Machine learning

Optimization

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Recollections

Since the beginning of the term we've seen

- Fitting different kinds of models
  - Least squares (global/linear and local/flexible)
  - Newton-Raphson for logistic regression / GLM / MLE
  - Defining SVMs via optimization problems
- Making models more complex
  - Adding variables
  - More flexible functions

This lecture: **optimization** as a unifying framework for ML

ML tasks as optimization problems

For a given **loss function** $L(x, y, g)$ and **probability model** $(X, Y) \sim P$, we want to minimize the **risk**

$$\text{minimize } R(g) = \mathbb{E}_P[L(X, Y, g)]$$

Sampling assumption: we have an i.i.d. sample from P

Then we focus on **empirical risk minimization** (ERM)

$$\text{minimize } \frac{1}{n}\sum_{i=1}^{n} L(x_i, y_i, g)$$

We also choose a **function class** (or parameter set), i.e. type of g, determining the domain of the optimization

Example: GLMs

- Probability model: the family of the GLM (e.g. binomial)
- Empirical loss function: negative log-likelihood (MLE)
- Function class: set of (parametric) functions of the form

$$f_\beta(\mathbf{x}) = g^{-1}(\mathbf{x}^T\beta)$$

for some $(p+1)$-dimensional vector of parameters, fixed link function g

- Make it more complex:
    - Add more predictors (new ones, or non-linear transformations, interactions, etc)
    - Localize it: for some flexible, non-linear h (e.g. `loess`)

$$f(\mathbf{x}) = g^{-1}(h(\mathbf{x}))$$

Parametric vs "non"-parametric

For GLM, Newton-Raphson gives us $\hat{\beta}$, i.e. $\hat{f}$

For `loess`, we choose (or use the default) `span` and then do local logistic regression to get $\hat{f}$

(using a multi-dimensional analogue of `loess` if necessary)

In both cases, we have computed the empirical risk minimizer $\hat{f}$ over some function class

Key optimization choice: which function class?

- Multivariate linear case: which predictors to include?
- `loess` case: what `span` value?

Example: SVM

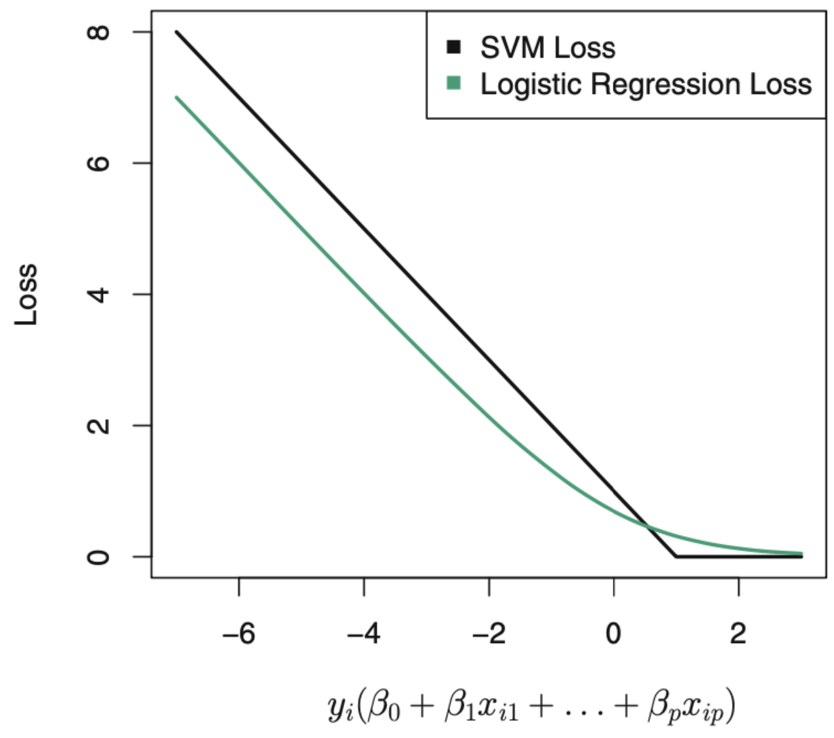
- Probability model: ...
- Empirical loss function: **hinge** loss, $[\ ]_+$ means positive part

$$\frac{1}{n}\sum_{i=1}^{n}[1 - y_i(\mathbf{x}_i^T\beta - \beta_0)]_+$$

Next slide: ISLR Figure 9.2 plot of $L(y_i\hat{y}_i) = [1 - y_i\hat{y}_i]_+$

- Function class: linear classifiers $f(\mathbf{x}) = \text{sign}(\mathbf{x}^T\beta + \beta_0)$
- Make it more complex
  - Add more predictors
  - Reduce constraint-violation budget (non-sep. case)
  - Make it flexibly non-linear (future lecture)

Example: SVM



Comparison: logistic vs SVM

- Similar classification performance possible with both
  - Compare "apples to apples," e.g. both non-linear
- Logistic advantage: inference
- SVM advantage: computation

Key optimization choice: which function class?

- Multivariate linear case
  - Which predictors to include?
  - What constraint budget value?
- Non-linear case: choosing the analogue of the `span` value

ML design choices

Pattern repeats as we introduce more ML methods (kernel methods, tree-based methods, neural networks, etc)

- Loss function (RSS, MLE, hinge, etc)
- Class of regression/classification functions (linear, parametric non-linear, some specific kind of non-parametric non-linear like `loess`, etc)
- Algorithm for fitting an optimal function *within* that class (choosing which predictors to include, estimating coefficients, choosing `span` or SVM constraint budget, etc)

Statistics ...often forgotten in ML! Key assumptions: **i.i.d.** data **sampled from desired probability distribution** (bias - "dataset/distribution shift")

Optimization strategies

Choosing predictor variables

Best subset selection

- Try all 2^p subsets of predictor variables
- Keep the best one (based on RSS or deviance or something)
- Problem: complexity exponential in p, over 10^9 models if $p = 30$

Forward stepwise/stagewise selection

"Greedy" approximation to best subset

1. Start with no predictors
2. At each step, find the one predictor (or a few, in stagewise) giving the best improvement (reduction in the loss function) over the current model
3. Add the best predictor(s) and iterate

- Greedy: not guaranteed to find the best model
- Computation: only $\binom{p}{2}$ models, e.g. 435 if $p = 30$
- **Problem**: when to stop adding more variables? After how many steps? (We'll come back to this)

Modeling assumption: sparsity

We might be willing to assume that a "true" (good enough) model contains only a few predictors

We call this **sparsity**, and may even refer to the number of variables as "the sparsity" of the model, or look for "the best 5-sparse model"

Motivation: Occam's razor / law of parsimony -- simpler models/theories are philosophically/scientifically preferable

Sparse best subsets

Now only $\sum_{k=1}^{s} \binom{p}{k}$ models to try, if sparsity assumed $\leq s$

e.g. about 174000 if $p = 30$ and $s = 5$

Coming soon: lasso

Another method to choose predictor variables

Based on sparsity assumption

Can think of it as a *less greedy* version of forward stepwise

Optimization strategies

Choosing tuning parameters

Degree of flexibility for non-linear methods, constraint budget for SVM, etc

Discretize and fit sequentially

- Start with a grid of values for the tuning parameter
- Fit the model for each value in this grid
- Pick the best fit (visually, or based on loss function value, or...)

e.g. For the `span` or fraction s in local regression, try $s \in \{0.1, 0.25, 0.5, 0.75, 0.9\}$ and visualize the result

e.g. For the budget ("soft margin") C in SVM, try $C \in \{2^k : k = -4, -2, 0, \dots, 10\}$

- **Problem**: When to stop increasing the complexity? (i.e. decreasing s or C)

Modeling assumption: smoothness

Version of simplicity/parsimony for flexible function classes

Linear functions are the smoothest

Smooth function classes: set of functions with some type of bound on second derivatives, for example

Cool math fact: can be related to sparsity by considering (rate of decay of) coefficients of function's Fourier transform (smoother functions have sparser representations when written in a basis of sine functions, for example)

Optimization strategies

"Scaling up" to "big data"

Calculus with the loss function, revisited

Downside of Newton-Raphson: requires second derivatives, including *inverting the $p \times p$ Hessian matrix* when optimizing over $p > 1$ parameters

If p is large, **second-order** optimization methods like Newton's are very costly

First order methods only require computing the $p \times 1$ gradient vector

Recall that the gradient is a vector in the *direction of steepest increase* in the parameter space

Gradient (steepest) descent

i.e. skiing as fast as possible. Notation, let

$$L(\beta) = L(\mathbf{X}, \mathbf{y}, g_\beta)$$

1. Start at an initial point $\beta^{(0)}$
2. For step $n = 1, \ldots$
   - Compute $\mathbf{d}_n = \nabla L(\beta^{(n-1)})$
   - Update $\beta^{(n)} = \beta^{(n-1)} - \gamma_n \mathbf{d}_n$
3. Until some convergence criteria is satisfied

Where the **step size** γ_n is made small enough to not "overshoot" and increase the loss, i.e. the loss only decreases

Coordinate descent

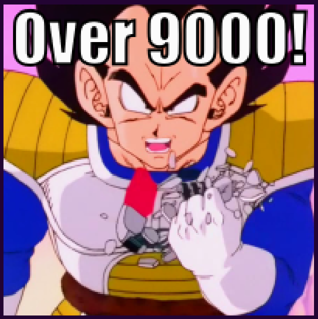
Update only one *coordinate* of β in each step

Cycle through coordinates until some convergence criteria is satisfied

Can combine with any strategy for univariate optimization -- e.g. one-dimensional Newton's method -- treating other parameters as constants

Optimization strategies

Scale up *more*! Bigger data!



Stochastic/random descent

- Instead of cycling through all coordinates in coordinate descent, just pick one randomly
- Instead of computing the gradient of the loss function on the entire dataset, compute it on a random sample

By identical distribution assumption, for any i', by linearity 🌠 of ∇ and $\mathbb{E}$ and $\sum$,

$$\mathbb{E}[\nabla L(\mathbf{x}_{i'}, \mathbf{y}_{i'}, g_\beta)] = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} \nabla L(\mathbf{x}_i, \mathbf{y}_i, g_\beta)\right]$$

Compute update using one randomly sampled observation

or a randomly sampled subset ("mini-batch SGD")

Optimization strategies

A few special topics in conclusion

Constrained optimization

Remember, some of our optimization problems have constraints on the parameters, e.g. SVM

Problem: What if the steps in these descent methods take us outside the parameter constraint region?

Solution strategy: Choose step sizes small enough to stay inside the constraint region

Solution strategy: *Project* from the updated point that is outside the constraint region to the *nearest* point inside the constraint region

Non-smooth optimization

Problem: What if the loss function is not (everywhere) differentiable?

And suppose it is *still* convex, e.g. hinge loss, absolute value, etc

Solution strategies: In this case there is not a well-defined gradient but there is still something called a *subgradient* which acts like a set of values that are all potential gradients--they all define tangent lines (surfaces) that *stay below the function*

Now if we're at a non-differentiable point we just need to compute any subgradient value and take a step in that direction

(Advanced topic, this slide non-examinable)

Early stopping

Optimization time = complexity

- For many optimization algorithms (including those on previous slides) the fitted model becomes more complex the longer the optimization algorithm runs
  - e.g. the more steps of (stochastic) gradient descent used in combination with a flexible function class
  - e.g. the more steps of forward stepwise (adding more predictor variables)

Idea: control model complexity by stopping the algorithm before convergence

This is early stopping -- we'll come back to it later

Optimization theory

- If the loss function is convex many of these methods have *guaranteed convergence* to the *global minimizer*
- If the loss function is non-convex, we lose mathematical guarantees
  - Possible convergence to local minimizer
  - Local minimizers may be much worse than the best possible model...
  - Or they might not be!

Deep learning: to hell with convexity 🤠 "it just works"

Conclusion: optimization in ML is a big topic

Strategies for specific problems

e.g. stepwise inclusion of variables, constraints, etc

Strategies for general loss/function classes

e.g. gradient methods, coordinate methods

Stopping at the right amount of complexity

Maybe the most important part! Next lecture