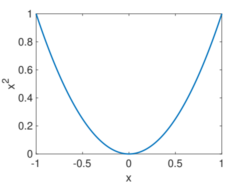
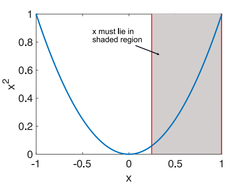
» Constrained Optimisation

* So far we've looked at unconstrained optimisation, e.g. minimise $f(x) = x^2$:



$x = 0$ minimises $f(x)$

* What if the allowed choices of x are constrained e.g. $0.25 \leq x \leq 1$:



now $x = 0.25$ minimises $f(x)$ for $x \geq 0.25$

* Adding constraints can change the value of x that is the minimiser

» Constrained Optimisation

Notation

* Unconstrained optimisation:

$$\min_{x} f(x)$$

* *Constrained optimisation*

$$\min_{x \in X} f(x)$$

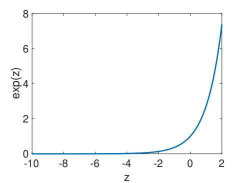
 with X the set of allowed values for vector x e.g. $X = \{x \in \mathbb{R} : x \geq 0.25\}$ or $X = \{x \in \mathbb{R}^2 : 0 \leq x_1 \leq 1, 0 \leq x_2 \leq 1\}$
    * Curly brackets $\{\}$ indicate its a set
    * $\mathbb{R}^2$ superscript 2 indicates that x is a vector with 2 elements, $\mathbb{R}$ means the elements are real valued
    * : reads as "such that"
    * So first example read: x is real-valued such that $x \geq 0.25$
    * Second example reads: x is a vector with 2 elements such that $0 \leq x_1 \leq 1$ and $0 \leq x_2 \leq 1$
    * See e.g. https://en.wikipedia.org/wiki/Set-builder_notation for set notation
* Special case is $X = \mathbb{R}^n$. The n superscript means its a vector with n elements, $\mathbb{R}$ means the elements are real-valued. Then we're back to an unconstrained optimisation and usually just drop X i.e. write

$$\min_{x \in \mathbb{R}^n} f(x) \text{ or } \min_{x} f(x)$$

» Change of Variables

Sometimes (if we're lucky) we can directly convert a constrained optimisation into an unconstrained optimisation

- Example: Suppose $f(x) = (x+2)^2$ and we require x to be non-negative i.e. $X = \{x \in \mathbb{R} : x \geq 0\}$. Make a *change of variable*:
  - Define $x = e^z$ and new function $g(z) = (e^z + 2)^2$. As z varies between $-\infty$ and $+\infty$, $x = e^z$ varies between 0 and $+\infty$ i.e. $x \in X$.



  - Solving unconstrained optimisation

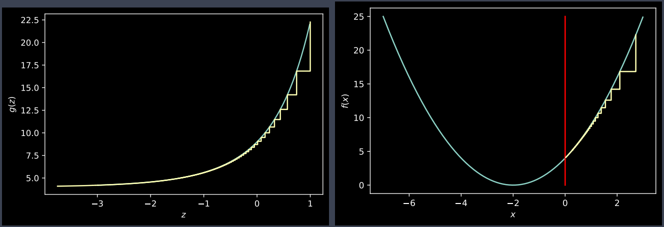
$$\min_z g(z) = (e^z + 2)^2$$

is now the same as solving constrained optimisation

$$\min_{x \geq 0} f(x) = (x+2)^2$$

» Change of Variables

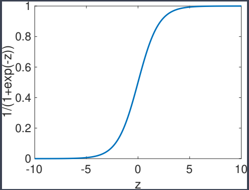
* $f(x) = (x+2)^2$, $g(z) = (e^z+2)^2$. Gradient descent, constant step size $\alpha = 0.05$:



* Left-hand plot: see that z updates so as to decrease $g(z)$. $g(z)$ is minimised by $z \to -\infty$ since $g(-\infty) = 2^2 = 4$
* Right-hand plot: see that $x = e^z$ heads to 0, but never goes negative (so stays within admissible set X). Function $f(x) \to 2^2 = 4$
* If no constraints then minimum would be $f(0) = 0$ when $x = -2$, but $x = -2$ lies outside set X

» Change of Variables

* Suppose we require x to be between 0 and 1 i.e. $X = \{x \in \mathbb{R} : 0 \leq x \leq 1\}$. Make change of variable: $x = \frac{1}{1+e^{-z}}$



* As z varies between $-\infty$ and $+\infty$, $x = \frac{1}{1+e^{-z}}$ varies between 0 and $+1$ i.e. $x \in X$.
* Example: suppose $f(x) = (x+2)^2$ then $g(z) = (\frac{1}{1+e^{-z}} + 2)^2$. Solving unconstrained optimisation

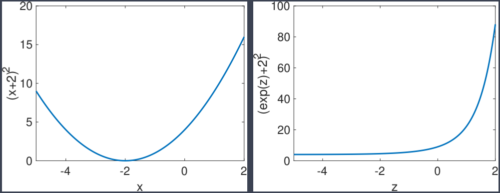
$$\min_z g(z) = (\frac{1}{1+e^{-z}} + 2)^2$$

is now the same as solving constrained optimisation

$$\min_{0 \leq x \leq 1} f(x) = (x+2)^2$$

» Change of Variables

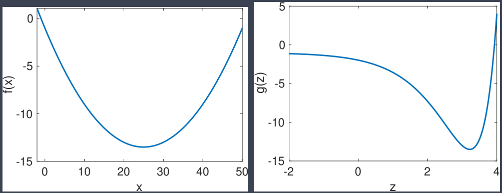
* Usually there no free lunch in optimisation ....
* By adding constraints we might expect that we make the optimisation problem "harder" i.e. it will take longer to find minimiser



* $f(x) = (x+2)^2$ is minimised by $x = -2$, $g(z) = (e^z + 2)^2$ is minimised by $z = -\infty$.
* Recall quadratic-like cost functions (strongly-convex cost functions) like $f(x) = (x+2)^2$ are easy/fast to minimise
* But *see that $g(z)$ has a large flat section on left-hand side of plot where gradient is getting smaller and smaller* $\rightarrow$ gradient descent algos will tend to converge slowly in this region.
* *Our change of variables has converted a strongly-convex optimistion into a harder one which is not strongly-convex*

» Change of Variables

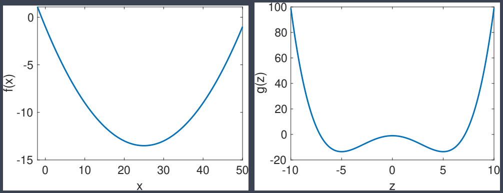
* Change of variables can also make a convex (“easy”) optimisation into a non-convex (“hard”) one ...
* E.g. suppose $f(x) = 0.02x^2 - x - 1$ and we change variable so $x = e^z$. Then $g(z) = 0.02(e^z)^2 - e^z - 1$:



* See that $g(z)$ is non-convex even though $f(x)$ is convex. The non-convexity is benign in this example (still just one global minimum, gradient descent will find it), but needn’t always be ...

» Change of Variables

- Another example. Suppose $f(x) = 0.02x^2 - x - 1$ again but now we change variable to $x = z^2$.
- As z varies between $-\infty$ and $+\infty$, $z^2 \geq 0$.
- $g(z) = 0.02z^4 - z^2 - 1$:



- See that $g(z)$ has *two* minima even though $f(x)$ only has one $\rightarrow$ that's because $5^2 = (-5)^2$
- This is why tend to prefer e^z rather than z^2 as change of var to ensure $x \geq 0$

» Projected Gradient Descent

* Usually we're not so lucky and can't just make a change of vars.
* Recall iterative gradient descent algorithm to minimise function $f(x)$:

for k in range(num_iters):

$$step_t = \alpha[\frac{\partial f}{\partial x_1}(x_t), \frac{\partial f}{\partial x_2}(x_t), \ldots, \frac{\partial f}{\partial x_n}(x_t)]$$
$$x_{t+1} = x_t - step_t$$

* *Projected gradient descent*: changes $x_{t+1} = x_t - step_t$ to:

$$z_{t+1} = x_t - step_t$$
$$x_{t+1} \in \arg\min_{x \in X} d(z_{t+1}, x)$$

* Here $\arg\min_{x \in X} d(z_{t+1}, x)$ is the set of x values (there might be more than one) that minimise function $d(z_{t+1}, x)$.
* Function $d(z, x)$ measures the distance between z and x e.g. Euclidean distance

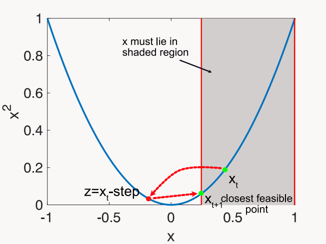
$$d(z, x) = \sum_{i=1}^{n}(z_i - x_i)^2$$

» Projected Gradient Descent

* *Projected gradient descent*: changes $x_{t+1} = x_t - step_t$ to:

  $z_{t+1} = x_t - step_t$
  $x_{t+1} \in \arg\min_{x \in X} d(z_{t+1}, x)$

* $\arg\min_{x \in X} d(z_{t+1}, x)$ is the set of x values (there might be more than one) that minimise $d(z_{t+1}, x)$
* $d(z, x)$ measures distance between z and x e.g. $d(z, x) = \sum_{i=1}^{n} (z_i - x_i)^2$
* z_{t+1} might lie outside set X is allowed values, so we choose x_{t+1} to be the value in X that is closest to z_{t+1}, e.g.



* Notation: usually simplified to: $x_{t+1} = P_X(x_t - step_t)$, called the *projection* of $x_t - step_t$ onto X.

» Examples Of Fast Projections

* In general, calculating $P_X(x_t - step_t)$ means solving an optimisation problem $\rightarrow$ computationally expensive and slow
* But in some common special cases we can write the answer directly. E.g:
* $X = \{x \in \mathbb{R} : x \geq 0\}$, $d(x, z)$ is Euclidean distance. Then

$$P_X(z) = \begin{cases} z & z \geq 0 \\ 0 & z < 0 \end{cases}$$

$\rightarrow$ *projection onto the set of positive values*

* $X = \{x \in \mathbb{R} : a \leq x \leq b\}$, $d(x, z)$ is Euclidean distance. Then

$$P_X(z) = \begin{cases} z & a \leq z \leq b \\ a & z < a \\ b & z > b \end{cases}$$

$\rightarrow$ *projection onto interval* $[a, b]$

» Examples Of Fast Projections

* x is a vector $x = [x_1, x_2, \ldots, x_n]$
* Have element-wise constraints $a_1 \le x_1 \le b_1$, $a_2 \le x_2 \le b_2, \ldots, a_n \le x_n \le b_n$.
* $d(x, z)$ is Euclidean distance.
* Then just separately project each element x_i onto interval $[a_i, b_i]$ i.e

$$[x_1, x_2, \ldots, x_n] = P_X([z_1, z_2, \ldots, z_n])$$

means

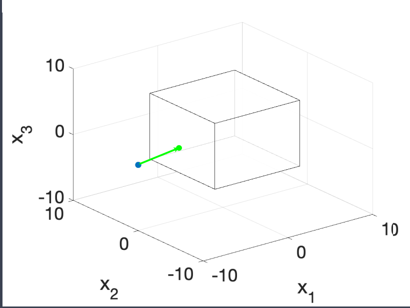
$$x_i = \begin{cases} z_i & a_i \le z_i \le b_i \\ a_i & z_i < a_i \\ b_i & {}_i z_i > b_i \end{cases}$$

for $i = 1, 2, \ldots, n$

$\rightarrow$ *projection onto a (hyper)cube*

» Examples Of Fast Projections

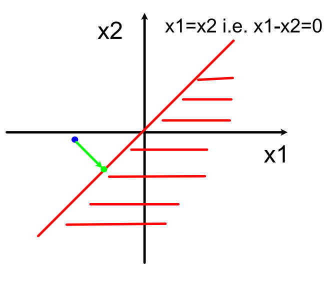
* *projection onto a (hyper)cube*
* e.g. $x = [x_1, x_2, x_3]$ and $a_i = -5, b_i = +5, i = 1, 2, 3$:



* Blue dot is projected onto the closest point (green dot) on face of cube that is nearest to it

» Examples Of Fast Projections

- What if sides of cube are not aligned with the axes?
- Simpler case first: suppose we restrict x to be on one side of a line, e.g $x_1 \leq x_2$:



shaded area indicates set where $x_1 \leq x_2$

- Blue dot is projected onto closest point on boundary (marked by green dot) $\rightarrow$ *Projection Onto Half-Plane*

» Examples Of Fast Projections

* When $x = [x_1, x_2, \ldots, x_n]$ the general equation of a boundary line/plane:

$$a^T x \leq b$$

where a is some vector and b is a scalar

* E.g.
  * $x = [x_1, x_2]$, $a = [1, -1]$, $b = 0$ corresponds to $x_1 - x_2 \leq 0$ i.e. $x_1 \leq x_2$
  * $x = [x_1, x_2]$, $a = [1, 0]$, $b = 1$ corresponds to $x_1 \leq 1$
  * $x = [x_1, x_2]$, $a = [-1, 0]$, $b = -1$ corresponds to $-x_1 \leq -1$ i.e. $x_1 \geq 1$
* $X = \{x \in \mathbb{R}^n : a^T x \leq b\}$, $d(x, z)$ is Euclidean distance. Then

$$P_X(z) = \begin{cases} z & a^T z \leq b \\ z - \frac{a^T z - b}{a^T a} a & a^T z > b \end{cases}$$

and recall $a^T a = \sum_{i=1}^n a_i^2$, $a^T z = \sum_{i=1}^n a_i z_i$

→ *Projection Onto Half-Plane*

» Examples Of Fast Projections

* $X = \{x \in \mathbb{R}^n : a^T x \le b\}$, $d(x,z)$ is Euclidean distance. Then

$$P_X(z) = \begin{cases} z & a^T z \le b \\ z - \frac{a^T z - b}{a^T a} a & a^T z > b \end{cases}$$

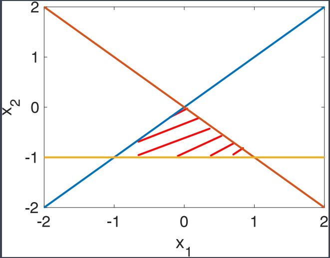
  and recall $a^T a = \sum_{i=1}^n a_i^2$, $a^T z = \sum_{i=1}^n a_i z_i$
* E.g. $x = [x_1, x_2]$, $a = [1, 0]$, $b = 1$ then $a^T x = [1, 0]^T [x_1, x_2] = x_1$ and constraint is $x_1 \le 0$.
* Projection is

$$P_X(z) = \begin{cases} z & z_1 \le 1 \\ z - \frac{z_1 - 1}{1}[1, 0] = [1, z_2] & z_1 > 1 \end{cases}$$

  i.e. if first element of z is greater than 1 we set it equal to 1
* Formula above also works when line/plane is not aligned with the axes e.g. when $x_1 \le x_2$. Then $a = [1, -1]$, $b = 0$. Will leave that to you to try out ...

» Examples Of Fast Projections

* A polytope is created from several intersecting lines e.g.

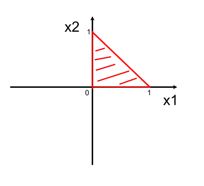


* red line: $x_2 = -x_1$, blue line: $x_1 = x_2$, yellow line: $x_1 = -1$
* Intersection of constraints $x_2 \leq -x_1$, $x_1 \leq x_2$, $x_1 \geq -1$ is the shaded triangle in the middle.
* By combining more lines we can make other shapes e.g. hexagon.
* *To project onto polytope just repeatedly use previous projection on half-plane formula (once for each boundary line of polytope)*

» Examples Of Fast Projections

Special case: *Projection Onto Simplex*

- $X = \{x \in \mathbb{R}^n : \sum_{i=1}^n x_1 \leq 1, x_1 \geq 0, x_2 \geq 0, \ldots, x_n \geq 0\}$

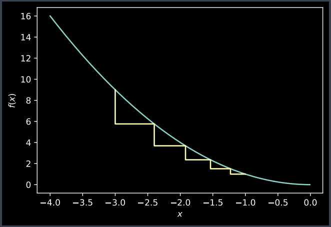


shaded area indicates set *X*

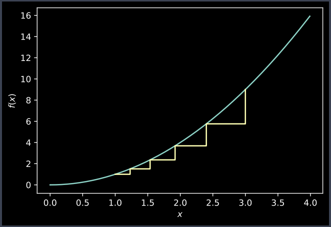
- Vectors in simplex *X* can be thought of as probability vectors (non-negative and elements sum to 1)
- See https://lcondat.github.io/publis/Condat_simplexproj.pdf for v fast algo

» Example

* $f(x) = x^2$ and we require x to be less than -1 i.e. $X = \{x \in \mathbb{R} : x \leq -1\}$. Projected gradient with constant step size $\alpha = 0.1$, initial $x = -3$:

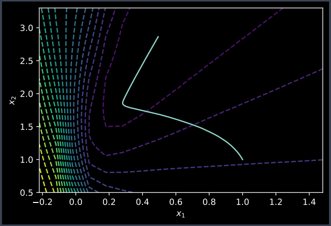


* See that x increases until $z_t = x_t - step_t$ starts to become bigger than -1, then x_{t+1} is snapped back to $x_{t+1} = -1$ by the projection, and thereafter stays there.
* And with $X = \{x \in \mathbb{R} : x \geq +1\}$, initial $x = +3$:

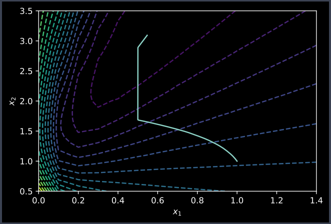


» Example

* Toy neural network and we require x_1 to be greater than 0.5 i.e. $X = \{x \in \mathbb{R}^2 : x_1 \geq 0.5\}$. Projected gradient with constant step size $\alpha = 0.75$, initial $x = [1, 1]$:



unconstrained



constrained

» Summary: Projected Gradient Descent

* *If can efficiently compute projection onto feasible set X*, then can use projected gradient descent to solve constrained optimisations
* We just looked at constant step sizes, what about using Polyak, Adagrad, RMSprop, Heavy Ball, Nesterov Acceleration, Adam with projected gradient descent?
* Adagrad can be used directly[1] with projected gradient descent
* Nesterov acceleration also carries over directly. Recall with gradient descent we used:
  $z_{t+1} = \beta z_t - \alpha \nabla f(x_t + \beta z_t)$, $x_{t+1} = x_t + z_{t+1}$
  See that $z_t = x_t - x_{t-1}$ and define $y_t = x_t + \beta z_t$. Then equivalently
  $y_t = x_t + \beta(x_t - x_{t-1})$, $x_{t+1} = y_t - \alpha \nabla f(y_t)$
  With projected gradient descent use:
  $y_t = x_t + \beta(x_t - x_{t-1})$, $x_{t+1} = P_X(y_t - \alpha \nabla f(y_t))$
  (sometimes called FISTA "Fast Iterative Shrinkage-Thresholding Algorithm" due to paper where originally proposed)
* *V little (no?) work on use of Polyak step size, RMSprop, Heavy Ball, Adam with projected gradient descent*

[1] https://www.jmlr.org/papers/volume12/duchi11a/duchi11a.pdf