Bi-Level Path Following for Cross Validated Solution of Kernel Quantile Regression

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Predictive modeling

- We are given a learning $\{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, with $\mathbf{x}_i \in \mathbb{R}^p$ and $y_i \in \mathbb{R}$ (or $y_i \in \{0, 1\}$), drawn i.i.d from $p(X, Y)$.

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  - Classification: estimate $f(\mathbf{x}) = P(Y = 1|X = \mathbf{x})$.
  - Regression: estimate $f(\mathbf{x}) = E(Y|X = \mathbf{x})$.
- What happens if we want to learn more about $P(Y|X)$ than just these expectations?

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- Define a loss function $L(y, f(\mathbf{x}))$ measuring how well $f(\mathbf{x})$ estimates y.
- Define a model complexity penalty $J(f)$
- Now let the optimal model $\hat{f}(\lambda)$ solve:

$$\min_{f \in \mathcal{F}} \sum_{i=1}^{n} L(y_i, f(\mathbf{x}_i)) + \lambda J(f)$$

Example: Kernel machines

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Can be solved efficiently because of the Representer Theorem.

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The optimal solution has the form: $\hat{f}(\lambda)(\mathbf{x}) = \sum_{j=1}^{n} \hat{\alpha}_j K(\mathbf{x}, \mathbf{x}_j)$.

The corresponding penalty is: $\|f\|^2_{\mathcal{H}_K} = \alpha^T K \alpha$.

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  - Using hold-out data (cross validation).

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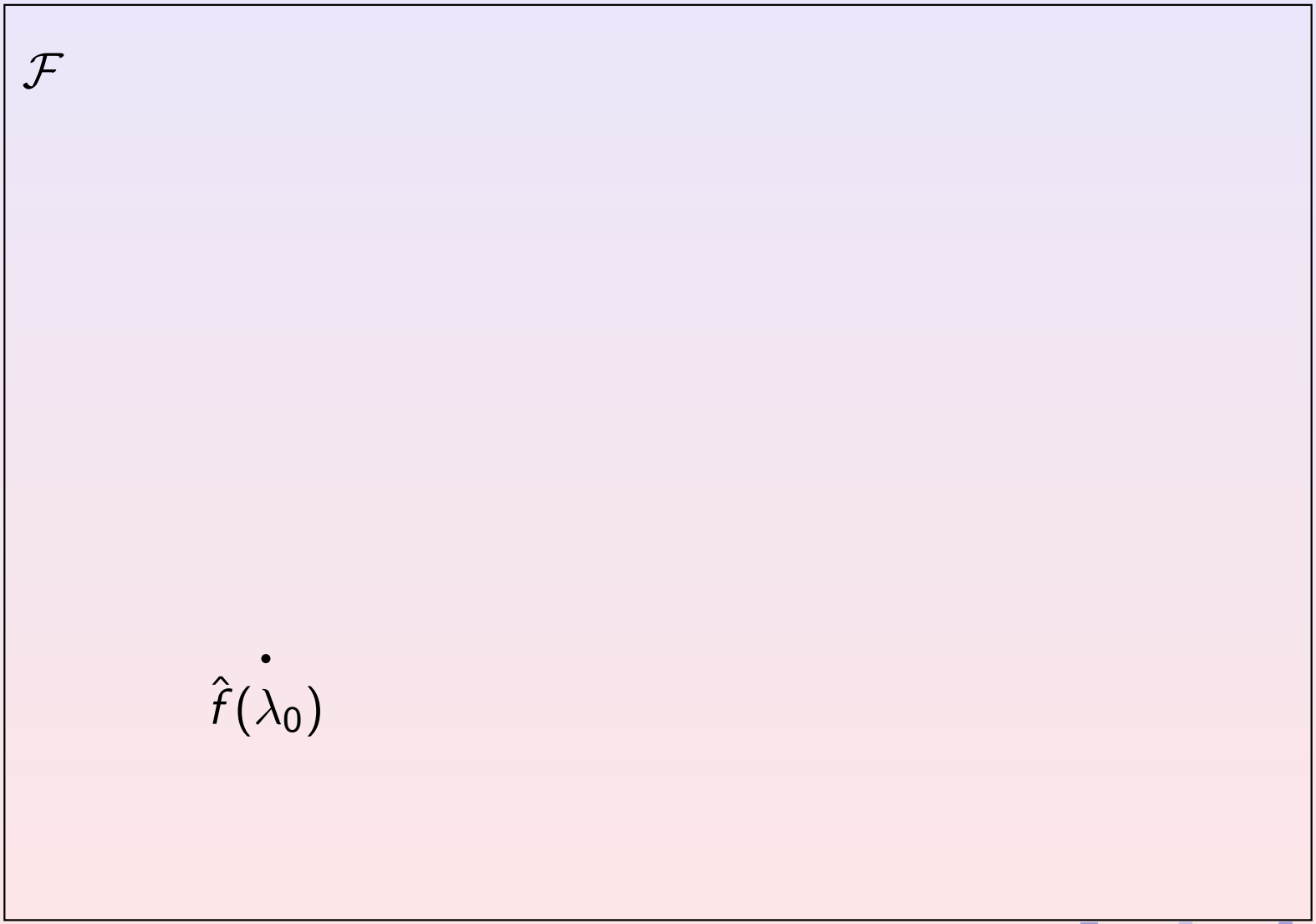
- This gives rise to homotopy methods for generating the whole set of solutions $\{\hat{f}(\lambda) : 0 \leq \lambda \leq \infty\}$ incrementally and efficiently.
- Such algorithms have been developed, among others, for:
  - Lasso (Efron et al. 2004)
  - Kernel SVM (Hastie et al. 2004)
  - Kernel quantile regression (Li et al. 2007)

Regularization path schematic



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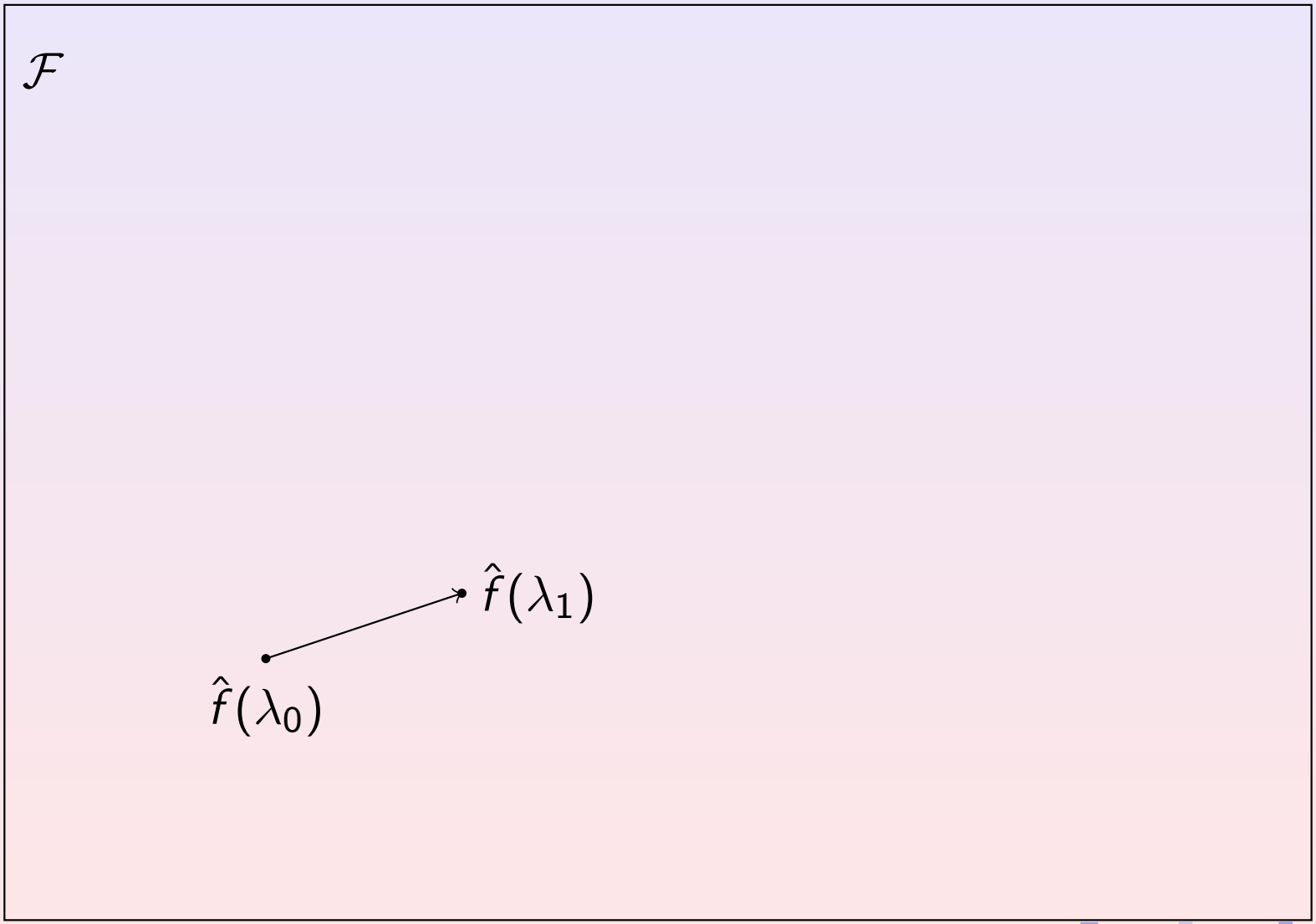

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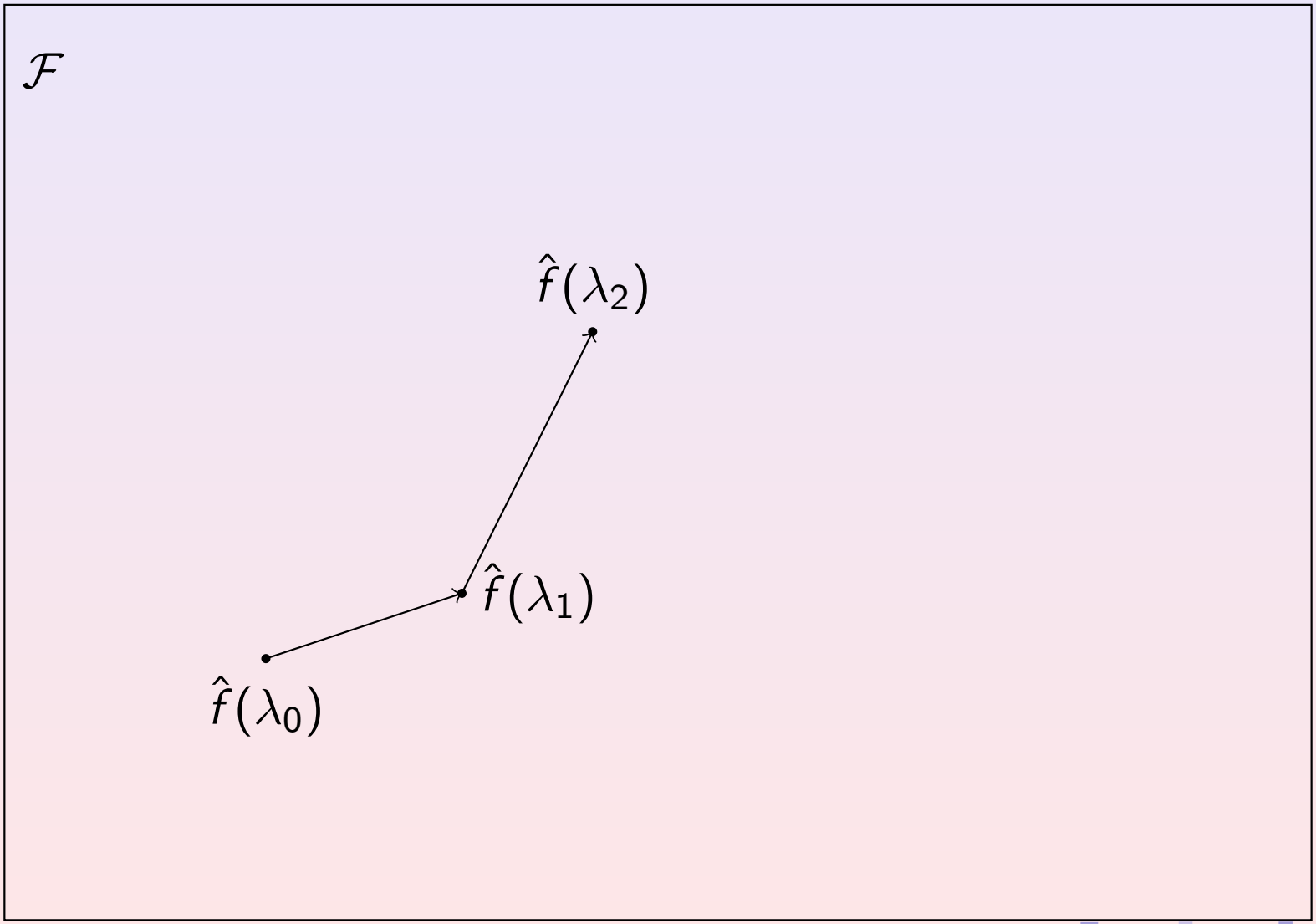

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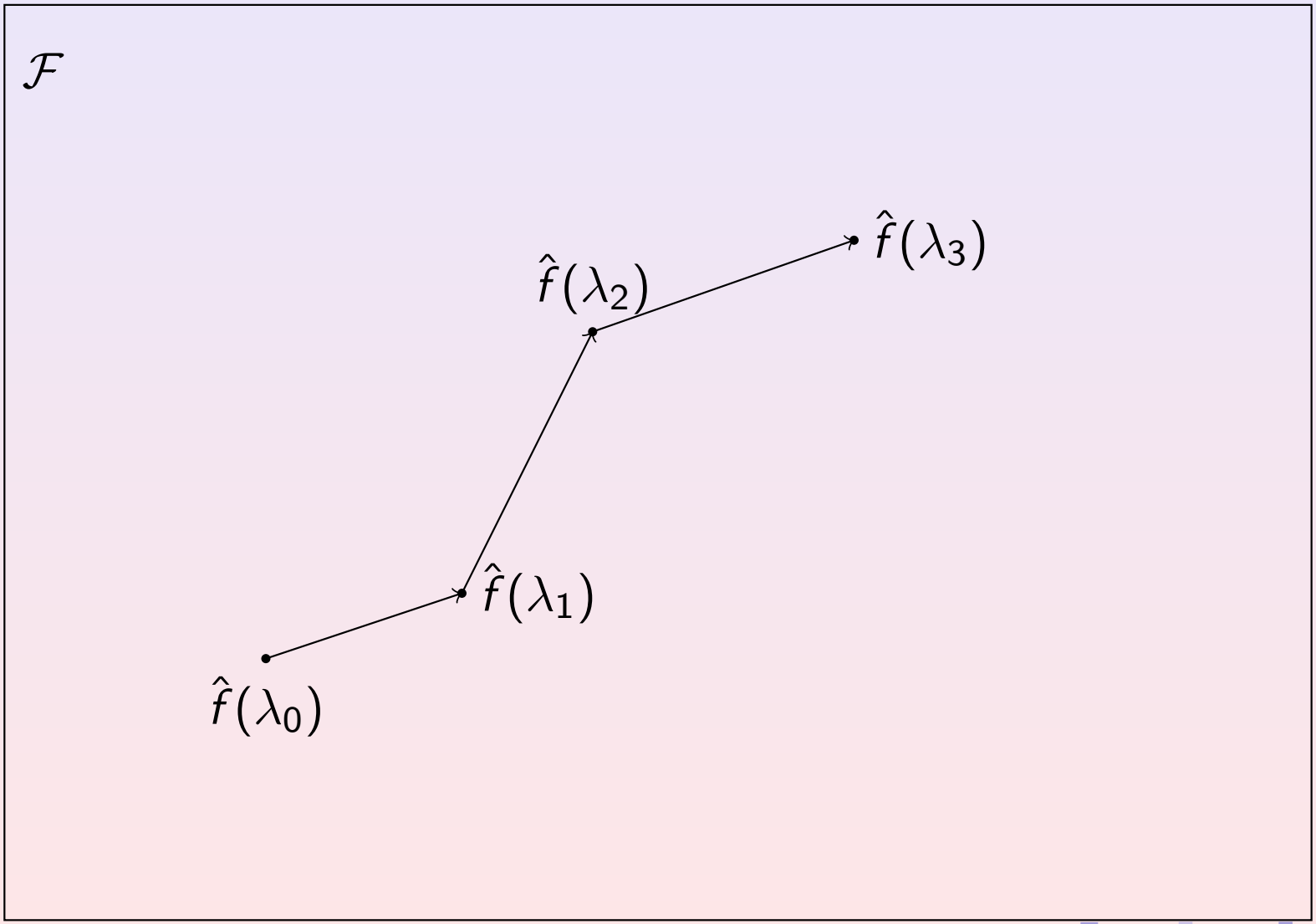

Cross validation as a bi-level programming problem

Assume we want to select a value for λ by comparing the Loss L of $\hat{f}(\lambda)$ for different values of λ on a holdout sample $\{(\tilde{\mathbf{x}}_1, \tilde{y}_1), ..., (\tilde{\mathbf{x}}_N, \tilde{y}_N)\}$:

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  - Naive solution: find the regularization path, and try many values of $\hat{f}(\lambda)$ on the holdout data.
  - Alternative: find a way to optimize the holdout loss efficiently.
  - Problem: even if the inner problem is convex for every λ, the bi-level problem is not convex!

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If $Y \in \mathbb{R}$, we may want to learn about $P(Y|X = \mathbf{x})$ through its quantiles $f_\tau(\mathbf{x})$ defined by: $P(Y \leq f_\tau(\mathbf{x})|X = \mathbf{x}) = \tau$.

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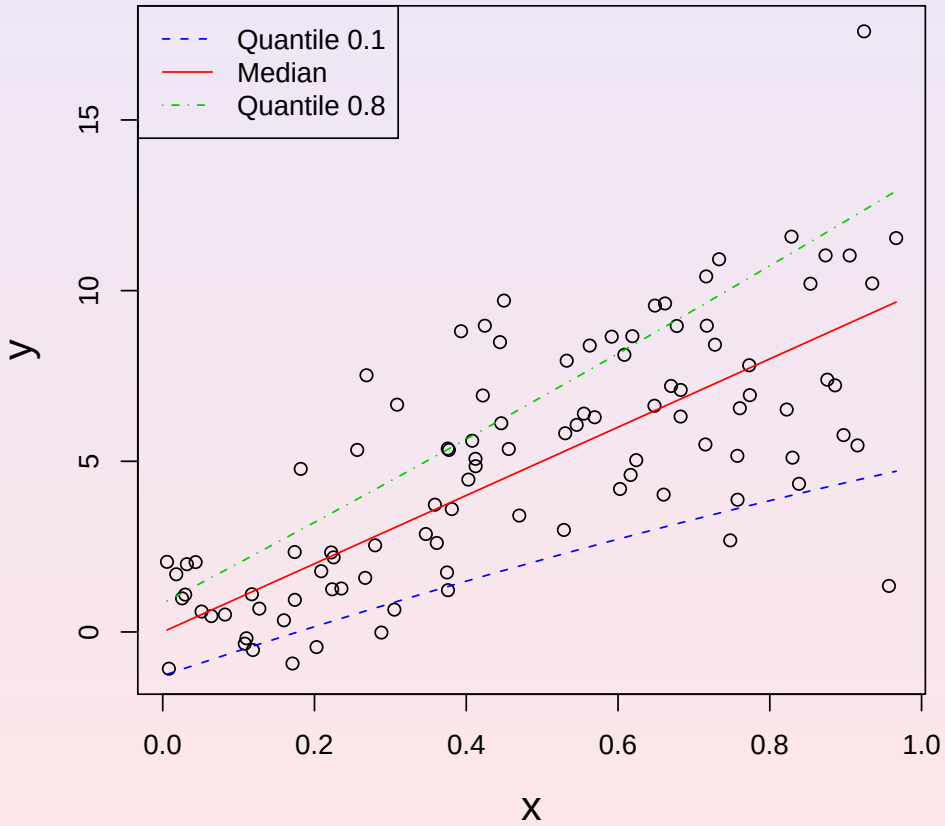
In simple cases, such as the classic model $Y = f(\mathbf{x}) + \epsilon$, ϵ i.i.d, modeling $f_\tau(\mathbf{x})$ for multiple values of τ is redundant.

Non-uniform noise ⇒ Non parallel quantiles

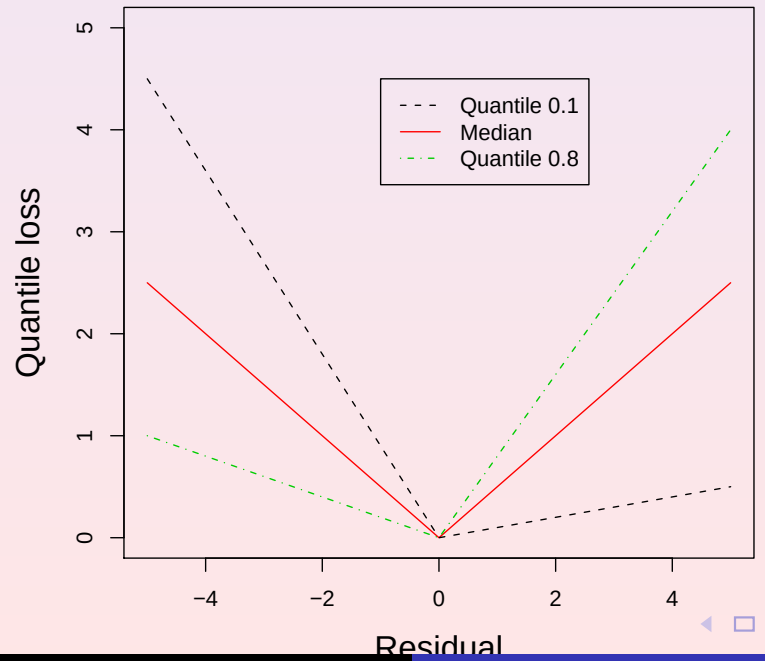


Quantile regression

The quantile loss function is:

$$L_\tau(r) = \begin{cases} r\tau & r \geq 0 \\ -r(1-\tau) & r < 0 \end{cases}$$

(where $r = y - f(\mathbf{x})$ is the residual)



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We are going to concentrate on the kernel quantile regression (KQR) version:

$$\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} L_\tau(y_i, -\sum_{j=1}^{n} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)) + \lambda \alpha^{\mathsf{T}} K \alpha$$

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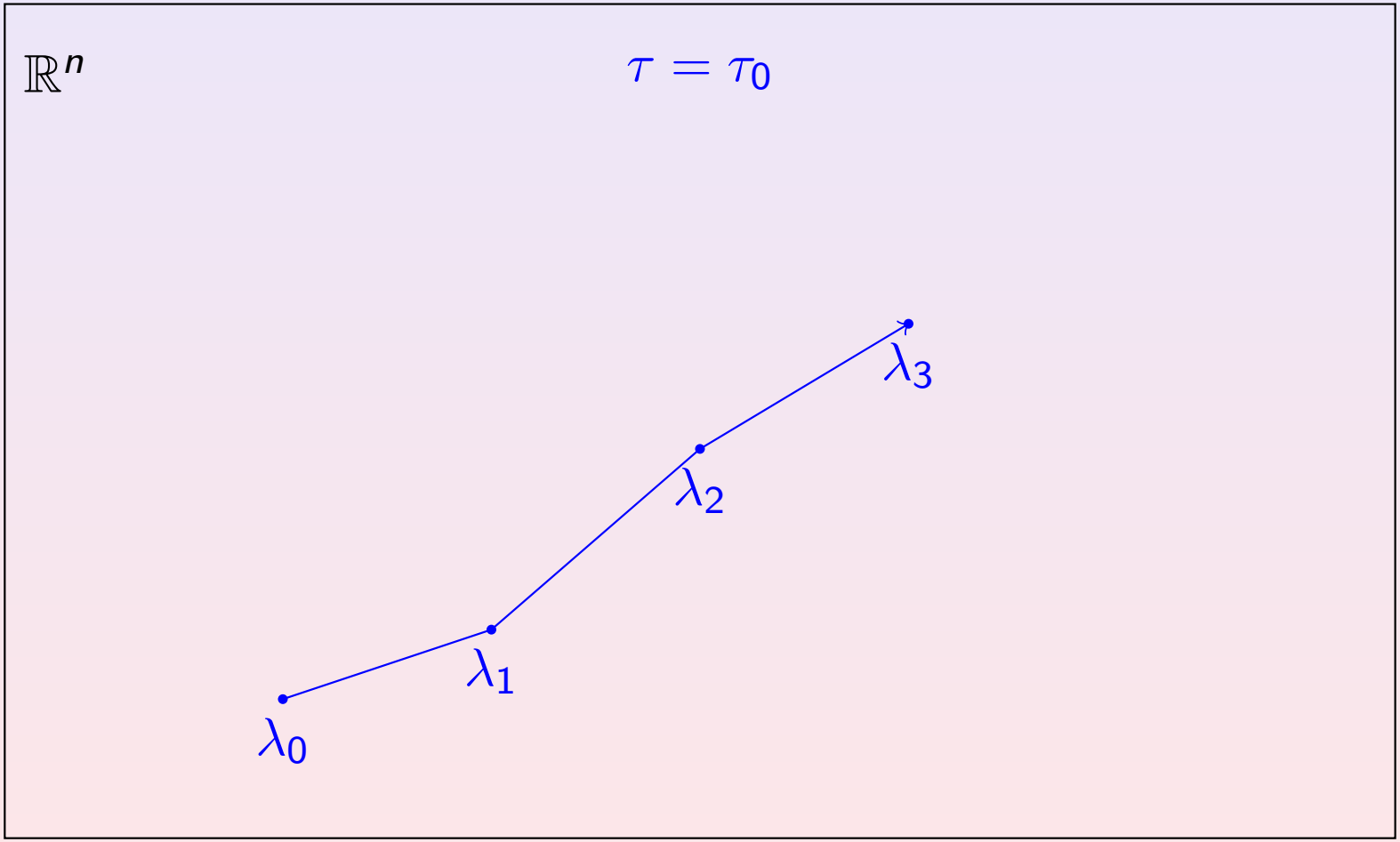
We would typically want to solve a bi-level problem to select an optimal regularizer for every quantile:

$$\lambda^*(\tau) = \arg\min_{\lambda} \sum_{i=1}^{N} L_\tau(\tilde{y}_i - \hat{f}(\lambda)(\tilde{\mathbf{x}}_i))$$

Regularization paths as τ and λ vary



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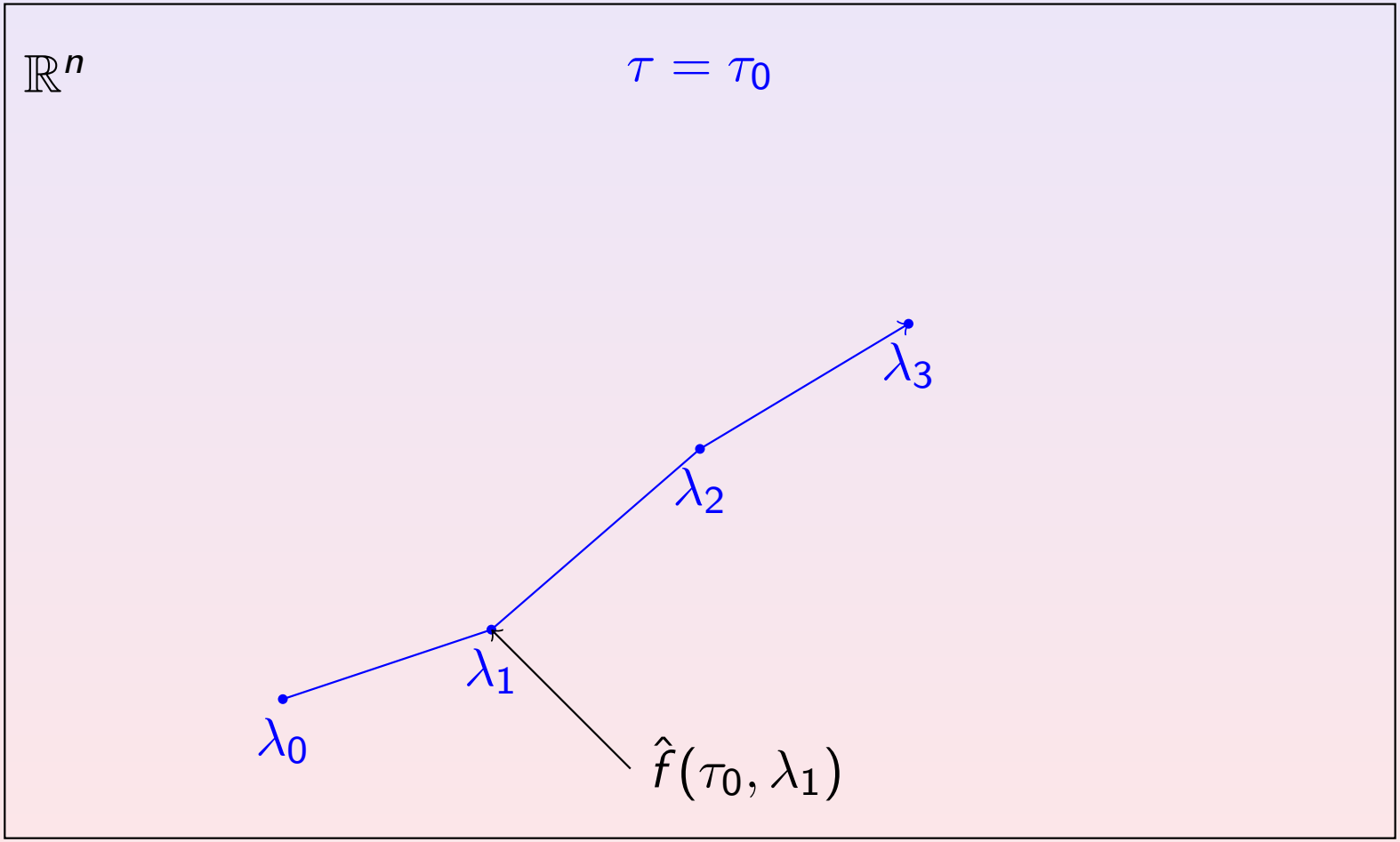

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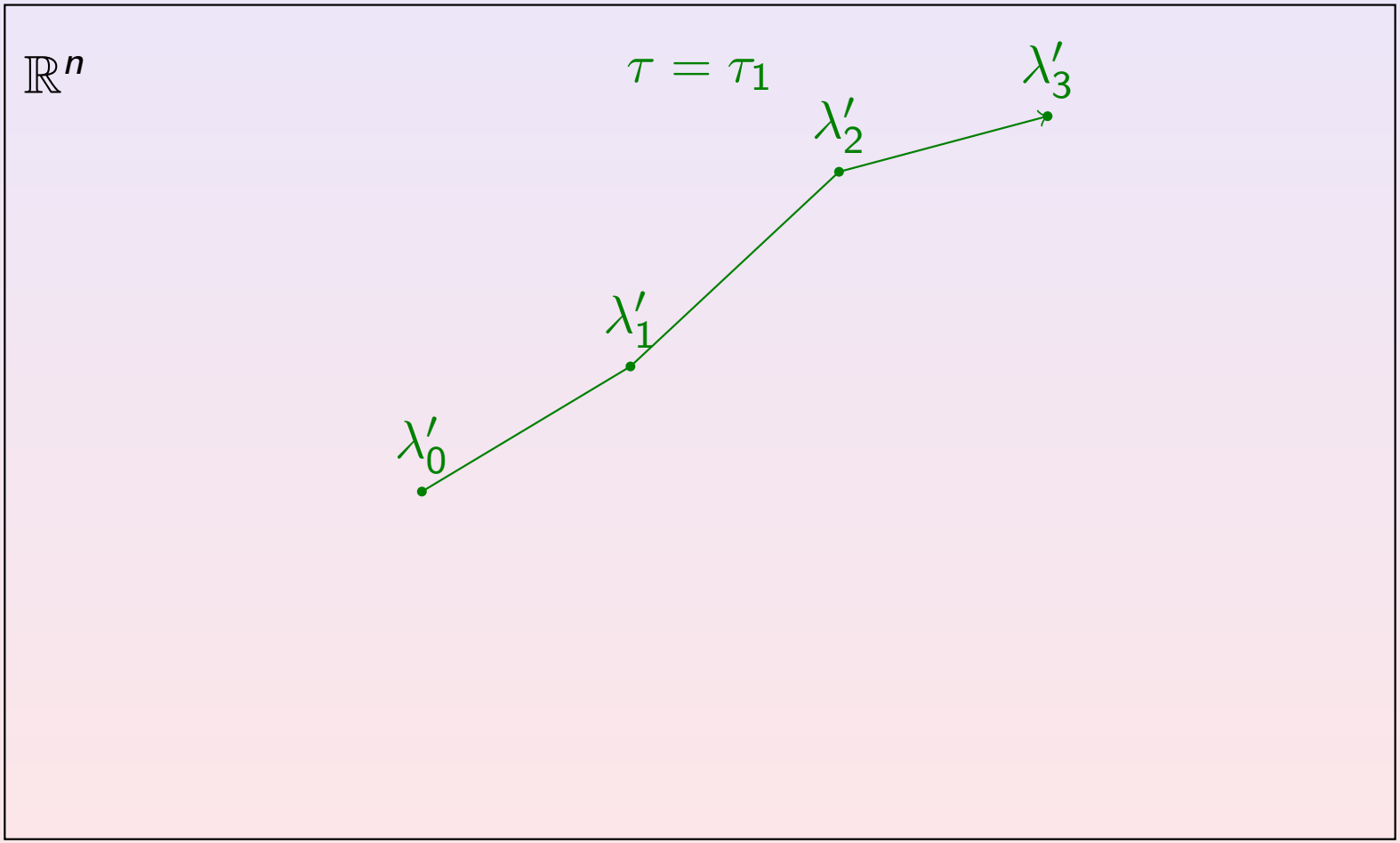

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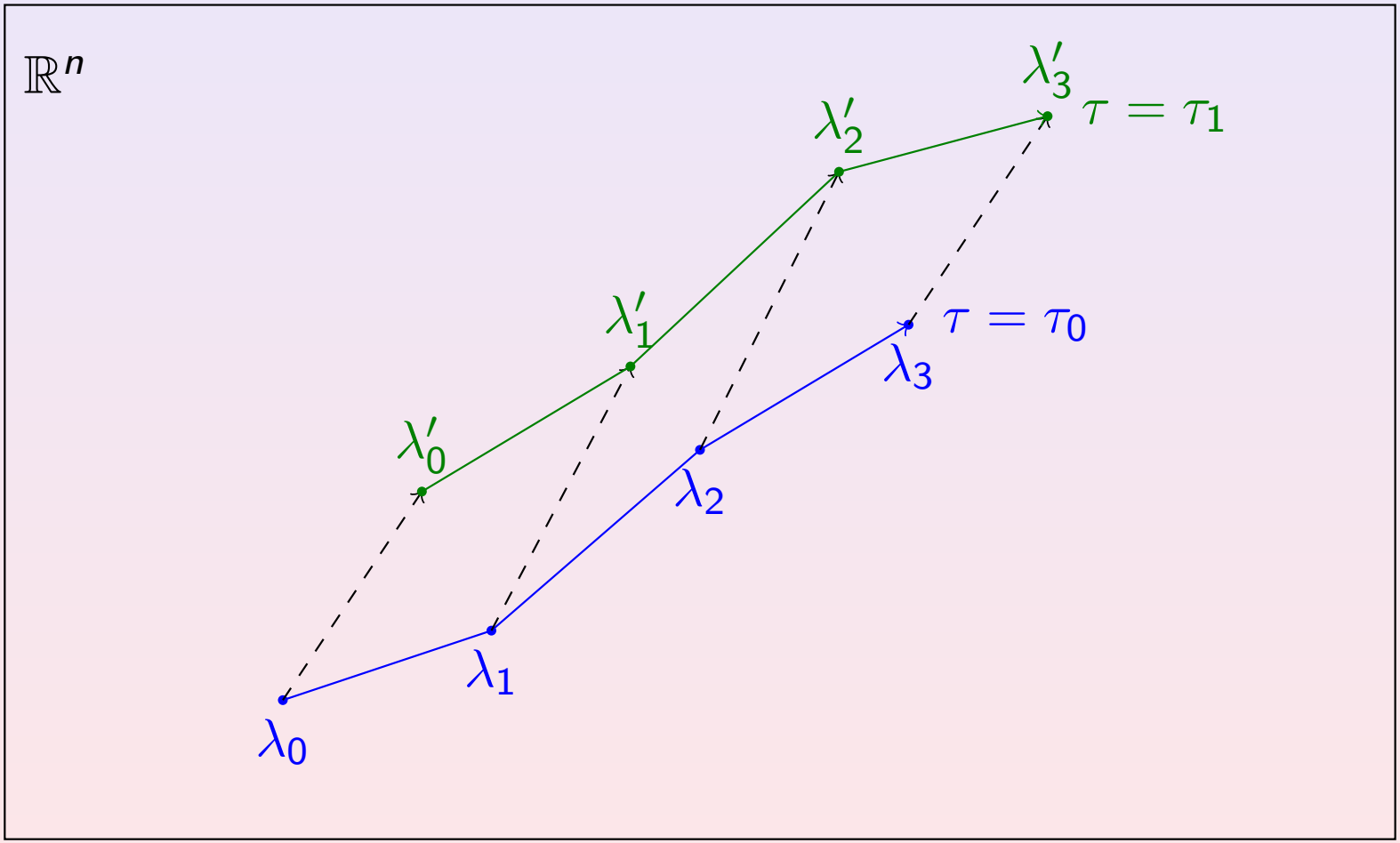

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- When each event happens, update directions of knots.

Knot evolution: some details

The KKT conditions for the KQR problem give us:

- Any knot λ_k moves linearly as τ changes.
- The regularization path at every τ can be fully described by the knots (in the appropriate representation).
- The fit at the moving knot:

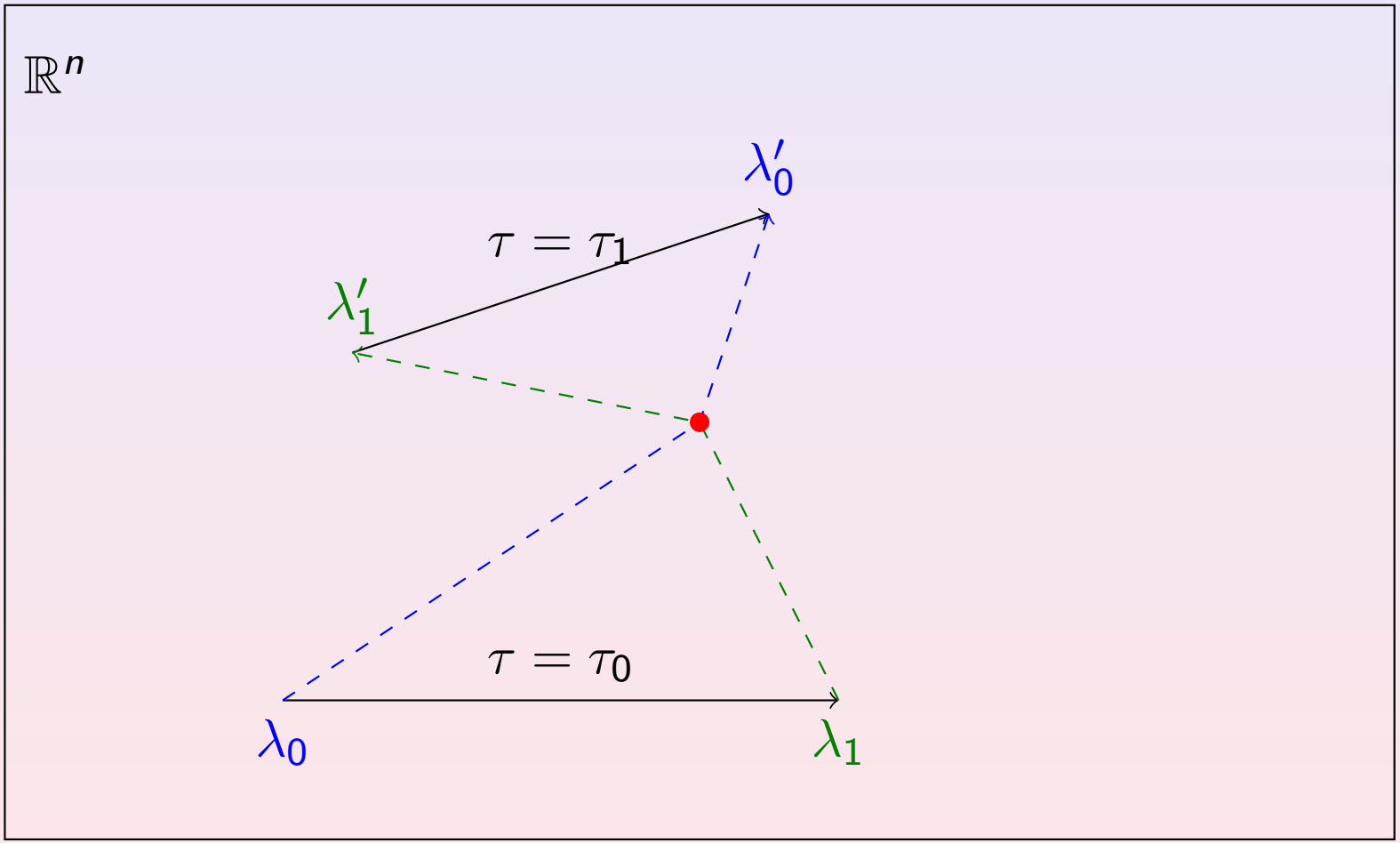
$$\hat{f}(\tau_0 + \delta, \lambda_k + c_k\delta) = \frac{1}{\lambda_k + c_k\delta}\left(\lambda_k \hat{f}(\lambda_k, \tau_0)(\mathbf{x}) + \delta h_k(\mathbf{x})\right)$$

$$h_k(\mathbf{x}) = \tilde{b}_0^k + \sum_{i \in \mathcal{E}_k - i_k} \tilde{b}_i^k K(\mathbf{x}, \mathbf{x}_i) + \sum_{i \in \mathcal{L} \cup \mathcal{R} \cup \{i_k\}} K(\mathbf{x}, \mathbf{x}_i)$$

- The direction $\tilde{\mathbf{b}}_k$ and rate c_k are determined by solving a set of linear equations:

$$\mathbf{B}^k \begin{pmatrix} \tilde{\mathbf{b}}^k \\ c_k \end{pmatrix} = \begin{pmatrix} -(|\mathcal{R}| + |\mathcal{L}| + 1) \\ -\mathbf{s}_{\mathcal{E}_k} \end{pmatrix}$$

Knot crossing example



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- However, optimal bi-level solutions can only occur in non-differentiability points of cross-validated objective (candidates):
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- As τ changes they stay in the same candidate for a while, then jump to another.

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- However, optimal bi-level solutions can only occur in non-differentiability points of cross-validated objective (candidates):
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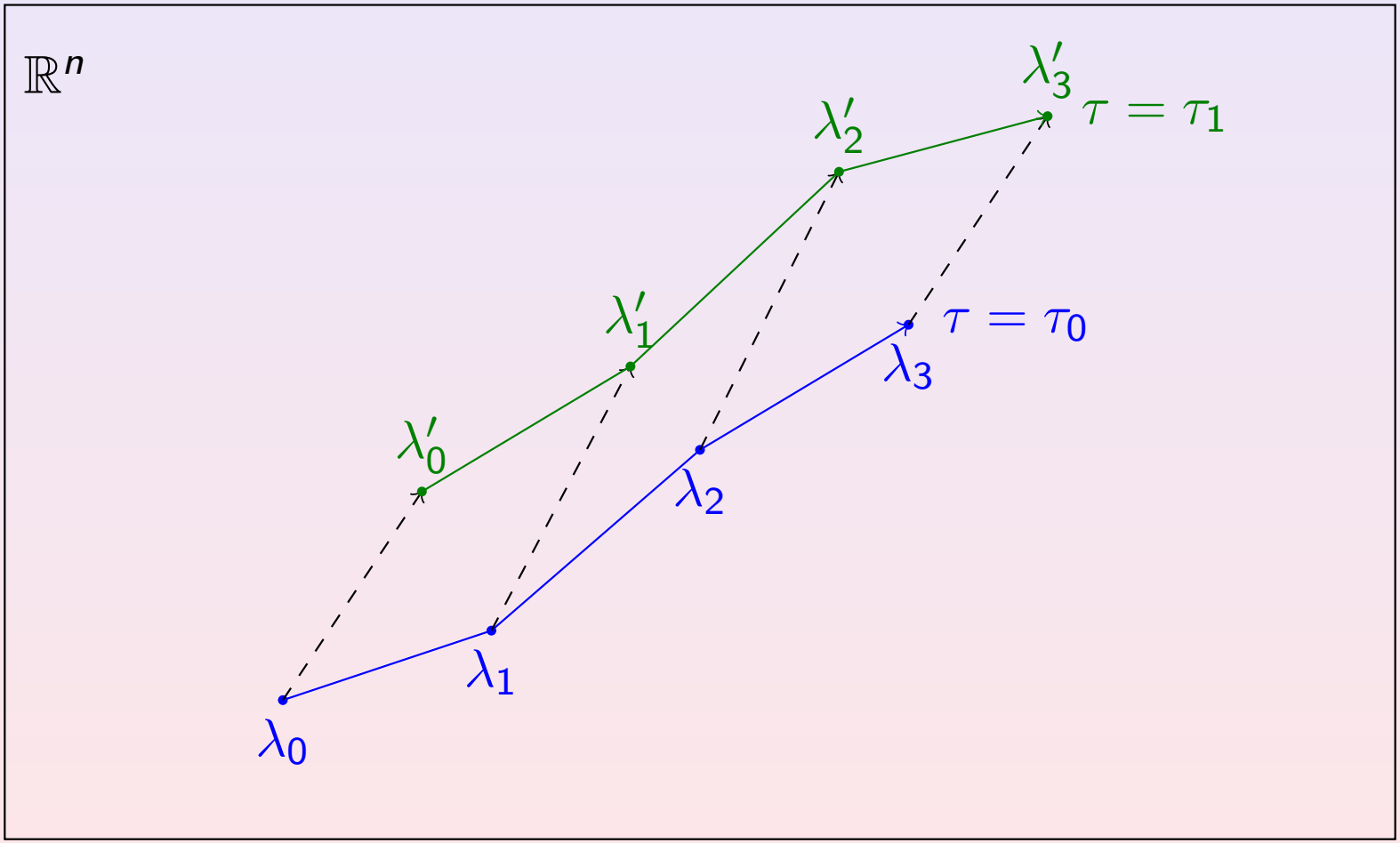
Evolution of bi-level solution



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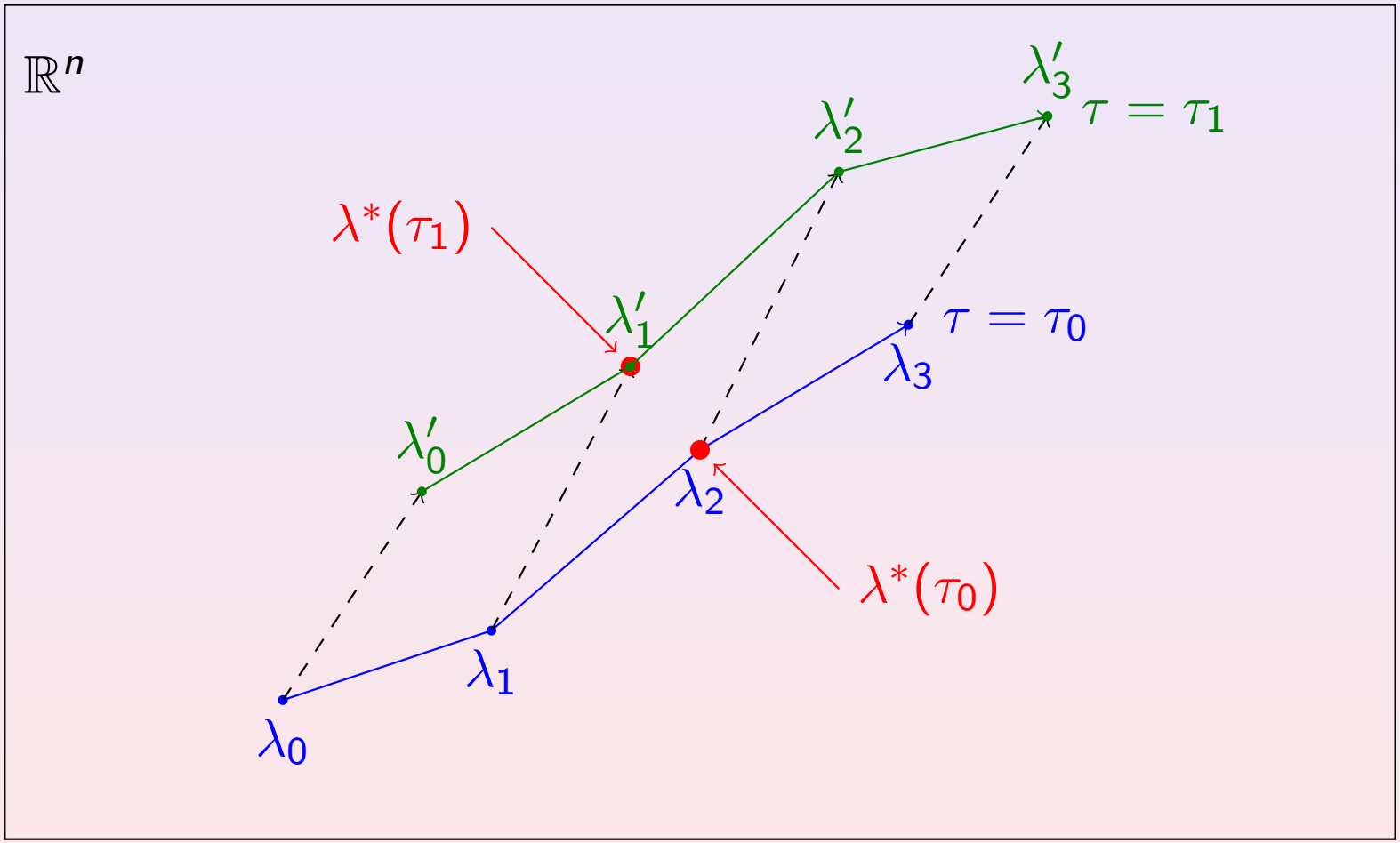

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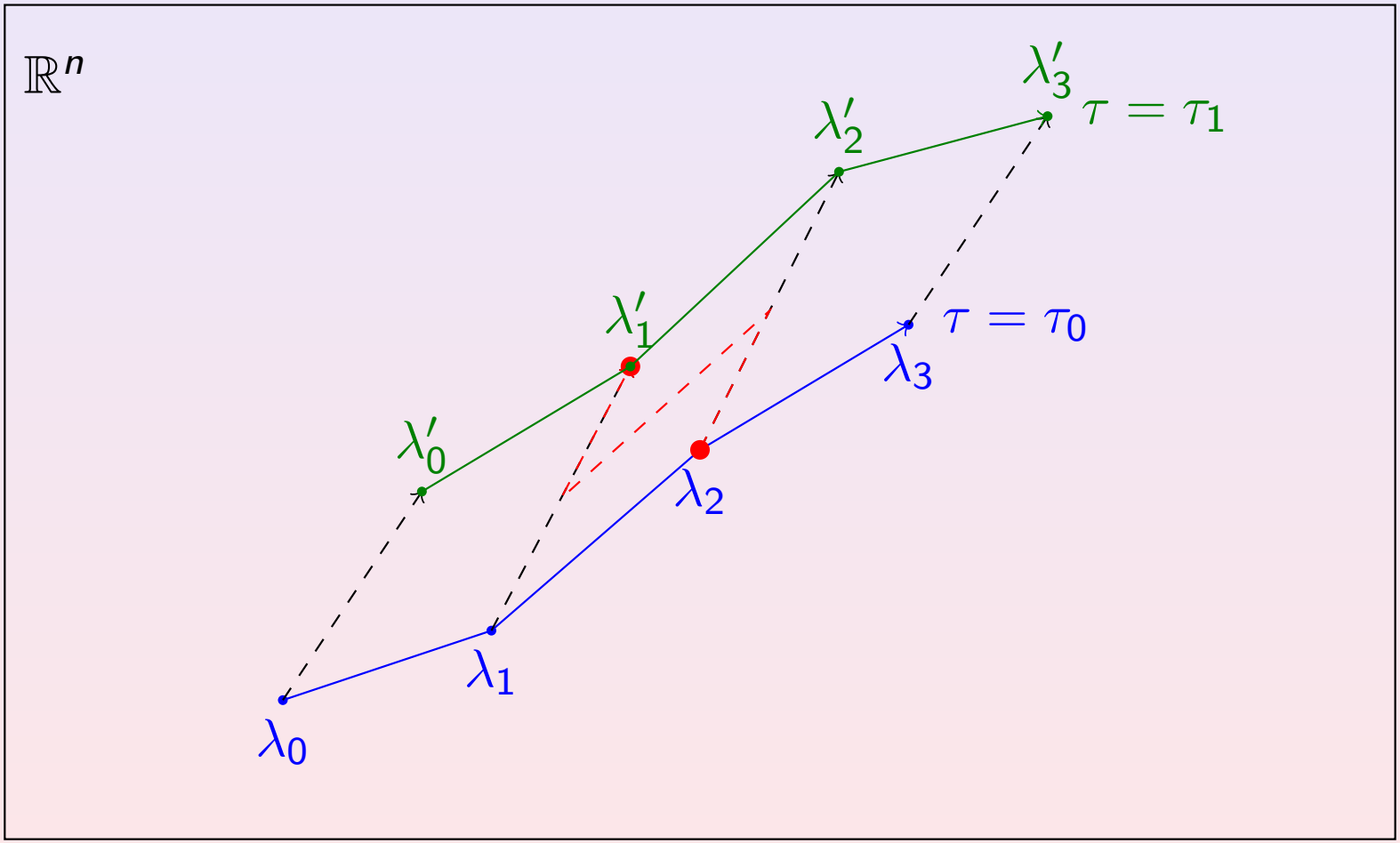

Schematic of complete algorithm

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- Based on various assumptions and approximations.
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Experiments show good computational performance relative to alternatives.

Example 1: parallel quantiles

- Take $x \in [0, 1]$ uniform.
- Let $f(x) = 2 \cdot \left(\exp(-30 \cdot (x - 0.25)^2) + \sin(\pi \cdot x^2)\right)$.
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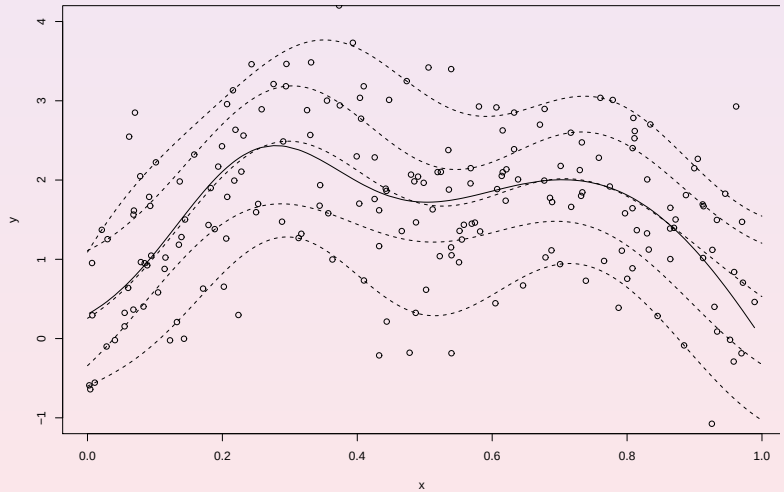

The plot shows the true mean/median $f(x)$ (solid) and the bi-level solutions for quantiles $0.1, 0.25, 0.5, 0.75, 0.9$.

Example 2: non-parallel quantiles

- Same $x, f(x)$.
- Now let $Y = f(x) + \epsilon$, with $\epsilon + (x+1)^2 \sim \exp(1/(x+1)^2)$.
- Errors are highly skewed and non-homogeneous.

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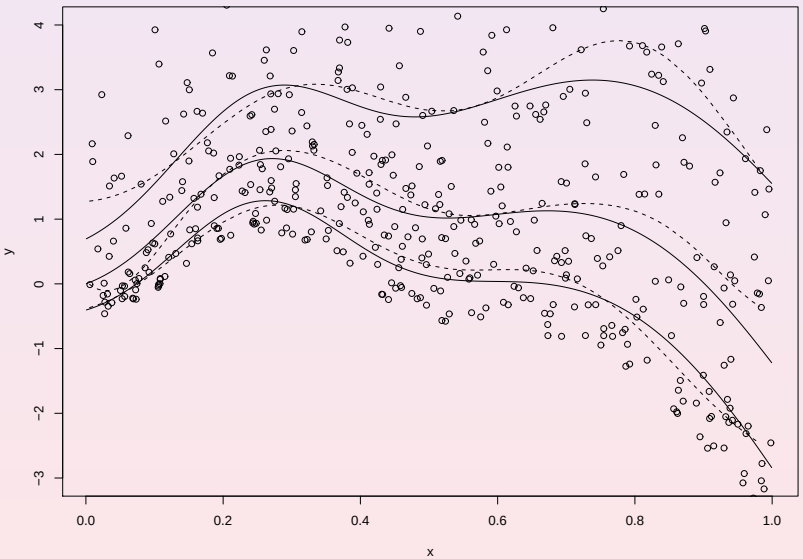

The plot shows the true (solid) and the bi-level solutions (dashed) for quantiles $0.25, 0.5, 0.75$.

Summary

Our work brings together traditional and emerging concepts in (Statistical) Machine Learning:

- Regularized optimization for predictive modeling, with kernel machines as an example.
- The importance of model selection.
- Path following for efficient solution.
- Quantile estimation as a flexible approach to regression modeling.

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Our work brings together traditional and emerging concepts in (Statistical) Machine Learning:

- Regularized optimization for predictive modeling, with kernel machines as an example.
- The importance of model selection.
- Path following for efficient solution.
- Quantile estimation as a flexible approach to regression modeling.

Main contributions:

- Mapping the whole solution surface $\hat{f}(\tau, \lambda)$.
- Path following algorithm for the bi-level solution $\lambda^*(\tau)$.

Thanks!

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