Lecture 5: Regularisation

Irrelevant / Multicolinear features

- Co-linearity between features
- Features not linearly independent
  - E.g. If x_1 and x_2 are the same $\Rightarrow$ perfectly correlated
- For linear model, feature X_j is irrelevant if
  - X_j is a linear combination of other columns

    $$X_{.j} = \Sigma_{l \neq j} \alpha_l X_{.l}$$

    for some scalars α_l
  - Equivalently: Some eigenvalue of $X'X$ is zero
- Problems
  1. The solution is not **unique**
     - Infinite number of solutions
  2. Lack of interpretability
     - cannot interpret the weights
  3. Optimising to learn parameter is **ill-posed problem**

Ill-posed problems

- Well-posed problem
  1. a solution exists
  2. the solution is unique
  3. the solution's behavior changes continuously with the initial condition
- If ill-posed, there is **no closed form solution**
  - Closed form solution $\hat{w} = (X'X)^{-1}X'y$
  - But if irrelevant, $X'X$ has no inverse (singular)
  - (Even near-irrelevance / colinearity can be problematic)

Re-conditioning the problem (Ridge Regression)

- Make it a well-posed solution and also prevent fitting noise / overfitting
- Original problem: minimise squared error

  $$||y - Xw||_2^2$$

- Regularised problem (L2, **Ridge regression**): minimise

  $$||y - Xw||_2^2 + \lambda ||w||_2^2 \text{ for } \lambda > 0$$

- Turns the ridge into a peak ($\Rightarrow$ unique solution)
- Adds λ to eigenvalues of $X'X$: makes invertible

Regulariser as a prior (Bayesian intepretation of ridge regression)

- Let prior distribution be:

$$W \sim N(0, 1/\lambda)$$

- Higher λ, more confidence at prior, therefore ignore data more
- Computing posterior and take **MAP**

$$\log(posterior) = \log(likelihood) + \log(prior) - \log(marg)$$

- can just ignore $\log(marg)$, since this term doesn't affect optimisation
- Arrive at the problem of minimising:

$$||y - Xw||_2^2 + \lambda||w||_2^2$$

- Become equivalent problem: Ridge Regression

Regularisation in non-linear models

- There is trade-off between **overfitting** and **underfitting**
- Right model class Θ will sacrifice some traininig error, for test error
- Choosing model complexity (2 Methods)
    1. Explicit model selection
        - Choosing degree of polynomial model by CV or held out validation
    2. Regularisation

Explicit model selection

- Using hold-out or CV to select the model

1. Split data into D_{train} and $D_{validate}$ sets
2. For each degree d (# of parameters), we have model f_d
    1. Train f_d on D_{train}
    2. Test (evaluate) f_d on $D_{validate}$
3. Pick degree $\hat{d}$ that gives the best test score
4. Re-train model $f_{\hat{d}}$ using all data (return this final model)

Regularisation

- Solving the problem:

$$\hat{\theta} \in \arg\min_{\theta \in \Theta}(L(data, \theta) + \lambda R(\theta))$$

- E.g. Ridge regression

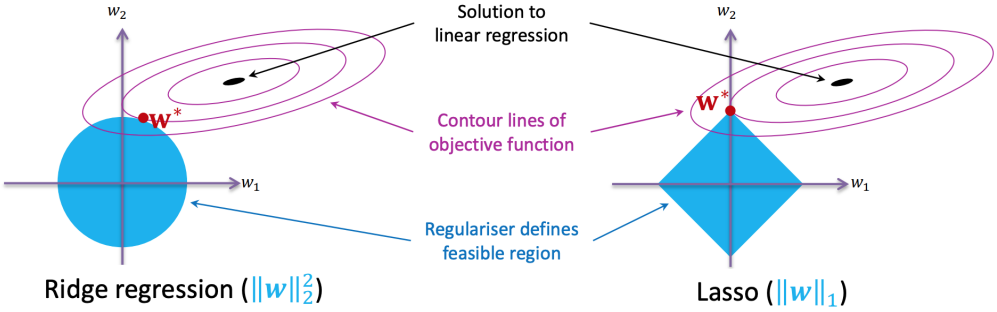
$$\hat{w} \in \arg\min_{w \in W} ||y - Xw||_2^2 + \lambda||w||_2^2$$

- Note: regulariser $R(\theta)$ doesn't depend on data
- Use held-out validation / cross validation to choose λ

Regulariser as a constraint

- Modified problem:

- minimise $||y - Xw||_2^2$ subject to $||w||_2^2 \leq \lambda$ for $\lambda > 0$



- w^* is the solution
- Lasso encourages solution to sit on the axes
  - Some of the weights are set to zero $\Rightarrow$ solution is sparse

Closed form solutions

1. Linear regression

$$(X'X)^{-1}X'y$$

2. Ridge regression

$$(X'X + \lambda I)^{-1}X'y$$

3. Lasso
   - No closed-form solution, but solutions are sparse and suitable for high-dim data

Bias-variance trade-off

- Model complexity is a major factor that influences the ability of the model to **generalise**
- Bias-variance decomposition
  - Risk / test error = $Bias^2 + Variance + IrreducibleError(noise)$

$$E[l(Y, \hat{f}(X_0))] = E[(Y - \hat{f})^2] = (E[Y] - E[\hat{f}])^2 + Var[\hat{f}] + Var[Y]$$

- Squared loss for supervised-regression

$$l(Y, f(\hat{X}_0)) = (Y - \hat{f}(X_0))^2$$

- Simple model $\Rightarrow$ high bias, low variance
- Complex model $\Rightarrow$ low bias, high variance

Lecture 6: Perceptron

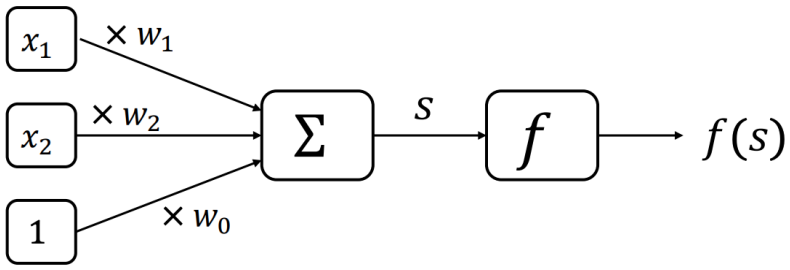
Artificial Neural Network (RNN, CNN, MLP)

- A network of processing elements
  - Each element converts inputs to output
  - Output: a (activation) function of a **weighted sum** of inputs (linear combination)
- To use ANN, we need
  - To design network topology
  - Adjust weights to given data

- Training an ANN $\Rightarrow$ adjusting weights for training data given a pre-defined network topology

Perceptron

- Perceptron is a binary classifier
  - $s = \sum_{i=0}^{m} x_i w_i$
    - Predict class A if $s \geq 0$
    - Predict class B if $s < 0$
- Loss function
  - Usually don't use 0-1 loss for training, since cannot calculate the gradient
  - Shouldn't give penalty for correctly classified examples
    - Penalty (loss) = s
  - Can be re-written as $L(s, y) = max(0, -sy)$



Stochastic gradient descent (SGD)

- Stochastic = Random: shuffling training examples
- Randomly shuffle / split all training examples in B batches
- Choose initial $\theta^{(1)}$
- For i from 1 to T (epochs)
  - For j from 1 to B (batches)
    - Do gradient descent update **using data from batch** j
- Advantage: computational feasibility for large datasets

Perceptron training algorithm (SDG with batch size 1)

- Choose initial guess $w^{(0)}$, $k = 0$
- For i from 1 to T (epochs)
  - For j from 1 to N (training examples)
    - Consider examples $\{\mathbf{x}_j, y_j\}$
    - Update: $w^{(k++)} = w^{(k)} - \eta \nabla L(w^{(k)})$
- Training rule (gradient descent)
  - Correct: We have $\frac{\partial L}{\partial w_i} = 0$ when $sy > 0$
  - Misclassified: We have $\frac{\partial L}{\partial w_i} = -x_i$ when y = 1 and $s < 0$
  - Misclassified: We have $\frac{\partial L}{\partial w_i} = x_i$ when y = -1 and $s > 0$
  - For sy = 0, we can do either of these (doesn't matter)
- When classified correctly, weights are unchanged
- When misclassified, update: $\mathbf{w}^{(k+1)} += -\eta(\pm\mathbf{x})$
  - $\pm x$ is gradient

- **Convergence theorem:** if the trianing data is linearly separable, the algorithm is guaranteed to **converge to a solution**. This is, there exist a finite K s.t. $L(\mathbf{w}^K) = 0$
- **Pros and cons:**
    - Pros: if data is linearly separable, the perceptron trianing algorithm will converge to a correct solution
    - Cons:
        - There are infinitely many possible solutions
        - If the data is not linearly separable, the training will fail completely rather than give some approx. solution