

Chapter 3 Numerical Methods

Part 2 3.2 Systems of Equations 3.3 Nonlinear and Constrained Optimization

Outline

- 3.2 Systems of Equations
- 3.3 Nonlinear and Constrained Optimization
- Summary



Outline

- 3.2 Systems of Equations
 - 3.2.1 Linear Systems
 - 3.2.2 Nonlinear Systems
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3.2.1.1 Square Systems

- You know this one already...
- Suppose H is square and:

$$\underline{z} = H\underline{x}$$

• The "solution" is:

$$\underline{x} = H^{-1}\underline{z}$$

- Use MATLAB and you're done.
- But how do you invert a matrix yourself?
- → Row operations do not change the solution of the linear system.

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Gaussian Elimination

• Consider three equations:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = y_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = y_2$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = y_3$$

 Multiply 2nd equation by a31/a21

$$a_{31}x_1 + \left(\frac{a_{31}}{a_{21}}\right)a_{22}x_2 + \left(\frac{a_{31}}{a_{21}}\right)a_{23}x_3 = \left(\frac{a_{31}}{a_{21}}\right)y_2$$

 Subtract this from 3rd equation:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = y_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = y_2$$

$$a_{32}^{(1)}x_2 + a_{33}^{(1)}x_3 = y_3^{(1)}$$

Gaussian Elimination

 Multiply 1st equation by a21/a11 and eliminate x1 from second equation:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = y_1$$
$$a_{22}^{(1)}x_2 + a_{23}^{(1)}x_3 = y_2^{(1)}$$
$$a_{32}^{(1)}x_2 + a_{33}^{(1)}x_3 = y_3^{(1)}$$

 Use same process to (new) 2nd and 3rd equations to eliminate x2:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = y_1$$
$$a_{22}^{(1)}x_2 + a_{23}^{(1)}x_3 = y_2^{(1)}$$
$$a_{33}^{(2)}x_3 = y_3^{(2)}$$



Gaussian Elimination

• Now we have:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = y_1$$
$$a_{22}^{(1)}x_2 + a_{23}^{(1)}x_3 = y_2^{(1)}$$
$$a_{33}^{(2)}x_3 = y_3^{(2)}$$

- Solve 3rd equation for x3, then 2nd equation for x2 etc.
- Notice:
 - Process generalizes to larger systems.
 - Process works for arbitrary matrices.



3.2.1.2 Left Pseudoinverse

- Consider again <u>z</u> = H<u>x</u> where H is m X n, m>n.
 Called an overdetermined system.
- Define the residual vector:

$$r(\underline{x}) = \underline{z} - H\underline{x}$$

- Define a cost function as its magnitude: $f(\underline{x}) = \frac{1}{2} \underline{r}^{T} (\underline{x}) \underline{r}(\underline{x})$
- Substitute the definition of residual:

$$f(\underline{x}) = \frac{1}{2}(\underline{z} - H\underline{x})^T(\underline{z} - H\underline{x})$$

3.2.1.2 Left Pseudoinverse

- Use the product rule to differentiate $yf(\underline{x}) = \frac{1}{2}(\underline{z} H\underline{x})^T(\underline{z} H\underline{x})$ x: $f_{\underline{x}} = (\underline{z} - H\underline{x})^T H$
- This will vanish at any local minimum:

$$(\underline{z} - H\underline{x}^*)^T H = 0$$

- Requires residual at minimizer to be orthogonal to the column space of H.
 - Hence, known as the "normal equations".
- The value of H<u>x</u>*:
 - Is in the column space of H
 - Has a residual (z-H \underline{x}^*) of minimum length.



3.2.1.2 Left Pseudoinverse

Move z to other side and solve:

$$H^T H \underline{x}^* = H^T \underline{z}$$

$$\underline{x}^* = (H^T H)^{-1} H^T \underline{z}$$

• The matrix:

$$H^{+} = (H^{T}H)^{-1}H^{T}$$

• ... is called the Left Pseudoinverse of H because...

$$H^{+}H = (H^{T}H)^{-1}H^{T}H = I_{n}$$
 m > n

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- Consider again <u>z</u> = H<u>x</u> where H is m X n, m<n.
 Called an underdetermined system.
- There are potentially an infinite number of solutions.
- Simple technique is to introduce a regularizer (cost function) to rank all solutions and pick the best.
- Define a cost function as the (squared) magnitude of x:

$$f(\underline{x}) = \frac{1}{2} \underline{x}^T \underline{x}$$

• Now form a constrained optimization problem:

optimize:
$$\underline{f}(\underline{x})$$
 $\underline{x} \in \mathfrak{R}^n$

subject to: $\underline{c}(\underline{x}) = \underline{z} - H\underline{x} = \underline{0} \quad \underline{h} \in \Re^m$

• Form the Lagrangian:

$$l(\underline{x},\underline{\lambda}) = \frac{1}{2}\underline{x}^{T}\underline{x} + \underline{\lambda}^{T}(\underline{z} - H\underline{x})$$

• First necessary condition is:

$$l_{\underline{x}}(\underline{x}, \underline{\lambda})^{T} = \underline{x} - H^{T}\underline{\lambda} = \underline{0} \Longrightarrow \underline{x} = H^{T}\underline{\lambda}$$

• Substitute into the second necessary condition (constraints): $l_{\lambda}(x, \lambda)^{T} = z - Hx = 0$

$$\underline{z} - HH^T \underline{\lambda} = \underline{0}$$
$$HH^T \underline{\lambda} = \underline{z}$$

• The solution for the multipliers is:

$$\underline{\lambda} = (HH^T)^{-1}\underline{z}$$



• Substitute back into the first equation:

$$\underline{x} = H^T \underline{\lambda} = H^T (HH^T)^{-1} \underline{z}$$

• The matrix:

$$H^+ = H^T (HH^T)^{-1}$$

• ... is known as the right pseudoinverse because ...

$$HH^{+} = HH^{T}(HH^{T})^{-1} = I_{m} \qquad m < n$$



3.2.1.4 About The Pseudoinverse

- Both LPI and RPI
 - reduce to the regular inverse when the matrix is square.
 - require H to be of full rank
 - invert a matrix whose dimension is the smaller of m and n
- It is possible to define "weighted" pseudoinverses (easy to re-derive). For example:

$$f(\underline{x}) = \frac{1}{2}\underline{r}^{T}(\underline{x})W\underline{r}(\underline{x})$$

Produces the Weighted LPI

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Standard Form

• The problem of solving: $\underline{g}(\underline{x}) = \underline{b}$

• Is equivalent to solving: $\underline{c}(\underline{x}) = \underline{g}(\underline{x}) - \underline{b} = 0$

- Often, <u>x</u> is really an unknown vector of parameters denoted as <u>p</u>.
- Note that:

$$\underline{c}_{\underline{x}} = \frac{\partial \underline{c}(\underline{x})}{\partial \underline{x}} = \frac{\partial \underline{g}(\underline{x})}{\partial \underline{x}} = \underline{g}_{\underline{x}}$$



3.2.2.1 Newton's Method

- Basic trick of numerical methods.....
- Linearize the constraints about a nonfeasible point $c(r + \Delta r) = c(r) + c \Delta r + c$

$$\underline{c}(\underline{x} + \Delta \underline{x}) = \underline{c}(\underline{x}) + \underline{c}_{\underline{x}} \Delta \underline{x} + \dots$$

• Require feasibility after perturbation:

$$\underline{c}(\underline{x} + \Delta \underline{x}) = 0$$

• Leads to: $c_{\underline{x}} \Delta \underline{x} = -c(\underline{x})$

The precise change which, when added to x, will produce a root of (the linearization of) $\underline{c}(\underline{x})$

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Basic iteration is:

$$\Delta \underline{x} = -\underline{c}_{\underline{x}}^{-1} \underline{c}(\underline{x}) = -\underline{c}_{\underline{x}}^{-1} [\underline{g}(\underline{x}) - \underline{b}]$$

Visualizing Newton's Method





- Nonlinear functions can have several roots each with its own radius of convergence.
- At an extremum (not at a root) the Jacobian is not invertible.
- Near an extremum, huge jumps to a different root are possible.

3.2.2.3 Numerical Derivatives

- Often its simpler, less error prone, and less computation to differentiate numerically.
- Compute the constraint vector one additional time at a perturbed location:

$$\frac{\partial \underline{c}}{\partial x_{i}} = \frac{\underline{c}(\underline{x} + \Delta \underline{x}_{i}) - \underline{c}(\underline{x})}{\Delta \underline{x}_{i}} \qquad \Delta \underline{x}_{i} = \begin{bmatrix} 0 & 0 & \dots & \Delta x_{i} & \dots & 0 \end{bmatrix}$$

i-th position

- This gives a numerical approximation for the i-th column of the Jacobian.
- Collect them all to get C_{-X}

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Isaac Newton

- English mathematician and scientist.
- Perhaps the greatest analytic thinker in human history.
- Graduated Trinity College Cambridge in 1665.
- Then came the Great Plague.
 - University shut down for 2 years.
- Worked at home on calculus, gravitation, and optics.
 - Figured them all out!
- We will use his calculus to solve nonlinear equations
 - and a few other things !!!



Isaac Newton 1643 -1727

3.3.1 Nonlinear Optimization

• The general nonlinear optimization problem:

minimize: $_{\underline{x}} f(\underline{x}) \qquad \underline{x} \in \Re^n$

 Numerical techniques produce a sequence of estimates such that:

$$f(\underline{x}_{k+1}) < f(\underline{x}_k)$$

- ...by controlling both the length and the direction of the steps.
- Two basic techniques:
 - 1) Line Search adjusts length after choosing direction.
 - 2) Trust Region adjusts direction after choosing length.

3.3.1.1 Line Search

- Often need to search the descent direction and that's expensive.
- Consider ways to be smart about this.....



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3.3.1.1 Line Search

- Given a descent direction d, converts to a 1D problem: $\minimize:_{\alpha}f(\underline{x} + \alpha \underline{d}) \quad \alpha \in \Re^{1}$
- Define the linearization of the scalar function:

 $f(\alpha \underline{d}) = f(\underline{x}) + f_{\underline{x}}(\alpha \underline{d})$

• Convergence is guaranteed if every iteration achieves sufficient decrease (relative to linear approximation)

$$\eta = \frac{f(\underline{x}) - f(\underline{x} + \alpha \underline{d})}{\hat{f}(\underline{0}) - \hat{f}(\alpha \underline{d})} > \eta_{\min} \qquad \eta_{\min}: \quad 0 < \eta_{\min} < 1$$

• For efficiency, try large steps and backtrack if necessary with: $\alpha_{k+1} = (2^{-i})\alpha_{k-1} = (1, 2, ...)$

Line Search Algorithm

```
00
     algorithm lineSearch ()
01
      \underline{x} \leftarrow \underline{x}_0 // initial guess
02 \eta_{min} \leftarrow const \in [0, 1/4]
03
     \alpha_{last} \leftarrow \alpha_0
04
      while (true)
05
            d \leftarrow findDirection(x)
            \alpha \leftarrow \alpha_{last} \times 4 // or \alpha \leftarrow l for Newton step
06
07
     while (true)
80
                  \eta \leftarrow (\text{see Equation 3.45})
                  if (\eta > \eta_{min}) break Accept step
09
10
                  \alpha \leftarrow \alpha \div 2
                                                  Reduce stepsize
11
           endwhile
            \underline{x} \leftarrow \underline{x} + \alpha \underline{d}; \alpha_{last} \leftarrow \alpha Move to new estimate
12
13
            if(finished()) break
14
       endwhile
15
       return
```

Algorithm 3.1: Line Search in a Descent Direction with Backtracking. The algorithm searches repeatedly in a descent direction.

3.3.1.1.2 Descent Direction: Gradient Descent

- Also called steepest descent.
- Consider, approximating the objective by degree 1 Taylor polynomial...

$$f(\underline{x} + \Delta \underline{x}) \approx f(\underline{x}) + f_{\underline{x}} \Delta \underline{x}$$

- Hence the increase in the objective is the projection of Δx onto the gradient f_x .
- Choose the negative gradient for max decrease:

$$\underline{d}^{T} = -f_{\underline{x}}$$

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3.3.1.1.3 Descent Direction: Newton Step

- Of course the gradient vanishes at a local minimum.
- Write Taylor series for the gradient. $f_{\underline{x}}(\underline{x} + \Delta \underline{x}) \approx f_{\underline{x}}(\underline{x}) + f_{\underline{x}\underline{x}}\Delta \underline{x} = \underline{0}^{T}$
- Hence the step is given by:

$$\mathbf{f}_{\underline{\mathbf{x}}\underline{\mathbf{x}}}\Delta\underline{\mathbf{x}} = -\mathbf{f}_{\underline{\mathbf{x}}}^{\mathrm{T}} \square \sum \Delta\underline{\mathbf{x}} = -\mathbf{f}_{\underline{\mathbf{x}}\underline{\mathbf{x}}}^{-1} \mathbf{f}_{\underline{\mathbf{x}}}^{\mathrm{T}}$$

Sometimes Called Newton-Raphson Method.

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• This is equivalent to fitting a parabola to f and computing the minimum of the parabola.

3.3.1.2 Descent Direction: Trust Region

- Solve this auxiliary constrained optimization problem: optimize: $\Delta \underline{x}$ $\hat{f}(\Delta \underline{x}) = f(\underline{x}) + f_{\underline{x}}\Delta \underline{x} + f_{\underline{x}\underline{x}}\frac{\Delta \underline{x}^2}{2}$ $\Delta \underline{x} \in \Re^n$ subject to: $\underline{g}(\Delta \underline{x}) = \Delta \underline{x}^T \Delta \underline{x} \le \rho_k^2$ Inequality constraint (stay in a circle)
- The solution is also a solution of:

$$(f_{\underline{x}\underline{x}} + \mu I)\Delta \underline{x}^* = -f_{\underline{x}}^T \quad \mu \ge 0$$

- When objective is locally quadratic μ is small.
- Otherwise μ is large and algorithm is reduced to gradient descent.
- Trust region is adapted based on ratio of actual and predicted reduction: $\eta = \frac{f(\underline{x}) f(\underline{x} + \Delta \underline{x})}{\hat{f}(0) \hat{f}(\Delta \underline{x})}$

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Levenberg-Marquardt Algorithm

```
algorithm Levenberg-Marquardt()
00
      \underline{x} \leftarrow \underline{x}_0 // \text{ initial guess}
01
02 \Delta \underline{x}_{max} \leftarrow const
03 \rho_{max} \leftarrow const
04 \rho \leftarrow \rho_0 \in [0, \rho_{max}]
05
     \eta_{min} \leftarrow const \in [0, 1/4]
06
      while (true)
07
           solve Equation 3.51 for \Delta x
80
           compute \eta using Equation 3.53
           if (\eta < \eta_{min}) then \Delta \underline{x} \leftarrow \theta Reject step
09
           x \leftarrow x + \Delta x // step to new point
10
           if (\eta < 1/4) \rho \leftarrow \rho/4 // decrease trust Reduce Trust
11
           else if (\eta > 3/4 and |\Delta \underline{x}| = \rho)
12
13
                 \rho \leftarrow min(2\rho, \rho_{max}) // increase trust Increase Trust
14
           endif
15
           if(finished()) break
16
      endwhile
17
      return
```

Algorithm 3.2: Levenberg-Marquardt. This is a popular optimization algorithm based on the trust region technique.

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Carl Friedrich Gauss

- German mathematician and scientist.
- Some say greatest mathematician in history.
- Famous for doing math in his head.
- Major contributions to number theory.
- "Proved" fundamental theorem of algebra.
- Invented method of least squares to predict orbital phenomena.



Carl Friedrich Gauss 1777 -855

3.3.1.3 Nonlinear Least Squares

• Consider nonlinear observations z of x:

 $\underline{z} = \underline{h}(\underline{x}) \ \underline{z} \in \Re^{m}, \underline{x} \in \Re^{n}, m > n$

Usually, not Satisfied exactly

• Define a residual and cost function:

$$\mathbf{r}(\mathbf{x}) = \mathbf{z} - \mathbf{h}(\mathbf{x})$$

 $f(\underline{x}) = \frac{1}{2} r^{T}(\underline{x}) W r(\underline{x})$ Assume a symmetric W

The weights can come from the inverse of the covariance:

$$W = R^{-1} = Exp(\underline{z}\underline{z}^{T})^{-1}$$

3.3.1.3.1 Derivatives $f(\underline{x}) = \frac{1}{2}\underline{r}^{T}(\underline{x})Wr(\underline{x})$

- Nonlinear \rightarrow must be solved by iterative methods.
- Gradient: Row $f_{\underline{x}} = \underline{r}^{T}(\underline{x})W_{\underline{x}}$ Jacobian Matrix • Also: $\underline{r}_{\underline{x}} = -\underline{h}_{\underline{x}}$

• Hessian: Matrix
$$f_{\underline{x}\underline{x}} = \underline{r}_{\underline{x}}^{T}W\underline{r}_{\underline{x}} + f_{\underline{x}\underline{x}}Wr(\underline{x})$$

• Also: $\underline{r}_{\underline{x}\underline{x}} = -\underline{h}_{\underline{x}\underline{x}}$

 Give these to any minimization algorithm (like Levenberg-Marquardt). Recall the Newton step:

$$\Delta \underline{\mathbf{x}} = -\mathbf{f}_{\underline{\mathbf{x}}\underline{\mathbf{x}}}^{-1} \mathbf{f}_{\underline{\mathbf{x}}}^{T}$$

3.3.1.3.2 Gauss Newton Algorithm

- From last slide: $f_{\underline{x}\underline{x}} = \underline{r}_{\underline{x}}^{T}W\underline{r}_{\underline{x}} + \underline{r}_{\underline{x}\underline{x}}W\underline{r}(\underline{x})$
- Residuals are often small since they are caused solely by noise.
- In that case <u>r(x)</u> can be neglected to give:

Gauss Newton Approximation to The Hessian

$$f_{\underline{x}\underline{x}} \approx \underline{r}_{\underline{x}}^{T} W \underline{r}_{\underline{x}}$$

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- This is a very cheap 2nd derivative computed from a 1st derivative (which you would need anyway).
- The Newton step becomes:

$$\Delta \underline{x} = -f_{\underline{x}\underline{x}}^{-1} f_{\underline{x}}^{T} = -r_{\underline{x}}^{T} W r_{\underline{x}} r_{\underline{x}}^{T} W r(\underline{x}) \qquad \text{Eqn } A$$

3.3.1.3.3 Rootfinding to a Minimum?

- The objective nearly vanishes at a minimum.
- Linearize observations and solve for the "root" of the gradient:

$$\mathbf{r}_{\mathbf{x}} \Delta \mathbf{x} = -\mathbf{r}(\mathbf{x})$$
 Overdetermine
System

• Solve iteratively with left pseudoinverse:

$$\underline{\mathbf{x}} = -[\underline{\mathbf{r}}_{\underline{\mathbf{x}}}^{\mathrm{T}}\underline{\mathbf{r}}_{\underline{\mathbf{x}}}^{\mathrm{T}}]^{-1}\underline{\mathbf{r}}_{\underline{\mathbf{x}}}^{\mathrm{T}}\underline{\mathbf{r}}(\underline{\mathbf{x}}) \qquad \begin{array}{l} \text{Same as Eqn A for} \\ \mathbf{W}=\mathbf{I} \\ \text{This is a valid} \\ \text{approach} \end{array}$$

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- To be safe, use this as a descent direction and use line search.
- Gauss Newton nonlinear least squares is equivalent to (gradient) rootfinding for small residuals.

Small Residuals

• Everything is fine as long as the minimum residual is small relative to the present one.



Large Residuals

- When the present residual is close to the minimum, the slope is near zero.
 - Eventually the update actually increases the residual.





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Constrained Optimization

• Problem Statement:

optimize:
$$f(x)$$
 $x \in \Re^n$ subject to: $c(x) = 0$ $c \in \Re^m$

• Recall the necessary conditions:

$$f_{\underline{x}}^{T} + \underline{c}_{\underline{x}}^{T} \lambda = 0 \quad \text{n eqns}$$
$$\underline{c}(\underline{x}) = 0 \quad \text{m eqns}$$

 These are n+m (generally nonlinear) equations in the n+m unknowns (x*,λ*).

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Compact Necessary Conditions

• Define the Lagrangian:

$$l(\underline{\mathbf{x}}, \underline{\lambda}) = f(\underline{\mathbf{x}}) + \underline{\lambda}^{\mathrm{T}} \underline{\mathbf{c}}(\underline{\mathbf{x}})$$

• Then, the necessary conditions become:

$$l_{\underline{x}}^{T} = 0 \qquad \text{n eqns} \\ l_{\underline{\lambda}}^{T} = 0 \qquad \text{m eqns}$$

• These are (the same) n+m (generally nonlinear) equations in the n+m unknowns (x*, λ *).

Constrained Newton Method

• Linearize of course!



- Where: $l_{\underline{x}} = f_{\underline{x}} + \lambda^{T} \underline{c}_{\underline{x}}$ $l_{\underline{x}\underline{x}} = f_{\underline{x}\underline{x}} + \lambda^{T} \underline{c}_{\underline{x}\underline{x}}$
- Efficient ways to invert this matrix were covered in the math section.
- Solution gives a descent direction for line search or trust region algorithm.

Initial Lagrange Multipliers

- An initial estimate of x is doable.
- What about λ ?
- One way is to solve the first (n) first order conditions for the (m) multipliers.

$$\mathbf{f}_{\mathbf{x}}^{T} + \mathbf{c}_{\mathbf{x}}^{T} \boldsymbol{\lambda} = \mathbf{0}$$

• They overdetermine λ so the solution is a left pseudoinverse (of $\underline{c}_{\underline{x}}^{T}$).

$$\lambda_{0} = -[\underline{c}_{\underline{x}}\underline{c}_{\underline{x}}^{T}]^{-1}\underline{c}_{\underline{x}}f_{\underline{x}}^{T}$$

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Constrained Gauss-Newton

 Consider the constrained nonlinear least squares problem:

minimize:
$$f(\underline{x}) = \frac{1}{2}r(\underline{x})^{T}r(\underline{x})$$

subject to: $\underline{g}(\underline{x}) = \underline{b}$

- The 1st and 2nd derivatives are:
 - $l_{\underline{x}\underline{x}} = f_{\underline{x}\underline{x}} + \lambda^{T} \underline{g}_{\underline{x}\underline{x}} = r_{\underline{x}}^{T} r_{\underline{x}} + \lambda^{T} \underline{g}_{\underline{x}\underline{x}}$ $l_{\underline{x}} = f_{\underline{x}} + \lambda^{T} \underline{g}_{\underline{x}} = r^{T} (\underline{x}) r_{\underline{x}} + \lambda^{T} \underline{g}_{\underline{x}}$

Small residuals Assumed here

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 Now go back and use the constrained Newton method on these to find a descent direction.

Penalty Function Approach

• Consider the following unconstrained problem:

$$f_k(\underline{x}) = f(\underline{x}) + \frac{1}{2} w_k \underline{c}(\underline{x})^T \underline{c}(\underline{x})$$

- Solve this for progressively increasing values of the weight w_k.
- Why do this?
 - Many constraints are soft and can be traded-off against the objective.
 - This has only n dof rather than n+m.
 - Can be used to get a good initial estimate for a constrained approach.

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Summary

- The inverse of a nonsquare matrix can be defined based on minimization of some suitable objective.
- The roots of nonlinear functions can be found by linearization and iteration. Newton's method converges quadratically.
- Minimization problems are very different from rootfinding.
 - Though they are easy to confuse when doing least squares.
 - Small residuals is a key assumption. Know when you are making it.

Summary

- Numerical methods for optimization either search for roots of the gradient or for local minima. Two techniques are:
 - Line search
 - Trust region
- Protected steps (line search) and backtracking are key ways to achieve robustness.

