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Adaptive Finite Element Methods for Partial Differential Equations

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Abstract

The numerical simulation of complex physical processes requires the use of economical discrete models. This lecture presents a general paradigm of deriving a posteriori error estimates for the Galerkin finite element approximation of nonlinear problems. Employing duality techniques as used in optimal control theory the error in the target quantities is estimated in terms of weighted 'primal' and 'dual' residuals. On the basis of the resulting local error indicators economical meshes can be constructed which are tailored to the particular goal of the computation. The performance of this *Dual Weighted Residual Method* is illustrated for a model situation in computational fluid mechanics: the computation of the drag of a body in a viscous flow, the drag minimization by boundary control and the investigation of the optimal solution's stability.

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1. Introduction

Suppose the goal of a simulation is the computation or optimization of a certain quantity $J(u)$ from the solution u of a continuous model with accuracy TOL, by using the solution u_h of a discrete model of dimension N,

$$\mathcal{A}(u) = 0, \qquad \mathcal{A}_h(u_h) = 0.$$

Then, the goal of adaptivity is the optimal use of computing resources, i.e., minimum work for prescribed accuracy, or maximum accuracy for prescribed work. In order

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to reach this goal, one uses *a posteriori* error estimates

$$|J(u)-J(u_h)| \approx \eta(u_h) := \sum_{K\in\mathbb{T}_h} \rho_K(u_h)\omega_K,$$

in terms of the local residuals $\rho_K(u_h)$ of the computed solution and weights ω_K obtained from the solution of a linearized *dual problem*. In the following, we will describe a general optimal control approach to such error estimates in Galerkin finite element methods. For earlier work on adaptivity, we refer to the survey articles [10], [1] and [7]. The contents of this paper is based on material from [5], [6] and [2], where also references to other recent work can be found.

2. Paradigm of a posteriori error analysis

We develop a general approach to a posteriori error estimation for Galerkin approximations of variational problems. The setting uses as little assumptions as possible. Let X be some function space and $L(\cdot)$ a differentiable functional on X. We are looking for stationary points of $L(\cdot)$ determined by

$$L'(x)(y) = 0 \qquad \forall y \in X,$$

and their Galerkin approximation in finite dimensional subspaces $X_h \subset X$,

$$L'(x_h)(y_h) = 0 \qquad \forall\, y_h \in X_h,$$

For this situation, we have the following general result:

Proposition 1 *There holds the a posteriori error representation*

$$L(x) - L(x_h) = \tfrac{1}{2}L'(x_h)(x-y_h) + R_h, \tag{2.1}$$

for arbitrary $y_h \in X_h$. *The remainder* R_h *is cubic in* $e := x-x_h$,

$$R_h := \tfrac{1}{2}\int_0^1 L'''(x_h+se)(e,e,e)\, s(s-1)\,\mathrm{ds}.$$

Proof. We sketch the rather elementary proof. First, we note that

$$L(x) - L(x_h) = \int_0^1 L'(x_h+se)(e)\,\mathrm{ds} - \tfrac{1}{2}\big\{L'(x_h)(e) + L'(x)(e)\big\} + \tfrac{1}{2}L'(x_h)(e).$$

Since x_h is a stationary point,

$$L'(x_h)(e) = L'(x_h)(x-y_h) + L'(x_h)(y_h-x_h) = L'(x_h)(x-y_h), \quad y_h \in X_h.$$

Finally, using the error representation of the trapezoidal rule,

$$\int_0^1 f(s)\,\mathrm{ds} - \tfrac{1}{2}\big\{f(0)+f(1)\big\} = \tfrac{1}{2}\int_0^1 f''(s)s(s-1)\,\mathrm{ds},$$

completes the proof. Notice that the derivation of the error representation (2.1) does not assume the uniqueness of the stationary points. But the a priori assumption $x_h \to x\ (h\to 0)$ makes this result meaningful.

3. Variational equations

We apply the result of Proposition 1 to the Galerkin approximation of *variational equations* posed in some function space V,

$$a(u)(\psi) = 0 \quad \forall \psi \in V, \tag{3.1}$$

Suppose that some functional output $J(u)$ of the solution u is to be computed using a Galerkin approximation in finite dimensional subspaces $V_h \subset V$,

$$a(u_h)(\psi_h) = 0 \quad \forall \psi_h \in V_h. \tag{3.2}$$

The goal is now to estimate the error $J(u)–J(u_h)$. To this end, we employ a formal Euler-Lagrange approach to embed the present situation into the general framework laid out above. Introducing a 'dual' variable z ('Lagrangian multiplier'), we define the Lagrangian functional $\mathcal{L}(u,z) := J(u) - a(u)(z)$. Then, stationary points $\{u,z\} \in V \times V$ of $\mathcal{L}(\cdot,\cdot)$ are determined by the system

$$\mathcal{L}'(u,z)(\varphi,\psi) = \left\{ \begin{array}{l} J'(u)(\varphi) - a'(u)(\varphi,z) \\ -a(u)(\psi) \end{array} \right\} = 0 \quad \forall \{\varphi,\psi\}.$$

The corresponding Galerkin approximation determines $\{u_h,z_h\} \in V_h \times V_h$ by

$$\mathcal{L}'(u_h,z_h)(\varphi_h,\psi_h) = \left\{ \begin{array}{l} J'(u_h)(\varphi_h) - a'(u_h)(\varphi_h,z_h)\rangle \\ -\langle a(u_h)(\psi_h) \end{array} \right\} = 0 \quad \forall \{\varphi_h,\psi_h\}.$$

Set $x := \{u,z\}$, $x_h := \{u_h,z_h\}$, and $L(x) := \mathcal{L}(u,z)$. Then,

$$J(u) - J(u_h) \;=\; L(x) + a(u)(z) - L(x_h) - a(u_h)(z_h).$$

Proposition 2 *With the 'primal' and 'dual' residuals*

$$\begin{aligned} \rho(u_h)(\cdot) &:= -a(u_h)(\cdot), \\ \rho^*(z_h)(\cdot) &:= J'(u_h)(\cdot) - a'(u_h)(\cdot,z_h), \end{aligned}$$

there holds the error identity

$$J(u) - J(u_h) \;=\; \tfrac{1}{2}\rho(u_h)(z-\psi_h) \;+\; \tfrac{1}{2}\rho^*(z_h)(u-\varphi_h) \;+\; \mathcal{R}_h, \tag{3.3}$$

for arbitrary $\varphi_h,\psi_h \in V_h$. The remainder $\mathcal{R}_h$ is cubic in the primal and dual errors $e^u := u-u_h$ and $e^z := z-z_h$.

The evaluation of the error identity (3.3) requires guesses for primal and dual solutions u and z which are usually generated by post-processing from the approximations u_h and z_h, respectively. The cubic remainder term $\mathcal{R}_h$ is neglected. We emphasize that the solution of the dual problem takes only a 'linear work unit' compared to the solution of the generally nonlinear primal problem.

4. Optimal control problems

Next, we apply Proposition 1 to the approximation of optimal control problems. Let V be the 'state space' and Q the 'control space' for the optimization problem

$$J(u,q) \to \min! \qquad a(u)(\psi) + b(q,\psi) = 0 \quad \forall \psi \in V. \tag{4.1}$$

Its Galerkin approximation uses subspaces $V_h \times Q_h \subset V \times Q$ as follows:

$$J(u_h,q_h) \to \min! \qquad a(u_h)(\psi_h) + b(q_h,\psi) = 0 \quad \forall \psi_h \in V_h. \tag{4.2}$$

For embedding this situation into our general framework, we again employ the Euler-Lagrange approach introducing the Lagrangian functional $\mathcal{L}(u,q,z) := J(u,q) - A(u)(z) - B(q,z)$. Corresponding stationary points $x := \{u,q,z\} \in X := V \times Q \times V$ are determined by the system ('first-order optimality condition')

$$\left\{ \begin{array}{l} J'_u(u,q)(\varphi) - a'(u)(\varphi,z) \\ J'_q(u,q)(\chi) - b(\chi,z) \\ -a(u)(\psi) - b(q,\psi) \end{array} \right\} = 0 \qquad \forall \{\varphi,\chi,\psi\}. \tag{4.3}$$

The Galerkin approximation detrmines $x_h := \{u_h,q_h,z_h\} \in X_h := V_h \times Q_h \times V_h$ in finite dimensional subspace $V_h \subset V$, $Q_h \subset Q$ by

$$\left\{ \begin{array}{l} J'_u(u_h,q_h)(\varphi_h) - a'(u_h)(\varphi_h,z_h) \\ J'_q(u_h,q_h)(\chi_h) - b(\chi_h,z_h) \\ -a(u_h)(\psi_h) - b(q_h,\psi_h) \end{array} \right\} = 0 \qquad \forall \{\varphi_h,\chi_h,\psi_h\}. \tag{4.4}$$

For estimating the accuracy in this discretization, we propose to use the natural 'cost functional' of the optimization problem, i.e., to estimate the error in terms of the difference $J(u,q) - J(u_h,q_h)$. Then, from Proposition 1, we immediately obtain the following result:

Proposition 3 *With the 'primal', 'dual' and 'control' residuals*

$$\begin{aligned} \rho^*(z_h)(\cdot) &:= J'_u(u_h,q_h)(\cdot) - a'(u_h)(\cdot,z_h), \\ \rho^q(q_h)(\cdot) &:= J'_q(u_h,q_h)(\cdot) - b(\cdot,z_h), \\ \rho(u_h)(\cdot) &:= -a(u_h)(\cdot) - b(q_h,\cdot), \end{aligned}$$

there holds the a posteriori error representation

$$\begin{aligned} J(u,q) - J(u_h,q_h) \; = \; & \tfrac{1}{2}\rho^*(z_h)(u-\varphi_h) + \tfrac{1}{2}\rho^q(q_h)(q-\chi_h) \\ & + \tfrac{1}{2}\rho(u_h)(z-\psi_h) \; + \; \mathcal{R}_h, \end{aligned} \tag{4.5}$$

for arbitrary $\varphi_h, \psi_h \in V_h$ and $\chi_h \in Q_h$. The remainder $\mathcal{R}_h$ is cubic in the errors $e^u := u - u_h$, $e^q := q - q_h$, $e^z := z - z_h$.

We note that error estimation in optimal control problems requires only the use of available information from the computed solution $\{u_h, q_h, z_h\}$, i.e., no extra dual problem has to be solve. This is typical for a situation where the discretization error is measured with respect to the 'generating' functional of the problem, i.e. the Lagrange functional in this case. In the practical solution process the mesh adaptation is nested with an outer Newton iteration leading to a successive 'model enrichment'. The 'optimal' solution $\{u_h^{\rm opt}, q_h^{\rm opt}\}$ obtained by the adapted discretization may satisfy the state equation only in a rather week sense. If more 'admissibility' is required, we may solve just the state equation with an better discretization (say on a finer mesh) using the computed optimal control q_h^{opt} as data.

5. Eigenvalue problems

Finally, we apply Proposition 1 to the Galerkin approximation of eigenvalue problems. Consider in a (complex) function space V the generalized eigenvalue problem

$$a(u,\psi) = \lambda\, m(u,\psi) \quad \forall \psi \in V, \qquad \lambda \in \mathbb{C},\ m(u,u) = 1, \tag{5.1}$$

where the form $a(\cdot,\cdot)$ is linear but not necessarily symmetric, and the eigenvalue form $m(\cdot,\cdot)$ is symmetric and positive semi-definit. The Galerkin approximation is defined in finite dimensional subspaces $V_h \subset V$,

$$a(u_h,\psi_h) = \lambda_h m(u_h,\psi_h) \quad \forall \psi_h \in V_h, \qquad \lambda_h \in \mathbb{C},\, m(u_h,u_h) = 1. \tag{5.2}$$

We want to control the error in the eigenvalues $\lambda - \lambda_h$. To this end, we embed this situation into the general framework of variational equations by introducing the spaces $\mathcal{V} := V \times \mathbb{C}$ and $\mathcal{V}_h := V_h \times \mathbb{C}$, consisting of elements $U := \{u, \lambda\}$ and $U_h := \{u_h, \lambda_h\}$, and the semi-linear form

$$A(U)(\Psi) := \lambda m(u,\psi) - a(u,\psi) + \overline{\mu}\big\{m(u,u) - 1\big\}, \quad \Psi = \{\psi, \mu\} \in \mathcal{V}.$$

Then, the eigenvalue problem (5.1) and its Galerkin approximation (5.2) can be written in the compact form

$$A(U)(\Psi) = 0 \qquad \forall \Psi \in \mathcal{V}, \tag{5.3}$$

$$A(U_h)(\Psi_h) = 0 \qquad \forall \Psi_h \in \mathcal{V}_h. \tag{5.4}$$

The error in this approximation will be estimated with respect to the functional

$$J(\Phi) := \mu\, m(\varphi,\varphi),$$

where $J(U) = \lambda$ since $m(u,u) = 1$. The corresponding continuous and discrete dual solutions $Z = \{z, \pi\} \in \mathcal{V}$ and $Z_h = \{z_h, \pi_h\} \in \mathcal{V}_h$ are determined by the problems

$$A'(U)(\Phi, Z) = J'(U)(\Phi) \qquad \forall \Phi \in \mathcal{V}, \tag{5.5}$$

$$A'(U_h)(\Phi_h, Z_h) = J'(U_h)(\Phi_h) \qquad \forall \Phi_h \in \mathcal{V}_h. \tag{5.6}$$

A straightforward calculation shows that these dual problems are equivalent to the *adjoint eigenvalue problems* associated to (5.1) and (5.2),

$$a(\varphi, z) = \pi\, m(\varphi, z) \qquad \forall \varphi \in V, \qquad m(u, z) = 1, \tag{5.7}$$

$$a(\varphi_h, z_h) = \pi_h\, m(\varphi_h, z_h) \quad \forall \varphi_h \in V_h, \quad m(u_h, z_h) = 1. \tag{5.8}$$

Then, application of Proposition 1 yields the following result:

Proposition 4 *With the 'primal' and 'dual' residuals*

$$\rho(u_h, \lambda_h)(\cdot) := a(u_h, \cdot) - \lambda_h\, m(u_h, \cdot),$$
$$\rho^*(z_h, \pi_h)(\cdot) := a(\cdot, z_h) - \pi_h\, m(\cdot, z_h),$$

there holds the a posteriori error representation

$$\lambda - \lambda_h \;=\; \tfrac{1}{2}\rho(u_h, \lambda_h)(z - \psi_h) + \tfrac{1}{2}\rho^*(z_h, \pi_h)(u - \varphi_h) - \mathcal{R}_h, \tag{5.9}$$

for arbitrary $\psi_h,\, \varphi_h \in V_h$*, with the remainder term*

$$\mathcal{R}_h \;=\; \tfrac{1}{2}(\lambda - \lambda_h)\, m(v - v_h, z - z_h).$$

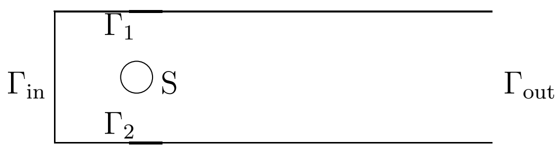
We note that in Proposition 4, no assumption about the multiplicity of the approximated eigenvalue λ has been made. In order to make the error representation (5.9) meaningful, we have to use a priori information about the convergence $\{\lambda_h, v_h\} \to \{\lambda, v\}$ as $h \to 0$. The simultaneous solution of primal and dual eigenvalue problems naturally occurs within an optimal multigrid solver of nonsymmetric eigenvalue problems. Further, error estimates with respect to functionals $J(u)$ of eigenfunctions can be derived following the general paradigm. Finally, in solving *stability eigenvalue problems* $\mathcal{A}'(\hat{u})v = \lambda \mathcal{M} v$, we can include the perturbation of the operator $\mathcal{A}'(\hat{u}_h) \approx \mathcal{A}'(\hat{u})$ in the a posteriori error estimate of the eigenvalues.

6. Application in fluid flow simulation

In order to illustrate the abstract theory developed so far, we present some results for the application of 'residual-driven' mesh adaptation for a model problem in computational fluid mechanics, namely 'channel flow around a cylinder' as shown in the figure below. The *stationary* Navier-Stokes system

$$\mathcal{A}(u) := \left\{ \begin{array}{c} -\nu\Delta v + v\cdot\nabla v + \nabla p \\ \nabla\cdot v \end{array} \right\} = 0$$

determines the pair $u := \{v, p\}$ of velocity vector v and scalar pressure p of a viscous incompressible fluid with viscosity ν and normalized density $\rho \equiv 1$. The physical boundary conditions are $v|_{\Gamma_{\rm rigid}} = 0$, $v|_{\Gamma_{\rm in}} = v^{\rm in}$, and $\nu\partial_n v - np|_{\Gamma_{\rm out}} = 0$, i.e., the flow is driven by the prescribed parabolic inflow $v^{\rm in}$. The Reynolds number is $\mathrm{Re} = \frac{\bar{\mathrm{U}}^2 \mathrm{D}}{\nu} = 20$, such that the flow is stationary.



Let the goal of the simulation be the accurate computation of the effective force in the main flow direction imposed on the cylinder, i.e. the so-called 'drag coefficient',

$$J(u) := c_{\text{drag}} = \frac{2}{\max |v^{\text{in}}|^2 D} \int_S n^T(2\nu\tau - pI)e_1 \, \mathrm{ds},$$

where S is the surface of the cylinder, D its diameter, and $\tau = \frac{1}{2}(\nabla v + \nabla v^T)$ the strain tensor. In practice, one uses a volume-oriented representation of c_{drag}.

Here, we cannot describe the standard variational formulation of the Navier-Stokes problem and its Galerkin finite element discretization in detail but rather refer to the literature; see [9], [6], and the references therein.

In the present situation the primal and dual residuals occuring in the a posteriori error representation (3.3) have the following explicit form:

$$\rho(u_h)(z - z_h) := \sum_{K \in \mathbb{T}_h} \Big\{ (R_h, z^v - z_h^v)_K + (r_h, z^v - z_h^v)_{\partial K} + (z^p - z_h^p, \nabla \cdot v_h)_K + \dots \Big\},$$

$$\rho^*(z_h)(u - u_h) := \sum_{K \in \mathbb{T}_h} \Big\{ (R_h^*, v - v_h)_K + (r_h^*, v - v_h)_{\partial K} + (p - p_h, \nabla \cdot z_h^v)_K + \dots \Big\},$$

with the cell and edge residuals defined by

$$\begin{aligned}
R_{h|K} &:= f + \nu\Delta v_h - v_h \cdot \nabla v_h - \nabla p, \\
R_{h|K}^* &:= j + \nu\Delta z_h^v + v_h \cdot \nabla z_h^v - \nabla v_h^T z_h^v + \nabla \cdot v_h z_h^v - \nabla z_h^p, \\
r_{h|\Gamma} &:= \left\{ \begin{array}{ll} \frac{1}{2}[\nu\partial_n v_h - n p_h], & \text{if } \Gamma \not\subset \partial\Omega \\ -\nu\partial_n v_h + n p_h, & \text{if } \Gamma \subset \Gamma_{\text{out}}, \quad (= 0 \text{ else}) \end{array} \right\}, \\
r_{h|\Gamma}^* &:= \left\{ \begin{array}{ll} \frac{1}{2}[\nu\partial_n z_h^v + n \cdot v_h z_h^v - z_h^p n], & \text{if } \Gamma \not\subset \partial\Omega \\ -\nu\partial_n z_h^v - n \cdot v_h z_h^v + z_h^p n, & \text{if } \Gamma \subset \Gamma_{\text{out}}, \quad (= 0 \text{ else}) \end{array} \right\},
\end{aligned}$$

where $[\dots]$ denotes the jump across edges Γ, and '...' stands for terms representing errors due to boundary and inflow approximation as well as stabilization.

Practical mesh adaptation on the basis of the a posteriori error estimates proceeds as follows: At first, the error functional may have to be regularized according to $\tilde{J}(u) = J(u) + \mathcal{O}(TOL)$. Then, after having computed the primal approximation u_h, the *linear* discrete dual problem is solved:

$$\langle \mathcal{A}'(u_h)^* z_h, \varphi_h \rangle = \tilde{J}'(u_h)(\varphi_h) \quad \forall \varphi_h \in V_h^*. \tag{6.1}$$

The error estimator is localized, $\eta_\omega = \sum_{K \in \mathbb{T}_h} \eta_K$, and approximation of the weights are computed by patch-wise higher-order interpolation: $(z - z_h)_{|K} \approx (I_{2h}^* z_h - z_h)_{|K}$.

Finally, the current mesh is adapted by 'error balancing' $\eta_K \approx \eta_\omega/\#\{K \in \mathbb{T}_h\}$. In the following, we show some results which have been obtained using mesh adaptation on the basis of the Dual Weighted Residual Method ('DWR method').

6.1. Drag computation (from [3])

The drag is computed on meshes generated by the DWR method and by an 'ad hoc' refinement criterion based on smoothness properties of the computed solution.

Table 1: *Results for drag computation on adapted meshes (1%-error in bold face).*

Computation of drag				
L	N	c_{drag}	η_{drag}	I_{eff}
4	984	5.66058	$1.1e{-}1$	0.76
5	**2244**	5.59431	$3.1e{-}2$	0.47
6	4368	5.58980	$1.8e{-}2$	0.58
6	7680	5.58507	$8.0e{-}3$	0.69
	∞	5.57953		

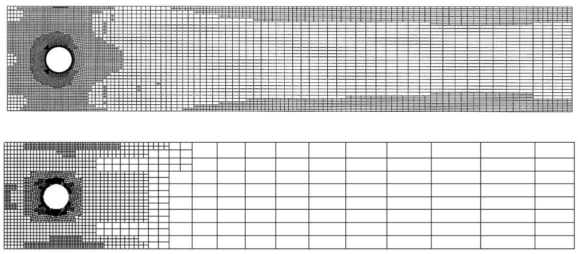


Figure 1: *Refined meshes by 'ad hoc' strategy (top) and DWR method (bottom).*

6.2. Drag minimization (from [4])

The drag coefficient is to be minimized by imposing a pressure drop at the two outlets Γ_i above and below the cylinder. In this case of 'boundary control' the control form is given by $b(q,\psi) := -(q, n{\cdot}\psi^v)_{\Gamma_1\cup\Gamma_2}$.

Table 2: *Uniform refinement versus adaptive refinement for* $\text{Re} = 40$.

Uniform refinement		Adaptive refinement	
N	J_{drag}	N	J_{drag}
10512	3.31321	1572	3.28625
41504	3.21096	4264	3.16723
164928	3.11800	11146	3.11972

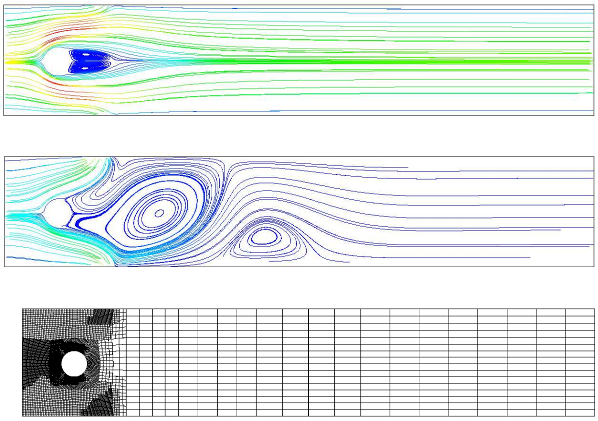


Figure 2: *Velocity of the uncontrolled flow (top), controlled flow (middle), corresponding adapted mesh (bottom).*

6.3. Stability of optimized flows (from [8])

We want to investigate the stability of the optimized solution $u^{\rm opt} = \{v^{\rm opt}, p^{\rm opt}\}$ by linear stability theory. This is a crucial question since in the present case the optimal solution is obtained by a *stationary* Newton iteration which may converge to physically unstable solutions. In this context, we have to consider the non-symmetric eigenvalue problem for $u := \{v, p\} \in V$ and $\lambda \in \mathbb{C}$:

$$\mathcal{A}'(u^{\rm opt})u := \left\{ \begin{array}{c} -\nu\Delta v + v^{\rm opt}\cdot\nabla v + v\cdot\nabla v^{\rm opt} + \nabla p \\ \nabla\cdot v \end{array} \right\} = \lambda \left\{ \begin{array}{c} v \\ 0 \end{array} \right\}.$$

If the real parts of all eigenvalues are positive, $\mathrm{Re}\,\lambda > 0$, then the (stationary) base flow $\{v^{\rm opt}, p^{\rm opt}\}$ is considered as stable (but with respect to possibly only very small perturbations). We find that the optimal solution is at the edge of being unstable.

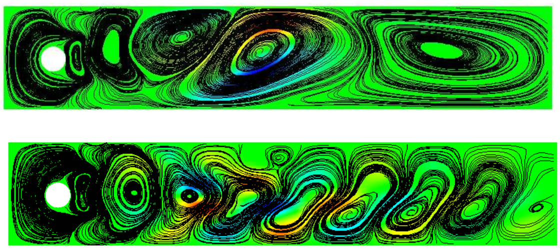


Figure 3: *Streamlines of real parts of the 'critical' eigenfunction shortly before the Hopf bifurcation and after, depending on the imposed pressure drop.*

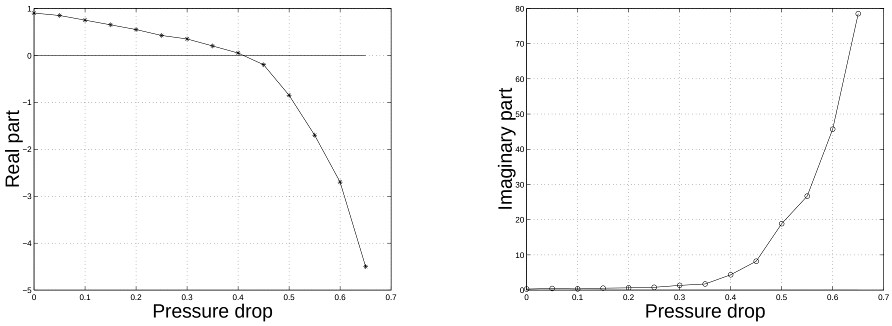


Figure 4: *Real and imaginary parts of the critical eigenvalue as function of the control variable.*

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