Numerical Optimal Control
Lecture 3: Newton method & SQP

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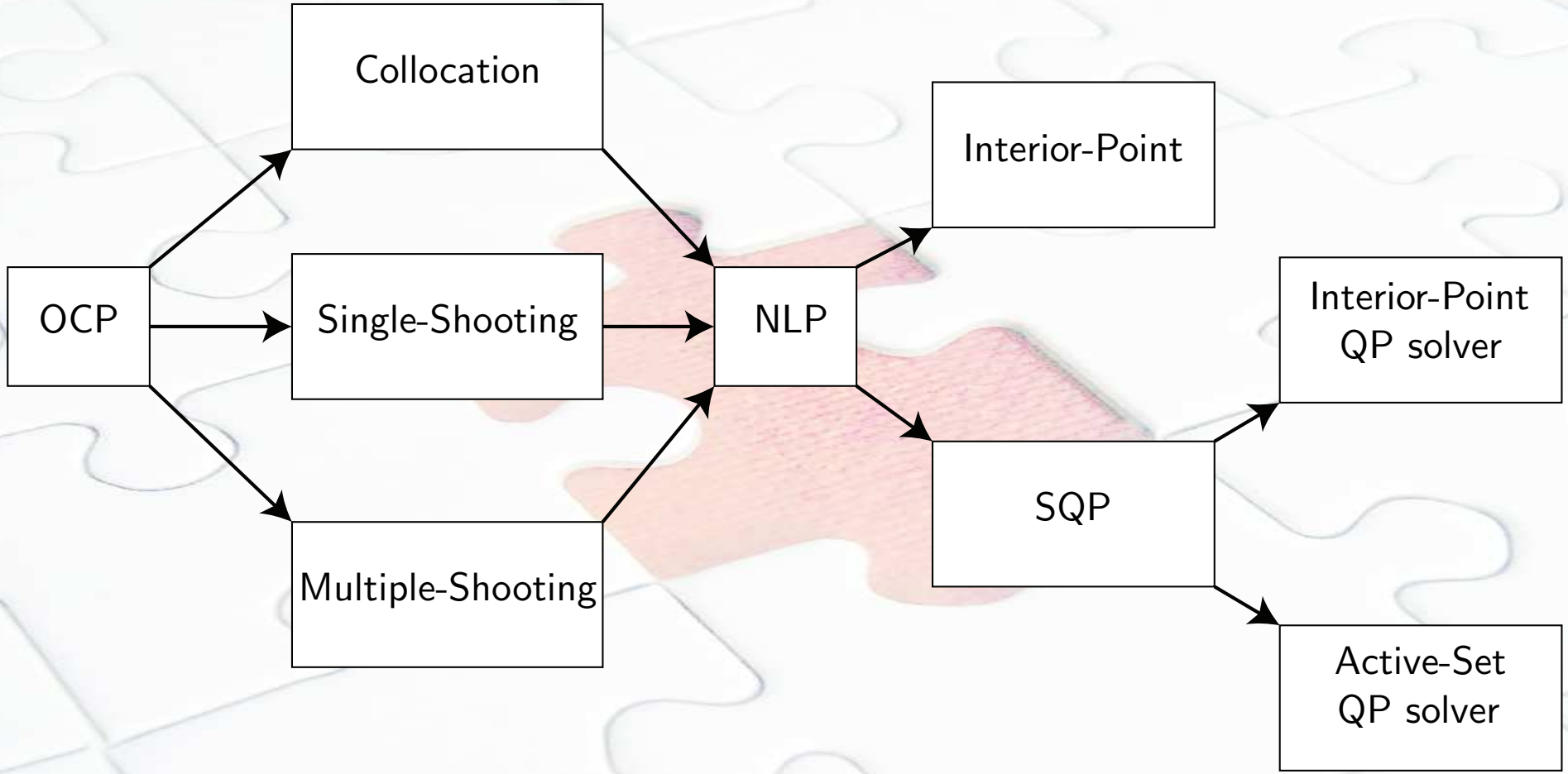
ITK NTNU

NTNU PhD course

Outline

1. The Newton method
2. Newton on the KKT conditions
3. The reduced Newton step (unconstrained problems)
4. The merit function - Line-search for constrained problems
5. Newton-type methods
6. Sequential Quadratic Programming

Survival map of Direct Optimal Control



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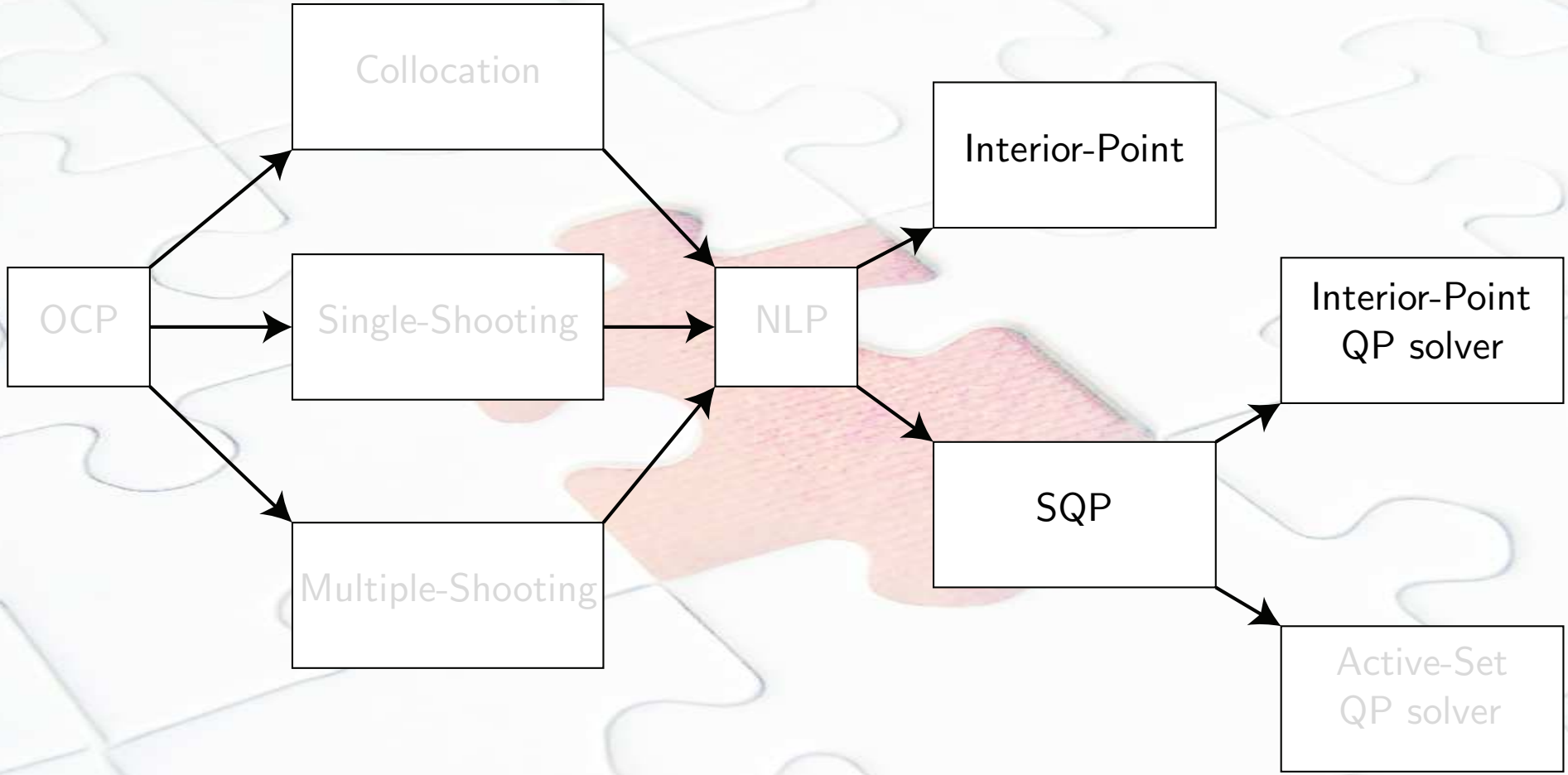

Newton - a general-purpose sledgehammer for algebraic equations...

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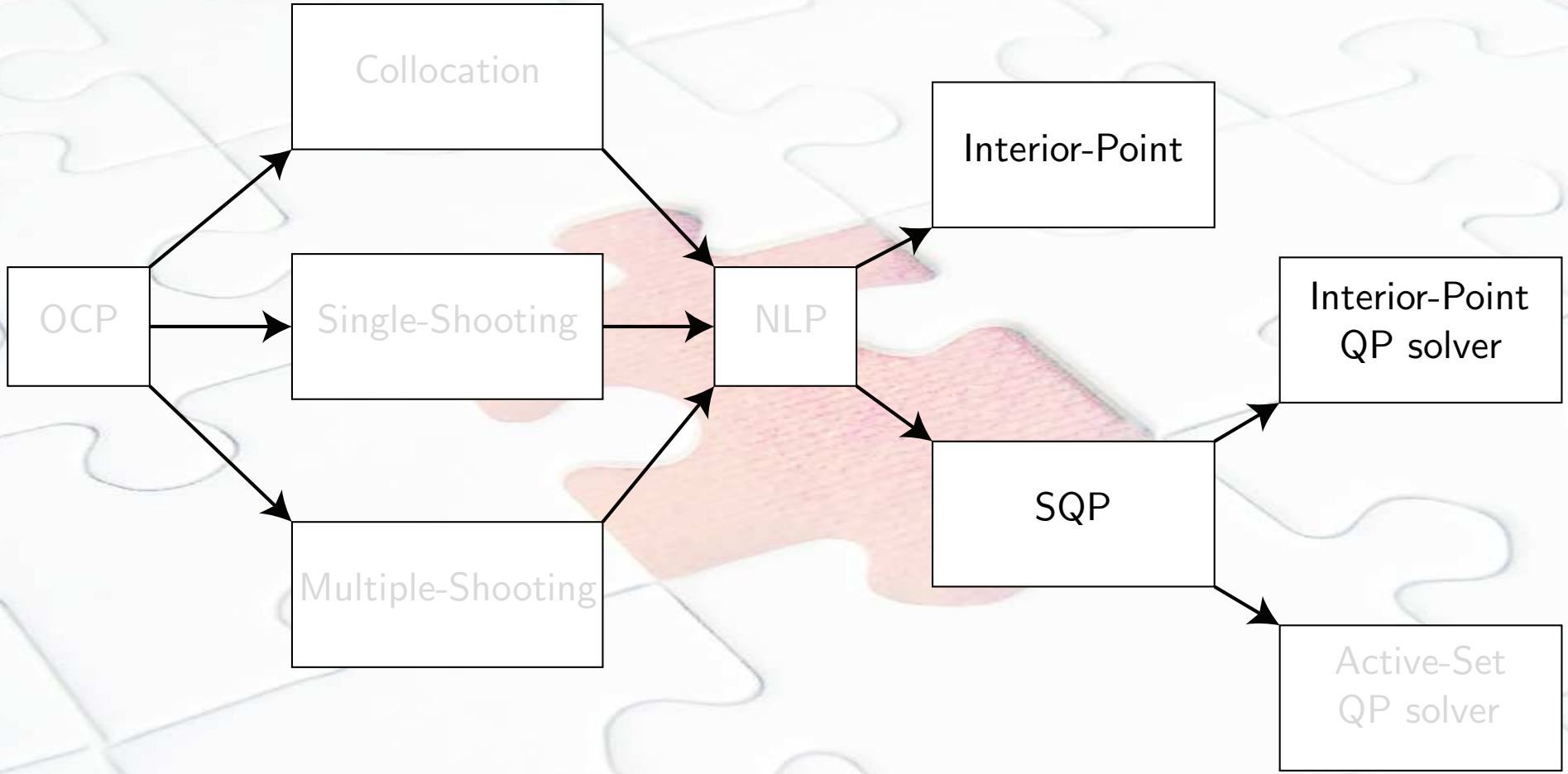

Newton - a general-purpose sledgehammer for algebraic equations...
... will be used to solve the KKT conditions !!

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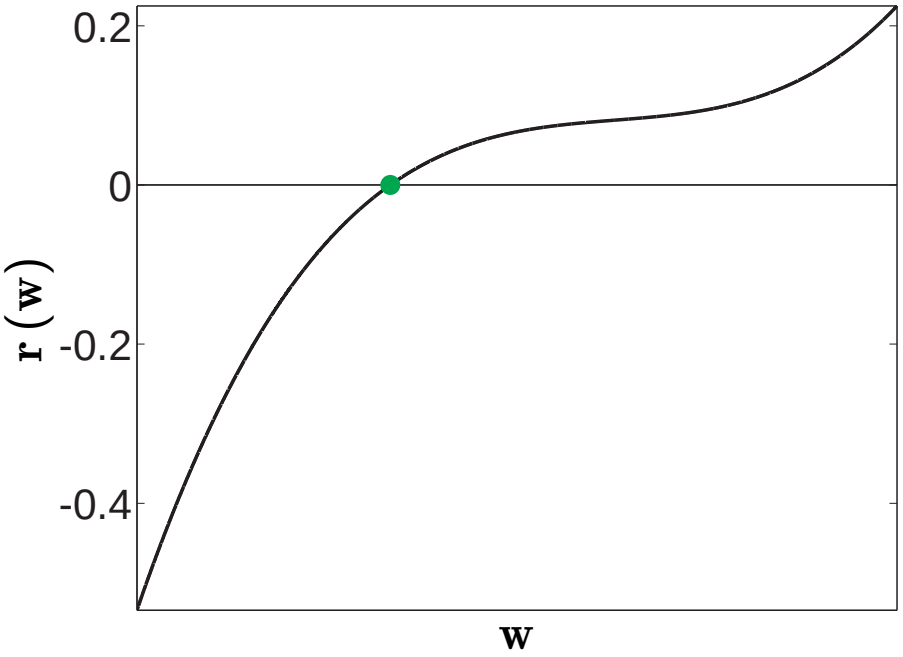
Goal: solve $\mathbf{r}(\mathbf{w}) = 0$... **how ?!?**



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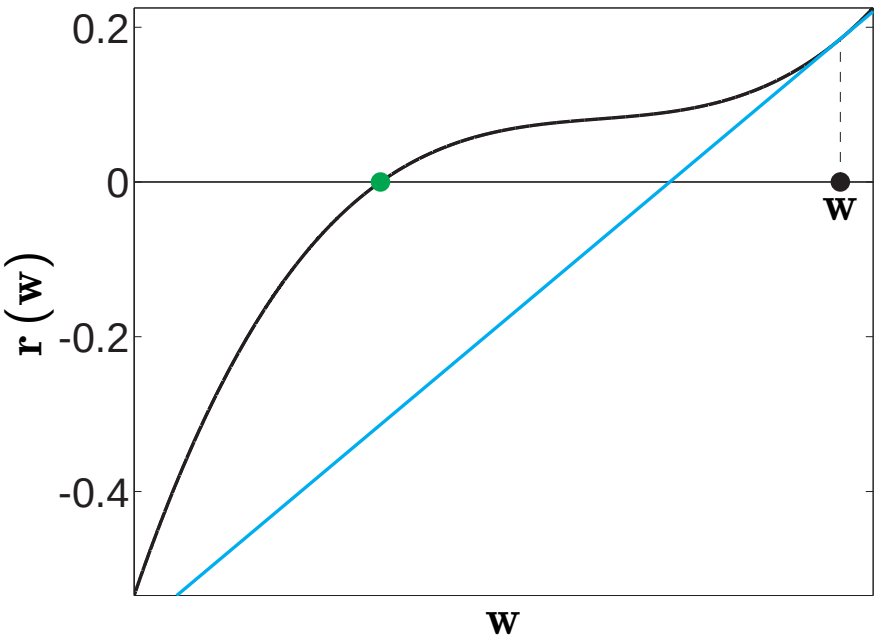

Key idea: guess $\mathbf{w}$, iterate the linear model:

$$\mathbf{r}(\mathbf{w} + \Delta\mathbf{w}) \approx \mathbf{r}(\mathbf{w}) + \nabla\mathbf{r}(\mathbf{w})^{\top} \Delta\mathbf{w} = 0$$

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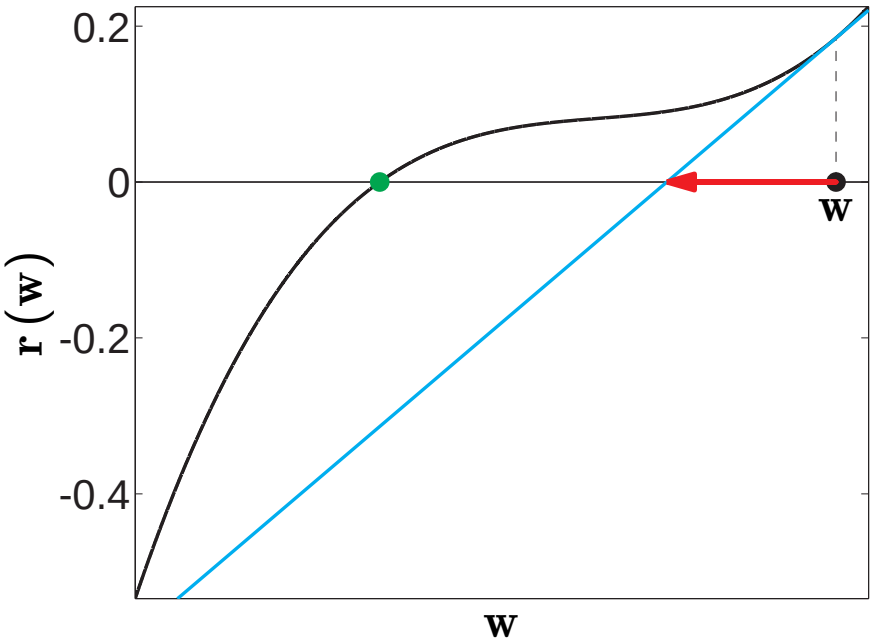

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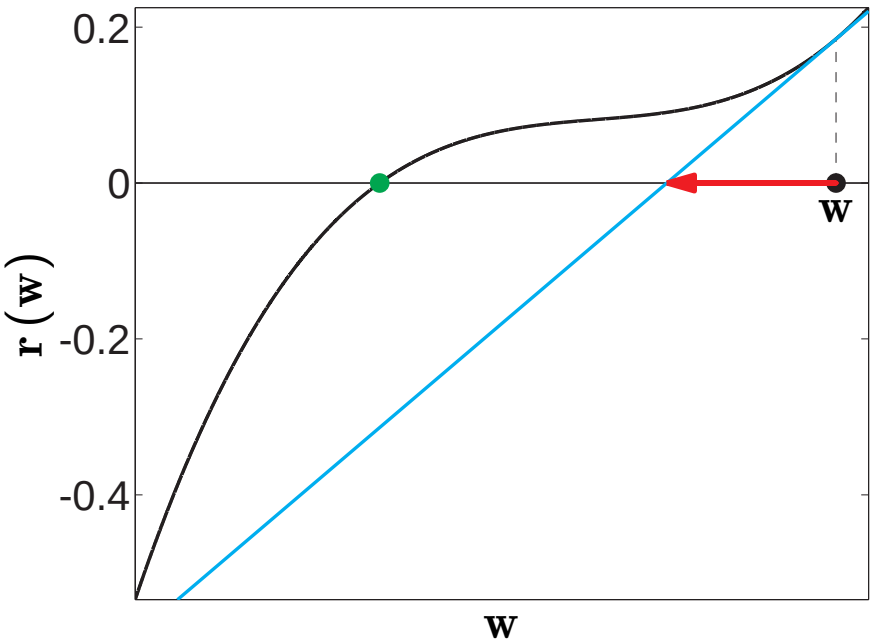

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Algorithm: Newton method

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$$\mathbf{r}(\mathbf{w}) \quad \text{and} \quad \nabla\mathbf{r}(\mathbf{w})$$

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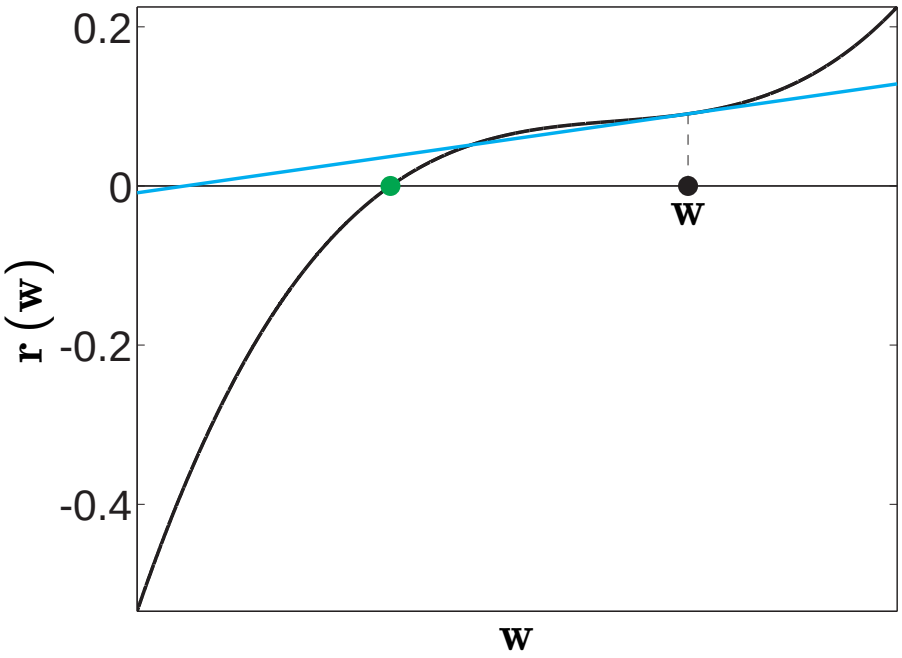

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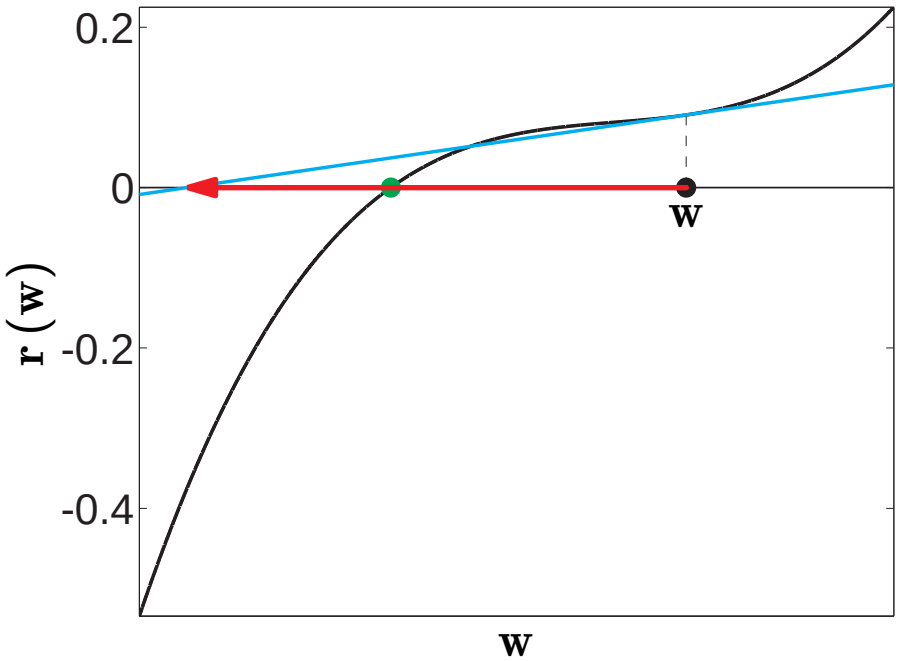

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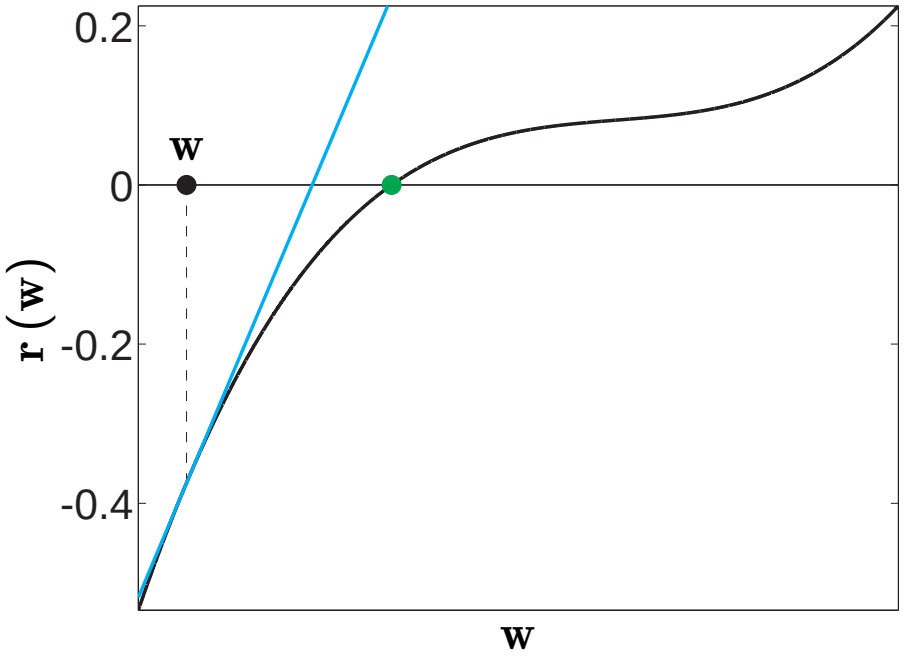

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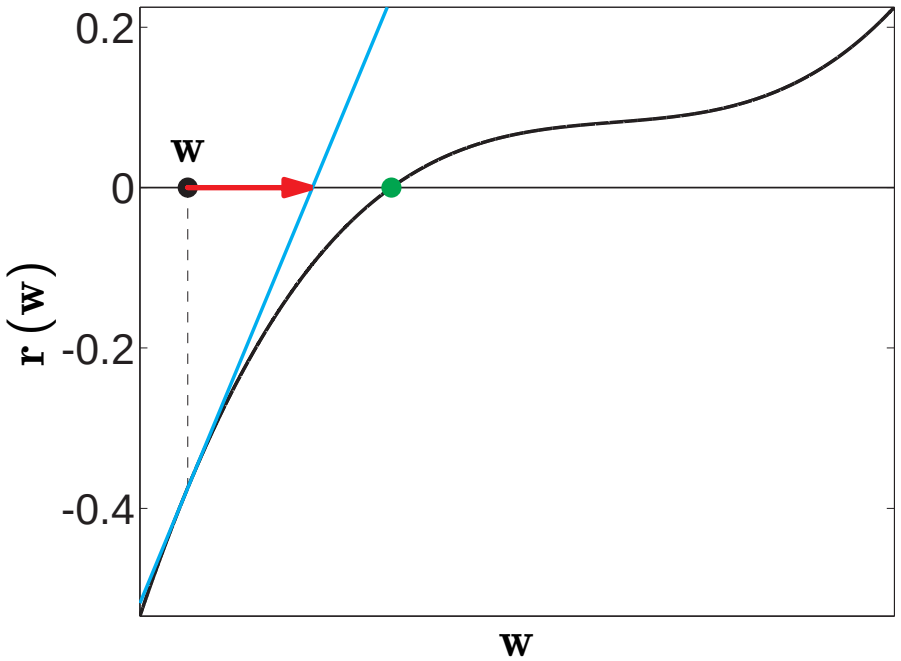

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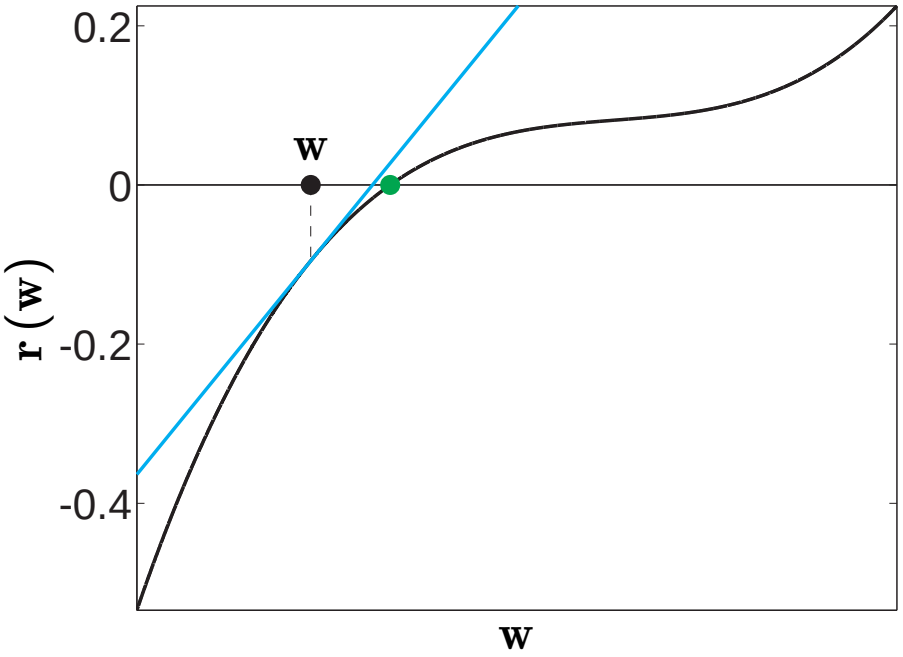

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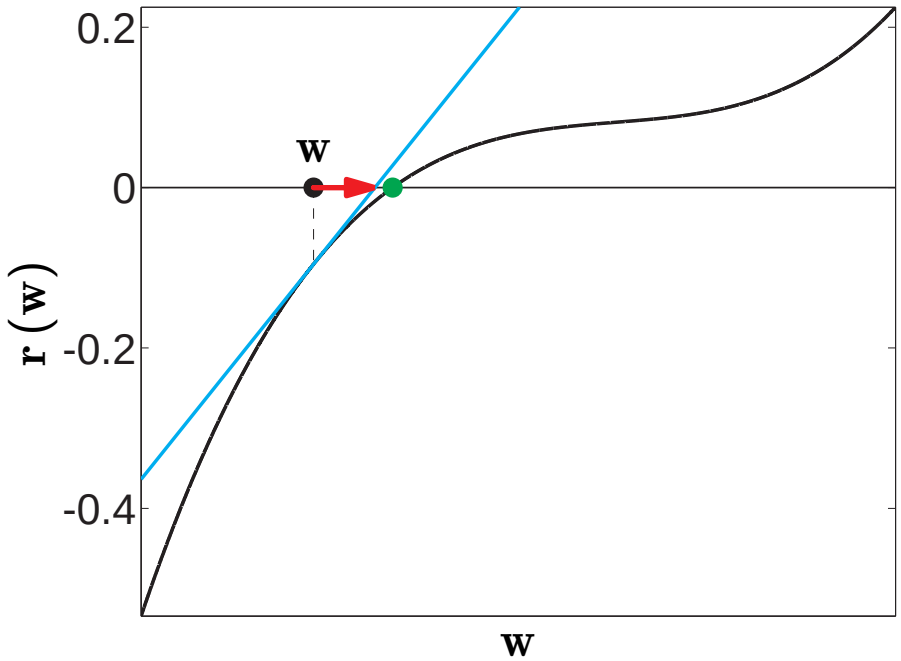

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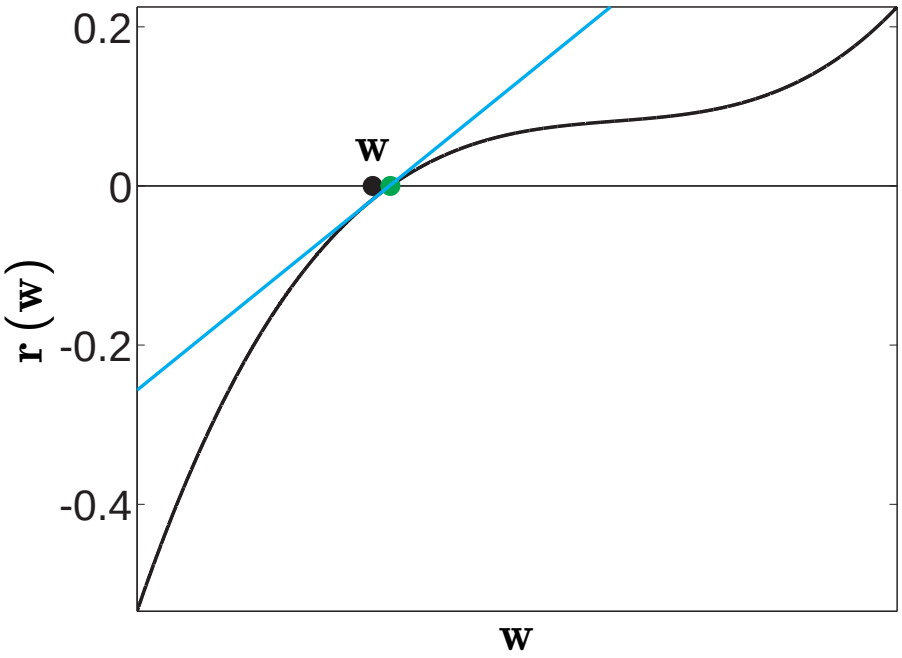

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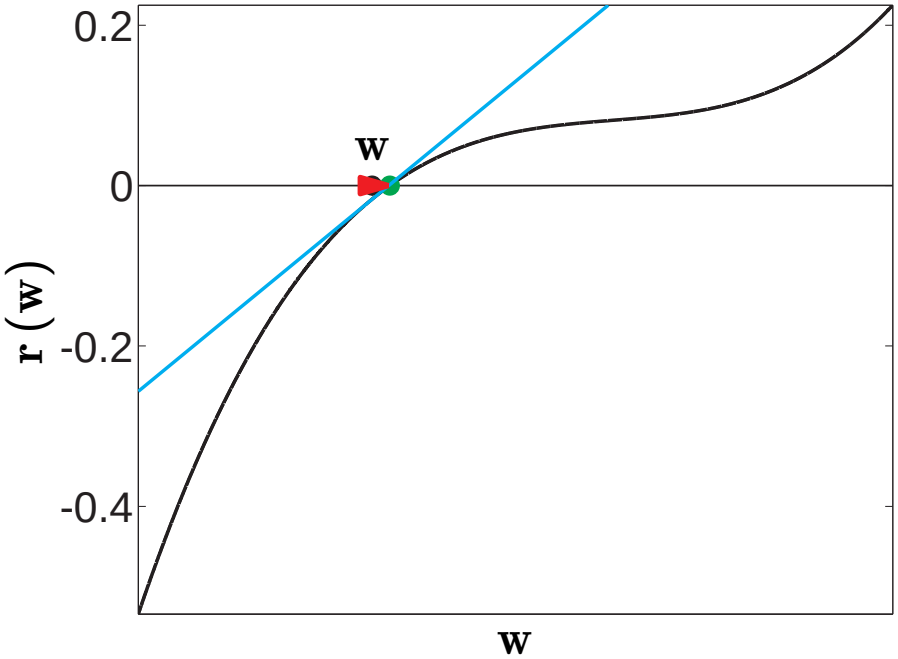

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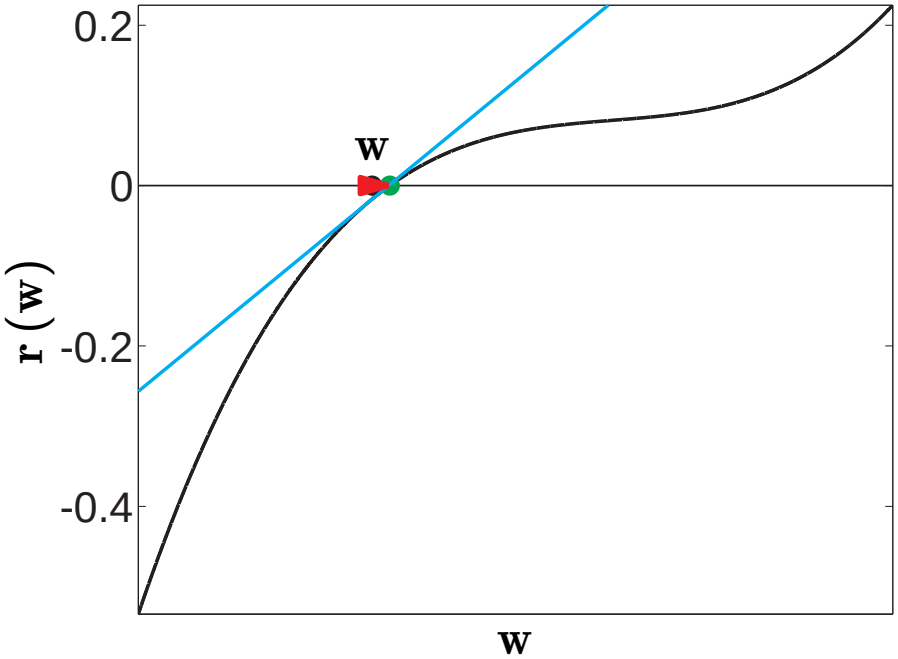

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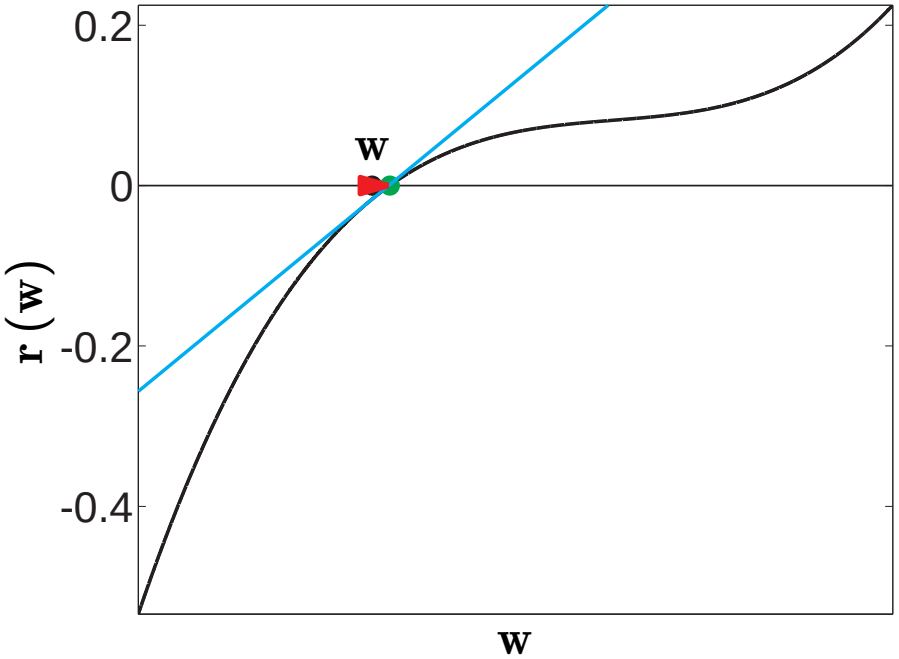

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Newton step, $t \in]0, 1]$

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- Reduced steps are often needed

Why reduced steps ?

Newton step with $t \in]0, 1]$:

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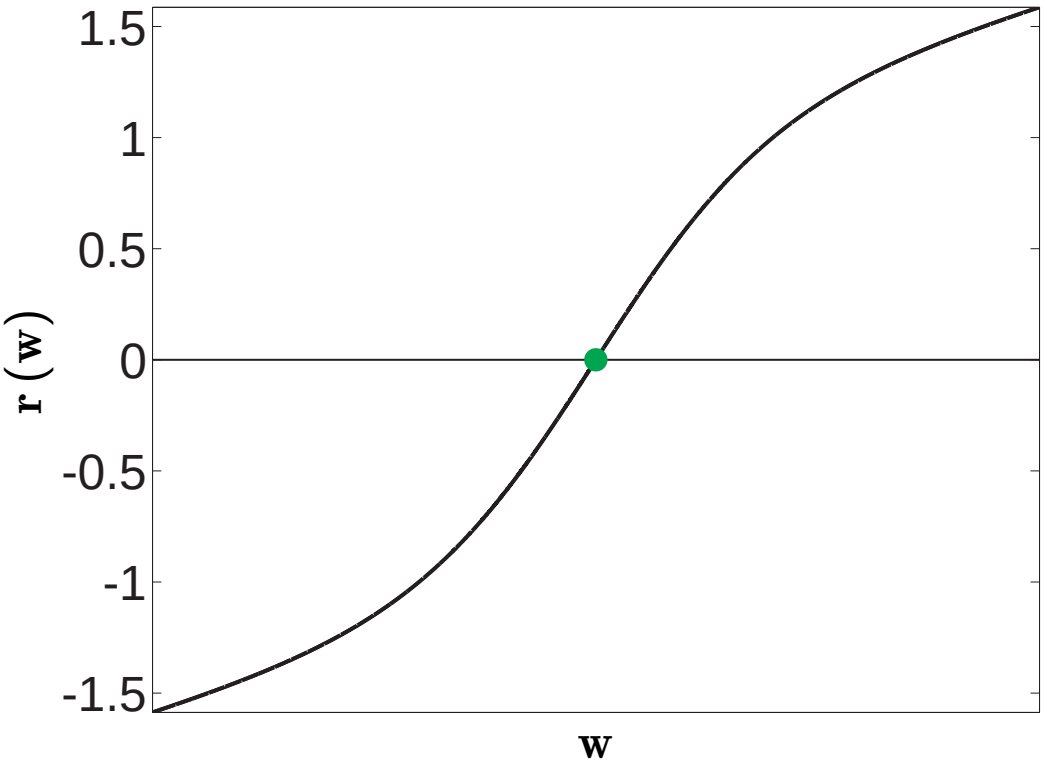

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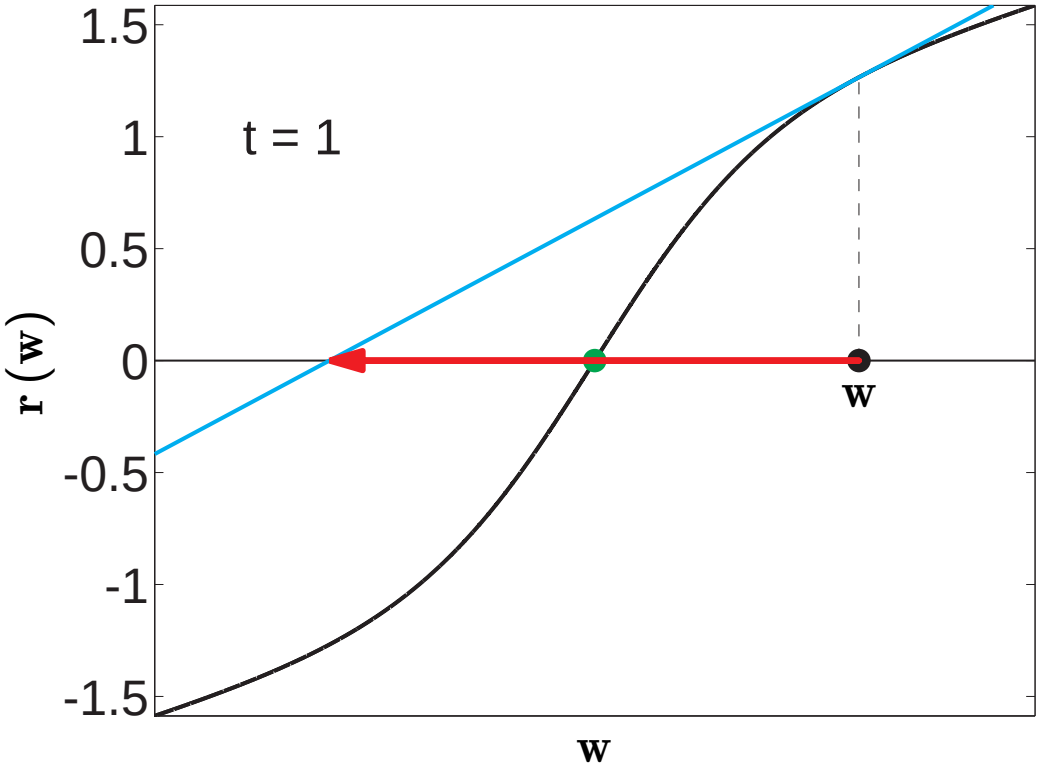

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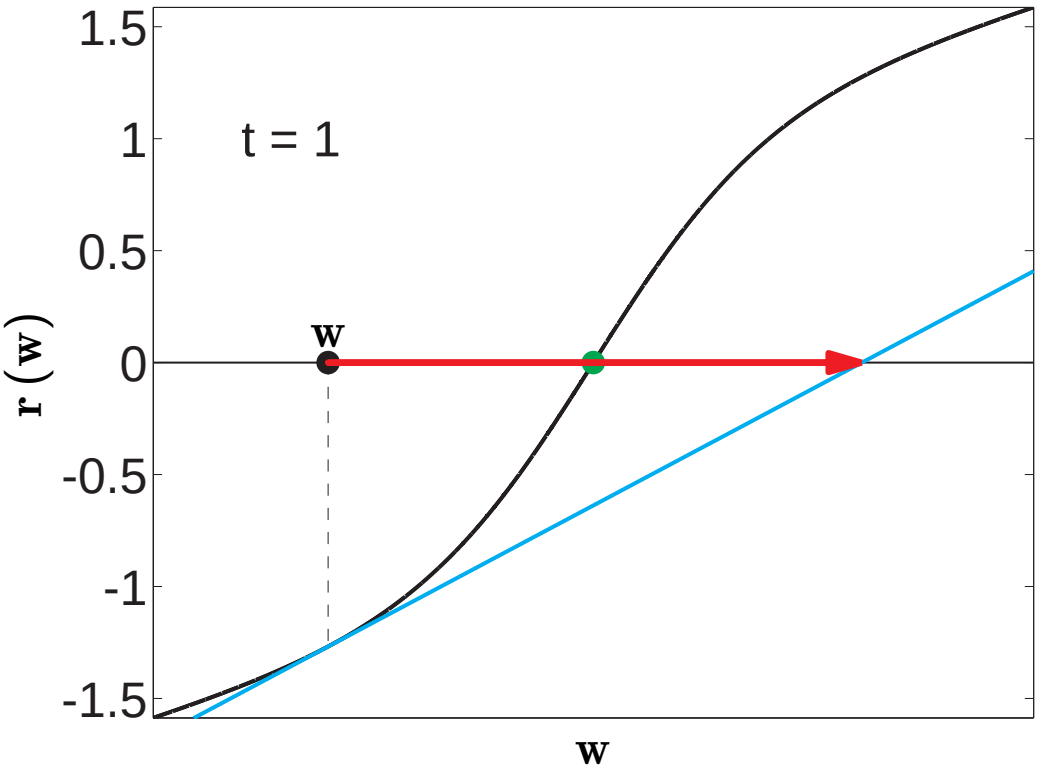

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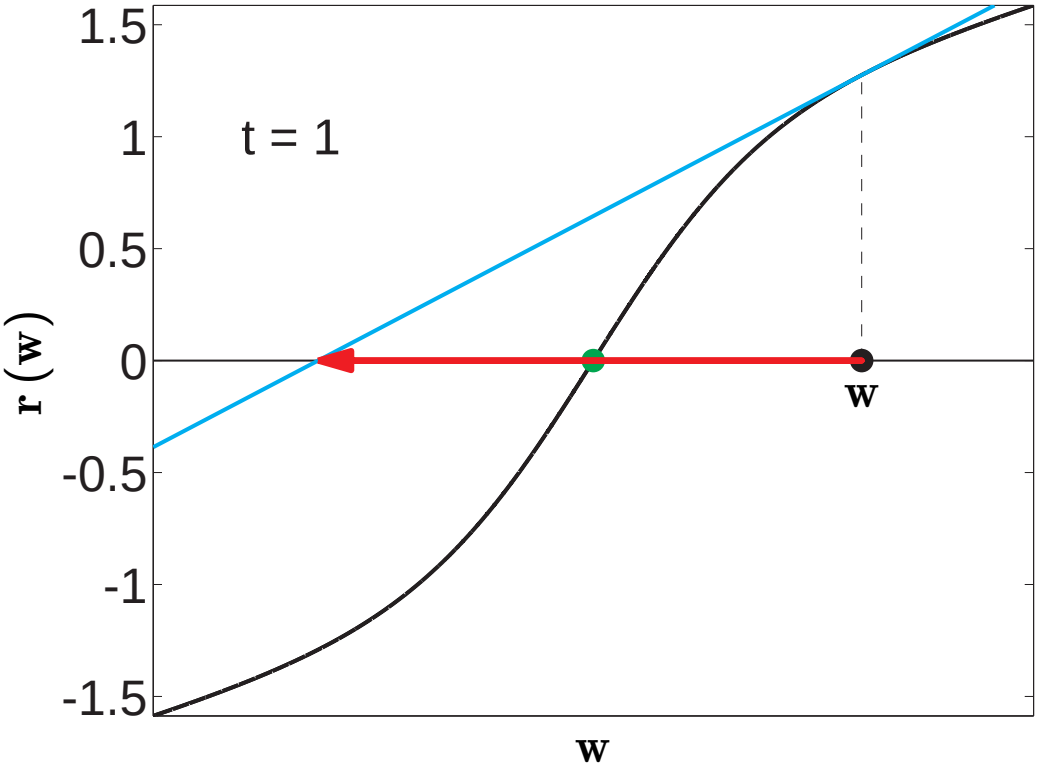

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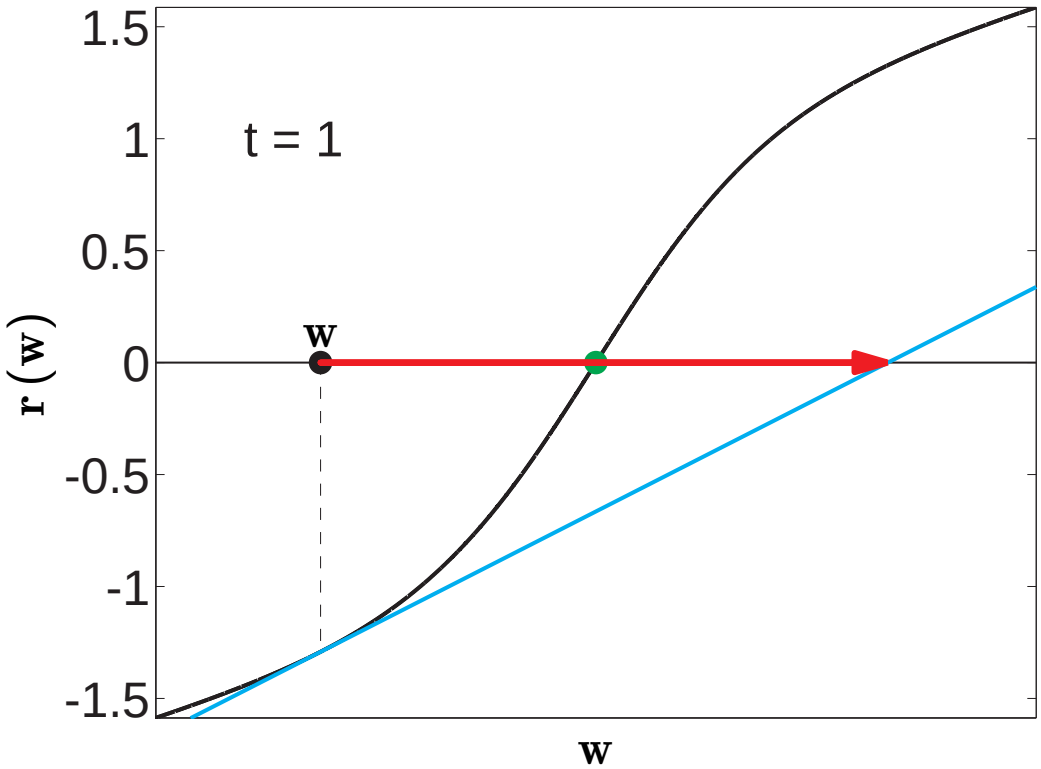

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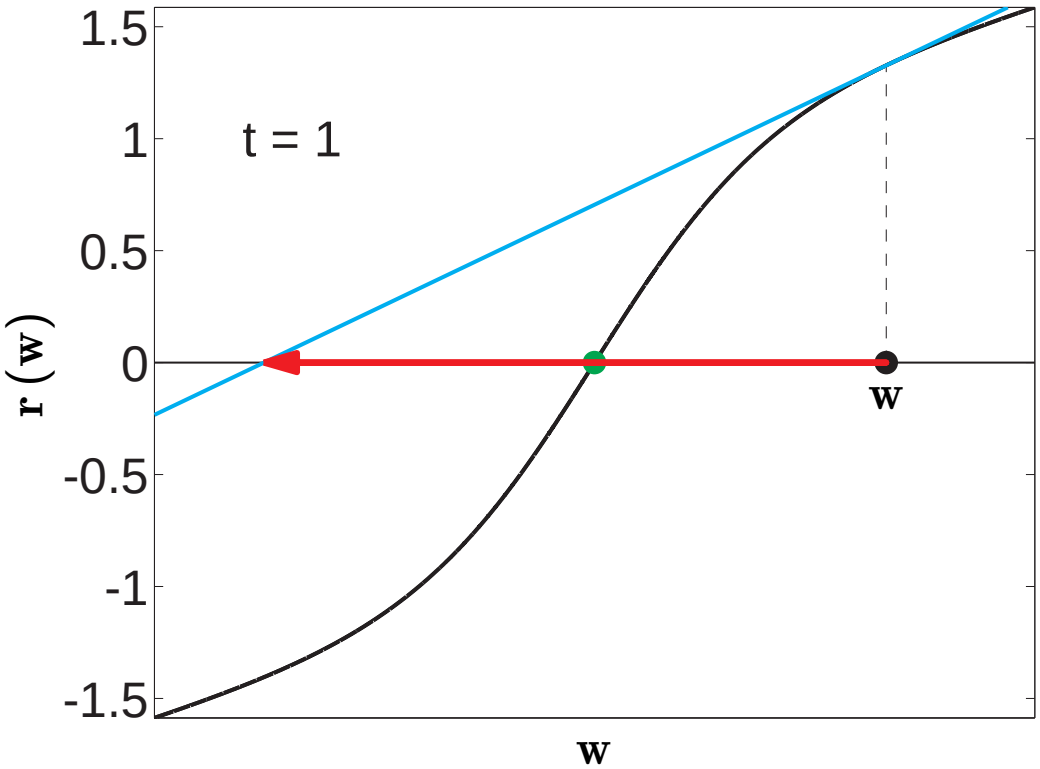

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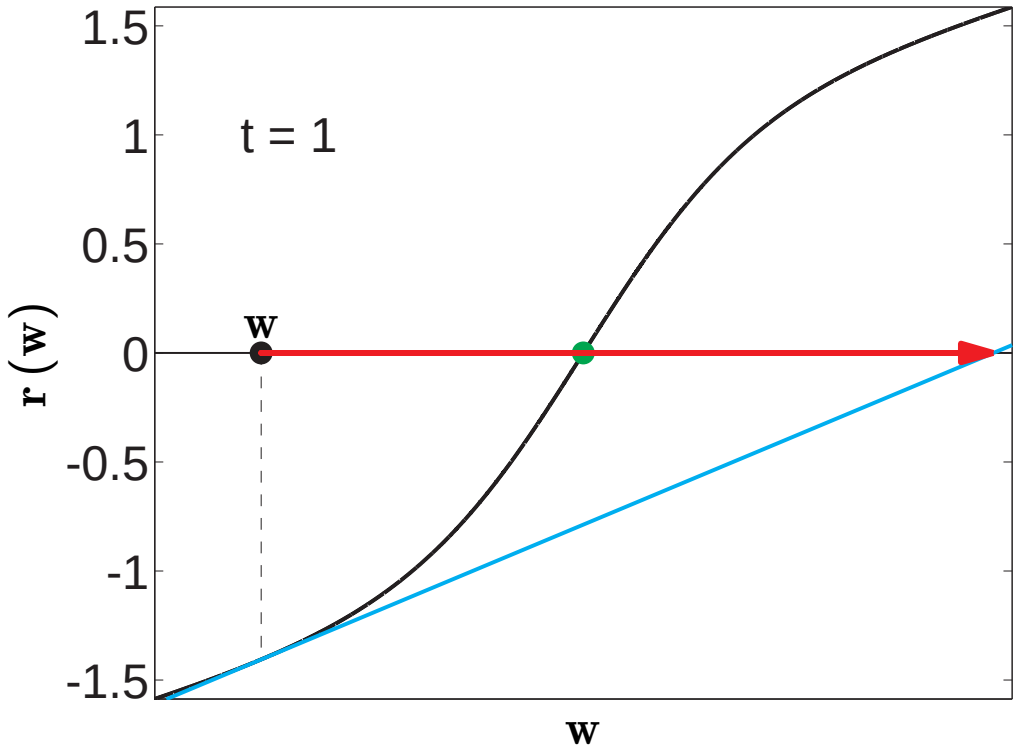

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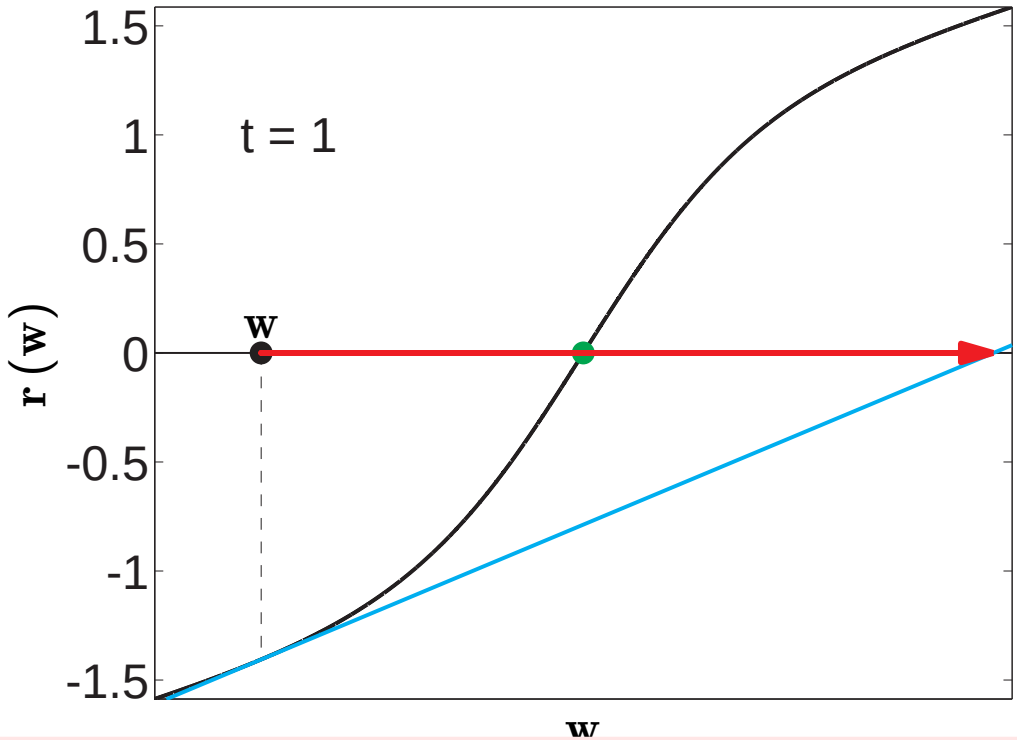

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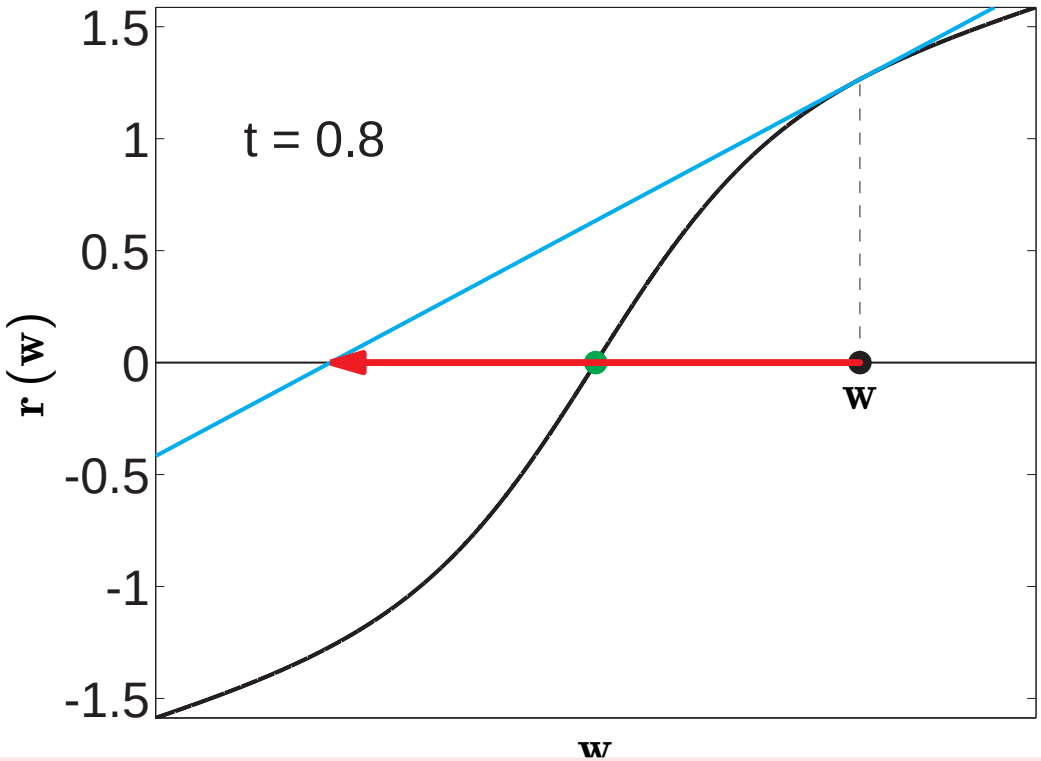

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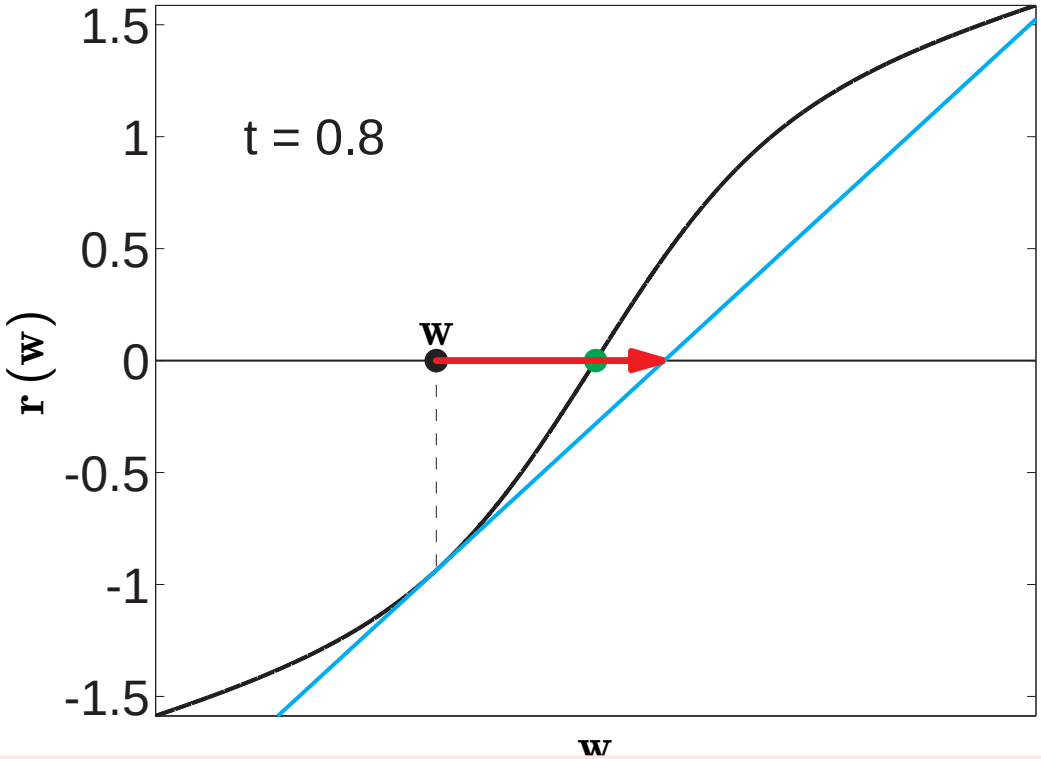

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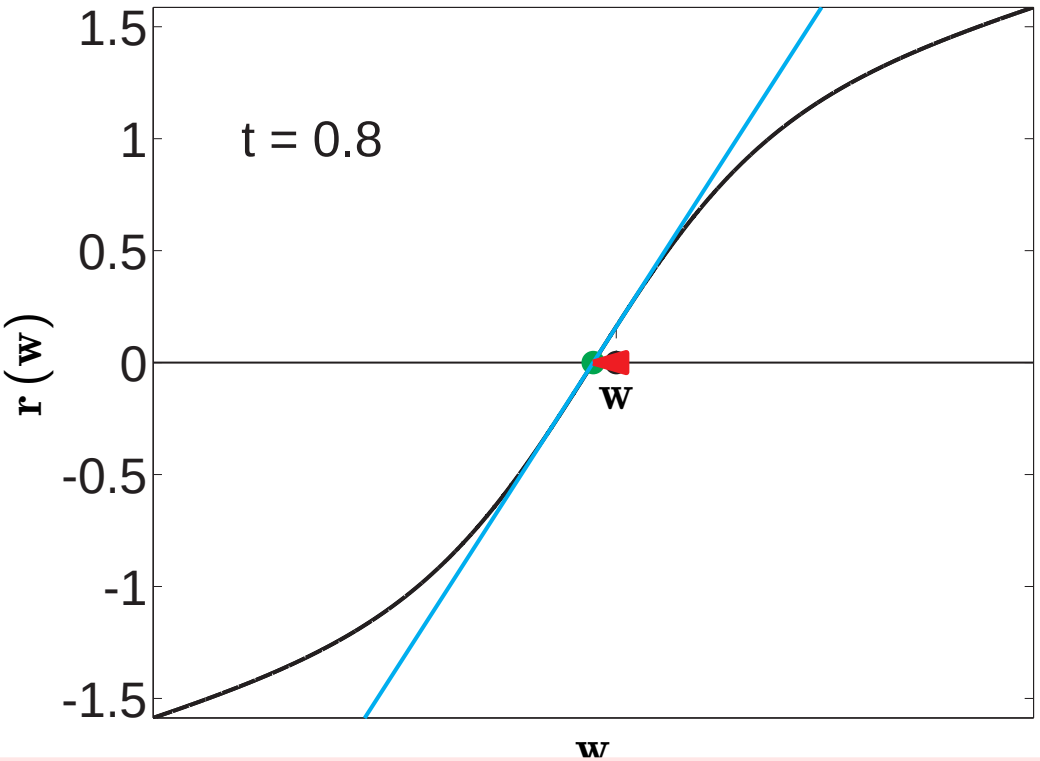

The full-step Newton iteration can be unstable !!

Why reduced steps ?

Newton step with $t \in]0, 1]$:

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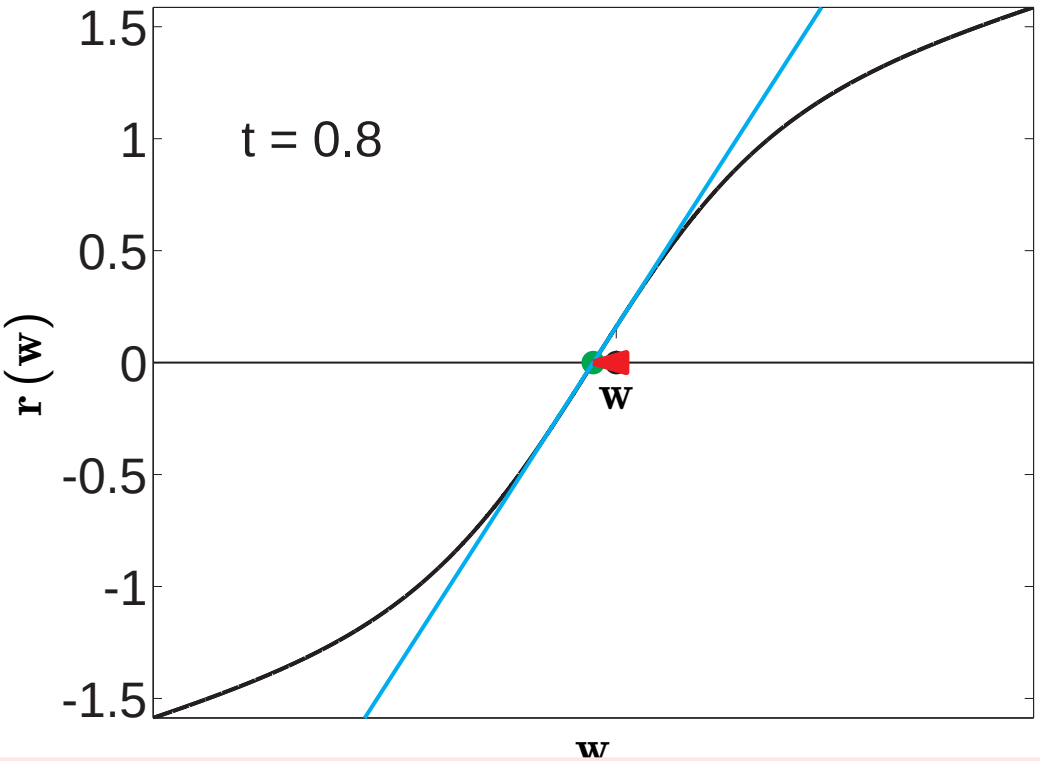

The full-step Newton iteration can be unstable !! Newton iteration with adequately reduced steps converges (does it ?)

Does Newton always work ?

Is there always a reduced Newton step $t\Delta\mathbf{w}$ "improving" $\mathbf{r}(\mathbf{w})$?

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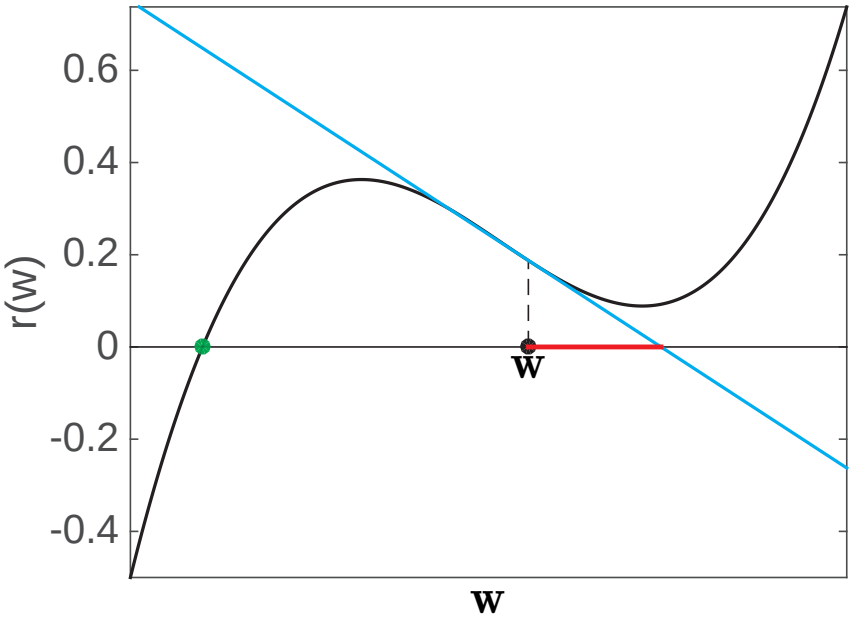
But still, Newton can fail...

Solve $\mathbf{r}(\mathbf{w}) = 0$



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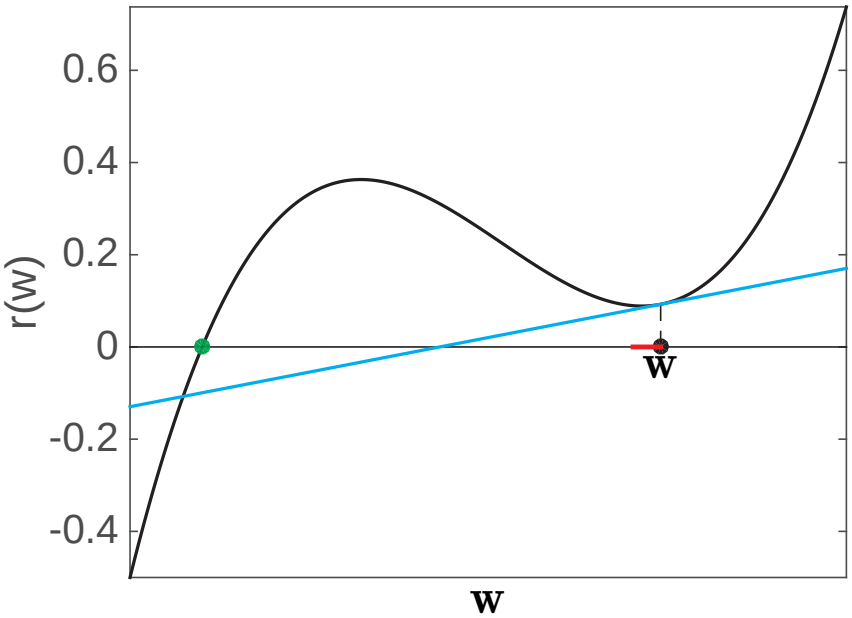

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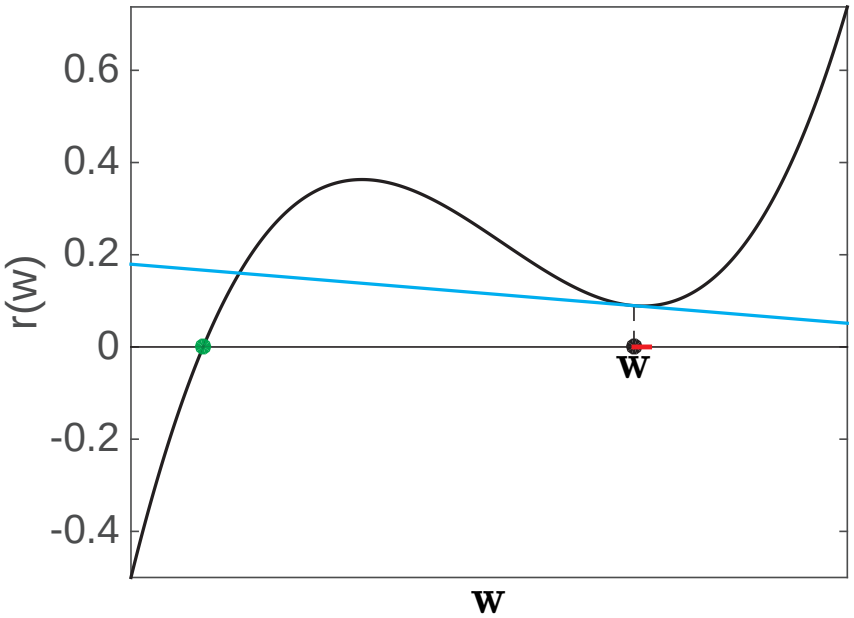

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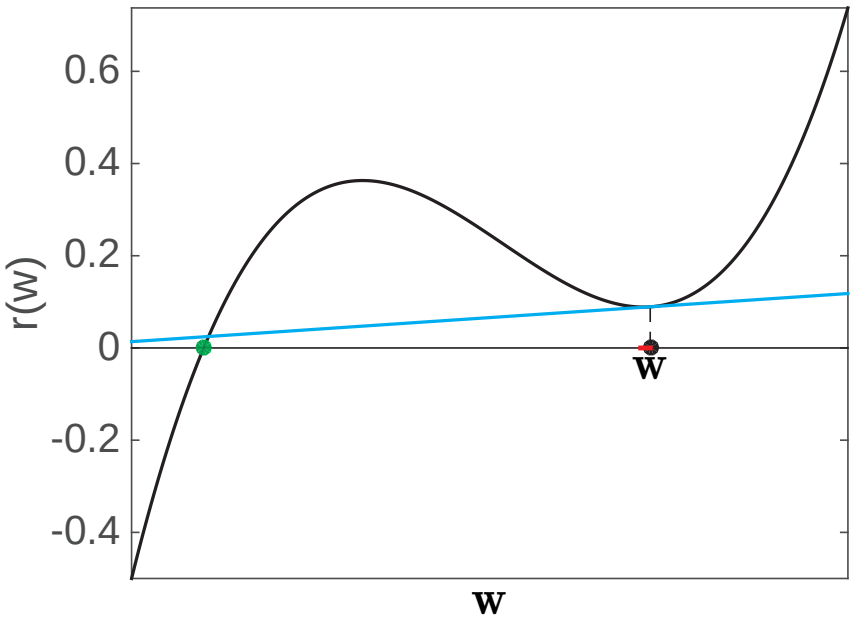

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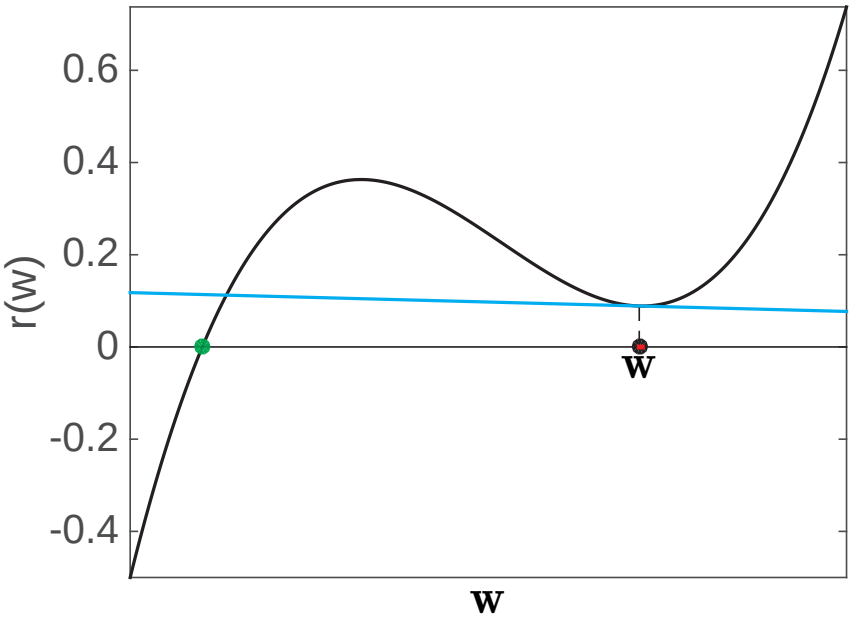

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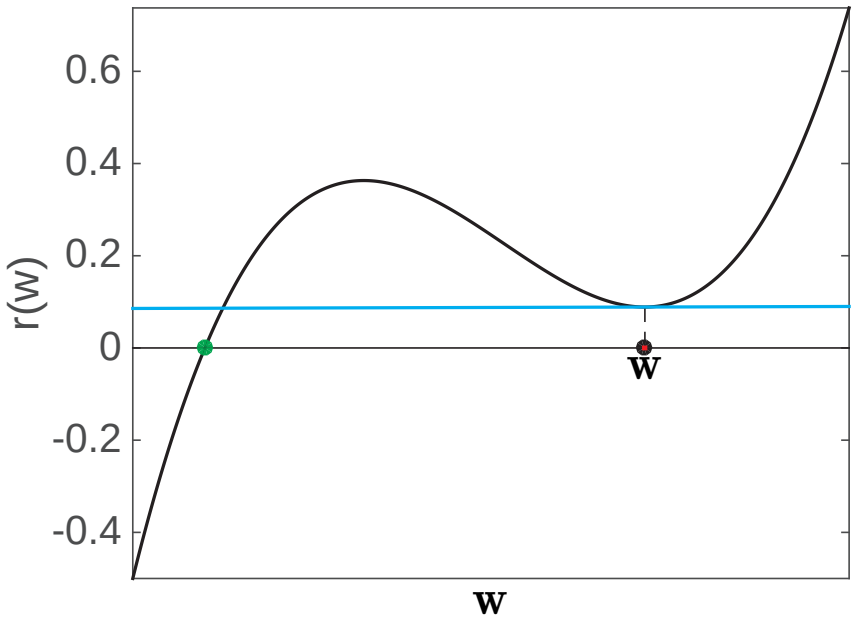

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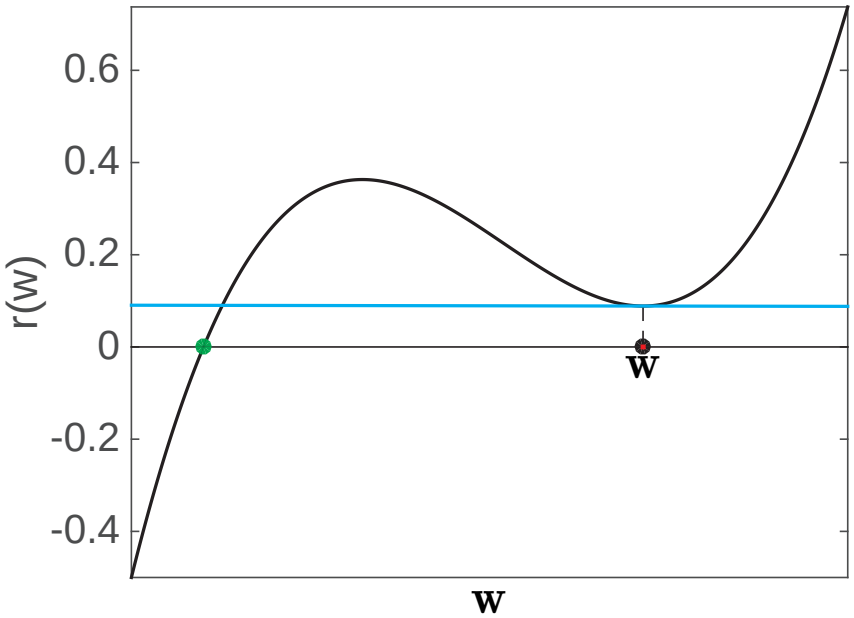

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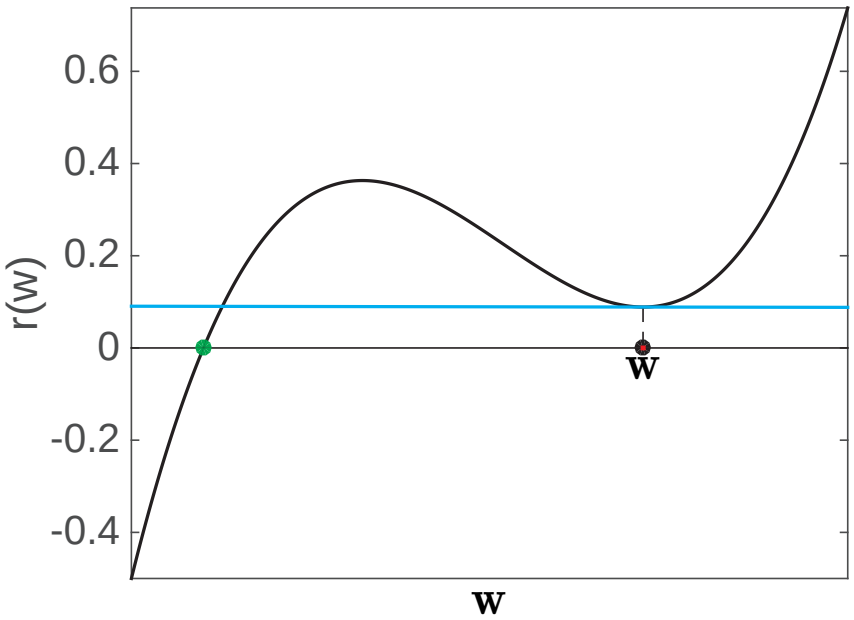

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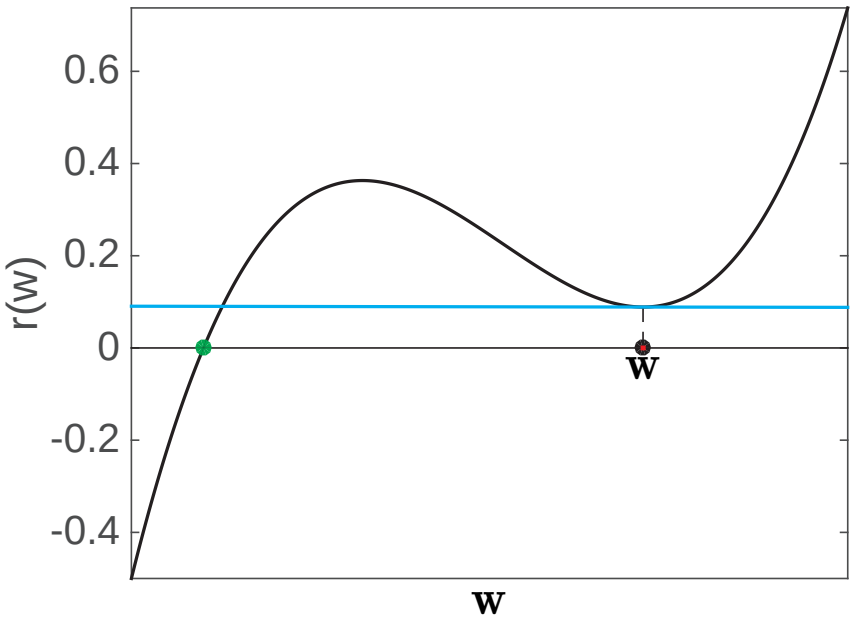

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Reduced-step Newton iteration converges to a solution of $\mathbf{r}(\mathbf{w}) = 0$ if $\nabla \mathbf{r}$ is full rank everywhere

Convergence of Newton methods & Inexact Jacobian

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Theorem: consider the Newton iteration $\mathbf{w}_{k+1} = \mathbf{w}_k - M_k^{-1}\mathbf{r}(\mathbf{w}_k)$ and assume

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Convergence of Newton methods

Theorem: consider the Newton iteration $\mathbf{w}_{k+1} = \mathbf{w}_k - M_k^{-1}\mathbf{r}(\mathbf{w}_k)$ and assume

- Lipschitz condition: $\|M_k^{-1}(\nabla \mathbf{r}(\mathbf{w})^\top - \nabla \mathbf{r}(\mathbf{w}^*))^\top\| \leq \omega \|\mathbf{w} - \mathbf{w}^*\|$
- Bound on the Jacobian approximation error $\|M_k^{-1}(\nabla \mathbf{r}(\mathbf{w}_k)^\top - M_k)\| \leq \kappa_k < \kappa < 1$
- Good initial guess $\|\mathbf{w}_0 - \mathbf{w}^*\| \leq \frac{2}{\omega}(1-\kappa)$

Then $\mathbf{w}_k \to \mathbf{w}^*$ with the following linear-quadratic contraction rate:

$$\|\mathbf{w}_{k+1} - \mathbf{w}^*\| \quad \leq \quad \left(\kappa_k + \frac{\omega}{2}\|\mathbf{w}_k - \mathbf{w}^*\|\right)\|\mathbf{w}_k - \mathbf{w}^*\|.$$

Proof

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Affine invariance of the (exact) Newton method

Affine change of coordinates

Consider: $\mathbf{w} = A\mathbf{v} + \mathbf{a}$ with $A \in \mathbb{R}^{n \times n}$ non-singular and $\mathbf{a} \in \mathbb{R}^n$.

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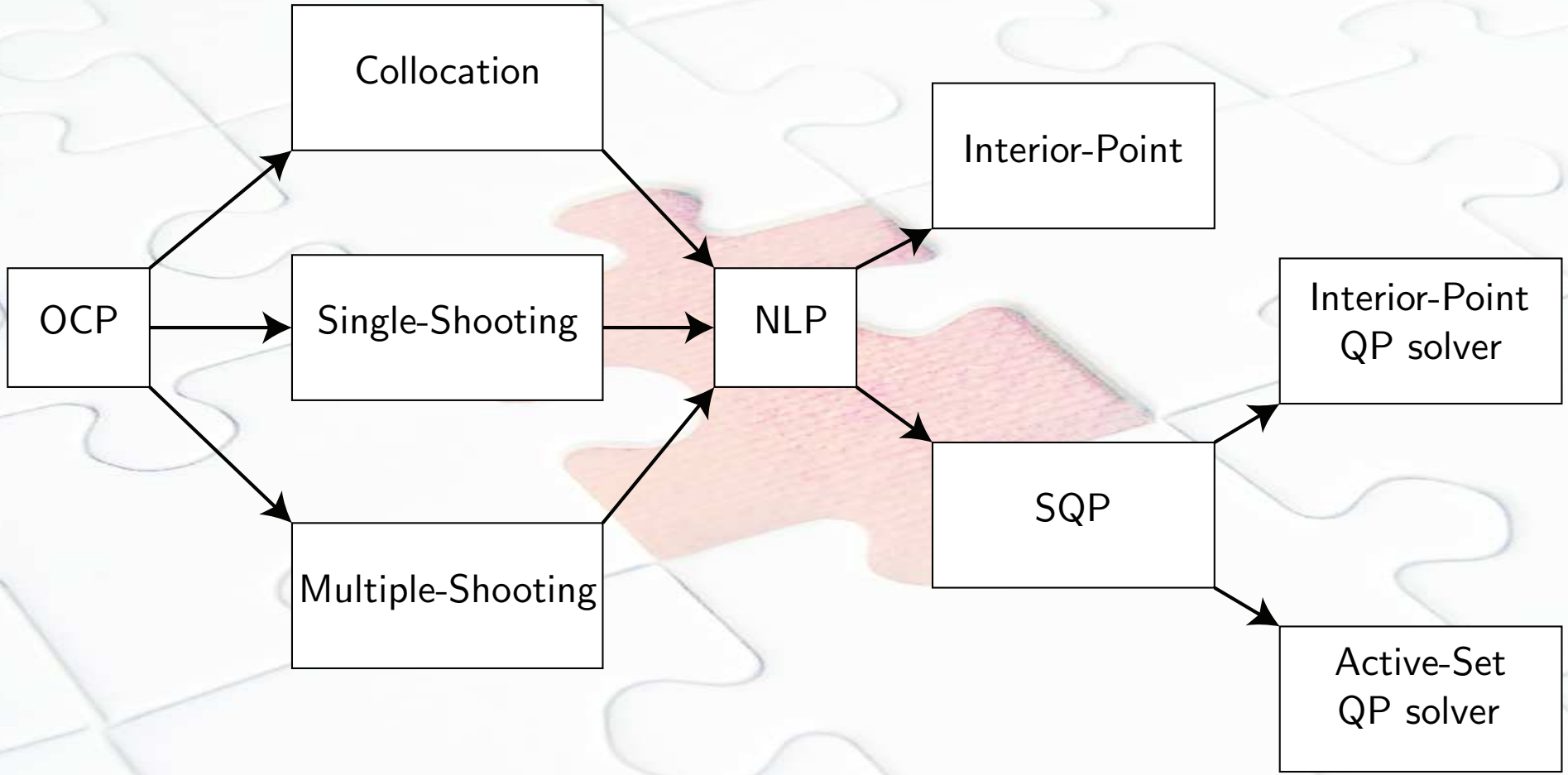
- **Rescaling** can still be very useful to **improve conditioning** of $\nabla_{\mathbf{w}} \mathbf{r}(\mathbf{w})$

Survival map of Direct Optimal Control



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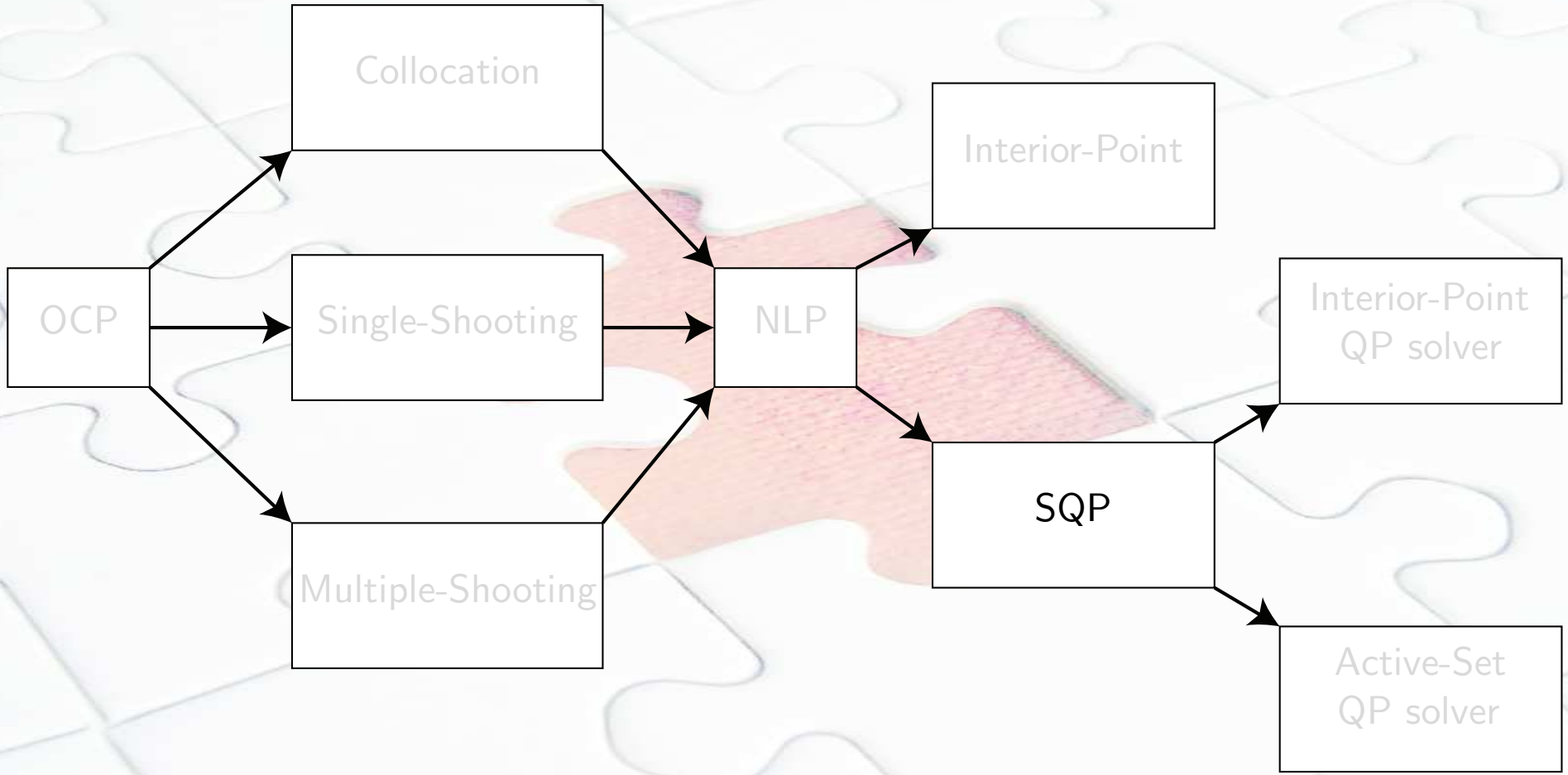

Let's approach the problem of solving the KKT conditions

Outline

1. The Newton method
2. Newton on the KKT conditions
3. The reduced Newton step (unconstrained problems)
4. The merit function - Line-search for constrained problems
5. Newton-type methods
6. Sequential Quadratic Programming

Core idea

A vast majority of solvers try to find a point $\mathbf{w}$, $\boldsymbol{\mu}$, $\boldsymbol{\lambda}$ satisfying the KKT conditions:

Primal Feasibility:	$\mathbf{g}(\mathbf{w}) = 0, \quad \mathbf{h}(\mathbf{w}) \leq 0,$
Dual Feasibility:	$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\mu}, \boldsymbol{\lambda}) = 0, \quad \boldsymbol{\mu} \geq 0,$
Complementarity Slackness:	$\mu_i \mathbf{h}_i(\mathbf{w}) = 0, \quad i = 1, \ldots$

where $\mathcal{L} = \Phi(\mathbf{w}) + \boldsymbol{\lambda}^{\top} \mathbf{g}(\mathbf{w}) + \boldsymbol{\mu}^{\top} \mathbf{h}(\mathbf{w})$

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Let's consider *for now* equality constrained problems, i.e. find $\mathbf{w}, \boldsymbol{\lambda}$ s.t.:

$$\begin{aligned} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) &= 0 \\ \mathbf{g}(\mathbf{w}) &= 0 \end{aligned}$$

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Idea: apply the Newton method on the KKT conditions, i.e.

Solve...

$$\mathbf{r}(\mathbf{w}, \boldsymbol{\lambda}) = \begin{bmatrix} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix} = 0$$

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... by iterating

$$\nabla \mathbf{r}(\mathbf{w}, \boldsymbol{\lambda})^{\top} \begin{bmatrix} \Delta \mathbf{w} \\ \Delta \boldsymbol{\lambda} \end{bmatrix} = -\mathbf{r}(\mathbf{w}, \boldsymbol{\lambda})$$

Newton method on the KKT conditions

KKT conditions:

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Newton iteration:

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Newton direction:

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Newton iteration:

$$\nabla \mathbf{r}\left(\mathbf{w}, \boldsymbol{\lambda}\right)^{\top} \begin{bmatrix} \Delta \mathbf{w} \\ \Delta \boldsymbol{\lambda} \end{bmatrix} = -\mathbf{r}\left(\mathbf{w}, \boldsymbol{\lambda}\right)$$

Newton direction: using $\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) = \nabla \Phi(\mathbf{w}) + \nabla \mathbf{g}(\mathbf{w}) \boldsymbol{\lambda}$

$$\begin{array}{rcll} \nabla_{\mathbf{w}}^2 \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) \Delta \mathbf{w} & + & \nabla \mathbf{g}(\mathbf{w}) \left(\boldsymbol{\lambda} + \Delta \boldsymbol{\lambda}\right) & = & -\nabla \Phi(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} \Delta \mathbf{w} & & & = & -\mathbf{g}(\mathbf{w}) \end{array}$$

Newton method on the KKT conditions

KKT conditions:

$$\begin{aligned} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) &= 0 \\ \mathbf{g}(\mathbf{w}) &= 0 \end{aligned}$$

Newton iteration:

$$\nabla \mathbf{r}(\mathbf{w}, \boldsymbol{\lambda})^{\top} \begin{bmatrix} \Delta \mathbf{w} \\ \Delta \boldsymbol{\lambda} \end{bmatrix} = -\mathbf{r}(\mathbf{w}, \boldsymbol{\lambda})$$

Newton direction: using $\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) = \nabla \Phi(\mathbf{w}) + \nabla \mathbf{g}(\mathbf{w}) \boldsymbol{\lambda}$

$$\begin{array}{rcl} \nabla_{\mathbf{w}}^2 \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) \Delta \mathbf{w} + \nabla \mathbf{g}(\mathbf{w}) (\boldsymbol{\lambda} + \Delta \boldsymbol{\lambda}) &=& -\nabla \Phi(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} \Delta \mathbf{w} &=& -\mathbf{g}(\mathbf{w}) \end{array}$$

The Newton direction on the KKT conditions

$$\begin{bmatrix} \nabla_{\mathbf{w}}^2 \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) & \nabla \mathbf{g}(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda} + \Delta \boldsymbol{\lambda} \end{bmatrix} = - \begin{bmatrix} \nabla \Phi(\mathbf{w}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix}$$

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Newton direction: using $\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) = \nabla \Phi(\mathbf{w}) + \nabla \mathbf{g}(\mathbf{w}) \boldsymbol{\lambda}$

$$\begin{array}{rcrcl} \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) \Delta \mathbf{w} & + & \nabla \mathbf{g}(\mathbf{w}) (\boldsymbol{\lambda} + \Delta \boldsymbol{\lambda}) & = & -\nabla \Phi(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} \Delta \mathbf{w} & & & = & -\mathbf{g}(\mathbf{w}) \end{array}$$

The Newton direction on the KKT conditions

$$\underbrace{\begin{bmatrix} H(\mathbf{w}, \boldsymbol{\lambda}) & \nabla \mathbf{g}(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} & 0 \end{bmatrix}}_{\text{KKT matrix (symmetric indefinite)}} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda} + \Delta \boldsymbol{\lambda} \end{bmatrix} = - \begin{bmatrix} \nabla \Phi(\mathbf{w}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix}$$

where $H(\mathbf{w}, \boldsymbol{\lambda}) = \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda})$ is the Hessian of the problem.

Newton method on the KKT conditions

KKT conditions:

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- In the following, we label $\boldsymbol{\lambda}^{+} = \boldsymbol{\lambda} + \Delta \boldsymbol{\lambda}$ (full dual Newton step)

Newton method on the KKT conditions

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- In the following, we label $\boldsymbol{\lambda}^{+} = \boldsymbol{\lambda} + \Delta \boldsymbol{\lambda}$ (full dual Newton step)
- $\mathcal{L}(\mathbf{w}, \boldsymbol{\lambda})$ enters only in the Hessian !

Newton method on the KKT conditions

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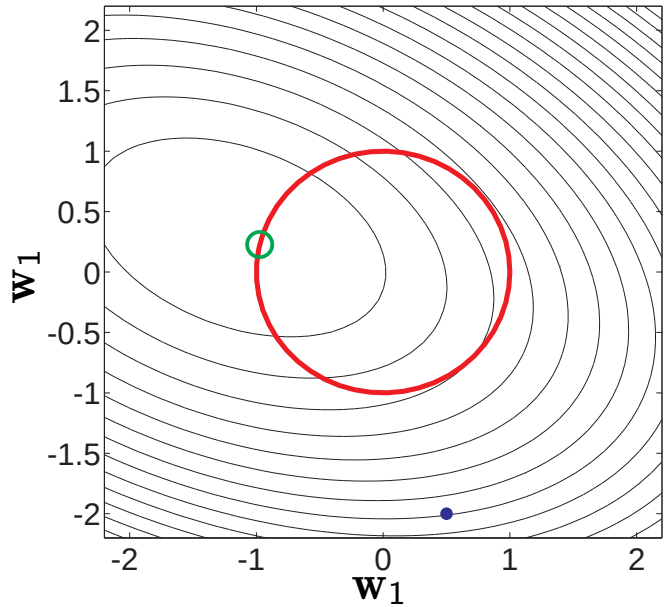
where $H(\mathbf{w}, \boldsymbol{\lambda}) = \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda})$ is the Hessian of the problem.

- In the following, we label $\boldsymbol{\lambda}^{+} = \boldsymbol{\lambda} + \Delta \boldsymbol{\lambda}$ (full dual Newton step)
- $\mathcal{L}(\mathbf{w}, \boldsymbol{\lambda})$ enters only in the Hessian !
- The updated multiplier $\boldsymbol{\lambda}^{+}$ is readily provided...

Newton Iteration for Optimization - Example

$$\min_{\mathbf{w}} \frac{1}{2}\mathbf{w}^T \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} \mathbf{w} + \mathbf{w}^T \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\text{s.t. } g(\mathbf{w}) = \mathbf{w}^T\mathbf{w} - 1 = 0$$



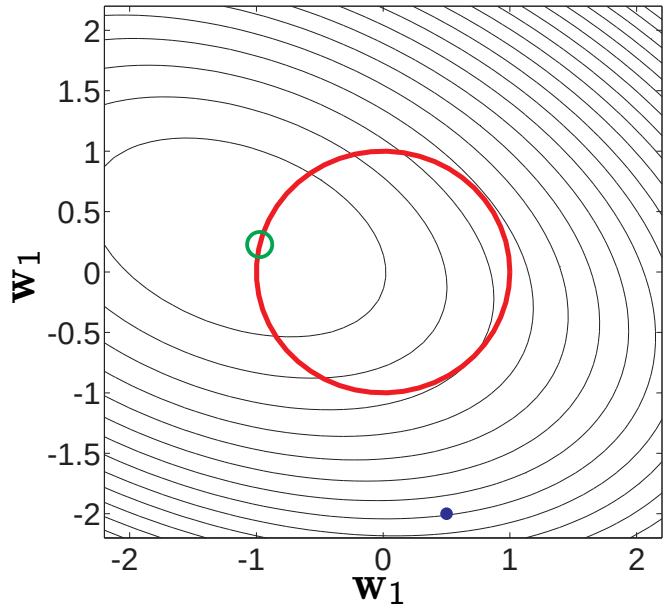
Newton Iteration for Optimization - Example

Iterate:

$$\begin{bmatrix} H & \nabla \mathbf{g} \\ \nabla \mathbf{g}^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda}^{+} \end{bmatrix} = - \begin{bmatrix} \nabla \Phi \\ \mathbf{g} \end{bmatrix}$$

$$\min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^{\mathsf{T}} \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} \mathbf{w} + \mathbf{w}^{\mathsf{T}} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\text{s.t. } g(\mathbf{w}) = \mathbf{w}^{\mathsf{T}} \mathbf{w} - 1 = 0$$



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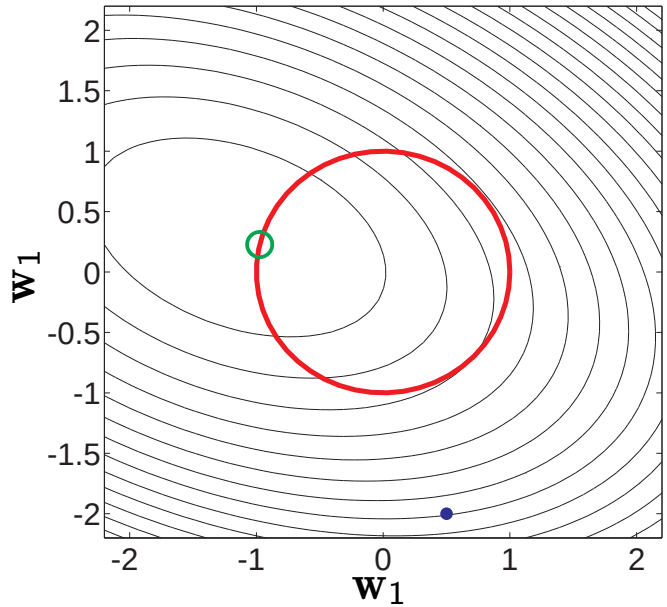
with:

$$\nabla g(\mathbf{w}) = 2\mathbf{w} = \begin{bmatrix} 2\mathbf{w}_1 \\ 2\mathbf{w}_2 \end{bmatrix}$$

$$\min_{\mathbf{w}} \frac{1}{2}\mathbf{w}^{\mathsf{T}} \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} \mathbf{w} + \mathbf{w}^{\mathsf{T}} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\text{s.t. } g(\mathbf{w}) = \mathbf{w}^{\mathsf{T}}\mathbf{w} - 1 = 0$$



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$$\mathcal{L}(\mathbf{w}, \lambda) = \Phi(\mathbf{w}) + \lambda g(\mathbf{w})$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \lambda) = \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} \mathbf{w} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 2\lambda \mathbf{w}$$

$$\min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^{\mathsf{T}} \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} \mathbf{w} + \mathbf{w}^{\mathsf{T}} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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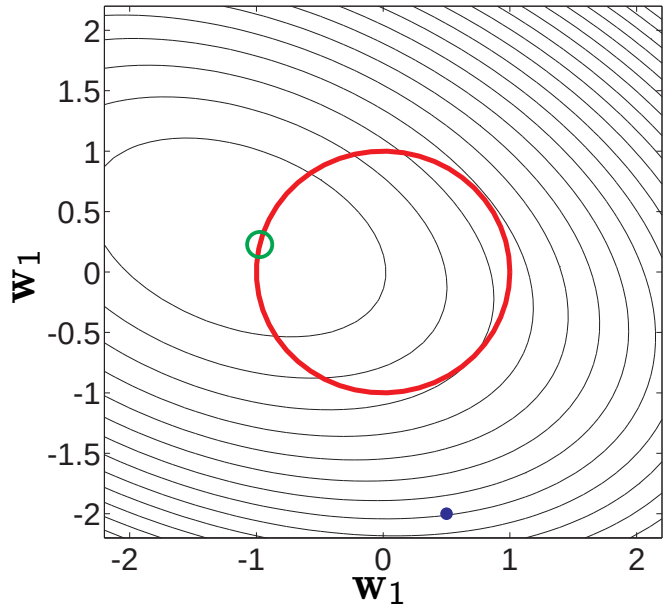


Newton Iteration for Optimization - Example

Iterate:

$$\begin{bmatrix} H & \nabla g \\ \nabla g^T & 0 \end{bmatrix} \begin{bmatrix} \Delta w \\ \lambda^+ \end{bmatrix} = - \begin{bmatrix} \nabla \Phi \\ g \end{bmatrix}$$

with:

$$\nabla g(w) = 2w = \begin{bmatrix} 2w_1 \\ 2w_2 \end{bmatrix}$$

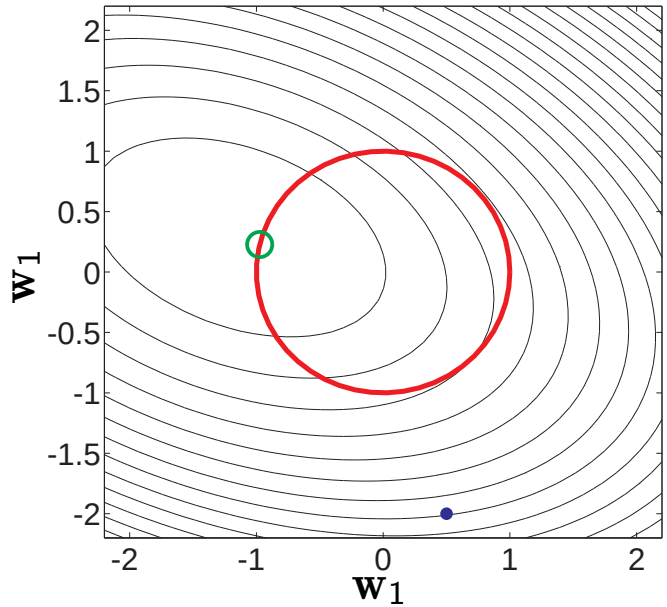
$$\mathcal{L}(w, \lambda) = \Phi(w) + \lambda g(w)$$

$$\nabla_w \mathcal{L}(w, \lambda) = \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} w + \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 2\lambda w$$

$$H(w, \lambda) = \begin{bmatrix} 2 + 2\lambda & 1 \\ 1 & 4 + 2\lambda \end{bmatrix}$$

$$\min_w \frac{1}{2} w^T \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} w + w^T \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\text{s.t. } g(w) = w^T w - 1 = 0$$



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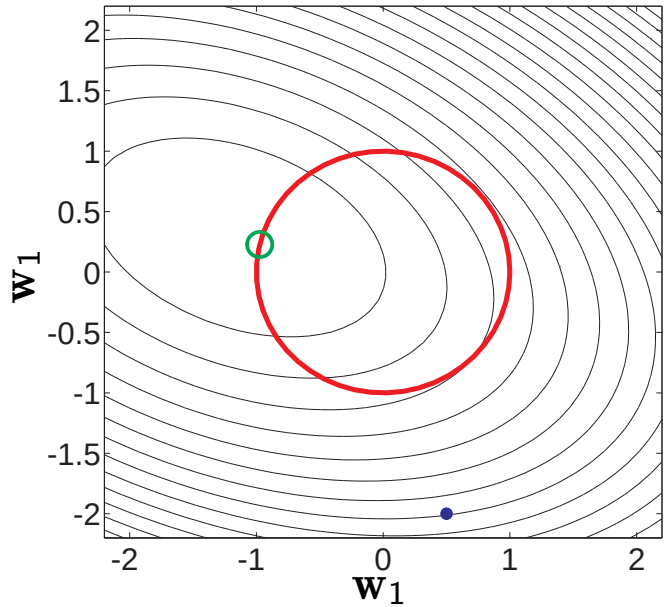
$$H(w, \lambda) = \begin{bmatrix} 2 + 2\lambda & 1 \\ 1 & 4 + 2\lambda \end{bmatrix}$$

$$\nabla \Phi(w) = \begin{bmatrix} 2w_1 + w_2 + 1 \\ w_1 + 4w_2 \end{bmatrix}$$

$$\min_w \frac{1}{2} w^T \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} w + w^T \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\text{s.t. } g(w) = w^T w - 1 = 0$$



Newton Iteration for Optimization - Example

Algorithm: Newton method

Input: guess $\mathbf{w}$, $\boldsymbol{\lambda}$

while $\|\nabla \mathcal{L}\|$ *or* $\|\mathbf{g}\| \geq \text{tol}$ **do**

Compute

$$H(\mathbf{w}, \boldsymbol{\lambda}),\ \nabla \mathbf{g}(\mathbf{w}),\ \nabla \Phi(\mathbf{w}),\ \mathbf{g}(\mathbf{w})$$

Compute Newton direction

$$\begin{bmatrix} H & \nabla \mathbf{g} \\ \nabla \mathbf{g}^T & 0 \end{bmatrix} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda}^+ \end{bmatrix} = - \begin{bmatrix} \nabla \Phi \\ \mathbf{g} \end{bmatrix}$$

$$\Delta \boldsymbol{\lambda} = \boldsymbol{\lambda}^+ - \boldsymbol{\lambda}$$

Compute Newton step, $t \in]0, 1]$

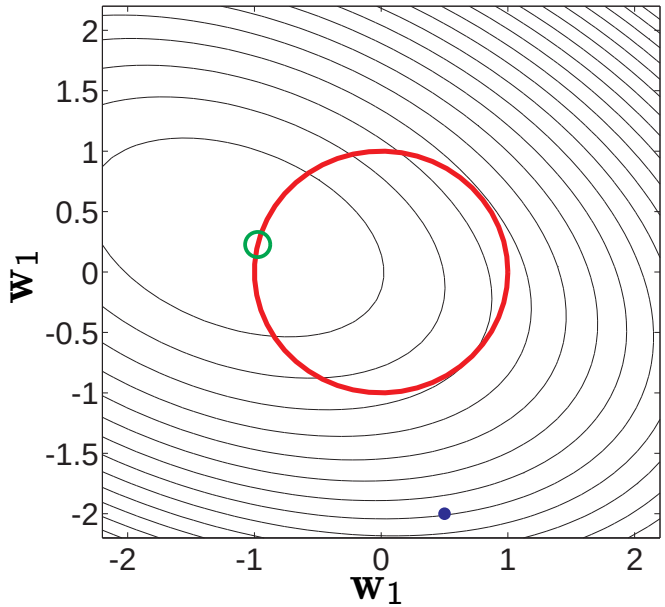
$$\mathbf{w} \leftarrow \mathbf{w} + t \Delta \mathbf{w}, \quad \boldsymbol{\lambda} \leftarrow \boldsymbol{\lambda} + t \Delta \boldsymbol{\lambda}$$

return $\mathbf{w}$, $\boldsymbol{\lambda}$

$$\min_{\mathbf{w}} \ \frac{1}{2} \mathbf{w}^T \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} \mathbf{w} + \mathbf{w}^T \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\text{s.t. } g(\mathbf{w}) = \mathbf{w}^T \mathbf{w} - 1 = 0$$

Guess $\lambda = 0$, step $t = 1$



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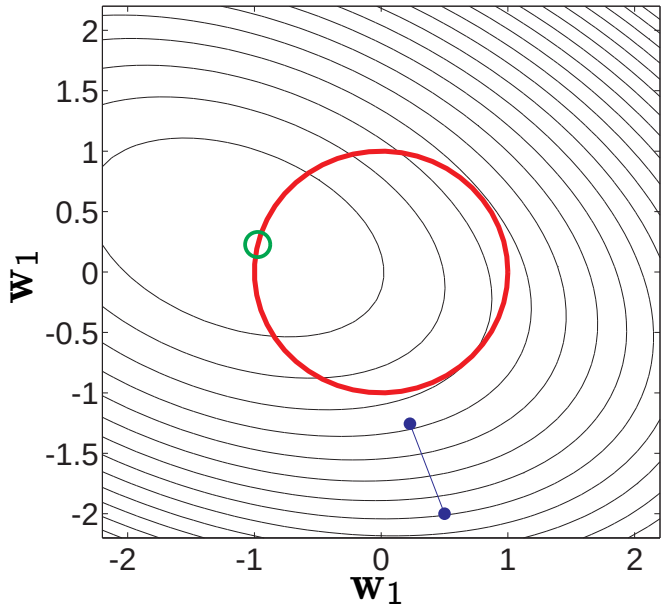

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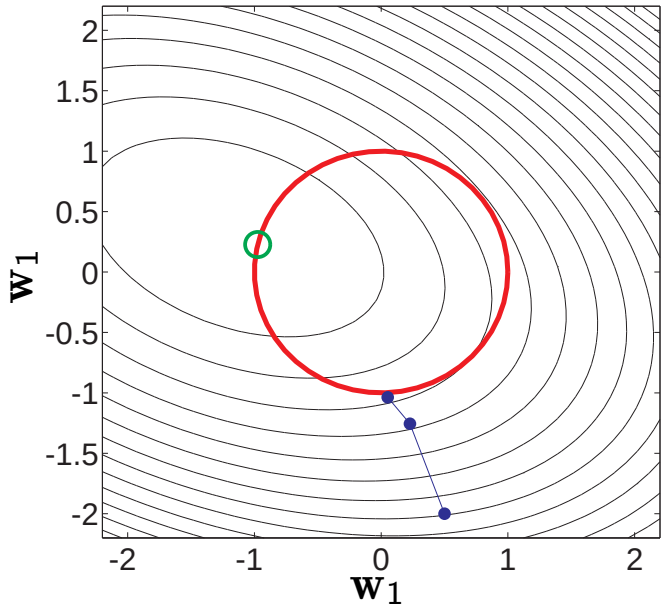

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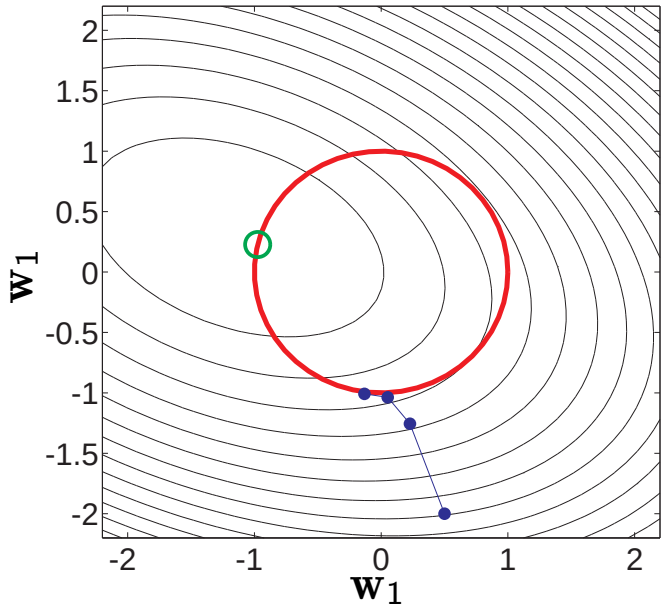

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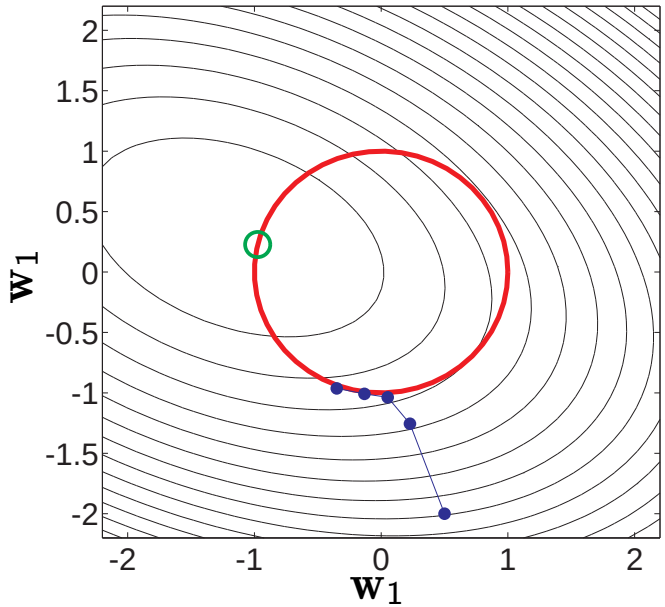
Guess $\lambda = 0$, step $t = 1$



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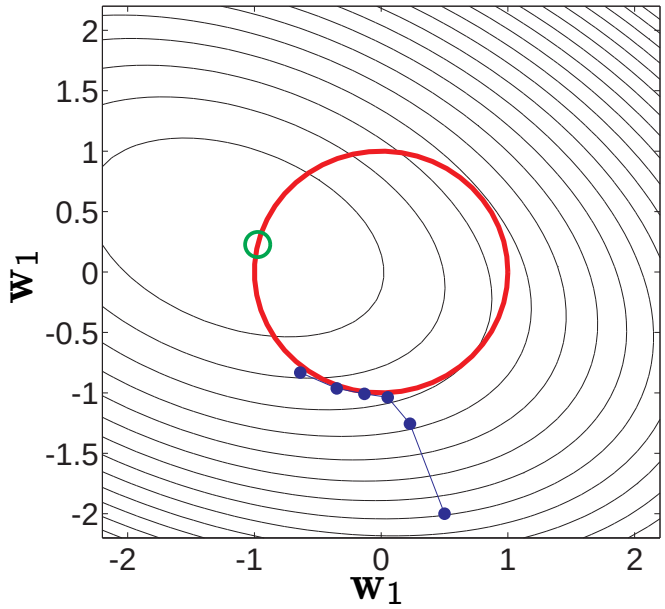

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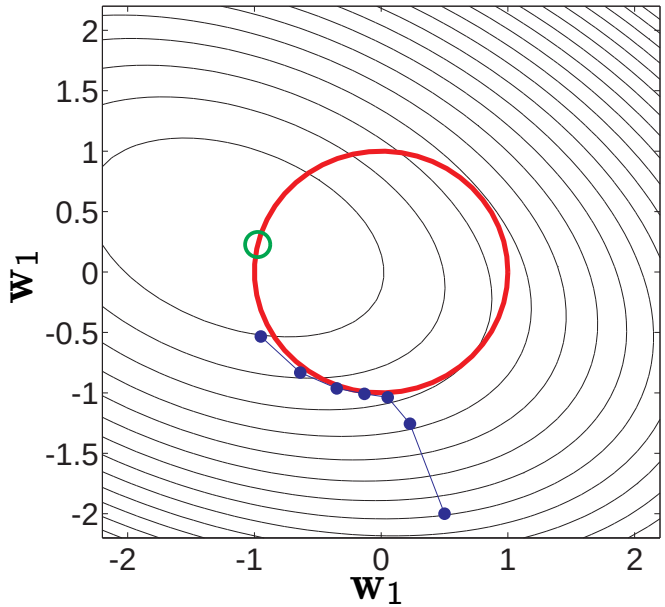

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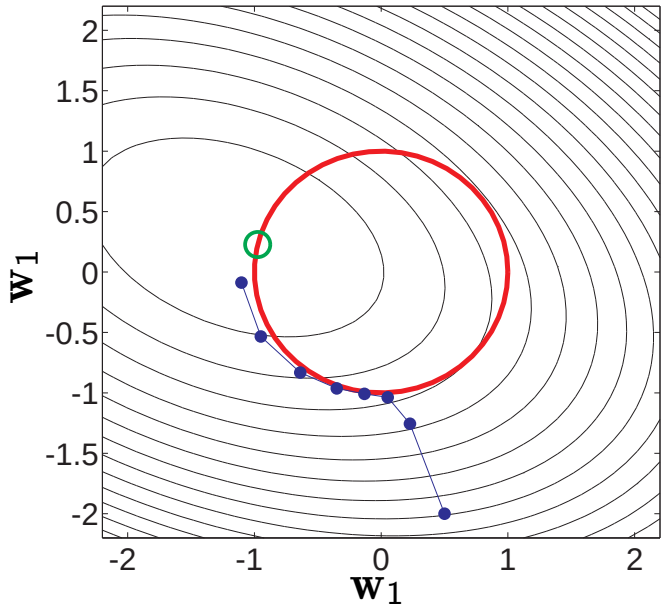

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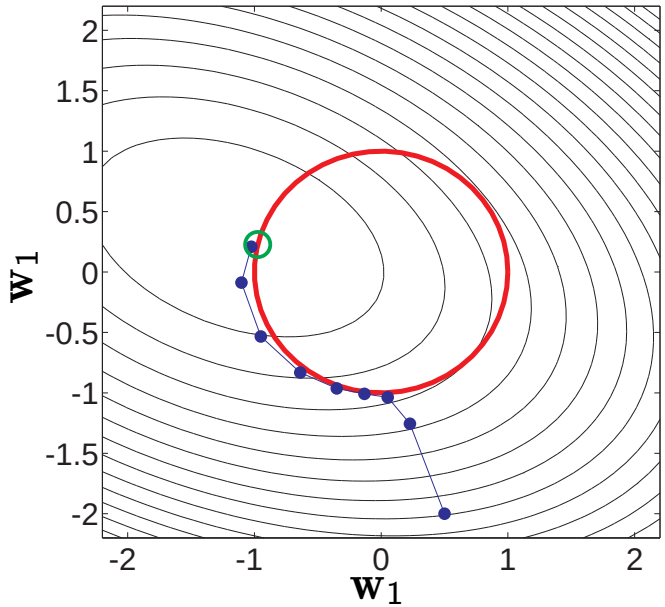

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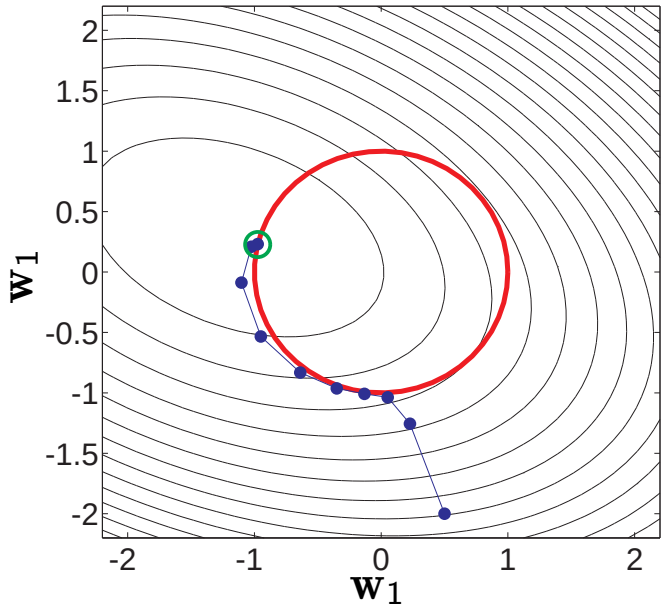

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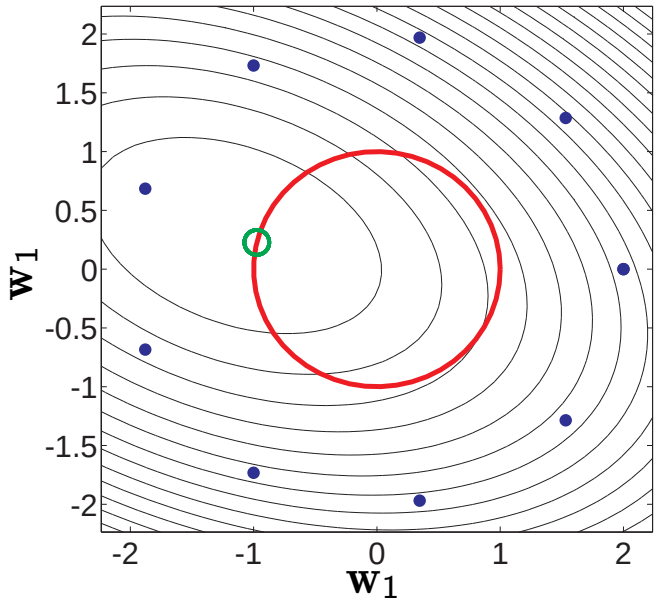

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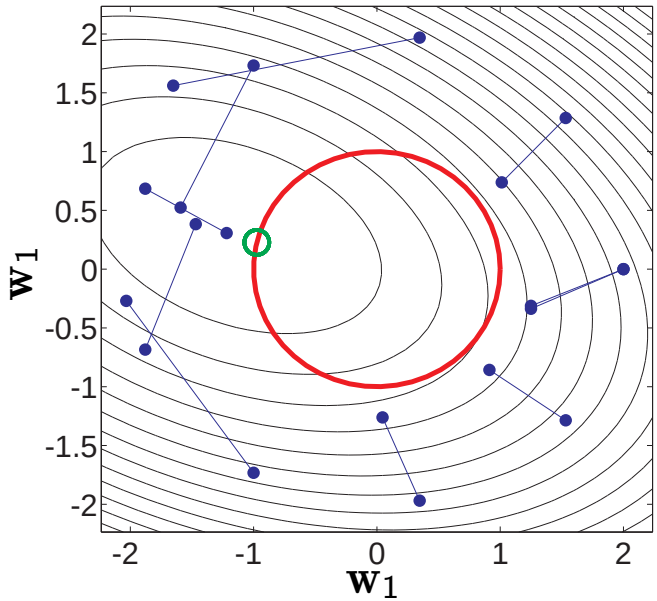

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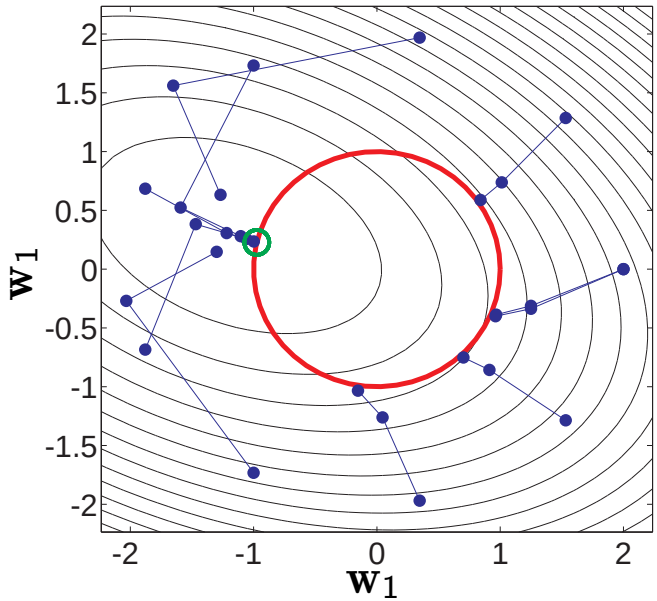

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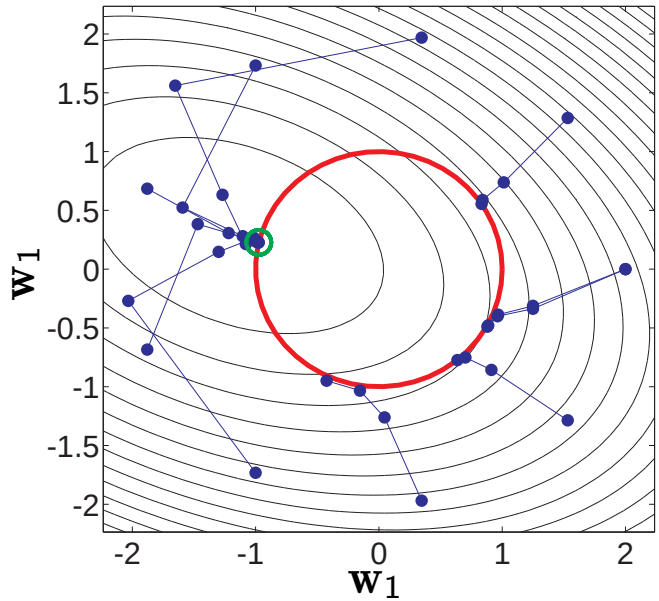

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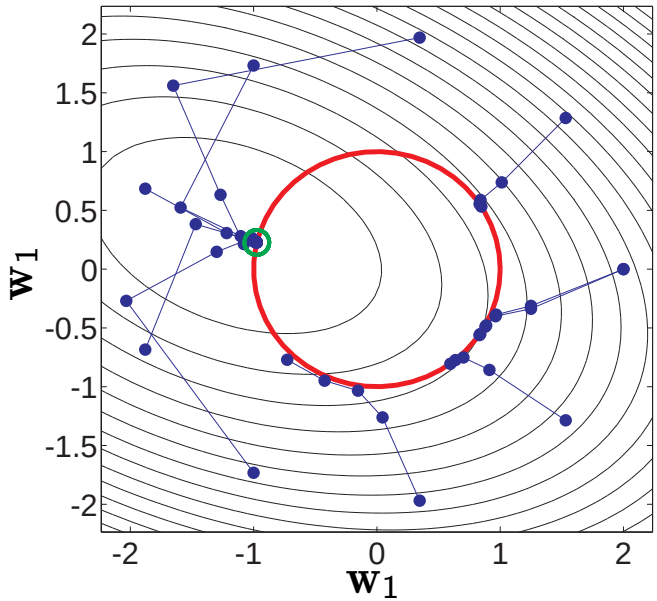

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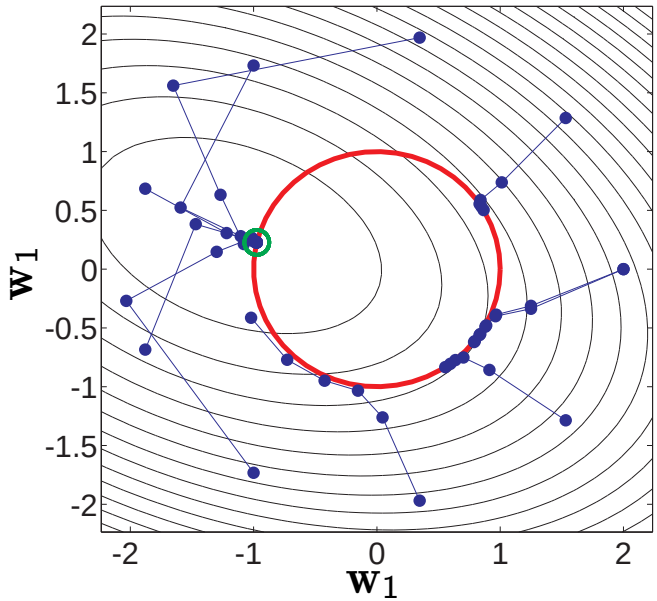

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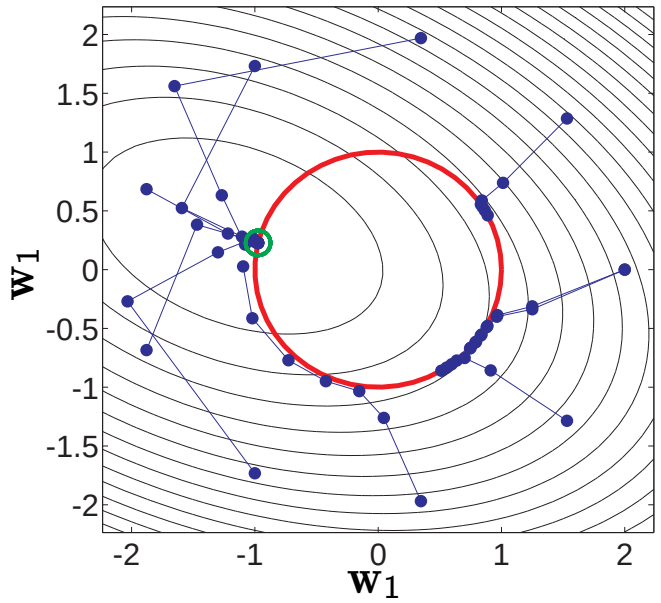

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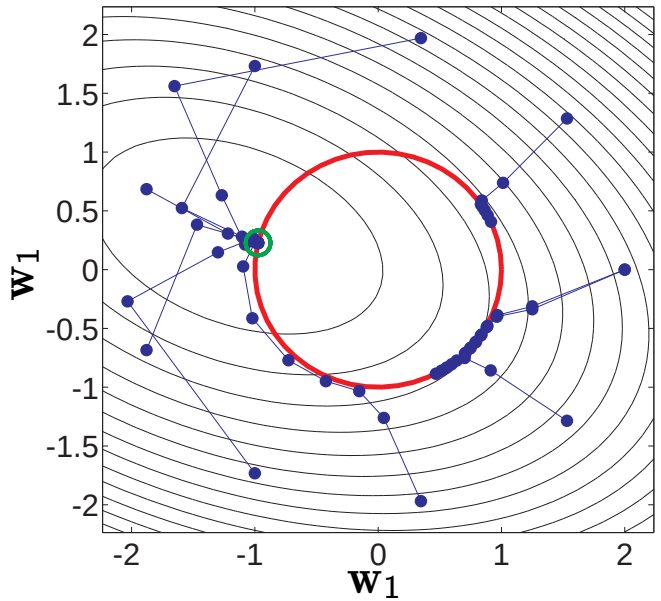

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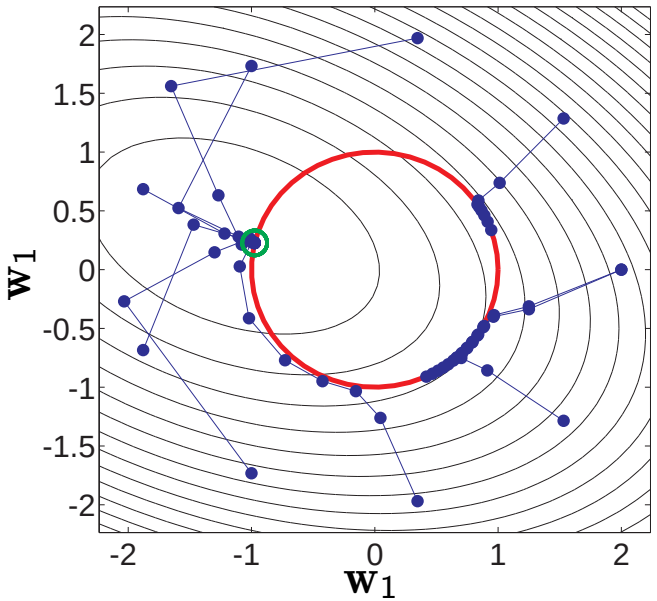

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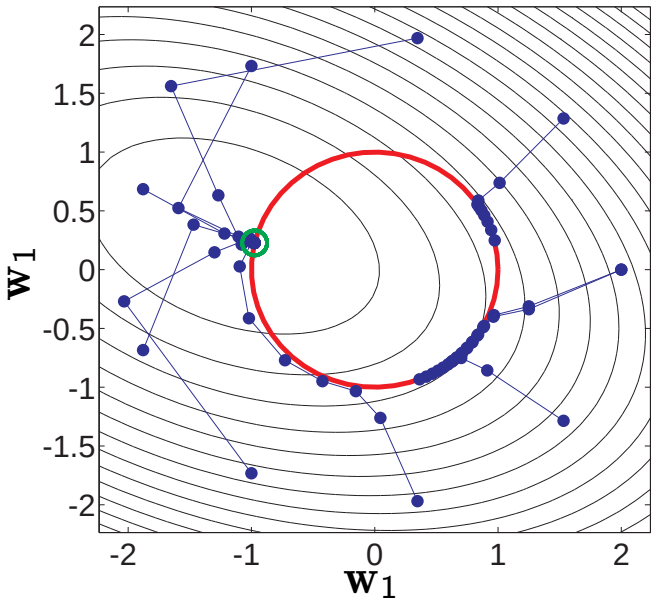

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Algorithm: Newton method

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while $\|\nabla \mathcal{L}\|$ *or* $\|\mathbf{g}\| \geq \text{tol}$ **do**

Compute

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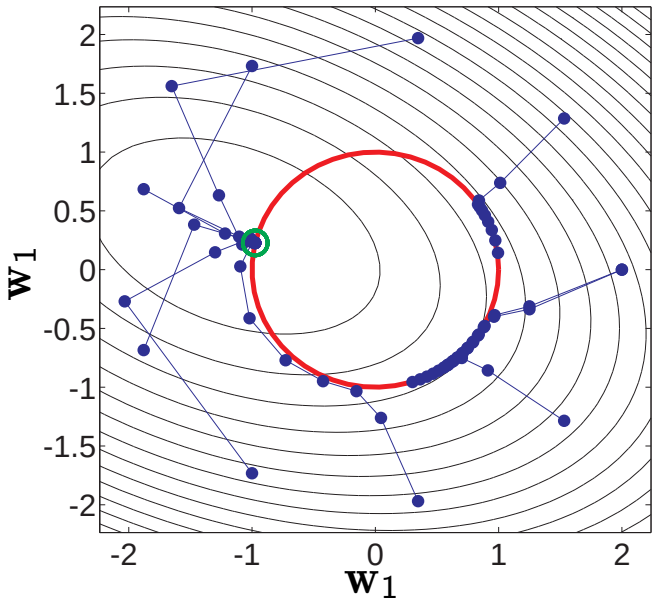

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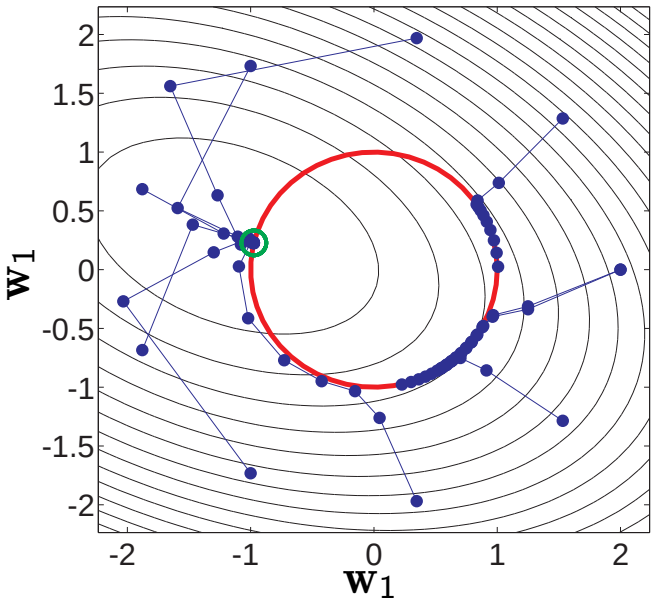

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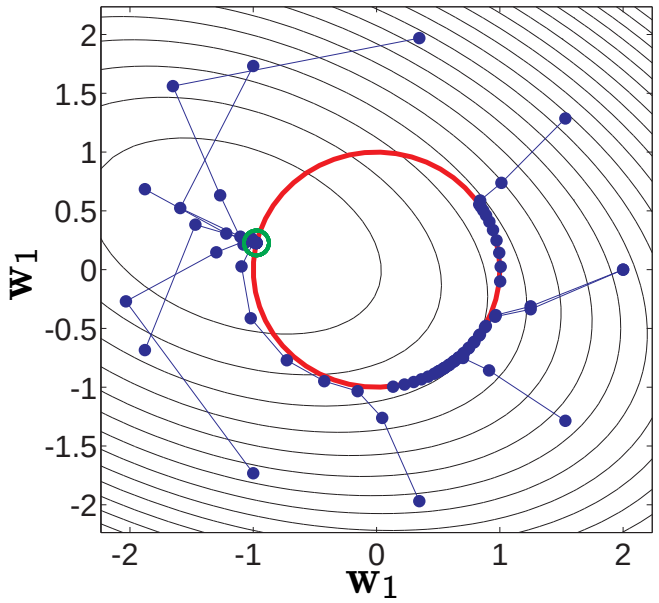

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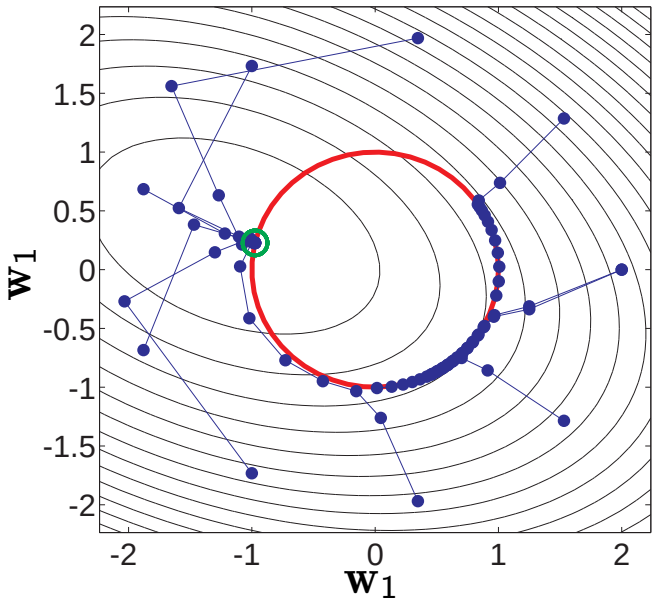

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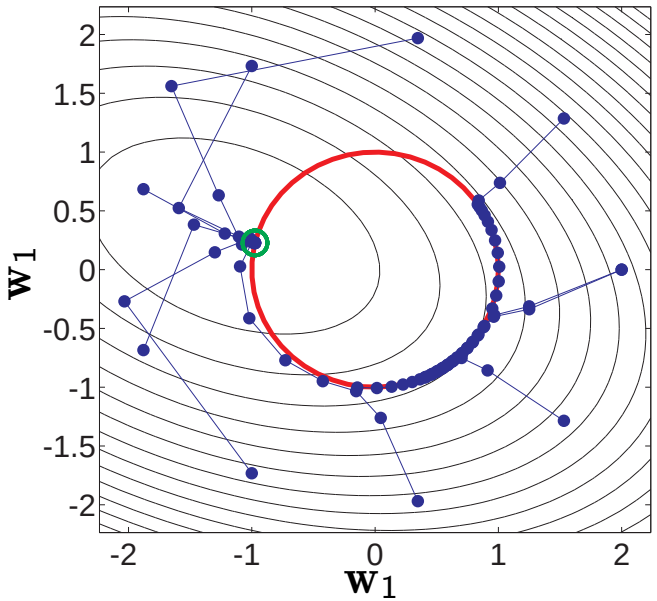

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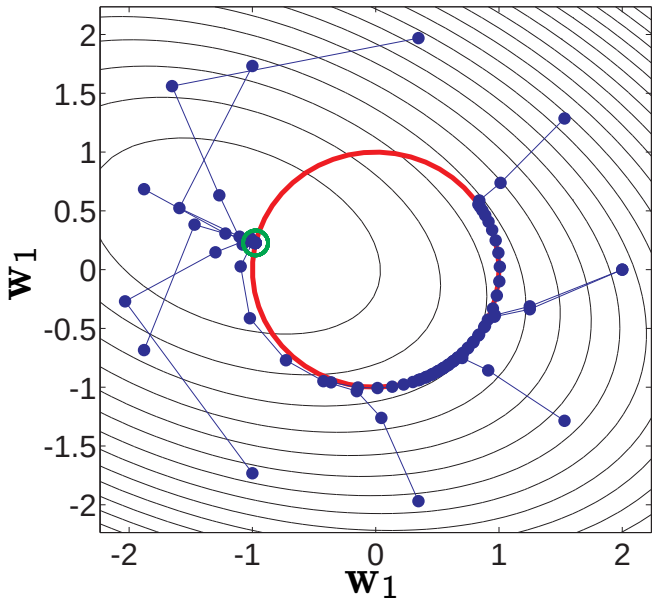

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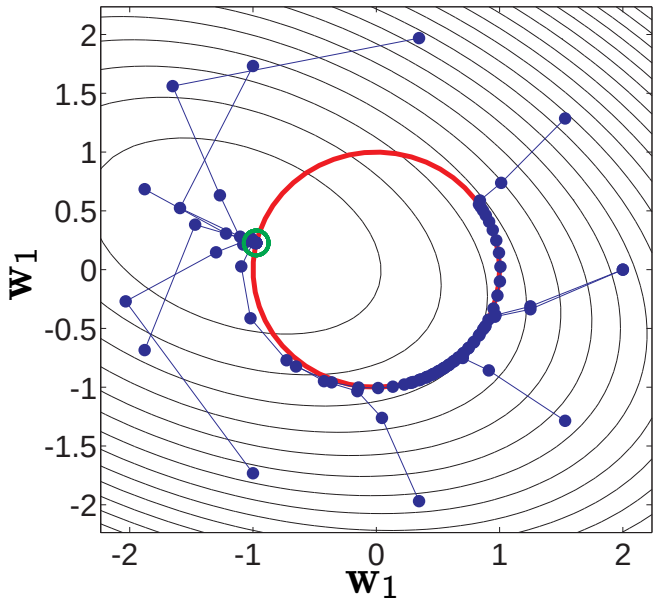

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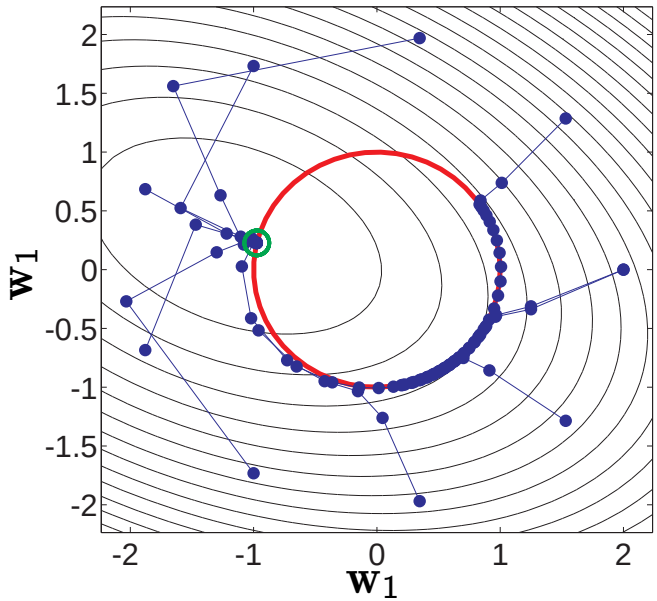

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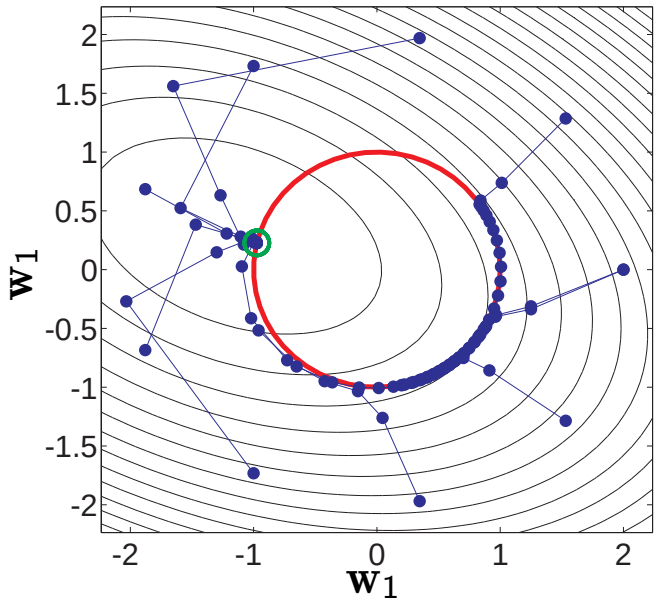

Your initial guess matters !!

Invertibility of the KKT matrix

The Newton direction of the KKT conditions

$$\underbrace{\begin{bmatrix} H(\mathbf{w},\boldsymbol{\lambda}) & \nabla \mathbf{g}(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} & 0 \end{bmatrix}}_{\text{KKT matrix (symmetric indefinite)}} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda}^{+} \end{bmatrix} = - \begin{bmatrix} \nabla \Phi(\mathbf{w}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix}$$

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The KKT matrix is invertible if (sufficient, not necessary)

- $\nabla \mathbf{g}(\mathbf{w})$ is full row rank (LICQ)
- $\forall \mathbf{d} \neq 0$, such that $\nabla \mathbf{g}(\mathbf{w})^{\top} \mathbf{d} = 0$

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Punchline: if you don't have LICQ/SOSC at $\mathbf{w}^*$, then the Newton iteration becomes (in general) ill-defined as you approach $\mathbf{w}^*$

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Matrix Inertia: # of positive, zero, negative eigenvalue (n_+, n_0, n_-)

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yields **KKT matrix:**

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Theorem: if SOSC and LICQ hold, then the inertia of M is $(n, 0, m)$

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- Hence

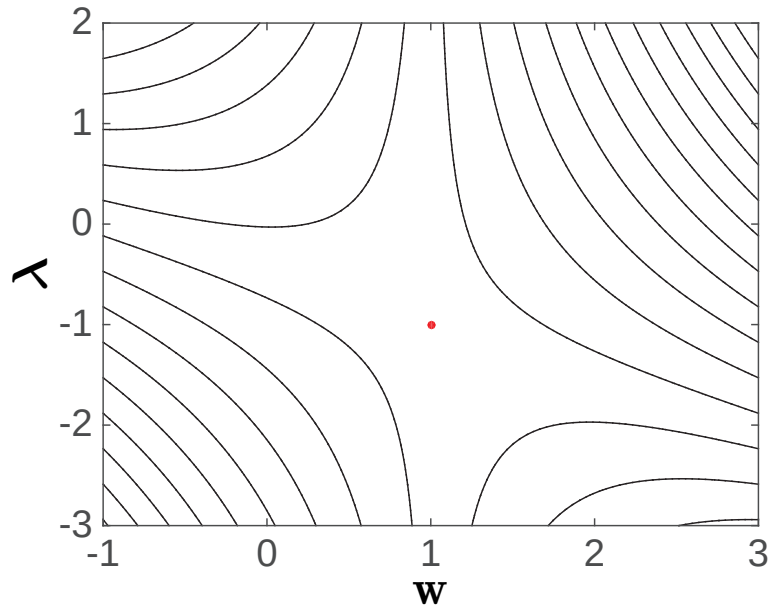
$$\nabla \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) = \begin{bmatrix} \nabla^2_{\mathbf{ww}} \mathcal{L} & \nabla_{\mathbf{w}\boldsymbol{\lambda}} \mathcal{L} \\ \nabla_{\boldsymbol{\lambda}\mathbf{w}} \mathcal{L} & \nabla_{\boldsymbol{\lambda}\boldsymbol{\lambda}} \mathcal{L} \end{bmatrix} = M$$

Theorem: if SOSC and LICQ hold, then the inertia of M is $(n, 0, m)$

Why ?

Solution is a saddle-point of $\mathcal{L}(\mathbf{w}, \boldsymbol{\lambda})$.

- Pos. eig. match n primal directions
- Neg. eig. match m dual directions



Quadratic model interpretation

Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \end{array}$$

The Newton direction is given by

$$\begin{bmatrix} H(\mathbf{w},\boldsymbol{\lambda}) & \nabla \mathbf{g}(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda}^{+} \end{bmatrix} = - \begin{bmatrix} \nabla \Phi(\mathbf{w}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix}$$

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Dual variables $\boldsymbol{\lambda}^+$ given by the dual variables of the QP, i.e. $\boldsymbol{\lambda}^+ = \boldsymbol{\lambda}_{\text{QP}}$

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Proof: KKT of the QP are equivalent to the KKT system.

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Proof: KKT of the QP are equivalent to the KKT system.

The Newton direction is given by solving a quadratic models of the original problem !!

Outline

1. The Newton method
2. Newton on the KKT conditions
3. The reduced Newton step (unconstrained problems)
4. The merit function - Line-search for constrained problems
5. Newton-type methods
6. Sequential Quadratic Programming

The Newton direction is a descent direction

Consider the unconstrained problem

$$\min_{\mathbf{w}} \quad \Phi(\mathbf{w})$$

The Newton direction $\Delta\mathbf{w}$ minimizes the quadratic model (unconstrained):

$$Q(\mathbf{w}, \Delta\mathbf{w}) = \Phi(\mathbf{w}) + \nabla\Phi(\mathbf{w})^{\mathsf{T}}\Delta\mathbf{w} + \frac{1}{2}\Delta\mathbf{w}^{\mathsf{T}} H(\mathbf{w})\Delta\mathbf{w}$$

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where $H(\mathbf{w}) = \nabla^2_{\mathbf{w}}\Phi(\mathbf{w})$. Step $\Delta\mathbf{w}$ reads as:

$$\Delta\mathbf{w} = -H(\mathbf{w})^{-1}\nabla\Phi(\mathbf{w})$$

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$$\Phi(\mathbf{w} + t\Delta\mathbf{w}) - \Phi(\mathbf{w}) = t\nabla\Phi(\mathbf{w})^{\mathsf{T}}\Delta\mathbf{w} = -t\nabla\Phi(\mathbf{w})^{\mathsf{T}} H(\mathbf{w})^{-1}\nabla\Phi(\mathbf{w}) < 0$$

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i.e. $\boxed{\Phi(\mathbf{w} + t\Delta\mathbf{w}) < \Phi(\mathbf{w}) \text{ for } t \in \mathbb{R}_+ \text{ sufficiently small.}}$

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i.e. $\boxed{\Phi(\mathbf{w} + t\Delta\mathbf{w}) < \Phi(\mathbf{w}) \text{ for } t \in \mathbb{R}_+ \text{ sufficiently small.}}$

However, there's no guarantee that $\Phi(\mathbf{w} + \Delta\mathbf{w}) < \Phi(\mathbf{w})$!!

Failure of the full Newton step

Newton direction $\Delta \mathbf{w}$ minimizes the quadratic model :

$$Q(\mathbf{w}, \Delta \mathbf{w}) = \Phi(\mathbf{w}) + \nabla \Phi(\mathbf{w})^T \Delta \mathbf{w} + \frac{1}{2} \Delta \mathbf{w}^T H(\mathbf{w}) \Delta \mathbf{w}$$

Given by:

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Full Newton step:

$$\mathbf{w} \leftarrow \mathbf{w} + \Delta \mathbf{w}$$

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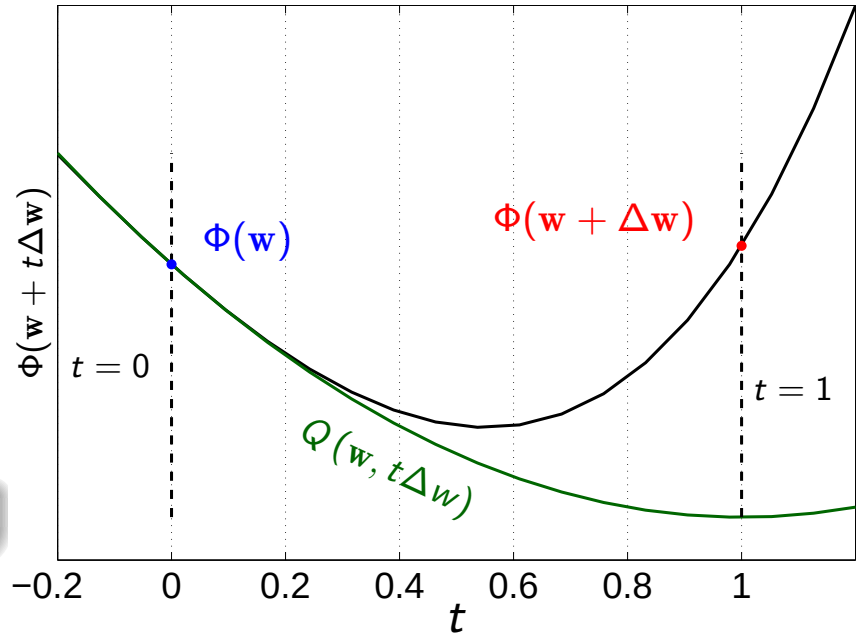

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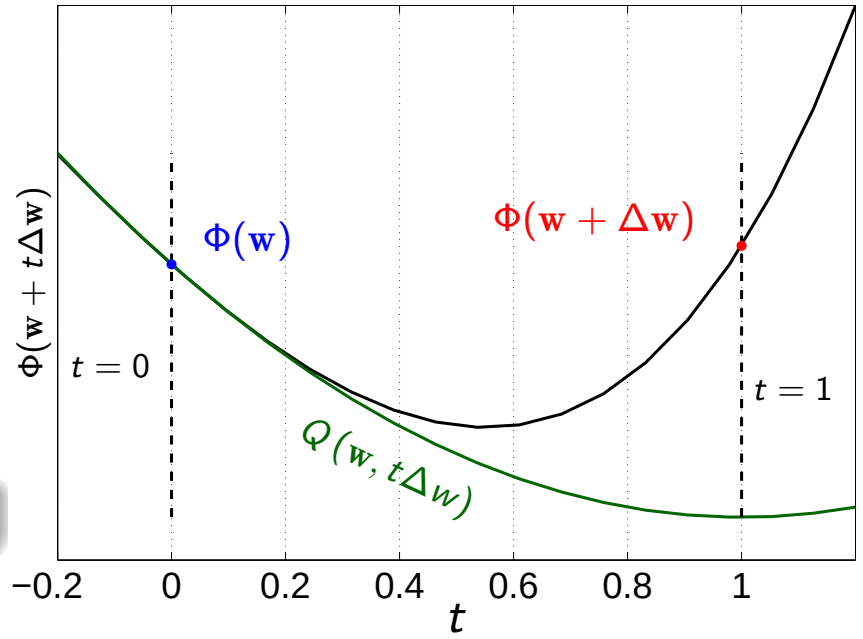


A situation with $\Phi(\mathbf{w} + \Delta \mathbf{w}) > \Phi(\mathbf{w})$ can easily occur...

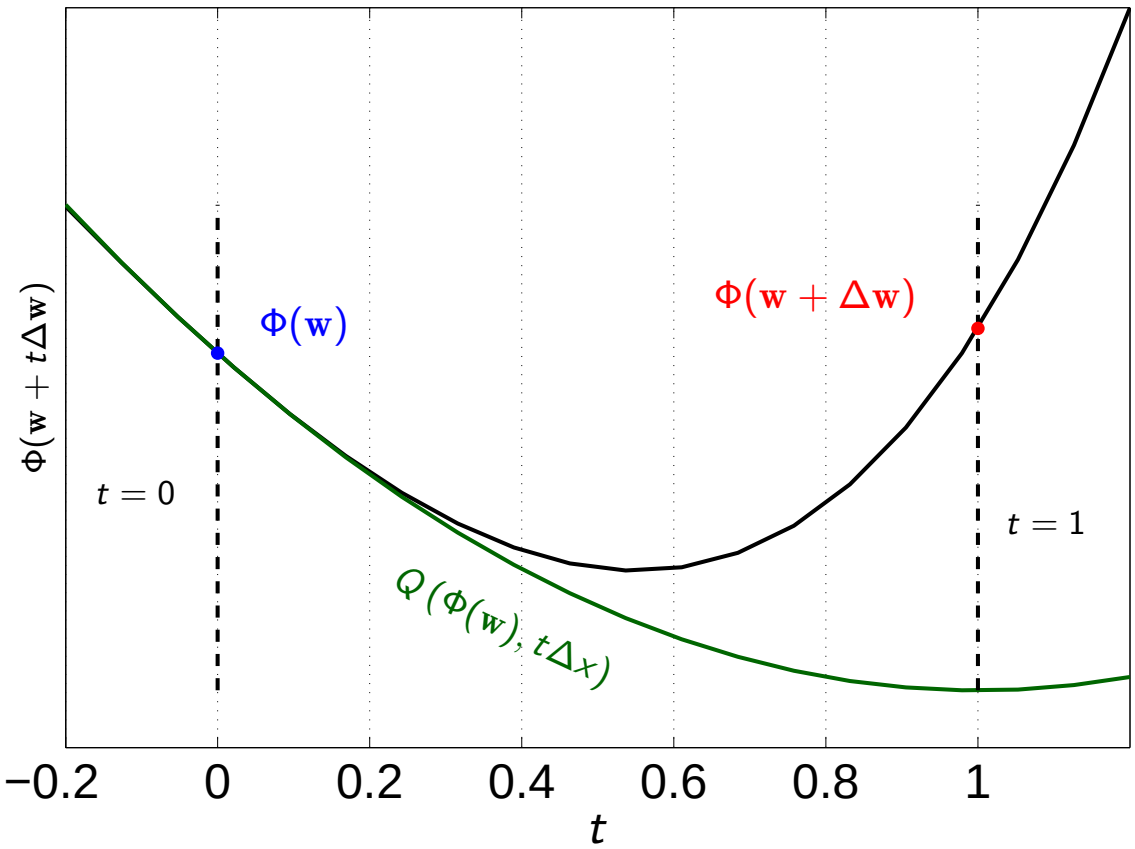
- Strong variation of H
- Nonlinear constraints (if the problem is constrained)

Globalization - Line search strategies

Exact line search (for unconstrained optimization)

Find the best step length:

$$t = \arg \min_{t \in]0,1]} \Phi(\mathbf{w} + t\Delta\mathbf{w})$$



Recap of last lecture

- Newton is a tool to solve nonlinear equations, will be used to solve the KKTs associated to an NLP
- Reduced-step Newton converges to a solution if $\nabla \mathbf{r}$ is full rank
- Convergence of full steps Newton is quadratic (fast), better when equations are "closer to linear"
- Rescaling the decision variables $\mathbf{w}$ has no effect on Newton, may help the linear algebra though
- Newton on KKT conditions has a specific structure, step well posed if LICQ & SOSC
- Newton step is equivalent to solving a QP forming a "linear-quadratic" approximation of the NLP
- In unconstrained optimization problems, this observation is equivalent to "minimizing a quadratic model of the cost", reduced steps are needed when that model validity is "locally limited"

Globalization - Line search strategies

"Armijo's" backtracking line search (for unconstrained optimization)

Given a primal direction $\Delta \mathbf{w}$, using $0 < \alpha \leq \frac{1}{2}$ and $0 < \beta < 1$, do $t = 1$:

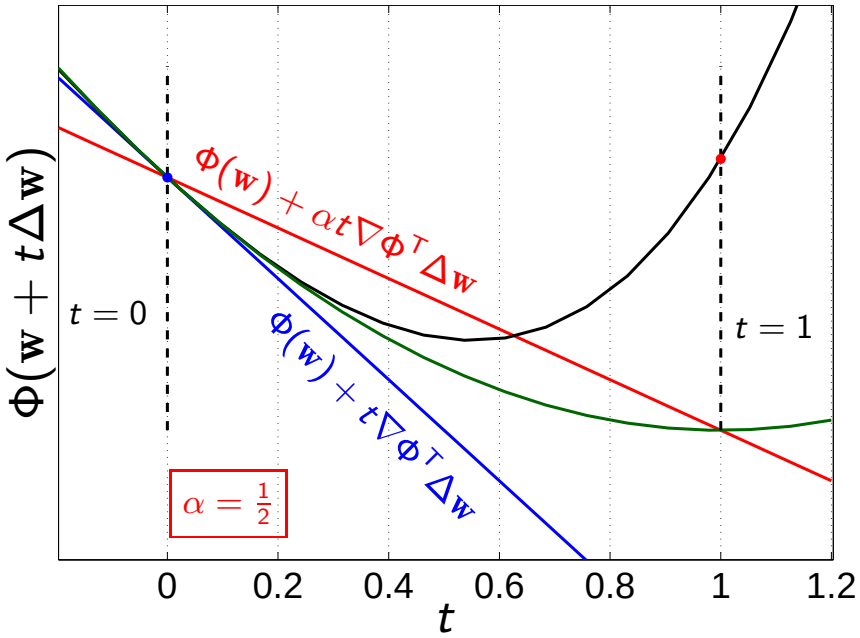
Algorithm: "Armijo's" backtracking

$t \leftarrow 1$

while $\Phi(\mathbf{w} + t\Delta\mathbf{w}) \geq \Phi(\mathbf{w}) + \alpha t \nabla \Phi(\mathbf{w})^T \Delta \mathbf{w}$ **do**

  $t \leftarrow \beta t$

return t



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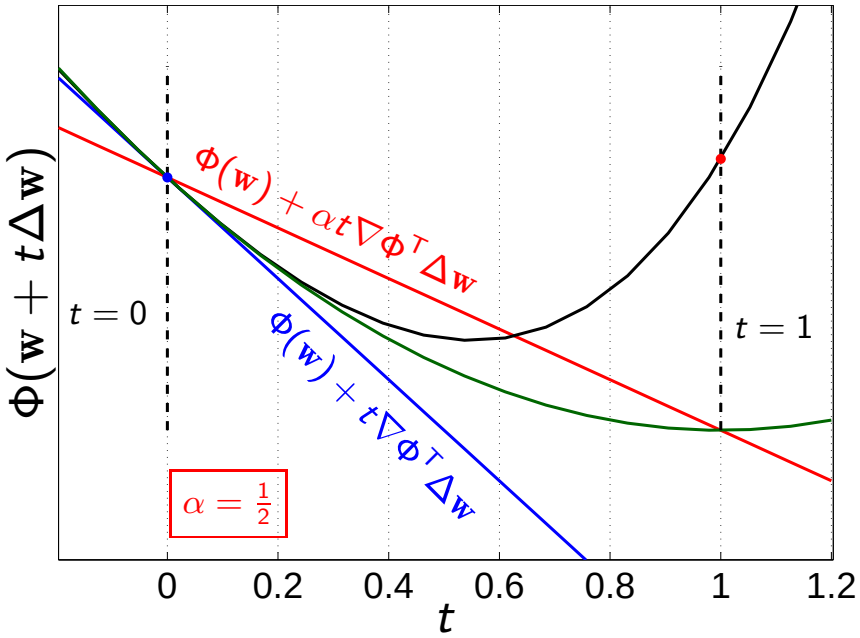

- If α too small we may accept steps yielding only mediocre improvement.
- If Φ is quadratic, we want full step, i.e. $\alpha \leq \frac{1}{2}$
- In practice $\alpha < \frac{1}{2}$ is usually preferred
- Additional conditions are sometimes used to yield a sufficiently large the step (c.f. Wolfe or Goldstein conditions)

Convergence of the Newton method with Line-search (unconstrained)

Theorem

Assume:

- Hessian is bounded $m \cdot I \leq \nabla^2 \Phi(\mathbf{w}) \leq M \cdot I$, with $m, M > 0$
- Hessian is Lipschitz, i.e. $\|\nabla^2 \Phi(\mathbf{w}) - \nabla^2 \Phi(\mathbf{y})\| \leq L\|\mathbf{w} - \mathbf{y}\|, \quad \forall \mathbf{w}, \mathbf{y}$

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then $\exists\ \eta, \gamma > 0$ with $\eta < \frac{m^2}{L}$ such that $\forall\ \mathbf{w}$:

Damped phase:				
$\Phi(\mathbf{w}^+) - \Phi(\mathbf{w})$	$\leq$	$-\gamma$	if	$\|\nabla \Phi(\mathbf{w})\| \geq \eta$
Quadratic phase:				
$\|\nabla \Phi(\mathbf{w}^+)\|$	$\leq$	$\frac{L}{2m^2}\|\nabla \Phi(\mathbf{w})\|^2$	if	$\|\nabla \Phi(\mathbf{w})\| < \eta$

where $\mathbf{w}^+ = \mathbf{w} + t\Delta\mathbf{w}$ is the (possibly) reduced Newton step

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Practical consequence: two-phase convergence

- If $\mathbf{w}$ is *far* from $\mathbf{w}^*$ $\Rightarrow$ Damped convergence (reduced steps)
- If $\mathbf{w}$ is *close* to $\mathbf{w}^*$ $\Rightarrow$ Quadratic convergence (full steps)
- Once Newton has entered the quadratic phase, it stays quadratic !!

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Practical consequence: region of quadratic convergence

- If L is large, then
  1. the quadratic region ($\|\nabla \Phi(\mathbf{w})\| < \eta$) is small
  2. the quadratic contraction rate is small

Convergence of the Newton method with Line-search (unconstrained)

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What if we have constraints ? Similar results, with $\nabla^2_{\mathbf{w}} \mathcal{L}$, $\nabla_{\mathbf{w}} \mathbf{g}$. However, Newton can fail on an infeasible point (no direction improving the constraints, c.f. "But still, Newton can fail...")

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Assessing convergence with constraints

Solve the NLP...

$$\begin{aligned} \min_{\mathbf{w}} \quad & \Phi(\mathbf{w}) \\ \text{s.t.} \quad & \mathbf{g}(\mathbf{w}) = 0 \end{aligned}$$

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... by satisfying the KKT conditions...

$$\mathbf{r}(\mathbf{w}, \boldsymbol{\lambda}) = \begin{bmatrix} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix} = 0$$

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... via taking Newton steps along the Newton directions.

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- We know that there exists a Newton step that improves $\|\mathbf{r}\|$, i.e.

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  for some $t \in]0, 1]$ (as long as $\nabla \mathbf{r}$ is non-singular). How to select t ?

Assessing convergence with constraints

Solve the NLP... ... by satisfying the KKT conditions...

$$\begin{aligned} \min_{\mathbf{w}} \quad & \Phi(\mathbf{w}) \\ \text{s.t.} \quad & \mathbf{g}(\mathbf{w}) = 0 \end{aligned}$$

$$\mathbf{r}(\mathbf{w}, \boldsymbol{\lambda}) = \begin{bmatrix} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix} = 0$$

... via taking Newton steps along the Newton directions.

The Newton directions are given by

$$\begin{bmatrix} H(\mathbf{w}, \boldsymbol{\lambda}) & \nabla \mathbf{g}(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^T & 0 \end{bmatrix} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda}^+ \end{bmatrix} = - \begin{bmatrix} \nabla \Phi(\mathbf{w}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix}$$

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- Could ensure the progress of $\|\mathbf{r}(\mathbf{w} + t\Delta \mathbf{w}, \boldsymbol{\lambda} + t\Delta \boldsymbol{\lambda})\|$
- Some caveats... e.g. need to evaluate $\nabla \mathbf{g}(\mathbf{w} + t\Delta \mathbf{w})$ each time we backtrack on t !! This can be computationally expensive...

Line-search with Equality Constraints

T_1 merit function...

... accounts for progress on Φ and $\mathbf{g}$

$$\boxed{T_1(\mathbf{w}) = \Phi(\mathbf{w}) + \nu \|\mathbf{g}(\mathbf{w})\|_1}$$

We would like $\min_{\mathbf{w}} T_1(\mathbf{w})$ to coincide with the solution of the NLP !!

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- If $\mathbf{w}^*, \boldsymbol{\lambda}^*$ is a regular KKT point with SOSC, then $\mathbf{w}^*$ is a (local) minimum of T_1 for $\nu > \|\boldsymbol{\lambda}^*\|_\infty$

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Similar results as in the unconstrained case if LICQ is respected !!

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Similar results as in the unconstrained case if LICQ is respected !!

Difficulty: $\boldsymbol{\lambda}^*$ is not know a priori. Parameter ν must be chosen adequately, possibly adjusted over the iterations !

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Theorem: for $\mathbf{g}_i(\mathbf{w}) \neq 0 \ \forall i$, then the Newton direction $(\mathbf{w}, \boldsymbol{\lambda})$

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and since $\nabla \mathbf{g}(\mathbf{w})^\top \Delta \mathbf{w} = -\mathbf{g}(\mathbf{w})$, we have:

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Moreover, $H\Delta \mathbf{w} + \nabla \mathbf{g} \boldsymbol{\lambda} = -\nabla \Phi$ yields $\Delta \mathbf{w}^\top H \Delta \mathbf{w} + \Delta \mathbf{w}^\top \nabla \mathbf{g} \boldsymbol{\lambda} = -\Delta \mathbf{w}^\top \nabla \Phi$

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Then, since $|\boldsymbol{\lambda} \mathbf{g}| \leq \|\boldsymbol{\lambda}\|_\infty \|\mathbf{g}\|_1$, we have:

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Then, since $|\boldsymbol{\lambda} \mathbf{g}| \leq \|\boldsymbol{\lambda}\|_\infty \|\mathbf{g}\|_1$, we have:

$$\frac{\mathrm{d}}{\mathrm{d}t} T_1(\mathbf{w} + t\Delta \mathbf{w})\Big|_{t=0} \leq -\Delta \mathbf{w}^\top H \Delta \mathbf{w} + \|\boldsymbol{\lambda}\|_\infty \|\mathbf{g}\|_1 - \nu \|\mathbf{g}(\mathbf{w})\|_1$$

.

Newton direction is a descent direction for T_1

Theorem: for $\mathbf{g}_i(\mathbf{w}) \neq 0 \ \forall i$, then the Newton direction $(\mathbf{w}, \boldsymbol{\lambda})$

$$\begin{bmatrix} H(\mathbf{w}, \boldsymbol{\lambda}) & \nabla \mathbf{g}(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^\top & 0 \end{bmatrix} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda} \end{bmatrix} = - \begin{bmatrix} \nabla \Phi(\mathbf{w}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix}$$

is a descent direction for the T_1 merit function $T_1 = \Phi(\mathbf{w}) + \nu \|\mathbf{g}(\mathbf{w})\|_1$.

Proof: $\Delta \mathbf{w}$ is a descent direction if

$$\frac{\mathrm{d}}{\mathrm{d}t} T_1(\mathbf{w} + t\Delta \mathbf{w})\Big|_{t=0} < 0$$

We have:

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i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t} T_1(\mathbf{w} + t\Delta \mathbf{w})\Big|_{t=0} \leq -\Delta \mathbf{w}^\top H \Delta \mathbf{w} + \left(\|\boldsymbol{\lambda}\|_\infty - \nu\right) \|\mathbf{g}(\mathbf{w})\|_1 < 0$$

holds if SOSC (reduced Hessian $Z^\top H Z \geq 0$) and $\|\boldsymbol{\lambda}\|_\infty > \nu$.

Outline

1. The Newton method
2. Newton on the KKT conditions
3. The reduced Newton step (unconstrained problems)
4. The merit function - Line-search for constrained problems
5. Newton-type methods
6. Sequential Quadratic Programming

Convergence of Newton-type methods

Computing $H = \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\lambda}, \boldsymbol{\mu})$ can be expensive, use an approximation instead !!

What happens to the convergence of the Newton method ?

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$$\mathbf{w}_{k+1} = \mathbf{w}_k - M_k^{-1} \mathbf{r}(\mathbf{w}_k), \qquad \text{with} \qquad M_k \text{ invertible, approximates } J = \frac{\partial \mathbf{r}(\mathbf{w})}{\partial \mathbf{w}}$$

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Then $\mathbf{w}_k \to \mathbf{w}^*$ with the following linear contraction in each iteration:

$$\|\mathbf{w}_{k+1} - \mathbf{w}^*\| \quad \leq \quad \left(\kappa_k + \frac{\omega}{2}\|\mathbf{w}_k - \mathbf{w}^*\|\right) \|\mathbf{w}_k - \mathbf{w}^*\|.$$

Newton-type Techniques (unconstrained)

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Local convergence for all Newton Methods

Assume

- $\mathbf{w}^*$ is **SOSC**
- **Lipschitz Hessian**: $\| M_k^{-1} \left(\nabla^2 \Phi(\mathbf{w}_k) - \nabla^2 \Phi(\mathbf{y}) \right) \| \leq \omega \| \mathbf{w}_k - \mathbf{y} \|$ holds on the iterations, $\forall \mathbf{y}$.
- **Compatibility**: $\| M_k^{-1} \left(\nabla^2 \Phi(\mathbf{w}_k) - M_k \right) \| \leq \kappa_k$ with $\kappa_k \leq \kappa < 1$

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Then if $\mathbf{w}_k$ is close to $\mathbf{w}^*$, $\mathbf{w}_k \to \mathbf{w}^*$ and convergence is

- Quadratic for $\kappa = 0$: $\| \mathbf{w}_{k+1} - \mathbf{w}^* \| \leq C \| \mathbf{w}_k - \mathbf{w}^* \|^2$ with $C = \omega / 2$
- Superlinear for $\kappa_k \to 0$: $\| \mathbf{w}_{k+1} - \mathbf{w}^* \| \leq C_k \| \mathbf{w}_k - \mathbf{w}^* \|$ with $C_k \to 0$
- Linear for $\kappa_k > \rho$: $\| \mathbf{w}_{k+1} - \mathbf{w}^* \| \leq C \| \mathbf{w}_k - \mathbf{w}^* \|$ with $C < 1$

Newton-type Methods (unconstrained)

Steepest descent

Use $M_k = \alpha_k^{-1} I$, then:

$$\Delta \mathbf{w}_k = -M_k^{-1} \nabla \Phi(\mathbf{w}_k) = -\alpha_k \nabla \Phi(\mathbf{w}_k)$$

Step size α_k is chosen sufficiently small by the line-search.

Convergence

- Compatibility: $\|\alpha_k \nabla^2 \Phi(\mathbf{w}_k) - I\| \leq \kappa_k$ with $\kappa_k \leq \kappa < 1$
- Constant κ_k does not converge to 0, i.e. $\kappa_k > \rho, \ \forall k$
- Linear convergence when $\mathbf{w}_k$ is close to $\mathbf{w}^*$

Newton-type Methods (unconstrained)

Cost function of the type $\Phi(\mathbf{w}) = \frac{1}{2}\|\mathbf{R}(\mathbf{w})\|^2$, with $\mathbf{R}(\mathbf{w}) \in \mathbb{R}^m$

Gauss-Newton Hessian approximation

Observe that

$$H(\mathbf{w}) = \frac{\partial}{\partial \mathbf{w}} \left(\nabla \mathbf{R}(\mathbf{w}) \mathbf{R}(\mathbf{w}) \right) = \nabla \mathbf{R}(\mathbf{w}) \nabla \mathbf{R}(\mathbf{w})^\top + \sum_{i=1}^{m} \nabla^2 \mathbf{R}_i(\mathbf{w}) \mathbf{R}_i(\mathbf{w})$$

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Gauss-Newton method proposes to use: $\boxed{B_k = \nabla \mathbf{R}(\mathbf{w}_k) \nabla \mathbf{R}(\mathbf{w}_k)^\top + \alpha_k I}$

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- all $\nabla^2 \mathbf{R}_i(\mathbf{w})$ are small ($\mathbf{R}$ close to linear), or
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Convergence

- If $\sum_{i=1}^{m} \nabla^2 \mathbf{R}_i(\mathbf{w}) \mathbf{R}_i(\mathbf{w}) \to 0$ then $\kappa_k \to 0$
- Superlinear convergence in some cases...

Newton-type Methods (unconstrained)

Compute $H(\mathbf{w})$ numerically in an efficient (iterative) way

BFGS

Define

$$\begin{aligned} \mathbf{s}_k &= \mathbf{w}_{k+1} - \mathbf{w}_k \\ \mathbf{y}_k &= \nabla\Phi(\mathbf{w}_{k+1}) - \nabla\Phi(\mathbf{w}_k) \end{aligned}$$

Idea: Update $M_k \rightarrow M_{k+1}$ such that $M_{k+1}\mathbf{s}_k = \mathbf{y}_k$ (secant condition)

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BFGS formula:

$$M_{k+1} = M_k - \frac{M_k \mathbf{s}\mathbf{s}^\top M_k}{\mathbf{s}^\top M_k \mathbf{s}} + \frac{\mathbf{y}\mathbf{y}^\top}{\mathbf{s}^\top \mathbf{y}}, \quad M_0 = I$$

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See "Powell's trick" ensure $M_{k+1} > 0$

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- It can be shown that $M_k \rightarrow H(\mathbf{w})$, then $\kappa_k \rightarrow 0$
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Obs: BFGS typically yields **dense Hessian** approximations, whereas the exact Hessian may be sparse. Factorization can become *unnecessarily* expensive !!

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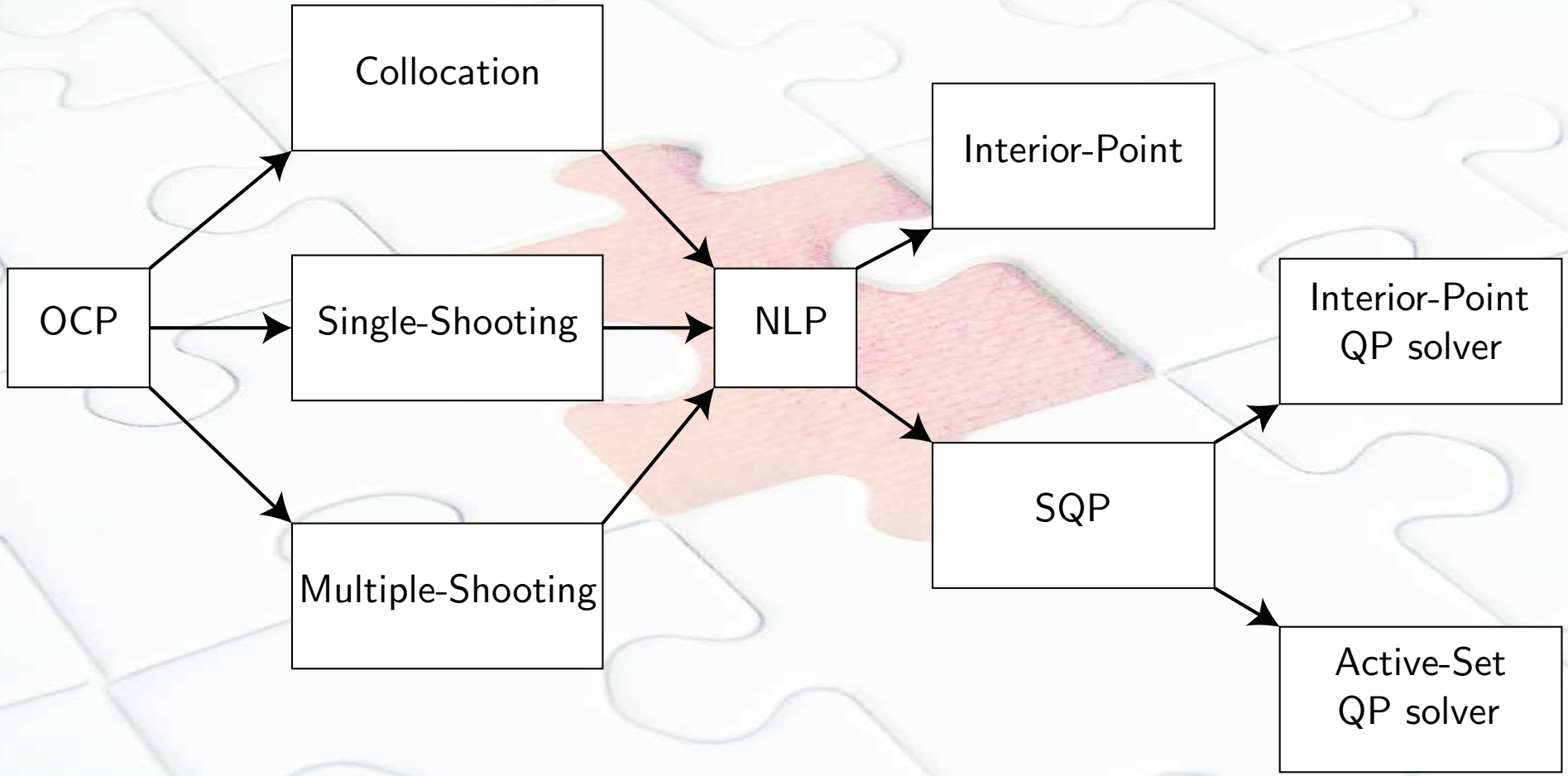
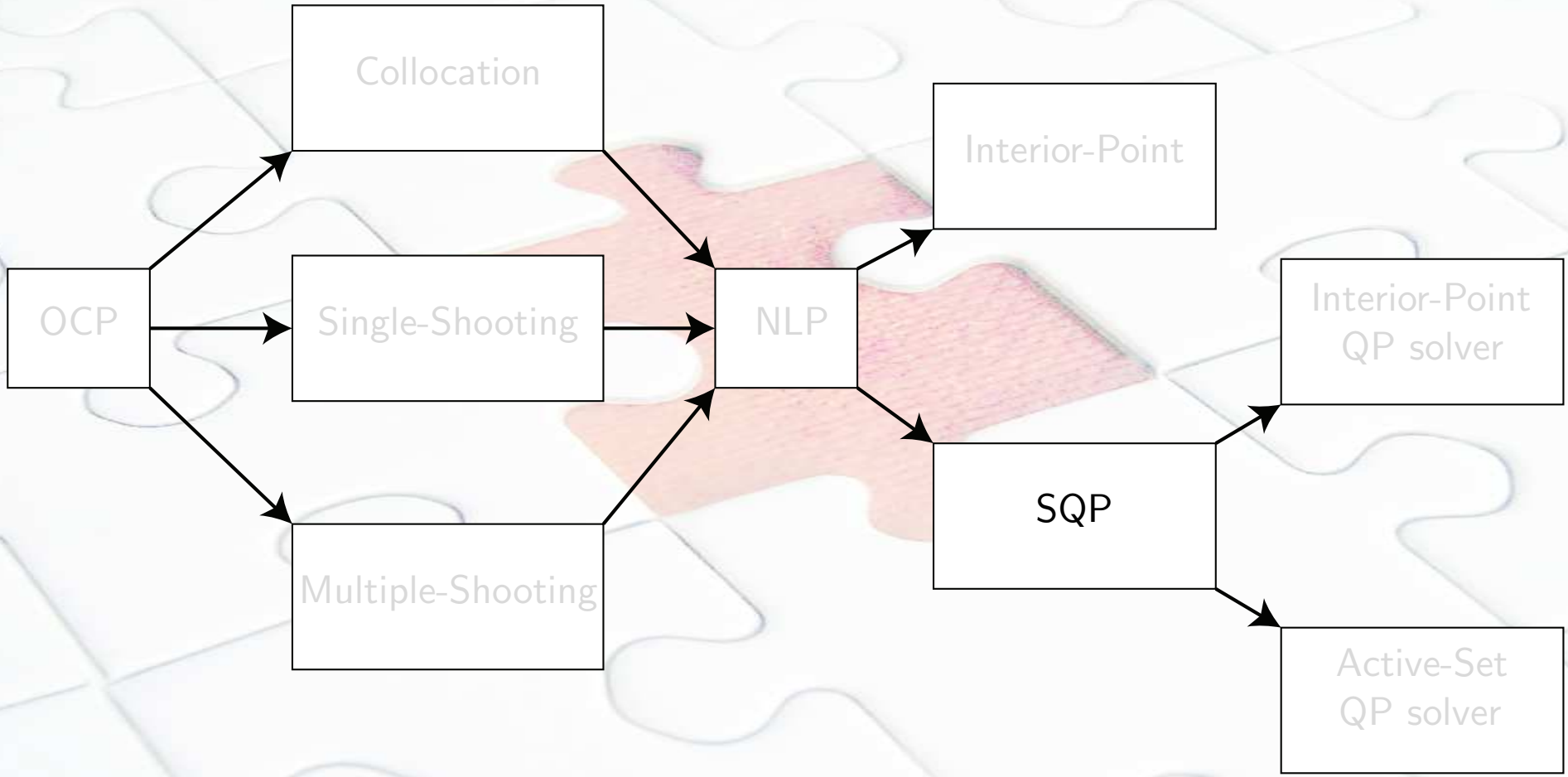
Survival map of Direct Optimal Control



Survival map of Direct Optimal Control



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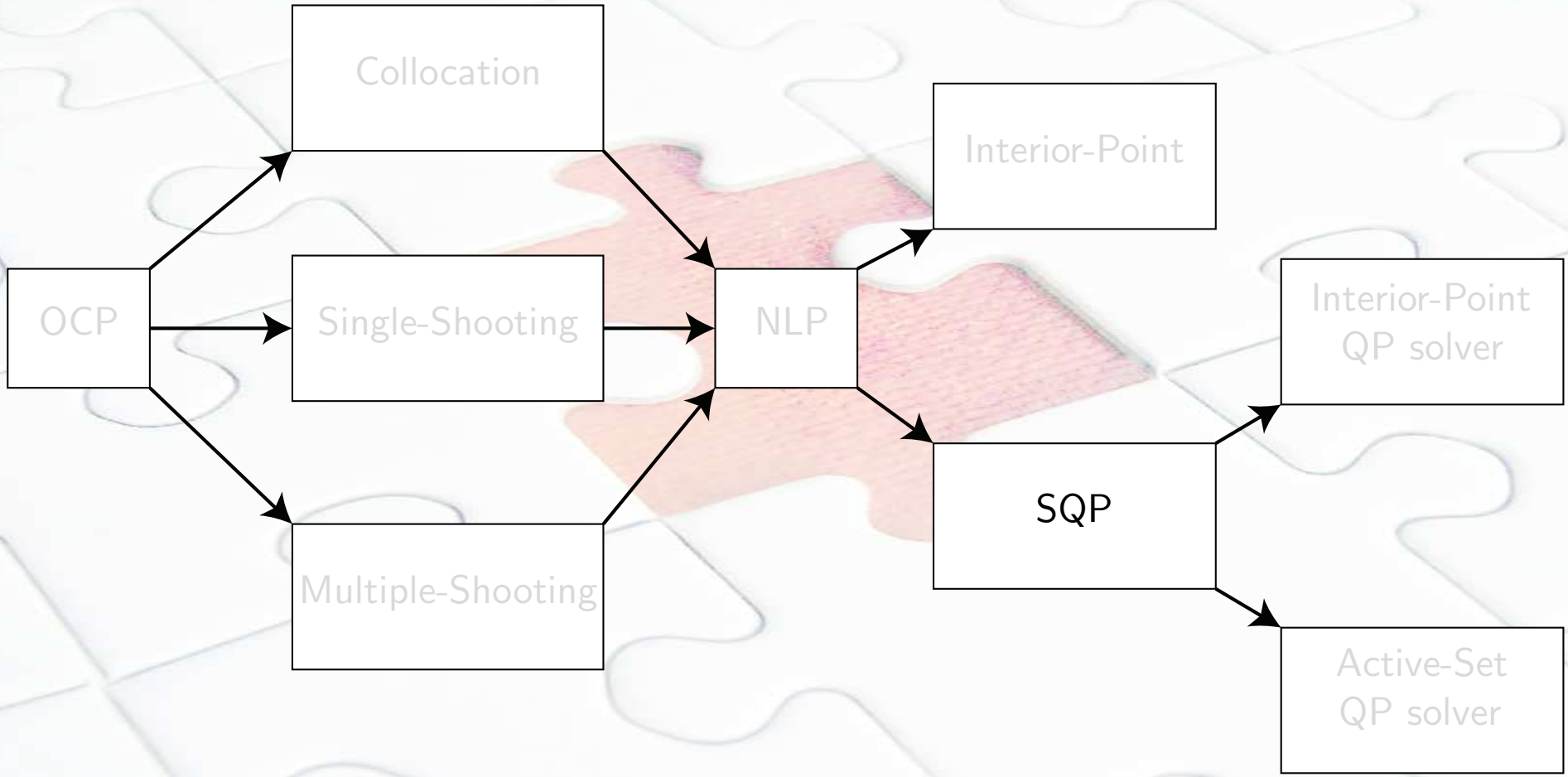

What about inequality constraints ?

Find the "primal-dual" variables $\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\lambda}$ such that:

Primal Feasibility:	$\mathbf{g}(\mathbf{w}) = 0, \quad \mathbf{h}(\mathbf{w}) \leq 0,$
Dual Feasibility:	$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \boldsymbol{\mu}, \boldsymbol{\lambda}) = 0, \quad \boldsymbol{\mu} \geq 0,$
Complementarity Slackness:	$\mu_i \mathbf{h}_i(\mathbf{w}) = 0, \quad i = 1, \ldots$

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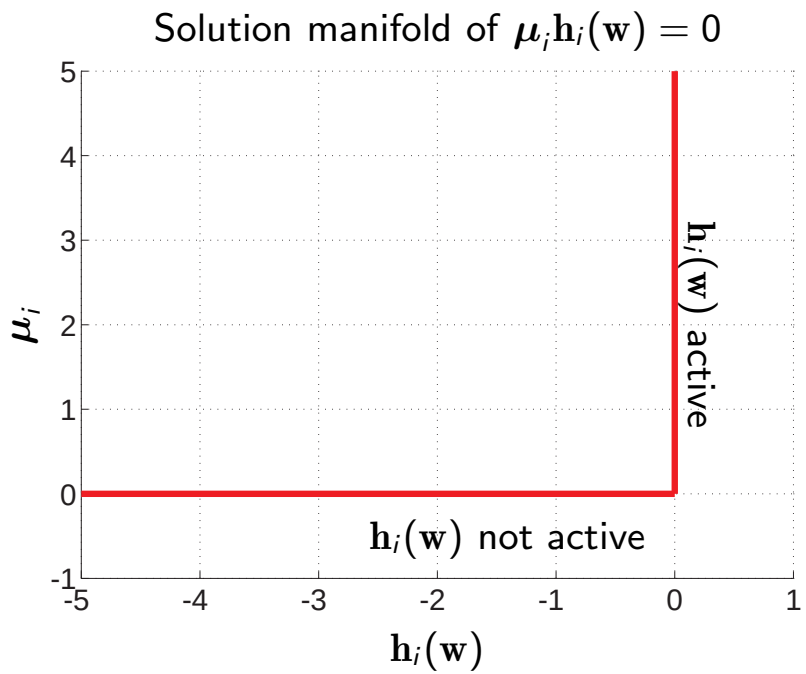

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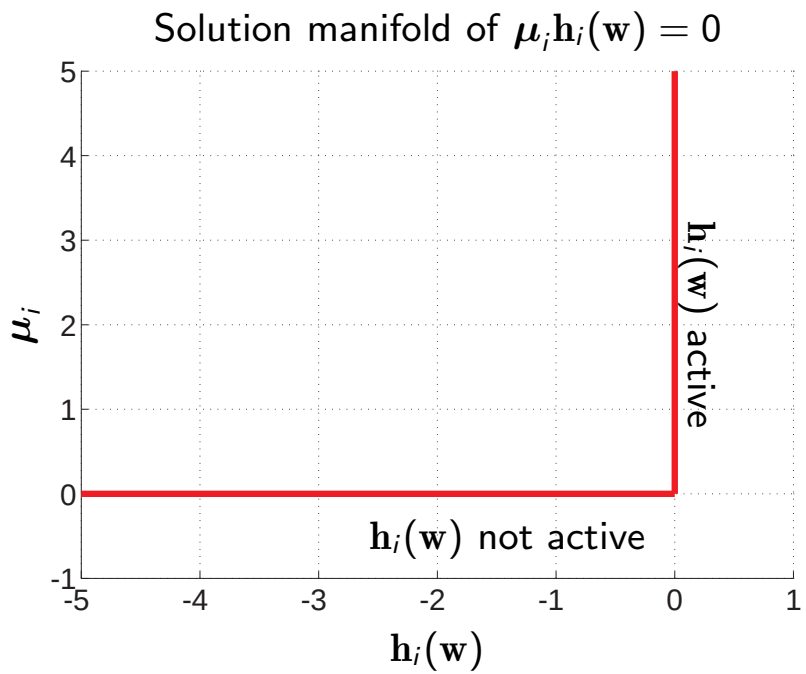

Manifold generated by the Complementarity Slackness condition is not-smooth, Newton can not be used !!

Quadratic model interpretation

Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \end{array}$$

The Newton direction is given by

$$\begin{bmatrix} H(\mathbf{w},\boldsymbol{\lambda}) & \nabla \mathbf{g}(\mathbf{w}) \\ \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \Delta \mathbf{w} \\ \boldsymbol{\lambda}^{+} \end{bmatrix} = - \begin{bmatrix} \nabla \Phi(\mathbf{w}) \\ \mathbf{g}(\mathbf{w}) \end{bmatrix}$$

with $H(\mathbf{w},\boldsymbol{\lambda}) = \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w},\boldsymbol{\lambda})$

Quadratic model interpretation

Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \end{array}$$

The Newton direction is given by

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with $H(\mathbf{w},\boldsymbol{\lambda}) = \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w},\boldsymbol{\lambda})$

The Newton direction is given by the Quadratic Program (QP):

$$\begin{array}{ll} \min\limits_{\Delta \mathbf{w}} & \frac{1}{2} \Delta \mathbf{w}^{\mathsf{T}} H(\mathbf{w},\boldsymbol{\lambda}) \Delta \mathbf{w} + \nabla \Phi(\mathbf{w})^{\mathsf{T}} \Delta \mathbf{w} \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) + \nabla \mathbf{g}(\mathbf{w})^{\mathsf{T}} \Delta \mathbf{w} = 0 \end{array}$$

Quadratic model interpretation

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$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \end{array}$$

The Newton direction is given by

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Dual variables $\boldsymbol{\lambda}^{+}$ given by the dual variables of the QP, i.e. $\boldsymbol{\lambda}^{+} = \boldsymbol{\lambda}_{\mathrm{QP}}$

Quadratic model interpretation

Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \end{array}$$

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Dual variables $\boldsymbol{\lambda}^{+}$ given by the dual variables of the QP, i.e. $\boldsymbol{\lambda}^{+} = \boldsymbol{\lambda}_{\mathrm{QP}}$

Proof: KKT of the QP are equivalent to the linearised KKT system of the original problem.

Quadratic interpretation for inequality constraints

Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \\ \text{s.t.} & \mathbf{h}(\mathbf{w}) \leq 0 \end{array}$$

Quadratic interpretation for inequality constraints

Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \\ \text{s.t.} & \mathbf{h}(\mathbf{w}) \leq 0 \end{array}$$

The Newton direction is given by the Quadratic Program (QP):

$$\begin{array}{ll} \min\limits_{\Delta\mathbf{w}} & \frac{1}{2}\Delta\mathbf{w}^{\mathsf{T}} H(\mathbf{w},\boldsymbol{\lambda},\boldsymbol{\mu})\Delta\mathbf{w} + \nabla\Phi(\mathbf{w})^{\mathsf{T}}\Delta\mathbf{w} \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) + \nabla\mathbf{g}(\mathbf{w})^{\mathsf{T}}\Delta\mathbf{w} = 0 \\ & \mathbf{h}(\mathbf{w}) + \nabla\mathbf{h}(\mathbf{w})^{\mathsf{T}}\Delta\mathbf{w} \leq 0 \end{array}$$

with $H(\mathbf{w},\boldsymbol{\lambda}) = \nabla^2_{\mathbf{w}}\mathcal{L}(\mathbf{w},\boldsymbol{\lambda})$

Quadratic interpretation for inequality constraints

Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & \Phi(\mathbf{w}) \\ \text{s.t.} & \mathbf{g}(\mathbf{w}) = 0 \\ \text{s.t.} & \mathbf{h}(\mathbf{w}) \leq 0 \end{array}$$

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with $H(\mathbf{w},\boldsymbol{\lambda}) = \nabla^2_{\mathbf{w}}\mathcal{L}(\mathbf{w},\boldsymbol{\lambda})$

Dual variables $\boldsymbol{\lambda}^+$ and $\boldsymbol{\mu}^+$ given by the dual variables of the QP, i.e.

$$\boldsymbol{\lambda}^+ = \boldsymbol{\lambda}_{\text{QP}}, \quad \boldsymbol{\mu}^+ = \boldsymbol{\mu}_{\text{QP}}$$

SQP - Monitoring progress with the T_1 merit function:

$$T_1(\mathbf{w}) = \Phi(\mathbf{w}) + \nu\|\mathbf{g}(\mathbf{w})\|_1 + \nu\sum_{i=1}^{m}\max(0, \mathbf{h}_i(\mathbf{w}))$$

Algorithm: SQP with line-search

Input: guess $\mathbf{w}$, $\boldsymbol{\lambda}$, $\boldsymbol{\mu}$

while $\|\nabla\mathcal{L}\|$ *or* $\|\mathbf{g}\|$ *or* $\max(0, \mathbf{h}) \geq \text{tol}$ **do**

Compute $\mathbf{g}$, $\mathbf{h}$, $\nabla\Phi(\mathbf{w})$, $\nabla\mathbf{g}(\mathbf{w})$, $\nabla\mathbf{h}(\mathbf{w})$, $H(\mathbf{w}, \boldsymbol{\mu}, \boldsymbol{\lambda})$

Compute Newton direction by solving the QP

$$\begin{aligned} \min_{\Delta\mathbf{w}} \quad & \frac{1}{2}\Delta\mathbf{w}^T H(\mathbf{w}, \boldsymbol{\lambda}, \boldsymbol{\mu})\Delta\mathbf{w} + \nabla\Phi(\mathbf{w})^T\Delta\mathbf{w} \\ \text{s.t.} \quad & \mathbf{g}(\mathbf{w}) + \nabla\mathbf{g}(\mathbf{w})^T\Delta\mathbf{w} = 0 \\ & \mathbf{h}(\mathbf{w}) + \nabla\mathbf{h}(\mathbf{w})^T\Delta\mathbf{w} \leq 0 \end{aligned}$$

Perform line-search on $T_1(\mathbf{w} + \alpha\Delta\mathbf{w})$, get step length α

Take primal step: $\mathbf{w} \leftarrow \mathbf{w} + \alpha\Delta\mathbf{w}$

Take dual step: $\boldsymbol{\lambda} \leftarrow (1-\alpha)\boldsymbol{\lambda} + \alpha\boldsymbol{\lambda}_{QP}$, $\boldsymbol{\mu} \leftarrow (1-\alpha)\boldsymbol{\mu} + \alpha\boldsymbol{\mu}_{QP}$

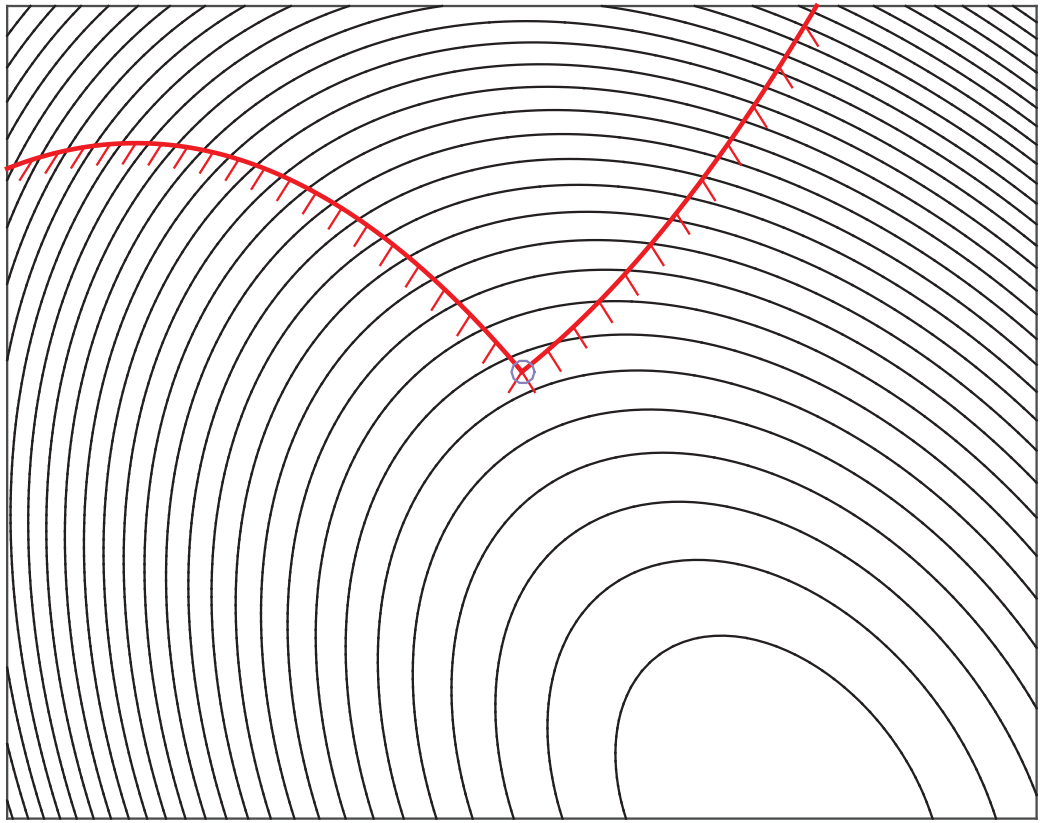
return $\mathbf{w}$, $\boldsymbol{\lambda}$, $\boldsymbol{\mu}$

If $H(\mathbf{x}_k, \boldsymbol{\mu}_k, \boldsymbol{\lambda}_k) \succ 0$ and $\nu > \max\left\{\|\boldsymbol{\mu}_{k+1}\|_\infty, \|\boldsymbol{\lambda}_{k+1}\|_\infty\right\}$ then $\Delta\mathbf{w}$ is a descent direction for $T_1(\mathbf{w})$

SQP - Illustration

NLP:

$$\begin{aligned} \min_{\mathbf{w}} \quad & \frac{1}{2} \left\| \mathbf{w} - \mathbf{w}_0 \right\|_Q^2 \\ \text{s.t.} \quad & \mathbf{h}\left(\mathbf{w}\right) \leq 0 \end{aligned}$$



QP:

$$\begin{aligned} \min_{\mathbf{w}} \quad & \frac{1}{2} \Delta \mathbf{w}^\top H\left(\mathbf{w}, \boldsymbol{\mu}\right) \Delta \mathbf{w} + \nabla \Phi\left(\mathbf{w}\right)^\top \Delta \mathbf{w} \\ \text{s.t.} \quad & \mathbf{h}\left(\mathbf{w}\right) + \nabla \mathbf{h}\left(\mathbf{w}\right)^\top \Delta \mathbf{w} \leq 0 \end{aligned}$$

Hessian:

$$H\left(\mathbf{w}, \boldsymbol{\mu}\right) = \nabla^2 \Phi\left(\mathbf{w}\right) + \nabla^2 \left(\boldsymbol{\mu}^\top \mathbf{h}\left(\mathbf{w}\right) \right)$$

SQP - Illustration

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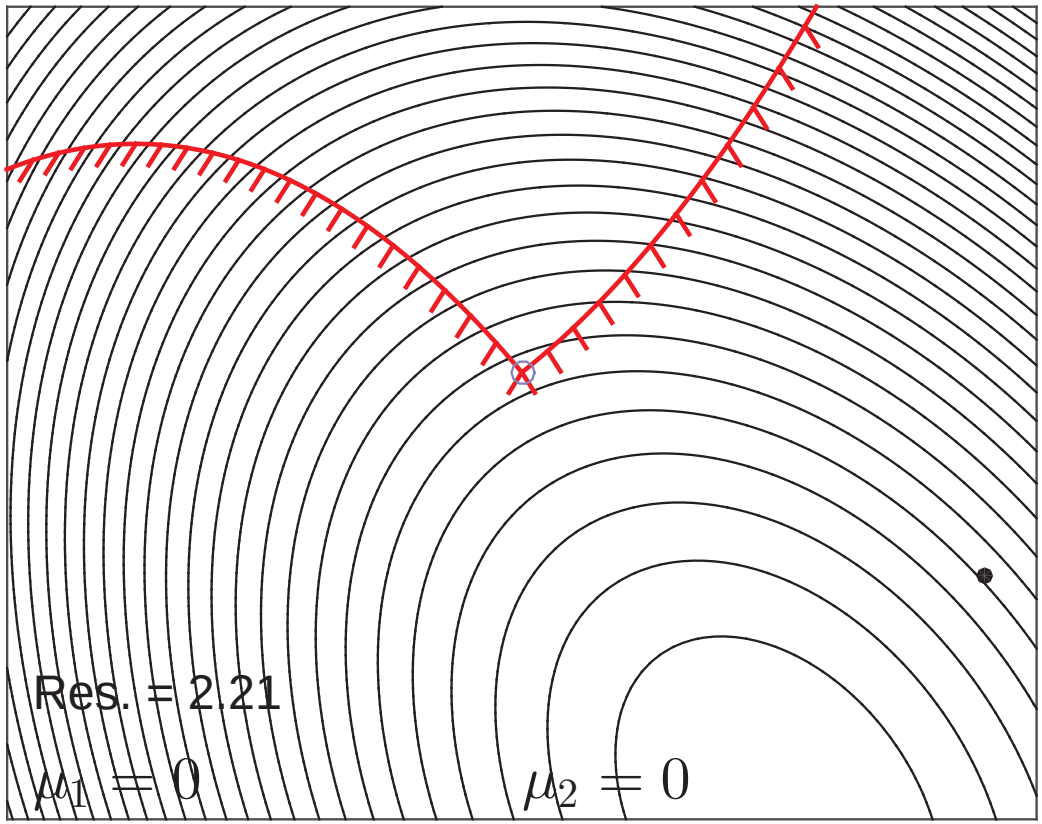

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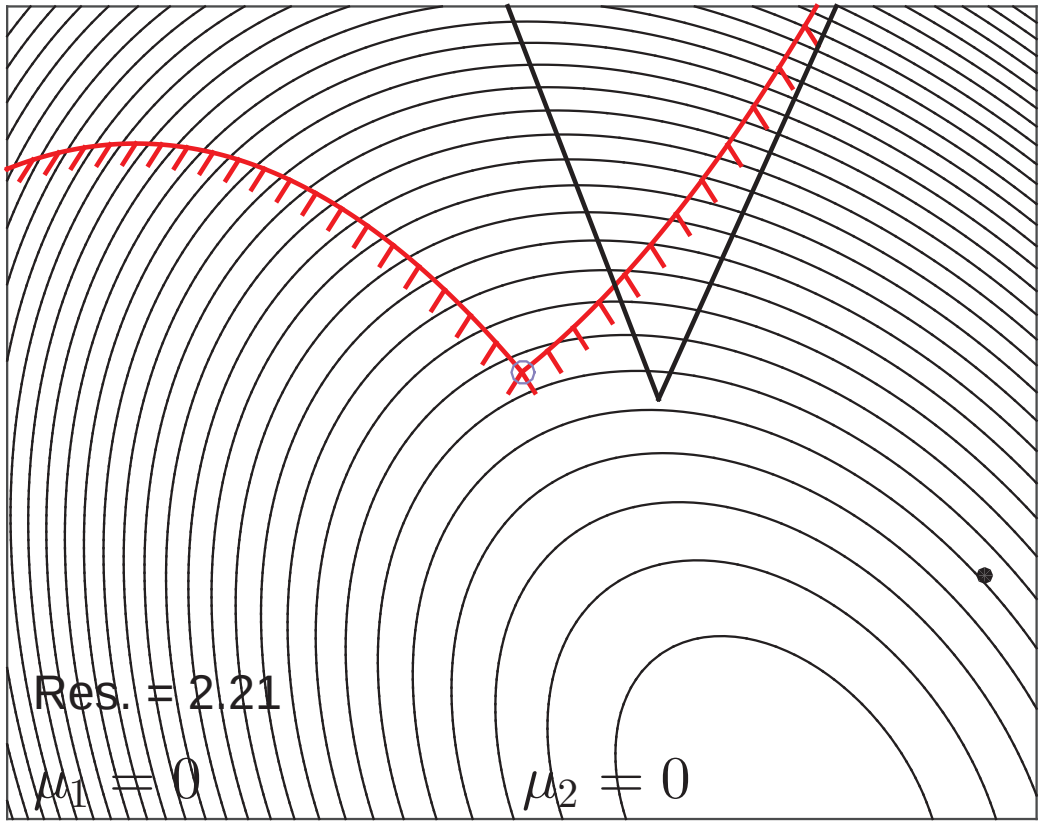
Linearized constraints



QP:

$$\begin{aligned} \min_{\mathbf{w}} \quad & \frac{1}{2} \Delta \mathbf{w}^\top H(\mathbf{w}, \boldsymbol{\mu}) \Delta \mathbf{w} + \nabla \Phi(\mathbf{w})^\top \Delta \mathbf{w} \\ \text{s.t.} \quad & \mathbf{h}(\mathbf{w}) + \nabla \mathbf{h}(\mathbf{w})^\top \Delta \mathbf{w} \leq 0 \end{aligned}$$

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SQP - Illustration

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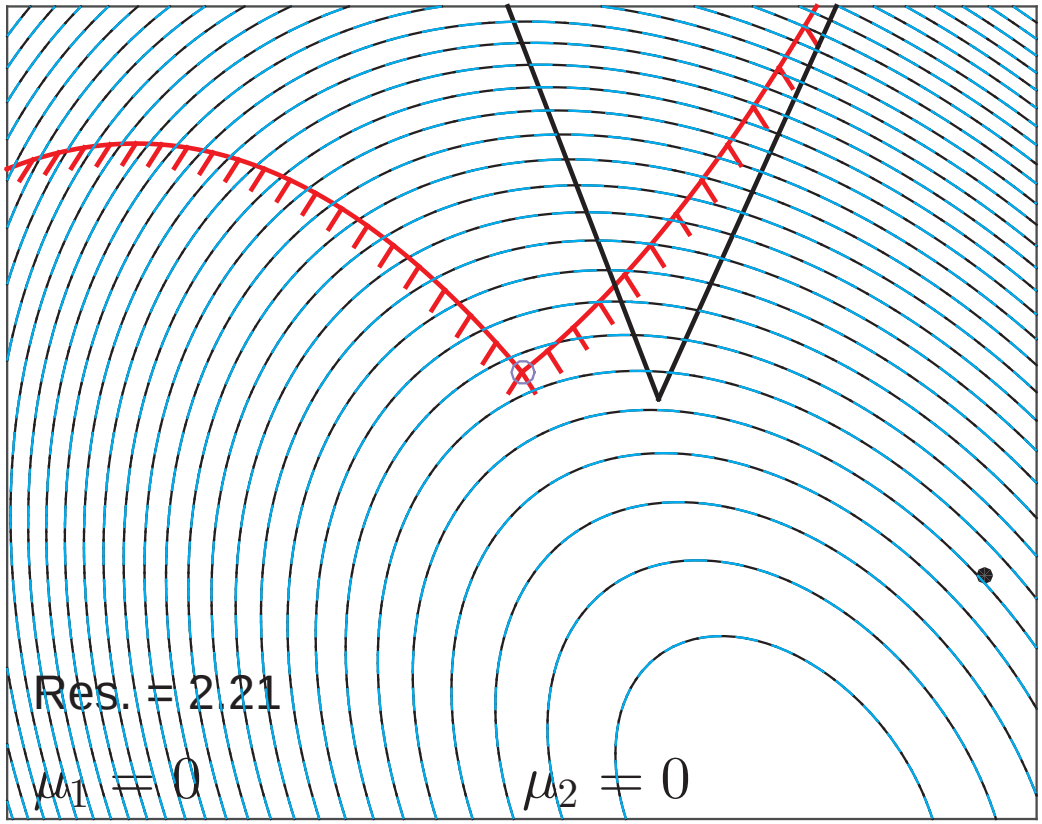
Contours of QP cost



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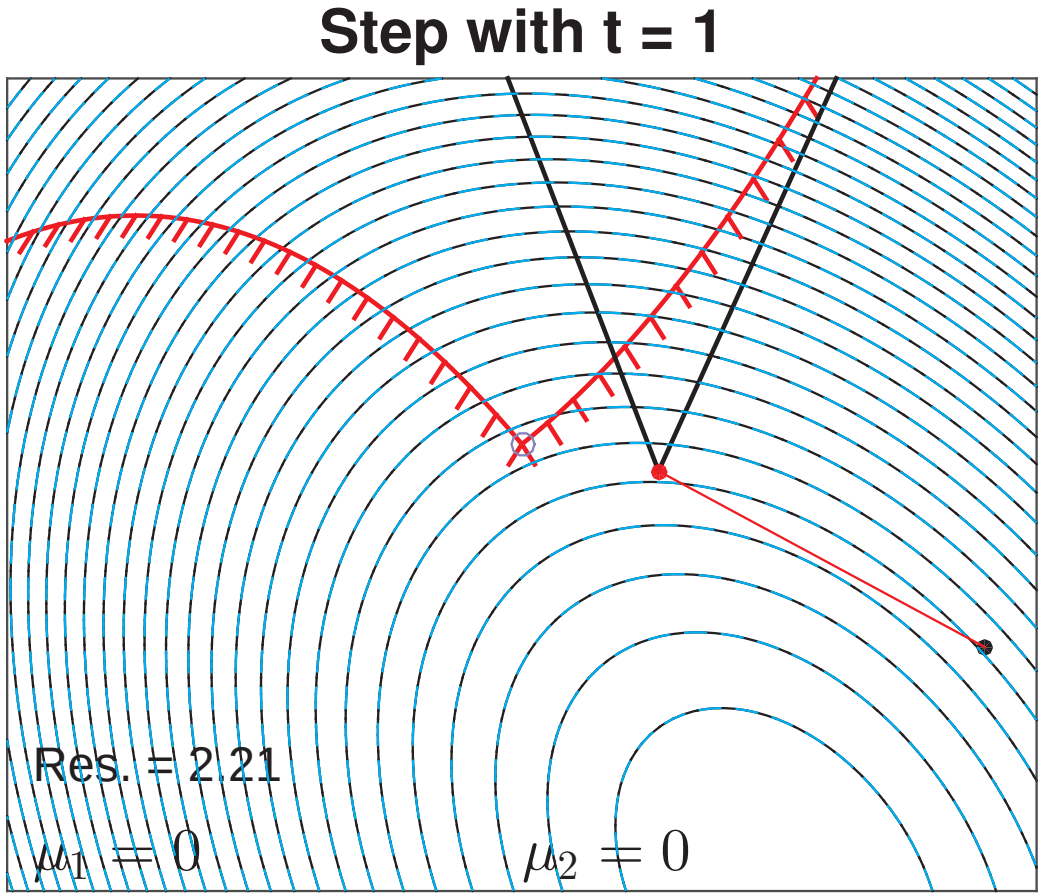

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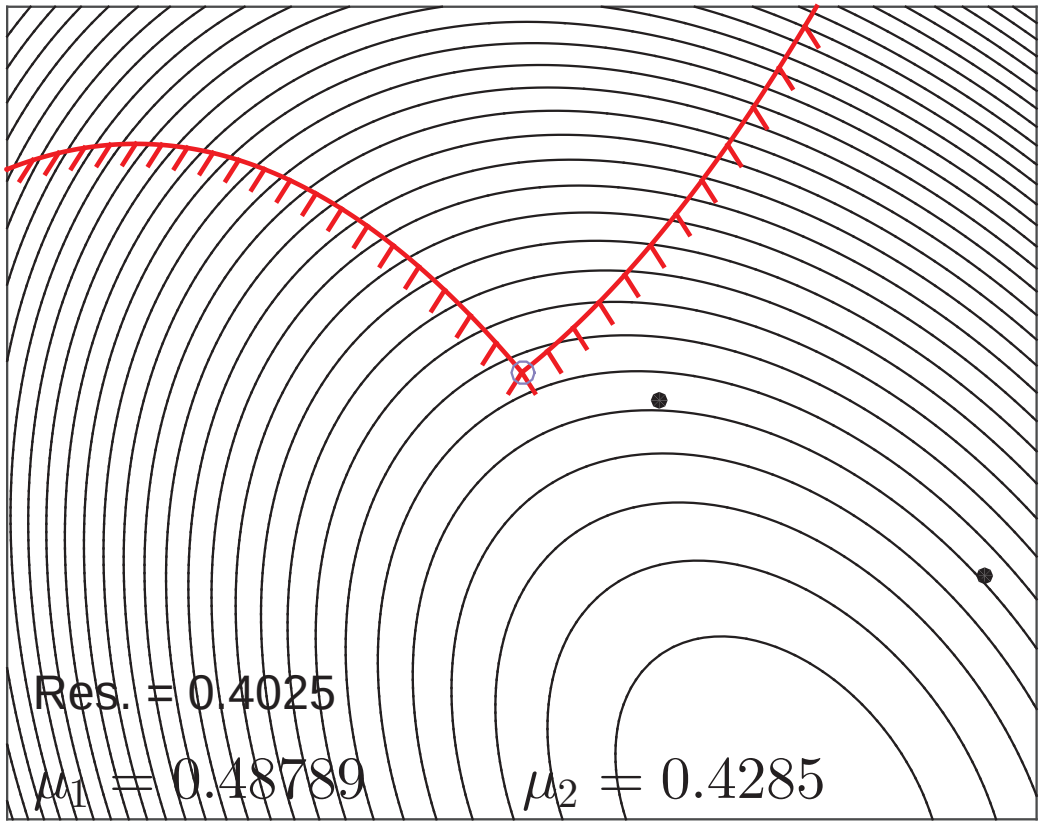

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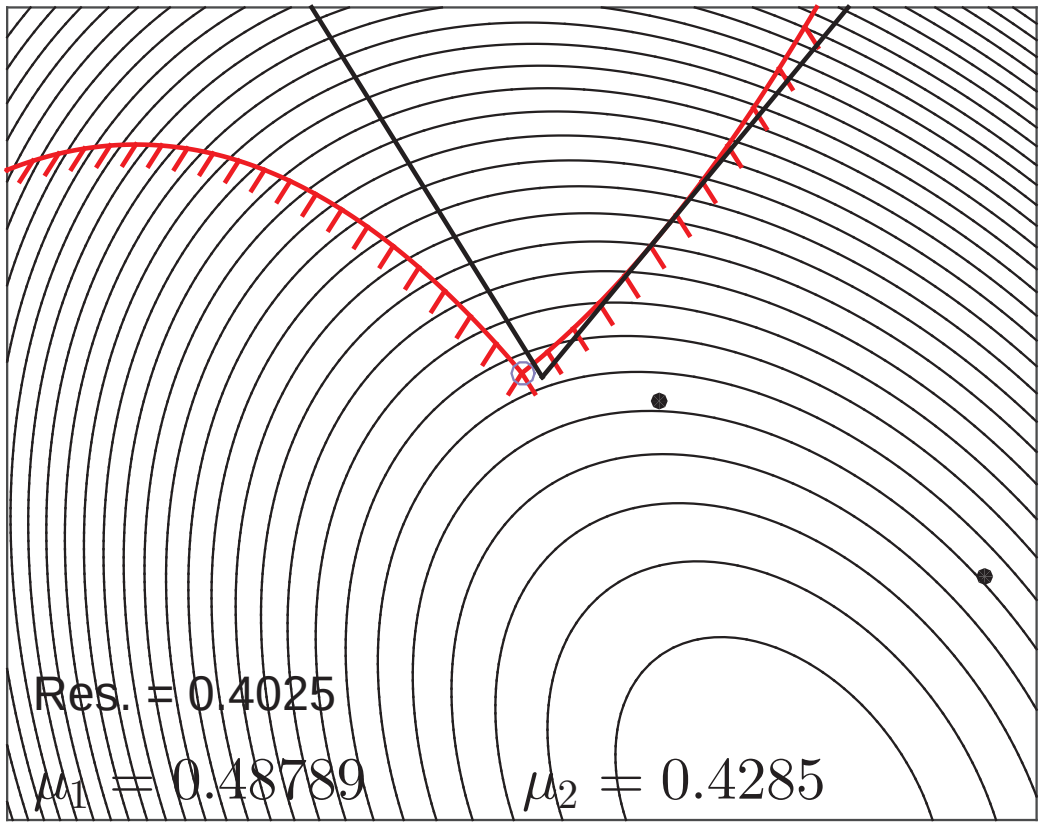

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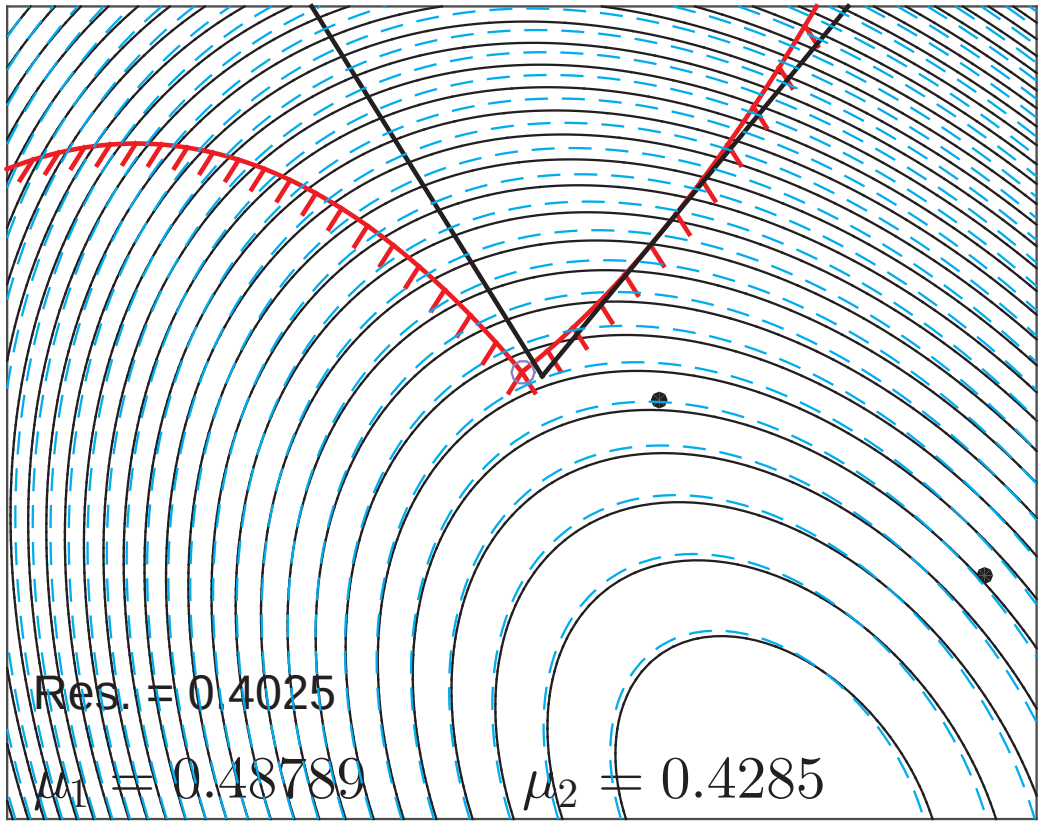
Contours of QP cost



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SQP - Illustration

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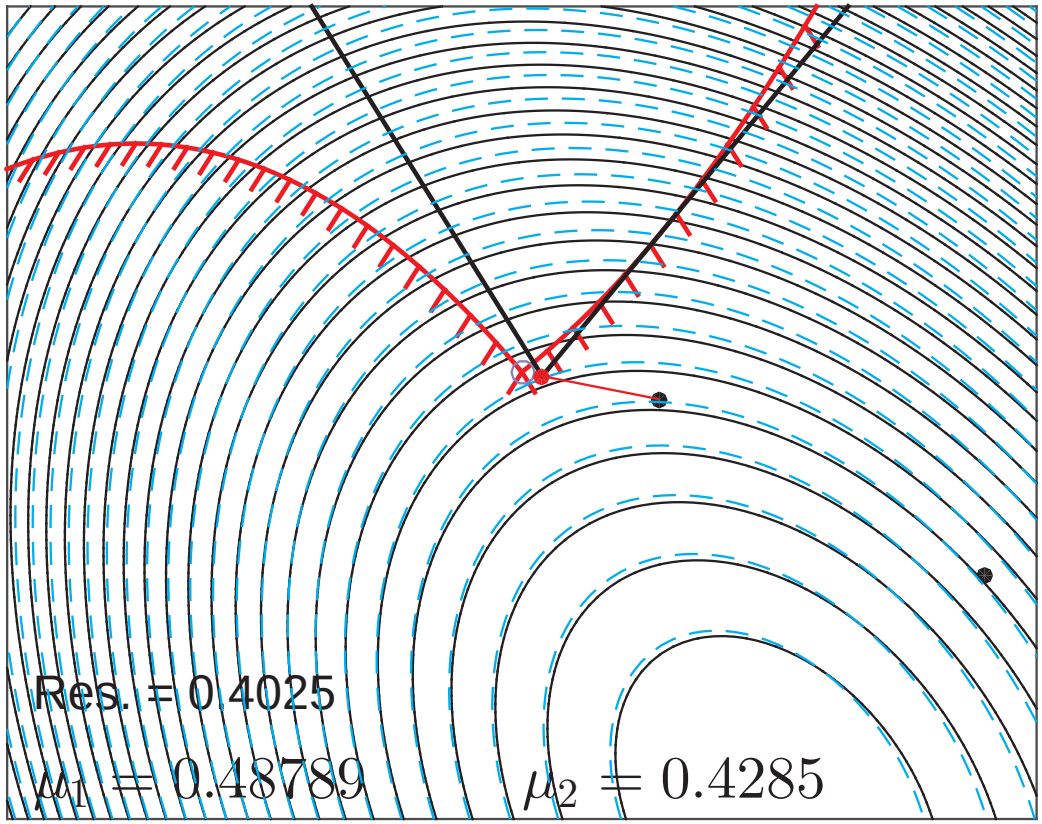
Step with t = 1



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SQP - Illustration

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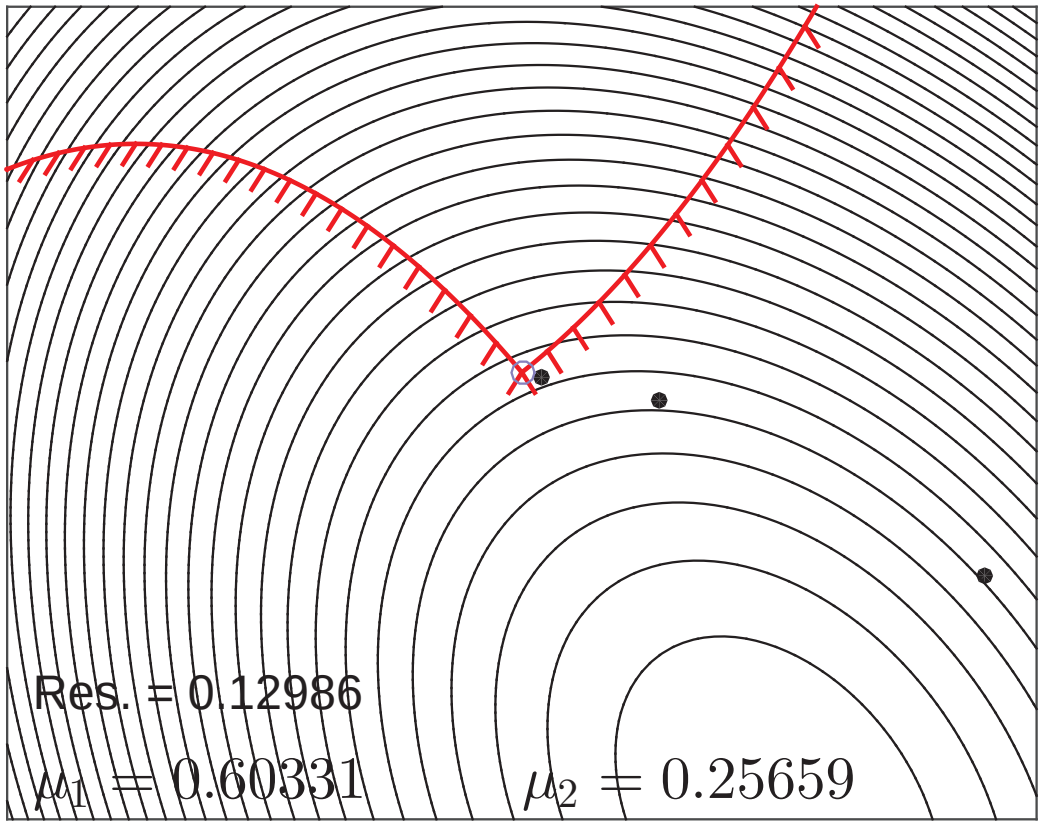

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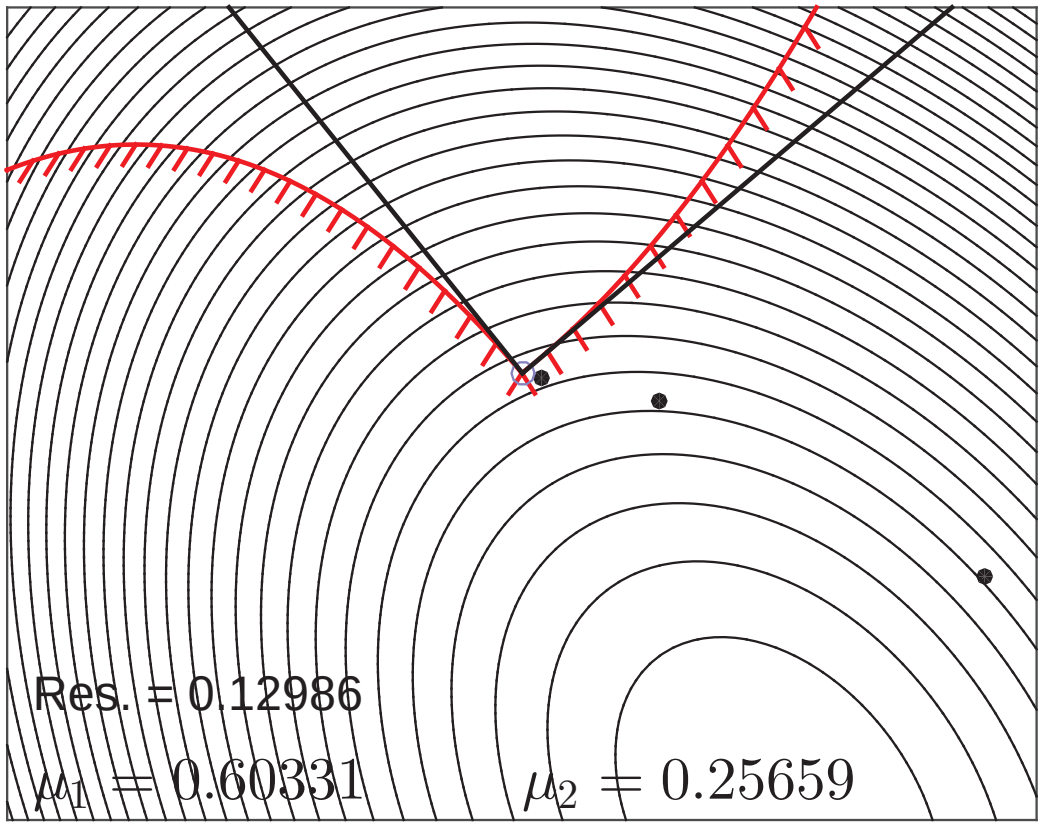

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SQP - Illustration

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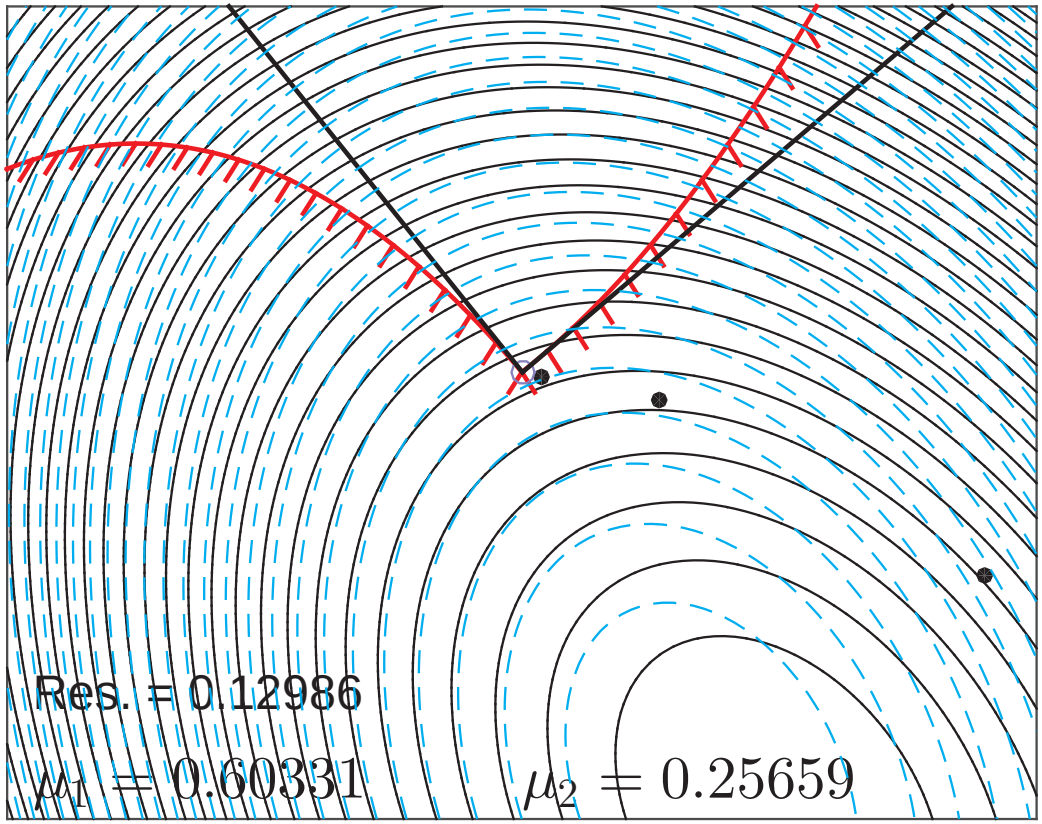
Contours of QP cost



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SQP - Illustration

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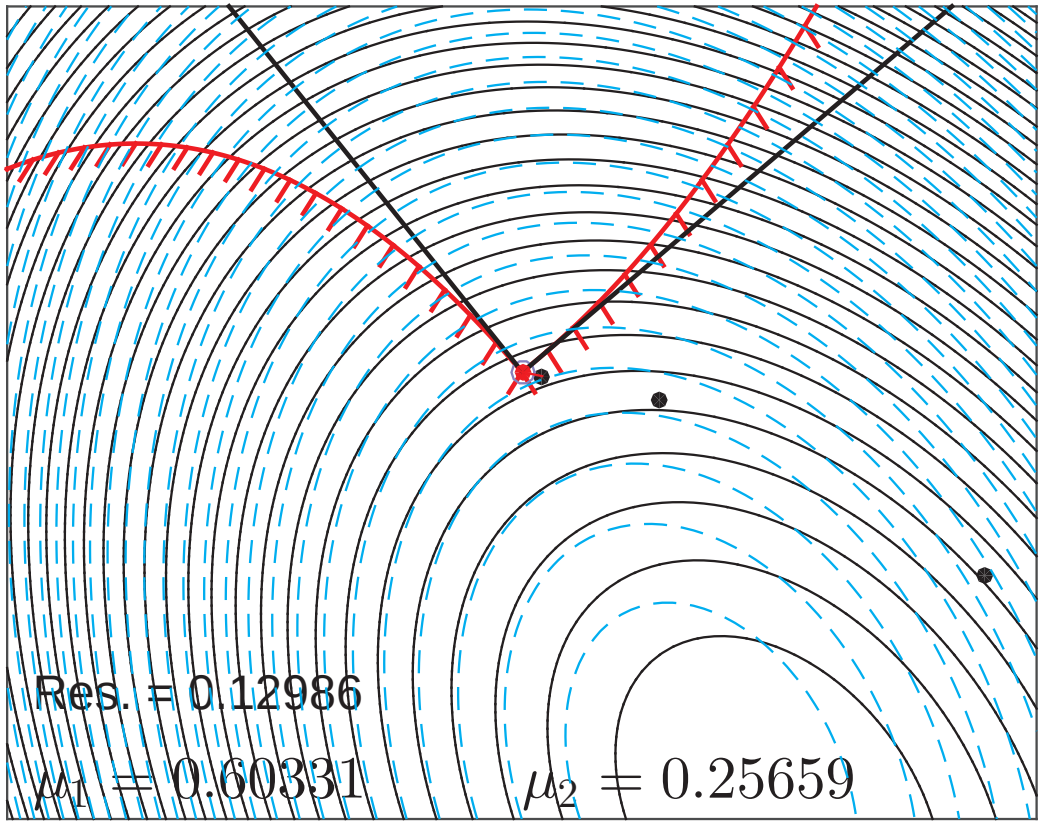
Step with t = 1



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SQP - Illustration

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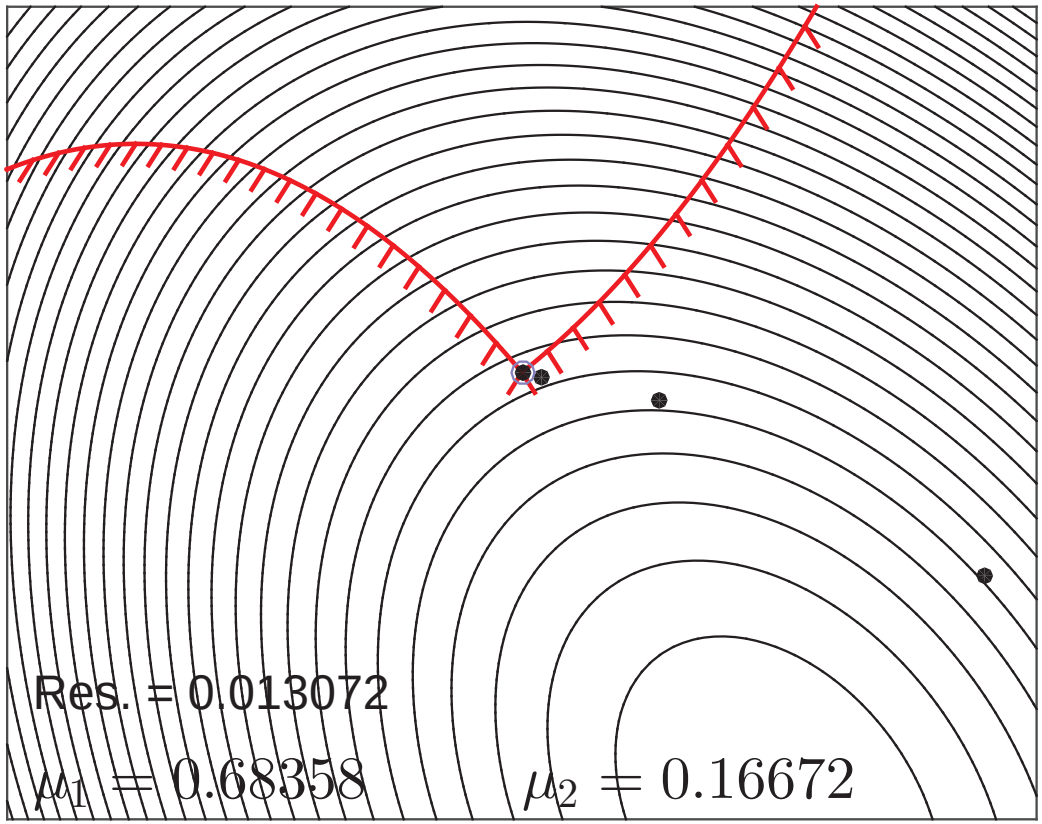
$$\begin{aligned} \min_{\mathbf{w}} \quad & \frac{1}{2} \left\| \mathbf{w} - \mathbf{w}_0 \right\|_Q^2 \\ \text{s.t.} \quad & \mathbf{h}(\mathbf{w}) \leq 0 \end{aligned}$$



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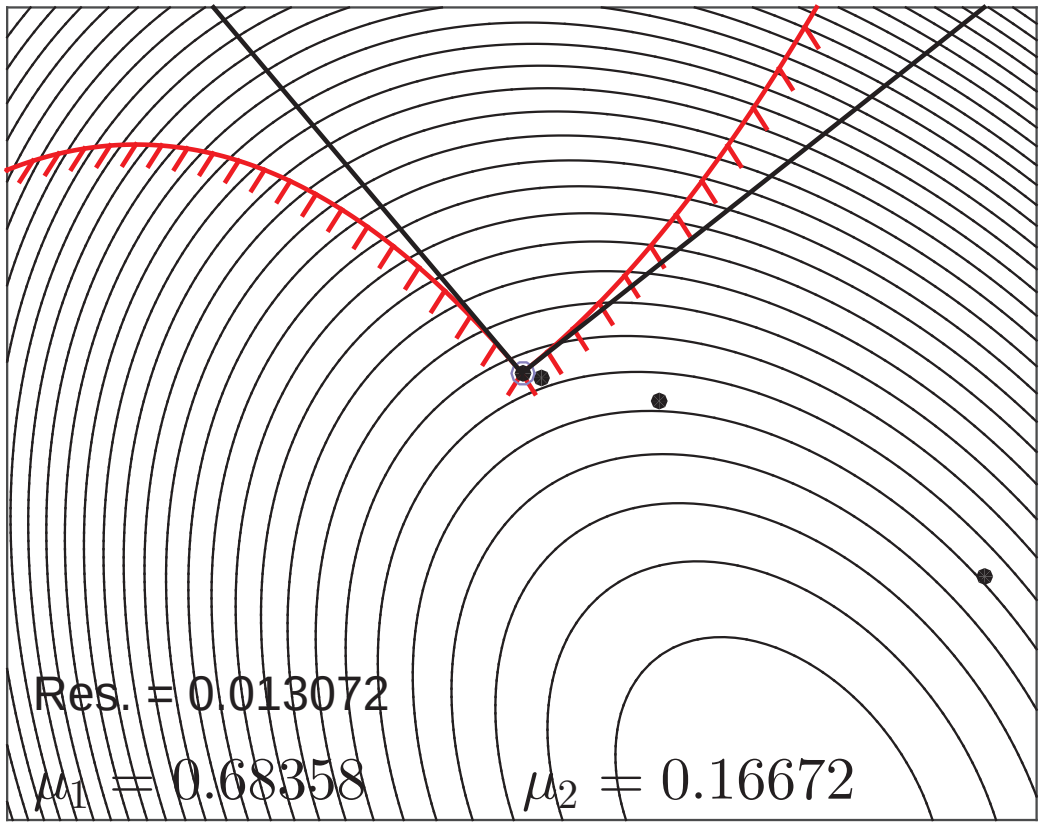

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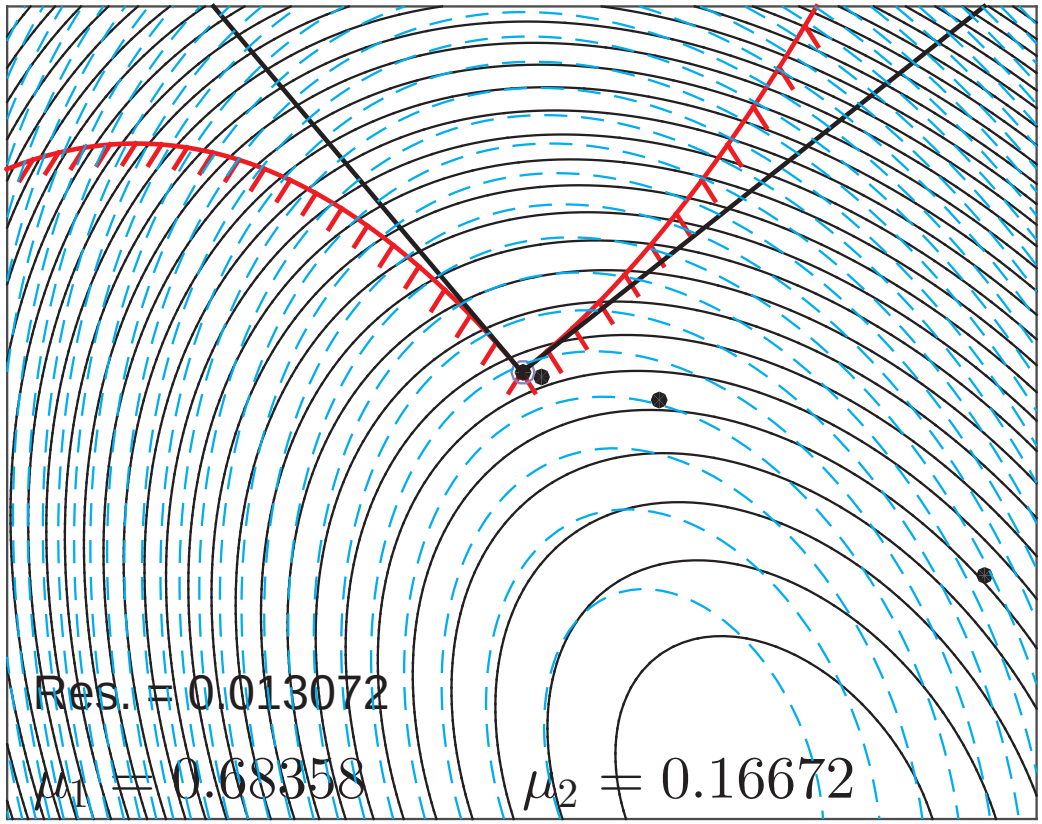

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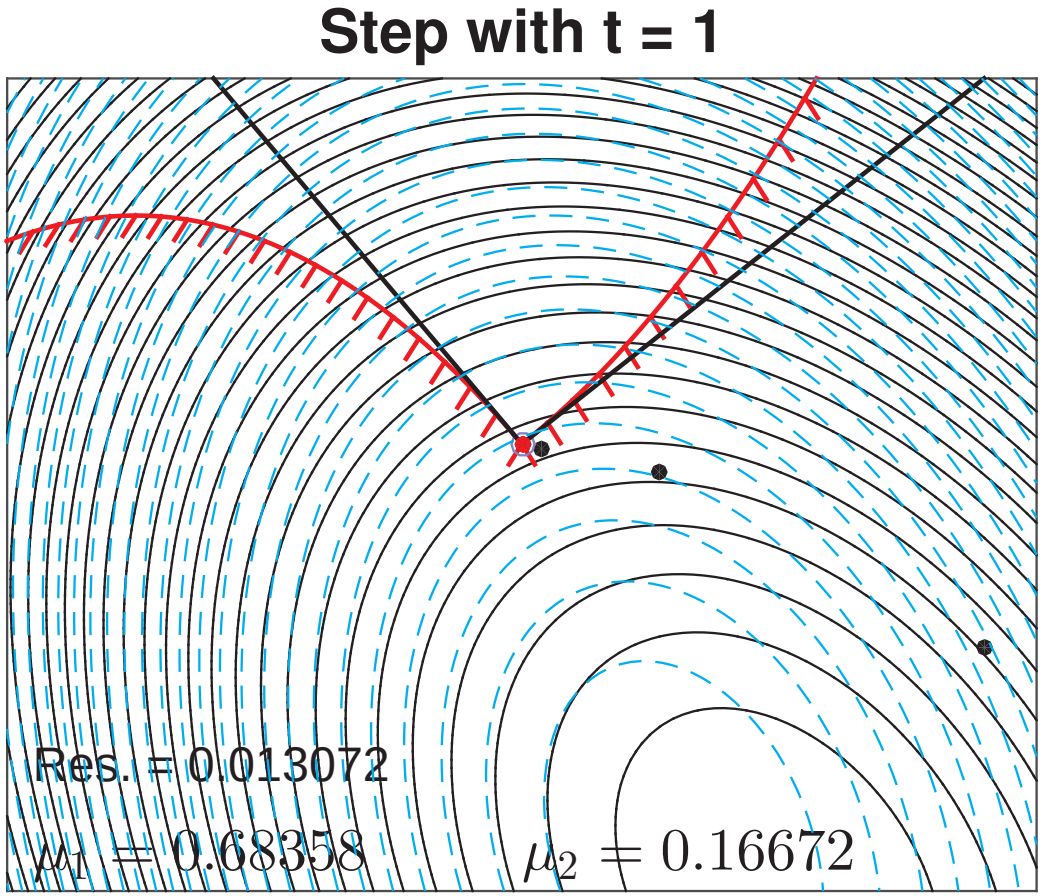

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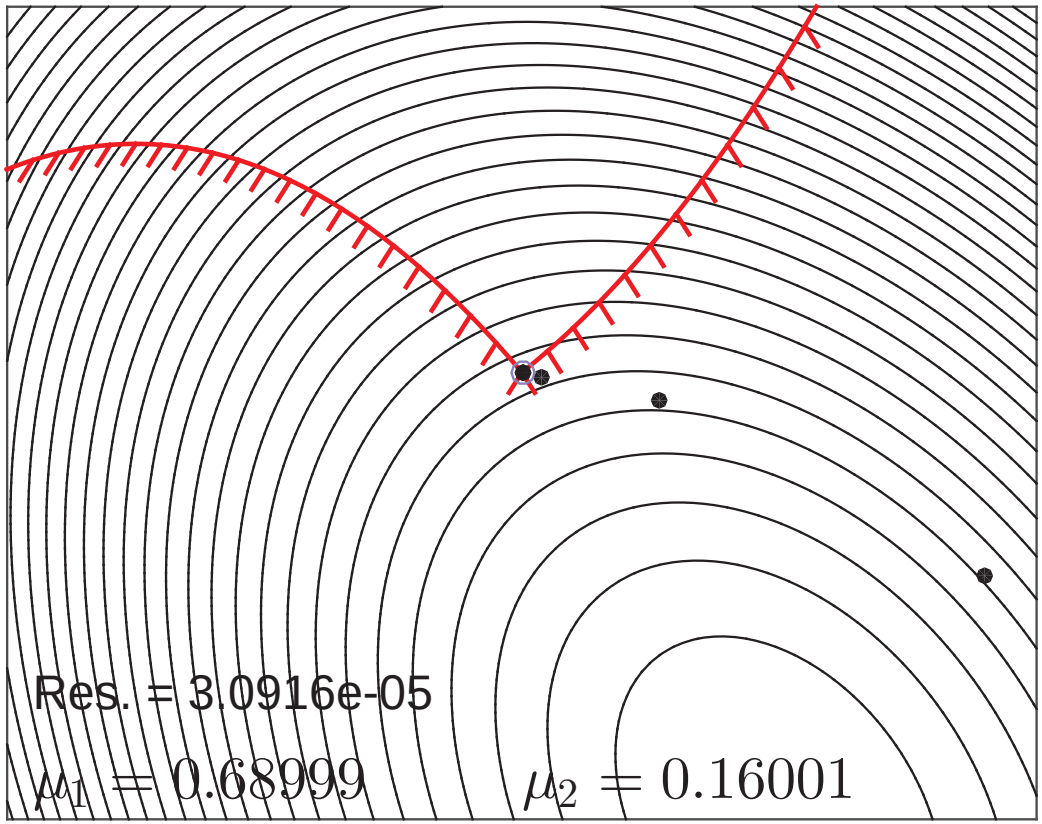

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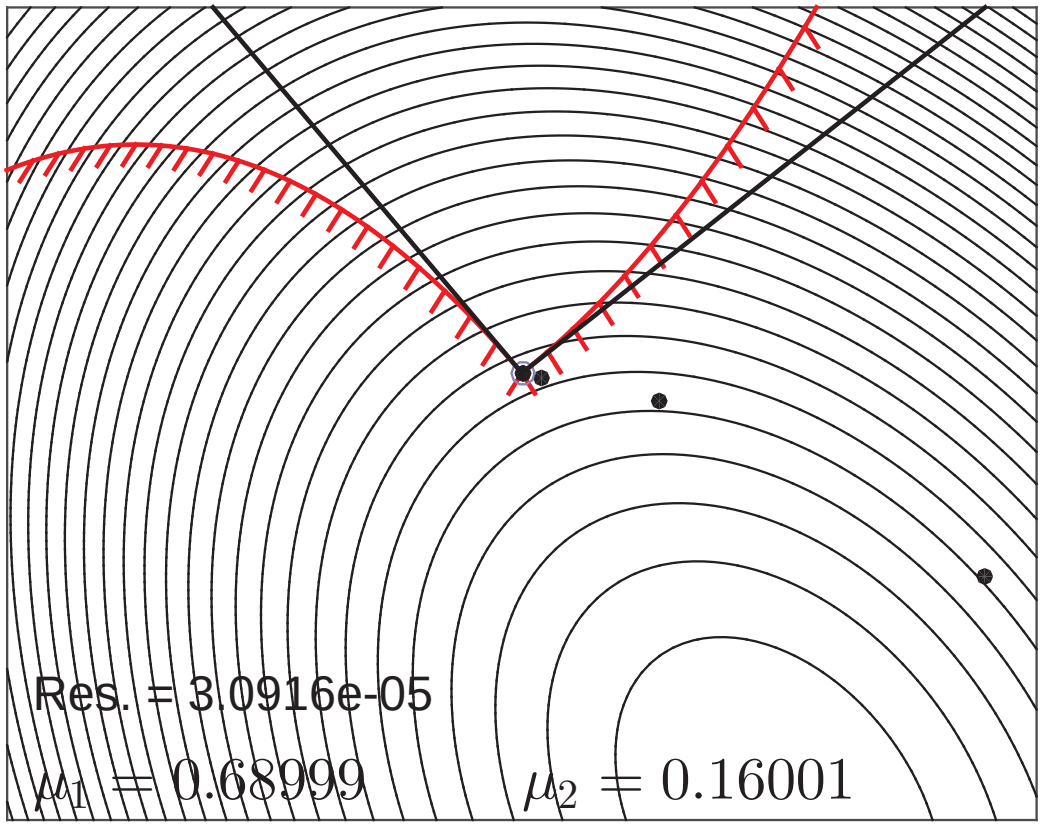

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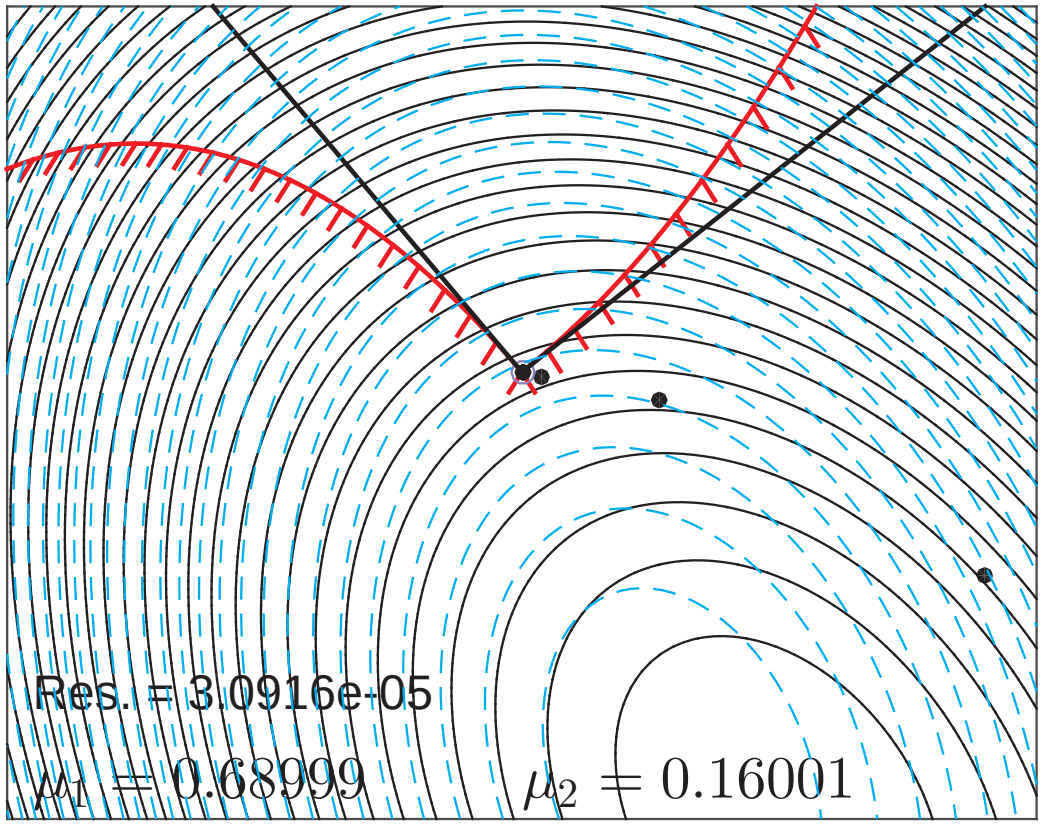

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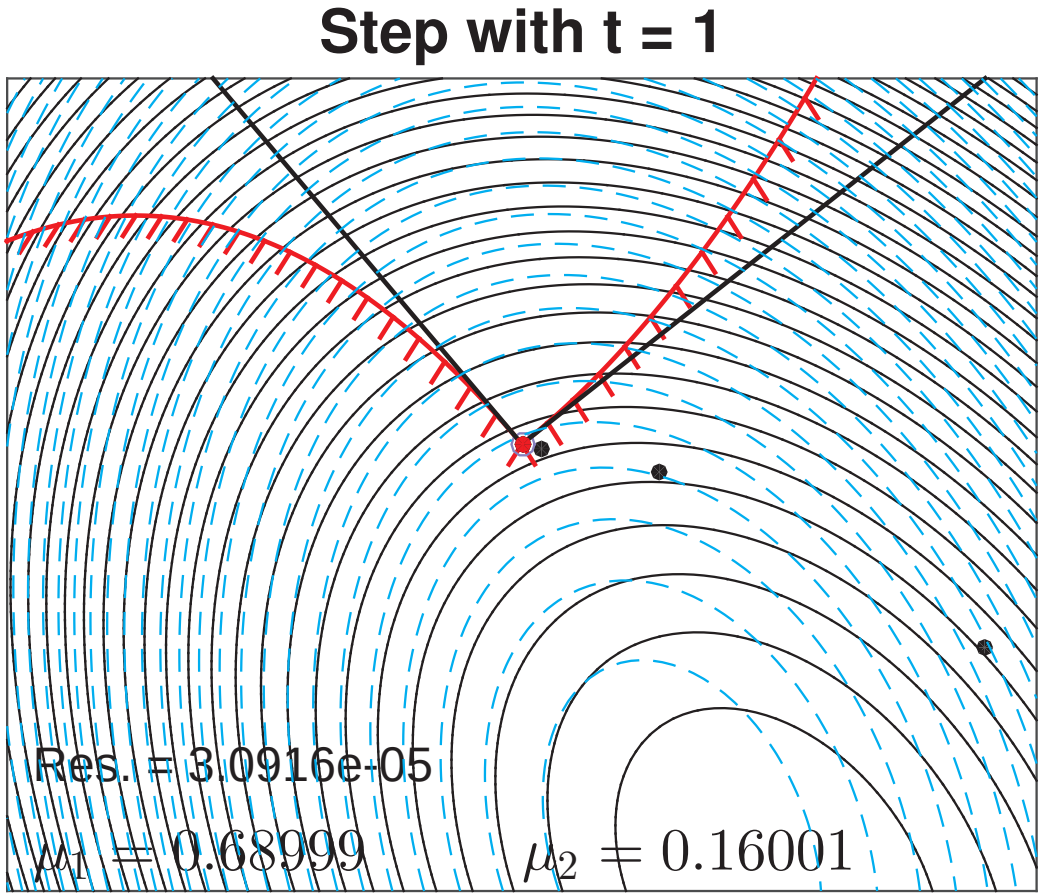

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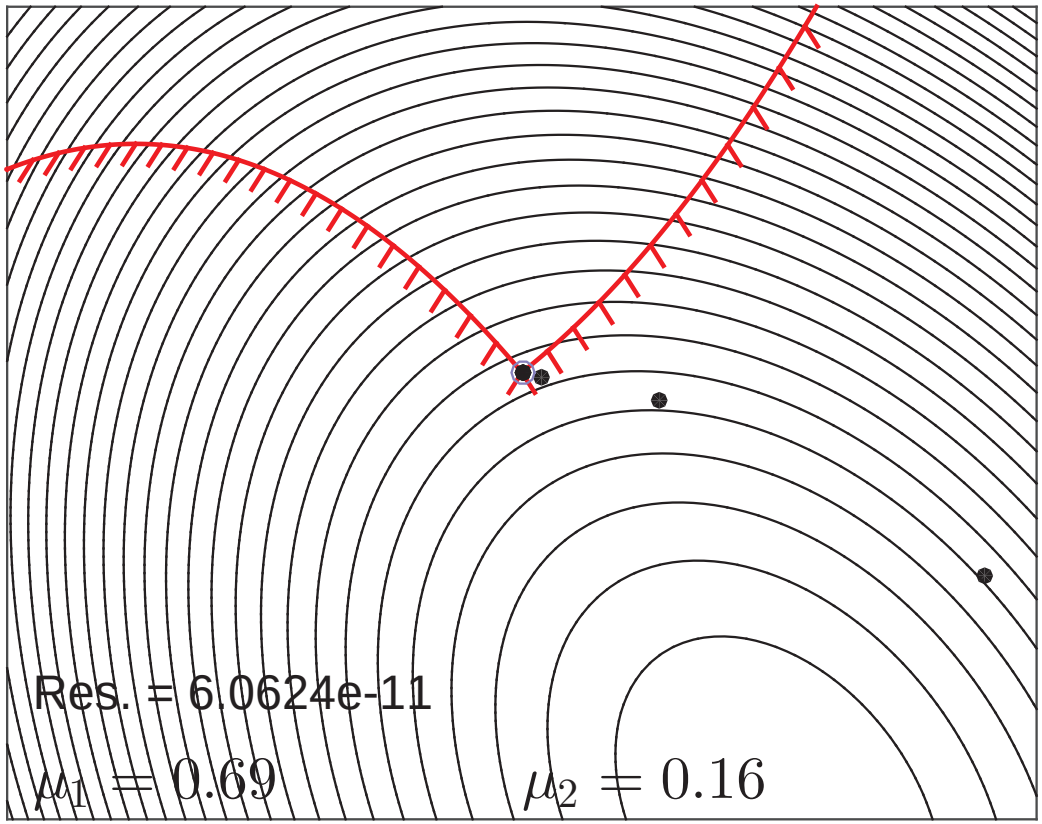

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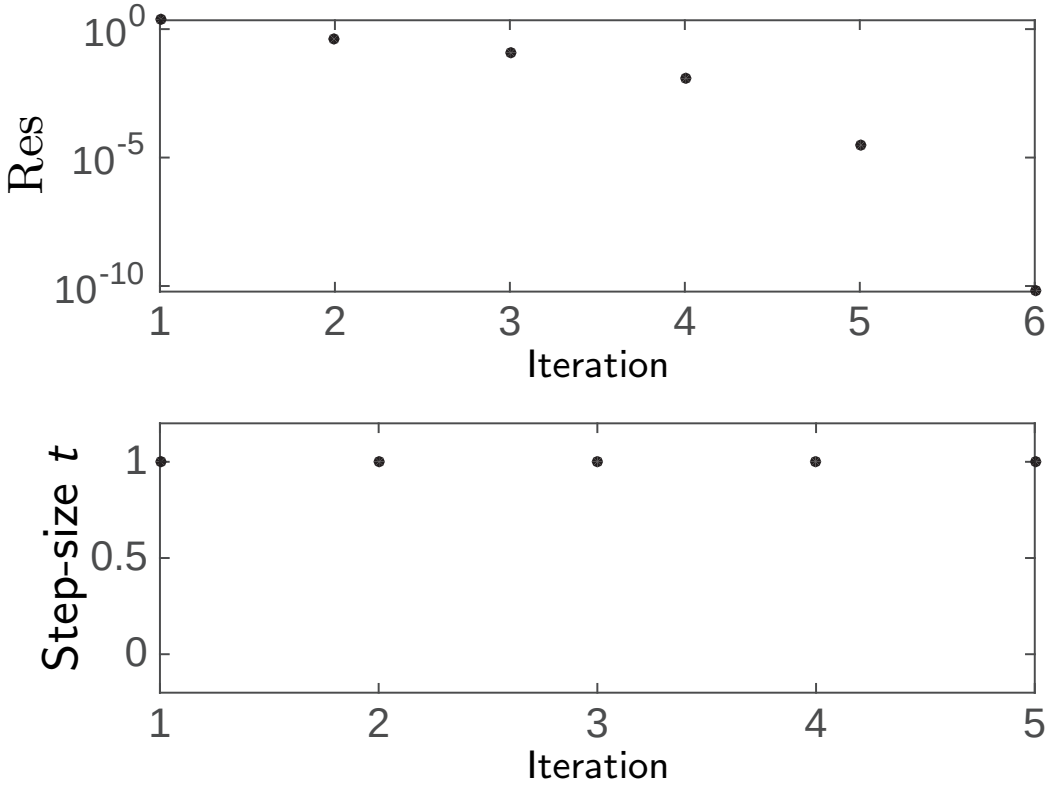

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Maratos effect

Consider the NLP :

$$\min_{u,v} \quad \Phi = 3v^2 - 2u$$

$$\text{s.t.} \quad g = u - v^2 = 0$$

Optimum: $\mathbf{w}^* = \begin{bmatrix} 0 & 0 \end{bmatrix}$.

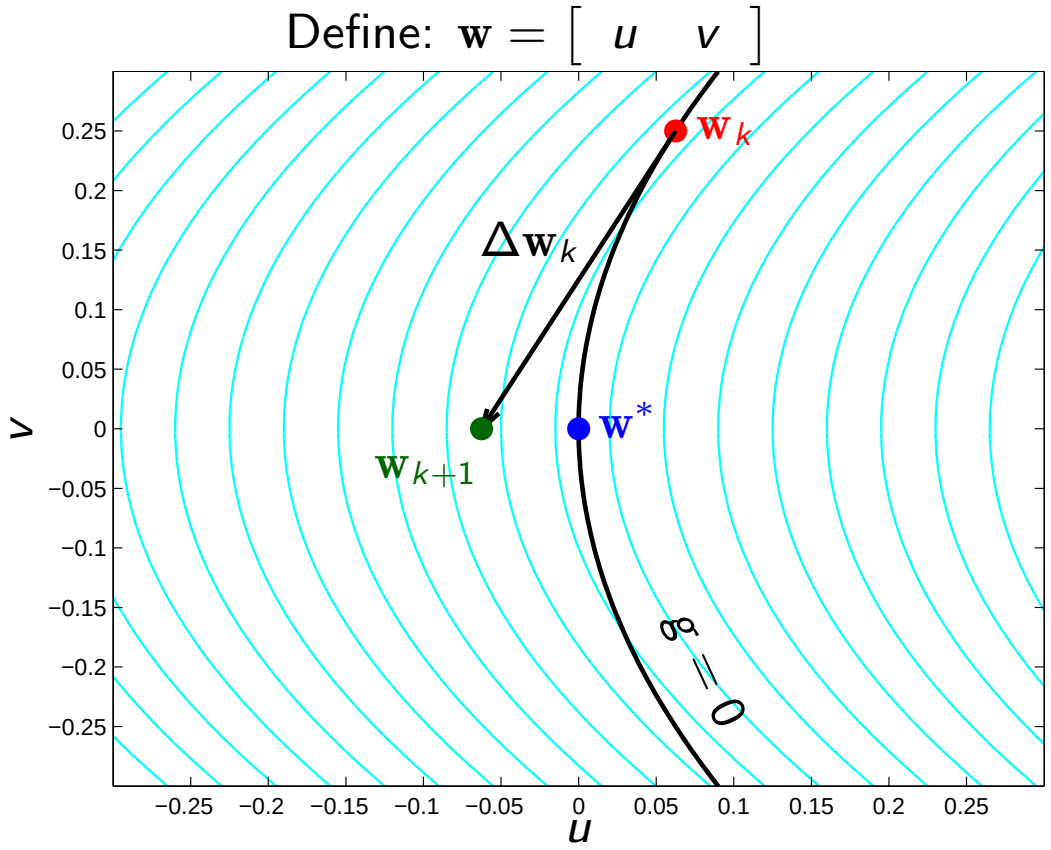
Consider the iterate:

$$\mathbf{w}_k = \begin{bmatrix} a^2 & a \end{bmatrix}$$

The Newton step is:

$$\Delta \mathbf{w}_k = -\begin{bmatrix} 2a^2 & a \end{bmatrix}$$

for $\lambda = 2$...



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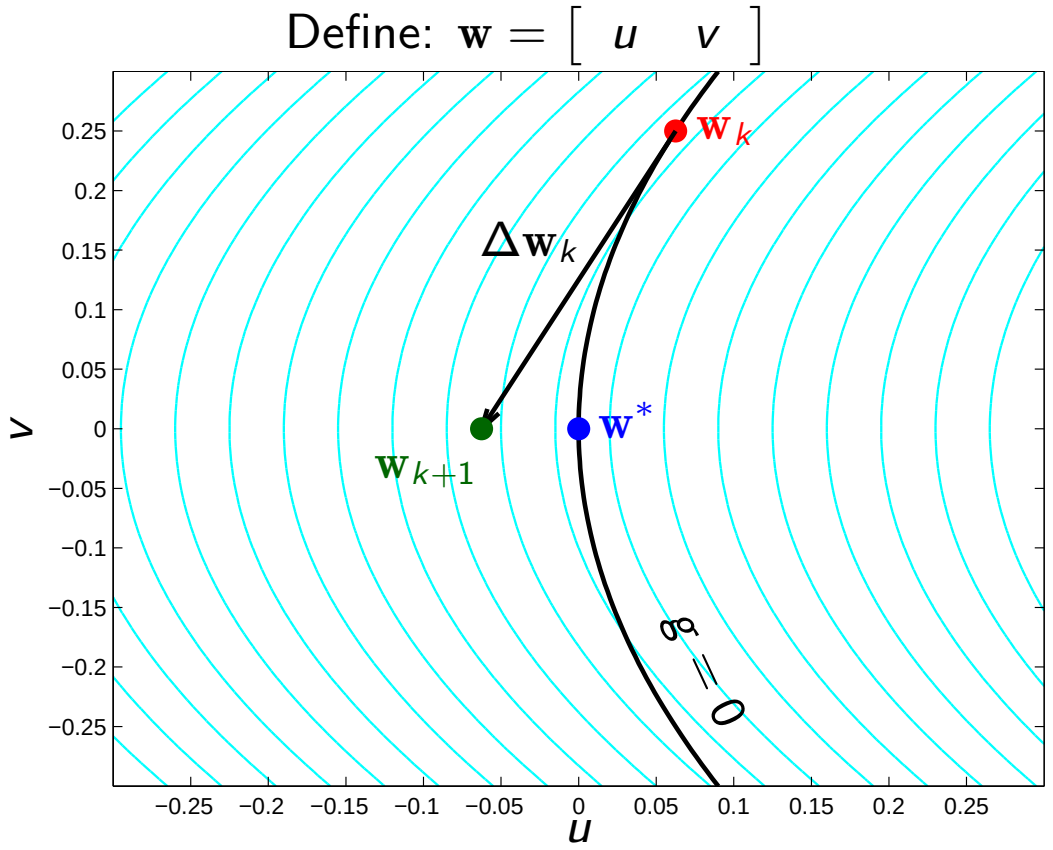

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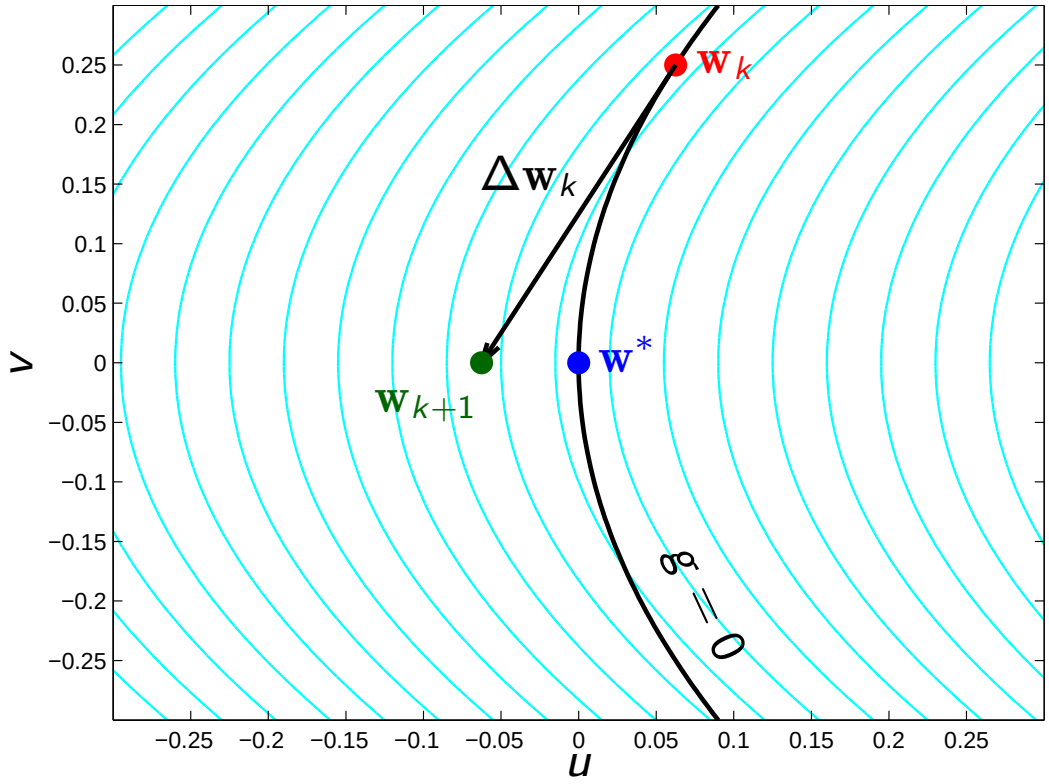
Define: $\mathbf{w} = \begin{bmatrix} u & v \end{bmatrix}$



But:
$\Phi(\mathbf{w}_{k+1}) > \Phi(\mathbf{w}_k)$
$|g(\mathbf{w}_{k+1})| > |g(\mathbf{w}_k)|$

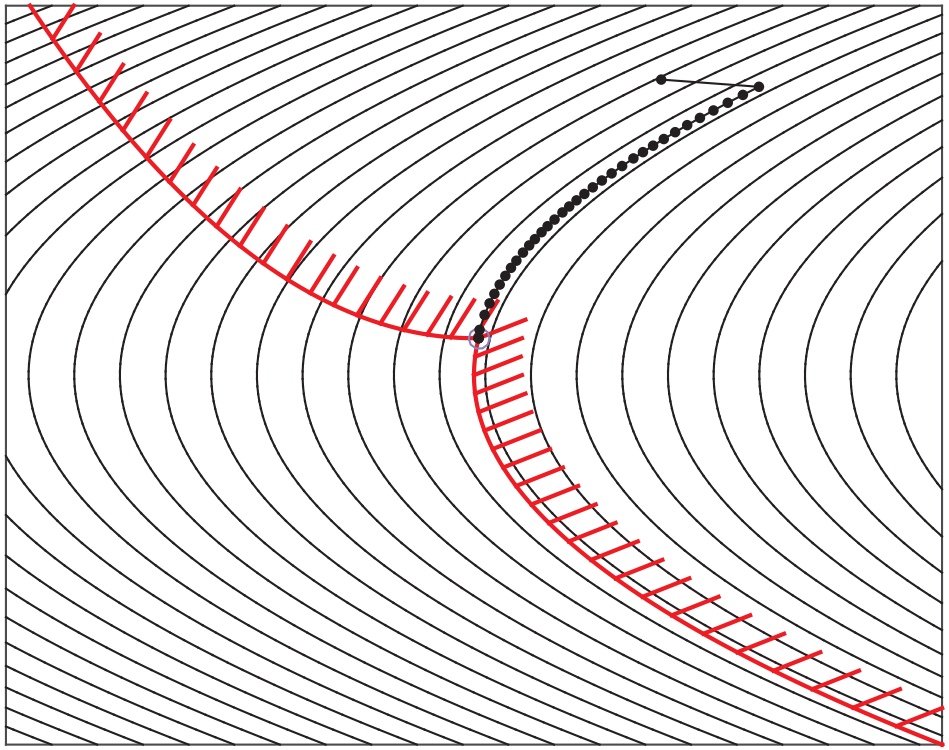
No penalty function can accept $\Delta \mathbf{w}_k$!!

Maratos effect - Illustration

Some NLPs can yield "creeping" convergence

NLP:

$$\begin{aligned} \min_{\mathbf{w}} \quad & \Phi(\mathbf{w}) \\ \text{s.t.} \quad & \mathbf{h}(\mathbf{w}) \leq 0 \end{aligned}$$



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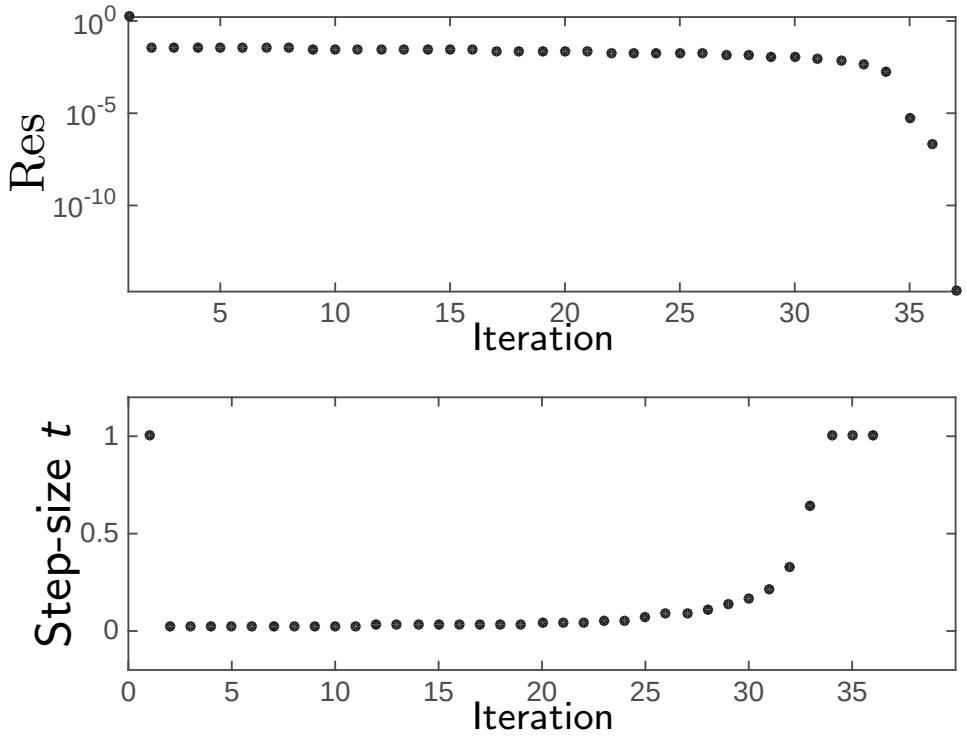
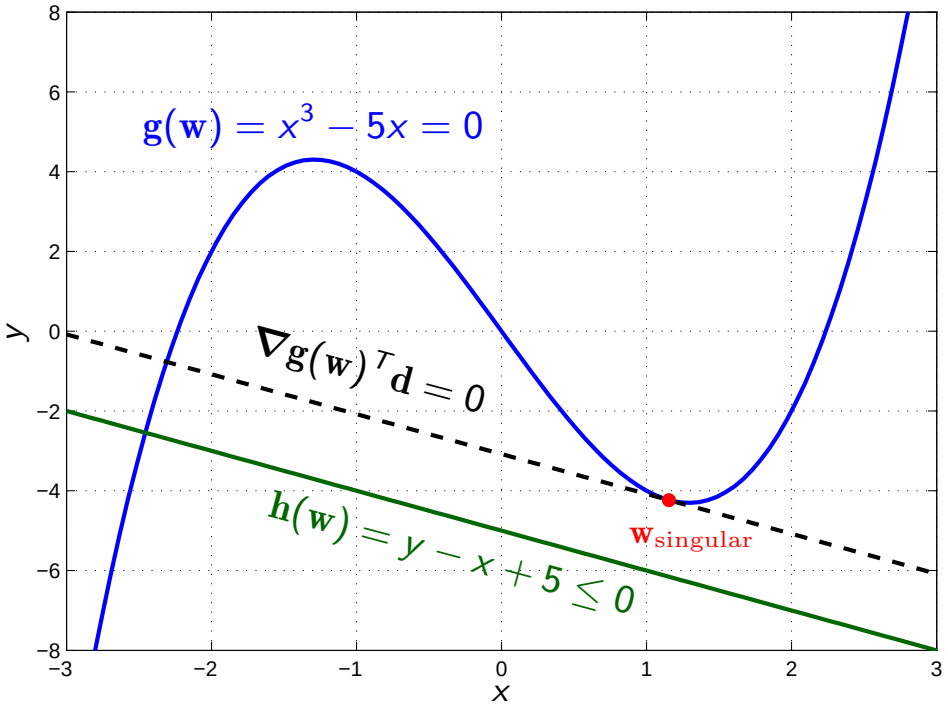


where $\mathrm{Res} = \left\| \begin{array}{c} \nabla \mathcal{L} \\ \max(\mathbf{h}, 0) \end{array} \right\|_{\infty}$

Failure of the Newton methods - Convergence to infeasible points



Problem:

$$\begin{array}{ll} \min\limits_{\mathbf{w}} & x^2 + y^2 \\ \text{s.t.} & x^3 - 5x = 0 \\ & y - x + 5 \leq 0 \end{array}$$

Vectors $\nabla \mathbf{g}(\mathbf{w})$ and $\nabla \mathbf{h}(\mathbf{w})$ are not Linearly Independent for some $\mathbf{w}$, i.e.

$\nexists \Delta \mathbf{w}$ such that:

$$\begin{bmatrix} \nabla \mathbf{g}(\mathbf{w})^\top \\ \nabla \mathbf{h}(\mathbf{w})^\top \end{bmatrix} \Delta \mathbf{w} + \begin{bmatrix} \mathbf{g}(\mathbf{w}) \\ \mathbf{h}(\mathbf{w}) \end{bmatrix} = 0$$

There is no feasible direction $\Delta \mathbf{w}$

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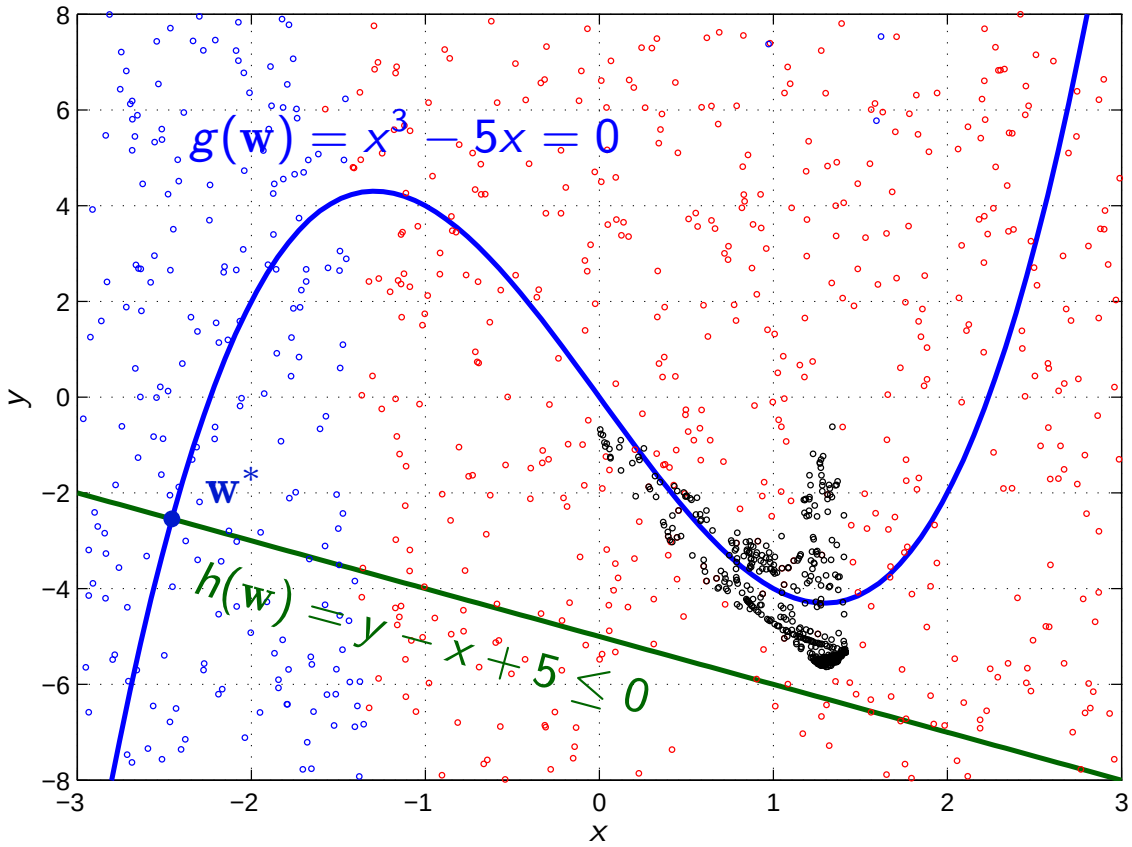

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Red dots: failed starting points $\rightarrow$ black dots

Blue dots: succesfull starting points $\rightarrow (-2.46, -2.54)$