Parameter Norm Penalties

Regularization Strategies

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Topics in Parameter Norm Penalties

1. Overview (limiting model capacity)
2. L^2 parameter regularization
3. L^1 regularization

Limiting Model Capacity

- Regularization has been used for decades prior to advent of deep learning
- Linear- and logistic-regression allow simple, straightforward and effective regularization strategies
  - Adding a parameter norm penalty $\Omega(\theta)$ to the objective function J:

$$\boxed{\tilde{J}(\boldsymbol{\theta}; X, y) = J(\boldsymbol{\theta}; X, y) + \alpha\Omega(\boldsymbol{\theta})}$$

    - where $\alpha \varepsilon [0, \theta)$ is a hyperparameter that weight the relative contribution of the norm penalty term Ω
      - Setting α to 0 results in no regularization. Larger values correspond to more regularization

Norm Penalty

- When our training algorithm minimizes the regularized objective function

$$\boxed{\tilde{J}(\boldsymbol{\theta}; X, y) = J(\boldsymbol{\theta}; X, y) + \alpha\Omega(\boldsymbol{\theta})}$$

  – it will decrease both the original objective J on the training data and some measure of the size of the parameters θ

- Different choices of the parameter norm Ω can result in different solutions preferred
  – We discuss effects of various norms

No penalty for biases

- Norm penalty Ω penalizes only weights at each layer and leaves biases unregularized
  - Biases require less data to fit than weights
  - Each weight specifies how variables interact
    - Fitting weights requires observing both variables in a variety of conditions
- Each bias controls only a single variable
  - We do not induce too much variance by leaving biases unregularized
- $\boldsymbol{w}$ indicates all weights affected by norm penalty
- $\boldsymbol{\theta}$ denotes both $\boldsymbol{w}$ and biases

Different or Same αs for layers?

- Sometimes it is desirable to use a separate penalty with a different α for each layer

$$\boxed{\tilde{J}(\theta; X, y) = J(\theta; X, y) + \alpha\Omega(\theta)}$$

- Invariance under linear transformation $\mathbf{T}$ is one case
  - i.e., we want neural net to perform the same when the inputs are transformed

- But this creates too many hyperparameters
  - Search space reduced by using same hyperparameters

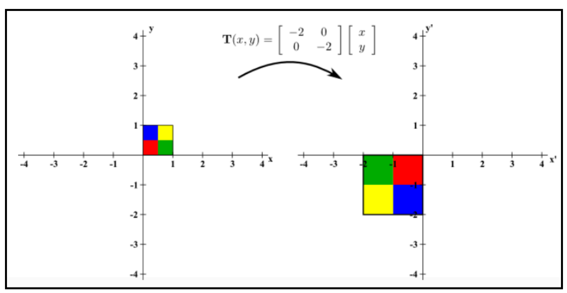
Linear Transformation T

- Consider a simple linear transformation of the input

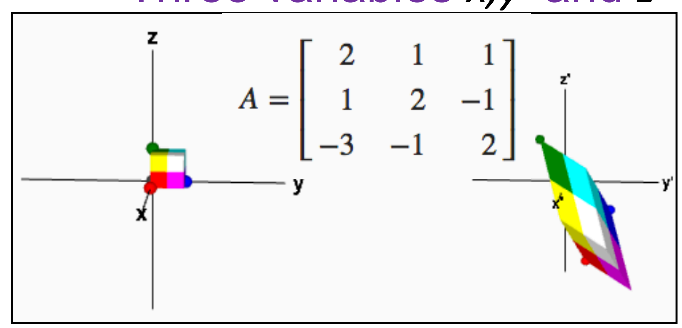
Two-variables
x and y

$$\mathbf{T}(x, y) = (ax + by, cx + dy) = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\boxed{\mathbf{T}(\mathbf{x}) = A\mathbf{x}}$$



Three variables *x,y* and *z*



Weight decay and invariance

- Suppose we train two 2-layer networks
  - *First network*: trained using original data: $\boldsymbol{x}=\{x_i\}$, $\boldsymbol{y}=\{y_k\}$
  - *Second network*: input and/or target variables are transformed by one of the linear transformations

$$\boxed{x_i \rightarrow \tilde{x}_i = a x_i + b} \qquad \boxed{y_k \rightarrow \tilde{y}_k = c y_k + d}$$

- Consistency requires that we should obtain equivalent networks that differ only by linear transformation of the weights

For first layer: And/or or second layer:

$\boxed{w_{ji} \rightarrow \frac{1}{a} w_{ji}}$ and/or $\boxed{w_{kj} \rightarrow c w_{kj}}$

Simple weight decay fails invariance

- Simple weight decay $\boxed{\tilde{E}(\boldsymbol{w}) = E(\boldsymbol{w}) + \frac{\alpha}{2}\boldsymbol{w}^{\mathrm{T}}\boldsymbol{w}}$
- Treats all weights and biases on equal footing
  - While resulting w_{ji} and w_{kj} should be treated differently
  - Consequently networks will have different weights and violate invariance
- We therefore look for a regularizer invariant under the linear transformations
  – Such a regularizer is $\boxed{\frac{\alpha_1}{2}\sum_{w \in W_1} w^2 + \frac{\alpha_2}{2}\sum_{w \in W_2} w^2}$
  - where W_1 are weights of first layer and
  - W_2 are the set of weights in the second layer
    – This regularizer remains unchanged under the weight transformations provided the parameters are rescaled using

$$\lambda_1 \to a^{1/2}\lambda_1 \quad \text{and} \quad \lambda_2 \to c^{-1/2}\lambda_2$$

Weight decay used in practice

- Because it can be expensive to search for the correct value of multiple hyperparameters, it is still reasonable to use same weight decay at all layers to reduce search space

L^2 parameter Regularization

- Simplest and most common kind
- Called *Weight decay*
- Drives weights closer to the origin
  - by adding a regularization term to the objectve function

$$\boxed{\Omega(\theta) = \frac{1}{2} \| w \|_2^2}$$

- In other communities also known as *ridge regression* or *Tikhonov regularization*

Gradient of Regularized Objective

- Objective function (with no bias parameter)

$$\boxed{\tilde{J}(w;X,y) = \frac{\alpha}{2} w^T w + J(w;X,y)}$$

- Corresponding parameter gradient

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

- To perform single gradient step, perform update:

$$\boxed{\boldsymbol{w} \leftarrow \boldsymbol{w} - \varepsilon\left(\alpha \boldsymbol{w} + \nabla_w J\left(\boldsymbol{w}; X, \boldsymbol{y}\right)\right)}$$

- Written another way, the update is

$$\boxed{\boldsymbol{w} \leftarrow (1-\varepsilon\alpha)\boldsymbol{w} - \varepsilon\nabla_w J\left(\boldsymbol{w}; X, \boldsymbol{y}\right)}$$

  – We have modified learning rule to shrink $\boldsymbol{w}$ by constant factor 1-$\varepsilon\alpha$ at each step

To study effect on entire training

- Make quadratic approximation to the objective function in the neighborhood of minimal unregularized cost $\boldsymbol{w}^*=\arg\min_{\boldsymbol{w}} J(\boldsymbol{w})$
- The approximation is given by

$$J(\boldsymbol{w}^*)+\tfrac{1}{2}(\boldsymbol{w}-\boldsymbol{w}^*)^T H(\boldsymbol{w}-\boldsymbol{w}^*)$$

- Where H is the Hessian matrix of J wrt $\boldsymbol{w}$ evaluated at $\boldsymbol{w}^*$

Effect of L^2 regularization on optimal w

Objective function: $\tilde{J}(w; X, y) = \frac{\alpha}{2} w^T w + J(w; X, y)$

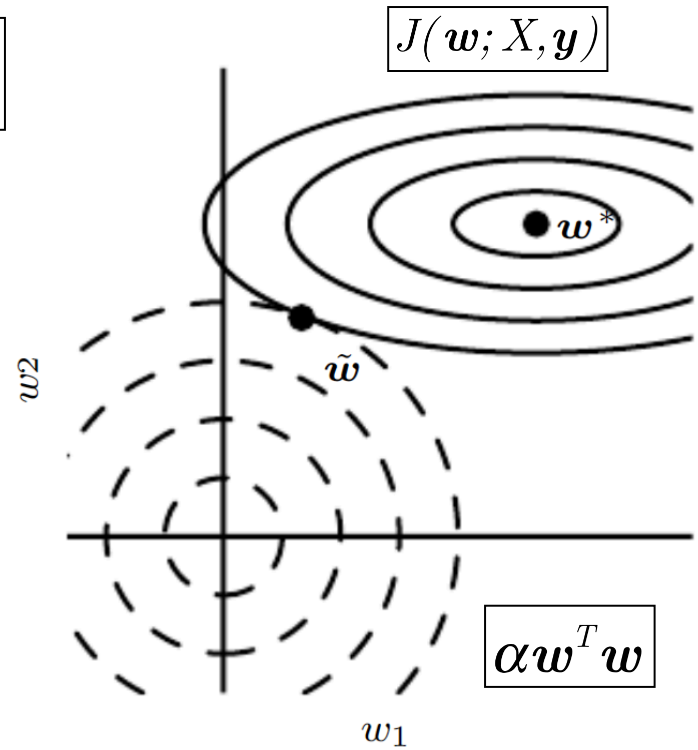
Solid ellipses:

contours of equal value of unregularized objective $J(\boldsymbol{w}; X, \boldsymbol{y})$

Dotted circles:

contours of equal value of L^2 regularizer $\alpha \boldsymbol{w}^T \boldsymbol{w}$

At point $\tilde{\boldsymbol{w}}$ competing objectives reach equilibrium



Along w_1, eigen value of Hessian of J is small. J does not increase much when moving horizontally away from $\boldsymbol{w}^*$. Because J does not have a strong preference along this direction, the regularizer has a strong effect on this axis. The regularizer pulls w_1 close to 0.

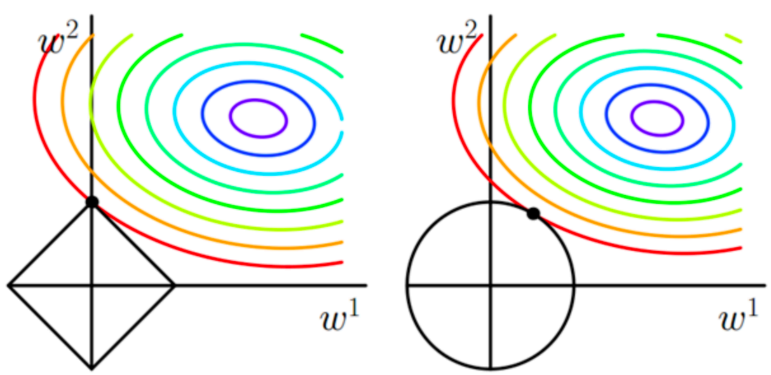
Along w_2, J is very sensitive to movements away from $\boldsymbol{w}^*$. The corresponding eigenvalue is large, indicating high curvature. As a result, weight decay affects the position of w_2 relatively little

L^1 Regularization

- L^2 weight decay is common weight decay
- Other ways to penalize model parameter size
- L^1 regularization is defined as

$$\boxed{\Omega(\boldsymbol{\theta}) = \|\boldsymbol{w}\|_1 = \sum_i |w_i|_1}$$

  – which sums the absolute values of parameters



(a) ℓ_1-ball meets quadratic function. ℓ_1-ball has corners. It's very likely that the meet-point is at one of the corners.

(b) ℓ_2-ball meets quadratic function. ℓ_2-ball has no corner. It is very unlikely that the meet-point is on any of axes.

Image Source: https://zhuanlan.zhihu.com/p/28023308

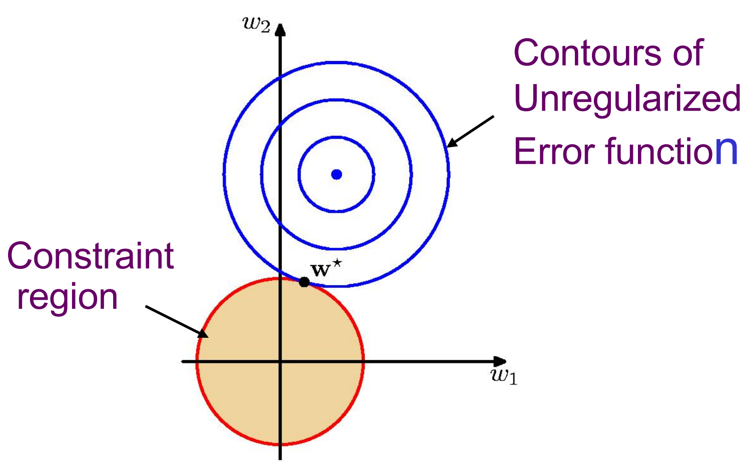
Sparsity and Feature Selection

- The sparsity property induced by L^1 regularization has been used extensively as a feature selection mechanism
  - Feature selection simplifies an ML problem by choosing subset of available features
- LASSO (Least Absolute Shrinkage and Selection Operator) integrates an L^1 penalty with a linear model and least squares cost function
  - The L^1 penalty causes a subset of the weights to become zero, suggesting that those features can be discarded

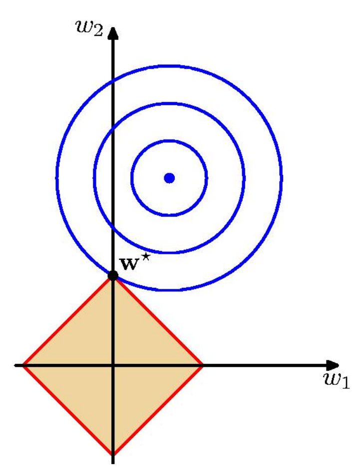
Sparsity with Lasso constraint

- With q=1 and λ is sufficiently large, some of the coefficients w_j are driven to zero
- Leads to a sparse model
  - where corresponding basis functions play no role
- Origin of sparsity is illustrated here:

Quadratic solution where w_1* and w_0* are nonzero



Minimization with Lasso Regularizer
A sparse solution with w_1*=0



Regularization with linear models

Norm Regularization:

$$Tikhonov: \quad \lambda \sum_{\forall i} w_i^2$$

$$Lasso: \quad \lambda \sum_{\forall i} |w_i|$$

$$Student-t: \quad \lambda \sum_{\forall i} \log(1+w_i^2)$$