In [30]:

```
# Set up environment with correct dependencies
using Pkg
Pkg.activate(".")
Pkg.instantiate()
```

```
 Activating environment at `~/GitHub/MathSys/teaching/MA934/MA934-slid
es/Project.toml`
```

In [31]:

```
using Plots
using LaTeXStrings
using Revise
using LinearAlgebra
using DualNumbers
using Random
using Distributions


pyplot()
# Set default fonts for all plots
#fnt = Plots.font("DejaVu Sans", 8.0)
#default(titlefont=fnt, guidefont=fnt, tickfont=fnt, legendfont=fnt)
```

Out[31]:

```
Plots.PyPlotBackend()
```

In [32]:

```julia
# Need Golden Section Search
include("files/code/gss.jl")

function gradient_descent_plot(f, gamma, xpos, ypos)
    n = 100
    x = range(-10.0,stop=10.0,length=n)
    y = range(-10.0,stop=10.0,length=n)

    xgrid = repeat(x',n,1)
    ygrid = repeat(y,1,n)
    z = zeros(n,n)

    for i in 1:n
        for j in 1:n
            z[i:i,j:j] .= f([x[j];y[i]], gamma)
        end
    end
    p = contour(xgrid, ygrid, z, colors="black", linewidth=1.0, colorbar=false,
    plot!(xpos, ypos, label="")
    scatter!(xpos, ypos, label="")
    return p
end

function gradient_descent_convergence_plot(xpos1, ypos1, xpos2, ypos2, labels)
    p=plot()
    n = length(xpos1)
    steps = 1:n
    dist = [sqrt(xpos1[i]^2+ypos1[i]^2) for i in steps]
    p = plot(steps, dist, yscale=:log10, label="", color=:blue, xlabel="# itera
    scatter!(steps, dist, color=:blue, label=labels[1])

    n = length(xpos2)
    steps = 1:n
    dist = [sqrt(xpos2[i]^2+ypos2[i]^2) for i in steps]
    plot!(steps, dist, yscale=:log10, label="", color=:green)
    scatter!(steps, dist, color=:green, label=labels[2])

    return p
end

function gradient_descent(f, df, gamma)
    x0 = [10.0, 1.0]

    g = df(x0, gamma)
    n = 0
    x = x0
    dx = - g / norm(g)

    steps = Int[]
    xposition = Float64[]
    yposition = Float64[]

    while n<20 && norm(g)>1E-5
        append!(steps,n); append!(xposition, x[1]); append!(yposition, x[2]);
        F(lambda) = f(x + lambda*dx, gamma)
        lmin = gss.minimise(F, [-100.0, 100.0, 0.0], 1.0E-6)
        x = x + lmin*dx
        g = df(x, gamma)
        dx = -g/norm(g)
        n+=1
    end
    return xposition, yposition
end

function gradient_descent(f, df, gamma)
    x0 = [10.0, 1.0]

    g = df(x0, gamma)
    n = 0
    x = x0
    dx = - g / norm(g)

    steps = Int[]
    xposition = Float64[]
    yposition = Float64[]

    while n<20 && norm(g)>1E-5
        append!(steps,n); append!(xposition, x[1]); append!(yposition, x[2]);
        F(lambda) = f(x + lambda*dx, gamma)
        lmin = gss.minimise(F, [-100.0, 0.0, 100.0], 1.0E-6)
        x = x + lmin*dx
        g = df(x, gamma)
        dx = -g/norm(g)
        n+=1
    end
    return xposition, yposition
end

function ADplot()
    xgrid1 = range(-1.0,stop=1.0,length=101)
    xgrid2 = range(-1.0,stop=1.0,length=51)
    z = [Dual(x, 1.0) for x in xgrid2]
    y = sin.(2*pi*xgrid1)
    yprime = 2*pi*cos.(2*pi*xgrid1)
    yz = sin.(2*pi*z)
    p = plot(xgrid1, y, label=L"y(x) = \sin(2\pi x)", color=:red, ylims=(-7,16)
    plot!(xgrid1, yprime, label=L"y(x) = 2\pi\,\cos(2\pi x)", color=:blue)
    scatter!(xgrid2, realpart.(yz), label="Real[y(z)]", color=:red)
    scatter!(xgrid2, dualpart.(yz), label="Dual[y(z)]", color=:blue)
    return p
end
```

```
WARNING: replacing module gss.
```

Out[32]:

```
ADplot (generic function with 1 method)
```

MA934

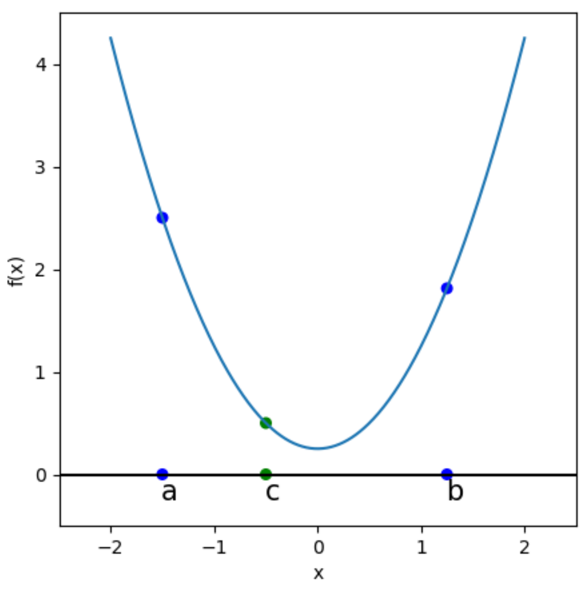
Nonlinear optimisation

Minimisation in 1 dimension

Given a function, $f(x)$ of a single variable, the task is to find a minimum of f.

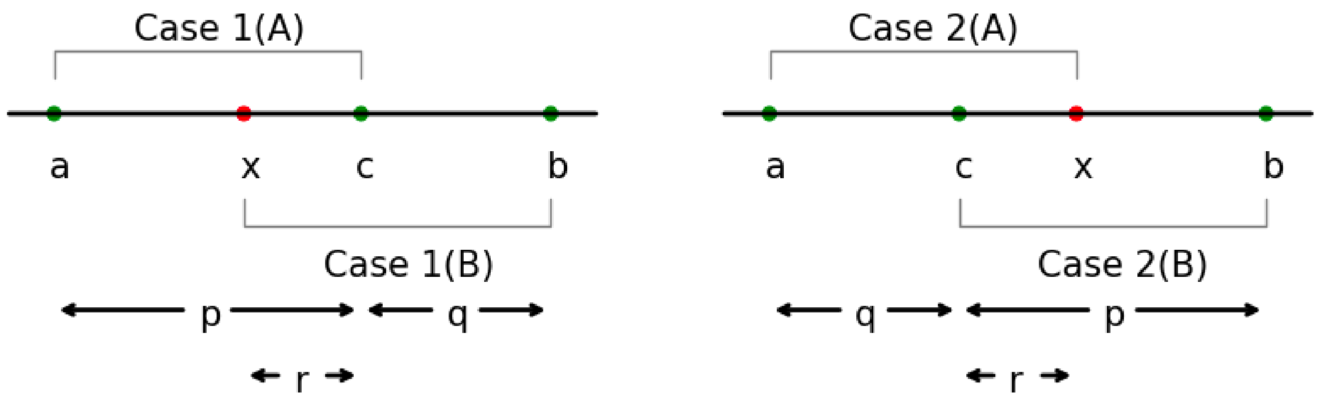
An ordered triple of points (a, c, b) is said to *bracket* a minimum of f if $f(c) < f(a)$ and $f(c) < f(b)$.

Line search: evaluate f at a new point, x, to construct a smaller bracketing triple. Iterate until a desired accuracy is reached.



Golden section search is a way to organise this search in an optimal way.

Golden section search



Most efficient to choose x in the larger of the two subintervals:

Golden section search: : choosing new point, x

Case 1: $[a, c]$ is the larger subinterval : new bracketing triple is either (a, x, c) or (x, c, b). Width of the new bracketing triple is independent of which outcome if :

$$c - a = b - x.$$

So we choose

$$x = a + b - c.$$

Case 2: if $[c, b]$ is the larger subinterval: new bracketing triple is either (a, c, x) or (c, x, b). Width of the new bracketing triple is independent of which outcome if :

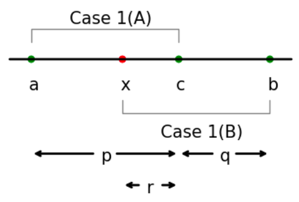
$$x - a = b - c.$$

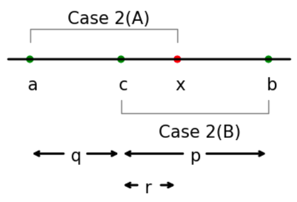
So we again choose

$$x = a + b - c.$$

Golden section search : choosing initial "shape"

Denote:





The idea is to choose c such that the ratio of the width of the shorter subinterval to the width of the longer one remains constant between iterations.

- p: width of the longer subinterval in the old triple
- q: width of the shorter subinterval in the old triple.
- r width of shorter subinterval in the *new* triple.

There are several cases:

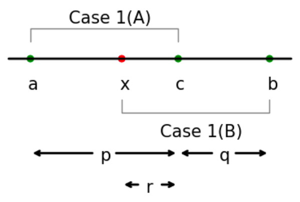
Golden section search : choosing initial "shape"

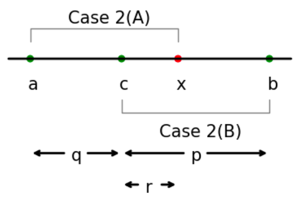
Case 1:

> Case 1(A) : $\frac{r}{p-r} = \frac{q}{p}$ Case 1(B) : $\frac{r}{q} = \frac{q}{p}$

Case 2: (get same equations)

> Case 2(A) : $\frac{r}{q} = \frac{q}{p}$
> Case 2(B) : $\frac{r}{p-r} = \frac{q}{p}$





Eliminating r gives

$$\left(\frac{q}{p}\right)^2 + \left(\frac{q}{p}\right) - 1 = 0$$
$$\Rightarrow \left(\frac{q}{p}\right) = \frac{\sqrt{5} \pm 1}{2}.$$

Golden section search

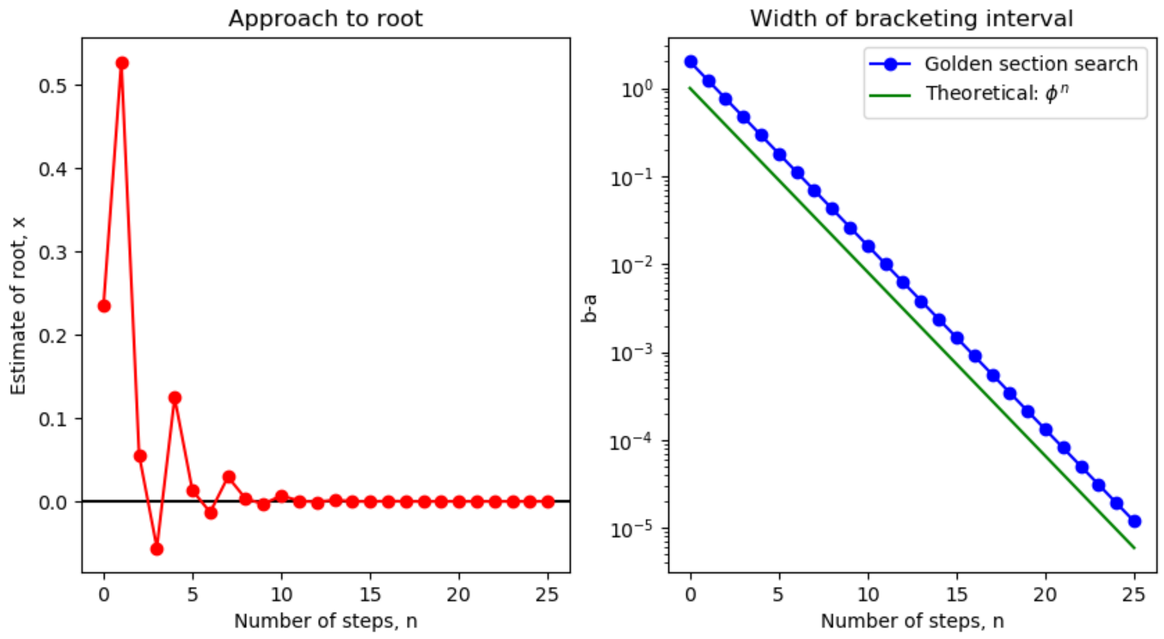
We choose the - sign since we assumed $\frac{q}{p} < 1$ ($\frac{q}{p} = \phi$, 1/golden ratio).

Since x is already determined, $x = a + b - c$, if we start with the correct ratio, $\frac{q}{p}$, this will be preserved when as we iterate.

Convergence is exponential in the number of iterations: width of interval after n iterations is $(b-a)\,\phi^n$.

Golden section search: convergence

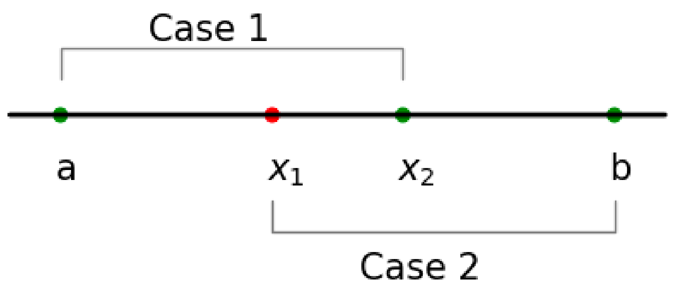
Finding the minimum of $f(x) = x^2$ at $x = 0$:



Golden section search : implementation

Implementation is simplified using temporary variables x_1 and x_2 to store the points x and c (in Case 1) or c and x (in Case 2) and f_1 and f_2 to store the associated function values.

Regardless of the order in which previous points were evaluated, the new triple will centre on the point with the smallest value of f found so far. Thus by comparing f_1 to f_2, there are only two cases:



Minimisation in $\mathbb{R}^n$: line minimisation

Given a function, $f : \mathbb{R}^n \to \mathbb{R}$, a position vector, $\mathbf{x} \in \mathbb{R}^n$, and a direction vector, $\mathbf{v} \in \mathbb{R}^n$, the *line minimiser* of f from $\mathbf{x}$ in the direction $\mathbf{v}$ is the point

$$\mathbf{x}^* = \mathbf{x} + \lambda^* \, \mathbf{v}$$

where

$$\lambda^* = \arg\min_{\lambda} f(\mathbf{x} + \lambda \, \mathbf{v}).$$

Note that although f is a function of n variables, this minimisation with respect to λ is one dimensional and can be done, for example, using Golden Section Search.

Minimisation in $\mathbb{R}^n$: gradient descent

Gradient descent is one a family of unconstrained optimisation algorithms that can be used when the gradient of the objective function is known or computable.

- Given $f : \mathbb{R}^n \to \mathbb{R}$ and any point, $\mathbf{x} \in \mathbb{R}^n$, $-\nabla f(\mathbf{x})$ points in the direction of steepest decrease of f at $\mathbf{x}$.
- Idea is to keep going "downhill" until a minimum is reached

Gradient descent algorithm

Start from a point, $\mathbf{x}_0$.

1. Calculate the unit direction vector
$$\mathbf{v}_n = -\frac{\nabla f(\mathbf{x}_n)}{|\nabla f(\mathbf{x}_n)|}.$$
2. Perform line minimisation in direction of $\mathbf{v}_n$:
$$\lambda^* = \arg\min_{\lambda} f(\mathbf{x}_n + \lambda \mathbf{v}_n)$$
3. Move to new position $\mathbf{x}_{n+1} = \mathbf{x}_n + \lambda^* \mathbf{v}_n$.
4. Repeat until $|\nabla f(\mathbf{x}_n)| < \epsilon_{\text{tol}}$.

Normalisation of $\mathbf{v}_n$ is not strictly necessary but helps keep accuracy as minimum is approached.

Note: any descent directions will work - gradient is the most efficient.

Gradient descent: example in $\mathbb{R}^2$

Consider the function
$$f(x, y) = \frac{1}{2}\left(x^2 + \gamma y^2\right).$$
The parameter $\gamma > 0$ controls the ellipticity. The gradient is
$$\nabla f(x, y) = (x, \gamma y)^T.$$

In [33]:

```
# Parameter to control ellipticity of
gamma = 10.0
# Define quadratic function of two va
f(x, gam) = 0.5*(x[1]^2.0 + gam*x[2]^
# Define corresponding gradient
df(x, gam) = [x[1], gam*x[2]]

```

Out[33]:

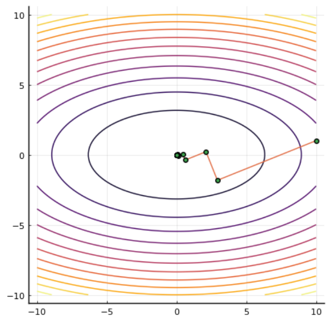
```
df (generic function with 1
method)
```

Gradient descent: example in $\mathbb{R}^2$

In [34]:

```
gamma=4.0
xpos1, ypos1 = gradient_descent(f, df
gradient_descent_plot(f, gamma, xpos1
```

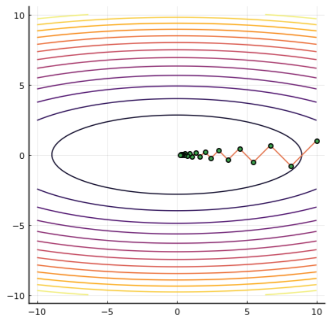
Out[34]:



In [35]:

```
gamma=10.0
xpos2, ypos2 = gradient_descent(f, df
gradient_descent_plot(f, gamma, xpos2
```

Out[35]:



Gradient descent: Why the zig zags?

Remember that $\mathbf{x}_{n+1}$ is a line minimiser of f from $\mathbf{x}_n$ in the direction of $\mathbf{v}_n$.

Letting $g(\lambda) = f(\mathbf{x}_n + \lambda\, \mathbf{v}_n)$, we must have

$$\begin{aligned} \frac{d\,g}{d\,\lambda}(\lambda^*) &= 0 \\ \Rightarrow \sum_{i=1}^{n} \frac{\partial\, f}{\partial\, x_i}(\mathbf{x}_n + \lambda^* \mathbf{v}_n)\, v_{n\,i} &= 0 \\ \Rightarrow \nabla\, f(\mathbf{x}_{n+1}) \cdot \mathbf{v}_n &= 0. \end{aligned}$$

Each step of the gradient descent algorithm is perpendicular to the previous one.

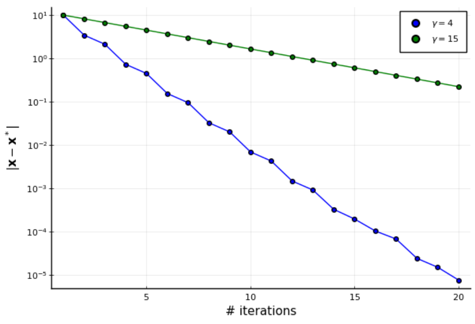
Gradient descent: convergence

- convergence is exponential but depends on γ.
- larger γ is harder - narrower valley requires more zig zags.
- this latter feature means vanilla gradient descent is rarely used in practice.

In [36]:

```
gradient_descent_convergence_plot(xpc
```

Out[36]:



Numerical calculation of derivatives

Explicit calculation of $\nabla\, f(\mathbf{x})$ is sometimes inconvenient. In such cases it is helpful to be able to calculate derivatives numerically. Several approaches:

- Finite difference approximation: the workhorse.
- Automatic differentiation: uses dual numbers
- Spectral methods: uses Fourier transforms

Dual Numbers: basic arithmetic

Dual numbers are of the form $z = x + \varepsilon\, y$ with x, $y \in \mathbb{R}$ and $\varepsilon^2 = 0$.

Addition rule:

$$\begin{aligned} z_1 + z_2 &= (x_1 + \varepsilon\, y_1) + (x_2 + \varepsilon\, y_2) \\ &= (x_1 + x_2) + \varepsilon\, (y_1 + y_2). \end{aligned}$$

Multiplication rule:

$$\begin{aligned} z_1 * z_2 &= (x_1 + \varepsilon\, y_1) * (x_2 + \varepsilon\, y_2) \\ &= (x_1 x_2) + \varepsilon\, (x_1\, y_2 + x_2\, y_1). \end{aligned}$$

Dual conjugate:

$$\bar{z} = x - \varepsilon\, y.$$

As with the complex numbers, $z\,\bar{z}$ is purely real:

$$z\,\bar{z} = (x + \varepsilon\, y) * (x - \varepsilon\, y) = x^2.$$

Dual numbers: division and powers

Division is defined using the conjugate:

$$\begin{aligned} \frac{z_1}{z_2} &= \frac{z_1\,\bar{z}_2}{z_2\,\bar{z}_2} \\ &= \frac{(x_1 + \varepsilon\, y_1)(x_2 - \varepsilon\, y_2)}{x_2^2} \\ &= \frac{x_1\, x_2 + \varepsilon\, (y_1\, x_2 - x_1\, y_2)}{x_2^2} \\ &= \frac{x_1}{x_2} + \varepsilon \left(\frac{y_1\, x_2 - x_1\, y_2}{x_2^2} \right). \end{aligned}$$

Division is not defined for $\mathrm{Re}(z_2) = 0$ so, unlike $\mathbb{C}$, the dual numbers do not form a field.

Powers are obtained using the binomial theorem:

$$\begin{aligned} (x + \varepsilon\, y)^n &= \sum_{k=0}^{n} \binom{n}{k}\, x^{n-k}\, (\varepsilon\, y)^k \\ &= \binom{n}{0} x^n + \binom{n}{1}\, x^{n-1}\, \varepsilon\, y \\ &= x^n + \varepsilon\, y\, n\, x^{n-1}. \end{aligned}$$

Dual numbers: automatic differentiation

Notice that for $f(x) = x^n$,

$$f(x + \varepsilon\, y) = f(x) + \varepsilon\, y\, f'(x).$$

Evaluating $f(x) = x^n$ at $x + \varepsilon$ gives the derivative of $f(x)$ as the dual component.

This is called *automatic differentiation*.

This property trivially extends to polynomial functions and *formally* extends to real analytic functions via their Taylor series:

$$\begin{aligned} f(x + \varepsilon\, y) &= \sum_{k=0}^{\infty} \frac{1}{k!}\, f^{(k)}(x)\, \varepsilon^k\, y^k \\ &= f(x) + \varepsilon\, y\, f'(x). \end{aligned}$$

Also the chain rule works (check). If $h(x) = f(g(x))$:

$$h(x + \varepsilon) = f(g(x)) + \varepsilon\, f'(g(x))\, g'(x).$$

Dual numbers in Julia

Advantages of automatic differentiation:

- no need to work out complicated analytic formulae for derivatives
- $\mathrm{Dual}[z]$ correct to the same precision as $\mathrm{Real}[z]$.

Dual arithmetic is supported in Julia by various packages, the most basic of which is DualNumbers.jl.

In [37]:

```julia
using DualNumbers
z1 = Dual(2.0,3.0)
z2 = Dual(1.0, 2.0)
z1*z2
```

Out[37]:

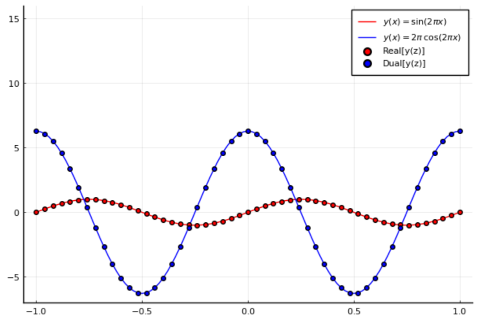
```
2.0 + 7.0ɛ
```

In [38]:

```julia
x = range(-1.0,stop=1.0,length=101)
z = [Dual(a, 1.0) for a in x]
y = sin.(2*pi*z)

ADplot()
```

Out[38]:



Automatic differentiation for multivariate functions

In the formulation presented above, automatic differentiation of multivariate functions requires a separate function evaluation for each partial derivative.

For a multivariate function $f : \mathbb{R}^n \to \mathbb{R}$, to calculate the partial derivative with respect to x_i, we have to add ε to the i^{th} component of the argument and then take the dual part. For example, in $\mathbb{R}^2$ we have

$$f(x+\varepsilon, y) = f(x,y) + \varepsilon\,\frac{\partial f}{\partial x}(x,y)$$
$$f(x, y+\varepsilon) = f(x,y) + \varepsilon\,\frac{\partial f}{\partial y}(x,y).$$

Minimisation of sums

Problems in statistical inference, ML and data science frequently produce optimisation problems that involve minimising a sum:

$$\min_{\beta} f(\beta) = \min_{\beta} \frac{1}{n}\sum_{i=1}^{n} L(\beta, \mathbf{x}_i).$$

Often β represents some model parameters, $\mathbf{x}_i$ represents the i^{th} observation in the training data set and L is a loss function of some kind.

Can be solved with GD by calculating the gradient with respect to β:

$$(\nabla f(\beta))_j = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial L}{\partial \beta_j}(\beta, \mathbf{x}_i)$$

Stochastic Gradient Descent

If the training data is large ($n \gg 1$), then calculating the gradient can become very expensive. Stochastic Gradient Descent addresses this issue.

Idea is to estimate the gradients as:

$$(\nabla f(\beta))_j \approx (\tilde{\nabla} f(\beta))_j = \frac{\partial L}{\partial \beta_j}(\beta, \tilde{\mathbf{x}}_i)$$

where $\tilde{\mathbf{x}}_i$ is the i^{th} training data point from the training data set having first undergone a random shuffle.

Stochastic Gradient Descent : learning rate

With SGD, we typically do not perform full line minimisations (due to sampling noise). Instead the basic update rule is

$$\beta_{n+1} = \beta_n - \zeta_n\, (\tilde{\nabla} f(\beta_n)).$$

ζ_n is a (decreasing) function of n often called the *learrning rate*. For example,

$$\zeta_n = \frac{\zeta_0}{1 + \zeta_1\, n}$$

ζ_0 and ζ_1 are *hyperparameters*. Note that $\sum_{n=1}^{\infty} \zeta_n$ is a divergent series. Prevents SGD from stalling.

Due to sampling noise, SGD only converges to a "noise ball" around the minimum of $f(\beta)$ rather than to the true minimum.

In [39]:

```
include("files/code/figures.jl")
pyplot()
```

```
WARNING: replacing module figures.
```

Out[39]:

```
Plots.PyPlotBackend()
```

Example: Logistic regression

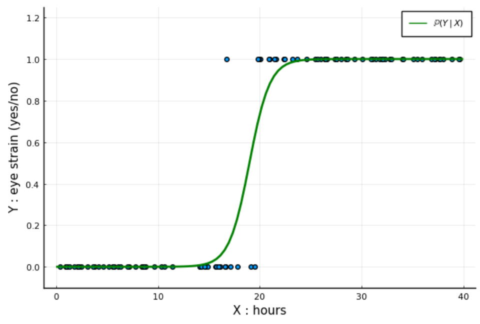
Binary variable, $Y \in \{0, 1\}$, explanatory variable, $X \in \mathbb{R}$.

Example: how is eye strain (Y) related to the number of hours per week (X) spent on MS Teams?

In [40]:

```
figures.plot_logistic_regression_data
```

Out[40]:



Assume $Y = \{Y_i, i = 1 \ldots n\}$ are id Bernoulli with parameters, p_i, depending on $X = \{X_i, i = 1 \ldots n\}$:

$$\mathbb{P}(Y|X) = \prod_{i=1}^{n} p(X_i)^{Y_i}\, (1 - p(X_i))^{1-Y_i}$$

Example: Logistic regression

How should Bernoulli parameter, p, vary with X?
Assume *log odds* are a linear function of X:

$$\log\left(\frac{p(X)}{1 - p(X)}\right) = \beta_0 + \beta_1\, X = \beta \cdot \mathbf{X}$$

where $\mathbf{X} = (1, X)$ and $\beta = (\beta_0, \beta_1)$.

Solve for $p(X)$:

$$p(X) = \sigma(\beta \cdot \mathbf{X}),$$

where $\sigma(x)$ is the sigmoid function:

$$\sigma(x) = \frac{1}{1 + \exp(-x)}.$$

Example: Logistic regression as an optimisation problem

Obviously cannot use least squares to select optimal values of β.

Instead maximise, $\mathbb{P}(Y|X)$ - *likelihood of Y given X* - with respect to β.

In fact easier to minimise $-\log \mathbb{P}(Y|X)$ because it turns task into a sum minimisation:

$$\beta_* = \arg\min_{\beta} \sum_{i=1}^{n} -Y_i \, \log(\sigma(\beta \cdot \mathbf{X}_i)) - (1 - Y_i) \, \log(1 - \sigma(\beta \cdot \mathbf{X}_i)).$$

Example: Logistic regression via gradient descent

We can solve this sum minimisation problem with GD or SGD. First we need the gradient of the objective function,

$$L(\beta) = \sum_{i=1}^{n} -Y_i \, \log(\sigma(\beta \cdot \mathbf{X}_i)) - (1 - Y_i) \, \log(1 - \sigma(\beta \cdot \mathbf{X}_i)).$$

Direct calculation gives (check)

$$(\nabla L(\beta))_k = \sum_{i=1}^{n} (\sigma(\beta \cdot \mathbf{X}_i)) - Y_i) \, (\mathbf{X}_i)_k$$

where $k \in \{0, 1\}$ and $(\mathbf{X}_i)_k$ is the k$^{\text{th}}$ component of $\mathbf{X}_i$.

Implementation: generate some test data

In [41]:

```julia
n = 1000 # Number of data points
xrange = [-20.0, 20.0] # Range of values for x
β0 = [1.0, 1.0] # True parameter values

sigmoid(x) = 1.0/(1.0+exp(-x))

# Generate some data
Random.seed!(2)
X = zeros(n,2)
X[:,1] .= 1.0
X[:,2] = rand(Uniform(xrange[1], xrange[2]), n)
Y = [rand(Bernoulli(sigmoid(β0⋅X[i,:]))) for i in 1:n]
```

Out[41]:

```
1000-element Array{Bool,1}:
 0
 1
 0
 1
 1
 1
 1
 0
 1
 1
 0
 1
 0
 ⋮
 0
 1
 0
 1
 0
 0
 1
 1
 0
 1
 0
 1
```

Implementation: define the objective function

Need negative log likelihood of the data $(\mathbf{X}, \mathbf{Y})$ for a given value of β.
First calculate the components of the sum as separate lists and then assemble them at end:

In [42]:

```
function L(β)
    S = [ sigmoid(β⋅X[i,:]) for i in 1:n]
    # It *can* happen that S[i]==0.0 or 1.0 due to finite precision. This needs
    # be handled separately to avoid log(0). Use the ? :  ternary operator
    A1 = [S[i] == 0.0 ? 0.0 : Y[i]*log(S[i]) for i in 1:n]
    A2 = [S[i] == 1.0 ? 0.0 : (1-Y[i])*log(1.0-S[i]) for i in 1:n]
    A = [A1[i] + A2[i] for i in 1:n]
    return -1.0*sum(A)
end
```

Out[42]:

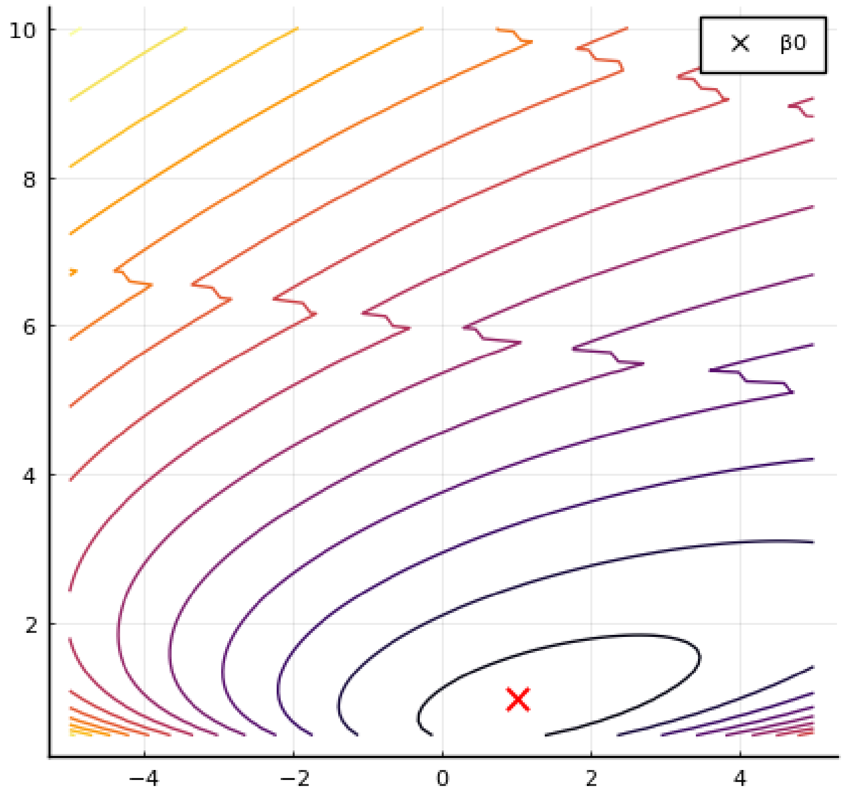
```
L (generic function with 1 method)
```

Plot of L(β)

In [43]:

```
p = figures.contour_plot(L, [-5.0,5.0], [0.5, 10.0])
scatter!([β0[1]],[β0[2]], marker=:x, markersize=8, label="β0",  color=:red)
```

Out[43]:



Implementation: define the gradient of the objective function

In [44]:

```
# Define the gradient of the likelihood function with respect to β
function dL(β)
    S = [ sigmoid(β⋅X[i,:]) for i in 1:n]
    A1 = [(S[i] - Y[i])*X[i,1] for i in 1:n]
    A2 = [(S[i] - Y[i])*X[i,2] for i in 1:n]
    return [sum(A1), sum(A2)]
end
```

Out[44]:

```
dL (generic function with 2 methods)
```

Implementation: define the partial gradient (for SGD)

In [45]:

```
# Define the ith partial gradient of the likelihood function with respect to β
function dL(β,i)
    S = sigmoid(β⋅X[i,:])
    A1 = (S - Y[i])*X[i,1]
    A2 = (S - Y[i])*X[i,2]
    return [A1, A2]
end

```

Out[45]:

```
dL (generic function with 2 methods)
```

Run gradient descent

This time we will use a pre-defined step size, $\eta_1(k)$, rather than doing full line minimisations.

In [46]:

```
include("files/code/GD.jl")
η1(k) = 1.0/(1.0 + k/2.0)
xpos, ypos = GD.gradient_descent(L, dL, [-5.0, 0.0], 1.0E-6, 200, η1)
println("GD: β = (", xpos[end], ", ", ypos[end],")." )
```

```
GD: β = (1.1777019786001126, 0.8687144958918414).

WARNING: replacing module GD.
```

Run stochastic gradient descent

In [47]:

```
η2(k) = 1.0/(1.0 + k/50.0)
xpos2, ypos2 = GD.stochastic_gradient_descent(L, dL, [-5.0, 0.0], 500, η2, n, 1)
println("SGD: β = (", xpos2[end], ", ", ypos2[end],")." )
```

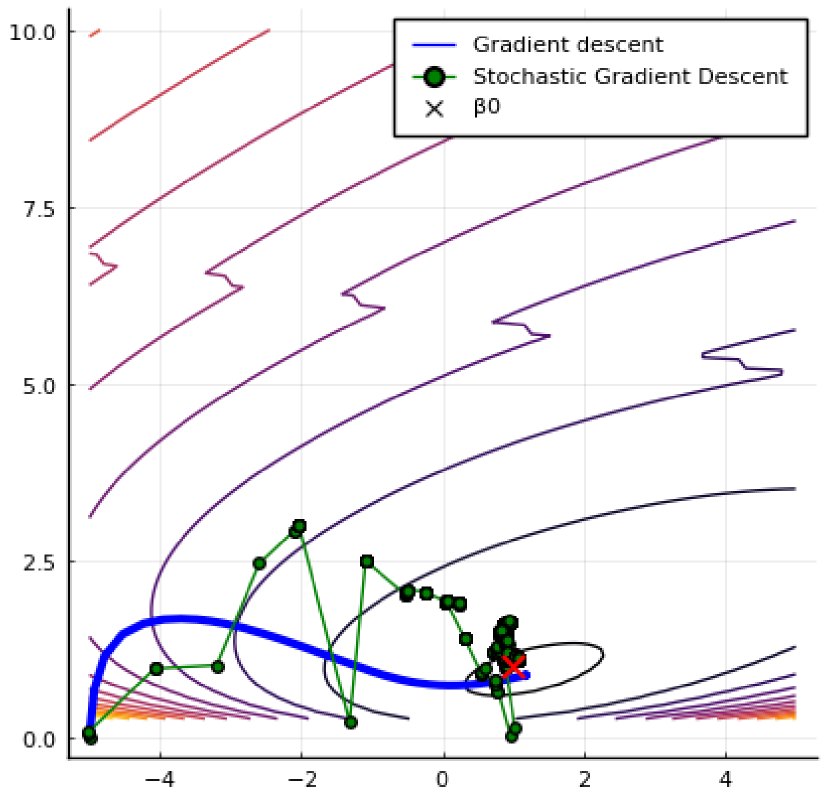
```
SGD: β = (1.0691395293705568, 1.118280854913653).
```

Comparison of results

In [48]:

```julia
p = figures.contour_plot(L, [-5.0,5.0], [0.25, 10.0])
plot!(xpos, ypos, label="Gradient descent", linewidth=3, color=:blue)
plot!(xpos2, ypos2, label="Stochastic Gradient Descent", marker=:circle, color=:
scatter!([β0[1]],[β0[2]], marker=:x, markersize=8, label="β0",  color=:red)
```

Out[48]:



Constrained nonlinear optimisation

Given $f(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$, we can combine what we have learned about gradient descent with what we have learned about linear programming to solve constrained nonlinear optimisation problems of the form:

$$\min_{\mathbf{x}\in C} f(\mathbf{x}),$$

where $C \subset \mathbb{R}^n$ is defined by a set of linear inequalities.

Clearly GD alone is insufficient since $\mathbf{x}_n$ could leave the feasible set, C.

Constrained nonlinear optimisation: Frank-Wolfe algorithm

Idea is to linearise $f(\mathbf{x})$ about $\mathbf{x}_n$ at each iteration of GD and solve the associated LP to obtain an $\mathbf{x}_{n+1}$, which cannot leave C by construction.

Given current point, $\mathbf{x}_n$,

$$f(\mathbf{x}) = f(\mathbf{x}_n) + (\mathbf{x} - \mathbf{x}_n) \cdot \nabla f(\mathbf{x}_n) + \mathcal{O}(|\mathbf{x} - \mathbf{x}_n|^2).$$

Neglecting the $\mathcal{O}(|\mathbf{x} - \mathbf{x}_n|^2)$ terms, minimisation of $f(\mathbf{x})$, is now a LP:

$$x^* = \arg\min_{\mathbf{x}\in C} \; [\mathbf{x} \cdot \nabla f(\mathbf{x}_n)]$$

Constrained nonlinear optimisation: Frank-Wolfe algorithm

Start from a point, $\mathbf{x}_0 \in C$. At each iteration, n:

1. Solve the linearised problem
$$x^* = \arg\min_{\mathbf{x} \in C} \; [\mathbf{x} \cdot \nabla f(\mathbf{x}_n)]$$
2. Perform *bounded* line minimisation of $f(\mathbf{x})$ from $\mathbf{x}_n$ in the direction of $\mathbf{x}^* - \mathbf{x}_n$:
$$\lambda^* = \arg \min_{\lambda \in [0,1]} f\left(\mathbf{x}_n + \lambda\,(\mathbf{x}^* - \mathbf{x}_n)\right)$$
3. Update
$$\mathbf{x}_{n+1} = \mathbf{x}_n + \lambda^*\,(\mathbf{x}^* - \mathbf{x}_n).$$
4. Repeat until desired tolerance is reached.