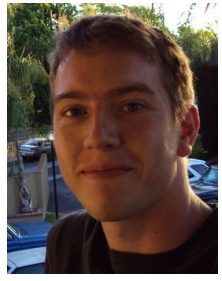
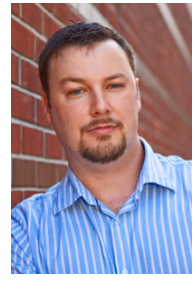
Early Stopping as Nonparametric Variational Inference

Dougal Maclaurin, David Duvenaud, Ryan Adams

Harvard University

June 15, 2015

Optimization as Inference

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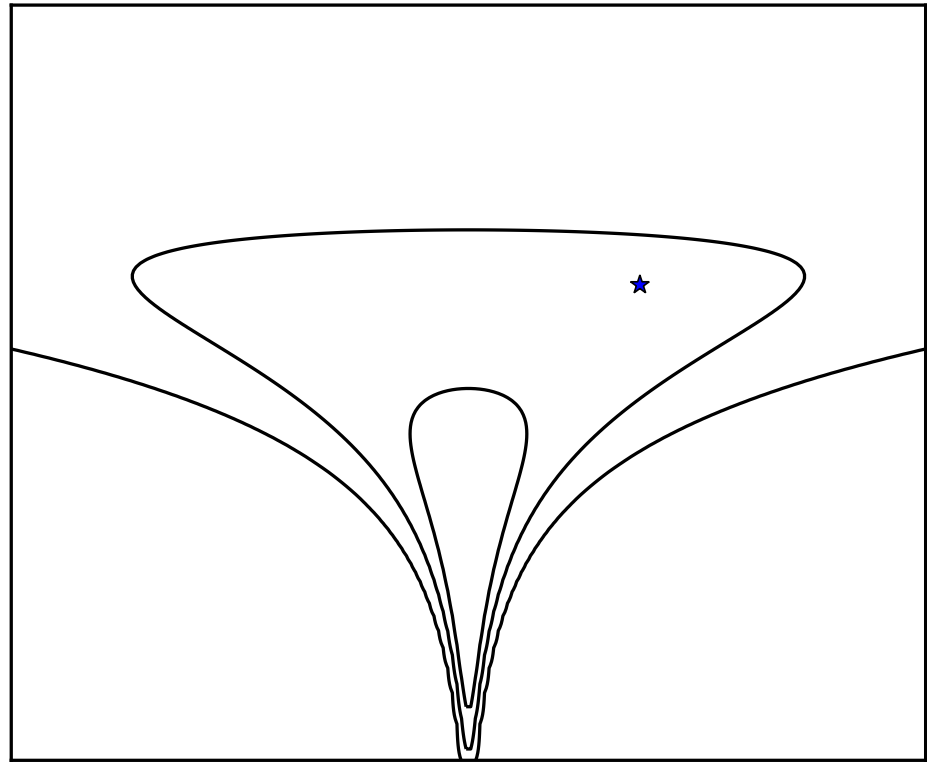

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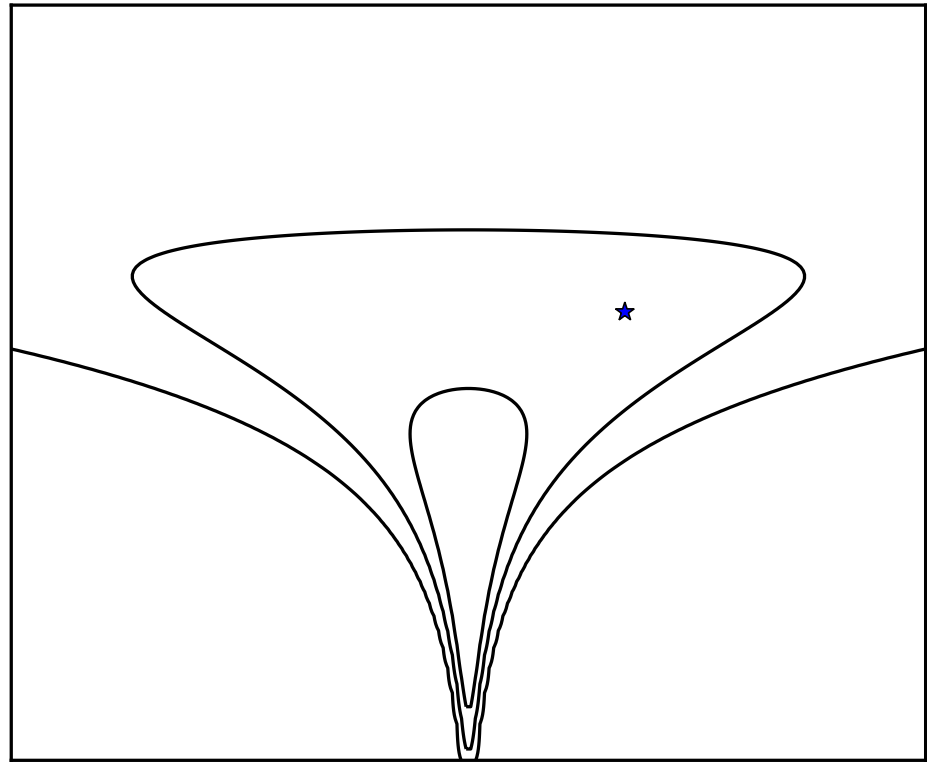

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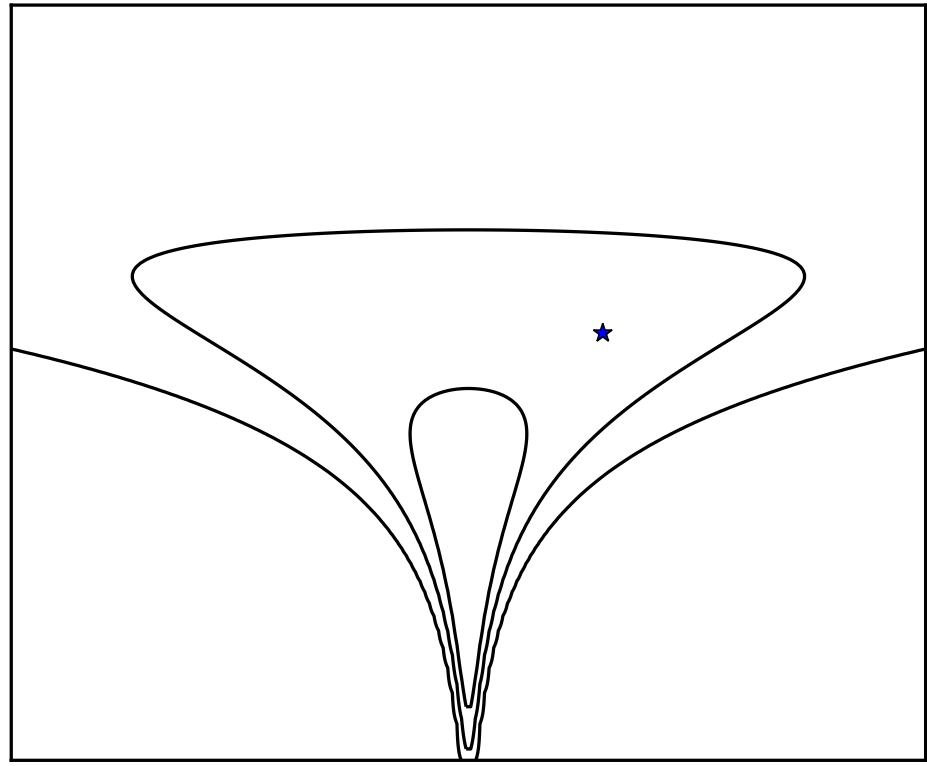

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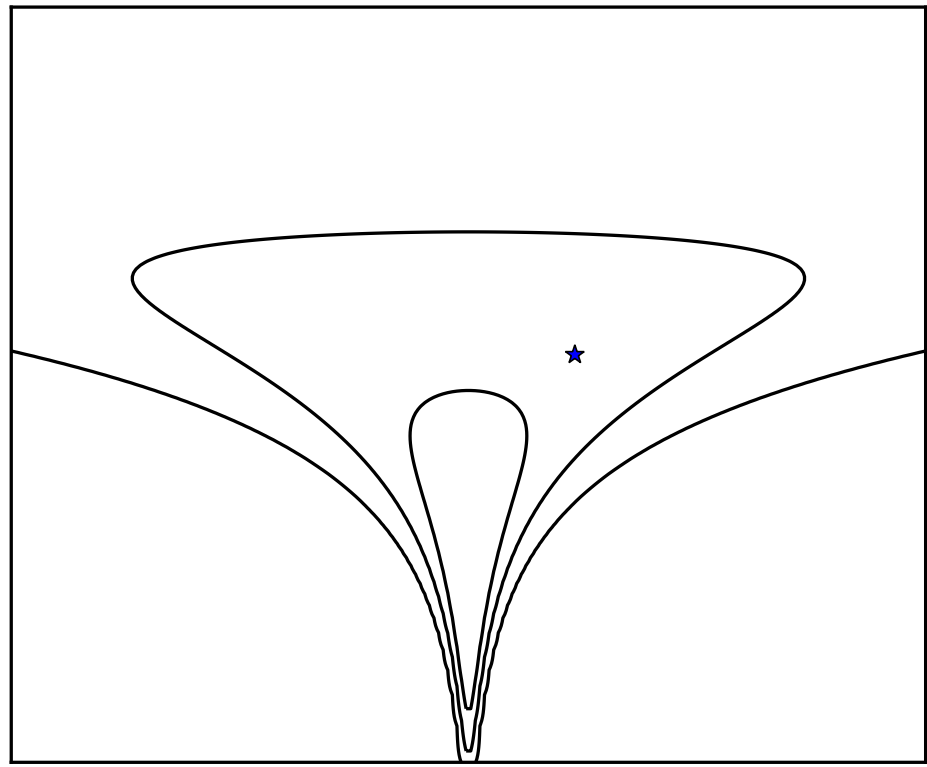

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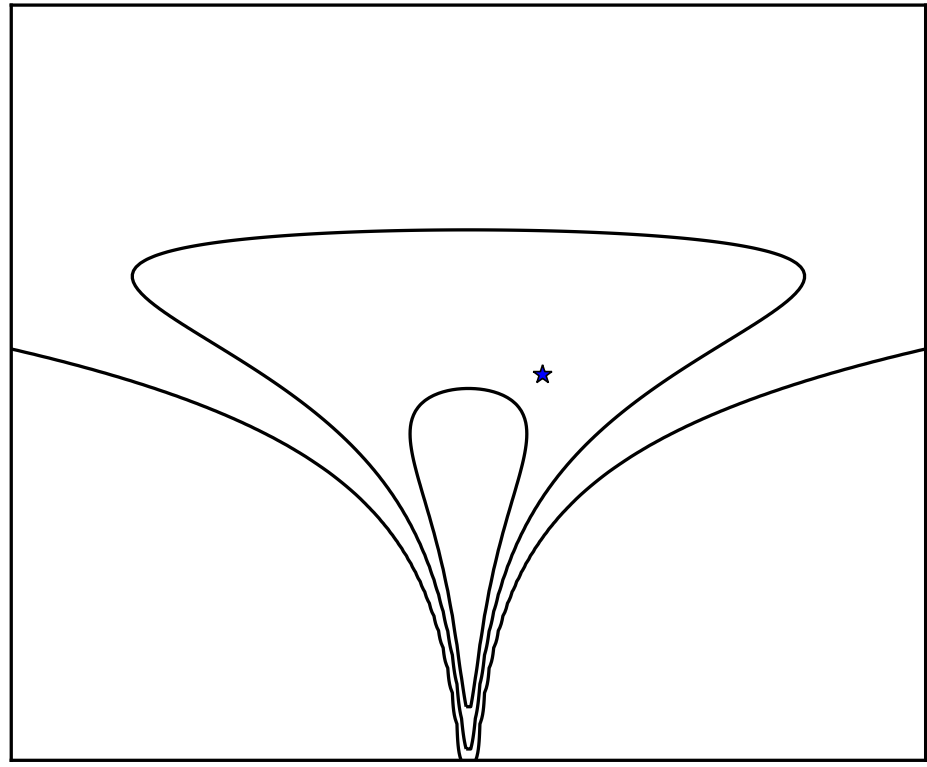

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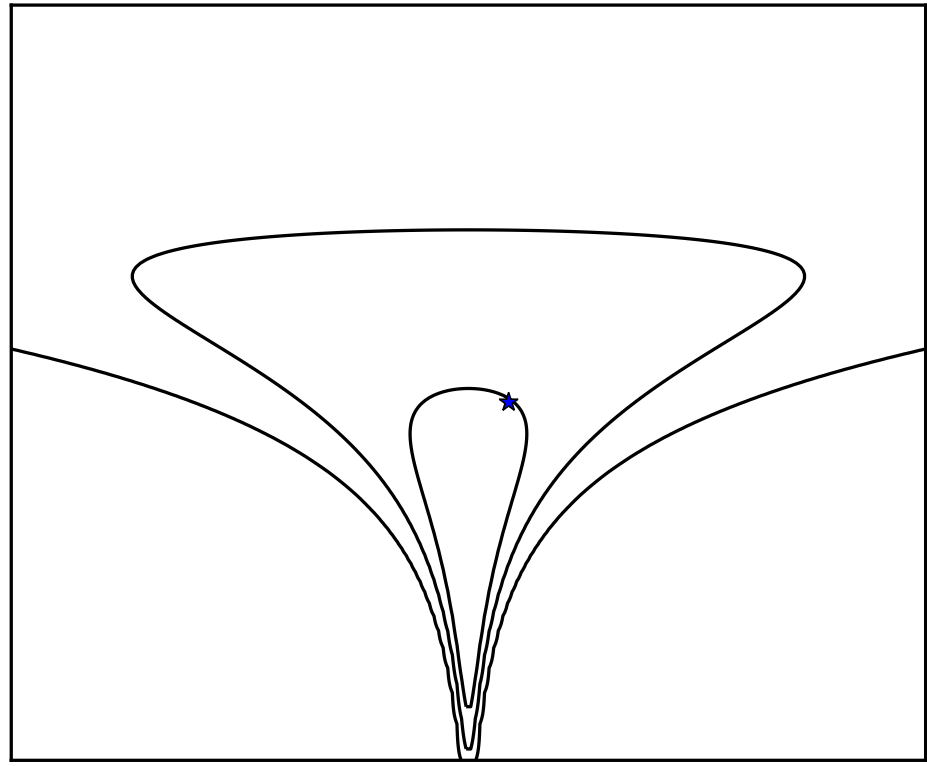

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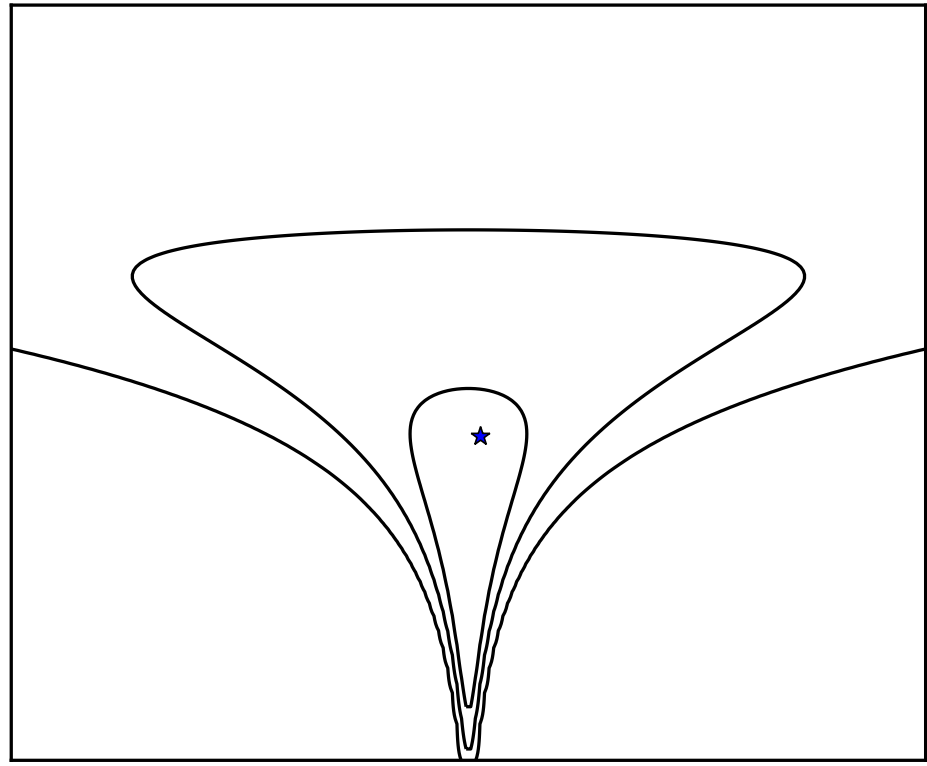

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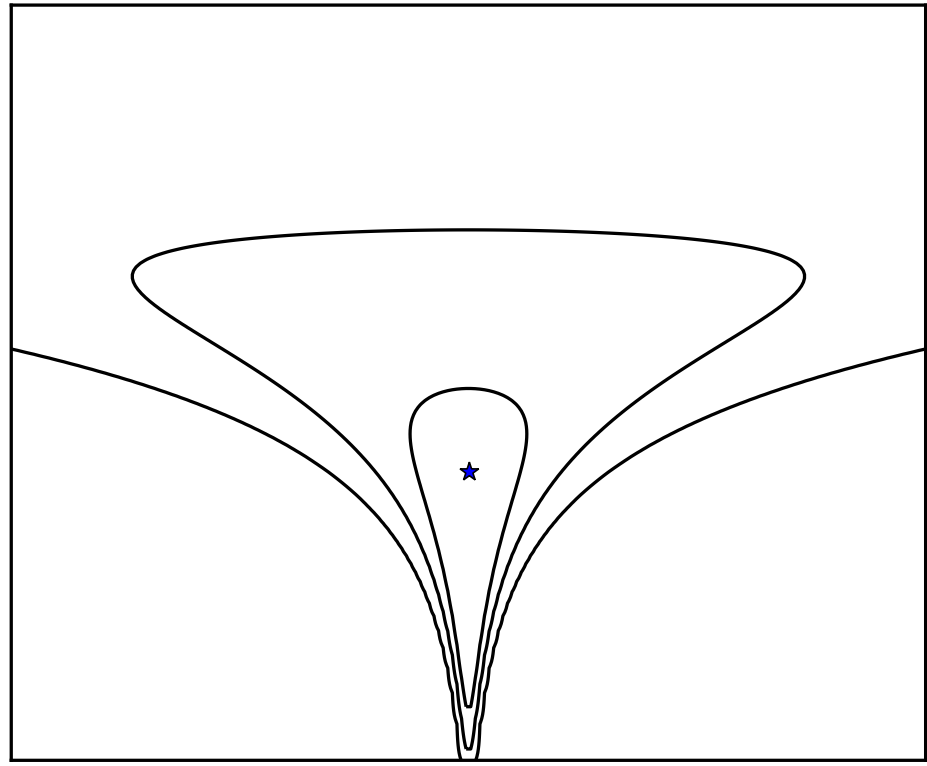

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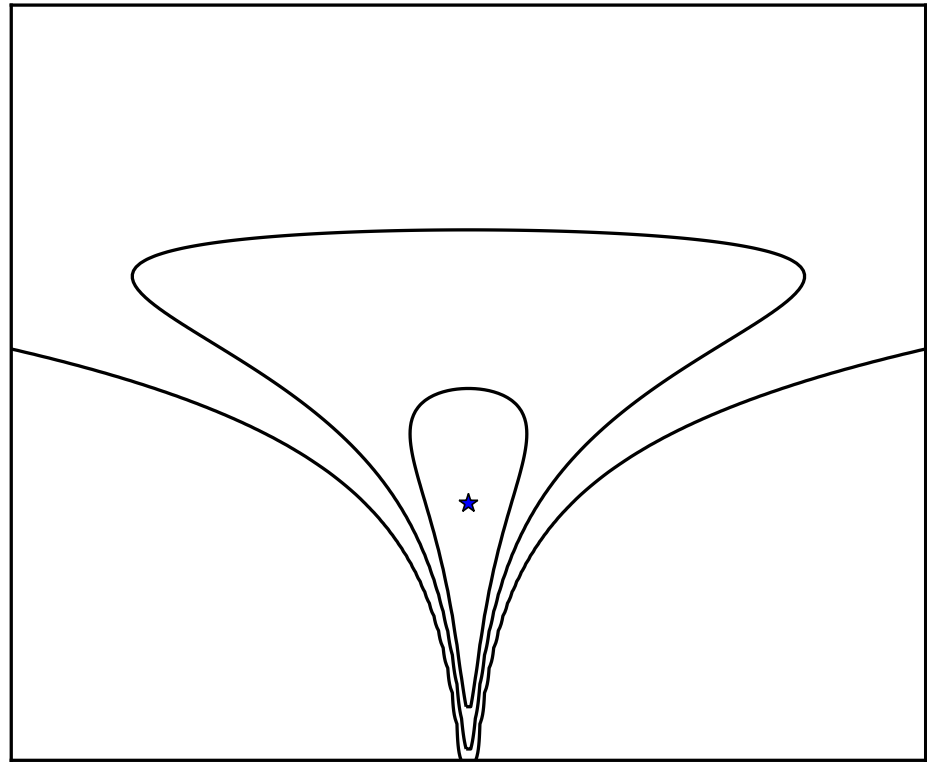

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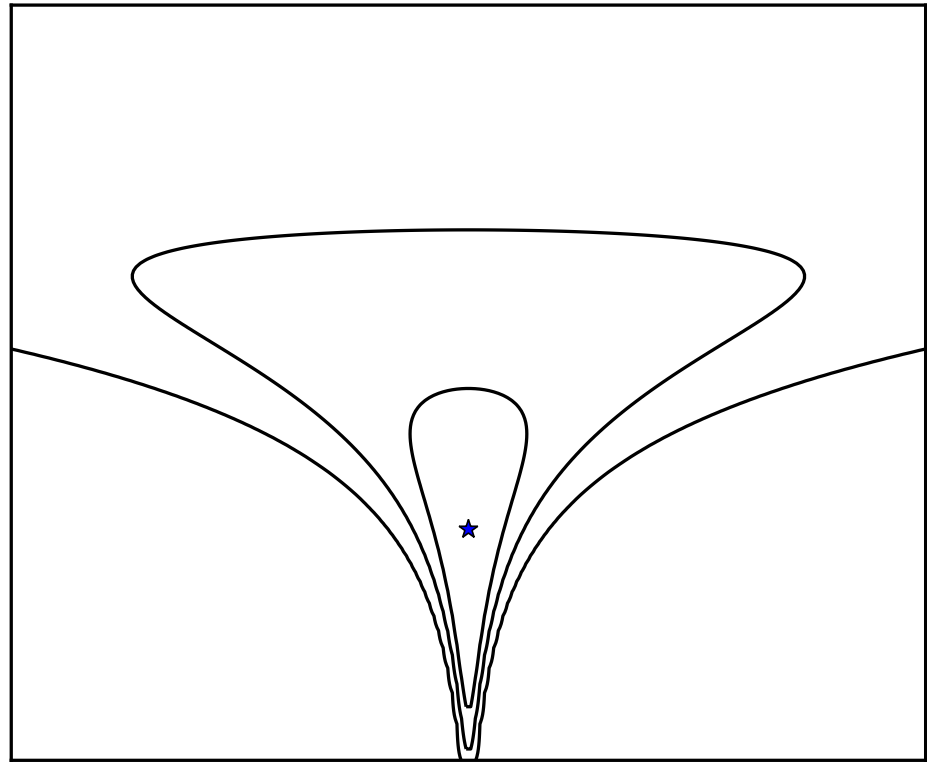

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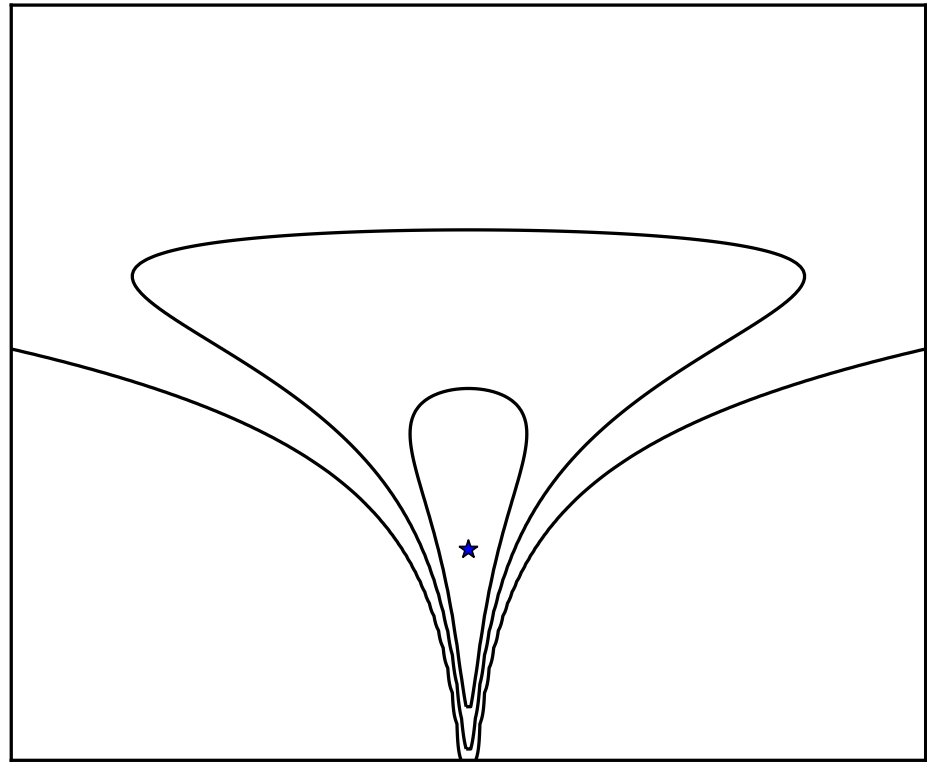

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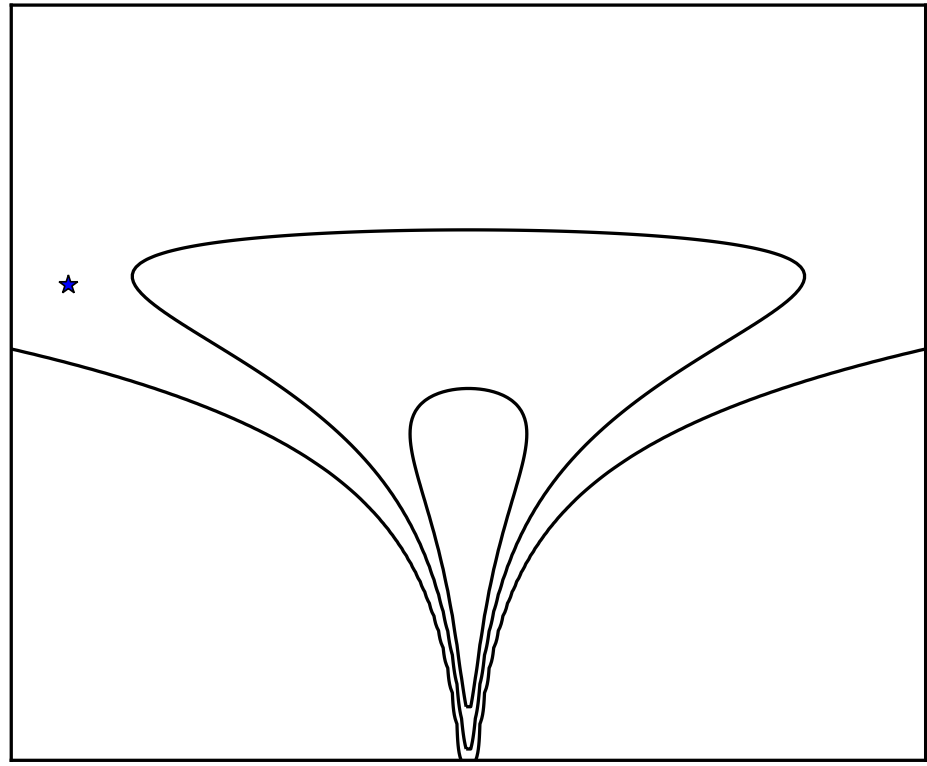

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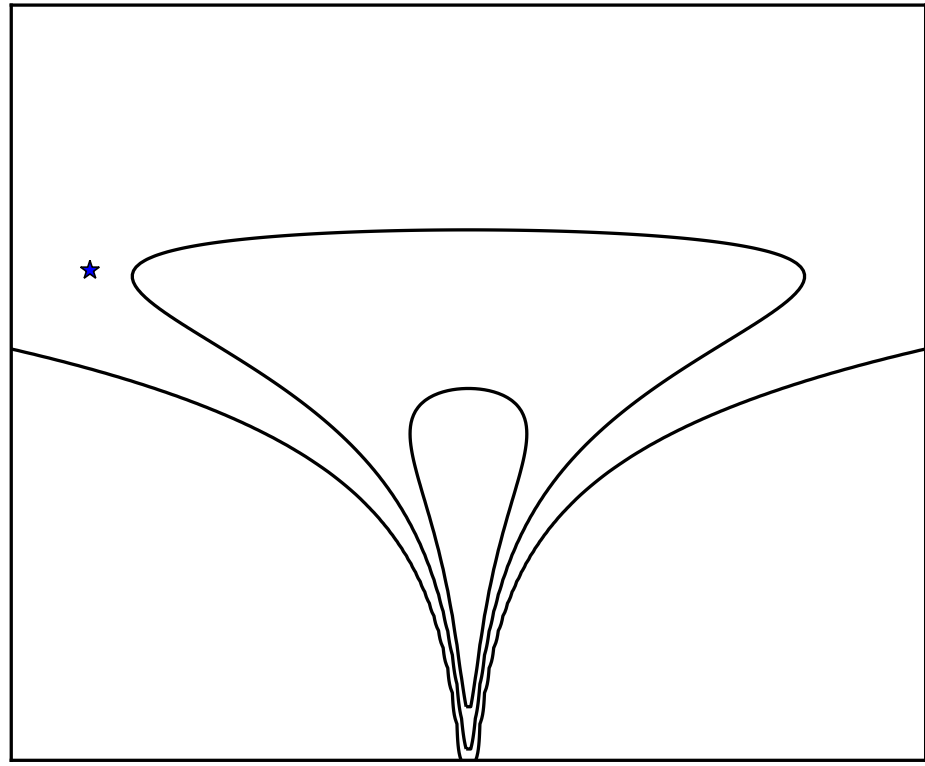

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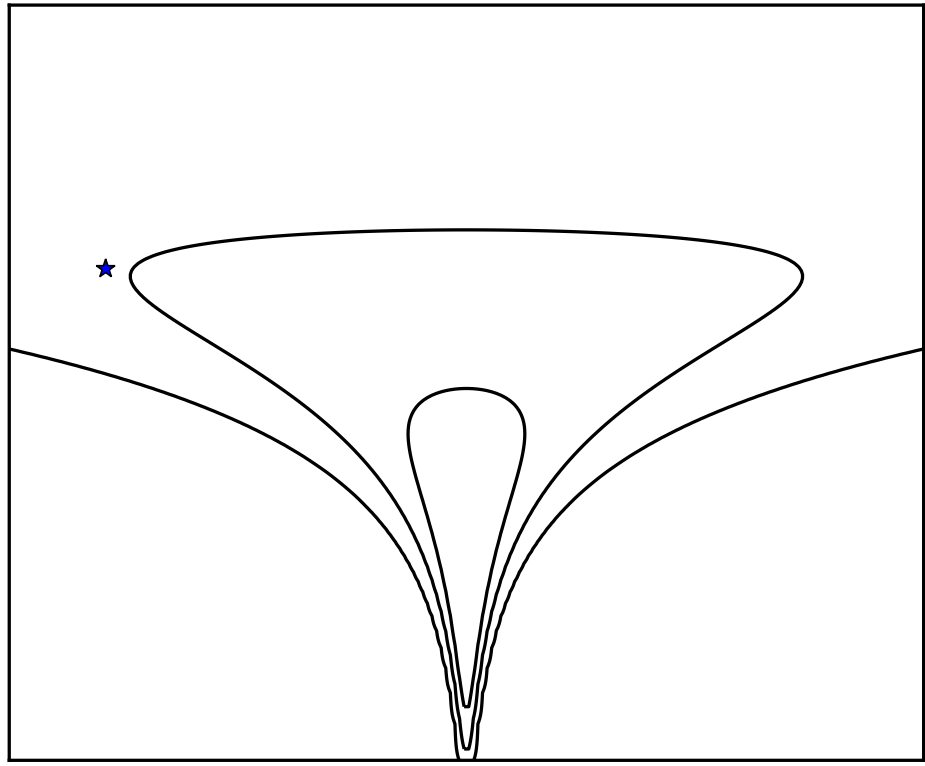

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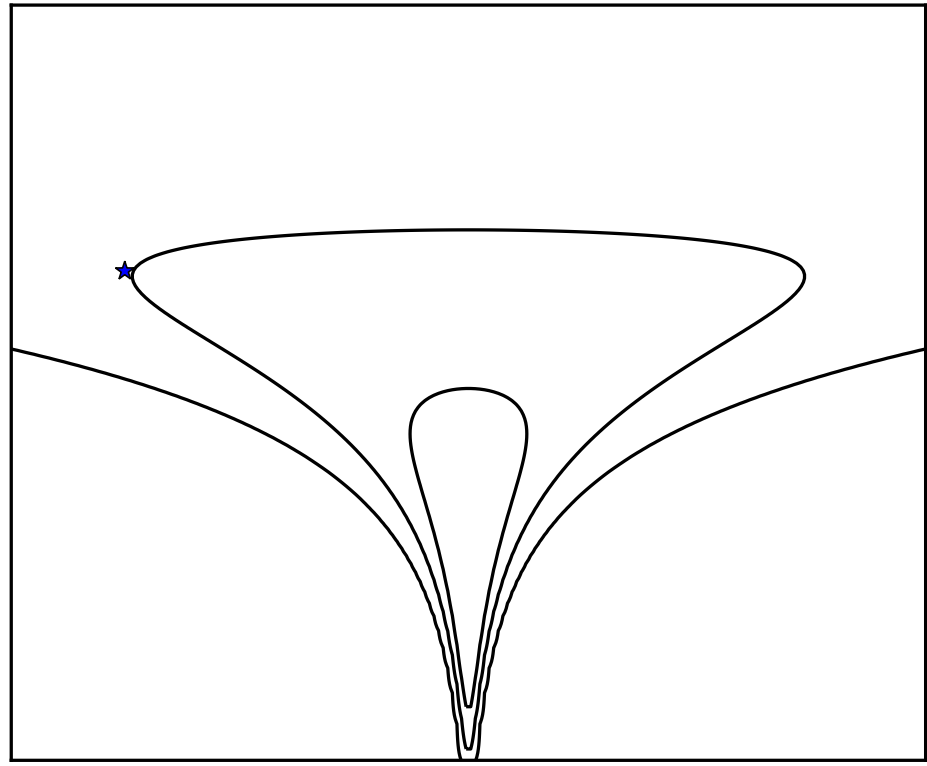

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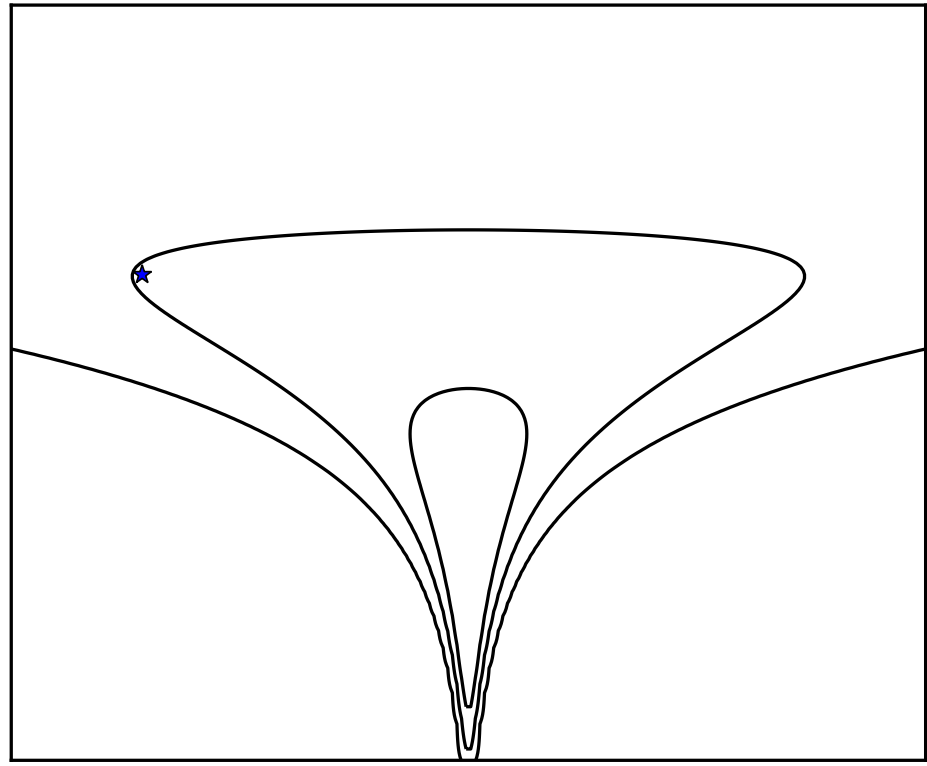

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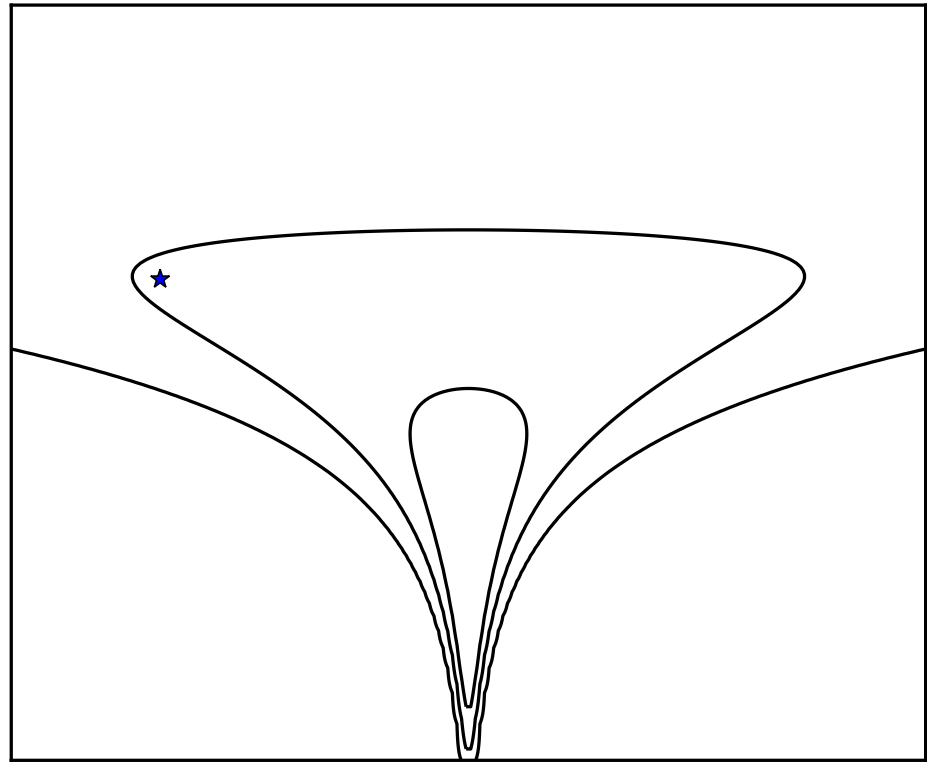

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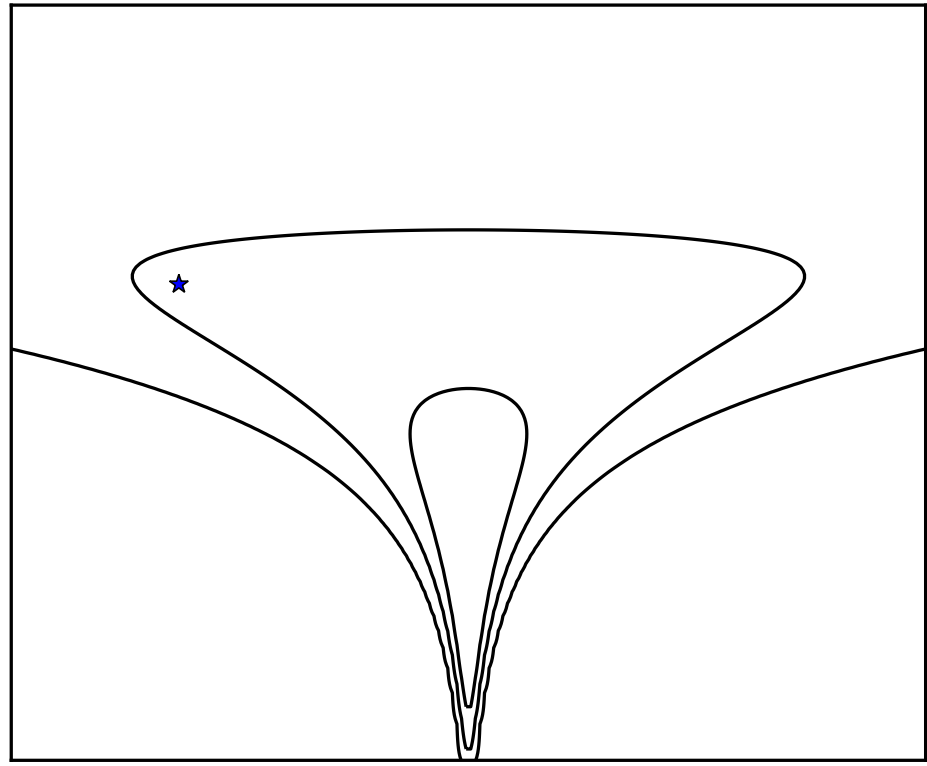

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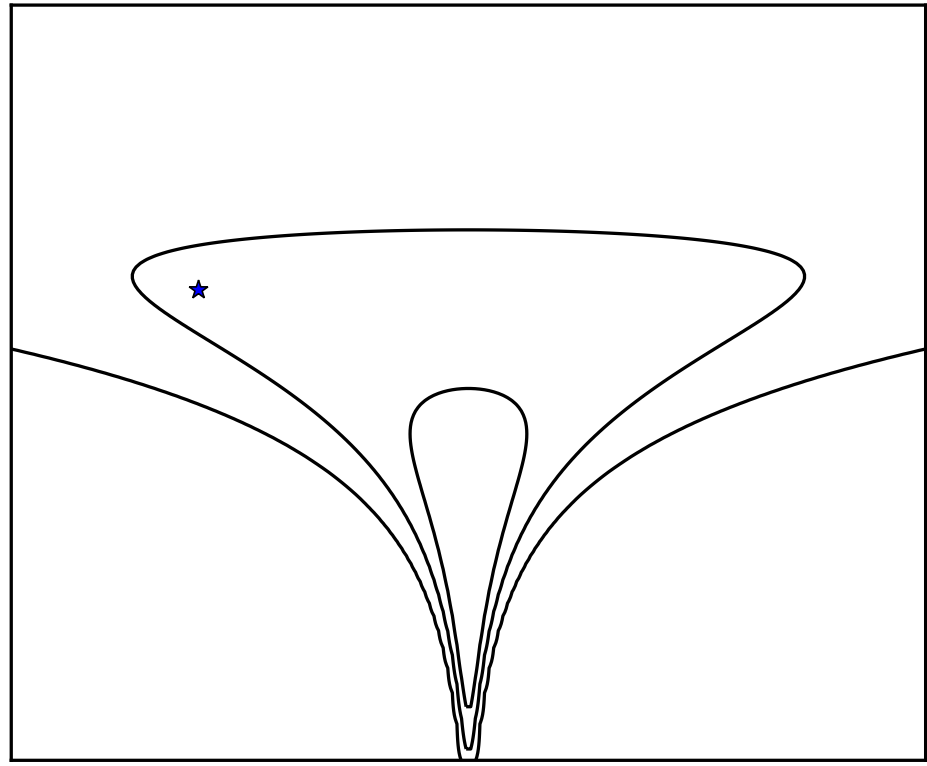

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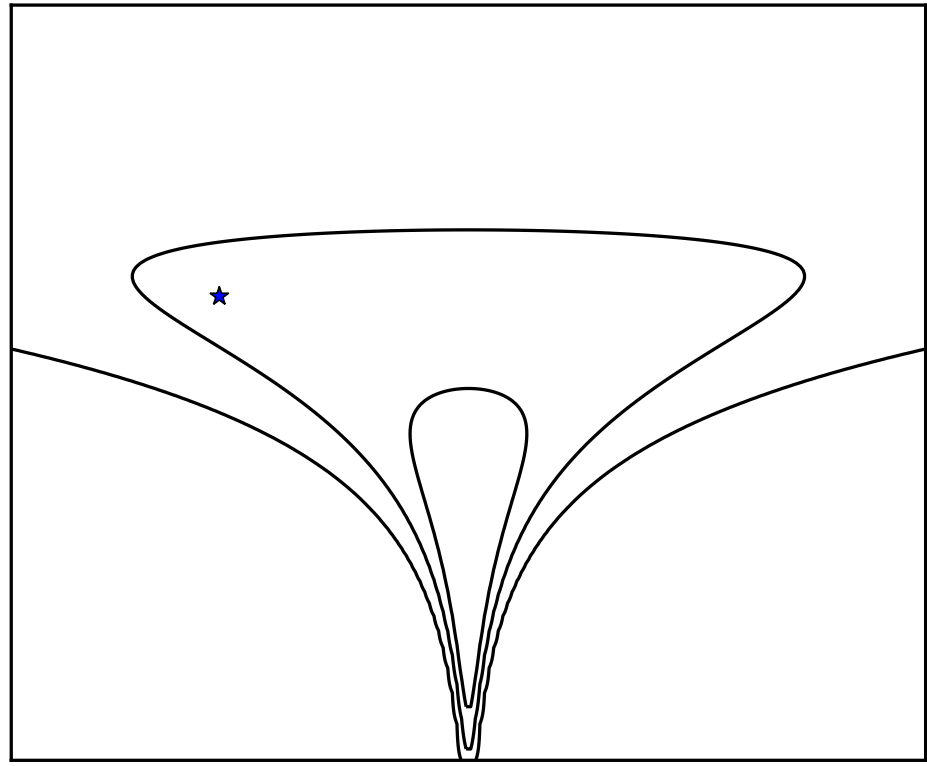

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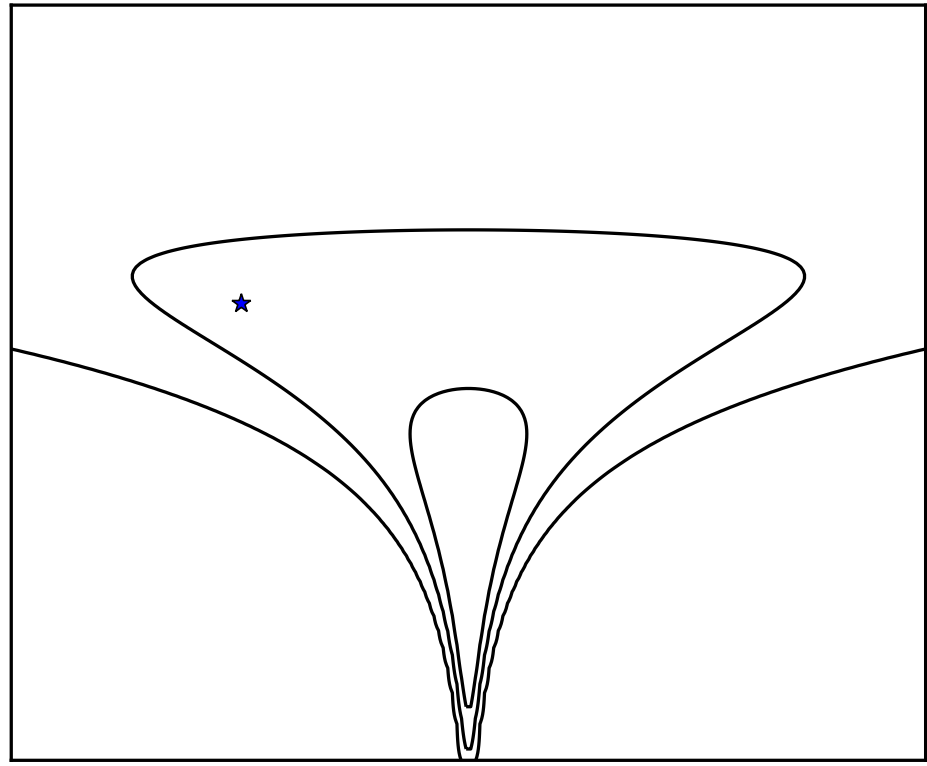

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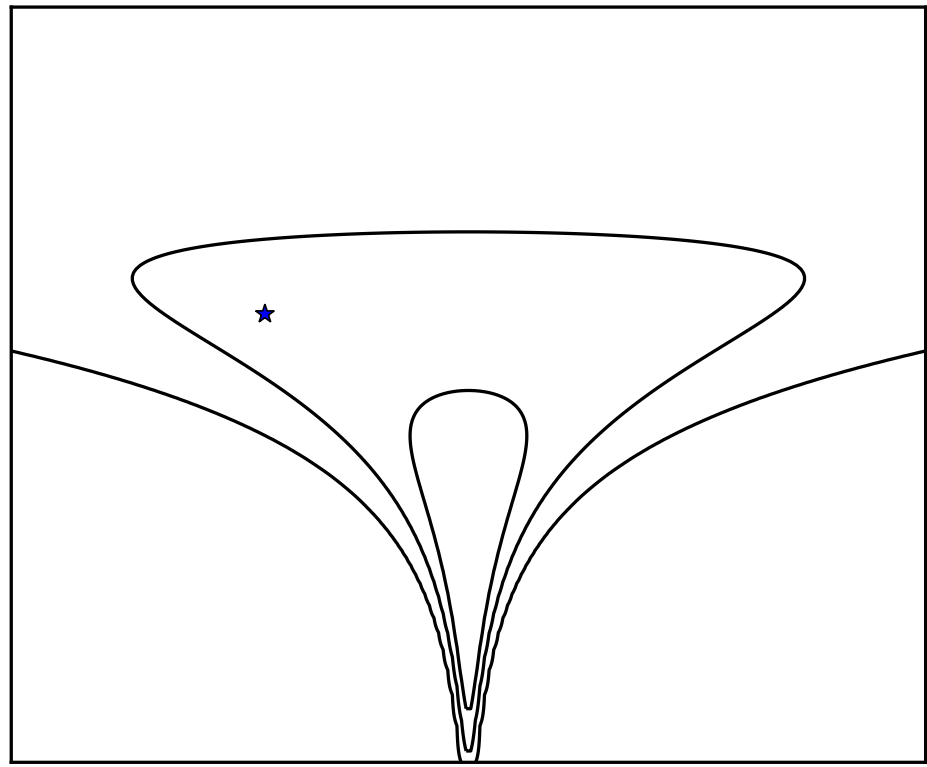

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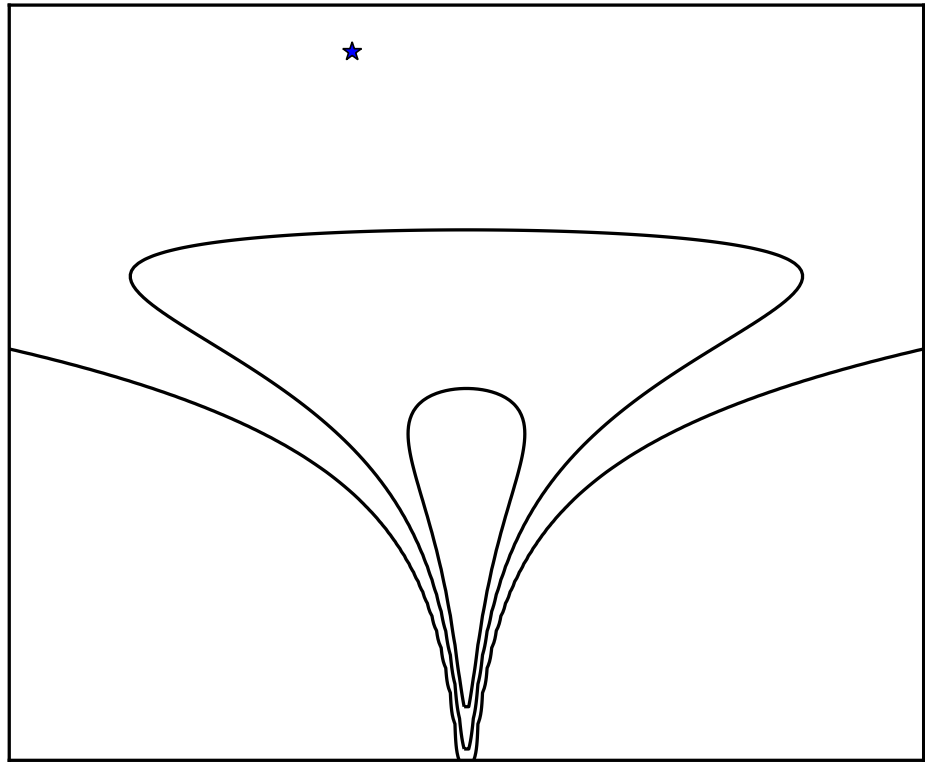

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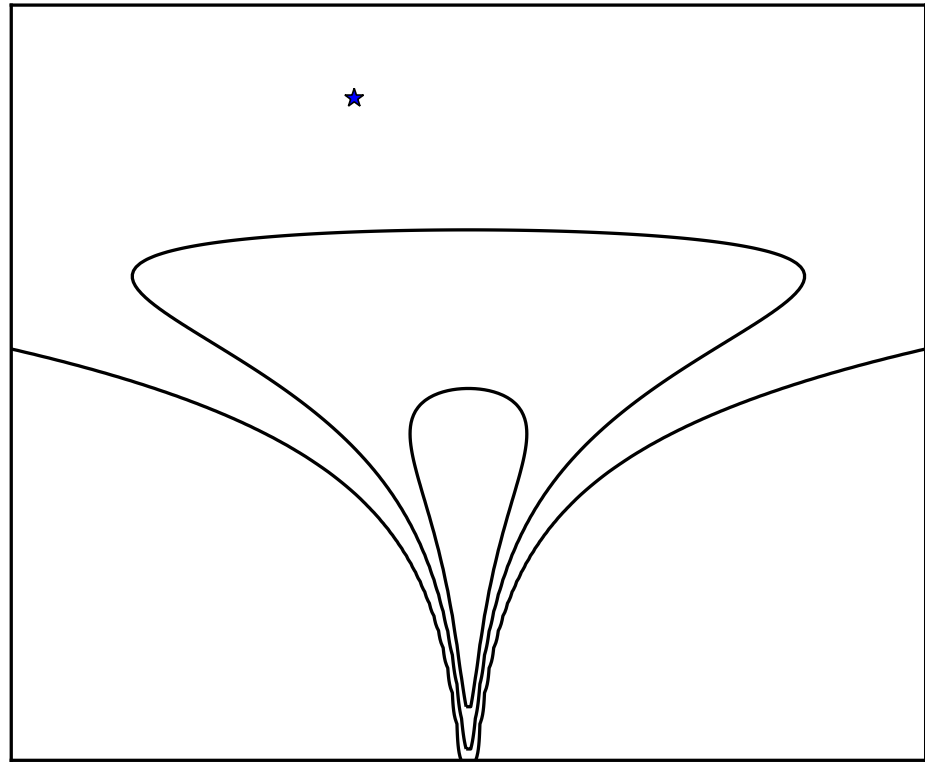

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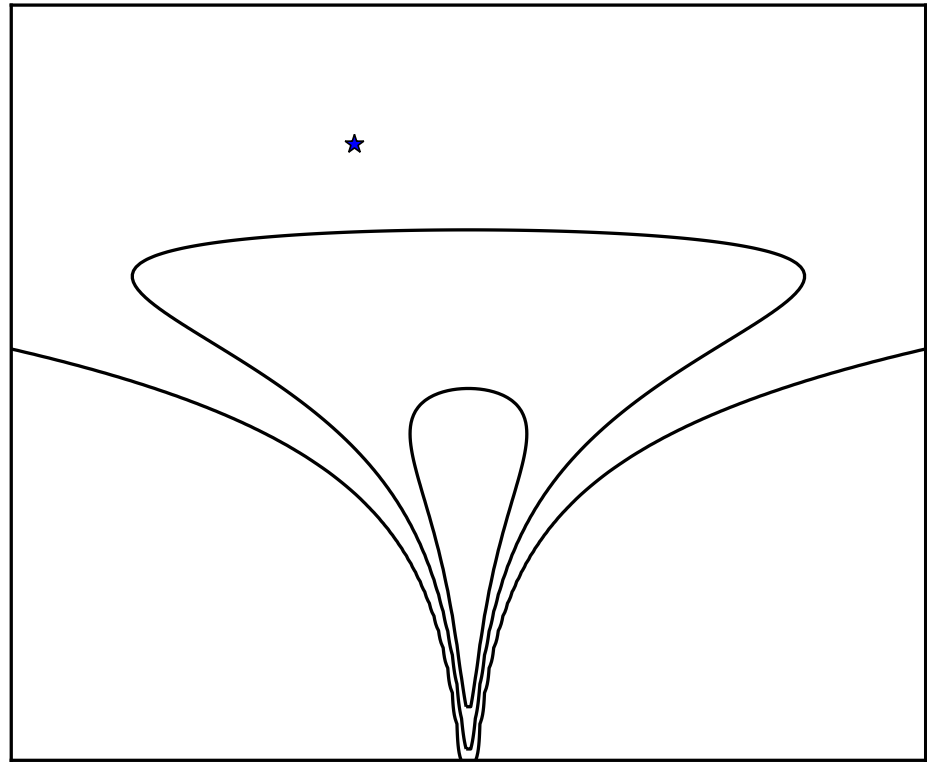

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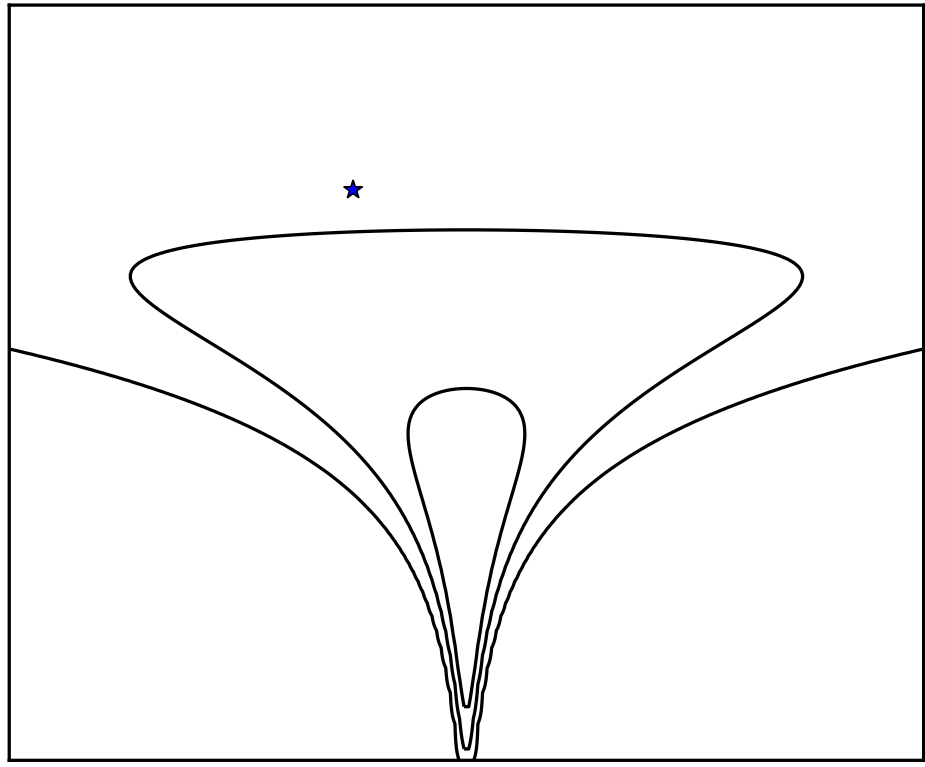

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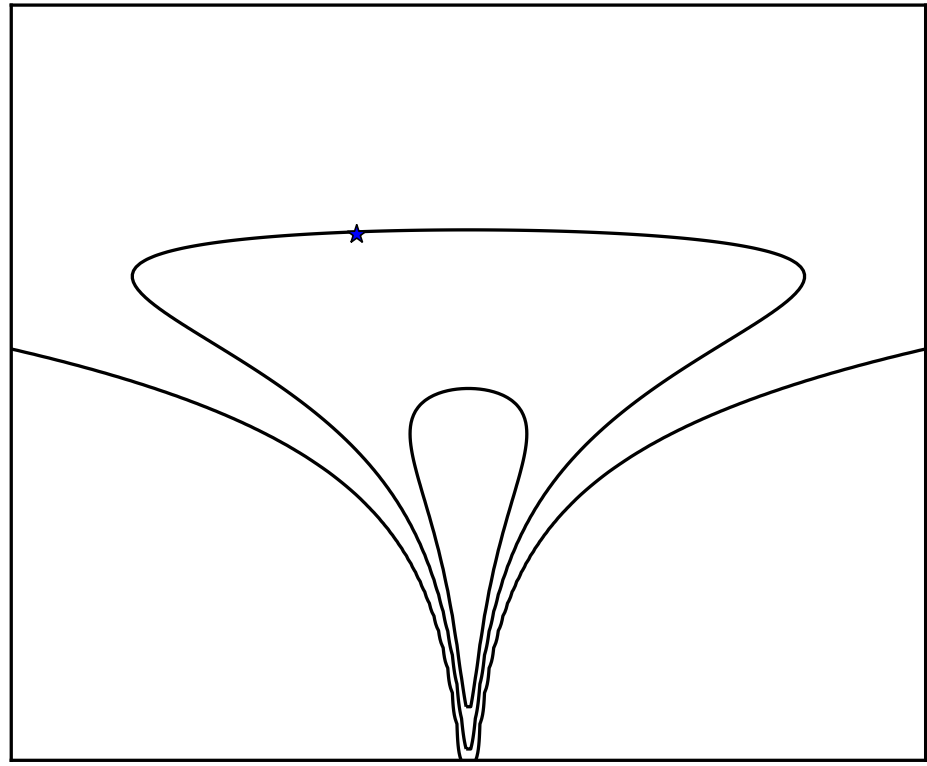

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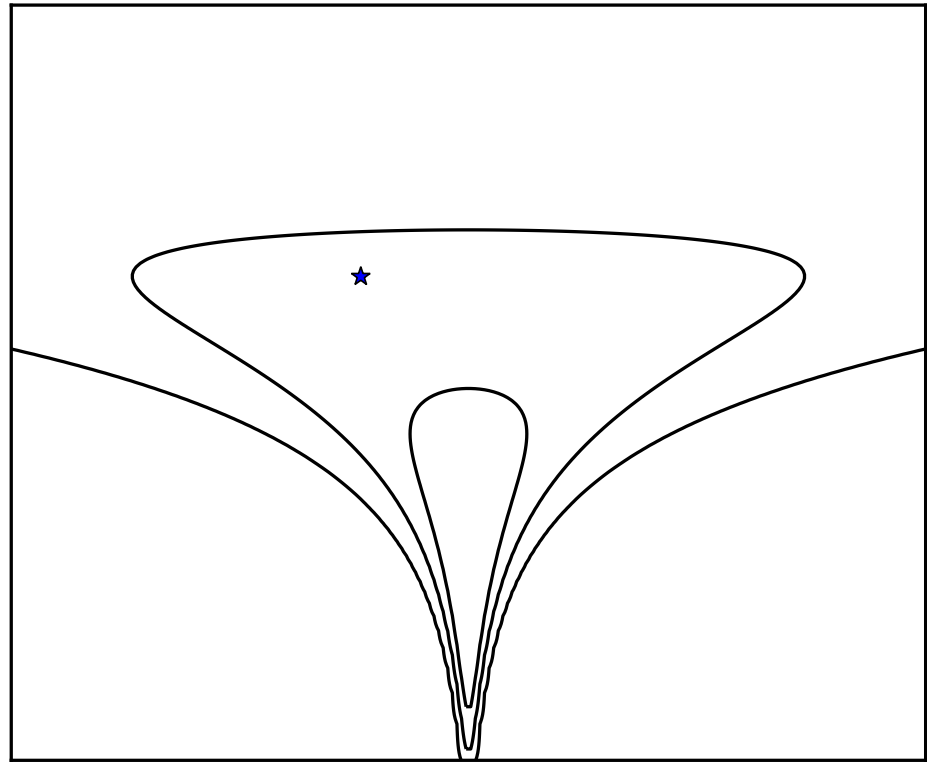

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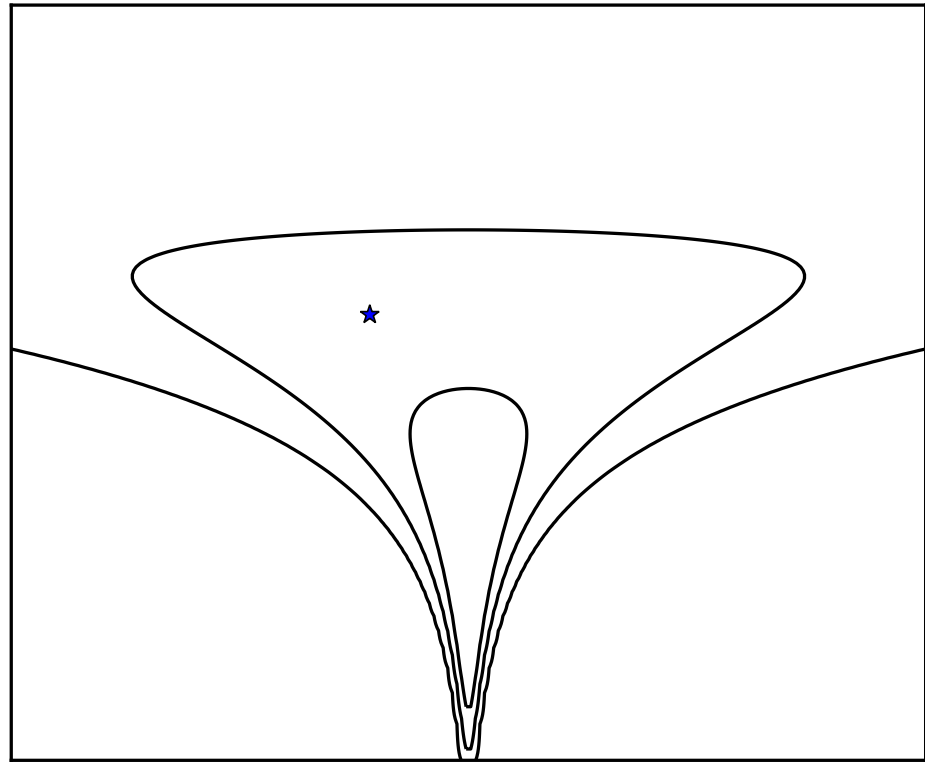

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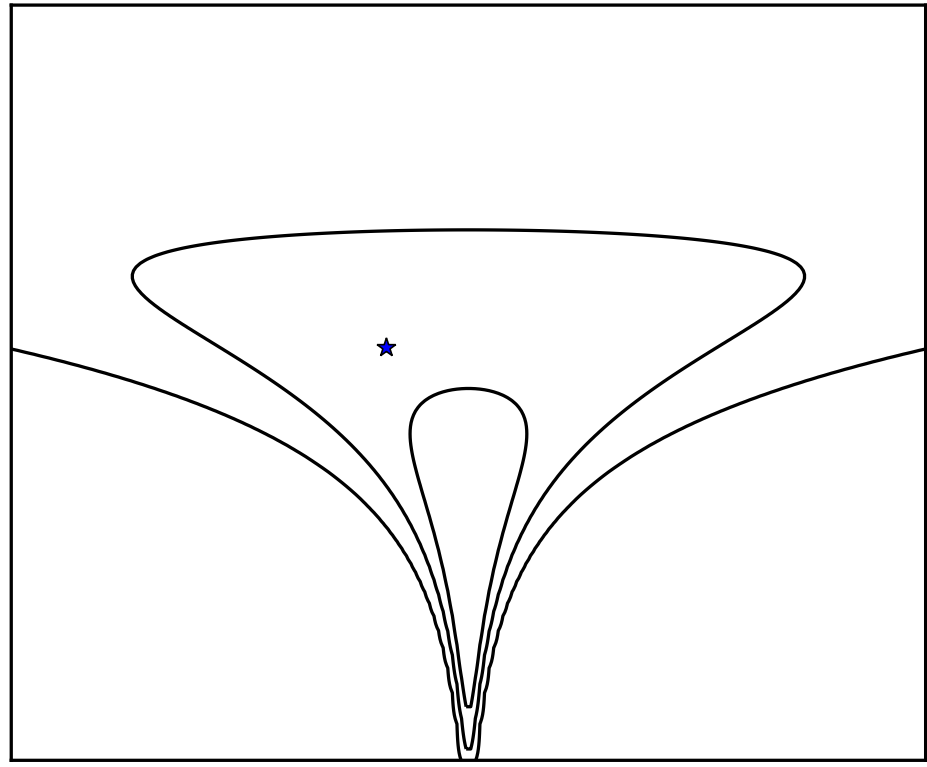

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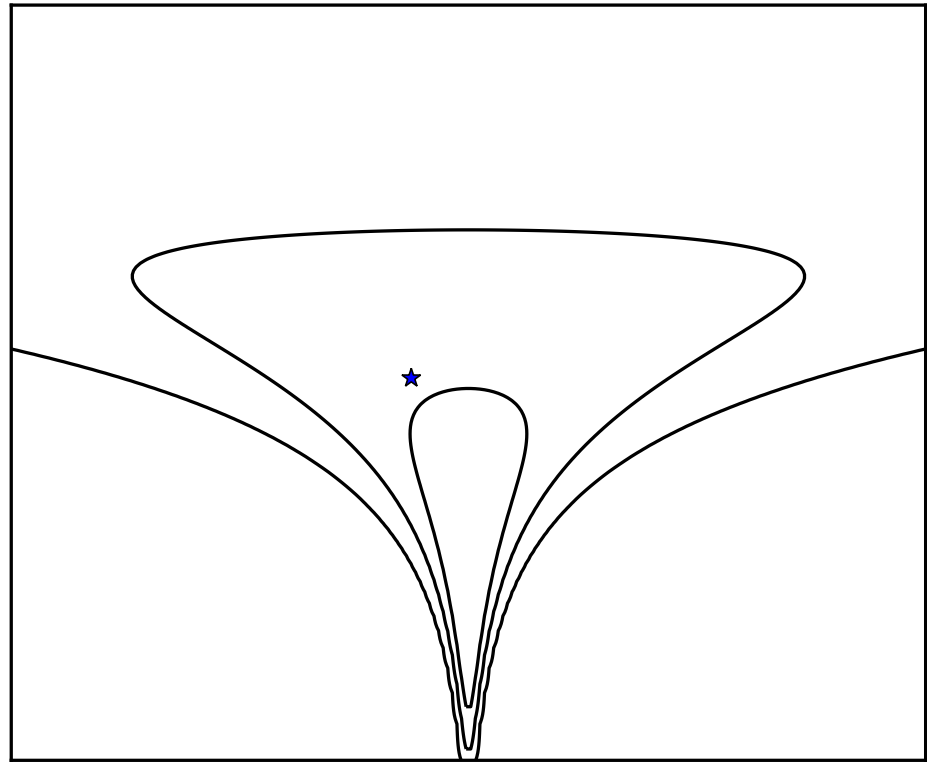

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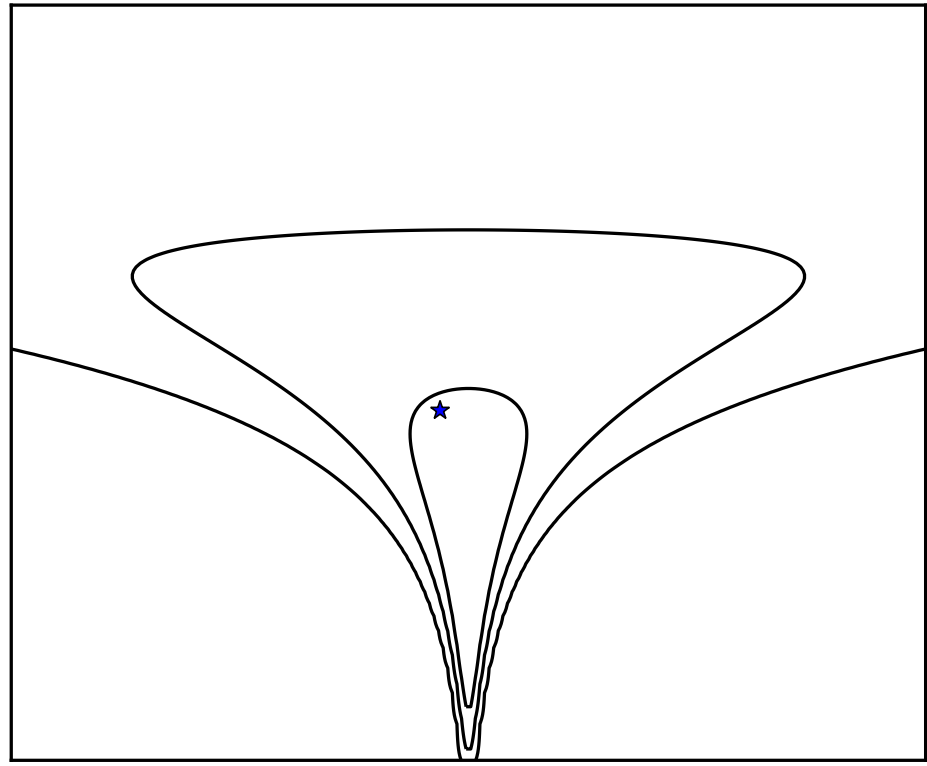

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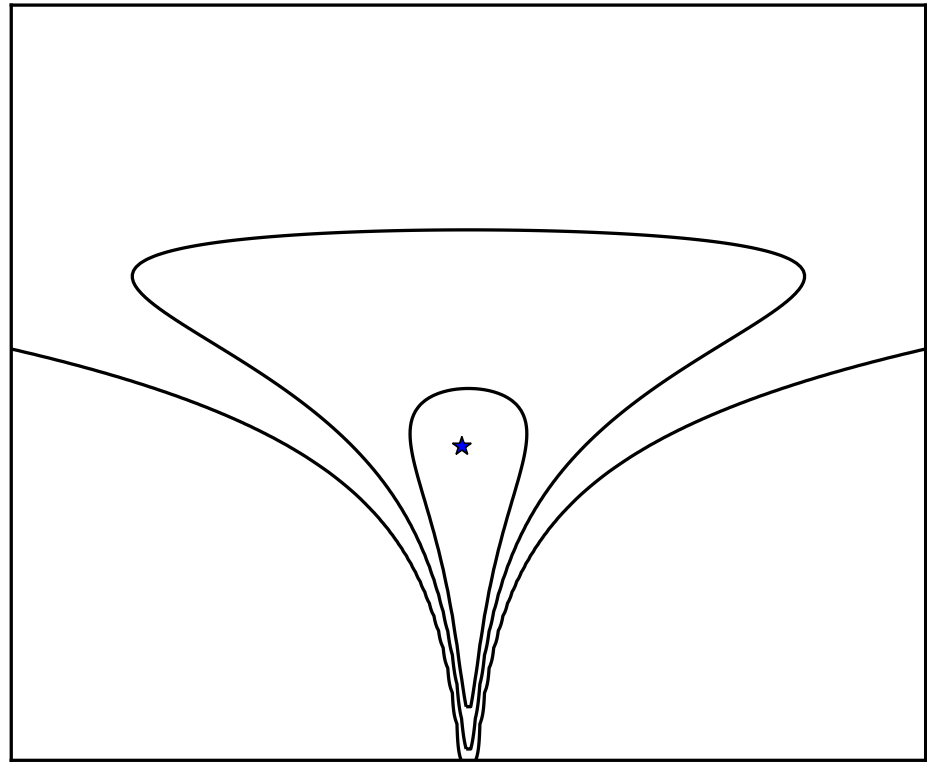

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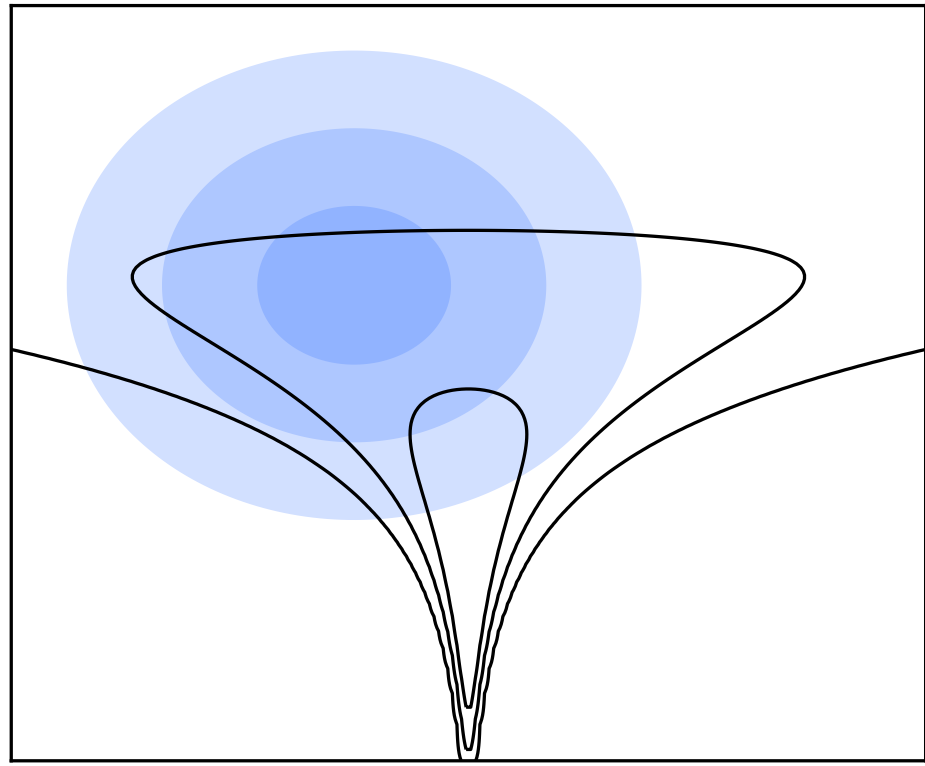

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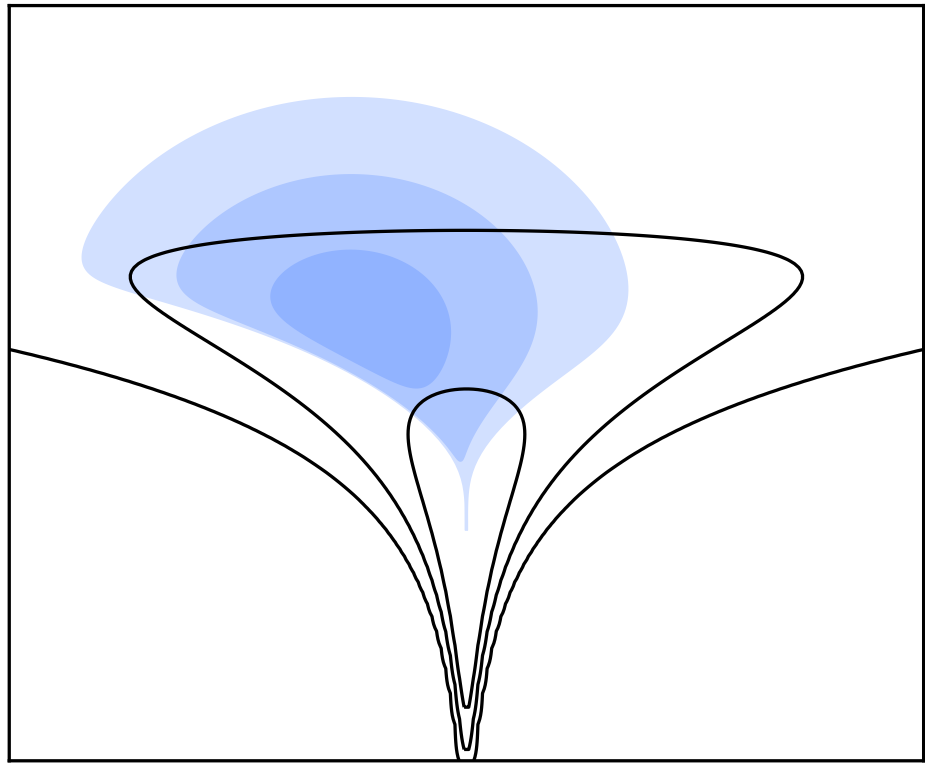

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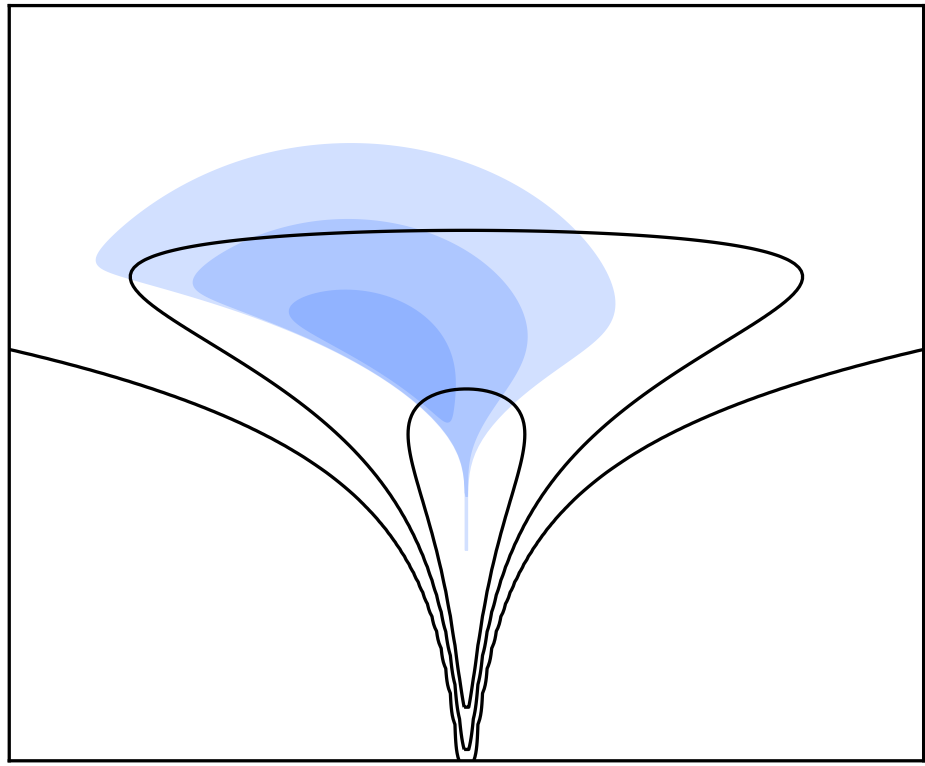

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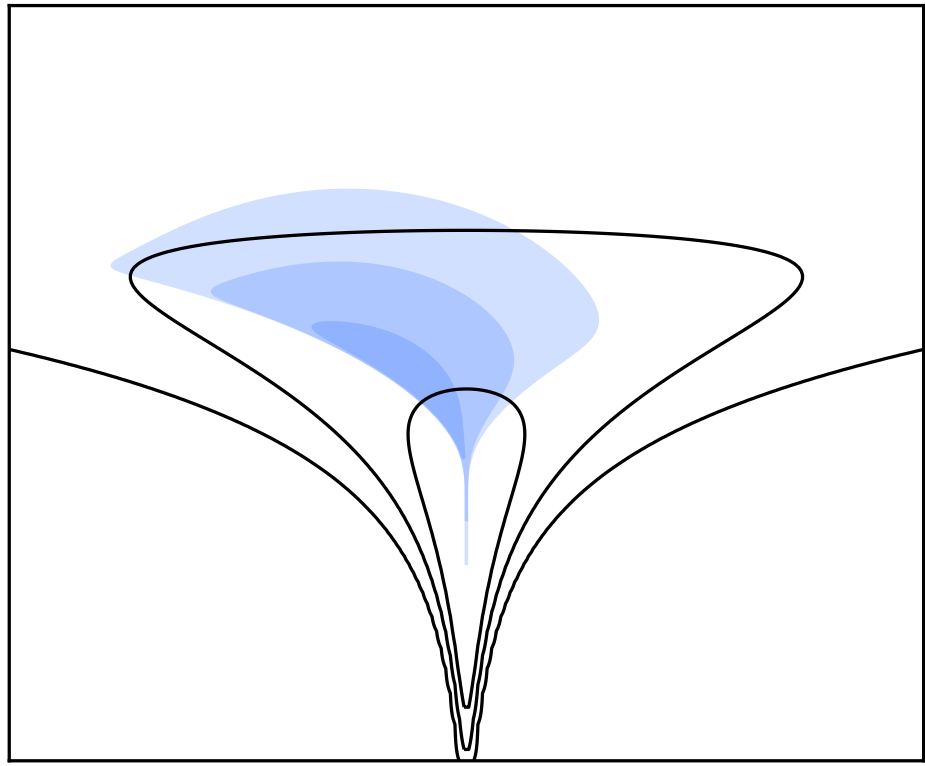

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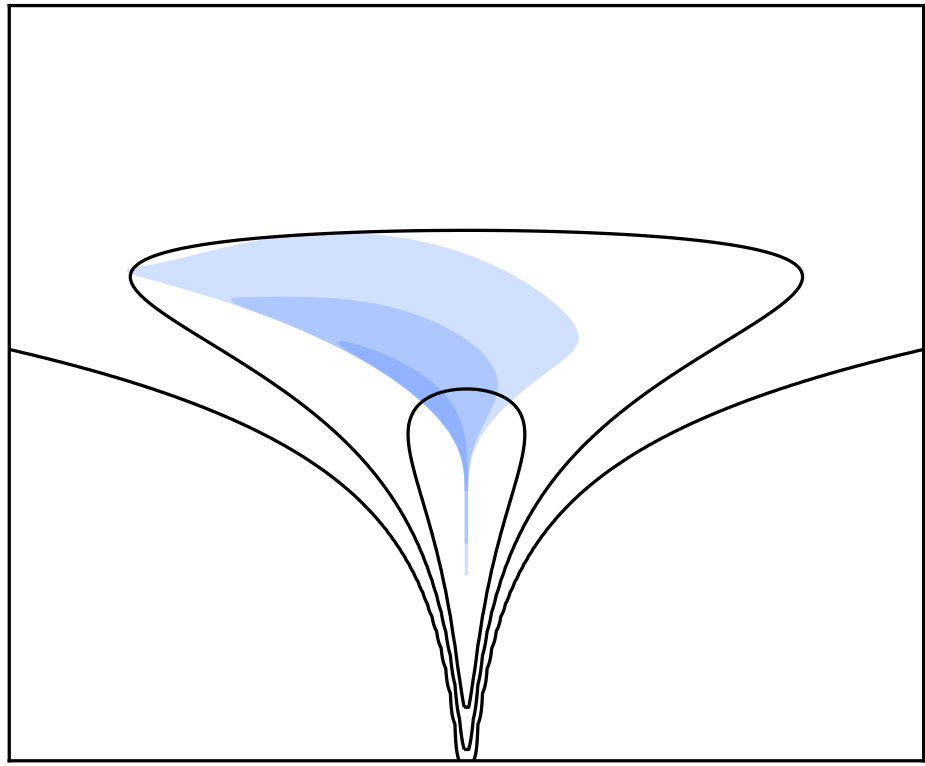

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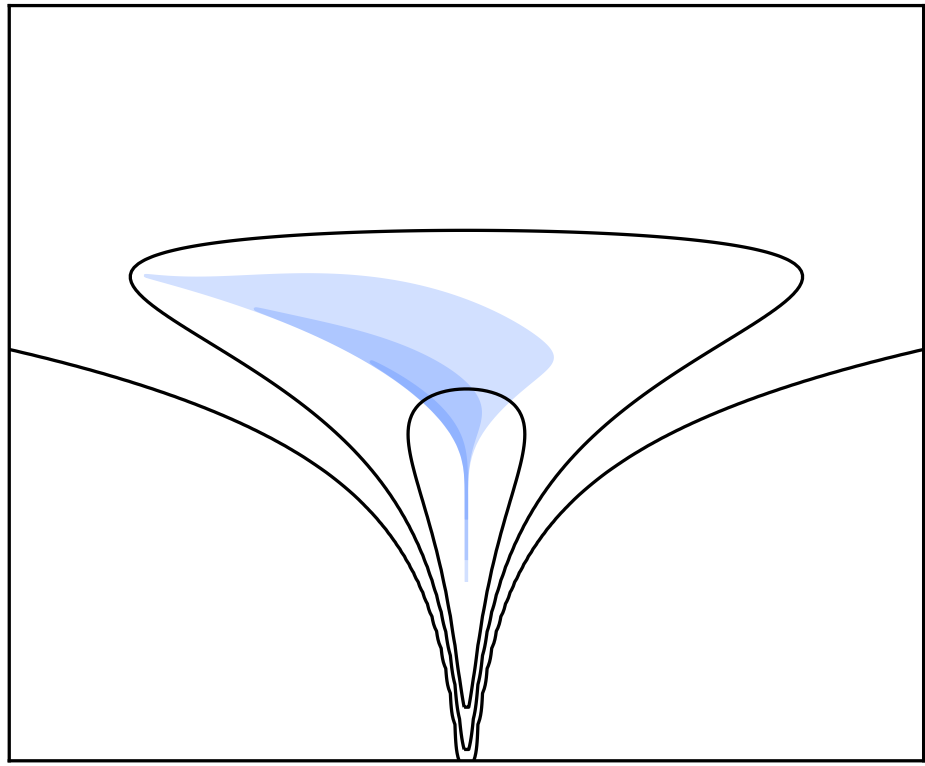

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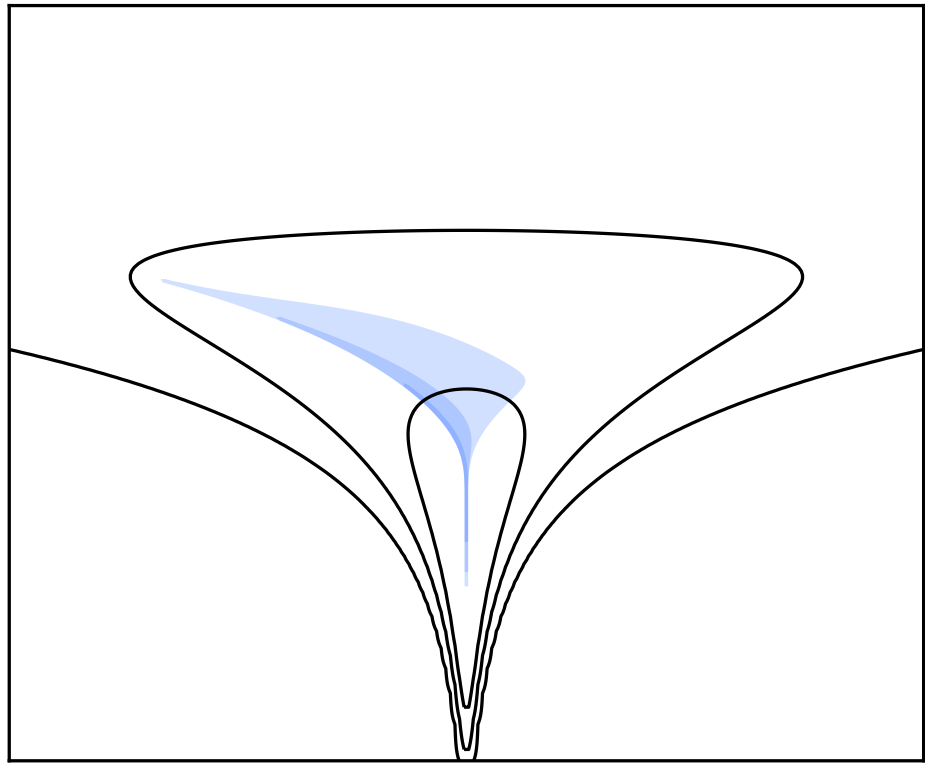

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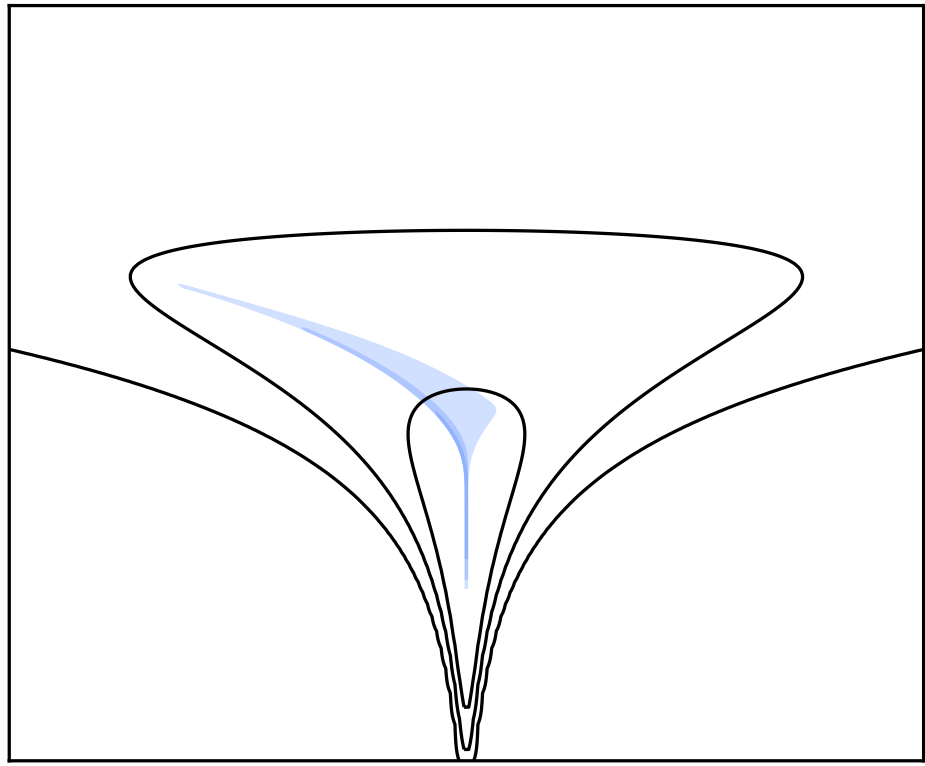

Main Idea

- What about the implicit distribution of parameters after optimizing for t steps?
- Starts as a bad approximation (prior dist)
- Ends as a bad approximation (point mass)
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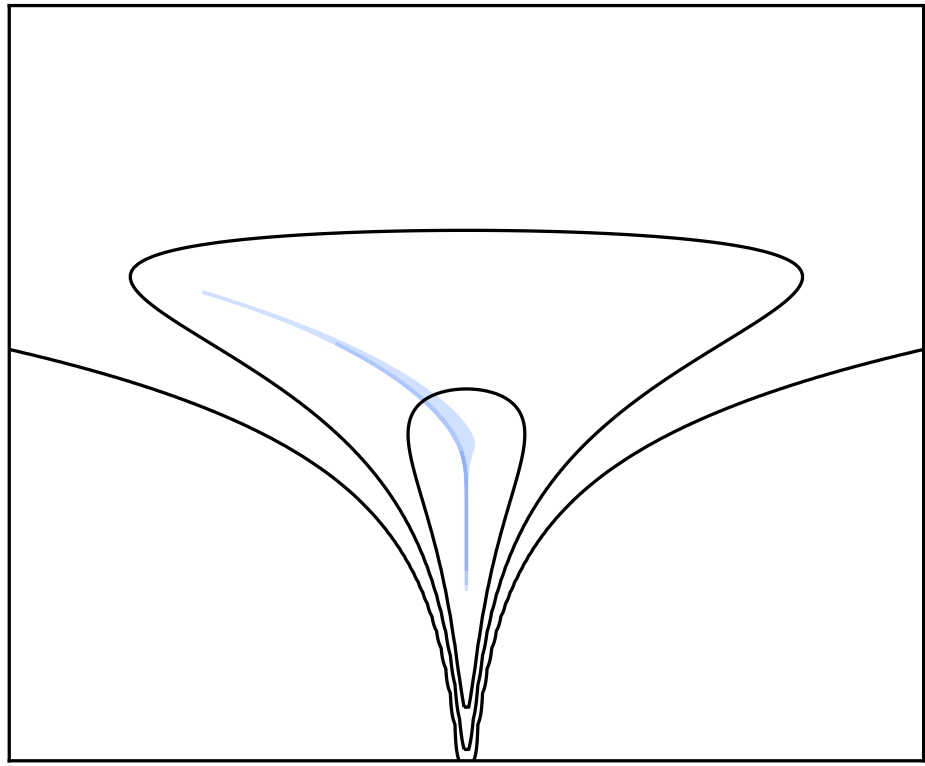

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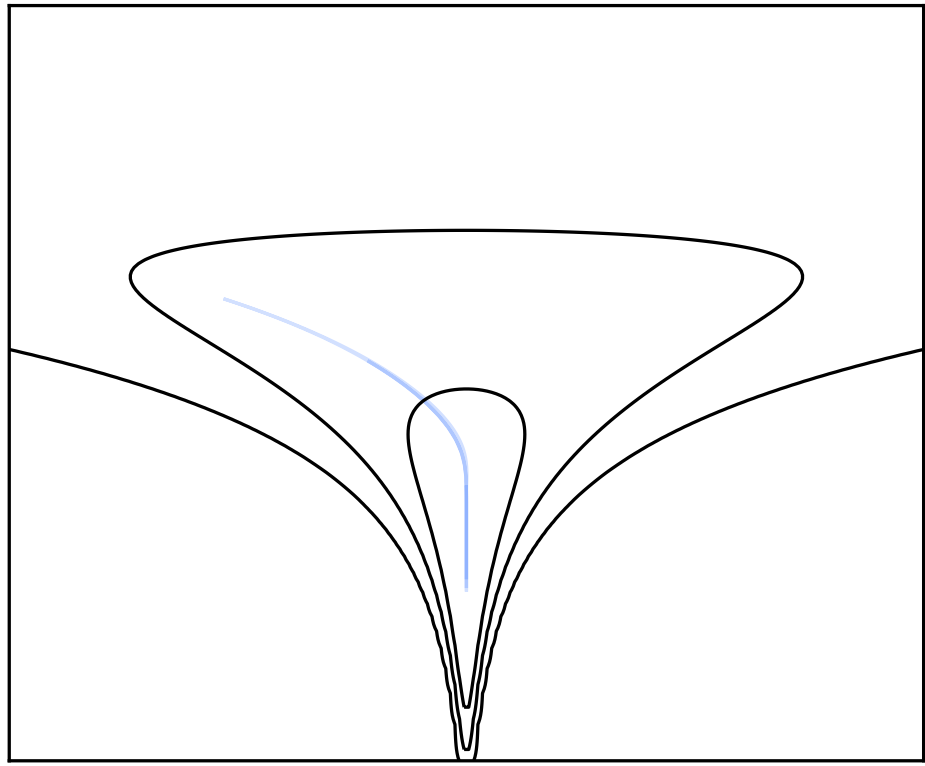

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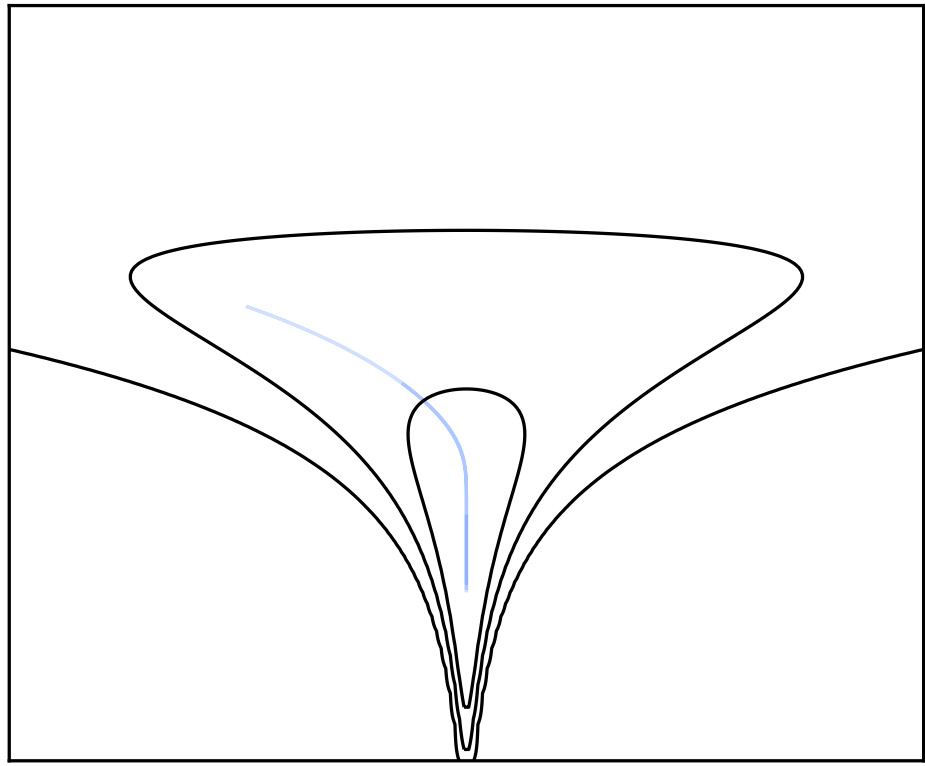
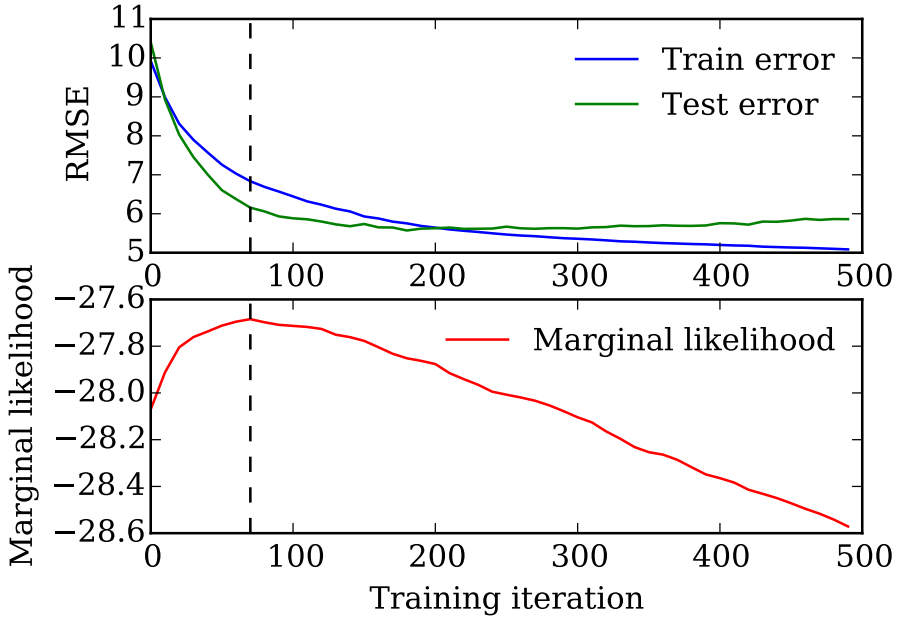


Cross Validation vs Marginal Likelihood

- What if we could evaluate marginal likelihood of implicit distribution?
- Currently, hyperparameters chosen by cross-validation
- Could choose model and learning hypers to maximize marginal likelihood
- No need for validation set

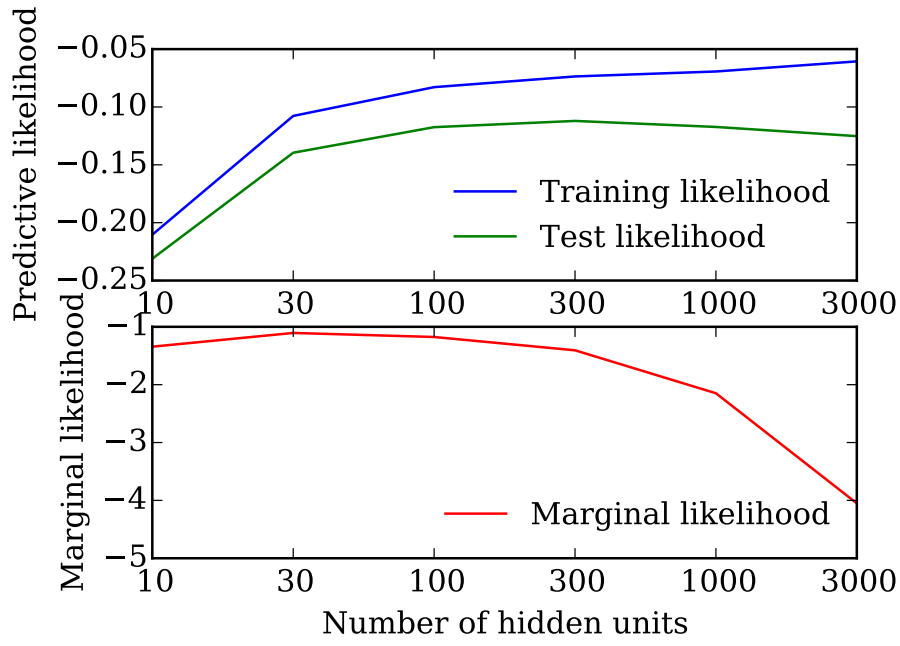
Experiments

- Early stopping
- Top: Training and test-set error on the Boston housing dataset.
- Bottom: Stochastic gradient descent marginal likelihood estimates.



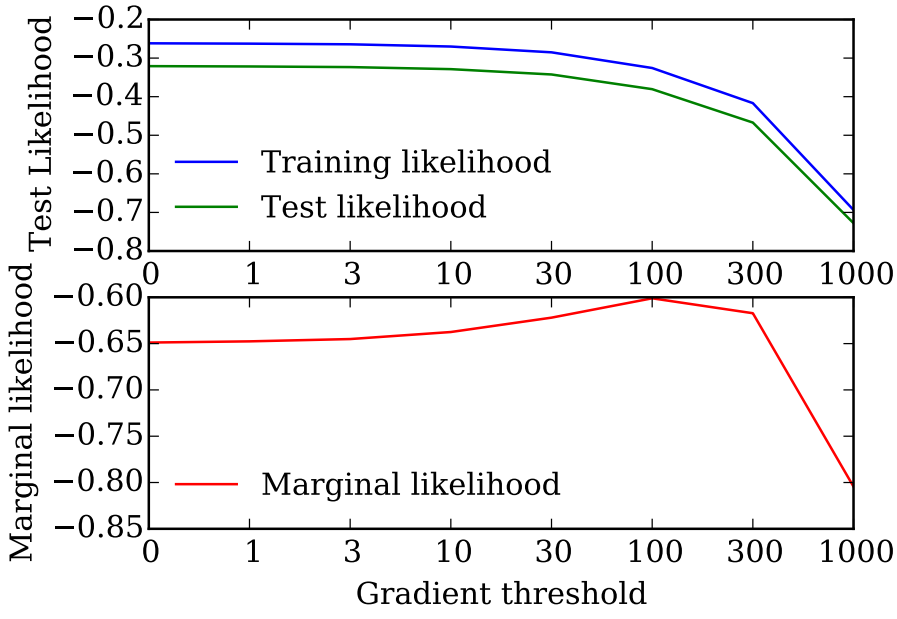
Experiments

- Choosing the number of hidden units
- Top: Training and test-set likelihood as a function of the number of hidden units in the first layer of a neural network.
- Bottom: Stochastic gradient descent marginal likelihood estimates.
- Side result: Looks like inter-sample variance is low, surprisngly!



Experiments

- Choosing the number of hidden units
- Top: Training and test-set likelihood as a function of the gradient threshold.
- Marginal likelihood as a function of the gradient threshold. A gradient threshold of zero corresponds to standard SGD.



Main Takeaways

- Optimization with random starts implies nonparametric intermediate distributions
- Can estimate lower bound on model evidence during optimization using minibatches