Figure S1: Distribution of each objective in bean SOM map (a). Distribution of each objective in maize SOM map (b). Region 1 corresponds to nodes with phenotypes with low carbon cost and root respiration. Region 2 corresponds to nodes with greatest biomass. Region 3 corresponds to nodes with greatest root length at depth. The mean of the objective in each node is represented. The change in color from blue to red show a change in magnitude of the value with red representing greatest values.
Figure S2: Mean value of objective in each node for bean optimal phenotypes in a region with sub-optimal N and P (a). The relative performance of the phenotypes in different objective in each node (b). Nodes 6, 8 and 9 have comparable biomass but vary in performance in other objectives. Some representative bean phenotypes with comparable biomass from nodes 6, 8 and 9 (c). Primary root is in black; Basal roots in red; Hypocotyl-borne roots in green.
Figure S3: Mean value of objective in each node for maize optimal phenotypes in a region with sub-optimal N and P (a). The relative performance of the phenotypes in different objective in each node (b). Nodes 1, 2, 3, 5 and 6 have comparable biomass but vary in performance in other objectives. Some representative phenotypes with comparable biomass from nodes 1, 2, 3, 5 and 6 (c). Primary root is in black; Seminal roots in red; Nodal roots in green.
Figure S4: Different primary root phenotypes found in optimal bean phenotypes (a) and optimal maize phenotypes (b). The primary root phenotype in bean and maize root system is defined by diameter and LRBD. Phenotypes with primary roots differing in both diameter and LRBD were found among the optimal solutions of both bean as well as maize. None of the optimal phenotypes had high values for both diameter and LRBD in bean or maize. Some phenotypes had very large diameter and some very high LRBD. Phenotypes with very high LRBD were seen in phenotypes optimal under low P in bean and in maize root systems.
Figure S5: Different hypocotyl-borne root phenotypes found in optimal bean phenotypes. The HBR phenotype is defined by the number of root axes, their diameter and LRBD, and phenotypes differing in all three of these phenes were found among the optimal solutions in bean. Phenotypes with more HBR as well as greater LRBD of HBR were found in optimal phenotypes evolved under low P. Some phenotypes did not have any HBR and were typically found in regions low in N and under very low P.
Figure S6: Different basal root phenotypes found in optimal bean phenotypes. Nodes in blue have phenotypes found in low N regions. Nodes in yellow have phenotypes found in low P regions. Nodes in grey have phenotypes found in low P as well as low N. The BR phenotype is defined by the number of root axes, and their angle, diameter and LRBD as well as the BRWN. Small diameter, highly branched, shallow basal roots were found almost exclusively in low P regions as well as in low N+P. Basal root phenotypes in low N are distinctly different from those expressed in low P conditions and typically had more basal roots with fewer lateral roots and had a wide range of root growth angles.
Figure S7: Different nodal root phenotypes found in optimal maize phenotypes. The NR phenotype is defined by the number of root axes, and their angle and diameter as well as time of emergence. Optimal phenotypes under low P had fewer NR while those under low N had more NR. Phenotypes with the greatest NR LRBD were found in the low P region.
The BORG MOEA provides SimRoot with a vector of root phene values. SimRoot returns the objective function values for the vector of root phene values. Stopping criteria – Number of evaluations:

- Optimized Objectives
- Phene values corresponding to the optimized objectives

Figure S8: Flow chart of the SimRoot-Borg loop. Vector of phene values is provided by the Borg MOEA to SimRoot as SimRoot inputs. The root architecture model is generated based on the input values by SimRoot and outputs obtained at the end of the model run are provided as objective function values to the Borg MOEA for evaluation.
Supplementary tables

Table S1: Range of input values for generating bean root phenotypes. PR – primary root; HBR-Hypocotyl-Borne-Root; BW – Basal Whorl; BW1, BW2, BW3, BW4, BW5 refer to the position of the basal whorl counted from basipetal to acropetal position; Dia – axial root diameter; Lat.Dia – lateral root diameter; LRBD – lateral root branching density.

|                         | Units | Min | Max | References       |
|-------------------------|-------|-----|-----|------------------|
| Number.BW1              | NA    | 0   | 4   | Miguel et al., 2013 |
| Number.BW2              | NA    | 0   | 4   |                  |
| Number.BW3              | NA    | 0   | 4   |                  |
| Number.BW4              | NA    | 0   | 4   |                  |
| Number.BW5              | NA    | 0   | 4   |                  |
| Number.HBR              | NA    | 0   | 30  | Miller et al., 2003 |
| PR.Dia                  | cm    | 0.08| 0.45| Henry et al., 2009 |
| BW1.Dia                 | cm    | 0   | 0.45|                  |
| BW2.Dia                 | cm    | 0   | 0.45|                  |
| BW3.Dia                 | cm    | 0   | 0.45|                  |
| BW4.Dia                 | cm    | 0   | 0.45|                  |
| BW5.Dia                 | cm    | 0   | 0.45|                  |
| HBR.Dia                 | cm    | 0   | 0.45|                  |
| BW1.Lat.Dia             | cm    | 0   | 0.03|                  |
| BW2.Lat.Dia             | cm    | 0   | 0.03|                  |
| BW3.Lat.Dia             | cm    | 0   | 0.03|                  |
| BW4.Lat.Dia             | cm    | 0   | 0.03|                  |
| BW5.Lat.Dia             | cm    | 0   | 0.03|                  |
| HBR.Lat.Dia             | cm    | 0   | 0.03|                  |
| PR.Lat.Dia              | cm    | 0   | 0.03|                  |
| BW1.LRBD                | cm⁻¹  | 0   | 40  | Miller et al., 2003 |
| BW2.LRBD                | cm⁻¹  | 0   | 40  |                  |
| BW3.LRBD                | cm⁻¹  | 0   | 40  |                  |
| BW4.LRBD                | cm⁻¹  | 0   | 40  |                  |
| BW5.LRBD                | cm⁻¹  | 0   | 40  |                  |
| PR.LRBD                 | cm⁻¹  | 0   | 40  |                  |
| HBR.LRBD                | cm⁻¹  | 0   | 40  |                  |
| BW1.Angle               | degree| 0   | 90  | Miguel et al., 2013 |
| BW2.Angle               | degree| 0   | 90  |                  |
| BW3.Angle               | degree| 0   | 90  |                  |
| BW4.Angle               | degree| 0   | 90  |                  |
| BW5.Angle               | degree| 0   | 90  |                  |
Table S2: Range of input values for generating maize root phenotypes. PR - Primary Root; SR - Seminal Root; NR - Nodal Root; NR1, NR2, NR3, NR4 refer to the nodal root position; Dia – axial root diameter; Lat.Dia – lateral root diameter; LRBD – lateral root branching density. *NR at different positions were considered to have similar parameters.

| Parameter       | Units | Min  | Max  | References                          |
|-----------------|-------|------|------|-------------------------------------|
| Number.SR       | NA    | 0    | 12   | Hochholdinger and Tuberosa, 2009    |
| Number.NR1      | NA    | 0    | 12   | Burton et al., 2013; York and Lynch, 2015 |
| Number.NR2      | NA    | 0    | 12   | Burton et al., 2013; York and Lynch, 2015 |
| Number.NR3      | NA    | 0    | 12   |                                     |
| Number.NR4      | NA    | 0    | 12   |                                     |
| PR.Dia          | cm    | 0.08 | 0.6  | Burton et al., 2013; York and Lynch, 2015 |
| SR.Dia          | cm    | 0    | 0.6  |                                     |
| NR1.Dia         | cm    | 0    | 0.6  |                                     |
| NR2.Dia         | cm    | 0    | 0.6  |                                     |
| NR3.Dia         | cm    | 0    | 0.6  |                                     |
| NR4.Dia         | cm    | 0    | 0.6  |                                     |
| PR.Lat.Dia      | cm    | 0    | 0.05 |                                     |
| SR.Lat.Dia      | cm    | 0    | 0.05 |                                     |
| NR1.Lat.Dia     | cm    | 0    | 0.05 |                                     |
| NR2.Lat.Dia     | cm    | 0    | 0.05 |                                     |
| NR3.Lat.Dia     | cm    | 0    | 0.05 |                                     |
| NR4.Lat.Dia     | cm    | 0    | 0.05 |                                     |
| PR.LRBD         | cm⁻¹  | 0    | 40   | Postma et al., 2014; York and Lynch, 2015 |
| SR.LRBD         | cm⁻¹  | 0    | 40   |                                     |
| NR1.LRBD        | cm⁻¹  | 0    | 40   |                                     |
| NR2.LRBD        | cm⁻¹  | 0    | 40   |                                     |
| NR3.LRBD        | cm⁻¹  | 0    | 40   |                                     |
| NR4.LRBD        | cm⁻¹  | 0    | 40   |                                     |
| SR.Angle        | degree| 0    | 90   | Liao et al., 2004; Zhu et al., 2005 |
| NR1.Angle       | degree| 0    | 90   |                                     |
| NR2.Angle       | degree| 0    | 90   |                                     |
| NR3.Angle       | degree| 0    | 90   |                                     |
| NR4.Angle       | degree| 0    | 90   |                                     |
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