Recent Additions to tidymodels

Max Kuhn

tidymodels and Me

I'm a statistician and software Engineer for RStudio working on modeling.

Formerly 6y in infectious disease diagnostics and 12y in drug discovery.

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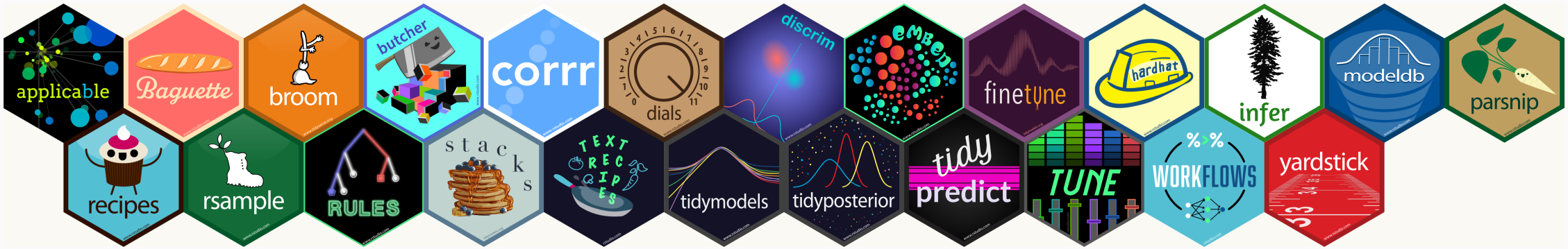
https://rstd.io/global2021/maxkuhn

tidymodels is a collection of modeling packages designed with the same principles as the tidyverse.



Recent Updates

Interfaces:

- `workflows` have a new interface for adding raw data columns (e.g. no formula or recipe)
- `recipes` now support all of the new `tidyselect` selectors
- `recipes` can now use `bake()` instead of `juice()` for the training set.
- The `autoplot()` method for `tune` objects works better for regular grids.

Today I'll be demonstrating a new package called **`finetune`**.

Efficiency:

- Parallel processing via PSOCK clusters on windows is less awful.
- `tune` can now use a larger number of parallel workers when tuning.
- For the 3 models that use them, sparse matrices can be passed from recipes to model functions.

Example Problem

For our example, the cell segmentation data are used to create a two-class classification model using a support vector machine (SVM).

- We'll tune this model over `cost` and `rbf_sigma`.

This talk is about new ways of **finding optimal values of these parameters**.

The data are resampled using 10-fold cross-validation.

The model definition and complete code set can be found at `https://rstd.io/global2021/maxkuhn` .

Climbing a Hill

We want to find good values of two tuning parameters (`cost` and `rbf_sigma`) that maximize the area under the ROC curve of the model. The true 2D surface:

Racing Methods

Racing methods can be used on pre-defined grids of tuning parameters.

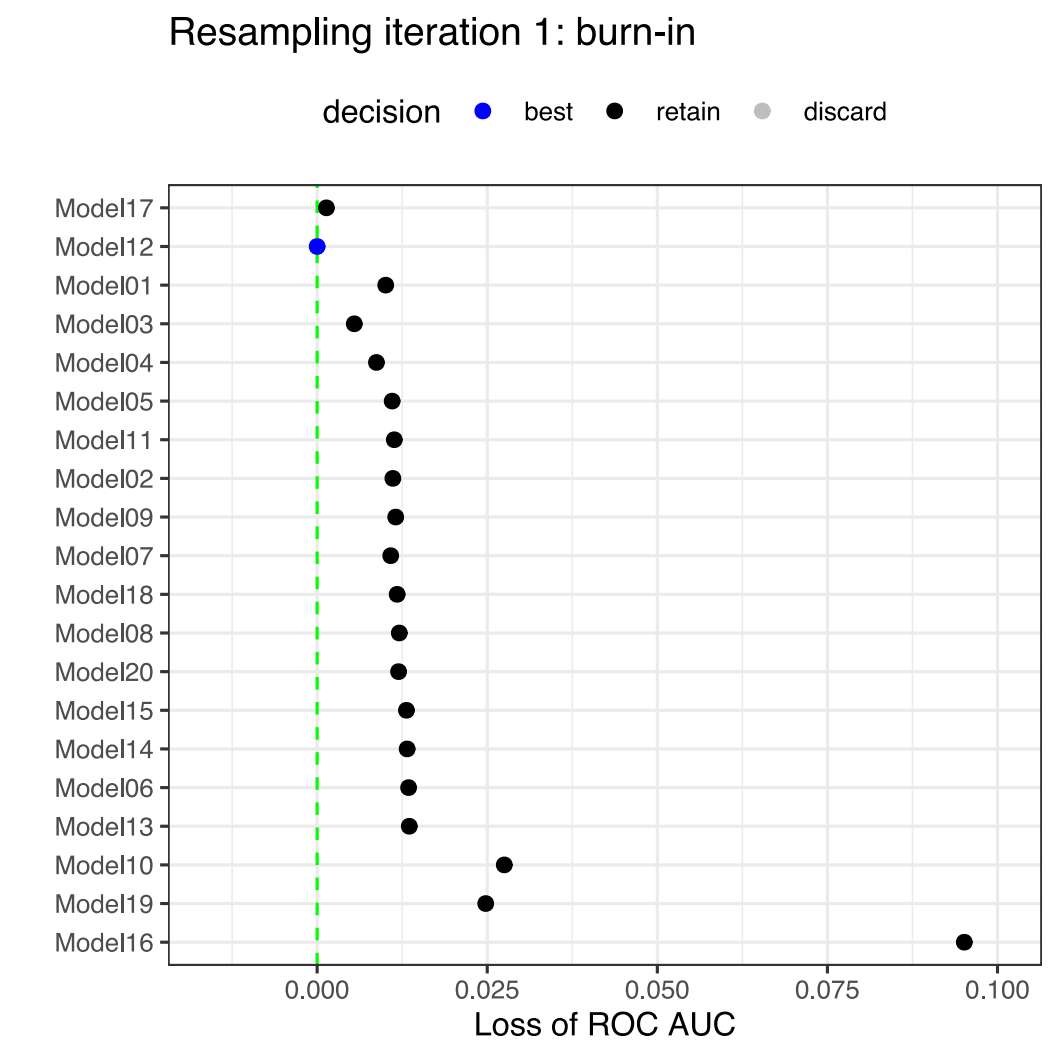
As the models are resampled (to compute performance), interim analyses are used to eliminate candidate parameters that have a low probability of of being the best.

The `finetune` package can use racing via ANOVA models that test for differences in parameters. A second method, based on win/loss statistics, can also be used.

- See *Futility Analysis in the Cross-Validation of Machine Learning Models* (Kuhn, 2014, *arXiv.org*)

Let's use a grid of 20 SVM tuning parameters generated using a space-filling design to demonstrate.

Illustrating the Race

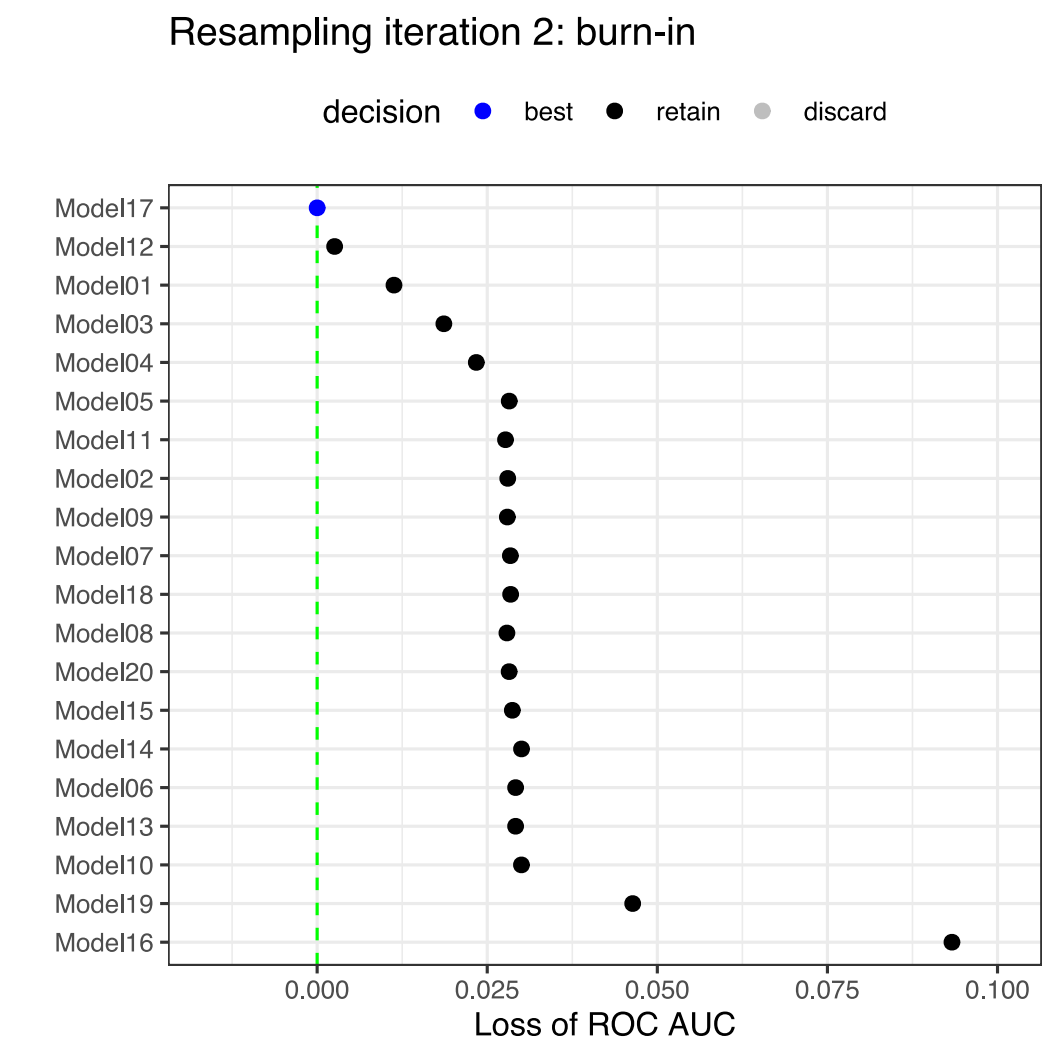


20 models go in... one comes out

The resampling method is simple 10-fold cross-validation.

Resampling iterations 1 and 2 proceed as normal.

Illustrating the Race



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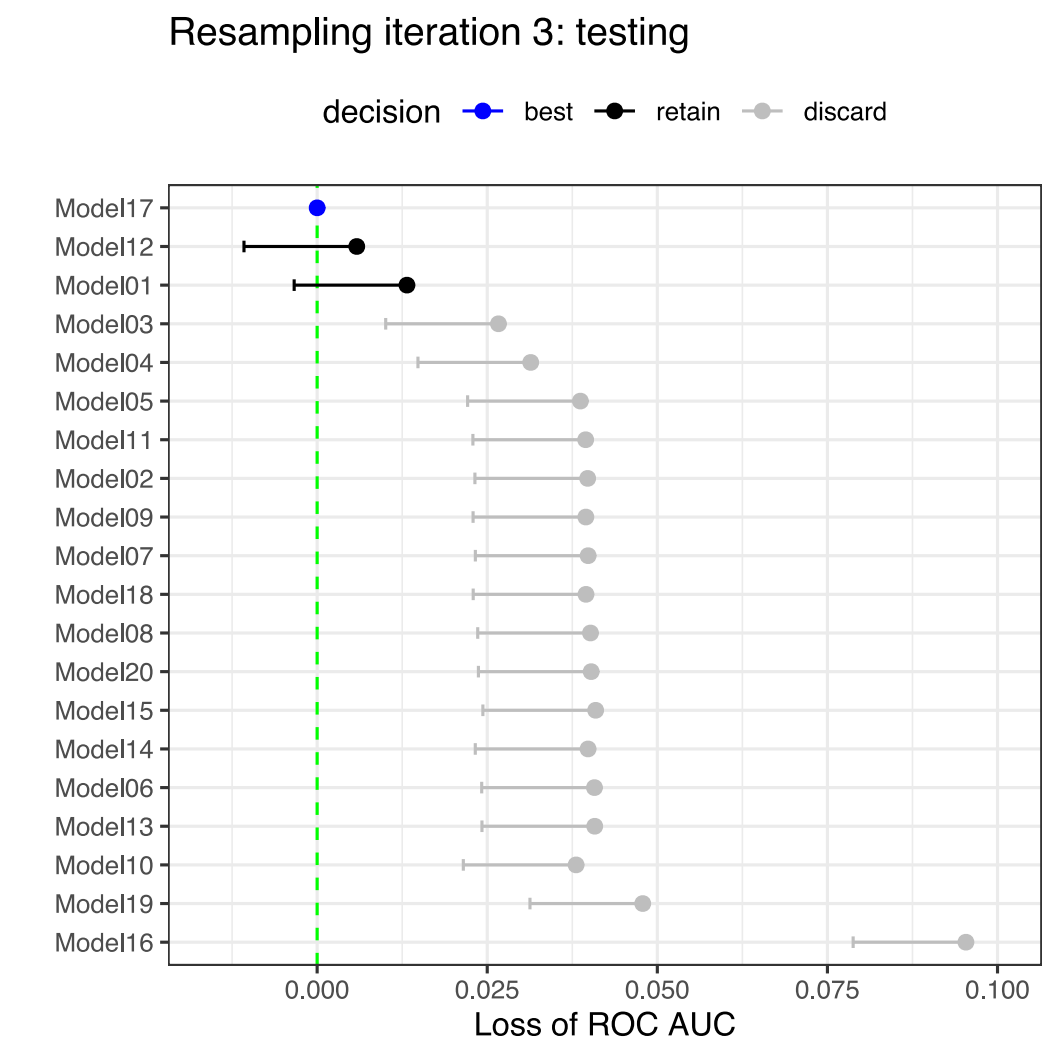

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At iteration 3, testing begins and many (poor) candidate models are removed.

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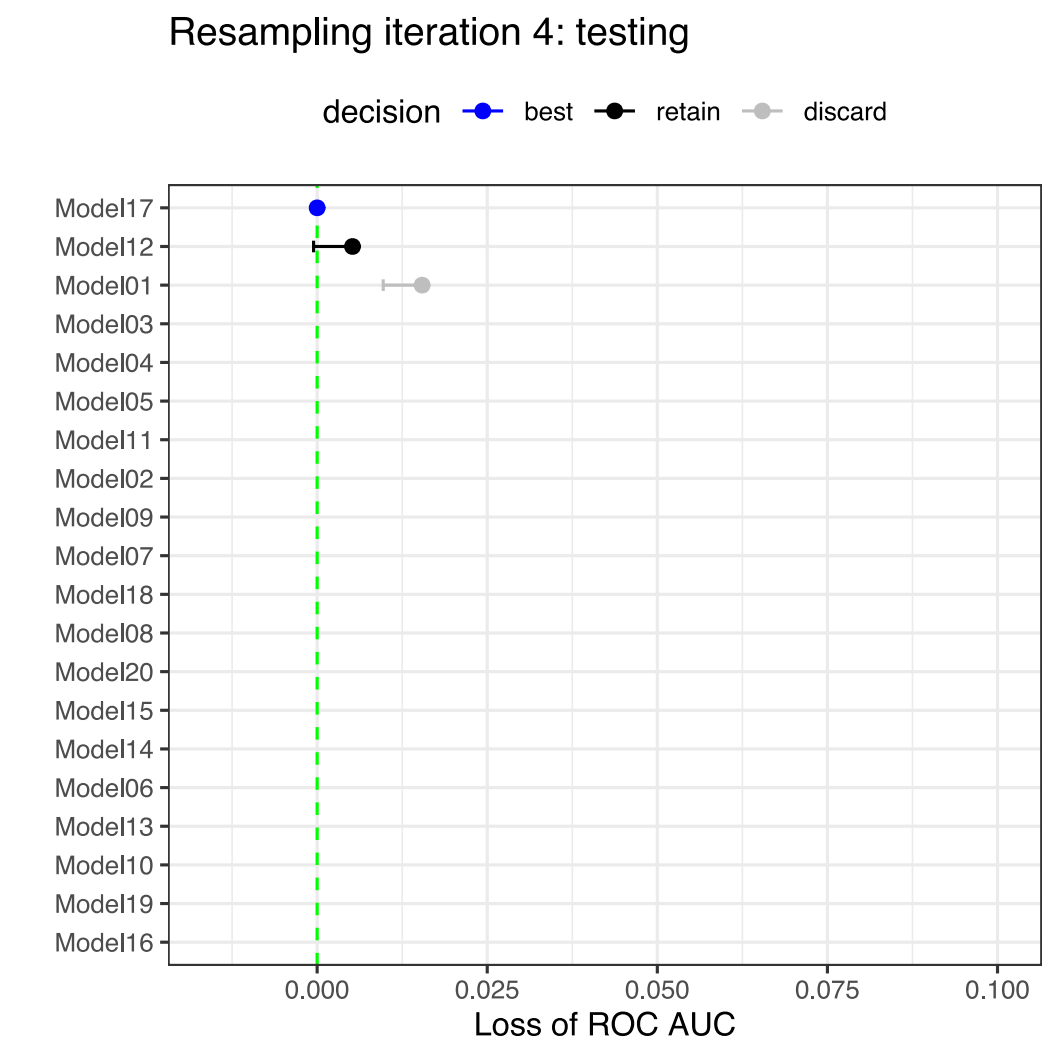

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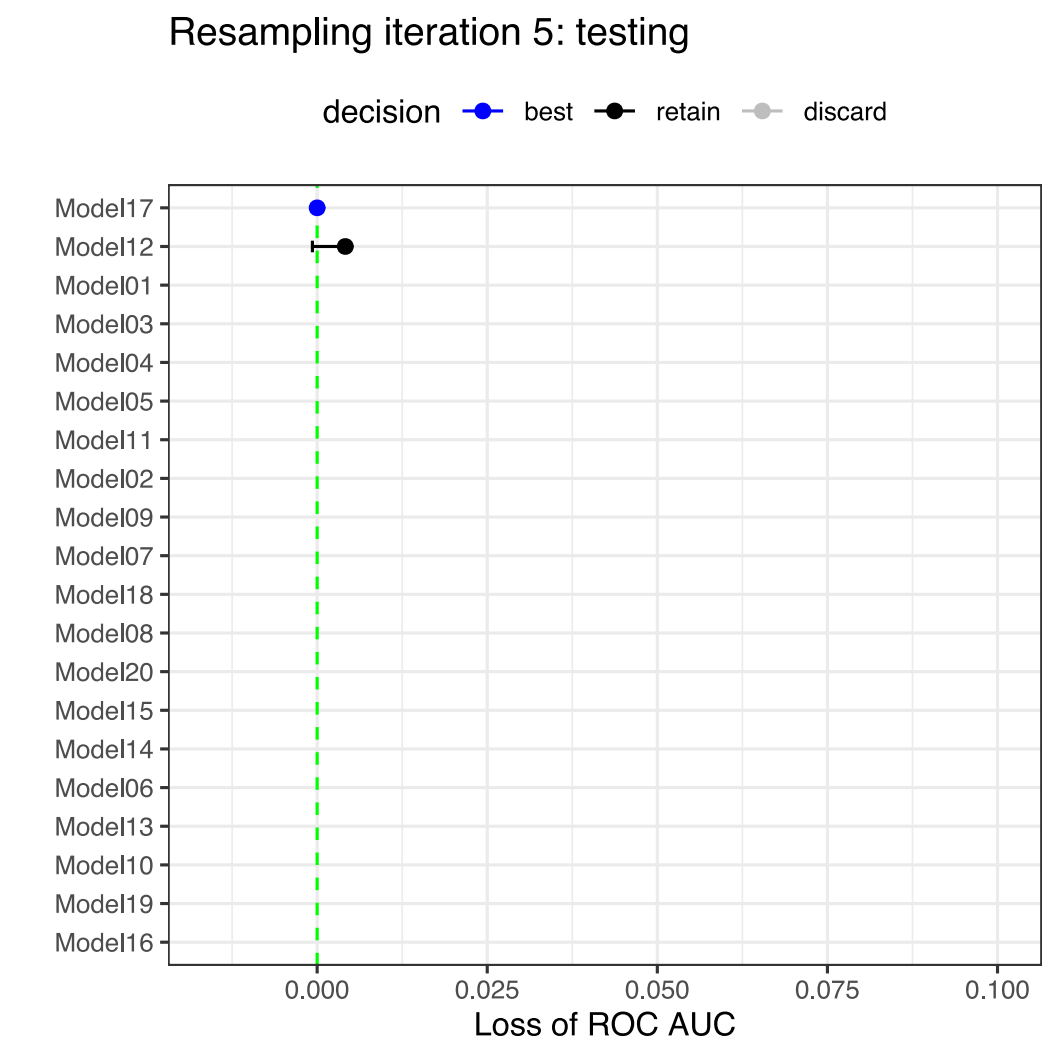

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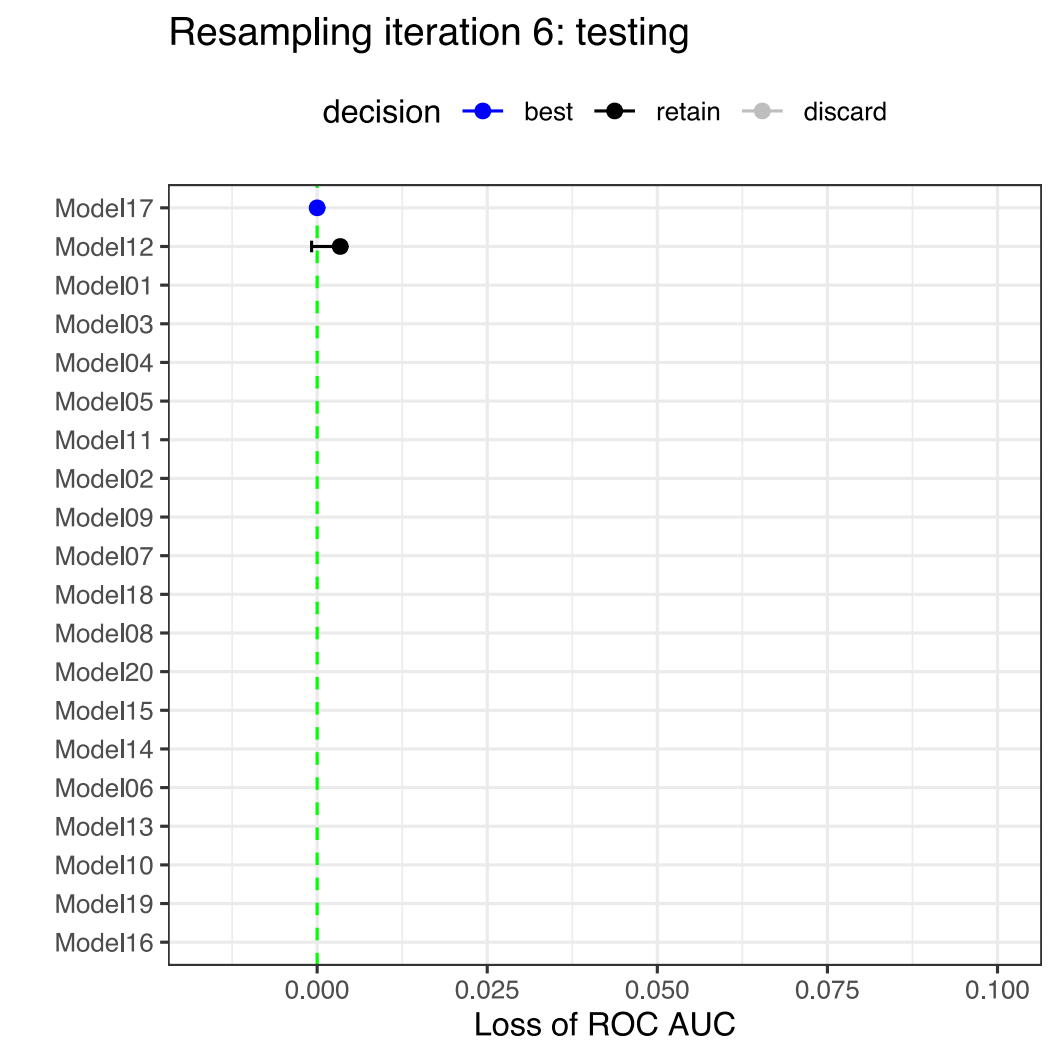

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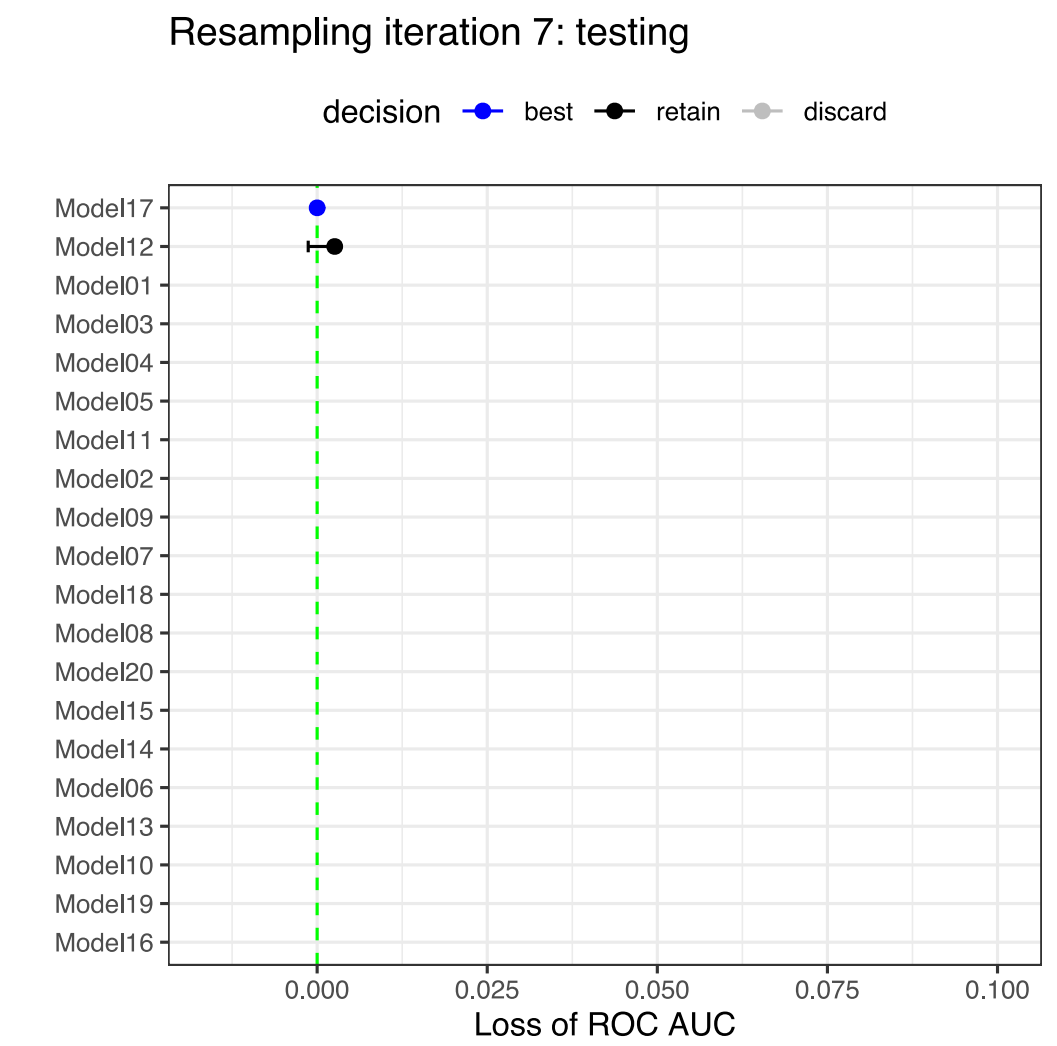

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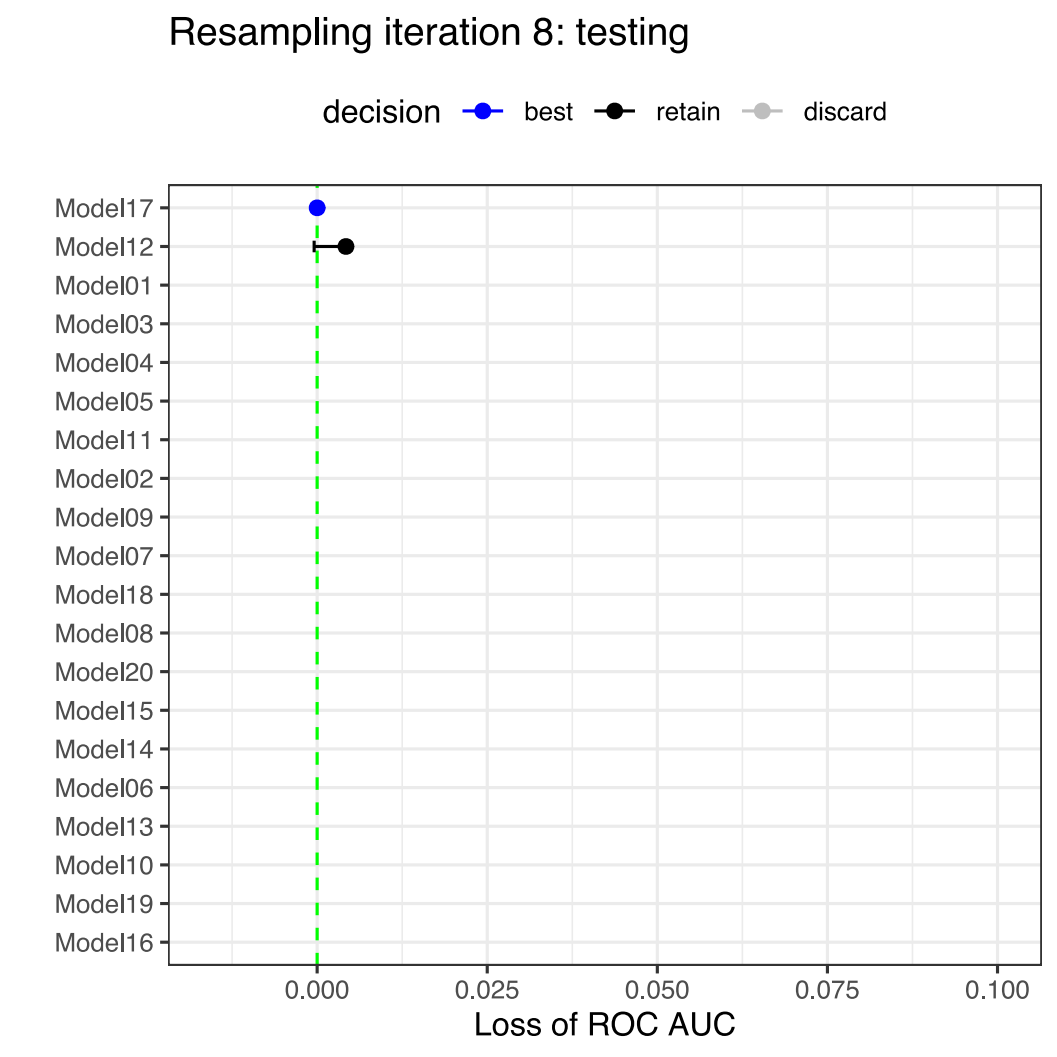

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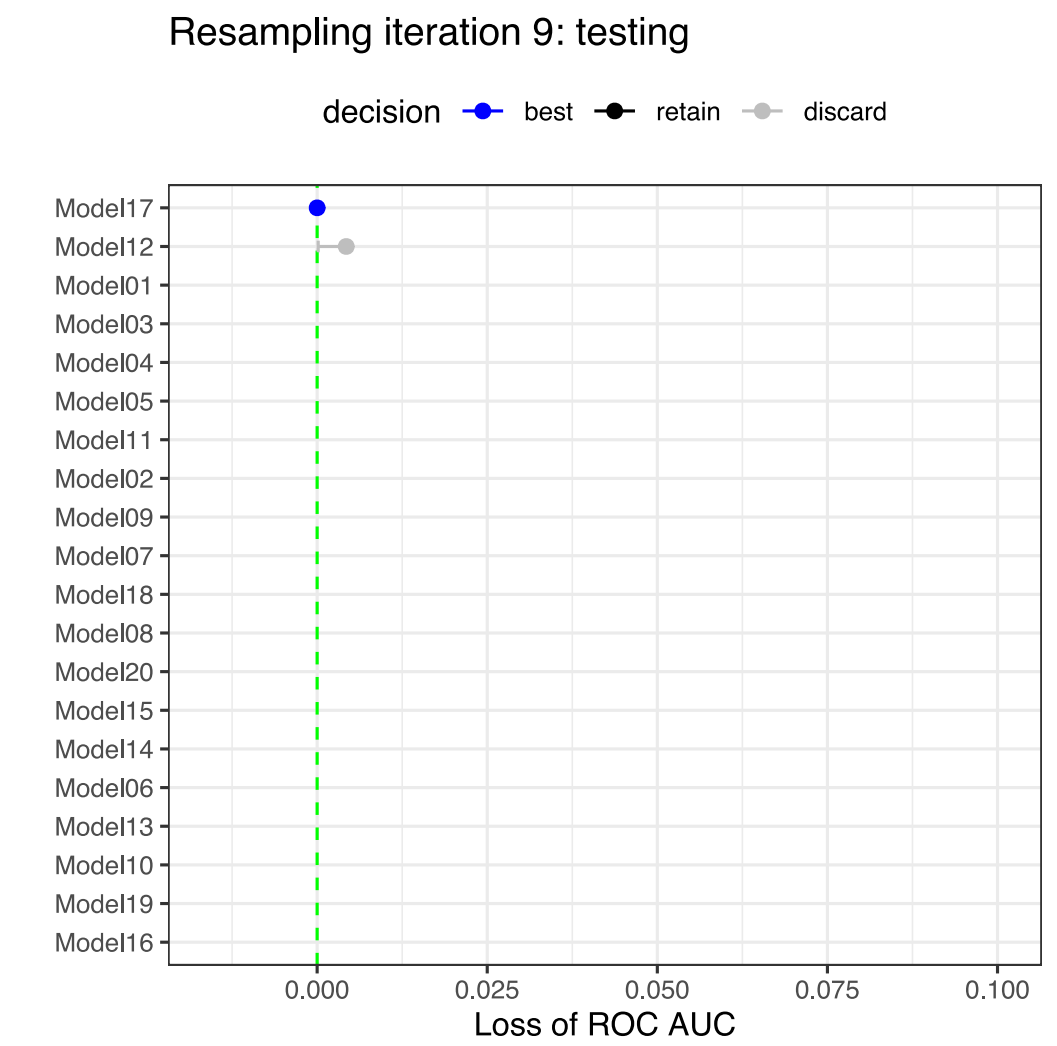


20 models go in... one comes out

The resampling method is simple 10-fold cross-validation.

The 9th iteration removes the last competitor.

Iteration 10 just resamples the single model that remains.

A total of 74 models were fit instead of 200 (=37%).

Example Code for Racing

```
set.seed(99)
svm_race <-
  svm_wflow %>%
  tune_race_anova(resamples = cell_folds, grid = 20)
```

Using the `verbose_elim` option:

```
ℹ Racing will maximize the roc_auc metric.
ℹ Resamples are analyzed in a random order.
ℹ Fold10: 17 eliminated;  3 candidates remain.
ℹ Fold09:  1 eliminated;  2 candidates remain.
ℹ Fold05:  0 eliminated;  2 candidates remain.
ℹ Fold01:  0 eliminated;  2 candidates remain.
ℹ Fold07:  0 eliminated;  2 candidates remain.
ℹ Fold03:  0 eliminated;  2 candidates remain.
ℹ Fold06: All but one parameter combination were eliminated.
```

`tune_race_win_loss()` can also be used.

Simulated Annealing Search

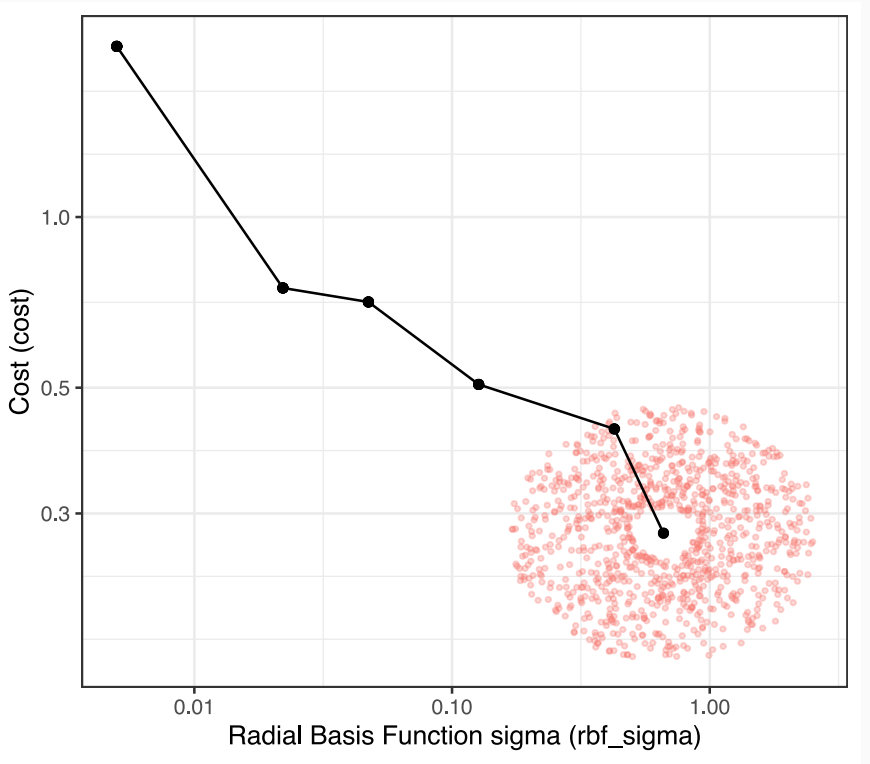
Simulated annealing (SA) is an old search routine that conducts a biased random walk around the tuning parameter space.

- The bias comes from the walk highly favoring steps that show better model results.

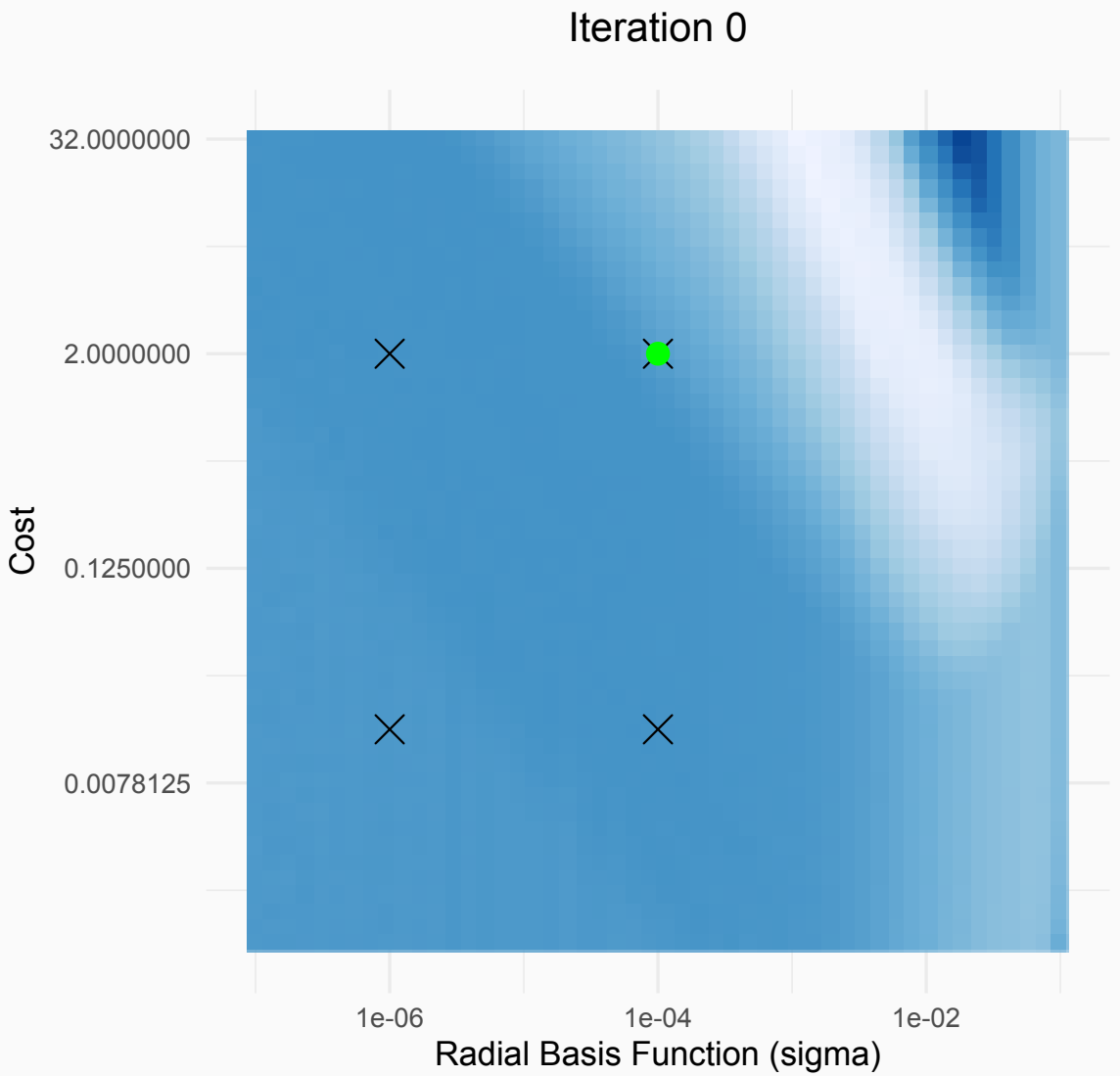
From an initial point, the next point is generated using a random value within a *neighborhood* of the current point.

- An example of candidate points in a neighborhood is shown 👉

SA accepts suboptimal results early in the search process and less as time goes on.



Simulated Annealing Search



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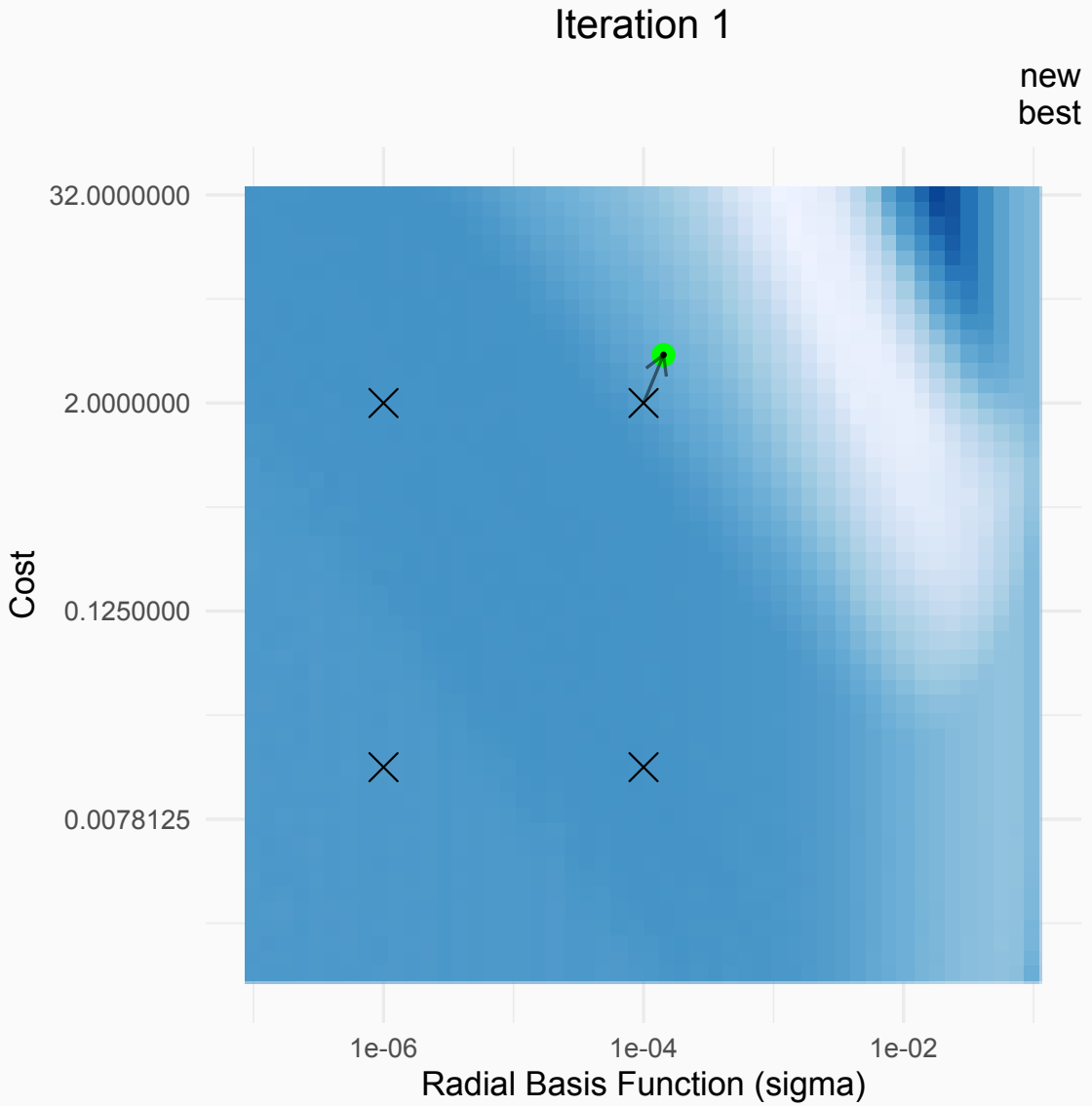

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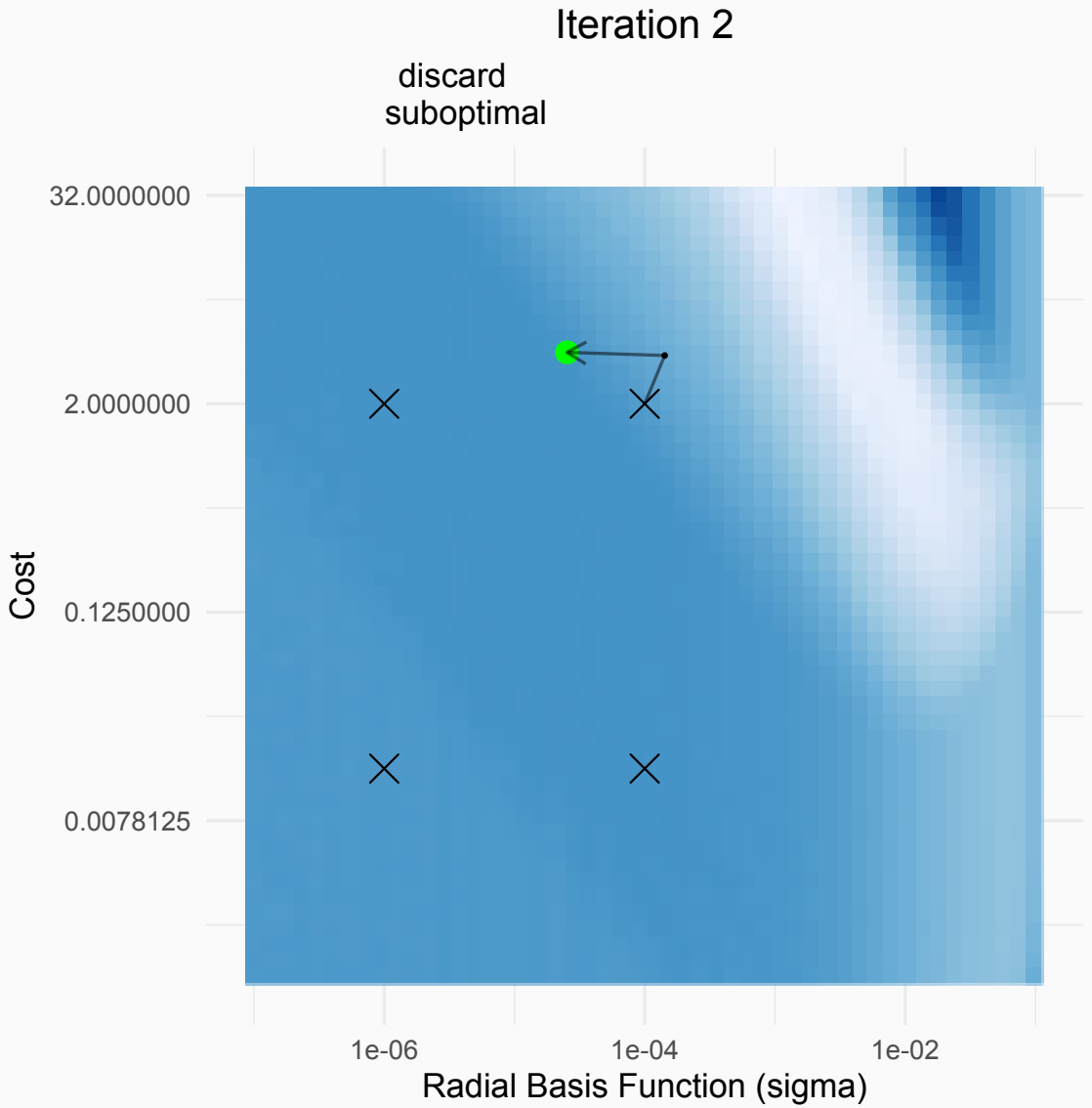

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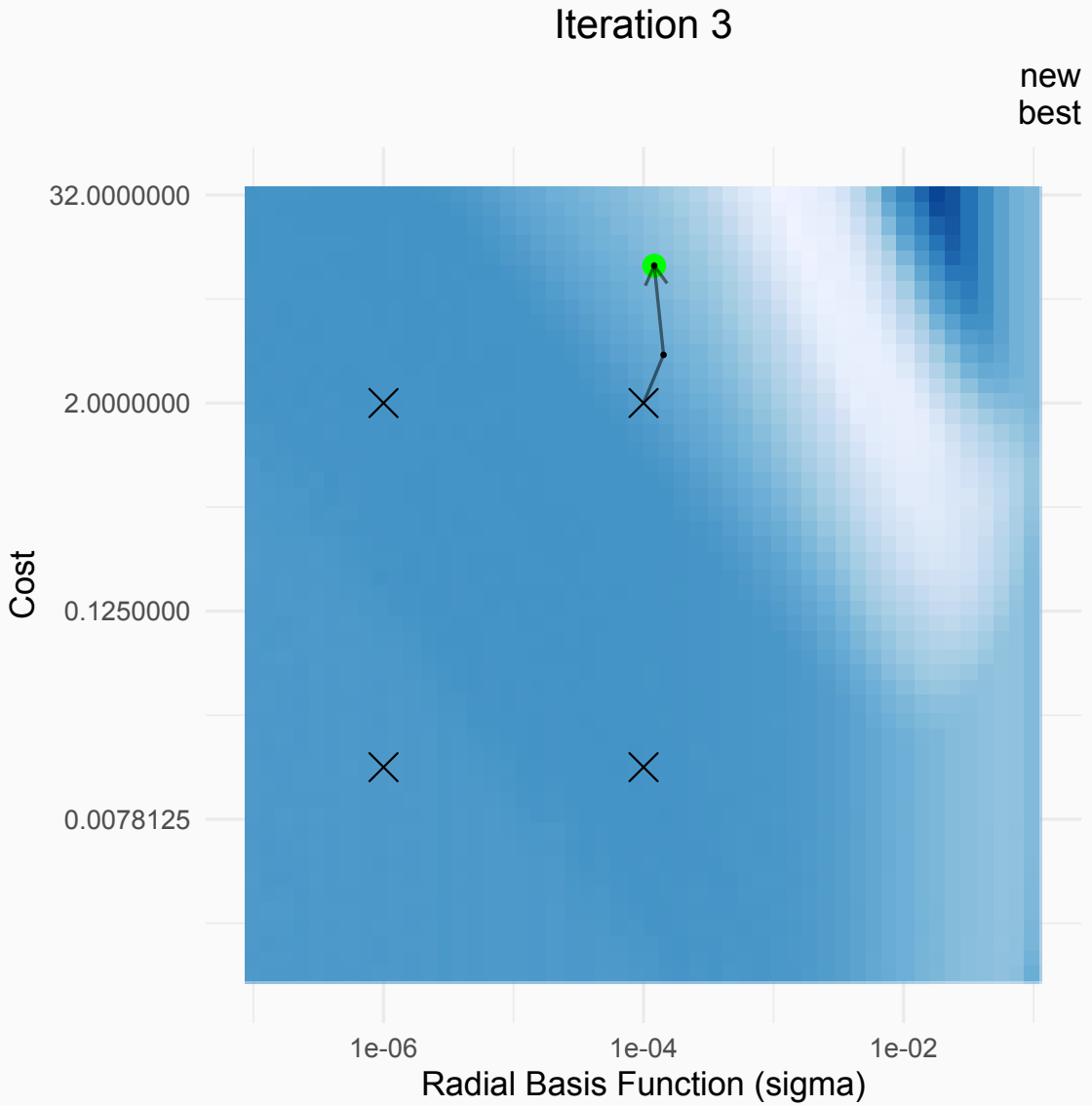

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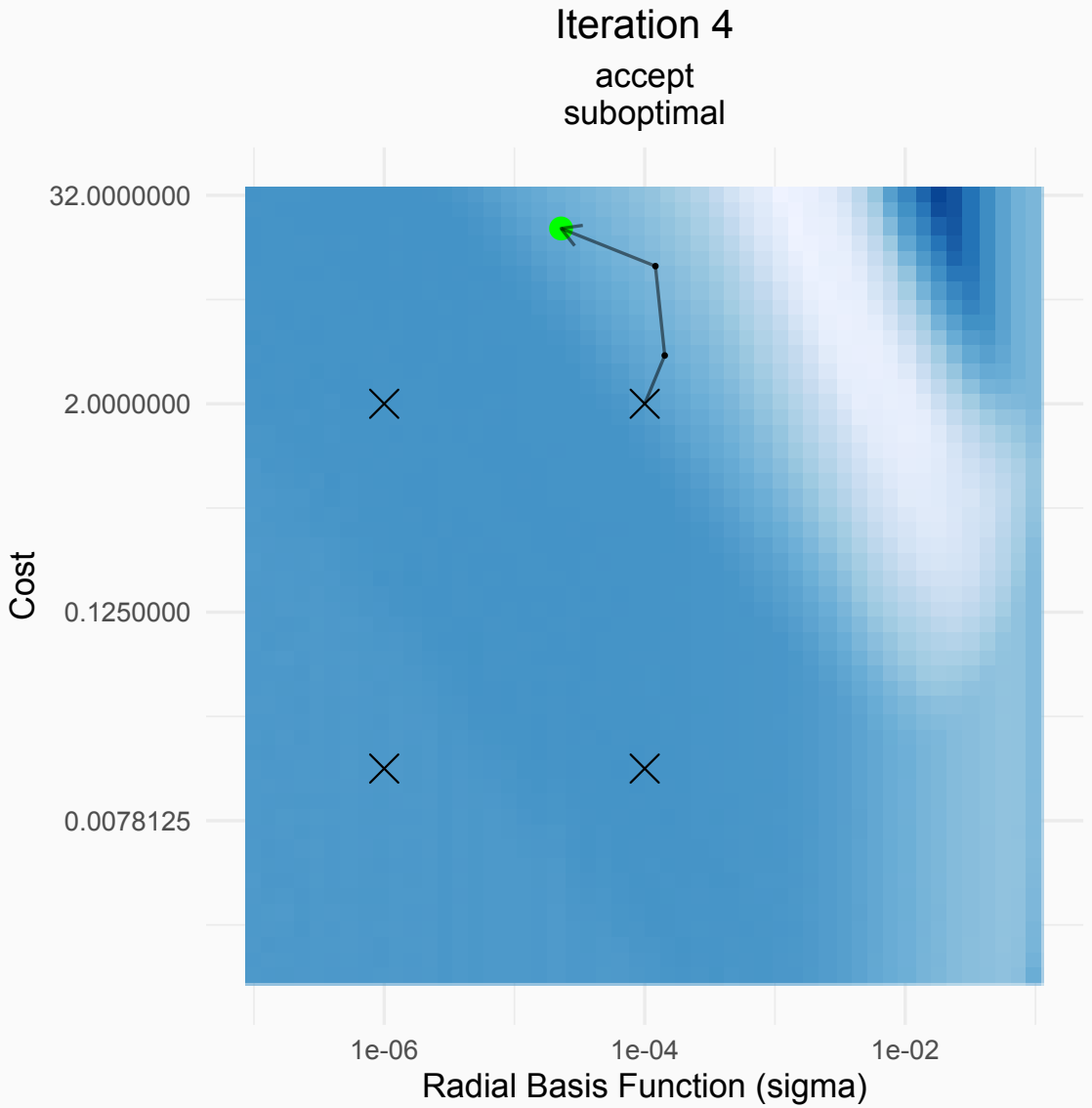

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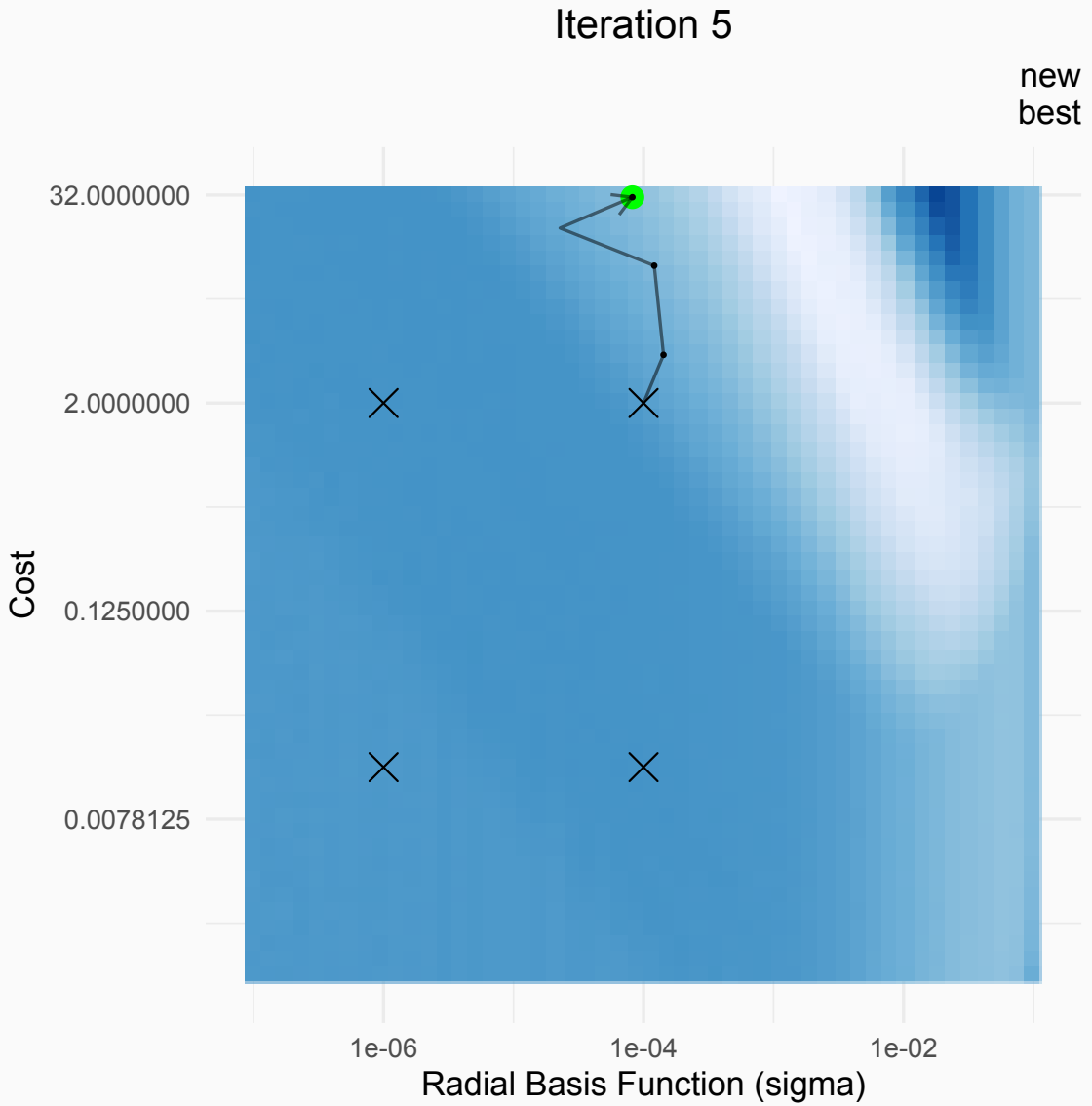

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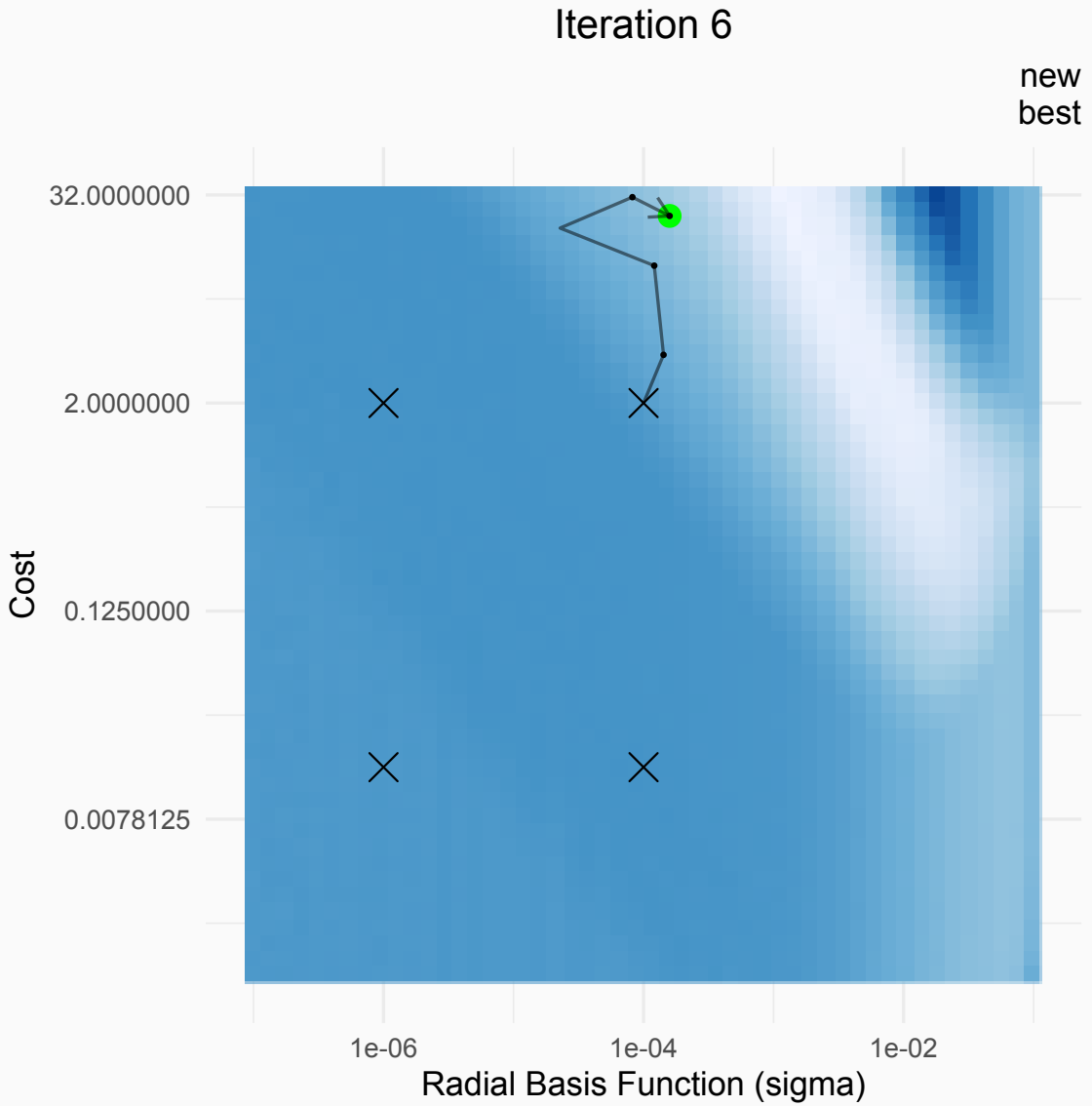

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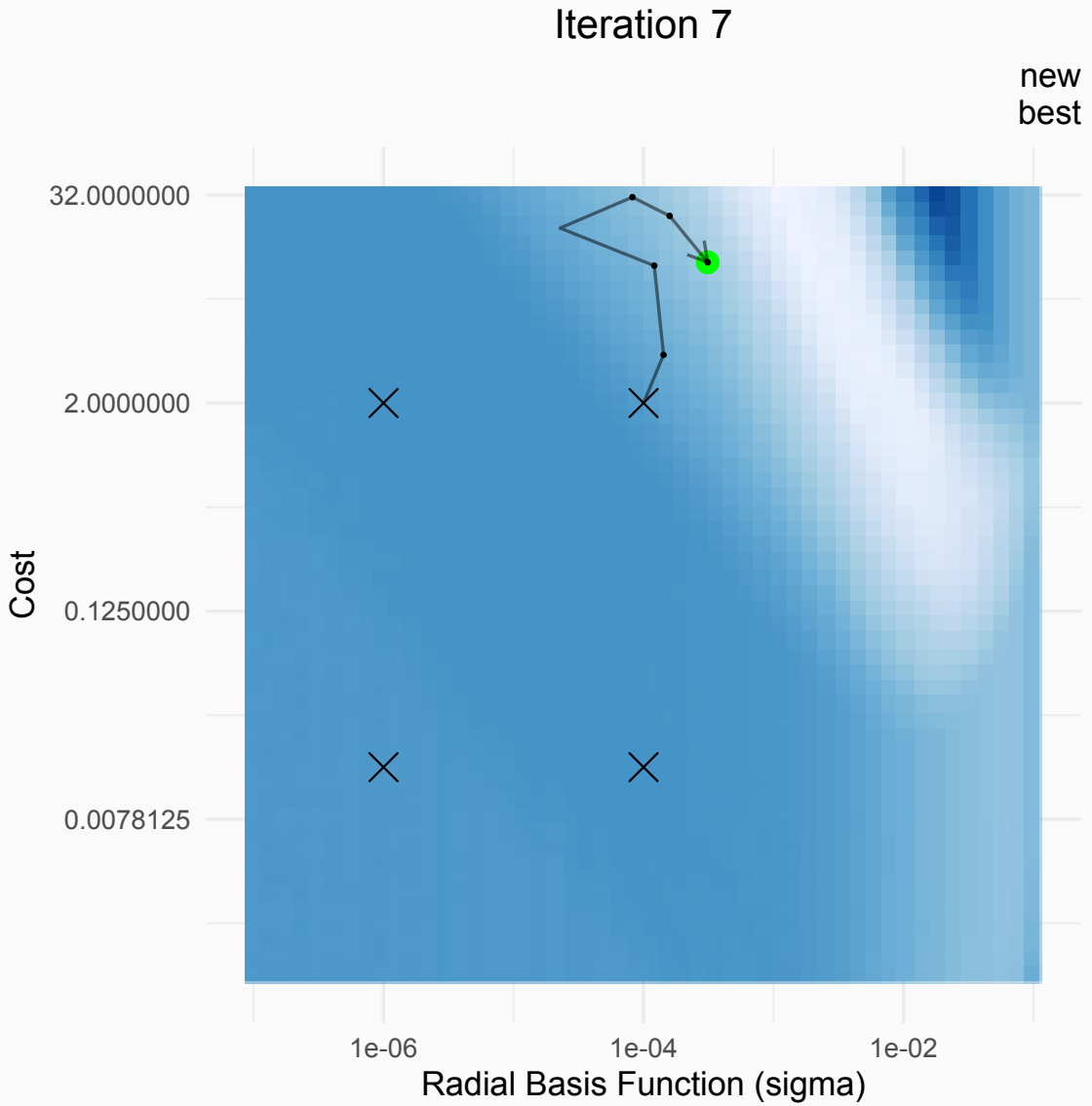

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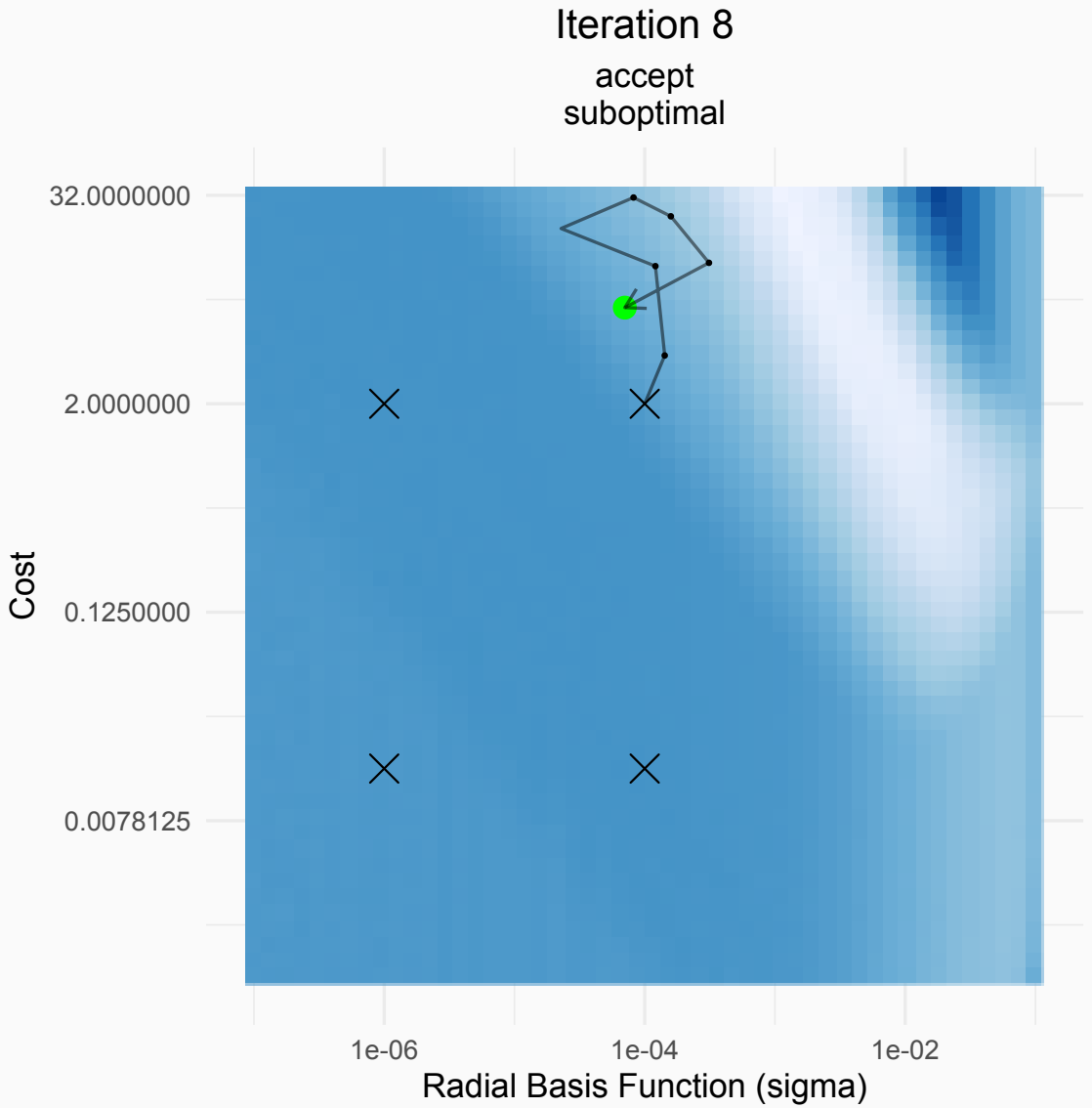

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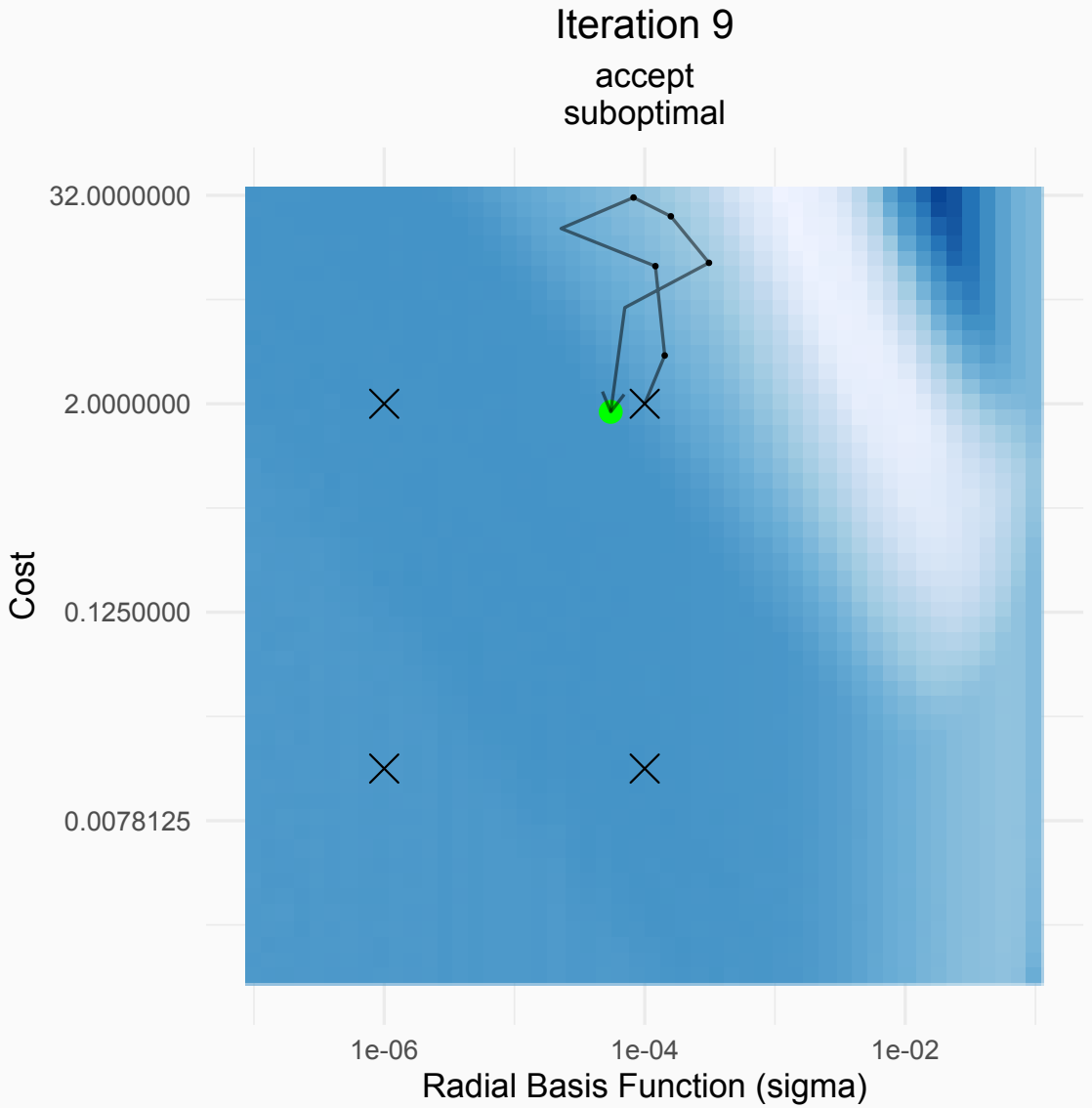

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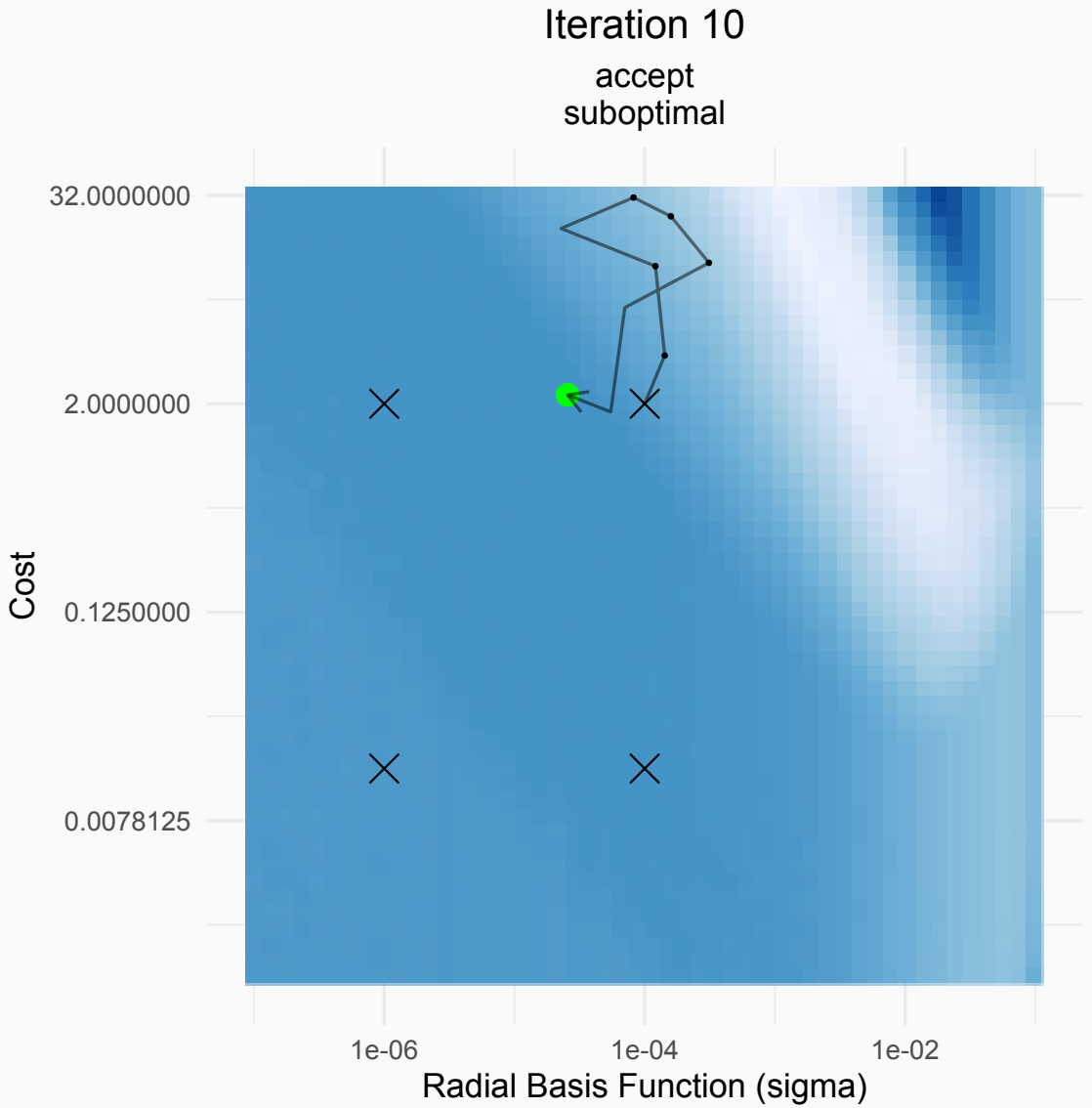

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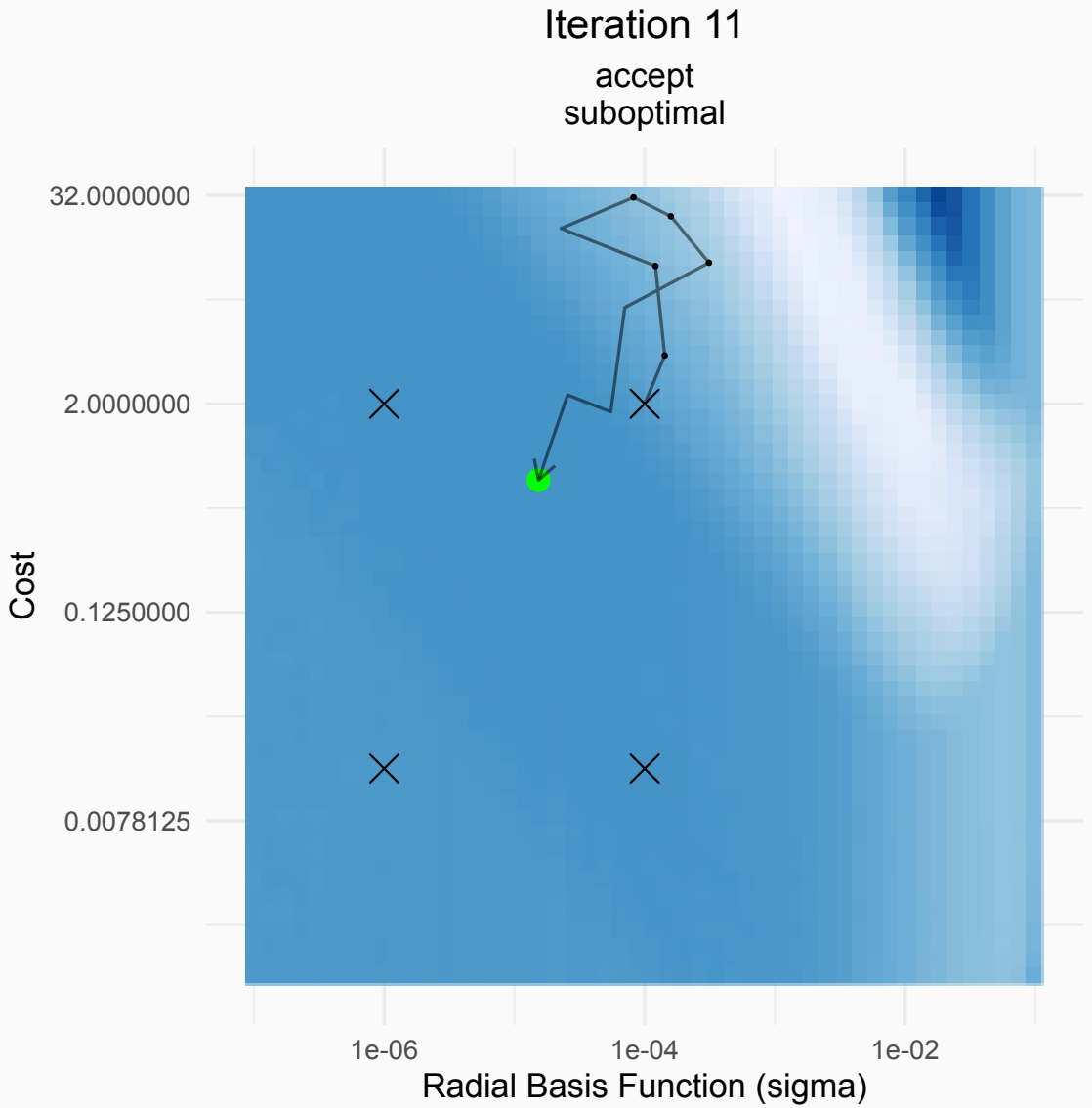

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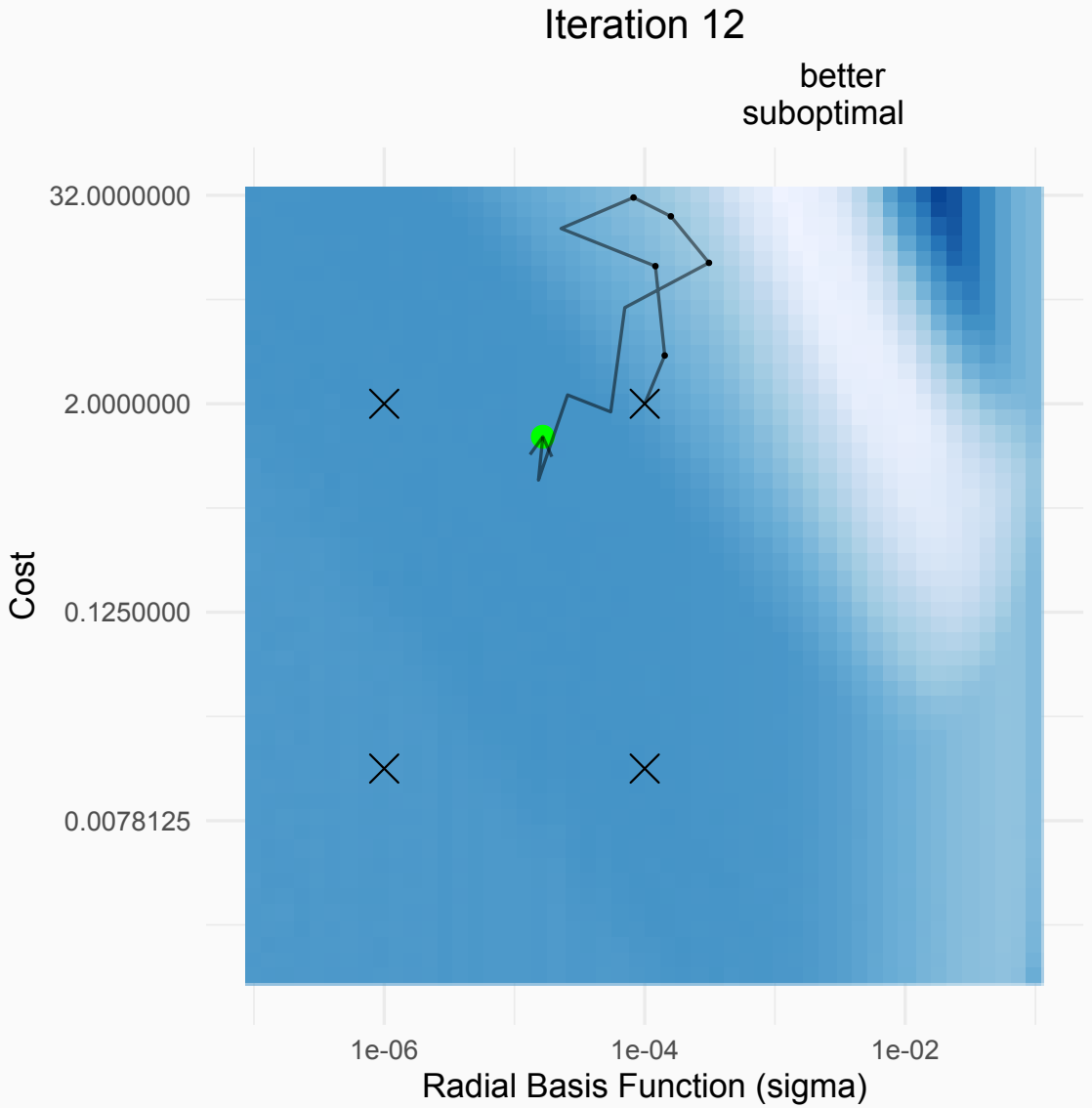

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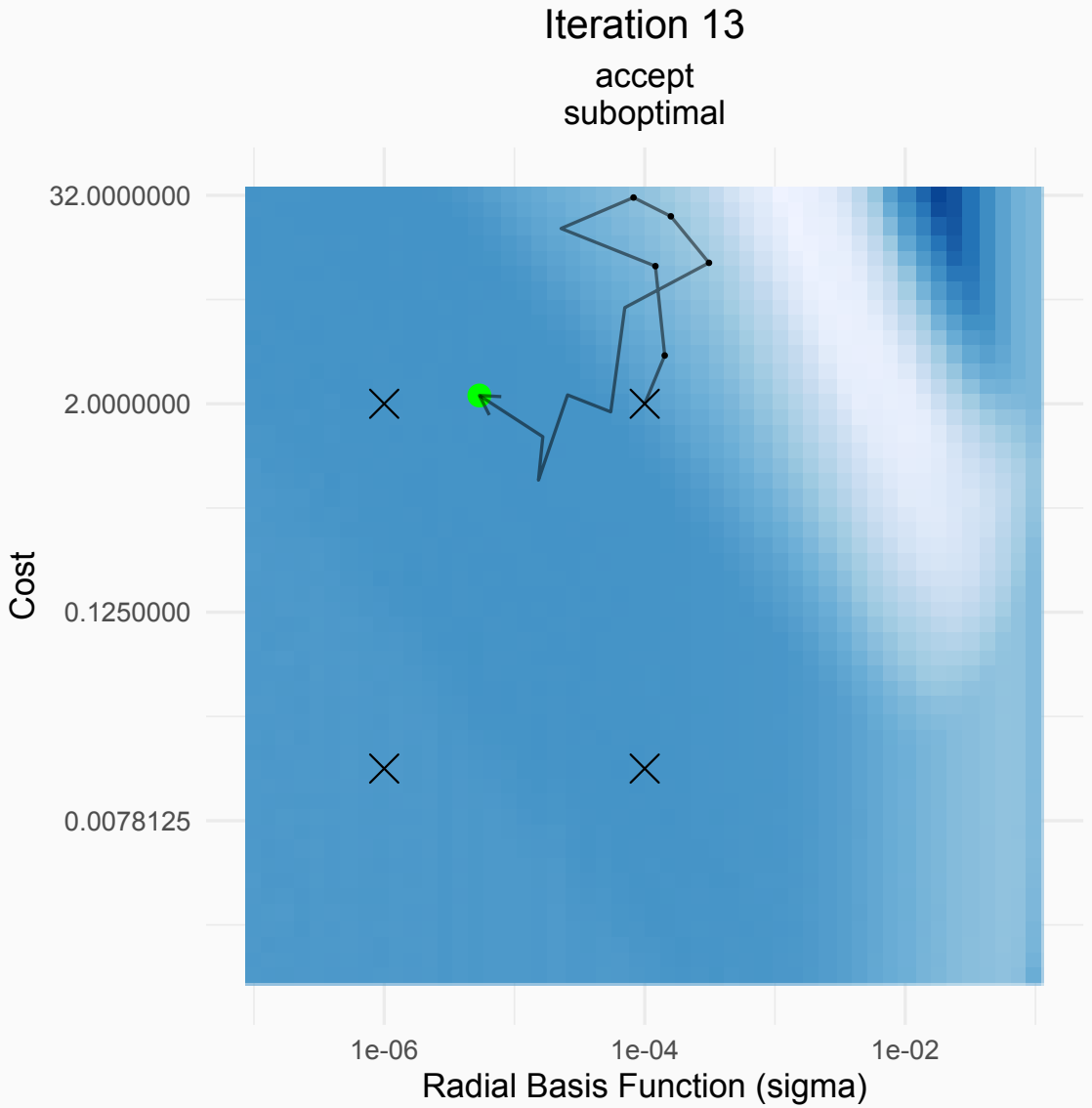

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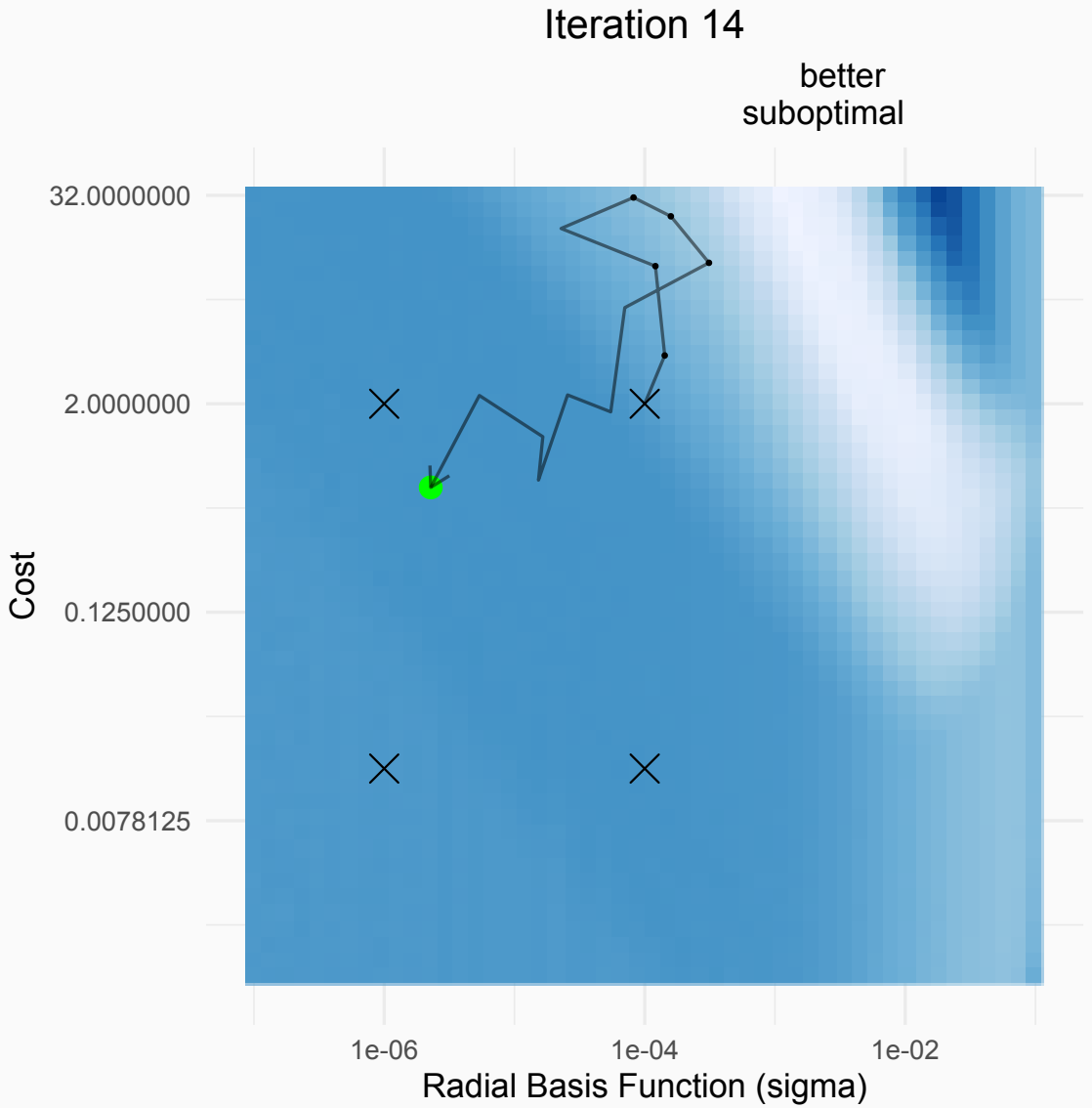

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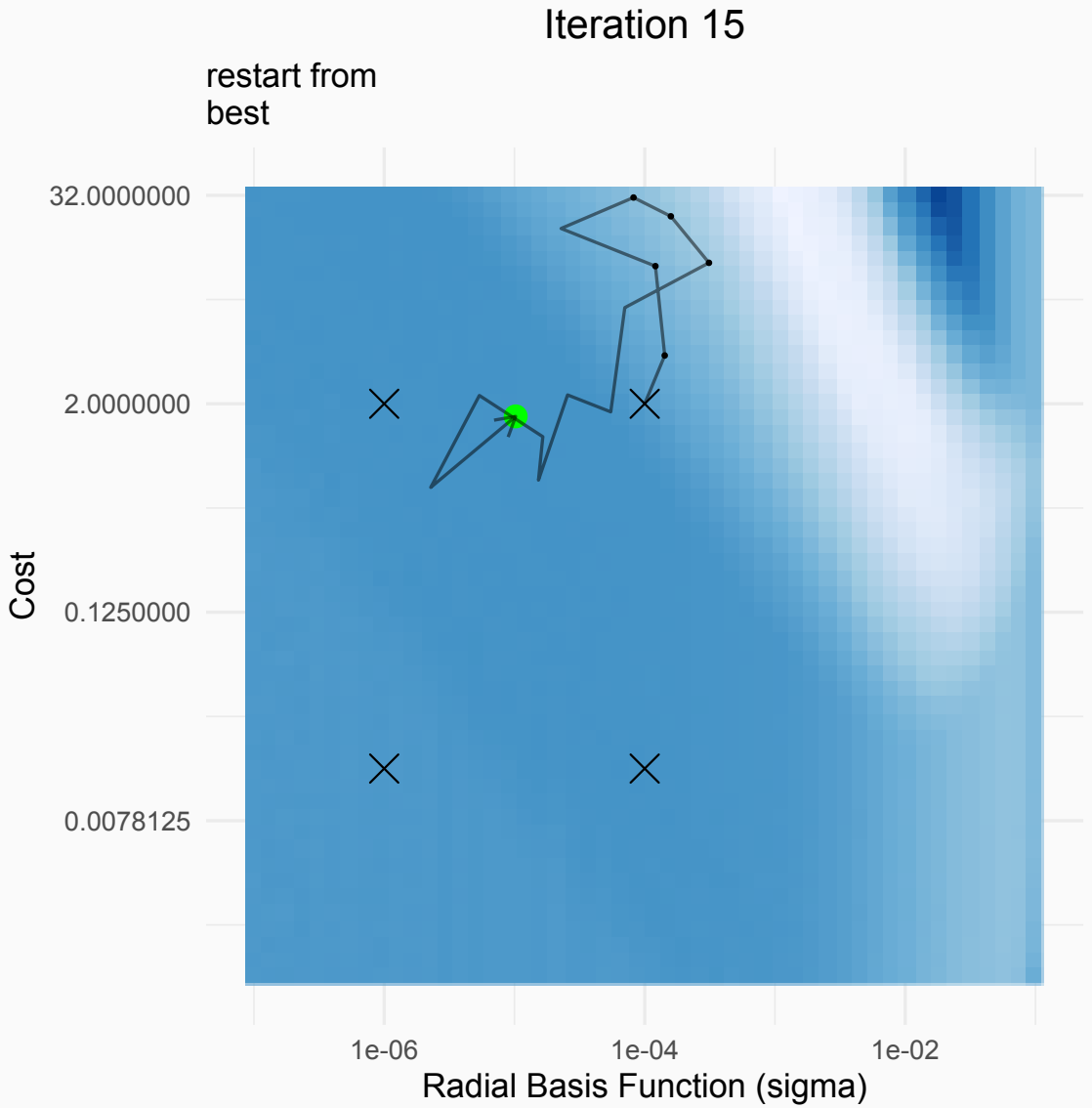

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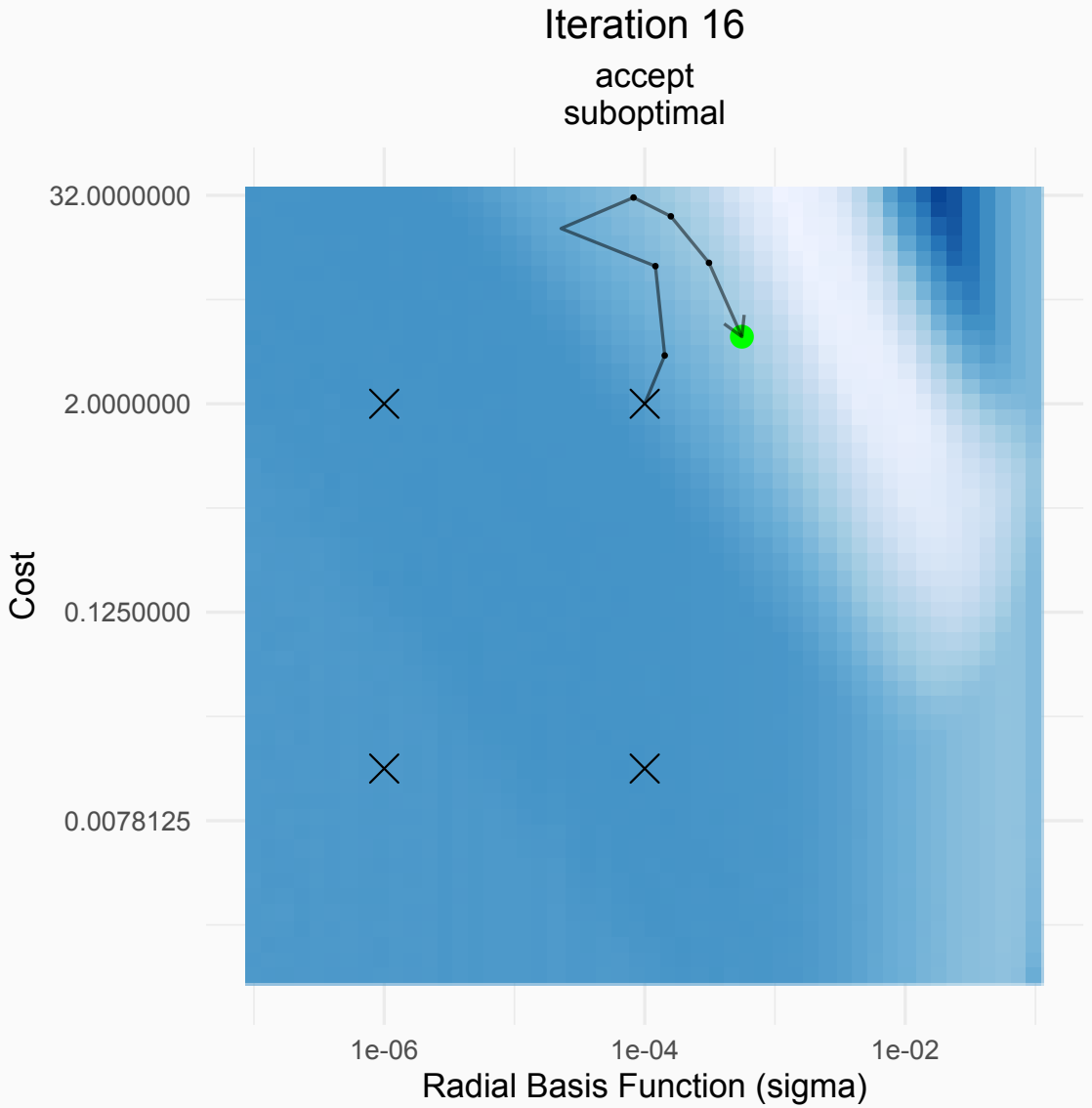

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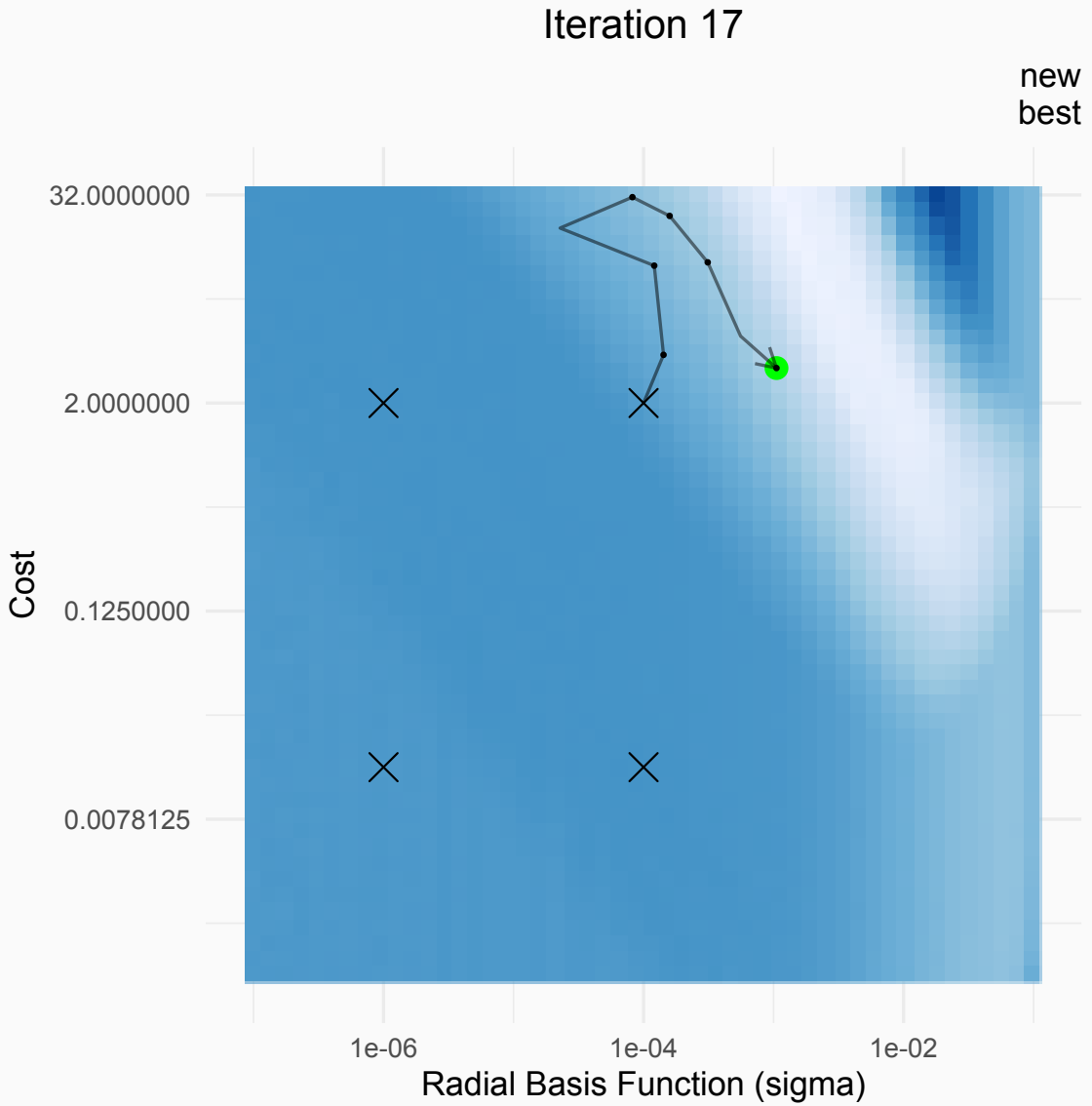

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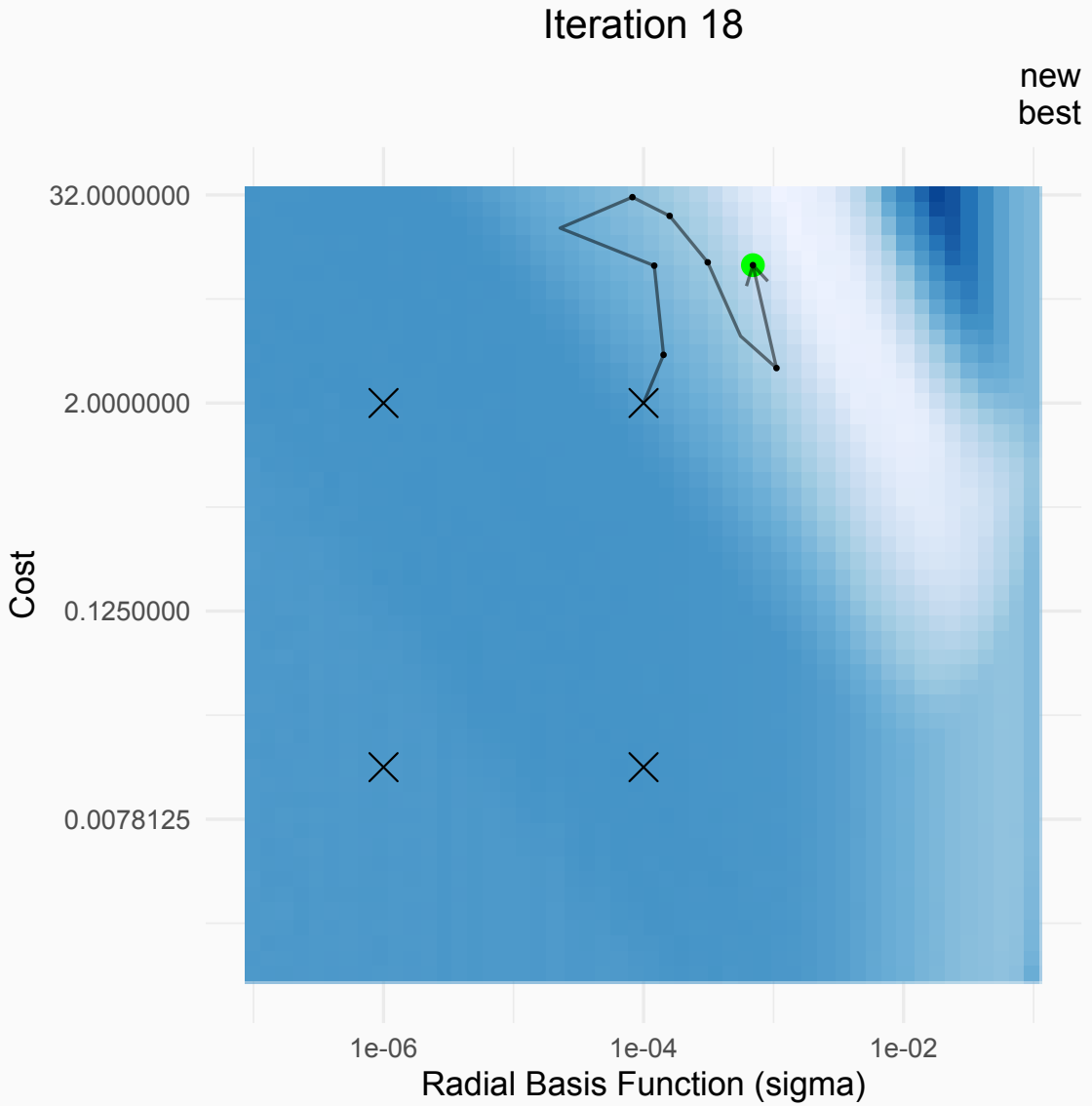

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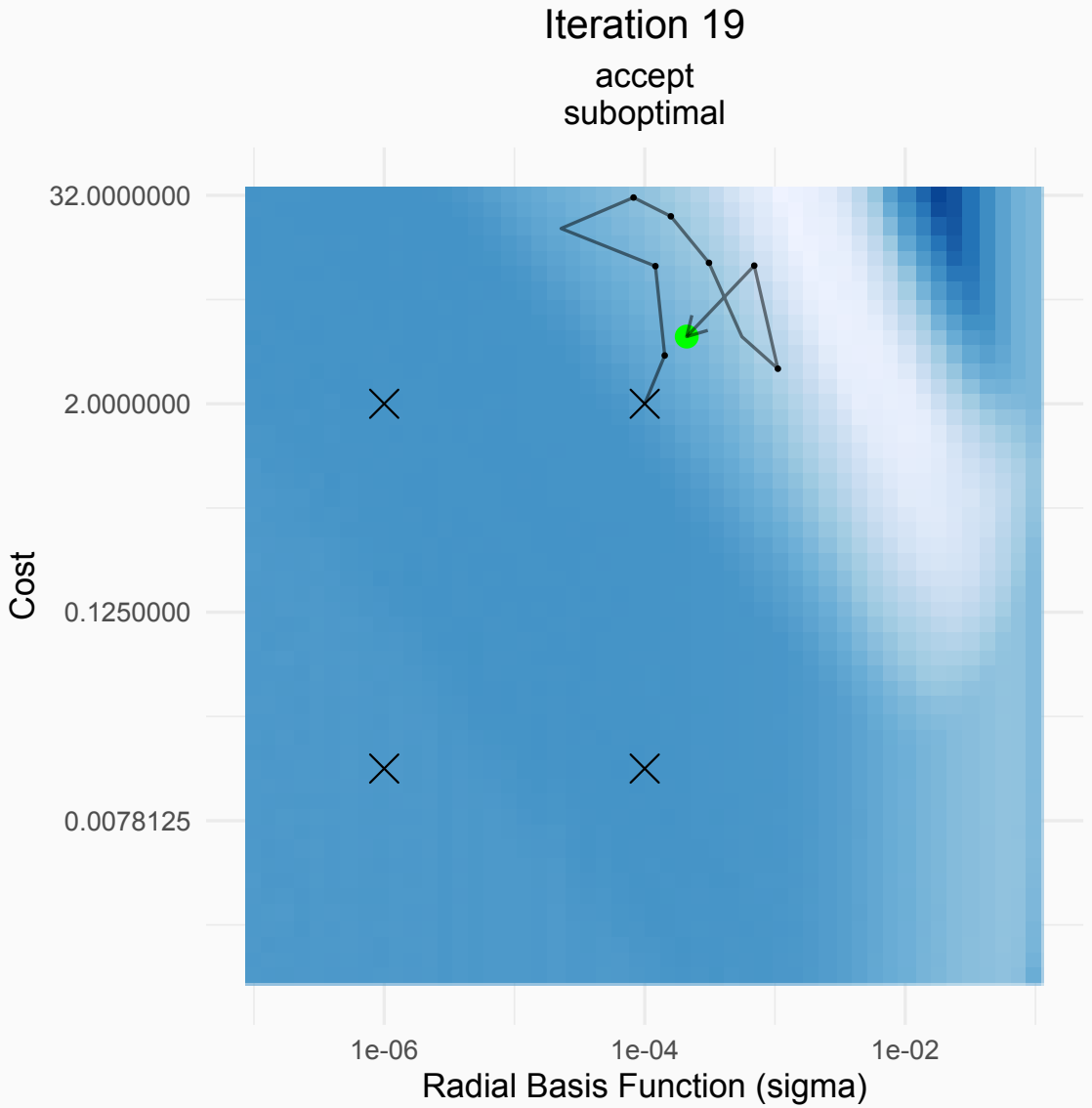

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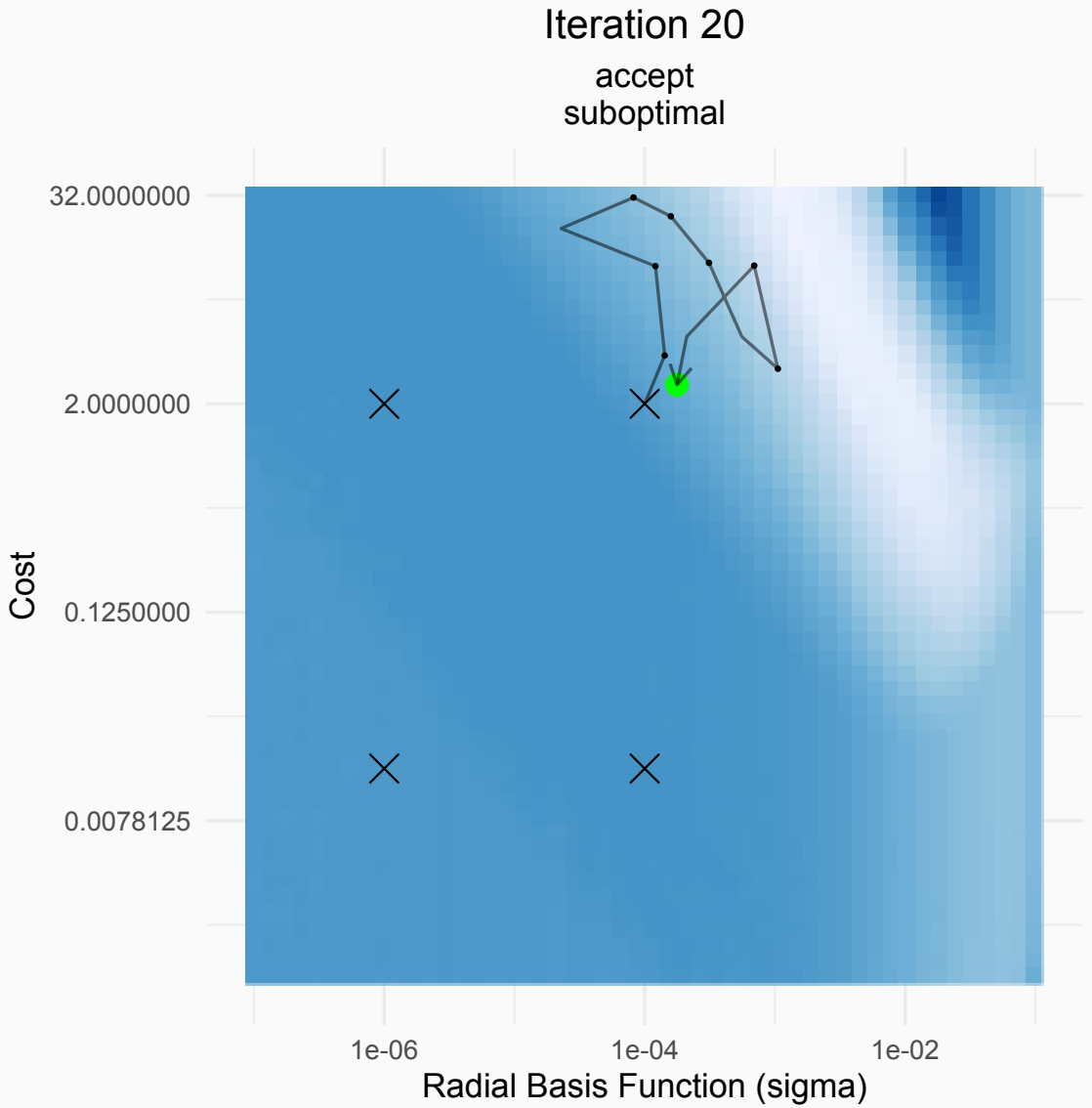

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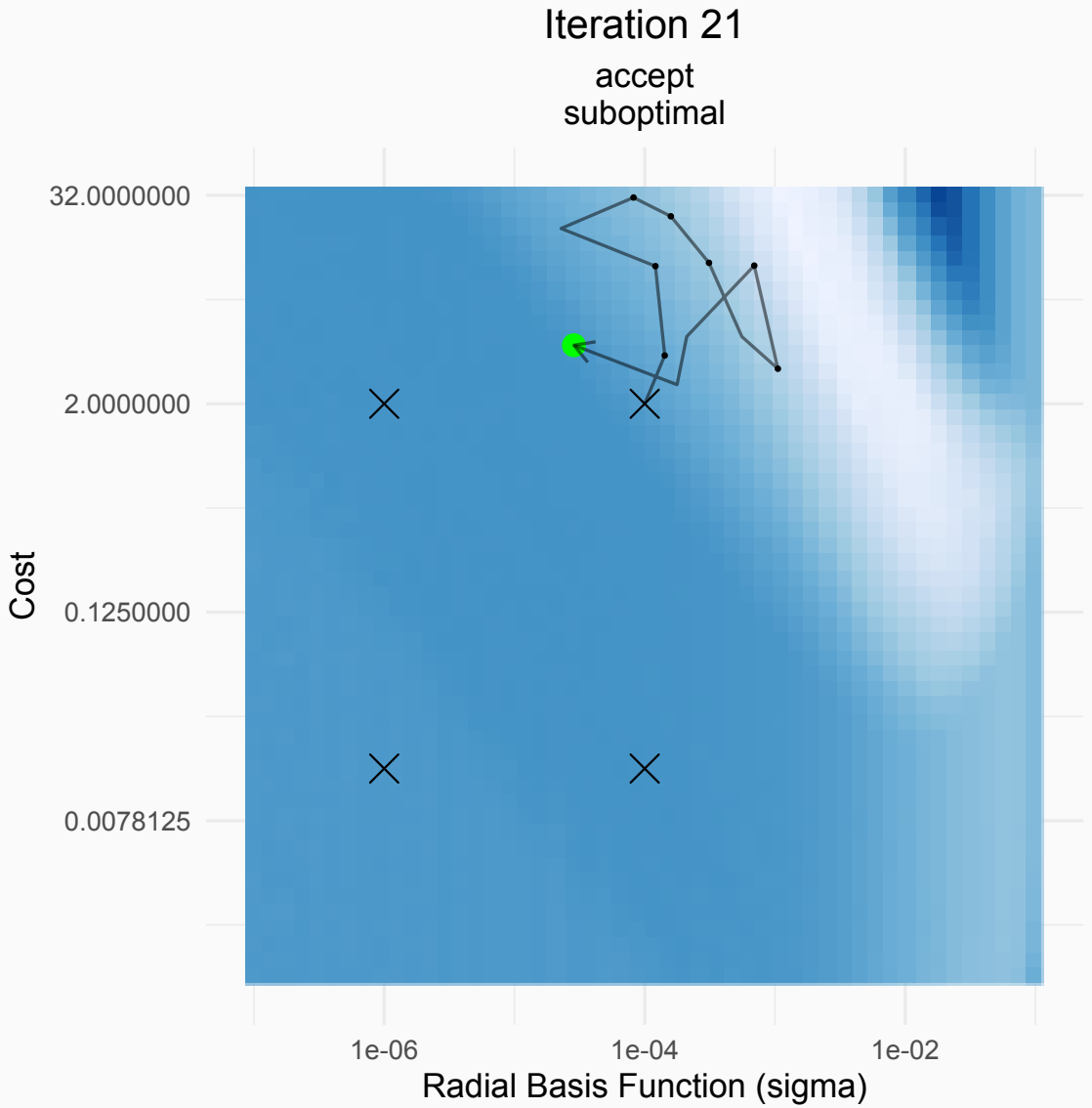

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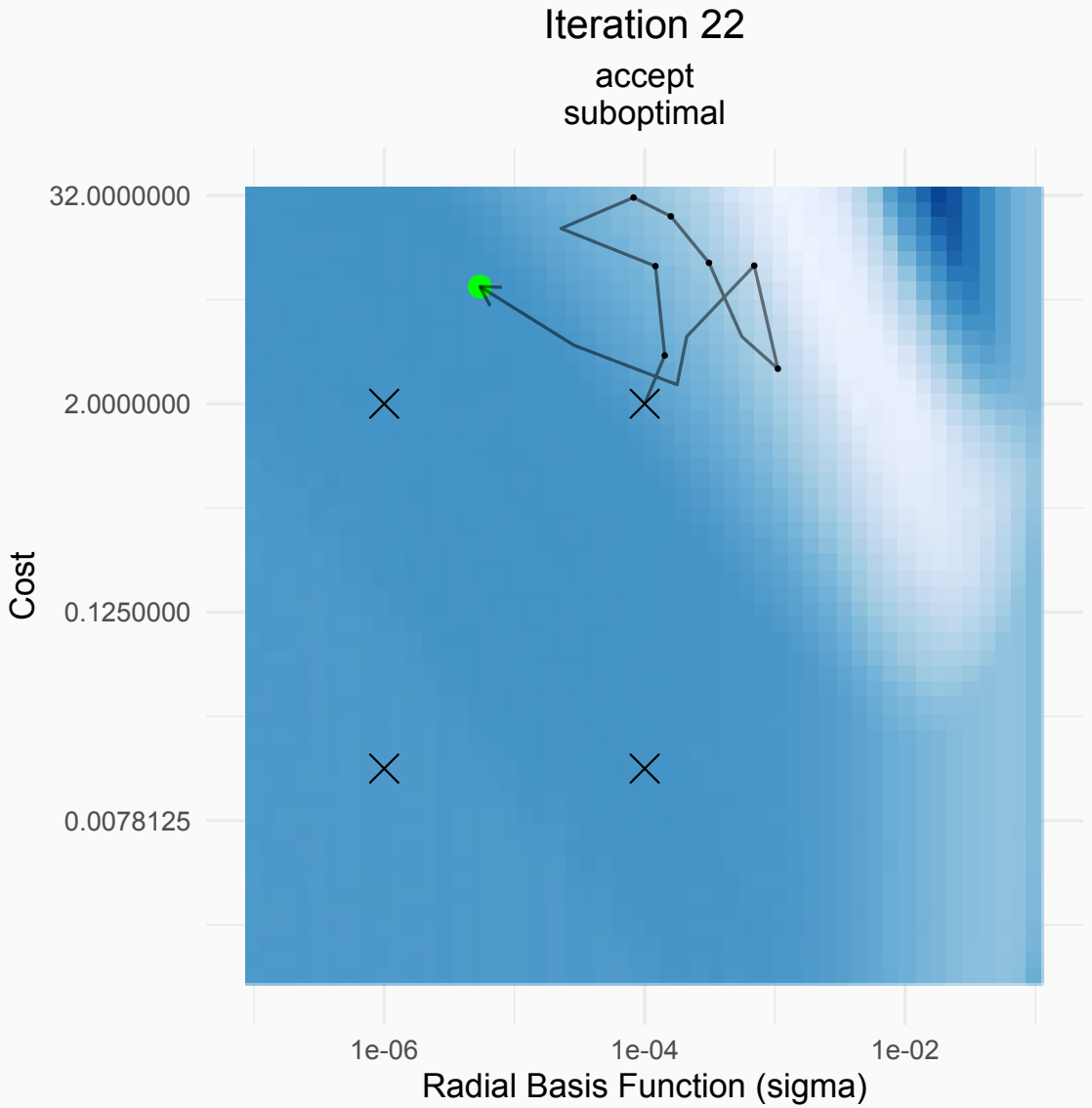

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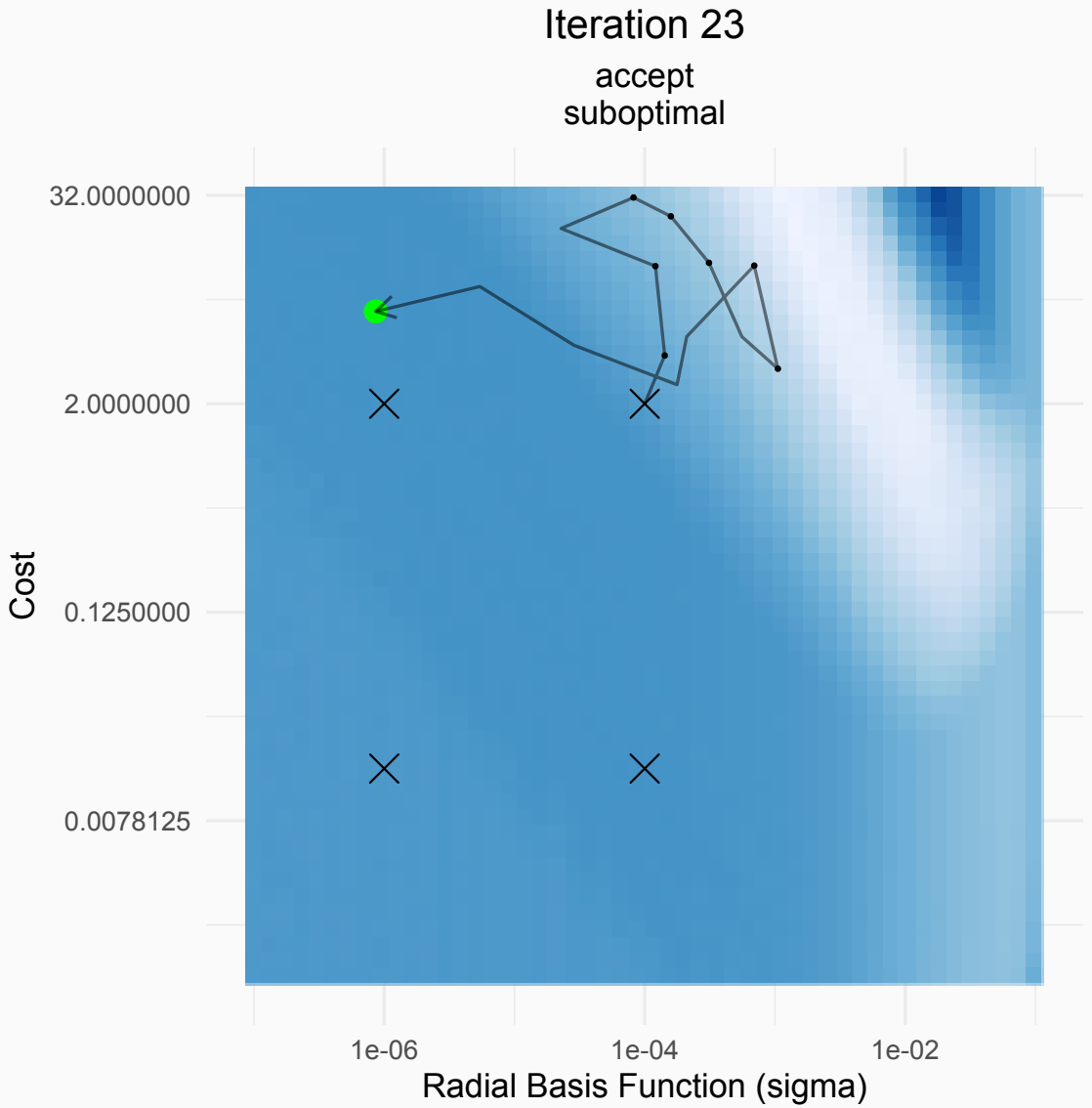

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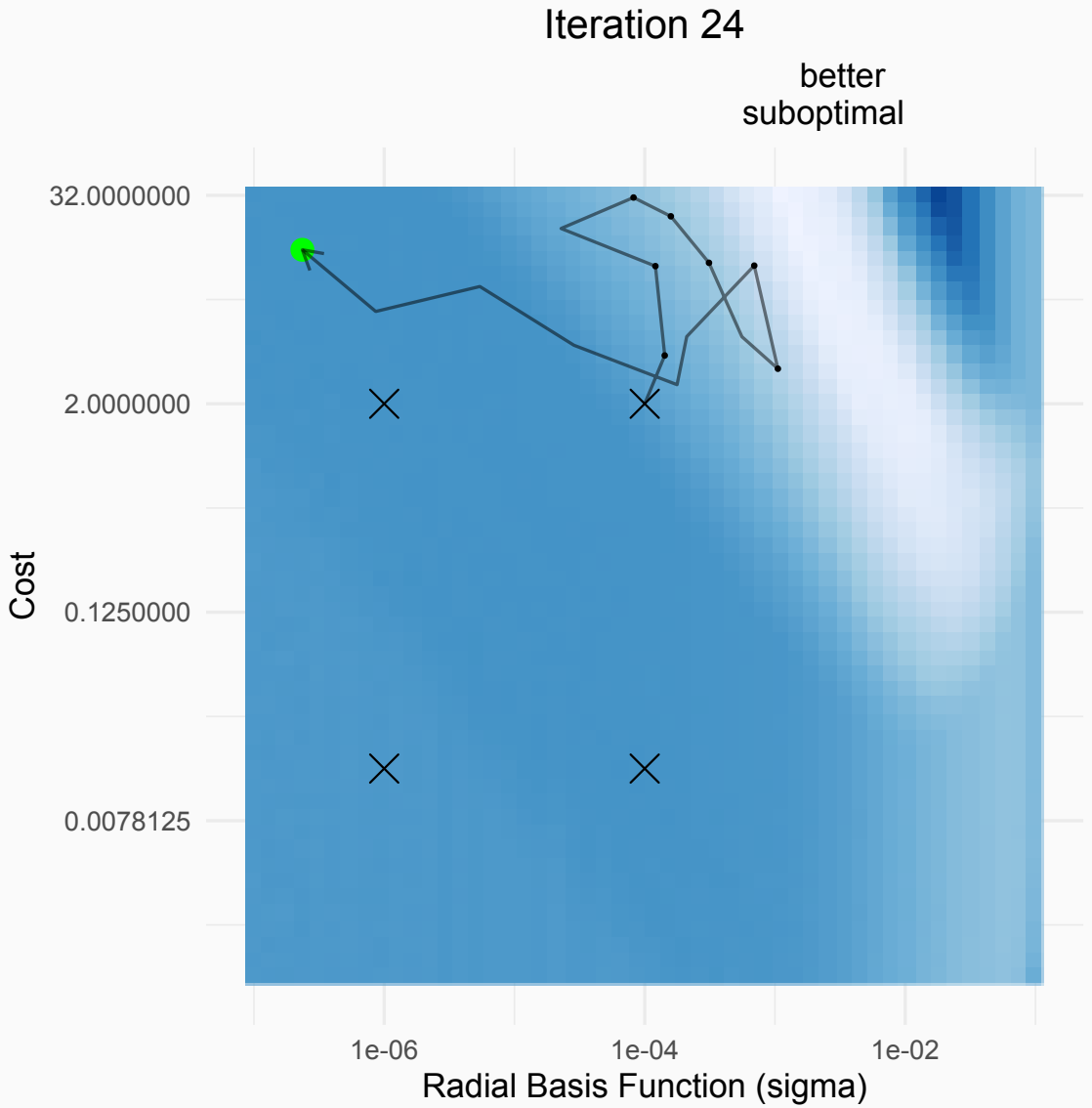

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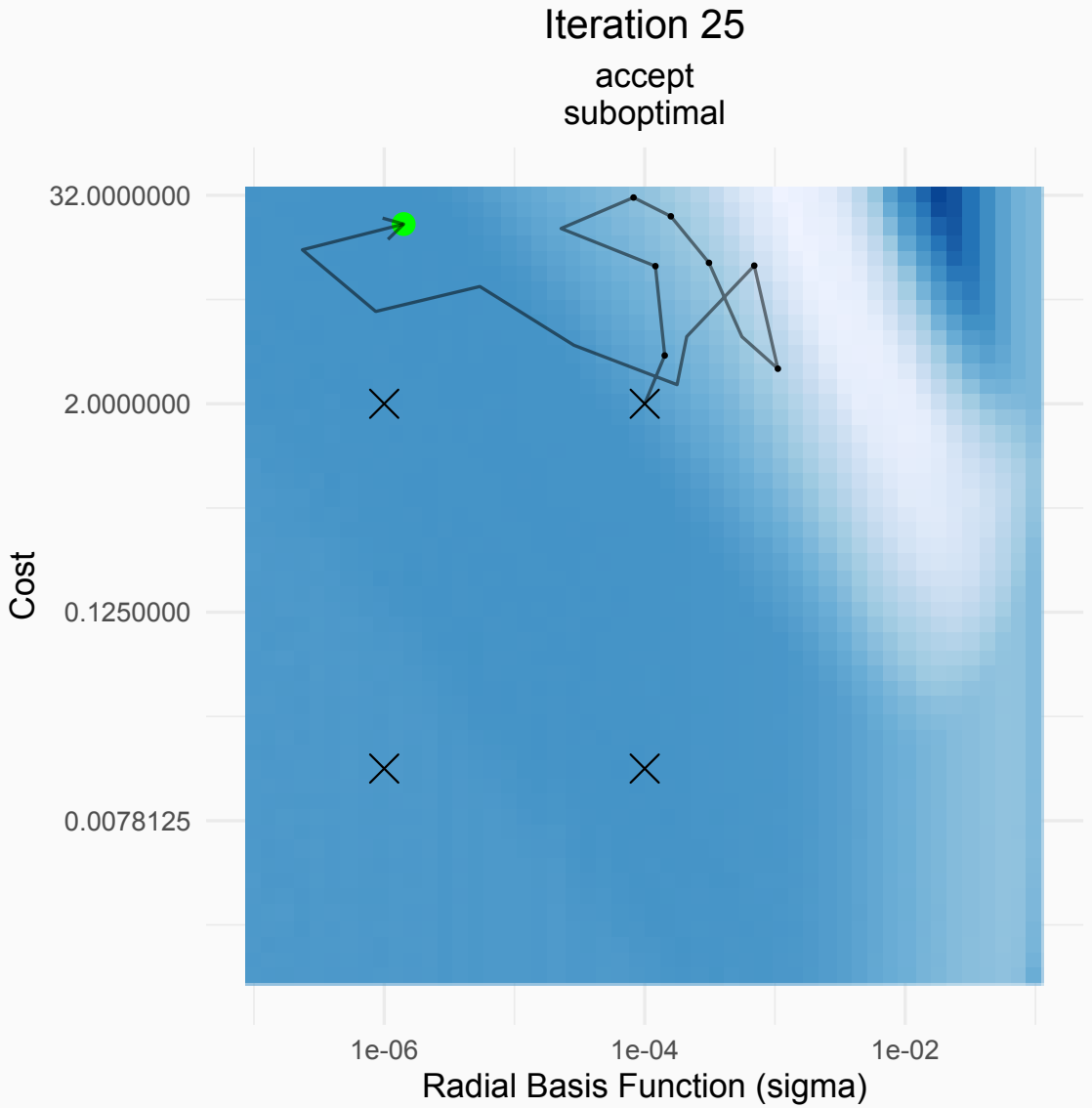

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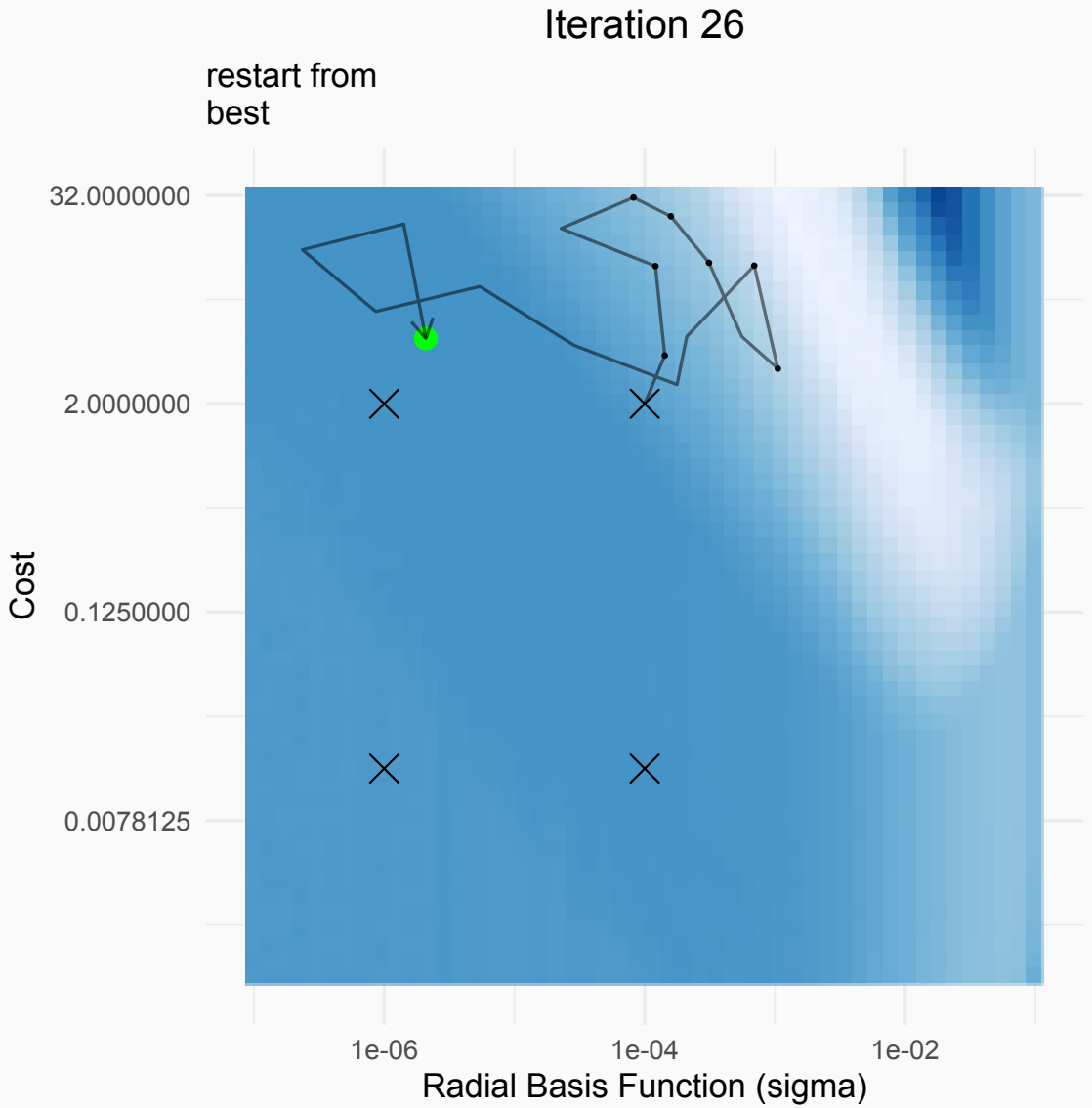

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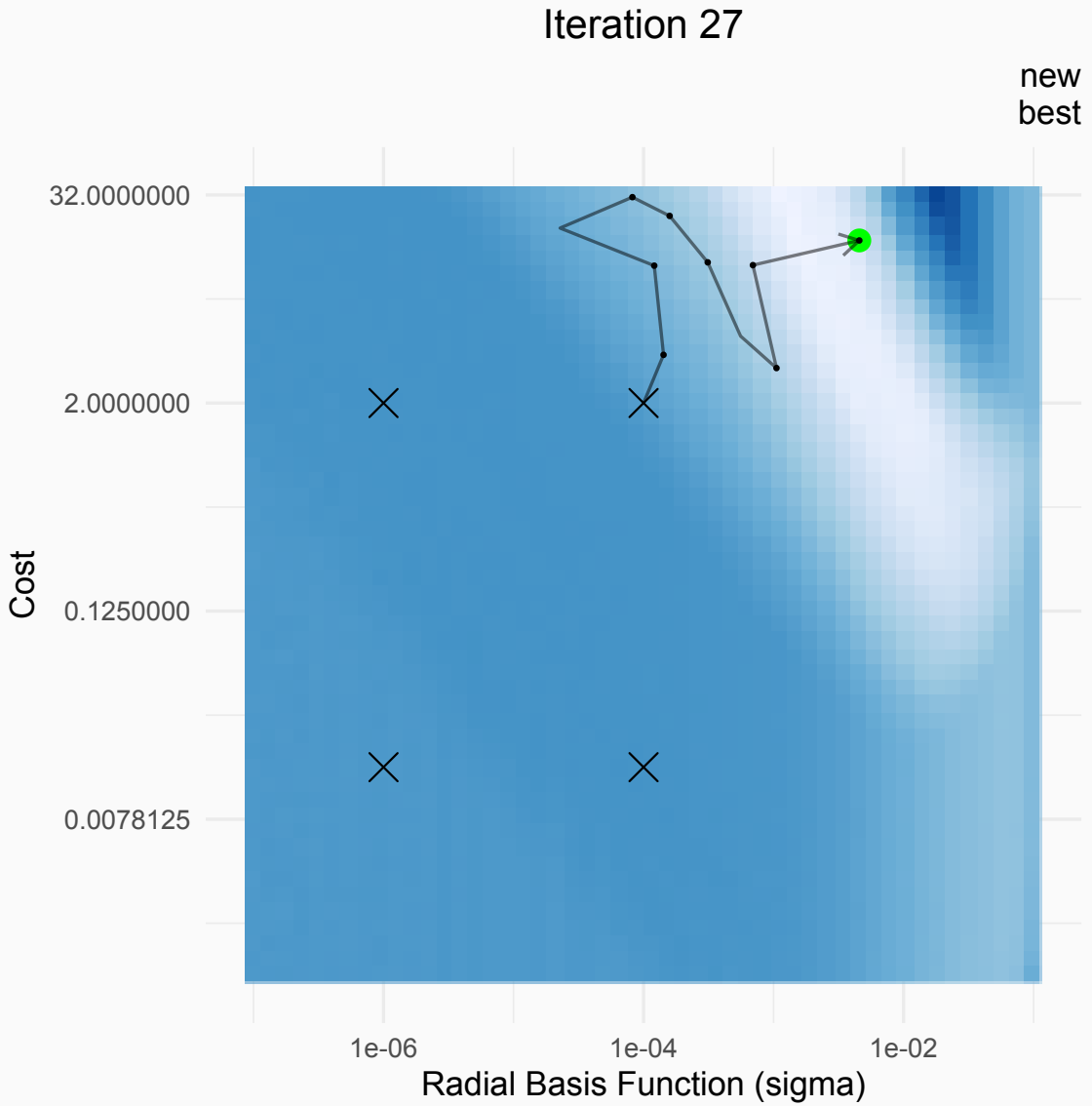

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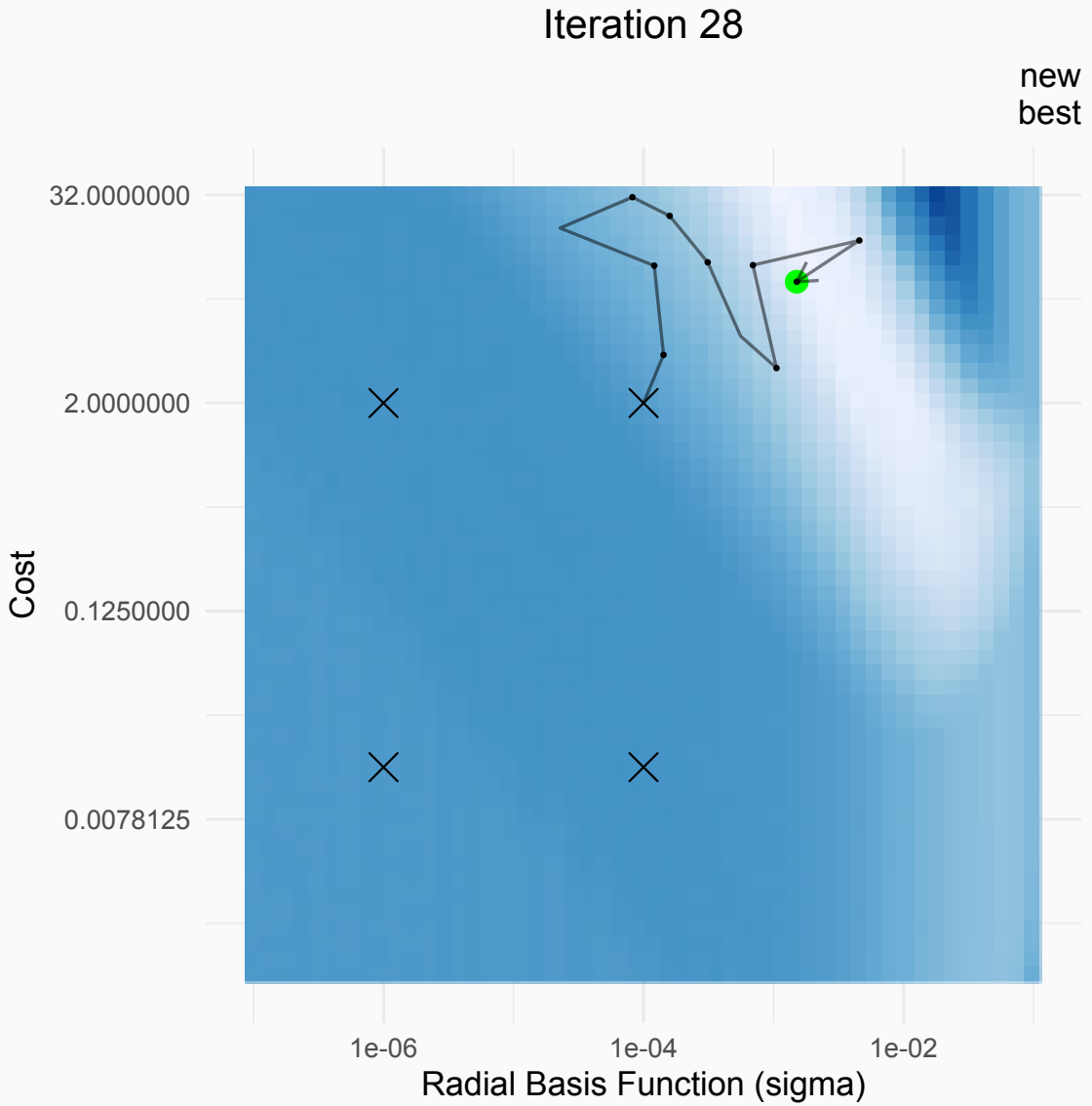

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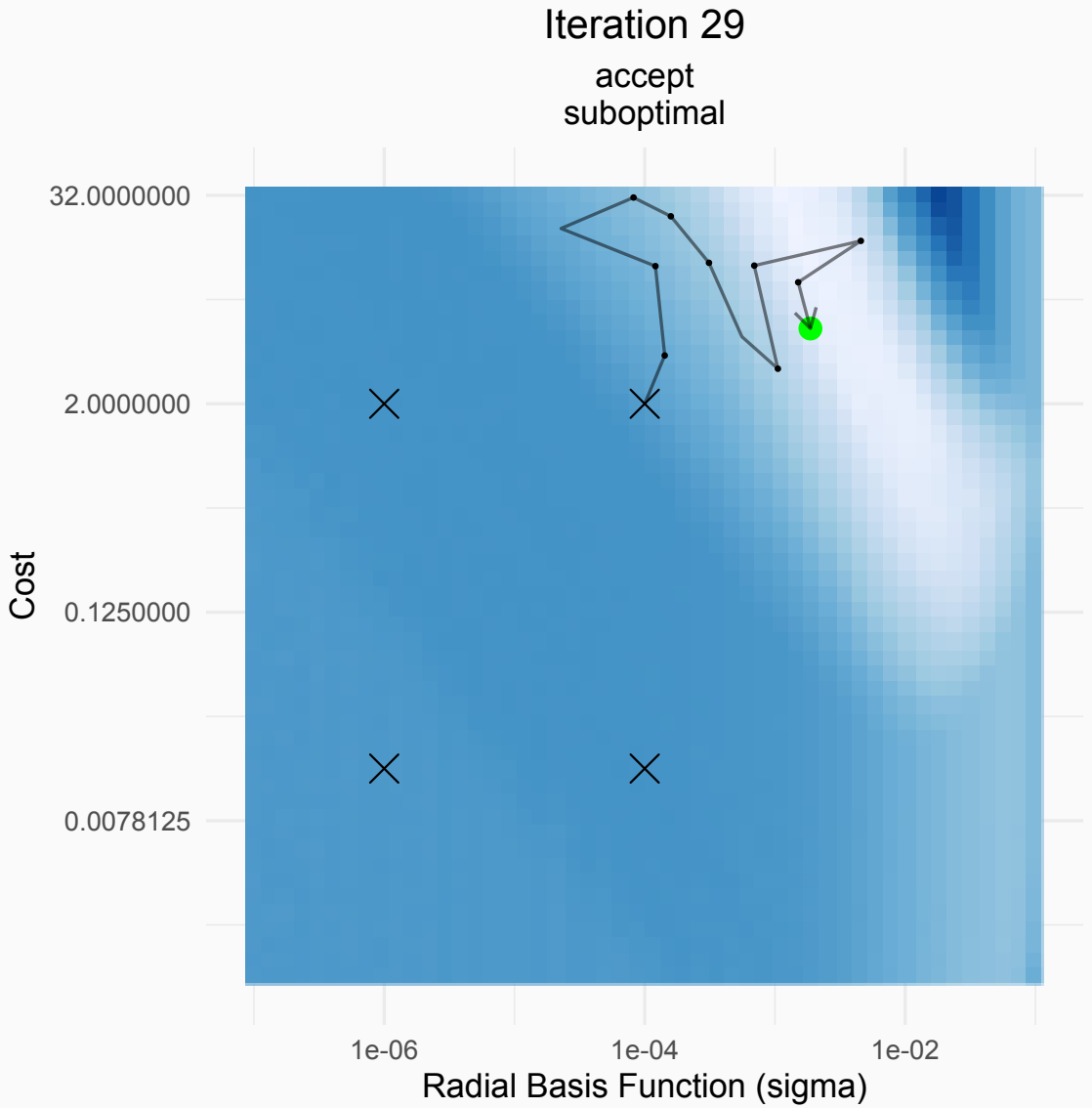

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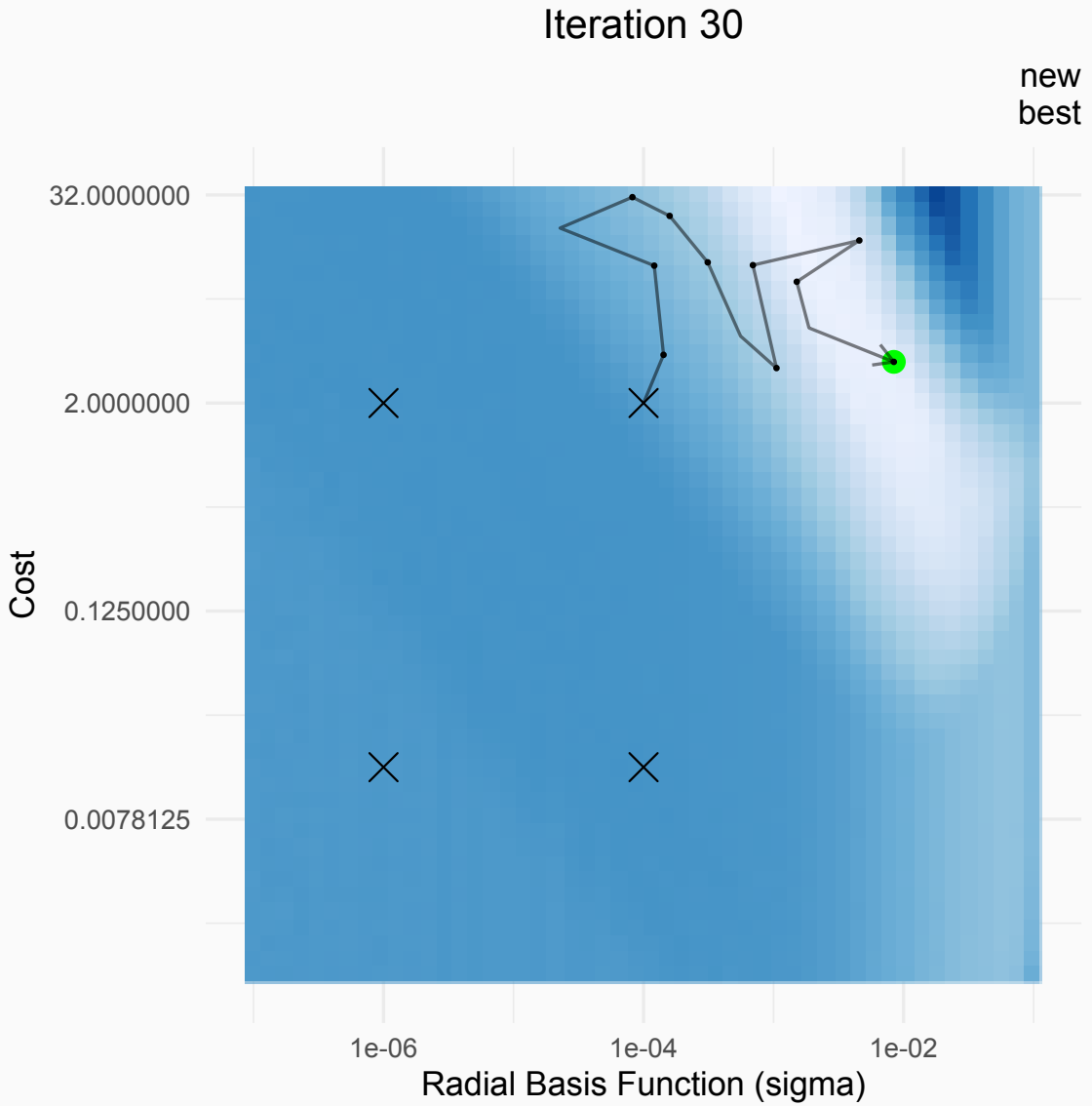

Example Code for Simulated Annealing

```
set.seed(1234)
svm_sa <-
  svm_wflow %>%
  tune_sim_anneal(
    resamples = cell_folds,
    initial = svm_initial,
    iter = 30
  )
```

With the option `verbose = TRUE`:

```
Optimizing roc_auc
Initial best: 0.86627
 1 ♥ new best           roc_auc=0.87157    (+/-0.007672)
 2 − discard suboptimal roc_auc=0.86362    (+/-0.008314)
 3 ♥ new best           roc_auc=0.87554    (+/-0.00752)
 4 ○ accept suboptimal  roc_auc=0.87044    (+/-0.0077)
 5 ♥ new best           roc_auc=0.87764    (+/-0.007252)
 6 ♥ new best           roc_auc=0.87999    (+/-0.007074)
 7 ♥ new best           roc_auc=0.88168    (+/-0.00707)
 8 ○ accept suboptimal  roc_auc=0.871      (+/-0.007702)
 9 ○ accept suboptimal  roc_auc=0.86378    (+/-0.008341)
```

Thanks for Watching!

Resources for learning more:

- `tidymodels.org`
- *Tidy Modeling with R* book
  - Chapter 13 (*Grid Search*) has details on racing methods
  - Chapter 14 (*Iterative search*) describes simulated annealing
- `finetune` webpage and blog post