

# STATS 230: Computational Statistics Optimization

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# Overview

- In this lecture, we discuss convex optimization problems
- We start by some general concepts and definitions for constrained optimization
- Next, we will discuss some computational methods for solving such problems
- At the end, we will focus on the application of these methods in statistics
- For the most part, this lecture is based on the book on Convex Optimization by Boyd and Vandenberghe (2004)

# Least squares regression models

- Consider the least squares problem we discussed before:

$$\text{minimize} \quad \text{RSS}(\beta) = \|y - x\beta\|^2$$

- For quadratic problems like this, we can solve the optimization problem by setting the gradient to zero

$$\begin{aligned}\nabla_{\beta} \text{RSS}(\beta) &= -2x^{\top}(y - x\hat{\beta}) = 0 \\ \hat{\beta} &= (x^{\top}x)^{-1}x^{\top}y\end{aligned}$$

assuming the Hessian is positive definite:

$$\nabla^2 \text{RSS}(\beta) = 2x^{\top}x \succ 0$$

which is true iff  $x$  has independent columns

# Regularized regression models

- Occasionally, we would like to solve the least squares problem while controlling the complexity of the resulting model by imposing constraints on the parameters
- One possible approach is to use Bridge regression models (Frank and Friedman, 1993)

$$\begin{array}{ll}\text{minimize} & \text{RSS}(\beta) = \|y - x\beta\|^2 \\ \text{subject to} & \sum_{j=1}^p |\beta_j|^\gamma \leq s\end{array}$$

- Two important special cases are ridge regression (Hoerl and Kennard, 1970)  $\gamma = 2$  and Lasso (Tibshirani, 1996)  $\gamma = 1$

# General optimization problems

- In general, optimization problems have the following form:

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0 \quad i = 1, \dots, m \\ & h_j(x) = 0 \quad j = 1, \dots, p\end{array}$$

- We are usually interested in *convex* optimization problems, where we minimize a convex objective function  $f_0(x)$  over a convex set with convex inequality constraints  $f_i(x)$  and affine equality constraints  $h_j(x) = Ax - b$ .

# Affine sets

- Affine set,  $C$ : lines through any two distinct points in  $C$  remains in  $C$ ,

$$\alpha x + \beta y \in C$$

$$\text{if } x, y \in C$$

$$\alpha, \beta \in \mathbb{R}$$

$$\alpha + \beta = 1$$

# Affine functions

- A function  $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}^m$  is an affine function if it is a sum of a linear function and a constant

$$f(x) = Ax + b$$

$$A \in \mathbb{R}^{m \times n}$$

$$b \in \mathbb{R}^m$$

# Convex sets

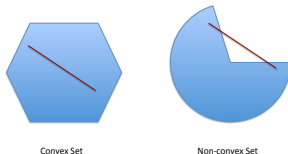
- Convex set,  $C$ : line segments between two points in  $C$  remains in  $C$ ,

$$\alpha x + \beta y \in C$$

$$\text{if } x, y \in C$$

$$0 \leq \alpha, \beta \leq 1$$

$$\alpha + \beta = 1$$



- If  $C$  is a convex set in  $\mathbb{R}^n$  and  $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}^m$  is an affine function, then  $f(C)$ , i.e., the image of  $C$  under  $f$  is also a convex set.



# Convex functions

- A function  $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}$  is convex if its domain is a convex set and

$$f(\alpha x + \beta y) \leq \alpha f(x) + \beta f(y)$$

$$\alpha \geq 0, \beta \geq 0, \alpha + \beta = 1$$

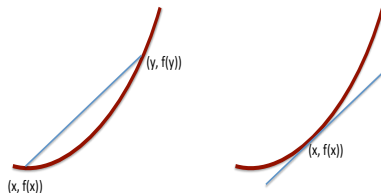
- In general, for convex function  $f(E[x]) \leq E[f(x)]$  (Jensen's inequality)
- For example, all norms are convex functions

$$\|x\|_p = \left( \sum_i |x_i|^p \right)^{1/p}, \quad p \geq 1$$

# Convex functions

- For convex functions,

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x), \quad \forall x, y \in D_f$$



- Also, the Hessian is positive semidefinite  $\nabla^2 f(x) \succeq 0$ ,  $\forall x \in D_f$

# Terminology and notations

- Optimal value  $p^* = \inf \{f_0(x) | f_i(x) \leq 0, h_j(x) = 0\}$
- $x$  is feasible if  $x \in D = \bigcap_{i=0}^m f_i \cap \bigcap_{i=1}^p h_i$  and satisfies the constraints
- A feasible  $x^*$  is optimal if  $f_0(x^*) = p^*$
- Assuming  $f_0$  is convex and differentiable,  $x$  is optimal iff its feasible and  $\nabla f_0(x)^\top (y - x) \geq 0$ , for all feasible  $y$
- For unconstrained problems,  $x$  is optimal iff  $\nabla f_0(x) = 0$

# Terminology and notations

- $x$  is locally optimal if for a given  $R > 0$ , it is optimal for

$$\begin{array}{ll}\text{minimize} & f_0(z) \\ \text{subject to} & f_i(z) \leq 0 \quad i = 1, \dots, m \\ & h_i(z) = 0 \quad j = 1, \dots, p \\ & \|z - x\| \leq R\end{array}$$

- In convex optimization problems, any locally optimal point is also globally optimal.

# Lagrangian

- Consider the following optimization problem:

$$\begin{aligned} & \text{minimize} && f_0(x) \\ & \text{subject to} && f_i(x) \leq 0 \quad i = 1, \dots, m \\ & && h_j(x) = 0 \quad j = 1, \dots, p \end{aligned}$$

- To take the constraints into account, we augment the objective function with a weighted sum of the constraints.
- Lagrangian:  $L : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \rightarrow \mathbb{R}$  defined as follows:

$$L(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) + \sum_{j=1}^p \nu_j h_j(x)$$

where  $\lambda$  and  $\nu$  are dual variables or Lagrange multipliers.

- This incorporates the constraints in the objective function

# Ridge regression

Original problem:

$$\begin{array}{ll}\text{minimize} & \text{RSS}(\beta) = \|y - x\beta\|^2 \\ \text{Subject to} & \|\beta\|^2 \leq s\end{array}$$

Lagrangian:

$$\begin{aligned}L &= (y - x\beta)^\top (y - x\beta) + \lambda \beta^\top \beta \\ \nabla_\beta L &= -2x^\top (y - x\hat{\beta}) + 2\lambda \hat{\beta} = 0 \\ -x^\top y + x^\top x \hat{\beta} + \lambda \hat{\beta} &= 0 \\ -x^\top y + (x^\top x + \lambda I) \hat{\beta} &= 0 \\ (x^\top x + \lambda I) \hat{\beta} &= x^\top y \\ \hat{\beta} &= (x^\top x + \lambda I)^{-1} x^\top y\end{aligned}$$

# Lagrange dual function

- We define the Lagrange dual function as follows:

$$g(\lambda, \nu) = \inf_{x \in D} L(x, \lambda, \nu)$$

- $g$  is concave in  $\lambda$  and  $\nu$  since it is a pointwise infimum of a family of affine functions in terms of  $(\lambda, \nu)$
- If  $\lambda \succeq 0$  then for each feasible point  $\tilde{x}$

$$\inf_{x \in D} L(x, \lambda, \nu) = g(\lambda, \nu) \leq L(\tilde{x}, \lambda, \nu) \leq f_0(\tilde{x})$$

- Therefore,  $g(\lambda, \nu) \leq p^*$  so  $g(\lambda, \nu)$  is a lower bound for the optimal value

# Lagrange dual function

- We define the **Lagrange dual problem** as follows:

$$\begin{array}{ll}\text{maximize} & g(\lambda, \nu) \\ \text{Subject to} & \lambda \succeq 0\end{array}$$

- Therefore, the above problem is also a convex optimization problem (i.e., minimizing  $-g$ )
- We denote the optimal value as  $d^*$ ; the corresponding solution  $(\lambda^*, \nu^*)$  is called the dual optimal point
- In contrast, the original problem is called the **primal problem**, whose solution  $x^*$  is called primal optimal



# Weak vs. strong duality

- $d^*$  is the best lower bound for  $p^*$
- $d^* \leq p^*$  is called weak duality
- $p^* - d^*$  is called the optimal duality gap
- Strong duality:  $d^* = p^*$

# Slater's condition

- Strong duality doesn't hold in general, but if the primal is convex, it usually holds under some conditions referred to as “constraint qualifications”
- A well known constraint qualification is Slater's condition which states that we have strong duality if besides convexity we also have strict feasibility

$$f_i(x) < 0 \quad \forall i, \quad Ax = b$$

# Complementary slackness

- Consider primal optimal  $x^*$  and dual optimal  $(\lambda^*, \nu^*)$  points
- If strong duality holds

$$\begin{aligned}f_0(x^*) &= g(\lambda^*, \nu^*) \\&= \inf_x [f_0(x) + \sum_{i=1}^m \lambda_i^* f_i(x) + \sum_{j=1}^p \nu_j^* h_j(x)] \\&\leq f_0(x^*) + \sum_{i=1}^m \lambda_i^* f_i(x^*) + \sum_{j=1}^p \nu_j^* h_j(x^*) \\&\leq f_0(x^*)\end{aligned}$$

- Therefore, these are all equalities

# Complementary slackness

- Conclusions:

- ▶  $x^*$  minimizes  $L(x, \lambda^*, \nu^*)$

- ▶  $\sum_{i=1}^m \lambda_i^* f_i(x^*) = 0$

- The latter called complementary slackness, which indicates:

$$\begin{aligned}\lambda_i^* > 0 &\Rightarrow f_i(x^*) = 0 \\ f_i(x^*) < 0 &\Rightarrow \lambda_i^* = 0\end{aligned}$$

- In theory, we can find  $(\lambda^*, \nu^*)$  from the dual problem (if it's easier to solve), then minimize  $L(x, \lambda^*, \nu^*)$
- For many practical problems in statistics, however, we use cross-validation to choose  $(\lambda, \nu)$

# Optimization through solving the dual problem

- When strong duality holds and a dual optimal exists,  $\lambda^*, \nu^*$ , then any primal optimal is also a minimizer of  $L(x, \lambda^*, \nu^*)$
- If the resulting solution is primal feasible then it is primal optimal
- We can use this fact to solve the optimization problem when the dual problem is easier to solve

# Entropy maximization

- In information theory, the information content for a specific outcome  $x$  is defined as

$$h(X = x) = \log \frac{1}{P(X = x)}$$

- For a set of possible outcomes,  $x_1, \dots, x_n$ , the entropy is defined as the expectation of information content:

$$H(X) = - \sum_{i=1}^n p_i \log p_i$$

where  $p_i = P(X = x_i)$

- We choose an optimal probability model by maximizing entropy, or equivalently, minimizing negative entropy

# Entropy maximization

- Primal:

$$\begin{aligned} &\text{Minimize} && \sum_{i=1}^n p_i \log p_i \\ &\text{Subject to} && \sum_{i=1}^n p_i = 1 \end{aligned}$$

For simplicity, I omitted the inequality constraints  $p_i \geq 0$

- Lagrangian

$$L(p, \nu) = \sum p_i \log p_i + \nu(\sum p_i - 1)$$

- We minimize  $L(p, \nu)$  by setting the gradient with respect to  $p$  to zero

$$\log \hat{p}_i + 1 + \nu = 0 \Rightarrow \hat{p}_i = \exp(-\nu - 1)$$

# Entropy maximization

- Therefore, the dual function is

$$\begin{aligned}g(\nu) &= (-\nu - 1) \sum \exp(-\nu - 1) + \nu([\sum \exp(-\nu - 1)] - 1) \\&= -n \exp(-\nu - 1) - \nu\end{aligned}$$

- Dual:

$$\text{Maximize } g(\nu) = -n \exp(-\nu - 1) - \nu$$

- We find the dual optimal

$$\begin{aligned}n \exp(-\nu^* - 1) - 1 &= 0 \\ \nu^* &= -1 - \log(1/n)\end{aligned}$$



# Entropy maximization

- We now minimize  $L(p, \nu^*)$

$$\log p_i^* + 1 + \nu^* = 0 \Rightarrow p_i^* = 1/n$$

- Therefore, the optimal probability model is the discrete uniform distribution
- Exercise: Show that maximizing the entropy while fixing the first  $k$  moments at  $m_1, \dots, m_k$  results in a member of the exponential family of distributions

# Karush-Kun-Tucker (KKT) optimality conditions

- Suppose the functions  $f_0, f_1, \dots, f_m, h_1, \dots, h_p$  are all differentiable; also  $x^*$  and  $(\lambda^*, \nu^*)$  primal and dual optimal points with zero duality gap
- Since  $x^*$  minimizes  $L(x, \lambda^*, \nu^*)$ , the gradient vanishes at  $x^*$

$$\nabla f_0(x^*) + \sum_{i=1}^m \lambda_i^* \nabla f_i(x^*) + \sum_{j=1}^p \nu_j^* \nabla h_j(x^*) = 0$$

- Additionally

$$f_i(x^*) \leq 0 \quad i = 1, \dots, m$$

$$h_j(x^*) = 0 \quad j = 1, \dots, p$$

$$\lambda_i^* \geq 0 \quad i = 1, \dots, m$$

$$\lambda_i^* f_i(x^*) = 0 \quad i = 1, \dots, m$$

- These are called Karush-Kun-Tucker (KKT) optimality conditions

# Karush-Kun-Tucker (KKT) optimality conditions

- When the primal is convex, then KKT conditions are sufficient for the points to be primal and dual optimal with zero duality gap
- Therefore, for convex optimization problems with differentiable functions that satisfy Slater's condition, then KKT provides the necessary and sufficient conditions for optimality
- Many convex optimization problems can be expressed as methods for solving KKT conditions

# Example

- Consider the following equality constrained quadratic problem:

$$\begin{array}{ll}\text{Minimize} & (1/2)x^\top Px + q^\top x + r; \quad P \succeq 0 \\ \text{Subject to} & Ax = b\end{array}$$

- KKT conditions:

$$\begin{aligned}Px^* + q + A^\top \nu^* &= 0 \\ Ax^* &= b\end{aligned}$$

- In the matrix form,

$$\begin{pmatrix} P & A^\top \\ A & 0 \end{pmatrix} \begin{pmatrix} x^* \\ \nu^* \end{pmatrix} = \begin{pmatrix} -q \\ b \end{pmatrix}$$

- To find  $x^*, \nu^*$ , we can solve the above system of  $n + m$  equations

# Descent methods

- We now focus on numerical solutions for unconstrained optimization problems

$$\text{Minimize } f(x)$$

with twice differentiable  $f : R^n \rightarrow R$

- In theory, we could find the optimal value by solving  $\nabla f(x^*) = 0$ ; in practice however, we need iterative methods to solve such problems
- To this end, we can use descent methods that produce a minimizing sequence  $x^{(k)}$ ,

$$f(x^{(k+1)}) < f(x^{(k)}), \quad k = 1, \dots$$

except when  $x^{(k)}$  is optimal.

# Descent methods

- We set up the sequence as

$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}, \quad t^{(k)} > 0$$

- $\Delta x^{(k)}$  is called the “step” or “search direction”;  $t^{(k)}$  is called the “step size”.
- Using the first order Taylor approximation, we have

$$f(x + t\Delta x) \approx f(x) + t\nabla f(x)^\top \Delta x$$

- To be a descent method, the search direction must satisfy

$$\nabla f(x^{(k)})^\top \Delta x^{(k)} < 0$$

- Note that for convex functions,

$$f(x + t\Delta x) \geq f(x) + t\nabla f(x)^\top \Delta x$$

so the first order Taylor approximation underestimates the function

# Backtracking

- To find the step size, suppose  $0 < \alpha < 0.5$  and  $0 < \beta < 1$ , then

$$f(x + t\Delta x) \approx f(x) + t\nabla f(x)^\top \Delta x < f(x) + \alpha t \nabla f(x)^\top \Delta x$$

We can then start with a relatively large step size and decrease it until it satisfies the above condition

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Set  $\alpha \in (0, 0.5)$ ,  $\beta \in (0, 1)$  and  $t := 1$

While  $f(x + t\Delta x) > f(x) + \alpha t \nabla f(x)^\top \Delta x$ , Set  $t := \beta t$

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# Gradient descent method

- A reasonable choice for the search direction is the negative gradient

$$\Delta x = -\nabla f(x)$$

- Combine with the backtracking method, we repeat these steps until a stopping criterion is satisfied

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Set  $\Delta x = -\nabla f(x)$

Set  $\alpha \in (0, 0.5)$ ,  $\beta \in (0, 1)$  and  $t := 1$

While  $f(x + t\Delta x) > f(x) + \alpha t \nabla f(x)^\top \Delta x$ , Set  $t := \beta t$

Set  $x \leftarrow x + t\Delta x$

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# Steepest descent method

- We can write the first-order Taylor approximation as follows

$$f(x + v) \approx f(x) + \nabla f(x)^\top v$$

where  $\nabla f(x)^\top v$  is the directional derivative of  $f$  at  $x$  in the direction of  $v$ .

- Note that  $v$  is assumed to be a descent direction:  $\nabla f(x)^\top v < 0$ .
- Our objective is to find  $v$ , where  $\|v\| = 1$ , such that the directional derivative is as negative as possible.
- This is called the *normalized steepest descent* direction,

$$\Delta x = \operatorname{argmin}\{\nabla f(x)^\top v \mid \|v\| = 1\}$$

# Steepest descent method

- The choice of the metric of course makes a difference.
- In general, given the metric  $P$  (i.e.,  $\|v\|_P = (v^\top P v)^{1/2}$ ), we can find the [unnormalized] steepest descent direction
- As discussed before, we use the change of variable  $z = P^{1/2}x$ , whose Euclidian norm,  $\|z\|$  is the same as the quadratic norm  $\|v\|_P$

$$x = P^{-1/2}z$$

$$\nabla_z f = P^{-1/2} \nabla_x f$$

- In the space of  $z$  with Euclidian norm, we set  $\Delta z = -\nabla_z f$  as before

$$\Delta z = -P^{-1/2} \nabla_x f$$

- For the original parameter, the corresponding step is

$$\Delta x = P^{-1/2}(-P^{-1/2} \nabla_x f) = -P^{-1} \nabla f(x)$$

# Newton's method

- If we use the Euclidean metric,  $P = I$ , the steepest descent direction is simply the negative gradient, and the steepest descent method simply becomes the gradient descent method.
- However, if we use the Hessian metric,  $P = \nabla^2 f(x)$ , the steepest descent method becomes Newton's method, with the following Newton step:

$$\Delta x = -[\nabla^2 f(x)]^{-1} \nabla f(x)$$

# Newton's method

- Newton's method can also be interpreted as the second-order Taylor approximation of  $f$  at  $x$ ,

$$\begin{aligned}f(x + \Delta x) &\approx f(x) + \nabla f(x)^\top \Delta x + \frac{1}{2} \Delta x^\top \nabla^2 f(x) \Delta x \\ &= \tilde{f}(x)\end{aligned}$$

- We find the optimal  $\Delta x$  by minimizing  $\tilde{f}(x)$  with respect to  $\Delta x$ ,

$$\Delta x = -[\nabla^2 f(x)]^{-1} \nabla f(x)$$

# The Newton decrement

- Because  $\nabla^2 f(x) \succ 0$

$$\nabla f(x)^\top \Delta x = -\nabla f(x)^\top [\nabla^2 f(x)]^{-1} \nabla f(x) < 0$$

- The term

$$\lambda(x) = (\nabla f(x)^\top [\nabla^2 f(x)]^{-1} \nabla f(x))^{1/2}$$

is called the Newton decrement, which measures the proximity of  $x$  to  $x^*$

- By plugging  $\Delta x$  in the second-order Taylor approximation,

$$\begin{aligned} f(x) - \min \tilde{f}(x) &= f(x) - (f(x) - \frac{1}{2} \nabla f(x)^\top [\nabla^2 f(x)]^{-1} \nabla f(x)) \\ &= \frac{1}{2} \lambda^2(x) \end{aligned}$$

# Newton's algorithm

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Specify the tolerance level  $\varepsilon$

Set  $\Delta x = -[\nabla^2 f(x)]^{-1} \nabla f(x)$

Calculate  $\lambda^2 = \nabla f(x)^\top [\nabla^2 f(x)]^{-1} \nabla f(x)$

If  $\lambda^2/2 \leq \varepsilon$  then quit; Otherwise

Set  $\alpha \in (0, 0.5)$ ,  $\beta \in (0, 1)$  and  $t := 1$

While  $f(x + t\Delta x) > f(x) + \alpha t \nabla f(x)^\top \Delta x$ , Set  $t := \beta t$

Set  $x \leftarrow x + t\Delta x$

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# Quasi-Newton method

- When finding the Hessian exactly is computationally expensive, we can approximate it with another positive definite matrix  $M \succ 0$  which is easier to use
- Then,

$$\Delta x = -M^{-1} \nabla f(x)$$

- One possible approach is to use a rank 1 update
- At each iteration, we find  $M^{(k+1)}$  based on its previous value  $M^{(k)}$

$$\begin{aligned}\Delta x &= x^{(k+1)} - x^{(k)} \\ y &= \nabla f(x^{(k+1)}) - \nabla f(x^{(k)}) \\ v &= y - M^{(k)} \Delta x\end{aligned}$$

# Quasi-Newton method

- Then,

$$M^{(k+1)} = M^{(k)} + vv^T / v^T \Delta x$$

- Note that in general for rank 1 updates we have (matrix inversion lemma)

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 + v^T A^{-1}u}$$

- Therefore, we can find the inverse of  $M^{(k+1)}$  directly from the previously computed inverse of  $M^{(k)}$
- The BFGS (Broyden-Fletcher-Goldfarb-Shanno) method uses a rank 2 update

$$M^{(k+1)} = M^{(k)} + \frac{yy^T}{y^T \Delta x} - \frac{M^{(k)} \Delta x (M^{(k)} \Delta x)^T}{\Delta x^T M^{(k)} \Delta x}$$



# Coordinate descent method

- For high dimensional problems, it would be easier to perform optimization one parameter at a time (Tseng, 2001)

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Start with  $x^{(0)} \in D_f$

At each iteration  $k$ , for  $i = 1, \dots, n$

$$x_i^{(k)} = \operatorname{argmin}_{x_i} f(x_1^{(k+1)}, x_2^{(k+1)}, \dots, x_i, x_{i+1}^{(k)}, \dots, x_n^{(k)})$$

Quit if  $\|x^{(k+1)} - x^{(k)}\| \leq \varepsilon$

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- The convergence to the optimal value  $x^*$  is guaranteed for strictly convex and differentiable functions

# Coordinate descent method

- Instead of “alternating optimization” approach discussed above, we could use a gradient descent in one direction at a time

$$f(x_1, \dots, x_n) = f_0(x_1, \dots, x_n) + \sum_{i=1}^n f_i(x_i)$$

where  $f_i$  is non-differentiable but convex, and  $f_0$  is convex and differentiable

- This condition for example holds for Lasso models

$$\text{Minimize } \|y - x\beta\|^2 + \lambda \|\beta\|_1$$

# Coordinate descent method

- When  $f$  is not differentiable, the convergence to the optimal solution is not guaranteed in general, but it works if the non-differentiable part of  $f$  is separable

$$x_i^{(k+1)} = x_i^{(k)} - t_{ki} \nabla_i f(x_1^{(k+1)}, \dots, x_i^{(k)}, \dots, x_n^{(k)})$$

- Also, instead of one coordinate at a time, we could update a block of coordinates; this is called “block coordinate descent”

# Newton's method with equality constraints

- We can use a modified version of Newton's method for optimization problems with equality constraints:

$$\begin{array}{ll}\text{minimize} & f(x) \\ \text{subject to} & Ax = b\end{array}$$

- We assume the the initial point is feasible:  $x^{(0)} \in D_f, Ax^{(0)} = b$ .
- Our goal is to modify the Newton step,  $\Delta x$ , by taking the equality constraints into account so the subsequent points are also feasible.
- For this, we need to have  $A\Delta x = 0$  so at each step  $A(x^{(k)} + \Delta x) = b$ .

# Newton's method with equality constraints

- To find  $\Delta x$ , we can replace the objective function with its second-order Taylor approximation at a given point  $x$  and rewrite the optimization problem as follows:

$$\begin{array}{ll}\text{minimize} & f(x + v) \approx f(x) + \nabla f(x)^\top v + \frac{1}{2} v^\top \nabla^2 f(x) v \\ \text{subject to} & Av = 0\end{array}$$

- The modified Newton step,  $\Delta x$ , is the solution for this optimization problem.
- This is of course an equality constrained quadratic problem (discussed above), for which we can use the KKT conditions to rewrite the optimization problem as a system of linear equations

$$\begin{pmatrix} \nabla^2 f(x) & A^\top \\ A & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \omega \end{pmatrix} = \begin{pmatrix} -\nabla f(x) \\ 0 \end{pmatrix}$$

# Newton's method with equality constraints

- Here we use  $\omega$  to denote the optimal dual variable for the approximate quadratic problem.
- If the original objective function,  $f(x)$ , is quadratic, then  $\omega$  is the same as  $\nu$ , the optimal dual variable for the original problem.
- After we find  $\Delta x$ , we follow the same Newton algorithm we discussed for the unconstrained problem.

# Newton's method with inequality constraints

- We now discuss Newton's method for convex optimization problems with inequality constraints:

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0 \quad i = 1, \dots, m \\ & Ax = b\end{array}$$

- We assume that Slater's constraint qualification holds: there exists  $x \in D$  for which  $Ax = b$  and  $f_i(x) < 0, i = 1, \dots, m$ .
- Therefore, the primal and dual optimal points satisfy the KKT conditions.

# Newton's method with inequality constraints

- For such problems, we can use Newton's methods based on *interior-point* algorithms.
- More specifically, we focus on a specific interior-point algorithm called the *barrier method*.
- In this approach, we bring the inequality constraints into the objective junction and rewrite the optimization problem as follows:

$$\begin{aligned} \text{minimize} \quad & f_0(x) + \sum_{i=1}^m l_-(f_i(x)) \\ \text{subject to} \quad & Ax = b \end{aligned}$$

where the indicator function is defined as

$$l_-(u) = \begin{cases} 0 & u \leq 0 \\ \infty & u > 0 \end{cases}$$



# Newton's method with inequality constraints

- This creates a barrier at 0 such that violating the inequality constraints adds an infinite cost to the objective function.
- The problem however is that the resulting objective function is not differentiable so we cannot use Newton's method.
- To solve this issue, we can use an approximate logarithmic barrier, which is smoother and differentiable, instead:

$$\hat{l}_-(u) = -\frac{1}{t} \log(-u)$$

where  $t > 0$  controls the accuracy of the approximation: higher  $t$ , better approximation.

# Newton's method with inequality constraints

- We can now rewrite our optimization problem as follows:

$$\begin{array}{ll}\text{minimize} & f_0(x) + \sum_{i=1}^m -\frac{1}{t} \log(-f_i(x)) \\ \text{subject to} & Ax = b\end{array}$$

- Or alternatively,

$$\begin{array}{ll}\text{minimize} & tf_0(x) + \phi(x) \\ \text{subject to} & Ax = b\end{array}$$

where  $\phi(x) = -\sum_{i=1}^m \log(-f_i(x))$ .

- We can now use Newton's method for this optimization problem as discussed before.

# Newton's method with inequality constraints

- The solution we find is of course for an approximation of the original problem.
- We can of course use very large  $t$  values to improve the quality of approximation, but this would lead to computational problems when we approach the boundary of the feasible set.
- To address this issue, we can start with a small value for  $t$  and gradually increase it to improve the approximation accuracy.
- This way, we will find a sequence of solutions  $x^*(t)$  for  $t > 0$ . This is called the *central path* for the original optimization problem.
- At each iteration  $k$ , we initialize Newton's method at  $x^*(t_{k-1})$  to find the new *central point*  $x^*(t_k)$ , where  $t_k > t_{k-1}$ .

# Optimization methods in statistics

- In the frequentist framework, we typically perform statistical inference by maximizing log-likelihood  $\ell(\theta)$ , or alternatively minimizing negative log-likelihood, which is also known as the energy function
- Additionally, we have
  - ▶ Score function:  $s(\theta) = \nabla_{\theta}\ell(\theta)$
  - ▶ Observed Fisher information:  $J(\theta) = -\nabla_{\theta}^2\ell(\theta)$
  - ▶ Fisher information:  $I(\theta) = E[-\nabla_{\theta}^2\ell(\theta)]$

- The step in Newton's method is

$$\Delta\theta = [J(\theta)]^{-1}s(\theta)$$

- That is, in iteration  $k$ ,

$$\theta^{(k+1)} = \theta^{(k)} + [J(\theta^{(k)})]^{-1}s(\theta^{(k)})$$

# Fisher scoring algorithm

- If instead of the observed information, we use the Fisher information (i.e., expectation of the observed information), the resulting method is called the *Fisher scoring* algorithm

$$\Delta\theta = [I(\theta)]^{-1}s(\theta)$$

- That is,

$$\theta^{(k+1)} = \theta^{(k)} + [I(\theta^{(k)})]^{-1}s(\theta^{(k)})$$

- In general, the Fisher scoring algorithm tends to be less sensitive to the initial guess. On the other hand, the Newton's method tends to converge faster
- For exponential family models with natural parameters and GLM with canonical links, the two methods are identical

# Exponential family and GLM

- Recall that the single parameter exponential family has the following general form:

$$P(y|\mu) = \exp\{g(\mu)t(y) + c(\mu) + h(y)\}$$

- For models with multiple parameters, we have

$$P(y|\mu) = \exp\left\{\sum_{k=1}^K g_k(\mu)t_k(y) + c(\mu) + h(y)\right\}$$

where  $g$ ,  $t$ ,  $c$ , and  $h$  are vectors.

- We can change the parameter using the transformation  $\phi_k = g_k(\mu)$ , and write the distribution in terms of natural parameter  $\phi$ :

$$P(y|\mu) = \exp\left\{\sum_{k=1}^K \phi_k t_k(y) + c^*(\phi) + h(y)\right\}$$

# Poisson model

- Consider the following Poisson model:

$$\begin{aligned}P(y_i|\mu) &= e^{-\mu_i} \mu_i^{y_i} / y_i! \\ &= \exp\{\log(\mu_i)y_i - \mu_i - \log(y_i!)\}\end{aligned}$$

where  $\phi_i = g(\mu_i) = \log(\mu_i)$ ,  $t(y_i) = y_i$ ,  $c(\mu_i) = -\mu_i$ , and  $h(y_i) = -\log(y_i!)$ .

- We have

$$\begin{aligned}\phi_i = \log(\mu_i) &\Rightarrow \mu_i = \exp(\phi_i) \\ c^*(\phi_i) &= \exp(\phi_i) \\ E_{\phi_i}[t(y_i)] = E(y_i) &= -\frac{\partial c^*(\phi_i)}{\partial \phi_i} = \exp(\phi_i) = \mu_i \\ \text{var}_{\phi_i}[t(y_i)] = \text{var}(y_i) &= -\frac{\partial^2 c^*(\phi_i)}{\partial \phi_i^2} = \exp(\phi_i) = \mu_i\end{aligned}$$

- The score function with respect to  $\phi_i$  can be obtained as follows:

$$\begin{aligned}s(\phi_i) &= \frac{\partial \ell(\phi_i)}{\partial \phi_i} \\&= t(y_i) + \frac{\partial c^*(\phi_i)}{\partial \phi_i} \\&= y_i - \exp(\phi_i) \\&= y_i - \mu_i\end{aligned}$$

- The total score function based on  $n$  observations is

$$s(\phi) = \sum_i y_i - \exp(\phi_i) = \sum_i y_i - \mu_i$$

- As the result, the likelihood equation is:

$$\sum_i y_i - \exp(\hat{\phi}_i) = \sum_i y_i - \hat{\mu}_i = 0$$



# Poisson model

- For Poisson regression model, we are of course interested in regression parameters  $\beta$ .
- Therefore, we would like to write the score function in terms of  $\beta$ .
- To do this, we first need to specify the link function.
- Suppose we use the log link function

$$g(\mu_i) = \log(\mu_i) = x_i\beta$$

- Since we have  $\phi_i = g(\mu_i)$ , we can write the link function as follows:

$$\phi_i = \log(\mu_i) = x_i\beta$$

- The link function that transforms the mean to the natural parameter is referred to as the *canonical link*.

# Poisson model

- Using the link function, we can now write the score function in terms of  $\beta$ .
- For the  $j^{th}$  element of  $\beta$ , we have

$$\begin{aligned}s(\beta_j) &= \sum_i \frac{\partial \ell(\beta)}{\partial \beta_j} \\&= \sum_i \frac{\partial \ell(\phi)}{\partial \phi_i} \frac{\partial \phi_i}{\partial \beta_j} \\&= \sum_i [y_i - \exp(x_i \beta)] x_{ij}\end{aligned}$$

- As the result, the likelihood equation in terms of  $\beta_j$  is

$$\sum_i [y_i - \exp(x_i \hat{\beta})] x_{ij} = 0$$

- We can now easily obtain the Fisher information matrix in terms of  $\beta$ .

$$\begin{aligned} I(\beta_j \beta_k) &= E\left[-\frac{\partial^2 \ell(\beta)}{\partial \beta_j \partial \beta_k}\right] \\ &= E\left[\sum_i x_{ij} x_{ik} \exp(x_i \beta)\right] \\ &= \sum_i x_{ij} x_{ik} \exp(x_i \beta) \end{aligned}$$

- In a matrix format

$$I(\beta) = X^T W X$$

where  $W$  is a diagonal matrix whose  $i^{th}$  element is  $\exp(x_i \beta)$ .

- In general, we can show that for the  $j$ th parameter

$$s(\beta_j) = \sum_i \frac{[y_i - \mu_i] x_{ij}}{\text{var}(y_i)} \frac{\partial \mu_i}{\partial \eta_i}$$

where  $\partial \mu_i / \partial \eta_i$  depends on the link function we choose

- It is also easy to show that for a general link function, the Fisher information matrix is

$$\begin{aligned} I(\beta_j, \beta_k) &= E\left(-\frac{\partial^2 \ell(\beta)}{\partial \beta_j \partial \beta_k}\right) \\ &= \sum_i \frac{x_{ij} x_{ik}}{\text{var}(y_i)} \left(\frac{\partial \mu_i}{\partial \eta_i}\right)^2 \\ I(\beta) &= \mathbf{x}^\top \mathbf{W} \mathbf{x} \\ W_{ii} &= \frac{\left(\frac{\partial \mu_i}{\partial \eta_i}\right)^2}{\text{var}(y_i)} \end{aligned}$$

# Iterative re-weighted least squares

- For GLM, Fisher scoring is related to the weighted least squares method (e.g., linear regression with non-constant variance for error terms)

- We can write the Fisher scoring algorithm for updating  $\beta$  as

$$I(\beta^{(k)})\beta^{(k+1)} = I(\beta^{(k)})\beta^{(k)} + s(\beta^{(k)})$$

- since  $I(\beta) = X^T W X$ ,

$$(X^T W^{(k)} X)\beta^{(k+1)} = (X^T W^{(k)} X)\beta^{(k)} + s(\beta^{(k)})$$

- After few simple steps, we have

$$(X^T W^{(k)} X)\beta^{(k+1)} = X^T W^{(k)} z^{(k)}$$

where

$$z_i^{(k)} = \eta_i^{(k)} + (y_i - \mu_i^{(k)}) \frac{\partial \eta_i^{(k)}}{\partial \mu_i^{(k)}}$$

# Iterative re-weighted least squares

- At each iteration, we can find the next estimate for  $\beta$  as follows:

$$\beta^{(k+1)} = (x^\top W^{(k)} x)^{-1} x^\top W^{(k)} z^{(k)}$$

- The above estimate is similar to the weighted least squares estimate. In this case,  $W^{(k)}$  is a diagonal matrix whose  $i^{th}$  element is

$$W_{ii}^{(k)} = \frac{\left(\frac{\partial \mu_i^{(k)}}{\partial \eta_i^{(k)}}\right)^2}{\text{var}(y_i)}$$

- Note that for GLM, the weights  $W$  and the response variable  $z$  change from one iteration to another based on the current estimate of  $\beta$ .
- We iteratively estimate  $\beta$  until the algorithm converges.