentation if the transformations known/easy to implement



# THANK YOU

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Matt Gormley, Elad Hazan, Tom Dietterich, and Pedro Domingos.