Regularization in Machine Learning

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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.

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

Overfitting example: regression using polynomials

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

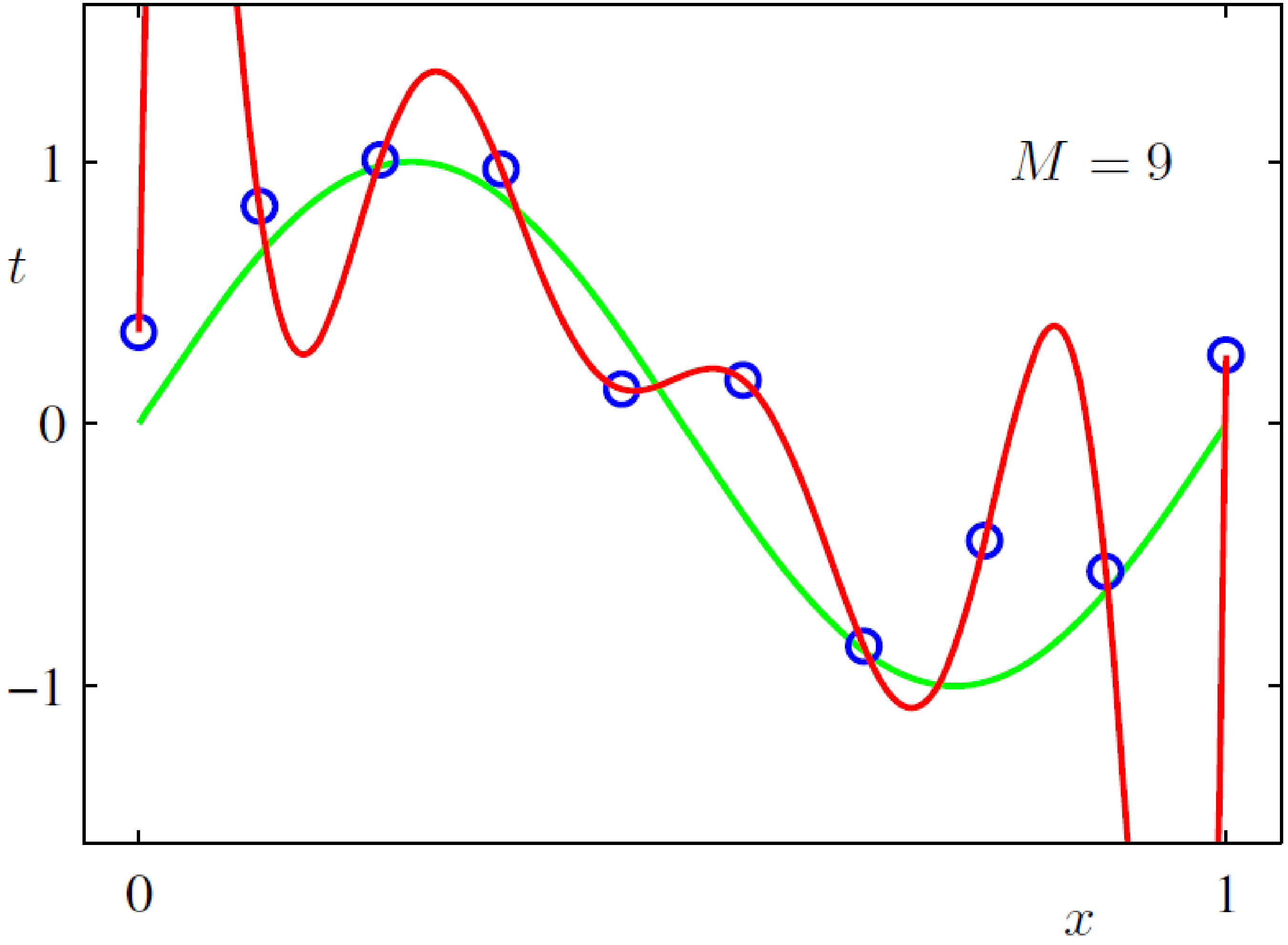


Figure from *Machine Learning and Pattern Recognition*, Bishop

Overfitting example: regression using polynomials

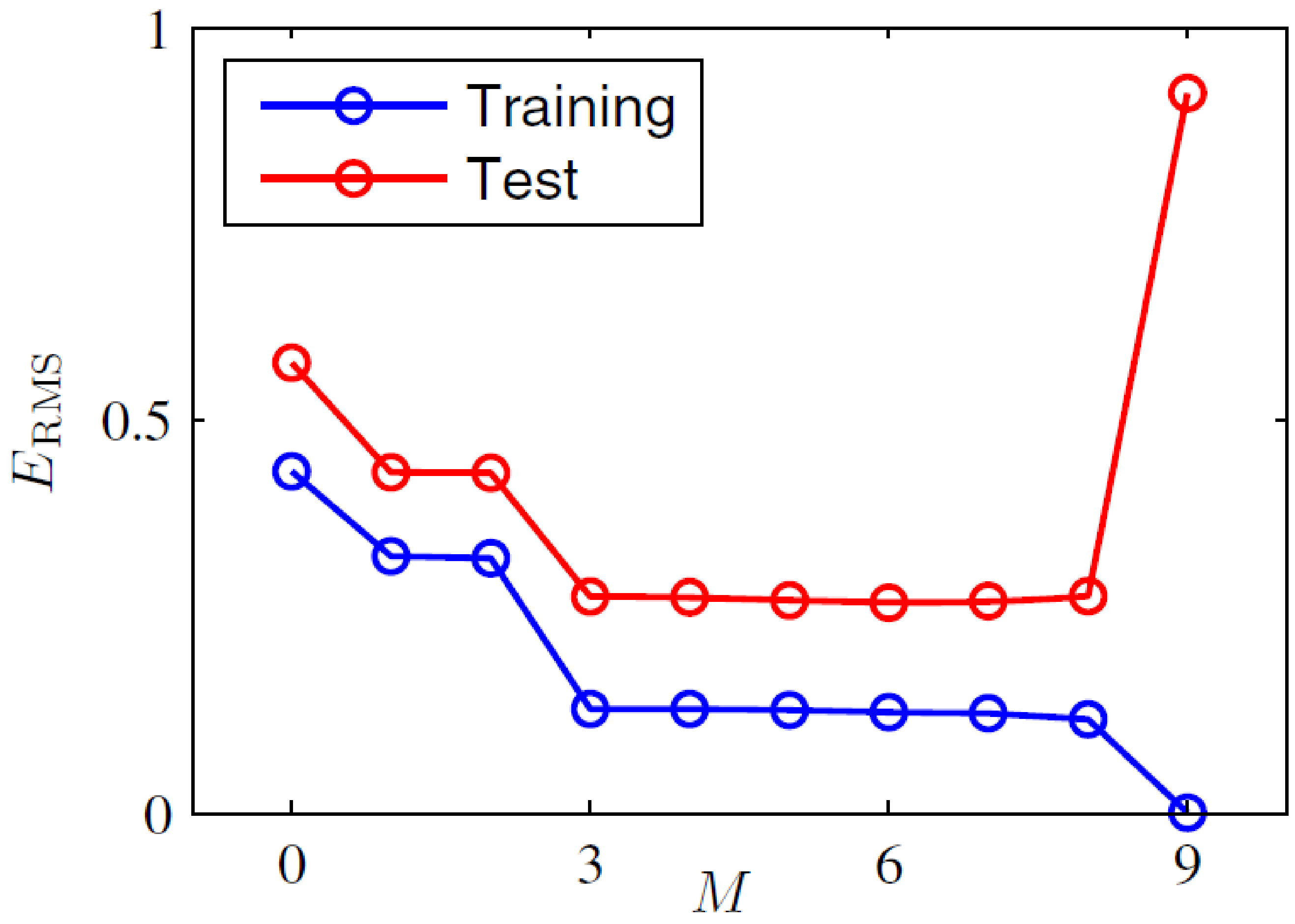


Figure from *Machine Learning and Pattern Recognition*, Bishop

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 Ω measured by some quantity R

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

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

- Example: l_2 regularization

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

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

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

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

- Suppose θ^* is the optimal for hard-constraint optimization

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

- Suppose λ^* is the corresponding optimal for max

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

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):

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

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 likelihood $p(x, y \mid \theta)$ 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

Three views

- 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 θ^*

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

- Since θ^* 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 θ_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

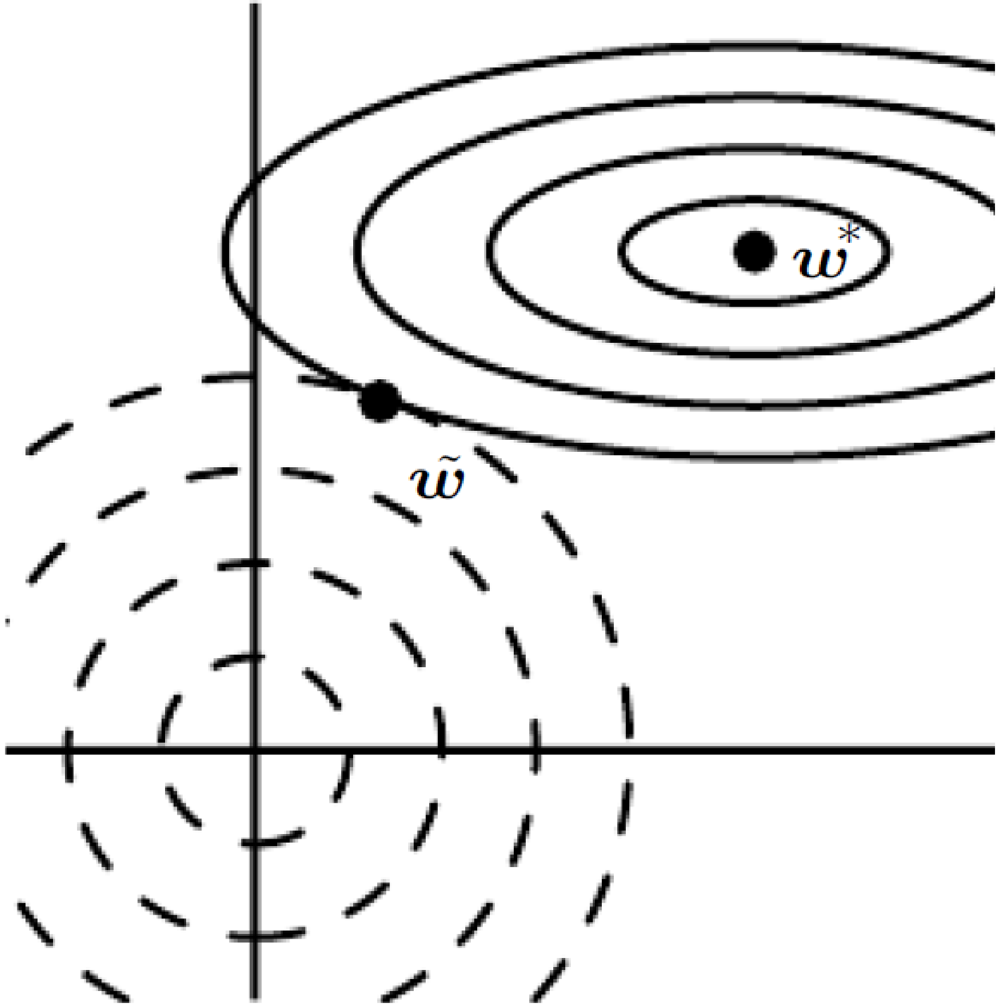
$$\theta_R^* \approx (H + \alpha I)^{-1} H \theta^*$$

- Suppose H has eigen-decomposition $H = Q \Lambda Q^T$

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

- Effect: rescale along eigenvectors of H

Effect on the optimal solution



Notations:

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

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 sign applies to each element in θ

- 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 θ^*

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

- Since θ^* 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)

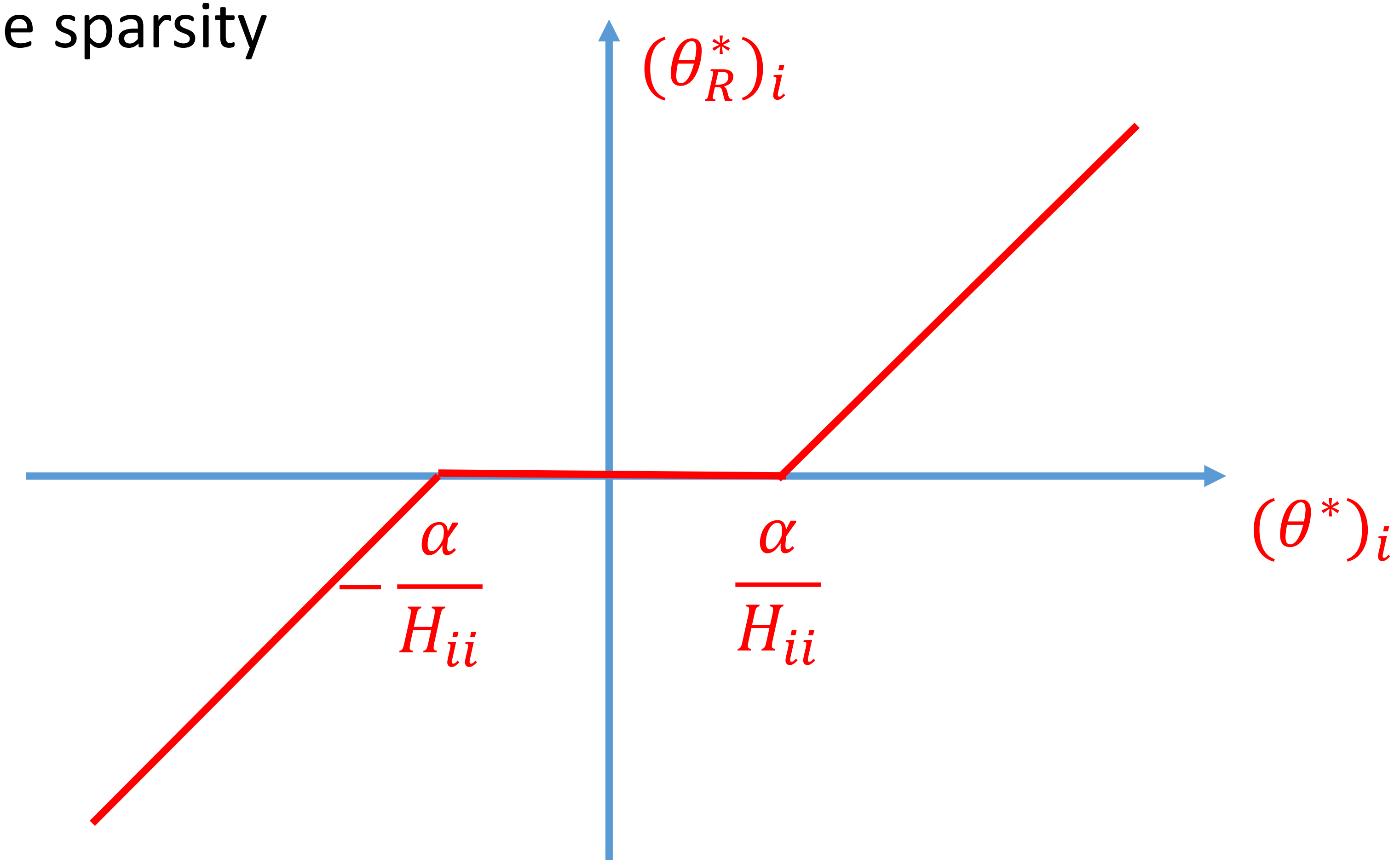
$$\hat{L}_R(\theta) \approx \sum_i \frac{1}{2} H_{ii}(\theta_i - \theta_i^*)^2 + \alpha\, |\theta_i|$$

- The optimal θ_R^*

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

Effect on the optimal solution

- Effect: induce sparsity



Effect on the optimal solution

- Further assume that H is diagonal
- Compact expression for the optimal θ_R^*

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

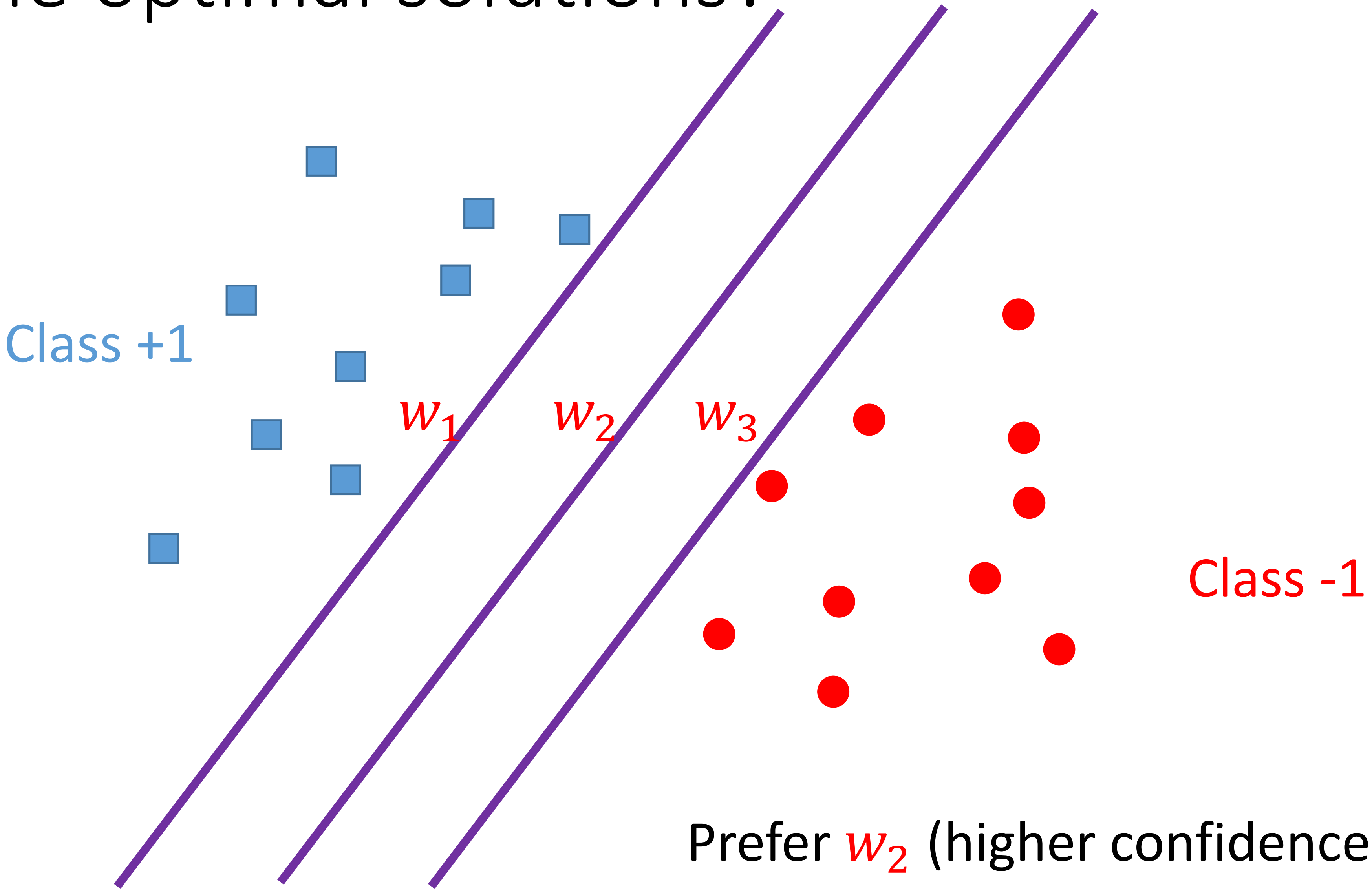
Bayesian view

- l_1 regularization corresponds to Laplacian prior

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

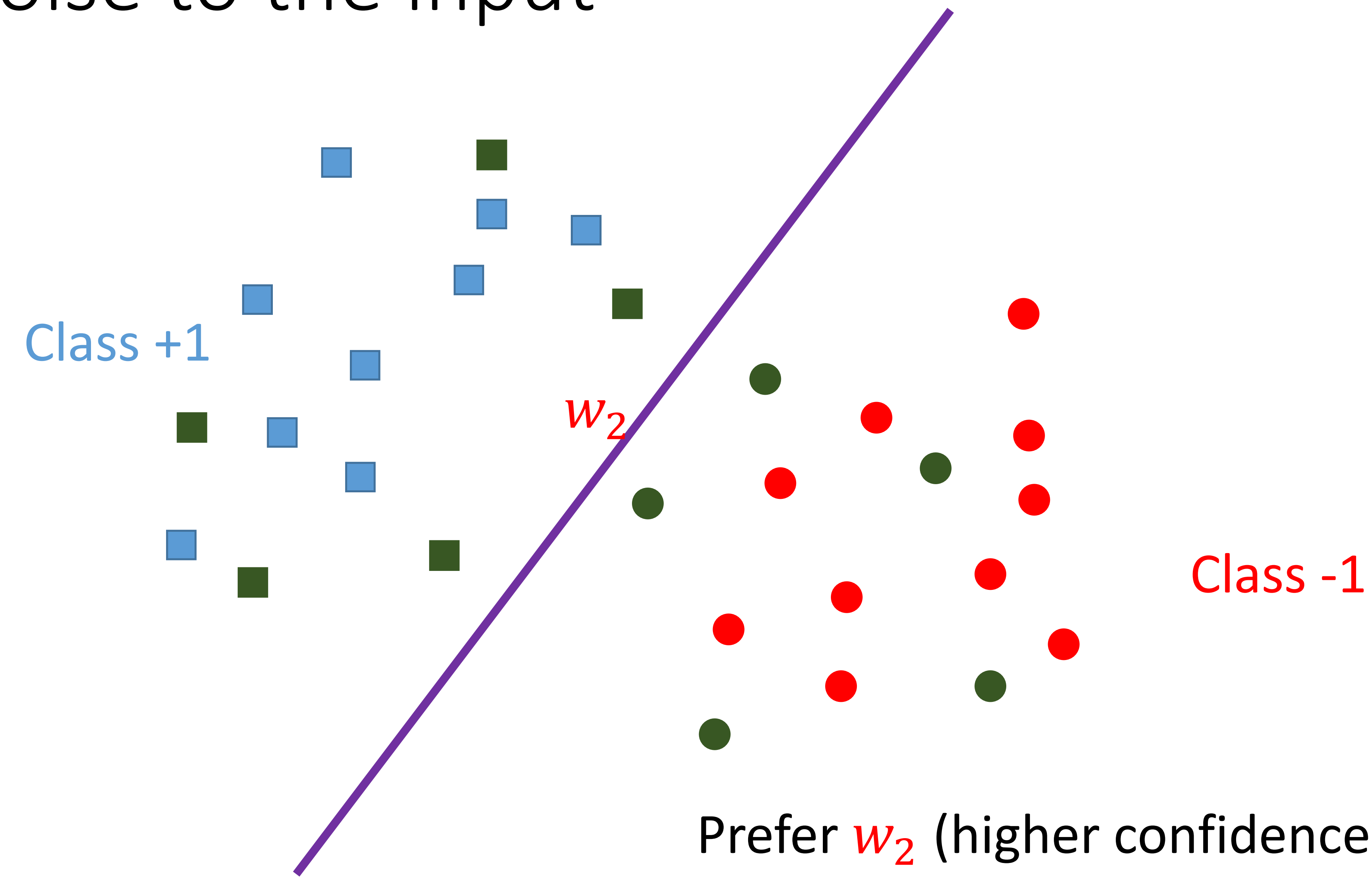
$$\log p(\theta) = \alpha \sum_i |\theta_i| + \text{constant} = \alpha ||\theta||_1 + \text{constant}$$

Multiple optimal solutions?



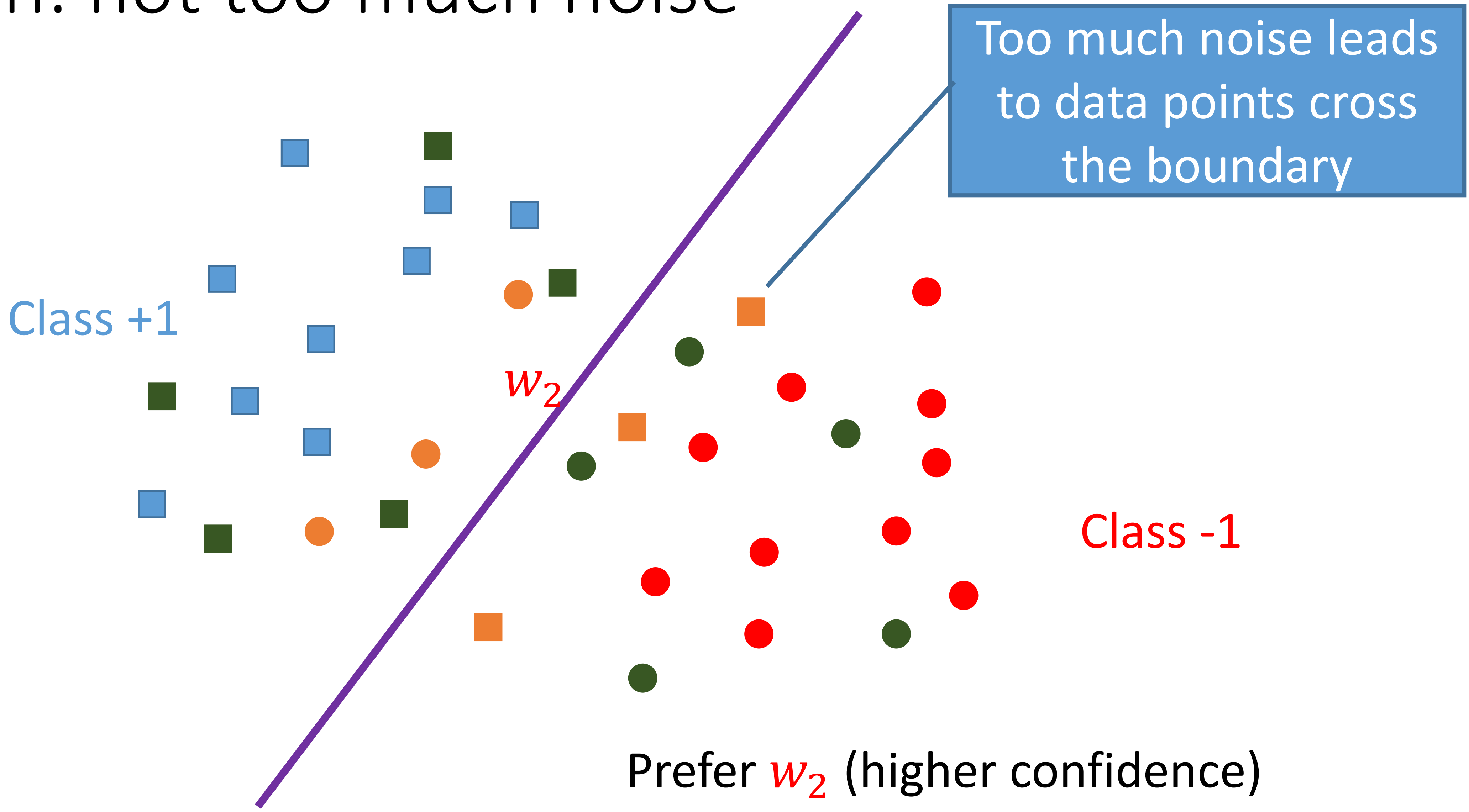
Prefer w_2 (higher confidence)

Add noise to the input



Prefer w_2 (higher confidence)

Caution: not too much noise



Prefer w_2 (higher confidence)

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

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

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

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

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
- $f_{w+\epsilon}(x) \approx f_w(x) + \epsilon^T \nabla f(x) + \frac{\epsilon^T \nabla^2 f(x) \epsilon}{2}$
- Plug in
- $L(f) \approx \mathbb{E}[f_w(x) - y]^2 + \eta\mathbb{E}[\underbrace{(f_w(x) - y)\nabla^2 f_w(x)}_{\text{Small so can be ignored}}] + \eta\underbrace{\mathbb{E}||\nabla f_w(x)||^2}_{\text{Regularization term}}$

Other types of regularizations

- Data augmentation
- Early stopping
- Dropout
- Batch Normalization

Data augmentation

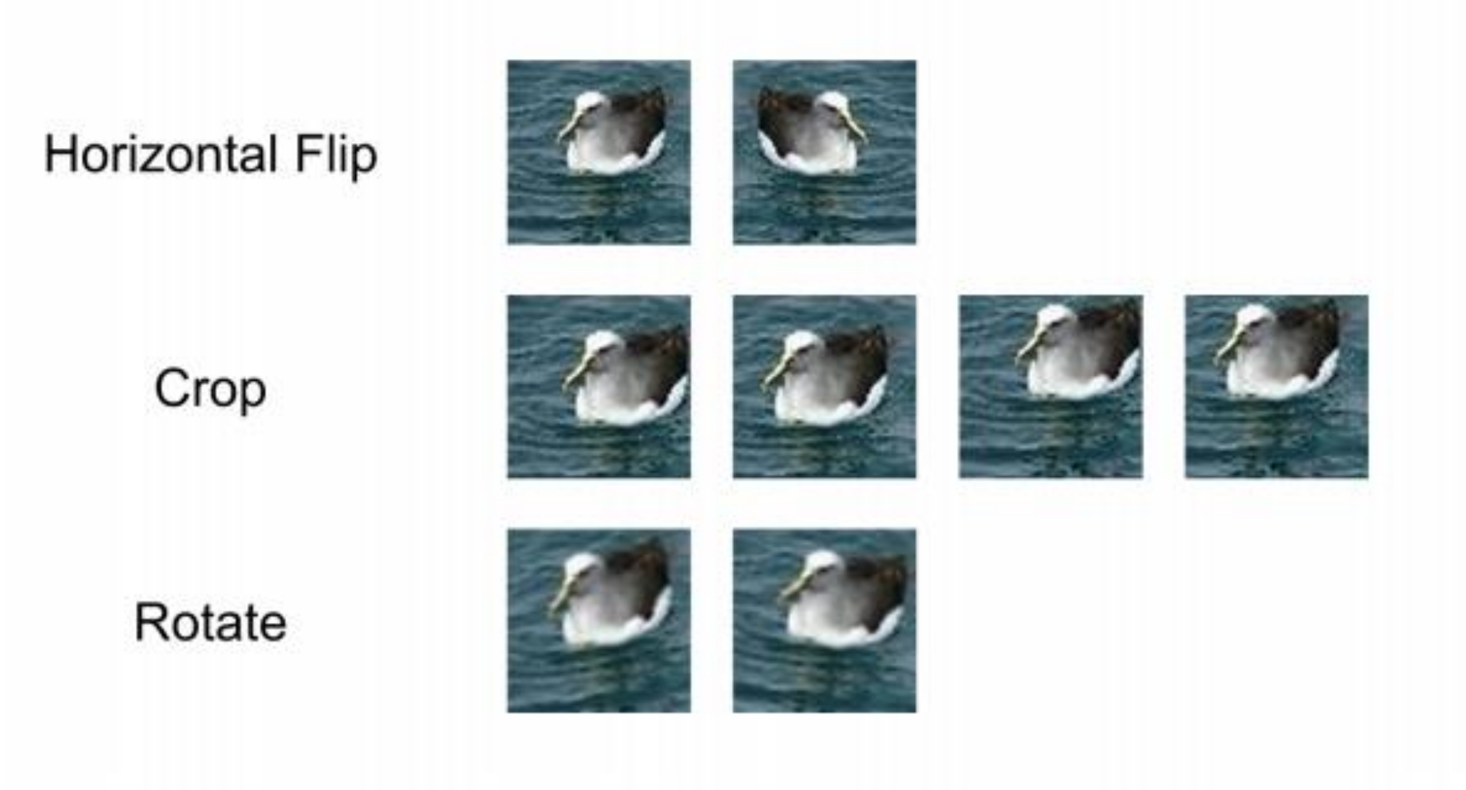


Figure from *Image Classification with Pyramid Representation and Rotated Data Augmentation on Torch 7,* by Keven Wang

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

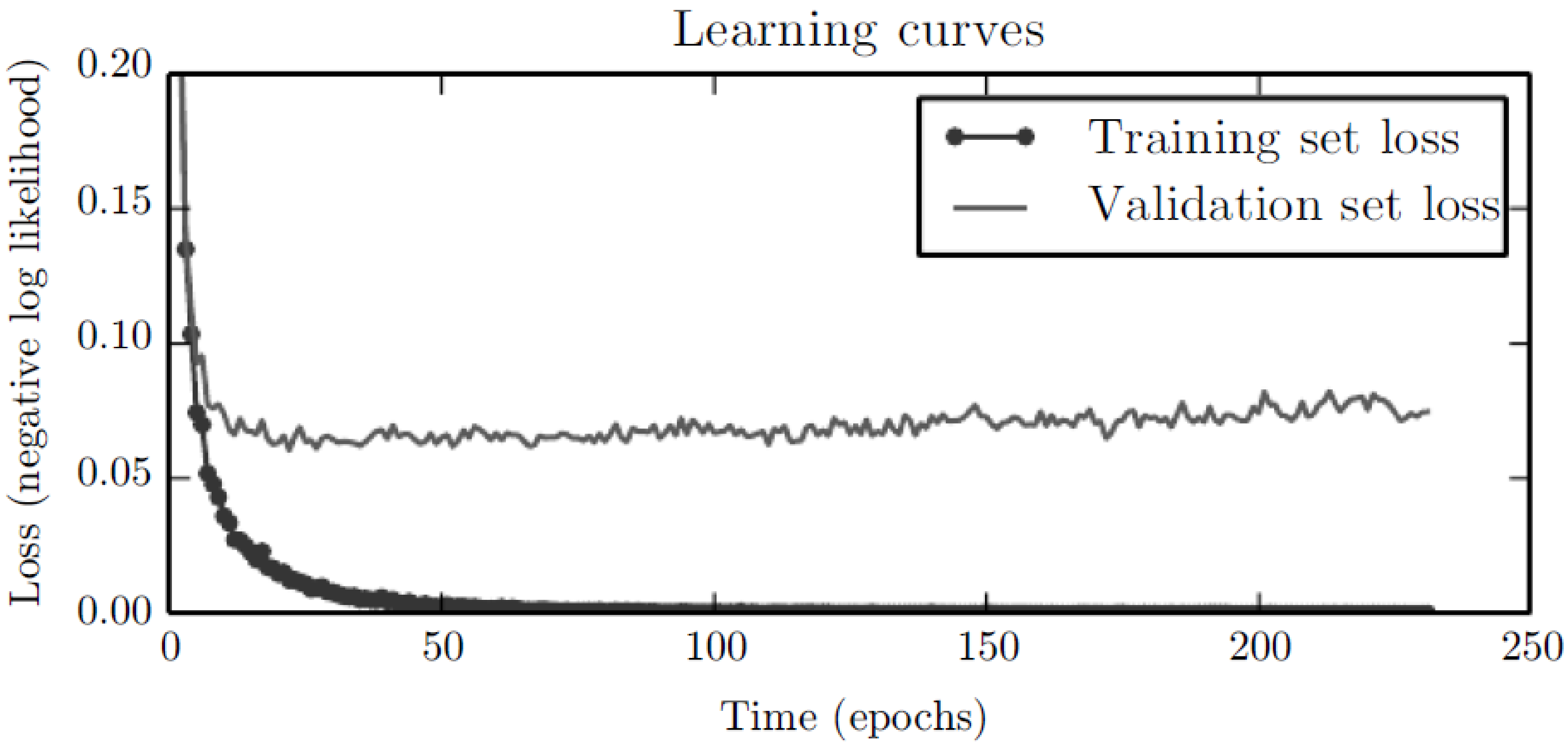


Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

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

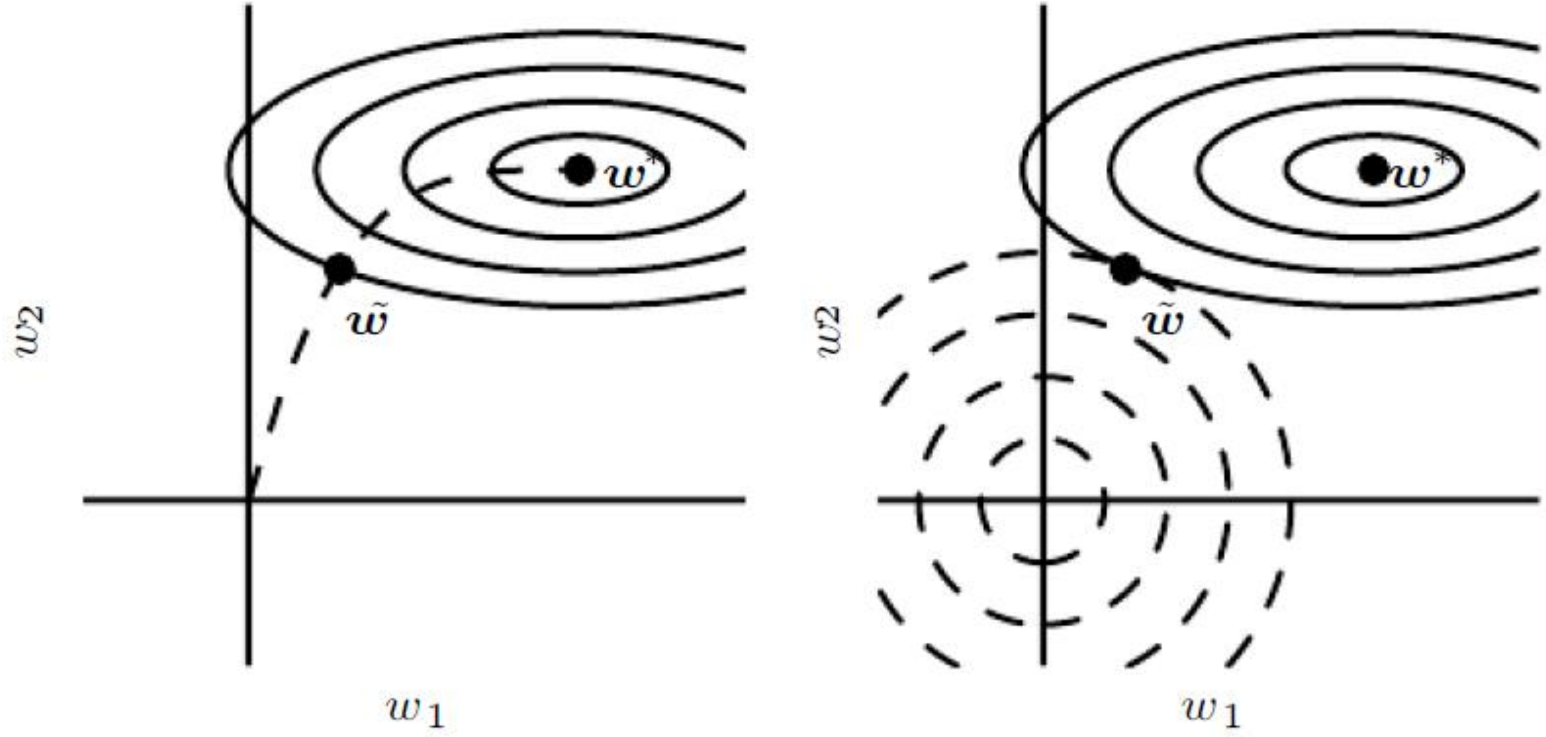


Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

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

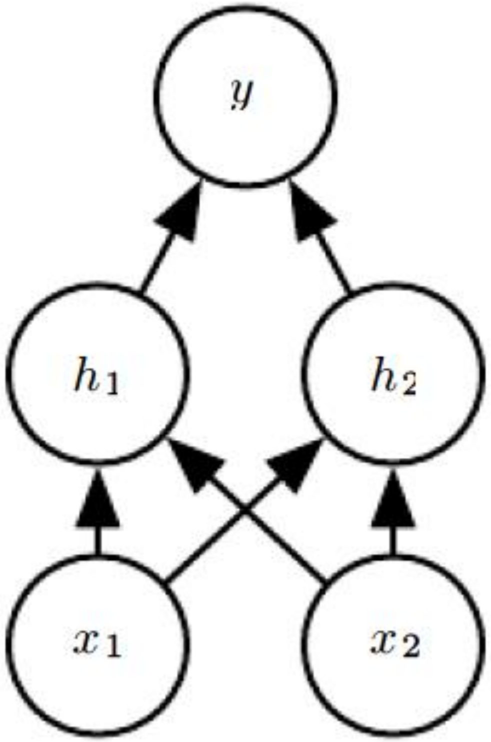


Figure from *Deep Learning*,
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Dropout

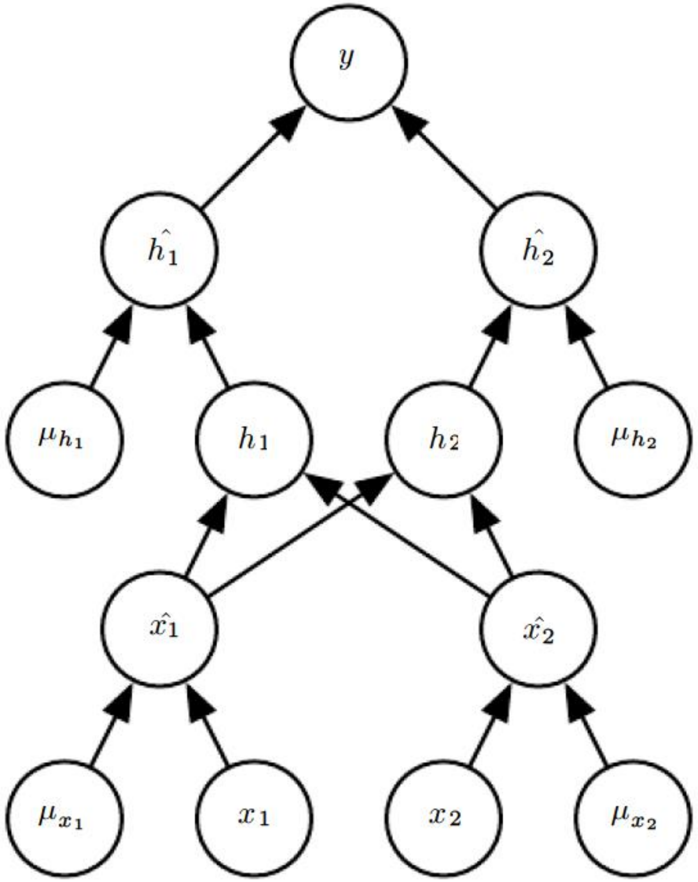

Figure from *Deep Learning*, Goodfellow, Bengio and Courville

Dropout

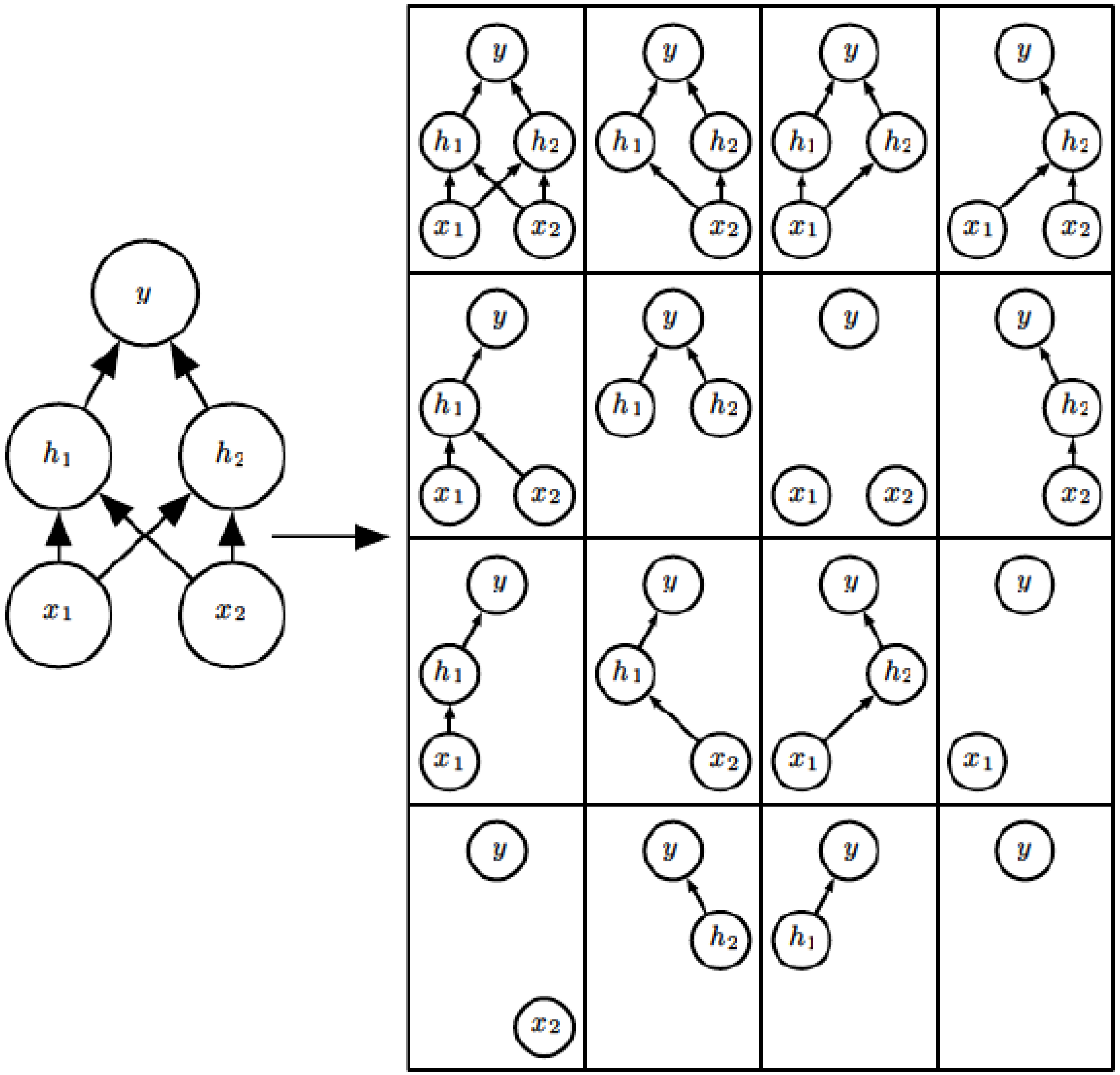

Figure from *Deep Learning*, Goodfellow, Bengio and Courville

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: γ, β

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

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

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

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

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

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