Regression

MLAI: Week 2

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Review

- Last time: Looked at Gaussian density and expectations under the Gaussian.
- Proved that maximum likelihood is minimum KL-diverence.
- This time: will begin fitting models to data.

Outline

Regression

Basis Functions

Regression Examples

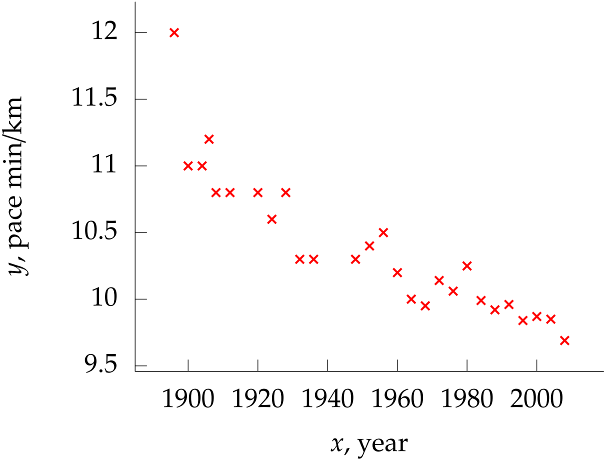
- Predict a real value, y_i given some inputs $\mathbf{x}_i$.
- Predict quality of meat given spectral measurements (Tecator data).
- Radiocarbon dating, the C14 calibration curve: predict age given quantity of C14 isotope.
- Predict quality of different Go or Backgammon moves given expert rated training data.

Olympic 100m Data

- Gold medal times for Olympic 100 m runners since 1896.

Image from Wikimedia Commons
http://bit.ly/191adDC

Olympic 100m Data



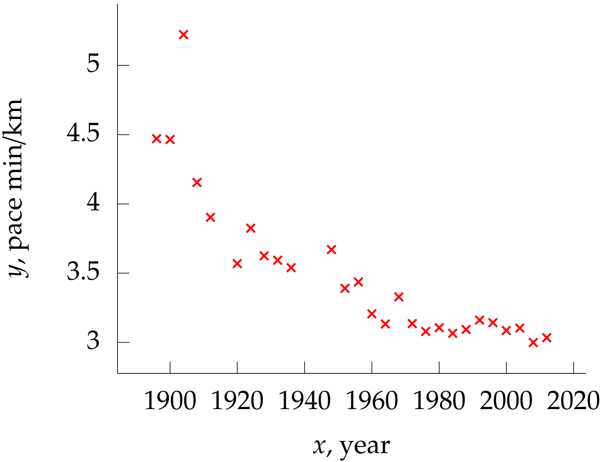
Olympic 100 m Data.

Olympic Marathon Data

- Gold medal times for Olympic Marathon since 1896.
- Marathons before 1924 didn't have a standardised distance.
- Present results using pace per km.
- In 1904 Marathon was badly organised leading to very slow times.

Image from Wikimedia Commons
http://bit.ly/16kMKHQ

Olympic Marathon Data



Olympic Marathon Data.

What is Machine Learning?

data

- data: observations, could be actively or passively acquired (meta-data).

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data +

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data + model

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- model: assumptions, based on previous experience (other data! transfer learning etc), or beliefs about the regularities of the universe. Inductive bias.

What is Machine Learning?

data + model =

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What is Machine Learning?

data + model = prediction

- data: observations, could be actively or passively acquired (meta-data).
- model: assumptions, based on previous experience (other data! transfer learning etc), or beliefs about the regularities of the universe. Inductive bias.
- prediction: an action to be taken or a categorization or a quality score.

Regression: Linear Releationship

$$y = mx + c$$

- y: winning time/pace.

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Regression: Linear Releationship

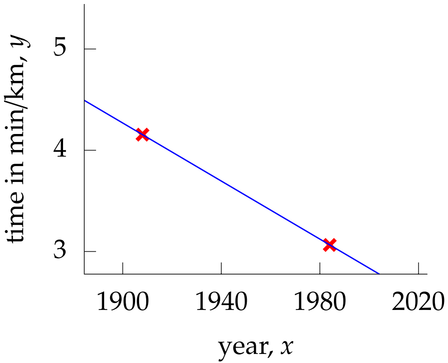
$$y = mx + c$$

- y: winning time/pace.
- x: year of Olympics.
- m: rate of improvement over time.
- c: winning time at year 0.

Two Simultaneous Equations

A system of two simultaneous equations with two unknowns.

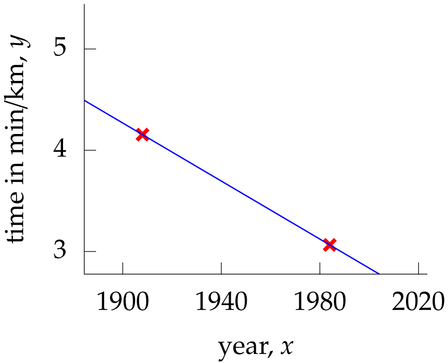
$$y_1 = mx_1 + c$$
$$y_2 = mx_2 + c$$



Two Simultaneous Equations

A system of two simultaneous equations with two unknowns.

$$y_1 - y_2 = m(x_1 - x_2)$$



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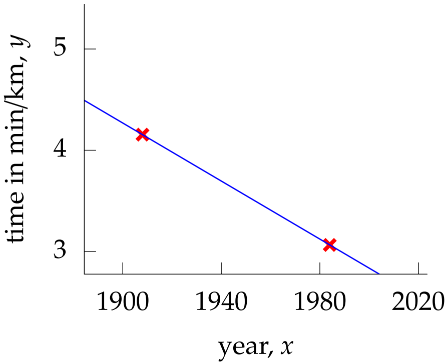
$$\frac{y_1 - y_2}{x_1 - x_2} = m$$

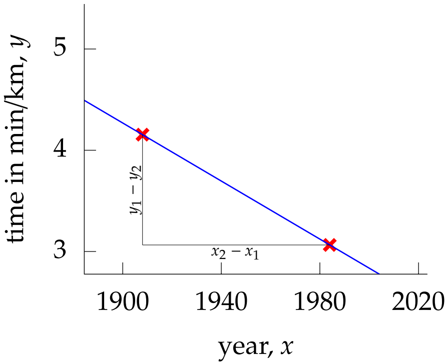


Two Simultaneous Equations

A system of two simultaneous equations with two unknowns.

$$m = \frac{y_2 - y_1}{x_2 - x_1}$$

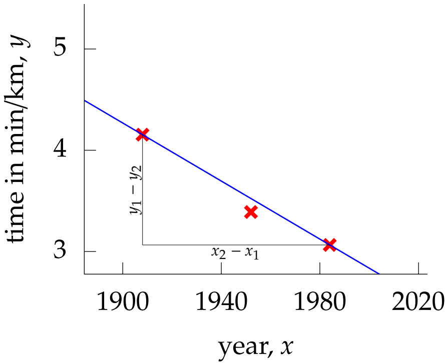
$$c = y_1 - m x_1$$



Two Simultaneous Equations

How do we deal with three simultaneous equations with only two unknowns?

$$y_1 = mx_1 + c$$
$$y_2 = mx_2 + c$$
$$y_3 = mx_3 + c$$



Overdetermined System

- With two unknowns and two observations:

$$y_1 = mx_1 + c$$
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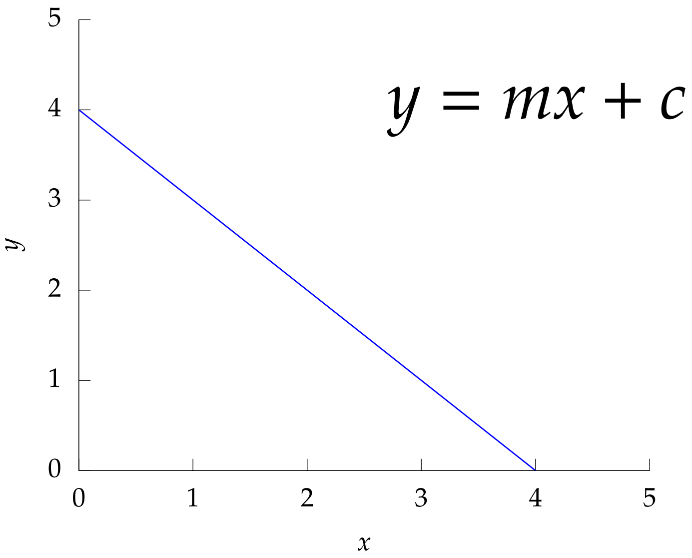
- This problem is solved through a noise model $\epsilon \sim \mathcal{N}\left(0, \sigma^2\right)$

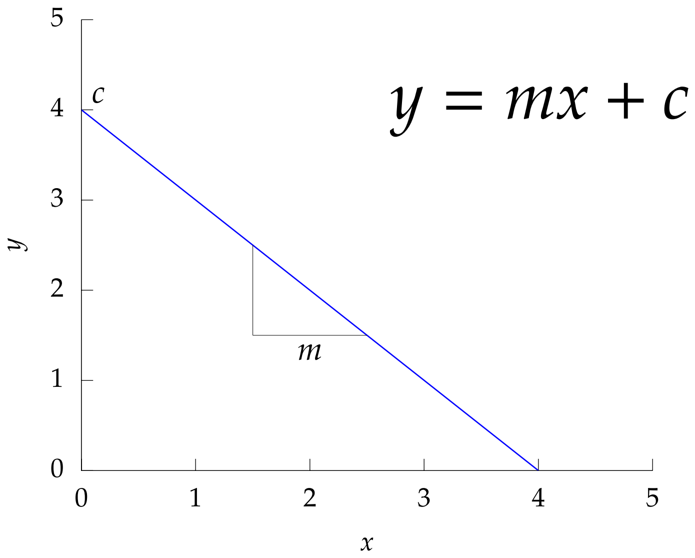
$$y_1 = mx_1 + c + \epsilon_1$$
$$y_2 = mx_2 + c + \epsilon_2$$
$$y_3 = mx_3 + c + \epsilon_3$$

Noise Models

- We aren't modeling entire system.
- Noise model gives mismatch between model and data.
- Gaussian model justified by appeal to central limit theorem.
- Other models also possible (Student-t for heavy tails).
- Maximum likelihood with Gaussian noise leads to *least squares*.

$$y = mx + c$$


$y = mx + c$
0
1
2
3
4
5
y
x



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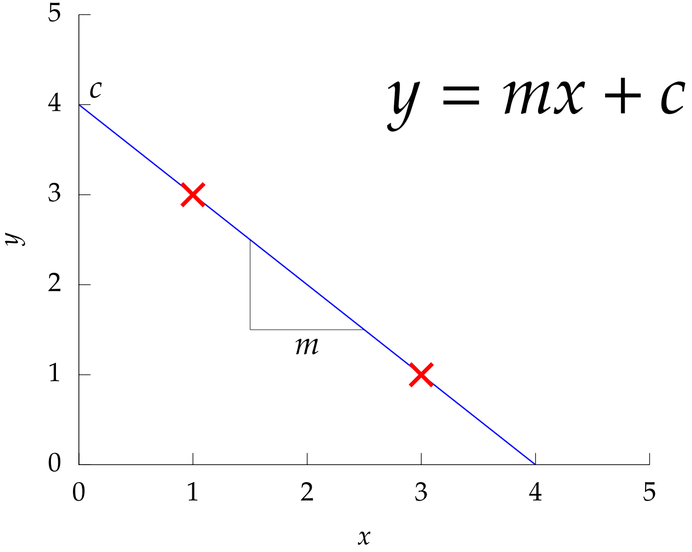
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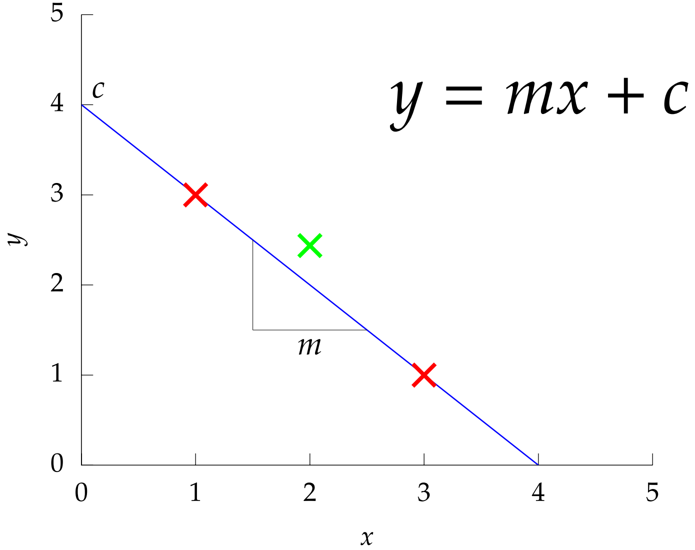

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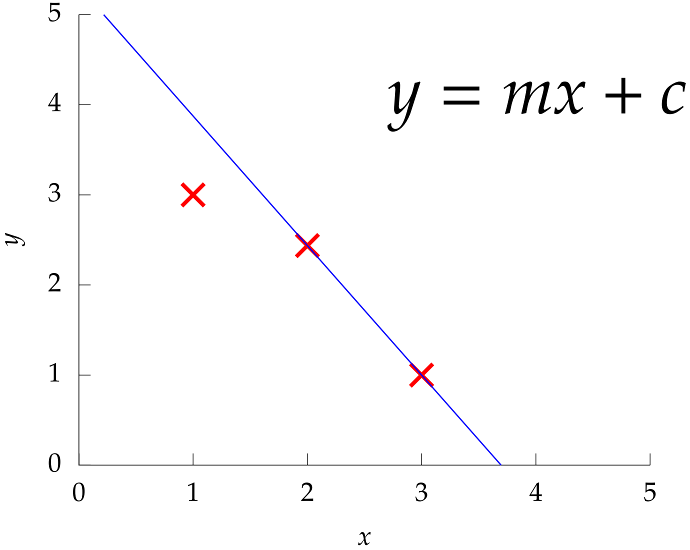

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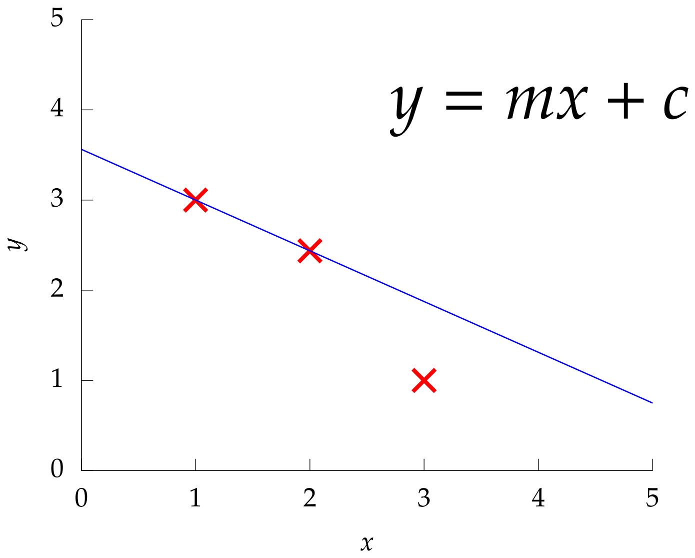
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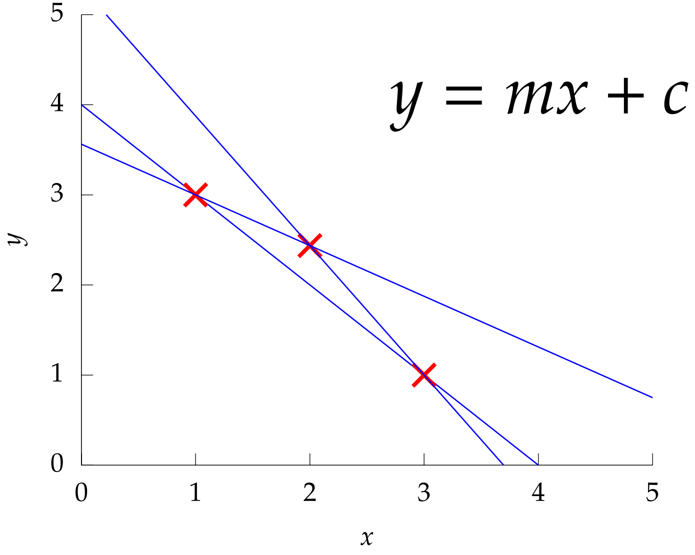


$y = mx + c$
5
4
3
2
1
0
0
1
2
3
4
5
y
x

point 1: $x = 1,\ y = 3$

$$3 = m + c$$

point 2: $x = 3,\ y = 1$

$$1 = 3m + c$$

point 3: $x = 2,\ y = 2.5$

$$2.5 = 2m + c$$

point 1: $x = 1$, $y = 3$

$$3 = m + c + \epsilon_1$$

point 2: $x = 3$, $y = 1$

$$1 = 3m + c + \epsilon_2$$

point 3: $x = 2$, $y = 2.5$

$$2.5 = 2m + c + \epsilon_3$$

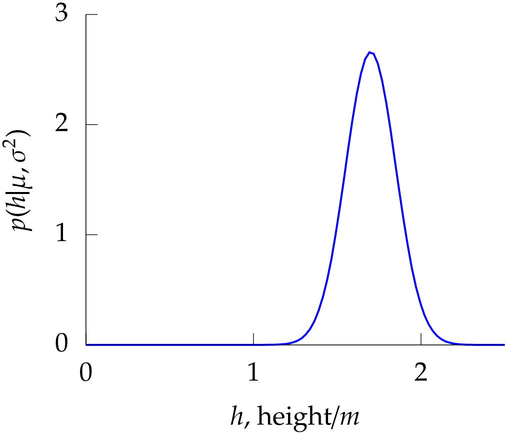
The Gaussian Density

- Perhaps the most common probability density.

$$
\begin{aligned}
p(y|\mu, \sigma^2) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right) \\
&\triangleq \mathcal{N}\left(y|\mu, \sigma^2\right)
\end{aligned}
$$

- The Gaussian density.

Gaussian Density



The Gaussian PDF with $\mu = 1.7$ and variance $\sigma^2 = 0.0225$. Mean shown as red line. It could represent the heights of a population of students.

Gaussian Density

$$\mathcal{N}\left(y|\mu,\sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$

σ^2 is the variance of the density and μ is the mean.

Two Important Gaussian Properties

Sum of Gaussians

- Sum of Gaussian variables is also Gaussian.

$$y_i \sim \mathcal{N}\left(\mu_i, \sigma_i^2\right)$$

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(*Aside*: As sum increases, sum of non-Gaussian, finite variance variables is also Gaussian [central limit theorem].)

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- Scaling a Gaussian leads to a Gaussian.

$$y \sim \mathcal{N}\left(\mu, \sigma^2\right)$$

And the scaled density is distributed as

$$wy \sim \mathcal{N}\left(w\mu, w^2\sigma^2\right)$$

A Probabilistic Process

- Set the mean of Gaussian to be a function.

$$p(y_i|x_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - f(x_i))^2}{2\sigma^2}\right).$$

- This gives us a 'noisy function'.
- This is known as a process.

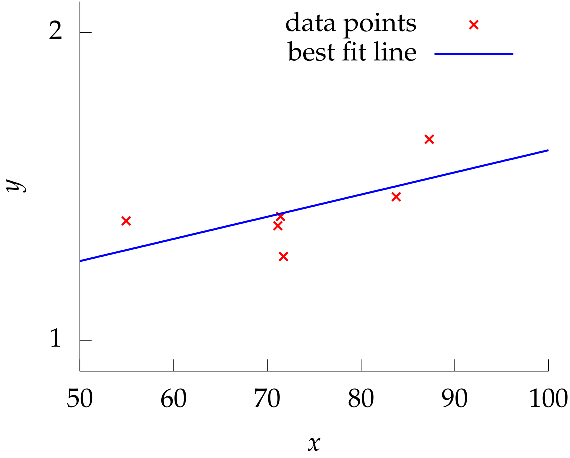
Height as a Function of Weight

- In the standard Gaussian, parametized by mean and variance.
- Make the mean a linear function of an *input*.
- This leads to a regression model.

$$
\begin{aligned}
y_i =& f(x_i) + \epsilon_i, \\
\epsilon_i \sim& \mathcal{N}\left(0, \sigma^2\right).
\end{aligned}
$$

- Assume y_i is height and x_i is weight.

Linear Function



A linear regression between x and y.

Data Point Likelihood

- Likelihood of an individual data point

$$p\left(y_i|x_i, m, c\right) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\left(y_i - mx_i - c\right)^2}{2\sigma^2}\right).$$

- Parameters are gradient, m, offset, c of the function and noise variance σ^2.

Data Set Likelihood

- If the noise, ϵ_i is sampled independently for each data point.
- Each data point is independent (given m and c).
- For independent variables:

$$p(\mathbf{y}) = \prod_{i=1}^{N} p(y_i)$$

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Data Set Likelihood

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$$p(\mathbf{y}|\mathbf{x}, m, c) = \frac{1}{(2\pi\sigma^2)^{\frac{N}{2}}} \exp\left(-\frac{\sum_{i=1}^{N} (y_i - mx_i - c)^2}{2\sigma^2}\right).$$

Log Likelihood Function

- Normally work with the log likelihood:

$$L(m, c, \sigma^2) = -\frac{N}{2}\log 2\pi - \frac{N}{2}\log \sigma^2 - \sum_{i=1}^{N} \frac{(y_i - mx_i - c)^2}{2\sigma^2}.$$

Consistency of Maximum Likelihood

- If data was really generated according to probability we specified.
- Correct parameters will be recovered in limit as $N \to \infty$.
- This can be proven through sample based approximations (law of large numbers) of "KL divergences".
- Mainstay of classical statistics.

Probabilistic Interpretation of the Error Function

- Probabilistic Interpretation for Error Function is Negative Log Likelihood.
- *Minimizing* error function is equivalent to *maximizing* log likelihood.
- Maximizing *log likelihood* is equivalent to maximizing the *likelihood* because log is monotonic.
- Probabilistic interpretation: Minimizing error function is equivalent to maximum likelihood with respect to parameters.

Error Function

- Negative log likelihood is the error function leading to an error function

$$E(m, c, \sigma^2) = \frac{N}{2} \log \sigma^2 + \frac{1}{2\sigma^2} \sum_{i=1}^{N} (y_i - mx_i - c)^2 .$$

- Learning proceeds by minimizing this error function for the data set provided.

Connection: Sum of Squares Error

- Ignoring terms which don't depend on m and c gives

$$E(m, c) \propto \sum_{i=1}^{N} (y_i - f(x_i))^2$$

  where $f(x_i) = mx_i + c$.
- This is known as the *sum of squares* error function.
- Commonly used and is closely associated with the Gaussian likelihood.

Mathematical Interpretation

- What is the mathematical interpretation?
  - There is a cost function.
  - It expresses mismatch between your prediction and reality.

$$E(\mathbf{w}) = \sum_{i=1}^{N} \left(y_i - mx_i + c - y_i\right)^2$$

  - This is known as the sum of squares error.

Learning is Optimization

- Learning is minimization of the cost function.
- At the minima the gradient is zero.
- Coordinate ascent, find gradient in each coordinate and set to zero.
$$\frac{\mathrm{d}E(m)}{\mathrm{d}m} = -2\sum_{i=1}^{N} x_i \left(y_i - mx_i - c\right)$$

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$$0 = -2 \sum_{i=1}^{N} x_i \left(y_i - m x_i - c\right)$$

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$$0 = -2\sum_{i=1}^{N} x_i y_i + 2\sum_{i=1}^{N} m x_i^2 + 2\sum_{i=1}^{N} c x_i$$

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$$m = \frac{\sum_{i=1}^{N} (y_i - c)\, x_i}{\sum_{i=1}^{N} x_i^2}$$

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$$\frac{\mathrm{d}E(c)}{\mathrm{d}c} = -2\sum_{i=1}^{N}(y_i - mx_i - c)$$

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$$0 = -2 \sum_{i=1}^{N} (y_i - mx_i - c)$$

Learning is Optimization

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$$0 = -2\sum_{i=1}^{N} y_i + 2\sum_{i=1}^{N} mx_i + 2Nc$$

Learning is Optimization

- Learning is minimization of the cost function.
- At the minima the gradient is zero.
- Coordinate ascent, find gradient in each coordinate and set to zero.

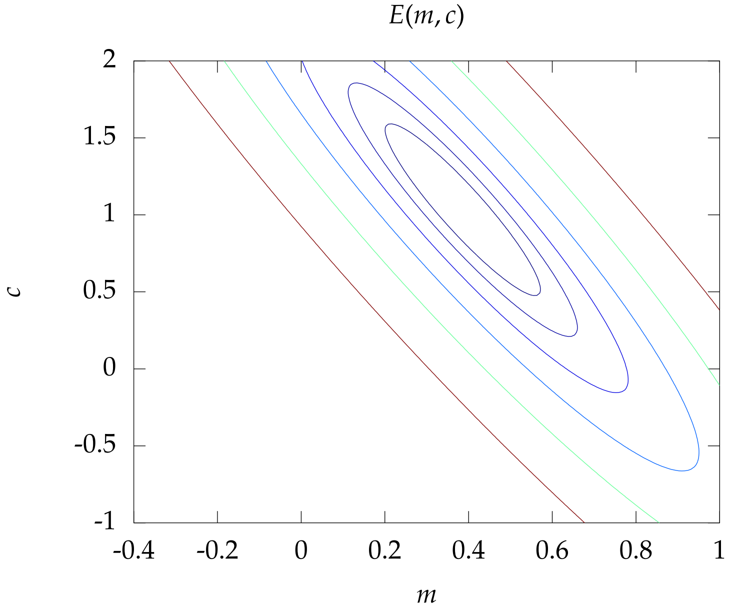
$$c = \frac{\sum_{i=1}^{N} (y_i - cx)}{N}$$

Fixed Point Updates

Worked example.

$$
\begin{aligned}
c^* &= \frac{\sum_{i=1}^{N} (y_i - m^* x_i)}{N}, \\
m^* &= \frac{\sum_{i=1}^{N} x_i (y_i - c^*)}{\sum_{i=1}^{N} x_i^2}, \\
\sigma^{2\,*} &= \frac{\sum_{i=1}^{N} (y_i - m^* x_i - c^*)^2}{N}
\end{aligned}
$$

Coordinate Descent



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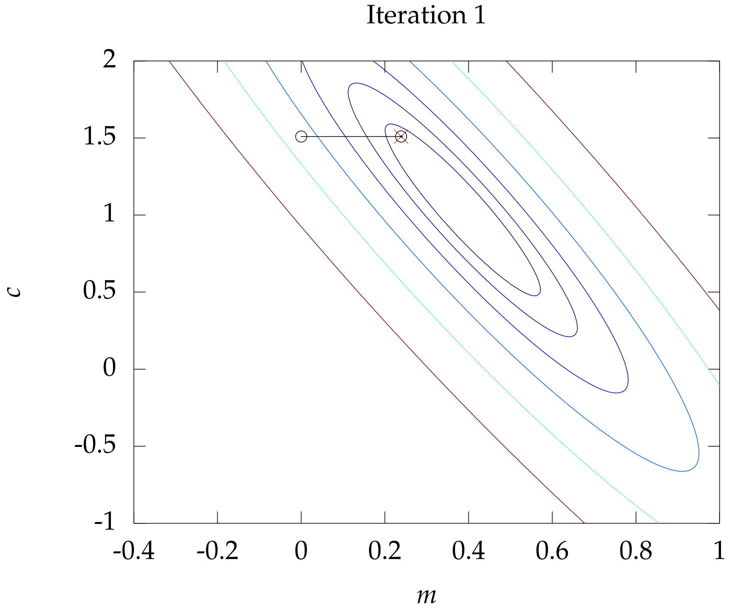

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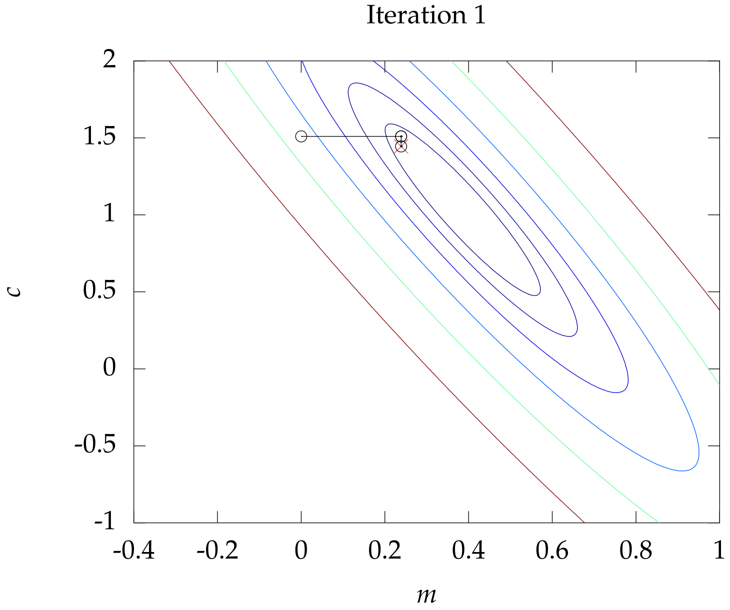

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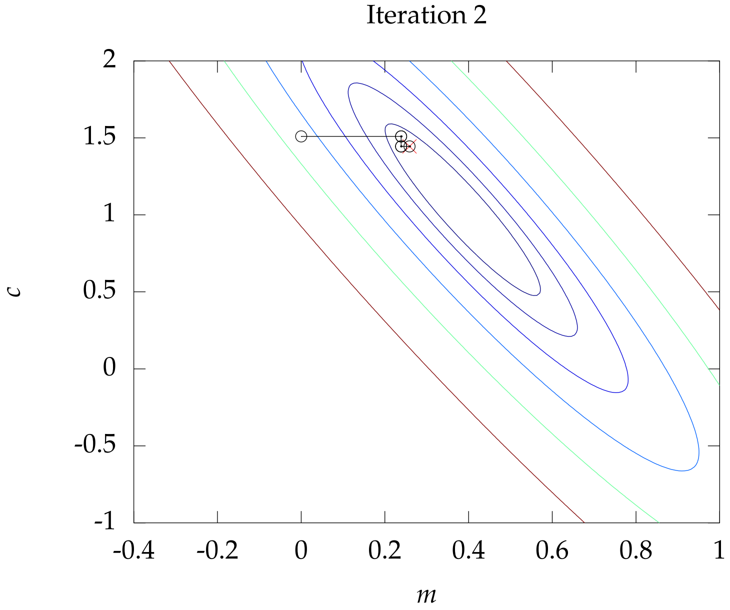

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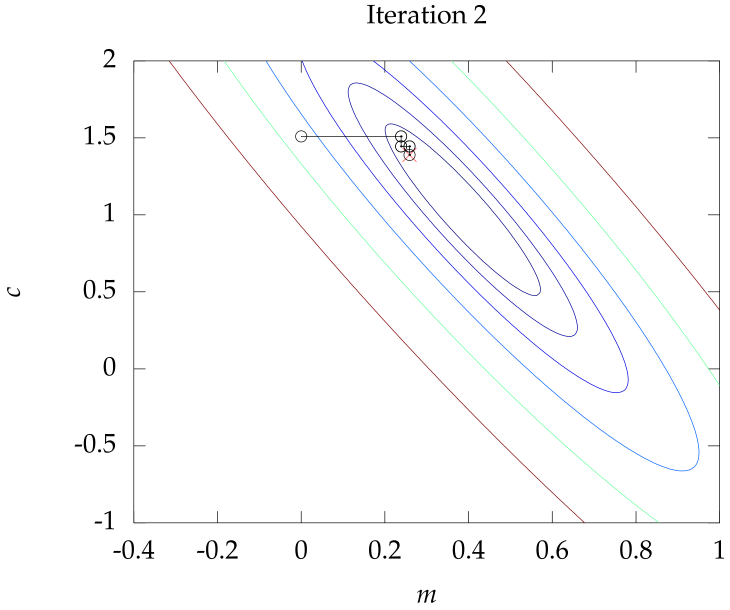

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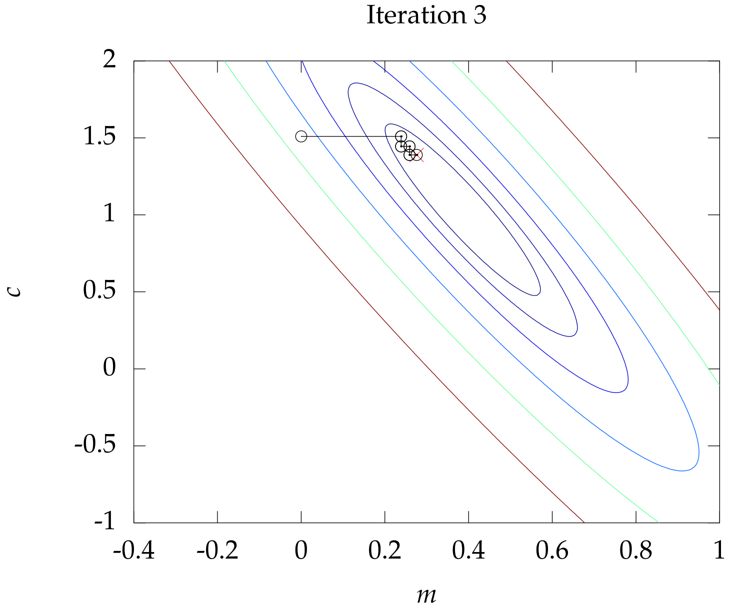

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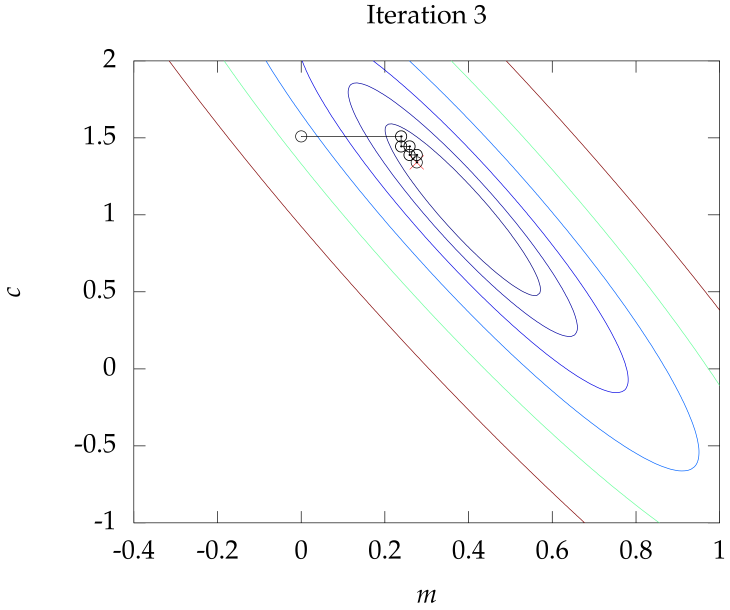

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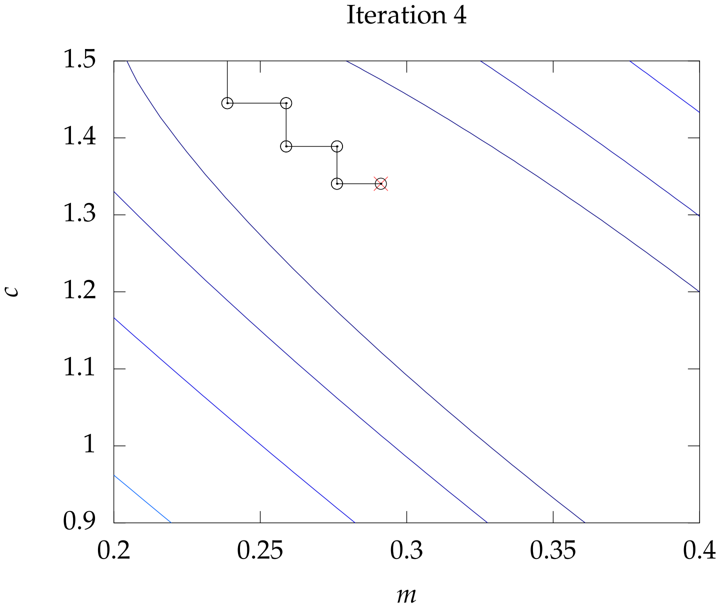

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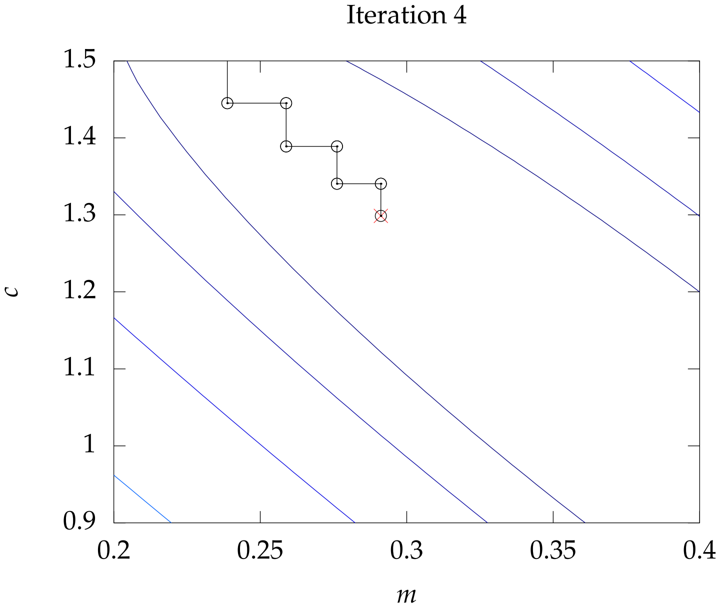

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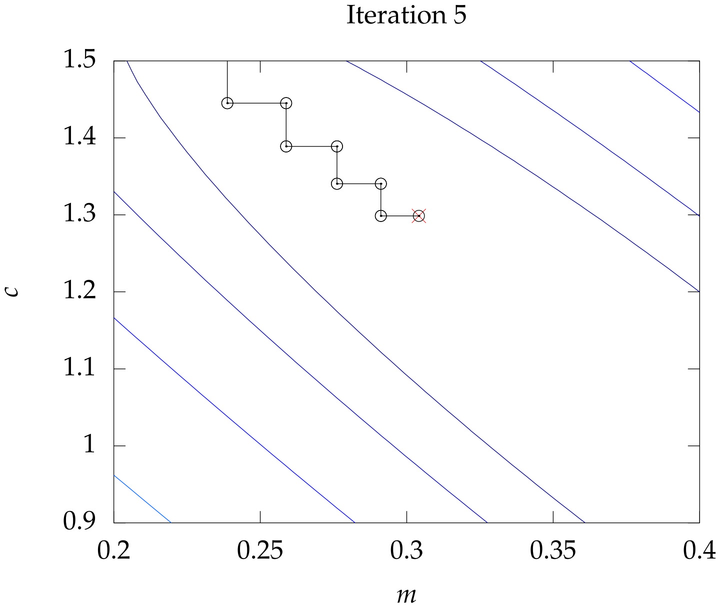

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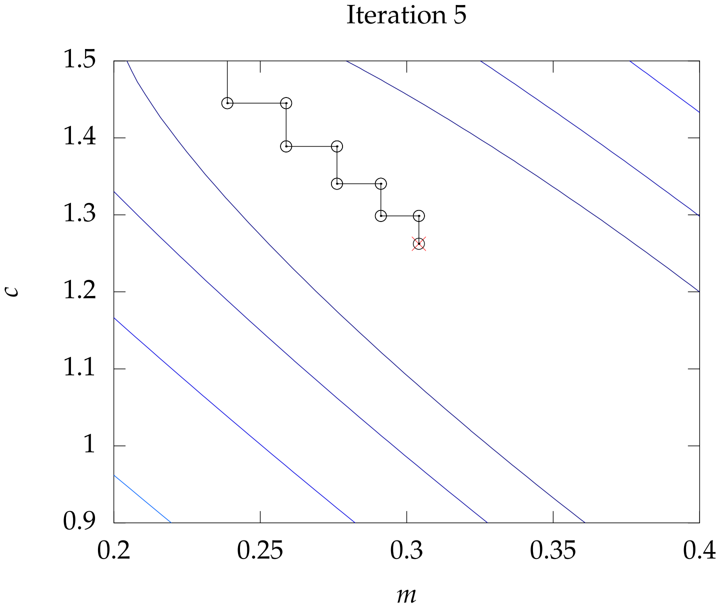

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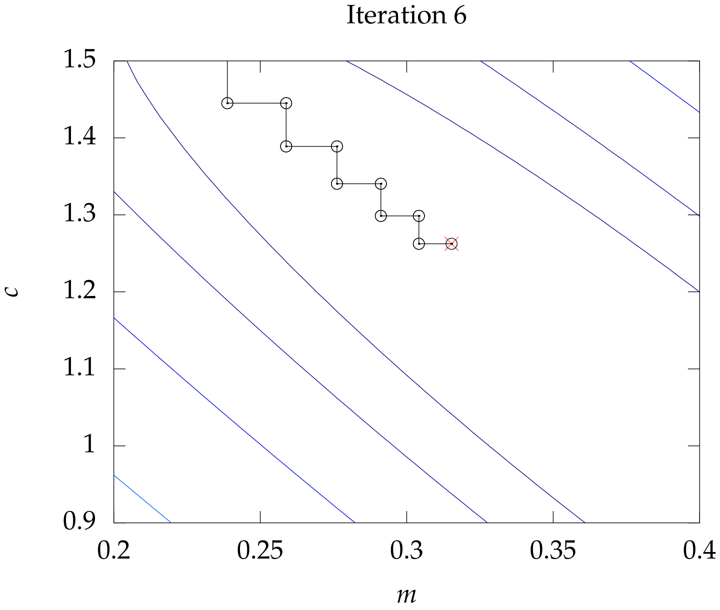

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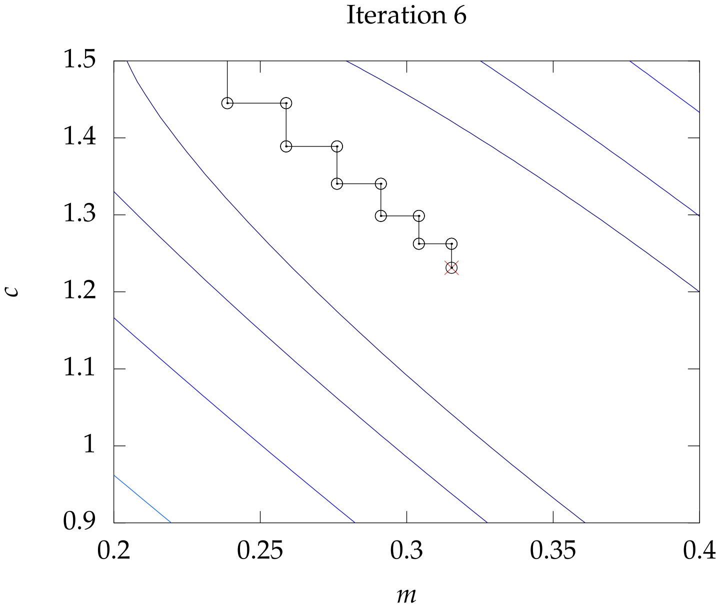

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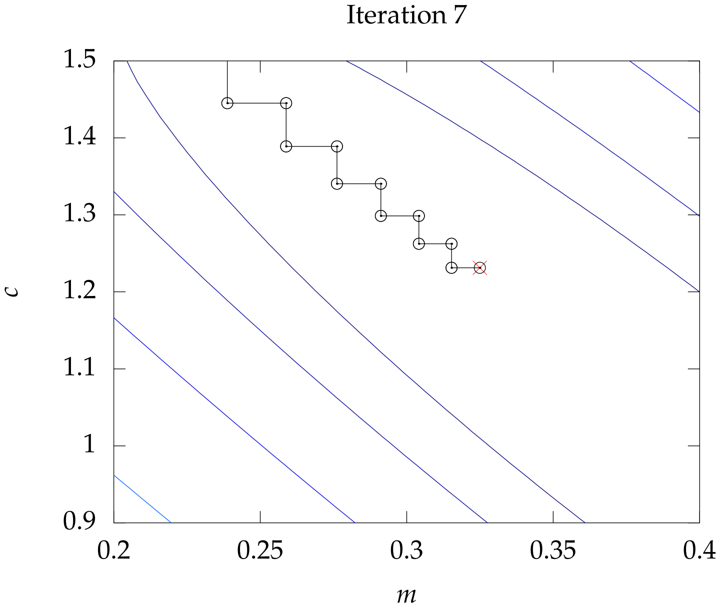

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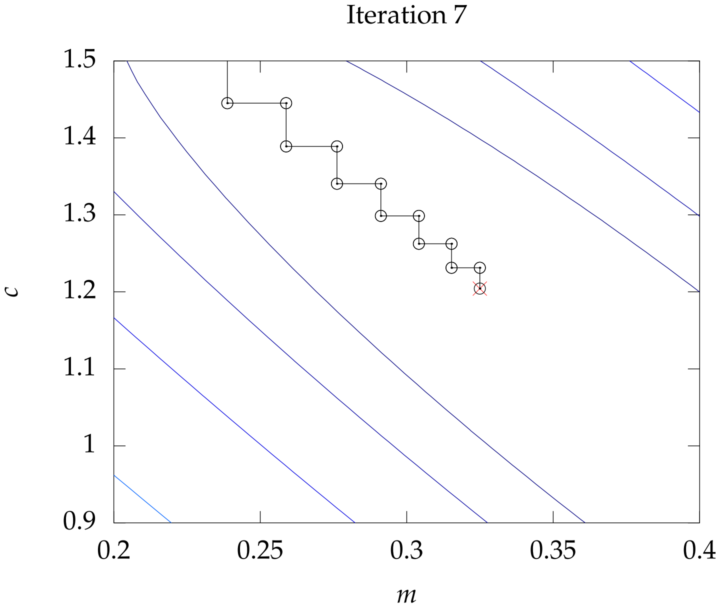

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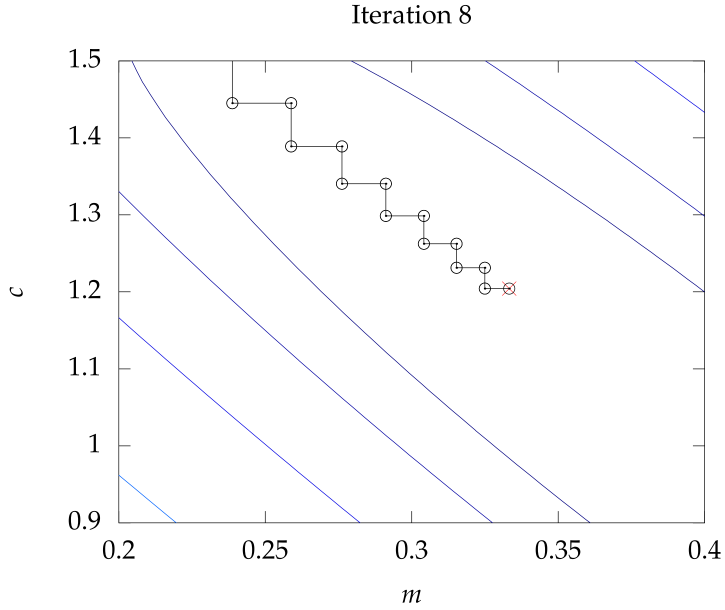

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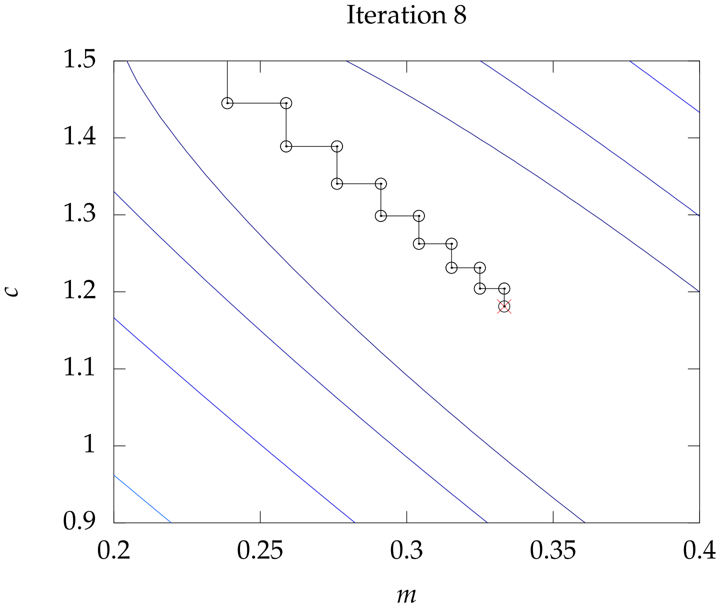

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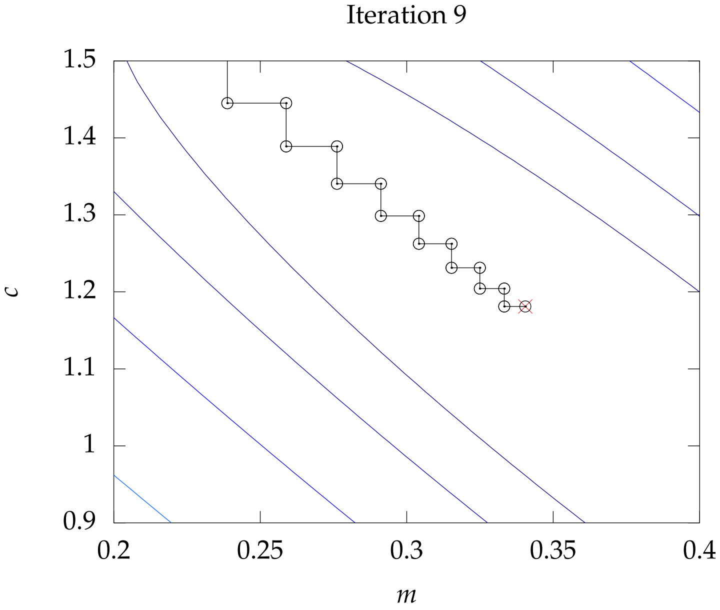

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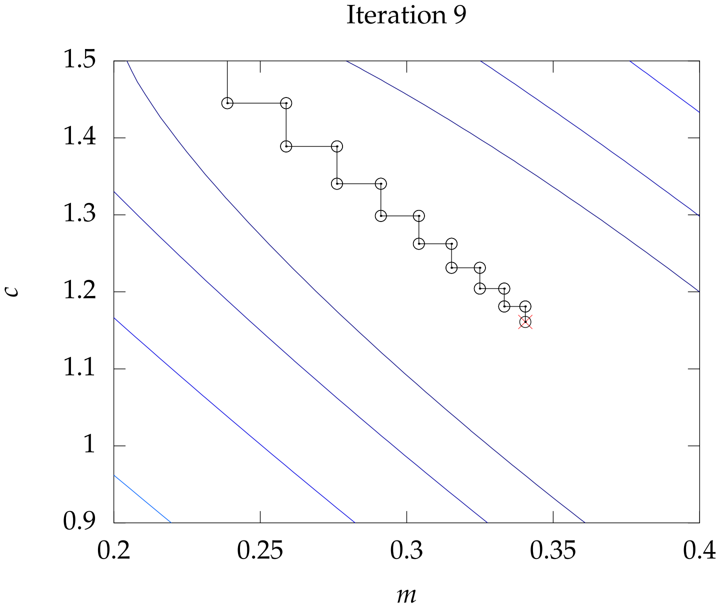

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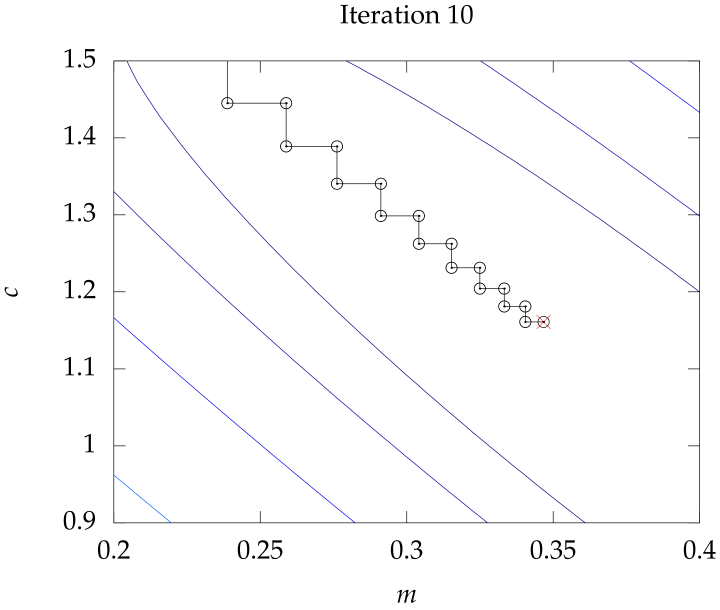

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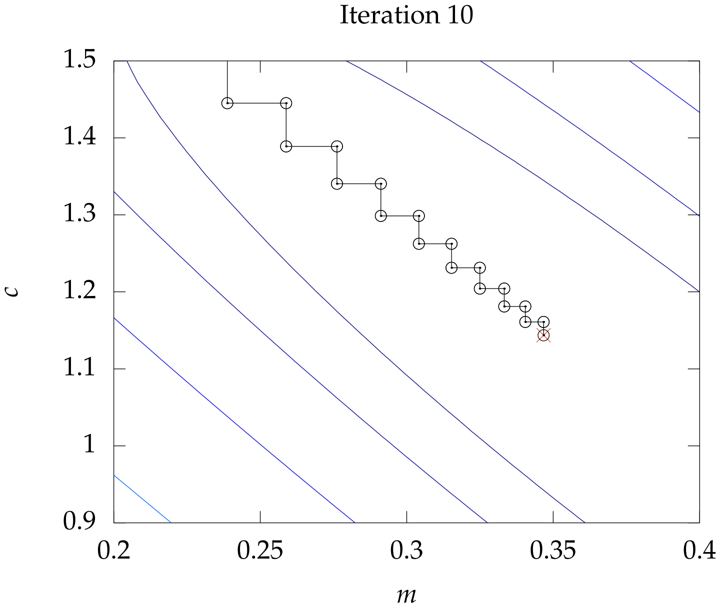

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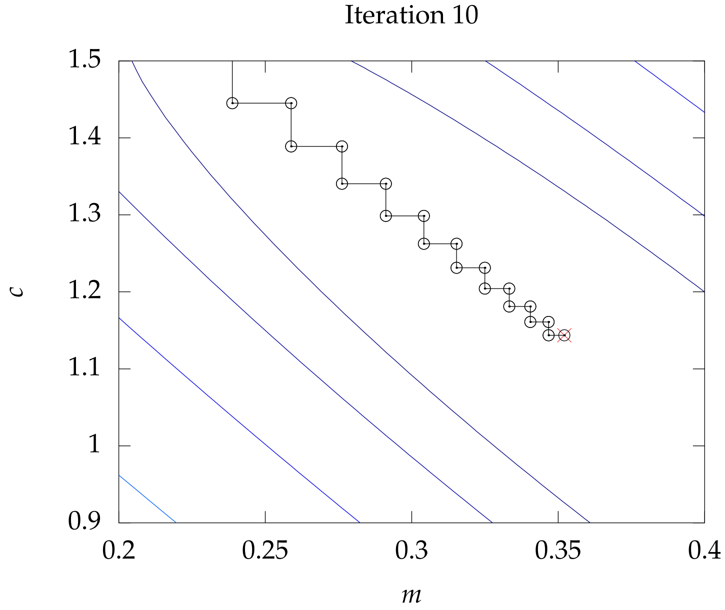

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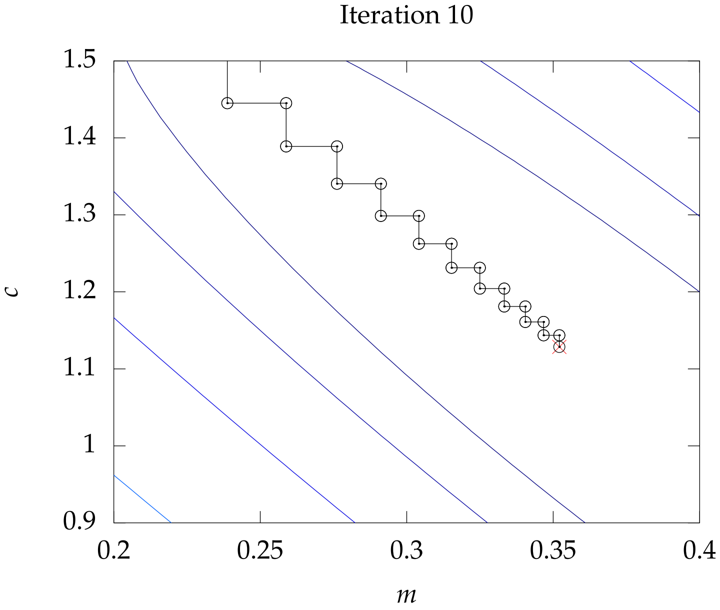

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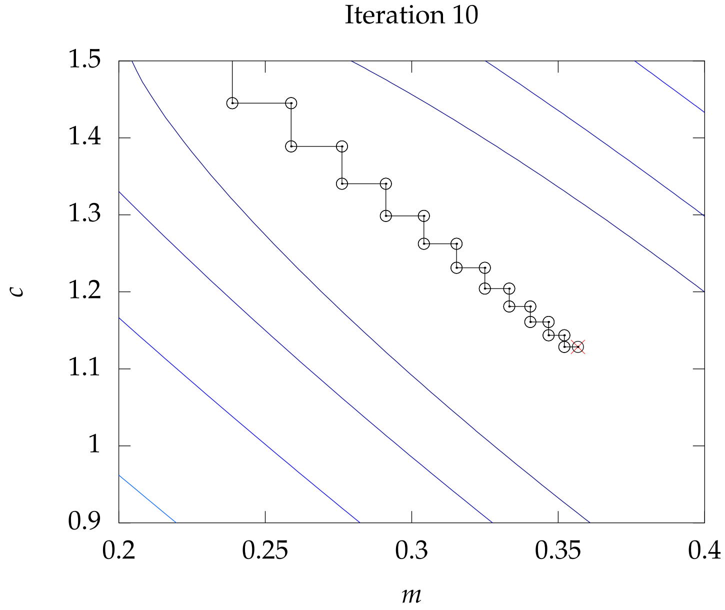

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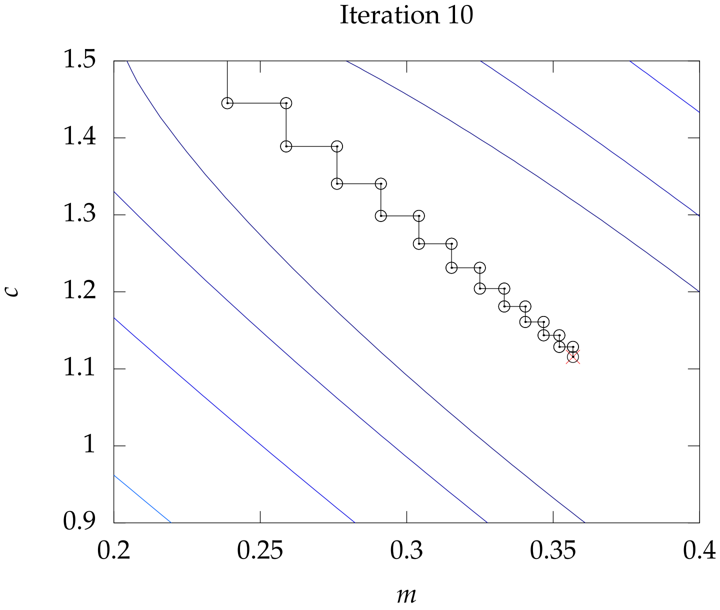

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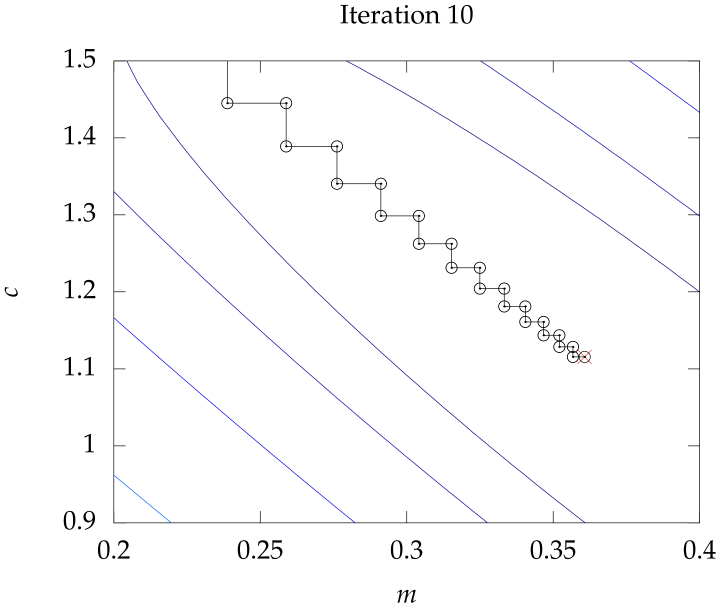

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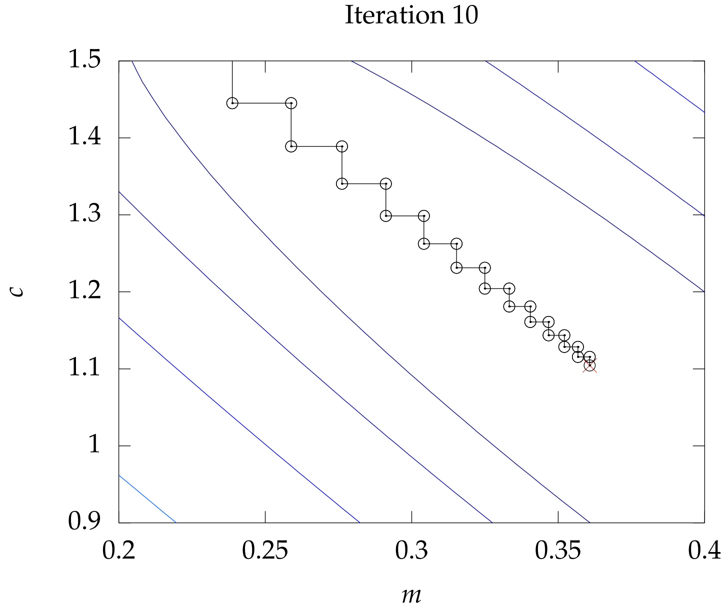

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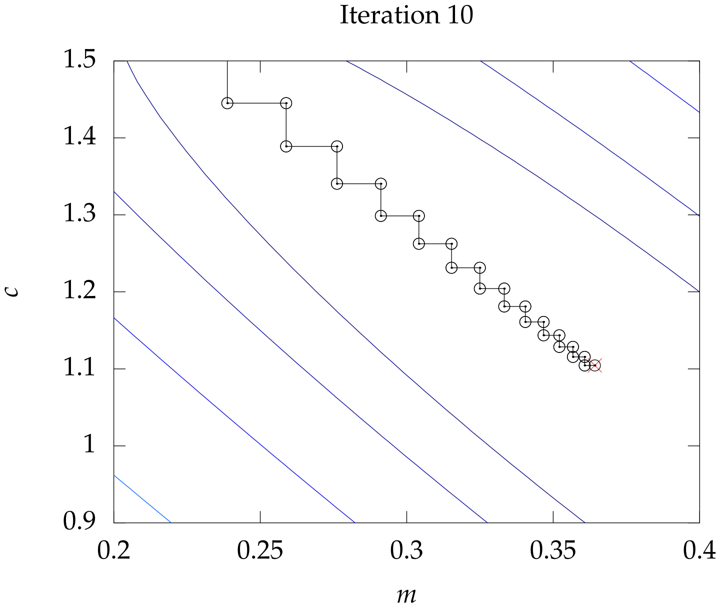

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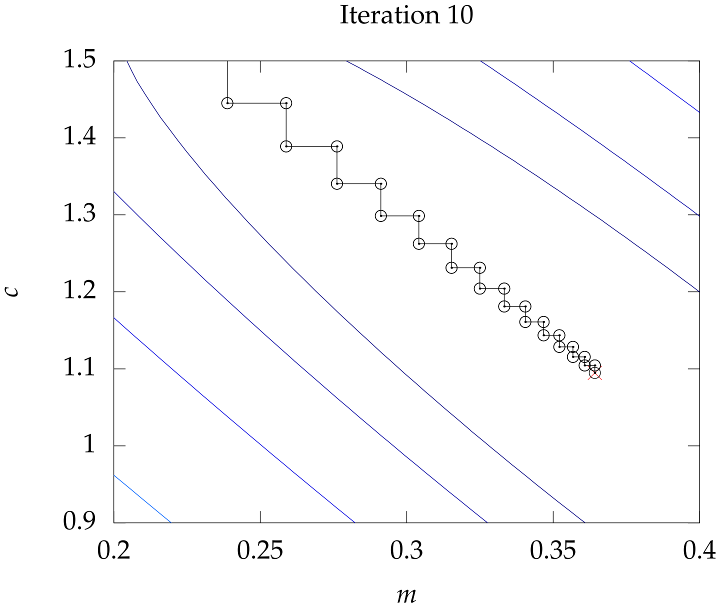

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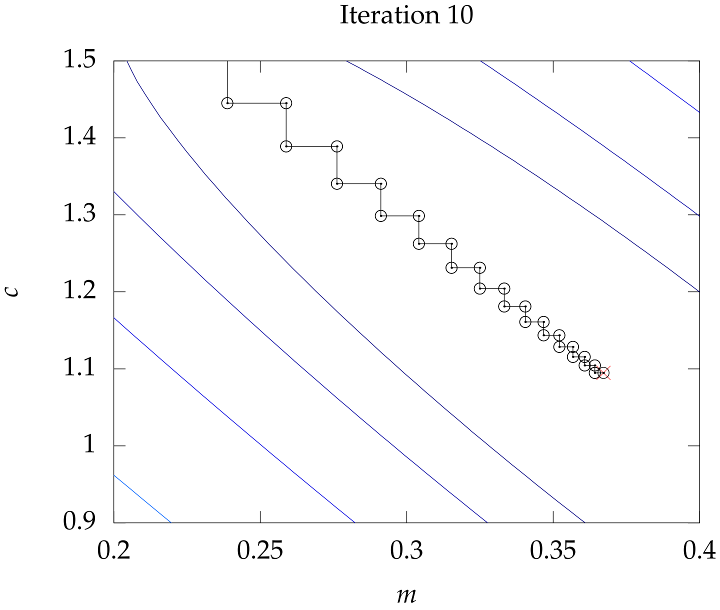

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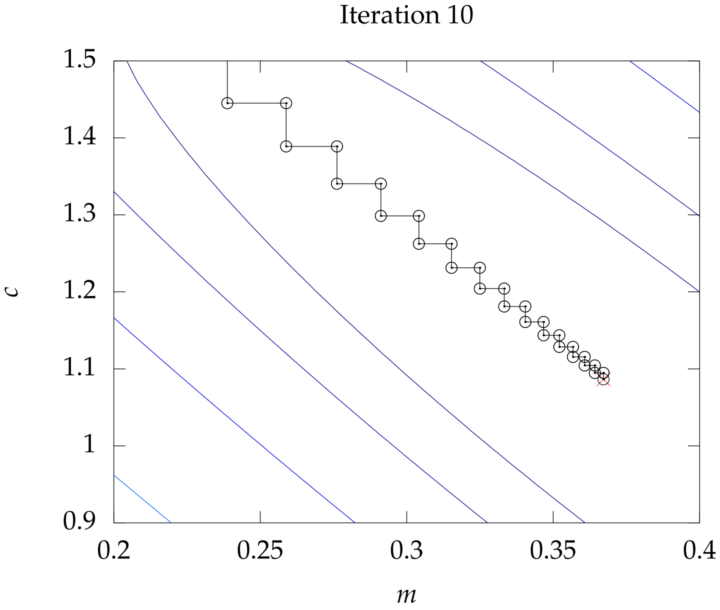

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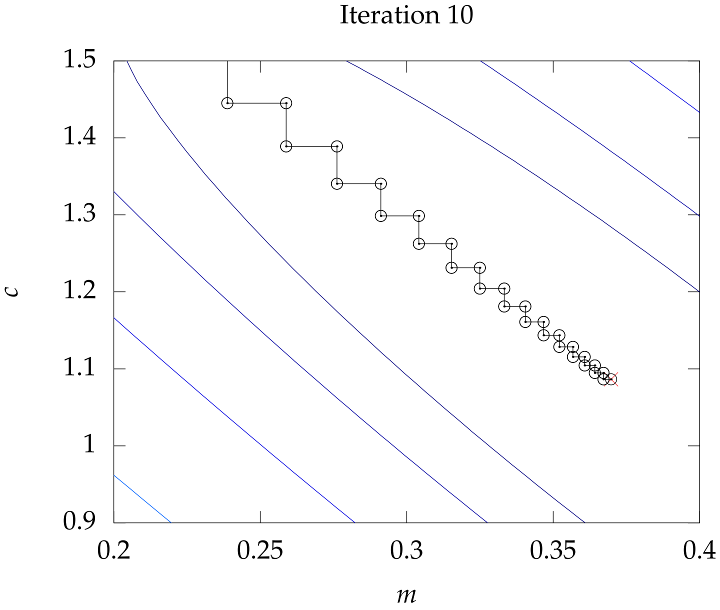

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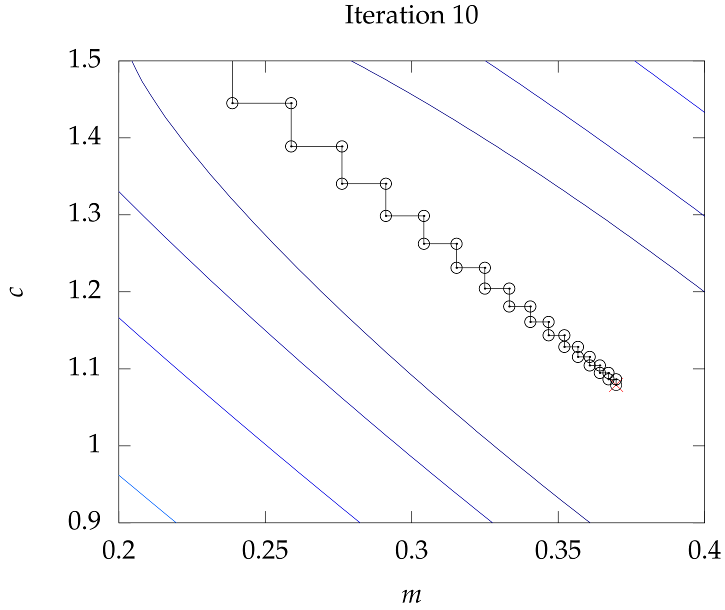

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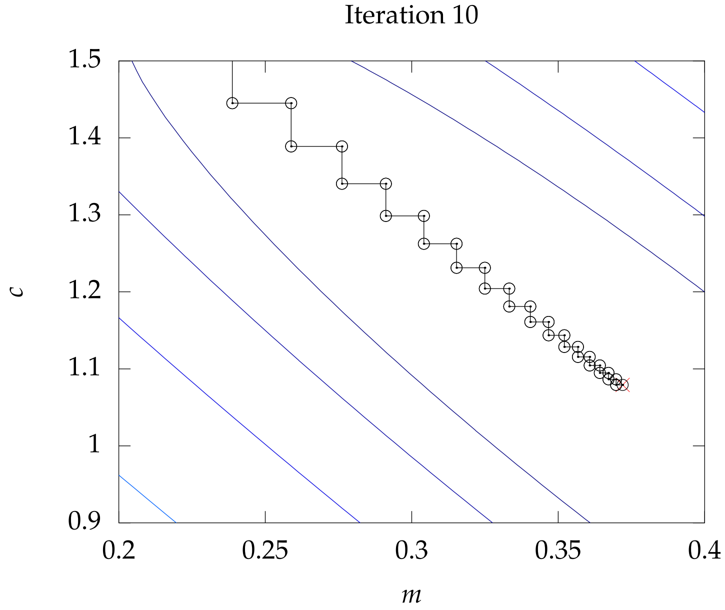

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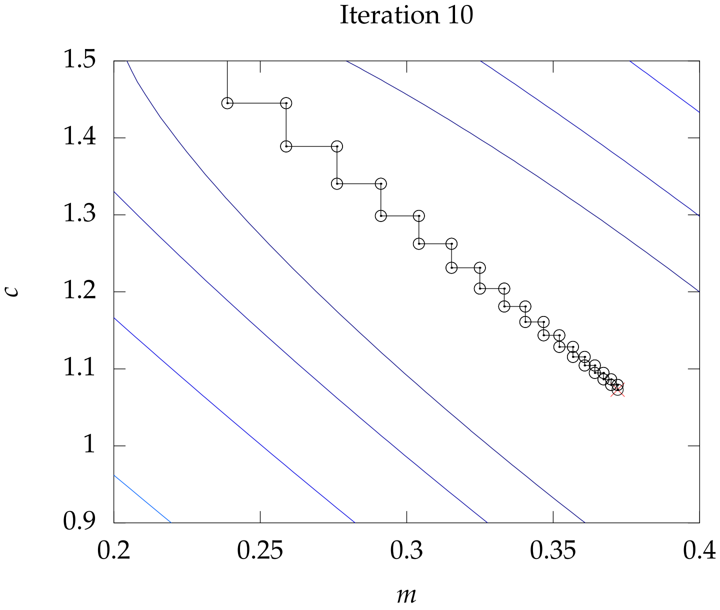

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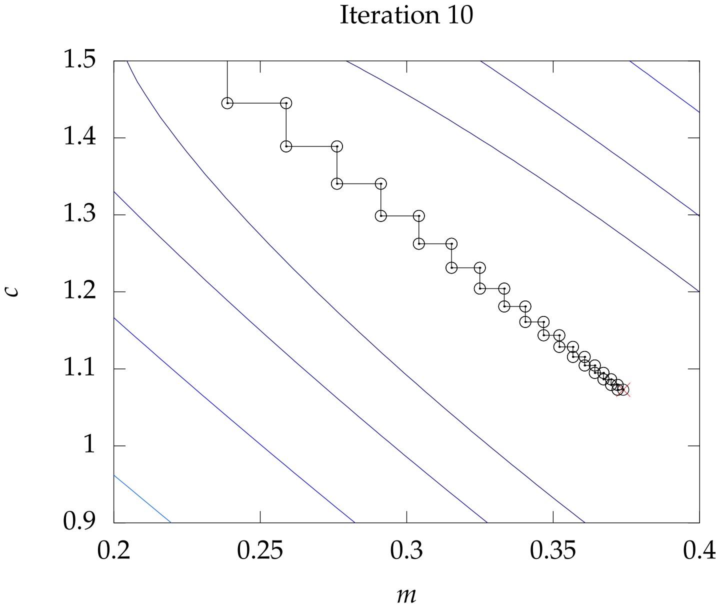

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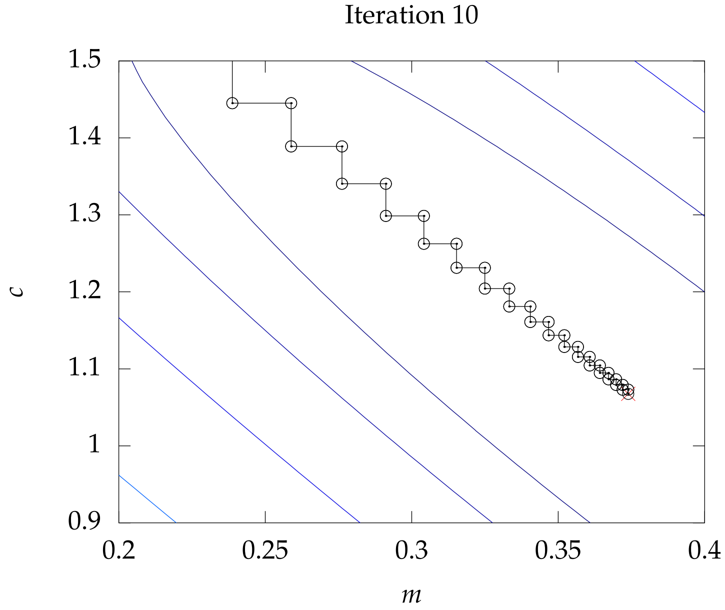

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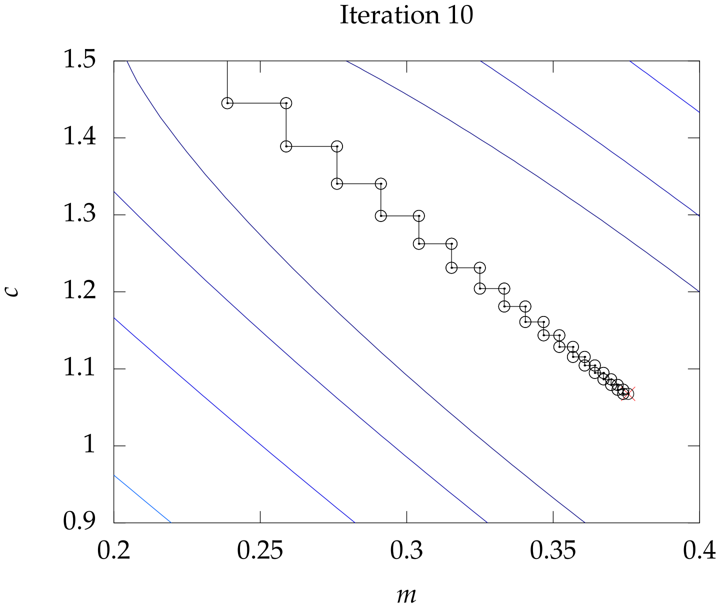

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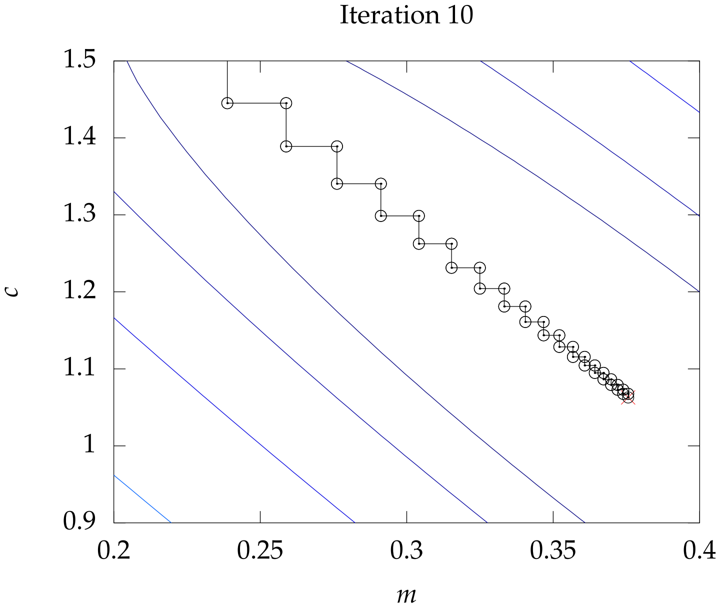

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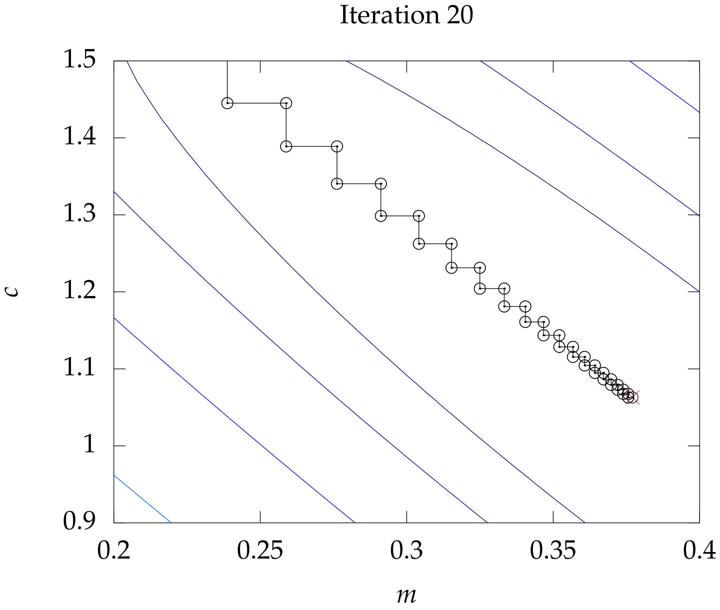

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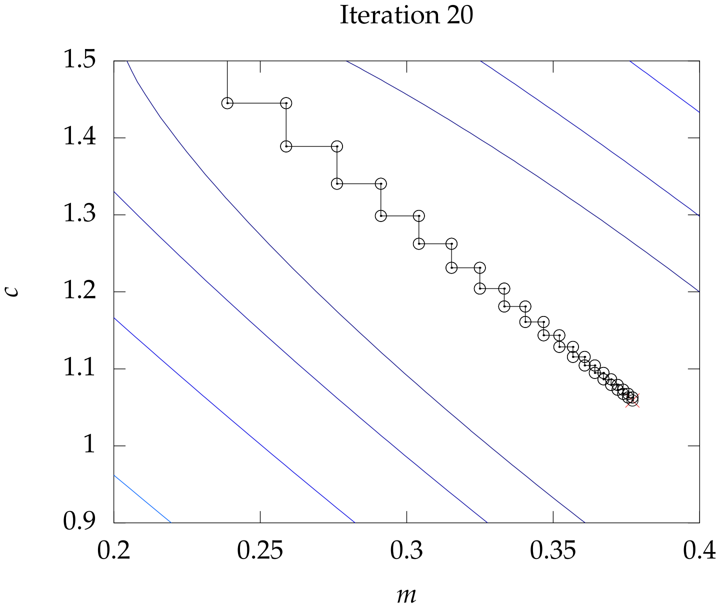

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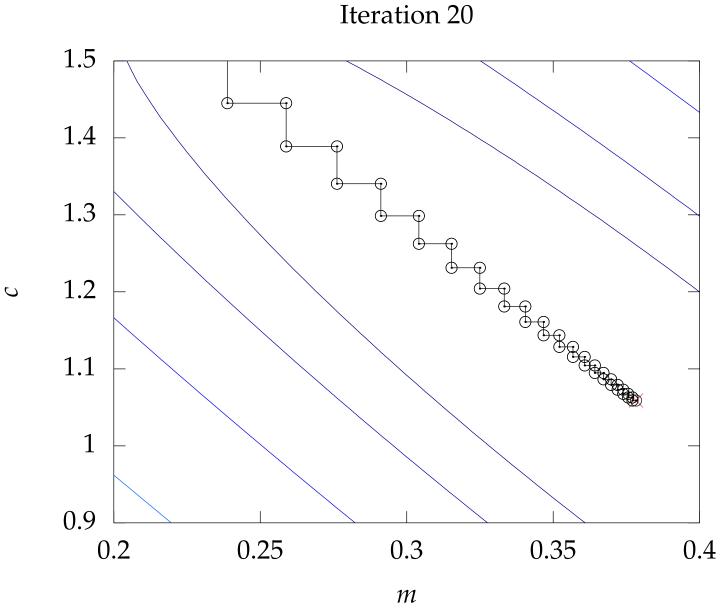

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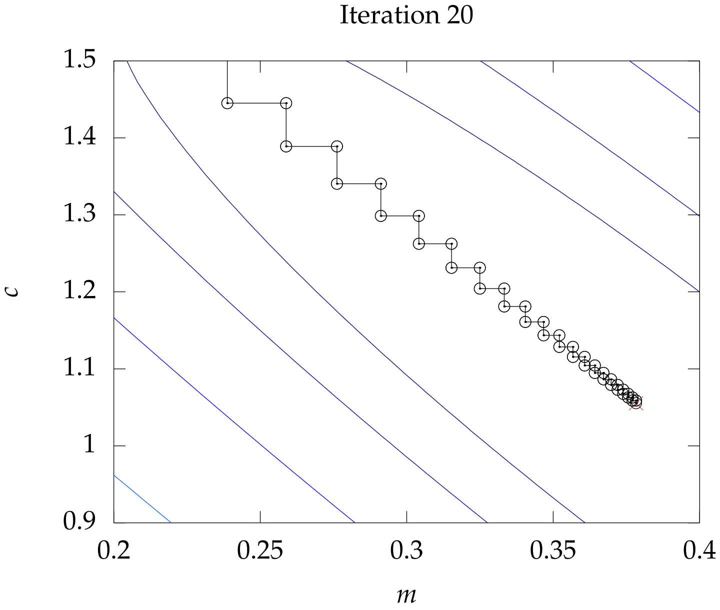

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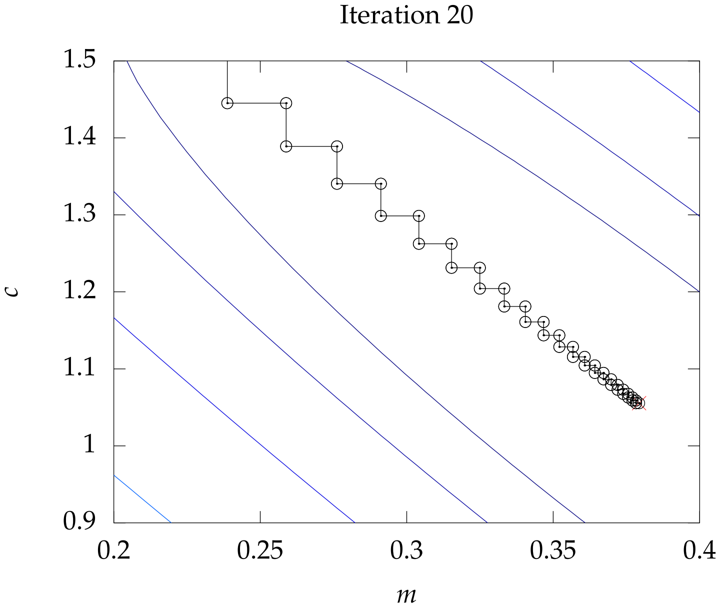

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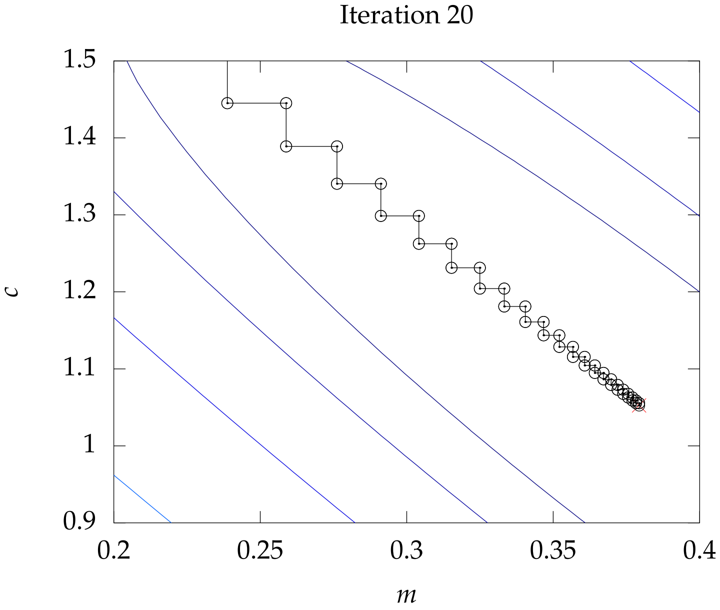

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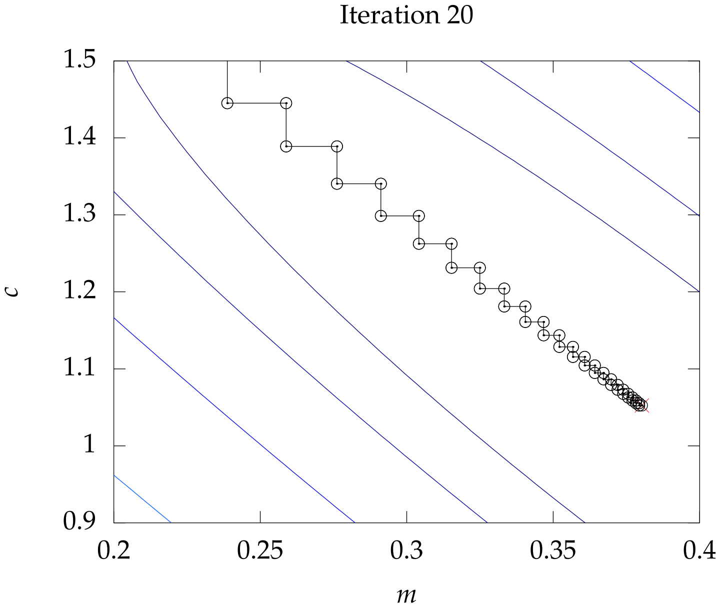

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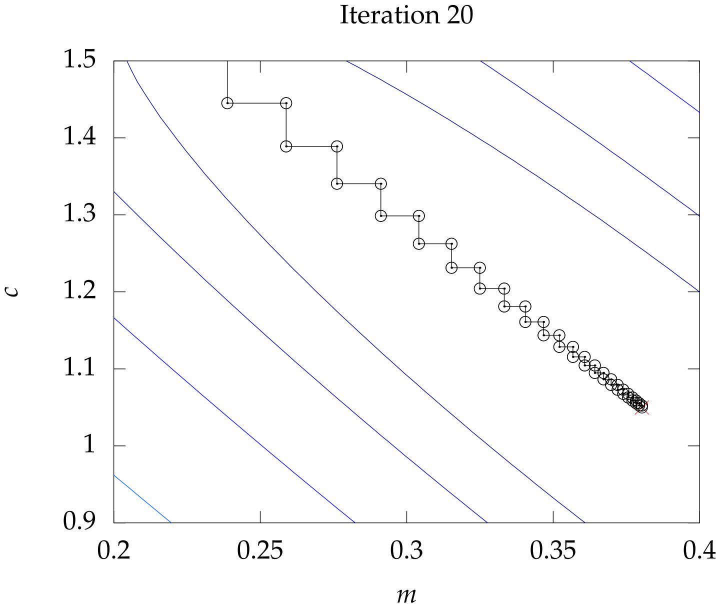

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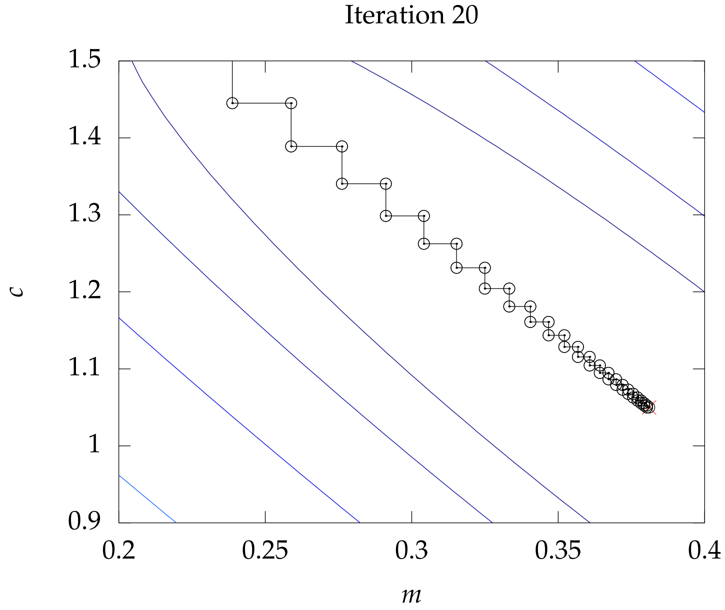

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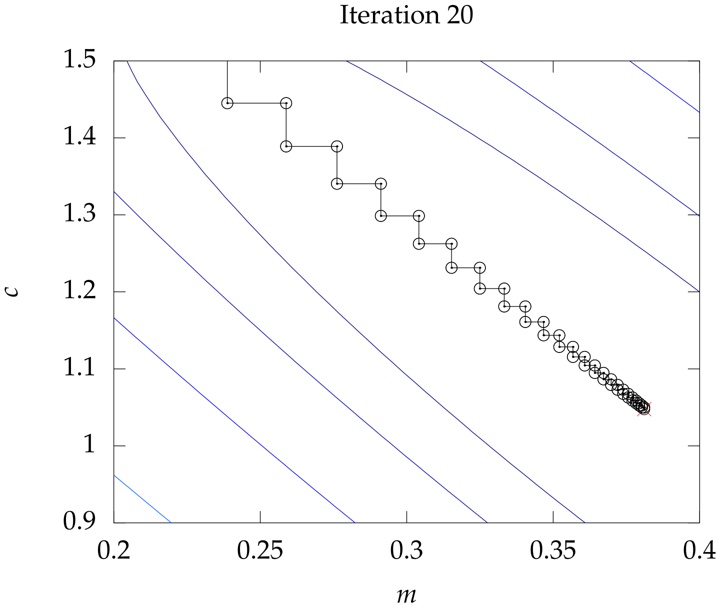

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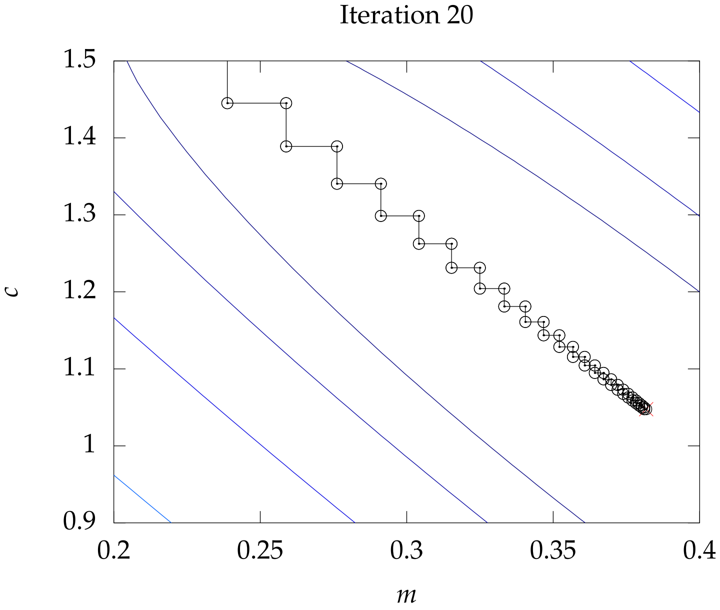

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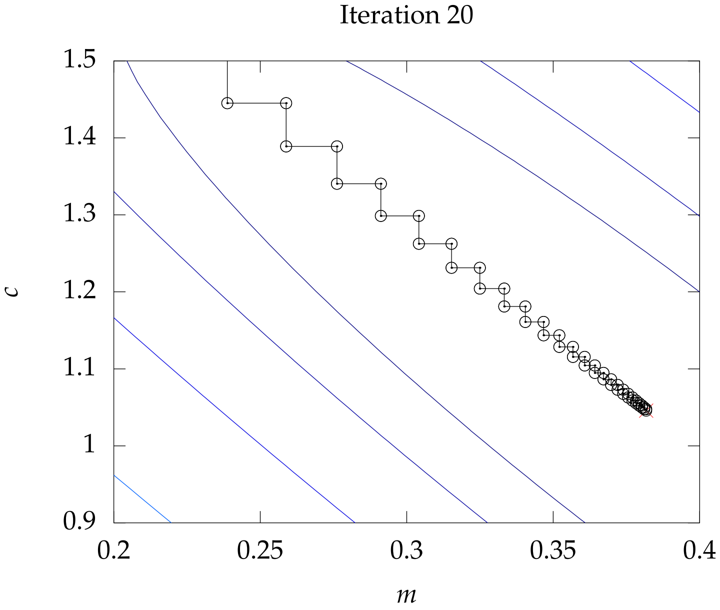

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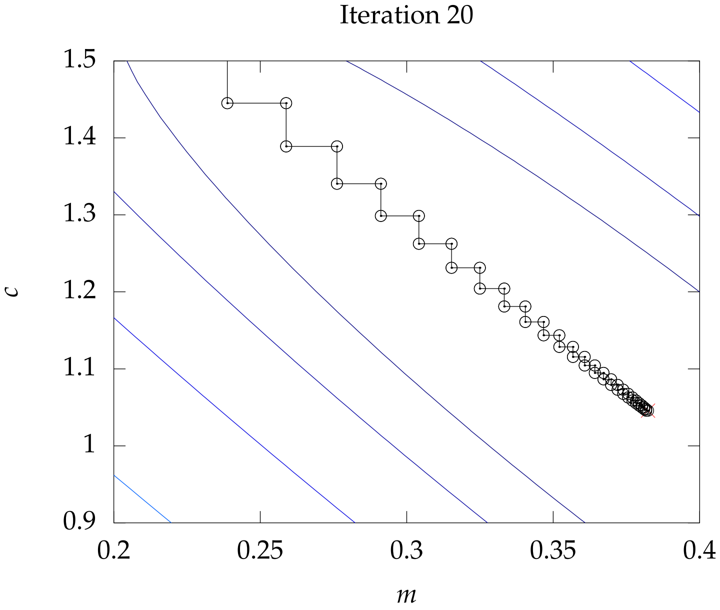

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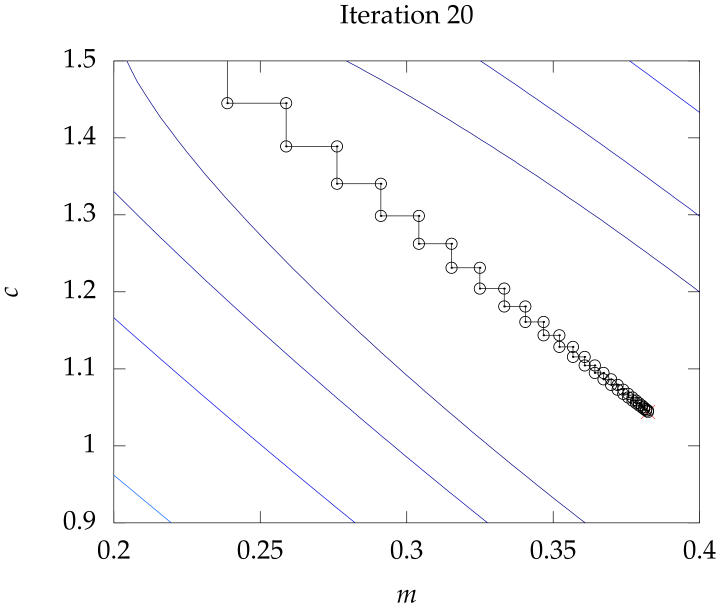

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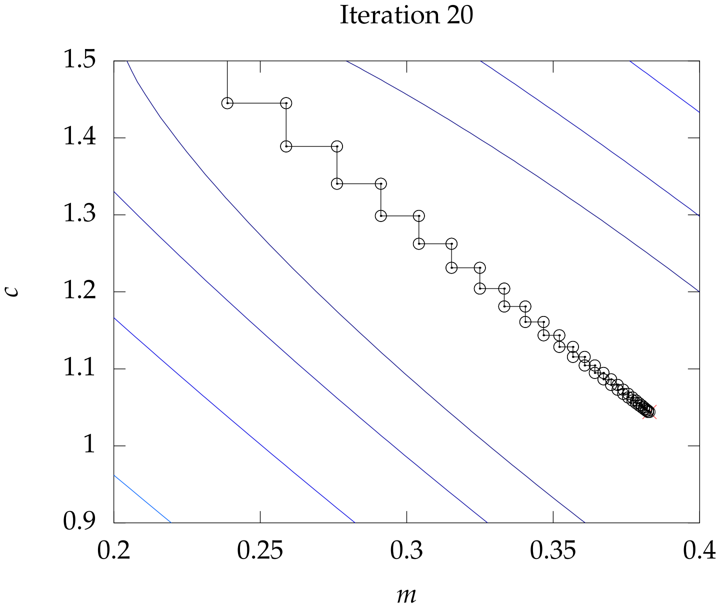

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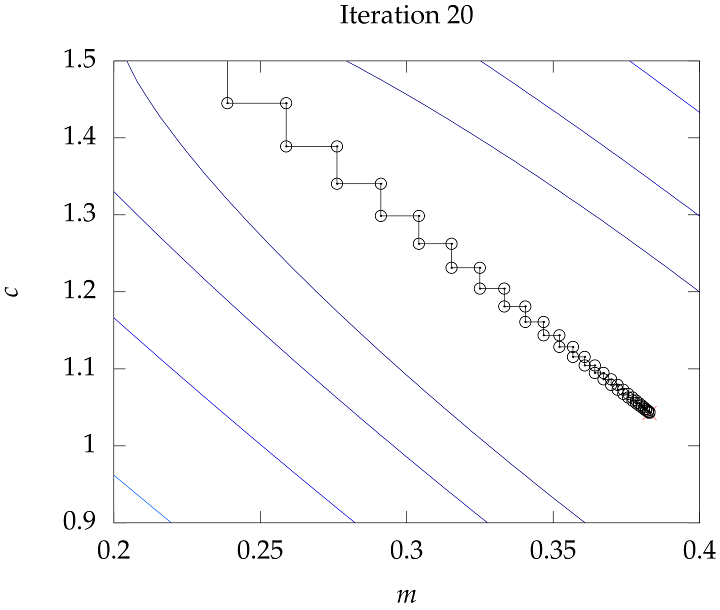

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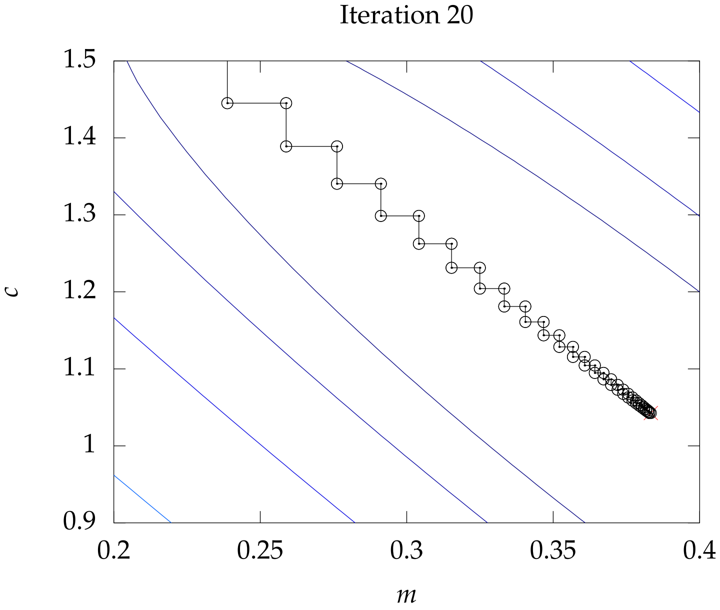

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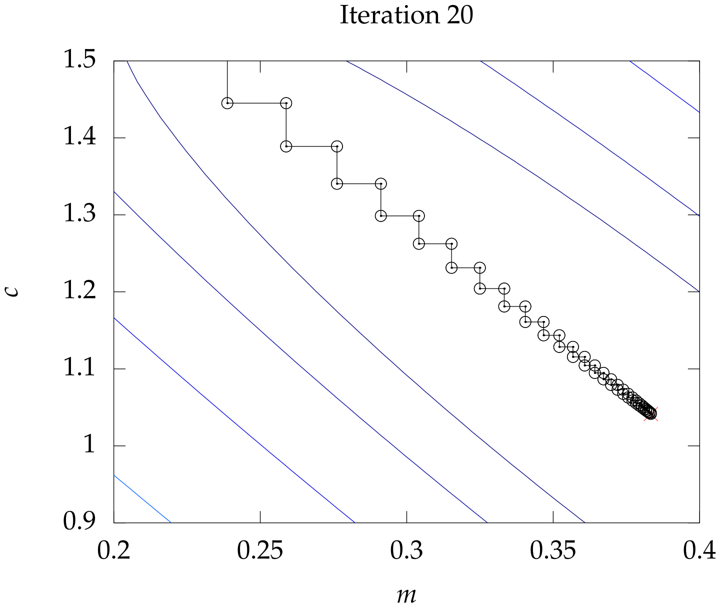

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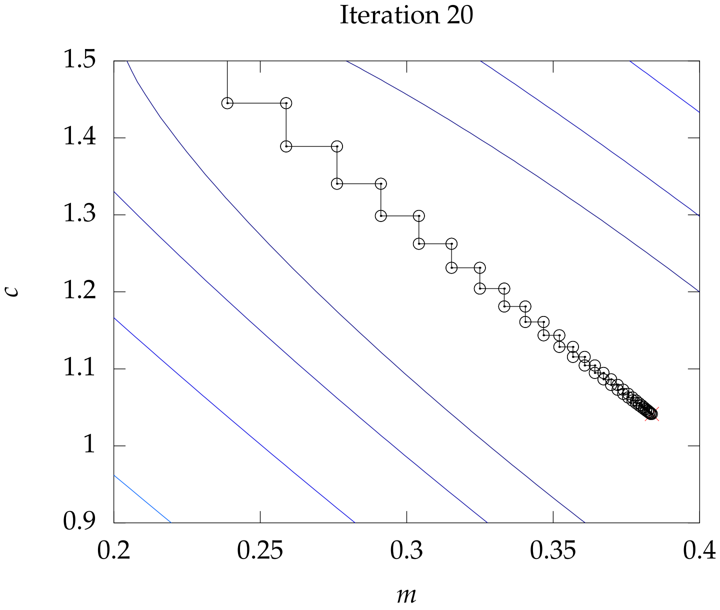

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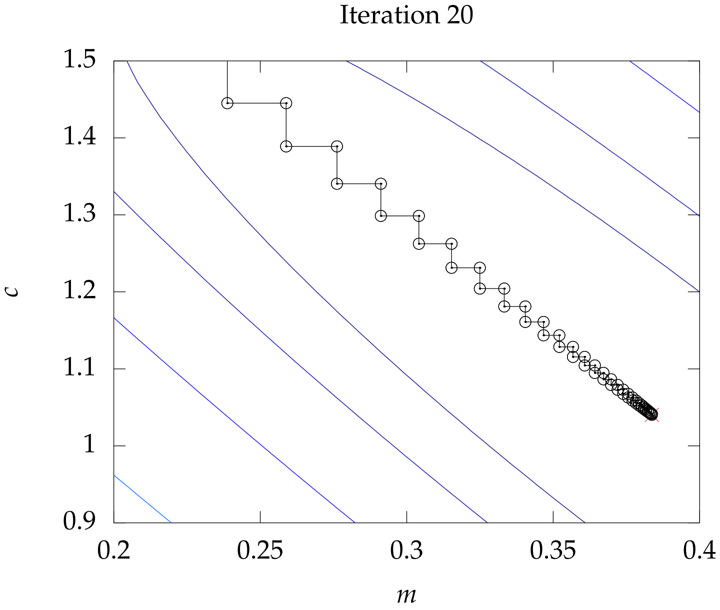

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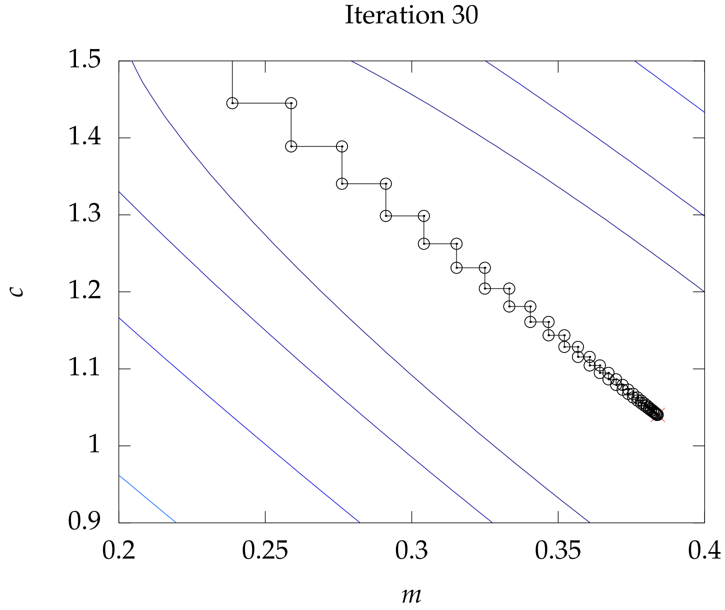

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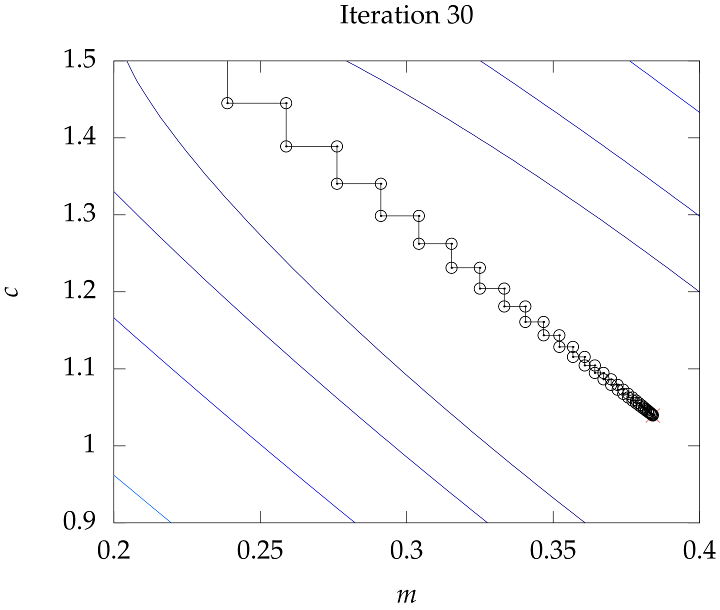

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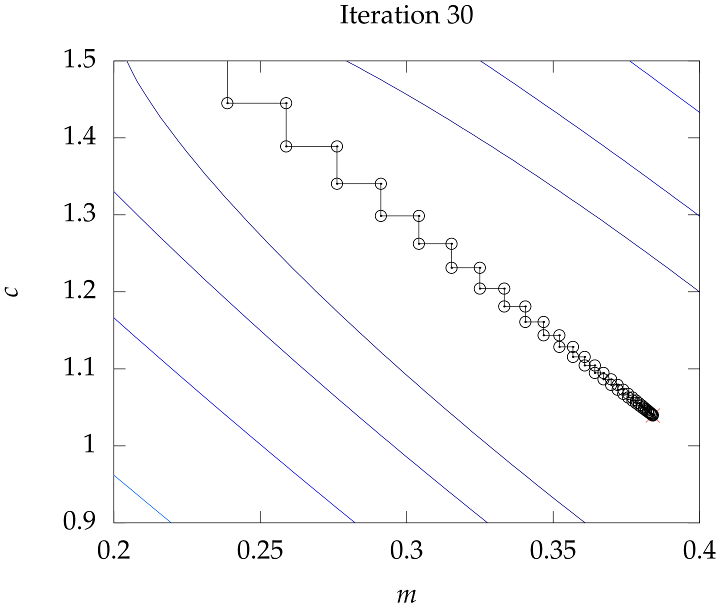
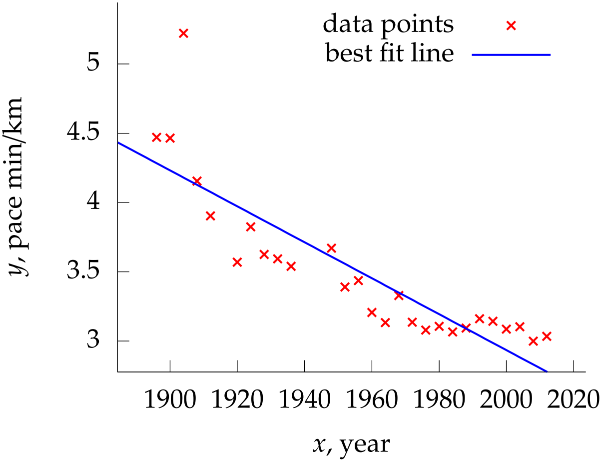


Important Concepts Not Covered

- Optimization methods.
  - Second order methods, conjugate gradient, quasi-Newton and Newton.
  - Effective heuristics such as momentum.
- Local vs global solutions.

Linear Function



Linear regression for Male Olympics Marathon Gold Medal times.

Reading

- Section 1.2.5 of Bishop up to equation 1.65.
- Section 1.1-1.2 of Rogers and Girolami for fitting linear models.

Multi-dimensional Inputs

- Multivariate functions involve more than one input.
- Height might be a function of weight and gender.
- There could be other contributory factors.
- Place these factors in a feature vector $\mathbf{x}_i$.
- Linear function is now defined as

$$f(\mathbf{x}_i) = \sum_{j=1}^{q} w_j x_{i,j} + c$$

Vector Notation

mo

- Write in vector notation,

$$f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i + c$$

- Can absorb c into $\mathbf{w}$ by assuming extra input x_0 which is always 1.

$$f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i$$

Log Likelihood for Multivariate Regression

- The likelihood of a single data point is

$$p\left(y_i|x_i\right) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\left(y_i - \mathbf{w}^\top \mathbf{x}_i\right)^2}{2\sigma^2}\right).$$

- Leading to a log likelihood for the data set of

$$L(\mathbf{w}, \sigma^2) = -\frac{N}{2}\log\sigma^2 - \frac{N}{2}\log 2\pi - \frac{\sum_{i=1}^{N}\left(y_i - \mathbf{w}^\top \mathbf{x}_i\right)^2}{2\sigma^2}.$$

- And a corresponding error function of

$$E(\mathbf{w}, \sigma^2) = \frac{N}{2}\log\sigma^2 + \frac{\sum_{i=1}^{N}\left(y_i - \mathbf{w}^\top \mathbf{x}_i\right)^2}{2\sigma^2}.$$

Expand the Brackets

$$
\begin{aligned}
E(\mathbf{w}, \sigma^2) =& \frac{N}{2}\log\sigma^2 + \frac{1}{2\sigma^2}\sum_{i=1}^{N} y_i^2 - \frac{1}{\sigma^2}\sum_{i=1}^{N} y_i \mathbf{w}^\top \mathbf{x}_i \\
&+ \frac{1}{2\sigma^2}\sum_{i=1}^{N} \mathbf{w}^\top \mathbf{x}_i \mathbf{x}_i^\top \mathbf{w} + \text{const.} \\
=& \frac{N}{2}\log\sigma^2 + \frac{1}{2\sigma^2}\sum_{i=1}^{N} y_i^2 - \frac{1}{\sigma^2}\mathbf{w}^\top \sum_{i=1}^{N} \mathbf{x}_i y_i \\
&+ \frac{1}{2\sigma^2}\mathbf{w}^\top \left[\sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^\top\right] \mathbf{w} + \text{const.}
\end{aligned}
$$

Multivariate Derivatives

- We will need some multivariate calculus.
- For now some simple multivariate differentiation:

$$\frac{\mathrm{d}\mathbf{a}^\top \mathbf{w}}{\mathrm{d}\mathbf{w}} = \mathbf{a}$$

and

$$\frac{\mathrm{d}\mathbf{w}^\top \mathbf{A}\mathbf{w}}{\mathrm{d}\mathbf{w}} = \left(\mathbf{A} + \mathbf{A}^\top\right)\mathbf{w}$$

or if $\mathbf{A}$ is symmetric (*i.e.* $\mathbf{A} = \mathbf{A}^\top$)

$$\frac{\mathrm{d}\mathbf{w}^\top \mathbf{A}\mathbf{w}}{\mathrm{d}\mathbf{w}} = 2\mathbf{A}\mathbf{w}.$$

Differentiate

Differentiating with respect to the vector **w** we obtain

$$\frac{\partial L(\mathbf{w}, \beta)}{\partial \mathbf{w}} = \beta \sum_{i=1}^{N} \mathbf{x}_i y_i - \beta \left[\sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^\top \right] \mathbf{w}$$

Leading to

$$\mathbf{w}^* = \left[\sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^\top \right]^{-1} \sum_{i=1}^{N} \mathbf{x}_i y_i,$$

Rewrite in matrix notation:

$$\sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^\top = \mathbf{X}^\top \mathbf{X}$$

$$\sum_{i=1}^{N} \mathbf{x}_i y_i = \mathbf{X}^\top \mathbf{y}$$

Update Equations

- Update for $\mathbf{w}^*$.

$$\mathbf{w}^* = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{y}$$

- The equation for ${\sigma^2}^*$ may also be found

$$ {\sigma^2}^* = \frac{\sum_{i=1}^{N} \left(y_i - {\mathbf{w}^*}^\top \mathbf{x}_i\right)^2}{N}. $$

Reading

- Section 1.3 of Rogers and Girolami for Matrix & Vector Review.

Outline

Regression

Basis Functions

- Problem with Linear Regression—$\mathbf{x}$ may not be linearly related to $\mathbf{y}$.
- Potential solution: create a feature space: define $\phi(\mathbf{x})$ where $\phi(\cdot)$ is a nonlinear function of $\mathbf{x}$.
- Model for target is a linear combination of these nonlinear functions

$$f(\mathbf{x}) = \sum_{j=1}^{K} w_j \phi_j(\mathbf{x}) \tag{1}$$

Quadratic Basis

- Basis functions can be global. E.g. quadratic basis:

$$[1, x, x^2]$$

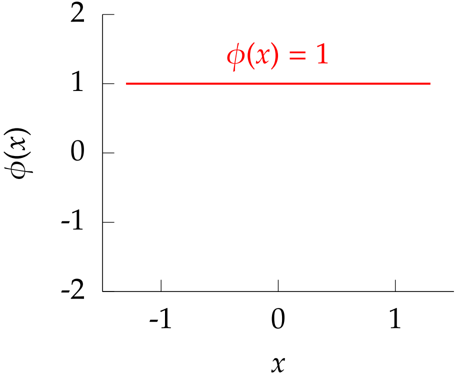


Figure: A quadratic basis.

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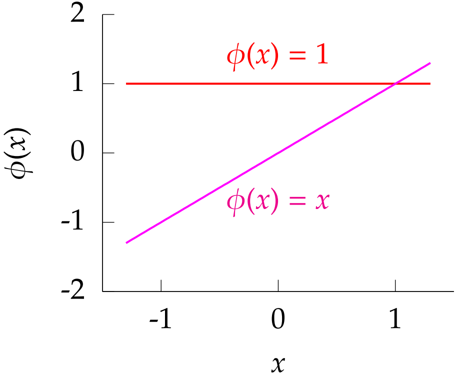

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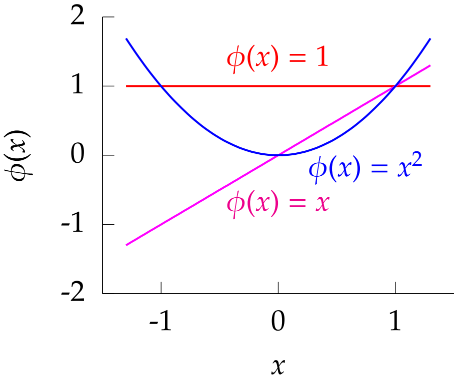

Figure: A quadratic basis.

Functions Derived from Quadratic Basis

$$f(x) = w_1 + w_2 x + w_3 x^2$$

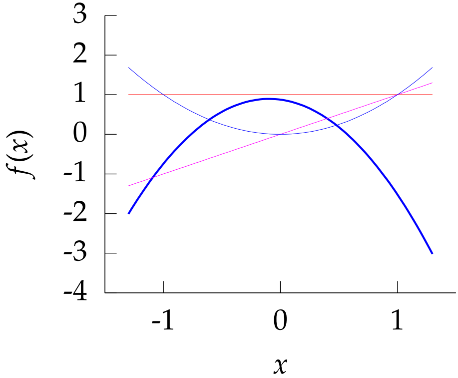

Figure: Function from quadratic basis with weights $w_1 = 0.87466$, $w_2 = -0.38835$, $w_3 = -2.0058$.

Functions Derived from Quadratic Basis

$$f(x) = w_1 + w_2 x + w_3 x^2$$

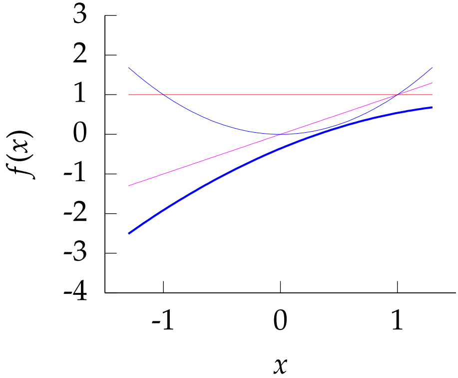

Figure: Function from quadratic basis with weights $w_1 = -0.35908$, $w_2 = 1.2274$, $w_3 = -0.32825$.

Functions Derived from Quadratic Basis

$$f(x) = w_1 + w_2 x + w_3 x^2$$

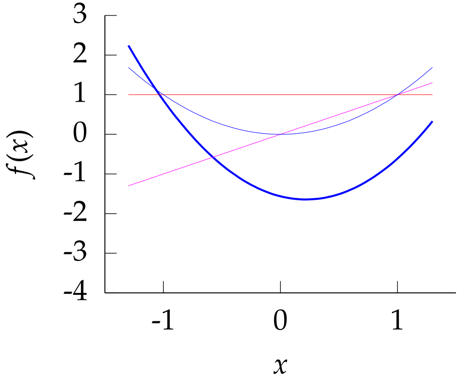

Figure: Function from quadratic basis with weights $w_1 = -1.5638$, $w_2 = -0.73577$, $w_3 = 1.6861$.

Radial Basis Functions

- Or they can be local. E.g. radial (or Gaussian) basis $\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{\ell^2}\right)$

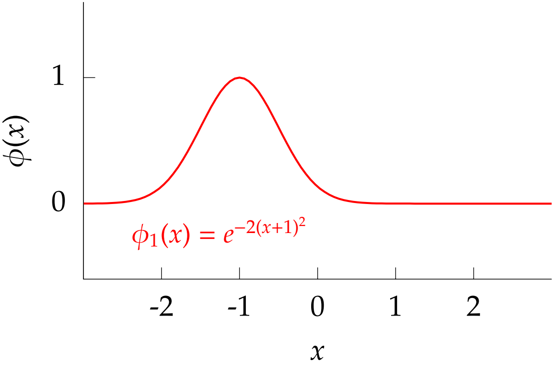

Figure: Radial basis functions.

Radial Basis Functions

- Or they can be local. E.g. radial (or Gaussian) basis $\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{\ell^2}\right)$

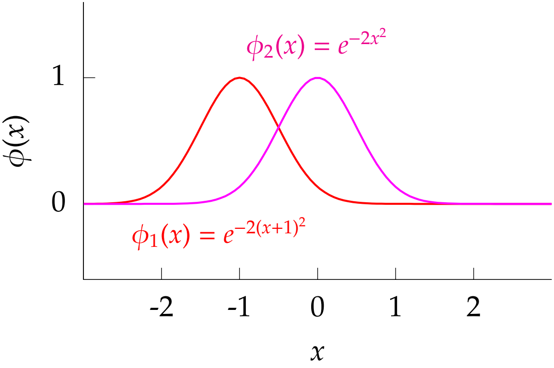

Figure: Radial basis functions.

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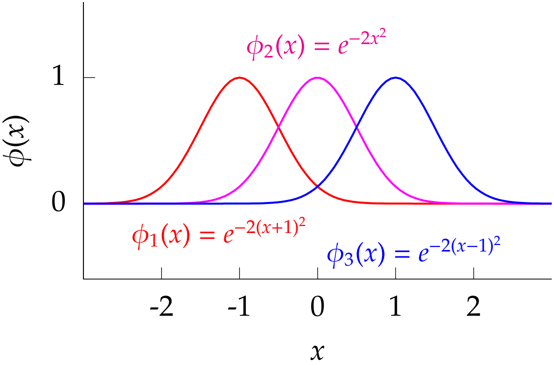

Figure: Radial basis functions.

Functions Derived from Radial Basis

$$f(x) = w_1 e^{-2(x+1)^2} + w_2 e^{-2x^2} + w_3 e^{-2(x-1)^2}$$

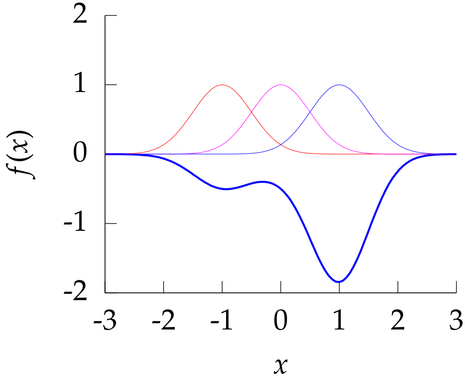

Figure: Function from radial basis with weights $w_1 = -0.47518$, $w_2 = -0.18924$, $w_3 = -1.8183$.

Functions Derived from Radial Basis

$$f(x) = w_1 e^{-2(x+1)^2} + w_2 e^{-2x^2} + w_3 e^{-2(x-1)^2}$$

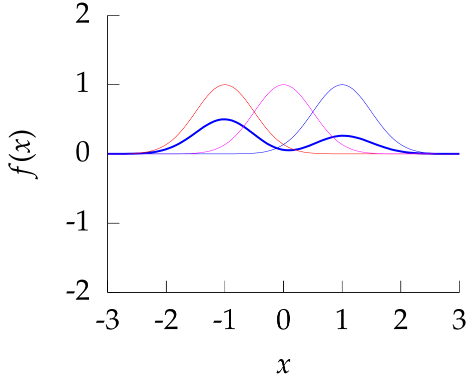

Figure: Function from radial basis with weights $w_1 = 0.50596$, $w_2 = -0.046315$, $w_3 = 0.26813$.

Functions Derived from Radial Basis

$$f(x) = w_1 e^{-2(x+1)^2} + w_2 e^{-2x^2} + w_3 e^{-2(x-1)^2}$$

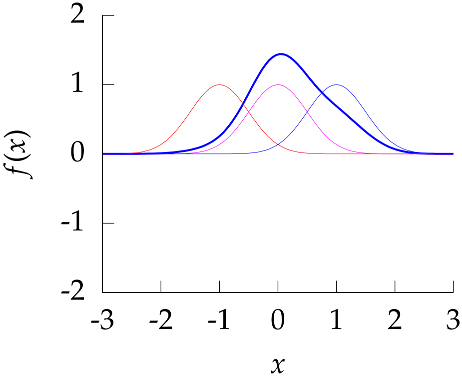

Figure: Function from radial basis with weights $w_1 = 0.07179$, $w_2 = 1.3591$, $w_3 = 0.50604$.

Reading

- Chapter 1, pg 1-6 of Bishop.
- Section 1.4 of Rogers and Girolami.
- Chapter 3, Section 3.1 of Bishop up to pg 143.

Reading Summary

- In Rogers and Girolami:
  - Section 1.1-1.2 for fitting linear models.
  - Section 1.3 for Matrix & Vector Review.
  - Section 1.4.
- In Bishop:
  - Chapter 1, pg 1-6.
  - Complete Section 1.2.4 (from last time), page 26–28 (don't worry about material on bias).
  - For material on information theory and KL divergence try Section 1.6 & 1.6.1 of (pg 48 onwards). Suggest skipping rest of Section 1.2.4, page 26–28 (don't worry about material on bias).
  - Section 1.2.5 of up to equation 1.65.
  - Section 1.1.
  - Chapter 3, Section 3.1 up to pg 143.

References I

C. M. Bishop. *Pattern Recognition and Machine Learning*. Springer-Verlag, 2006. [Google Books] .

S. Rogers and M. Girolami. *A First Course in Machine Learning*. CRC Press, 2011. [Google Books] .