Optimization

Machine Learning and Pattern Recognition

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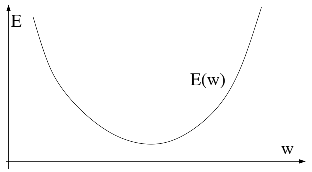
(These slides have been adapted from previous versions by Charles Sutton, Amos Storkey, David Barber, and from Sam Roweis (1972-2010))

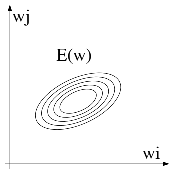
Outline

- Unconstrained Optimization Problems
  - Gradient descent
  - Second order methods
- Constrained Optimization Problems
  - Linear programming
  - Quadratic programming
- Non-convexity
- Reading: Murphy 8.3.2, 8.3.3, 8.5.2.3, 7.3.3.
  Barber A.3, A.4, A.5 up to end A.5.1, A.5.7, 17.4.1 pp 379-381.

Why Numerical Optimization?

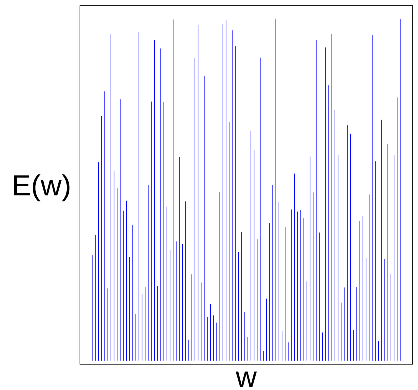
- Logistic regression and neural networks both result in likelihoods that we cannot maximize in closed form.
- End result: an "error function" $E(\mathbf{w})$ which we want to minimize.
- Note $\operatorname{argmin} f(\mathbf{x}) = \operatorname{argmax} - f(\mathbf{x})$
- e.g., $E(\mathbf{w})$ can be the negative of the log likelihood.
- Consider a fixed training set; think in weight (not input) space. At each setting of the weights there is some error (given the fixed training set): this defines an error surface in weight space.
- Learning $\equiv$ descending the error surface.





Role of Smoothness

If E completely unconstrained, minimization is impossible.



All we could do is search through all possible values $\mathbf{w}$.

Key idea: If E is continuous, then measuring $E(\mathbf{w})$ gives information about E at many nearby values.

Role of Derivatives

- Another powerful tool that we have is the gradient

$$\nabla E = (\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \ldots, \frac{\partial E}{\partial w_D})^T.$$

- Two ways to think of this:
  - Each $\frac{\partial E}{\partial w_k}$ says: If we wiggle w_k and keep everything else the same, does the error get better or worse?
  - The function

    $$f(\mathbf{w}) = E(\mathbf{w}_0) + (\mathbf{w} - \mathbf{w}_0)^\top \nabla E|_{\mathbf{w}_0}$$

    is a linear function of $\mathbf{w}$ that approximates E well in a neighbourhood around $\mathbf{w}_0$. (Taylor's theorem)
- Gradient points in the direction of steepest error ascent in weight space.

Numerical Optimization Algorithms

- **Numerical optimization** algorithms try to solve the general problem

$$\min_{\mathbf{w}} E(\mathbf{w})$$

- Different types of optimization algorithms expect different inputs
  - Zero-th order: Requires only a procedure that computes $E(\mathbf{w})$. These are basically search algorithms.
  - First order: Also requires the gradient ∇E
  - Second order: Also requires the Hessian matrix $\nabla\nabla E$
  - High order: Uses higher order derivatives. Rarely useful.
  - Constrained optimization: Only a subset of $\mathbf{w}$ values are legal.
- Today we'll discuss first order, second order, and constrained optimization

Optimization Algorithm Cartoon

- Basically, numerical optimization algorithms are iterative. They generate a sequence of points

$$\mathbf{w}_0, \mathbf{w}_1, \mathbf{w}_2, \ldots$$
$$E(\mathbf{w}_0), E(\mathbf{w}_1), E(\mathbf{w}_2), \ldots$$
$$\nabla E(\mathbf{w}_0), \nabla E(\mathbf{w}_1), \nabla E(\mathbf{w}_2), \ldots$$

- Basic optimization algorithm is

initialize $\mathbf{w}$
while $E(\mathbf{w})$ is unacceptably high
    calculate $\mathbf{g} = \nabla E$
    Compute direction $\mathbf{d}$ from $\mathbf{w}$, $E(\mathbf{w})$, $\mathbf{g}$
        (can use previous gradients as well...)
    $\mathbf{w} \leftarrow \mathbf{w} - \eta\, \mathbf{d}$
end while
return $\mathbf{w}$

Gradient Descent

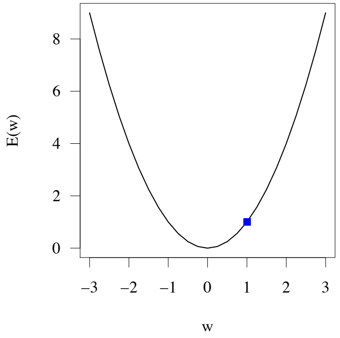
- Locally the direction of steepest descent is the gradient.
- Simple gradient descent algorithm:

initialize $\mathbf{w}$
while $E(\mathbf{w})$ is unacceptably high
    calculate $\mathbf{g} \leftarrow \frac{\partial E}{\partial \mathbf{w}}$
    $\mathbf{w} \leftarrow \mathbf{w} - \eta\, \mathbf{g}$
end while
return $\mathbf{w}$

- η is known as the *step size* (sometimes called *learning rate*)
  - We must choose $\eta > 0$.
  - η too small $\rightarrow$ too slow
  - η too large $\rightarrow$ instability

Effect of Step Size

Goal: Minimize
$E(w) = w^2$

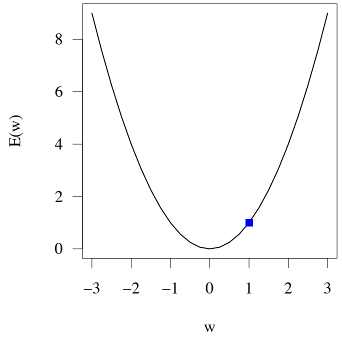


- Take $\eta = 0.1$. Works well.

$$
\begin{aligned}
w_0 &= 1.0 \\
w_1 &= \mathbf{w}_0 - 0.1 \cdot 2w_0 = 0.8 \\
w_2 &= \mathbf{w}_1 - 0.1 \cdot 2w_1 = 0.64 \\
w_3 &= \mathbf{w}_2 - 0.1 \cdot 2w_2 = 0.512 \\
&\cdots \\
w_{25} &= 0.0047
\end{aligned}
$$

Effect of Step Size

Goal: Minimize
$E(w) = w^2$



- Take $\eta = 1.1$. Not so good. If you step too far, you can leap over the region that contains the minimum

$$
\begin{aligned}
w_0 &= 1.0 \\
w_1 &= \mathbf{w}_0 - 1.1 \cdot 2w_0 = -1.2 \\
w_2 &= \mathbf{w}_1 - 1.1 \cdot 2w_1 = 1.44 \\
w_3 &= \mathbf{w}_2 - 1.1 \cdot 2w_2 = -1.72 \\
&\cdots \\
w_{25} &= 79.50
\end{aligned}
$$

- Finally, take $\eta = 0.000001$. What happens here?

Batch vs online

- So far all the objective functions we have seen look like:

$$E(\mathbf{w}; D) = \sum_{n=1}^{n} E^n(\mathbf{w}; y^n, \mathbf{x}^n).$$

$D = \{(\mathbf{x}^1, y^1), (\mathbf{x}^2, y^2), \ldots (\mathbf{x}^n, y^n)\}$ is the training set.
- Each term sum depends on only one training instance
- The gradient in this case is always

$$\frac{\partial E}{\partial \mathbf{w}} = \sum_{n=1}^{N} \frac{\partial E^n}{\partial \mathbf{w}}$$

- The algorithm on slide 8 scans *all* the training instances before changing the parameters.
- Seems dumb if we have millions of training instances. Surely we can get a gradient that is "good enough" from fewer instances, e.g., a couple thousand? Or maybe even from just one?

Batch vs online

- **Batch** learning: use all patterns in training set, and update weights after calculating

$$\frac{\partial E}{\partial \mathbf{w}} = \sum_{n=1}^{N} \frac{\partial E^n}{\partial \mathbf{w}}$$

- **On-line** learning: adapt weights after each pattern presentation, using $\frac{\partial E^n}{\partial \mathbf{w}}$
- **Batch** more powerful optimization methods
- **Batch** easier to analyze
- **On-line** more feasible for huge or continually growing datasets
- **On-line** may have ability to jump over local optima

Algorithms for Batch Gradient Descent

- Here is batch gradient descent.

  initialize $\mathbf{w}$
  while $E(\mathbf{w})$ is unacceptably high
  calculate $\mathbf{g} \leftarrow \sum_{n=1}^{N} \frac{\partial E^n}{\partial \mathbf{w}}$
  $\mathbf{w} \leftarrow \mathbf{w} - \eta\,\mathbf{g}$
  end while
  return $\mathbf{w}$

- This is just the algorithm we have seen before. We have just "substituted in" the fact that $E = \sum_{n=1}^{N} E^n$.

Algorithms for Online Gradient Descent

- Here is (a particular type of) online gradient descent algorithm

  initialize $\mathbf{w}$
  while $E(\mathbf{w})$ is unacceptably high
  Pick j as uniform random integer in $1 \ldots N$
  calculate $\mathbf{g} \leftarrow \frac{\partial E^j}{\partial \mathbf{w}}$
  $\mathbf{w} \leftarrow \mathbf{w} - \eta\,\mathbf{g}$
  end while
  return $\mathbf{w}$

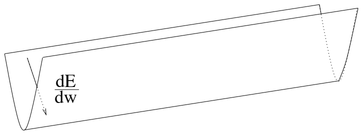
- This version is also called "stochastic gradient ascent" because we have picked the training instance randomly.
- There are other variants of online gradient descent.

Problems With Gradient Descent

- Setting the step size η
- Shallow valleys
- Highly curved error surfaces
- Local minima

Shallow Valleys

- Typical gradient descent can be fooled in several ways, which is why more sophisticated methods are used when possible. One problem:



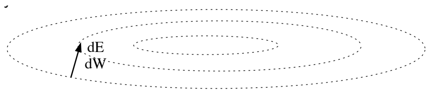
- Gradient descent goes very slowly once it hits the shallow valley.
- One hack to deal with this is *momentum*

$$\mathbf{d}_t = \beta \mathbf{d}_{t-1} + (1-\beta)\eta \nabla E(\mathbf{w}_t)$$

- Now you have to set both η and β. Can be difficult and irritating.

Curved Error Surfaces

- A second problem with gradient descent is that the gradient might not point towards the optimum. This is because of curvature



- Note: gradient is the *locally* steepest direction. Need not directly point toward local optimum.
- Local curvature is measured by the Hessian matrix: $H_{ij} = \partial^2 E / \partial w_i w_j$.
- By the way, do these ellipses remind you of anything?

Second Order Information

- Taylor expansion

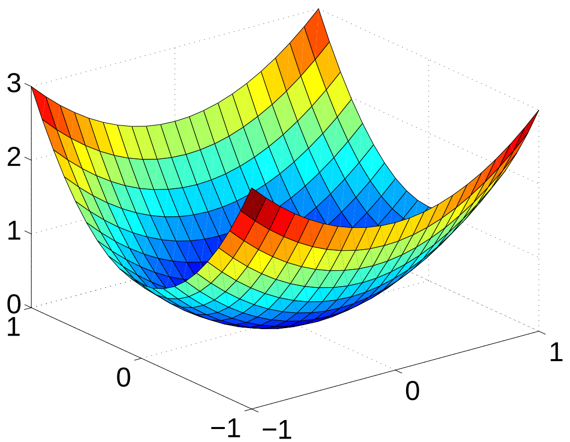
$$E(\mathbf{w} + \boldsymbol{\delta}) \simeq E(\mathbf{w}) + \boldsymbol{\delta}^T \nabla_{\mathbf{w}} E + \frac{1}{2} \boldsymbol{\delta}^T H \boldsymbol{\delta}$$

where

$$H_{ij} = \frac{\partial^2 E}{\partial w_i \partial w_j}$$

- H is called the Hessian.
- If H is positive definite, this models the error surface as a quadratic bowl.

Quadratic Bowl



Direct Optimization

- A quadratic function

$$E(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T H \mathbf{w} + \mathbf{b}^T \mathbf{w}$$

can be minimised directly using

$$\mathbf{w} = -H^{-1} \mathbf{b}$$

but this requires
  - Knowing/computing H, which has size $O(D^2)$ for a D-dimensional parameter space
  - Inverting H, $O(D^3)$

Newton's Method

- Use the second order Taylor expansion

$$E(\mathbf{w} + \boldsymbol{\delta}) \simeq E(\mathbf{w}) + \boldsymbol{\delta}^T \nabla_{\mathbf{w}} E + \frac{1}{2} \boldsymbol{\delta}^T H \boldsymbol{\delta}$$

- From the last slide, the minimum of the approximation is $\boldsymbol{\delta}^* = -H^{-1} \nabla_{\mathbf{w}} E$
- Use that as the direction in steepest descent
- This is called *Newton's method*.
- You may have heard of Newton's method for finding a root, i.e., a point x such that $f(x) = 0$. Similar thing, we are finding zeros of ∇f.
- Compare Newton step to gradient descent $\boldsymbol{\delta} = -\eta \nabla_{\mathbf{w}} E$

Advanced First Order Methods

- Newton's method is fast in that once you are close enough to a minimum.
- What we mean by this is that it needs very few iterations to get close to the optimum (You can actually prove this if you take an optimization course)
- If you have a not-too-large number of parameters and instances, this is probably method of choice.
- But for most ML problems, it is slow. Why? How many second derivatives are there?
- Instead we use "fancy" first-order methods that try to approximate second order information using only gradients.
- These are the state of the art *for batch methods*
  - One type: Quasi-Newton methods (I like one called *limited memory BFGS*).
  - Conjugate gradient
  - We won't discuss how these work, but you should know that they exist so that you can use them.

Constrained problems

- Constraints: e.g. $f(\mathbf{w}) < 0$.
- Example: Observe the points $\{0.5, 1.0\}$ from a Gaussian with known mean $\mu = 0.8$ and unknown standard deviation σ. Want to estimate σ by maximum likelihood.
- Constraint: σ must be positive.
- In this case to find the maximum likelihood solution, the optimization problem is

$$\max_{\sigma} \sum_{i=1}^{2} [-\frac{1}{2\sigma^2}(x^i - \mu)^2 - \frac{1}{2}\log(2\pi\sigma^2)]$$

subject to $\sigma > 0$

- In this case: solution can be done analytically. More complex cases require a numerical method for constrained optimization.

Constrained problems

Either remove constraints by re-parameterization. E.g. $\mathbf{w} > 0$. Set $\phi = \log(\mathbf{w})$. Now ϕ unconstrained.

Or use a constrained optimization method, e.g. for linear programming, quadratic programming.

Linear Programming

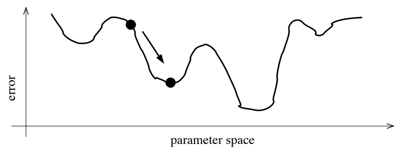
- Find optimum, within a (potentially unbounded) polytope, of a linear function
- Polytope = polygon or higher dimensional generalization thereof.
- Easy: maximum (if it exists) must be at vertex of polytope (or on a convex set containing such a vertex). Hill climb on vertices using an adjacency walk (Simplex algorithm)

Quadratic Programming

- Find optimum, within a (potentially unbounded) polytope, of a quadratic form
- Interior point methods, Active set methods.
- Second order methods for convex quadratic functions Newton-Raphson, Conjugate Gradient variants.
- A number of machine learning methods are cast as quadratic programming problems (e.g. Support Vector Machines).

Non-convexity and local minima

- If you follow the gradient, where will you end up? Once you hit a local minimum, gradient is 0, so you stop.



- Certain nice functions, such as the likelihood for linear and logistic regression are *convex*, meaning that the second derivative is always positive. This implies that any local minimum is global.

- Dealing with local minima: Train multiple models from different starting places, and then choose best (or combine in some way).
- No guarantees. Unrealistic to believe this will find global mimimum.
- Local minima occur, e.g. for neural networks
- Bayesian interpretation, where $E(\mathbf{w}) = -\log p(\mathbf{w}|D)$
- Finding local minima of $E(\mathbf{w})$ as a way of approximating integration over the posterior by finding local maxima of $p(\mathbf{w}|D)$

Convex Functions

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if for $\alpha \in [0,1]$

$$f(\alpha \mathbf{x} + (1-\alpha)\mathbf{y}) \le \alpha f(\mathbf{x}) + (1-\alpha) f(\mathbf{y})$$

  Essentially "bowl shaped"
- Examples:

$$f(x) = x^2 \qquad f(x) = -\log x \qquad f(\mathbf{x}) = \log\left(\sum_d \exp\{x_d\}\right)$$

- If f differentiable, this implies

$$f(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0)^\top \nabla f|_{\mathbf{x}_0} \le f(\mathbf{x})$$

  for all $\mathbf{x}$ and $\mathbf{x}_0$. (To see this: take limit of above as $\mathbf{x} \to \mathbf{y}$.)
- This implies that any local minimum is a global one!

Convex Optimization Problems

- A convex optimization problem is one that can be written as

$$\begin{aligned} &\min \ f_0(\mathbf{x}) \\ \text{subject to } & f_i(\mathbf{x}) \le 0 \qquad i \in \{1 \dots N\} \end{aligned}$$

  for some choice of functions $f_0 \dots f_N$ where each f_i is convex
- Optimise convex function over a convex set...
- Unconstrained problems: Use methods from before. You'll find a global optimum!
- Convexity means any local optimum is also global optimum.
- Constrained convex problems: Interior point methods, Active set methods.
- Most convex optimization problems can be solved efficiently in practice.
- (How high a scale you can reach depends on the type of problem you have)

Optimization: Summary

- Complex mathematical area. Do not implement your own optimization algorithms if you can help it!
- My advice: For unconstrained problems
  - Batch is less hassle than online. But if you have big data, you must use online. Batch is too slow
  - (For neural networks, typically online methods are method of choice.)
  - If online, you use gradient descent. Forget about second order stuff.
  - If batch, use one of the fancy first-order methods (quasi-Newton or conjugate gradients). DO NOT implement either of these yourself!
- If you have a constrained problem
  - Linear programs are easy. Use off the shelf tools.
  - More than that: Try to convert into unconstrained problem.
- Convex problems: Global minimum. Non-convex: *Local* optima.

What you should take away

- Complex mathematical area. Do not implement your own optimization algorithms if you can help it!
- Stuff you should understand:
  - How and why we convert learning problems into optimization problems
  - *Modularity* between modelling and optimization
  - Gradient descent
  - Why gradient descent can run into problems
  - Especially local minima
- Methods of choice: Fancy first-order methods (e.g., quasi-Newton, CG) for moderate amounts of data. Stochastic gradient for large amounts of data.