Machine Learning 410

Lesson 2

Regularization for Deep Learning

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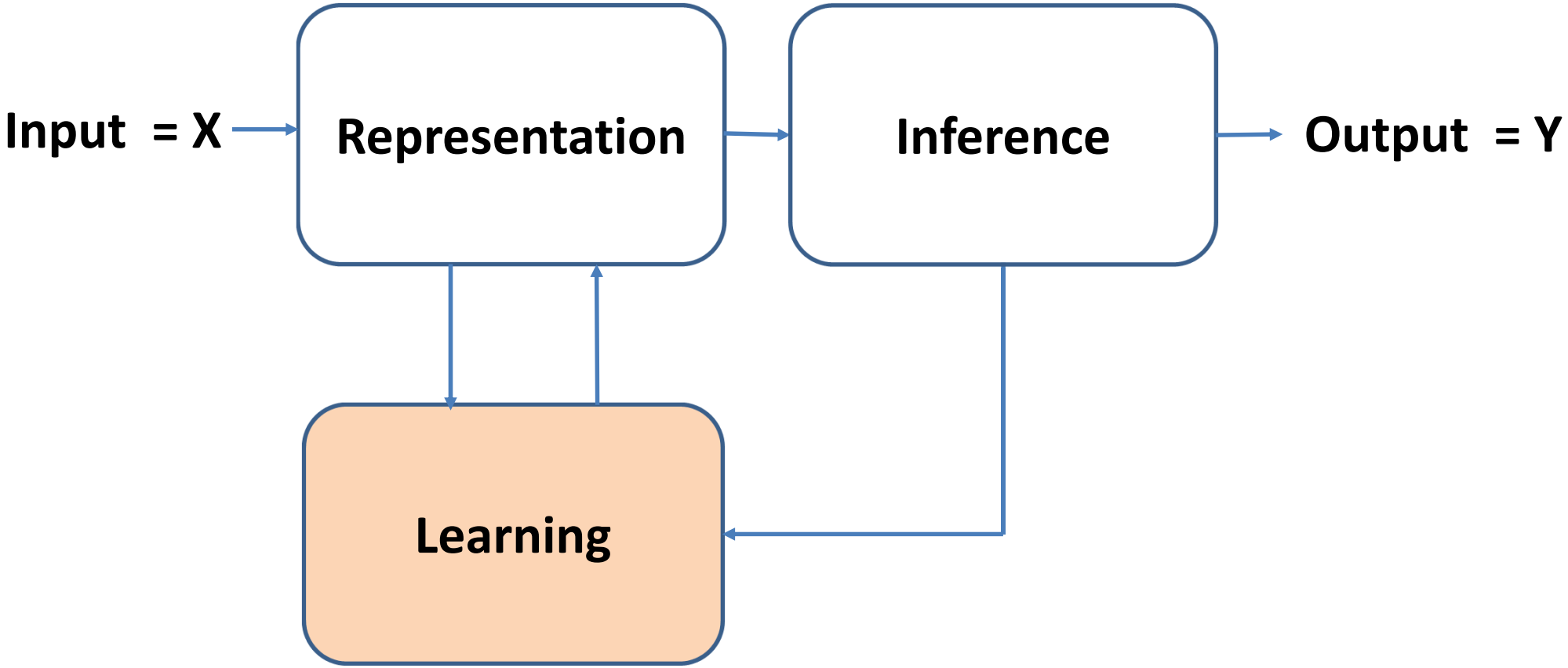
Introduction to Regularization for Deep Learning



Introduction to Regularization for Deep Learning

- Deep learning models have very large numbers of parameters which must be learned.
  - Even with large training datasets there may only be a few samples per parameters
- Large number of parameters leads to high chance of **over-fitting** deep learning models
  - Over-fit models do not generalize
  - Over-fit models have poor response to input noise
- To prevent over-fitting we apply **regularization methods**

Introduction to Regularization for Deep Learning

- Bias-variance trade-off
- l2 regularization
- l1 regularization
- Early stopping
- Dropout regularization
- Batch normalization

The Bias-Variance Trade-Off

- High capacity models fit training data well
  - Exhibit high variance
  - Do not generalize well; exhibit **brittle behavior**
  - $\text{Error}_{\text{training}} << \text{Error}_{\text{test}}$
- Low capacity models have high bias
  - Generalize well
  - Do not fit data well
- Regularization adds bias
  - Strong regularization adds significant bias
  - Weak regularization leads to high variance

The Bias-Variance Trade-Off

- How can we understand the bias-variance trade-off?
- We start with the error:

$$\Delta y = E\left[Y - \hat{f}(X)\right]$$

Where:

$Y =$ the label vector.

$X =$ the feature matrix.

$\hat{f}(x) =$ the trained model.

The Bias-Variance Trade-Off

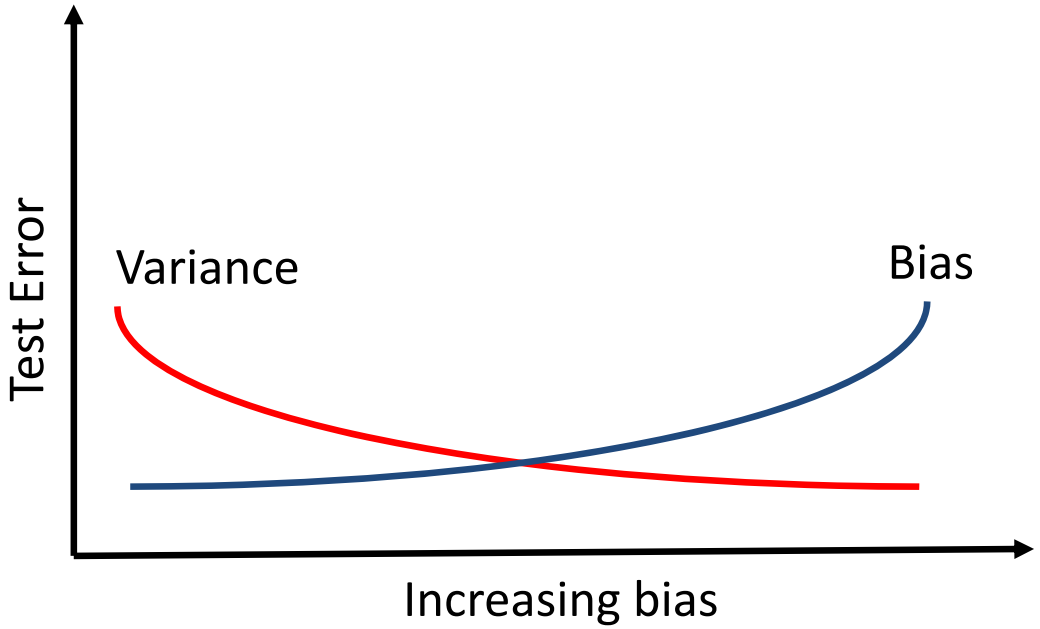
- We can expand the error term

$$\Delta x = \left(E[\hat{f}(X)] - \hat{f}(X)\right)^2 + E\left[(\hat{f}(X) - E[\hat{f}(X)])^2\right] + \sigma^2$$

$$\Delta x = Bias^2 + Variance + Irreducible\ Error$$

- Increasing bias decreases variance
- Notice that even if the bias and variance are 0 there is still irreducible error

The Bias-Variance Trade-Off



l2 Regularization

- Over-fit models tend to have parameters (weights) with extreme values
- One way to regularize models is to limit the values of the parameters
- We add a small bias term to (greatly) reduce the variance

l2 Regularization

- One way to limit the size of the model parameters is to constrain the **l2** or **Euclidian norm**:

$$||W||^2 = \left(w_1^2 + w_2^2 + \ldots + w_n^2\right)^{\frac{1}{2}} = \left(\sum_{i=1}^{n} w_i^2\right)^{\frac{1}{2}}$$

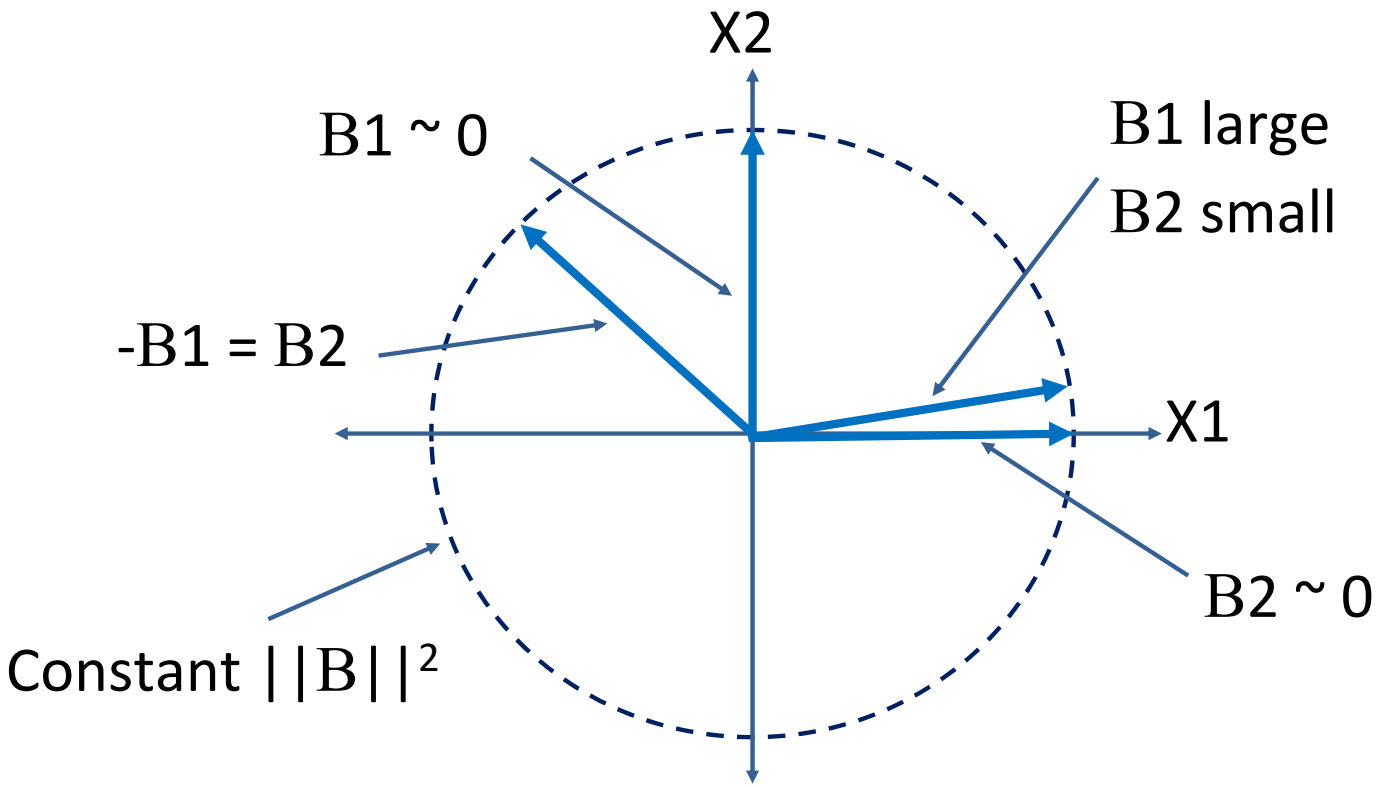
- The regularized loss function is then:

$$J(W) = J_{MLE}(W) + \lambda||W||^2$$

- Where λ is the regularization hyperparameter
  - Large λ increases bias but reduces variance
  - Small λ decreases bias and increases variance

l2 Regularization

How can you gain some intuition about l2 regularization?



l2 regularization is considered a **soft constraint**

l2 Regularization

- l2 regularization goes by many names
- Is called Euclidian norm regularization
- First published by Andrey Tikhonov regularization, in late 1940s
  - Only published in English in 1977
  - Is known as **Tikhonov regularization**
- In the statistics literature the method is often called **ridge regression**
- In the engineering literature is referred to as **pre-whitening**

l2 Regularization

Plaque commemorating Andrey Tikhonov at Moscow Institute of Mathematics

Review of Eigenvalues

Eigenvalues are characteristic roots or characteristic values of a linear system

- Start with a square n x n matrix *A*, and vector *x*:

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- Then, an **eigenvalue** of *A* has the property:

$$Ax = \lambda x$$

Review of Eigenvalues

Eigenvalues are characteristic roots or characteristic values of a linear system

- Rewrite the eigenvalue relationship:

$$Ax = \lambda x$$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- To see that λ is a root of A we can rearrange as follows:

$$Ax - \lambda x = 0$$

$$(A - I\lambda)x = 0$$

Review of Eigenvalues

Eigenvalues are characteristic roots or characteristic values of a linear system

- An n x n matrix A will have **n eigenvalues**
- Find eigenvalues by solving

$$(A - I\lambda)x = 0$$

- Solve n equations involving the **determinant**:

$$det(A - x) = 0$$

- For more detail on determinants see: https://en.wikipedia.org/wiki/Determinant

Review of Eigenvalues and Eigenvectors

Each eigenvalue of a square matrix is associated with an **eigenvector**

- There is a left and right eigenvector for each eigenvalue
- The **right eigenvector** has the following relationship to the matrix *A* and eigenvalue λ:

$$Ax_r = \lambda_r x_r$$

$$(A - I\lambda_r)x_r = 0$$

- Notice that the right eigenvector is to the right of the matrix

Review of Eigenvalues and Eigenvectors

Each eigenvalue of a square matrix is associated with an **eigenvector**

- There is also a **left eigenvector** with the following relationship to the matrix A and eigenvalue λ:

$$x_l A = \lambda_l x_l$$

$$(x_l A)^T = \lambda_l x_l^T$$

$$(A^T - I\lambda_l)x_l^T = 0$$

- Notice that the right eigenvector is to the right of the matrix

Review of Eigenvalues and Eigenvectors

Each eigenvalue of a square matrix is associated with an **eigenvector**

- The **l2 norm** of any eigenvector is 1:

$$||x||^2 = (x_1^2 + x_2^2 \dots x_n^2)^{1/2} = 1$$

- This property means that the matrix of n eigenvectors, *Q*, is **unitary**
- For a **full rank** matrix, each eigenvector is **orthogonal** to every other eigenvector, and **linearly independent**
- Thus, for diagonal matrix of n eigenvalues, Λ, an n x n matrix, *A*, can be **factored**:

$$A = Q\Lambda Q^{-1}$$

Review of Eigenvalues and Eigenvectors

Each eigenvalue of a square matrix is associated with an **eigenvector**

- Given the eigenvalue-eigenvector **factorization** of the matrix *A*:

$$A = Q\Lambda Q^{-1}$$

- The **inverse** of *A* can be found:

$$A^{-1} = Q\Lambda^{-1}Q^{-1}$$

- And, A to the **Nth power** can be computed:

$$A^{N} = Q\Lambda^{N}Q^{-1}$$

- You can find more on eigenvalue-eigenvector decomposition: https://en.wikipedia.org/wiki/Eigendecomposition_of_a_matrix

Eigenvalues and Regularization

l2 regularization with eigenvalue-eigenvector decomposition

- A linear model with feature matrix, *A*, labels, *x*, and parameter vector *b* is written:

$$x = Ab$$

- We want to find a solution:

$$b = A^{-1}x$$

- The **normal equations** represent a computationally efficient approach:

$$b = (A^T A)^{-1} A^T x$$

Eigenvalues and Regularization

l2 regularization with eigenvalue-eigenvector decomposition

- The n coefficients of the linear model are found with the normal equations:

$$b = (A^T A)^{-1} A^T x$$

- The solution requires finding the inverse of a **symmetric n x n matrix**
- This matrix can be represented by its eigenvalue-eigenvector decomposition:

$$A^T A = Q \Lambda Q^{-1}$$

Eigenvalues and Regularization

l2 regularization with eigenvalue-eigenvector decomposition

- We need the inverse of the symmetric matrix with decomposition:

$$A^T A = Q \Lambda Q^{-1}$$

$$(A^T A)^{-1} = Q \Lambda^{-1} Q^{-1}$$

- Where

$$\Lambda^{-1} = \begin{bmatrix} \frac{1}{\lambda_1} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\lambda_2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & \frac{1}{\lambda_n} \end{bmatrix}$$

Eigenvalues and Regularization

l2 regularization with eigenvalue-eigenvector decomposition

- Can compute the inverse of the symmetric matrix with decomposition:

$$(A^T A)^{-1} = Q\Lambda^{-1}Q^{-1}$$

- But, $(A^TA)^{-1}$ can be **rank deficient**!
- In practice, many machine learning problems are rank deficient
- A the eigenvectors of a rank deficient matrix are **not linearly independent**
- A rank deficient matrix has some **zero eigenvalues**
- A matrix with m nonzero eigenvalues is said to have **rank m**

Eigenvalues and Regularization

l2 regularization with eigenvalue-eigenvector decomposition

- For l2 regularization we introduce a small bias term, α^2
- The least-squares, or l2 minimization problem, is then:

$$min[\| A \cdot x - b \| + \| \alpha^2 \cdot I \|]$$

- With solution

$$b = (A^T A + \alpha^2 \cdot I)^{-1} A^T x$$

Eigenvalues and Regularization

l2 regularization with eigenvalue-eigenvector decomposition

- For the inverse $(A^T A + \alpha^2 \cdot I)^{-1}$ the eigenvalue matrix is:

$$\Lambda^{+}_{Tikhonov} = \begin{bmatrix} \frac{1}{\lambda_1 + \alpha^2} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\lambda_2 + \alpha^2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & \frac{1}{\lambda_m + \alpha^2} \end{bmatrix}$$

- Even for an eigenvalue, λ, of 0, the biased inverse becomes $1/\alpha^2$
- Thus, the bias term, α^2, creates a 'ridge' of nonzero values on the diagonal ensuring the inverse exists and is stable.

Eigenvalues and Regularization

l2 regularization with eigenvalue-eigenvector decomposition

- Consider the bias-variance trade off of the solution:

$$b = (A^T A + \alpha^2 \cdot I)^{-1} A^T x$$

- For $\alpha^2 = 0$, there is no bias, but variance can be high
- For a large value of α^2 , the inverse is stable and the variance is low, but the bias can be high

Bayesian View of l2 Regularization

How can l2 regularization be interpreted in terms of a prior?

- For data X and label values, Y the posterior distribution of the weights, W is:

$$p(W \mid \{X, Y\}) = \frac{p(W)\, p(\{X, Y\} \mid W)}{p(\{X, Y\})}$$

- The likelihood of the data and labels given the weights is:

$$p(\{X, Y\} \mid W)$$

- The prior distribution of the weights is $p(W)$

Bayesian View of l2 Regularization

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- The likelihood of the data and labels given the weights is:

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Bayesian View of l2 Regularization

How can l2 regularization be interpreted in terms of a prior?

- Starting from:

$$p(W \mid \{X, Y\}) = \frac{p(W)\, p(\{X, Y\} \mid W)}{p(\{X, Y\})}$$

- Take logs of both sides to find the maximum a postirori (MAP) value of W:

- The prior distribution of the weights is $p(W)$

l1 Regularization

- Regularization can be performed with other norms
- The **l1 (min-max) norm** is another common choice
- Conceptually, l1 norm limits the sum of the absolute values of the weights:

$$\|W\|^1 = \left(|w_1| + |w_2| + \ldots + |w_n|\right) = \left(\sum_{i=1}^{n} |w_i|\right)^1$$

- The l1 norm is also known as the **Manhattan distance** or **taxi cab distance**, since it is the distance traveled on a grid between two points.

l1 Regularization

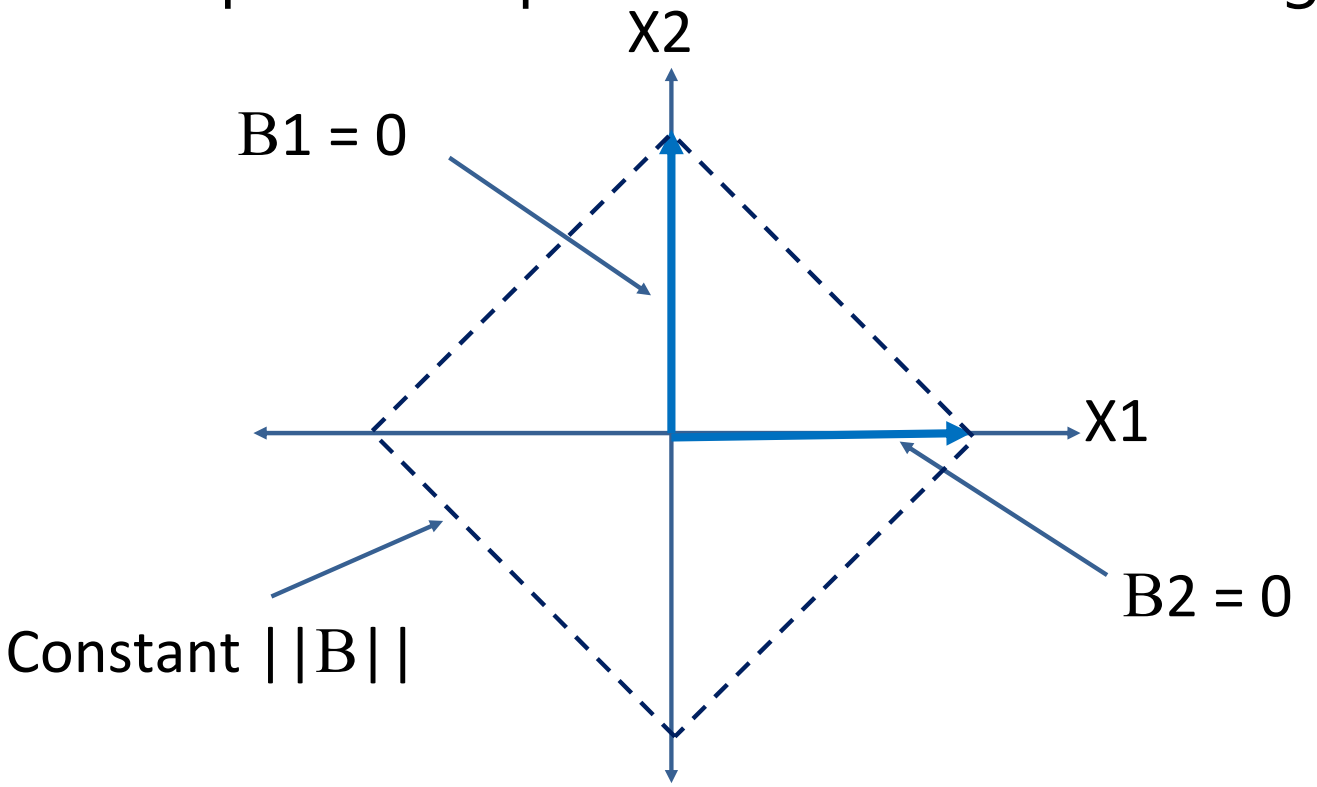
- Given the l1 norm of the weights, the loss function becomes:

$$J(W) = J_{MLE}(W) + \alpha ||W||^1$$

- Where α is the regularization hyperparameter
  - Large α increases bias but reduces variance
  - Small α decreases bias and increases variance
- The l1 constraint drives some weights to exactly 0
  - This behavior leads to the term **lasso regularization**

l1 Regularization

A diagram helps develop some intuition on l1 regularization:



L1 regularization is a **hard constraint** on the weights

Early Stopping

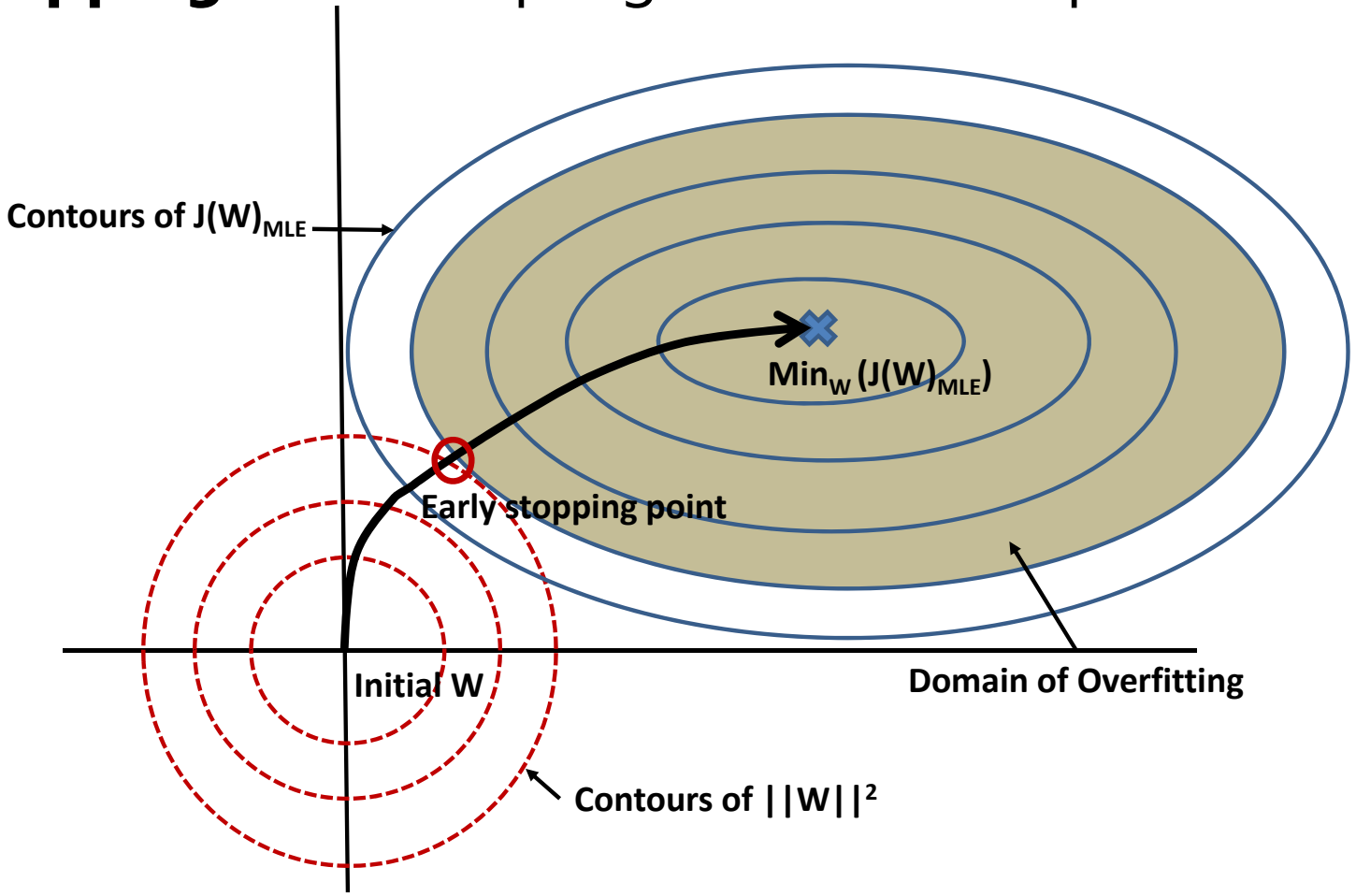
- **Early stopping** is an old and simple idea
- Stop updating the model weights before the model becomes overfit
- Early stopping is analogous to l2 regularization
- We can formulate the regularized loss function as:

$$argmin_W J(W) = J(W)_{MLE} + \alpha ||W||^2$$

- Where α is the regularization hyperparameter

Early Stopping

Early stopping has a simple geometric interpretation



Dropout regularization

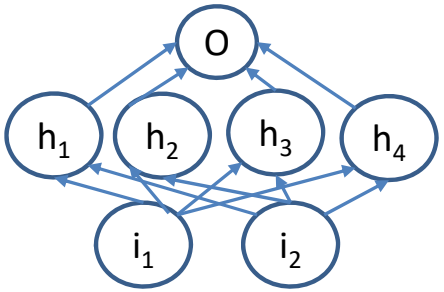
- Overfit deep network models tend to suffer from a problem of co-adaptation
  - With limited training data weight tensors become adapted to the training data
  - Such a model is unlikely to generalize
- We need a way to break the co-adaptation of the weight tensor

Dropout regularization

- **Dropout regularization** is a conceptually simple method unique to deep learning
  - At each step of the gradient decent some **fraction, p, of the weights are dropped-out** of each layer
  - The result is a series of models trained for each dropout sample
  - The final model is a **geometric mean** of the individual models
- Weight values are clipped in a small range as a further regularization
- For full details see the readable paper by Srivastava et. al., 2014 http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf

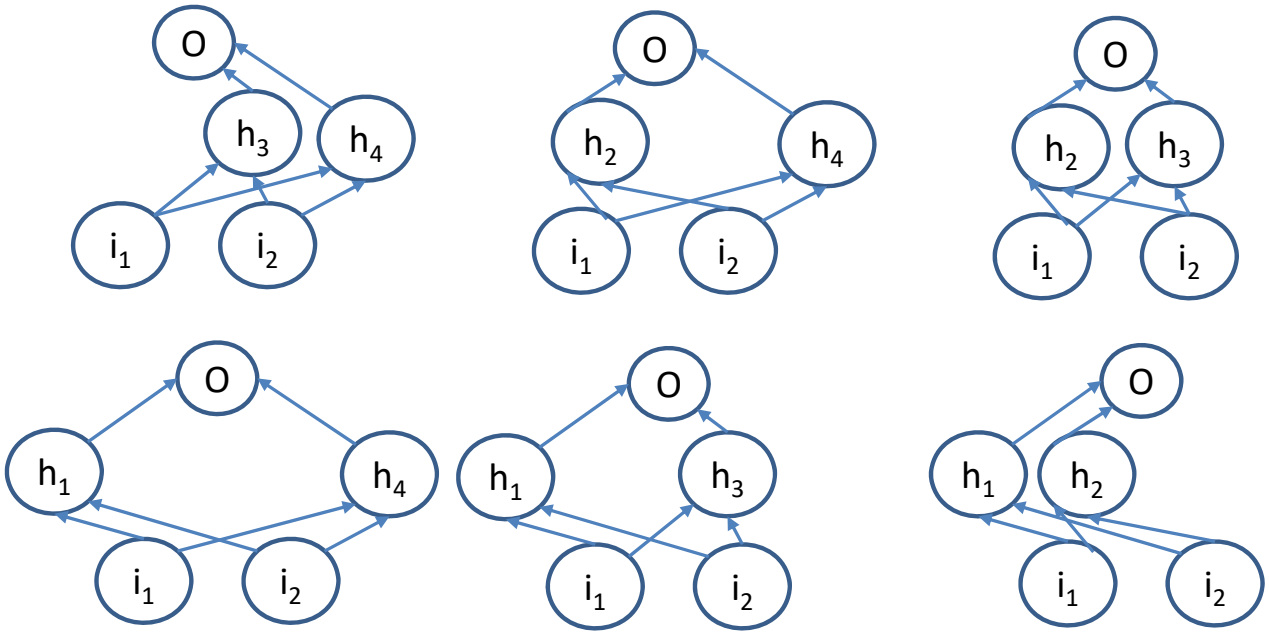
Dropout regularization

- Let's look at a simple example of a network with one hidden layer:



Dropout regularization

- For p = 0.5 here are six of the possible samples:



Batch Normalization

- In deep neural networks there is a high chance that units in a hidden layer have a **large range of output values**
  - Causes shifts in the covariance of the output values
  - Leads to difficulty computing the gradient
  - Slows convergence
- A solution is to normalize the output of the hidden layers in the network as a batch
- This simple idea can be really effective
- For more details see Sergey and Szegedy, 2015: https://arxiv.org/pdf/1502.03167.pdf