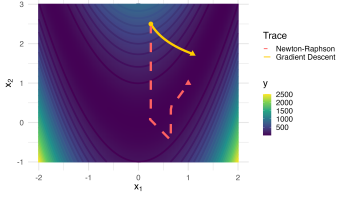
Optimization in Machine Learning

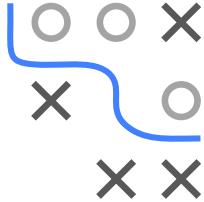
Second order methods
Newton-Raphson vs Gradient Descent



Learning goals

- Comparison of Newton-Raphson and Gradient Descent
- Pure Newton vs relaxed Newton with step size

NEWTON-RAPHSON AND GD (RECAP)



- Gradient Descent: **first order method**
  $\Rightarrow$ *Gradient* information, i.e., first derivatives
- Newton-Raphson: **second order method**
  $\Rightarrow$ *Hessian* information, i.e., second derivatives

Gradient Descent:

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha \nabla f(\boldsymbol{\theta}^{[t]})$$

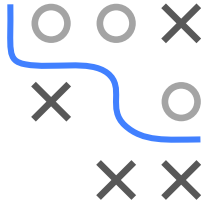
Pure Newton-Raphson:

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - (\nabla^2 f(\boldsymbol{\theta}^{[t]}))^{-1} \nabla f(\boldsymbol{\theta}^{[t]})$$

Relaxed/Damped Newton-Raphson:

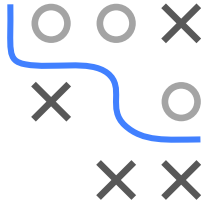
$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha (\nabla^2 f(\boldsymbol{\theta}^{[t]}))^{-1} \nabla f(\boldsymbol{\theta}^{[t]})$$

COMPARISON SIMULATION SET-UP

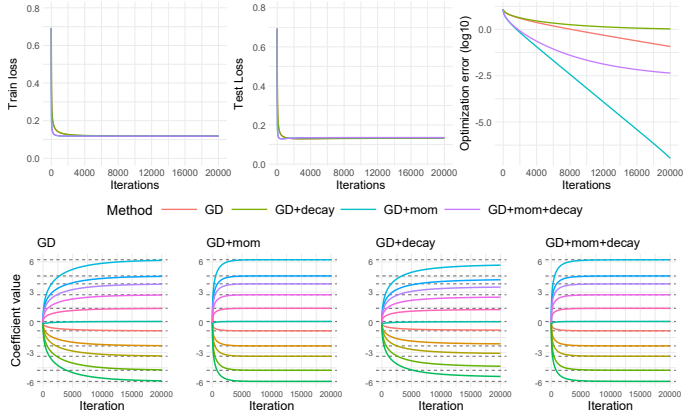


- Comparison of Newton-Raphson, relaxed NR and GD+momentum:
- **Logistic regression** (log loss) simulation with $n = 500$ samples and $p = 11$ features, where $\boldsymbol{\theta}^* = (-5, -4, \ldots 0, \ldots, 4, 5)^T$, and $\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \Sigma)$ for $\Sigma = \boldsymbol{I}$ (i.i.d.) or $\Sigma_{i,j} = 0.99^{|i-j|}$ (corr. features)
- To simulate response, we set $y^{(i)} \sim \mathcal{B}(\pi^{(i)}), \pi^{(i)} = \frac{1}{1+e^{-(\boldsymbol{x}^{(i)})^T \boldsymbol{\theta}^*}}$
- Indep. features result in a condition number of ≈ 2.9 while corr. features yield (moderately) bad condition number ≈ 600
- ERM has unique global minimizer (convexity) but no closed-form solution. We can approximate $\hat{\boldsymbol{\theta}}$ using `glm` solution
- We also track the optimization error $||\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}||_2$
- For relaxed NR we use $\alpha = 0.7$ and for GD we set $\alpha = 1$, momentum to 0.8 and use no step size control

LOGISTIC REGRESSION (GD VARIANTS RECAP)



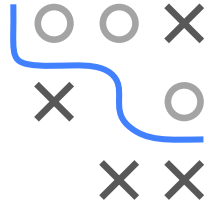
- Recall comparison of GD variants on log. reg. in last chapter:



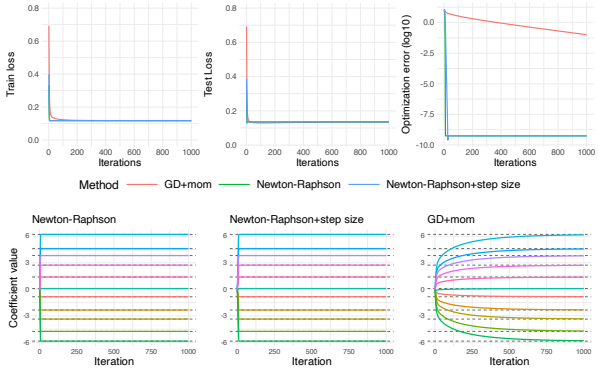
Dotted lines indicate global minimizers.

- **GD+momentum** was fastest $\Rightarrow$ now compare w/ Newton-Raphson
- **NB**: GD+momentum only converges after several thousand steps

LOGISTIC REGRESSION (GD VS. NR)



- Let's run GD vs. NR for 1000 **steps** (independent features):

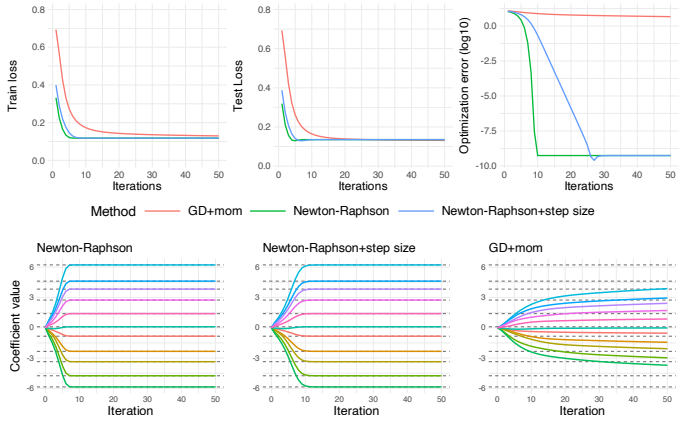


Dotted lines indicate global minimizers.

- **NR** and **relaxed NR** $\Rightarrow$ almost instantaneous convergence (see optimization error)
- Using $\alpha < 1$ slightly slows down **relaxed NR**
- **GD+mom** several orders of magnitude slower than NR

LOGISTIC REGRESSION (GD VS. NR)

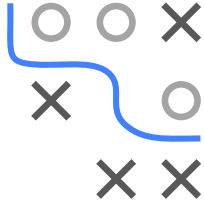
- Let's run the same configuration only for 50 **steps** to see clearer picture:



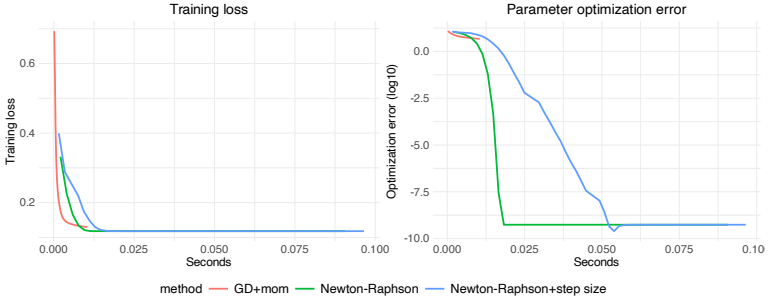
Dotted lines indicate global minimizers.

- **NR** takes ≈ 10 steps to reach same optimization error as **GD+mom** after $20,000$ steps!
- **Relaxed NR** with $\alpha < 1$ shows no advantage here

RUNTIME COMPARISON (INDEP.)



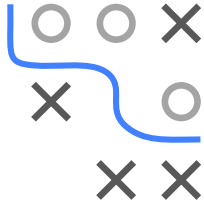
- Clearly, NR makes more progress than GD per iteration
- OTOH Newton steps are much more expensive than GD updates
- $\Rightarrow$ How do NR and GD compare wrt runtime instead of iterations (50 steps)?



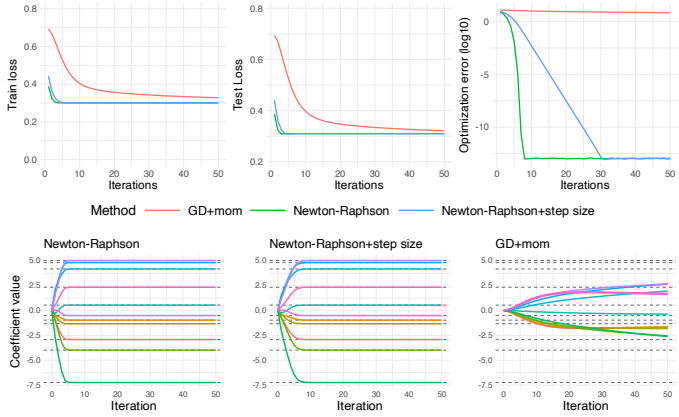
Observations:

- **NR** steps are indeed slower than **GD** steps ($\approx 3\times$ here)
- But each NR step is so much better than GD ($\approx 2000\times$) that per-iteration runtime advantage of GD becomes **irrelevant**

LOGISTIC REGRESSION (CORR.)



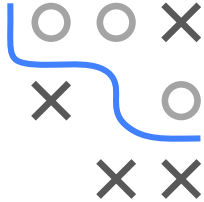
- In case of correlated features the results are very similar:



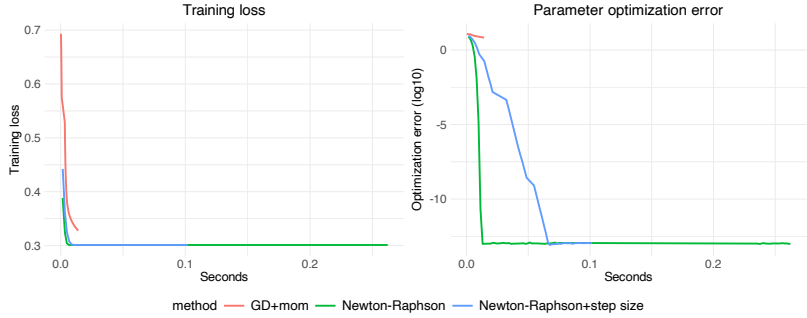
Dotted lines indicate global minimizers.

- **NR**'s performance is unaffected by feature correlation
- **GD** iterates become "warped" compared to before

RUNTIME COMPARISON (CORR.)



- Previous conclusions on runtime comparison for independent features carry over to correlated feature case:



Observations:

- **NR** steps are indeed slower than **GD** steps ($\approx 4\times$ here)
- Overall **NR** is strongly superior to **GD** wrt optim error and speed