Neural Network Part 2:
Regularization

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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

\[ t = \sin(2\pi x) + \epsilon \]
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

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

subject to: \( f \in \mathcal{H} \)

• When parametrized

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

subject to: \( \theta \in \Omega \)
Regularization as hard constraint

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

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

subject to: $R(\theta) \leq r$

• Example: $l_2$ regularization

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

subject to: $||\theta||_2^2 \leq r^2$
Regularization as soft constraint

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

\[
\begin{align*}
\min_\theta \hat{L}_R(\theta) &= \frac{1}{n} \sum_{i=1}^{n} l(\theta, x_i, y_i) + \lambda^* R(\theta)
\end{align*}
\]

for some regularization parameter \( \lambda^* > 0 \)

• Example: \( l_2 \) regularization

\[
\begin{align*}
\min_\theta \hat{L}_R(\theta) &= \frac{1}{n} \sum_{i=1}^{n} l(\theta, x_i, y_i) + \lambda^* \|\theta\|_2^2
\end{align*}
\]
Regularization as soft constraint

• Showed by Lagrangian multiplier method

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

• Suppose \( \theta^* \) is the optimal for hard-constraint optimization

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

• Suppose \( \lambda^* \) is the corresponding optimal for max

\[ \theta^* = \arg \min_{\theta} \mathcal{L}(\theta, \lambda^*) := \hat{L}(\theta) + \lambda^*[R(\theta) - r] \]
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: $p(\{x_i, y_i\}\mid\theta)$

- Bayesian rule:

$$p(\theta \mid \{x_i, y_i\}) = \frac{p(\theta)p(\{x_i, y_i\}\mid\theta)}{p(\{x_i, y_i\})}$$
Regularization as Bayesian prior

- Bayesian rule:
  \[ p(\theta \mid \{x_i, y_i\}) = \frac{p(\theta)p(\{x_i, y_i\} \mid \theta)}{p(\{x_i, y_i\})} \]

- Maximum A Posteriori (MAP):
  \[ \max_{\theta} \log p(\theta \mid \{x_i, y_i\}) = \max_{\theta} \log p(\theta) + \log p(\{x_i, y_i\} \mid \theta) \]

  Regularization  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 $p(x, y | \theta)$ 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 $\theta^*$

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

• 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 \( H = Q \Lambda Q^T \)

\[ \theta^*_R \approx (H + \alpha I)^{-1} H \theta^* = Q(\Lambda + \alpha I)^{-1} \Lambda Q^T \theta^* \]

• 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

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

where \text{sign} applies to each element in \( \theta \)

• Gradient descent update

$$\theta \leftarrow \theta - \eta \nabla \hat{L}_R(\theta) = \theta - \eta \nabla \hat{L}(\theta) - \eta \alpha \text{sign}(\theta)$$
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 $\theta_R^*$
  \[
  (\theta_R^*)_i \approx \begin{cases} 
  \max \{ \theta_i^* - \frac{\alpha}{H_{ii}}, 0 \} & \text{if } \theta_i^* \geq 0 \\
  \min \{ \theta_i^* + \frac{\alpha}{H_{ii}}, 0 \} & \text{if } \theta_i^* < 0 
  \end{cases}
  \]
Effect on the optimal solution

- Effect: induce sparsity

\[
\alpha \frac{H_{ii}}{\theta^*_R} \to \alpha \frac{H_{ii}}{\theta^*_i}
\]
Effect on the optimal solution

• Further assume that $H$ is diagonal
• Compact expression for the optimal $\theta_R^*$

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

Class +1

Class -1

Prefer $w_2$ (higher confidence)
Add noise to the input

Class +1

Class -1

Prefer $w_2$ (higher confidence)
Caution: not too much noise

Too much noise leads to data points cross the boundary

Class +1

Class -1

$\mathbf{w}_2$

Prefer $\mathbf{w}_2$ (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

\[ L(f) \approx \mathbb{E}[f_w(x) - y]^2 + \eta \mathbb{E}[(f_w(x) - y)\nabla^2 f_w(x)] + \eta \mathbb{E}[||\nabla f_w(x)||^2] \]

Small so can be ignored

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

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

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

\[
\hat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}} \quad \text{// normalize}
\]

\[
y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i) \quad \text{// scale and shift}
\]

**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