Numerical optimization and logistic regression

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Recall, that we can transform any maximization problem into a minimization problem.

Example I

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As the FOC is none-linear in x, this optimization problem has no closed form solution

Aim for the first half of the lecture

Introduce you to numerical methods used to solve optimization problems

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1. Gradient based (our focus)
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Gradient based optimizers include (not conclusive):

- Newton's method
- BFGS
- BHHH
- Gradient descent

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- Idea: A second order polynomial has a closed form solution. So, let's approximate $f(x)$ by a 2nd order Taylor polynomial in the point x_0

$$\min_{x \in \mathbb{R}^k} \quad f(x_0) + (x - x_0)^T \nabla f(x_0) + \tfrac{1}{2}(x - x_0)^T \nabla^2 f(x_0)(x - x_0)$$

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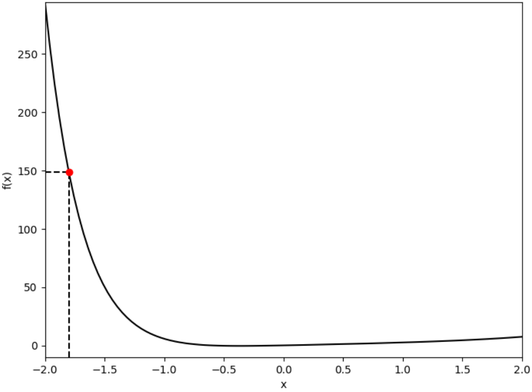
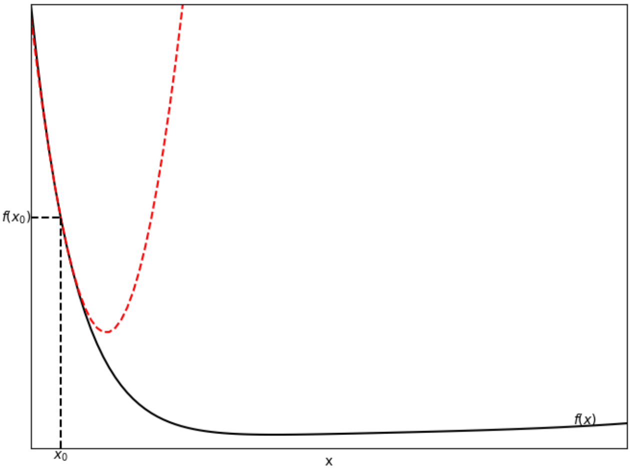
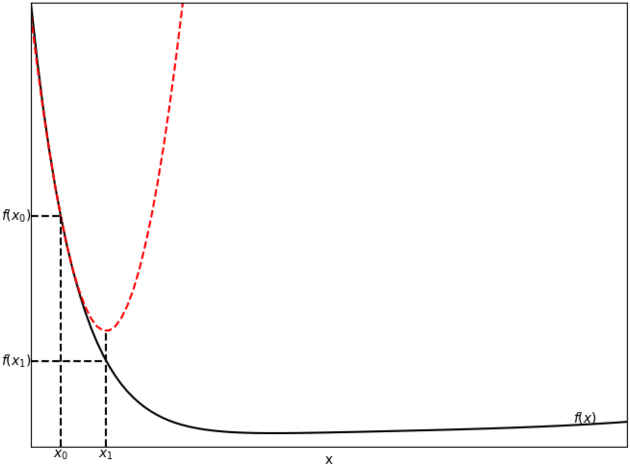


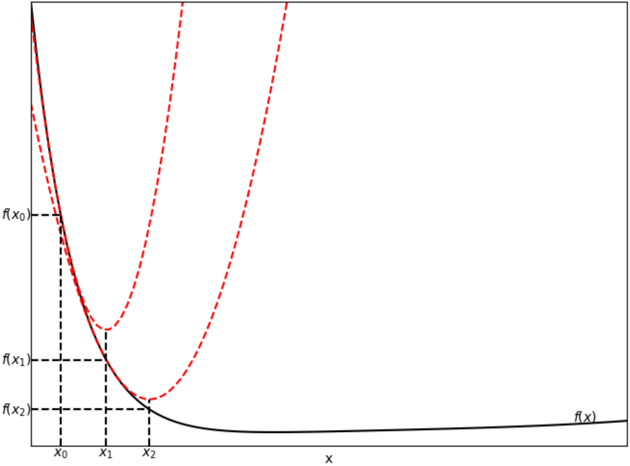
Example I: Approximate the function by the 2nd order Taylor approximation



Example I: Find the minimum of the 2nd order Taylor approximation



Example I: Repeat



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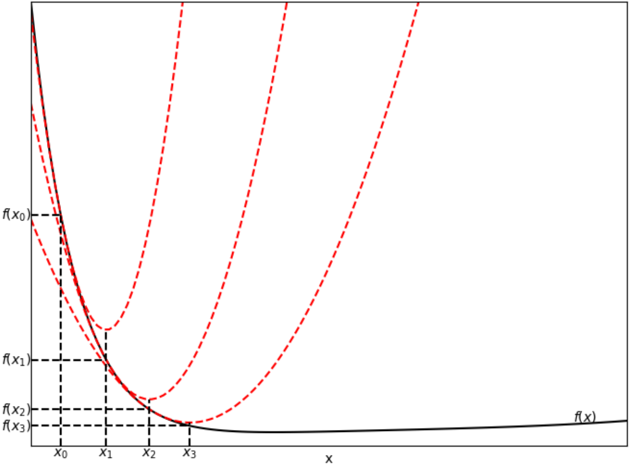

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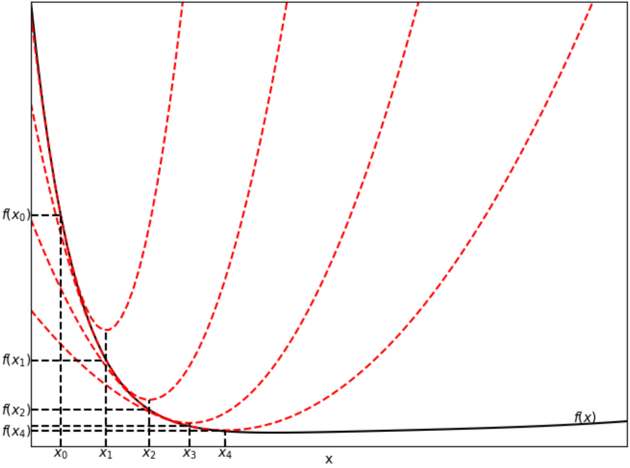

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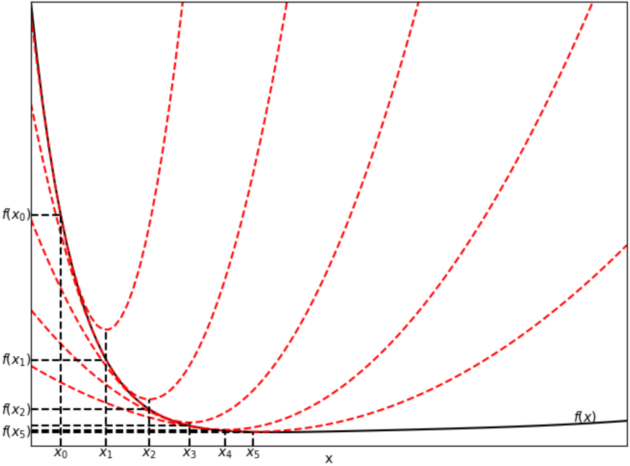

Newton's method

The simplest implementation of Newton's method starts from an initial guess, x_0, and then iterative update the solution of the FOC

$$x_{k+1} = x_k - [\nabla^2 f(x_k)]^{-1} \nabla f(x_k),$$

until the norm of the gradient is sufficiently close to zero, $\|\nabla f(x_k)\| < \varepsilon$.

Simple implementation of the Newton's method

```
def NewtonsMethod(x,grad,hess):
  convergence = 'failed'
  for k in range(1000):
    gradx = grad(x) #evaluate the gradient in x_{k}

    norm_grad = np.sum(np.abs(gradx), axis=None) #calculate the norm of the gradient
    if norm_grad < 1e-10: #stop if gradient close to zero
      convergence = 'converged'
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    dx =-np.linalg.solve(hess(x), gradx) #calculate the newton step
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Let's take a closer look at how this works

Under- and over shooting

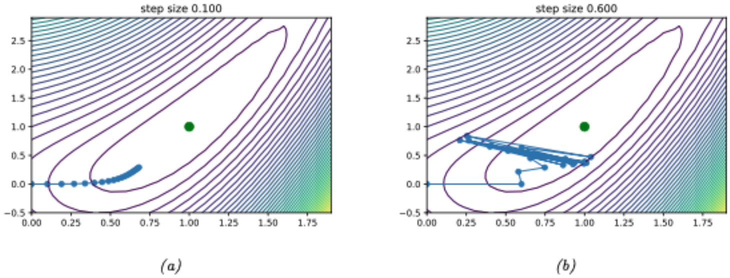

Figure 8.11: Steepest descent on a simple convex function, starting from $(0, 0)$*, for 20 steps, using a fixed step size. The global minimum is at* $(1, 1)$*. (a)* $\eta = 0.1$*. (b)* $\eta = 0.6$*. Generated by steepestDescentDemo.ipynb.*

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- Inexact line search just tries to find an adequately t

Backtracking line search

Backtracking line search is a very simple inexact line search algorithm based on the Armijo–Goldstein condition

$$
\begin{aligned}
& f(x_k) - f(x_k + t\Delta x) > t\gamma, \\
\Leftrightarrow & f(x_k + t\Delta x) < f(x_k) - t\gamma,
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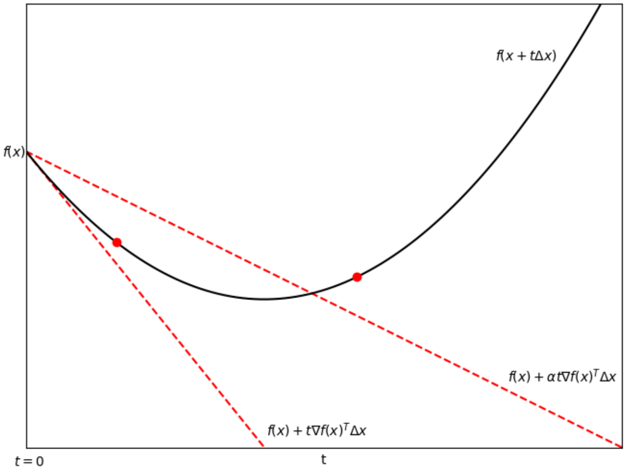
Backtracking line search with $\alpha < 1$



Implementation of Newton's method with backtracking

```
def NewtonsMethodBacktracking(fun,x0,grad,hess):
  convergence = 'failed'
  a, b = 0.2, 0.6 #backtracking parameters
  for k in range(1000):
    fun0 = fun(x0) #evaluate the function value in x_{k}
    grad0 = grad(x0) #evaluate the gradient in x_{k}

    norm_grad = np.sum(np.abs(grad0), axis=None) #calculate the norm of the gradient
    if norm_grad < 1e-10: #stop if gradient close to zero
      convergence = 'converged'
      break

    dx =-np.linalg.solve(hess(x0), grad0) #calculate the newton step

    t = 1 #initiate t step length
    x1 = x0 + dx #calculate initial x_{k+1}
    while (fun(x1) > fun0 + a * t * grad0 * dx): # Armijo-Goldstein condition
      t = b * t #update t if predicted improvement in f(x) is not adequately large
      x1 = x0 + t * dx #update x_{k+1}

    norm_step = np.sum(np.abs(t * dx), axis=None) #calculate the norm of the step size
    if norm_step < 1e-12: #stop if step is close to zero
      convergence = 'stopped early'
      break
  return x1, convergence
```

Calculating the gradient and hessian

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As the hessian, $\nabla^2 f(x)$, is the second derivative we can also use numerical and automatic differentiation to calculate the hessian by simply applying the method twice.

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\begin{aligned}
H_{k+1} &= H_k + \frac{yy^T}{y^T s} - \frac{H_k s s^T H_k^T}{s^T H_k s}, \\
y &\equiv \nabla f(x_{k+1}) - \nabla f(x_k), \\
s &\equiv x_{k+1} - x_k
\end{aligned}
$$

where H_0 typically is set to the identity matrix, $H_0 = I$

Stochastic Gradient descent

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The stochastic gradient descent method iteratively updates

$$x_{k+1} = x_k - t\nabla F(x_k, B_k),$$

Multinomial logistic regression

Multinomial logistic regression can be used as a classification model

$$p(y = c|x, \theta) = \frac{e^{a_c}}{\sum_{c'=1}^{C} e^{a_{c'}}},$$
$$a = b + Wx,$$

where $\theta = (b, W)$.

Maximum likelihood estimation

We can then estimate θ by maximum likelihood estimation (MLE) by maximizing the log-likelihood function

$$\hat{\theta} = \underset{\theta \in \mathbb{R}^{(C-1)D}}{\arg\max} \prod_{i=1}^{N} \prod_{c=1}^{C} p(y_i = c | x_i, \theta)^{y_i}.$$

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Let's take a look at a practical example

Decision rule

If the loss for misclassifying each class is the same, then the optimal decision rule is to predict $\hat{y} = c$ iff class c is the most likely class

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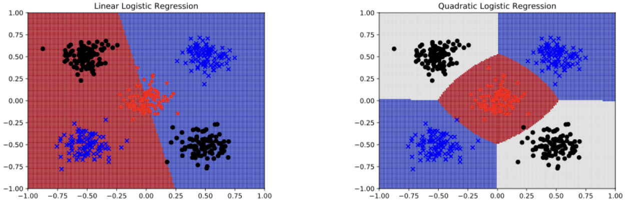
$$\hat{y} = \underset{c=1,\ldots,C}{\arg\max}\, p(y = c|x, \theta)$$



(a) *(b)*

Figure 10.7: Example of 3-class logistic regression with 2d inputs. (a) Original features. (b) Quadratic features. Generated by logreg_multiclass_demo.ipynb.

Overfit

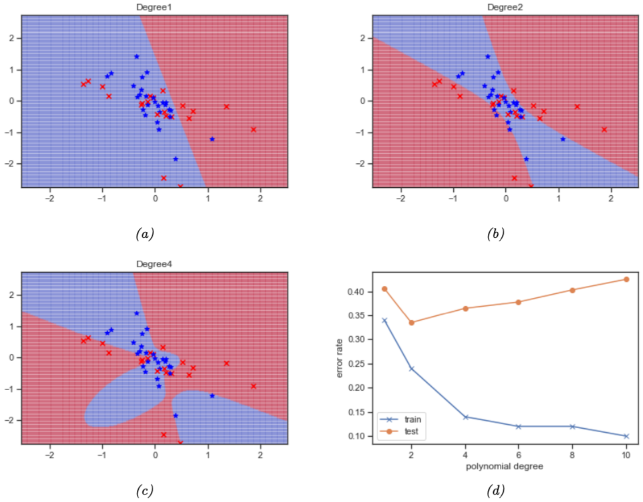


Figure 10.4: Polynomial feature expansion applied to a two-class, two-dimensional logistic regression problem. (a) Degree $K = 1$. (b) Degree $K = 2$. (c) Degree $K = 4$. (d) Train and test error vs degree. Generated by logreg_poly_demo.ipynb.

Regularization

Simplest regularization

$$\hat{\theta} = \underset{\theta \in \mathbb{R}^{(C-1)D}}{\arg\min} -\frac{1}{N} \sum_{i=1}^{N} \sum_{c=1}^{C} y_i \log p(y_i = c | x_i, \theta) + \lambda ||\theta||_2^2.$$

Important to standardize the features (mean 0 and variance 1). Alternatively, use min-max scaling of the features (the features lie in the [0,1]).

Thank you for today :)